# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:56 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 4UB6 / pdb_00004ub6 |
| Title | : | Native structure of photosystem II (dataset-1) by a femtosecond X-ray laser |
| Authors | : | Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R. |
| Deposited on | : | 2014-08-12 |
| Resolution | : | 1.95 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:

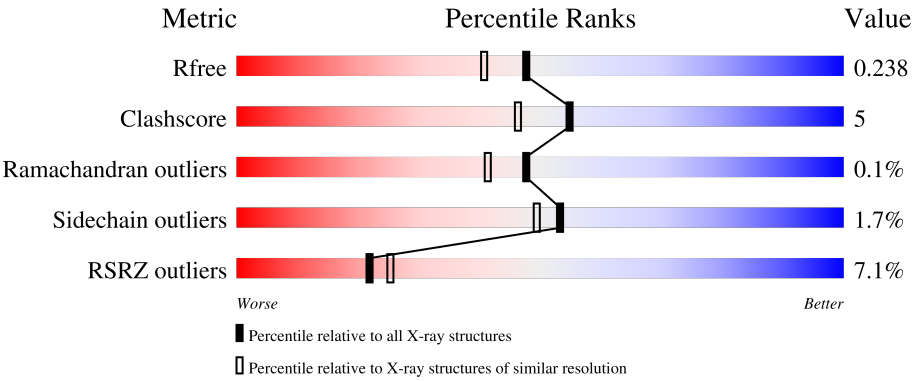
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.010 (Gargrove) |
| Density-Fitness | : | 1.0.12 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 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 1.95 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)) |
|---|---|---|
| $R_{free}$ | 180053 | 3494 (1.96-1.96) |
| Clashscore | 190562 | 3612 (1.96-1.96) |
| Ramachandran outliers | 187476 | 3587 (1.96-1.96) |
| Sidechain outliers | 187428 | 3587 (1.96-1.96) |
| RSRZ outliers | 180081 | 3495 (1.96-1.96) |

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 | 344 | 2% 91% 6% · |
| 1 | a | 344 | 3% 86% 11% · |
| 2 | B | 505 | 4% 92% 8% |
| 2 | b | 505 | 6% 91% 8% |
| 3 | C | 455 | 4% 90% 9% · |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | c | 455 | 4% 93% 7% |
| 4 | D | 342 | % 92% 8% |
| 4 | d | 342 | % 92% 8% |
| 5 | E | 84 | 10% 88% 8% |
| 5 | e | 84 | 20% 80% 15% |
| 6 | F | 44 | 9% 61% 14% 23% |
| 6 | f | 44 | 7% 50% 23% 27% |
| 7 | H | 65 | 6% 95% 5% |
| 7 | h | 65 | 11% 97% |
| 8 | I | 38 | 16% 87% 13% |
| 8 | i | 38 | 16% 89% 8% |
| 9 | J | 39 | 15% 90% 8% |
| 9 | j | 39 | 18% 87% 10% |
| 10 | K | 37 | 8% 86% 14% |
| 10 | k | 37 | 14% 81% 19% |
| 11 | L | 37 | 8% 84% 11% 5% |
| 11 | l | 37 | 5% 86% 14% |
| 12 | M | 36 | 8% 75% 19% 6% |
| 12 | m | 36 | 6% 75% 14% 6% 6% |
| 13 | O | 244 | 7% 88% 12% |
| 13 | o | 244 | 13% 86% 13% |
| 14 | T | 32 | 6% 88% 6% 6% |
| 14 | t | 32 | 6% 88% 6% |
| 15 | U | 104 | 4% 89% 7% |
| 15 | u | 104 | 2% 86% 7% 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 16 | V | 137 | 4% 97% |
| 16 | v | 137 | 4% 93% 7% |
| 17 | Y | 30 | 33% 77% 20% |
| 17 | y | 30 | 47% 67% 27% |
| 18 | X | 40 | 20% 95% |
| 18 | x | 40 | 18% 98% |
| 19 | Z | 62 | 34% 85% 15% |
| 19 | z | 62 | 45% 90% 10% |
| 20 | R | 34 | 79% 88% 9% |

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 | CL | U | 201 | - | - | X | - |
| 22 | CL | v | 201 | - | - | X | - |
| 24 | CLA | A | 405 | X | - | - | - |
| 24 | CLA | A | 406 | X | - | - | - |
| 24 | CLA | B | 602 | X | - | - | - |
| 24 | CLA | B | 603 | X | - | - | - |
| 24 | CLA | B | 604 | X | - | - | - |
| 24 | CLA | B | 605 | X | - | - | - |
| 24 | CLA | B | 606 | X | - | - | - |
| 24 | CLA | B | 607 | X | - | - | - |
| 24 | CLA | B | 608 | X | - | - | - |
| 24 | CLA | B | 610 | X | - | - | - |
| 24 | CLA | B | 611 | X | - | - | - |
| 24 | CLA | B | 612 | X | - | - | - |
| 24 | CLA | B | 613 | X | - | - | - |
| 24 | CLA | B | 614 | X | - | - | - |
| 24 | CLA | B | 615 | X | - | - | - |
| 24 | CLA | B | 616 | X | - | - | - |
| 24 | CLA | B | 617 | X | - | - | - |
| 24 | CLA | C | 502 | X | - | - | - |
| 24 | CLA | C | 504 | X | - | - | - |
| 24 | CLA | C | 505 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 24 | CLA | C | 506 | X | - | - | - |
| 24 | CLA | C | 507 | X | - | - | - |
| 24 | CLA | C | 508 | X | - | - | - |
| 24 | CLA | C | 510 | X | - | - | - |
| 24 | CLA | C | 511 | X | - | - | - |
| 24 | CLA | C | 512 | X | - | - | - |
| 24 | CLA | C | 513 | X | - | - | - |
| 24 | CLA | D | 401 | X | - | - | - |
| 24 | CLA | D | 402 | X | - | - | - |
| 24 | CLA | a | 406 | X | - | - | - |
| 24 | CLA | a | 409 | X | - | - | - |
| 24 | CLA | b | 605 | X | - | - | - |
| 24 | CLA | b | 606 | X | - | - | - |
| 24 | CLA | b | 607 | X | - | - | - |
| 24 | CLA | b | 608 | X | - | - | - |
| 24 | CLA | b | 609 | X | - | - | - |
| 24 | CLA | b | 610 | X | - | - | - |
| 24 | CLA | b | 611 | X | - | - | - |
| 24 | CLA | b | 613 | X | - | - | - |
| 24 | CLA | b | 614 | X | - | - | - |
| 24 | CLA | b | 615 | X | - | - | - |
| 24 | CLA | b | 616 | X | - | - | - |
| 24 | CLA | b | 617 | X | - | - | - |
| 24 | CLA | b | 618 | X | - | - | - |
| 24 | CLA | b | 619 | X | - | - | - |
| 24 | CLA | b | 620 | X | - | - | - |
| 24 | CLA | c | 902 | X | - | - | - |
| 24 | CLA | c | 903 | X | - | - | - |
| 24 | CLA | c | 904 | X | - | - | - |
| 24 | CLA | c | 905 | X | - | - | - |
| 24 | CLA | c | 906 | X | - | - | - |
| 24 | CLA | c | 907 | X | - | - | - |
| 24 | CLA | c | 908 | X | - | - | - |
| 24 | CLA | c | 909 | X | - | - | - |
| 24 | CLA | c | 910 | X | - | - | - |
| 24 | CLA | c | 911 | X | - | - | - |
| 24 | CLA | c | 912 | X | - | - | - |
| 24 | CLA | c | 913 | X | - | - | - |
| 24 | CLA | c | 914 | X | - | - | - |
| 24 | CLA | d | 401 | X | - | - | - |
| 24 | CLA | d | 402 | X | - | - | - |

# 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 334 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 2634 | 1728 | 432 | 459 | 15 | | | |
| 1 | a | 334 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 2645 | 1737 | 432 | 461 | 15 | | | |

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 504 | Total | C | N | O | S | 0 | 11 | 0 |
| | | | 4027 | 2643 | 668 | 703 | 13 | | | |
| 2 | b | 504 | Total | C | N | O | S | 0 | 12 | 0 |
| | | | 4033 | 2650 | 668 | 702 | 13 | | | |

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 451 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 3501 | 2291 | 584 | 613 | 13 | | | |
| 3 | c | 455 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 3544 | 2323 | 589 | 619 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 342 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2729 | 1807 | 445 | 465 | 12 | | | |
| 4 | d | 341 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2720 | 1802 | 444 | 462 | 12 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 81 | Total<br>668 | C<br>436 | N<br>107 | O<br>125 | 0 | 2 | 0 |
| 5 | e | 81 | Total<br>670 | C<br>439 | N<br>107 | O<br>124 | 0 | 2 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 34 | Total<br>275 | C<br>187 | N<br>45 | O<br>42 | S<br>1 | 0 | 0 | 0 |
| 6 | f | 32 | Total<br>257 | C<br>175 | N<br>43 | O<br>38 | S<br>1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | H | 65 | Total<br>519 | C<br>346 | N<br>85 | O<br>86 | S<br>2 | 0 | 1 | 0 |
| 7 | h | 65 | Total<br>511 | C<br>341 | N<br>82 | O<br>86 | S<br>2 | 0 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 38 | Total<br>272 | C<br>182 | N<br>42 | O<br>47 | S<br>1 | 0 | 0 | 0 |
| 9 | j | 39 | Total<br>280 | C<br>187 | N<br>43 | O<br>48 | S<br>2 | 0 | 0 | 0 |

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | L | 37 | Total<br>309 | C<br>207 | N<br>48 | O<br>53 | S<br>1 | 0 | 1 | 0 |
| 11 | l | 37 | Total<br>309 | C<br>207 | N<br>48 | O<br>53 | S<br>1 | 0 | 1 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | M | 34 | Total<br>274 | C<br>184 | N<br>40 | O<br>49 | S<br>1 | 0 | 1 | 0 |
| 12 | m | 34 | Total<br>269 | C<br>179 | N<br>40 | O<br>49 | S<br>1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | O | 243 | Total<br>1903 | C<br>1191 | N<br>315 | O<br>392 | S<br>5 | 0 | 8 | 0 |
| 13 | o | 243 | Total<br>1891 | C<br>1183 | N<br>315 | O<br>388 | S<br>5 | 0 | 5 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | T | 30 | Total<br>264 | C<br>185 | N<br>36 | O<br>41 | S<br>2 | 0 | 1 | 0 |
| 14 | t | 30 | Total<br>264 | C<br>185 | N<br>36 | O<br>41 | S<br>2 | 0 | 1 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | V | 137 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 1072 | 680 | 180 | 208 | 4 | | | |
| 16 | v | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1064 | 675 | 177 | 208 | 4 | | | |

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | Y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |
| 17 | y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | X | 39 | Total | C | N | O | 0 | 0 | 0 |
| | | | 287 | 191 | 46 | 50 | | | |
| 18 | x | 39 | Total | C | N | O | 0 | 0 | 0 |
| | | | 287 | 191 | 46 | 50 | | | |

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

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

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

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

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

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

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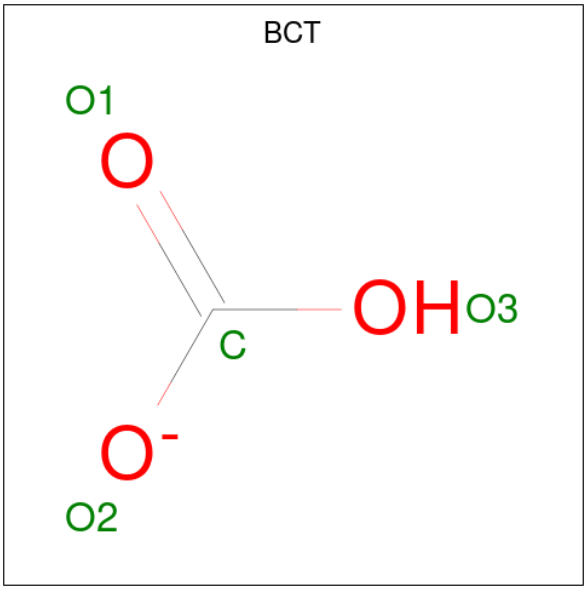
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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 21 | a | 1 | Total Fe<br>1 1 | 0 | 0 |

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

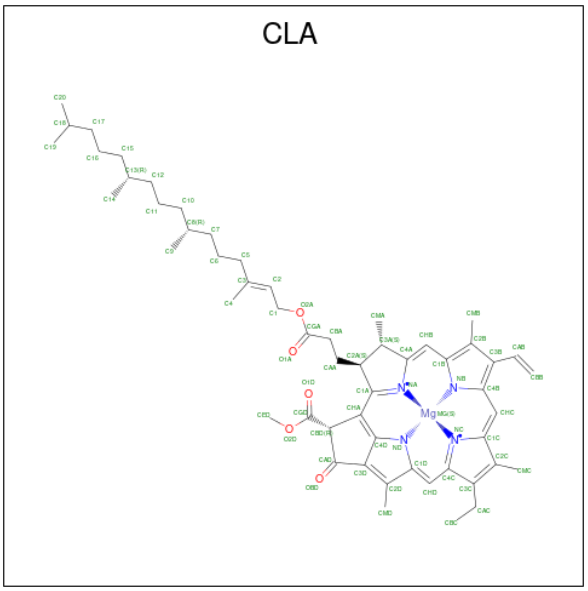
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 22 | A | 2 | Total Cl<br>2 2 | 0 | 0 |
| 22 | U | 1 | Total Cl<br>1 1 | 0 | 0 |
| 22 | a | 2 | Total Cl<br>2 2 | 0 | 0 |
| 22 | v | 1 | Total Cl<br>1 1 | 0 | 0 |

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: $CHO_3$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 23 | A | 1 | Total C O<br>4 1 3 | 0 | 0 |
| 23 | a | 1 | Total C O<br>4 1 3 | 0 | 0 |

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 24 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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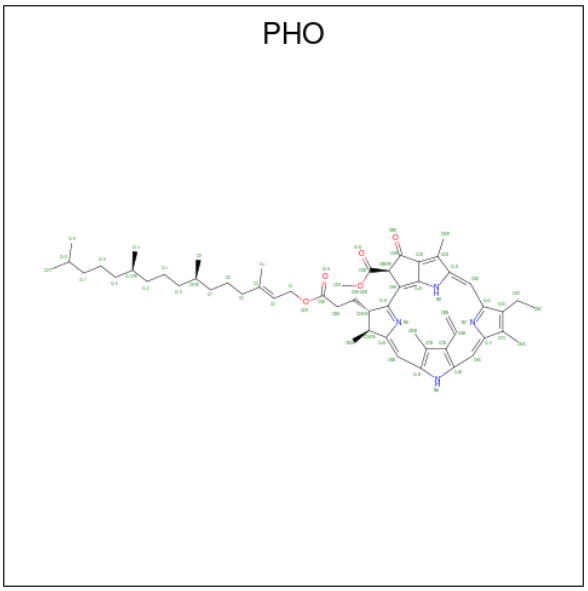
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 24 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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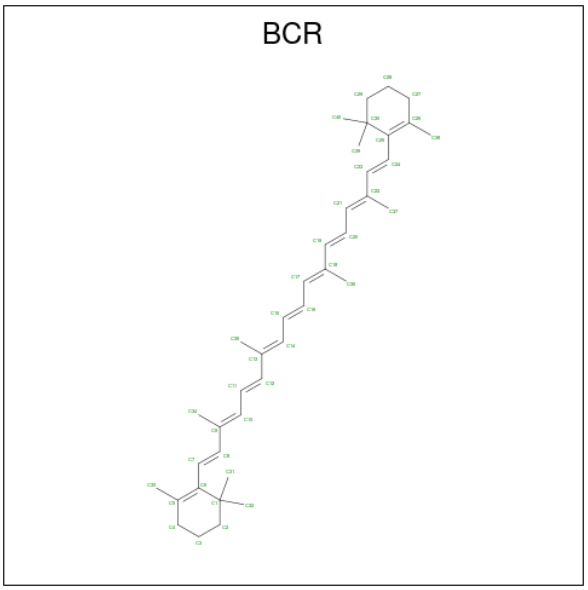
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



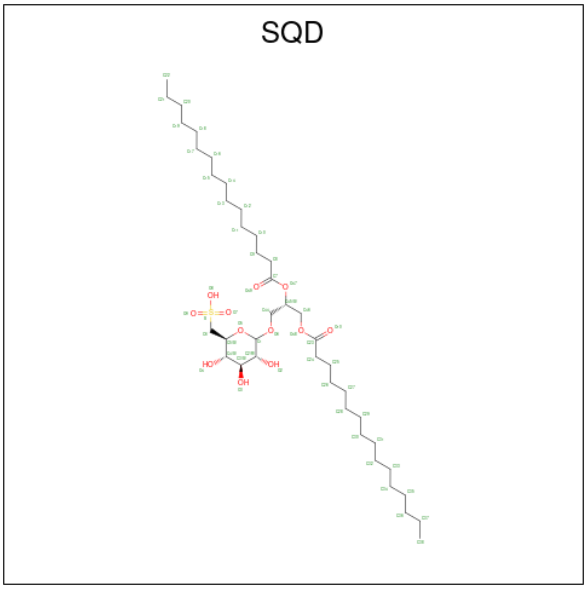

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 25 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 25 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 25 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



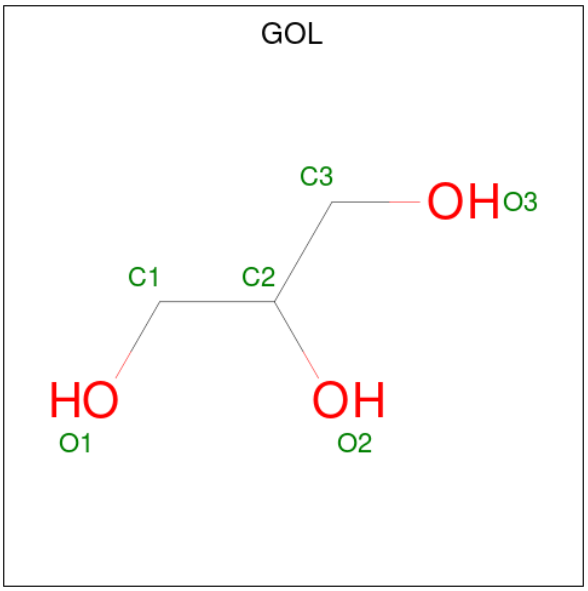
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 26 | A | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | B | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | B | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | B | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | C | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | C | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | D | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | H | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | K | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | K | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | T | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | a | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | b | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | b | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | b | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | c | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | d | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | h | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | k | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | k | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | t | 1 | Total C<br>40 40 | 0 | 0 |
| 26 | y | 1 | Total C<br>40 40 | 0 | 0 |

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 27 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | F | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 27 | L | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | f | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | F | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | O | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

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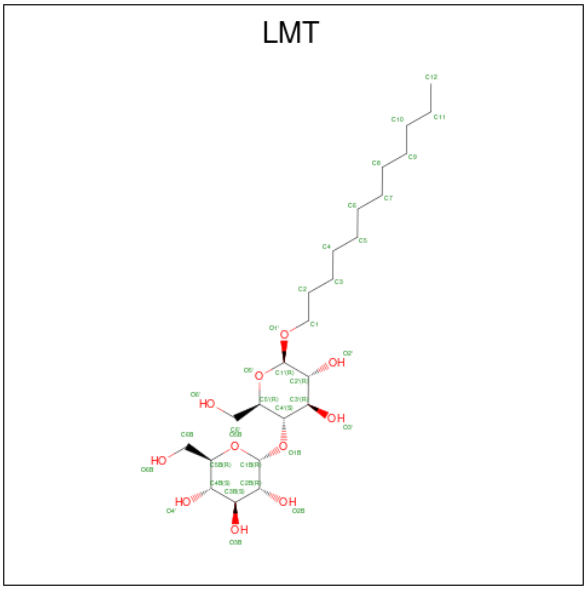
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 28 | T | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | T | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | V | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | V | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | V | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | V | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | a | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | a | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | a | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | b | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | b | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | b | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | b | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | b | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | b | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | c | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | c | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | f | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | o | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | t | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | v | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 28 | v | 1 | Total C O<br>6 3 3 | 0 | 0 |
| 28 | v | 1 | Total C O<br>6 3 3 | 0 | 0 |

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



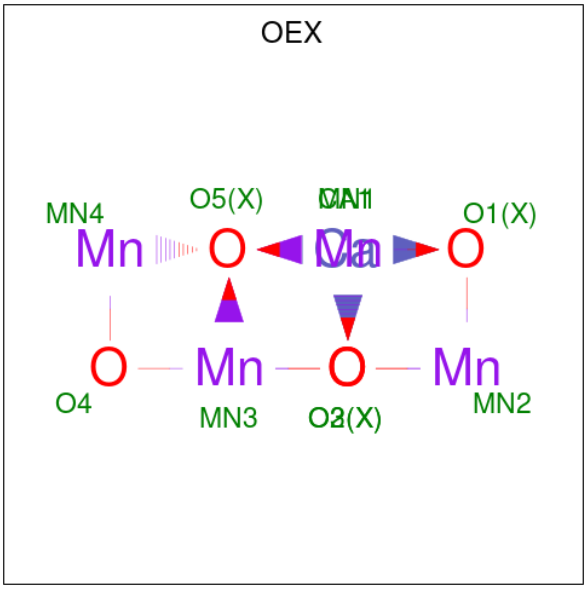

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 29 | A | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | B | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | B | 1 | Total C O<br>25 19 6 | 0 | 0 |
| 29 | C | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | E | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | M | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | a | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | b | 1 | Total C O<br>25 19 6 | 0 | 0 |
| 29 | b | 1 | Total C O<br>25 19 6 | 0 | 0 |

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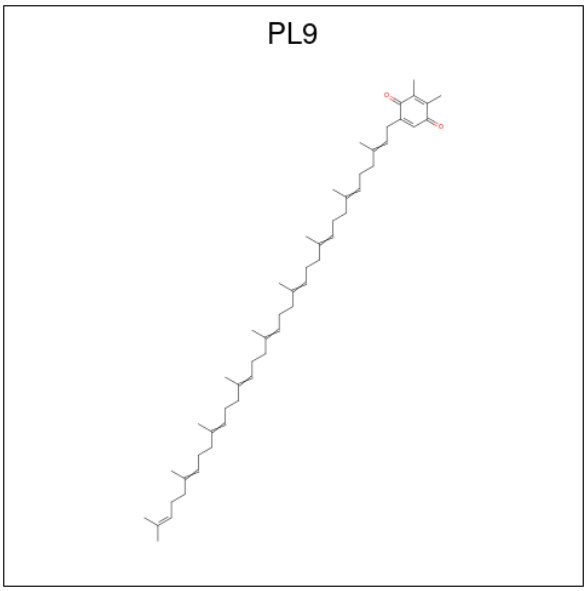
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 29 | c | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | f | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | m | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | m | 1 | Total C O<br>35 24 11 | 0 | 0 |
| 29 | m | 1 | Total C O<br>35 24 11 | 0 | 0 |

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).




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

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




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 31 | A | 1 | Total C O<br>55 53 2 | 0 | 0 |
| 31 | D | 1 | Total C O<br>55 53 2 | 0 | 0 |
| 31 | a | 1 | Total C O<br>55 53 2 | 0 | 0 |
| 31 | d | 1 | Total C O<br>55 53 2 | 0 | 0 |

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 32 | A | 1 | Total C O<br>28 23 5 | 0 | 0 |
| 32 | B | 1 | Total C O<br>33 28 5 | 0 | 0 |
| 32 | D | 2 | Total C O<br>57 51 6 | 0 | 0 |
| 32 | I | 1 | Total C O<br>40 35 5 | 0 | 0 |
| 32 | J | 1 | Total C<br>10 10 | 0 | 0 |
| 32 | K | 1 | Total C O<br>34 29 5 | 0 | 0 |
| 32 | M | 1 | Total C<br>10 10 | 0 | 0 |
| 32 | X | 1 | Total C O<br>18 16 2 | 0 | 0 |

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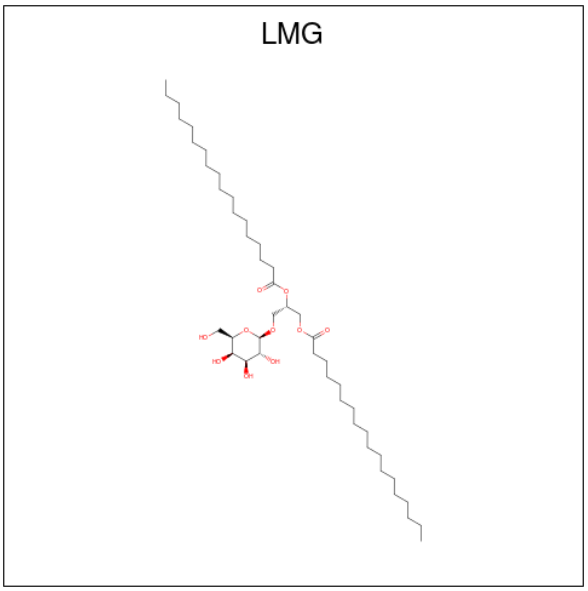
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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 32 | a | 1 | Total C O<br>30 25 5 | 0 | 0 |
| 32 | b | 1 | Total C O<br>33 28 5 | 0 | 0 |
| 32 | c | 1 | Total C O<br>32 27 5 | 0 | 0 |
| 32 | d | 3 | Total C O<br>71 63 8 | 0 | 0 |
| 32 | i | 1 | Total C O<br>40 35 5 | 0 | 0 |
| 32 | j | 1 | Total C<br>10 10 | 0 | 0 |
| 32 | m | 1 | Total C<br>10 10 | 0 | 0 |

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

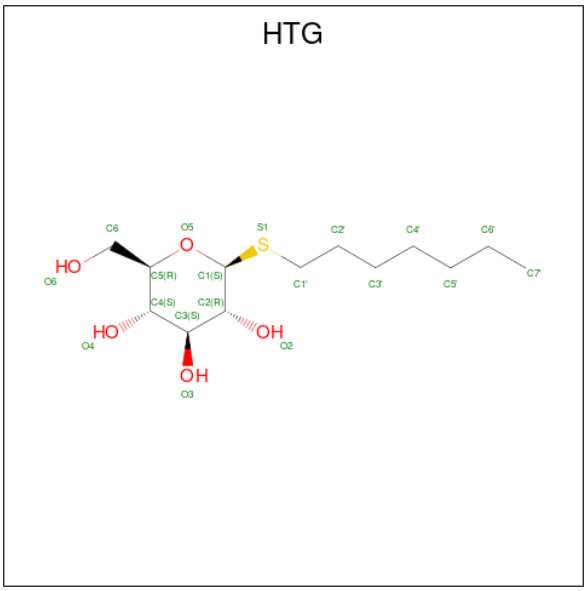
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 33 | B | 1 | Total Ca<br>1 1 | 0 | 0 |
| 33 | F | 1 | Total Ca<br>1 1 | 0 | 0 |
| 33 | O | 1 | Total Ca<br>1 1 | 0 | 0 |
| 33 | b | 1 | Total Ca<br>1 1 | 0 | 0 |
| 33 | c | 1 | Total Ca<br>1 1 | 0 | 0 |
| 33 | f | 1 | Total Ca<br>1 1 | 0 | 0 |
| 33 | o | 1 | Total Ca<br>1 1 | 0 | 0 |

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 34 | B | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | C | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | C | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | C | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | J | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | Z | 1 | Total C O<br>37 27 10 | 0 | 0 |
| 34 | a | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | b | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | c | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | c | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | j | 1 | Total C O<br>51 41 10 | 0 | 0 |
| 34 | z | 1 | Total C O<br>39 29 10 | 0 | 0 |

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



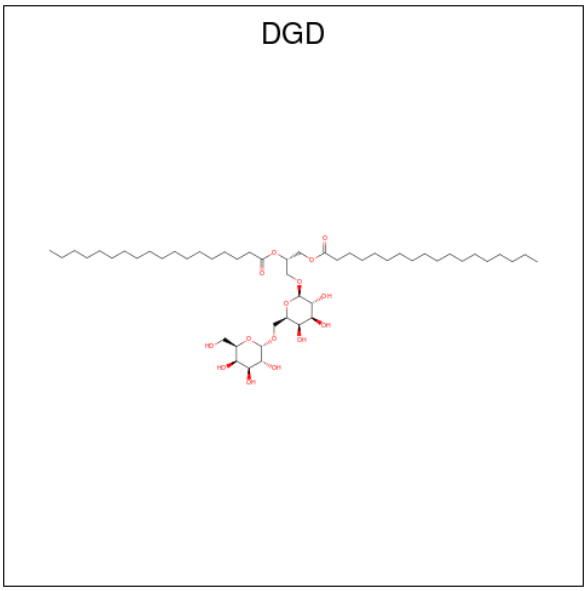

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | C | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | C | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | D | 1 | Total | C | O | S | 0 | 0 |
| | | | 16 | 10 | 5 | 1 | | |
| 35 | O | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | V | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 35 | c | 1 | Total C O S<br>19 13 5 1 | 0 | 0 |
| 35 | c | 1 | Total C O S<br>19 13 5 1 | 0 | 0 |
| 35 | d | 1 | Total C O S<br>16 10 5 1 | 0 | 0 |

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



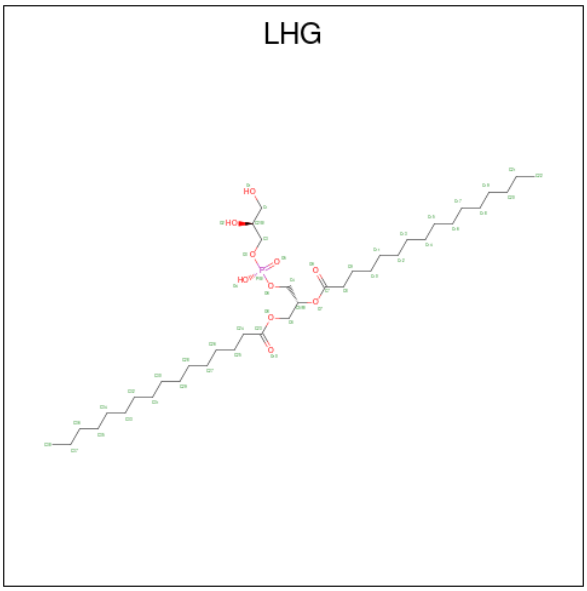

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 36 | C | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | C | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | C | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | D | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | H | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | c | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | c | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | c | 1 | Total C O<br>62 47 15 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 36 | d | 1 | Total C O<br>62 47 15 | 0 | 0 |
| 36 | h | 1 | Total C O<br>62 47 15 | 0 | 0 |

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



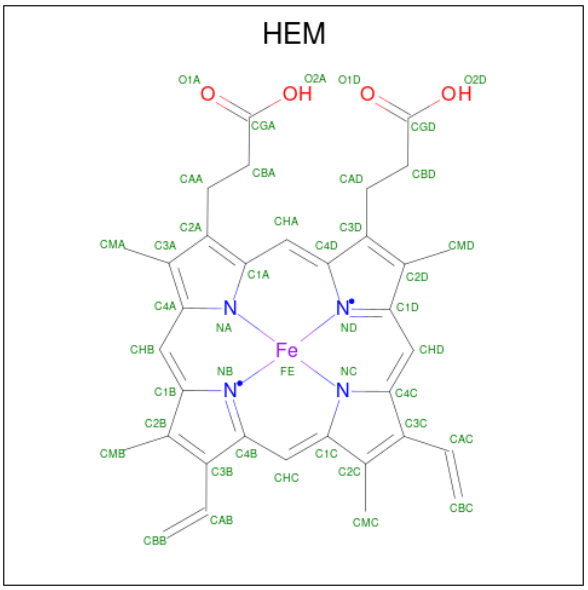

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 37 | D | 1 | Total C O P<br>49 38 10 1 | 0 | 0 |
| 37 | D | 1 | Total C O P<br>49 38 10 1 | 0 | 0 |
| 37 | D | 1 | Total C O P<br>49 38 10 1 | 0 | 0 |
| 37 | E | 1 | Total C O P<br>42 31 10 1 | 0 | 0 |
| 37 | L | 1 | Total C O P<br>49 38 10 1 | 0 | 0 |
| 37 | d | 1 | Total C O P<br>49 38 10 1 | 0 | 0 |
| 37 | d | 1 | Total C O P<br>49 38 10 1 | 0 | 0 |
| 37 | d | 1 | Total C O P<br>49 38 10 1 | 0 | 0 |
| 37 | e | 1 | Total C O P<br>42 31 10 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | l | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |

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

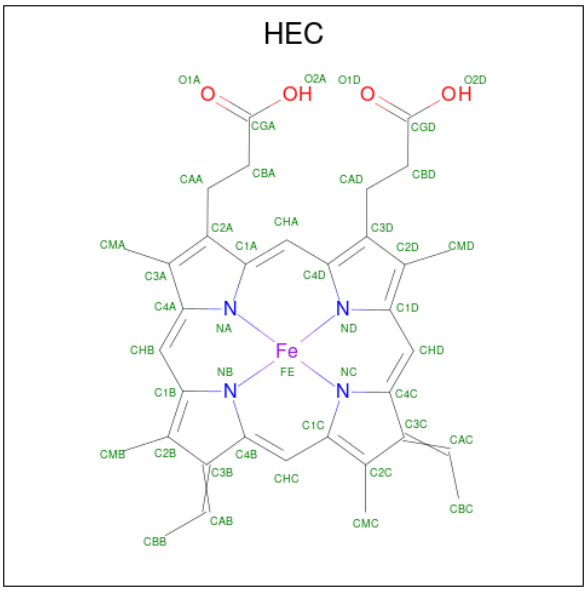



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 38 | E | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |
| 38 | e | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).




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

- Molecule 41 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 41 | A | 165 | Total | O | 0 | 2 |
| | | | 167 | 167 | | |
| 41 | B | 289 | Total | O | 0 | 4 |
| | | | 293 | 293 | | |
| 41 | C | 233 | Total | O | 0 | 2 |
| | | | 235 | 235 | | |
| 41 | D | 138 | Total | O | 0 | 5 |
| | | | 143 | 143 | | |
| 41 | E | 31 | Total | O | 0 | 0 |
| | | | 31 | 31 | | |
| 41 | F | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 41 | H | 48 | Total | O | 0 | 1 |
| | | | 49 | 49 | | |
| 41 | I | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 41 | J | 13 | Total | O | 0 | 0 |
| | | | 13 | 13 | | |
| 41 | K | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 41 | L | 16 | Total O<br>17 17 | 0 | 1 |
| 41 | M | 8 | Total O<br>8 8 | 0 | 0 |
| 41 | O | 188 | Total O<br>191 191 | 0 | 3 |
| 41 | T | 16 | Total O<br>17 17 | 0 | 1 |
| 41 | U | 81 | Total O<br>81 81 | 0 | 0 |
| 41 | V | 116 | Total O<br>118 118 | 0 | 2 |
| 41 | Y | 4 | Total O<br>4 4 | 0 | 0 |
| 41 | X | 9 | Total O<br>9 9 | 0 | 0 |
| 41 | Z | 1 | Total O<br>1 1 | 0 | 0 |
| 41 | a | 153 | Total O<br>154 154 | 0 | 1 |
| 41 | b | 261 | Total O<br>264 264 | 0 | 3 |
| 41 | c | 197 | Total O<br>199 199 | 0 | 2 |
| 41 | d | 132 | Total O<br>137 137 | 0 | 5 |
| 41 | e | 17 | Total O<br>17 17 | 0 | 0 |
| 41 | f | 5 | Total O<br>5 5 | 0 | 0 |
| 41 | h | 41 | Total O<br>41 41 | 0 | 0 |
| 41 | i | 6 | Total O<br>6 6 | 0 | 0 |
| 41 | j | 7 | Total O<br>7 7 | 0 | 0 |
| 41 | k | 6 | Total O<br>6 6 | 0 | 0 |
| 41 | l | 10 | Total O<br>10 10 | 0 | 0 |
| 41 | m | 18 | Total O<br>18 18 | 0 | 0 |

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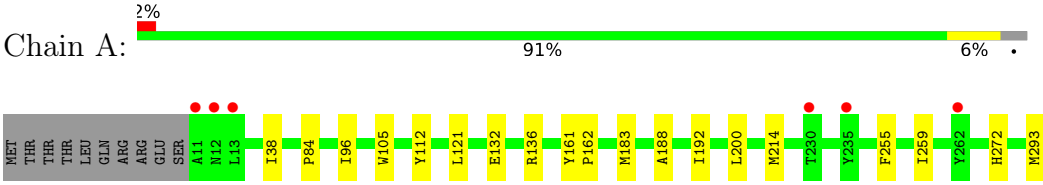
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 41 | o | 154 | Total O<br>155 155 | 0 | 1 |
| 41 | t | 12 | Total O<br>12 12 | 0 | 0 |
| 41 | u | 97 | Total O<br>97 97 | 0 | 0 |
| 41 | v | 89 | Total O<br>90 90 | 0 | 1 |
| 41 | y | 4 | Total O<br>4 4 | 0 | 0 |
| 41 | x | 4 | Total O<br>4 4 | 0 | 0 |

# 3 Residue-property plots (i)

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

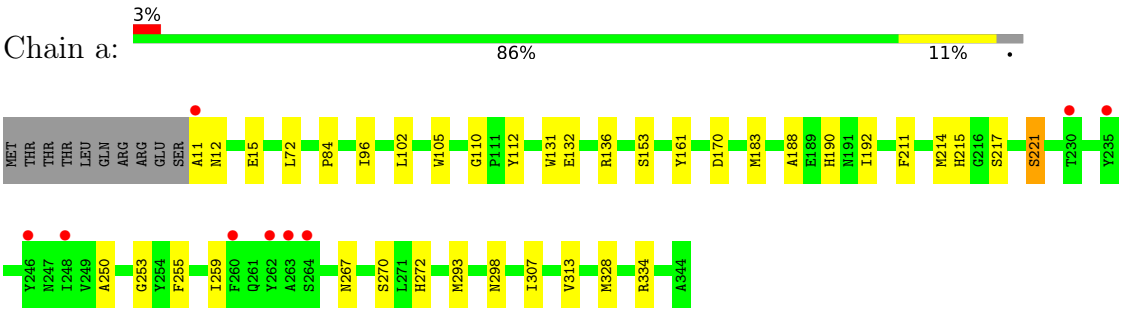
• Molecule 1: Photosystem Q(B) protein

Chain A:



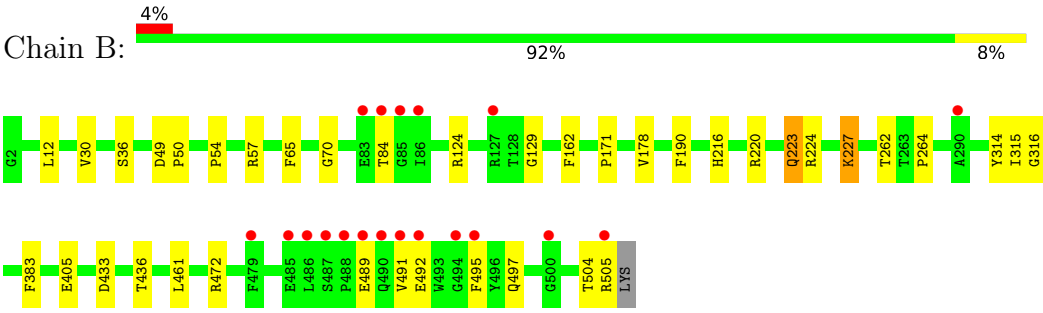

• Molecule 1: Photosystem Q(B) protein

Chain a:



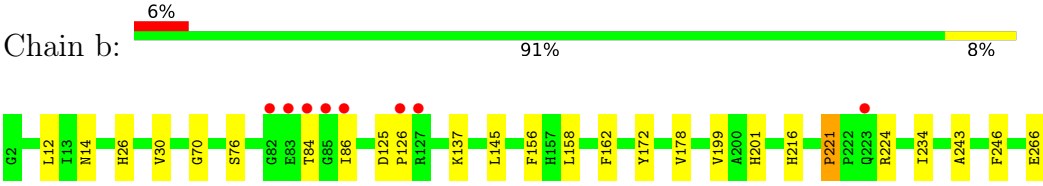

• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

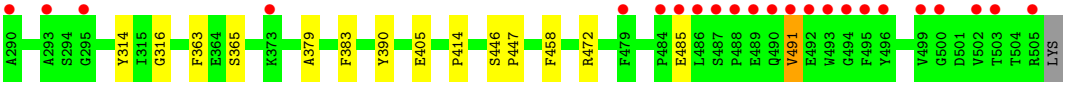
Chain B:



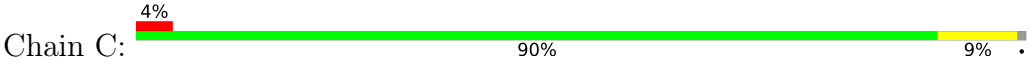

• Molecule 2: Photosystem II CP47 chlorophyll apoprotein

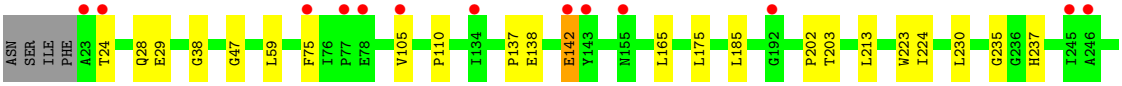
Chain b:

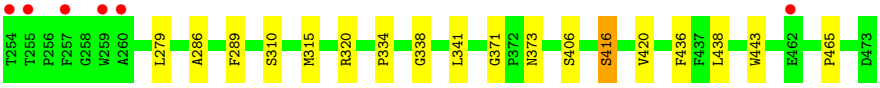





• Molecule 3: Photosystem II 44 kDa reaction center protein

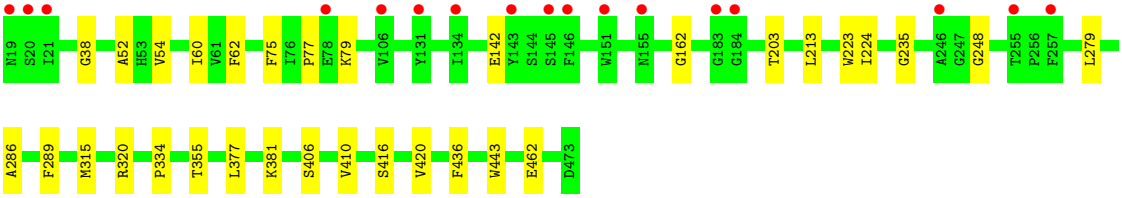


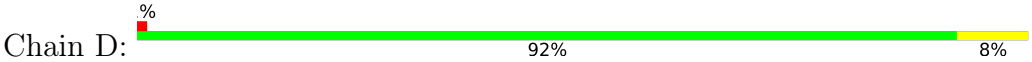




• Molecule 3: Photosystem II 44 kDa reaction center protein



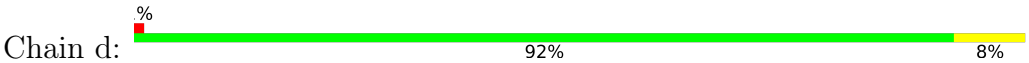

• Molecule 4: Photosystem II D2 protein







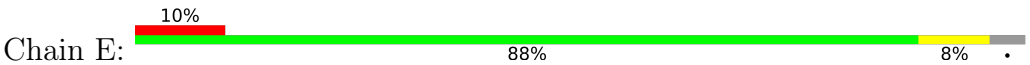
• Molecule 4: Photosystem II D2 protein

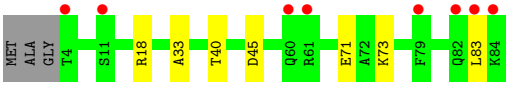






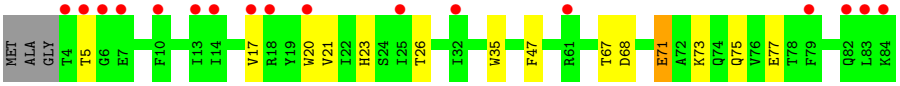
• Molecule 5: Cytochrome b559 subunit alpha



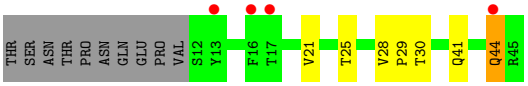

• Molecule 5: Cytochrome b559 subunit alpha





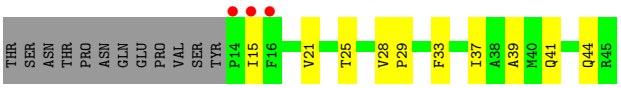

• Molecule 6: Cytochrome b559 subunit beta



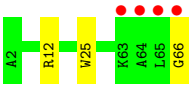

• Molecule 6: Cytochrome b559 subunit beta



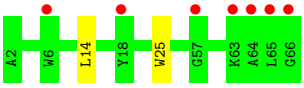

• Molecule 7: Photosystem II reaction center protein H



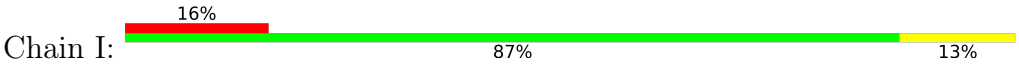



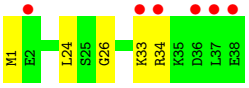

• Molecule 7: Photosystem II reaction center protein H



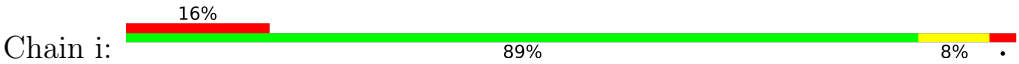



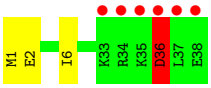

• Molecule 8: Photosystem II reaction center protein I



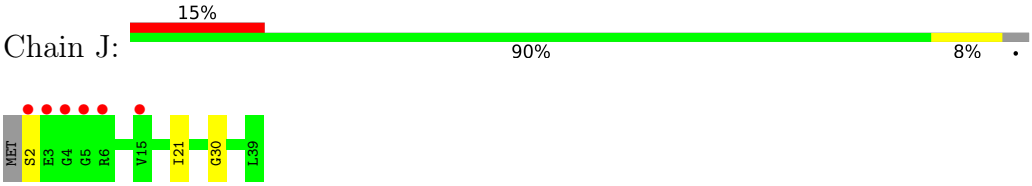

• Molecule 8: Photosystem II reaction center protein I



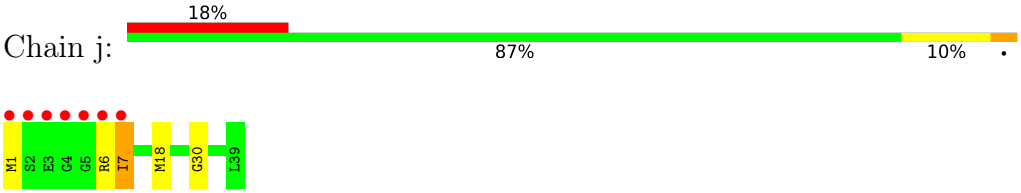

• Molecule 9: Photosystem II reaction center protein J

Chain J:



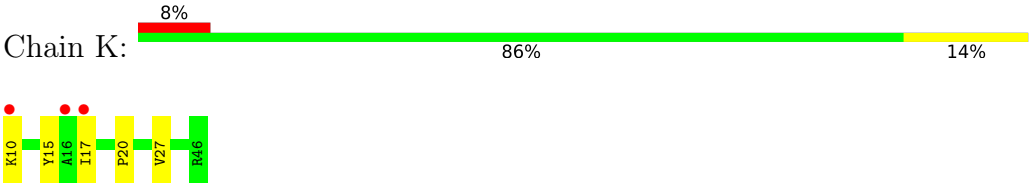

• Molecule 9: Photosystem II reaction center protein J

Chain j:



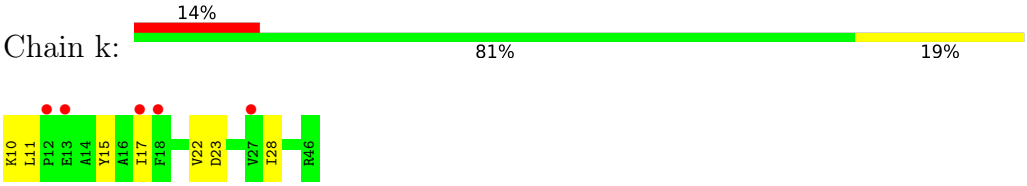

• Molecule 10: Photosystem II reaction center protein K

Chain K:



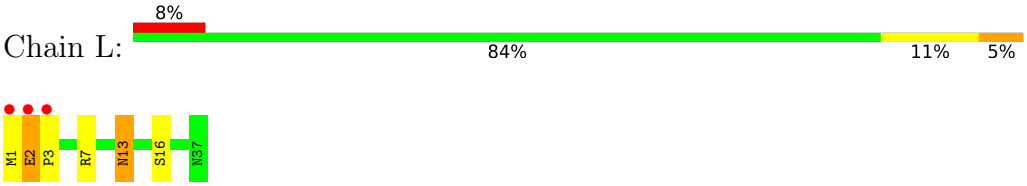

• Molecule 10: Photosystem II reaction center protein K

Chain k:



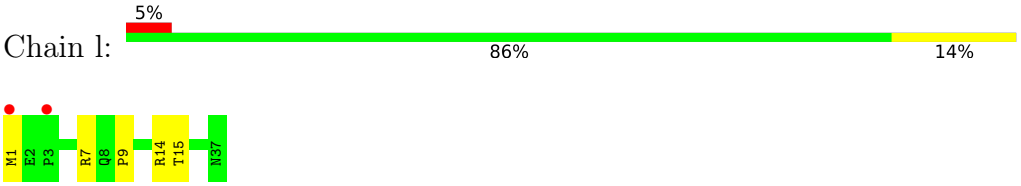

• Molecule 11: Photosystem II reaction center protein L

Chain L:



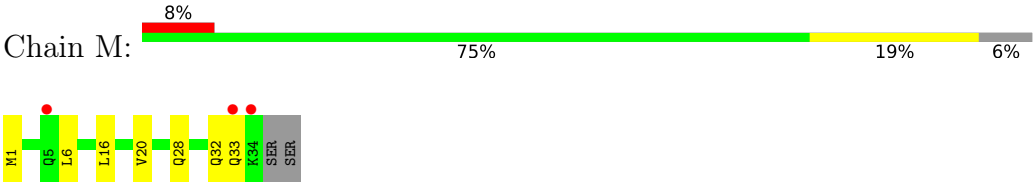

• Molecule 11: Photosystem II reaction center protein L

Chain l:




• Molecule 12: Photosystem II reaction center protein M

Chain M:



• Molecule 12: Photosystem II reaction center protein M

Chain m:



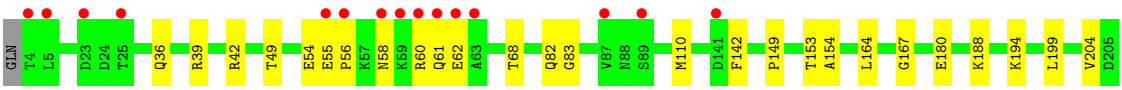


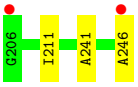


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



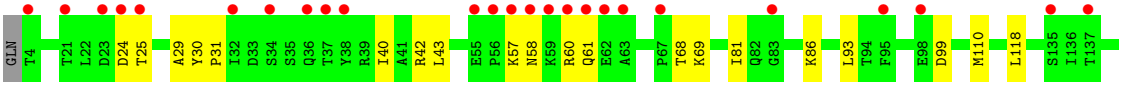



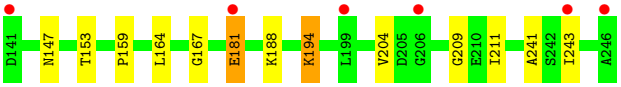




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



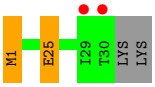




• Molecule 14: Photosystem II reaction center protein T

Chain T:

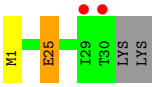



• Molecule 14: Photosystem II reaction center protein T

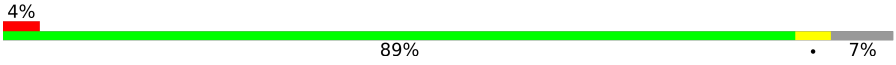
Chain t:

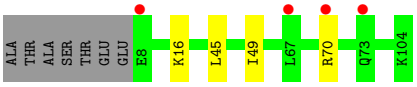



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:






• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

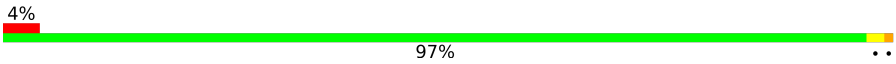


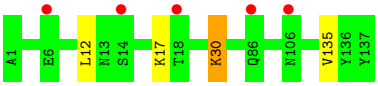




• Molecule 16: Cytochrome c-550

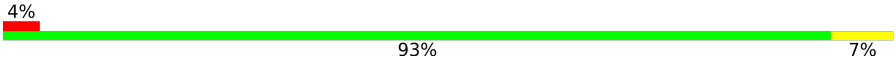
Chain V:

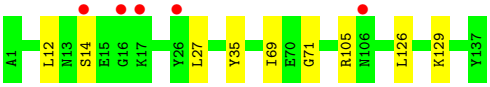



• Molecule 16: Cytochrome c-550

Chain v:

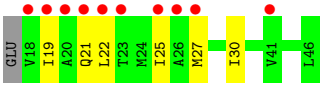



• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:

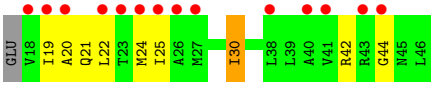



• Molecule 17: Photosystem II reaction center protein Ycf12

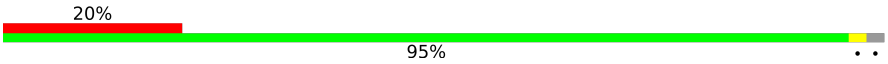
Chain y:

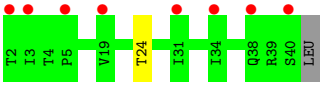



• Molecule 18: Photosystem II reaction center protein X

Chain X:

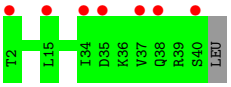



• Molecule 18: Photosystem II reaction center protein X

Chain x:

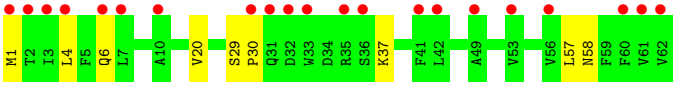



• Molecule 19: Photosystem II reaction center protein Z

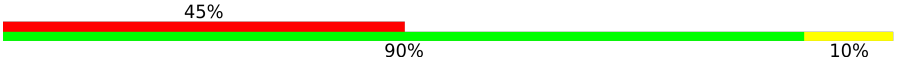
Chain Z:

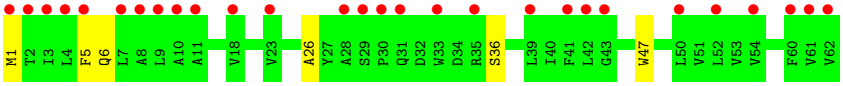



• Molecule 19: Photosystem II reaction center protein Z

Chain z:

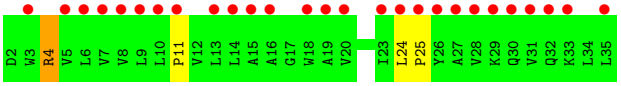



• Molecule 20: Photosystem II protein Y

Chain R:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 123.74Å 229.99Å 288.34Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 62.29 – 1.95<br>62.29 – 1.95 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.3 (62.29-1.95)<br>92.2 (62.29-1.95) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.67 (at 1.95Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8_1069) | Depositor |
| R, $R_{free}$ | 0.198 , 0.238<br>0.198 , 0.238 | Depositor<br>DCC |
| $R_{free}$ test set | 29338 reflections (3.64%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 20.2 | Xtriage |
| Anisotropy | 0.622 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.36 , 64.3 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 54195 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 34.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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

## 5.1 Standard geometry

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

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 | 0.66 | 0/2728 | 0.85 | 0/3719 |
| 1 | a | 0.65 | 0/2748 | 0.84 | 0/3746 |
| 2 | B | 0.60 | 0/4200 | 0.82 | 0/5721 |
| 2 | b | 0.57 | 0/4209 | 0.83 | 2/5734 (0.0%) |
| 3 | C | 0.56 | 1/3626 (0.0%) | 0.83 | 2/4936 (0.0%) |
| 3 | c | 0.56 | 1/3676 (0.0%) | 0.82 | 0/5004 |
| 4 | D | 0.65 | 0/2827 | 0.84 | 0/3852 |
| 4 | d | 0.63 | 0/2818 | 0.83 | 4/3840 (0.1%) |
| 5 | E | 0.47 | 0/693 | 0.87 | 1/944 (0.1%) |
| 5 | e | 0.45 | 0/695 | 0.78 | 0/948 |
| 6 | F | 0.52 | 0/284 | 0.79 | 0/387 |
| 6 | f | 0.56 | 0/265 | 0.85 | 0/360 |
| 7 | H | 0.51 | 0/535 | 0.84 | 0/728 |
| 7 | h | 0.47 | 0/524 | 0.78 | 0/713 |
| 8 | I | 0.43 | 0/311 | 0.85 | 0/419 |
| 8 | i | 0.48 | 0/311 | 0.79 | 0/419 |
| 9 | J | 0.53 | 0/278 | 0.81 | 0/376 |
| 9 | j | 0.51 | 0/286 | 0.86 | 2/386 (0.5%) |
| 10 | K | 0.47 | 0/303 | 0.80 | 0/416 |
| 10 | k | 0.57 | 0/303 | 0.78 | 0/416 |
| 11 | L | 0.58 | 0/319 | 0.73 | 0/433 |
| 11 | l | 0.53 | 0/319 | 0.75 | 0/433 |
| 12 | M | 0.61 | 0/270 | 0.89 | 0/368 |
| 12 | m | 0.74 | 0/262 | 0.95 | 0/357 |
| 13 | O | 0.50 | 0/1958 | 0.82 | 3/2654 (0.1%) |
| 13 | o | 0.48 | 0/1937 | 0.81 | 0/2625 |
| 14 | T | 0.63 | 0/266 | 0.81 | 0/362 |
| 14 | t | 0.69 | 0/266 | 0.71 | 0/362 |
| 15 | U | 0.54 | 0/785 | 0.80 | 0/1064 |
| 15 | u | 0.52 | 0/785 | 0.77 | 0/1064 |
| 16 | V | 0.56 | 0/1096 | 0.80 | 0/1487 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | v | 0.51 | 0/1085 | 0.82 | 1/1473 (0.1%) |
| 17 | Y | 0.46 | 0/216 | 0.80 | 0/289 |
| 17 | y | 0.45 | 0/216 | 0.85 | 0/289 |
| 18 | X | 0.46 | 0/290 | 0.73 | 0/392 |
| 18 | x | 0.42 | 0/290 | 0.76 | 0/392 |
| 19 | Z | 0.43 | 0/490 | 0.76 | 0/669 |
| 19 | z | 0.45 | 0/490 | 0.85 | 0/669 |
| 20 | R | 0.38 | 0/279 | 0.73 | 0/383 |
| All | All | 0.57 | 2/43239 (0.0%) | 0.82 | 15/58829 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | c | 410 | VAL | CA-CB | 5.56 | 1.59 | 1.54 |
| 3 | C | 310 | SER | C-O | 5.41 | 1.30 | 1.24 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | v | 105 | ARG | N-CA-C | 6.89 | 119.63 | 111.71 |
| 2 | b | 221 | PRO | O-C-N | 6.03 | 123.98 | 121.15 |
| 4 | d | 170 | ALA | CA-C-N | -5.69 | 114.07 | 119.76 |
| 4 | d | 170 | ALA | C-N-CA | -5.69 | 114.07 | 119.76 |
| 4 | d | 55 | VAL | N-CA-C | 5.51 | 116.92 | 108.71 |
| 3 | C | 371 | GLY | CA-C-N | 5.50 | 125.84 | 119.47 |
| 3 | C | 371 | GLY | C-N-CA | 5.50 | 125.84 | 119.47 |
| 9 | j | 7 | ILE | CA-C-N | 5.32 | 125.62 | 119.93 |
| 9 | j | 7 | ILE | C-N-CA | 5.32 | 125.62 | 119.93 |
| 4 | d | 330 | ALA | N-CA-C | 5.21 | 120.02 | 113.25 |
| 5 | E | 83 | LEU | N-CA-C | -5.17 | 107.49 | 112.97 |
| 13 | O | 55 | GLU | CA-C-N | 5.09 | 125.02 | 119.78 |
| 13 | O | 55 | GLU | C-N-CA | 5.09 | 125.02 | 119.78 |
| 13 | O | 154 | ALA | N-CA-C | 5.03 | 117.49 | 111.71 |
| 2 | b | 414 | PRO | N-CA-C | 5.03 | 116.83 | 110.70 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2634 | 0 | 2546 | 13 | 0 |
| 1 | a | 2645 | 0 | 2567 | 29 | 0 |
| 2 | B | 4027 | 0 | 3906 | 27 | 0 |
| 2 | b | 4033 | 0 | 3921 | 35 | 0 |
| 3 | C | 3501 | 0 | 3428 | 26 | 0 |
| 3 | c | 3544 | 0 | 3480 | 22 | 0 |
| 4 | D | 2729 | 0 | 2632 | 22 | 0 |
| 4 | d | 2720 | 0 | 2626 | 21 | 0 |
| 5 | E | 668 | 0 | 658 | 6 | 0 |
| 5 | e | 670 | 0 | 664 | 11 | 0 |
| 6 | F | 275 | 0 | 282 | 5 | 0 |
| 6 | f | 257 | 0 | 269 | 5 | 0 |
| 7 | H | 519 | 0 | 545 | 4 | 0 |
| 7 | h | 511 | 0 | 532 | 5 | 0 |
| 8 | I | 314 | 0 | 328 | 4 | 0 |
| 8 | i | 314 | 0 | 328 | 2 | 0 |
| 9 | J | 272 | 0 | 279 | 3 | 0 |
| 9 | j | 280 | 0 | 291 | 4 | 0 |
| 10 | K | 293 | 0 | 305 | 5 | 0 |
| 10 | k | 293 | 0 | 305 | 5 | 0 |
| 11 | L | 309 | 0 | 327 | 5 | 0 |
| 11 | l | 309 | 0 | 327 | 5 | 0 |
| 12 | M | 274 | 0 | 299 | 7 | 0 |
| 12 | m | 269 | 0 | 288 | 8 | 0 |
| 13 | O | 1903 | 0 | 1886 | 16 | 0 |
| 13 | o | 1891 | 0 | 1870 | 18 | 0 |
| 14 | T | 264 | 0 | 267 | 2 | 0 |
| 14 | t | 264 | 0 | 267 | 1 | 0 |
| 15 | U | 774 | 0 | 773 | 2 | 0 |
| 15 | u | 774 | 0 | 773 | 5 | 0 |
| 16 | V | 1072 | 0 | 1086 | 3 | 0 |
| 16 | v | 1064 | 0 | 1073 | 6 | 0 |
| 17 | Y | 215 | 0 | 246 | 3 | 0 |
| 17 | y | 215 | 0 | 246 | 5 | 0 |
| 18 | X | 287 | 0 | 317 | 1 | 0 |
| 18 | x | 287 | 0 | 317 | 0 | 0 |
| 19 | Z | 479 | 0 | 516 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 19 | z | 479 | 0 | 516 | 4 | 0 |
| 20 | R | 273 | 0 | 305 | 4 | 0 |
| 21 | A | 1 | 0 | 0 | 0 | 0 |
| 21 | a | 1 | 0 | 0 | 0 | 0 |
| 22 | A | 2 | 0 | 0 | 0 | 0 |
| 22 | U | 1 | 0 | 0 | 3 | 0 |
| 22 | a | 2 | 0 | 0 | 0 | 0 |
| 22 | v | 1 | 0 | 0 | 2 | 0 |
| 23 | A | 4 | 0 | 0 | 0 | 0 |
| 23 | a | 4 | 0 | 0 | 0 | 0 |
| 24 | A | 260 | 0 | 288 | 8 | 0 |
| 24 | B | 1040 | 0 | 1152 | 28 | 0 |
| 24 | C | 845 | 0 | 936 | 29 | 0 |
| 24 | D | 130 | 0 | 144 | 3 | 0 |
| 24 | a | 195 | 0 | 216 | 5 | 0 |
| 24 | b | 1040 | 0 | 1152 | 23 | 0 |
| 24 | c | 845 | 0 | 936 | 25 | 0 |
| 24 | d | 195 | 0 | 216 | 5 | 0 |
| 25 | A | 128 | 0 | 148 | 1 | 0 |
| 25 | a | 128 | 0 | 148 | 1 | 0 |
| 26 | A | 40 | 0 | 56 | 1 | 0 |
| 26 | B | 120 | 0 | 168 | 7 | 0 |
| 26 | C | 80 | 0 | 112 | 1 | 0 |
| 26 | D | 40 | 0 | 56 | 2 | 0 |
| 26 | H | 40 | 0 | 56 | 3 | 0 |
| 26 | K | 80 | 0 | 112 | 4 | 0 |
| 26 | T | 40 | 0 | 56 | 4 | 0 |
| 26 | a | 40 | 0 | 56 | 3 | 0 |
| 26 | b | 120 | 0 | 168 | 6 | 0 |
| 26 | c | 40 | 0 | 56 | 2 | 0 |
| 26 | d | 40 | 0 | 56 | 4 | 0 |
| 26 | h | 40 | 0 | 56 | 2 | 0 |
| 26 | k | 80 | 0 | 112 | 6 | 0 |
| 26 | t | 40 | 0 | 56 | 7 | 0 |
| 26 | y | 40 | 0 | 56 | 2 | 0 |
| 27 | A | 108 | 0 | 156 | 7 | 0 |
| 27 | B | 54 | 0 | 78 | 3 | 0 |
| 27 | F | 43 | 0 | 52 | 3 | 0 |
| 27 | L | 54 | 0 | 78 | 2 | 0 |
| 27 | a | 108 | 0 | 156 | 4 | 0 |
| 27 | f | 43 | 0 | 53 | 0 | 0 |
| 28 | A | 18 | 0 | 24 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 28 | B | 42 | 0 | 56 | 4 | 0 |
| 28 | C | 12 | 0 | 16 | 2 | 0 |
| 28 | F | 6 | 0 | 7 | 0 | 0 |
| 28 | O | 6 | 0 | 8 | 0 | 0 |
| 28 | T | 12 | 0 | 16 | 4 | 0 |
| 28 | V | 24 | 0 | 32 | 0 | 0 |
| 28 | a | 18 | 0 | 24 | 2 | 0 |
| 28 | b | 36 | 0 | 48 | 4 | 0 |
| 28 | c | 12 | 0 | 16 | 2 | 0 |
| 28 | f | 6 | 0 | 6 | 1 | 0 |
| 28 | o | 6 | 0 | 8 | 0 | 0 |
| 28 | t | 6 | 0 | 8 | 0 | 0 |
| 28 | v | 18 | 0 | 24 | 2 | 0 |
| 29 | A | 35 | 0 | 46 | 0 | 0 |
| 29 | B | 60 | 0 | 81 | 2 | 0 |
| 29 | C | 35 | 0 | 46 | 2 | 0 |
| 29 | E | 35 | 0 | 46 | 1 | 0 |
| 29 | M | 35 | 0 | 46 | 3 | 0 |
| 29 | a | 35 | 0 | 46 | 2 | 0 |
| 29 | b | 50 | 0 | 70 | 4 | 0 |
| 29 | c | 35 | 0 | 46 | 1 | 0 |
| 29 | f | 35 | 0 | 46 | 1 | 0 |
| 29 | m | 105 | 0 | 138 | 7 | 0 |
| 30 | A | 10 | 0 | 0 | 0 | 0 |
| 30 | a | 10 | 0 | 0 | 0 | 0 |
| 31 | A | 55 | 0 | 80 | 5 | 0 |
| 31 | D | 55 | 0 | 80 | 1 | 0 |
| 31 | a | 55 | 0 | 80 | 5 | 0 |
| 31 | d | 55 | 0 | 80 | 1 | 0 |
| 32 | A | 28 | 0 | 0 | 0 | 0 |
| 32 | B | 33 | 0 | 0 | 0 | 0 |
| 32 | D | 57 | 0 | 0 | 0 | 0 |
| 32 | I | 40 | 0 | 0 | 0 | 0 |
| 32 | J | 10 | 0 | 0 | 0 | 0 |
| 32 | K | 34 | 0 | 0 | 0 | 0 |
| 32 | M | 10 | 0 | 0 | 0 | 0 |
| 32 | X | 18 | 0 | 0 | 0 | 0 |
| 32 | a | 30 | 0 | 0 | 0 | 0 |
| 32 | b | 33 | 0 | 0 | 0 | 0 |
| 32 | c | 32 | 0 | 0 | 0 | 0 |
| 32 | d | 71 | 0 | 0 | 0 | 0 |
| 32 | i | 40 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 32 | j | 10 | 0 | 0 | 0 | 0 |
| 32 | m | 10 | 0 | 0 | 0 | 0 |
| 33 | B | 1 | 0 | 0 | 0 | 0 |
| 33 | F | 1 | 0 | 0 | 0 | 0 |
| 33 | O | 1 | 0 | 0 | 0 | 0 |
| 33 | b | 1 | 0 | 0 | 0 | 0 |
| 33 | c | 1 | 0 | 0 | 0 | 0 |
| 33 | f | 1 | 0 | 0 | 0 | 0 |
| 33 | o | 1 | 0 | 0 | 0 | 0 |
| 34 | B | 51 | 0 | 72 | 2 | 0 |
| 34 | C | 153 | 0 | 216 | 7 | 0 |
| 34 | J | 51 | 0 | 72 | 3 | 0 |
| 34 | Z | 37 | 0 | 44 | 3 | 0 |
| 34 | a | 51 | 0 | 72 | 3 | 0 |
| 34 | b | 51 | 0 | 72 | 2 | 0 |
| 34 | c | 102 | 0 | 144 | 2 | 0 |
| 34 | j | 51 | 0 | 72 | 5 | 0 |
| 34 | z | 39 | 0 | 48 | 2 | 0 |
| 35 | B | 95 | 0 | 130 | 3 | 0 |
| 35 | C | 38 | 0 | 52 | 1 | 0 |
| 35 | D | 16 | 0 | 17 | 3 | 0 |
| 35 | O | 19 | 0 | 26 | 1 | 0 |
| 35 | V | 19 | 0 | 26 | 0 | 0 |
| 35 | b | 76 | 0 | 104 | 0 | 0 |
| 35 | c | 38 | 0 | 52 | 1 | 0 |
| 35 | d | 16 | 0 | 17 | 2 | 0 |
| 36 | C | 186 | 0 | 246 | 8 | 0 |
| 36 | D | 62 | 0 | 82 | 5 | 0 |
| 36 | H | 62 | 0 | 82 | 1 | 0 |
| 36 | c | 186 | 0 | 246 | 5 | 0 |
| 36 | d | 62 | 0 | 82 | 6 | 0 |
| 36 | h | 62 | 0 | 82 | 0 | 0 |
| 37 | D | 147 | 0 | 222 | 9 | 0 |
| 37 | E | 42 | 0 | 57 | 2 | 0 |
| 37 | L | 49 | 0 | 74 | 1 | 0 |
| 37 | d | 147 | 0 | 222 | 8 | 0 |
| 37 | e | 42 | 0 | 57 | 1 | 0 |
| 37 | l | 49 | 0 | 74 | 2 | 0 |
| 38 | E | 43 | 0 | 30 | 0 | 0 |
| 38 | e | 43 | 0 | 30 | 2 | 0 |
| 39 | J | 1 | 0 | 0 | 0 | 0 |
| 39 | j | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | V | 43 | 0 | 30 | 0 | 0 |
| 40 | v | 43 | 0 | 30 | 0 | 0 |
| 41 | A | 167 | 0 | 0 | 0 | 0 |
| 41 | B | 293 | 0 | 0 | 2 | 0 |
| 41 | C | 235 | 0 | 0 | 1 | 0 |
| 41 | D | 143 | 0 | 0 | 2 | 0 |
| 41 | E | 31 | 0 | 0 | 0 | 0 |
| 41 | F | 9 | 0 | 0 | 0 | 0 |
| 41 | H | 49 | 0 | 0 | 0 | 0 |
| 41 | I | 4 | 0 | 0 | 0 | 0 |
| 41 | J | 13 | 0 | 0 | 1 | 0 |
| 41 | K | 8 | 0 | 0 | 1 | 0 |
| 41 | L | 17 | 0 | 0 | 0 | 0 |
| 41 | M | 8 | 0 | 0 | 0 | 0 |
| 41 | O | 191 | 0 | 0 | 4 | 0 |
| 41 | T | 17 | 0 | 0 | 0 | 0 |
| 41 | U | 81 | 0 | 0 | 3 | 0 |
| 41 | V | 118 | 0 | 0 | 1 | 0 |
| 41 | X | 9 | 0 | 0 | 0 | 0 |
| 41 | Y | 4 | 0 | 0 | 0 | 0 |
| 41 | Z | 1 | 0 | 0 | 1 | 0 |
| 41 | a | 154 | 0 | 0 | 3 | 0 |
| 41 | b | 264 | 0 | 0 | 2 | 0 |
| 41 | c | 199 | 0 | 0 | 1 | 0 |
| 41 | d | 137 | 0 | 0 | 2 | 0 |
| 41 | e | 17 | 0 | 0 | 0 | 0 |
| 41 | f | 5 | 0 | 0 | 0 | 0 |
| 41 | h | 41 | 0 | 0 | 0 | 0 |
| 41 | i | 6 | 0 | 0 | 0 | 0 |
| 41 | j | 7 | 0 | 0 | 0 | 0 |
| 41 | k | 6 | 0 | 0 | 0 | 0 |
| 41 | l | 10 | 0 | 0 | 0 | 0 |
| 41 | m | 18 | 0 | 0 | 0 | 0 |
| 41 | o | 155 | 0 | 0 | 0 | 0 |
| 41 | t | 12 | 0 | 0 | 0 | 0 |
| 41 | u | 97 | 0 | 0 | 2 | 0 |
| 41 | v | 90 | 0 | 0 | 0 | 0 |
| 41 | x | 4 | 0 | 0 | 0 | 0 |
| 41 | y | 4 | 0 | 0 | 1 | 0 |
| All | All | 54195 | 0 | 52838 | 501 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (501) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:214:MET:HG2 | 31:A:419:PL9:H102 | 1.48 | 0.95 |
| 5:e:67:THR:H | 5:e:75:GLN:HE22 | 1.13 | 0.94 |
| 12:M:16[C]:LEU:HD23 | 12:m:16:LEU:HD12 | 1.55 | 0.88 |
| 1:a:253:GLY:HA3 | 2:b:491:VAL:HG12 | 1.55 | 0.87 |
| 1:a:214:MET:HG2 | 31:a:417:PL9:H102 | 1.55 | 0.85 |
| 22:U:201:CL:CL | 41:U:305:HOH:O | 2.35 | 0.82 |
| 1:a:250:ALA:HA | 2:b:491:VAL:HG11 | 1.63 | 0.81 |
| 24:C:514:CLA:H202 | 34:C:521:LMG:H402 | 1.66 | 0.76 |
| 26:T:102:BCR:H19C | 26:b:622:BCR:H363 | 1.67 | 0.76 |
| 12:M:6:LEU:HD11 | 29:m:102:LMT:H21 | 1.68 | 0.76 |
| 28:a:414:GOL:H11 | 12:m:1:FME:HG2 | 1.69 | 0.73 |
| 28:A:414:GOL:H11 | 12:M:1:FME:HG2 | 1.71 | 0.73 |
| 41:b:754:HOH:O | 22:v:201:CL:CL | 2.43 | 0.73 |
| 14:T:25[A]:GLU:HG3 | 28:T:101:GOL:H2 | 1.70 | 0.72 |
| 37:D:408:LHG:H372 | 37:D:408:LHG:H132 | 1.72 | 0.72 |
| 34:j:101:LMG:H342 | 34:j:101:LMG:H241 | 1.72 | 0.72 |
| 22:U:201:CL:CL | 41:V:407:HOH:O | 2.46 | 0.70 |
| 2:B:223[B]:GLN:NE2 | 41:B:943:HOH:O | 2.23 | 0.70 |
| 10:K:15:TYR:OH | 19:Z:58:ASN:ND2 | 2.23 | 0.69 |
| 3:C:286:ALA:HB2 | 24:C:503:CLA:HMD1 | 1.75 | 0.69 |
| 27:A:412:SQD:H251 | 37:D:408:LHG:H131 | 1.74 | 0.68 |
| 36:D:405:DGD:O1B | 36:D:405:DGD:O2D | 2.11 | 0.68 |
| 5:E:45:ASP:OD2 | 20:R:4:ARG:NH2 | 2.27 | 0.68 |
| 34:j:101:LMG:H321 | 34:j:101:LMG:H221 | 1.75 | 0.68 |
| 3:c:279:LEU:HD22 | 24:c:910:CLA:HED2 | 1.75 | 0.68 |
| 22:U:201:CL:CL | 41:U:331:HOH:O | 2.49 | 0.67 |
| 36:C:519:DGD:HA32 | 34:J:101:LMG:H121 | 1.77 | 0.67 |
| 24:c:903:CLA:H61 | 24:c:913:CLA:H42 | 1.76 | 0.66 |
| 28:T:103:GOL:H2 | 29:b:601:LMT:H2' | 1.76 | 0.66 |
| 2:b:266:GLU:HB3 | 28:b:633:GOL:H11 | 1.78 | 0.66 |
| 24:C:509:CLA:H92 | 37:D:408:LHG:H371 | 1.77 | 0.65 |
| 34:c:920:LMG:H391 | 34:c:920:LMG:H232 | 1.77 | 0.65 |
| 41:u:242:HOH:O | 22:v:201:CL:CL | 2.52 | 0.65 |
| 4:D:139:ARG:NH2 | 41:D:629:HOH:O | 2.30 | 0.65 |
| 24:b:615:CLA:H142 | 37:l:101:LHG:H361 | 1.78 | 0.65 |
| 26:K:102:BCR:H321 | 26:K:102:BCR:HC8 | 1.80 | 0.64 |
| 26:H:101:BCR:HC8 | 26:H:101:BCR:H331 | 1.79 | 0.63 |
| 13:o:40:ILE:HG12 | 13:o:243:ILE:HD13 | 1.80 | 0.63 |
| 15:U:16:LYS:NZ | 41:U:347:HOH:O | 2.30 | 0.62 |
| 24:a:409:CLA:H152 | 24:c:907:CLA:H142 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:j:101:LMG:H292 | 34:j:101:LMG:H142 | 1.81 | 0.61 |
| 11:L:2:GLU:HG2 | 11:L:3:PRO:HD2 | 1.82 | 0.61 |
| 24:c:911:CLA:H41 | 37:d:409:LHG:H383 | 1.83 | 0.61 |
| 2:b:224:ARG:HH11 | 29:b:625:LMT:H1' | 1.66 | 0.61 |
| 4:d:192:THR:HG23 | 24:d:402:CLA:HBC2 | 1.83 | 0.61 |
| 2:b:224:ARG:NH1 | 29:b:625:LMT:H1' | 2.15 | 0.60 |
| 16:v:71:GLY:HA2 | 28:v:203:GOL:H32 | 1.83 | 0.60 |
| 6:F:30:THR:HG21 | 34:J:101:LMG:H412 | 1.82 | 0.60 |
| 12:M:16[C]:LEU:CD2 | 12:m:16:LEU:HD12 | 2.29 | 0.60 |
| 36:D:405:DGD:HD4 | 5:E:45:ASP:HB3 | 1.83 | 0.60 |
| 28:a:414:GOL:O1 | 41:a:523:HOH:O | 2.16 | 0.59 |
| 1:A:121[B]:LEU:HD11 | 24:C:506:CLA:H122 | 1.85 | 0.59 |
| 12:M:16[C]:LEU:HD23 | 12:m:16:LEU:CD1 | 2.28 | 0.59 |
| 24:C:507:CLA:HMC2 | 24:C:508:CLA:H102 | 1.83 | 0.58 |
| 28:T:103:GOL:H12 | 29:m:104:LMT:H12 | 1.85 | 0.58 |
| 24:b:613:CLA:HHC | 24:b:613:CLA:HBB1 | 1.84 | 0.58 |
| 1:a:298:ASN:ND2 | 41:a:578:HOH:O | 2.33 | 0.58 |
| 12:m:6:LEU:HD11 | 29:m:104:LMT:H11 | 1.84 | 0.58 |
| 1:a:211:PHE:CE2 | 31:a:417:PL9:H13 | 2.38 | 0.58 |
| 24:C:503:CLA:H61 | 24:C:513:CLA:H42 | 1.85 | 0.58 |
| 29:B:636:LMT:H2' | 28:B:637:GOL:H2 | 1.85 | 0.57 |
| 36:D:405:DGD:HA42 | 36:D:405:DGD:HB22 | 1.86 | 0.57 |
| 16:V:12:LEU:HD23 | 16:V:17:LYS:HD3 | 1.85 | 0.57 |
| 24:b:619:CLA:H2 | 24:b:620:CLA:HBB2 | 1.86 | 0.57 |
| 24:B:602:CLA:H12 | 24:B:602:CLA:H71 | 1.85 | 0.57 |
| 24:B:616:CLA:H71 | 24:B:617:CLA:H192 | 1.85 | 0.57 |
| 3:c:443:TRP:CE2 | 24:c:909:CLA:HMD2 | 2.40 | 0.57 |
| 3:c:54:VAL:HG22 | 24:c:914:CLA:HBB1 | 1.87 | 0.57 |
| 24:C:510:CLA:HMB1 | 24:C:510:CLA:HBB1 | 1.87 | 0.56 |
| 4:d:101:PHE:HB3 | 36:d:406:DGD:HG2 | 1.86 | 0.56 |
| 11:L:13:ASN:C | 11:L:13:ASN:HD22 | 2.14 | 0.56 |
| 2:b:234:ILE:HB | 28:b:632:GOL:H31 | 1.86 | 0.56 |
| 13:o:204:VAL:HG22 | 13:o:211:ILE:HG22 | 1.87 | 0.56 |
| 36:d:406:DGD:O1B | 36:d:406:DGD:O2D | 2.25 | 0.55 |
| 3:c:320:ARG:HB2 | 28:c:925:GOL:H32 | 1.88 | 0.55 |
| 3:C:320:ARG:HB2 | 28:C:525:GOL:H32 | 1.88 | 0.55 |
| 11:L:13:ASN:ND2 | 11:L:16:SER:H | 2.03 | 0.55 |
| 24:B:605:CLA:HBB1 | 24:B:605:CLA:HMB1 | 1.89 | 0.55 |
| 28:B:637:GOL:H12 | 29:m:102:LMT:H11 | 1.88 | 0.55 |
| 3:C:406:SER:HA | 3:C:420:VAL:HG23 | 1.89 | 0.55 |
| 16:v:14:SER:OG | 28:v:203:GOL:O1 | 2.24 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:307[B]:ILE:HG22 | 1:a:313:VAL:HA | 1.89 | 0.55 |
| 24:B:617:CLA:H121 | 26:B:620:BCR:H12C | 1.89 | 0.55 |
| 37:d:409:LHG:H381 | 37:d:409:LHG:H122 | 1.88 | 0.55 |
| 1:A:214:MET:HE2 | 1:A:255:PHE:CE1 | 2.41 | 0.55 |
| 31:a:417:PL9:H28 | 37:e:101:LHG:H222 | 1.89 | 0.55 |
| 34:C:501:LMG:H161 | 36:C:517:DGD:HA62 | 1.89 | 0.55 |
| 34:c:920:LMG:H321 | 26:k:101:BCR:H342 | 1.87 | 0.54 |
| 24:c:907:CLA:HMC2 | 24:c:908:CLA:H102 | 1.89 | 0.54 |
| 8:i:36:ASP:OD1 | 8:i:36:ASP:N | 2.38 | 0.54 |
| 28:B:637:GOL:H31 | 29:m:102:LMT:H6D | 1.88 | 0.54 |
| 27:L:102:SQD:H1 | 27:L:102:SQD:H462 | 1.88 | 0.54 |
| 26:y:101:BCR:H321 | 26:y:101:BCR:HC8 | 1.89 | 0.54 |
| 25:A:409:PHO:HBC3 | 4:D:279:LEU:HD22 | 1.90 | 0.54 |
| 13:O:82:GLN:NE2 | 41:O:566:HOH:O | 2.40 | 0.53 |
| 3:c:377:LEU:HG | 3:c:381:LYS:HE3 | 1.89 | 0.53 |
| 28:f:101:GOL:H11 | 16:v:27:LEU:HD21 | 1.90 | 0.53 |
| 24:A:410:CLA:H193 | 24:C:507:CLA:H93 | 1.91 | 0.53 |
| 1:A:84:PRO:HA | 1:A:112:TYR:CG | 2.44 | 0.53 |
| 4:d:103:ARG:HH21 | 5:e:77:GLU:HG3 | 1.73 | 0.53 |
| 24:C:509:CLA:HBC3 | 24:C:511:CLA:H71 | 1.90 | 0.53 |
| 29:M:101:LMT:H6'1 | 11:l:9:PRO:HB3 | 1.91 | 0.53 |
| 3:C:465:PRO:HG3 | 8:I:33:LYS:HE2 | 1.91 | 0.52 |
| 3:c:334:PRO:HA | 13:o:153:THR:OG1 | 2.10 | 0.52 |
| 35:B:633:HTG:H61 | 1:a:102:LEU:HD12 | 1.90 | 0.52 |
| 26:H:101:BCR:H331 | 26:H:101:BCR:C8 | 2.37 | 0.52 |
| 34:B:622:LMG:HC5 | 29:m:102:LMT:H12 | 1.91 | 0.52 |
| 24:A:410:CLA:H171 | 24:C:507:CLA:H142 | 1.90 | 0.52 |
| 24:c:913:CLA:O2D | 24:c:914:CLA:HBB2 | 2.10 | 0.52 |
| 24:C:511:CLA:H43 | 37:D:408:LHG:H383 | 1.92 | 0.52 |
| 34:J:101:LMG:H152 | 34:J:101:LMG:H292 | 1.92 | 0.52 |
| 28:b:631:GOL:H11 | 15:u:22:GLY:HA2 | 1.92 | 0.52 |
| 1:A:183:MET:HA | 24:A:405:CLA:HMD1 | 1.91 | 0.52 |
| 31:A:419:PL9:H502 | 4:D:39:PRO:HG3 | 1.93 | 0.51 |
| 34:C:501:LMG:H382 | 36:C:517:DGD:HB51 | 1.91 | 0.51 |
| 3:C:438:LEU:HD11 | 24:C:506:CLA:HBB1 | 1.92 | 0.51 |
| 2:b:70:GLY:HA2 | 2:b:178:VAL:HG21 | 1.91 | 0.51 |
| 3:c:213[B]:LEU:HD11 | 26:c:915:BCR:H373 | 1.93 | 0.51 |
| 6:f:41:GLN:OE1 | 9:j:30:GLY:HA3 | 2.10 | 0.51 |
| 24:B:609:CLA:HBB2 | 4:D:150:ILE:HD12 | 1.91 | 0.51 |
| 13:O:60:ARG:NH1 | 2:b:405:GLU:O | 2.44 | 0.51 |
| 4:D:123:ILE:HD11 | 36:H:102:DGD:HAE1 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:Z:4:LEU:HD22 | 19:Z:57:LEU:HD11 | 1.93 | 0.51 |
| 29:f:103:LMT:O3' | 29:f:103:LMT:O2B | 2.27 | 0.51 |
| 24:C:511:CLA:H192 | 24:C:511:CLA:HBC3 | 1.92 | 0.51 |
| 2:B:30:VAL:HG12 | 24:B:606:CLA:HHD | 1.93 | 0.51 |
| 2:b:383:PHE:CZ | 13:o:167:GLY:HA2 | 2.45 | 0.51 |
| 26:B:619:BCR:H363 | 26:t:101:BCR:H19C | 1.93 | 0.50 |
| 2:b:145:LEU:HD22 | 24:b:608:CLA:H192 | 1.92 | 0.50 |
| 29:M:101:LMT:H6'2 | 12:m:32:GLN:HG2 | 1.92 | 0.50 |
| 8:i:2:GLU:O | 8:i:6:ILE:HG12 | 2.12 | 0.50 |
| 26:B:620:BCR:H331 | 26:B:620:BCR:C8 | 2.42 | 0.50 |
| 2:b:86[B]:ILE:HD13 | 2:b:86[B]:ILE:H | 1.76 | 0.50 |
| 36:d:406:DGD:HBT2 | 5:e:47:PHE:HZ | 1.76 | 0.50 |
| 27:A:412:SQD:H381 | 9:J:21:ILE:HD11 | 1.93 | 0.50 |
| 2:B:162:PHE:O | 24:B:607:CLA:HHD | 2.11 | 0.50 |
| 1:a:188:ALA:HB2 | 1:a:328:MET:HB2 | 1.92 | 0.50 |
| 4:d:139:ARG:NH2 | 41:d:627:HOH:O | 2.43 | 0.50 |
| 2:B:383:PHE:CZ | 13:O:167:GLY:HA2 | 2.45 | 0.50 |
| 3:C:279:LEU:HD22 | 24:C:510:CLA:HED2 | 1.93 | 0.50 |
| 3:c:443:TRP:CD2 | 24:c:909:CLA:HMD2 | 2.46 | 0.50 |
| 3:C:223:TRP:CG | 3:C:224:ILE:H | 2.30 | 0.50 |
| 29:B:623:LMT:O6' | 4:D:16:ASP:OD2 | 2.30 | 0.50 |
| 2:b:201:HIS:HB2 | 24:b:606:CLA:CHB | 2.42 | 0.49 |
| 24:c:902:CLA:C4D | 24:c:904:CLA:H2 | 2.42 | 0.49 |
| 6:F:21:VAL:O | 6:F:25:THR:HG23 | 2.12 | 0.49 |
| 2:b:491:VAL:HG13 | 4:d:136:VAL:HG13 | 1.95 | 0.49 |
| 3:c:381:LYS:NZ | 13:o:99:ASP:OD2 | 2.42 | 0.49 |
| 2:b:224:ARG:HD3 | 7:h:25:TRP:CE2 | 2.46 | 0.49 |
| 2:b:216:HIS:HE1 | 24:b:613:CLA:C1A | 2.25 | 0.49 |
| 1:a:214:MET:HE2 | 1:a:255:PHE:CE1 | 2.48 | 0.49 |
| 1:a:267:ASN:HB3 | 1:a:270[B]:SER:OG | 2.13 | 0.49 |
| 17:y:20:ALA:O | 17:y:24:MET:HG2 | 2.13 | 0.49 |
| 2:B:497:GLN:HB2 | 2:B:504:THR:HB | 1.95 | 0.49 |
| 2:b:12:LEU:HB2 | 24:b:616:CLA:HMC2 | 1.94 | 0.49 |
| 13:o:181[A]:GLU:H | 13:o:181[A]:GLU:CD | 2.20 | 0.49 |
| 1:A:38:ILE:HG12 | 27:A:416:SQD:H142 | 1.94 | 0.49 |
| 24:c:910:CLA:H191 | 24:c:913:CLA:HAC1 | 1.95 | 0.48 |
| 4:D:103:ARG:HG3 | 5:E:73:LYS:HE2 | 1.96 | 0.48 |
| 13:o:58:ASN:HD21 | 13:o:61:GLN:HB2 | 1.76 | 0.48 |
| 2:B:49:ASP:OD1 | 13:o:57:LYS:NZ | 2.44 | 0.48 |
| 2:B:489:GLU:HB3 | 2:B:495:PHE:CD1 | 2.48 | 0.48 |
| 26:d:404:BCR:HC22 | 36:d:406:DGD:HA71 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:D:408:LHG:H382 | 37:D:408:LHG:H112 | 1.96 | 0.48 |
| 12:M:20:VAL:HG22 | 12:m:20:VAL:HG11 | 1.95 | 0.48 |
| 27:B:621:SQD:H462 | 27:B:621:SQD:H1 | 1.94 | 0.48 |
| 19:z:47:TRP:CE2 | 34:z:101:LMG:H241 | 2.48 | 0.48 |
| 3:C:185:LEU:HB2 | 3:C:230:LEU:HD13 | 1.95 | 0.48 |
| 29:C:522:LMT:H6'1 | 8:I:26:GLY:HA3 | 1.95 | 0.48 |
| 25:a:420:PHO:NC | 25:a:420:PHO:ND | 2.61 | 0.48 |
| 26:b:622:BCR:H331 | 26:b:622:BCR:C8 | 2.44 | 0.48 |
| 13:O:42:ARG:O | 13:O:241:ALA:HA | 2.14 | 0.48 |
| 27:a:411:SQD:H321 | 24:c:909:CLA:H71 | 1.95 | 0.48 |
| 24:c:903:CLA:H193 | 35:c:922:HTG:H3'1 | 1.95 | 0.48 |
| 36:d:406:DGD:HE3 | 36:d:406:DGD:HD4 | 1.96 | 0.48 |
| 37:d:409:LHG:H302 | 37:d:409:LHG:H332 | 1.38 | 0.48 |
| 13:o:42:ARG:O | 13:o:241:ALA:HA | 2.14 | 0.48 |
| 2:B:341:LYS:HA | 2:B:405[A]:GLU:HG2 | 1.96 | 0.47 |
| 24:a:406:CLA:HBB1 | 24:a:406:CLA:HMB3 | 1.95 | 0.47 |
| 35:O:303:HTG:HO6 | 2:b:76[A]:SER:HG | 1.63 | 0.47 |
| 2:B:216:HIS:HE1 | 24:B:610:CLA:C1A | 2.27 | 0.47 |
| 26:k:102:BCR:H24C | 26:k:102:BCR:H371 | 1.64 | 0.47 |
| 6:F:28:VAL:HB | 6:F:29:PRO:HD3 | 1.96 | 0.47 |
| 27:a:411:SQD:H251 | 37:d:409:LHG:H132 | 1.95 | 0.47 |
| 36:c:917:DGD:HB61 | 36:c:917:DGD:HB32 | 1.62 | 0.47 |
| 26:d:404:BCR:H381 | 34:j:101:LMG:H232 | 1.96 | 0.47 |
| 5:e:35:TRP:CD2 | 6:f:39:ALA:HB2 | 2.50 | 0.47 |
| 4:D:49:LEU:HD13 | 26:D:403:BCR:C15 | 2.44 | 0.47 |
| 4:d:85:MET:HE1 | 4:d:96:GLU:HG2 | 1.97 | 0.47 |
| 35:d:412:HTG:H1 | 7:h:25:TRP:CD1 | 2.49 | 0.47 |
| 17:y:44:GLY:O | 41:y:203:HOH:O | 2.20 | 0.47 |
| 9:j:6:ARG:HA | 9:j:6:ARG:NH2 | 2.30 | 0.47 |
| 1:a:132:GLU:O | 1:a:136:ARG:HG2 | 2.15 | 0.47 |
| 9:j:18:MET:HE1 | 17:y:30:ILE:HD12 | 1.97 | 0.47 |
| 27:a:402:SQD:H142 | 26:t:101:BCR:HC41 | 1.96 | 0.47 |
| 16:v:12:LEU:HD12 | 16:v:69:ILE:HB | 1.97 | 0.47 |
| 24:B:617:CLA:HED2 | 24:B:617:CLA:H43 | 1.96 | 0.47 |
| 3:C:24:THR:HB | 3:C:138:GLU:OE1 | 2.15 | 0.47 |
| 13:O:68:THR:HG22 | 13:O:110[B]:MET:HG2 | 1.97 | 0.47 |
| 26:T:102:BCR:HC8 | 26:T:102:BCR:H311 | 1.96 | 0.47 |
| 37:d:409:LHG:H331 | 37:d:409:LHG:H361 | 1.67 | 0.47 |
| 2:B:224:ARG:HD3 | 7:H:25:TRP:CE2 | 2.50 | 0.46 |
| 3:C:203:THR:O | 3:C:235:GLY:HA3 | 2.15 | 0.46 |
| 4:D:27:PHE:HD1 | 37:E:101:LHG:HC12 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:a:272:HIS:CD2 | 4:d:218:VAL:HG21 | 2.50 | 0.46 |
| 29:C:522:LMT:H31 | 8:I:24:LEU:HD13 | 1.98 | 0.46 |
| 1:a:96:ILE:HG12 | 1:a:105:TRP:CE2 | 2.51 | 0.46 |
| 10:K:20:PRO:HB3 | 17:Y:21:GLN:HG3 | 1.96 | 0.46 |
| 4:d:101:PHE:HB2 | 36:d:406:DGD:HA41 | 1.97 | 0.46 |
| 19:z:26:ALA:HB1 | 19:z:36:SER:HB3 | 1.98 | 0.46 |
| 1:a:153:SER:HB2 | 24:a:406:CLA:H43 | 1.97 | 0.46 |
| 36:C:518:DGD:HA81 | 36:C:518:DGD:HAE2 | 1.61 | 0.46 |
| 34:C:520:LMG:H192 | 10:K:27:VAL:HG11 | 1.97 | 0.46 |
| 34:C:521:LMG:HC1 | 34:C:521:LMG:HC8 | 1.74 | 0.46 |
| 1:a:84:PRO:HA | 1:a:112:TYR:CG | 2.51 | 0.46 |
| 13:o:30:TYR:CD1 | 13:o:209:GLY:HA2 | 2.51 | 0.46 |
| 27:A:412:SQD:O7 | 3:C:28:GLN:NE2 | 2.30 | 0.46 |
| 3:C:59:LEU:HD21 | 26:K:103:BCR:H372 | 1.97 | 0.46 |
| 24:D:402:CLA:HAC1 | 27:F:101:SQD:H383 | 1.98 | 0.46 |
| 26:K:103:BCR:H24C | 26:K:103:BCR:H371 | 1.73 | 0.46 |
| 24:d:403:CLA:H142 | 24:d:403:CLA:H112 | 1.71 | 0.46 |
| 17:Y:22:LEU:HA | 17:Y:25:ILE:HG22 | 1.98 | 0.46 |
| 1:a:183:MET:HA | 24:a:406:CLA:HMD1 | 1.98 | 0.46 |
| 19:z:47:TRP:CE3 | 34:z:101:LMG:H221 | 2.51 | 0.46 |
| 37:D:406:LHG:H101 | 37:D:406:LHG:H351 | 1.98 | 0.46 |
| 11:L:13:ASN:HD22 | 11:L:16:SER:H | 1.64 | 0.46 |
| 1:a:131:TRP:CH2 | 24:c:906:CLA:HAA2 | 2.51 | 0.46 |
| 3:C:38:GLY:HA3 | 24:C:512:CLA:HMD2 | 1.98 | 0.45 |
| 27:L:102:SQD:H62 | 11:l:7:ARG:NH1 | 2.31 | 0.45 |
| 4:d:223:PHE:CZ | 4:d:245:SER:HB2 | 2.51 | 0.45 |
| 4:d:341:PHE:O | 41:d:614:HOH:O | 2.21 | 0.45 |
| 26:h:101:BCR:H24C | 26:h:101:BCR:H371 | 1.70 | 0.45 |
| 31:A:419:PL9:H251 | 31:A:419:PL9:H271 | 1.62 | 0.45 |
| 24:B:614:CLA:H143 | 24:B:614:CLA:H111 | 1.84 | 0.45 |
| 4:D:304:ARG:NH1 | 41:D:504:HOH:O | 2.29 | 0.45 |
| 26:H:101:BCR:H24C | 26:H:101:BCR:H371 | 1.76 | 0.45 |
| 2:b:156:PHE:HB3 | 2:b:162:PHE:HB3 | 1.98 | 0.45 |
| 24:b:605:CLA:H202 | 26:h:101:BCR:H353 | 1.97 | 0.45 |
| 3:c:62:PHE:HZ | 10:k:28:ILE:HD12 | 1.80 | 0.45 |
| 1:A:272:HIS:CD2 | 4:D:218:VAL:HG21 | 2.50 | 0.45 |
| 3:C:436:PHE:CE1 | 24:C:505:CLA:H161 | 2.51 | 0.45 |
| 29:E:102:LMT:O3' | 29:E:102:LMT:O2B | 2.30 | 0.45 |
| 1:a:72:LEU:HD11 | 29:a:401:LMT:H52 | 1.98 | 0.45 |
| 37:d:408:LHG:HC62 | 11:l:15:THR:HG23 | 1.99 | 0.45 |
| 37:d:409:LHG:H151 | 37:d:409:LHG:H342 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:C:518:DGD:HA31 | 36:C:518:DGD:HA62 | 1.80 | 0.45 |
| 24:b:619:CLA:H2 | 24:b:620:CLA:CBB | 2.46 | 0.45 |
| 15:u:45:LEU:HD21 | 15:u:71:GLN:HB3 | 1.98 | 0.45 |
| 2:B:220:ARG:NH1 | 41:B:703:HOH:O | 2.44 | 0.45 |
| 24:B:616:CLA:H112 | 24:B:616:CLA:H152 | 1.63 | 0.45 |
| 19:Z:30:PRO:HD2 | 41:Z:201:HOH:O | 2.16 | 0.45 |
| 3:c:406:SER:HA | 3:c:420:VAL:HG23 | 1.97 | 0.45 |
| 1:A:132:GLU:O | 1:A:136:ARG:HG2 | 2.17 | 0.45 |
| 13:o:29:ALA:O | 13:o:31:PRO:HD3 | 2.17 | 0.45 |
| 1:A:200:LEU:HG | 36:C:519:DGD:HAT2 | 1.98 | 0.45 |
| 24:A:410:CLA:H61 | 24:A:410:CLA:H41 | 1.76 | 0.45 |
| 2:B:171:PRO:HD3 | 7:H:66:GLY:HA2 | 1.99 | 0.45 |
| 26:T:102:BCR:HC8 | 26:T:102:BCR:H321 | 1.99 | 0.45 |
| 15:U:45:LEU:O | 15:U:49:ILE:HG13 | 2.17 | 0.45 |
| 3:C:47:GLY:HA3 | 3:C:137:PRO:O | 2.17 | 0.45 |
| 24:C:508:CLA:H92 | 24:C:508:CLA:H61 | 1.84 | 0.45 |
| 28:C:525:GOL:H2 | 41:C:708:HOH:O | 2.16 | 0.45 |
| 2:b:172:TYR:CE1 | 2:b:283:GLU:HB2 | 2.52 | 0.45 |
| 24:c:909:CLA:H92 | 37:d:409:LHG:H371 | 1.99 | 0.45 |
| 13:o:43:LEU:HB3 | 13:o:81:ILE:HB | 1.98 | 0.45 |
| 1:A:96:ILE:HG12 | 1:A:105:TRP:CE2 | 2.52 | 0.45 |
| 4:D:13:GLY:HA3 | 35:D:411:HTG:H62 | 1.99 | 0.45 |
| 10:K:10:LYS:N | 41:K:204:HOH:O | 2.50 | 0.45 |
| 3:c:223:TRP:CG | 3:c:224:ILE:H | 2.34 | 0.45 |
| 35:D:411:HTG:H1 | 7:H:25:TRP:CD1 | 2.52 | 0.45 |
| 27:F:101:SQD:H331 | 18:X:24:THR:HA | 1.99 | 0.45 |
| 2:b:363:PHE:HB3 | 2:b:365:SER:O | 2.16 | 0.45 |
| 10:k:11:LEU:HD11 | 10:k:22:VAL:HG21 | 1.99 | 0.45 |
| 2:B:65:PHE:HE1 | 24:B:605:CLA:HED2 | 1.83 | 0.44 |
| 27:B:621:SQD:H383 | 27:B:621:SQD:H352 | 1.78 | 0.44 |
| 4:D:14:TRP:CD1 | 35:D:411:HTG:HO6 | 2.35 | 0.44 |
| 4:D:192:THR:HG23 | 24:D:401:CLA:HBC2 | 1.99 | 0.44 |
| 4:d:49:LEU:HD13 | 26:d:404:BCR:C15 | 2.46 | 0.44 |
| 3:C:223:TRP:CE3 | 3:C:224:ILE:HG12 | 2.52 | 0.44 |
| 12:M:28:GLN:O | 12:M:32:GLN:HG3 | 2.18 | 0.44 |
| 3:c:79:LYS:HD2 | 16:v:35:TYR:HE1 | 1.82 | 0.44 |
| 24:c:911:CLA:H161 | 24:c:911:CLA:H121 | 1.88 | 0.44 |
| 11:l:14:ARG:HB3 | 14:t:25[A]:GLU:HG2 | 1.99 | 0.44 |
| 13:o:68:THR:HG22 | 13:o:110[B]:MET:HG2 | 1.98 | 0.44 |
| 26:t:101:BCR:H24C | 26:t:101:BCR:H371 | 1.82 | 0.44 |
| 26:B:619:BCR:H331 | 26:B:619:BCR:C8 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:C:520:LMG:H172 | 17:Y:25:ILE:HG12 | 2.00 | 0.44 |
| 13:O:39:ARG:HG3 | 13:O:83:GLY:O | 2.18 | 0.44 |
| 2:b:158:LEU:HB3 | 2:b:199:VAL:HG22 | 1.99 | 0.44 |
| 24:b:610:CLA:H162 | 24:b:610:CLA:H122 | 1.43 | 0.44 |
| 24:c:902:CLA:H202 | 24:c:908:CLA:HBB1 | 2.00 | 0.44 |
| 4:D:213:ILE:HD11 | 4:D:253:TRP:CH2 | 2.53 | 0.44 |
| 3:c:38:GLY:HA3 | 24:c:912:CLA:HMD2 | 1.98 | 0.44 |
| 2:B:124:ARG:HD2 | 2:B:129:GLY:O | 2.18 | 0.44 |
| 2:B:461:LEU:HD22 | 37:D:406:LHG:H301 | 1.99 | 0.44 |
| 13:O:36:GLN:O | 41:O:557:HOH:O | 2.20 | 0.44 |
| 35:B:633:HTG:O2 | 35:B:634:HTG:S1 | 2.58 | 0.44 |
| 24:C:502:CLA:H192 | 24:C:507:CLA:C1B | 2.47 | 0.44 |
| 34:a:412:LMG:H172 | 34:a:412:LMG:H201 | 1.73 | 0.44 |
| 24:c:906:CLA:H112 | 24:c:906:CLA:H72 | 1.83 | 0.44 |
| 1:A:192:ILE:HG13 | 1:A:293:MET:HE1 | 1.99 | 0.44 |
| 1:a:105:TRP:NE1 | 1:a:110:GLY:HA3 | 2.33 | 0.44 |
| 1:a:334:ARG:NH2 | 13:o:159:PRO:HA | 2.33 | 0.44 |
| 4:d:85:MET:CE | 4:d:96:GLU:HG2 | 2.48 | 0.44 |
| 2:B:50:PRO:HB2 | 28:B:631:GOL:H12 | 2.00 | 0.44 |
| 3:C:334:PRO:HA | 13:O:153:THR:OG1 | 2.18 | 0.44 |
| 4:D:102:THR:OG1 | 36:D:405:DGD:HG31 | 2.18 | 0.44 |
| 26:a:410:BCR:H24C | 26:a:410:BCR:H371 | 1.73 | 0.44 |
| 2:b:379:ALA:HA | 2:b:390:TYR:HB3 | 1.99 | 0.44 |
| 5:e:23:HIS:CD2 | 38:e:102:HEM:NC | 2.84 | 0.44 |
| 26:t:101:BCR:H331 | 26:t:101:BCR:HC7 | 1.55 | 0.44 |
| 16:v:126:LEU:HB3 | 16:v:129:LYS:HB2 | 1.99 | 0.44 |
| 24:C:507:CLA:HBB1 | 24:C:507:CLA:HMB3 | 2.00 | 0.43 |
| 36:C:517:DGD:HAH1 | 36:C:517:DGD:HAT2 | 1.78 | 0.43 |
| 24:b:612:CLA:HAB | 4:d:123:ILE:HG12 | 2.00 | 0.43 |
| 2:B:12:LEU:HB2 | 24:B:613:CLA:HMC2 | 2.00 | 0.43 |
| 6:F:44:GLN:HE21 | 6:F:44:GLN:HB2 | 1.60 | 0.43 |
| 13:O:204:VAL:HG22 | 13:O:211:ILE:HG22 | 2.00 | 0.43 |
| 15:u:58:VAL:HG12 | 15:u:79:LEU:HD22 | 2.00 | 0.43 |
| 26:y:101:BCR:H15C | 26:y:101:BCR:H351 | 1.78 | 0.43 |
| 1:A:188:ALA:HB2 | 1:A:328:MET:HB2 | 2.00 | 0.43 |
| 3:c:203:THR:O | 3:c:235:GLY:HA3 | 2.17 | 0.43 |
| 4:d:103:ARG:HG3 | 5:e:73:LYS:HG3 | 2.00 | 0.43 |
| 26:k:101:BCR:H24C | 26:k:101:BCR:H371 | 1.72 | 0.43 |
| 5:E:40:THR:HB | 20:R:4:ARG:HG2 | 1.99 | 0.43 |
| 2:b:201:HIS:HB2 | 24:b:606:CLA:C1B | 2.48 | 0.43 |
| 26:t:101:BCR:H321 | 26:t:101:BCR:HC8 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:491:VAL:HG12 | 4:D:136:VAL:HG13 | 2.00 | 0.43 |
| 24:B:603:CLA:H203 | 24:B:603:CLA:H162 | 1.83 | 0.43 |
| 13:O:164:LEU:HB2 | 13:O:188:LYS:HB2 | 2.01 | 0.43 |
| 13:O:180:GLU:CD | 13:O:180:GLU:H | 2.26 | 0.43 |
| 26:a:410:BCR:H15C | 26:a:410:BCR:H351 | 1.91 | 0.43 |
| 36:c:917:DGD:HBE1 | 36:c:917:DGD:HBF2 | 1.62 | 0.43 |
| 26:B:618:BCR:H11C | 26:B:618:BCR:H341 | 1.89 | 0.43 |
| 2:b:30:VAL:HG12 | 24:b:609:CLA:HHD | 1.99 | 0.43 |
| 3:C:175:LEU:HD23 | 3:C:237:HIS:CG | 2.53 | 0.43 |
| 24:C:510:CLA:H191 | 24:C:513:CLA:HAC1 | 2.01 | 0.43 |
| 26:T:102:BCR:H331 | 26:T:102:BCR:HC7 | 1.51 | 0.43 |
| 34:a:412:LMG:H201 | 36:c:916:DGD:HA81 | 2.01 | 0.43 |
| 2:b:446:SER:HB2 | 2:b:447:PRO:HD2 | 2.00 | 0.43 |
| 36:c:917:DGD:HA81 | 36:c:917:DGD:HAF1 | 2.01 | 0.43 |
| 27:A:412:SQD:H171 | 37:D:408:LHG:H181 | 2.01 | 0.43 |
| 6:f:21:VAL:O | 6:f:25:THR:HG23 | 2.19 | 0.43 |
| 26:k:101:BCR:H11C | 26:k:101:BCR:H341 | 1.91 | 0.43 |
| 12:m:28:GLN:O | 12:m:32:GLN:HG3 | 2.19 | 0.43 |
| 26:t:101:BCR:H23C | 26:t:101:BCR:H382 | 2.00 | 0.43 |
| 2:B:54:PRO:HD2 | 2:B:57:ARG:HG3 | 2.01 | 0.43 |
| 3:C:202:PRO:HD2 | 35:C:524:HTG:H62 | 1.99 | 0.43 |
| 13:O:54:GLU:O | 13:O:56:PRO:HD3 | 2.19 | 0.43 |
| 20:R:24:LEU:N | 20:R:25:PRO:HD2 | 2.34 | 0.43 |
| 1:a:153:SER:CB | 24:a:406:CLA:H43 | 2.48 | 0.43 |
| 2:b:137:LYS:HD2 | 7:h:14:LEU:O | 2.19 | 0.43 |
| 4:D:343:GLU:HG2 | 16:V:135:VAL:HG11 | 2.00 | 0.43 |
| 5:E:33:ALA:HB2 | 20:R:11:PRO:HB2 | 2.00 | 0.43 |
| 34:b:624:LMG:H421 | 37:l:101:LHG:H371 | 2.01 | 0.43 |
| 4:d:272:LEU:C | 4:d:272:LEU:HD23 | 2.43 | 0.43 |
| 2:B:224:ARG:HD3 | 7:H:25:TRP:CD2 | 2.54 | 0.42 |
| 4:D:160:TYR:HA | 4:D:290:ALA:HB2 | 2.01 | 0.42 |
| 15:u:27:LEU:HD22 | 15:u:49:ILE:HG21 | 2.00 | 0.42 |
| 2:B:314:TYR:CE2 | 2:B:316:GLY:HA3 | 2.53 | 0.42 |
| 5:e:68:ASP:OD1 | 5:e:71:GLU:HB2 | 2.19 | 0.42 |
| 10:k:15:TYR:CZ | 19:z:5:PHE:HZ | 2.37 | 0.42 |
| 17:y:22:LEU:HA | 17:y:25:ILE:HG22 | 2.01 | 0.42 |
| 28:T:103:GOL:H32 | 29:m:104:LMT:H21 | 2.01 | 0.42 |
| 1:a:215:HIS:HA | 31:a:417:PL9:O1 | 2.19 | 0.42 |
| 24:d:402:CLA:H201 | 34:j:101:LMG:H222 | 2.00 | 0.42 |
| 15:u:86:GLU:HG2 | 41:u:293:HOH:O | 2.18 | 0.42 |
| 24:A:405:CLA:CBD | 24:A:406:CLA:HAC2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:B:609:CLA:H162 | 24:D:402:CLA:H3A | 2.01 | 0.42 |
| 24:B:610:CLA:HHC | 24:B:610:CLA:HBB1 | 2.02 | 0.42 |
| 3:C:110:PRO:HG3 | 34:C:521:LMG:H121 | 2.01 | 0.42 |
| 31:a:417:PL9:H251 | 31:a:417:PL9:H272 | 1.87 | 0.42 |
| 24:b:618:CLA:H41 | 24:b:618:CLA:H62 | 1.64 | 0.42 |
| 3:C:373:ASN:HB3 | 41:O:558:HOH:O | 2.19 | 0.42 |
| 26:a:410:BCR:H11C | 26:a:410:BCR:H341 | 1.94 | 0.42 |
| 24:b:605:CLA:H93 | 24:b:605:CLA:H111 | 1.88 | 0.42 |
| 2:B:190:PHE:CZ | 24:B:603:CLA:HBB1 | 2.54 | 0.42 |
| 24:C:514:CLA:HBA1 | 24:C:514:CLA:H3A | 1.67 | 0.42 |
| 24:C:514:CLA:HBC1 | 34:Z:101:LMG:H171 | 2.02 | 0.42 |
| 1:a:170:ASP:CG | 41:a:527:HOH:O | 2.61 | 0.42 |
| 2:b:221:PRO:HA | 24:b:613:CLA:HED3 | 2.02 | 0.42 |
| 24:b:609:CLA:HHC | 24:b:609:CLA:HBB1 | 2.02 | 0.42 |
| 6:f:33:PHE:O | 6:f:37:ILE:HG13 | 2.20 | 0.42 |
| 26:C:515:BCR:H24C | 26:C:515:BCR:H371 | 1.88 | 0.42 |
| 4:D:27:PHE:CD1 | 37:E:101:LHG:HC12 | 2.54 | 0.42 |
| 8:I:33:LYS:HB3 | 8:I:34:ARG:H | 1.51 | 0.42 |
| 4:d:186:GLN:HB2 | 24:d:402:CLA:HBC1 | 2.01 | 0.42 |
| 24:A:406:CLA:H203 | 24:A:406:CLA:H162 | 1.80 | 0.42 |
| 31:A:419:PL9:H28 | 31:A:419:PL9:H321 | 1.87 | 0.42 |
| 2:B:433:ASP:OD1 | 2:B:436:THR:OG1 | 2.36 | 0.42 |
| 24:B:608:CLA:C4A | 24:B:608:CLA:HBA2 | 2.49 | 0.42 |
| 2:b:243:ALA:HA | 2:b:246:PHE:CE2 | 2.54 | 0.42 |
| 24:b:607:CLA:CGA | 24:b:607:CLA:H3A | 2.50 | 0.42 |
| 3:c:162:GLY:HA2 | 3:c:248:GLY:HA2 | 2.02 | 0.42 |
| 4:d:202:ALA:HB2 | 31:d:405:PL9:H353 | 2.01 | 0.42 |
| 24:d:401:CLA:H203 | 24:d:401:CLA:H162 | 1.73 | 0.42 |
| 5:e:17:VAL:O | 5:e:21:VAL:HG23 | 2.20 | 0.42 |
| 24:A:406:CLA:C4A | 24:A:406:CLA:HBA1 | 2.49 | 0.42 |
| 26:K:103:BCR:H15C | 26:K:103:BCR:H351 | 1.90 | 0.42 |
| 27:a:411:SQD:H312 | 27:a:411:SQD:H342 | 1.69 | 0.42 |
| 26:b:623:BCR:H15C | 26:b:623:BCR:H351 | 1.92 | 0.42 |
| 3:c:286:ALA:HB2 | 24:c:903:CLA:HMD2 | 2.02 | 0.42 |
| 26:c:915:BCR:H15C | 26:c:915:BCR:H351 | 1.87 | 0.42 |
| 4:d:190:ASN:HB2 | 4:d:296:TYR:CD1 | 2.54 | 0.42 |
| 13:o:86:LYS:O | 13:o:93:LEU:HA | 2.20 | 0.42 |
| 13:o:147:ASN:ND2 | 13:o:194:LYS:HE2 | 2.34 | 0.42 |
| 24:B:614:CLA:H162 | 24:B:614:CLA:H121 | 1.67 | 0.42 |
| 5:E:18:ARG:H | 9:J:2:SER:N | 2.18 | 0.42 |
| 24:b:605:CLA:C1B | 24:b:605:CLA:H143 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:b:621:BCR:H24C | 26:b:621:BCR:H371 | 1.77 | 0.42 |
| 2:B:36[A]:SER:OG | 26:B:619:BCR:H362 | 2.19 | 0.41 |
| 24:B:617:CLA:H91 | 24:B:617:CLA:H112 | 1.60 | 0.41 |
| 24:C:506:CLA:HAA1 | 24:C:506:CLA:HBD | 2.02 | 0.41 |
| 41:J:206:HOH:O | 16:V:30:LYS:HE3 | 2.20 | 0.41 |
| 13:O:142:PHE:HB2 | 13:O:199:LEU:HD12 | 2.02 | 0.41 |
| 14:T:1:FME:HCN | 29:b:601:LMT:H11 | 2.01 | 0.41 |
| 24:b:619:CLA:H112 | 24:b:619:CLA:H152 | 1.80 | 0.41 |
| 28:c:925:GOL:H2 | 41:c:1107:HOH:O | 2.19 | 0.41 |
| 26:A:411:BCR:H24C | 26:A:411:BCR:H371 | 1.80 | 0.41 |
| 24:B:602:CLA:C4A | 24:B:602:CLA:HBA2 | 2.50 | 0.41 |
| 35:B:625:HTG:H2'2 | 35:B:625:HTG:H1 | 1.88 | 0.41 |
| 34:a:412:LMG:H211 | 34:a:412:LMG:H241 | 1.77 | 0.41 |
| 24:c:914:CLA:C4B | 26:k:101:BCR:H383 | 2.50 | 0.41 |
| 3:C:75:PHE:CZ | 3:C:105:VAL:HG21 | 2.55 | 0.41 |
| 24:C:508:CLA:H61 | 24:C:508:CLA:H41 | 1.87 | 0.41 |
| 13:O:58:ASN:HD21 | 13:O:61:GLN:HB2 | 1.86 | 0.41 |
| 2:b:125:ASP:HA | 2:b:126:PRO:HD3 | 1.93 | 0.41 |
| 26:b:621:BCR:H12C | 34:b:624:LMG:C43 | 2.51 | 0.41 |
| 4:d:26:ARG:HA | 5:e:5:THR:HB | 2.03 | 0.41 |
| 10:k:10:LYS:HD2 | 10:k:10:LYS:N | 2.35 | 0.41 |
| 31:A:419:PL9:H512 | 27:F:101:SQD:H302 | 2.02 | 0.41 |
| 36:C:517:DGD:HAE1 | 36:C:517:DGD:HA81 | 1.79 | 0.41 |
| 2:b:26:HIS:CE1 | 24:b:616:CLA:HMA2 | 2.56 | 0.41 |
| 27:A:412:SQD:H152 | 27:A:412:SQD:H122 | 1.61 | 0.41 |
| 4:D:85:MET:CE | 4:D:96:GLU:HG2 | 2.51 | 0.41 |
| 2:b:224:ARG:HD3 | 7:h:25:TRP:CD2 | 2.55 | 0.41 |
| 5:e:26:THR:HB | 38:e:102:HEM:HAB | 2.03 | 0.41 |
| 13:o:164:LEU:HB2 | 13:o:188:LYS:HB2 | 2.02 | 0.41 |
| 24:B:602:CLA:H142 | 24:B:602:CLA:H112 | 1.80 | 0.41 |
| 3:C:142:GLU:CD | 3:C:142:GLU:H | 2.28 | 0.41 |
| 3:C:165:LEU:HD21 | 24:C:507:CLA:CAB | 2.51 | 0.41 |
| 3:C:338:GLY:HA3 | 3:C:341:LEU:O | 2.20 | 0.41 |
| 4:D:190:ASN:HB2 | 4:D:296:TYR:CD1 | 2.55 | 0.41 |
| 13:O:149:PRO:HB2 | 41:O:409:HOH:O | 2.21 | 0.41 |
| 1:a:11:ALA:HA | 1:a:15:GLU:OE2 | 2.20 | 0.41 |
| 35:d:412:HTG:H1 | 7:h:25:TRP:CG | 2.56 | 0.41 |
| 24:B:607:CLA:H122 | 24:B:607:CLA:H161 | 1.81 | 0.41 |
| 26:D:403:BCR:H11C | 26:D:403:BCR:H341 | 1.93 | 0.41 |
| 34:Z:101:LMG:H111 | 34:Z:101:LMG:HC8 | 1.64 | 0.41 |
| 28:b:632:GOL:H32 | 41:b:961:HOH:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:B:614:CLA:H122 | 34:B:622:LMG:H232 | 2.02 | 0.41 |
| 24:C:506:CLA:H93 | 24:C:506:CLA:H111 | 1.87 | 0.41 |
| 24:C:508:CLA:HAA2 | 24:C:508:CLA:HBD | 2.02 | 0.41 |
| 13:O:39:ARG:HB2 | 13:O:246:ALA:HB2 | 2.02 | 0.41 |
| 3:c:52:ALA:HB2 | 24:c:912:CLA:HMA2 | 2.02 | 0.41 |
| 4:d:47:GLY:C | 4:d:114:ILE:HD11 | 2.46 | 0.41 |
| 6:f:28:VAL:HB | 6:f:29:PRO:HD3 | 2.03 | 0.41 |
| 2:B:70:GLY:HA2 | 2:B:178:VAL:HG21 | 2.02 | 0.41 |
| 2:B:223[A]:GLN:OE1 | 2:B:227:LYS:HD2 | 2.21 | 0.41 |
| 24:B:602:CLA:HAA1 | 24:B:602:CLA:HBD | 2.02 | 0.41 |
| 24:B:612:CLA:H142 | 37:L:101:LHG:H362 | 2.02 | 0.41 |
| 24:B:617:CLA:H152 | 24:B:617:CLA:H111 | 1.75 | 0.41 |
| 36:D:405:DGD:HBT1 | 36:D:405:DGD:HBH1 | 1.85 | 0.41 |
| 37:D:408:LHG:H112 | 37:D:408:LHG:C38 | 2.51 | 0.41 |
| 1:a:217:SER:O | 1:a:221[A]:SER:HB3 | 2.20 | 0.41 |
| 1:a:221[A]:SER:HB2 | 4:d:139:ARG:O | 2.21 | 0.41 |
| 2:b:458:PHE:HB3 | 24:b:608:CLA:HBC2 | 2.02 | 0.41 |
| 3:c:436:PHE:CE1 | 24:c:905:CLA:H161 | 2.55 | 0.41 |
| 36:c:917:DGD:HA81 | 36:c:917:DGD:HAE2 | 1.80 | 0.41 |
| 29:c:921:LMT:H72 | 29:c:921:LMT:H102 | 1.89 | 0.41 |
| 26:k:101:BCR:H351 | 26:k:101:BCR:H15C | 1.78 | 0.41 |
| 24:B:604:CLA:CGA | 24:B:604:CLA:H3A | 2.51 | 0.41 |
| 3:C:443:TRP:CE2 | 24:C:509:CLA:HMD2 | 2.56 | 0.41 |
| 10:K:10:LYS:N | 10:K:10:LYS:HD2 | 2.36 | 0.41 |
| 19:Z:29:SER:HA | 19:Z:30:PRO:HD3 | 1.88 | 0.41 |
| 1:a:72:LEU:HD13 | 29:a:401:LMT:H11 | 2.02 | 0.41 |
| 3:c:75:PHE:CZ | 3:c:77:PRO:HA | 2.55 | 0.41 |
| 5:e:20:TRP:HD1 | 9:j:7:ILE:HD12 | 1.85 | 0.41 |
| 2:B:262:THR:C | 2:B:264:PRO:HD3 | 2.45 | 0.40 |
| 1:a:192:ILE:HG13 | 1:a:293:MET:HE1 | 2.02 | 0.40 |
| 24:b:605:CLA:H142 | 24:b:605:CLA:H112 | 1.80 | 0.40 |
| 3:c:213[A]:LEU:HG | 24:c:907:CLA:H202 | 2.03 | 0.40 |
| 26:B:619:BCR:H371 | 26:B:619:BCR:H24C | 1.77 | 0.40 |
| 19:Z:37:LYS:NZ | 34:Z:101:LMG:HC61 | 2.36 | 0.40 |
| 2:b:86[A]:ILE:H | 2:b:86[A]:ILE:HG13 | 1.77 | 0.40 |
| 2:b:314:TYR:CE2 | 2:b:316:GLY:HA3 | 2.55 | 0.40 |
| 26:d:404:BCR:H15C | 26:d:404:BCR:H351 | 1.85 | 0.40 |
| 1:A:161:TYR:HB3 | 1:A:162:PRO:HD3 | 2.04 | 0.40 |
| 24:A:406:CLA:H192 | 27:A:416:SQD:H223 | 2.02 | 0.40 |
| 27:B:621:SQD:O8 | 11:L:7:ARG:HD3 | 2.21 | 0.40 |
| 24:C:513:CLA:H101 | 24:C:514:CLA:H141 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:b:623:BCR:C8 | 26:b:623:BCR:H331 | 2.51 | 0.40 |
| 31:D:404:PL9:H422 | 31:D:404:PL9:H401 | 1.74 | 0.40 |
| 29:M:101:LMT:H6D | 11:l:9:PRO:HA | 2.03 | 0.40 |
| 1:a:161:TYR:OH | 1:a:190:HIS:NE2 | 2.35 | 0.40 |
| 3:c:60:ILE:HG22 | 24:c:904:CLA:HHD | 2.03 | 0.40 |
| 10:k:23:ASP:OD2 | 17:y:21:GLN:NE2 | 2.53 | 0.40 |
| 26:t:101:BCR:H11C | 26:t:101:BCR:H341 | 1.97 | 0.40 |
| 6:F:41:GLN:OE1 | 9:J:30:GLY:HA3 | 2.21 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 335/344 (97%) | 331 (99%) | 3 (1%) | 1 (0%) | 36 | 28 |
| 1 | a | 338/344 (98%) | 333 (98%) | 4 (1%) | 1 (0%) | 36 | 28 |
| 2 | B | 513/505 (102%) | 506 (99%) | 7 (1%) | 0 | 100 | 100 |
| 2 | b | 514/505 (102%) | 506 (98%) | 8 (2%) | 0 | 100 | 100 |
| 3 | C | 453/455 (100%) | 441 (97%) | 10 (2%) | 2 (0%) | 30 | 21 |
| 3 | c | 459/455 (101%) | 445 (97%) | 12 (3%) | 2 (0%) | 30 | 21 |
| 4 | D | 341/342 (100%) | 334 (98%) | 7 (2%) | 0 | 100 | 100 |
| 4 | d | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 5 | E | 81/84 (96%) | 81 (100%) | 0 | 0 | 100 | 100 |
| 5 | e | 81/84 (96%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | F | 32/44 (73%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 30/44 (68%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 64/65 (98%) | 61 (95%) | 3 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 7 | h | 63/65 (97%) | 59 (94%) | 4 (6%) | 0 | 100 | 100 |
| 8 | I | 36/38 (95%) | 33 (92%) | 3 (8%) | 0 | 100 | 100 |
| 8 | i | 36/38 (95%) | 33 (92%) | 2 (6%) | 1 (3%) | 4 | 1 |
| 9 | J | 36/39 (92%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 9 | j | 37/39 (95%) | 37 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 10 | k | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | L | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 33/36 (92%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 32/36 (89%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 13 | O | 249/244 (102%) | 240 (96%) | 8 (3%) | 1 (0%) | 30 | 21 |
| 13 | o | 246/244 (101%) | 237 (96%) | 9 (4%) | 0 | 100 | 100 |
| 14 | T | 29/32 (91%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 14 | t | 29/32 (91%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 15 | U | 95/104 (91%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 15 | u | 95/104 (91%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | V | 136/137 (99%) | 132 (97%) | 4 (3%) | 0 | 100 | 100 |
| 16 | v | 135/137 (98%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 17 | Y | 27/30 (90%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 17 | y | 27/30 (90%) | 26 (96%) | 1 (4%) | 0 | 100 | 100 |
| 18 | X | 37/40 (92%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | x | 37/40 (92%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 19 | Z | 60/62 (97%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 19 | z | 60/62 (97%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 20 | R | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| All | All | 5290/5384 (98%) | 5170 (98%) | 112 (2%) | 8 (0%) | 48 | 36 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 416[A] | SER |
| 3 | C | 416[B] | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | c | 416[A] | SER |
| 3 | c | 416[B] | SER |
| 13 | O | 62 | GLU |
| 8 | i | 36 | ASP |
| 1 | a | 259 | ILE |
| 1 | A | 259 | ILE |

### 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 | 272/279 (98%) | 272 (100%) | 0 | 100 100 |
| 1 | a | 275/279 (99%) | 272 (99%) | 3 (1%) | 65 64 |
| 2 | B | 413/403 (102%) | 404 (98%) | 9 (2%) | 45 40 |
| 2 | b | 414/403 (103%) | 409 (99%) | 5 (1%) | 63 61 |
| 3 | C | 356/356 (100%) | 349 (98%) | 7 (2%) | 48 43 |
| 3 | c | 362/356 (102%) | 356 (98%) | 6 (2%) | 53 49 |
| 4 | D | 278/277 (100%) | 275 (99%) | 3 (1%) | 65 64 |
| 4 | d | 277/277 (100%) | 274 (99%) | 3 (1%) | 65 64 |
| 5 | E | 74/73 (101%) | 73 (99%) | 1 (1%) | 59 56 |
| 5 | e | 74/73 (101%) | 73 (99%) | 1 (1%) | 59 56 |
| 6 | F | 28/38 (74%) | 27 (96%) | 1 (4%) | 31 21 |
| 6 | f | 26/38 (68%) | 24 (92%) | 2 (8%) | 12 3 |
| 7 | H | 55/54 (102%) | 53 (96%) | 2 (4%) | 31 21 |
| 7 | h | 54/54 (100%) | 54 (100%) | 0 | 100 100 |
| 8 | I | 34/34 (100%) | 34 (100%) | 0 | 100 100 |
| 8 | i | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 29 |
| 9 | J | 26/27 (96%) | 26 (100%) | 0 | 100 100 |
| 9 | j | 27/27 (100%) | 26 (96%) | 1 (4%) | 30 20 |
| 10 | K | 30/30 (100%) | 29 (97%) | 1 (3%) | 33 24 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 10 | k | 30/30 (100%) | 29 (97%) | 1 (3%) | 33 24 |
| 11 | L | 36/35 (103%) | 33 (92%) | 3 (8%) | 10 3 |
| 11 | l | 36/35 (103%) | 35 (97%) | 1 (3%) | 38 30 |
| 12 | M | 31/32 (97%) | 30 (97%) | 1 (3%) | 34 25 |
| 12 | m | 30/32 (94%) | 28 (93%) | 2 (7%) | 15 5 |
| 13 | O | 214/207 (103%) | 211 (99%) | 3 (1%) | 59 56 |
| 13 | o | 211/207 (102%) | 204 (97%) | 7 (3%) | 33 24 |
| 14 | T | 27/28 (96%) | 25 (93%) | 2 (7%) | 13 4 |
| 14 | t | 27/28 (96%) | 25 (93%) | 2 (7%) | 13 4 |
| 15 | U | 84/89 (94%) | 83 (99%) | 1 (1%) | 63 61 |
| 15 | u | 84/89 (94%) | 83 (99%) | 1 (1%) | 63 61 |
| 16 | V | 118/117 (101%) | 117 (99%) | 1 (1%) | 73 74 |
| 16 | v | 117/117 (100%) | 117 (100%) | 0 | 100 100 |
| 17 | Y | 22/23 (96%) | 19 (86%) | 3 (14%) | 3 0 |
| 17 | y | 22/23 (96%) | 19 (86%) | 3 (14%) | 3 0 |
| 18 | X | 32/33 (97%) | 32 (100%) | 0 | 100 100 |
| 18 | x | 32/33 (97%) | 32 (100%) | 0 | 100 100 |
| 19 | Z | 52/52 (100%) | 49 (94%) | 3 (6%) | 18 7 |
| 19 | z | 52/52 (100%) | 50 (96%) | 2 (4%) | 29 19 |
| 20 | R | 29/29 (100%) | 28 (97%) | 1 (3%) | 32 23 |
| All | All | 4395/4403 (100%) | 4312 (98%) | 83 (2%) | 53 45 |

All (83) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 84 | THR |
| 2 | B | 223[A] | GLN |
| 2 | B | 223[B] | GLN |
| 2 | B | 227 | LYS |
| 2 | B | 315 | ILE |
| 2 | B | 362 | PHE |
| 2 | B | 472 | ARG |
| 2 | B | 492 | GLU |
| 2 | B | 505 | ARG |
| 3 | C | 29 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 142 | GLU |
| 3 | C | 213 | LEU |
| 3 | C | 289 | PHE |
| 3 | C | 315 | MET |
| 3 | C | 416[A] | SER |
| 3 | C | 416[B] | SER |
| 4 | D | 90 | LEU |
| 4 | D | 150 | ILE |
| 4 | D | 329 | MET |
| 5 | E | 71 | GLU |
| 6 | F | 44 | GLN |
| 7 | H | 12[A] | ARG |
| 7 | H | 12[B] | ARG |
| 10 | K | 17 | ILE |
| 11 | L | 1 | MET |
| 11 | L | 2 | GLU |
| 11 | L | 13 | ASN |
| 12 | M | 33 | GLN |
| 13 | O | 49[A] | THR |
| 13 | O | 49[B] | THR |
| 13 | O | 194 | LYS |
| 14 | T | 25[A] | GLU |
| 14 | T | 25[B] | GLU |
| 15 | U | 70 | ARG |
| 16 | V | 30 | LYS |
| 17 | Y | 19 | ILE |
| 17 | Y | 27 | MET |
| 17 | Y | 30 | ILE |
| 19 | Z | 1 | MET |
| 19 | Z | 6 | GLN |
| 19 | Z | 20 | VAL |
| 20 | R | 4 | ARG |
| 1 | a | 12 | ASN |
| 1 | a | 221[A] | SER |
| 1 | a | 221[B] | SER |
| 2 | b | 14 | ASN |
| 2 | b | 84 | THR |
| 2 | b | 472 | ARG |
| 2 | b | 485 | GLU |
| 2 | b | 491 | VAL |
| 3 | c | 142 | GLU |
| 3 | c | 289 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | c | 315 | MET |
| 3 | c | 355 | THR |
| 3 | c | 462[A] | GLU |
| 3 | c | 462[B] | GLU |
| 4 | d | 90 | LEU |
| 4 | d | 150 | ILE |
| 4 | d | 329 | MET |
| 5 | e | 71 | GLU |
| 6 | f | 15 | ILE |
| 6 | f | 44 | GLN |
| 8 | i | 36 | ASP |
| 9 | j | 1 | MET |
| 10 | k | 17 | ILE |
| 11 | l | 1 | MET |
| 12 | m | 16 | LEU |
| 12 | m | 33 | GLN |
| 13 | o | 24 | ASP |
| 13 | o | 25 | THR |
| 13 | o | 69 | LYS |
| 13 | o | 118 | LEU |
| 13 | o | 181[A] | GLU |
| 13 | o | 181[B] | GLU |
| 13 | o | 194 | LYS |
| 14 | t | 25[A] | GLU |
| 14 | t | 25[B] | GLU |
| 15 | u | 86 | GLU |
| 17 | y | 19 | ILE |
| 17 | y | 30 | ILE |
| 17 | y | 42 | ARG |
| 19 | z | 1 | MET |
| 19 | z | 6 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 165 | GLN |
| 3 | C | 418 | ASN |
| 4 | D | 83 | ASN |
| 4 | D | 301 | GLN |
| 4 | D | 332 | GLN |
| 6 | F | 44 | GLN |
| 11 | L | 13 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | O | 124 | ASN |
| 13 | O | 147 | ASN |
| 19 | Z | 31 | GLN |
| 19 | Z | 58 | ASN |
| 1 | a | 165 | GLN |
| 1 | a | 296 | ASN |
| 2 | b | 53 | ASN |
| 2 | b | 490 | GLN |
| 3 | c | 201 | ASN |
| 3 | c | 373 | ASN |
| 4 | d | 83 | ASN |
| 4 | d | 186 | GLN |
| 4 | d | 332 | GLN |
| 4 | d | 350 | ASN |
| 5 | e | 75 | GLN |
| 6 | f | 44 | GLN |
| 10 | k | 40 | GLN |
| 11 | l | 6 | ASN |
| 13 | o | 124 | ASN |
| 13 | o | 147 | ASN |
| 13 | o | 155 | ASN |
| 16 | v | 118 | HIS |
| 19 | z | 6 | GLN |
| 19 | z | 31 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 8 | FME | I | 1 | 8 | 8,9,10 | 0.61 | 0 | 8,9,11 | 1.32 | 2 (25%) |
| 14 | FME | t | 1 | 14 | 8,9,10 | 0.66 | 0 | 8,9,11 | 1.90 | 3 (37%) |
| 12 | FME | M | 1 | 12 | 8,9,10 | 0.69 | 0 | 8,9,11 | 1.05 | 0 |
| 8 | FME | i | 1 | 8 | 8,9,10 | 0.73 | 0 | 8,9,11 | 1.29 | 1 (12%) |
| 14 | FME | T | 1 | 14 | 8,9,10 | 0.68 | 0 | 8,9,11 | 1.87 | 3 (37%) |
| 12 | FME | m | 1 | 12 | 8,9,10 | 0.76 | 0 | 8,9,11 | 1.09 | 1 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 8 | FME | I | 1 | 8 | - | 1/7/9/11 | - |
| 14 | FME | t | 1 | 14 | - | 3/7/9/11 | - |
| 12 | FME | M | 1 | 12 | - | 1/7/9/11 | - |
| 8 | FME | i | 1 | 8 | - | 0/7/9/11 | - |
| 14 | FME | T | 1 | 14 | - | 3/7/9/11 | - |
| 12 | FME | m | 1 | 12 | - | 0/7/9/11 | - |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | T | 1 | FME | CB-CA-N | -3.37 | 104.39 | 110.52 |
| 14 | t | 1 | FME | C-CA-N | 2.99 | 115.27 | 109.50 |
| 14 | t | 1 | FME | O-C-CA | -2.68 | 117.88 | 124.77 |
| 14 | T | 1 | FME | C-CA-N | 2.62 | 114.55 | 109.50 |
| 14 | t | 1 | FME | CA-N-CN | -2.56 | 118.89 | 122.82 |
| 8 | I | 1 | FME | O-C-CA | -2.40 | 118.59 | 124.77 |
| 8 | i | 1 | FME | CA-N-CN | -2.29 | 119.30 | 122.82 |
| 12 | m | 1 | FME | O-C-CA | -2.20 | 119.12 | 124.77 |
| 8 | I | 1 | FME | CA-N-CN | -2.19 | 119.45 | 122.82 |
| 14 | T | 1 | FME | O-C-CA | -2.01 | 119.59 | 124.77 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 14 | T | 1 | FME | N-CA-CB-CG |
| 14 | t | 1 | FME | O1-CN-N-CA |
| 14 | T | 1 | FME | C-CA-CB-CG |
| 12 | M | 1 | FME | CA-CB-CG-SD |
| 14 | T | 1 | FME | CB-CG-SD-CE |
| 8 | I | 1 | FME | CA-CB-CG-SD |
| 14 | t | 1 | FME | CB-CG-SD-CE |
| 14 | t | 1 | FME | CB-CA-N-CN |

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 12 | M | 1 | FME | 1 | 0 |
| 14 | T | 1 | FME | 1 | 0 |
| 12 | m | 1 | FME | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 251 ligands modelled in this entry, 17 are monoatomic and 18 are unknown - leaving 216 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 | $\#\|Z\| > 2$ |
| 24 | CLA | B | 606 | - | 69,73,73 | 1.99 | 20 (28%) | 82,113,113 | 2.61 | 30 (36%) |
| 26 | BCR | a | 410 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.27 | 5 (8%) |
| 28 | GOL | b | 633 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.38 | 0 |
| 35 | HTG | c | 922 | - | 19,19,19 | 0.83 | 1 (5%) | 23,24,24 | 1.19 | 1 (4%) |
| 28 | GOL | A | 414 | - | 5,5,5 | 0.45 | 0 | 5,5,5 | 0.37 | 0 |
| 28 | GOL | B | 632 | - | 5,5,5 | 0.35 | 0 | 5,5,5 | 0.40 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 28 | GOL | v | 203 | - | 5,5,5 | 0.29 | 0 | 5,5,5 | 0.65 | 0 |
| 24 | CLA | b | 611 | 41 | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.74 | 32 (39%) |
| 24 | CLA | b | 616 | - | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.67 | 30 (36%) |
| 28 | GOL | b | 631 | - | 5,5,5 | 0.34 | 0 | 5,5,5 | 0.49 | 0 |
| 24 | CLA | c | 912 | 3 | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.58 | 29 (35%) |
| 35 | HTG | C | 523 | - | 19,19,19 | 0.90 | 2 (10%) | 23,24,24 | 1.24 | 2 (8%) |
| 28 | GOL | V | 204 | - | 5,5,5 | 0.44 | 0 | 5,5,5 | 0.46 | 0 |
| 35 | HTG | C | 524 | - | 19,19,19 | 0.94 | 1 (5%) | 23,24,24 | 1.54 | 4 (17%) |
| 38 | HEM | E | 103 | 6,5 | 50,50,50 | 1.51 | 6 (12%) | 67,82,82 | 1.67 | 13 (19%) |
| 24 | CLA | c | 914 | - | 69,73,73 | 2.03 | 21 (30%) | 82,113,113 | 2.67 | 31 (37%) |
| 35 | HTG | B | 624 | - | 19,19,19 | 1.04 | 1 (5%) | 23,24,24 | 1.31 | 1 (4%) |
| 34 | LMG | j | 101 | 39 | 51,51,55 | 0.90 | 2 (3%) | 59,59,63 | 0.99 | 4 (6%) |
| 24 | CLA | B | 608 | 41 | 69,73,73 | 2.00 | 20 (28%) | 82,113,113 | 2.56 | 31 (37%) |
| 28 | GOL | V | 203 | - | 5,5,5 | 0.39 | 0 | 5,5,5 | 0.17 | 0 |
| 35 | HTG | B | 625 | - | 19,19,19 | 0.77 | 1 (5%) | 23,24,24 | 1.11 | 2 (8%) |
| 28 | GOL | a | 413 | - | 5,5,5 | 0.31 | 0 | 5,5,5 | 0.69 | 0 |
| 24 | CLA | D | 401 | - | 69,73,73 | 1.97 | 19 (27%) | 82,113,113 | 2.64 | 31 (37%) |
| 37 | LHG | D | 407 | - | 48,48,48 | 0.88 | 2 (4%) | 51,54,54 | 0.86 | 2 (3%) |
| 24 | CLA | B | 603 | - | 69,73,73 | 2.03 | 19 (27%) | 82,113,113 | 2.76 | 36 (43%) |
| 28 | GOL | A | 415 | - | 5,5,5 | 0.43 | 0 | 5,5,5 | 0.29 | 0 |
| 29 | LMT | E | 102 | - | 36,36,36 | 0.49 | 0 | 47,47,47 | 0.87 | 0 |
| 34 | LMG | C | 501 | - | 51,51,55 | 0.96 | 2 (3%) | 59,59,63 | 1.11 | 5 (8%) |
| 26 | BCR | T | 102 | - | 41,41,41 | 0.99 | 1 (2%) | 56,56,56 | 1.40 | 11 (19%) |
| 35 | HTG | B | 633 | - | 19,19,19 | 1.02 | 2 (10%) | 23,24,24 | 1.18 | 1 (4%) |
| 36 | DGD | d | 406 | - | 63,63,67 | 0.93 | 3 (4%) | 77,77,81 | 1.23 | 7 (9%) |
| 28 | GOL | O | 302 | - | 5,5,5 | 0.32 | 0 | 5,5,5 | 0.49 | 0 |
| 24 | CLA | b | 615 | - | 69,73,73 | 1.98 | 20 (28%) | 82,113,113 | 2.74 | 29 (35%) |
| 37 | LHG | d | 407 | - | 48,48,48 | 0.93 | 2 (4%) | 51,54,54 | 1.02 | 4 (7%) |
| 34 | LMG | c | 920 | - | 51,51,55 | 0.95 | 2 (3%) | 59,59,63 | 1.22 | 7 (11%) |
| 38 | HEM | e | 102 | 6,5 | 50,50,50 | 1.58 | 8 (16%) | 67,82,82 | 1.66 | 17 (25%) |
| 35 | HTG | O | 303 | - | 19,19,19 | 0.88 | 1 (5%) | 23,24,24 | 0.67 | 0 |
| 24 | CLA | B | 611 | 41 | 69,73,73 | 2.07 | 20 (28%) | 82,113,113 | 2.62 | 33 (40%) |
| 24 | CLA | c | 903 | - | 69,73,73 | 2.01 | 19 (27%) | 82,113,113 | 2.63 | 28 (34%) |
| 24 | CLA | d | 401 | 41 | 69,73,73 | 2.03 | 19 (27%) | 82,113,113 | 2.71 | 32 (39%) |
| 24 | CLA | C | 510 | - | 69,73,73 | 2.07 | 19 (27%) | 82,113,113 | 2.67 | 34 (41%) |
| 28 | GOL | V | 205 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.41 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | LHG | D | 408 | - | 48,48,48 | 0.88 | 2 (4%) | 51,54,54 | 1.07 | 4 (7%) |
| 24 | CLA | C | 505 | 41 | 69,73,73 | 2.05 | 20 (28%) | 82,113,113 | 2.74 | 29 (35%) |
| 37 | LHG | l | 101 | - | 48,48,48 | 0.93 | 2 (4%) | 51,54,54 | 1.14 | 4 (7%) |
| 24 | CLA | A | 405 | - | 69,73,73 | 2.01 | 19 (27%) | 82,113,113 | 2.65 | 27 (32%) |
| 24 | CLA | B | 613 | - | 69,73,73 | 1.98 | 20 (28%) | 82,113,113 | 2.56 | 27 (32%) |
| 24 | CLA | B | 604 | - | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.76 | 30 (36%) |
| 24 | CLA | b | 619 | - | 69,73,73 | 1.99 | 18 (26%) | 82,113,113 | 2.62 | 30 (36%) |
| 24 | CLA | b | 610 | - | 69,73,73 | 1.97 | 20 (28%) | 82,113,113 | 2.75 | 32 (39%) |
| 24 | CLA | b | 609 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.77 | 31 (37%) |
| 24 | CLA | B | 607 | - | 69,73,73 | 2.02 | 19 (27%) | 82,113,113 | 2.79 | 32 (39%) |
| 26 | BCR | C | 515 | - | 41,41,41 | 1.09 | 1 (2%) | 56,56,56 | 1.33 | 4 (7%) |
| 28 | GOL | c | 924 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.34 | 0 |
| 24 | CLA | c | 902 | - | 69,73,73 | 1.97 | 19 (27%) | 82,113,113 | 2.62 | 29 (35%) |
| 24 | CLA | a | 407 | 41 | 69,73,73 | 2.04 | 20 (28%) | 82,113,113 | 2.72 | 35 (42%) |
| 24 | CLA | B | 612 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.71 | 31 (37%) |
| 26 | BCR | H | 101 | - | 41,41,41 | 1.08 | 1 (2%) | 56,56,56 | 1.39 | 7 (12%) |
| 28 | GOL | T | 103 | - | 5,5,5 | 0.40 | 0 | 5,5,5 | 0.20 | 0 |
| 24 | CLA | A | 406 | 41 | 69,73,73 | 1.97 | 17 (24%) | 82,113,113 | 2.88 | 35 (42%) |
| 23 | BCT | a | 419 | 21 | 3,3,3 | 1.50 | 1 (33%) | 2,3,3 | 0.27 | 0 |
| 29 | LMT | C | 522 | - | 36,36,36 | 0.49 | 0 | 47,47,47 | 1.29 | 5 (10%) |
| 26 | BCR | t | 101 | - | 41,41,41 | 1.09 | 1 (2%) | 56,56,56 | 1.38 | 9 (16%) |
| 29 | LMT | b | 601 | - | 25,25,36 | 0.46 | 0 | 30,30,47 | 1.36 | 3 (10%) |
| 24 | CLA | c | 905 | 41 | 69,73,73 | 2.01 | 20 (28%) | 82,113,113 | 2.67 | 32 (39%) |
| 28 | GOL | B | 631 | - | 5,5,5 | 0.43 | 0 | 5,5,5 | 0.47 | 0 |
| 27 | SQD | a | 402 | - | 52,54,54 | 0.98 | 2 (3%) | 62,65,65 | 1.15 | 6 (9%) |
| 26 | BCR | b | 621 | - | 41,41,41 | 1.13 | 1 (2%) | 56,56,56 | 1.19 | 3 (5%) |
| 37 | LHG | e | 101 | - | 41,41,48 | 1.02 | 2 (4%) | 44,47,54 | 0.99 | 2 (4%) |
| 34 | LMG | z | 101 | - | 39,39,55 | 1.10 | 2 (5%) | 47,47,63 | 1.46 | 7 (14%) |
| 24 | CLA | C | 506 | - | 69,73,73 | 2.04 | 19 (27%) | 82,113,113 | 2.62 | 31 (37%) |
| 24 | CLA | b | 618 | - | 69,73,73 | 2.01 | 20 (28%) | 82,113,113 | 2.81 | 33 (40%) |
| 28 | GOL | B | 637 | - | 5,5,5 | 0.41 | 0 | 5,5,5 | 0.30 | 0 |
| 36 | DGD | D | 405 | - | 63,63,67 | 0.98 | 4 (6%) | 77,77,81 | 1.24 | 7 (9%) |
| 24 | CLA | c | 913 | - | 69,73,73 | 1.98 | 20 (28%) | 82,113,113 | 2.73 | 33 (40%) |
| 28 | GOL | T | 101 | - | 5,5,5 | 0.42 | 0 | 5,5,5 | 0.35 | 0 |
| 24 | CLA | a | 406 | - | 69,73,73 | 2.02 | 19 (27%) | 82,113,113 | 2.66 | 34 (41%) |
| 37 | LHG | d | 408 | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 0.92 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 28 | GOL | B | 630 | - | 5,5,5 | 0.34 | 0 | 5,5,5 | 0.40 | 0 |
| 29 | LMT | M | 101 | - | 36,36,36 | 0.41 | 0 | 47,47,47 | 0.91 | 2 (4%) |
| 24 | CLA | c | 909 | - | 69,73,73 | 2.01 | 20 (28%) | 82,113,113 | 2.61 | 28 (34%) |
| 24 | CLA | c | 908 | 41 | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.66 | 32 (39%) |
| 24 | CLA | C | 507 | - | 69,73,73 | 2.05 | 19 (27%) | 82,113,113 | 2.62 | 32 (39%) |
| 24 | CLA | A | 410 | - | 69,73,73 | 2.04 | 19 (27%) | 82,113,113 | 2.63 | 31 (37%) |
| 26 | BCR | B | 618 | - | 41,41,41 | 1.09 | 1 (2%) | 56,56,56 | 1.21 | 8 (14%) |
| 24 | CLA | B | 614 | - | 69,73,73 | 1.98 | 18 (26%) | 82,113,113 | 2.67 | 31 (37%) |
| 24 | CLA | B | 609 | - | 69,73,73 | 2.05 | 21 (30%) | 82,113,113 | 2.62 | 32 (39%) |
| 24 | CLA | B | 610 | - | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.68 | 34 (41%) |
| 28 | GOL | F | 103 | 33 | 5,5,5 | 0.32 | 0 | 5,5,5 | 0.34 | 0 |
| 35 | HTG | B | 634 | - | 19,19,19 | 0.96 | 1 (5%) | 23,24,24 | 1.44 | 3 (13%) |
| 28 | GOL | c | 925 | - | 5,5,5 | 0.36 | 0 | 5,5,5 | 0.60 | 0 |
| 35 | HTG | b | 627 | - | 19,19,19 | 1.01 | 1 (5%) | 23,24,24 | 1.86 | 4 (17%) |
| 35 | HTG | b | 626 | - | 19,19,19 | 0.83 | 1 (5%) | 23,24,24 | 1.32 | 3 (13%) |
| 27 | SQD | L | 102 | - | 52,54,54 | 0.98 | 2 (3%) | 62,65,65 | 1.52 | 10 (16%) |
| 24 | CLA | C | 509 | - | 69,73,73 | 2.01 | 20 (28%) | 82,113,113 | 2.71 | 31 (37%) |
| 24 | CLA | c | 911 | - | 69,73,73 | 2.05 | 20 (28%) | 82,113,113 | 2.53 | 32 (39%) |
| 24 | CLA | b | 605 | 41 | 69,73,73 | 2.04 | 19 (27%) | 82,113,113 | 2.62 | 27 (32%) |
| 24 | CLA | c | 910 | - | 69,73,73 | 2.05 | 20 (28%) | 82,113,113 | 2.65 | 30 (36%) |
| 28 | GOL | a | 414 | - | 5,5,5 | 0.39 | 0 | 5,5,5 | 0.46 | 0 |
| 37 | LHG | L | 101 | - | 48,48,48 | 0.91 | 2 (4%) | 51,54,54 | 1.05 | 4 (7%) |
| 28 | GOL | C | 525 | - | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.65 | 0 |
| 26 | BCR | c | 915 | - | 41,41,41 | 1.09 | 1 (2%) | 56,56,56 | 1.43 | 8 (14%) |
| 26 | BCR | B | 620 | - | 41,41,41 | 1.11 | 1 (2%) | 56,56,56 | 1.24 | 5 (8%) |
| 24 | CLA | B | 616 | - | 69,73,73 | 1.96 | 21 (30%) | 82,113,113 | 2.67 | 32 (39%) |
| 24 | CLA | b | 608 | - | 69,73,73 | 2.02 | 19 (27%) | 82,113,113 | 2.58 | 28 (34%) |
| 28 | GOL | b | 629 | - | 5,5,5 | 0.35 | 0 | 5,5,5 | 0.16 | 0 |
| 35 | HTG | b | 603 | - | 19,19,19 | 0.94 | 2 (10%) | 23,24,24 | 1.31 | 2 (8%) |
| 36 | DGD | C | 518 | - | 63,63,67 | 0.85 | 2 (3%) | 77,77,81 | 1.03 | 6 (7%) |
| 24 | CLA | b | 607 | - | 69,73,73 | 2.04 | 20 (28%) | 82,113,113 | 2.73 | 33 (40%) |
| 24 | CLA | A | 407 | 41 | 69,73,73 | 2.06 | 19 (27%) | 82,113,113 | 2.73 | 34 (41%) |
| 29 | LMT | m | 103 | - | 36,36,36 | 0.48 | 0 | 47,47,47 | 1.00 | 2 (4%) |
| 26 | BCR | B | 619 | - | 41,41,41 | 1.07 | 1 (2%) | 56,56,56 | 1.24 | 5 (8%) |
| 24 | CLA | c | 906 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.61 | 28 (34%) |
| 34 | LMG | b | 624 | - | 51,51,55 | 0.92 | 3 (5%) | 59,59,63 | 1.06 | 4 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 35 | HTG | b | 602 | - | 19,19,19 | 1.04 | 2 (10%) | 23,24,24 | 1.13 | 1 (4%) |
| 28 | GOL | o | 302 | - | 5,5,5 | 0.40 | 0 | 5,5,5 | 0.51 | 0 |
| 26 | BCR | C | 516 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.41 | 7 (12%) |
| 26 | BCR | k | 102 | - | 41,41,41 | 1.07 | 1 (2%) | 56,56,56 | 1.37 | 6 (10%) |
| 23 | BCT | A | 404 | 21 | 3,3,3 | 1.42 | 1 (33%) | 2,3,3 | 0.50 | 0 |
| 26 | BCR | b | 622 | - | 41,41,41 | 1.07 | 1 (2%) | 56,56,56 | 1.28 | 5 (8%) |
| 35 | HTG | B | 626 | - | 19,19,19 | 0.92 | 1 (5%) | 23,24,24 | 1.52 | 2 (8%) |
| 24 | CLA | C | 504 | - | 69,73,73 | 2.00 | 20 (28%) | 82,113,113 | 2.70 | 29 (35%) |
| 24 | CLA | c | 907 | - | 69,73,73 | 2.01 | 19 (27%) | 82,113,113 | 2.61 | 32 (39%) |
| 27 | SQD | A | 412 | - | 52,54,54 | 0.93 | 2 (3%) | 62,65,65 | 1.76 | 12 (19%) |
| 29 | LMT | m | 104 | - | 36,36,36 | 0.51 | 0 | 47,47,47 | 1.02 | 2 (4%) |
| 28 | GOL | b | 628 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.33 | 0 |
| 40 | HEC | v | 202 | 16 | 46,50,50 | 1.70 | 9 (19%) | 58,82,82 | 1.52 | 11 (18%) |
| 24 | CLA | d | 403 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.66 | 32 (39%) |
| 26 | BCR | y | 101 | - | 41,41,41 | 1.06 | 1 (2%) | 56,56,56 | 1.63 | 11 (19%) |
| 28 | GOL | A | 413 | - | 5,5,5 | 0.26 | 0 | 5,5,5 | 0.54 | 0 |
| 28 | GOL | f | 101 | 33 | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.41 | 0 |
| 24 | CLA | C | 502 | - | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.71 | 31 (37%) |
| 24 | CLA | b | 617 | - | 69,73,73 | 1.99 | 20 (28%) | 82,113,113 | 2.61 | 34 (41%) |
| 36 | DGD | h | 102 | - | 63,63,67 | 0.93 | 3 (4%) | 77,77,81 | 0.99 | 6 (7%) |
| 34 | LMG | C | 520 | - | 51,51,55 | 0.96 | 2 (3%) | 59,59,63 | 1.08 | 4 (6%) |
| 28 | GOL | a | 415 | - | 5,5,5 | 0.41 | 0 | 5,5,5 | 0.50 | 0 |
| 24 | CLA | a | 409 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.61 | 35 (42%) |
| 37 | LHG | D | 406 | - | 48,48,48 | 0.87 | 2 (4%) | 51,54,54 | 1.11 | 5 (9%) |
| 24 | CLA | D | 402 | - | 69,73,73 | 2.01 | 19 (27%) | 82,113,113 | 2.61 | 28 (34%) |
| 24 | CLA | C | 508 | 41 | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.55 | 29 (35%) |
| 36 | DGD | c | 916 | - | 63,63,67 | 0.83 | 2 (3%) | 77,77,81 | 1.10 | 6 (7%) |
| 28 | GOL | t | 102 | - | 5,5,5 | 0.41 | 0 | 5,5,5 | 0.25 | 0 |
| 37 | LHG | E | 101 | - | 41,41,48 | 1.06 | 2 (4%) | 44,47,54 | 1.11 | 3 (6%) |
| 24 | CLA | C | 503 | - | 69,73,73 | 2.04 | 20 (28%) | 82,113,113 | 2.57 | 31 (37%) |
| 24 | CLA | B | 602 | 41 | 69,73,73 | 2.03 | 19 (27%) | 82,113,113 | 2.69 | 32 (39%) |
| 36 | DGD | c | 917 | - | 63,63,67 | 0.89 | 2 (3%) | 77,77,81 | 1.01 | 3 (3%) |
| 28 | GOL | B | 629 | - | 5,5,5 | 0.41 | 0 | 5,5,5 | 0.60 | 0 |
| 24 | CLA | B | 615 | - | 69,73,73 | 2.02 | 19 (27%) | 82,113,113 | 2.84 | 33 (40%) |
| 28 | GOL | B | 627 | - | 5,5,5 | 0.42 | 0 | 5,5,5 | 0.62 | 0 |
| 28 | GOL | B | 628 | - | 5,5,5 | 0.28 | 0 | 5,5,5 | 0.46 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 34 | LMG | J | 101 | 39 | 51,51,55 | 0.88 | 2 (3%) | 59,59,63 | 0.89 | 3 (5%) |
| 35 | HTG | c | 923 | - | 19,19,19 | 1.04 | 2 (10%) | 23,24,24 | 1.71 | 5 (21%) |
| 36 | DGD | c | 918 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 0.95 | 4 (5%) |
| 25 | PHO | a | 420 | - | 58,69,69 | 2.84 | 12 (20%) | 55,99,99 | 2.85 | 15 (27%) |
| 29 | LMT | f | 103 | - | 36,36,36 | 0.54 | 1 (2%) | 47,47,47 | 0.94 | 4 (8%) |
| 31 | PL9 | D | 404 | - | 55,55,55 | 0.74 | 2 (3%) | 68,69,69 | 1.58 | 15 (22%) |
| 24 | CLA | C | 513 | - | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.70 | 35 (42%) |
| 34 | LMG | C | 521 | - | 51,51,55 | 0.96 | 2 (3%) | 59,59,63 | 1.07 | 4 (6%) |
| 34 | LMG | a | 412 | - | 51,51,55 | 0.91 | 2 (3%) | 59,59,63 | 1.15 | 6 (10%) |
| 29 | LMT | b | 625 | - | 25,25,36 | 0.53 | 1 (4%) | 30,30,47 | 0.60 | 0 |
| 28 | GOL | b | 632 | - | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.58 | 0 |
| 27 | SQD | F | 101 | - | 41,43,54 | 1.11 | 2 (4%) | 51,54,65 | 1.93 | 10 (19%) |
| 40 | HEC | V | 201 | 16 | 46,50,50 | 1.73 | 10 (21%) | 58,82,82 | 1.63 | 10 (17%) |
| 27 | SQD | A | 416 | - | 52,54,54 | 0.96 | 2 (3%) | 62,65,65 | 1.19 | 5 (8%) |
| 28 | GOL | v | 205 | - | 5,5,5 | 0.40 | 0 | 5,5,5 | 0.38 | 0 |
| 35 | HTG | D | 411 | - | 16,16,19 | 1.06 | 2 (12%) | 20,21,24 | 0.90 | 1 (5%) |
| 24 | CLA | d | 402 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.77 | 29 (35%) |
| 28 | GOL | b | 630 | - | 5,5,5 | 0.33 | 0 | 5,5,5 | 0.57 | 0 |
| 25 | PHO | A | 409 | - | 58,69,69 | 2.86 | 14 (24%) | 55,99,99 | 2.88 | 15 (27%) |
| 26 | BCR | K | 102 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.43 | 7 (12%) |
| 24 | CLA | B | 605 | - | 69,73,73 | 1.92 | 18 (26%) | 82,113,113 | 2.62 | 28 (34%) |
| 24 | CLA | C | 512 | 3 | 69,73,73 | 2.03 | 20 (28%) | 82,113,113 | 2.60 | 29 (35%) |
| 30 | OEX | a | 416 | 1,41,3 | 0,15,15 | - | - | - | | |
| 31 | PL9 | a | 417 | - | 55,55,55 | 0.65 | 2 (3%) | 68,69,69 | 1.93 | 19 (27%) |
| 25 | PHO | A | 408 | - | 58,69,69 | 2.75 | 11 (18%) | 55,99,99 | 3.05 | 13 (23%) |
| 29 | LMT | B | 636 | - | 25,25,36 | 0.43 | 0 | 30,30,47 | 0.66 | 0 |
| 27 | SQD | a | 411 | - | 52,54,54 | 0.89 | 2 (3%) | 62,65,65 | 1.59 | 9 (14%) |
| 29 | LMT | c | 921 | - | 36,36,36 | 0.45 | 0 | 47,47,47 | 0.83 | 1 (2%) |
| 29 | LMT | m | 102 | - | 36,36,36 | 0.48 | 0 | 47,47,47 | 0.92 | 2 (4%) |
| 36 | DGD | C | 517 | - | 63,63,67 | 0.87 | 3 (4%) | 77,77,81 | 1.05 | 5 (6%) |
| 34 | LMG | B | 622 | - | 51,51,55 | 0.92 | 2 (3%) | 59,59,63 | 1.17 | 3 (5%) |
| 24 | CLA | b | 612 | - | 69,73,73 | 2.06 | 20 (28%) | 82,113,113 | 2.60 | 31 (37%) |
| 25 | PHO | a | 408 | - | 58,69,69 | 2.67 | 12 (20%) | 55,99,99 | 2.88 | 13 (23%) |
| 24 | CLA | B | 617 | - | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.67 | 29 (35%) |
| 27 | SQD | B | 621 | - | 52,54,54 | 1.00 | 3 (5%) | 62,65,65 | 1.45 | 9 (14%) |
| 28 | GOL | C | 526 | - | 5,5,5 | 0.22 | 0 | 5,5,5 | 0.47 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 31 | PL9 | A | 419 | - | 55,55,55 | 0.65 | 2 (3%) | 68,69,69 | 1.85 | 22 (32%) |
| 35 | HTG | V | 202 | - | 19,19,19 | 0.92 | 2 (10%) | 23,24,24 | 1.43 | 3 (13%) |
| 28 | GOL | v | 204 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.41 | 0 |
| 34 | LMG | c | 919 | - | 51,51,55 | 0.97 | 3 (5%) | 59,59,63 | 1.02 | 2 (3%) |
| 24 | CLA | b | 613 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.68 | 31 (37%) |
| 26 | BCR | h | 101 | - | 41,41,41 | 1.08 | 1 (2%) | 56,56,56 | 1.29 | 5 (8%) |
| 26 | BCR | b | 623 | - | 41,41,41 | 1.01 | 1 (2%) | 56,56,56 | 1.45 | 9 (16%) |
| 24 | CLA | c | 904 | - | 69,73,73 | 2.01 | 20 (28%) | 82,113,113 | 2.61 | 30 (36%) |
| 24 | CLA | C | 511 | - | 69,73,73 | 2.04 | 20 (28%) | 82,113,113 | 2.57 | 30 (36%) |
| 29 | LMT | A | 417 | - | 36,36,36 | 0.50 | 1 (2%) | 47,47,47 | 1.08 | 2 (4%) |
| 29 | LMT | a | 401 | - | 36,36,36 | 0.53 | 1 (2%) | 47,47,47 | 0.96 | 2 (4%) |
| 29 | LMT | B | 623 | - | 36,36,36 | 0.43 | 0 | 47,47,47 | 1.42 | 5 (10%) |
| 37 | LHG | d | 409 | - | 48,48,48 | 0.96 | 2 (4%) | 51,54,54 | 1.06 | 4 (7%) |
| 34 | LMG | Z | 101 | - | 37,37,55 | 1.00 | 2 (5%) | 45,45,63 | 1.32 | 6 (13%) |
| 24 | CLA | C | 514 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.66 | 30 (36%) |
| 26 | BCR | k | 101 | - | 41,41,41 | 1.11 | 1 (2%) | 56,56,56 | 1.45 | 10 (17%) |
| 27 | SQD | f | 102 | - | 41,43,54 | 1.10 | 2 (4%) | 51,54,65 | 1.42 | 8 (15%) |
| 24 | CLA | b | 606 | - | 69,73,73 | 2.00 | 21 (30%) | 82,113,113 | 2.72 | 31 (37%) |
| 26 | BCR | K | 103 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.42 | 7 (12%) |
| 26 | BCR | A | 411 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.21 | 5 (8%) |
| 30 | OEX | A | 418 | 1,41,3 | 0,15,15 | - | - | - | | |
| 36 | DGD | H | 102 | - | 63,63,67 | 0.95 | 4 (6%) | 77,77,81 | 0.93 | 4 (5%) |
| 36 | DGD | C | 519 | - | 63,63,67 | 0.84 | 3 (4%) | 77,77,81 | 0.96 | 5 (6%) |
| 26 | BCR | d | 404 | - | 41,41,41 | 1.07 | 1 (2%) | 56,56,56 | 1.80 | 17 (30%) |
| 31 | PL9 | d | 405 | - | 55,55,55 | 0.75 | 2 (3%) | 68,69,69 | 1.53 | 13 (19%) |
| 24 | CLA | b | 614 | 41 | 69,73,73 | 2.04 | 20 (28%) | 82,113,113 | 2.63 | 35 (42%) |
| 35 | HTG | d | 412 | - | 16,16,19 | 1.01 | 2 (12%) | 20,21,24 | 1.24 | 1 (5%) |
| 26 | BCR | D | 403 | - | 41,41,41 | 1.07 | 1 (2%) | 56,56,56 | 1.75 | 13 (23%) |
| 24 | CLA | b | 620 | - | 69,73,73 | 2.00 | 21 (30%) | 82,113,113 | 2.60 | 27 (32%) |
| 28 | GOL | V | 206 | - | 5,5,5 | 0.33 | 0 | 5,5,5 | 0.33 | 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 |
|---|---|---|---|---|---|---|---|
| 24 | CLA | B | 606 | - | 1/1/15/20 | 8/39/115/115 | - |
| 26 | BCR | a | 410 | - | - | 0/29/63/63 | 0/2/2/2 |
| 28 | GOL | b | 633 | - | - | 2/4/4/4 | - |
| 35 | HTG | c | 922 | - | - | 4/10/30/30 | 0/1/1/1 |
| 28 | GOL | A | 414 | - | - | 2/4/4/4 | - |
| 28 | GOL | B | 632 | - | - | 2/4/4/4 | - |
| 28 | GOL | v | 203 | - | - | 3/4/4/4 | - |
| 24 | CLA | b | 611 | 41 | 1/1/15/20 | 4/39/115/115 | - |
| 24 | CLA | b | 616 | - | 1/1/15/20 | 1/39/115/115 | - |
| 28 | GOL | b | 631 | - | - | 2/4/4/4 | - |
| 24 | CLA | c | 912 | 3 | 1/1/15/20 | 4/39/115/115 | - |
| 35 | HTG | C | 523 | - | - | 1/10/30/30 | 0/1/1/1 |
| 28 | GOL | V | 204 | - | - | 2/4/4/4 | - |
| 35 | HTG | C | 524 | - | - | 2/10/30/30 | 0/1/1/1 |
| 38 | HEM | E | 103 | 6,5 | - | 4/14/54/54 | - |
| 24 | CLA | c | 914 | - | 1/1/15/20 | 10/39/115/115 | - |
| 35 | HTG | B | 624 | - | - | 1/10/30/30 | 0/1/1/1 |
| 34 | LMG | j | 101 | 39 | - | 11/46/66/70 | 0/1/1/1 |
| 24 | CLA | B | 608 | 41 | 1/1/15/20 | 1/39/115/115 | - |
| 28 | GOL | V | 203 | - | - | 4/4/4/4 | - |
| 35 | HTG | B | 625 | - | - | 3/10/30/30 | 0/1/1/1 |
| 28 | GOL | a | 413 | - | - | 0/4/4/4 | - |
| 24 | CLA | D | 401 | - | 1/1/15/20 | 2/39/115/115 | - |
| 37 | LHG | D | 407 | - | - | 5/53/53/53 | - |
| 24 | CLA | B | 603 | - | 1/1/15/20 | 5/39/115/115 | - |
| 28 | GOL | A | 415 | - | - | 2/4/4/4 | - |
| 29 | LMT | E | 102 | - | - | 7/21/61/61 | 0/2/2/2 |
| 34 | LMG | C | 501 | - | - | 20/46/66/70 | 0/1/1/1 |
| 26 | BCR | T | 102 | - | - | 1/29/63/63 | 0/2/2/2 |
| 35 | HTG | B | 633 | - | - | 3/10/30/30 | 0/1/1/1 |
| 36 | DGD | d | 406 | - | - | 28/51/91/95 | 0/2/2/2 |
| 28 | GOL | O | 302 | - | - | 2/4/4/4 | - |
| 24 | CLA | b | 615 | - | 1/1/15/20 | 5/39/115/115 | - |
| 37 | LHG | d | 407 | - | - | 9/53/53/53 | - |
| 34 | LMG | c | 920 | - | - | 4/46/66/70 | 0/1/1/1 |
| 38 | HEM | e | 102 | 6,5 | - | 5/14/54/54 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 35 | HTG | O | 303 | - | - | 1/10/30/30 | 0/1/1/1 |
| 24 | CLA | B | 611 | 41 | 1/1/15/20 | 6/39/115/115 | - |
| 24 | CLA | c | 903 | - | 1/1/15/20 | 6/39/115/115 | - |
| 24 | CLA | d | 401 | 41 | 1/1/15/20 | 5/39/115/115 | - |
| 24 | CLA | C | 510 | - | 1/1/15/20 | 7/39/115/115 | - |
| 28 | GOL | V | 205 | - | - | 1/4/4/4 | - |
| 37 | LHG | D | 408 | - | - | 11/53/53/53 | - |
| 24 | CLA | C | 505 | 41 | 1/1/15/20 | 6/39/115/115 | - |
| 37 | LHG | l | 101 | - | - | 16/53/53/53 | - |
| 24 | CLA | A | 405 | - | 1/1/15/20 | 2/39/115/115 | - |
| 24 | CLA | B | 613 | - | 1/1/15/20 | 4/39/115/115 | - |
| 24 | CLA | B | 604 | - | 1/1/15/20 | 5/39/115/115 | - |
| 24 | CLA | b | 619 | - | 1/1/15/20 | 4/39/115/115 | - |
| 24 | CLA | b | 610 | - | 1/1/15/20 | 16/39/115/115 | - |
| 24 | CLA | b | 609 | - | 1/1/15/20 | 8/39/115/115 | - |
| 24 | CLA | B | 607 | - | 1/1/15/20 | 5/39/115/115 | - |
| 26 | BCR | C | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 28 | GOL | c | 924 | - | - | 0/4/4/4 | - |
| 24 | CLA | c | 902 | - | 1/1/15/20 | 3/39/115/115 | - |
| 24 | CLA | a | 407 | 41 | - | 4/39/115/115 | - |
| 24 | CLA | B | 612 | - | 1/1/15/20 | 2/39/115/115 | - |
| 26 | BCR | H | 101 | - | - | 3/29/63/63 | 0/2/2/2 |
| 28 | GOL | T | 103 | - | - | 4/4/4/4 | - |
| 24 | CLA | A | 406 | 41 | 1/1/15/20 | 2/39/115/115 | - |
| 29 | LMT | C | 522 | - | - | 10/21/61/61 | 0/2/2/2 |
| 26 | BCR | t | 101 | - | - | 1/29/63/63 | 0/2/2/2 |
| 29 | LMT | b | 601 | - | - | 8/17/37/61 | 0/1/1/2 |
| 24 | CLA | c | 905 | 41 | 1/1/15/20 | 4/39/115/115 | - |
| 28 | GOL | B | 631 | - | - | 4/4/4/4 | - |
| 27 | SQD | a | 402 | - | - | 14/49/69/69 | 0/1/1/1 |
| 26 | BCR | b | 621 | - | - | 2/29/63/63 | 0/2/2/2 |
| 37 | LHG | e | 101 | - | - | 10/46/46/53 | - |
| 34 | LMG | z | 101 | - | - | 10/34/54/70 | 0/1/1/1 |
| 24 | CLA | C | 506 | - | 1/1/15/20 | 8/39/115/115 | - |
| 24 | CLA | b | 618 | - | 1/1/15/20 | 13/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 28 | GOL | B | 637 | - | - | 2/4/4/4 | - |
| 36 | DGD | D | 405 | - | - | 22/51/91/95 | 0/2/2/2 |
| 24 | CLA | c | 913 | - | 1/1/15/20 | 7/39/115/115 | - |
| 28 | GOL | T | 101 | - | - | 0/4/4/4 | - |
| 24 | CLA | a | 406 | - | 1/1/15/20 | 2/39/115/115 | - |
| 37 | LHG | d | 408 | - | - | 11/53/53/53 | - |
| 28 | GOL | B | 630 | - | - | 0/4/4/4 | - |
| 29 | LMT | M | 101 | - | - | 6/21/61/61 | 0/2/2/2 |
| 24 | CLA | c | 909 | - | 1/1/15/20 | 1/39/115/115 | - |
| 24 | CLA | c | 908 | 41 | 1/1/15/20 | 4/39/115/115 | - |
| 24 | CLA | C | 507 | - | 1/1/15/20 | 10/39/115/115 | - |
| 24 | CLA | A | 410 | - | - | 10/39/115/115 | - |
| 26 | BCR | B | 618 | - | - | 2/29/63/63 | 0/2/2/2 |
| 24 | CLA | B | 614 | - | 1/1/15/20 | 7/39/115/115 | - |
| 24 | CLA | B | 609 | - | - | 0/39/115/115 | - |
| 24 | CLA | B | 610 | - | 1/1/15/20 | 1/39/115/115 | - |
| 28 | GOL | F | 103 | 33 | - | 2/4/4/4 | - |
| 35 | HTG | B | 634 | - | - | 2/10/30/30 | 0/1/1/1 |
| 28 | GOL | c | 925 | - | - | 0/4/4/4 | - |
| 35 | HTG | b | 627 | - | - | 2/10/30/30 | 0/1/1/1 |
| 35 | HTG | b | 626 | - | - | 1/10/30/30 | 0/1/1/1 |
| 27 | SQD | L | 102 | - | - | 25/49/69/69 | 0/1/1/1 |
| 24 | CLA | C | 509 | - | - | 5/39/115/115 | - |
| 24 | CLA | c | 911 | - | 1/1/15/20 | 8/39/115/115 | - |
| 24 | CLA | b | 605 | 41 | 1/1/15/20 | 11/39/115/115 | - |
| 24 | CLA | c | 910 | - | 1/1/15/20 | 7/39/115/115 | - |
| 28 | GOL | a | 414 | - | - | 1/4/4/4 | - |
| 37 | LHG | L | 101 | - | - | 15/53/53/53 | - |
| 28 | GOL | C | 525 | - | - | 0/4/4/4 | - |
| 26 | BCR | c | 915 | - | - | 4/29/63/63 | 0/2/2/2 |
| 26 | BCR | B | 620 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | CLA | B | 616 | - | 1/1/15/20 | 10/39/115/115 | - |
| 24 | CLA | b | 608 | - | 1/1/15/20 | 6/39/115/115 | - |
| 28 | GOL | b | 629 | - | - | 0/4/4/4 | - |
| 35 | HTG | b | 603 | - | - | 0/10/30/30 | 0/1/1/1 |
| 36 | DGD | C | 518 | - | - | 14/51/91/95 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | CLA | b | 607 | - | 1/1/15/20 | 4/39/115/115 | - |
| 24 | CLA | A | 407 | 41 | - | 2/39/115/115 | - |
| 29 | LMT | m | 103 | - | - | 2/21/61/61 | 0/2/2/2 |
| 26 | BCR | B | 619 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | CLA | c | 906 | - | 1/1/15/20 | 3/39/115/115 | - |
| 34 | LMG | b | 624 | - | - | 14/46/66/70 | 0/1/1/1 |
| 35 | HTG | b | 602 | - | - | 1/10/30/30 | 0/1/1/1 |
| 28 | GOL | o | 302 | - | - | 2/4/4/4 | - |
| 26 | BCR | C | 516 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | k | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 35 | HTG | B | 626 | - | - | 4/10/30/30 | 0/1/1/1 |
| 26 | BCR | b | 622 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | CLA | C | 504 | - | 1/1/15/20 | 6/39/115/115 | - |
| 24 | CLA | c | 907 | - | 1/1/15/20 | 8/39/115/115 | - |
| 27 | SQD | A | 412 | - | - | 11/49/69/69 | 0/1/1/1 |
| 29 | LMT | m | 104 | - | - | 7/21/61/61 | 0/2/2/2 |
| 28 | GOL | b | 628 | - | - | 2/4/4/4 | - |
| 40 | HEC | v | 202 | 16 | - | 6/14/54/54 | - |
| 24 | CLA | d | 403 | - | - | 6/39/115/115 | - |
| 26 | BCR | y | 101 | - | - | 3/29/63/63 | 0/2/2/2 |
| 28 | GOL | A | 413 | - | - | 2/4/4/4 | - |
| 28 | GOL | f | 101 | 33 | - | 4/4/4/4 | - |
| 24 | CLA | C | 502 | - | 1/1/15/20 | 9/39/115/115 | - |
| 24 | CLA | b | 617 | - | 1/1/15/20 | 4/39/115/115 | - |
| 36 | DGD | h | 102 | - | - | 14/51/91/95 | 0/2/2/2 |
| 34 | LMG | C | 520 | - | - | 11/46/66/70 | 0/1/1/1 |
| 28 | GOL | a | 415 | - | - | 2/4/4/4 | - |
| 24 | CLA | a | 409 | - | 1/1/15/20 | 7/39/115/115 | - |
| 37 | LHG | D | 406 | - | - | 6/53/53/53 | - |
| 24 | CLA | D | 402 | - | 1/1/15/20 | 10/39/115/115 | - |
| 24 | CLA | C | 508 | 41 | 1/1/15/20 | 6/39/115/115 | - |
| 36 | DGD | c | 916 | - | - | 10/51/91/95 | 0/2/2/2 |
| 28 | GOL | t | 102 | - | - | 0/4/4/4 | - |
| 37 | LHG | E | 101 | - | - | 20/46/46/53 | - |
| 24 | CLA | C | 503 | - | - | 5/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | CLA | B | 602 | 41 | 1/1/15/20 | 14/39/115/115 | - |
| 36 | DGD | c | 917 | - | - | 14/51/91/95 | 0/2/2/2 |
| 28 | GOL | B | 629 | - | - | 2/4/4/4 | - |
| 24 | CLA | B | 615 | - | 1/1/15/20 | 16/39/115/115 | - |
| 28 | GOL | B | 627 | - | - | 1/4/4/4 | - |
| 28 | GOL | B | 628 | - | - | 2/4/4/4 | - |
| 34 | LMG | J | 101 | 39 | - | 13/46/66/70 | 0/1/1/1 |
| 35 | HTG | c | 923 | - | - | 0/10/30/30 | 0/1/1/1 |
| 36 | DGD | c | 918 | - | - | 17/51/91/95 | 0/2/2/2 |
| 25 | PHO | a | 420 | - | - | 2/37/103/103 | 0/5/6/6 |
| 29 | LMT | f | 103 | - | - | 9/21/61/61 | 0/2/2/2 |
| 31 | PL9 | D | 404 | - | - | 3/53/73/73 | 0/1/1/1 |
| 24 | CLA | C | 513 | - | 1/1/15/20 | 11/39/115/115 | - |
| 34 | LMG | C | 521 | - | - | 12/46/66/70 | 0/1/1/1 |
| 34 | LMG | a | 412 | - | - | 9/46/66/70 | 0/1/1/1 |
| 29 | LMT | b | 625 | - | - | 4/17/37/61 | 0/1/1/2 |
| 28 | GOL | b | 632 | - | - | 2/4/4/4 | - |
| 27 | SQD | F | 101 | - | - | 14/38/58/69 | 0/1/1/1 |
| 40 | HEC | V | 201 | 16 | - | 6/14/54/54 | - |
| 27 | SQD | A | 416 | - | - | 14/49/69/69 | 0/1/1/1 |
| 28 | GOL | v | 205 | - | - | 2/4/4/4 | - |
| 35 | HTG | D | 411 | - | - | 1/7/27/30 | 0/1/1/1 |
| 24 | CLA | d | 402 | - | 1/1/15/20 | 2/39/115/115 | - |
| 28 | GOL | b | 630 | - | - | 0/4/4/4 | - |
| 25 | PHO | A | 409 | - | - | 0/37/103/103 | 0/5/6/6 |
| 26 | BCR | K | 102 | - | - | 4/29/63/63 | 0/2/2/2 |
| 24 | CLA | B | 605 | - | 1/1/15/20 | 2/39/115/115 | - |
| 24 | CLA | C | 512 | 3 | 1/1/15/20 | 2/39/115/115 | - |
| 31 | PL9 | a | 417 | - | - | 12/53/73/73 | 0/1/1/1 |
| 25 | PHO | A | 408 | - | - | 4/37/103/103 | 0/5/6/6 |
| 29 | LMT | B | 636 | - | - | 8/17/37/61 | 0/1/1/2 |
| 27 | SQD | a | 411 | - | - | 12/49/69/69 | 0/1/1/1 |
| 29 | LMT | c | 921 | - | - | 4/21/61/61 | 0/2/2/2 |
| 29 | LMT | m | 102 | - | - | 6/21/61/61 | 0/2/2/2 |
| 36 | DGD | C | 517 | - | - | 16/51/91/95 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 34 | LMG | B | 622 | - | - | 12/46/66/70 | 0/1/1/1 |
| 24 | CLA | b | 612 | - | - | 3/39/115/115 | - |
| 25 | PHO | a | 408 | - | - | 1/37/103/103 | 0/5/6/6 |
| 24 | CLA | B | 617 | - | 1/1/15/20 | 11/39/115/115 | - |
| 27 | SQD | B | 621 | - | - | 25/49/69/69 | 0/1/1/1 |
| 28 | GOL | C | 526 | - | - | 0/4/4/4 | - |
| 31 | PL9 | A | 419 | - | - | 7/53/73/73 | 0/1/1/1 |
| 35 | HTG | V | 202 | - | - | 5/10/30/30 | 0/1/1/1 |
| 28 | GOL | v | 204 | - | - | 2/4/4/4 | - |
| 34 | LMG | c | 919 | - | - | 17/46/66/70 | 0/1/1/1 |
| 24 | CLA | b | 613 | - | 1/1/15/20 | 0/39/115/115 | - |
| 26 | BCR | h | 101 | - | - | 3/29/63/63 | 0/2/2/2 |
| 26 | BCR | b | 623 | - | - | 2/29/63/63 | 0/2/2/2 |
| 24 | CLA | c | 904 | - | 1/1/15/20 | 3/39/115/115 | - |
| 24 | CLA | C | 511 | - | 1/1/15/20 | 10/39/115/115 | - |
| 29 | LMT | A | 417 | - | - | 5/21/61/61 | 0/2/2/2 |
| 29 | LMT | a | 401 | - | - | 11/21/61/61 | 0/2/2/2 |
| 29 | LMT | B | 623 | - | - | 7/21/61/61 | 0/2/2/2 |
| 37 | LHG | d | 409 | - | - | 12/53/53/53 | - |
| 34 | LMG | Z | 101 | - | - | 12/31/51/70 | 0/1/1/1 |
| 24 | CLA | C | 514 | - | - | 2/39/115/115 | - |
| 26 | BCR | k | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | SQD | f | 102 | - | - | 15/38/58/69 | 0/1/1/1 |
| 24 | CLA | b | 606 | - | 1/1/15/20 | 1/39/115/115 | - |
| 26 | BCR | K | 103 | - | - | 2/29/63/63 | 0/2/2/2 |
| 26 | BCR | A | 411 | - | - | 0/29/63/63 | 0/2/2/2 |
| 36 | DGD | H | 102 | - | - | 10/51/91/95 | 0/2/2/2 |
| 36 | DGD | C | 519 | - | - | 8/51/91/95 | 0/2/2/2 |
| 26 | BCR | d | 404 | - | - | 4/29/63/63 | 0/2/2/2 |
| 31 | PL9 | d | 405 | - | - | 2/53/73/73 | 0/1/1/1 |
| 24 | CLA | b | 614 | 41 | 1/1/15/20 | 5/39/115/115 | - |
| 35 | HTG | d | 412 | - | - | 0/7/27/30 | 0/1/1/1 |
| 26 | BCR | D | 403 | - | - | 6/29/63/63 | 0/2/2/2 |
| 24 | CLA | b | 620 | - | 1/1/15/20 | 8/39/115/115 | - |
| 28 | GOL | V | 206 | - | - | 1/4/4/4 | - |

All (1595) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | a | 408 | PHO | C1D-C2D | 9.35 | 1.49 | 1.39 |
| 25 | A | 409 | PHO | C1B-C2B | 9.30 | 1.49 | 1.39 |
| 25 | a | 420 | PHO | C1B-C2B | 9.19 | 1.49 | 1.39 |
| 25 | A | 408 | PHO | C1B-C2B | 8.92 | 1.49 | 1.39 |
| 25 | a | 408 | PHO | C1B-C2B | 8.78 | 1.49 | 1.39 |
| 25 | a | 420 | PHO | C1D-C2D | 8.62 | 1.49 | 1.39 |
| 25 | A | 409 | PHO | C3B-C4B | 8.55 | 1.50 | 1.41 |
| 25 | A | 408 | PHO | C3B-C4B | 8.39 | 1.50 | 1.41 |
| 25 | A | 408 | PHO | C1D-C2D | 8.35 | 1.48 | 1.39 |
| 25 | a | 420 | PHO | C3B-C4B | 8.16 | 1.49 | 1.41 |
| 25 | A | 409 | PHO | C1D-C2D | 8.13 | 1.48 | 1.39 |
| 25 | a | 420 | PHO | C4D-CHA | 7.78 | 1.51 | 1.39 |
| 25 | a | 408 | PHO | C3B-C4B | 7.13 | 1.48 | 1.41 |
| 25 | A | 408 | PHO | C4D-CHA | 7.05 | 1.50 | 1.39 |
| 25 | a | 420 | PHO | C3B-C2B | 6.89 | 1.49 | 1.40 |
| 25 | A | 409 | PHO | C3B-C2B | 6.78 | 1.49 | 1.40 |
| 25 | A | 409 | PHO | C4D-CHA | 6.73 | 1.49 | 1.39 |
| 25 | A | 408 | PHO | C3B-C2B | 6.36 | 1.49 | 1.40 |
| 25 | a | 408 | PHO | C4D-CHA | 6.30 | 1.49 | 1.39 |
| 25 | a | 408 | PHO | C3B-C2B | 6.11 | 1.48 | 1.40 |
| 25 | A | 409 | PHO | C3D-C2D | 5.88 | 1.49 | 1.39 |
| 24 | B | 611 | CLA | C3C-C2C | 5.67 | 1.49 | 1.36 |
| 24 | b | 605 | CLA | C3C-C2C | 5.61 | 1.48 | 1.36 |
| 25 | a | 420 | PHO | C3D-C2D | 5.60 | 1.49 | 1.39 |
| 24 | A | 407 | CLA | C3C-C2C | 5.55 | 1.48 | 1.36 |
| 38 | e | 102 | HEM | FE-NB | 5.49 | 2.11 | 1.94 |
| 24 | C | 504 | CLA | C3C-C2C | 5.45 | 1.48 | 1.36 |
| 24 | b | 618 | CLA | C3C-C2C | 5.43 | 1.48 | 1.36 |
| 24 | C | 507 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 24 | b | 612 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 24 | D | 402 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 24 | B | 609 | CLA | C3C-C2C | 5.37 | 1.48 | 1.36 |
| 24 | C | 511 | CLA | C3C-C2C | 5.37 | 1.48 | 1.36 |
| 24 | C | 513 | CLA | C3C-C2C | 5.35 | 1.48 | 1.36 |
| 24 | b | 614 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 24 | B | 604 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 24 | B | 614 | CLA | C3C-C2C | 5.32 | 1.48 | 1.36 |
| 24 | d | 401 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 24 | C | 506 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 24 | C | 514 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 24 | b | 617 | CLA | O2D-CGD | 5.29 | 1.46 | 1.33 |
| 24 | b | 607 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 24 | a | 406 | CLA | C3C-C2C | 5.27 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 913 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 24 | c | 909 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 24 | A | 410 | CLA | C3C-C2C | 5.23 | 1.48 | 1.36 |
| 24 | c | 911 | CLA | C3C-C2C | 5.23 | 1.48 | 1.36 |
| 25 | A | 408 | PHO | OBD-CAD | 5.23 | 1.29 | 1.22 |
| 24 | a | 409 | CLA | C3C-C2C | 5.22 | 1.48 | 1.36 |
| 24 | C | 503 | CLA | C3C-C2C | 5.21 | 1.48 | 1.36 |
| 24 | c | 907 | CLA | O2D-CGD | 5.20 | 1.46 | 1.33 |
| 24 | C | 505 | CLA | C3C-C2C | 5.19 | 1.48 | 1.36 |
| 24 | B | 603 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 24 | C | 510 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 24 | A | 407 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 24 | c | 903 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 24 | c | 904 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 24 | A | 407 | CLA | CHC-C1C | 5.13 | 1.48 | 1.38 |
| 24 | b | 605 | CLA | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 24 | b | 616 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 24 | B | 603 | CLA | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 26 | k | 101 | BCR | C23-C22 | -5.12 | 1.35 | 1.46 |
| 24 | a | 409 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 24 | b | 611 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 24 | B | 608 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 24 | A | 405 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 24 | c | 912 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 24 | d | 401 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 24 | a | 407 | CLA | CHC-C1C | 5.09 | 1.48 | 1.38 |
| 24 | c | 910 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 24 | C | 510 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 38 | E | 103 | HEM | FE-NB | 5.09 | 2.10 | 1.94 |
| 26 | t | 101 | BCR | C23-C22 | -5.08 | 1.35 | 1.46 |
| 25 | A | 409 | PHO | OBD-CAD | 5.08 | 1.29 | 1.22 |
| 25 | a | 408 | PHO | C3D-C2D | 5.08 | 1.48 | 1.39 |
| 24 | c | 914 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 24 | a | 406 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 24 | b | 613 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 24 | b | 620 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 24 | A | 410 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 24 | B | 602 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 24 | c | 905 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 24 | b | 606 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 24 | C | 506 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 24 | B | 617 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 26 | B | 620 | BCR | C23-C22 | -5.03 | 1.35 | 1.46 |
| 24 | C | 503 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 24 | a | 407 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 24 | b | 616 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 26 | b | 622 | BCR | C23-C22 | -5.02 | 1.35 | 1.46 |
| 24 | c | 914 | CLA | CHC-C1C | 5.02 | 1.48 | 1.38 |
| 24 | A | 406 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 24 | a | 407 | CLA | C1D-ND | 5.01 | 1.44 | 1.37 |
| 24 | c | 908 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 24 | b | 617 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 24 | B | 610 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 25 | a | 420 | PHO | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 24 | c | 910 | CLA | C3C-C2C | 5.00 | 1.47 | 1.36 |
| 24 | d | 403 | CLA | C3C-C2C | 5.00 | 1.47 | 1.36 |
| 24 | B | 605 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 24 | c | 905 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 24 | C | 507 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 24 | b | 611 | CLA | CHC-C1C | 4.99 | 1.48 | 1.38 |
| 24 | c | 910 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 24 | C | 513 | CLA | CHC-C1C | 4.98 | 1.48 | 1.38 |
| 24 | c | 906 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 24 | B | 602 | CLA | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 24 | C | 509 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 24 | C | 509 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 26 | k | 102 | BCR | C23-C22 | -4.96 | 1.35 | 1.46 |
| 24 | b | 618 | CLA | CHC-C1C | 4.96 | 1.48 | 1.38 |
| 24 | c | 902 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 24 | b | 607 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 24 | c | 911 | CLA | CHC-C1C | 4.95 | 1.48 | 1.38 |
| 24 | B | 608 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 24 | D | 402 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 24 | B | 612 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 24 | b | 606 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 24 | B | 615 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 24 | b | 609 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 24 | b | 610 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 24 | b | 615 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 24 | c | 907 | CLA | C3C-C2C | 4.92 | 1.47 | 1.36 |
| 24 | C | 510 | CLA | C3C-C2C | 4.92 | 1.47 | 1.36 |
| 24 | C | 512 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 24 | B | 616 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 904 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 24 | c | 903 | CLA | CHC-C1C | 4.91 | 1.48 | 1.38 |
| 24 | A | 405 | CLA | CHC-C1C | 4.91 | 1.48 | 1.38 |
| 24 | c | 913 | CLA | CHC-C1C | 4.90 | 1.48 | 1.38 |
| 24 | b | 616 | CLA | CHC-C1C | 4.90 | 1.48 | 1.38 |
| 24 | b | 620 | CLA | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 24 | B | 604 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 24 | B | 613 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 24 | B | 607 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 24 | D | 402 | CLA | CHC-C1C | 4.89 | 1.48 | 1.38 |
| 24 | A | 405 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 24 | C | 508 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |
| 24 | B | 612 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 24 | B | 606 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 24 | B | 611 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 24 | B | 613 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 24 | c | 904 | CLA | CHC-C1C | 4.86 | 1.48 | 1.38 |
| 24 | B | 616 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 24 | b | 613 | CLA | CHC-C1C | 4.86 | 1.48 | 1.38 |
| 26 | d | 404 | BCR | C23-C22 | -4.86 | 1.35 | 1.46 |
| 24 | B | 607 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 24 | B | 606 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 26 | D | 403 | BCR | C23-C22 | -4.85 | 1.35 | 1.46 |
| 24 | A | 406 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 24 | B | 614 | CLA | CHC-C1C | 4.85 | 1.48 | 1.38 |
| 25 | A | 408 | PHO | C3D-C2D | 4.84 | 1.47 | 1.39 |
| 24 | c | 907 | CLA | C1D-ND | 4.84 | 1.44 | 1.37 |
| 24 | C | 505 | CLA | CHC-C1C | 4.84 | 1.48 | 1.38 |
| 24 | C | 513 | CLA | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | CHC-C1C | 4.83 | 1.48 | 1.38 |
| 24 | B | 615 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 24 | c | 903 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 24 | b | 608 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 24 | b | 605 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 24 | c | 909 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 24 | d | 403 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 25 | A | 408 | PHO | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 24 | b | 608 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 26 | C | 515 | BCR | C23-C22 | -4.81 | 1.35 | 1.46 |
| 24 | b | 619 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 24 | C | 512 | CLA | C3C-C2C | 4.81 | 1.47 | 1.36 |
| 24 | c | 914 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 906 | CLA | C3C-C2C | 4.80 | 1.47 | 1.36 |
| 26 | C | 516 | BCR | C23-C22 | -4.80 | 1.35 | 1.46 |
| 24 | D | 401 | CLA | C3C-C2C | 4.80 | 1.47 | 1.36 |
| 24 | d | 402 | CLA | C3C-C2C | 4.80 | 1.47 | 1.36 |
| 24 | B | 604 | CLA | CHC-C1C | 4.80 | 1.48 | 1.38 |
| 24 | c | 913 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 24 | b | 609 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 24 | C | 514 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 24 | b | 607 | CLA | CHC-C1C | 4.78 | 1.48 | 1.38 |
| 24 | C | 502 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 24 | B | 616 | CLA | C3C-C2C | 4.78 | 1.47 | 1.36 |
| 24 | c | 912 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 24 | c | 911 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 24 | c | 909 | CLA | C1D-ND | 4.77 | 1.44 | 1.37 |
| 26 | h | 101 | BCR | C23-C22 | -4.76 | 1.35 | 1.46 |
| 24 | C | 502 | CLA | C3C-C2C | 4.76 | 1.47 | 1.36 |
| 24 | B | 610 | CLA | CHC-C1C | 4.76 | 1.48 | 1.38 |
| 24 | B | 603 | CLA | CHC-C1C | 4.76 | 1.48 | 1.38 |
| 24 | A | 410 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 24 | c | 912 | CLA | C1D-ND | 4.75 | 1.44 | 1.37 |
| 24 | B | 609 | CLA | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 24 | b | 608 | CLA | CHC-C1C | 4.74 | 1.48 | 1.38 |
| 24 | B | 614 | CLA | O2D-CGD | 4.74 | 1.44 | 1.33 |
| 24 | B | 604 | CLA | O2D-CGD | 4.74 | 1.44 | 1.33 |
| 24 | c | 910 | CLA | CHC-C1C | 4.74 | 1.48 | 1.38 |
| 26 | b | 623 | BCR | C23-C22 | -4.74 | 1.35 | 1.46 |
| 24 | B | 613 | CLA | CHC-C1C | 4.73 | 1.48 | 1.38 |
| 24 | c | 908 | CLA | O2D-CGD | 4.73 | 1.44 | 1.33 |
| 24 | B | 602 | CLA | CHC-C1C | 4.73 | 1.48 | 1.38 |
| 26 | K | 103 | BCR | C23-C22 | -4.72 | 1.35 | 1.46 |
| 24 | B | 612 | CLA | C1D-ND | 4.72 | 1.44 | 1.37 |
| 24 | A | 406 | CLA | O2D-CGD | 4.72 | 1.44 | 1.33 |
| 40 | V | 201 | HEC | CAC-C3C | 4.71 | 1.50 | 1.35 |
| 24 | c | 912 | CLA | CHC-C1C | 4.71 | 1.47 | 1.38 |
| 24 | b | 614 | CLA | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 24 | C | 514 | CLA | C1D-ND | 4.71 | 1.44 | 1.37 |
| 24 | b | 605 | CLA | CHC-C1C | 4.71 | 1.47 | 1.38 |
| 24 | D | 402 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 24 | b | 619 | CLA | C3C-C2C | 4.70 | 1.46 | 1.36 |
| 24 | b | 609 | CLA | CHC-C1C | 4.69 | 1.47 | 1.38 |
| 24 | B | 602 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | b | 617 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 24 | B | 612 | CLA | CHC-C1C | 4.68 | 1.47 | 1.38 |
| 24 | C | 503 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 24 | C | 507 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 24 | b | 618 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 24 | b | 610 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 24 | c | 903 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 24 | b | 615 | CLA | C3C-C2C | 4.65 | 1.46 | 1.36 |
| 24 | d | 403 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 26 | y | 101 | BCR | C23-C22 | -4.65 | 1.36 | 1.46 |
| 24 | b | 613 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 26 | b | 621 | BCR | C23-C22 | -4.65 | 1.36 | 1.46 |
| 25 | A | 409 | PHO | O2D-CGD | 4.64 | 1.44 | 1.33 |
| 24 | C | 504 | CLA | C1D-ND | 4.64 | 1.44 | 1.37 |
| 24 | B | 617 | CLA | O2D-CGD | 4.64 | 1.44 | 1.33 |
| 24 | b | 614 | CLA | CHC-C1C | 4.63 | 1.47 | 1.38 |
| 24 | B | 603 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 24 | C | 505 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 24 | b | 617 | CLA | CHC-C1C | 4.63 | 1.47 | 1.38 |
| 24 | C | 508 | CLA | CHC-C1C | 4.63 | 1.47 | 1.38 |
| 37 | E | 101 | LHG | O8-C23 | 4.62 | 1.46 | 1.33 |
| 24 | b | 606 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 24 | C | 511 | CLA | C1D-ND | 4.61 | 1.43 | 1.37 |
| 24 | C | 506 | CLA | CHC-C1C | 4.61 | 1.47 | 1.38 |
| 24 | c | 908 | CLA | O2A-CGA | 4.61 | 1.46 | 1.33 |
| 24 | d | 401 | CLA | O2D-CGD | 4.61 | 1.44 | 1.33 |
| 36 | D | 405 | DGD | O1G-C1A | 4.60 | 1.46 | 1.33 |
| 24 | C | 507 | CLA | CHD-C1D | 4.60 | 1.47 | 1.38 |
| 26 | H | 101 | BCR | C23-C22 | -4.60 | 1.36 | 1.46 |
| 24 | B | 611 | CLA | O2D-CGD | 4.60 | 1.44 | 1.33 |
| 24 | b | 609 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 24 | C | 512 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 24 | C | 511 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 24 | b | 610 | CLA | CHC-C1C | 4.59 | 1.47 | 1.38 |
| 24 | b | 611 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 24 | C | 504 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 24 | C | 505 | CLA | O2A-CGA | 4.59 | 1.46 | 1.33 |
| 24 | B | 615 | CLA | O2D-CGD | 4.58 | 1.44 | 1.33 |
| 24 | B | 616 | CLA | CHC-C1C | 4.58 | 1.47 | 1.38 |
| 24 | b | 620 | CLA | CHC-C1C | 4.57 | 1.47 | 1.38 |
| 24 | b | 613 | CLA | C3C-C2C | 4.57 | 1.46 | 1.36 |
| 24 | A | 407 | CLA | C1D-ND | 4.57 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 911 | CLA | C1D-ND | 4.57 | 1.43 | 1.37 |
| 24 | C | 503 | CLA | CHD-C1D | 4.56 | 1.47 | 1.38 |
| 24 | c | 905 | CLA | CHC-C1C | 4.56 | 1.47 | 1.38 |
| 24 | c | 902 | CLA | O2D-CGD | 4.56 | 1.44 | 1.33 |
| 24 | b | 614 | CLA | CHD-C1D | 4.56 | 1.47 | 1.38 |
| 24 | B | 603 | CLA | CHD-C1D | 4.56 | 1.47 | 1.38 |
| 24 | b | 606 | CLA | CHC-C1C | 4.56 | 1.47 | 1.38 |
| 26 | c | 915 | BCR | C23-C22 | -4.56 | 1.36 | 1.46 |
| 24 | b | 615 | CLA | C1D-ND | 4.55 | 1.43 | 1.37 |
| 24 | d | 403 | CLA | CHC-C1C | 4.55 | 1.47 | 1.38 |
| 24 | B | 615 | CLA | O2A-CGA | 4.54 | 1.46 | 1.33 |
| 24 | a | 406 | CLA | O2D-CGD | 4.54 | 1.44 | 1.33 |
| 24 | B | 610 | CLA | C1D-ND | 4.54 | 1.43 | 1.37 |
| 24 | b | 618 | CLA | O2D-CGD | 4.54 | 1.44 | 1.33 |
| 24 | D | 401 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 24 | b | 611 | CLA | O2A-CGA | 4.53 | 1.46 | 1.33 |
| 24 | C | 514 | CLA | CHC-C1C | 4.53 | 1.47 | 1.38 |
| 24 | c | 914 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 27 | a | 402 | SQD | O48-C23 | 4.53 | 1.46 | 1.33 |
| 34 | z | 101 | LMG | O8-C28 | 4.53 | 1.46 | 1.33 |
| 24 | B | 615 | CLA | CHC-C1C | 4.53 | 1.47 | 1.38 |
| 24 | C | 511 | CLA | CHD-C1D | 4.53 | 1.47 | 1.38 |
| 24 | C | 510 | CLA | O2A-CGA | 4.52 | 1.46 | 1.33 |
| 24 | b | 608 | CLA | CHD-C1D | 4.52 | 1.47 | 1.38 |
| 27 | B | 621 | SQD | O47-C7 | 4.52 | 1.47 | 1.34 |
| 26 | T | 102 | BCR | C23-C22 | -4.52 | 1.36 | 1.46 |
| 24 | A | 410 | CLA | CHC-C1C | 4.51 | 1.47 | 1.38 |
| 24 | b | 616 | CLA | C1D-ND | 4.51 | 1.43 | 1.37 |
| 26 | A | 411 | BCR | C23-C22 | -4.50 | 1.36 | 1.46 |
| 34 | c | 919 | LMG | O8-C28 | 4.50 | 1.46 | 1.33 |
| 24 | c | 910 | CLA | CHD-C1D | 4.50 | 1.47 | 1.38 |
| 24 | C | 512 | CLA | CHC-C1C | 4.50 | 1.47 | 1.38 |
| 24 | A | 405 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 24 | B | 610 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 24 | c | 908 | CLA | CHC-C1C | 4.49 | 1.47 | 1.38 |
| 24 | a | 407 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 24 | a | 409 | CLA | CHC-C1C | 4.49 | 1.47 | 1.38 |
| 24 | C | 511 | CLA | CHC-C1C | 4.48 | 1.47 | 1.38 |
| 24 | C | 502 | CLA | C1D-ND | 4.48 | 1.43 | 1.37 |
| 24 | B | 605 | CLA | O2D-CGD | 4.48 | 1.44 | 1.33 |
| 27 | f | 102 | SQD | O47-C7 | 4.48 | 1.46 | 1.34 |
| 24 | c | 908 | CLA | C1D-ND | 4.48 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 613 | CLA | CHD-C1D | 4.48 | 1.47 | 1.38 |
| 24 | B | 602 | CLA | O2A-CGA | 4.47 | 1.46 | 1.33 |
| 24 | C | 508 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |
| 26 | B | 619 | BCR | C23-C22 | -4.47 | 1.36 | 1.46 |
| 24 | b | 607 | CLA | CHD-C1D | 4.47 | 1.47 | 1.38 |
| 27 | F | 101 | SQD | O47-C7 | 4.47 | 1.46 | 1.34 |
| 24 | c | 906 | CLA | C1D-ND | 4.46 | 1.43 | 1.37 |
| 24 | b | 620 | CLA | C1D-ND | 4.46 | 1.43 | 1.37 |
| 26 | a | 410 | BCR | C23-C22 | -4.46 | 1.36 | 1.46 |
| 24 | B | 608 | CLA | OBD-CAD | 4.46 | 1.30 | 1.22 |
| 24 | c | 902 | CLA | CHC-C1C | 4.46 | 1.47 | 1.38 |
| 24 | c | 904 | CLA | CHD-C1D | 4.46 | 1.47 | 1.38 |
| 24 | B | 605 | CLA | CHC-C1C | 4.45 | 1.47 | 1.38 |
| 24 | C | 503 | CLA | CHC-C1C | 4.45 | 1.47 | 1.38 |
| 24 | C | 509 | CLA | C3D-C2D | 4.45 | 1.51 | 1.39 |
| 34 | C | 520 | LMG | O8-C28 | 4.45 | 1.46 | 1.33 |
| 24 | b | 607 | CLA | O2A-CGA | 4.45 | 1.46 | 1.33 |
| 24 | B | 608 | CLA | CHC-C1C | 4.45 | 1.47 | 1.38 |
| 24 | B | 617 | CLA | CHC-C1C | 4.45 | 1.47 | 1.38 |
| 24 | C | 506 | CLA | CHD-C1D | 4.44 | 1.47 | 1.38 |
| 24 | C | 507 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |
| 24 | B | 605 | CLA | C1D-ND | 4.44 | 1.43 | 1.37 |
| 24 | B | 614 | CLA | C1D-ND | 4.44 | 1.43 | 1.37 |
| 24 | a | 406 | CLA | CHB-C1B | 4.44 | 1.49 | 1.39 |
| 24 | C | 509 | CLA | CHD-C1D | 4.43 | 1.47 | 1.38 |
| 24 | c | 906 | CLA | CHC-C1C | 4.43 | 1.47 | 1.38 |
| 24 | d | 401 | CLA | CHD-C1D | 4.43 | 1.47 | 1.38 |
| 24 | b | 609 | CLA | O2A-CGA | 4.43 | 1.46 | 1.33 |
| 25 | a | 408 | PHO | O2D-CGD | 4.43 | 1.44 | 1.33 |
| 24 | d | 402 | CLA | O2A-CGA | 4.42 | 1.46 | 1.33 |
| 24 | C | 504 | CLA | CHC-C1C | 4.41 | 1.47 | 1.38 |
| 24 | b | 614 | CLA | C1D-ND | 4.41 | 1.43 | 1.37 |
| 24 | C | 505 | CLA | O2D-CGD | 4.41 | 1.44 | 1.33 |
| 24 | c | 906 | CLA | CHD-C1D | 4.41 | 1.47 | 1.38 |
| 24 | C | 513 | CLA | C1D-ND | 4.39 | 1.43 | 1.37 |
| 24 | b | 608 | CLA | C1D-ND | 4.39 | 1.43 | 1.37 |
| 24 | b | 619 | CLA | C3D-C2D | 4.39 | 1.51 | 1.39 |
| 24 | C | 510 | CLA | CHC-C1C | 4.38 | 1.47 | 1.38 |
| 24 | B | 607 | CLA | C1D-ND | 4.38 | 1.43 | 1.37 |
| 24 | b | 607 | CLA | C1D-ND | 4.37 | 1.43 | 1.37 |
| 24 | b | 619 | CLA | CHD-C1D | 4.37 | 1.46 | 1.38 |
| 26 | K | 102 | BCR | C23-C22 | -4.36 | 1.36 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | d | 401 | CLA | CHC-C1C | 4.36 | 1.47 | 1.38 |
| 40 | v | 202 | HEC | CAC-C3C | 4.36 | 1.49 | 1.35 |
| 24 | c | 907 | CLA | CHD-C1D | 4.36 | 1.46 | 1.38 |
| 24 | d | 402 | CLA | O2D-CGD | 4.36 | 1.43 | 1.33 |
| 24 | b | 611 | CLA | CHD-C1D | 4.35 | 1.46 | 1.38 |
| 24 | c | 911 | CLA | CHB-C1B | 4.35 | 1.49 | 1.39 |
| 24 | C | 510 | CLA | CHD-C1D | 4.35 | 1.46 | 1.38 |
| 24 | b | 620 | CLA | CHD-C1D | 4.35 | 1.46 | 1.38 |
| 24 | B | 607 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 24 | c | 914 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 24 | B | 611 | CLA | CHC-C1C | 4.34 | 1.47 | 1.38 |
| 24 | b | 615 | CLA | CHC-C1C | 4.34 | 1.47 | 1.38 |
| 24 | C | 502 | CLA | CHC-C1C | 4.34 | 1.47 | 1.38 |
| 24 | a | 406 | CLA | CHC-C1C | 4.33 | 1.47 | 1.38 |
| 24 | C | 513 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 24 | C | 512 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 24 | c | 911 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 24 | B | 609 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 36 | D | 405 | DGD | O2G-C1B | 4.32 | 1.46 | 1.34 |
| 24 | C | 508 | CLA | O2D-CGD | 4.32 | 1.43 | 1.33 |
| 24 | C | 509 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 34 | C | 521 | LMG | O7-C10 | 4.31 | 1.46 | 1.34 |
| 24 | B | 610 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 36 | d | 406 | DGD | O2G-C1B | 4.31 | 1.46 | 1.34 |
| 37 | d | 409 | LHG | O8-C23 | 4.31 | 1.45 | 1.33 |
| 24 | B | 617 | CLA | C1D-ND | 4.31 | 1.43 | 1.37 |
| 24 | B | 609 | CLA | C1D-ND | 4.31 | 1.43 | 1.37 |
| 24 | B | 611 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 24 | C | 509 | CLA | CHC-C1C | 4.31 | 1.47 | 1.38 |
| 24 | c | 909 | CLA | CHC-C1C | 4.31 | 1.47 | 1.38 |
| 24 | c | 904 | CLA | O2D-CGD | 4.31 | 1.43 | 1.33 |
| 24 | A | 406 | CLA | C3D-C2D | 4.30 | 1.50 | 1.39 |
| 24 | b | 619 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 34 | C | 501 | LMG | O7-C10 | 4.30 | 1.46 | 1.34 |
| 24 | c | 914 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 24 | D | 401 | CLA | CHC-C1C | 4.30 | 1.47 | 1.38 |
| 34 | b | 624 | LMG | O8-C28 | 4.29 | 1.45 | 1.33 |
| 24 | c | 914 | CLA | CHD-C4C | 4.29 | 1.49 | 1.39 |
| 34 | C | 501 | LMG | O8-C28 | 4.29 | 1.45 | 1.33 |
| 24 | B | 609 | CLA | C3D-C2D | 4.29 | 1.50 | 1.39 |
| 24 | C | 506 | CLA | C1D-ND | 4.29 | 1.43 | 1.37 |
| 24 | C | 502 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 34 | c | 920 | LMG | O8-C28 | 4.28 | 1.45 | 1.33 |
| 24 | D | 401 | CLA | O2D-CGD | 4.27 | 1.43 | 1.33 |
| 24 | c | 905 | CLA | C1D-ND | 4.27 | 1.43 | 1.37 |
| 34 | Z | 101 | LMG | O7-C10 | 4.27 | 1.46 | 1.34 |
| 24 | B | 610 | CLA | CHD-C1D | 4.27 | 1.46 | 1.38 |
| 24 | c | 909 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 24 | b | 605 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 24 | D | 402 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | CHD-C1D | 4.27 | 1.46 | 1.38 |
| 27 | A | 416 | SQD | O47-C7 | 4.26 | 1.46 | 1.34 |
| 24 | A | 407 | CLA | CHD-C1D | 4.26 | 1.46 | 1.38 |
| 40 | v | 202 | HEC | CBC-CAC | -4.26 | 1.33 | 1.49 |
| 24 | C | 508 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 24 | B | 606 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 24 | b | 619 | CLA | CHC-C1C | 4.25 | 1.47 | 1.38 |
| 24 | c | 906 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 24 | C | 506 | CLA | OBD-CAD | 4.25 | 1.29 | 1.22 |
| 24 | B | 609 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 24 | B | 607 | CLA | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 25 | a | 408 | PHO | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 36 | d | 406 | DGD | O1G-C1A | 4.25 | 1.45 | 1.33 |
| 24 | b | 618 | CLA | CHB-C1B | 4.25 | 1.48 | 1.39 |
| 24 | b | 610 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 34 | C | 521 | LMG | O8-C28 | 4.24 | 1.45 | 1.33 |
| 24 | D | 402 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 37 | e | 101 | LHG | O8-C23 | 4.24 | 1.45 | 1.33 |
| 27 | A | 412 | SQD | O48-C23 | 4.24 | 1.45 | 1.33 |
| 24 | b | 619 | CLA | C1D-ND | 4.24 | 1.43 | 1.37 |
| 27 | L | 102 | SQD | O47-C7 | 4.24 | 1.46 | 1.34 |
| 34 | B | 622 | LMG | O8-C28 | 4.24 | 1.45 | 1.33 |
| 24 | B | 606 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 24 | c | 910 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 24 | A | 410 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 24 | a | 409 | CLA | C1D-ND | 4.23 | 1.43 | 1.37 |
| 27 | A | 416 | SQD | O48-C23 | 4.23 | 1.45 | 1.33 |
| 36 | h | 102 | DGD | O2G-C1B | 4.22 | 1.46 | 1.34 |
| 24 | b | 618 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 24 | C | 511 | CLA | CHC-C4B | 4.21 | 1.48 | 1.39 |
| 24 | C | 512 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 40 | V | 201 | HEC | CAB-C3B | 4.21 | 1.48 | 1.35 |
| 24 | b | 620 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | a | 420 | PHO | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 27 | F | 101 | SQD | O48-C23 | 4.21 | 1.45 | 1.33 |
| 24 | a | 406 | CLA | CHD-C4C | 4.21 | 1.48 | 1.39 |
| 24 | C | 503 | CLA | C3D-C2D | 4.21 | 1.50 | 1.39 |
| 24 | B | 603 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 27 | a | 411 | SQD | O48-C23 | 4.21 | 1.45 | 1.33 |
| 24 | C | 507 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 24 | a | 407 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 24 | c | 913 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 24 | b | 610 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 24 | B | 608 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 24 | c | 902 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 24 | b | 615 | CLA | CHB-C1B | 4.20 | 1.48 | 1.39 |
| 24 | C | 502 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 24 | B | 615 | CLA | CHB-C1B | 4.20 | 1.48 | 1.39 |
| 24 | C | 514 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 24 | b | 613 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 24 | d | 402 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 27 | f | 102 | SQD | O48-C23 | 4.19 | 1.45 | 1.33 |
| 24 | B | 602 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 24 | B | 607 | CLA | CHC-C1C | 4.19 | 1.46 | 1.38 |
| 34 | c | 920 | LMG | O7-C10 | 4.19 | 1.46 | 1.34 |
| 24 | A | 407 | CLA | CHD-C4C | 4.19 | 1.48 | 1.39 |
| 24 | c | 912 | CLA | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 24 | a | 407 | CLA | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 24 | d | 403 | CLA | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 24 | b | 606 | CLA | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 40 | v | 202 | HEC | CAB-C3B | 4.18 | 1.48 | 1.35 |
| 24 | b | 610 | CLA | C1D-ND | 4.18 | 1.43 | 1.37 |
| 24 | c | 912 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 24 | C | 505 | CLA | OBD-CAD | 4.17 | 1.29 | 1.22 |
| 24 | c | 907 | CLA | CHC-C1C | 4.17 | 1.46 | 1.38 |
| 24 | C | 514 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 38 | E | 103 | HEM | FE-NC | 4.17 | 2.08 | 1.95 |
| 24 | B | 609 | CLA | CHC-C1C | 4.17 | 1.46 | 1.38 |
| 24 | c | 902 | CLA | CHB-C1B | 4.16 | 1.48 | 1.39 |
| 24 | b | 605 | CLA | CHD-C4C | 4.16 | 1.48 | 1.39 |
| 24 | b | 616 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 24 | C | 504 | CLA | CHD-C1D | 4.16 | 1.46 | 1.38 |
| 24 | C | 505 | CLA | CHD-C1D | 4.16 | 1.46 | 1.38 |
| 38 | e | 102 | HEM | FE-NC | 4.15 | 2.08 | 1.95 |
| 24 | B | 617 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 611 | CLA | CHB-C1B | 4.15 | 1.48 | 1.39 |
| 24 | c | 902 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 24 | D | 401 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 24 | b | 605 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 34 | a | 412 | LMG | O8-C28 | 4.14 | 1.45 | 1.33 |
| 24 | B | 602 | CLA | CHD-C4C | 4.14 | 1.48 | 1.39 |
| 40 | V | 201 | HEC | CBC-CAC | -4.13 | 1.34 | 1.49 |
| 24 | b | 605 | CLA | C3D-C2D | 4.13 | 1.50 | 1.39 |
| 25 | a | 420 | PHO | OBD-CAD | 4.13 | 1.27 | 1.22 |
| 24 | c | 913 | CLA | C1D-ND | 4.13 | 1.43 | 1.37 |
| 24 | A | 405 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 24 | C | 507 | CLA | CHB-C1B | 4.12 | 1.48 | 1.39 |
| 24 | c | 908 | CLA | CHD-C1D | 4.12 | 1.46 | 1.38 |
| 24 | B | 608 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 24 | B | 612 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 24 | d | 402 | CLA | C1D-ND | 4.11 | 1.43 | 1.37 |
| 24 | B | 606 | CLA | C1D-ND | 4.11 | 1.43 | 1.37 |
| 24 | B | 606 | CLA | CHC-C1C | 4.11 | 1.46 | 1.38 |
| 24 | a | 406 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |
| 37 | l | 101 | LHG | O7-C7 | 4.10 | 1.45 | 1.34 |
| 24 | B | 602 | CLA | C3D-C2D | 4.10 | 1.50 | 1.39 |
| 37 | e | 101 | LHG | O7-C7 | 4.10 | 1.45 | 1.34 |
| 27 | L | 102 | SQD | O48-C23 | 4.10 | 1.45 | 1.33 |
| 24 | D | 401 | CLA | CHB-C1B | 4.10 | 1.48 | 1.39 |
| 24 | C | 510 | CLA | C3D-C2D | 4.09 | 1.50 | 1.39 |
| 24 | c | 902 | CLA | C1D-ND | 4.09 | 1.43 | 1.37 |
| 24 | B | 616 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 24 | c | 903 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | CHC-C4B | 4.09 | 1.48 | 1.39 |
| 24 | c | 904 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 24 | c | 909 | CLA | C3D-C2D | 4.08 | 1.50 | 1.39 |
| 24 | C | 511 | CLA | C3D-C2D | 4.08 | 1.50 | 1.39 |
| 24 | a | 409 | CLA | CHD-C1D | 4.08 | 1.46 | 1.38 |
| 24 | B | 616 | CLA | C3D-C2D | 4.08 | 1.50 | 1.39 |
| 37 | D | 408 | LHG | O7-C7 | 4.08 | 1.45 | 1.34 |
| 24 | A | 406 | CLA | CHC-C1C | 4.08 | 1.46 | 1.38 |
| 24 | c | 905 | CLA | C3D-C2D | 4.08 | 1.50 | 1.39 |
| 24 | b | 607 | CLA | CHD-C4C | 4.07 | 1.48 | 1.39 |
| 24 | C | 505 | CLA | CHB-C1B | 4.07 | 1.48 | 1.39 |
| 24 | A | 410 | CLA | C3D-C2D | 4.07 | 1.50 | 1.39 |
| 24 | c | 905 | CLA | O2A-CGA | 4.07 | 1.45 | 1.33 |
| 24 | C | 512 | CLA | CHD-C4C | 4.06 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | d | 407 | LHG | O8-C23 | 4.06 | 1.45 | 1.33 |
| 24 | d | 401 | CLA | C3D-C2D | 4.06 | 1.50 | 1.39 |
| 24 | B | 604 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 24 | d | 401 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 24 | a | 409 | CLA | C3D-C2D | 4.05 | 1.50 | 1.39 |
| 24 | b | 614 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 24 | d | 403 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 24 | B | 611 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 25 | a | 408 | PHO | OBD-CAD | 4.04 | 1.27 | 1.22 |
| 24 | C | 508 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 24 | C | 511 | CLA | CHB-C1B | 4.04 | 1.48 | 1.39 |
| 24 | C | 507 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 24 | B | 613 | CLA | C3D-C2D | 4.04 | 1.50 | 1.39 |
| 24 | B | 605 | CLA | CHB-C1B | 4.04 | 1.48 | 1.39 |
| 24 | C | 503 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 24 | C | 504 | CLA | CHD-C4C | 4.03 | 1.48 | 1.39 |
| 24 | B | 615 | CLA | CHD-C1D | 4.03 | 1.46 | 1.38 |
| 24 | c | 907 | CLA | CHD-C4C | 4.03 | 1.48 | 1.39 |
| 26 | B | 618 | BCR | C23-C22 | -4.03 | 1.37 | 1.46 |
| 24 | A | 407 | CLA | CHC-C4B | 4.03 | 1.48 | 1.39 |
| 24 | d | 402 | CLA | CHC-C1C | 4.03 | 1.46 | 1.38 |
| 37 | E | 101 | LHG | O7-C7 | 4.03 | 1.45 | 1.34 |
| 34 | z | 101 | LMG | O7-C10 | 4.03 | 1.45 | 1.34 |
| 24 | a | 407 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 40 | v | 202 | HEC | CBB-CAB | -4.02 | 1.34 | 1.49 |
| 24 | C | 508 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |
| 24 | b | 615 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 24 | c | 907 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 24 | b | 608 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 27 | a | 402 | SQD | O47-C7 | 4.01 | 1.45 | 1.34 |
| 24 | c | 912 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 36 | c | 918 | DGD | O1G-C1A | 4.00 | 1.45 | 1.33 |
| 24 | b | 618 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 36 | c | 917 | DGD | O1G-C1A | 4.00 | 1.45 | 1.33 |
| 24 | A | 410 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 24 | a | 409 | CLA | O2A-CGA | 4.00 | 1.45 | 1.33 |
| 24 | A | 410 | CLA | CHD-C4C | 4.00 | 1.48 | 1.39 |
| 34 | B | 622 | LMG | O7-C10 | 3.99 | 1.45 | 1.34 |
| 24 | c | 910 | CLA | C3D-C2D | 3.99 | 1.49 | 1.39 |
| 24 | A | 406 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 24 | b | 618 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 24 | c | 905 | CLA | CHD-C1D | 3.99 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 617 | CLA | CHD-C1D | 3.98 | 1.46 | 1.38 |
| 24 | b | 614 | CLA | O2A-CGA | 3.98 | 1.45 | 1.33 |
| 24 | D | 401 | CLA | CHD-C1D | 3.98 | 1.46 | 1.38 |
| 34 | C | 520 | LMG | O7-C10 | 3.98 | 1.45 | 1.34 |
| 24 | C | 512 | CLA | CHB-C1B | 3.98 | 1.48 | 1.39 |
| 24 | c | 904 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |
| 25 | A | 408 | PHO | O2A-CGA | 3.97 | 1.44 | 1.33 |
| 24 | C | 509 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 24 | b | 616 | CLA | CHB-C1B | 3.96 | 1.48 | 1.39 |
| 24 | B | 611 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 24 | B | 610 | CLA | C3D-C2D | 3.96 | 1.49 | 1.39 |
| 24 | C | 513 | CLA | C3D-C2D | 3.96 | 1.49 | 1.39 |
| 34 | a | 412 | LMG | O7-C10 | 3.96 | 1.45 | 1.34 |
| 24 | c | 911 | CLA | O2A-CGA | 3.96 | 1.44 | 1.33 |
| 24 | C | 503 | CLA | CHB-C1B | 3.96 | 1.48 | 1.39 |
| 24 | c | 907 | CLA | C3D-C2D | 3.96 | 1.49 | 1.39 |
| 24 | c | 908 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 24 | B | 606 | CLA | C3D-C2D | 3.96 | 1.49 | 1.39 |
| 24 | B | 611 | CLA | C3D-C2D | 3.95 | 1.49 | 1.39 |
| 24 | C | 511 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 36 | H | 102 | DGD | O2G-C1B | 3.95 | 1.45 | 1.34 |
| 24 | C | 504 | CLA | O2A-CGA | 3.95 | 1.44 | 1.33 |
| 24 | c | 910 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 24 | C | 505 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 37 | d | 409 | LHG | O7-C7 | 3.95 | 1.45 | 1.34 |
| 24 | B | 612 | CLA | CHC-C4B | 3.95 | 1.48 | 1.39 |
| 24 | B | 609 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 24 | A | 410 | CLA | OBD-CAD | 3.95 | 1.29 | 1.22 |
| 34 | c | 919 | LMG | O7-C10 | 3.95 | 1.45 | 1.34 |
| 24 | B | 615 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 40 | V | 201 | HEC | CBB-CAB | -3.94 | 1.34 | 1.49 |
| 24 | c | 903 | CLA | CHD-C1D | 3.94 | 1.46 | 1.38 |
| 24 | C | 507 | CLA | C3D-C2D | 3.94 | 1.49 | 1.39 |
| 24 | b | 620 | CLA | C3D-C2D | 3.94 | 1.49 | 1.39 |
| 24 | B | 609 | CLA | OBD-CAD | 3.93 | 1.29 | 1.22 |
| 24 | b | 611 | CLA | OBD-CAD | 3.93 | 1.29 | 1.22 |
| 24 | B | 612 | CLA | CHD-C4C | 3.93 | 1.48 | 1.39 |
| 24 | B | 605 | CLA | CHD-C1D | 3.93 | 1.46 | 1.38 |
| 24 | c | 903 | CLA | C3D-C2D | 3.93 | 1.49 | 1.39 |
| 27 | B | 621 | SQD | O48-C23 | 3.92 | 1.44 | 1.33 |
| 24 | A | 405 | CLA | CHB-C1B | 3.92 | 1.48 | 1.39 |
| 36 | H | 102 | DGD | O1G-C1A | 3.92 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 608 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 24 | b | 609 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 24 | C | 506 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 24 | B | 606 | CLA | CHB-C1B | 3.91 | 1.48 | 1.39 |
| 24 | b | 608 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 24 | B | 617 | CLA | OBD-CAD | 3.91 | 1.29 | 1.22 |
| 24 | b | 613 | CLA | CHB-C1B | 3.91 | 1.48 | 1.39 |
| 36 | C | 519 | DGD | O1G-C1A | 3.91 | 1.44 | 1.33 |
| 37 | L | 101 | LHG | O8-C23 | 3.91 | 1.44 | 1.33 |
| 24 | C | 506 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 24 | D | 401 | CLA | C3D-C2D | 3.90 | 1.49 | 1.39 |
| 24 | B | 612 | CLA | C3D-C2D | 3.90 | 1.49 | 1.39 |
| 24 | C | 508 | CLA | C3D-C2D | 3.90 | 1.49 | 1.39 |
| 24 | B | 614 | CLA | C3D-C2D | 3.90 | 1.49 | 1.39 |
| 24 | A | 407 | CLA | C3D-C2D | 3.90 | 1.49 | 1.39 |
| 24 | c | 905 | CLA | OBD-CAD | 3.90 | 1.29 | 1.22 |
| 24 | b | 613 | CLA | CHC-C4B | 3.89 | 1.48 | 1.39 |
| 24 | c | 911 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 24 | C | 514 | CLA | C3D-C2D | 3.89 | 1.49 | 1.39 |
| 36 | C | 518 | DGD | O1G-C1A | 3.89 | 1.44 | 1.33 |
| 34 | j | 101 | LMG | O8-C28 | 3.89 | 1.44 | 1.33 |
| 36 | c | 917 | DGD | O2G-C1B | 3.89 | 1.45 | 1.34 |
| 24 | C | 510 | CLA | CHB-C1B | 3.89 | 1.48 | 1.39 |
| 24 | d | 403 | CLA | C3D-C2D | 3.89 | 1.49 | 1.39 |
| 24 | b | 610 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 37 | D | 406 | LHG | O8-C23 | 3.89 | 1.44 | 1.33 |
| 36 | c | 916 | DGD | O1G-C1A | 3.89 | 1.44 | 1.33 |
| 24 | B | 605 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 24 | c | 903 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 24 | b | 620 | CLA | CHB-C1B | 3.89 | 1.48 | 1.39 |
| 24 | A | 405 | CLA | C3D-C2D | 3.89 | 1.49 | 1.39 |
| 37 | d | 408 | LHG | O7-C7 | 3.88 | 1.45 | 1.34 |
| 24 | B | 610 | CLA | CHB-C1B | 3.88 | 1.48 | 1.39 |
| 24 | C | 503 | CLA | O2A-CGA | 3.88 | 1.44 | 1.33 |
| 37 | l | 101 | LHG | O8-C23 | 3.88 | 1.44 | 1.33 |
| 24 | B | 617 | CLA | CHB-C1B | 3.88 | 1.48 | 1.39 |
| 24 | c | 911 | CLA | CHC-C4B | 3.88 | 1.48 | 1.39 |
| 24 | b | 612 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 24 | b | 610 | CLA | C3D-C2D | 3.87 | 1.49 | 1.39 |
| 24 | b | 617 | CLA | C3D-C2D | 3.87 | 1.49 | 1.39 |
| 24 | A | 410 | CLA | CHC-C4B | 3.87 | 1.48 | 1.39 |
| 24 | c | 903 | CLA | CHB-C1B | 3.87 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | b | 617 | CLA | O2A-CGA | 3.87 | 1.44 | 1.33 |
| 24 | d | 403 | CLA | CHB-C1B | 3.86 | 1.48 | 1.39 |
| 24 | B | 605 | CLA | O2A-CGA | 3.86 | 1.44 | 1.33 |
| 24 | C | 509 | CLA | O2A-CGA | 3.86 | 1.44 | 1.33 |
| 36 | h | 102 | DGD | O1G-C1A | 3.86 | 1.44 | 1.33 |
| 35 | b | 602 | HTG | C1'-S1 | -3.86 | 1.76 | 1.81 |
| 24 | C | 502 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 24 | A | 407 | CLA | O2A-CGA | 3.86 | 1.44 | 1.33 |
| 24 | B | 612 | CLA | CHD-C1D | 3.86 | 1.45 | 1.38 |
| 34 | j | 101 | LMG | O7-C10 | 3.86 | 1.45 | 1.34 |
| 36 | C | 519 | DGD | O2G-C1B | 3.85 | 1.45 | 1.34 |
| 24 | b | 615 | CLA | C3D-C2D | 3.85 | 1.49 | 1.39 |
| 24 | d | 401 | CLA | OBD-CAD | 3.85 | 1.29 | 1.22 |
| 35 | B | 624 | HTG | C1'-S1 | -3.85 | 1.76 | 1.81 |
| 24 | b | 614 | CLA | CHB-C1B | 3.85 | 1.48 | 1.39 |
| 24 | b | 606 | CLA | CHB-C1B | 3.85 | 1.48 | 1.39 |
| 34 | J | 101 | LMG | O8-C28 | 3.84 | 1.44 | 1.33 |
| 24 | B | 617 | CLA | C3D-C2D | 3.84 | 1.49 | 1.39 |
| 24 | B | 613 | CLA | O2A-CGA | 3.84 | 1.44 | 1.33 |
| 24 | b | 609 | CLA | CHB-C1B | 3.84 | 1.48 | 1.39 |
| 24 | a | 406 | CLA | C3D-C2D | 3.84 | 1.49 | 1.39 |
| 24 | C | 506 | CLA | CHC-C4B | 3.84 | 1.48 | 1.39 |
| 36 | c | 918 | DGD | O2G-C1B | 3.84 | 1.45 | 1.34 |
| 24 | b | 609 | CLA | OBD-CAD | 3.84 | 1.29 | 1.22 |
| 27 | A | 412 | SQD | O47-C7 | 3.84 | 1.45 | 1.34 |
| 24 | C | 504 | CLA | C3D-C2D | 3.84 | 1.49 | 1.39 |
| 24 | c | 912 | CLA | C3D-C2D | 3.84 | 1.49 | 1.39 |
| 24 | c | 910 | CLA | CHC-C4B | 3.84 | 1.48 | 1.39 |
| 24 | c | 913 | CLA | CHD-C1D | 3.84 | 1.45 | 1.38 |
| 37 | D | 407 | LHG | O7-C7 | 3.84 | 1.45 | 1.34 |
| 24 | B | 604 | CLA | CHD-C1D | 3.83 | 1.45 | 1.38 |
| 24 | C | 510 | CLA | CHD-C4C | 3.83 | 1.47 | 1.39 |
| 24 | b | 606 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 24 | b | 613 | CLA | CHD-C4C | 3.83 | 1.47 | 1.39 |
| 24 | a | 407 | CLA | CHC-C4B | 3.83 | 1.48 | 1.39 |
| 24 | B | 614 | CLA | CHD-C1D | 3.83 | 1.45 | 1.38 |
| 24 | B | 614 | CLA | O2A-CGA | 3.83 | 1.44 | 1.33 |
| 24 | B | 613 | CLA | OBD-CAD | 3.83 | 1.29 | 1.22 |
| 36 | C | 517 | DGD | O2G-C1B | 3.83 | 1.45 | 1.34 |
| 24 | C | 505 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 24 | C | 502 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 24 | b | 619 | CLA | OBD-CAD | 3.83 | 1.29 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 912 | CLA | CHB-C1B | 3.83 | 1.48 | 1.39 |
| 24 | a | 407 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 24 | B | 612 | CLA | CHB-C1B | 3.83 | 1.48 | 1.39 |
| 24 | c | 906 | CLA | CHB-C1B | 3.83 | 1.48 | 1.39 |
| 24 | c | 908 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 25 | A | 409 | PHO | O2A-CGA | 3.83 | 1.44 | 1.33 |
| 24 | c | 913 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 34 | J | 101 | LMG | O7-C10 | 3.82 | 1.45 | 1.34 |
| 24 | B | 607 | CLA | OBD-CAD | 3.82 | 1.29 | 1.22 |
| 24 | C | 509 | CLA | CHB-C1B | 3.82 | 1.48 | 1.39 |
| 24 | b | 608 | CLA | CHC-C4B | 3.82 | 1.48 | 1.39 |
| 24 | c | 903 | CLA | OBD-CAD | 3.82 | 1.29 | 1.22 |
| 24 | B | 603 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 24 | c | 907 | CLA | CHB-C1B | 3.82 | 1.48 | 1.39 |
| 24 | c | 903 | CLA | CHC-C4B | 3.82 | 1.48 | 1.39 |
| 24 | c | 908 | CLA | CHB-C1B | 3.82 | 1.48 | 1.39 |
| 24 | c | 902 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 37 | L | 101 | LHG | O7-C7 | 3.81 | 1.45 | 1.34 |
| 24 | C | 512 | CLA | OBD-CAD | 3.81 | 1.29 | 1.22 |
| 24 | b | 615 | CLA | CHD-C1D | 3.81 | 1.45 | 1.38 |
| 36 | C | 517 | DGD | O1G-C1A | 3.81 | 1.44 | 1.33 |
| 24 | B | 611 | CLA | CHC-C4B | 3.81 | 1.48 | 1.39 |
| 24 | d | 401 | CLA | CHB-C1B | 3.81 | 1.48 | 1.39 |
| 24 | b | 612 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 24 | B | 616 | CLA | CHD-C1D | 3.81 | 1.45 | 1.38 |
| 24 | C | 511 | CLA | O2A-CGA | 3.80 | 1.44 | 1.33 |
| 24 | c | 904 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 24 | c | 909 | CLA | CHD-C1D | 3.80 | 1.45 | 1.38 |
| 24 | c | 913 | CLA | CHC-C4B | 3.80 | 1.47 | 1.39 |
| 24 | A | 406 | CLA | CHD-C1D | 3.79 | 1.45 | 1.38 |
| 24 | b | 614 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 24 | C | 514 | CLA | CHB-C1B | 3.79 | 1.47 | 1.39 |
| 24 | B | 606 | CLA | OBD-CAD | 3.79 | 1.29 | 1.22 |
| 24 | b | 605 | CLA | CHC-C4B | 3.79 | 1.47 | 1.39 |
| 24 | B | 604 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 24 | A | 407 | CLA | OBD-CAD | 3.78 | 1.29 | 1.22 |
| 24 | C | 514 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 36 | c | 916 | DGD | O2G-C1B | 3.78 | 1.44 | 1.34 |
| 24 | b | 617 | CLA | CHD-C1D | 3.78 | 1.45 | 1.38 |
| 24 | a | 409 | CLA | OBD-CAD | 3.77 | 1.29 | 1.22 |
| 24 | B | 603 | CLA | CHB-C1B | 3.77 | 1.47 | 1.39 |
| 24 | c | 911 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 603 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 24 | d | 403 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 24 | A | 405 | CLA | CHC-C4B | 3.77 | 1.47 | 1.39 |
| 24 | c | 906 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 24 | D | 402 | CLA | CHB-C1B | 3.76 | 1.47 | 1.39 |
| 24 | A | 405 | CLA | CHD-C1D | 3.76 | 1.45 | 1.38 |
| 24 | C | 502 | CLA | CHC-C4B | 3.76 | 1.47 | 1.39 |
| 36 | C | 518 | DGD | O2G-C1B | 3.76 | 1.44 | 1.34 |
| 24 | b | 619 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 24 | d | 401 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 24 | c | 904 | CLA | CHC-C4B | 3.76 | 1.47 | 1.39 |
| 24 | c | 913 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 24 | b | 620 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 24 | b | 617 | CLA | CHB-C1B | 3.76 | 1.47 | 1.39 |
| 24 | B | 607 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 34 | b | 624 | LMG | O7-C10 | 3.75 | 1.44 | 1.34 |
| 24 | A | 407 | CLA | CHB-C1B | 3.75 | 1.47 | 1.39 |
| 24 | c | 905 | CLA | CHB-C1B | 3.75 | 1.47 | 1.39 |
| 24 | B | 608 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 24 | b | 616 | CLA | CHD-C1D | 3.75 | 1.45 | 1.38 |
| 27 | a | 411 | SQD | O47-C7 | 3.74 | 1.44 | 1.34 |
| 24 | B | 615 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 24 | b | 609 | CLA | CHD-C1D | 3.74 | 1.45 | 1.38 |
| 24 | b | 613 | CLA | O2A-CGA | 3.74 | 1.44 | 1.33 |
| 24 | B | 615 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 24 | b | 606 | CLA | O2A-CGA | 3.73 | 1.44 | 1.33 |
| 24 | B | 613 | CLA | CHB-C1B | 3.73 | 1.47 | 1.39 |
| 24 | A | 406 | CLA | O2A-CGA | 3.73 | 1.44 | 1.33 |
| 24 | b | 614 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 24 | C | 513 | CLA | CHD-C1D | 3.72 | 1.45 | 1.38 |
| 24 | B | 602 | CLA | CHC-C4B | 3.72 | 1.47 | 1.39 |
| 24 | a | 406 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 24 | B | 604 | CLA | CHC-C4B | 3.71 | 1.47 | 1.39 |
| 24 | D | 402 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 24 | C | 502 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 24 | B | 614 | CLA | CHB-C1B | 3.70 | 1.47 | 1.39 |
| 24 | B | 613 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 24 | b | 609 | CLA | CHC-C4B | 3.70 | 1.47 | 1.39 |
| 24 | b | 614 | CLA | CHC-C4B | 3.70 | 1.47 | 1.39 |
| 24 | c | 906 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 24 | d | 402 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 24 | b | 606 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 912 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 24 | C | 512 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 24 | b | 611 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 24 | C | 508 | CLA | CHC-C4B | 3.69 | 1.47 | 1.39 |
| 24 | b | 611 | CLA | CHB-C1B | 3.69 | 1.47 | 1.39 |
| 24 | b | 613 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 24 | b | 612 | CLA | CHB-C1B | 3.69 | 1.47 | 1.39 |
| 24 | b | 616 | CLA | CHC-C4B | 3.69 | 1.47 | 1.39 |
| 24 | B | 616 | CLA | CHD-C4C | 3.69 | 1.47 | 1.39 |
| 24 | B | 610 | CLA | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 24 | B | 610 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 24 | c | 914 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 24 | a | 409 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 24 | c | 909 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 24 | c | 910 | CLA | CHB-C1B | 3.68 | 1.47 | 1.39 |
| 24 | B | 608 | CLA | CHC-C4B | 3.68 | 1.47 | 1.39 |
| 24 | C | 502 | CLA | CHB-C1B | 3.67 | 1.47 | 1.39 |
| 24 | b | 608 | CLA | CHB-C1B | 3.67 | 1.47 | 1.39 |
| 24 | B | 614 | CLA | CHD-C4C | 3.67 | 1.47 | 1.39 |
| 24 | C | 513 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 24 | b | 608 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 24 | C | 510 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 24 | c | 911 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 24 | B | 605 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 24 | B | 608 | CLA | CHB-C1B | 3.66 | 1.47 | 1.39 |
| 24 | b | 607 | CLA | CHC-C4B | 3.65 | 1.47 | 1.39 |
| 24 | c | 910 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 24 | B | 610 | CLA | CHC-C4B | 3.65 | 1.47 | 1.39 |
| 24 | C | 513 | CLA | CHD-C4C | 3.65 | 1.47 | 1.39 |
| 37 | d | 407 | LHG | O7-C7 | 3.65 | 1.44 | 1.34 |
| 24 | C | 509 | CLA | CHC-C4B | 3.65 | 1.47 | 1.39 |
| 24 | B | 604 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |
| 24 | c | 909 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 24 | c | 902 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |
| 24 | C | 508 | CLA | CHB-C1B | 3.64 | 1.47 | 1.39 |
| 24 | B | 603 | CLA | CHC-C4B | 3.63 | 1.47 | 1.39 |
| 24 | B | 607 | CLA | C3D-C2D | 3.63 | 1.48 | 1.39 |
| 24 | B | 614 | CLA | CHC-C4B | 3.63 | 1.47 | 1.39 |
| 24 | B | 612 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 24 | c | 904 | CLA | CHB-C1B | 3.62 | 1.47 | 1.39 |
| 24 | b | 611 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 24 | D | 402 | CLA | CHD-C4C | 3.62 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | a | 407 | CLA | CHB-C1B | 3.62 | 1.47 | 1.39 |
| 24 | A | 410 | CLA | CHB-C1B | 3.62 | 1.47 | 1.39 |
| 24 | C | 503 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 24 | D | 402 | CLA | CHC-C4B | 3.61 | 1.47 | 1.39 |
| 24 | C | 508 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 24 | b | 605 | CLA | CHB-C1B | 3.61 | 1.47 | 1.39 |
| 24 | B | 616 | CLA | CHC-C4B | 3.61 | 1.47 | 1.39 |
| 24 | b | 613 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 24 | c | 912 | CLA | CHC-C4B | 3.61 | 1.47 | 1.39 |
| 24 | d | 402 | CLA | C1B-NB | -3.61 | 1.33 | 1.37 |
| 35 | c | 923 | HTG | C1'-S1 | -3.60 | 1.76 | 1.81 |
| 24 | B | 613 | CLA | CHC-C4B | 3.60 | 1.47 | 1.39 |
| 24 | d | 402 | CLA | CHD-C4C | 3.60 | 1.47 | 1.39 |
| 24 | a | 406 | CLA | O2A-CGA | 3.60 | 1.43 | 1.33 |
| 24 | d | 402 | CLA | CHC-C4B | 3.59 | 1.47 | 1.39 |
| 37 | d | 408 | LHG | O8-C23 | 3.59 | 1.43 | 1.33 |
| 24 | A | 406 | CLA | CHC-C4B | 3.59 | 1.47 | 1.39 |
| 37 | D | 408 | LHG | O8-C23 | 3.59 | 1.43 | 1.33 |
| 24 | b | 609 | CLA | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 24 | D | 401 | CLA | CHD-C4C | 3.59 | 1.47 | 1.39 |
| 24 | C | 505 | CLA | CHC-C4B | 3.58 | 1.47 | 1.39 |
| 24 | b | 611 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 24 | C | 504 | CLA | CHC-C4B | 3.58 | 1.47 | 1.39 |
| 24 | c | 914 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 24 | B | 607 | CLA | CHB-C1B | 3.58 | 1.47 | 1.39 |
| 24 | C | 506 | CLA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 24 | b | 612 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 24 | b | 616 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 24 | b | 615 | CLA | CHD-C4C | 3.57 | 1.47 | 1.39 |
| 24 | B | 604 | CLA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 24 | d | 402 | CLA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 24 | C | 506 | CLA | C1B-NB | -3.56 | 1.33 | 1.37 |
| 24 | d | 403 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 24 | a | 406 | CLA | CHC-C4B | 3.56 | 1.47 | 1.39 |
| 24 | B | 613 | CLA | CHD-C4C | 3.56 | 1.47 | 1.39 |
| 24 | c | 914 | CLA | CHC-C4B | 3.56 | 1.47 | 1.39 |
| 24 | b | 618 | CLA | CHC-C4B | 3.55 | 1.47 | 1.39 |
| 24 | B | 608 | CLA | C3D-C2D | 3.55 | 1.48 | 1.39 |
| 24 | b | 618 | CLA | C3D-C2D | 3.55 | 1.48 | 1.39 |
| 38 | e | 102 | HEM | C4D-ND | -3.54 | 1.34 | 1.40 |
| 24 | B | 617 | CLA | C4B-NB | -3.54 | 1.33 | 1.37 |
| 24 | c | 905 | CLA | CHD-C4C | 3.54 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | A | 405 | CLA | CHD-C4C | 3.54 | 1.47 | 1.39 |
| 24 | C | 513 | CLA | CHB-C1B | 3.54 | 1.47 | 1.39 |
| 24 | b | 617 | CLA | CHC-C4B | 3.54 | 1.47 | 1.39 |
| 35 | B | 633 | HTG | C1'-S1 | -3.53 | 1.76 | 1.81 |
| 24 | b | 615 | CLA | CHC-C4B | 3.53 | 1.47 | 1.39 |
| 24 | B | 602 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 24 | c | 908 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 24 | b | 616 | CLA | C3D-C2D | 3.52 | 1.48 | 1.39 |
| 24 | a | 407 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 24 | b | 607 | CLA | C3D-C2D | 3.52 | 1.48 | 1.39 |
| 24 | c | 909 | CLA | CHC-C4B | 3.52 | 1.47 | 1.39 |
| 24 | B | 604 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 24 | B | 606 | CLA | CHC-C4B | 3.51 | 1.47 | 1.39 |
| 24 | b | 606 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 24 | c | 909 | CLA | CHB-C1B | 3.51 | 1.47 | 1.39 |
| 24 | C | 504 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 37 | D | 407 | LHG | O8-C23 | 3.50 | 1.43 | 1.33 |
| 24 | b | 605 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 24 | b | 618 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 24 | c | 907 | CLA | C1B-NB | -3.50 | 1.33 | 1.37 |
| 24 | d | 403 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 24 | b | 617 | CLA | CHD-C4C | 3.49 | 1.47 | 1.39 |
| 24 | c | 913 | CLA | CHB-C1B | 3.48 | 1.47 | 1.39 |
| 24 | b | 617 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 24 | B | 607 | CLA | C1B-NB | -3.48 | 1.33 | 1.37 |
| 35 | D | 411 | HTG | C1'-S1 | -3.47 | 1.76 | 1.81 |
| 24 | a | 409 | CLA | CHB-C1B | 3.47 | 1.47 | 1.39 |
| 24 | b | 611 | CLA | CHD-C4C | 3.47 | 1.47 | 1.39 |
| 24 | C | 512 | CLA | C4B-NB | -3.46 | 1.33 | 1.37 |
| 24 | C | 507 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 24 | b | 615 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 24 | b | 606 | CLA | CHC-C4B | 3.44 | 1.47 | 1.39 |
| 24 | C | 506 | CLA | C3D-C2D | 3.44 | 1.48 | 1.39 |
| 24 | b | 610 | CLA | CHC-C4B | 3.44 | 1.47 | 1.39 |
| 24 | b | 620 | CLA | CHC-C4B | 3.44 | 1.47 | 1.39 |
| 24 | b | 610 | CLA | OBD-CAD | 3.44 | 1.28 | 1.22 |
| 24 | C | 514 | CLA | CHC-C4B | 3.43 | 1.47 | 1.39 |
| 24 | d | 401 | CLA | CHC-C4B | 3.43 | 1.47 | 1.39 |
| 24 | c | 914 | CLA | CHB-C1B | 3.43 | 1.47 | 1.39 |
| 24 | b | 607 | CLA | CHB-C1B | 3.43 | 1.47 | 1.39 |
| 24 | D | 401 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 24 | c | 905 | CLA | CHC-C4B | 3.42 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | d | 401 | CLA | C1B-C2B | 3.42 | 1.51 | 1.43 |
| 24 | b | 619 | CLA | CHB-C1B | 3.41 | 1.47 | 1.39 |
| 35 | B | 634 | HTG | C1'-S1 | -3.41 | 1.76 | 1.81 |
| 35 | b | 627 | HTG | C1'-S1 | -3.41 | 1.76 | 1.81 |
| 24 | D | 402 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 24 | a | 409 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 24 | c | 907 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 24 | b | 615 | CLA | C1B-C2B | 3.40 | 1.51 | 1.43 |
| 24 | B | 603 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 24 | B | 602 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 24 | C | 513 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 24 | c | 907 | CLA | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 24 | c | 906 | CLA | C3D-C2D | 3.38 | 1.48 | 1.39 |
| 24 | B | 607 | CLA | C4B-NB | -3.37 | 1.33 | 1.37 |
| 24 | B | 609 | CLA | C4B-NB | -3.37 | 1.33 | 1.37 |
| 24 | B | 615 | CLA | C4B-NB | -3.37 | 1.33 | 1.37 |
| 24 | B | 609 | CLA | CHC-C4B | 3.36 | 1.46 | 1.39 |
| 24 | B | 609 | CLA | C1B-NB | -3.35 | 1.33 | 1.37 |
| 24 | B | 611 | CLA | C1B-NB | -3.35 | 1.33 | 1.37 |
| 24 | c | 913 | CLA | OBD-CAD | 3.35 | 1.28 | 1.22 |
| 24 | C | 514 | CLA | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 38 | E | 103 | HEM | C4D-ND | -3.34 | 1.34 | 1.40 |
| 24 | b | 619 | CLA | C1B-C2B | 3.33 | 1.50 | 1.43 |
| 24 | b | 613 | CLA | C1B-NB | -3.33 | 1.33 | 1.37 |
| 24 | B | 614 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 24 | B | 607 | CLA | CHC-C4B | 3.32 | 1.46 | 1.39 |
| 24 | D | 401 | CLA | CHC-C4B | 3.32 | 1.46 | 1.39 |
| 24 | b | 619 | CLA | CHC-C4B | 3.31 | 1.46 | 1.39 |
| 24 | b | 611 | CLA | C1B-C2B | 3.30 | 1.50 | 1.43 |
| 24 | b | 611 | CLA | C1B-NB | -3.30 | 1.33 | 1.37 |
| 24 | c | 906 | CLA | C1B-C2B | 3.30 | 1.50 | 1.43 |
| 24 | B | 617 | CLA | CHC-C4B | 3.30 | 1.46 | 1.39 |
| 24 | b | 620 | CLA | OBD-CAD | 3.29 | 1.28 | 1.22 |
| 24 | c | 904 | CLA | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 24 | C | 507 | CLA | CHC-C4B | 3.28 | 1.46 | 1.39 |
| 24 | C | 510 | CLA | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 24 | B | 605 | CLA | C3D-C2D | 3.28 | 1.47 | 1.39 |
| 24 | C | 509 | CLA | OBD-CAD | 3.27 | 1.28 | 1.22 |
| 24 | c | 905 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |
| 24 | B | 617 | CLA | CHD-C4C | 3.27 | 1.46 | 1.39 |
| 24 | b | 607 | CLA | C1B-NB | -3.26 | 1.33 | 1.37 |
| 24 | b | 610 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | b | 608 | CLA | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 25 | A | 409 | PHO | CHA-CBD | -3.24 | 1.47 | 1.51 |
| 37 | D | 406 | LHG | O7-C7 | 3.24 | 1.43 | 1.34 |
| 24 | C | 512 | CLA | C1B-C2B | 3.23 | 1.50 | 1.43 |
| 24 | C | 503 | CLA | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 24 | c | 908 | CLA | CHC-C4B | 3.21 | 1.46 | 1.39 |
| 24 | c | 911 | CLA | C1B-NB | -3.21 | 1.33 | 1.37 |
| 24 | c | 902 | CLA | OBD-CAD | 3.21 | 1.28 | 1.22 |
| 24 | C | 504 | CLA | CHB-C1B | 3.20 | 1.46 | 1.39 |
| 24 | B | 606 | CLA | CHD-C4C | 3.20 | 1.46 | 1.39 |
| 24 | C | 512 | CLA | CHC-C4B | 3.20 | 1.46 | 1.39 |
| 24 | B | 615 | CLA | CHC-C4B | 3.20 | 1.46 | 1.39 |
| 38 | E | 103 | HEM | C1B-NB | -3.19 | 1.34 | 1.40 |
| 24 | b | 616 | CLA | CHD-C4C | 3.19 | 1.46 | 1.39 |
| 35 | b | 603 | HTG | C1'-S1 | -3.18 | 1.76 | 1.81 |
| 24 | c | 902 | CLA | CHC-C4B | 3.17 | 1.46 | 1.39 |
| 35 | C | 524 | HTG | C1'-S1 | -3.17 | 1.77 | 1.81 |
| 24 | C | 514 | CLA | C4B-NB | -3.17 | 1.33 | 1.37 |
| 24 | D | 401 | CLA | C1B-C2B | 3.16 | 1.50 | 1.43 |
| 35 | d | 412 | HTG | C1'-S1 | -3.16 | 1.77 | 1.81 |
| 24 | b | 607 | CLA | OBD-CAD | 3.16 | 1.27 | 1.22 |
| 24 | b | 608 | CLA | C4C-C3C | 3.16 | 1.50 | 1.45 |
| 24 | C | 510 | CLA | C4B-NB | -3.15 | 1.33 | 1.37 |
| 24 | c | 909 | CLA | C1B-C2B | 3.15 | 1.50 | 1.43 |
| 35 | B | 626 | HTG | C1'-S1 | -3.15 | 1.77 | 1.81 |
| 24 | A | 405 | CLA | OBD-CAD | 3.15 | 1.27 | 1.22 |
| 24 | A | 406 | CLA | C4B-NB | -3.15 | 1.33 | 1.37 |
| 24 | c | 908 | CLA | C4B-NB | -3.15 | 1.33 | 1.37 |
| 24 | c | 912 | CLA | C4B-NB | -3.14 | 1.33 | 1.37 |
| 24 | B | 604 | CLA | C4B-NB | -3.13 | 1.33 | 1.37 |
| 24 | c | 902 | CLA | C1B-NB | -3.13 | 1.33 | 1.37 |
| 24 | d | 401 | CLA | C1B-NB | -3.12 | 1.33 | 1.37 |
| 24 | B | 616 | CLA | CHB-C1B | 3.12 | 1.46 | 1.39 |
| 24 | B | 611 | CLA | C1B-C2B | 3.12 | 1.50 | 1.43 |
| 24 | c | 906 | CLA | CHC-C4B | 3.12 | 1.46 | 1.39 |
| 24 | C | 511 | CLA | OBD-CAD | 3.11 | 1.27 | 1.22 |
| 24 | C | 504 | CLA | C4B-NB | -3.11 | 1.33 | 1.37 |
| 24 | D | 402 | CLA | C1B-C2B | 3.11 | 1.50 | 1.43 |
| 35 | V | 202 | HTG | C1'-S1 | -3.11 | 1.77 | 1.81 |
| 24 | B | 609 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 24 | a | 409 | CLA | C1B-C2B | 3.10 | 1.50 | 1.43 |
| 24 | B | 608 | CLA | C4C-C3C | 3.09 | 1.50 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 912 | CLA | C1B-NB | -3.09 | 1.33 | 1.37 |
| 24 | C | 508 | CLA | C4B-NB | -3.08 | 1.33 | 1.37 |
| 24 | B | 614 | CLA | C4D-CHA | 3.08 | 1.48 | 1.38 |
| 25 | a | 420 | PHO | C3A-C2A | -3.08 | 1.52 | 1.54 |
| 24 | B | 611 | CLA | C4D-CHA | 3.07 | 1.48 | 1.38 |
| 24 | A | 406 | CLA | CHB-C1B | 3.07 | 1.46 | 1.39 |
| 24 | b | 610 | CLA | C1B-C2B | 3.07 | 1.50 | 1.43 |
| 24 | c | 906 | CLA | C4C-C3C | 3.07 | 1.50 | 1.45 |
| 24 | b | 619 | CLA | C4D-CHA | 3.06 | 1.48 | 1.38 |
| 24 | C | 507 | CLA | C4B-NB | -3.06 | 1.33 | 1.37 |
| 24 | B | 616 | CLA | C1B-NB | -3.05 | 1.33 | 1.37 |
| 24 | a | 409 | CLA | C4B-NB | -3.05 | 1.33 | 1.37 |
| 24 | A | 406 | CLA | C1B-NB | -3.05 | 1.33 | 1.37 |
| 24 | b | 606 | CLA | C1B-C2B | 3.04 | 1.50 | 1.43 |
| 35 | C | 523 | HTG | C1'-S1 | -3.04 | 1.77 | 1.81 |
| 24 | B | 613 | CLA | C1B-NB | -3.03 | 1.33 | 1.37 |
| 24 | b | 610 | CLA | C1B-NB | -3.03 | 1.33 | 1.37 |
| 38 | e | 102 | HEM | C1B-NB | -3.02 | 1.35 | 1.40 |
| 24 | c | 914 | CLA | C1B-NB | -3.02 | 1.33 | 1.37 |
| 24 | c | 908 | CLA | C4D-CHA | 3.02 | 1.48 | 1.38 |
| 24 | c | 910 | CLA | C1B-NB | -3.01 | 1.33 | 1.37 |
| 24 | A | 406 | CLA | OBD-CAD | 3.01 | 1.27 | 1.22 |
| 24 | B | 606 | CLA | C1B-NB | -3.01 | 1.33 | 1.37 |
| 24 | C | 507 | CLA | C1B-C2B | 3.01 | 1.50 | 1.43 |
| 24 | B | 606 | CLA | C1B-C2B | 3.00 | 1.50 | 1.43 |
| 24 | C | 510 | CLA | C4C-C3C | 3.00 | 1.50 | 1.45 |
| 24 | C | 510 | CLA | C1B-NB | -3.00 | 1.33 | 1.37 |
| 24 | C | 508 | CLA | C1B-C2B | 3.00 | 1.50 | 1.43 |
| 24 | d | 403 | CLA | C1B-C2B | 3.00 | 1.50 | 1.43 |
| 24 | a | 409 | CLA | C1B-NB | -3.00 | 1.33 | 1.37 |
| 24 | b | 618 | CLA | C1B-C2B | 3.00 | 1.50 | 1.43 |
| 24 | b | 605 | CLA | C1B-NB | -2.99 | 1.33 | 1.37 |
| 24 | B | 605 | CLA | OBD-CAD | 2.99 | 1.27 | 1.22 |
| 24 | C | 503 | CLA | C4D-CHA | 2.99 | 1.48 | 1.38 |
| 24 | B | 602 | CLA | C4B-NB | -2.98 | 1.33 | 1.37 |
| 24 | b | 616 | CLA | C4B-NB | -2.98 | 1.33 | 1.37 |
| 24 | a | 407 | CLA | C4D-CHA | 2.98 | 1.48 | 1.38 |
| 24 | C | 511 | CLA | C1B-NB | -2.98 | 1.33 | 1.37 |
| 24 | A | 406 | CLA | C4D-CHA | 2.97 | 1.48 | 1.38 |
| 24 | c | 908 | CLA | C1B-C2B | 2.97 | 1.50 | 1.43 |
| 24 | b | 618 | CLA | C1B-NB | -2.97 | 1.34 | 1.37 |
| 24 | C | 509 | CLA | C4C-C3C | 2.96 | 1.50 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 35 | O | 303 | HTG | C1'-S1 | -2.96 | 1.77 | 1.81 |
| 24 | b | 608 | CLA | C4D-CHA | 2.96 | 1.48 | 1.38 |
| 24 | b | 620 | CLA | C4B-NB | -2.96 | 1.34 | 1.37 |
| 24 | A | 410 | CLA | C1B-C2B | 2.96 | 1.50 | 1.43 |
| 24 | C | 503 | CLA | C1B-C2B | 2.95 | 1.50 | 1.43 |
| 35 | b | 626 | HTG | C1'-S1 | -2.95 | 1.77 | 1.81 |
| 24 | A | 410 | CLA | C4D-CHA | 2.94 | 1.48 | 1.38 |
| 24 | A | 405 | CLA | C1B-NB | -2.94 | 1.34 | 1.37 |
| 40 | V | 201 | HEC | C1B-NB | -2.94 | 1.34 | 1.39 |
| 24 | a | 407 | CLA | C4B-NB | -2.93 | 1.34 | 1.37 |
| 24 | C | 505 | CLA | C1B-NB | -2.93 | 1.34 | 1.37 |
| 24 | D | 401 | CLA | C4C-C3C | 2.93 | 1.50 | 1.45 |
| 24 | b | 608 | CLA | C1C-C2C | 2.93 | 1.50 | 1.44 |
| 24 | b | 609 | CLA | C4D-CHA | 2.92 | 1.48 | 1.38 |
| 24 | b | 617 | CLA | C4B-NB | -2.92 | 1.34 | 1.37 |
| 24 | C | 507 | CLA | C1B-NB | -2.92 | 1.34 | 1.37 |
| 24 | c | 907 | CLA | C4B-NB | -2.91 | 1.34 | 1.37 |
| 24 | C | 510 | CLA | C4D-CHA | 2.91 | 1.48 | 1.38 |
| 24 | b | 616 | CLA | C1B-NB | -2.91 | 1.34 | 1.37 |
| 24 | C | 506 | CLA | C4C-C3C | 2.91 | 1.50 | 1.45 |
| 24 | b | 608 | CLA | C1B-C2B | 2.91 | 1.50 | 1.43 |
| 24 | B | 608 | CLA | C4D-CHA | 2.91 | 1.48 | 1.38 |
| 24 | d | 403 | CLA | C1B-NB | -2.90 | 1.34 | 1.37 |
| 24 | b | 610 | CLA | C1C-C2C | 2.90 | 1.50 | 1.44 |
| 24 | B | 608 | CLA | C1B-NB | -2.90 | 1.34 | 1.37 |
| 24 | C | 505 | CLA | C1B-C2B | 2.90 | 1.49 | 1.43 |
| 24 | B | 615 | CLA | C4D-CHA | 2.89 | 1.48 | 1.38 |
| 24 | B | 607 | CLA | C4C-C3C | 2.89 | 1.49 | 1.45 |
| 24 | b | 614 | CLA | C1B-NB | -2.89 | 1.34 | 1.37 |
| 24 | A | 410 | CLA | C1B-NB | -2.89 | 1.34 | 1.37 |
| 24 | B | 611 | CLA | OBD-CAD | 2.89 | 1.27 | 1.22 |
| 24 | B | 615 | CLA | C1B-C2B | 2.88 | 1.49 | 1.43 |
| 24 | B | 612 | CLA | C1B-C2B | 2.88 | 1.49 | 1.43 |
| 24 | b | 612 | CLA | C1B-C2B | 2.87 | 1.49 | 1.43 |
| 24 | c | 903 | CLA | C1B-NB | -2.87 | 1.34 | 1.37 |
| 24 | b | 612 | CLA | C4D-CHA | 2.86 | 1.48 | 1.38 |
| 24 | C | 510 | CLA | C1B-C2B | 2.86 | 1.49 | 1.43 |
| 24 | c | 909 | CLA | C4C-C3C | 2.86 | 1.49 | 1.45 |
| 24 | B | 610 | CLA | C1B-C2B | 2.86 | 1.49 | 1.43 |
| 24 | c | 911 | CLA | C1B-C2B | 2.86 | 1.49 | 1.43 |
| 24 | c | 902 | CLA | C4D-CHA | 2.86 | 1.48 | 1.38 |
| 24 | a | 406 | CLA | C1B-C2B | 2.86 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 910 | CLA | C4D-CHA | 2.86 | 1.48 | 1.38 |
| 24 | C | 503 | CLA | C1B-NB | -2.85 | 1.34 | 1.37 |
| 35 | B | 625 | HTG | C1'-S1 | -2.85 | 1.77 | 1.81 |
| 24 | b | 615 | CLA | C1B-NB | -2.85 | 1.34 | 1.37 |
| 24 | B | 604 | CLA | C1B-NB | -2.84 | 1.34 | 1.37 |
| 24 | C | 512 | CLA | C4D-CHA | 2.84 | 1.48 | 1.38 |
| 24 | c | 910 | CLA | C4B-NB | -2.83 | 1.34 | 1.37 |
| 24 | c | 904 | CLA | C4C-C3C | 2.83 | 1.49 | 1.45 |
| 24 | C | 513 | CLA | C1B-NB | -2.83 | 1.34 | 1.37 |
| 24 | B | 606 | CLA | C4C-C3C | 2.83 | 1.49 | 1.45 |
| 24 | a | 406 | CLA | C4C-C3C | 2.83 | 1.49 | 1.45 |
| 24 | b | 613 | CLA | C1C-C2C | 2.82 | 1.50 | 1.44 |
| 24 | B | 616 | CLA | OBD-CAD | 2.82 | 1.27 | 1.22 |
| 24 | b | 612 | CLA | C1B-NB | -2.82 | 1.34 | 1.37 |
| 31 | A | 419 | PL9 | C6-C5 | 2.82 | 1.49 | 1.35 |
| 31 | a | 417 | PL9 | C6-C5 | 2.82 | 1.49 | 1.35 |
| 24 | D | 401 | CLA | C4D-CHA | 2.82 | 1.48 | 1.38 |
| 24 | B | 617 | CLA | C1B-C2B | 2.81 | 1.49 | 1.43 |
| 24 | b | 620 | CLA | C1B-C2B | 2.81 | 1.49 | 1.43 |
| 24 | B | 616 | CLA | C1B-C2B | 2.81 | 1.49 | 1.43 |
| 24 | c | 909 | CLA | C4D-CHA | 2.81 | 1.48 | 1.38 |
| 24 | c | 906 | CLA | C1B-NB | -2.80 | 1.34 | 1.37 |
| 24 | B | 612 | CLA | C4C-C3C | 2.80 | 1.49 | 1.45 |
| 24 | C | 514 | CLA | C1B-C2B | 2.80 | 1.49 | 1.43 |
| 24 | B | 612 | CLA | C4D-CHA | 2.80 | 1.48 | 1.38 |
| 24 | a | 409 | CLA | C4D-CHA | 2.80 | 1.48 | 1.38 |
| 24 | D | 402 | CLA | C4C-C3C | 2.80 | 1.49 | 1.45 |
| 24 | B | 617 | CLA | C4D-CHA | 2.80 | 1.48 | 1.38 |
| 24 | c | 902 | CLA | C1B-C2B | 2.80 | 1.49 | 1.43 |
| 24 | b | 609 | CLA | C1C-C2C | 2.79 | 1.50 | 1.44 |
| 24 | b | 609 | CLA | C1B-C2B | 2.79 | 1.49 | 1.43 |
| 24 | C | 514 | CLA | C1B-NB | -2.79 | 1.34 | 1.37 |
| 36 | H | 102 | DGD | O5D-C1E | 2.79 | 1.44 | 1.40 |
| 24 | b | 619 | CLA | C4B-NB | -2.79 | 1.34 | 1.37 |
| 24 | c | 902 | CLA | C4B-NB | -2.79 | 1.34 | 1.37 |
| 24 | b | 617 | CLA | C4D-CHA | 2.78 | 1.47 | 1.38 |
| 24 | a | 407 | CLA | C3D-C4D | -2.78 | 1.37 | 1.44 |
| 24 | C | 502 | CLA | C4D-CHA | 2.78 | 1.47 | 1.38 |
| 24 | d | 402 | CLA | C4C-C3C | 2.78 | 1.49 | 1.45 |
| 24 | C | 502 | CLA | C1B-NB | -2.78 | 1.34 | 1.37 |
| 24 | C | 513 | CLA | C1C-C2C | 2.78 | 1.50 | 1.44 |
| 31 | d | 405 | PL9 | C6-C5 | 2.78 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 31 | D | 404 | PL9 | C6-C5 | 2.78 | 1.48 | 1.35 |
| 24 | A | 410 | CLA | C4B-NB | -2.78 | 1.34 | 1.37 |
| 24 | C | 502 | CLA | C1B-C2B | 2.78 | 1.49 | 1.43 |
| 24 | c | 907 | CLA | C4D-CHA | 2.78 | 1.47 | 1.38 |
| 24 | c | 913 | CLA | C1B-C2B | 2.78 | 1.49 | 1.43 |
| 24 | C | 503 | CLA | C4C-C3C | 2.78 | 1.49 | 1.45 |
| 24 | C | 504 | CLA | C1B-NB | -2.77 | 1.34 | 1.37 |
| 24 | c | 914 | CLA | C1B-C2B | 2.77 | 1.49 | 1.43 |
| 24 | B | 617 | CLA | C1B-NB | -2.76 | 1.34 | 1.37 |
| 24 | c | 913 | CLA | C1B-NB | -2.76 | 1.34 | 1.37 |
| 24 | c | 906 | CLA | C4D-CHA | 2.76 | 1.47 | 1.38 |
| 24 | B | 603 | CLA | C4B-NB | -2.76 | 1.34 | 1.37 |
| 24 | B | 602 | CLA | C4D-CHA | 2.75 | 1.47 | 1.38 |
| 24 | B | 611 | CLA | C4B-NB | -2.75 | 1.34 | 1.37 |
| 24 | B | 603 | CLA | C4D-CHA | 2.75 | 1.47 | 1.38 |
| 24 | C | 511 | CLA | C4D-CHA | 2.75 | 1.47 | 1.38 |
| 24 | c | 905 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 24 | C | 508 | CLA | C1B-NB | -2.75 | 1.34 | 1.37 |
| 24 | A | 405 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 24 | C | 505 | CLA | C4B-NB | -2.75 | 1.34 | 1.37 |
| 24 | c | 905 | CLA | C1C-C2C | 2.75 | 1.50 | 1.44 |
| 40 | v | 202 | HEC | C1D-ND | -2.75 | 1.34 | 1.39 |
| 34 | Z | 101 | LMG | O8-C28 | 2.74 | 1.46 | 1.33 |
| 24 | C | 504 | CLA | C4C-C3C | 2.74 | 1.49 | 1.45 |
| 24 | C | 509 | CLA | C1B-NB | -2.74 | 1.34 | 1.37 |
| 24 | b | 614 | CLA | C1B-C2B | 2.74 | 1.49 | 1.43 |
| 24 | A | 407 | CLA | C1B-C2B | 2.73 | 1.49 | 1.43 |
| 24 | c | 905 | CLA | C1B-NB | -2.73 | 1.34 | 1.37 |
| 24 | b | 610 | CLA | C4D-CHA | 2.73 | 1.47 | 1.38 |
| 24 | b | 619 | CLA | C1B-NB | -2.73 | 1.34 | 1.37 |
| 24 | c | 911 | CLA | C4D-CHA | 2.73 | 1.47 | 1.38 |
| 24 | d | 402 | CLA | OBD-CAD | 2.73 | 1.27 | 1.22 |
| 24 | c | 909 | CLA | C1B-NB | -2.72 | 1.34 | 1.37 |
| 24 | C | 511 | CLA | C1B-C2B | 2.72 | 1.49 | 1.43 |
| 24 | C | 503 | CLA | C4B-NB | -2.72 | 1.34 | 1.37 |
| 24 | C | 506 | CLA | C1B-C2B | 2.72 | 1.49 | 1.43 |
| 25 | A | 409 | PHO | C3A-C2A | -2.72 | 1.52 | 1.54 |
| 24 | d | 402 | CLA | C4D-CHA | 2.72 | 1.47 | 1.38 |
| 24 | c | 906 | CLA | C4B-NB | -2.72 | 1.34 | 1.37 |
| 24 | B | 603 | CLA | C1B-NB | -2.71 | 1.34 | 1.37 |
| 24 | A | 407 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 24 | B | 602 | CLA | C1B-NB | -2.71 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | b | 607 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 24 | C | 511 | CLA | C1C-C2C | 2.71 | 1.50 | 1.44 |
| 24 | b | 611 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 24 | c | 913 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 35 | c | 922 | HTG | C1'-S1 | -2.71 | 1.77 | 1.81 |
| 24 | B | 603 | CLA | C3D-C4D | -2.70 | 1.38 | 1.44 |
| 24 | b | 617 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 24 | c | 912 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 24 | b | 605 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 24 | B | 609 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 24 | C | 507 | CLA | C4C-C3C | 2.70 | 1.49 | 1.45 |
| 24 | B | 613 | CLA | C1C-C2C | 2.70 | 1.50 | 1.44 |
| 24 | A | 407 | CLA | C1B-NB | -2.70 | 1.34 | 1.37 |
| 24 | B | 613 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 24 | C | 505 | CLA | C1C-C2C | 2.70 | 1.50 | 1.44 |
| 24 | C | 503 | CLA | C1C-C2C | 2.70 | 1.50 | 1.44 |
| 24 | B | 607 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 24 | c | 910 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 24 | c | 904 | CLA | C1B-NB | -2.69 | 1.34 | 1.37 |
| 24 | C | 504 | CLA | C1C-C2C | 2.69 | 1.50 | 1.44 |
| 24 | c | 905 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 24 | B | 614 | CLA | C4C-C3C | 2.69 | 1.49 | 1.45 |
| 24 | B | 615 | CLA | C1B-NB | -2.68 | 1.34 | 1.37 |
| 24 | B | 603 | CLA | C1C-C2C | 2.68 | 1.50 | 1.44 |
| 24 | C | 508 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 24 | b | 620 | CLA | C1B-NB | -2.67 | 1.34 | 1.37 |
| 24 | c | 904 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 24 | b | 606 | CLA | C1B-NB | -2.67 | 1.34 | 1.37 |
| 24 | d | 402 | CLA | C4B-NB | -2.67 | 1.34 | 1.37 |
| 24 | C | 513 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 24 | d | 403 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 24 | A | 405 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 24 | b | 614 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 24 | B | 606 | CLA | C4B-NB | -2.66 | 1.34 | 1.37 |
| 24 | C | 509 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 24 | B | 611 | CLA | C4C-C3C | 2.66 | 1.49 | 1.45 |
| 24 | B | 609 | CLA | C4C-C3C | 2.65 | 1.49 | 1.45 |
| 24 | c | 913 | CLA | C1C-C2C | 2.65 | 1.49 | 1.44 |
| 24 | b | 616 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 24 | B | 607 | CLA | C1C-C2C | 2.64 | 1.49 | 1.44 |
| 24 | B | 610 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 24 | B | 605 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 612 | CLA | C1B-NB | -2.64 | 1.34 | 1.37 |
| 24 | B | 616 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 24 | b | 609 | CLA | C3D-C4D | -2.64 | 1.38 | 1.44 |
| 24 | B | 614 | CLA | C3B-C2B | 2.64 | 1.50 | 1.41 |
| 24 | C | 502 | CLA | C1C-C2C | 2.63 | 1.49 | 1.44 |
| 24 | b | 606 | CLA | C4B-NB | -2.63 | 1.34 | 1.37 |
| 24 | b | 605 | CLA | C3B-C4B | 2.63 | 1.50 | 1.42 |
| 24 | D | 401 | CLA | C3D-C4D | -2.63 | 1.38 | 1.44 |
| 24 | b | 620 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 24 | c | 910 | CLA | C1C-C2C | 2.62 | 1.49 | 1.44 |
| 24 | b | 616 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 24 | b | 611 | CLA | C1C-C2C | 2.62 | 1.49 | 1.44 |
| 24 | C | 512 | CLA | C1B-NB | -2.62 | 1.34 | 1.37 |
| 24 | B | 604 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 24 | B | 614 | CLA | C1C-C2C | 2.62 | 1.49 | 1.44 |
| 24 | d | 403 | CLA | C4B-NB | -2.62 | 1.34 | 1.37 |
| 24 | D | 402 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 24 | c | 903 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 24 | B | 605 | CLA | C1B-NB | -2.61 | 1.34 | 1.37 |
| 24 | C | 506 | CLA | C4B-NB | -2.61 | 1.34 | 1.37 |
| 24 | b | 619 | CLA | C4C-C3C | 2.61 | 1.49 | 1.45 |
| 24 | b | 607 | CLA | C3D-C4D | -2.61 | 1.38 | 1.44 |
| 24 | B | 615 | CLA | C1C-C2C | 2.61 | 1.49 | 1.44 |
| 24 | b | 607 | CLA | C4C-C3C | 2.60 | 1.49 | 1.45 |
| 24 | B | 614 | CLA | C4B-NB | -2.60 | 1.34 | 1.37 |
| 24 | B | 606 | CLA | C3D-C4D | -2.60 | 1.38 | 1.44 |
| 24 | b | 606 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 25 | A | 408 | PHO | CHA-CBD | -2.60 | 1.48 | 1.51 |
| 24 | C | 507 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 24 | d | 402 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 24 | b | 617 | CLA | C1B-NB | -2.59 | 1.34 | 1.37 |
| 36 | h | 102 | DGD | O5D-C1E | 2.59 | 1.44 | 1.40 |
| 24 | B | 603 | CLA | C4C-C3C | 2.59 | 1.49 | 1.45 |
| 24 | C | 505 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 24 | B | 605 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 24 | A | 407 | CLA | C3B-C4B | 2.58 | 1.50 | 1.42 |
| 24 | B | 602 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 24 | A | 405 | CLA | C4B-NB | -2.58 | 1.34 | 1.37 |
| 24 | b | 607 | CLA | C4B-NB | -2.58 | 1.34 | 1.37 |
| 24 | B | 608 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 24 | c | 903 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 24 | c | 914 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | b | 615 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 24 | B | 607 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 24 | C | 510 | CLA | C1C-C2C | 2.57 | 1.49 | 1.44 |
| 24 | c | 907 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 24 | C | 509 | CLA | C4B-NB | -2.57 | 1.34 | 1.37 |
| 24 | C | 511 | CLA | C4C-C3C | 2.57 | 1.49 | 1.45 |
| 24 | b | 612 | CLA | C4C-C3C | 2.57 | 1.49 | 1.45 |
| 24 | b | 618 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 24 | C | 502 | CLA | C4C-C3C | 2.56 | 1.49 | 1.45 |
| 24 | a | 406 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 24 | C | 513 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 24 | B | 613 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 24 | C | 502 | CLA | C4B-NB | -2.56 | 1.34 | 1.37 |
| 24 | D | 401 | CLA | C1B-NB | -2.56 | 1.34 | 1.37 |
| 24 | C | 509 | CLA | C1B-C2B | 2.56 | 1.49 | 1.43 |
| 24 | B | 604 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 24 | C | 506 | CLA | C3D-C4D | -2.55 | 1.38 | 1.44 |
| 24 | b | 616 | CLA | C1C-C2C | 2.55 | 1.49 | 1.44 |
| 24 | b | 610 | CLA | C4B-NB | -2.55 | 1.34 | 1.37 |
| 24 | C | 504 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 24 | c | 911 | CLA | C4B-NB | -2.55 | 1.34 | 1.37 |
| 24 | a | 407 | CLA | C3B-C4B | 2.55 | 1.50 | 1.42 |
| 24 | b | 617 | CLA | C1C-C2C | 2.55 | 1.49 | 1.44 |
| 24 | c | 914 | CLA | C1C-C2C | 2.55 | 1.49 | 1.44 |
| 24 | b | 607 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 24 | B | 609 | CLA | C1C-C2C | 2.54 | 1.49 | 1.44 |
| 24 | b | 606 | CLA | C1C-C2C | 2.54 | 1.49 | 1.44 |
| 24 | b | 620 | CLA | C3B-C2B | 2.54 | 1.49 | 1.41 |
| 24 | b | 615 | CLA | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 24 | a | 406 | CLA | C3B-C2B | 2.54 | 1.49 | 1.41 |
| 24 | a | 407 | CLA | C1B-NB | -2.53 | 1.34 | 1.37 |
| 24 | B | 617 | CLA | C3B-C2B | 2.53 | 1.49 | 1.41 |
| 24 | b | 613 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 24 | C | 506 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 24 | b | 614 | CLA | C4C-C3C | 2.53 | 1.49 | 1.45 |
| 24 | c | 902 | CLA | C4C-C3C | 2.53 | 1.49 | 1.45 |
| 24 | B | 605 | CLA | C1C-C2C | 2.53 | 1.49 | 1.44 |
| 24 | c | 908 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |
| 24 | C | 503 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 24 | c | 904 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 24 | C | 514 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 24 | C | 512 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | c | 906 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 24 | c | 911 | CLA | C1C-C2C | 2.52 | 1.49 | 1.44 |
| 24 | b | 613 | CLA | C3B-C4B | 2.52 | 1.50 | 1.42 |
| 24 | D | 402 | CLA | C3B-C4B | 2.51 | 1.50 | 1.42 |
| 24 | c | 913 | CLA | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 24 | b | 611 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 24 | B | 604 | CLA | C1C-C2C | 2.51 | 1.49 | 1.44 |
| 24 | b | 616 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 40 | V | 201 | HEC | C1D-ND | -2.51 | 1.34 | 1.39 |
| 24 | d | 401 | CLA | C4B-NB | -2.51 | 1.34 | 1.37 |
| 24 | C | 505 | CLA | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 24 | D | 402 | CLA | C1C-C2C | 2.51 | 1.49 | 1.44 |
| 24 | c | 906 | CLA | C1C-C2C | 2.51 | 1.49 | 1.44 |
| 24 | C | 510 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 24 | b | 607 | CLA | C3B-C4B | 2.50 | 1.50 | 1.42 |
| 25 | a | 408 | PHO | C1D-ND | -2.50 | 1.34 | 1.38 |
| 24 | c | 904 | CLA | C4B-NB | -2.50 | 1.34 | 1.37 |
| 24 | c | 913 | CLA | C3B-C4B | 2.50 | 1.50 | 1.42 |
| 24 | a | 407 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 24 | d | 403 | CLA | C4C-C3C | 2.50 | 1.49 | 1.45 |
| 24 | c | 910 | CLA | C3B-C2B | 2.50 | 1.49 | 1.41 |
| 24 | B | 613 | CLA | C4B-NB | -2.49 | 1.34 | 1.37 |
| 24 | b | 617 | CLA | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 24 | c | 903 | CLA | C4B-NB | -2.49 | 1.34 | 1.37 |
| 24 | c | 904 | CLA | C1C-C2C | 2.49 | 1.49 | 1.44 |
| 24 | A | 407 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 24 | c | 902 | CLA | C1C-C2C | 2.49 | 1.49 | 1.44 |
| 24 | C | 509 | CLA | C1C-C2C | 2.48 | 1.49 | 1.44 |
| 24 | c | 904 | CLA | C1B-C2B | 2.48 | 1.49 | 1.43 |
| 24 | b | 618 | CLA | C1C-C2C | 2.48 | 1.49 | 1.44 |
| 24 | b | 605 | CLA | C1B-C2B | 2.48 | 1.48 | 1.43 |
| 24 | c | 912 | CLA | C4D-CHA | 2.48 | 1.46 | 1.38 |
| 24 | B | 616 | CLA | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 24 | B | 604 | CLA | C3B-C2B | 2.47 | 1.49 | 1.41 |
| 24 | c | 905 | CLA | C4C-C3C | 2.47 | 1.49 | 1.45 |
| 24 | B | 602 | CLA | C3B-C4B | 2.47 | 1.49 | 1.42 |
| 24 | b | 612 | CLA | C4B-NB | -2.47 | 1.34 | 1.37 |
| 29 | a | 401 | LMT | O1'-C1' | 2.47 | 1.44 | 1.40 |
| 24 | C | 510 | CLA | C3B-C2B | 2.47 | 1.49 | 1.41 |
| 40 | v | 202 | HEC | C1B-NB | -2.47 | 1.35 | 1.39 |
| 24 | b | 615 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 24 | C | 514 | CLA | C3B-C2B | 2.46 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | b | 614 | CLA | C4B-NB | -2.46 | 1.34 | 1.37 |
| 24 | c | 903 | CLA | C3D-C4D | -2.46 | 1.38 | 1.44 |
| 24 | c | 908 | CLA | C1B-NB | -2.46 | 1.34 | 1.37 |
| 24 | c | 914 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 24 | B | 614 | CLA | C1B-NB | -2.45 | 1.34 | 1.37 |
| 24 | b | 606 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 24 | A | 406 | CLA | C1B-C2B | 2.45 | 1.48 | 1.43 |
| 24 | c | 911 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 24 | B | 604 | CLA | C3D-C4D | -2.45 | 1.38 | 1.44 |
| 24 | C | 511 | CLA | C4B-NB | -2.45 | 1.34 | 1.37 |
| 24 | c | 909 | CLA | C4B-NB | -2.45 | 1.34 | 1.37 |
| 24 | C | 511 | CLA | C3B-C2B | 2.45 | 1.49 | 1.41 |
| 38 | e | 102 | HEM | C1C-C2C | -2.45 | 1.40 | 1.45 |
| 24 | C | 506 | CLA | C1C-C2C | 2.44 | 1.49 | 1.44 |
| 36 | D | 405 | DGD | O3G-C1D | 2.44 | 1.44 | 1.40 |
| 24 | b | 608 | CLA | C3B-C2B | 2.44 | 1.49 | 1.41 |
| 24 | A | 410 | CLA | C1C-C2C | 2.44 | 1.49 | 1.44 |
| 24 | B | 603 | CLA | C1B-C2B | 2.44 | 1.48 | 1.43 |
| 24 | b | 607 | CLA | C1C-C2C | 2.44 | 1.49 | 1.44 |
| 38 | e | 102 | HEM | C1D-ND | -2.44 | 1.34 | 1.38 |
| 24 | C | 504 | CLA | C1B-C2B | 2.44 | 1.48 | 1.43 |
| 24 | B | 613 | CLA | C3B-C2B | 2.44 | 1.49 | 1.41 |
| 24 | c | 902 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 24 | a | 406 | CLA | C1B-NB | -2.43 | 1.34 | 1.37 |
| 24 | b | 608 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 24 | A | 405 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 24 | b | 609 | CLA | C1B-NB | -2.43 | 1.34 | 1.37 |
| 24 | d | 401 | CLA | C4D-CHA | 2.43 | 1.46 | 1.38 |
| 35 | c | 923 | HTG | C1-S1 | -2.43 | 1.76 | 1.80 |
| 24 | B | 608 | CLA | C4B-NB | -2.42 | 1.34 | 1.37 |
| 24 | B | 605 | CLA | C3B-C2B | 2.42 | 1.49 | 1.41 |
| 24 | b | 612 | CLA | C3B-C4B | 2.42 | 1.49 | 1.42 |
| 24 | c | 913 | CLA | C4B-NB | -2.42 | 1.34 | 1.37 |
| 24 | b | 615 | CLA | C4B-NB | -2.42 | 1.34 | 1.37 |
| 24 | B | 617 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 24 | a | 406 | CLA | C4B-NB | -2.41 | 1.34 | 1.37 |
| 24 | b | 618 | CLA | C4C-C3C | 2.41 | 1.49 | 1.45 |
| 24 | B | 606 | CLA | C1C-C2C | 2.41 | 1.49 | 1.44 |
| 24 | c | 903 | CLA | C1C-C2C | 2.40 | 1.49 | 1.44 |
| 24 | B | 610 | CLA | C1C-C2C | 2.40 | 1.49 | 1.44 |
| 24 | C | 513 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 24 | B | 611 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | A | 409 | PHO | CBD-CGD | -2.40 | 1.49 | 1.52 |
| 24 | c | 914 | CLA | C4B-NB | -2.40 | 1.34 | 1.37 |
| 24 | C | 514 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 24 | b | 612 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 24 | B | 610 | CLA | C1B-NB | -2.39 | 1.34 | 1.37 |
| 24 | d | 403 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 24 | b | 619 | CLA | C3B-C2B | 2.39 | 1.49 | 1.41 |
| 24 | c | 909 | CLA | C3B-C2B | 2.39 | 1.49 | 1.41 |
| 35 | B | 633 | HTG | C1-S1 | -2.39 | 1.76 | 1.80 |
| 24 | B | 614 | CLA | C1B-C2B | 2.39 | 1.48 | 1.43 |
| 24 | d | 402 | CLA | C1C-C2C | 2.39 | 1.49 | 1.44 |
| 40 | V | 201 | HEC | C4B-NB | -2.39 | 1.35 | 1.39 |
| 40 | v | 202 | HEC | C4D-ND | -2.38 | 1.35 | 1.39 |
| 24 | C | 502 | CLA | C3B-C2B | 2.38 | 1.49 | 1.41 |
| 24 | B | 609 | CLA | C1B-C2B | 2.38 | 1.48 | 1.43 |
| 24 | b | 620 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 24 | b | 618 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 24 | c | 911 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 24 | c | 913 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 24 | b | 618 | CLA | C4B-NB | -2.37 | 1.34 | 1.37 |
| 24 | B | 610 | CLA | C3B-C4B | 2.37 | 1.49 | 1.42 |
| 24 | B | 609 | CLA | C3B-C2B | 2.37 | 1.49 | 1.41 |
| 24 | b | 609 | CLA | C3B-C4B | 2.37 | 1.49 | 1.42 |
| 24 | d | 403 | CLA | C3B-C2B | 2.37 | 1.49 | 1.41 |
| 24 | c | 908 | CLA | C1C-C2C | 2.37 | 1.49 | 1.44 |
| 24 | c | 905 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 24 | c | 907 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 24 | b | 614 | CLA | C1C-C2C | 2.37 | 1.49 | 1.44 |
| 27 | B | 621 | SQD | O6-C1 | 2.36 | 1.44 | 1.40 |
| 24 | D | 402 | CLA | C1B-NB | -2.36 | 1.34 | 1.37 |
| 24 | C | 508 | CLA | C1C-C2C | 2.36 | 1.49 | 1.44 |
| 24 | B | 606 | CLA | C4D-CHA | 2.36 | 1.46 | 1.38 |
| 24 | C | 505 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 24 | b | 610 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 24 | c | 912 | CLA | C1D-C2D | 2.36 | 1.50 | 1.45 |
| 24 | b | 614 | CLA | C3B-C2B | 2.36 | 1.49 | 1.41 |
| 24 | b | 617 | CLA | C3B-C2B | 2.35 | 1.49 | 1.41 |
| 24 | B | 615 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 24 | B | 612 | CLA | C4B-NB | -2.35 | 1.34 | 1.37 |
| 24 | B | 607 | CLA | C3B-C2B | 2.34 | 1.49 | 1.41 |
| 24 | a | 407 | CLA | C4C-C3C | 2.34 | 1.49 | 1.45 |
| 25 | A | 409 | PHO | C1D-ND | -2.34 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | b | 612 | CLA | C1C-C2C | 2.34 | 1.49 | 1.44 |
| 24 | C | 508 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 24 | B | 604 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 24 | c | 910 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 24 | C | 514 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 24 | b | 608 | CLA | C1B-NB | -2.32 | 1.34 | 1.37 |
| 24 | b | 617 | CLA | C3D-C4D | -2.32 | 1.39 | 1.44 |
| 24 | A | 406 | CLA | C3D-C4D | -2.32 | 1.39 | 1.44 |
| 24 | b | 615 | CLA | C3B-C2B | 2.32 | 1.49 | 1.41 |
| 24 | a | 407 | CLA | C1C-C2C | 2.32 | 1.49 | 1.44 |
| 24 | c | 907 | CLA | C4C-C3C | 2.31 | 1.49 | 1.45 |
| 38 | E | 103 | HEM | C1D-ND | -2.31 | 1.34 | 1.38 |
| 24 | C | 511 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 24 | b | 614 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 24 | c | 902 | CLA | C3B-C2B | 2.31 | 1.49 | 1.41 |
| 24 | C | 511 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 24 | b | 613 | CLA | C1B-C2B | 2.31 | 1.48 | 1.43 |
| 24 | B | 612 | CLA | C3B-C2B | 2.31 | 1.48 | 1.41 |
| 24 | C | 503 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 24 | B | 611 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 24 | D | 401 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 38 | E | 103 | HEM | C1C-C2C | -2.30 | 1.40 | 1.45 |
| 24 | A | 406 | CLA | C3B-C2B | 2.30 | 1.48 | 1.41 |
| 24 | C | 513 | CLA | C4B-NB | -2.30 | 1.34 | 1.37 |
| 24 | C | 512 | CLA | C1C-NC | -2.30 | 1.34 | 1.37 |
| 24 | C | 504 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 24 | C | 509 | CLA | C3B-C2B | 2.30 | 1.48 | 1.41 |
| 24 | b | 616 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 29 | A | 417 | LMT | O1'-C1' | 2.29 | 1.44 | 1.40 |
| 25 | a | 408 | PHO | C4B-NB | -2.29 | 1.34 | 1.38 |
| 24 | c | 912 | CLA | C3B-C2B | 2.29 | 1.48 | 1.41 |
| 24 | c | 909 | CLA | C1C-C2C | 2.29 | 1.49 | 1.44 |
| 24 | C | 507 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 24 | b | 606 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 24 | b | 605 | CLA | C4B-NB | -2.28 | 1.34 | 1.37 |
| 24 | B | 609 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 24 | B | 616 | CLA | C4B-NB | -2.28 | 1.34 | 1.37 |
| 24 | B | 605 | CLA | C4B-NB | -2.28 | 1.34 | 1.37 |
| 24 | c | 909 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 24 | b | 610 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 35 | d | 412 | HTG | C1-S1 | -2.28 | 1.76 | 1.80 |
| 24 | C | 512 | CLA | C1C-C2C | 2.27 | 1.49 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | C | 508 | CLA | C4C-C3C | 2.27 | 1.48 | 1.45 |
| 24 | b | 615 | CLA | C1C-C2C | 2.27 | 1.49 | 1.44 |
| 24 | b | 606 | CLA | C3B-C2B | 2.27 | 1.48 | 1.41 |
| 24 | b | 613 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 24 | c | 914 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 24 | B | 607 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 24 | a | 409 | CLA | C1C-C2C | 2.26 | 1.49 | 1.44 |
| 40 | v | 202 | HEC | C4B-NB | -2.26 | 1.35 | 1.39 |
| 24 | d | 401 | CLA | C1D-C2D | 2.26 | 1.49 | 1.45 |
| 24 | B | 613 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 24 | c | 914 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 31 | a | 417 | PL9 | C2-C3 | 2.25 | 1.40 | 1.34 |
| 24 | c | 914 | CLA | C1D-C2D | 2.25 | 1.49 | 1.45 |
| 24 | A | 410 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 24 | c | 910 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 24 | b | 607 | CLA | C3B-C2B | 2.25 | 1.48 | 1.41 |
| 24 | A | 405 | CLA | C1C-C2C | 2.25 | 1.49 | 1.44 |
| 24 | C | 507 | CLA | C3B-C2B | 2.25 | 1.48 | 1.41 |
| 24 | B | 602 | CLA | C4C-C3C | 2.25 | 1.48 | 1.45 |
| 24 | B | 605 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 24 | A | 405 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 24 | b | 611 | CLA | C4C-C3C | 2.24 | 1.48 | 1.45 |
| 24 | b | 605 | CLA | C1C-C2C | 2.24 | 1.49 | 1.44 |
| 24 | c | 905 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 24 | A | 407 | CLA | C1C-C2C | 2.23 | 1.49 | 1.44 |
| 24 | B | 612 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 23 | a | 419 | BCT | O1-C | 2.23 | 1.33 | 1.25 |
| 24 | b | 616 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 24 | C | 512 | CLA | C3B-C2B | 2.23 | 1.48 | 1.41 |
| 24 | B | 603 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 24 | B | 611 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 24 | B | 616 | CLA | C1C-C2C | 2.22 | 1.49 | 1.44 |
| 24 | B | 606 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 31 | D | 404 | PL9 | C2-C3 | 2.22 | 1.40 | 1.34 |
| 24 | C | 512 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 24 | c | 907 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 24 | B | 608 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 24 | A | 410 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 24 | A | 407 | CLA | C4B-NB | -2.22 | 1.34 | 1.37 |
| 24 | C | 504 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 34 | b | 624 | LMG | O7-C8 | -2.21 | 1.41 | 1.46 |
| 24 | C | 504 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 616 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 25 | A | 409 | PHO | C4B-NB | -2.21 | 1.34 | 1.38 |
| 24 | b | 613 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 24 | c | 911 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 40 | V | 201 | HEC | C4A-C3A | -2.21 | 1.41 | 1.45 |
| 24 | A | 407 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 24 | D | 401 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 24 | a | 406 | CLA | C1C-C2C | 2.20 | 1.49 | 1.44 |
| 24 | b | 612 | CLA | C3B-C2B | 2.20 | 1.48 | 1.41 |
| 24 | C | 513 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 24 | b | 606 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 24 | c | 912 | CLA | C3D-C4D | -2.20 | 1.39 | 1.44 |
| 24 | C | 502 | CLA | C3D-C4D | -2.19 | 1.39 | 1.44 |
| 40 | V | 201 | HEC | C4D-ND | -2.19 | 1.35 | 1.39 |
| 24 | b | 614 | CLA | C3D-C4D | -2.19 | 1.39 | 1.44 |
| 24 | d | 401 | CLA | C3D-C4D | -2.19 | 1.39 | 1.44 |
| 24 | B | 616 | CLA | C4C-C3C | 2.19 | 1.48 | 1.45 |
| 24 | C | 507 | CLA | C1C-C2C | 2.19 | 1.49 | 1.44 |
| 24 | C | 513 | CLA | C3B-C2B | 2.19 | 1.48 | 1.41 |
| 24 | c | 903 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 24 | B | 609 | CLA | C1C-NC | -2.19 | 1.34 | 1.37 |
| 24 | b | 611 | CLA | C3B-C2B | 2.19 | 1.48 | 1.41 |
| 24 | D | 401 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 24 | a | 409 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 24 | B | 617 | CLA | C1C-NC | -2.18 | 1.34 | 1.37 |
| 24 | d | 402 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 24 | c | 911 | CLA | C3B-C2B | 2.17 | 1.48 | 1.41 |
| 25 | a | 420 | PHO | CHA-CBD | -2.17 | 1.49 | 1.51 |
| 24 | b | 609 | CLA | C4B-NB | -2.17 | 1.35 | 1.37 |
| 24 | b | 608 | CLA | C3B-C4B | 2.16 | 1.49 | 1.42 |
| 24 | b | 618 | CLA | C3B-C4B | 2.16 | 1.49 | 1.42 |
| 40 | v | 202 | HEC | C1D-C2D | 2.16 | 1.48 | 1.43 |
| 31 | A | 419 | PL9 | C2-C3 | 2.16 | 1.40 | 1.34 |
| 24 | b | 615 | CLA | C3B-C4B | 2.16 | 1.49 | 1.42 |
| 36 | C | 517 | DGD | O5D-C1E | 2.16 | 1.43 | 1.40 |
| 24 | b | 620 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 36 | C | 519 | DGD | O2G-C2G | -2.16 | 1.41 | 1.46 |
| 24 | C | 505 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 24 | c | 912 | CLA | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 24 | C | 509 | CLA | C3D-C4D | -2.15 | 1.39 | 1.44 |
| 24 | b | 610 | CLA | C3B-C2B | 2.15 | 1.48 | 1.41 |
| 25 | a | 420 | PHO | C4B-NB | -2.15 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 23 | A | 404 | BCT | O1-C | 2.15 | 1.33 | 1.25 |
| 26 | a | 410 | BCR | C12-C13 | 2.15 | 1.50 | 1.46 |
| 24 | d | 402 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 24 | C | 514 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 38 | e | 102 | HEM | C3C-C4C | -2.14 | 1.42 | 1.46 |
| 24 | B | 611 | CLA | C1C-NC | -2.14 | 1.34 | 1.37 |
| 24 | c | 905 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 24 | A | 405 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 24 | B | 602 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 24 | c | 908 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 24 | b | 605 | CLA | C3B-C2B | 2.13 | 1.48 | 1.41 |
| 31 | d | 405 | PL9 | C2-C3 | 2.13 | 1.40 | 1.34 |
| 24 | B | 609 | CLA | C3B-C4B | 2.13 | 1.49 | 1.42 |
| 24 | B | 608 | CLA | C3B-C4B | 2.13 | 1.48 | 1.42 |
| 24 | b | 617 | CLA | C1C-NC | -2.13 | 1.34 | 1.37 |
| 38 | e | 102 | HEM | C3B-C4B | 2.12 | 1.49 | 1.44 |
| 24 | a | 406 | CLA | C3D-C4D | -2.12 | 1.39 | 1.44 |
| 24 | b | 613 | CLA | C4B-NB | -2.12 | 1.35 | 1.37 |
| 24 | c | 914 | CLA | C3B-C2B | 2.12 | 1.48 | 1.41 |
| 24 | c | 907 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 24 | d | 401 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 24 | b | 605 | CLA | C3D-C4D | -2.12 | 1.39 | 1.44 |
| 24 | B | 608 | CLA | C3D-C4D | -2.11 | 1.39 | 1.44 |
| 24 | c | 909 | CLA | C3B-C4B | 2.11 | 1.48 | 1.42 |
| 24 | c | 910 | CLA | C3B-C4B | 2.11 | 1.48 | 1.42 |
| 24 | C | 505 | CLA | C3D-C4D | -2.11 | 1.39 | 1.44 |
| 35 | V | 202 | HTG | C1-S1 | -2.11 | 1.77 | 1.80 |
| 24 | c | 904 | CLA | C3B-C2B | 2.11 | 1.48 | 1.41 |
| 24 | B | 613 | CLA | C4C-C3C | 2.10 | 1.48 | 1.45 |
| 36 | d | 406 | DGD | O5D-C1E | 2.10 | 1.43 | 1.40 |
| 24 | B | 602 | CLA | C3D-C4D | -2.10 | 1.39 | 1.44 |
| 24 | b | 609 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 24 | c | 908 | CLA | C3D-C4D | -2.10 | 1.39 | 1.44 |
| 24 | C | 506 | CLA | C3B-C2B | 2.09 | 1.48 | 1.41 |
| 24 | C | 503 | CLA | C3B-C2B | 2.09 | 1.48 | 1.41 |
| 24 | C | 508 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 24 | a | 407 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 24 | d | 403 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 24 | D | 402 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 29 | f | 103 | LMT | O1'-C1' | 2.08 | 1.43 | 1.40 |
| 24 | B | 610 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 24 | b | 618 | CLA | C3B-C2B | 2.07 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | b | 625 | LMT | O1'-C1' | 2.07 | 1.43 | 1.40 |
| 24 | b | 611 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 24 | B | 616 | CLA | C3B-C2B | 2.07 | 1.48 | 1.41 |
| 35 | b | 602 | HTG | C1-S1 | -2.07 | 1.77 | 1.80 |
| 36 | H | 102 | DGD | O2G-C2G | -2.06 | 1.41 | 1.46 |
| 24 | a | 409 | CLA | C3B-C4B | 2.06 | 1.48 | 1.42 |
| 24 | c | 912 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 24 | B | 608 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 35 | D | 411 | HTG | C1-S1 | -2.06 | 1.77 | 1.80 |
| 24 | b | 611 | CLA | C3B-C4B | 2.06 | 1.48 | 1.42 |
| 24 | B | 615 | CLA | C1C-NC | -2.05 | 1.34 | 1.37 |
| 24 | b | 620 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 34 | c | 919 | LMG | O1-C1 | 2.05 | 1.43 | 1.40 |
| 24 | b | 619 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 40 | V | 201 | HEC | C3B-C4B | 2.05 | 1.49 | 1.46 |
| 24 | B | 616 | CLA | C1C-NC | -2.05 | 1.34 | 1.37 |
| 24 | B | 612 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 24 | a | 409 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 24 | B | 604 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 24 | B | 613 | CLA | C3B-C4B | 2.04 | 1.48 | 1.42 |
| 24 | c | 903 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 24 | d | 401 | CLA | C3B-C2B | 2.03 | 1.48 | 1.41 |
| 24 | C | 509 | CLA | C3B-C4B | 2.03 | 1.48 | 1.42 |
| 35 | b | 603 | HTG | C1-S1 | -2.03 | 1.77 | 1.80 |
| 24 | b | 606 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 24 | B | 610 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 24 | c | 904 | CLA | C3B-C4B | 2.03 | 1.48 | 1.42 |
| 24 | b | 620 | CLA | C3B-C4B | 2.02 | 1.48 | 1.42 |
| 25 | a | 408 | PHO | CHA-CBD | -2.02 | 1.49 | 1.51 |
| 25 | A | 408 | PHO | C4B-NB | -2.02 | 1.35 | 1.38 |
| 24 | c | 906 | CLA | C3B-C4B | 2.02 | 1.48 | 1.42 |
| 24 | B | 606 | CLA | C3B-C2B | 2.01 | 1.48 | 1.41 |
| 24 | c | 913 | CLA | C3B-C2B | 2.01 | 1.48 | 1.41 |
| 24 | b | 620 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 24 | B | 615 | CLA | C3B-C2B | 2.01 | 1.48 | 1.41 |
| 36 | D | 405 | DGD | O5D-C1E | 2.01 | 1.43 | 1.40 |
| 35 | C | 523 | HTG | C1-S1 | -2.01 | 1.77 | 1.80 |
| 24 | A | 410 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 24 | b | 610 | CLA | C4C-C3C | 2.00 | 1.48 | 1.45 |
| 24 | D | 402 | CLA | C4B-NB | -2.00 | 1.35 | 1.37 |

All (2794) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | a | 408 | PHO | C2D-C1D-ND | 12.30 | 118.32 | 109.43 |
| 25 | A | 408 | PHO | C2D-C1D-ND | 11.57 | 117.79 | 109.43 |
| 25 | A | 409 | PHO | C2D-C1D-ND | 11.06 | 117.42 | 109.43 |
| 25 | a | 420 | PHO | C2D-C1D-ND | 10.97 | 117.36 | 109.43 |
| 24 | B | 612 | CLA | C1D-ND-C4D | -10.09 | 99.23 | 106.31 |
| 24 | C | 505 | CLA | C1D-ND-C4D | -10.06 | 99.26 | 106.31 |
| 25 | A | 408 | PHO | O2D-CGD-CBD | 10.01 | 121.95 | 110.95 |
| 24 | B | 615 | CLA | C1D-ND-C4D | -9.95 | 99.33 | 106.31 |
| 24 | c | 914 | CLA | C1D-ND-C4D | -9.93 | 99.34 | 106.31 |
| 24 | C | 504 | CLA | C1D-ND-C4D | -9.82 | 99.43 | 106.31 |
| 24 | A | 406 | CLA | C1D-ND-C4D | -9.68 | 99.52 | 106.31 |
| 24 | b | 609 | CLA | C1D-ND-C4D | -9.67 | 99.53 | 106.31 |
| 24 | b | 618 | CLA | C1D-ND-C4D | -9.65 | 99.54 | 106.31 |
| 24 | B | 603 | CLA | C1D-ND-C4D | -9.65 | 99.54 | 106.31 |
| 24 | B | 605 | CLA | C1D-ND-C4D | -9.64 | 99.55 | 106.31 |
| 24 | B | 610 | CLA | C1D-ND-C4D | -9.60 | 99.57 | 106.31 |
| 24 | A | 407 | CLA | C1D-ND-C4D | -9.59 | 99.58 | 106.31 |
| 24 | c | 913 | CLA | C1D-ND-C4D | -9.57 | 99.60 | 106.31 |
| 24 | b | 611 | CLA | C1D-ND-C4D | -9.51 | 99.64 | 106.31 |
| 24 | C | 514 | CLA | C1D-ND-C4D | -9.49 | 99.65 | 106.31 |
| 24 | B | 602 | CLA | C1D-ND-C4D | -9.46 | 99.67 | 106.31 |
| 24 | D | 402 | CLA | C1D-ND-C4D | -9.45 | 99.68 | 106.31 |
| 24 | d | 402 | CLA | C1D-ND-C4D | -9.44 | 99.69 | 106.31 |
| 24 | B | 604 | CLA | C1D-ND-C4D | -9.43 | 99.70 | 106.31 |
| 24 | b | 615 | CLA | C1D-ND-C4D | -9.41 | 99.71 | 106.31 |
| 24 | b | 616 | CLA | C1D-ND-C4D | -9.39 | 99.72 | 106.31 |
| 24 | b | 613 | CLA | C1D-ND-C4D | -9.39 | 99.72 | 106.31 |
| 25 | a | 420 | PHO | O2D-CGD-CBD | 9.30 | 121.16 | 110.95 |
| 24 | a | 406 | CLA | C1D-ND-C4D | -9.29 | 99.79 | 106.31 |
| 24 | c | 909 | CLA | C1D-ND-C4D | -9.19 | 99.86 | 106.31 |
| 24 | B | 614 | CLA | C1D-ND-C4D | -9.18 | 99.87 | 106.31 |
| 24 | b | 605 | CLA | C1D-ND-C4D | -9.17 | 99.88 | 106.31 |
| 24 | C | 513 | CLA | C1D-ND-C4D | -9.14 | 99.90 | 106.31 |
| 24 | A | 410 | CLA | C1D-ND-C4D | -9.11 | 99.92 | 106.31 |
| 24 | c | 912 | CLA | C1D-ND-C4D | -9.10 | 99.92 | 106.31 |
| 24 | c | 910 | CLA | C1D-ND-C4D | -9.09 | 99.94 | 106.31 |
| 24 | d | 403 | CLA | C1D-ND-C4D | -9.08 | 99.94 | 106.31 |
| 24 | C | 502 | CLA | C1D-ND-C4D | -9.04 | 99.97 | 106.31 |
| 24 | C | 509 | CLA | C1D-ND-C4D | -8.99 | 100.01 | 106.31 |
| 24 | C | 512 | CLA | C1D-ND-C4D | -8.95 | 100.03 | 106.31 |
| 24 | B | 617 | CLA | C1D-ND-C4D | -8.94 | 100.04 | 106.31 |
| 24 | d | 401 | CLA | C1D-ND-C4D | -8.93 | 100.05 | 106.31 |
| 24 | b | 606 | CLA | C1D-ND-C4D | -8.91 | 100.06 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 609 | CLA | C1D-ND-C4D | -8.89 | 100.07 | 106.31 |
| 24 | A | 405 | CLA | C1D-ND-C4D | -8.89 | 100.08 | 106.31 |
| 24 | c | 902 | CLA | C1D-ND-C4D | -8.88 | 100.08 | 106.31 |
| 24 | c | 905 | CLA | C1D-ND-C4D | -8.86 | 100.09 | 106.31 |
| 24 | a | 407 | CLA | C1D-ND-C4D | -8.82 | 100.13 | 106.31 |
| 24 | c | 903 | CLA | C1D-ND-C4D | -8.77 | 100.16 | 106.31 |
| 24 | b | 610 | CLA | C1D-ND-C4D | -8.65 | 100.24 | 106.31 |
| 24 | b | 614 | CLA | C1D-ND-C4D | -8.64 | 100.25 | 106.31 |
| 24 | c | 906 | CLA | C1D-ND-C4D | -8.63 | 100.25 | 106.31 |
| 24 | c | 904 | CLA | C1D-ND-C4D | -8.63 | 100.26 | 106.31 |
| 24 | c | 911 | CLA | C1D-ND-C4D | -8.61 | 100.27 | 106.31 |
| 24 | B | 616 | CLA | C1D-ND-C4D | -8.60 | 100.28 | 106.31 |
| 24 | C | 510 | CLA | C1D-ND-C4D | -8.60 | 100.28 | 106.31 |
| 24 | D | 401 | CLA | C1D-ND-C4D | -8.59 | 100.28 | 106.31 |
| 24 | B | 606 | CLA | C1D-ND-C4D | -8.54 | 100.32 | 106.31 |
| 24 | B | 608 | CLA | C1D-ND-C4D | -8.50 | 100.35 | 106.31 |
| 24 | b | 620 | CLA | C1D-ND-C4D | -8.49 | 100.35 | 106.31 |
| 24 | C | 507 | CLA | C1D-ND-C4D | -8.49 | 100.36 | 106.31 |
| 24 | b | 612 | CLA | C1D-ND-C4D | -8.39 | 100.42 | 106.31 |
| 24 | c | 908 | CLA | C1D-ND-C4D | -8.35 | 100.45 | 106.31 |
| 24 | C | 506 | CLA | C1D-ND-C4D | -8.34 | 100.46 | 106.31 |
| 24 | b | 617 | CLA | C1D-ND-C4D | -8.31 | 100.48 | 106.31 |
| 24 | B | 607 | CLA | C1D-ND-C4D | -8.27 | 100.51 | 106.31 |
| 24 | C | 511 | CLA | C1D-ND-C4D | -8.25 | 100.53 | 106.31 |
| 24 | C | 503 | CLA | C1D-ND-C4D | -8.23 | 100.54 | 106.31 |
| 24 | C | 508 | CLA | C1D-ND-C4D | -8.21 | 100.55 | 106.31 |
| 24 | b | 607 | CLA | C1D-ND-C4D | -8.15 | 100.60 | 106.31 |
| 24 | B | 613 | CLA | C1D-ND-C4D | -8.11 | 100.62 | 106.31 |
| 24 | b | 619 | CLA | C1D-ND-C4D | -8.03 | 100.68 | 106.31 |
| 24 | a | 409 | CLA | C1D-ND-C4D | -7.98 | 100.71 | 106.31 |
| 24 | b | 608 | CLA | C1D-ND-C4D | -7.88 | 100.78 | 106.31 |
| 25 | a | 408 | PHO | O2D-CGD-CBD | 7.83 | 119.55 | 110.95 |
| 25 | A | 408 | PHO | C3B-C4B-NB | 7.82 | 112.56 | 107.46 |
| 24 | c | 907 | CLA | C1D-ND-C4D | -7.78 | 100.85 | 106.31 |
| 24 | B | 611 | CLA | C1D-ND-C4D | -7.76 | 100.86 | 106.31 |
| 24 | B | 607 | CLA | C4A-NA-C1A | -7.61 | 103.21 | 106.68 |
| 25 | A | 409 | PHO | C3B-C4B-NB | 7.60 | 112.42 | 107.46 |
| 25 | a | 408 | PHO | C3B-C4B-NB | 7.55 | 112.38 | 107.46 |
| 24 | B | 607 | CLA | CMD-C2D-C1D | 7.36 | 137.68 | 124.73 |
| 24 | d | 402 | CLA | C4A-NA-C1A | -7.35 | 103.33 | 106.68 |
| 24 | b | 613 | CLA | C4A-NA-C1A | -7.12 | 103.43 | 106.68 |
| 24 | b | 611 | CLA | CMD-C2D-C1D | 7.07 | 137.18 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 908 | CLA | O2D-CGD-CBD | 7.04 | 123.54 | 111.23 |
| 24 | C | 506 | CLA | CMD-C2D-C1D | 7.02 | 137.09 | 124.73 |
| 24 | a | 407 | CLA | CMD-C2D-C1D | 6.99 | 137.04 | 124.73 |
| 24 | A | 406 | CLA | C2D-C1D-ND | 6.95 | 117.00 | 110.13 |
| 25 | A | 409 | PHO | O2D-CGD-CBD | 6.94 | 118.58 | 110.95 |
| 24 | B | 616 | CLA | C4A-NA-C1A | -6.93 | 103.52 | 106.68 |
| 24 | C | 510 | CLA | CMD-C2D-C1D | 6.92 | 136.91 | 124.73 |
| 24 | B | 615 | CLA | CMD-C2D-C1D | 6.91 | 136.89 | 124.73 |
| 27 | F | 101 | SQD | O6-C1-C2 | 6.86 | 118.69 | 108.27 |
| 24 | A | 405 | CLA | C4A-NA-C1A | -6.78 | 103.59 | 106.68 |
| 24 | c | 914 | CLA | CMD-C2D-C1D | 6.74 | 136.60 | 124.73 |
| 24 | b | 609 | CLA | CHD-C4C-C3C | -6.73 | 114.96 | 124.77 |
| 24 | b | 618 | CLA | CMD-C2D-C1D | 6.69 | 136.52 | 124.73 |
| 24 | b | 611 | CLA | CHD-C4C-C3C | -6.68 | 115.04 | 124.77 |
| 24 | C | 502 | CLA | CMD-C2D-C1D | 6.67 | 136.48 | 124.73 |
| 24 | C | 513 | CLA | CHD-C4C-C3C | -6.65 | 115.08 | 124.77 |
| 25 | a | 420 | PHO | C3B-C4B-NB | 6.64 | 111.79 | 107.46 |
| 24 | B | 615 | CLA | CHD-C4C-C3C | -6.62 | 115.12 | 124.77 |
| 24 | C | 509 | CLA | C4A-NA-C1A | -6.60 | 103.67 | 106.68 |
| 24 | b | 607 | CLA | CMD-C2D-C1D | 6.59 | 136.34 | 124.73 |
| 24 | C | 512 | CLA | CMD-C2D-C1D | 6.59 | 136.34 | 124.73 |
| 24 | C | 505 | CLA | C2D-C1D-ND | 6.57 | 116.63 | 110.13 |
| 24 | b | 607 | CLA | C4A-NA-C1A | -6.57 | 103.68 | 106.68 |
| 24 | C | 513 | CLA | C2D-C1D-ND | 6.55 | 116.61 | 110.13 |
| 24 | B | 611 | CLA | CMD-C2D-C1D | 6.52 | 136.21 | 124.73 |
| 24 | b | 612 | CLA | CMD-C2D-C1D | 6.51 | 136.19 | 124.73 |
| 24 | c | 913 | CLA | C2D-C1D-ND | 6.51 | 116.57 | 110.13 |
| 24 | B | 615 | CLA | C2D-C1D-ND | 6.49 | 116.55 | 110.13 |
| 24 | B | 617 | CLA | CHD-C4C-C3C | -6.48 | 115.32 | 124.77 |
| 24 | d | 403 | CLA | CMD-C2D-C1D | 6.48 | 136.14 | 124.73 |
| 24 | d | 401 | CLA | CMD-C2D-C1D | 6.45 | 136.09 | 124.73 |
| 24 | b | 609 | CLA | C2D-C1D-ND | 6.44 | 116.50 | 110.13 |
| 24 | b | 615 | CLA | C2D-C1D-ND | 6.43 | 116.49 | 110.13 |
| 24 | B | 617 | CLA | O2D-CGD-CBD | 6.42 | 122.46 | 111.23 |
| 24 | C | 505 | CLA | CMD-C2D-C1D | 6.42 | 136.04 | 124.73 |
| 24 | c | 907 | CLA | CMD-C2D-C1D | 6.42 | 136.03 | 124.73 |
| 24 | B | 612 | CLA | C2D-C1D-ND | 6.42 | 116.48 | 110.13 |
| 24 | b | 605 | CLA | CHD-C4C-C3C | -6.41 | 115.43 | 124.77 |
| 24 | b | 608 | CLA | CMD-C2D-C1D | 6.41 | 136.01 | 124.73 |
| 24 | C | 507 | CLA | CMD-C2D-C1D | 6.39 | 135.98 | 124.73 |
| 24 | B | 614 | CLA | C2D-C1D-ND | 6.36 | 116.42 | 110.13 |
| 24 | c | 905 | CLA | CMD-C2D-C1D | 6.36 | 135.92 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 615 | CLA | CMD-C2D-C1D | 6.35 | 135.91 | 124.73 |
| 24 | b | 615 | CLA | CHD-C4C-C3C | -6.35 | 115.51 | 124.77 |
| 24 | B | 603 | CLA | C2D-C1D-ND | 6.35 | 116.41 | 110.13 |
| 24 | a | 406 | CLA | CMD-C2D-C1D | 6.33 | 135.88 | 124.73 |
| 24 | b | 610 | CLA | C4A-NA-C1A | -6.33 | 103.79 | 106.68 |
| 24 | B | 604 | CLA | CHD-C4C-C3C | -6.33 | 115.55 | 124.77 |
| 24 | B | 605 | CLA | CHD-C4C-C3C | -6.30 | 115.58 | 124.77 |
| 24 | B | 603 | CLA | CHD-C4C-C3C | -6.29 | 115.59 | 124.77 |
| 24 | b | 610 | CLA | CMD-C2D-C1D | 6.29 | 135.81 | 124.73 |
| 24 | D | 402 | CLA | C2D-C1D-ND | 6.29 | 116.35 | 110.13 |
| 24 | b | 610 | CLA | O2D-CGD-CBD | 6.28 | 122.21 | 111.23 |
| 24 | b | 606 | CLA | CHD-C4C-C3C | -6.27 | 115.62 | 124.77 |
| 24 | C | 506 | CLA | C4A-NA-C1A | -6.27 | 103.82 | 106.68 |
| 24 | D | 402 | CLA | CMD-C2D-C1D | 6.27 | 135.76 | 124.73 |
| 24 | c | 912 | CLA | CMD-C2D-C1D | 6.27 | 135.76 | 124.73 |
| 24 | b | 611 | CLA | C2D-C1D-ND | 6.26 | 116.32 | 110.13 |
| 24 | c | 903 | CLA | CMD-C2D-C1D | 6.26 | 135.75 | 124.73 |
| 24 | a | 407 | CLA | C4A-NA-C1A | -6.25 | 103.83 | 106.68 |
| 24 | A | 405 | CLA | CMD-C2D-C1D | 6.25 | 135.73 | 124.73 |
| 24 | B | 610 | CLA | CHD-C4C-C3C | -6.24 | 115.68 | 124.77 |
| 24 | B | 604 | CLA | CMD-C2D-C1D | 6.23 | 135.70 | 124.73 |
| 24 | C | 509 | CLA | O2D-CGD-CBD | 6.22 | 122.11 | 111.23 |
| 24 | b | 618 | CLA | CHD-C4C-C3C | -6.22 | 115.71 | 124.77 |
| 24 | B | 614 | CLA | CMD-C2D-C1D | 6.21 | 135.67 | 124.73 |
| 24 | b | 609 | CLA | CMD-C2D-C1D | 6.21 | 135.66 | 124.73 |
| 24 | b | 605 | CLA | CMD-C2D-C1D | 6.20 | 135.66 | 124.73 |
| 24 | c | 906 | CLA | CMD-C2D-C1D | 6.20 | 135.65 | 124.73 |
| 24 | c | 904 | CLA | CMD-C2D-C1D | 6.20 | 135.65 | 124.73 |
| 24 | B | 610 | CLA | C2D-C1D-ND | 6.19 | 116.26 | 110.13 |
| 24 | B | 616 | CLA | CHD-C4C-C3C | -6.18 | 115.76 | 124.77 |
| 24 | a | 409 | CLA | CHD-C4C-C3C | -6.18 | 115.76 | 124.77 |
| 24 | b | 616 | CLA | C2D-C1D-ND | 6.18 | 116.24 | 110.13 |
| 24 | B | 605 | CLA | C2D-C1D-ND | 6.18 | 116.24 | 110.13 |
| 24 | c | 905 | CLA | C2D-C1D-ND | 6.17 | 116.23 | 110.13 |
| 24 | b | 618 | CLA | C2D-C1D-ND | 6.16 | 116.22 | 110.13 |
| 24 | c | 904 | CLA | C4A-NA-C1A | -6.15 | 103.87 | 106.68 |
| 24 | d | 402 | CLA | C2D-C1D-ND | 6.15 | 116.21 | 110.13 |
| 24 | b | 620 | CLA | C2D-C1D-ND | 6.15 | 116.21 | 110.13 |
| 24 | C | 504 | CLA | CMD-C2D-C1D | 6.15 | 135.55 | 124.73 |
| 24 | C | 514 | CLA | C2D-C1D-ND | 6.15 | 116.21 | 110.13 |
| 24 | C | 504 | CLA | C2D-C1D-ND | 6.14 | 116.21 | 110.13 |
| 24 | b | 614 | CLA | CMD-C2D-C1D | 6.14 | 135.54 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | a | 408 | PHO | C4D-ND-C1D | -6.14 | 101.52 | 108.87 |
| 24 | A | 410 | CLA | C2D-C1D-ND | 6.13 | 116.19 | 110.13 |
| 24 | D | 401 | CLA | CMD-C2D-C1D | 6.13 | 135.53 | 124.73 |
| 24 | B | 617 | CLA | C2D-C1D-ND | 6.13 | 116.19 | 110.13 |
| 24 | b | 608 | CLA | O2D-CGD-CBD | 6.13 | 121.94 | 111.23 |
| 24 | A | 410 | CLA | CHD-C4C-C3C | -6.11 | 115.87 | 124.77 |
| 24 | c | 908 | CLA | C2D-C1D-ND | 6.10 | 116.17 | 110.13 |
| 24 | c | 909 | CLA | C2D-C1D-ND | 6.10 | 116.17 | 110.13 |
| 24 | b | 606 | CLA | CMD-C2D-C1D | 6.10 | 135.47 | 124.73 |
| 24 | A | 406 | CLA | CHD-C4C-C3C | -6.10 | 115.88 | 124.77 |
| 25 | A | 409 | PHO | C2B-C1B-NB | 6.10 | 113.84 | 109.43 |
| 24 | B | 602 | CLA | C2D-C1D-ND | 6.09 | 116.15 | 110.13 |
| 24 | B | 606 | CLA | C2C-C1C-NC | 6.08 | 116.37 | 109.98 |
| 24 | b | 613 | CLA | CMD-C2D-C1D | 6.08 | 135.44 | 124.73 |
| 24 | c | 902 | CLA | C2D-C1D-ND | 6.08 | 116.14 | 110.13 |
| 24 | b | 618 | CLA | O2D-CGD-CBD | 6.07 | 121.85 | 111.23 |
| 24 | b | 619 | CLA | C4A-NA-C1A | -6.06 | 103.91 | 106.68 |
| 24 | B | 612 | CLA | CMD-C2D-C1D | 6.06 | 135.40 | 124.73 |
| 24 | c | 902 | CLA | CMD-C2D-C1D | 6.05 | 135.39 | 124.73 |
| 24 | d | 402 | CLA | CMD-C2D-C1D | 6.05 | 135.38 | 124.73 |
| 24 | B | 608 | CLA | C2D-C1D-ND | 6.05 | 116.11 | 110.13 |
| 24 | c | 913 | CLA | CHD-C4C-C3C | -6.05 | 115.95 | 124.77 |
| 24 | c | 908 | CLA | CMD-C2D-C1D | 6.04 | 135.37 | 124.73 |
| 24 | B | 613 | CLA | O2D-CGD-CBD | 6.04 | 121.79 | 111.23 |
| 24 | C | 508 | CLA | CHD-C4C-C3C | -6.04 | 115.96 | 124.77 |
| 24 | b | 617 | CLA | CMD-C2D-C1D | 6.03 | 135.35 | 124.73 |
| 24 | B | 616 | CLA | C2D-C1D-ND | 6.03 | 116.09 | 110.13 |
| 24 | b | 616 | CLA | CHD-C4C-C3C | -6.01 | 116.00 | 124.77 |
| 24 | A | 410 | CLA | CMD-C2D-C1D | 6.01 | 135.32 | 124.73 |
| 24 | C | 514 | CLA | CMD-C2D-C1D | 6.00 | 135.29 | 124.73 |
| 24 | c | 903 | CLA | CHD-C4C-C3C | -6.00 | 116.03 | 124.77 |
| 24 | a | 407 | CLA | CHD-C4C-C3C | -5.98 | 116.05 | 124.77 |
| 24 | b | 607 | CLA | O2D-CGD-CBD | 5.98 | 121.68 | 111.23 |
| 24 | b | 613 | CLA | CHD-C4C-C3C | -5.97 | 116.07 | 124.77 |
| 24 | B | 603 | CLA | CMD-C2D-C1D | 5.97 | 135.24 | 124.73 |
| 24 | C | 511 | CLA | O2D-CGD-CBD | 5.95 | 121.63 | 111.23 |
| 24 | C | 511 | CLA | CHD-C4C-C3C | -5.95 | 116.10 | 124.77 |
| 24 | B | 609 | CLA | C4A-NA-C1A | -5.95 | 103.97 | 106.68 |
| 25 | A | 408 | PHO | C4D-ND-C1D | -5.95 | 101.75 | 108.87 |
| 24 | C | 505 | CLA | O2D-CGD-CBD | 5.94 | 121.62 | 111.23 |
| 24 | C | 504 | CLA | C4A-NA-C1A | -5.93 | 103.97 | 106.68 |
| 24 | b | 617 | CLA | CHD-C4C-C3C | -5.93 | 116.13 | 124.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 910 | CLA | CMD-C2D-C1D | 5.92 | 135.16 | 124.73 |
| 24 | c | 902 | CLA | CHD-C4C-C3C | -5.91 | 116.15 | 124.77 |
| 24 | d | 403 | CLA | CHD-C4C-C3C | -5.90 | 116.17 | 124.77 |
| 24 | B | 605 | CLA | CMD-C2D-C1D | 5.90 | 135.12 | 124.73 |
| 24 | C | 512 | CLA | CHD-C4C-C3C | -5.90 | 116.17 | 124.77 |
| 24 | c | 910 | CLA | C2D-C1D-ND | 5.90 | 115.96 | 110.13 |
| 24 | b | 610 | CLA | C2D-C1D-ND | 5.89 | 115.96 | 110.13 |
| 24 | b | 606 | CLA | C2D-C1D-ND | 5.89 | 115.95 | 110.13 |
| 24 | A | 407 | CLA | C2D-C1D-ND | 5.88 | 115.94 | 110.13 |
| 24 | c | 911 | CLA | CHD-C4C-C3C | -5.88 | 116.20 | 124.77 |
| 24 | b | 610 | CLA | CHD-C4C-C3C | -5.87 | 116.22 | 124.77 |
| 24 | D | 401 | CLA | C4A-NA-C1A | -5.86 | 104.00 | 106.68 |
| 24 | C | 504 | CLA | CHD-C4C-C3C | -5.86 | 116.22 | 124.77 |
| 24 | c | 905 | CLA | O2D-CGD-CBD | 5.86 | 121.48 | 111.23 |
| 24 | A | 405 | CLA | C2D-C1D-ND | 5.86 | 115.92 | 110.13 |
| 24 | D | 402 | CLA | CHD-C4C-C3C | -5.86 | 116.23 | 124.77 |
| 24 | d | 403 | CLA | C2D-C1D-ND | 5.85 | 115.92 | 110.13 |
| 24 | c | 906 | CLA | O2D-CGD-CBD | 5.85 | 121.46 | 111.23 |
| 24 | c | 912 | CLA | CHD-C4C-C3C | -5.85 | 116.24 | 124.77 |
| 24 | C | 506 | CLA | O2D-CGD-CBD | 5.85 | 121.45 | 111.23 |
| 24 | c | 914 | CLA | C2D-C1D-ND | 5.85 | 115.91 | 110.13 |
| 25 | A | 409 | PHO | C4D-ND-C1D | -5.84 | 101.87 | 108.87 |
| 24 | B | 607 | CLA | C2C-C1C-NC | 5.84 | 116.12 | 109.98 |
| 24 | b | 617 | CLA | C2D-C1D-ND | 5.84 | 115.91 | 110.13 |
| 24 | b | 613 | CLA | C2D-C1D-ND | 5.84 | 115.91 | 110.13 |
| 24 | c | 910 | CLA | CHD-C4C-C3C | -5.84 | 116.27 | 124.77 |
| 24 | A | 407 | CLA | C4A-NA-C1A | -5.83 | 104.02 | 106.68 |
| 24 | B | 602 | CLA | CMD-C2D-C1D | 5.83 | 134.99 | 124.73 |
| 24 | A | 407 | CLA | CHD-C4C-C3C | -5.82 | 116.29 | 124.77 |
| 24 | C | 502 | CLA | C2D-C1D-ND | 5.82 | 115.88 | 110.13 |
| 24 | B | 606 | CLA | CHD-C4C-C3C | -5.81 | 116.30 | 124.77 |
| 24 | b | 616 | CLA | CMD-C2D-C1D | 5.81 | 134.97 | 124.73 |
| 24 | B | 604 | CLA | C2D-C1D-ND | 5.79 | 115.86 | 110.13 |
| 24 | B | 608 | CLA | CMD-C2D-C1D | 5.78 | 134.91 | 124.73 |
| 24 | B | 616 | CLA | CMD-C2D-C1D | 5.78 | 134.91 | 124.73 |
| 24 | C | 508 | CLA | CMD-C2D-C1D | 5.77 | 134.89 | 124.73 |
| 24 | B | 608 | CLA | C4A-NA-C1A | -5.77 | 104.05 | 106.68 |
| 24 | b | 620 | CLA | CHD-C4C-C3C | -5.77 | 116.36 | 124.77 |
| 24 | C | 512 | CLA | C2D-C1D-ND | 5.77 | 115.83 | 110.13 |
| 24 | b | 612 | CLA | C4A-NA-C1A | -5.76 | 104.05 | 106.68 |
| 24 | C | 509 | CLA | C2D-C1D-ND | 5.76 | 115.83 | 110.13 |
| 24 | B | 606 | CLA | C2D-C1D-ND | 5.76 | 115.83 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | D | 401 | CLA | C2C-C1C-NC | 5.76 | 116.03 | 109.98 |
| 24 | c | 904 | CLA | CHD-C4C-C3C | -5.75 | 116.39 | 124.77 |
| 25 | A | 408 | PHO | C2B-C1B-NB | 5.75 | 113.59 | 109.43 |
| 24 | B | 602 | CLA | O2D-CGD-CBD | 5.73 | 121.24 | 111.23 |
| 24 | C | 502 | CLA | O2D-CGD-CBD | 5.73 | 121.24 | 111.23 |
| 24 | a | 406 | CLA | C2C-C1C-NC | 5.73 | 116.00 | 109.98 |
| 24 | A | 406 | CLA | CMD-C2D-C1D | 5.71 | 134.79 | 124.73 |
| 24 | c | 906 | CLA | C2C-C1C-NC | 5.71 | 115.98 | 109.98 |
| 24 | B | 612 | CLA | CHD-C4C-C3C | -5.70 | 116.46 | 124.77 |
| 24 | C | 503 | CLA | CHD-C4C-C3C | -5.70 | 116.46 | 124.77 |
| 24 | c | 908 | CLA | CHD-C4C-C3C | -5.70 | 116.46 | 124.77 |
| 24 | b | 612 | CLA | CHD-C4C-C3C | -5.70 | 116.46 | 124.77 |
| 24 | b | 605 | CLA | C2D-C1D-ND | 5.69 | 115.76 | 110.13 |
| 24 | B | 602 | CLA | CHD-C4C-C3C | -5.68 | 116.50 | 124.77 |
| 24 | b | 619 | CLA | C2D-C1D-ND | 5.68 | 115.74 | 110.13 |
| 24 | c | 913 | CLA | CMD-C2D-C1D | 5.67 | 134.72 | 124.73 |
| 24 | C | 509 | CLA | CHD-C4C-C3C | -5.67 | 116.50 | 124.77 |
| 24 | b | 617 | CLA | C2C-C1C-NC | 5.67 | 115.94 | 109.98 |
| 24 | B | 609 | CLA | C2C-C1C-NC | 5.67 | 115.94 | 109.98 |
| 24 | c | 903 | CLA | C2D-C1D-ND | 5.66 | 115.73 | 110.13 |
| 24 | B | 613 | CLA | C4A-NA-C1A | -5.65 | 104.10 | 106.68 |
| 24 | b | 620 | CLA | C4A-NA-C1A | -5.65 | 104.10 | 106.68 |
| 24 | A | 405 | CLA | CHD-C4C-C3C | -5.64 | 116.54 | 124.77 |
| 24 | C | 503 | CLA | C2D-C1D-ND | 5.64 | 115.71 | 110.13 |
| 24 | C | 510 | CLA | C2D-C1D-ND | 5.64 | 115.71 | 110.13 |
| 24 | c | 910 | CLA | O2D-CGD-CBD | 5.64 | 121.09 | 111.23 |
| 24 | A | 407 | CLA | CMD-C2D-C1D | 5.64 | 134.66 | 124.73 |
| 24 | B | 609 | CLA | C2D-C1D-ND | 5.64 | 115.70 | 110.13 |
| 24 | B | 610 | CLA | C4A-NA-C1A | -5.62 | 104.11 | 106.68 |
| 24 | d | 401 | CLA | C2C-C1C-NC | 5.62 | 115.89 | 109.98 |
| 24 | d | 403 | CLA | C2C-C1C-NC | 5.62 | 115.88 | 109.98 |
| 24 | B | 611 | CLA | CHD-C4C-C3C | -5.61 | 116.59 | 124.77 |
| 24 | c | 902 | CLA | O2D-CGD-CBD | 5.61 | 121.03 | 111.23 |
| 24 | C | 508 | CLA | O2D-CGD-CBD | 5.61 | 121.03 | 111.23 |
| 24 | b | 616 | CLA | O2D-CGD-CBD | 5.60 | 121.03 | 111.23 |
| 24 | B | 610 | CLA | CMD-C2D-C1D | 5.60 | 134.59 | 124.73 |
| 24 | c | 914 | CLA | CHD-C4C-C3C | -5.60 | 116.61 | 124.77 |
| 24 | B | 617 | CLA | CMD-C2D-C1D | 5.59 | 134.58 | 124.73 |
| 24 | C | 514 | CLA | CHD-C4C-C3C | -5.59 | 116.62 | 124.77 |
| 25 | A | 409 | PHO | C3D-C4D-ND | 5.58 | 114.86 | 107.71 |
| 24 | C | 507 | CLA | C2C-C1C-NC | 5.57 | 115.83 | 109.98 |
| 24 | c | 905 | CLA | CHD-C4C-C3C | -5.57 | 116.65 | 124.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A | 405 | CLA | C2C-C1C-NC | 5.56 | 115.83 | 109.98 |
| 24 | B | 603 | CLA | C4A-NA-C1A | -5.56 | 104.14 | 106.68 |
| 24 | D | 401 | CLA | C2D-C1D-ND | 5.56 | 115.63 | 110.13 |
| 24 | c | 904 | CLA | C2D-C1D-ND | 5.56 | 115.63 | 110.13 |
| 24 | B | 614 | CLA | CHD-C4C-C3C | -5.56 | 116.67 | 124.77 |
| 24 | C | 509 | CLA | C2C-C1C-NC | 5.55 | 115.81 | 109.98 |
| 24 | b | 614 | CLA | C2D-C1D-ND | 5.54 | 115.61 | 110.13 |
| 24 | B | 608 | CLA | C2C-C1C-NC | 5.54 | 115.80 | 109.98 |
| 24 | d | 401 | CLA | C2D-C1D-ND | 5.54 | 115.61 | 110.13 |
| 24 | b | 614 | CLA | CHD-C4C-C3C | -5.53 | 116.71 | 124.77 |
| 35 | B | 626 | HTG | C1'-S1-C1 | 5.53 | 112.39 | 100.45 |
| 24 | a | 407 | CLA | C2D-C1D-ND | 5.53 | 115.60 | 110.13 |
| 24 | b | 606 | CLA | O2D-CGD-CBD | 5.53 | 120.89 | 111.23 |
| 24 | C | 502 | CLA | CHD-C4C-C3C | -5.53 | 116.72 | 124.77 |
| 24 | B | 614 | CLA | C4A-NA-C1A | -5.52 | 104.16 | 106.68 |
| 24 | c | 908 | CLA | C2C-C1C-NC | 5.52 | 115.78 | 109.98 |
| 24 | d | 402 | CLA | C2C-C1C-NC | 5.50 | 115.76 | 109.98 |
| 24 | C | 506 | CLA | CHD-C4C-C3C | -5.50 | 116.75 | 124.77 |
| 27 | a | 411 | SQD | O6-C1-C2 | 5.50 | 116.62 | 108.27 |
| 24 | b | 619 | CLA | C2C-C1C-NC | 5.50 | 115.76 | 109.98 |
| 24 | C | 511 | CLA | CMD-C2D-C1D | 5.50 | 134.41 | 124.73 |
| 24 | B | 609 | CLA | CHD-C4C-C3C | -5.49 | 116.77 | 124.77 |
| 24 | B | 613 | CLA | CHD-C4C-C3C | -5.49 | 116.77 | 124.77 |
| 24 | B | 611 | CLA | C4A-NA-C1A | -5.48 | 104.18 | 106.68 |
| 24 | c | 906 | CLA | CHD-C4C-C3C | -5.48 | 116.79 | 124.77 |
| 24 | c | 909 | CLA | CHD-C4C-C3C | -5.46 | 116.81 | 124.77 |
| 24 | B | 607 | CLA | O2D-CGD-CBD | 5.46 | 120.77 | 111.23 |
| 24 | C | 508 | CLA | C2D-C1D-ND | 5.46 | 115.53 | 110.13 |
| 24 | c | 911 | CLA | CMD-C2D-C1D | 5.45 | 134.33 | 124.73 |
| 25 | a | 420 | PHO | C4D-ND-C1D | -5.45 | 102.34 | 108.87 |
| 38 | E | 103 | HEM | CHC-C4B-NB | 5.45 | 130.29 | 124.42 |
| 24 | b | 605 | CLA | O2D-CGD-CBD | 5.45 | 120.76 | 111.23 |
| 24 | c | 907 | CLA | C2C-C1C-NC | 5.44 | 115.70 | 109.98 |
| 24 | a | 406 | CLA | C2D-C1D-ND | 5.44 | 115.51 | 110.13 |
| 24 | A | 406 | CLA | C3D-C2D-C1D | -5.43 | 98.42 | 105.83 |
| 24 | c | 907 | CLA | CHD-C4C-C3C | -5.43 | 116.86 | 124.77 |
| 24 | C | 511 | CLA | C4A-NA-C1A | -5.42 | 104.21 | 106.68 |
| 24 | c | 907 | CLA | C2D-C1D-ND | 5.42 | 115.49 | 110.13 |
| 24 | C | 510 | CLA | CHD-C4C-C3C | -5.42 | 116.88 | 124.77 |
| 24 | B | 604 | CLA | O2D-CGD-CBD | 5.41 | 120.70 | 111.23 |
| 27 | A | 412 | SQD | O6-C1-C2 | 5.41 | 116.49 | 108.27 |
| 24 | c | 903 | CLA | O2D-CGD-CBD | 5.40 | 120.68 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 615 | CLA | O2D-CGD-CBD | 5.40 | 120.67 | 111.23 |
| 24 | b | 609 | CLA | O2D-CGD-CBD | 5.40 | 120.67 | 111.23 |
| 24 | b | 620 | CLA | O2D-CGD-CBD | 5.39 | 120.66 | 111.23 |
| 24 | b | 608 | CLA | C2C-C1C-NC | 5.39 | 115.64 | 109.98 |
| 24 | B | 611 | CLA | C2D-C1D-ND | 5.39 | 115.46 | 110.13 |
| 24 | d | 401 | CLA | CHD-C4C-C3C | -5.38 | 116.93 | 124.77 |
| 24 | b | 606 | CLA | C4A-NA-C1A | -5.37 | 104.23 | 106.68 |
| 24 | C | 507 | CLA | C2D-C1D-ND | 5.36 | 115.44 | 110.13 |
| 24 | a | 409 | CLA | C2D-C1D-ND | 5.36 | 115.43 | 110.13 |
| 24 | B | 613 | CLA | C2D-C1D-ND | 5.36 | 115.43 | 110.13 |
| 24 | C | 512 | CLA | C2C-C1C-NC | 5.34 | 115.59 | 109.98 |
| 27 | a | 411 | SQD | O47-C7-C8 | 5.34 | 123.03 | 111.48 |
| 24 | b | 614 | CLA | C2C-C1C-NC | 5.34 | 115.59 | 109.98 |
| 24 | b | 611 | CLA | C2C-C1C-NC | 5.34 | 115.59 | 109.98 |
| 24 | c | 903 | CLA | C4A-NA-C1A | -5.32 | 104.25 | 106.68 |
| 24 | b | 616 | CLA | C4A-NA-C1A | -5.32 | 104.25 | 106.68 |
| 24 | C | 513 | CLA | CMD-C2D-C1D | 5.32 | 134.10 | 124.73 |
| 24 | d | 402 | CLA | CHD-C4C-C3C | -5.32 | 117.02 | 124.77 |
| 25 | a | 408 | PHO | C2B-C1B-NB | 5.32 | 113.27 | 109.43 |
| 25 | a | 408 | PHO | C3D-C4D-ND | 5.31 | 114.52 | 107.71 |
| 24 | c | 913 | CLA | O2D-CGD-CBD | 5.31 | 120.51 | 111.23 |
| 24 | a | 407 | CLA | O2D-CGD-CBD | 5.30 | 120.49 | 111.23 |
| 25 | a | 420 | PHO | C2B-C1B-NB | 5.30 | 113.26 | 109.43 |
| 24 | b | 615 | CLA | C2C-C1C-NC | 5.29 | 115.54 | 109.98 |
| 24 | B | 603 | CLA | O2D-CGD-CBD | 5.28 | 120.46 | 111.23 |
| 24 | b | 618 | CLA | C4A-NA-C1A | -5.28 | 104.27 | 106.68 |
| 24 | c | 912 | CLA | C4A-NA-C1A | -5.28 | 104.27 | 106.68 |
| 24 | C | 510 | CLA | O2D-CGD-CBD | 5.28 | 120.46 | 111.23 |
| 24 | B | 607 | CLA | CHD-C4C-C3C | -5.27 | 117.09 | 124.77 |
| 24 | c | 912 | CLA | C3B-C2B-C1B | -5.27 | 100.96 | 107.17 |
| 24 | C | 505 | CLA | CHD-C4C-C3C | -5.26 | 117.10 | 124.77 |
| 24 | a | 409 | CLA | C3B-C2B-C1B | -5.26 | 100.97 | 107.17 |
| 24 | C | 510 | CLA | C2C-C1C-NC | 5.26 | 115.50 | 109.98 |
| 24 | A | 406 | CLA | C2B-C1B-NB | 5.26 | 115.78 | 110.33 |
| 24 | c | 902 | CLA | C2C-C1C-NC | 5.26 | 115.50 | 109.98 |
| 24 | B | 607 | CLA | C2D-C1D-ND | 5.24 | 115.31 | 110.13 |
| 24 | B | 602 | CLA | C2B-C1B-NB | 5.24 | 115.76 | 110.33 |
| 24 | c | 904 | CLA | C2C-C1C-NC | 5.23 | 115.48 | 109.98 |
| 24 | C | 513 | CLA | O2D-CGD-CBD | 5.23 | 120.37 | 111.23 |
| 24 | C | 502 | CLA | C2C-C1C-NC | 5.21 | 115.45 | 109.98 |
| 24 | b | 614 | CLA | C4A-NA-C1A | -5.20 | 104.31 | 106.68 |
| 24 | C | 506 | CLA | C2C-C1C-NC | 5.19 | 115.44 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 913 | CLA | C4A-NA-C1A | -5.18 | 104.32 | 106.68 |
| 24 | A | 410 | CLA | C3B-C2B-C1B | -5.18 | 101.06 | 107.17 |
| 24 | b | 608 | CLA | CHD-C4C-C3C | -5.18 | 117.22 | 124.77 |
| 24 | B | 611 | CLA | C2C-C1C-NC | 5.18 | 115.42 | 109.98 |
| 27 | f | 102 | SQD | O47-C7-C8 | 5.17 | 122.67 | 111.48 |
| 24 | C | 511 | CLA | C2D-C1D-ND | 5.17 | 115.24 | 110.13 |
| 24 | C | 514 | CLA | C3B-C2B-C1B | -5.17 | 101.08 | 107.17 |
| 24 | c | 912 | CLA | C2D-C1D-ND | 5.17 | 115.24 | 110.13 |
| 24 | a | 409 | CLA | CMD-C2D-C1D | 5.16 | 133.82 | 124.73 |
| 24 | B | 614 | CLA | C2C-C1C-NC | 5.16 | 115.41 | 109.98 |
| 24 | C | 508 | CLA | C3B-C2B-C1B | -5.16 | 101.09 | 107.17 |
| 25 | A | 408 | PHO | C3D-C4D-ND | 5.15 | 114.31 | 107.71 |
| 24 | c | 909 | CLA | C2C-C1C-NC | 5.14 | 115.38 | 109.98 |
| 24 | B | 615 | CLA | C4A-NA-C1A | -5.14 | 104.33 | 106.68 |
| 24 | B | 615 | CLA | C2C-C1C-NC | 5.13 | 115.37 | 109.98 |
| 24 | A | 406 | CLA | C3B-C2B-C1B | -5.13 | 101.12 | 107.17 |
| 27 | A | 412 | SQD | O47-C7-C8 | 5.12 | 122.56 | 111.48 |
| 24 | c | 909 | CLA | CMD-C2D-C1D | 5.11 | 133.73 | 124.73 |
| 24 | C | 508 | CLA | C2C-C1C-NC | 5.11 | 115.35 | 109.98 |
| 24 | b | 607 | CLA | CHD-C4C-C3C | -5.11 | 117.32 | 124.77 |
| 24 | a | 407 | CLA | C3B-C2B-C1B | -5.11 | 101.15 | 107.17 |
| 24 | c | 911 | CLA | C2D-C1D-ND | 5.11 | 115.18 | 110.13 |
| 24 | b | 620 | CLA | CMD-C2D-C1D | 5.10 | 133.72 | 124.73 |
| 24 | C | 505 | CLA | C4A-NA-C1A | -5.10 | 104.35 | 106.68 |
| 26 | K | 103 | BCR | C7-C8-C9 | -5.09 | 118.70 | 126.23 |
| 24 | C | 513 | CLA | C3B-C2B-C1B | -5.09 | 101.17 | 107.17 |
| 24 | B | 612 | CLA | C4A-NA-C1A | -5.09 | 104.36 | 106.68 |
| 24 | b | 615 | CLA | C3D-C2D-C1D | -5.09 | 98.89 | 105.83 |
| 24 | B | 605 | CLA | C2C-C1C-NC | 5.09 | 115.32 | 109.98 |
| 24 | b | 605 | CLA | C4A-NA-C1A | -5.08 | 104.36 | 106.68 |
| 24 | C | 504 | CLA | C2B-C1B-NB | 5.08 | 115.60 | 110.33 |
| 24 | B | 617 | CLA | C3B-C2B-C1B | -5.08 | 101.18 | 107.17 |
| 24 | c | 913 | CLA | C2B-C1B-NB | 5.08 | 115.59 | 110.33 |
| 24 | c | 909 | CLA | O2D-CGD-CBD | 5.08 | 120.11 | 111.23 |
| 24 | C | 507 | CLA | CHD-C4C-C3C | -5.08 | 117.37 | 124.77 |
| 36 | d | 406 | DGD | O6E-C5E-C4E | 5.08 | 118.85 | 109.70 |
| 24 | B | 613 | CLA | CMD-C2D-C1D | 5.08 | 133.67 | 124.73 |
| 24 | C | 504 | CLA | C3B-C2B-C1B | -5.08 | 101.19 | 107.17 |
| 24 | B | 609 | CLA | C2B-C1B-NB | 5.07 | 115.59 | 110.33 |
| 24 | C | 513 | CLA | C3D-C2D-C1D | -5.07 | 98.91 | 105.83 |
| 24 | B | 603 | CLA | C3B-C2B-C1B | -5.07 | 101.19 | 107.17 |
| 24 | b | 611 | CLA | O2D-CGD-CBD | 5.07 | 120.09 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 604 | CLA | C3B-C2B-C1B | -5.07 | 101.20 | 107.17 |
| 24 | B | 609 | CLA | C3B-C2B-C1B | -5.07 | 101.20 | 107.17 |
| 24 | D | 401 | CLA | O2D-CGD-CBD | 5.06 | 120.08 | 111.23 |
| 24 | a | 409 | CLA | C2C-C1C-NC | 5.06 | 115.30 | 109.98 |
| 24 | b | 609 | CLA | C3D-C2D-C1D | -5.06 | 98.92 | 105.83 |
| 25 | A | 409 | PHO | C1-C2-C3 | -5.05 | 117.92 | 126.20 |
| 24 | b | 609 | CLA | C4A-NA-C1A | -5.05 | 104.37 | 106.68 |
| 24 | b | 619 | CLA | CHD-C4C-C3C | -5.05 | 117.41 | 124.77 |
| 35 | B | 634 | HTG | C1'-S1-C1 | 5.04 | 111.33 | 100.45 |
| 24 | B | 606 | CLA | O2D-CGD-CBD | 5.04 | 120.03 | 111.23 |
| 24 | C | 513 | CLA | C4A-NA-C1A | -5.03 | 104.38 | 106.68 |
| 24 | b | 612 | CLA | C2D-C1D-ND | 5.03 | 115.11 | 110.13 |
| 27 | F | 101 | SQD | O47-C7-C8 | 5.03 | 122.37 | 111.48 |
| 24 | b | 615 | CLA | O2D-CGD-CBD | 5.03 | 120.03 | 111.23 |
| 24 | B | 602 | CLA | C3B-C2B-C1B | -5.03 | 101.24 | 107.17 |
| 24 | b | 619 | CLA | CMD-C2D-C1D | 5.03 | 133.58 | 124.73 |
| 24 | d | 401 | CLA | C3B-C4B-NB | 5.02 | 115.01 | 110.53 |
| 24 | c | 908 | CLA | C3D-C2D-C1D | -5.02 | 98.98 | 105.83 |
| 24 | B | 615 | CLA | C3D-C2D-C1D | -5.02 | 98.98 | 105.83 |
| 24 | B | 616 | CLA | C3D-C2D-C1D | -5.01 | 98.99 | 105.83 |
| 24 | B | 615 | CLA | C3B-C2B-C1B | -5.01 | 101.26 | 107.17 |
| 24 | C | 513 | CLA | C2B-C1B-NB | 5.01 | 115.52 | 110.33 |
| 24 | c | 905 | CLA | C3D-C2D-C1D | -5.00 | 99.01 | 105.83 |
| 24 | B | 609 | CLA | CMD-C2D-C1D | 4.99 | 133.52 | 124.73 |
| 24 | c | 906 | CLA | C2D-C1D-ND | 4.99 | 115.06 | 110.13 |
| 24 | b | 612 | CLA | C2C-C1C-NC | 4.99 | 115.22 | 109.98 |
| 24 | a | 407 | CLA | C2B-C1B-NB | 4.98 | 115.49 | 110.33 |
| 24 | B | 611 | CLA | C3D-C2D-C1D | -4.98 | 99.04 | 105.83 |
| 24 | C | 503 | CLA | C2C-C1C-NC | 4.98 | 115.21 | 109.98 |
| 24 | d | 402 | CLA | O2D-CGD-CBD | 4.98 | 119.93 | 111.23 |
| 40 | V | 201 | HEC | CBB-CAB-C3B | -4.98 | 117.49 | 127.43 |
| 24 | c | 913 | CLA | C3B-C2B-C1B | -4.97 | 101.31 | 107.17 |
| 24 | b | 610 | CLA | C3B-C2B-C1B | -4.97 | 101.31 | 107.17 |
| 27 | B | 621 | SQD | O6-C1-C2 | 4.97 | 115.82 | 108.27 |
| 24 | d | 403 | CLA | C3B-C2B-C1B | -4.97 | 101.31 | 107.17 |
| 24 | C | 503 | CLA | CMD-C2D-C1D | 4.97 | 133.47 | 124.73 |
| 24 | c | 908 | CLA | C3B-C2B-C1B | -4.96 | 101.32 | 107.17 |
| 24 | b | 617 | CLA | C3B-C2B-C1B | -4.96 | 101.32 | 107.17 |
| 24 | C | 503 | CLA | C3B-C2B-C1B | -4.96 | 101.33 | 107.17 |
| 24 | c | 903 | CLA | C3B-C2B-C1B | -4.96 | 101.33 | 107.17 |
| 24 | b | 607 | CLA | C2B-C1B-NB | 4.95 | 115.46 | 110.33 |
| 24 | D | 402 | CLA | C3D-C2D-C1D | -4.95 | 99.07 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 603 | CLA | C3D-C2D-C1D | -4.95 | 99.08 | 105.83 |
| 24 | b | 620 | CLA | C3D-C2D-C1D | -4.94 | 99.09 | 105.83 |
| 24 | c | 910 | CLA | C3B-C2B-C1B | -4.94 | 101.35 | 107.17 |
| 24 | b | 618 | CLA | C2C-C1C-NC | 4.94 | 115.17 | 109.98 |
| 24 | b | 619 | CLA | C3B-C4B-NB | 4.93 | 114.93 | 110.53 |
| 24 | B | 606 | CLA | C4A-NA-C1A | -4.93 | 104.43 | 106.68 |
| 24 | C | 512 | CLA | C3B-C2B-C1B | -4.93 | 101.36 | 107.17 |
| 24 | c | 905 | CLA | C2C-C1C-NC | 4.93 | 115.16 | 109.98 |
| 24 | b | 606 | CLA | C3B-C2B-C1B | -4.92 | 101.37 | 107.17 |
| 24 | b | 619 | CLA | C3B-C2B-C1B | -4.92 | 101.37 | 107.17 |
| 24 | B | 616 | CLA | C3B-C2B-C1B | -4.91 | 101.38 | 107.17 |
| 24 | b | 611 | CLA | C3C-C4C-NC | 4.91 | 116.72 | 110.43 |
| 24 | D | 401 | CLA | CHD-C4C-C3C | -4.91 | 117.62 | 124.77 |
| 24 | C | 508 | CLA | C4A-NA-C1A | -4.91 | 104.44 | 106.68 |
| 24 | c | 905 | CLA | C3B-C2B-C1B | -4.91 | 101.39 | 107.17 |
| 24 | C | 510 | CLA | C3B-C2B-C1B | -4.90 | 101.39 | 107.17 |
| 24 | B | 604 | CLA | C2B-C1B-NB | 4.90 | 115.41 | 110.33 |
| 24 | b | 620 | CLA | C2C-C1C-NC | 4.90 | 115.12 | 109.98 |
| 24 | B | 606 | CLA | CMD-C2D-C1D | 4.90 | 133.35 | 124.73 |
| 24 | B | 607 | CLA | C3B-C2B-C1B | -4.90 | 101.40 | 107.17 |
| 24 | b | 618 | CLA | C1-C2-C3 | -4.90 | 118.18 | 126.20 |
| 24 | C | 514 | CLA | O2D-CGD-CBD | 4.89 | 119.79 | 111.23 |
| 24 | C | 505 | CLA | C2C-C1C-NC | 4.89 | 115.12 | 109.98 |
| 24 | c | 914 | CLA | C3D-C4D-ND | 4.89 | 117.94 | 109.99 |
| 24 | B | 603 | CLA | C2C-C1C-NC | 4.88 | 115.11 | 109.98 |
| 24 | c | 910 | CLA | C4A-NA-C1A | -4.88 | 104.45 | 106.68 |
| 24 | c | 914 | CLA | C3B-C2B-C1B | -4.87 | 101.42 | 107.17 |
| 24 | C | 505 | CLA | C3D-C2D-C1D | -4.87 | 99.19 | 105.83 |
| 24 | A | 407 | CLA | C2B-C1B-NB | 4.87 | 115.38 | 110.33 |
| 24 | b | 611 | CLA | C3D-C2D-C1D | -4.87 | 99.19 | 105.83 |
| 24 | C | 514 | CLA | C3D-C2D-C1D | -4.87 | 99.19 | 105.83 |
| 24 | A | 406 | CLA | C2C-C1C-NC | 4.86 | 115.09 | 109.98 |
| 24 | C | 507 | CLA | C3B-C2B-C1B | -4.86 | 101.44 | 107.17 |
| 24 | b | 612 | CLA | C3B-C2B-C1B | -4.84 | 101.46 | 107.17 |
| 24 | d | 403 | CLA | C3D-C2D-C1D | -4.84 | 99.23 | 105.83 |
| 26 | D | 403 | BCR | C7-C8-C9 | -4.84 | 119.08 | 126.23 |
| 24 | B | 610 | CLA | CMB-C2B-C1B | 4.83 | 132.78 | 125.42 |
| 24 | b | 614 | CLA | O2D-CGD-CBD | 4.83 | 119.68 | 111.23 |
| 24 | b | 609 | CLA | C2C-C1C-NC | 4.83 | 115.05 | 109.98 |
| 24 | C | 506 | CLA | C3B-C2B-C1B | -4.83 | 101.48 | 107.17 |
| 24 | b | 608 | CLA | C2D-C1D-ND | 4.82 | 114.89 | 110.13 |
| 24 | b | 615 | CLA | C3B-C2B-C1B | -4.81 | 101.50 | 107.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 913 | CLA | C3D-C2D-C1D | -4.81 | 99.27 | 105.83 |
| 24 | C | 509 | CLA | C3D-C4D-ND | 4.81 | 117.80 | 109.99 |
| 35 | c | 923 | HTG | C1'-S1-C1 | 4.81 | 110.83 | 100.45 |
| 24 | C | 507 | CLA | O2D-CGD-CBD | 4.80 | 119.62 | 111.23 |
| 24 | B | 612 | CLA | C2C-C1C-NC | 4.80 | 115.02 | 109.98 |
| 24 | b | 607 | CLA | C2D-C1D-ND | 4.80 | 114.87 | 110.13 |
| 24 | a | 407 | CLA | C3D-C2D-C1D | -4.79 | 99.29 | 105.83 |
| 27 | B | 621 | SQD | O47-C7-C8 | 4.79 | 121.85 | 111.48 |
| 24 | A | 405 | CLA | C3B-C2B-C1B | -4.79 | 101.53 | 107.17 |
| 24 | B | 602 | CLA | C2C-C1C-NC | 4.79 | 115.01 | 109.98 |
| 24 | c | 907 | CLA | O2D-CGD-CBD | 4.79 | 119.60 | 111.23 |
| 24 | b | 615 | CLA | C4A-NA-C1A | -4.78 | 104.50 | 106.68 |
| 24 | b | 620 | CLA | C3B-C2B-C1B | -4.78 | 101.53 | 107.17 |
| 24 | c | 904 | CLA | C3B-C2B-C1B | -4.78 | 101.53 | 107.17 |
| 24 | c | 910 | CLA | C2C-C1C-NC | 4.78 | 115.00 | 109.98 |
| 24 | B | 608 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 24 | C | 510 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 24 | b | 606 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 24 | C | 514 | CLA | C2C-C1C-NC | 4.77 | 115.00 | 109.98 |
| 24 | C | 504 | CLA | C2C-C1C-NC | 4.77 | 114.99 | 109.98 |
| 24 | A | 410 | CLA | C2B-C1B-NB | 4.77 | 115.27 | 110.33 |
| 24 | B | 616 | CLA | C2B-C1B-NB | 4.77 | 115.27 | 110.33 |
| 24 | B | 604 | CLA | C4A-NA-C1A | -4.77 | 104.50 | 106.68 |
| 24 | b | 608 | CLA | C3B-C2B-C1B | -4.77 | 101.55 | 107.17 |
| 24 | b | 610 | CLA | C2B-C1B-NB | 4.76 | 115.27 | 110.33 |
| 24 | c | 903 | CLA | C2B-C1B-NB | 4.76 | 115.27 | 110.33 |
| 24 | B | 612 | CLA | C3B-C2B-C1B | -4.76 | 101.56 | 107.17 |
| 24 | c | 907 | CLA | C3D-C2D-C1D | -4.76 | 99.34 | 105.83 |
| 35 | b | 603 | HTG | C1'-S1-C1 | 4.75 | 110.71 | 100.45 |
| 24 | A | 407 | CLA | O2D-CGD-CBD | 4.75 | 119.53 | 111.23 |
| 24 | d | 401 | CLA | O2D-CGD-CBD | 4.74 | 119.52 | 111.23 |
| 24 | c | 902 | CLA | C3D-C2D-C1D | -4.74 | 99.36 | 105.83 |
| 24 | B | 606 | CLA | C3C-C4C-NC | 4.74 | 116.50 | 110.43 |
| 24 | a | 409 | CLA | O2D-CGD-CBD | 4.74 | 119.52 | 111.23 |
| 24 | d | 401 | CLA | C3D-C2D-C1D | -4.74 | 99.36 | 105.83 |
| 24 | c | 909 | CLA | C3D-C2D-C1D | -4.74 | 99.36 | 105.83 |
| 24 | C | 502 | CLA | C3B-C2B-C1B | -4.74 | 101.58 | 107.17 |
| 24 | b | 618 | CLA | C3D-C2D-C1D | -4.73 | 99.37 | 105.83 |
| 24 | b | 609 | CLA | C3B-C2B-C1B | -4.73 | 101.59 | 107.17 |
| 24 | A | 406 | CLA | O2D-CGD-CBD | 4.73 | 119.50 | 111.23 |
| 24 | A | 405 | CLA | C2B-C1B-NB | 4.73 | 115.23 | 110.33 |
| 24 | B | 612 | CLA | O2D-CGD-CBD | 4.73 | 119.49 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 504 | CLA | O2D-CGD-CBD | 4.73 | 119.49 | 111.23 |
| 24 | b | 610 | CLA | C3D-C2D-C1D | -4.72 | 99.38 | 105.83 |
| 27 | L | 102 | SQD | O6-C1-C2 | 4.72 | 115.44 | 108.27 |
| 24 | b | 605 | CLA | C2B-C1B-NB | 4.72 | 115.22 | 110.33 |
| 24 | A | 410 | CLA | C3D-C2D-C1D | -4.72 | 99.39 | 105.83 |
| 24 | A | 407 | CLA | C3D-C4D-ND | 4.72 | 117.66 | 109.99 |
| 24 | c | 914 | CLA | C2B-C1B-NB | 4.72 | 115.22 | 110.33 |
| 35 | b | 627 | HTG | C1-O5-C5 | 4.72 | 121.02 | 112.56 |
| 24 | B | 613 | CLA | C3B-C2B-C1B | -4.72 | 101.61 | 107.17 |
| 24 | d | 403 | CLA | C4A-NA-C1A | -4.71 | 104.53 | 106.68 |
| 24 | B | 614 | CLA | C3D-C2D-C1D | -4.71 | 99.40 | 105.83 |
| 24 | c | 911 | CLA | C2C-C1C-NC | 4.71 | 114.93 | 109.98 |
| 24 | c | 906 | CLA | C3B-C2B-C1B | -4.71 | 101.62 | 107.17 |
| 24 | B | 606 | CLA | C3B-C2B-C1B | -4.71 | 101.62 | 107.17 |
| 24 | c | 904 | CLA | C3D-C2D-C1D | -4.71 | 99.41 | 105.83 |
| 24 | C | 503 | CLA | C3D-C2D-C1D | -4.70 | 99.41 | 105.83 |
| 24 | a | 406 | CLA | C1C-C2C-C3C | -4.70 | 102.03 | 106.98 |
| 24 | c | 914 | CLA | CHD-C1D-ND | -4.70 | 118.19 | 124.80 |
| 24 | C | 512 | CLA | C3D-C2D-C1D | -4.70 | 99.42 | 105.83 |
| 24 | c | 904 | CLA | C2B-C1B-NB | 4.70 | 115.20 | 110.33 |
| 27 | A | 412 | SQD | C45-O47-C7 | -4.70 | 106.55 | 117.80 |
| 24 | a | 409 | CLA | C2B-C1B-NB | 4.70 | 115.20 | 110.33 |
| 26 | K | 102 | BCR | C33-C5-C6 | -4.69 | 119.36 | 124.48 |
| 24 | B | 612 | CLA | C3D-C2D-C1D | -4.69 | 99.43 | 105.83 |
| 24 | B | 603 | CLA | C2B-C1B-NB | 4.69 | 115.19 | 110.33 |
| 24 | c | 909 | CLA | C3B-C2B-C1B | -4.69 | 101.64 | 107.17 |
| 24 | B | 605 | CLA | O2D-CGD-CBD | 4.69 | 119.43 | 111.23 |
| 24 | b | 607 | CLA | C2C-C1C-NC | 4.69 | 114.91 | 109.98 |
| 24 | c | 911 | CLA | O2D-CGD-CBD | 4.69 | 119.42 | 111.23 |
| 29 | b | 601 | LMT | C1'-O5'-C5' | 4.68 | 122.87 | 113.72 |
| 24 | b | 612 | CLA | C2B-C1B-NB | 4.68 | 115.18 | 110.33 |
| 24 | B | 602 | CLA | C3D-C4D-ND | 4.68 | 117.59 | 109.99 |
| 24 | b | 606 | CLA | C2C-C1C-NC | 4.68 | 114.89 | 109.98 |
| 24 | B | 617 | CLA | C3D-C2D-C1D | -4.68 | 99.45 | 105.83 |
| 24 | C | 511 | CLA | C2C-C1C-NC | 4.67 | 114.88 | 109.98 |
| 24 | c | 902 | CLA | O2D-CGD-O1D | -4.67 | 114.77 | 123.85 |
| 24 | B | 616 | CLA | C2C-C1C-NC | 4.66 | 114.88 | 109.98 |
| 24 | C | 504 | CLA | C3D-C4D-ND | 4.65 | 117.55 | 109.99 |
| 24 | B | 613 | CLA | C2C-C1C-NC | 4.65 | 114.87 | 109.98 |
| 24 | b | 613 | CLA | O2D-CGD-CBD | 4.65 | 119.36 | 111.23 |
| 24 | b | 617 | CLA | C3D-C2D-C1D | -4.65 | 99.48 | 105.83 |
| 24 | C | 502 | CLA | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 610 | CLA | C2C-C1C-NC | 4.63 | 114.85 | 109.98 |
| 24 | c | 903 | CLA | C2C-C1C-NC | 4.63 | 114.85 | 109.98 |
| 24 | A | 406 | CLA | C1C-C2C-C3C | -4.63 | 102.11 | 106.98 |
| 24 | B | 604 | CLA | C2C-C1C-NC | 4.63 | 114.84 | 109.98 |
| 24 | B | 605 | CLA | C3B-C2B-C1B | -4.63 | 101.71 | 107.17 |
| 24 | B | 609 | CLA | C3D-C4D-ND | 4.63 | 117.51 | 109.99 |
| 24 | a | 406 | CLA | C3D-C4D-ND | 4.62 | 117.50 | 109.99 |
| 24 | B | 610 | CLA | C3D-C4D-ND | 4.62 | 117.50 | 109.99 |
| 27 | L | 102 | SQD | O47-C7-C8 | 4.62 | 121.47 | 111.48 |
| 24 | B | 615 | CLA | C1D-CHD-C4C | -4.62 | 116.21 | 126.02 |
| 24 | C | 507 | CLA | C3D-C2D-C1D | -4.61 | 99.53 | 105.83 |
| 24 | B | 602 | CLA | C3D-C2D-C1D | -4.61 | 99.55 | 105.83 |
| 24 | c | 912 | CLA | C3D-C4D-ND | 4.60 | 117.47 | 109.99 |
| 36 | D | 405 | DGD | O2G-C1B-C2B | 4.60 | 121.44 | 111.48 |
| 24 | B | 612 | CLA | C3D-C4D-ND | 4.60 | 117.47 | 109.99 |
| 24 | c | 905 | CLA | C2B-C1B-NB | 4.60 | 115.09 | 110.33 |
| 24 | C | 504 | CLA | C3D-C2D-C1D | -4.60 | 99.56 | 105.83 |
| 24 | C | 509 | CLA | CMD-C2D-C1D | 4.60 | 132.82 | 124.73 |
| 25 | A | 408 | PHO | C1A-C2A-C3A | -4.59 | 98.47 | 102.84 |
| 24 | D | 401 | CLA | C3D-C2D-C1D | -4.59 | 99.56 | 105.83 |
| 24 | c | 914 | CLA | C2C-C1C-NC | 4.59 | 114.80 | 109.98 |
| 24 | C | 511 | CLA | C3B-C2B-C1B | -4.59 | 101.76 | 107.17 |
| 24 | b | 605 | CLA | C3D-C4D-ND | 4.59 | 117.45 | 109.99 |
| 24 | B | 615 | CLA | C1C-C2C-C3C | -4.59 | 102.16 | 106.98 |
| 24 | B | 614 | CLA | C2B-C1B-NB | 4.58 | 115.08 | 110.33 |
| 24 | c | 912 | CLA | C2B-C1B-NB | 4.58 | 115.08 | 110.33 |
| 24 | C | 503 | CLA | C2B-C1B-NB | 4.58 | 115.08 | 110.33 |
| 24 | C | 503 | CLA | C4A-NA-C1A | -4.58 | 104.59 | 106.68 |
| 24 | b | 616 | CLA | C3B-C2B-C1B | -4.58 | 101.77 | 107.17 |
| 35 | b | 627 | HTG | O5-C1-C2 | 4.57 | 116.62 | 110.32 |
| 24 | b | 616 | CLA | C3C-C4C-NC | 4.57 | 116.29 | 110.43 |
| 26 | C | 516 | BCR | C7-C8-C9 | -4.57 | 119.47 | 126.23 |
| 24 | C | 507 | CLA | C1C-C2C-C3C | -4.57 | 102.17 | 106.98 |
| 24 | A | 407 | CLA | C3B-C2B-C1B | -4.57 | 101.78 | 107.17 |
| 24 | b | 609 | CLA | C2B-C1B-NB | 4.57 | 115.07 | 110.33 |
| 24 | B | 614 | CLA | C3B-C2B-C1B | -4.57 | 101.78 | 107.17 |
| 24 | c | 903 | CLA | C3D-C2D-C1D | -4.57 | 99.60 | 105.83 |
| 27 | L | 102 | SQD | O7-S-C6 | 4.57 | 113.57 | 106.76 |
| 26 | y | 101 | BCR | C33-C5-C6 | -4.56 | 119.50 | 124.48 |
| 24 | c | 910 | CLA | C2B-C1B-NB | 4.56 | 115.06 | 110.33 |
| 24 | b | 615 | CLA | C3C-C4C-NC | 4.56 | 116.27 | 110.43 |
| 24 | B | 608 | CLA | O2D-CGD-CBD | 4.56 | 119.20 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 502 | CLA | C4A-NA-C1A | -4.56 | 104.60 | 106.68 |
| 24 | c | 910 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 24 | b | 616 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 24 | D | 402 | CLA | C2C-C1C-NC | 4.55 | 114.76 | 109.98 |
| 24 | C | 505 | CLA | C3D-C4D-ND | 4.54 | 117.37 | 109.99 |
| 24 | B | 606 | CLA | C3D-C2D-C1D | -4.54 | 99.64 | 105.83 |
| 24 | C | 508 | CLA | C3D-C2D-C1D | -4.53 | 99.65 | 105.83 |
| 24 | B | 610 | CLA | C3D-C2D-C1D | -4.53 | 99.65 | 105.83 |
| 24 | c | 913 | CLA | C2C-C1C-NC | 4.53 | 114.74 | 109.98 |
| 24 | B | 604 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 24 | B | 607 | CLA | C1C-C2C-C3C | -4.52 | 102.22 | 106.98 |
| 24 | b | 606 | CLA | C3C-C4C-NC | 4.51 | 116.21 | 110.43 |
| 24 | C | 512 | CLA | C3B-C4B-NB | 4.51 | 114.56 | 110.53 |
| 24 | C | 509 | CLA | C3B-C2B-C1B | -4.51 | 101.85 | 107.17 |
| 24 | c | 906 | CLA | C3B-C4B-NB | 4.51 | 114.56 | 110.53 |
| 24 | b | 607 | CLA | C3B-C2B-C1B | -4.51 | 101.86 | 107.17 |
| 24 | a | 406 | CLA | CHD-C4C-C3C | -4.51 | 118.20 | 124.77 |
| 24 | c | 911 | CLA | C1-C2-C3 | -4.51 | 118.81 | 126.20 |
| 24 | B | 614 | CLA | C3B-C4B-NB | 4.51 | 114.55 | 110.53 |
| 24 | A | 407 | CLA | C3D-C2D-C1D | -4.50 | 99.68 | 105.83 |
| 24 | D | 402 | CLA | C3B-C2B-C1B | -4.50 | 101.87 | 107.17 |
| 24 | c | 911 | CLA | C4A-NA-C1A | -4.50 | 104.63 | 106.68 |
| 24 | C | 505 | CLA | CHD-C1D-ND | -4.50 | 118.47 | 124.80 |
| 24 | B | 610 | CLA | C2C-C1C-NC | 4.50 | 114.70 | 109.98 |
| 24 | c | 914 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 24 | d | 401 | CLA | C3B-C2B-C1B | -4.49 | 101.87 | 107.17 |
| 24 | A | 410 | CLA | C2C-C1C-NC | 4.49 | 114.70 | 109.98 |
| 24 | B | 605 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 24 | b | 606 | CLA | C2B-C1B-NB | 4.49 | 114.98 | 110.33 |
| 24 | d | 401 | CLA | C3D-C4D-ND | 4.49 | 117.29 | 109.99 |
| 24 | b | 618 | CLA | C3C-C4C-NC | 4.49 | 116.18 | 110.43 |
| 38 | e | 102 | HEM | CHC-C4B-NB | 4.49 | 129.25 | 124.42 |
| 26 | d | 404 | BCR | C28-C27-C26 | -4.49 | 106.05 | 114.06 |
| 24 | b | 618 | CLA | C3B-C2B-C1B | -4.49 | 101.88 | 107.17 |
| 24 | C | 502 | CLA | C2B-C1B-NB | 4.48 | 114.98 | 110.33 |
| 24 | C | 503 | CLA | C1-C2-C3 | -4.48 | 118.86 | 126.20 |
| 24 | B | 617 | CLA | C2C-C1C-NC | 4.48 | 114.69 | 109.98 |
| 24 | B | 609 | CLA | O2D-CGD-CBD | 4.48 | 119.06 | 111.23 |
| 24 | a | 409 | CLA | C1-C2-C3 | -4.47 | 118.87 | 126.20 |
| 31 | a | 417 | PL9 | C32-C33-C34 | -4.47 | 117.38 | 127.62 |
| 24 | d | 402 | CLA | C3B-C2B-C1B | -4.47 | 101.89 | 107.17 |
| 24 | c | 912 | CLA | C2C-C1C-NC | 4.47 | 114.68 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | d | 402 | CLA | C3D-C2D-C1D | -4.47 | 99.73 | 105.83 |
| 24 | d | 402 | CLA | C3D-C4D-ND | 4.47 | 117.26 | 109.99 |
| 34 | c | 920 | LMG | O7-C10-C11 | 4.47 | 121.15 | 111.48 |
| 25 | a | 420 | PHO | C3D-C4D-ND | 4.47 | 113.43 | 107.71 |
| 24 | B | 607 | CLA | C2B-C1B-NB | 4.46 | 114.96 | 110.33 |
| 24 | A | 405 | CLA | C3D-C2D-C1D | -4.46 | 99.74 | 105.83 |
| 24 | b | 605 | CLA | CHD-C1D-ND | -4.46 | 118.52 | 124.80 |
| 24 | B | 608 | CLA | CHD-C4C-C3C | -4.46 | 118.27 | 124.77 |
| 24 | b | 614 | CLA | C3D-C2D-C1D | -4.46 | 99.74 | 105.83 |
| 24 | c | 909 | CLA | C3D-C4D-ND | 4.46 | 117.23 | 109.99 |
| 24 | B | 611 | CLA | O2D-CGD-CBD | 4.46 | 119.02 | 111.23 |
| 24 | A | 405 | CLA | C3C-C4C-NC | 4.45 | 116.14 | 110.43 |
| 24 | b | 614 | CLA | C3B-C2B-C1B | -4.45 | 101.92 | 107.17 |
| 35 | b | 626 | HTG | C1'-S1-C1 | 4.45 | 110.06 | 100.45 |
| 24 | B | 617 | CLA | C1D-CHD-C4C | -4.45 | 116.56 | 126.02 |
| 24 | c | 909 | CLA | C2B-C1B-NB | 4.45 | 114.94 | 110.33 |
| 24 | C | 511 | CLA | C2B-C1B-NB | 4.45 | 114.94 | 110.33 |
| 24 | C | 514 | CLA | C3D-C4D-ND | 4.45 | 117.21 | 109.99 |
| 24 | d | 401 | CLA | C1C-C2C-C3C | -4.45 | 102.30 | 106.98 |
| 24 | C | 514 | CLA | C2B-C1B-NB | 4.45 | 114.94 | 110.33 |
| 24 | C | 506 | CLA | C2D-C1D-ND | 4.44 | 114.52 | 110.13 |
| 24 | D | 402 | CLA | C2B-C1B-NB | 4.43 | 114.92 | 110.33 |
| 24 | B | 609 | CLA | C1C-C2C-C3C | -4.43 | 102.32 | 106.98 |
| 24 | c | 904 | CLA | C1D-CHD-C4C | -4.43 | 116.61 | 126.02 |
| 24 | b | 619 | CLA | O2D-CGD-CBD | 4.43 | 118.97 | 111.23 |
| 24 | B | 605 | CLA | C1C-C2C-C3C | -4.42 | 102.33 | 106.98 |
| 24 | B | 604 | CLA | C3D-C4D-ND | 4.42 | 117.18 | 109.99 |
| 24 | b | 605 | CLA | C3B-C2B-C1B | -4.42 | 101.96 | 107.17 |
| 24 | a | 407 | CLA | C1D-CHD-C4C | -4.41 | 116.64 | 126.02 |
| 24 | b | 619 | CLA | C2B-C1B-NB | 4.41 | 114.90 | 110.33 |
| 29 | B | 623 | LMT | O1B-C4'-C3' | 4.41 | 118.44 | 107.23 |
| 24 | B | 607 | CLA | CHD-C1D-ND | -4.41 | 118.60 | 124.80 |
| 24 | C | 505 | CLA | C3B-C2B-C1B | -4.40 | 101.98 | 107.17 |
| 24 | b | 605 | CLA | C2C-C1C-NC | 4.40 | 114.61 | 109.98 |
| 24 | d | 403 | CLA | C2B-C1B-NB | 4.40 | 114.88 | 110.33 |
| 24 | a | 406 | CLA | C3B-C2B-C1B | -4.39 | 101.99 | 107.17 |
| 24 | c | 909 | CLA | C3B-C4B-NB | 4.39 | 114.45 | 110.53 |
| 24 | c | 906 | CLA | C2B-C1B-NB | 4.39 | 114.88 | 110.33 |
| 24 | B | 607 | CLA | C3D-C2D-C1D | -4.39 | 99.84 | 105.83 |
| 24 | B | 613 | CLA | C2B-C1B-NB | 4.39 | 114.88 | 110.33 |
| 24 | b | 613 | CLA | C3D-C2D-C1D | -4.39 | 99.85 | 105.83 |
| 26 | y | 101 | BCR | C15-C14-C13 | -4.38 | 121.13 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | z | 101 | LMG | C3-C4-C5 | 4.38 | 118.17 | 110.23 |
| 24 | b | 605 | CLA | C3D-C2D-C1D | -4.38 | 99.86 | 105.83 |
| 26 | t | 101 | BCR | C33-C5-C6 | -4.38 | 119.71 | 124.48 |
| 24 | b | 619 | CLA | C3D-C2D-C1D | -4.37 | 99.86 | 105.83 |
| 24 | b | 613 | CLA | C3D-C4D-ND | 4.37 | 117.09 | 109.99 |
| 24 | d | 403 | CLA | C3D-C4D-ND | 4.37 | 117.09 | 109.99 |
| 35 | C | 524 | HTG | C1-O5-C5 | 4.37 | 120.40 | 112.56 |
| 24 | C | 502 | CLA | C3D-C4D-ND | 4.37 | 117.09 | 109.99 |
| 25 | a | 420 | PHO | O2D-CGD-O1D | -4.37 | 115.35 | 123.85 |
| 24 | c | 913 | CLA | C3D-C4D-ND | 4.36 | 117.08 | 109.99 |
| 24 | D | 402 | CLA | C3D-C4D-ND | 4.36 | 117.08 | 109.99 |
| 24 | c | 907 | CLA | C4A-NA-C1A | -4.36 | 104.69 | 106.68 |
| 24 | A | 406 | CLA | C3B-C4B-NB | 4.35 | 114.42 | 110.53 |
| 24 | C | 506 | CLA | C3D-C4D-ND | 4.35 | 117.06 | 109.99 |
| 24 | A | 406 | CLA | C3D-C4D-ND | 4.35 | 117.06 | 109.99 |
| 35 | c | 922 | HTG | C1'-S1-C1 | 4.35 | 109.84 | 100.45 |
| 24 | B | 615 | CLA | C3D-C4D-ND | 4.35 | 117.05 | 109.99 |
| 24 | c | 911 | CLA | C3D-C4D-ND | 4.34 | 117.05 | 109.99 |
| 36 | d | 406 | DGD | O2G-C1B-C2B | 4.34 | 120.88 | 111.48 |
| 24 | a | 406 | CLA | C4A-NA-C1A | -4.34 | 104.70 | 106.68 |
| 24 | b | 611 | CLA | C3D-C4D-ND | 4.34 | 117.04 | 109.99 |
| 24 | B | 608 | CLA | C1C-C2C-C3C | -4.33 | 102.42 | 106.98 |
| 26 | D | 403 | BCR | C24-C23-C22 | -4.33 | 119.83 | 126.23 |
| 34 | C | 521 | LMG | O7-C10-C11 | 4.32 | 120.83 | 111.48 |
| 24 | b | 608 | CLA | C4A-NA-C1A | -4.32 | 104.71 | 106.68 |
| 24 | b | 616 | CLA | C2B-C1B-NB | 4.32 | 114.81 | 110.33 |
| 40 | v | 202 | HEC | CHC-C4B-NB | 4.32 | 129.15 | 124.45 |
| 24 | D | 401 | CLA | C3D-C4D-ND | 4.32 | 117.00 | 109.99 |
| 24 | B | 612 | CLA | C2B-C1B-NB | 4.31 | 114.80 | 110.33 |
| 24 | B | 603 | CLA | C3D-C4D-ND | 4.31 | 117.00 | 109.99 |
| 24 | B | 610 | CLA | O2D-CGD-CBD | 4.31 | 118.77 | 111.23 |
| 24 | B | 617 | CLA | C4A-NA-C1A | -4.31 | 104.71 | 106.68 |
| 24 | b | 617 | CLA | C3C-C4C-NC | 4.31 | 115.95 | 110.43 |
| 24 | b | 608 | CLA | C2B-C1B-NB | 4.31 | 114.79 | 110.33 |
| 24 | C | 513 | CLA | C2C-C1C-NC | 4.31 | 114.50 | 109.98 |
| 36 | c | 917 | DGD | O2G-C1B-C2B | 4.30 | 120.79 | 111.48 |
| 24 | c | 907 | CLA | C3B-C2B-C1B | -4.30 | 102.10 | 107.17 |
| 24 | C | 506 | CLA | C2B-C1B-NB | 4.30 | 114.79 | 110.33 |
| 24 | A | 410 | CLA | C3D-C4D-ND | 4.30 | 116.98 | 109.99 |
| 24 | b | 609 | CLA | C3C-C4C-NC | 4.30 | 115.94 | 110.43 |
| 24 | b | 612 | CLA | O2D-CGD-CBD | 4.30 | 118.74 | 111.23 |
| 24 | c | 905 | CLA | C3D-C4D-ND | 4.30 | 116.97 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 618 | CLA | O2D-CGD-O1D | -4.30 | 115.48 | 123.85 |
| 24 | B | 605 | CLA | C2B-C1B-NB | 4.29 | 114.78 | 110.33 |
| 24 | B | 615 | CLA | C2B-C1B-NB | 4.29 | 114.78 | 110.33 |
| 24 | C | 509 | CLA | C2B-C1B-NB | 4.29 | 114.77 | 110.33 |
| 24 | B | 613 | CLA | C3C-C4C-NC | 4.29 | 115.92 | 110.43 |
| 34 | C | 501 | LMG | O7-C10-C11 | 4.29 | 120.76 | 111.48 |
| 24 | B | 611 | CLA | C3B-C2B-C1B | -4.29 | 102.12 | 107.17 |
| 24 | A | 410 | CLA | CHD-C1D-ND | -4.28 | 118.77 | 124.80 |
| 24 | b | 610 | CLA | CHD-C1D-ND | -4.28 | 118.77 | 124.80 |
| 24 | B | 612 | CLA | CHD-C1D-ND | -4.28 | 118.78 | 124.80 |
| 24 | C | 504 | CLA | CHD-C1D-ND | -4.28 | 118.78 | 124.80 |
| 24 | b | 618 | CLA | C3D-C4D-ND | 4.28 | 116.94 | 109.99 |
| 24 | b | 614 | CLA | C3D-C4D-ND | 4.28 | 116.94 | 109.99 |
| 24 | d | 402 | CLA | C3C-C4C-NC | 4.28 | 115.91 | 110.43 |
| 24 | b | 620 | CLA | C2B-C1B-NB | 4.28 | 114.76 | 110.33 |
| 24 | D | 402 | CLA | CHD-C1D-ND | -4.27 | 118.79 | 124.80 |
| 24 | A | 410 | CLA | C4A-NA-C1A | -4.27 | 104.73 | 106.68 |
| 24 | D | 401 | CLA | C3B-C4B-NB | 4.27 | 114.34 | 110.53 |
| 24 | b | 618 | CLA | C2B-C1B-NB | 4.27 | 114.75 | 110.33 |
| 24 | D | 402 | CLA | O2D-CGD-CBD | 4.27 | 118.69 | 111.23 |
| 31 | A | 419 | PL9 | C27-C28-C29 | -4.27 | 117.86 | 127.62 |
| 24 | C | 505 | CLA | C2B-C1B-NB | 4.27 | 114.75 | 110.33 |
| 24 | c | 905 | CLA | CHD-C1D-ND | -4.27 | 118.80 | 124.80 |
| 24 | C | 503 | CLA | O2D-CGD-CBD | 4.27 | 118.69 | 111.23 |
| 24 | d | 401 | CLA | CHD-C1D-ND | -4.26 | 118.80 | 124.80 |
| 24 | a | 409 | CLA | C3D-C2D-C1D | -4.26 | 100.01 | 105.83 |
| 24 | b | 613 | CLA | C2C-C1C-NC | 4.26 | 114.46 | 109.98 |
| 24 | C | 509 | CLA | C1C-C2C-C3C | -4.26 | 102.50 | 106.98 |
| 24 | c | 914 | CLA | C4A-NA-C1A | -4.25 | 104.74 | 106.68 |
| 24 | C | 511 | CLA | C3D-C4D-ND | 4.25 | 116.89 | 109.99 |
| 24 | b | 608 | CLA | C1-C2-C3 | -4.25 | 119.24 | 126.20 |
| 31 | a | 417 | PL9 | C37-C38-C39 | -4.24 | 117.92 | 127.62 |
| 24 | b | 612 | CLA | C3D-C2D-C1D | -4.24 | 100.04 | 105.83 |
| 24 | B | 615 | CLA | CHD-C1D-ND | -4.24 | 118.83 | 124.80 |
| 24 | B | 603 | CLA | CHD-C1D-ND | -4.24 | 118.84 | 124.80 |
| 24 | B | 604 | CLA | C1D-CHD-C4C | -4.24 | 117.01 | 126.02 |
| 24 | B | 606 | CLA | C3D-C4D-ND | 4.24 | 116.87 | 109.99 |
| 24 | B | 613 | CLA | C3D-C4D-ND | 4.23 | 116.87 | 109.99 |
| 24 | c | 906 | CLA | C3C-C4C-NC | 4.23 | 115.85 | 110.43 |
| 24 | b | 614 | CLA | C2B-C1B-NB | 4.23 | 114.72 | 110.33 |
| 31 | a | 417 | PL9 | C15-C14-C16 | 4.23 | 122.57 | 115.23 |
| 24 | B | 602 | CLA | C4A-NA-C1A | -4.23 | 104.75 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 606 | CLA | C3D-C4D-ND | 4.23 | 116.86 | 109.99 |
| 24 | C | 510 | CLA | C1-C2-C3 | -4.23 | 119.27 | 126.20 |
| 24 | d | 401 | CLA | C4A-NA-C1A | -4.22 | 104.75 | 106.68 |
| 31 | A | 419 | PL9 | C37-C38-C39 | -4.22 | 117.96 | 127.62 |
| 24 | b | 619 | CLA | CAC-C3C-C4C | 4.22 | 130.28 | 124.79 |
| 24 | b | 615 | CLA | C2B-C1B-NB | 4.22 | 114.70 | 110.33 |
| 24 | c | 903 | CLA | C3D-C4D-ND | 4.22 | 116.85 | 109.99 |
| 24 | c | 902 | CLA | C3B-C2B-C1B | -4.22 | 102.20 | 107.17 |
| 24 | a | 406 | CLA | C3D-C2D-C1D | -4.21 | 100.08 | 105.83 |
| 37 | l | 101 | LHG | O7-C7-C8 | 4.21 | 120.59 | 111.48 |
| 24 | d | 402 | CLA | C2B-C1B-NB | 4.20 | 114.68 | 110.33 |
| 24 | b | 615 | CLA | C3D-C4D-ND | 4.20 | 116.81 | 109.99 |
| 24 | c | 905 | CLA | C4A-NA-C1A | -4.20 | 104.76 | 106.68 |
| 24 | A | 410 | CLA | C1C-C2C-C3C | -4.20 | 102.56 | 106.98 |
| 24 | c | 904 | CLA | O2D-CGD-CBD | 4.20 | 118.57 | 111.23 |
| 24 | C | 509 | CLA | O2D-CGD-O1D | -4.20 | 115.68 | 123.85 |
| 24 | b | 612 | CLA | C3D-C4D-ND | 4.19 | 116.81 | 109.99 |
| 24 | b | 609 | CLA | C1D-CHD-C4C | -4.19 | 117.10 | 126.02 |
| 24 | b | 617 | CLA | C2B-C1B-NB | 4.19 | 114.67 | 110.33 |
| 35 | c | 923 | HTG | C1-O5-C5 | 4.18 | 120.07 | 112.56 |
| 24 | C | 512 | CLA | C2B-C1B-NB | 4.18 | 114.66 | 110.33 |
| 24 | d | 401 | CLA | CMB-C2B-C1B | 4.18 | 131.78 | 125.42 |
| 24 | B | 615 | CLA | O2D-CGD-O1D | -4.18 | 115.72 | 123.85 |
| 24 | C | 507 | CLA | C3D-C4D-ND | 4.17 | 116.77 | 109.99 |
| 24 | c | 906 | CLA | C3D-C4D-ND | 4.17 | 116.77 | 109.99 |
| 24 | d | 403 | CLA | C3B-C4B-NB | 4.17 | 114.26 | 110.53 |
| 24 | C | 507 | CLA | C2B-C1B-NB | 4.17 | 114.65 | 110.33 |
| 24 | C | 510 | CLA | C2B-C1B-NB | 4.17 | 114.65 | 110.33 |
| 24 | C | 502 | CLA | C1C-C2C-C3C | -4.17 | 102.60 | 106.98 |
| 24 | c | 910 | CLA | C3D-C4D-ND | 4.17 | 116.76 | 109.99 |
| 24 | B | 614 | CLA | CHD-C1D-ND | -4.17 | 118.94 | 124.80 |
| 24 | C | 510 | CLA | C4A-NA-C1A | -4.16 | 104.78 | 106.68 |
| 24 | C | 512 | CLA | C4A-NA-C1A | -4.16 | 104.78 | 106.68 |
| 34 | Z | 101 | LMG | O7-C10-C11 | 4.16 | 120.49 | 111.48 |
| 24 | C | 514 | CLA | C4A-NA-C1A | -4.16 | 104.78 | 106.68 |
| 24 | b | 610 | CLA | CMC-C2C-C1C | 4.16 | 131.54 | 125.03 |
| 24 | A | 406 | CLA | C1D-CHD-C4C | -4.16 | 117.17 | 126.02 |
| 24 | a | 407 | CLA | C2C-C1C-NC | 4.16 | 114.35 | 109.98 |
| 24 | B | 614 | CLA | C3D-C4D-ND | 4.16 | 116.75 | 109.99 |
| 24 | b | 608 | CLA | C1C-C2C-C3C | -4.16 | 102.61 | 106.98 |
| 24 | C | 512 | CLA | C3D-C4D-ND | 4.16 | 116.74 | 109.99 |
| 24 | c | 902 | CLA | C3D-C4D-ND | 4.15 | 116.74 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 502 | CLA | CBC-CAC-C3C | -4.15 | 101.16 | 112.42 |
| 24 | D | 401 | CLA | C3C-C4C-NC | 4.15 | 115.75 | 110.43 |
| 24 | b | 610 | CLA | C3D-C4D-ND | 4.15 | 116.73 | 109.99 |
| 24 | D | 401 | CLA | CHD-C1D-ND | -4.15 | 118.96 | 124.80 |
| 24 | C | 502 | CLA | CHD-C1D-ND | -4.15 | 118.97 | 124.80 |
| 24 | c | 907 | CLA | C1C-C2C-C3C | -4.15 | 102.62 | 106.98 |
| 24 | C | 509 | CLA | C3D-C2D-C1D | -4.15 | 100.17 | 105.83 |
| 24 | b | 620 | CLA | C3C-C4C-NC | 4.14 | 115.74 | 110.43 |
| 24 | B | 605 | CLA | C3C-C4C-NC | 4.14 | 115.74 | 110.43 |
| 24 | b | 613 | CLA | CHD-C1D-ND | -4.14 | 118.98 | 124.80 |
| 24 | c | 912 | CLA | CHD-C1D-ND | -4.14 | 118.98 | 124.80 |
| 24 | c | 911 | CLA | C3B-C2B-C1B | -4.14 | 102.29 | 107.17 |
| 24 | B | 609 | CLA | C3D-C2D-C1D | -4.14 | 100.19 | 105.83 |
| 24 | c | 909 | CLA | C3C-C4C-NC | 4.14 | 115.73 | 110.43 |
| 24 | A | 405 | CLA | C3D-C4D-ND | 4.13 | 116.70 | 109.99 |
| 24 | b | 611 | CLA | CHD-C1D-ND | -4.13 | 118.99 | 124.80 |
| 24 | c | 908 | CLA | C1C-C2C-C3C | -4.13 | 102.64 | 106.98 |
| 35 | b | 627 | HTG | C1'-S1-C1 | 4.13 | 109.36 | 100.45 |
| 24 | b | 608 | CLA | C3D-C2D-C1D | -4.13 | 100.20 | 105.83 |
| 25 | A | 408 | PHO | O1D-CGD-CBD | -4.13 | 118.47 | 124.72 |
| 24 | b | 610 | CLA | C1C-C2C-C3C | -4.13 | 102.64 | 106.98 |
| 24 | b | 609 | CLA | C3D-C4D-ND | 4.13 | 116.69 | 109.99 |
| 24 | c | 905 | CLA | C1C-C2C-C3C | -4.12 | 102.64 | 106.98 |
| 24 | B | 617 | CLA | C3C-C4C-NC | 4.12 | 115.71 | 110.43 |
| 24 | B | 606 | CLA | O2D-CGD-O1D | -4.12 | 115.83 | 123.85 |
| 24 | a | 406 | CLA | C3B-C4B-NB | 4.12 | 114.21 | 110.53 |
| 24 | B | 605 | CLA | C3D-C4D-ND | 4.12 | 116.69 | 109.99 |
| 25 | a | 420 | PHO | C1-C2-C3 | -4.12 | 119.45 | 126.20 |
| 24 | d | 403 | CLA | C1C-C2C-C3C | -4.12 | 102.65 | 106.98 |
| 24 | b | 615 | CLA | CAC-C3C-C4C | 4.12 | 130.15 | 124.79 |
| 24 | C | 508 | CLA | C1D-CHD-C4C | -4.12 | 117.27 | 126.02 |
| 24 | b | 609 | CLA | O2D-CGD-O1D | -4.11 | 115.84 | 123.85 |
| 24 | C | 512 | CLA | C1D-CHD-C4C | -4.11 | 117.28 | 126.02 |
| 24 | B | 617 | CLA | C2B-C1B-NB | 4.11 | 114.58 | 110.33 |
| 24 | C | 507 | CLA | CHD-C1D-ND | -4.11 | 119.03 | 124.80 |
| 34 | a | 412 | LMG | O7-C10-C11 | 4.10 | 120.36 | 111.48 |
| 24 | D | 401 | CLA | C1-C2-C3 | -4.10 | 119.48 | 126.20 |
| 24 | a | 407 | CLA | C3D-C4D-ND | 4.10 | 116.65 | 109.99 |
| 24 | B | 602 | CLA | CHD-C1D-ND | -4.10 | 119.04 | 124.80 |
| 24 | B | 607 | CLA | C3C-C4C-NC | 4.10 | 115.68 | 110.43 |
| 24 | B | 611 | CLA | C1D-CHD-C4C | -4.09 | 117.32 | 126.02 |
| 24 | B | 603 | CLA | C3C-C4C-NC | 4.09 | 115.67 | 110.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 504 | CLA | C3C-C4C-NC | 4.09 | 115.67 | 110.43 |
| 34 | B | 622 | LMG | O7-C10-C11 | 4.09 | 120.32 | 111.48 |
| 24 | b | 607 | CLA | C3D-C2D-C1D | -4.09 | 100.26 | 105.83 |
| 24 | b | 611 | CLA | C3B-C2B-C1B | -4.09 | 102.35 | 107.17 |
| 24 | A | 407 | CLA | CBC-CAC-C3C | -4.08 | 101.35 | 112.42 |
| 24 | C | 508 | CLA | C2B-C1B-NB | 4.08 | 114.56 | 110.33 |
| 24 | D | 402 | CLA | C3C-C4C-NC | 4.08 | 115.66 | 110.43 |
| 35 | C | 523 | HTG | C1'-S1-C1 | 4.08 | 109.26 | 100.45 |
| 24 | B | 606 | CLA | C1D-CHD-C4C | -4.08 | 117.35 | 126.02 |
| 24 | b | 619 | CLA | C3D-C4D-ND | 4.07 | 116.61 | 109.99 |
| 24 | C | 503 | CLA | C3D-C4D-ND | 4.07 | 116.61 | 109.99 |
| 24 | B | 604 | CLA | C3C-C4C-NC | 4.07 | 115.64 | 110.43 |
| 26 | c | 915 | BCR | C7-C8-C9 | -4.07 | 120.21 | 126.23 |
| 24 | C | 505 | CLA | C1C-C2C-C3C | -4.07 | 102.70 | 106.98 |
| 24 | b | 616 | CLA | C2C-C1C-NC | 4.07 | 114.26 | 109.98 |
| 24 | A | 407 | CLA | C1D-CHD-C4C | -4.07 | 117.37 | 126.02 |
| 24 | A | 406 | CLA | CMA-C3A-C4A | -4.07 | 100.84 | 111.77 |
| 24 | d | 402 | CLA | CHD-C1D-ND | -4.07 | 119.08 | 124.80 |
| 24 | A | 405 | CLA | CHD-C1D-ND | -4.07 | 119.08 | 124.80 |
| 24 | C | 513 | CLA | C3D-C4D-ND | 4.07 | 116.60 | 109.99 |
| 24 | c | 908 | CLA | C3C-C4C-NC | 4.06 | 115.64 | 110.43 |
| 24 | b | 617 | CLA | C1C-C2C-C3C | -4.06 | 102.71 | 106.98 |
| 24 | c | 902 | CLA | C1C-C2C-C3C | -4.06 | 102.71 | 106.98 |
| 24 | C | 513 | CLA | C1D-CHD-C4C | -4.06 | 117.38 | 126.02 |
| 35 | C | 524 | HTG | C1'-S1-C1 | 4.06 | 109.22 | 100.45 |
| 24 | D | 402 | CLA | CMB-C2B-C1B | 4.06 | 131.60 | 125.42 |
| 24 | C | 507 | CLA | C4A-NA-C1A | -4.06 | 104.83 | 106.68 |
| 24 | b | 607 | CLA | O2D-CGD-O1D | -4.06 | 115.95 | 123.85 |
| 24 | b | 616 | CLA | C3D-C4D-ND | 4.05 | 116.58 | 109.99 |
| 24 | C | 504 | CLA | C1-C2-C3 | -4.05 | 119.56 | 126.20 |
| 26 | T | 102 | BCR | C33-C5-C6 | -4.05 | 120.06 | 124.48 |
| 24 | a | 409 | CLA | C3C-C4C-NC | 4.05 | 115.61 | 110.43 |
| 24 | c | 912 | CLA | C3D-C2D-C1D | -4.05 | 100.31 | 105.83 |
| 24 | C | 503 | CLA | C3C-C4C-NC | 4.04 | 115.61 | 110.43 |
| 24 | b | 607 | CLA | C3D-C4D-ND | 4.04 | 116.56 | 109.99 |
| 24 | A | 406 | CLA | CHD-C1D-ND | -4.04 | 119.12 | 124.80 |
| 24 | c | 907 | CLA | C3B-C4B-NB | 4.04 | 114.14 | 110.53 |
| 24 | B | 606 | CLA | C2B-C1B-NB | 4.04 | 114.52 | 110.33 |
| 26 | C | 515 | BCR | C7-C8-C9 | -4.04 | 120.26 | 126.23 |
| 40 | v | 202 | HEC | CBB-CAB-C3B | -4.04 | 119.36 | 127.43 |
| 24 | A | 406 | CLA | C4-C3-C5 | 4.04 | 122.24 | 115.23 |
| 24 | c | 907 | CLA | C2B-C1B-NB | 4.04 | 114.51 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 511 | CLA | C3D-C2D-C1D | -4.03 | 100.33 | 105.83 |
| 24 | C | 513 | CLA | C3C-C4C-NC | 4.03 | 115.59 | 110.43 |
| 35 | d | 412 | HTG | C1'-S1-C1 | 4.03 | 109.15 | 100.45 |
| 24 | C | 507 | CLA | C3B-C4B-NB | 4.03 | 114.12 | 110.53 |
| 24 | C | 514 | CLA | CHD-C1D-ND | -4.03 | 119.14 | 124.80 |
| 24 | B | 617 | CLA | C3D-C4D-ND | 4.03 | 116.53 | 109.99 |
| 24 | C | 504 | CLA | C1D-CHD-C4C | -4.02 | 117.47 | 126.02 |
| 37 | d | 409 | LHG | O7-C7-C8 | 4.02 | 120.17 | 111.48 |
| 36 | C | 517 | DGD | O2G-C1B-C2B | 4.02 | 120.17 | 111.48 |
| 24 | B | 614 | CLA | C3C-C4C-NC | 4.02 | 115.58 | 110.43 |
| 24 | B | 613 | CLA | C3D-C2D-C1D | -4.01 | 100.35 | 105.83 |
| 24 | c | 902 | CLA | C3C-C4C-NC | 4.01 | 115.57 | 110.43 |
| 24 | d | 402 | CLA | O2D-CGD-O1D | -4.01 | 116.04 | 123.85 |
| 24 | B | 610 | CLA | C1D-CHD-C4C | -4.01 | 117.50 | 126.02 |
| 24 | b | 613 | CLA | CMC-C2C-C1C | 4.01 | 131.29 | 125.03 |
| 24 | C | 506 | CLA | C3C-C4C-NC | 4.00 | 115.55 | 110.43 |
| 24 | c | 911 | CLA | C1D-CHD-C4C | -4.00 | 117.53 | 126.02 |
| 24 | c | 912 | CLA | O2D-CGD-CBD | 4.00 | 118.22 | 111.23 |
| 24 | C | 508 | CLA | C3C-C4C-NC | 4.00 | 115.55 | 110.43 |
| 24 | c | 903 | CLA | C3C-C4C-NC | 4.00 | 115.55 | 110.43 |
| 24 | B | 607 | CLA | C3B-C4B-NB | 3.99 | 114.09 | 110.53 |
| 24 | b | 613 | CLA | C3C-C4C-NC | 3.99 | 115.55 | 110.43 |
| 24 | c | 913 | CLA | C1C-C2C-C3C | -3.99 | 102.78 | 106.98 |
| 24 | B | 607 | CLA | C3D-C4D-ND | 3.99 | 116.48 | 109.99 |
| 24 | d | 403 | CLA | CHD-C1D-ND | -3.99 | 119.19 | 124.80 |
| 24 | C | 510 | CLA | CAC-C3C-C4C | 3.99 | 129.98 | 124.79 |
| 24 | C | 510 | CLA | C3D-C4D-ND | 3.99 | 116.47 | 109.99 |
| 24 | b | 607 | CLA | C1D-CHD-C4C | -3.99 | 117.54 | 126.02 |
| 24 | C | 514 | CLA | C1-C2-C3 | -3.99 | 119.66 | 126.20 |
| 24 | a | 409 | CLA | C1D-CHD-C4C | -3.99 | 117.54 | 126.02 |
| 24 | c | 904 | CLA | C3D-C4D-ND | 3.99 | 116.47 | 109.99 |
| 24 | d | 402 | CLA | CAC-C3C-C4C | 3.99 | 129.98 | 124.79 |
| 24 | a | 409 | CLA | C1C-C2C-C3C | -3.99 | 102.79 | 106.98 |
| 24 | B | 608 | CLA | C3B-C2B-C1B | -3.99 | 102.47 | 107.17 |
| 29 | C | 522 | LMT | O1B-C4'-C3' | 3.99 | 117.36 | 107.23 |
| 24 | c | 908 | CLA | C1D-CHD-C4C | -3.98 | 117.56 | 126.02 |
| 24 | c | 906 | CLA | CAC-C3C-C4C | 3.98 | 129.97 | 124.79 |
| 27 | A | 412 | SQD | C1-O5-C5 | -3.98 | 105.96 | 113.72 |
| 38 | E | 103 | HEM | CHD-C4C-NC | 3.97 | 128.78 | 124.45 |
| 24 | a | 409 | CLA | C3D-C4D-ND | 3.97 | 116.44 | 109.99 |
| 24 | c | 908 | CLA | C4A-NA-C1A | -3.97 | 104.87 | 106.68 |
| 24 | b | 608 | CLA | CAC-C3C-C4C | 3.97 | 129.95 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | h | 101 | BCR | C38-C26-C25 | -3.97 | 120.15 | 124.48 |
| 24 | B | 611 | CLA | C2B-C1B-NB | 3.97 | 114.44 | 110.33 |
| 24 | c | 902 | CLA | C4A-NA-C1A | -3.97 | 104.87 | 106.68 |
| 24 | b | 620 | CLA | C3B-C4B-NB | 3.96 | 114.07 | 110.53 |
| 24 | B | 606 | CLA | C1C-C2C-C3C | -3.96 | 102.81 | 106.98 |
| 24 | B | 614 | CLA | C1C-C2C-C3C | -3.96 | 102.81 | 106.98 |
| 26 | B | 620 | BCR | C38-C26-C25 | -3.96 | 120.16 | 124.48 |
| 24 | A | 406 | CLA | C4A-NA-C1A | -3.96 | 104.87 | 106.68 |
| 24 | C | 508 | CLA | C1C-C2C-C3C | -3.96 | 102.81 | 106.98 |
| 24 | B | 610 | CLA | C3C-C4C-NC | 3.96 | 115.50 | 110.43 |
| 29 | C | 522 | LMT | C1'-O5'-C5' | 3.95 | 121.43 | 113.72 |
| 24 | b | 608 | CLA | C3C-C4C-NC | 3.95 | 115.49 | 110.43 |
| 24 | a | 406 | CLA | CHD-C1D-ND | -3.95 | 119.25 | 124.80 |
| 24 | b | 609 | CLA | C1C-C2C-C3C | -3.94 | 102.83 | 106.98 |
| 24 | b | 606 | CLA | CAA-C2A-C3A | -3.94 | 102.34 | 113.00 |
| 24 | c | 908 | CLA | C2B-C1B-NB | 3.94 | 114.41 | 110.33 |
| 24 | b | 605 | CLA | C1C-C2C-C3C | -3.94 | 102.83 | 106.98 |
| 24 | b | 609 | CLA | CMB-C2B-C1B | 3.94 | 131.42 | 125.42 |
| 24 | C | 508 | CLA | C3D-C4D-ND | 3.94 | 116.38 | 109.99 |
| 24 | d | 401 | CLA | C2B-C1B-NB | 3.93 | 114.41 | 110.33 |
| 24 | b | 607 | CLA | CHD-C1D-ND | -3.93 | 119.28 | 124.80 |
| 26 | D | 403 | BCR | C28-C27-C26 | -3.93 | 107.06 | 114.06 |
| 24 | b | 620 | CLA | C1D-CHD-C4C | -3.92 | 117.68 | 126.02 |
| 25 | A | 408 | PHO | C1-C2-C3 | -3.92 | 119.77 | 126.20 |
| 27 | F | 101 | SQD | C44-O6-C1 | -3.92 | 105.38 | 113.80 |
| 24 | C | 502 | CLA | C3B-C4B-NB | 3.92 | 114.03 | 110.53 |
| 24 | C | 510 | CLA | CHD-C1D-ND | -3.92 | 119.29 | 124.80 |
| 24 | A | 405 | CLA | C1C-C2C-C3C | -3.92 | 102.86 | 106.98 |
| 24 | B | 605 | CLA | C4A-NA-C1A | -3.91 | 104.89 | 106.68 |
| 24 | b | 620 | CLA | C3D-C4D-ND | 3.91 | 116.35 | 109.99 |
| 24 | B | 608 | CLA | C3D-C4D-ND | 3.91 | 116.35 | 109.99 |
| 24 | b | 615 | CLA | C3B-C4B-NB | 3.91 | 114.02 | 110.53 |
| 24 | B | 611 | CLA | C3B-C4B-NB | 3.91 | 114.02 | 110.53 |
| 24 | c | 906 | CLA | C3D-C2D-C1D | -3.91 | 100.50 | 105.83 |
| 24 | B | 602 | CLA | C1D-CHD-C4C | -3.91 | 117.72 | 126.02 |
| 24 | b | 606 | CLA | C1D-CHD-C4C | -3.90 | 117.72 | 126.02 |
| 24 | d | 403 | CLA | C3C-C4C-NC | 3.90 | 115.43 | 110.43 |
| 26 | b | 621 | BCR | C33-C5-C6 | -3.90 | 120.23 | 124.48 |
| 24 | b | 618 | CLA | C1D-CHD-C4C | -3.90 | 117.73 | 126.02 |
| 24 | c | 904 | CLA | C3C-C4C-NC | 3.90 | 115.42 | 110.43 |
| 24 | c | 911 | CLA | C2B-C1B-NB | 3.90 | 114.37 | 110.33 |
| 24 | b | 608 | CLA | C3D-C4D-ND | 3.90 | 116.32 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | d | 404 | BCR | C7-C8-C9 | -3.89 | 120.48 | 126.23 |
| 24 | D | 401 | CLA | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 24 | A | 405 | CLA | CAA-C2A-C3A | -3.88 | 102.50 | 113.00 |
| 24 | C | 514 | CLA | C1D-CHD-C4C | -3.88 | 117.78 | 126.02 |
| 24 | c | 910 | CLA | C1D-CHD-C4C | -3.88 | 117.78 | 126.02 |
| 24 | B | 616 | CLA | CHD-C1D-ND | -3.88 | 119.35 | 124.80 |
| 40 | V | 201 | HEC | CHC-C4B-NB | 3.87 | 128.67 | 124.45 |
| 24 | b | 615 | CLA | C1D-CHD-C4C | -3.87 | 117.80 | 126.02 |
| 24 | c | 902 | CLA | CHD-C1D-ND | -3.87 | 119.36 | 124.80 |
| 24 | b | 612 | CLA | C1C-C2C-C3C | -3.86 | 102.92 | 106.98 |
| 24 | c | 902 | CLA | C3B-C4B-NB | 3.86 | 113.98 | 110.53 |
| 27 | F | 101 | SQD | C1-C2-C3 | -3.86 | 101.88 | 110.01 |
| 24 | b | 610 | CLA | C3C-C4C-NC | 3.86 | 115.38 | 110.43 |
| 24 | b | 613 | CLA | C2B-C1B-NB | 3.86 | 114.33 | 110.33 |
| 24 | C | 512 | CLA | C3C-C4C-NC | 3.85 | 115.36 | 110.43 |
| 24 | c | 911 | CLA | C3D-C2D-C1D | -3.85 | 100.58 | 105.83 |
| 24 | A | 407 | CLA | C2C-C1C-NC | 3.85 | 114.02 | 109.98 |
| 24 | c | 905 | CLA | C3C-C4C-NC | 3.85 | 115.36 | 110.43 |
| 24 | A | 405 | CLA | C1D-CHD-C4C | -3.84 | 117.85 | 126.02 |
| 24 | b | 614 | CLA | C3C-C4C-NC | 3.84 | 115.35 | 110.43 |
| 24 | c | 910 | CLA | C1C-C2C-C3C | -3.84 | 102.94 | 106.98 |
| 24 | B | 611 | CLA | C3C-C4C-NC | 3.84 | 115.35 | 110.43 |
| 24 | b | 605 | CLA | C1D-CHD-C4C | -3.84 | 117.87 | 126.02 |
| 24 | c | 907 | CLA | C1D-CHD-C4C | -3.83 | 117.87 | 126.02 |
| 35 | B | 633 | HTG | C1'-S1-C1 | 3.83 | 108.73 | 100.45 |
| 24 | b | 617 | CLA | O2D-CGD-CBD | 3.83 | 117.93 | 111.23 |
| 24 | b | 611 | CLA | C3B-C4B-NB | 3.83 | 113.95 | 110.53 |
| 24 | c | 911 | CLA | C3C-C4C-NC | 3.82 | 115.33 | 110.43 |
| 24 | a | 406 | CLA | C2B-C1B-NB | 3.82 | 114.29 | 110.33 |
| 24 | B | 616 | CLA | O2D-CGD-CBD | 3.82 | 117.91 | 111.23 |
| 24 | C | 511 | CLA | C3C-C4C-NC | 3.82 | 115.32 | 110.43 |
| 31 | a | 417 | PL9 | C27-C28-C29 | -3.82 | 118.88 | 127.62 |
| 24 | c | 907 | CLA | C1-C2-C3 | -3.82 | 119.94 | 126.20 |
| 24 | b | 616 | CLA | C4C-C3C-C2C | -3.82 | 101.33 | 106.89 |
| 24 | C | 509 | CLA | CHD-C1D-ND | -3.82 | 119.43 | 124.80 |
| 24 | b | 611 | CLA | C1C-C2C-C3C | -3.82 | 102.97 | 106.98 |
| 24 | a | 409 | CLA | CAA-C2A-C3A | -3.81 | 102.69 | 113.00 |
| 24 | C | 511 | CLA | C1-C2-C3 | -3.81 | 119.95 | 126.20 |
| 24 | B | 616 | CLA | C1D-CHD-C4C | -3.81 | 117.92 | 126.02 |
| 24 | b | 614 | CLA | C1D-CHD-C4C | -3.81 | 117.92 | 126.02 |
| 24 | b | 614 | CLA | C1C-C2C-C3C | -3.81 | 102.97 | 106.98 |
| 24 | b | 612 | CLA | C1D-CHD-C4C | -3.81 | 117.93 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A | 407 | CLA | CMB-C2B-C1B | 3.81 | 131.21 | 125.42 |
| 24 | b | 611 | CLA | C2B-C1B-NB | 3.80 | 114.27 | 110.33 |
| 24 | B | 605 | CLA | C1D-CHD-C4C | -3.80 | 117.94 | 126.02 |
| 24 | B | 609 | CLA | C3C-C4C-NC | 3.80 | 115.30 | 110.43 |
| 24 | B | 616 | CLA | C3D-C4D-ND | 3.80 | 116.16 | 109.99 |
| 24 | a | 406 | CLA | CAC-C3C-C4C | 3.80 | 129.73 | 124.79 |
| 24 | b | 619 | CLA | C1-C2-C3 | -3.80 | 119.98 | 126.20 |
| 24 | b | 607 | CLA | CAA-C2A-C3A | -3.79 | 102.75 | 113.00 |
| 24 | B | 608 | CLA | C2B-C1B-NB | 3.79 | 114.26 | 110.33 |
| 24 | C | 503 | CLA | C1C-C2C-C3C | -3.79 | 103.00 | 106.98 |
| 24 | c | 908 | CLA | C3D-C4D-ND | 3.79 | 116.14 | 109.99 |
| 24 | b | 609 | CLA | CHD-C1D-ND | -3.79 | 119.47 | 124.80 |
| 36 | d | 406 | DGD | C3E-C4E-C5E | 3.79 | 117.10 | 110.23 |
| 24 | c | 910 | CLA | CHD-C1D-ND | -3.79 | 119.47 | 124.80 |
| 24 | B | 613 | CLA | CAC-C3C-C4C | 3.79 | 129.72 | 124.79 |
| 24 | C | 512 | CLA | CHD-C1D-ND | -3.78 | 119.48 | 124.80 |
| 24 | b | 606 | CLA | C4C-C3C-C2C | -3.78 | 101.39 | 106.89 |
| 24 | B | 617 | CLA | CAC-C3C-C4C | 3.78 | 129.71 | 124.79 |
| 24 | B | 610 | CLA | CHD-C1D-ND | -3.78 | 119.48 | 124.80 |
| 24 | C | 510 | CLA | C1C-C2C-C3C | -3.78 | 103.00 | 106.98 |
| 24 | c | 912 | CLA | C1D-CHD-C4C | -3.78 | 117.99 | 126.02 |
| 24 | c | 909 | CLA | C1-C2-C3 | -3.78 | 120.01 | 126.20 |
| 24 | C | 503 | CLA | CMB-C2B-C1B | 3.78 | 131.17 | 125.42 |
| 24 | B | 603 | CLA | C1C-C2C-C3C | -3.78 | 103.01 | 106.98 |
| 24 | C | 505 | CLA | C3B-C4B-NB | 3.77 | 113.90 | 110.53 |
| 24 | c | 913 | CLA | CHD-C1D-ND | -3.77 | 119.49 | 124.80 |
| 24 | B | 617 | CLA | C3B-C4B-NB | 3.77 | 113.90 | 110.53 |
| 29 | B | 623 | LMT | C3B-C4B-C5B | 3.77 | 117.06 | 110.23 |
| 24 | C | 503 | CLA | C1D-CHD-C4C | -3.77 | 118.01 | 126.02 |
| 24 | B | 617 | CLA | O2D-CGD-O1D | -3.76 | 116.52 | 123.85 |
| 24 | B | 615 | CLA | C3B-C4B-NB | 3.76 | 113.89 | 110.53 |
| 24 | c | 914 | CLA | C1C-C2C-C3C | -3.76 | 103.02 | 106.98 |
| 37 | D | 408 | LHG | O7-C7-C8 | 3.76 | 119.62 | 111.48 |
| 24 | b | 610 | CLA | C1D-CHD-C4C | -3.76 | 118.03 | 126.02 |
| 24 | B | 613 | CLA | CMC-C2C-C1C | 3.76 | 130.91 | 125.03 |
| 24 | C | 506 | CLA | C1C-C2C-C3C | -3.76 | 103.03 | 106.98 |
| 24 | C | 511 | CLA | C1D-CHD-C4C | -3.76 | 118.03 | 126.02 |
| 24 | a | 406 | CLA | C1D-CHD-C4C | -3.75 | 118.04 | 126.02 |
| 24 | B | 602 | CLA | C1C-C2C-C3C | -3.75 | 103.03 | 106.98 |
| 24 | c | 904 | CLA | C1C-C2C-C3C | -3.75 | 103.03 | 106.98 |
| 24 | B | 604 | CLA | CHD-C1D-ND | -3.75 | 119.53 | 124.80 |
| 24 | c | 914 | CLA | O2D-CGD-CBD | 3.75 | 117.78 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | z | 101 | LMG | O6-C5-C4 | 3.75 | 116.45 | 109.70 |
| 27 | A | 416 | SQD | O47-C7-C8 | 3.74 | 119.57 | 111.48 |
| 24 | b | 612 | CLA | CHD-C1D-ND | -3.74 | 119.54 | 124.80 |
| 24 | b | 619 | CLA | CHD-C1D-ND | -3.74 | 119.55 | 124.80 |
| 34 | B | 622 | LMG | O8-C28-C29 | 3.74 | 123.22 | 111.83 |
| 24 | c | 910 | CLA | C1-C2-C3 | -3.73 | 120.08 | 126.20 |
| 24 | D | 402 | CLA | C4A-NA-C1A | -3.73 | 104.98 | 106.68 |
| 24 | C | 514 | CLA | C3C-C4C-NC | 3.73 | 115.21 | 110.43 |
| 24 | A | 407 | CLA | CHD-C1D-ND | -3.73 | 119.55 | 124.80 |
| 24 | d | 403 | CLA | O2D-CGD-CBD | 3.73 | 117.75 | 111.23 |
| 24 | c | 913 | CLA | C1D-CHD-C4C | -3.73 | 118.10 | 126.02 |
| 24 | b | 617 | CLA | C1D-CHD-C4C | -3.72 | 118.10 | 126.02 |
| 24 | b | 606 | CLA | CHD-C1D-ND | -3.72 | 119.56 | 124.80 |
| 24 | b | 606 | CLA | CAC-C3C-C4C | 3.72 | 129.63 | 124.79 |
| 24 | B | 604 | CLA | C4-C3-C5 | 3.72 | 121.69 | 115.23 |
| 24 | b | 618 | CLA | C3B-C4B-NB | 3.72 | 113.85 | 110.53 |
| 27 | A | 412 | SQD | C1-C2-C3 | -3.72 | 102.18 | 110.01 |
| 26 | B | 618 | BCR | C33-C5-C6 | -3.72 | 120.42 | 124.48 |
| 24 | B | 609 | CLA | C3B-C4B-NB | 3.72 | 113.85 | 110.53 |
| 24 | c | 909 | CLA | CAC-C3C-C4C | 3.72 | 129.63 | 124.79 |
| 24 | d | 401 | CLA | C1D-CHD-C4C | -3.72 | 118.12 | 126.02 |
| 24 | B | 606 | CLA | CMB-C2B-C1B | 3.72 | 131.08 | 125.42 |
| 24 | A | 406 | CLA | CBC-CAC-C3C | -3.71 | 102.36 | 112.42 |
| 24 | B | 608 | CLA | CHD-C1D-ND | -3.71 | 119.58 | 124.80 |
| 24 | B | 612 | CLA | C1D-CHD-C4C | -3.71 | 118.13 | 126.02 |
| 24 | C | 511 | CLA | C1C-C2C-C3C | -3.71 | 103.08 | 106.98 |
| 24 | b | 611 | CLA | CAA-C2A-C3A | -3.71 | 102.97 | 113.00 |
| 27 | a | 411 | SQD | C1-O5-C5 | -3.71 | 106.48 | 113.72 |
| 24 | b | 619 | CLA | C3C-C4C-NC | 3.70 | 115.17 | 110.43 |
| 24 | C | 505 | CLA | C1D-CHD-C4C | -3.70 | 118.15 | 126.02 |
| 24 | b | 613 | CLA | C3B-C2B-C1B | -3.70 | 102.81 | 107.17 |
| 24 | C | 513 | CLA | C1C-C2C-C3C | -3.70 | 103.09 | 106.98 |
| 24 | B | 611 | CLA | C3D-C4D-ND | 3.70 | 116.00 | 109.99 |
| 26 | k | 102 | BCR | C20-C21-C22 | -3.70 | 122.09 | 127.28 |
| 24 | C | 505 | CLA | O2D-CGD-O1D | -3.70 | 116.65 | 123.85 |
| 24 | c | 910 | CLA | O2D-CGD-O1D | -3.70 | 116.65 | 123.85 |
| 24 | A | 406 | CLA | CHD-C4C-NC | 3.70 | 129.96 | 124.23 |
| 27 | A | 416 | SQD | O48-C23-C24 | 3.70 | 123.10 | 111.83 |
| 24 | c | 910 | CLA | C3C-C4C-NC | 3.69 | 115.16 | 110.43 |
| 25 | a | 408 | PHO | CMA-C3A-C4A | -3.69 | 106.66 | 114.61 |
| 26 | H | 101 | BCR | C38-C26-C25 | -3.69 | 120.46 | 124.48 |
| 24 | B | 609 | CLA | C1D-CHD-C4C | -3.69 | 118.18 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | d | 403 | CLA | C1D-CHD-C4C | -3.69 | 118.18 | 126.02 |
| 24 | C | 509 | CLA | C3C-C4C-NC | 3.69 | 115.16 | 110.43 |
| 24 | b | 614 | CLA | CHD-C1D-ND | -3.69 | 119.61 | 124.80 |
| 24 | B | 604 | CLA | CAA-C2A-C3A | -3.69 | 103.04 | 113.00 |
| 24 | c | 907 | CLA | CHD-C1D-ND | -3.69 | 119.61 | 124.80 |
| 34 | z | 101 | LMG | O7-C10-C11 | 3.68 | 119.45 | 111.48 |
| 24 | c | 912 | CLA | C3C-C4C-NC | 3.68 | 115.15 | 110.43 |
| 24 | B | 612 | CLA | C1-C2-C3 | -3.68 | 120.16 | 126.20 |
| 24 | B | 605 | CLA | CHD-C1D-ND | -3.68 | 119.62 | 124.80 |
| 24 | b | 617 | CLA | C3D-C4D-ND | 3.68 | 115.97 | 109.99 |
| 24 | C | 509 | CLA | C1D-CHD-C4C | -3.68 | 118.19 | 126.02 |
| 24 | b | 620 | CLA | CAC-C3C-C4C | 3.68 | 129.58 | 124.79 |
| 24 | B | 616 | CLA | C3C-C4C-NC | 3.68 | 115.14 | 110.43 |
| 24 | b | 611 | CLA | C4A-NA-C1A | -3.68 | 105.00 | 106.68 |
| 24 | b | 616 | CLA | C1D-CHD-C4C | -3.68 | 118.20 | 126.02 |
| 36 | c | 918 | DGD | O2G-C1B-C2B | 3.68 | 119.44 | 111.48 |
| 27 | a | 411 | SQD | C45-O47-C7 | -3.68 | 108.99 | 117.80 |
| 24 | c | 914 | CLA | C1D-CHD-C4C | -3.68 | 118.21 | 126.02 |
| 24 | b | 610 | CLA | O2D-CGD-O1D | -3.67 | 116.70 | 123.85 |
| 24 | c | 907 | CLA | C3D-C4D-ND | 3.67 | 115.96 | 109.99 |
| 24 | B | 603 | CLA | C1D-CHD-C4C | -3.67 | 118.22 | 126.02 |
| 24 | c | 911 | CLA | C3B-C4B-NB | 3.67 | 113.80 | 110.53 |
| 24 | C | 510 | CLA | C3B-C4B-NB | 3.67 | 113.80 | 110.53 |
| 24 | B | 614 | CLA | C1-C2-C3 | -3.67 | 120.19 | 126.20 |
| 35 | V | 202 | HTG | C1-C2-C3 | -3.67 | 103.38 | 110.55 |
| 24 | A | 410 | CLA | C1D-CHD-C4C | -3.66 | 118.23 | 126.02 |
| 24 | c | 903 | CLA | CHD-C1D-ND | -3.66 | 119.65 | 124.80 |
| 24 | B | 611 | CLA | C4C-C3C-C2C | -3.66 | 101.56 | 106.89 |
| 24 | b | 617 | CLA | C1-C2-C3 | -3.66 | 120.20 | 126.20 |
| 24 | C | 510 | CLA | C3C-C4C-NC | 3.66 | 115.12 | 110.43 |
| 24 | B | 615 | CLA | C3C-C4C-NC | 3.66 | 115.12 | 110.43 |
| 24 | c | 905 | CLA | C3B-C4B-NB | 3.66 | 113.80 | 110.53 |
| 24 | B | 607 | CLA | C1D-CHD-C4C | -3.66 | 118.25 | 126.02 |
| 24 | B | 609 | CLA | CHD-C1D-ND | -3.65 | 119.66 | 124.80 |
| 24 | b | 615 | CLA | CHD-C1D-ND | -3.65 | 119.66 | 124.80 |
| 24 | B | 617 | CLA | C4C-C3C-C2C | -3.65 | 101.58 | 106.89 |
| 24 | c | 903 | CLA | CMB-C2B-C1B | 3.65 | 130.98 | 125.42 |
| 24 | c | 906 | CLA | C1D-CHD-C4C | -3.65 | 118.27 | 126.02 |
| 24 | d | 402 | CLA | C3B-C4B-NB | 3.65 | 113.79 | 110.53 |
| 24 | b | 607 | CLA | O2A-CGA-CBA | 3.65 | 122.96 | 111.83 |
| 24 | c | 908 | CLA | C3B-C4B-NB | 3.65 | 113.78 | 110.53 |
| 24 | b | 607 | CLA | C3B-C4B-NB | 3.64 | 113.78 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | B | 619 | BCR | C29-C30-C25 | 3.64 | 115.73 | 110.44 |
| 24 | b | 613 | CLA | CAC-C3C-C4C | 3.64 | 129.53 | 124.79 |
| 31 | a | 417 | PL9 | C22-C23-C24 | -3.64 | 119.29 | 127.62 |
| 29 | b | 601 | LMT | O5'-C5'-C4' | 3.64 | 117.25 | 109.72 |
| 26 | D | 403 | BCR | C38-C26-C25 | -3.64 | 120.51 | 124.48 |
| 24 | B | 605 | CLA | C1-C2-C3 | -3.64 | 120.24 | 126.20 |
| 24 | C | 507 | CLA | C1D-CHD-C4C | -3.64 | 118.29 | 126.02 |
| 24 | c | 903 | CLA | C1C-C2C-C3C | -3.63 | 103.16 | 106.98 |
| 24 | c | 904 | CLA | CHD-C1D-ND | -3.63 | 119.69 | 124.80 |
| 24 | C | 509 | CLA | C1-C2-C3 | -3.63 | 120.25 | 126.20 |
| 24 | C | 506 | CLA | C1D-CHD-C4C | -3.63 | 118.31 | 126.02 |
| 26 | a | 410 | BCR | C7-C8-C9 | -3.63 | 120.87 | 126.23 |
| 26 | K | 103 | BCR | C20-C21-C22 | -3.63 | 122.19 | 127.28 |
| 24 | b | 606 | CLA | C3B-C4B-NB | 3.63 | 113.77 | 110.53 |
| 24 | C | 502 | CLA | C1D-CHD-C4C | -3.63 | 118.31 | 126.02 |
| 24 | B | 604 | CLA | C1C-C2C-C3C | -3.62 | 103.17 | 106.98 |
| 24 | a | 407 | CLA | CAC-C3C-C4C | 3.62 | 129.50 | 124.79 |
| 24 | a | 406 | CLA | CAA-C2A-C3A | -3.62 | 103.21 | 113.00 |
| 24 | c | 906 | CLA | C1C-C2C-C3C | -3.62 | 103.17 | 106.98 |
| 38 | e | 102 | HEM | CHD-C4C-NC | 3.62 | 128.40 | 124.45 |
| 27 | L | 102 | SQD | C3-C4-C5 | 3.62 | 116.80 | 110.23 |
| 24 | A | 406 | CLA | CAA-C2A-C3A | -3.62 | 103.23 | 113.00 |
| 24 | a | 407 | CLA | C3C-C4C-NC | 3.61 | 115.06 | 110.43 |
| 24 | B | 604 | CLA | O2D-CGD-O1D | -3.61 | 116.82 | 123.85 |
| 24 | C | 506 | CLA | CHD-C1D-ND | -3.61 | 119.72 | 124.80 |
| 24 | c | 913 | CLA | CMB-C2B-C1B | 3.61 | 130.91 | 125.42 |
| 24 | c | 913 | CLA | C3C-C4C-NC | 3.60 | 115.05 | 110.43 |
| 26 | k | 101 | BCR | C15-C14-C13 | -3.60 | 122.23 | 127.28 |
| 24 | B | 608 | CLA | CAA-C2A-C3A | -3.60 | 103.28 | 113.00 |
| 24 | b | 617 | CLA | C3B-C4B-NB | 3.60 | 113.74 | 110.53 |
| 24 | C | 502 | CLA | CMC-C2C-C1C | 3.60 | 130.65 | 125.03 |
| 24 | A | 407 | CLA | CAC-C3C-C4C | 3.59 | 129.47 | 124.79 |
| 24 | b | 607 | CLA | O2A-CGA-O1A | -3.59 | 114.64 | 123.63 |
| 24 | b | 608 | CLA | CHD-C1D-ND | -3.59 | 119.75 | 124.80 |
| 24 | C | 505 | CLA | C3C-C4C-NC | 3.59 | 115.03 | 110.43 |
| 24 | b | 618 | CLA | CHD-C1D-ND | -3.59 | 119.75 | 124.80 |
| 24 | D | 401 | CLA | C4B-C3B-C2B | -3.59 | 102.84 | 107.30 |
| 24 | C | 510 | CLA | C1D-CHD-C4C | -3.59 | 118.40 | 126.02 |
| 24 | C | 502 | CLA | C3C-C4C-NC | 3.59 | 115.02 | 110.43 |
| 24 | c | 914 | CLA | C3C-C4C-NC | 3.59 | 115.02 | 110.43 |
| 25 | A | 409 | PHO | C1A-C2A-C3A | -3.58 | 99.43 | 102.84 |
| 24 | B | 608 | CLA | C3B-C4B-NB | 3.58 | 113.73 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 612 | CLA | C1C-C2C-C3C | -3.58 | 103.21 | 106.98 |
| 24 | c | 903 | CLA | C1D-CHD-C4C | -3.58 | 118.41 | 126.02 |
| 24 | B | 611 | CLA | CHD-C1D-ND | -3.58 | 119.76 | 124.80 |
| 27 | F | 101 | SQD | C1-O5-C5 | -3.58 | 106.73 | 113.72 |
| 24 | c | 908 | CLA | O2D-CGD-O1D | -3.58 | 116.88 | 123.85 |
| 24 | b | 619 | CLA | C1D-CHD-C4C | -3.58 | 118.42 | 126.02 |
| 24 | B | 612 | CLA | C3B-C4B-NB | 3.58 | 113.72 | 110.53 |
| 36 | c | 916 | DGD | O2G-C1B-C2B | 3.58 | 119.22 | 111.48 |
| 24 | c | 911 | CLA | C1C-C2C-C3C | -3.57 | 103.23 | 106.98 |
| 24 | c | 907 | CLA | CBC-CAC-C3C | -3.57 | 102.75 | 112.42 |
| 24 | b | 619 | CLA | C1C-C2C-C3C | -3.57 | 103.23 | 106.98 |
| 24 | c | 903 | CLA | O2D-CGD-O1D | -3.57 | 116.91 | 123.85 |
| 24 | a | 409 | CLA | C3B-C4B-NB | 3.57 | 113.71 | 110.53 |
| 24 | b | 612 | CLA | C3C-C4C-NC | 3.56 | 114.99 | 110.43 |
| 24 | B | 610 | CLA | C2B-C1B-NB | 3.56 | 114.02 | 110.33 |
| 24 | b | 607 | CLA | C3C-C4C-NC | 3.56 | 114.99 | 110.43 |
| 24 | a | 407 | CLA | O2D-CGD-O1D | -3.56 | 116.92 | 123.85 |
| 24 | a | 407 | CLA | CHD-C1D-ND | -3.56 | 119.79 | 124.80 |
| 38 | E | 103 | HEM | CBD-CAD-C3D | -3.56 | 102.69 | 112.53 |
| 24 | D | 401 | CLA | C3B-C2B-C1B | -3.56 | 102.97 | 107.17 |
| 37 | E | 101 | LHG | O7-C7-C8 | 3.56 | 119.17 | 111.48 |
| 24 | B | 603 | CLA | CAA-C2A-C3A | -3.55 | 103.39 | 113.00 |
| 24 | C | 506 | CLA | O2D-CGD-O1D | -3.55 | 116.93 | 123.85 |
| 24 | C | 509 | CLA | C3B-C4B-NB | 3.55 | 113.70 | 110.53 |
| 26 | b | 623 | BCR | C3-C4-C5 | -3.55 | 107.72 | 114.06 |
| 24 | b | 620 | CLA | C4C-C3C-C2C | -3.55 | 101.73 | 106.89 |
| 24 | A | 410 | CLA | CMC-C2C-C1C | 3.55 | 130.58 | 125.03 |
| 24 | C | 512 | CLA | CAC-C3C-C4C | 3.55 | 129.41 | 124.79 |
| 24 | B | 610 | CLA | C3B-C2B-C1B | -3.54 | 102.99 | 107.17 |
| 24 | C | 512 | CLA | C1C-C2C-C3C | -3.54 | 103.25 | 106.98 |
| 24 | c | 902 | CLA | C1D-CHD-C4C | -3.54 | 118.49 | 126.02 |
| 24 | B | 615 | CLA | CHD-C4C-NC | 3.54 | 129.72 | 124.23 |
| 24 | b | 605 | CLA | CHD-C4C-NC | 3.54 | 129.72 | 124.23 |
| 24 | c | 908 | CLA | CHD-C1D-ND | -3.54 | 119.82 | 124.80 |
| 34 | c | 919 | LMG | O7-C10-C11 | 3.54 | 119.14 | 111.48 |
| 24 | B | 606 | CLA | CAC-C3C-C4C | 3.54 | 129.39 | 124.79 |
| 36 | D | 405 | DGD | C1D-C2D-C3D | 3.53 | 117.44 | 110.01 |
| 24 | A | 405 | CLA | C3B-C4B-NB | 3.53 | 113.68 | 110.53 |
| 24 | C | 514 | CLA | C1C-C2C-C3C | -3.53 | 103.27 | 106.98 |
| 24 | b | 618 | CLA | C4C-C3C-C2C | -3.53 | 101.76 | 106.89 |
| 24 | b | 607 | CLA | C4-C3-C5 | 3.52 | 121.34 | 115.23 |
| 24 | B | 604 | CLA | C3B-C4B-NB | 3.52 | 113.67 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | C | 515 | BCR | C38-C26-C25 | -3.51 | 120.65 | 124.48 |
| 24 | C | 504 | CLA | C3B-C4B-NB | 3.51 | 113.67 | 110.53 |
| 24 | B | 604 | CLA | O2A-CGA-O1A | -3.51 | 114.85 | 123.63 |
| 24 | b | 613 | CLA | C1-C2-C3 | -3.51 | 120.45 | 126.20 |
| 37 | e | 101 | LHG | O7-C7-C8 | 3.51 | 119.07 | 111.48 |
| 24 | B | 612 | CLA | CAC-C3C-C4C | 3.50 | 129.35 | 124.79 |
| 24 | B | 610 | CLA | C1C-C2C-C3C | -3.50 | 103.30 | 106.98 |
| 24 | B | 608 | CLA | C3C-C4C-NC | 3.50 | 114.91 | 110.43 |
| 24 | c | 909 | CLA | C1D-CHD-C4C | -3.49 | 118.59 | 126.02 |
| 24 | c | 909 | CLA | C1C-C2C-C3C | -3.49 | 103.31 | 106.98 |
| 24 | b | 615 | CLA | C4C-C3C-C2C | -3.49 | 101.81 | 106.89 |
| 24 | B | 616 | CLA | C1C-C2C-C3C | -3.49 | 103.31 | 106.98 |
| 24 | B | 611 | CLA | CHC-C1C-C2C | -3.49 | 117.04 | 126.95 |
| 37 | D | 406 | LHG | O8-C23-O10 | -3.49 | 114.91 | 123.63 |
| 26 | c | 915 | BCR | C33-C5-C6 | -3.49 | 120.68 | 124.48 |
| 24 | a | 406 | CLA | CHC-C1C-C2C | -3.49 | 117.04 | 126.95 |
| 34 | C | 520 | LMG | O8-C28-C29 | 3.49 | 122.46 | 111.83 |
| 24 | b | 615 | CLA | CMB-C2B-C1B | 3.48 | 130.72 | 125.42 |
| 24 | b | 619 | CLA | C4-C3-C5 | 3.48 | 121.27 | 115.23 |
| 24 | B | 602 | CLA | C3C-C4C-NC | 3.48 | 114.89 | 110.43 |
| 24 | d | 402 | CLA | C1C-C2C-C3C | -3.48 | 103.32 | 106.98 |
| 24 | c | 907 | CLA | C3C-C4C-NC | 3.48 | 114.88 | 110.43 |
| 24 | b | 611 | CLA | C1D-CHD-C4C | -3.47 | 118.64 | 126.02 |
| 24 | b | 607 | CLA | C1C-C2C-C3C | -3.47 | 103.33 | 106.98 |
| 24 | C | 514 | CLA | C3B-C4B-NB | 3.47 | 113.62 | 110.53 |
| 24 | B | 613 | CLA | C3B-C4B-NB | 3.46 | 113.62 | 110.53 |
| 27 | a | 411 | SQD | O47-C7-O49 | -3.46 | 115.61 | 123.70 |
| 24 | C | 506 | CLA | C3D-C2D-C1D | -3.46 | 101.11 | 105.83 |
| 24 | b | 610 | CLA | C3B-C4B-NB | 3.46 | 113.62 | 110.53 |
| 24 | A | 406 | CLA | O2A-CGA-O1A | -3.46 | 114.98 | 123.63 |
| 26 | k | 102 | BCR | C24-C23-C22 | -3.45 | 121.13 | 126.23 |
| 24 | B | 605 | CLA | C3B-C4B-NB | 3.45 | 113.61 | 110.53 |
| 24 | d | 402 | CLA | C1D-CHD-C4C | -3.45 | 118.69 | 126.02 |
| 24 | c | 910 | CLA | C3B-C4B-NB | 3.45 | 113.61 | 110.53 |
| 24 | C | 506 | CLA | CAC-C3C-C4C | 3.45 | 129.28 | 124.79 |
| 24 | C | 508 | CLA | CHD-C1D-ND | -3.45 | 119.95 | 124.80 |
| 24 | b | 605 | CLA | C3C-C4C-NC | 3.44 | 114.84 | 110.43 |
| 24 | C | 511 | CLA | CHD-C1D-ND | -3.44 | 119.96 | 124.80 |
| 24 | d | 402 | CLA | O2A-CGA-CBA | 3.44 | 122.33 | 111.83 |
| 24 | b | 619 | CLA | CHC-C1C-C2C | -3.44 | 117.17 | 126.95 |
| 31 | A | 419 | PL9 | C7-C8-C9 | -3.44 | 120.90 | 126.83 |
| 24 | C | 507 | CLA | C1-C2-C3 | -3.44 | 120.56 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 511 | CLA | O2D-CGD-O1D | -3.44 | 117.15 | 123.85 |
| 24 | c | 905 | CLA | C1-C2-C3 | -3.44 | 120.56 | 126.20 |
| 24 | b | 608 | CLA | CMC-C2C-C1C | 3.44 | 130.40 | 125.03 |
| 24 | B | 607 | CLA | CMC-C2C-C1C | 3.43 | 130.40 | 125.03 |
| 24 | c | 906 | CLA | O2D-CGD-O1D | -3.42 | 117.18 | 123.85 |
| 24 | A | 410 | CLA | CHD-C4C-NC | 3.41 | 129.52 | 124.23 |
| 24 | b | 616 | CLA | O2D-CGD-O1D | -3.41 | 117.21 | 123.85 |
| 24 | A | 407 | CLA | C4-C3-C5 | 3.41 | 121.15 | 115.23 |
| 24 | C | 502 | CLA | O2D-CGD-O1D | -3.41 | 117.21 | 123.85 |
| 27 | f | 102 | SQD | C1-O5-C5 | 3.41 | 120.38 | 113.72 |
| 24 | B | 613 | CLA | C1C-C2C-C3C | -3.41 | 103.39 | 106.98 |
| 24 | c | 907 | CLA | CAC-C3C-C4C | 3.41 | 129.22 | 124.79 |
| 24 | c | 909 | CLA | C4C-C3C-C2C | -3.41 | 101.93 | 106.89 |
| 24 | C | 513 | CLA | CHD-C1D-ND | -3.41 | 120.01 | 124.80 |
| 24 | C | 505 | CLA | C4-C3-C5 | 3.41 | 121.14 | 115.23 |
| 24 | C | 504 | CLA | C4C-C3C-C2C | -3.41 | 101.93 | 106.89 |
| 31 | D | 404 | PL9 | C7-C8-C9 | -3.41 | 120.96 | 126.83 |
| 29 | B | 623 | LMT | C4B-C3B-C2B | 3.40 | 116.81 | 110.83 |
| 26 | d | 404 | BCR | C29-C30-C25 | 3.40 | 115.38 | 110.44 |
| 24 | b | 611 | CLA | C4C-C3C-C2C | -3.40 | 101.94 | 106.89 |
| 34 | C | 520 | LMG | O7-C10-C11 | 3.40 | 118.84 | 111.48 |
| 24 | C | 502 | CLA | CAC-C3C-C4C | 3.40 | 129.22 | 124.79 |
| 24 | D | 402 | CLA | C4C-C3C-C2C | -3.40 | 101.95 | 106.89 |
| 31 | A | 419 | PL9 | C22-C23-C24 | -3.39 | 119.86 | 127.62 |
| 24 | b | 614 | CLA | CMA-C3A-C4A | -3.39 | 102.66 | 111.77 |
| 24 | D | 401 | CLA | C2B-C1B-NB | 3.39 | 113.84 | 110.33 |
| 24 | B | 606 | CLA | C4C-C3C-C2C | -3.39 | 101.96 | 106.89 |
| 35 | V | 202 | HTG | C1'-S1-C1 | 3.39 | 107.76 | 100.45 |
| 25 | a | 420 | PHO | C4-C3-C5 | 3.39 | 121.11 | 115.23 |
| 26 | K | 102 | BCR | C38-C26-C25 | -3.38 | 120.79 | 124.48 |
| 26 | b | 623 | BCR | C38-C26-C25 | -3.38 | 120.80 | 124.48 |
| 24 | B | 613 | CLA | CHD-C1D-ND | -3.38 | 120.05 | 124.80 |
| 27 | F | 101 | SQD | O7-S-C6 | 3.38 | 111.80 | 106.76 |
| 24 | b | 613 | CLA | C1C-C2C-C3C | -3.38 | 103.43 | 106.98 |
| 24 | c | 906 | CLA | C4A-NA-C1A | -3.37 | 105.14 | 106.68 |
| 24 | a | 407 | CLA | CBC-CAC-C3C | -3.37 | 103.28 | 112.42 |
| 34 | c | 919 | LMG | O8-C28-C29 | 3.37 | 122.11 | 111.83 |
| 24 | d | 402 | CLA | C4C-C3C-C2C | -3.37 | 101.99 | 106.89 |
| 38 | E | 103 | HEM | CAD-CBD-CGD | 3.37 | 122.60 | 113.67 |
| 24 | B | 611 | CLA | C4B-C3B-C2B | -3.37 | 103.11 | 107.30 |
| 24 | b | 615 | CLA | C1C-C2C-C3C | -3.37 | 103.44 | 106.98 |
| 24 | B | 614 | CLA | C4B-C3B-C2B | -3.37 | 103.11 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 616 | CLA | CAC-C3C-C4C | 3.37 | 129.17 | 124.79 |
| 24 | b | 616 | CLA | CMB-C2B-C1B | 3.37 | 130.54 | 125.42 |
| 24 | B | 611 | CLA | CAC-C3C-C4C | 3.36 | 129.17 | 124.79 |
| 26 | d | 404 | BCR | C33-C5-C6 | -3.36 | 120.81 | 124.48 |
| 24 | C | 510 | CLA | O2D-CGD-O1D | -3.36 | 117.31 | 123.85 |
| 24 | C | 507 | CLA | CBC-CAC-C3C | -3.36 | 103.32 | 112.42 |
| 24 | c | 907 | CLA | C4B-C3B-C2B | -3.36 | 103.13 | 107.30 |
| 25 | a | 408 | PHO | C1A-C2A-C3A | -3.36 | 99.65 | 102.84 |
| 24 | b | 607 | CLA | CAC-C3C-C4C | 3.35 | 129.15 | 124.79 |
| 24 | C | 511 | CLA | C3B-C4B-NB | 3.35 | 113.52 | 110.53 |
| 24 | b | 618 | CLA | C1C-C2C-C3C | -3.35 | 103.46 | 106.98 |
| 24 | D | 402 | CLA | C1D-CHD-C4C | -3.35 | 118.91 | 126.02 |
| 24 | B | 610 | CLA | C3B-C4B-NB | 3.34 | 113.52 | 110.53 |
| 24 | c | 904 | CLA | C3B-C4B-NB | 3.34 | 113.52 | 110.53 |
| 24 | d | 401 | CLA | CHC-C1C-C2C | -3.34 | 117.44 | 126.95 |
| 24 | C | 507 | CLA | CHC-C1C-C2C | -3.34 | 117.45 | 126.95 |
| 37 | D | 406 | LHG | O8-C23-C24 | 3.34 | 122.03 | 111.83 |
| 24 | a | 409 | CLA | C4A-NA-C1A | -3.34 | 105.16 | 106.68 |
| 34 | c | 920 | LMG | C3-C4-C5 | 3.34 | 116.29 | 110.23 |
| 24 | B | 612 | CLA | C3C-C4C-NC | 3.34 | 114.71 | 110.43 |
| 24 | b | 616 | CLA | CHD-C1D-ND | -3.34 | 120.11 | 124.80 |
| 24 | c | 904 | CLA | CAC-C3C-C4C | 3.33 | 129.13 | 124.79 |
| 24 | b | 616 | CLA | C1-C2-C3 | -3.33 | 120.74 | 126.20 |
| 27 | A | 412 | SQD | O48-C23-C24 | 3.33 | 121.99 | 111.83 |
| 24 | A | 410 | CLA | O2D-CGD-CBD | 3.33 | 117.05 | 111.23 |
| 24 | c | 912 | CLA | C1-C2-C3 | -3.33 | 120.74 | 126.20 |
| 24 | B | 616 | CLA | CMB-C2B-C1B | 3.33 | 130.48 | 125.42 |
| 40 | V | 201 | HEC | CHA-C1A-NA | 3.32 | 128.07 | 124.45 |
| 24 | c | 902 | CLA | C2B-C1B-NB | 3.32 | 113.77 | 110.33 |
| 24 | C | 506 | CLA | CMB-C2B-C1B | 3.32 | 130.48 | 125.42 |
| 24 | b | 607 | CLA | C4B-C3B-C2B | -3.32 | 103.17 | 107.30 |
| 24 | c | 914 | CLA | CAC-C3C-C4C | 3.32 | 129.11 | 124.79 |
| 24 | B | 608 | CLA | C4B-C3B-C2B | -3.32 | 103.18 | 107.30 |
| 24 | D | 401 | CLA | O2D-CGD-O1D | -3.32 | 117.39 | 123.85 |
| 24 | B | 602 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 110.53 |
| 24 | D | 402 | CLA | C3B-C4B-NB | 3.31 | 113.48 | 110.53 |
| 37 | E | 101 | LHG | O8-C23-C24 | 3.30 | 121.91 | 111.83 |
| 24 | b | 620 | CLA | CHD-C1D-ND | -3.30 | 120.16 | 124.80 |
| 27 | B | 621 | SQD | O7-S-C6 | 3.30 | 111.68 | 106.76 |
| 24 | C | 513 | CLA | C1-C2-C3 | -3.29 | 120.80 | 126.20 |
| 36 | C | 518 | DGD | O2G-C1B-C2B | 3.29 | 118.60 | 111.48 |
| 24 | C | 504 | CLA | C1C-C2C-C3C | -3.29 | 103.52 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | b | 624 | LMG | O8-C28-C29 | 3.29 | 121.86 | 111.83 |
| 24 | C | 513 | CLA | CHD-C4C-NC | 3.29 | 129.33 | 124.23 |
| 24 | B | 602 | CLA | O2A-CGA-CBA | 3.29 | 121.86 | 111.83 |
| 24 | b | 619 | CLA | O2D-CGD-O1D | -3.29 | 117.45 | 123.85 |
| 24 | c | 911 | CLA | C4B-C3B-C2B | -3.29 | 103.22 | 107.30 |
| 31 | d | 405 | PL9 | C10-C9-C11 | 3.28 | 120.93 | 115.23 |
| 24 | b | 617 | CLA | C4A-NA-C1A | -3.28 | 105.18 | 106.68 |
| 27 | a | 402 | SQD | O47-C7-C8 | 3.28 | 118.58 | 111.48 |
| 24 | C | 512 | CLA | O2D-CGD-CBD | 3.28 | 116.96 | 111.23 |
| 38 | e | 102 | HEM | C1B-NB-C4B | 3.28 | 109.09 | 105.21 |
| 27 | a | 402 | SQD | O48-C23-C24 | 3.28 | 121.82 | 111.83 |
| 31 | d | 405 | PL9 | C53-C6-C1 | 3.28 | 121.98 | 115.28 |
| 24 | c | 912 | CLA | C4C-C3C-C2C | -3.27 | 102.13 | 106.89 |
| 24 | b | 612 | CLA | O2A-CGA-CBA | 3.27 | 121.81 | 111.83 |
| 24 | B | 613 | CLA | C1D-CHD-C4C | -3.27 | 119.07 | 126.02 |
| 24 | B | 604 | CLA | O2A-CGA-CBA | 3.27 | 121.80 | 111.83 |
| 24 | b | 614 | CLA | C3B-C4B-NB | 3.27 | 113.44 | 110.53 |
| 24 | d | 401 | CLA | C3C-C4C-NC | 3.26 | 114.61 | 110.43 |
| 24 | b | 613 | CLA | C1D-CHD-C4C | -3.26 | 119.08 | 126.02 |
| 24 | b | 612 | CLA | C1-C2-C3 | -3.26 | 120.86 | 126.20 |
| 24 | A | 410 | CLA | C3C-C4C-NC | 3.26 | 114.61 | 110.43 |
| 24 | B | 613 | CLA | O2D-CGD-O1D | -3.26 | 117.50 | 123.85 |
| 24 | c | 910 | CLA | CMC-C2C-C1C | 3.25 | 130.12 | 125.03 |
| 24 | c | 906 | CLA | C4C-C3C-C2C | -3.25 | 102.16 | 106.89 |
| 24 | c | 905 | CLA | C1D-CHD-C4C | -3.25 | 119.11 | 126.02 |
| 24 | c | 906 | CLA | CHD-C1D-ND | -3.25 | 120.23 | 124.80 |
| 31 | d | 405 | PL9 | C7-C8-C9 | -3.25 | 121.24 | 126.83 |
| 24 | A | 410 | CLA | C3B-C4B-NB | 3.24 | 113.43 | 110.53 |
| 31 | D | 404 | PL9 | C53-C6-C1 | 3.24 | 121.92 | 115.28 |
| 24 | d | 401 | CLA | C2A-C1A-CHA | -3.24 | 118.24 | 123.87 |
| 24 | b | 608 | CLA | C1D-CHD-C4C | -3.24 | 119.14 | 126.02 |
| 31 | a | 417 | PL9 | C17-C18-C19 | -3.24 | 120.21 | 127.62 |
| 24 | D | 402 | CLA | C1C-C2C-C3C | -3.24 | 103.58 | 106.98 |
| 37 | d | 407 | LHG | O7-C7-C8 | 3.23 | 118.47 | 111.48 |
| 31 | A | 419 | PL9 | C32-C33-C34 | -3.23 | 120.23 | 127.62 |
| 26 | D | 403 | BCR | C15-C14-C13 | -3.23 | 122.75 | 127.28 |
| 24 | B | 607 | CLA | CAC-C3C-C4C | 3.23 | 128.99 | 124.79 |
| 24 | c | 907 | CLA | CHC-C1C-C2C | -3.23 | 117.78 | 126.95 |
| 38 | e | 102 | HEM | CAD-CBD-CGD | 3.23 | 122.22 | 113.67 |
| 24 | C | 509 | CLA | C2A-C1A-CHA | -3.22 | 118.28 | 123.87 |
| 24 | D | 401 | CLA | C4C-C3C-C2C | -3.22 | 102.20 | 106.89 |
| 31 | A | 419 | PL9 | C20-C19-C21 | 3.22 | 120.82 | 115.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | f | 102 | SQD | O5-C5-C4 | 3.22 | 115.50 | 109.70 |
| 24 | c | 912 | CLA | C3B-C4B-NB | 3.22 | 113.40 | 110.53 |
| 37 | D | 407 | LHG | O7-C7-C8 | 3.21 | 118.44 | 111.48 |
| 38 | E | 103 | HEM | C1B-NB-C4B | 3.21 | 109.01 | 105.21 |
| 31 | a | 417 | PL9 | C42-C43-C44 | -3.21 | 120.27 | 127.62 |
| 24 | C | 507 | CLA | O2D-CGD-O1D | -3.21 | 117.60 | 123.85 |
| 24 | d | 403 | CLA | CAC-C3C-C4C | 3.21 | 128.97 | 124.79 |
| 24 | A | 407 | CLA | C3C-C4C-NC | 3.21 | 114.54 | 110.43 |
| 24 | d | 401 | CLA | C4B-C3B-C2B | -3.21 | 103.31 | 107.30 |
| 24 | b | 617 | CLA | C4C-C3C-C2C | -3.21 | 102.22 | 106.89 |
| 24 | b | 615 | CLA | C1-C2-C3 | -3.21 | 120.94 | 126.20 |
| 24 | C | 512 | CLA | C4C-C3C-C2C | -3.21 | 102.22 | 106.89 |
| 24 | c | 906 | CLA | CHC-C1C-C2C | -3.21 | 117.84 | 126.95 |
| 24 | b | 609 | CLA | CMC-C2C-C1C | 3.20 | 130.04 | 125.03 |
| 24 | a | 407 | CLA | C1C-C2C-C3C | -3.20 | 103.61 | 106.98 |
| 26 | c | 915 | BCR | C38-C26-C25 | -3.20 | 120.99 | 124.48 |
| 24 | c | 908 | CLA | CMB-C2B-C1B | 3.20 | 130.29 | 125.42 |
| 24 | a | 406 | CLA | O2A-CGA-CBA | 3.20 | 121.59 | 111.83 |
| 24 | B | 615 | CLA | CMC-C2C-C1C | 3.20 | 130.03 | 125.03 |
| 24 | D | 402 | CLA | C4-C3-C5 | 3.20 | 120.78 | 115.23 |
| 24 | b | 611 | CLA | C4B-C3B-C2B | -3.20 | 103.33 | 107.30 |
| 24 | c | 906 | CLA | CMB-C2B-C1B | 3.19 | 130.28 | 125.42 |
| 37 | d | 408 | LHG | O7-C7-C8 | 3.19 | 118.38 | 111.48 |
| 24 | B | 604 | CLA | C4C-C3C-C2C | -3.19 | 102.25 | 106.89 |
| 24 | b | 610 | CLA | C4-C3-C5 | 3.19 | 120.76 | 115.23 |
| 24 | A | 407 | CLA | C3B-C4B-NB | 3.18 | 113.37 | 110.53 |
| 24 | A | 407 | CLA | CHD-C4C-NC | 3.18 | 129.17 | 124.23 |
| 24 | B | 610 | CLA | O2A-CGA-CBA | 3.18 | 121.53 | 111.83 |
| 24 | B | 614 | CLA | C4C-C3C-C2C | -3.18 | 102.27 | 106.89 |
| 38 | e | 102 | HEM | CBA-CAA-C2A | -3.18 | 103.75 | 112.53 |
| 24 | B | 610 | CLA | CMC-C2C-C1C | 3.17 | 129.99 | 125.03 |
| 24 | B | 608 | CLA | C1D-CHD-C4C | -3.17 | 119.28 | 126.02 |
| 24 | C | 505 | CLA | C4B-C3B-C2B | -3.17 | 103.36 | 107.30 |
| 24 | A | 405 | CLA | C4C-C3C-C2C | -3.17 | 102.28 | 106.89 |
| 24 | d | 401 | CLA | CBC-CAC-C3C | -3.17 | 103.83 | 112.42 |
| 24 | b | 608 | CLA | C3B-C4B-NB | 3.17 | 113.36 | 110.53 |
| 24 | B | 607 | CLA | C4-C3-C5 | 3.17 | 120.72 | 115.23 |
| 26 | b | 622 | BCR | C29-C30-C25 | 3.17 | 115.04 | 110.44 |
| 24 | c | 905 | CLA | CMC-C2C-C1C | 3.17 | 129.98 | 125.03 |
| 24 | B | 602 | CLA | CMB-C2B-C1B | 3.16 | 130.24 | 125.42 |
| 24 | C | 507 | CLA | CMB-C2B-C1B | 3.16 | 130.24 | 125.42 |
| 38 | e | 102 | HEM | CHD-C1D-ND | 3.16 | 127.83 | 124.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 503 | CLA | C3B-C4B-NB | 3.16 | 113.35 | 110.53 |
| 24 | B | 611 | CLA | C1C-C2C-C3C | -3.16 | 103.66 | 106.98 |
| 24 | B | 616 | CLA | CAC-C3C-C4C | 3.16 | 128.90 | 124.79 |
| 24 | A | 406 | CLA | CHC-C1C-C2C | -3.16 | 117.98 | 126.95 |
| 24 | A | 405 | CLA | CAC-C3C-C4C | 3.16 | 128.90 | 124.79 |
| 24 | b | 617 | CLA | CAC-C3C-C4C | 3.16 | 128.90 | 124.79 |
| 24 | d | 403 | CLA | CHC-C1C-C2C | -3.16 | 117.98 | 126.95 |
| 24 | C | 503 | CLA | CAC-C3C-C4C | 3.16 | 128.90 | 124.79 |
| 24 | C | 514 | CLA | C4C-C3C-C2C | -3.15 | 102.30 | 106.89 |
| 24 | a | 406 | CLA | O2A-CGA-O1A | -3.15 | 115.74 | 123.63 |
| 24 | D | 401 | CLA | CHC-C1C-C2C | -3.15 | 117.99 | 126.95 |
| 24 | a | 406 | CLA | C2A-C1A-CHA | -3.15 | 118.40 | 123.87 |
| 31 | a | 417 | PL9 | C7-C8-C9 | -3.15 | 121.41 | 126.83 |
| 24 | b | 618 | CLA | CAC-C3C-C4C | 3.15 | 128.89 | 124.79 |
| 24 | B | 611 | CLA | CAA-C2A-C3A | -3.15 | 104.49 | 113.00 |
| 24 | c | 909 | CLA | C4B-C3B-C2B | -3.15 | 103.39 | 107.30 |
| 31 | A | 419 | PL9 | C53-C6-C1 | 3.15 | 121.72 | 115.28 |
| 24 | c | 911 | CLA | CHD-C1D-ND | -3.14 | 120.38 | 124.80 |
| 26 | d | 404 | BCR | C3-C4-C5 | -3.14 | 108.45 | 114.06 |
| 24 | A | 407 | CLA | C1C-C2C-C3C | -3.14 | 103.68 | 106.98 |
| 24 | b | 609 | CLA | CHD-C4C-NC | 3.14 | 129.10 | 124.23 |
| 24 | a | 406 | CLA | C4B-C3B-C2B | -3.14 | 103.40 | 107.30 |
| 24 | c | 909 | CLA | C4-C3-C5 | 3.14 | 120.68 | 115.23 |
| 24 | B | 605 | CLA | O2A-CGA-O1A | -3.14 | 115.77 | 123.63 |
| 24 | b | 609 | CLA | C4-C3-C5 | 3.14 | 120.68 | 115.23 |
| 24 | c | 909 | CLA | CHD-C1D-ND | -3.14 | 120.39 | 124.80 |
| 24 | b | 612 | CLA | C3B-C4B-NB | 3.14 | 113.33 | 110.53 |
| 24 | B | 616 | CLA | O2D-CGD-O1D | -3.14 | 117.74 | 123.85 |
| 24 | C | 503 | CLA | O2D-CGD-O1D | -3.14 | 117.75 | 123.85 |
| 24 | B | 616 | CLA | CHD-C4C-NC | 3.13 | 129.09 | 124.23 |
| 24 | c | 909 | CLA | CHC-C1C-C2C | -3.13 | 118.04 | 126.95 |
| 24 | b | 619 | CLA | C4B-C3B-C2B | -3.13 | 103.41 | 107.30 |
| 31 | d | 405 | PL9 | C27-C28-C29 | -3.13 | 120.46 | 127.62 |
| 24 | c | 902 | CLA | C4B-C3B-C2B | -3.13 | 103.41 | 107.30 |
| 40 | V | 201 | HEC | C2A-C1A-NA | -3.13 | 107.31 | 110.32 |
| 24 | b | 614 | CLA | C1-C2-C3 | -3.12 | 121.08 | 126.20 |
| 24 | A | 410 | CLA | C4-C3-C5 | 3.12 | 120.64 | 115.23 |
| 26 | k | 101 | BCR | C33-C5-C6 | -3.12 | 121.08 | 124.48 |
| 24 | b | 616 | CLA | C4-C3-C5 | 3.12 | 120.64 | 115.23 |
| 24 | C | 506 | CLA | C4C-C3C-C2C | -3.12 | 102.36 | 106.89 |
| 24 | b | 613 | CLA | C4B-C3B-C2B | -3.11 | 103.44 | 107.30 |
| 24 | c | 914 | CLA | CMC-C2C-C1C | 3.11 | 129.89 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 910 | CLA | CAC-C3C-C4C | 3.11 | 128.83 | 124.79 |
| 24 | B | 614 | CLA | O2A-CGA-CBA | 3.11 | 121.31 | 111.83 |
| 24 | A | 407 | CLA | CAA-C2A-C3A | -3.11 | 104.60 | 113.00 |
| 24 | d | 401 | CLA | CAA-C2A-C3A | -3.11 | 104.60 | 113.00 |
| 24 | d | 402 | CLA | CHC-C1C-C2C | -3.10 | 118.13 | 126.95 |
| 26 | y | 101 | BCR | C40-C30-C25 | -3.10 | 105.38 | 110.24 |
| 24 | c | 913 | CLA | C1-C2-C3 | -3.10 | 121.12 | 126.20 |
| 24 | b | 616 | CLA | C3B-C4B-NB | 3.10 | 113.30 | 110.53 |
| 24 | b | 610 | CLA | CBC-CAC-C3C | -3.10 | 104.02 | 112.42 |
| 24 | b | 614 | CLA | O2A-CGA-CBA | 3.10 | 121.28 | 111.83 |
| 24 | B | 613 | CLA | C4C-C3C-C2C | -3.10 | 102.38 | 106.89 |
| 31 | D | 404 | PL9 | C27-C28-C29 | -3.10 | 120.53 | 127.62 |
| 25 | A | 408 | PHO | CMA-C3A-C4A | -3.10 | 107.94 | 114.61 |
| 24 | B | 607 | CLA | C4B-C3B-C2B | -3.10 | 103.45 | 107.30 |
| 24 | d | 402 | CLA | C1-C2-C3 | -3.09 | 121.13 | 126.20 |
| 38 | E | 103 | HEM | CHB-C1B-NB | 3.09 | 128.19 | 124.37 |
| 24 | A | 410 | CLA | CMB-C2B-C1B | 3.09 | 130.13 | 125.42 |
| 24 | a | 406 | CLA | CAA-C2A-C1A | -3.09 | 101.85 | 111.97 |
| 29 | m | 104 | LMT | C1'-O5'-C5' | 3.09 | 119.75 | 113.72 |
| 24 | C | 504 | CLA | CAC-C3C-C4C | 3.09 | 128.81 | 124.79 |
| 24 | b | 620 | CLA | C1-C2-C3 | -3.09 | 121.14 | 126.20 |
| 26 | b | 622 | BCR | C28-C27-C26 | -3.09 | 108.55 | 114.06 |
| 24 | C | 508 | CLA | O2D-CGD-O1D | -3.08 | 117.85 | 123.85 |
| 24 | B | 611 | CLA | O2A-CGA-CBA | 3.08 | 121.24 | 111.83 |
| 24 | b | 618 | CLA | C2A-C1A-CHA | -3.08 | 118.52 | 123.87 |
| 24 | C | 509 | CLA | CHC-C1C-C2C | -3.08 | 118.19 | 126.95 |
| 24 | B | 603 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 24 | b | 619 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 24 | b | 617 | CLA | CMC-C2C-C1C | 3.08 | 129.84 | 125.03 |
| 24 | C | 513 | CLA | C1-O2A-CGA | 3.08 | 124.10 | 116.65 |
| 24 | D | 401 | CLA | CMB-C2B-C1B | 3.08 | 130.10 | 125.42 |
| 24 | B | 610 | CLA | CAC-C3C-C4C | 3.07 | 128.79 | 124.79 |
| 24 | c | 913 | CLA | CHD-C4C-NC | 3.07 | 129.00 | 124.23 |
| 24 | a | 407 | CLA | C4C-C3C-C2C | -3.07 | 102.42 | 106.89 |
| 24 | b | 614 | CLA | CAC-C3C-C4C | 3.07 | 128.79 | 124.79 |
| 24 | c | 912 | CLA | CAC-C3C-C4C | 3.07 | 128.79 | 124.79 |
| 24 | C | 514 | CLA | O2D-CGD-O1D | -3.07 | 117.87 | 123.85 |
| 26 | d | 404 | BCR | C38-C26-C25 | -3.07 | 121.13 | 124.48 |
| 27 | A | 412 | SQD | C44-O6-C1 | -3.07 | 107.21 | 113.80 |
| 24 | C | 505 | CLA | CMC-C2C-C1C | 3.07 | 129.83 | 125.03 |
| 35 | B | 624 | HTG | C1'-S1-C1 | 3.07 | 107.08 | 100.45 |
| 31 | a | 417 | PL9 | C10-C9-C11 | 3.07 | 120.55 | 115.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 610 | CLA | C4B-C3B-C2B | -3.07 | 103.49 | 107.30 |
| 24 | C | 503 | CLA | CHD-C1D-ND | -3.06 | 120.49 | 124.80 |
| 24 | B | 616 | CLA | C3B-C4B-NB | 3.06 | 113.26 | 110.53 |
| 24 | b | 614 | CLA | C4C-C3C-C2C | -3.06 | 102.44 | 106.89 |
| 24 | d | 402 | CLA | C4B-C3B-C2B | -3.06 | 103.50 | 107.30 |
| 24 | B | 611 | CLA | CMB-C2B-C1B | 3.06 | 130.08 | 125.42 |
| 24 | b | 615 | CLA | O2D-CGD-O1D | -3.06 | 117.90 | 123.85 |
| 24 | C | 508 | CLA | CMB-C2B-C1B | 3.06 | 130.07 | 125.42 |
| 35 | b | 602 | HTG | C1'-S1-C1 | 3.06 | 107.05 | 100.45 |
| 26 | b | 623 | BCR | C37-C22-C23 | 3.06 | 122.75 | 118.09 |
| 24 | c | 908 | CLA | CAC-C3C-C4C | 3.05 | 128.76 | 124.79 |
| 24 | B | 617 | CLA | CHD-C4C-NC | 3.05 | 128.97 | 124.23 |
| 24 | c | 903 | CLA | C4C-C3C-C2C | -3.05 | 102.45 | 106.89 |
| 24 | c | 914 | CLA | O2A-CGA-CBA | 3.05 | 121.14 | 111.83 |
| 26 | H | 101 | BCR | C16-C17-C18 | -3.05 | 123.00 | 127.28 |
| 24 | C | 511 | CLA | C4B-C3B-C2B | -3.05 | 103.51 | 107.30 |
| 24 | c | 913 | CLA | C3B-C4B-NB | 3.05 | 113.25 | 110.53 |
| 24 | B | 608 | CLA | CAC-C3C-C4C | 3.05 | 128.76 | 124.79 |
| 24 | b | 612 | CLA | O2A-CGA-O1A | -3.05 | 116.00 | 123.63 |
| 24 | b | 620 | CLA | C1C-C2C-C3C | -3.05 | 103.77 | 106.98 |
| 24 | B | 609 | CLA | C4B-C3B-C2B | -3.05 | 103.51 | 107.30 |
| 24 | b | 610 | CLA | O2A-CGA-O1A | -3.05 | 116.01 | 123.63 |
| 29 | C | 522 | LMT | C2'-C3'-C4' | -3.05 | 102.77 | 109.68 |
| 24 | b | 620 | CLA | C4B-C3B-C2B | -3.05 | 103.51 | 107.30 |
| 36 | H | 102 | DGD | O1G-C1A-O1A | -3.05 | 116.01 | 123.63 |
| 24 | B | 616 | CLA | C1-C2-C3 | -3.05 | 121.21 | 126.20 |
| 24 | b | 605 | CLA | O2D-CGD-O1D | -3.04 | 117.93 | 123.85 |
| 24 | c | 903 | CLA | CAC-C3C-C4C | 3.04 | 128.75 | 124.79 |
| 26 | h | 101 | BCR | C7-C8-C9 | -3.04 | 121.74 | 126.23 |
| 24 | B | 615 | CLA | CBC-CAC-C3C | -3.04 | 104.18 | 112.42 |
| 24 | A | 406 | CLA | C4B-C3B-C2B | -3.04 | 103.52 | 107.30 |
| 24 | B | 603 | CLA | C3B-C4B-NB | 3.04 | 113.24 | 110.53 |
| 24 | C | 512 | CLA | C4-C3-C5 | 3.04 | 120.50 | 115.23 |
| 35 | c | 923 | HTG | O5-C1-C2 | 3.04 | 114.50 | 110.32 |
| 24 | a | 409 | CLA | CBC-CAC-C3C | -3.04 | 104.19 | 112.42 |
| 24 | C | 504 | CLA | C4-C3-C5 | 3.04 | 120.50 | 115.23 |
| 24 | A | 406 | CLA | CMC-C2C-C1C | 3.04 | 129.78 | 125.03 |
| 24 | C | 513 | CLA | C3B-C4B-NB | 3.03 | 113.24 | 110.53 |
| 31 | a | 417 | PL9 | C30-C29-C31 | 3.03 | 120.49 | 115.23 |
| 24 | c | 908 | CLA | C4C-C3C-C2C | -3.03 | 102.48 | 106.89 |
| 24 | B | 616 | CLA | C4C-C3C-C2C | -3.03 | 102.48 | 106.89 |
| 24 | b | 606 | CLA | O2D-CGD-O1D | -3.03 | 117.95 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 914 | CLA | C3B-C4B-NB | 3.03 | 113.23 | 110.53 |
| 24 | b | 613 | CLA | O2A-CGA-O1A | -3.02 | 116.06 | 123.63 |
| 24 | B | 613 | CLA | C2A-C1A-CHA | -3.02 | 118.62 | 123.87 |
| 24 | C | 503 | CLA | C4C-C3C-C2C | -3.02 | 102.49 | 106.89 |
| 24 | c | 912 | CLA | C1C-C2C-C3C | -3.02 | 103.80 | 106.98 |
| 24 | B | 612 | CLA | CHC-C1C-C2C | -3.02 | 118.37 | 126.95 |
| 24 | C | 507 | CLA | C3C-C4C-NC | 3.02 | 114.30 | 110.43 |
| 24 | a | 409 | CLA | C4C-C3C-C2C | -3.02 | 102.50 | 106.89 |
| 24 | b | 614 | CLA | C4B-C3B-C2B | -3.02 | 103.55 | 107.30 |
| 24 | a | 406 | CLA | O2D-CGD-CBD | 3.02 | 116.50 | 111.23 |
| 24 | c | 902 | CLA | CHC-C1C-C2C | -3.01 | 118.38 | 126.95 |
| 24 | D | 401 | CLA | O2A-CGA-CBA | 3.01 | 121.02 | 111.83 |
| 24 | a | 409 | CLA | CHD-C1D-ND | -3.01 | 120.57 | 124.80 |
| 24 | a | 407 | CLA | CHD-C4C-NC | 3.01 | 128.89 | 124.23 |
| 24 | B | 608 | CLA | CHC-C1C-C2C | -3.01 | 118.41 | 126.95 |
| 31 | D | 404 | PL9 | C10-C9-C11 | 3.00 | 120.44 | 115.23 |
| 24 | b | 612 | CLA | O2D-CGD-O1D | -3.00 | 118.01 | 123.85 |
| 24 | B | 602 | CLA | CAC-C3C-C4C | 3.00 | 128.69 | 124.79 |
| 24 | b | 614 | CLA | CHC-C1C-C2C | -3.00 | 118.42 | 126.95 |
| 24 | b | 615 | CLA | CHC-C1C-C2C | -3.00 | 118.42 | 126.95 |
| 24 | b | 617 | CLA | O2A-CGA-CBA | 3.00 | 120.98 | 111.83 |
| 24 | B | 616 | CLA | CBC-CAC-C3C | -3.00 | 104.30 | 112.42 |
| 24 | a | 406 | CLA | C3C-C4C-NC | 3.00 | 114.27 | 110.43 |
| 24 | a | 409 | CLA | CMB-C2B-C1B | 3.00 | 129.98 | 125.42 |
| 24 | b | 605 | CLA | C4-C3-C5 | 3.00 | 120.43 | 115.23 |
| 24 | D | 401 | CLA | CAC-C3C-C4C | 2.99 | 128.69 | 124.79 |
| 24 | B | 615 | CLA | CHC-C1C-C2C | -2.99 | 118.44 | 126.95 |
| 24 | C | 502 | CLA | C1-C2-C3 | -2.99 | 121.30 | 126.20 |
| 24 | c | 911 | CLA | CAC-C3C-C4C | 2.99 | 128.68 | 124.79 |
| 24 | B | 606 | CLA | CHC-C1C-C2C | -2.99 | 118.45 | 126.95 |
| 24 | C | 509 | CLA | C4-C3-C5 | 2.99 | 120.41 | 115.23 |
| 24 | B | 612 | CLA | C4-C3-C5 | 2.99 | 120.41 | 115.23 |
| 24 | c | 913 | CLA | CBC-CAC-C3C | -2.99 | 104.32 | 112.42 |
| 24 | c | 914 | CLA | CMB-C2B-C1B | 2.99 | 129.97 | 125.42 |
| 24 | c | 908 | CLA | CHC-C1C-C2C | -2.98 | 118.47 | 126.95 |
| 31 | D | 404 | PL9 | C42-C43-C44 | -2.98 | 120.79 | 127.62 |
| 24 | c | 911 | CLA | C4C-C3C-C2C | -2.98 | 102.55 | 106.89 |
| 24 | C | 510 | CLA | CHC-C1C-C2C | -2.98 | 118.47 | 126.95 |
| 24 | B | 614 | CLA | C4-C3-C5 | 2.98 | 120.41 | 115.23 |
| 24 | B | 602 | CLA | CHC-C1C-C2C | -2.98 | 118.49 | 126.95 |
| 26 | B | 620 | BCR | C24-C23-C22 | -2.98 | 121.83 | 126.23 |
| 24 | b | 617 | CLA | CMB-C2B-C1B | 2.98 | 129.95 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 607 | CLA | C4C-C3C-C2C | -2.98 | 102.56 | 106.89 |
| 24 | C | 505 | CLA | CAC-C3C-C4C | 2.97 | 128.66 | 124.79 |
| 24 | c | 909 | CLA | C4A-NA-C1A | -2.97 | 105.32 | 106.68 |
| 29 | A | 417 | LMT | O5'-C5'-C4' | 2.97 | 115.87 | 109.72 |
| 24 | c | 902 | CLA | C4C-C3C-C2C | -2.97 | 102.56 | 106.89 |
| 24 | C | 503 | CLA | O2A-CGA-O1A | -2.97 | 116.19 | 123.63 |
| 24 | C | 512 | CLA | CHC-C1C-C2C | -2.97 | 118.50 | 126.95 |
| 24 | a | 407 | CLA | CAA-C2A-C3A | -2.97 | 104.97 | 113.00 |
| 36 | h | 102 | DGD | O1G-C1A-C2A | 2.97 | 120.89 | 111.83 |
| 37 | D | 406 | LHG | O7-C7-C8 | 2.97 | 117.91 | 111.48 |
| 24 | C | 514 | CLA | CHC-C1C-C2C | -2.97 | 118.52 | 126.95 |
| 24 | b | 612 | CLA | CHC-C1C-C2C | -2.97 | 118.52 | 126.95 |
| 24 | C | 502 | CLA | C4B-C3B-C2B | -2.97 | 103.61 | 107.30 |
| 24 | A | 407 | CLA | C4C-C3C-C2C | -2.96 | 102.58 | 106.89 |
| 24 | a | 407 | CLA | O2A-CGA-CBA | 2.96 | 120.87 | 111.83 |
| 24 | C | 506 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.95 |
| 24 | C | 509 | CLA | O2A-CGA-O1A | -2.96 | 116.22 | 123.63 |
| 24 | C | 502 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.95 |
| 24 | c | 902 | CLA | C1-O2A-CGA | 2.96 | 123.82 | 116.65 |
| 24 | b | 605 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.95 |
| 24 | b | 617 | CLA | CHD-C1D-ND | -2.96 | 120.64 | 124.80 |
| 24 | c | 905 | CLA | CAC-C3C-C4C | 2.96 | 128.64 | 124.79 |
| 24 | B | 610 | CLA | CHD-C4C-NC | 2.96 | 128.82 | 124.23 |
| 24 | C | 512 | CLA | C1-O2A-CGA | 2.96 | 123.81 | 116.65 |
| 24 | B | 609 | CLA | C4C-C3C-C2C | -2.96 | 102.59 | 106.89 |
| 26 | b | 621 | BCR | C7-C8-C9 | -2.96 | 121.86 | 126.23 |
| 24 | C | 507 | CLA | CAC-C3C-C4C | 2.96 | 128.63 | 124.79 |
| 37 | L | 101 | LHG | O7-C7-C8 | 2.95 | 117.87 | 111.48 |
| 24 | d | 401 | CLA | CAC-C3C-C4C | 2.95 | 128.63 | 124.79 |
| 24 | B | 605 | CLA | CHC-C1C-C2C | -2.95 | 118.56 | 126.95 |
| 24 | c | 909 | CLA | O2D-CGD-O1D | -2.95 | 118.11 | 123.85 |
| 24 | B | 604 | CLA | CHD-C4C-NC | 2.95 | 128.81 | 124.23 |
| 24 | B | 614 | CLA | C1D-CHD-C4C | -2.95 | 119.75 | 126.02 |
| 24 | A | 405 | CLA | CAA-C2A-C1A | -2.95 | 102.31 | 111.97 |
| 24 | B | 609 | CLA | O2A-CGA-CBA | 2.95 | 120.83 | 111.83 |
| 24 | b | 611 | CLA | CAA-CBA-CGA | 2.95 | 121.58 | 113.21 |
| 24 | C | 513 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 24 | C | 508 | CLA | CHC-C1C-C2C | -2.95 | 118.57 | 126.95 |
| 24 | b | 620 | CLA | CHC-C1C-C2C | -2.95 | 118.57 | 126.95 |
| 24 | b | 613 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 24 | B | 612 | CLA | CHD-C4C-NC | 2.94 | 128.80 | 124.23 |
| 24 | c | 905 | CLA | O2D-CGD-O1D | -2.94 | 118.12 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 512 | CLA | C4B-C3B-C2B | -2.94 | 103.64 | 107.30 |
| 24 | b | 613 | CLA | O2D-CGD-O1D | -2.94 | 118.12 | 123.85 |
| 26 | C | 516 | BCR | C15-C14-C13 | -2.94 | 123.15 | 127.28 |
| 24 | b | 608 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.95 |
| 24 | C | 509 | CLA | C4B-C3B-C2B | -2.94 | 103.64 | 107.30 |
| 24 | B | 616 | CLA | C11-C10-C8 | -2.94 | 106.19 | 115.97 |
| 24 | B | 610 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.89 |
| 24 | a | 409 | CLA | O2D-CGD-O1D | -2.94 | 118.13 | 123.85 |
| 27 | B | 621 | SQD | O48-C23-C24 | 2.94 | 120.79 | 111.83 |
| 24 | C | 510 | CLA | C4C-C3C-C2C | -2.94 | 102.62 | 106.89 |
| 24 | a | 409 | CLA | CHC-C1C-C2C | -2.94 | 118.60 | 126.95 |
| 37 | d | 407 | LHG | O8-C23-C24 | 2.94 | 120.79 | 111.83 |
| 24 | c | 913 | CLA | CMC-C2C-C1C | 2.94 | 129.62 | 125.03 |
| 24 | B | 603 | CLA | CHC-C1C-C2C | -2.93 | 118.61 | 126.95 |
| 24 | c | 904 | CLA | CMC-C2C-C1C | 2.93 | 129.62 | 125.03 |
| 31 | A | 419 | PL9 | C15-C14-C16 | 2.93 | 120.32 | 115.23 |
| 26 | b | 623 | BCR | C2-C1-C6 | 2.93 | 114.69 | 110.44 |
| 24 | C | 506 | CLA | C4-C3-C5 | 2.93 | 120.31 | 115.23 |
| 24 | C | 508 | CLA | C4C-C3C-C2C | -2.93 | 102.63 | 106.89 |
| 25 | A | 409 | PHO | C4-C3-C5 | 2.93 | 120.31 | 115.23 |
| 26 | B | 619 | BCR | C2-C1-C6 | 2.93 | 114.69 | 110.44 |
| 24 | b | 609 | CLA | C4C-C3C-C2C | -2.92 | 102.64 | 106.89 |
| 24 | b | 618 | CLA | C4B-C3B-C2B | -2.92 | 103.67 | 107.30 |
| 24 | C | 514 | CLA | CAC-C3C-C4C | 2.92 | 128.59 | 124.79 |
| 34 | a | 412 | LMG | C8-O7-C10 | -2.92 | 110.81 | 117.80 |
| 24 | C | 505 | CLA | CBC-CAC-C3C | -2.92 | 104.51 | 112.42 |
| 24 | b | 618 | CLA | O2A-CGA-CBA | 2.92 | 120.73 | 111.83 |
| 24 | B | 613 | CLA | C4B-C3B-C2B | -2.92 | 103.67 | 107.30 |
| 24 | B | 604 | CLA | C4B-C3B-C2B | -2.92 | 103.68 | 107.30 |
| 24 | c | 914 | CLA | CAA-C2A-C3A | -2.91 | 105.13 | 113.00 |
| 24 | A | 406 | CLA | C3C-C4C-NC | 2.91 | 114.16 | 110.43 |
| 24 | B | 615 | CLA | O2A-CGA-CBA | 2.91 | 120.71 | 111.83 |
| 26 | t | 101 | BCR | C15-C16-C17 | -2.91 | 117.56 | 123.52 |
| 26 | C | 516 | BCR | C33-C5-C6 | -2.91 | 121.31 | 124.48 |
| 24 | C | 511 | CLA | C4C-C3C-C2C | -2.91 | 102.66 | 106.89 |
| 29 | f | 103 | LMT | C1B-O5B-C5B | 2.91 | 119.40 | 113.72 |
| 24 | A | 407 | CLA | C1-C2-C3 | -2.91 | 121.43 | 126.20 |
| 24 | C | 510 | CLA | C4B-C3B-C2B | -2.91 | 103.69 | 107.30 |
| 24 | b | 605 | CLA | C4B-C3B-C2B | -2.91 | 103.69 | 107.30 |
| 24 | c | 907 | CLA | O2D-CGD-O1D | -2.91 | 118.19 | 123.85 |
| 24 | A | 410 | CLA | CBC-CAC-C3C | -2.91 | 104.54 | 112.42 |
| 24 | b | 609 | CLA | C3B-C4B-NB | 2.90 | 113.12 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | L | 101 | LHG | O8-C23-C24 | 2.90 | 120.69 | 111.83 |
| 24 | B | 607 | CLA | CHC-C1C-C2C | -2.90 | 118.70 | 126.95 |
| 26 | d | 404 | BCR | C16-C17-C18 | -2.90 | 123.21 | 127.28 |
| 35 | V | 202 | HTG | O5-C1-C2 | -2.90 | 106.32 | 110.32 |
| 24 | B | 603 | CLA | CHD-C4C-NC | 2.90 | 128.72 | 124.23 |
| 24 | B | 602 | CLA | C1-C2-C3 | -2.89 | 121.46 | 126.20 |
| 27 | A | 416 | SQD | O48-C23-O10 | -2.89 | 116.39 | 123.63 |
| 24 | C | 514 | CLA | C4-C3-C5 | 2.89 | 120.25 | 115.23 |
| 24 | B | 615 | CLA | C2A-C1A-CHA | -2.89 | 118.85 | 123.87 |
| 24 | c | 912 | CLA | O2A-CGA-CBA | 2.89 | 120.64 | 111.83 |
| 24 | c | 907 | CLA | CAA-C2A-C3A | -2.89 | 105.19 | 113.00 |
| 24 | B | 606 | CLA | C3B-C4B-NB | 2.89 | 113.11 | 110.53 |
| 24 | B | 610 | CLA | O2D-CGD-O1D | -2.89 | 118.23 | 123.85 |
| 24 | c | 904 | CLA | CMB-C2B-C1B | 2.89 | 129.81 | 125.42 |
| 24 | c | 904 | CLA | C4C-C3C-C2C | -2.89 | 102.69 | 106.89 |
| 24 | B | 609 | CLA | O2D-CGD-O1D | -2.89 | 118.23 | 123.85 |
| 25 | a | 420 | PHO | C1A-C2A-C3A | -2.88 | 100.10 | 102.84 |
| 24 | b | 620 | CLA | O2D-CGD-O1D | -2.88 | 118.24 | 123.85 |
| 24 | c | 908 | CLA | O2A-CGA-CBA | 2.88 | 120.62 | 111.83 |
| 24 | B | 607 | CLA | C1-C2-C3 | -2.88 | 121.48 | 126.20 |
| 24 | B | 611 | CLA | C1-C2-C3 | -2.88 | 121.48 | 126.20 |
| 24 | C | 508 | CLA | C3B-C4B-NB | 2.88 | 113.10 | 110.53 |
| 24 | B | 602 | CLA | C4C-C3C-C2C | -2.88 | 102.70 | 106.89 |
| 36 | D | 405 | DGD | C4D-C3D-C2D | 2.88 | 115.88 | 110.83 |
| 37 | D | 408 | LHG | O8-C23-O10 | -2.88 | 116.43 | 123.63 |
| 29 | C | 522 | LMT | C1B-O5B-C5B | 2.88 | 119.34 | 113.72 |
| 34 | J | 101 | LMG | O7-C10-C11 | 2.88 | 117.70 | 111.48 |
| 24 | c | 903 | CLA | O2A-CGA-CBA | 2.88 | 120.60 | 111.83 |
| 24 | a | 409 | CLA | CHB-C4A-NA | 2.87 | 128.55 | 124.40 |
| 24 | c | 910 | CLA | C4B-C3B-C2B | -2.87 | 103.73 | 107.30 |
| 24 | c | 902 | CLA | CAC-C3C-C4C | 2.87 | 128.53 | 124.79 |
| 24 | b | 611 | CLA | CMC-C2C-C1C | 2.87 | 129.52 | 125.03 |
| 24 | c | 907 | CLA | CMC-C2C-C1C | 2.87 | 129.52 | 125.03 |
| 24 | b | 615 | CLA | CMC-C2C-C1C | 2.87 | 129.51 | 125.03 |
| 36 | h | 102 | DGD | O2G-C1B-C2B | 2.87 | 117.68 | 111.48 |
| 24 | c | 912 | CLA | CHC-C1C-C2C | -2.86 | 118.81 | 126.95 |
| 24 | b | 614 | CLA | CMB-C2B-C1B | 2.86 | 129.78 | 125.42 |
| 24 | B | 605 | CLA | CHD-C4C-NC | 2.86 | 128.67 | 124.23 |
| 24 | c | 906 | CLA | C4B-C3B-C2B | -2.86 | 103.74 | 107.30 |
| 24 | B | 606 | CLA | C1-O2A-CGA | 2.86 | 123.58 | 116.65 |
| 24 | C | 503 | CLA | CHC-C1C-C2C | -2.86 | 118.82 | 126.95 |
| 24 | d | 403 | CLA | C4C-C3C-C2C | -2.86 | 102.73 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 617 | CLA | CMB-C2B-C1B | 2.86 | 129.77 | 125.42 |
| 24 | B | 617 | CLA | CHC-C1C-C2C | -2.86 | 118.83 | 126.95 |
| 26 | D | 403 | BCR | C29-C30-C25 | 2.86 | 114.59 | 110.44 |
| 26 | d | 404 | BCR | C21-C20-C19 | -2.86 | 114.92 | 123.20 |
| 24 | b | 618 | CLA | CHC-C1C-C2C | -2.86 | 118.83 | 126.95 |
| 31 | A | 419 | PL9 | C10-C9-C11 | 2.86 | 120.19 | 115.23 |
| 24 | b | 612 | CLA | C4C-C3C-C2C | -2.86 | 102.73 | 106.89 |
| 24 | b | 610 | CLA | CAA-C2A-C3A | -2.86 | 105.28 | 113.00 |
| 24 | b | 608 | CLA | O2D-CGD-O1D | -2.85 | 118.30 | 123.85 |
| 24 | b | 611 | CLA | CHC-C1C-C2C | -2.85 | 118.85 | 126.95 |
| 24 | c | 906 | CLA | C1-C2-C3 | -2.85 | 121.53 | 126.20 |
| 31 | A | 419 | PL9 | C42-C43-C44 | -2.85 | 121.11 | 127.62 |
| 24 | B | 617 | CLA | CHD-C1D-ND | -2.84 | 120.80 | 124.80 |
| 24 | B | 612 | CLA | C4C-C3C-C2C | -2.84 | 102.75 | 106.89 |
| 24 | B | 606 | CLA | O2A-CGA-O1A | -2.84 | 116.52 | 123.63 |
| 26 | b | 622 | BCR | C38-C26-C25 | -2.84 | 121.39 | 124.48 |
| 24 | b | 615 | CLA | C4B-C3B-C2B | -2.84 | 103.78 | 107.30 |
| 24 | A | 407 | CLA | CED-O2D-CGD | 2.84 | 122.35 | 115.92 |
| 24 | b | 610 | CLA | O2A-CGA-CBA | 2.83 | 120.48 | 111.83 |
| 24 | d | 403 | CLA | CMC-C2C-C1C | 2.83 | 129.46 | 125.03 |
| 24 | C | 507 | CLA | C4B-C3B-C2B | -2.83 | 103.78 | 107.30 |
| 24 | b | 620 | CLA | O2A-CGA-CBA | 2.83 | 120.47 | 111.83 |
| 24 | a | 409 | CLA | CHD-C4C-NC | 2.83 | 128.62 | 124.23 |
| 24 | b | 616 | CLA | O2A-CGA-CBA | 2.83 | 120.47 | 111.83 |
| 24 | A | 405 | CLA | CMC-C2C-C1C | 2.83 | 129.46 | 125.03 |
| 24 | b | 607 | CLA | CHC-C1C-C2C | -2.83 | 118.91 | 126.95 |
| 24 | b | 605 | CLA | O2A-CGA-CBA | 2.83 | 120.46 | 111.83 |
| 24 | B | 602 | CLA | CHD-C4C-NC | 2.83 | 128.62 | 124.23 |
| 24 | B | 610 | CLA | CHC-C1C-C2C | -2.83 | 118.91 | 126.95 |
| 24 | B | 614 | CLA | O2A-CGA-O1A | -2.83 | 116.56 | 123.63 |
| 24 | C | 506 | CLA | C3B-C4B-NB | 2.83 | 113.05 | 110.53 |
| 29 | m | 102 | LMT | O5'-C5'-C4' | 2.83 | 115.57 | 109.72 |
| 36 | C | 519 | DGD | O3G-C3G-C2G | -2.83 | 103.95 | 110.82 |
| 24 | c | 912 | CLA | CHD-C4C-NC | 2.82 | 128.61 | 124.23 |
| 24 | c | 911 | CLA | C4-C3-C5 | 2.82 | 120.13 | 115.23 |
| 24 | A | 405 | CLA | CHC-C1C-C2C | -2.82 | 118.93 | 126.95 |
| 36 | H | 102 | DGD | O2G-C1B-C2B | 2.82 | 117.58 | 111.48 |
| 26 | T | 102 | BCR | C21-C20-C19 | -2.82 | 115.03 | 123.20 |
| 24 | B | 614 | CLA | CHC-C1C-C2C | -2.82 | 118.94 | 126.95 |
| 24 | d | 402 | CLA | C2A-C1A-CHA | -2.82 | 118.98 | 123.87 |
| 34 | z | 101 | LMG | O8-C28-C29 | 2.82 | 120.42 | 111.83 |
| 24 | A | 405 | CLA | C4B-C3B-C2B | -2.81 | 103.80 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A | 406 | CLA | CED-O2D-CGD | 2.81 | 122.30 | 115.92 |
| 35 | B | 625 | HTG | C1'-S1-C1 | 2.81 | 106.52 | 100.45 |
| 24 | C | 507 | CLA | CAA-C2A-C3A | -2.81 | 105.41 | 113.00 |
| 24 | D | 401 | CLA | O2A-CGA-O1A | -2.81 | 116.60 | 123.63 |
| 24 | c | 914 | CLA | C2A-C1A-CHA | -2.81 | 118.99 | 123.87 |
| 36 | D | 405 | DGD | O1G-C1A-C2A | 2.81 | 120.40 | 111.83 |
| 24 | b | 616 | CLA | C2A-C1A-CHA | -2.81 | 119.00 | 123.87 |
| 36 | C | 517 | DGD | O3G-C3G-C2G | -2.81 | 103.99 | 110.82 |
| 24 | B | 606 | CLA | CHD-C1D-ND | -2.81 | 120.85 | 124.80 |
| 24 | b | 610 | CLA | CMB-C2B-C1B | 2.80 | 129.69 | 125.42 |
| 24 | b | 607 | CLA | C5-C3-C2 | -2.80 | 114.88 | 121.17 |
| 24 | d | 403 | CLA | C4B-C3B-C2B | -2.80 | 103.82 | 107.30 |
| 24 | c | 911 | CLA | CHC-C1C-C2C | -2.80 | 118.98 | 126.95 |
| 24 | C | 511 | CLA | CHD-C4C-NC | 2.80 | 128.57 | 124.23 |
| 24 | A | 407 | CLA | CHC-C1C-C2C | -2.80 | 118.99 | 126.95 |
| 24 | c | 910 | CLA | CHD-C4C-NC | 2.80 | 128.57 | 124.23 |
| 24 | D | 402 | CLA | CHC-C1C-C2C | -2.80 | 118.99 | 126.95 |
| 24 | B | 609 | CLA | CMC-C2C-C1C | 2.80 | 129.41 | 125.03 |
| 24 | c | 904 | CLA | CHC-C1C-C2C | -2.80 | 118.99 | 126.95 |
| 24 | B | 611 | CLA | C4-C3-C5 | 2.80 | 120.08 | 115.23 |
| 24 | b | 608 | CLA | O2A-CGA-CBA | 2.80 | 120.36 | 111.83 |
| 24 | B | 616 | CLA | CMC-C2C-C1C | 2.80 | 129.40 | 125.03 |
| 24 | B | 605 | CLA | C4B-C3B-C2B | -2.80 | 103.83 | 107.30 |
| 24 | C | 511 | CLA | CMC-C2C-C1C | 2.80 | 129.40 | 125.03 |
| 31 | D | 404 | PL9 | C40-C39-C41 | 2.80 | 120.08 | 115.23 |
| 27 | L | 102 | SQD | O48-C23-C24 | 2.79 | 120.35 | 111.83 |
| 24 | B | 606 | CLA | C2A-C1A-CHA | -2.79 | 119.02 | 123.87 |
| 38 | e | 102 | HEM | CHB-C1B-NB | 2.79 | 127.82 | 124.37 |
| 34 | C | 521 | LMG | C8-O7-C10 | -2.79 | 111.12 | 117.80 |
| 26 | h | 101 | BCR | C24-C23-C22 | -2.79 | 122.11 | 126.23 |
| 27 | f | 102 | SQD | O48-C23-C24 | 2.79 | 120.34 | 111.83 |
| 24 | B | 602 | CLA | O2D-CGD-O1D | -2.79 | 118.42 | 123.85 |
| 24 | d | 402 | CLA | CAA-C2A-C3A | -2.79 | 105.47 | 113.00 |
| 24 | B | 616 | CLA | CHC-C1C-C2C | -2.79 | 119.03 | 126.95 |
| 24 | c | 905 | CLA | C4C-C3C-C2C | -2.79 | 102.84 | 106.89 |
| 24 | B | 612 | CLA | CMB-C2B-C1B | 2.79 | 129.66 | 125.42 |
| 24 | C | 508 | CLA | CBC-CAC-C3C | -2.78 | 104.87 | 112.42 |
| 24 | c | 905 | CLA | C4B-C3B-C2B | -2.78 | 103.84 | 107.30 |
| 34 | c | 920 | LMG | O6-C5-C4 | 2.78 | 114.71 | 109.70 |
| 24 | B | 617 | CLA | C4B-C3B-C2B | -2.78 | 103.84 | 107.30 |
| 24 | b | 612 | CLA | CHD-C4C-NC | 2.78 | 128.54 | 124.23 |
| 26 | T | 102 | BCR | C7-C6-C5 | -2.78 | 115.15 | 121.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 906 | CLA | C1-O2A-CGA | 2.78 | 123.37 | 116.65 |
| 34 | c | 920 | LMG | O8-C28-C29 | 2.78 | 120.30 | 111.83 |
| 24 | b | 613 | CLA | C2A-C1A-CHA | -2.77 | 119.05 | 123.87 |
| 34 | J | 101 | LMG | O8-C28-O10 | -2.77 | 116.69 | 123.63 |
| 31 | a | 417 | PL9 | C53-C6-C1 | 2.77 | 120.96 | 115.28 |
| 24 | A | 410 | CLA | CHC-C1C-C2C | -2.77 | 119.07 | 126.95 |
| 24 | d | 401 | CLA | CMA-C3A-C2A | -2.77 | 103.27 | 113.98 |
| 24 | C | 504 | CLA | CHC-C1C-C2C | -2.77 | 119.08 | 126.95 |
| 24 | c | 904 | CLA | O2D-CGD-O1D | -2.77 | 118.46 | 123.85 |
| 24 | C | 509 | CLA | C4C-C3C-C2C | -2.77 | 102.86 | 106.89 |
| 31 | D | 404 | PL9 | C20-C19-C21 | 2.76 | 120.03 | 115.23 |
| 24 | c | 913 | CLA | C4-C3-C5 | 2.76 | 120.02 | 115.23 |
| 24 | C | 503 | CLA | C4-C3-C5 | 2.76 | 120.02 | 115.23 |
| 24 | b | 606 | CLA | C1C-C2C-C3C | -2.76 | 104.08 | 106.98 |
| 40 | V | 201 | HEC | CHD-C4C-NC | 2.76 | 127.46 | 124.45 |
| 24 | c | 903 | CLA | C1-C2-C3 | -2.76 | 121.67 | 126.20 |
| 27 | a | 402 | SQD | O5-C5-C4 | 2.76 | 114.67 | 109.70 |
| 24 | c | 914 | CLA | C4C-C3C-C2C | -2.76 | 102.88 | 106.89 |
| 24 | A | 407 | CLA | C4B-C3B-C2B | -2.76 | 103.88 | 107.30 |
| 24 | B | 615 | CLA | C4-C3-C5 | 2.75 | 120.01 | 115.23 |
| 24 | a | 407 | CLA | C1-C2-C3 | -2.75 | 121.69 | 126.20 |
| 24 | c | 905 | CLA | CHC-C1C-C2C | -2.75 | 119.12 | 126.95 |
| 24 | A | 405 | CLA | C2A-C1A-CHA | -2.75 | 119.09 | 123.87 |
| 24 | b | 616 | CLA | C1C-C2C-C3C | -2.75 | 104.09 | 106.98 |
| 24 | B | 614 | CLA | CED-O2D-CGD | 2.75 | 122.16 | 115.92 |
| 24 | C | 513 | CLA | CHC-C1C-C2C | -2.75 | 119.13 | 126.95 |
| 24 | b | 606 | CLA | CHC-C1C-C2C | -2.75 | 119.13 | 126.95 |
| 24 | B | 612 | CLA | CMC-C2C-C1C | 2.75 | 129.33 | 125.03 |
| 27 | A | 412 | SQD | O47-C7-O49 | -2.75 | 117.28 | 123.70 |
| 34 | b | 624 | LMG | O7-C10-C11 | 2.75 | 117.42 | 111.48 |
| 24 | c | 902 | CLA | CMC-C2C-C1C | 2.75 | 129.33 | 125.03 |
| 24 | c | 904 | CLA | C4-C3-C5 | 2.75 | 120.00 | 115.23 |
| 24 | a | 406 | CLA | C4-C3-C5 | 2.75 | 119.99 | 115.23 |
| 24 | b | 605 | CLA | C3B-C4B-NB | 2.75 | 112.98 | 110.53 |
| 26 | t | 101 | BCR | C1-C6-C7 | 2.75 | 123.10 | 115.65 |
| 24 | a | 407 | CLA | CMB-C2B-C1B | 2.74 | 129.60 | 125.42 |
| 24 | C | 510 | CLA | CMB-C2B-C1B | 2.74 | 129.60 | 125.42 |
| 31 | a | 417 | PL9 | C7-C3-C4 | 2.74 | 119.17 | 116.91 |
| 24 | B | 610 | CLA | CBC-CAC-C3C | -2.74 | 104.99 | 112.42 |
| 24 | a | 406 | CLA | O2D-CGD-O1D | -2.74 | 118.51 | 123.85 |
| 24 | c | 903 | CLA | CHC-C1C-C2C | -2.74 | 119.16 | 126.95 |
| 24 | C | 508 | CLA | CHD-C4C-NC | 2.74 | 128.47 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | d | 402 | CLA | C4-C3-C5 | 2.74 | 119.98 | 115.23 |
| 31 | d | 405 | PL9 | C42-C43-C44 | -2.74 | 121.36 | 127.62 |
| 40 | v | 202 | HEC | CHD-C4C-NC | 2.73 | 127.43 | 124.45 |
| 24 | b | 616 | CLA | C4B-C3B-C2B | -2.73 | 103.90 | 107.30 |
| 24 | c | 910 | CLA | C4C-C3C-C2C | -2.73 | 102.91 | 106.89 |
| 24 | c | 905 | CLA | C4-C3-C5 | 2.73 | 119.97 | 115.23 |
| 24 | c | 911 | CLA | CHD-C4C-NC | 2.73 | 128.47 | 124.23 |
| 26 | y | 101 | BCR | C10-C11-C12 | -2.73 | 115.29 | 123.20 |
| 26 | a | 410 | BCR | C2-C1-C6 | 2.73 | 114.40 | 110.44 |
| 24 | c | 911 | CLA | CMC-C2C-C1C | 2.73 | 129.30 | 125.03 |
| 24 | C | 512 | CLA | CHD-C4C-NC | 2.73 | 128.46 | 124.23 |
| 24 | d | 401 | CLA | CHD-C4C-NC | 2.73 | 128.46 | 124.23 |
| 31 | a | 417 | PL9 | C25-C24-C26 | 2.73 | 119.96 | 115.23 |
| 24 | A | 410 | CLA | CAA-C2A-C3A | -2.73 | 105.63 | 113.00 |
| 24 | C | 511 | CLA | O2A-CGA-CBA | 2.73 | 120.14 | 111.83 |
| 38 | e | 102 | HEM | CHA-C1A-NA | 2.72 | 128.79 | 123.86 |
| 24 | C | 504 | CLA | O2D-CGD-O1D | -2.72 | 118.55 | 123.85 |
| 24 | a | 406 | CLA | CMA-C3A-C2A | -2.72 | 103.47 | 113.98 |
| 26 | k | 101 | BCR | C24-C23-C22 | -2.72 | 122.21 | 126.23 |
| 24 | C | 504 | CLA | C4B-C3B-C2B | -2.72 | 103.92 | 107.30 |
| 24 | B | 607 | CLA | CAA-C2A-C3A | -2.72 | 105.66 | 113.00 |
| 24 | A | 410 | CLA | O2A-CGA-CBA | 2.72 | 120.12 | 111.83 |
| 24 | c | 910 | CLA | CHC-C1C-C2C | -2.72 | 119.23 | 126.95 |
| 24 | d | 401 | CLA | O2A-CGA-O1A | -2.72 | 116.83 | 123.63 |
| 24 | b | 608 | CLA | C4C-C3C-C2C | -2.72 | 102.94 | 106.89 |
| 24 | c | 903 | CLA | C3B-C4B-NB | 2.71 | 112.95 | 110.53 |
| 24 | b | 611 | CLA | C4-C3-C5 | 2.71 | 119.93 | 115.23 |
| 24 | b | 606 | CLA | CMB-C2B-C1B | 2.71 | 129.55 | 125.42 |
| 24 | A | 406 | CLA | CHB-C4A-NA | 2.71 | 128.31 | 124.40 |
| 24 | B | 605 | CLA | O2A-CGA-CBA | 2.71 | 120.09 | 111.83 |
| 24 | c | 904 | CLA | O2A-CGA-CBA | 2.71 | 120.09 | 111.83 |
| 24 | B | 611 | CLA | O2D-CGD-O1D | -2.71 | 118.58 | 123.85 |
| 24 | B | 609 | CLA | CHC-C1C-C2C | -2.70 | 119.26 | 126.95 |
| 24 | b | 617 | CLA | CMA-C3A-C4A | -2.70 | 104.50 | 111.77 |
| 24 | c | 903 | CLA | CHD-C4C-NC | 2.70 | 128.42 | 124.23 |
| 34 | J | 101 | LMG | O8-C28-C29 | 2.70 | 120.06 | 111.83 |
| 24 | B | 606 | CLA | O2A-CGA-CBA | 2.70 | 120.06 | 111.83 |
| 24 | a | 407 | CLA | CHC-C1C-C2C | -2.70 | 119.28 | 126.95 |
| 24 | c | 914 | CLA | CHC-C1C-C2C | -2.70 | 119.29 | 126.95 |
| 24 | c | 913 | CLA | C4C-C3C-C2C | -2.69 | 102.97 | 106.89 |
| 24 | C | 510 | CLA | C1-O2A-CGA | 2.69 | 123.17 | 116.65 |
| 34 | B | 622 | LMG | O8-C28-O10 | -2.69 | 116.89 | 123.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 612 | CLA | CAC-C3C-C4C | 2.69 | 128.29 | 124.79 |
| 35 | B | 634 | HTG | C1-O5-C5 | 2.69 | 117.39 | 112.56 |
| 24 | b | 610 | CLA | CHD-C4C-NC | 2.69 | 128.40 | 124.23 |
| 27 | F | 101 | SQD | O48-C23-C24 | 2.69 | 120.04 | 111.83 |
| 27 | F | 101 | SQD | C3-C4-C5 | 2.69 | 115.11 | 110.23 |
| 24 | B | 612 | CLA | C4B-C3B-C2B | -2.69 | 103.96 | 107.30 |
| 24 | b | 606 | CLA | C4B-C3B-C2B | -2.69 | 103.96 | 107.30 |
| 24 | b | 610 | CLA | C4B-C3B-C2B | -2.69 | 103.96 | 107.30 |
| 24 | C | 505 | CLA | CHC-C1C-C2C | -2.69 | 119.31 | 126.95 |
| 24 | d | 401 | CLA | CHB-C1B-NB | -2.69 | 120.02 | 124.05 |
| 37 | D | 408 | LHG | O8-C23-C24 | 2.68 | 120.02 | 111.83 |
| 24 | c | 913 | CLA | O2D-CGD-O1D | -2.68 | 118.62 | 123.85 |
| 31 | a | 417 | PL9 | C20-C19-C21 | 2.68 | 119.89 | 115.23 |
| 31 | A | 419 | PL9 | C8-C7-C3 | 2.68 | 118.97 | 112.03 |
| 36 | h | 102 | DGD | O1G-C1A-O1A | -2.68 | 116.92 | 123.63 |
| 24 | B | 607 | CLA | C4C-C3C-C2C | -2.68 | 102.99 | 106.89 |
| 26 | t | 101 | BCR | C7-C6-C5 | -2.68 | 115.38 | 121.56 |
| 24 | B | 609 | CLA | CMA-C3A-C4A | -2.68 | 104.57 | 111.77 |
| 24 | b | 613 | CLA | CHD-C4C-NC | 2.68 | 128.38 | 124.23 |
| 24 | d | 403 | CLA | CHD-C4C-NC | 2.68 | 128.38 | 124.23 |
| 24 | C | 514 | CLA | C2A-C1A-CHA | -2.68 | 119.22 | 123.87 |
| 34 | Z | 101 | LMG | O6-C5-C4 | 2.68 | 114.52 | 109.70 |
| 24 | d | 402 | CLA | O2A-CGA-O1A | -2.68 | 116.94 | 123.63 |
| 24 | c | 907 | CLA | C4-C3-C5 | 2.67 | 119.87 | 115.23 |
| 24 | c | 913 | CLA | CED-O2D-CGD | 2.67 | 121.98 | 115.92 |
| 36 | d | 406 | DGD | C1E-O6E-C5E | 2.67 | 118.94 | 113.72 |
| 31 | A | 419 | PL9 | C7-C3-C4 | 2.67 | 119.11 | 116.91 |
| 24 | b | 614 | CLA | C4-C3-C5 | 2.67 | 119.86 | 115.23 |
| 24 | B | 612 | CLA | C2A-C1A-CHA | -2.67 | 119.23 | 123.87 |
| 24 | a | 409 | CLA | CMA-C3A-C4A | -2.67 | 104.60 | 111.77 |
| 31 | A | 419 | PL9 | C25-C24-C26 | 2.67 | 119.86 | 115.23 |
| 26 | A | 411 | BCR | C33-C5-C6 | -2.67 | 121.58 | 124.48 |
| 24 | b | 605 | CLA | C4C-C3C-C2C | -2.66 | 103.01 | 106.89 |
| 24 | c | 913 | CLA | CHC-C1C-C2C | -2.66 | 119.38 | 126.95 |
| 24 | B | 608 | CLA | C4C-C3C-C2C | -2.66 | 103.02 | 106.89 |
| 24 | b | 612 | CLA | C4B-C3B-C2B | -2.66 | 103.99 | 107.30 |
| 24 | B | 614 | CLA | CAC-C3C-C4C | 2.66 | 128.25 | 124.79 |
| 24 | b | 609 | CLA | O2A-CGA-O1A | -2.66 | 116.97 | 123.63 |
| 38 | e | 102 | HEM | CHA-C4D-ND | 2.66 | 127.66 | 124.37 |
| 24 | b | 606 | CLA | C1-C2-C3 | -2.66 | 121.84 | 126.20 |
| 24 | c | 914 | CLA | CHD-C4C-NC | 2.66 | 128.35 | 124.23 |
| 24 | B | 605 | CLA | C4C-C3C-C2C | -2.66 | 103.03 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 615 | CLA | CMB-C2B-C1B | 2.66 | 129.46 | 125.42 |
| 24 | C | 513 | CLA | CMC-C2C-C1C | 2.65 | 129.18 | 125.03 |
| 24 | C | 509 | CLA | CHD-C4C-NC | 2.65 | 128.34 | 124.23 |
| 24 | b | 609 | CLA | CHC-C1C-C2C | -2.65 | 119.41 | 126.95 |
| 24 | b | 607 | CLA | C2A-C1A-CHA | -2.65 | 119.27 | 123.87 |
| 24 | C | 511 | CLA | CHC-C1C-C2C | -2.65 | 119.42 | 126.95 |
| 24 | c | 908 | CLA | CMC-C2C-C1C | 2.65 | 129.17 | 125.03 |
| 24 | b | 617 | CLA | CHC-C1C-C2C | -2.65 | 119.43 | 126.95 |
| 24 | C | 507 | CLA | CHD-C4C-NC | 2.64 | 128.33 | 124.23 |
| 31 | d | 405 | PL9 | C15-C14-C16 | 2.64 | 119.82 | 115.23 |
| 24 | c | 907 | CLA | O2A-CGA-O1A | -2.64 | 117.02 | 123.63 |
| 24 | B | 604 | CLA | CHC-C1C-C2C | -2.64 | 119.44 | 126.95 |
| 24 | C | 511 | CLA | C4-C3-C5 | 2.64 | 119.81 | 115.23 |
| 26 | K | 103 | BCR | C15-C14-C13 | -2.64 | 123.57 | 127.28 |
| 24 | D | 402 | CLA | C4B-C3B-C2B | -2.64 | 104.02 | 107.30 |
| 24 | B | 617 | CLA | C1C-C2C-C3C | -2.64 | 104.20 | 106.98 |
| 24 | A | 406 | CLA | CMA-C3A-C2A | -2.64 | 103.77 | 113.98 |
| 24 | c | 903 | CLA | CMC-C2C-C1C | 2.64 | 129.16 | 125.03 |
| 24 | b | 609 | CLA | C2A-C1A-CHA | -2.64 | 119.28 | 123.87 |
| 31 | a | 417 | PL9 | C37-C36-C34 | -2.64 | 104.44 | 113.19 |
| 26 | H | 101 | BCR | C37-C22-C21 | -2.64 | 118.54 | 122.82 |
| 24 | C | 507 | CLA | C4-C3-C5 | 2.64 | 119.81 | 115.23 |
| 24 | b | 617 | CLA | O2A-CGA-O1A | -2.64 | 117.03 | 123.63 |
| 31 | A | 419 | PL9 | C35-C34-C36 | 2.64 | 119.81 | 115.23 |
| 24 | C | 505 | CLA | C4C-C3C-C2C | -2.64 | 103.05 | 106.89 |
| 24 | c | 903 | CLA | O2A-CGA-O1A | -2.64 | 117.03 | 123.63 |
| 24 | D | 402 | CLA | C2A-C1A-CHA | -2.64 | 119.29 | 123.87 |
| 27 | f | 102 | SQD | O7-S-C6 | 2.63 | 110.69 | 106.76 |
| 24 | c | 910 | CLA | O2A-CGA-CBA | 2.63 | 119.86 | 111.83 |
| 26 | k | 101 | BCR | C7-C8-C9 | -2.63 | 122.34 | 126.23 |
| 34 | c | 920 | LMG | C8-O7-C10 | -2.63 | 111.50 | 117.80 |
| 24 | B | 608 | CLA | O2D-CGD-O1D | -2.63 | 118.73 | 123.85 |
| 36 | c | 918 | DGD | O1G-C1A-C2A | 2.63 | 119.85 | 111.83 |
| 26 | T | 102 | BCR | C1-C6-C7 | 2.63 | 122.78 | 115.65 |
| 24 | D | 402 | CLA | CAC-C3C-C4C | 2.63 | 128.21 | 124.79 |
| 24 | b | 609 | CLA | O2A-CGA-CBA | 2.63 | 119.84 | 111.83 |
| 26 | b | 623 | BCR | C15-C14-C13 | -2.63 | 123.59 | 127.28 |
| 24 | B | 617 | CLA | O2A-CGA-CBA | 2.63 | 119.84 | 111.83 |
| 25 | A | 409 | PHO | CMB-C2B-C3B | 2.62 | 129.92 | 124.68 |
| 37 | L | 101 | LHG | O8-C23-O10 | -2.62 | 117.08 | 123.63 |
| 24 | B | 604 | CLA | CBC-CAC-C3C | -2.62 | 105.32 | 112.42 |
| 35 | B | 626 | HTG | O5-C1-C2 | 2.62 | 113.93 | 110.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 913 | CLA | O2A-CGA-CBA | 2.62 | 119.81 | 111.83 |
| 25 | a | 408 | PHO | CBC-CAC-C3C | -2.62 | 109.13 | 112.87 |
| 24 | C | 514 | CLA | C4B-C3B-C2B | -2.61 | 104.05 | 107.30 |
| 24 | B | 613 | CLA | CHC-C1C-C2C | -2.61 | 119.52 | 126.95 |
| 24 | B | 608 | CLA | C1-O2A-CGA | 2.61 | 122.98 | 116.65 |
| 29 | A | 417 | LMT | C1'-O5'-C5' | 2.61 | 118.82 | 113.72 |
| 24 | C | 511 | CLA | O2A-CGA-O1A | -2.61 | 117.09 | 123.63 |
| 24 | C | 513 | CLA | C4-C3-C5 | 2.61 | 119.76 | 115.23 |
| 24 | c | 902 | CLA | CBC-CAC-C3C | -2.61 | 105.34 | 112.42 |
| 36 | H | 102 | DGD | O1G-C1A-C2A | 2.61 | 119.79 | 111.83 |
| 36 | d | 406 | DGD | O1G-C1A-C2A | 2.61 | 119.79 | 111.83 |
| 24 | C | 512 | CLA | CMB-C2B-C1B | 2.61 | 129.39 | 125.42 |
| 24 | c | 905 | CLA | CMB-C2B-C1B | 2.61 | 129.39 | 125.42 |
| 24 | c | 902 | CLA | CHD-C4C-NC | 2.61 | 128.27 | 124.23 |
| 26 | c | 915 | BCR | C3-C4-C5 | -2.60 | 109.41 | 114.06 |
| 24 | B | 612 | CLA | O2A-CGA-CBA | 2.60 | 119.77 | 111.83 |
| 34 | a | 412 | LMG | O8-C28-C29 | 2.60 | 119.77 | 111.83 |
| 37 | d | 409 | LHG | O8-C23-C24 | 2.60 | 119.76 | 111.83 |
| 26 | D | 403 | BCR | C10-C11-C12 | -2.60 | 115.67 | 123.20 |
| 24 | b | 608 | CLA | CMB-C2B-C1B | 2.60 | 129.38 | 125.42 |
| 24 | c | 907 | CLA | CHD-C4C-NC | 2.60 | 128.26 | 124.23 |
| 24 | C | 513 | CLA | O2A-CGA-CBA | 2.60 | 119.75 | 111.83 |
| 24 | C | 502 | CLA | CHD-C4C-NC | 2.59 | 128.25 | 124.23 |
| 24 | C | 510 | CLA | CMC-C2C-C1C | 2.59 | 129.09 | 125.03 |
| 24 | B | 607 | CLA | C1-O2A-CGA | 2.59 | 122.93 | 116.65 |
| 24 | B | 609 | CLA | CAA-C2A-C3A | -2.59 | 106.00 | 113.00 |
| 24 | c | 904 | CLA | C4B-C3B-C2B | -2.59 | 104.08 | 107.30 |
| 26 | k | 101 | BCR | C38-C26-C25 | -2.59 | 121.66 | 124.48 |
| 26 | K | 102 | BCR | C16-C17-C18 | -2.59 | 123.65 | 127.28 |
| 24 | c | 912 | CLA | O2D-CGD-O1D | -2.58 | 118.82 | 123.85 |
| 26 | t | 101 | BCR | C21-C20-C19 | -2.58 | 115.71 | 123.20 |
| 31 | d | 405 | PL9 | C45-C44-C46 | 2.58 | 119.71 | 115.23 |
| 24 | c | 903 | CLA | C2A-C1A-CHA | -2.58 | 119.38 | 123.87 |
| 24 | C | 508 | CLA | CAC-C3C-C4C | 2.58 | 128.15 | 124.79 |
| 24 | b | 615 | CLA | O2A-CGA-O1A | -2.58 | 117.17 | 123.63 |
| 24 | c | 911 | CLA | O2A-CGA-CBA | 2.58 | 119.70 | 111.83 |
| 31 | a | 417 | PL9 | C40-C39-C41 | 2.58 | 119.71 | 115.23 |
| 24 | b | 611 | CLA | CHD-C4C-NC | 2.58 | 128.23 | 124.23 |
| 24 | C | 510 | CLA | C4-C3-C5 | 2.58 | 119.71 | 115.23 |
| 26 | D | 403 | BCR | C33-C5-C6 | -2.58 | 121.67 | 124.48 |
| 24 | A | 405 | CLA | O2A-CGA-CBA | 2.58 | 119.70 | 111.83 |
| 26 | K | 102 | BCR | C24-C23-C22 | -2.58 | 122.42 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 27 | f | 102 | SQD | O47-C7-O49 | -2.58 | 117.67 | 123.70 |
| 26 | h | 101 | BCR | C10-C11-C12 | -2.58 | 115.73 | 123.20 |
| 35 | b | 627 | HTG | C1-C2-C3 | 2.58 | 115.59 | 110.55 |
| 25 | A | 408 | PHO | CMB-C2B-C3B | 2.58 | 129.84 | 124.68 |
| 31 | A | 419 | PL9 | C45-C44-C46 | 2.58 | 119.70 | 115.23 |
| 24 | A | 407 | CLA | C2A-C1A-CHA | -2.58 | 119.39 | 123.87 |
| 24 | b | 616 | CLA | CMC-C2C-C1C | 2.58 | 129.06 | 125.03 |
| 34 | a | 412 | LMG | C7-O1-C1 | -2.58 | 108.28 | 113.80 |
| 24 | c | 912 | CLA | C4-C3-C5 | 2.57 | 119.69 | 115.23 |
| 24 | b | 606 | CLA | O2A-CGA-CBA | 2.57 | 119.67 | 111.83 |
| 24 | b | 615 | CLA | CHD-C4C-NC | 2.57 | 128.21 | 124.23 |
| 24 | c | 906 | CLA | CMC-C2C-C1C | 2.57 | 129.04 | 125.03 |
| 24 | b | 612 | CLA | C2A-C1A-CHA | -2.57 | 119.41 | 123.87 |
| 24 | C | 506 | CLA | CMD-C2D-C3D | -2.57 | 121.81 | 127.69 |
| 24 | B | 609 | CLA | CAC-C3C-C4C | 2.56 | 128.13 | 124.79 |
| 26 | y | 101 | BCR | C21-C20-C19 | -2.56 | 115.77 | 123.20 |
| 26 | d | 404 | BCR | C15-C14-C13 | -2.56 | 123.69 | 127.28 |
| 24 | b | 608 | CLA | C4B-C3B-C2B | -2.56 | 104.12 | 107.30 |
| 24 | C | 503 | CLA | O2A-CGA-CBA | 2.56 | 119.64 | 111.83 |
| 24 | B | 606 | CLA | C4-C3-C5 | 2.56 | 119.67 | 115.23 |
| 24 | B | 615 | CLA | C1-C2-C3 | -2.56 | 122.00 | 126.20 |
| 24 | B | 608 | CLA | C2A-C1A-CHA | -2.56 | 119.43 | 123.87 |
| 24 | b | 617 | CLA | C4B-C3B-C2B | -2.56 | 104.12 | 107.30 |
| 24 | b | 613 | CLA | O2A-CGA-CBA | 2.56 | 119.64 | 111.83 |
| 24 | B | 614 | CLA | CHB-C4A-NA | 2.56 | 128.09 | 124.40 |
| 24 | B | 602 | CLA | C4B-C3B-C2B | -2.56 | 104.12 | 107.30 |
| 24 | d | 401 | CLA | O2D-CGD-O1D | -2.56 | 118.87 | 123.85 |
| 24 | a | 409 | CLA | O2A-CGA-CBA | 2.55 | 119.62 | 111.83 |
| 31 | D | 404 | PL9 | C7-C3-C4 | 2.55 | 119.01 | 116.91 |
| 24 | c | 914 | CLA | C4B-C3B-C2B | -2.55 | 104.13 | 107.30 |
| 24 | C | 509 | CLA | CAC-C3C-C4C | 2.55 | 128.11 | 124.79 |
| 26 | H | 101 | BCR | C7-C8-C9 | -2.55 | 122.46 | 126.23 |
| 26 | d | 404 | BCR | C24-C23-C22 | -2.55 | 122.47 | 126.23 |
| 34 | Z | 101 | LMG | C8-O7-C10 | -2.55 | 111.70 | 117.80 |
| 24 | d | 402 | CLA | CMB-C2B-C1B | 2.55 | 129.30 | 125.42 |
| 24 | B | 611 | CLA | OBD-CAD-C3D | -2.55 | 122.46 | 128.42 |
| 26 | k | 102 | BCR | C33-C5-C6 | -2.55 | 121.70 | 124.48 |
| 24 | c | 904 | CLA | CHD-C4C-NC | 2.55 | 128.18 | 124.23 |
| 24 | C | 503 | CLA | CBC-CAC-C3C | -2.55 | 105.52 | 112.42 |
| 24 | B | 609 | CLA | CHB-C4A-NA | 2.55 | 128.07 | 124.40 |
| 24 | b | 616 | CLA | O2A-CGA-O1A | -2.55 | 117.26 | 123.63 |
| 24 | a | 409 | CLA | C4-C3-C5 | 2.54 | 119.64 | 115.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | c | 915 | BCR | C15-C14-C13 | -2.54 | 123.71 | 127.28 |
| 26 | K | 103 | BCR | C38-C26-C25 | -2.54 | 121.71 | 124.48 |
| 24 | b | 618 | CLA | CMC-C2C-C1C | 2.54 | 129.00 | 125.03 |
| 29 | m | 104 | LMT | O5'-C5'-C4' | 2.54 | 114.98 | 109.72 |
| 24 | B | 603 | CLA | CMA-C3A-C4A | -2.54 | 104.95 | 111.77 |
| 24 | b | 619 | CLA | CMB-C2B-C1B | 2.54 | 129.28 | 125.42 |
| 24 | C | 514 | CLA | CHD-C4C-NC | 2.54 | 128.17 | 124.23 |
| 24 | b | 610 | CLA | CHC-C1C-C2C | -2.54 | 119.73 | 126.95 |
| 24 | c | 907 | CLA | C4C-C3C-C2C | -2.54 | 103.20 | 106.89 |
| 40 | v | 202 | HEC | CHA-C1A-NA | 2.53 | 127.21 | 124.45 |
| 24 | B | 607 | CLA | C2A-C1A-CHA | -2.53 | 119.47 | 123.87 |
| 24 | C | 503 | CLA | OBD-CAD-C3D | -2.53 | 122.50 | 128.42 |
| 24 | B | 603 | CLA | CBC-CAC-C3C | -2.53 | 105.55 | 112.42 |
| 24 | b | 606 | CLA | C4-C3-C5 | 2.53 | 119.62 | 115.23 |
| 24 | c | 914 | CLA | C4-C3-C5 | 2.53 | 119.62 | 115.23 |
| 24 | c | 902 | CLA | CMB-C2B-C1B | 2.53 | 129.27 | 125.42 |
| 24 | b | 616 | CLA | OBD-CAD-C3D | -2.53 | 122.50 | 128.42 |
| 24 | b | 610 | CLA | C4C-C3C-C2C | -2.53 | 103.21 | 106.89 |
| 25 | a | 420 | PHO | O2A-CGA-CBA | 2.53 | 119.55 | 111.83 |
| 38 | E | 103 | HEM | CHD-C1D-ND | 2.53 | 127.14 | 124.42 |
| 24 | c | 909 | CLA | CAA-C2A-C3A | -2.53 | 106.17 | 113.00 |
| 24 | b | 606 | CLA | CHD-C4C-NC | 2.53 | 128.15 | 124.23 |
| 36 | d | 406 | DGD | O5D-C1E-C2E | 2.53 | 112.11 | 108.27 |
| 24 | b | 609 | CLA | OBD-CAD-C3D | -2.53 | 122.51 | 128.42 |
| 37 | d | 408 | LHG | O8-C23-O10 | -2.53 | 117.31 | 123.63 |
| 31 | d | 405 | PL9 | C40-C39-C41 | 2.52 | 119.61 | 115.23 |
| 27 | a | 411 | SQD | C44-O6-C1 | -2.52 | 108.38 | 113.80 |
| 27 | L | 102 | SQD | O47-C7-O49 | -2.52 | 117.81 | 123.70 |
| 24 | C | 503 | CLA | C2A-C1A-CHA | -2.52 | 119.49 | 123.87 |
| 36 | C | 519 | DGD | O1G-C1A-C2A | 2.52 | 119.53 | 111.83 |
| 24 | a | 407 | CLA | C2A-C1A-CHA | -2.52 | 119.49 | 123.87 |
| 24 | C | 508 | CLA | O2A-CGA-CBA | 2.52 | 119.52 | 111.83 |
| 24 | a | 409 | CLA | CAC-C3C-C4C | 2.52 | 128.07 | 124.79 |
| 24 | b | 618 | CLA | CAA-C2A-C3A | -2.52 | 106.19 | 113.00 |
| 24 | B | 604 | CLA | C2A-C1A-CHA | -2.52 | 119.49 | 123.87 |
| 24 | d | 401 | CLA | C4C-C3C-C2C | -2.52 | 103.22 | 106.89 |
| 24 | C | 506 | CLA | C4B-C3B-C2B | -2.52 | 104.17 | 107.30 |
| 26 | t | 101 | BCR | C29-C28-C27 | -2.52 | 105.75 | 111.28 |
| 26 | y | 101 | BCR | C16-C17-C18 | -2.52 | 123.75 | 127.28 |
| 34 | j | 101 | LMG | O8-C28-O10 | -2.52 | 117.34 | 123.63 |
| 26 | C | 515 | BCR | C33-C5-C6 | -2.51 | 121.74 | 124.48 |
| 24 | c | 908 | CLA | O1D-CGD-CBD | -2.51 | 119.56 | 124.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 606 | CLA | CMC-C2C-C1C | 2.51 | 128.96 | 125.03 |
| 24 | c | 905 | CLA | C2A-C1A-CHA | -2.51 | 119.50 | 123.87 |
| 29 | a | 401 | LMT | O5'-C5'-C4' | 2.51 | 114.92 | 109.72 |
| 40 | v | 202 | HEC | CHB-C1B-NB | 2.51 | 128.42 | 123.86 |
| 24 | C | 513 | CLA | CBC-CAC-C3C | -2.51 | 105.61 | 112.42 |
| 26 | d | 404 | BCR | C38-C26-C27 | 2.51 | 118.95 | 113.60 |
| 31 | d | 405 | PL9 | C32-C33-C34 | -2.51 | 121.88 | 127.62 |
| 36 | D | 405 | DGD | C3D-C4D-C5D | 2.51 | 114.78 | 110.23 |
| 24 | B | 603 | CLA | CMB-C2B-C1B | 2.51 | 129.24 | 125.42 |
| 36 | c | 916 | DGD | C2G-O2G-C1B | -2.51 | 111.80 | 117.80 |
| 27 | A | 412 | SQD | O48-C23-O10 | -2.51 | 117.36 | 123.63 |
| 24 | b | 618 | CLA | CMB-C2B-C1B | 2.50 | 129.23 | 125.42 |
| 36 | C | 519 | DGD | O2G-C1B-C2B | 2.50 | 116.90 | 111.48 |
| 24 | b | 617 | CLA | C4-C3-C5 | 2.50 | 119.57 | 115.23 |
| 24 | C | 503 | CLA | C4B-C3B-C2B | -2.50 | 104.19 | 107.30 |
| 26 | b | 623 | BCR | C16-C15-C14 | -2.50 | 118.40 | 123.52 |
| 24 | B | 613 | CLA | C4-C3-C5 | 2.50 | 119.57 | 115.23 |
| 40 | v | 202 | HEC | CHA-C4D-ND | 2.50 | 128.39 | 123.86 |
| 24 | D | 402 | CLA | CHD-C4C-NC | 2.50 | 128.11 | 124.23 |
| 38 | E | 103 | HEM | CBA-CAA-C2A | -2.50 | 105.62 | 112.53 |
| 24 | C | 513 | CLA | CMB-C2B-C1B | 2.50 | 129.22 | 125.42 |
| 24 | C | 504 | CLA | CHD-C4C-NC | 2.50 | 128.11 | 124.23 |
| 24 | b | 618 | CLA | O2A-CGA-O1A | -2.50 | 117.38 | 123.63 |
| 24 | B | 615 | CLA | C4B-C3B-C2B | -2.50 | 104.19 | 107.30 |
| 24 | C | 505 | CLA | C2A-C1A-CHA | -2.50 | 119.53 | 123.87 |
| 24 | c | 910 | CLA | C4-C3-C5 | 2.50 | 119.56 | 115.23 |
| 24 | B | 608 | CLA | C4-C3-C5 | 2.50 | 119.56 | 115.23 |
| 27 | L | 102 | SQD | C1-C2-C3 | -2.50 | 104.75 | 110.01 |
| 26 | D | 403 | BCR | C29-C28-C27 | -2.50 | 105.79 | 111.28 |
| 24 | b | 618 | CLA | CHD-C4C-NC | 2.50 | 128.10 | 124.23 |
| 27 | a | 411 | SQD | O48-C23-C24 | 2.50 | 119.44 | 111.83 |
| 24 | c | 909 | CLA | CMB-C2B-C1B | 2.49 | 129.22 | 125.42 |
| 24 | C | 502 | CLA | C4C-C3C-C2C | -2.49 | 103.26 | 106.89 |
| 24 | B | 614 | CLA | CMA-C3A-C4A | -2.49 | 105.08 | 111.77 |
| 24 | B | 605 | CLA | CMC-C2C-C1C | 2.49 | 128.93 | 125.03 |
| 37 | l | 101 | LHG | O8-C23-C24 | 2.49 | 119.43 | 111.83 |
| 26 | y | 101 | BCR | C28-C27-C26 | -2.49 | 109.62 | 114.06 |
| 24 | B | 606 | CLA | C4B-C3B-C2B | -2.49 | 104.21 | 107.30 |
| 25 | A | 409 | PHO | C4A-C3A-C2A | -2.49 | 100.47 | 102.84 |
| 24 | C | 508 | CLA | CMC-C2C-C1C | 2.49 | 128.92 | 125.03 |
| 24 | B | 615 | CLA | CAA-C2A-C3A | -2.49 | 106.28 | 113.00 |
| 31 | d | 405 | PL9 | C37-C38-C39 | -2.49 | 121.94 | 127.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | l | 101 | LHG | O7-C7-O9 | -2.49 | 117.89 | 123.70 |
| 24 | B | 615 | CLA | C4C-C3C-C2C | -2.48 | 103.28 | 106.89 |
| 24 | B | 617 | CLA | C1-O2A-CGA | 2.48 | 122.66 | 116.65 |
| 26 | T | 102 | BCR | C11-C10-C9 | -2.48 | 123.80 | 127.28 |
| 27 | A | 412 | SQD | O8-S-C6 | 2.48 | 110.77 | 105.97 |
| 24 | c | 913 | CLA | C4B-C3B-C2B | -2.48 | 104.22 | 107.30 |
| 35 | c | 923 | HTG | O5-C5-C4 | 2.48 | 114.17 | 109.70 |
| 37 | d | 409 | LHG | O7-C7-O9 | -2.48 | 117.90 | 123.70 |
| 25 | A | 409 | PHO | O2D-CGD-O1D | -2.48 | 119.02 | 123.85 |
| 24 | a | 407 | CLA | C3B-C4B-NB | 2.48 | 112.74 | 110.53 |
| 38 | e | 102 | HEM | C3B-C4B-NB | -2.48 | 107.69 | 109.47 |
| 35 | C | 524 | HTG | O5-C5-C4 | 2.48 | 114.17 | 109.70 |
| 24 | B | 616 | CLA | C4B-C3B-C2B | -2.48 | 104.22 | 107.30 |
| 24 | C | 514 | CLA | O2A-CGA-CBA | 2.48 | 119.39 | 111.83 |
| 24 | B | 603 | CLA | O2A-CGA-CBA | 2.48 | 119.39 | 111.83 |
| 24 | B | 611 | CLA | CHD-C4C-NC | 2.47 | 128.06 | 124.23 |
| 26 | B | 618 | BCR | C29-C30-C25 | 2.47 | 114.03 | 110.44 |
| 25 | a | 408 | PHO | O1D-CGD-CBD | -2.47 | 120.97 | 124.72 |
| 24 | b | 615 | CLA | C2A-C1A-CHA | -2.47 | 119.58 | 123.87 |
| 24 | b | 613 | CLA | CHC-C1C-C2C | -2.47 | 119.92 | 126.95 |
| 24 | b | 615 | CLA | O2A-CGA-CBA | 2.47 | 119.37 | 111.83 |
| 24 | a | 407 | CLA | O2A-CGA-O1A | -2.47 | 117.45 | 123.63 |
| 24 | D | 402 | CLA | C1-C2-C3 | -2.47 | 122.16 | 126.20 |
| 24 | B | 604 | CLA | CMC-C2C-C1C | 2.47 | 128.89 | 125.03 |
| 24 | b | 614 | CLA | CAA-C2A-C3A | -2.46 | 106.34 | 113.00 |
| 24 | A | 410 | CLA | C4B-C3B-C2B | -2.46 | 104.24 | 107.30 |
| 24 | D | 401 | CLA | C1D-CHD-C4C | -2.46 | 120.79 | 126.02 |
| 26 | B | 618 | BCR | C7-C8-C9 | -2.46 | 122.59 | 126.23 |
| 24 | b | 608 | CLA | O1D-CGD-CBD | -2.46 | 119.66 | 124.52 |
| 24 | b | 609 | CLA | CAA-C2A-C3A | -2.46 | 106.35 | 113.00 |
| 24 | a | 409 | CLA | CMA-C3A-C2A | -2.46 | 104.47 | 113.98 |
| 31 | D | 404 | PL9 | C22-C23-C24 | -2.46 | 121.99 | 127.62 |
| 29 | m | 103 | LMT | C1'-C2'-C3' | 2.46 | 115.18 | 110.01 |
| 24 | b | 607 | CLA | CMC-C2C-C1C | 2.45 | 128.87 | 125.03 |
| 29 | B | 623 | LMT | O1B-C4'-C5' | -2.45 | 103.04 | 109.48 |
| 24 | B | 602 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 34 | z | 101 | LMG | O1-C1-C2 | 2.45 | 112.00 | 108.27 |
| 24 | A | 405 | CLA | CMB-C2B-C1B | 2.45 | 129.15 | 125.42 |
| 24 | B | 604 | CLA | CAC-C3C-C4C | 2.45 | 127.98 | 124.79 |
| 24 | B | 617 | CLA | C2A-C1A-CHA | -2.45 | 119.61 | 123.87 |
| 24 | b | 611 | CLA | O2D-CGD-O1D | -2.45 | 119.08 | 123.85 |
| 24 | d | 403 | CLA | CMB-C2B-C1B | 2.45 | 129.15 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 607 | CLA | O1D-CGD-CBD | -2.45 | 119.69 | 124.52 |
| 31 | D | 404 | PL9 | C12-C13-C14 | -2.45 | 122.02 | 127.62 |
| 24 | b | 613 | CLA | CMA-C3A-C2A | -2.45 | 104.52 | 113.98 |
| 26 | k | 102 | BCR | C2-C1-C6 | 2.45 | 113.99 | 110.44 |
| 24 | C | 509 | CLA | O2A-CGA-CBA | 2.45 | 119.29 | 111.83 |
| 24 | A | 405 | CLA | O2D-CGD-CBD | 2.45 | 115.50 | 111.23 |
| 24 | B | 602 | CLA | C4-C3-C5 | 2.44 | 119.47 | 115.23 |
| 27 | F | 101 | SQD | O47-C7-O49 | -2.44 | 117.99 | 123.70 |
| 24 | B | 614 | CLA | O2D-CGD-CBD | 2.44 | 115.50 | 111.23 |
| 26 | B | 620 | BCR | C39-C30-C25 | -2.44 | 106.42 | 110.24 |
| 24 | C | 502 | CLA | O2A-CGA-CBA | 2.44 | 119.28 | 111.83 |
| 24 | B | 603 | CLA | O2D-CGD-O1D | -2.44 | 119.10 | 123.85 |
| 24 | b | 617 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 24 | A | 407 | CLA | CMA-C3A-C2A | -2.44 | 104.56 | 113.98 |
| 24 | b | 605 | CLA | CBC-CAC-C3C | -2.44 | 105.81 | 112.42 |
| 24 | c | 904 | CLA | O2A-CGA-O1A | -2.44 | 117.53 | 123.63 |
| 24 | b | 609 | CLA | C1-C2-C3 | -2.44 | 122.20 | 126.20 |
| 24 | B | 607 | CLA | O2A-CGA-CBA | 2.44 | 119.26 | 111.83 |
| 24 | A | 406 | CLA | CAA-CBA-CGA | 2.44 | 120.12 | 113.21 |
| 24 | B | 613 | CLA | C1-C2-C3 | -2.44 | 122.21 | 126.20 |
| 24 | B | 603 | CLA | CAA-CBA-CGA | -2.43 | 106.30 | 113.21 |
| 24 | C | 510 | CLA | CHD-C4C-NC | 2.43 | 128.00 | 124.23 |
| 27 | a | 411 | SQD | O8-S-C6 | 2.43 | 110.67 | 105.97 |
| 24 | c | 911 | CLA | O2A-CGA-O1A | -2.43 | 117.55 | 123.63 |
| 35 | B | 634 | HTG | O5-C5-C4 | 2.43 | 114.08 | 109.70 |
| 24 | b | 609 | CLA | C4B-C3B-C2B | -2.43 | 104.28 | 107.30 |
| 29 | f | 103 | LMT | O5B-C5B-C4B | 2.43 | 114.08 | 109.70 |
| 24 | b | 610 | CLA | CAC-C3C-C4C | 2.43 | 127.95 | 124.79 |
| 24 | B | 610 | CLA | O2A-CGA-O1A | -2.43 | 117.56 | 123.63 |
| 26 | a | 410 | BCR | C3-C4-C5 | -2.43 | 109.73 | 114.06 |
| 24 | B | 603 | CLA | C4-C3-C5 | 2.43 | 119.44 | 115.23 |
| 24 | C | 503 | CLA | CMC-C2C-C1C | 2.43 | 128.82 | 125.03 |
| 29 | b | 601 | LMT | O5'-C1'-C2' | 2.43 | 115.35 | 110.37 |
| 24 | A | 410 | CLA | CMA-C3A-C4A | -2.43 | 105.25 | 111.77 |
| 36 | C | 518 | DGD | O1G-C1A-C2A | 2.42 | 119.22 | 111.83 |
| 24 | c | 908 | CLA | C4B-C3B-C2B | -2.42 | 104.29 | 107.30 |
| 24 | C | 512 | CLA | O2D-CGD-O1D | -2.42 | 119.13 | 123.85 |
| 24 | c | 905 | CLA | CHD-C4C-NC | 2.42 | 127.99 | 124.23 |
| 24 | a | 409 | CLA | CMC-C2C-C1C | 2.42 | 128.82 | 125.03 |
| 31 | d | 405 | PL9 | C35-C34-C36 | 2.42 | 119.43 | 115.23 |
| 26 | b | 623 | BCR | C10-C11-C12 | -2.42 | 116.19 | 123.20 |
| 24 | B | 605 | CLA | O2D-CGD-O1D | -2.42 | 119.14 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | C | 515 | BCR | C2-C1-C6 | 2.42 | 113.95 | 110.44 |
| 24 | B | 603 | CLA | C1-C2-C3 | -2.42 | 122.24 | 126.20 |
| 24 | C | 502 | CLA | C2A-C1A-CHA | -2.42 | 119.67 | 123.87 |
| 24 | c | 912 | CLA | C4B-C3B-C2B | -2.41 | 104.30 | 107.30 |
| 36 | c | 916 | DGD | O5D-C6D-C5D | -2.41 | 103.98 | 109.42 |
| 26 | B | 619 | BCR | C28-C27-C26 | -2.41 | 109.75 | 114.06 |
| 25 | a | 408 | PHO | CMC-C2C-C1C | 2.41 | 129.07 | 124.73 |
| 40 | V | 201 | HEC | C4B-NB-C1B | 2.41 | 109.75 | 105.82 |
| 26 | k | 101 | BCR | C21-C20-C19 | -2.41 | 116.22 | 123.20 |
| 24 | c | 907 | CLA | CGD-CBD-CAD | -2.41 | 103.05 | 110.85 |
| 24 | A | 410 | CLA | CMA-C3A-C2A | -2.41 | 104.68 | 113.98 |
| 24 | C | 513 | CLA | O2D-CGD-O1D | -2.40 | 119.17 | 123.85 |
| 24 | b | 614 | CLA | O2A-CGA-O1A | -2.40 | 117.61 | 123.63 |
| 24 | b | 618 | CLA | OBD-CAD-C3D | -2.40 | 122.80 | 128.42 |
| 24 | B | 610 | CLA | CGD-CBD-CAD | -2.40 | 103.07 | 110.85 |
| 24 | B | 610 | CLA | C2A-C1A-CHA | -2.40 | 119.70 | 123.87 |
| 26 | c | 915 | BCR | C15-C16-C17 | -2.40 | 118.61 | 123.52 |
| 38 | E | 103 | HEM | O2A-CGA-CBA | 2.40 | 121.59 | 114.00 |
| 24 | C | 513 | CLA | C4B-C3B-C2B | -2.40 | 104.32 | 107.30 |
| 24 | b | 605 | CLA | C2A-C1A-CHA | -2.40 | 119.70 | 123.87 |
| 24 | b | 616 | CLA | CHC-C1C-C2C | -2.40 | 120.13 | 126.95 |
| 31 | d | 405 | PL9 | C20-C19-C21 | 2.40 | 119.39 | 115.23 |
| 24 | c | 912 | CLA | C2A-C1A-CHA | -2.40 | 119.71 | 123.87 |
| 24 | b | 614 | CLA | CHD-C4C-NC | 2.39 | 127.94 | 124.23 |
| 24 | C | 506 | CLA | CMC-C2C-C1C | 2.39 | 128.77 | 125.03 |
| 24 | B | 612 | CLA | O2A-CGA-O1A | -2.39 | 117.65 | 123.63 |
| 24 | B | 609 | CLA | CHD-C4C-NC | 2.39 | 127.94 | 124.23 |
| 24 | b | 608 | CLA | C4-C3-C5 | 2.39 | 119.37 | 115.23 |
| 38 | e | 102 | HEM | CBD-CAD-C3D | -2.39 | 105.93 | 112.53 |
| 35 | D | 411 | HTG | C1'-S1-C1 | 2.39 | 105.61 | 100.45 |
| 35 | b | 603 | HTG | C1-O5-C5 | 2.39 | 116.84 | 112.56 |
| 24 | C | 503 | CLA | CHD-C4C-NC | 2.39 | 127.93 | 124.23 |
| 24 | C | 506 | CLA | O2A-CGA-CBA | 2.39 | 119.11 | 111.83 |
| 31 | D | 404 | PL9 | C37-C38-C39 | -2.39 | 122.16 | 127.62 |
| 26 | d | 404 | BCR | C30-C25-C26 | -2.39 | 119.38 | 122.64 |
| 24 | C | 504 | CLA | C2A-C1A-CHA | -2.39 | 119.73 | 123.87 |
| 24 | B | 602 | CLA | CBC-CAC-C3C | -2.39 | 105.95 | 112.42 |
| 24 | B | 608 | CLA | CMC-C2C-C1C | 2.39 | 128.76 | 125.03 |
| 24 | C | 507 | CLA | C4C-C3C-C2C | -2.38 | 103.42 | 106.89 |
| 24 | c | 909 | CLA | C2A-C1A-CHA | -2.38 | 119.73 | 123.87 |
| 24 | C | 507 | CLA | CMC-C2C-C1C | 2.38 | 128.76 | 125.03 |
| 24 | B | 605 | CLA | CMB-C2B-C1B | 2.38 | 129.05 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | a | 407 | CLA | CMC-C2C-C1C | 2.38 | 128.76 | 125.03 |
| 25 | A | 408 | PHO | C4-C3-C5 | 2.38 | 119.36 | 115.23 |
| 24 | C | 502 | CLA | O2A-CGA-O1A | -2.38 | 117.67 | 123.63 |
| 24 | c | 913 | CLA | CBA-CAA-C2A | -2.38 | 106.71 | 113.79 |
| 26 | k | 102 | BCR | C36-C18-C19 | 2.38 | 121.72 | 118.09 |
| 24 | d | 403 | CLA | O2D-CGD-O1D | -2.38 | 119.22 | 123.85 |
| 26 | D | 403 | BCR | C16-C17-C18 | -2.38 | 123.94 | 127.28 |
| 24 | b | 617 | CLA | CHD-C4C-NC | 2.38 | 127.92 | 124.23 |
| 24 | d | 402 | CLA | C1-O2A-CGA | 2.37 | 122.39 | 116.65 |
| 24 | C | 511 | CLA | C2A-C1A-CHA | -2.37 | 119.75 | 123.87 |
| 24 | b | 612 | CLA | CMC-C2C-C1C | 2.37 | 128.74 | 125.03 |
| 24 | b | 619 | CLA | CBC-CAC-C3C | -2.37 | 106.00 | 112.42 |
| 24 | b | 611 | CLA | CAC-C3C-C4C | 2.37 | 127.87 | 124.79 |
| 34 | z | 101 | LMG | C7-O1-C1 | -2.37 | 108.72 | 113.80 |
| 24 | c | 904 | CLA | C1-C2-C3 | -2.37 | 122.32 | 126.20 |
| 24 | b | 606 | CLA | O2A-CGA-O1A | -2.37 | 117.71 | 123.63 |
| 24 | B | 610 | CLA | CMA-C3A-C4A | -2.37 | 105.41 | 111.77 |
| 36 | c | 918 | DGD | O1G-C1A-O1A | -2.37 | 117.71 | 123.63 |
| 26 | K | 102 | BCR | C10-C11-C12 | -2.37 | 116.34 | 123.20 |
| 24 | b | 620 | CLA | CHD-C4C-NC | 2.36 | 127.89 | 124.23 |
| 24 | B | 603 | CLA | C4B-C3B-C2B | -2.36 | 104.36 | 107.30 |
| 24 | c | 912 | CLA | C1-O2A-CGA | 2.36 | 122.37 | 116.65 |
| 24 | C | 505 | CLA | CAA-C2A-C3A | -2.36 | 106.62 | 113.00 |
| 37 | D | 406 | LHG | O7-C7-O9 | -2.36 | 118.19 | 123.70 |
| 40 | V | 201 | HEC | CHB-C1B-NB | 2.36 | 128.13 | 123.86 |
| 24 | C | 513 | CLA | CMA-C3A-C4A | -2.35 | 105.44 | 111.77 |
| 24 | B | 608 | CLA | O2A-CGA-CBA | 2.35 | 119.01 | 111.83 |
| 24 | c | 908 | CLA | CHD-C4C-NC | 2.35 | 127.88 | 124.23 |
| 24 | c | 910 | CLA | C2A-C1A-CHA | -2.35 | 119.78 | 123.87 |
| 34 | a | 412 | LMG | O1-C1-C2 | 2.35 | 111.84 | 108.27 |
| 27 | B | 621 | SQD | C1-C2-C3 | -2.35 | 105.07 | 110.01 |
| 25 | a | 420 | PHO | CMB-C2B-C3B | 2.35 | 129.38 | 124.68 |
| 34 | C | 520 | LMG | C8-O7-C10 | -2.35 | 112.17 | 117.80 |
| 24 | D | 401 | CLA | CBC-CAC-C3C | -2.35 | 106.05 | 112.42 |
| 24 | C | 505 | CLA | CHD-C4C-NC | 2.35 | 127.87 | 124.23 |
| 31 | A | 419 | PL9 | C30-C29-C31 | 2.35 | 119.30 | 115.23 |
| 26 | d | 404 | BCR | C40-C30-C25 | -2.35 | 106.56 | 110.24 |
| 35 | C | 524 | HTG | O5-C1-C2 | 2.34 | 113.55 | 110.32 |
| 40 | v | 202 | HEC | C4B-NB-C1B | 2.34 | 109.64 | 105.82 |
| 24 | C | 504 | CLA | CMB-C2B-C1B | 2.34 | 128.99 | 125.42 |
| 25 | a | 408 | PHO | CBA-CAA-C2A | -2.34 | 106.87 | 113.78 |
| 26 | b | 623 | BCR | C21-C20-C19 | -2.34 | 116.41 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | a | 417 | PL9 | C51-C49-C50 | 2.34 | 119.97 | 114.59 |
| 24 | a | 407 | CLA | CMA-C3A-C2A | -2.34 | 104.94 | 113.98 |
| 24 | B | 607 | CLA | CBC-CAC-C3C | -2.34 | 106.08 | 112.42 |
| 24 | B | 609 | CLA | O2A-CGA-O1A | -2.34 | 117.78 | 123.63 |
| 37 | D | 406 | LHG | O4-P-O5 | 2.34 | 123.32 | 112.44 |
| 24 | C | 514 | CLA | C1-O2A-CGA | 2.34 | 122.30 | 116.65 |
| 24 | B | 603 | CLA | C2A-C1A-CHA | -2.34 | 119.81 | 123.87 |
| 24 | a | 409 | CLA | C4B-C3B-C2B | -2.34 | 104.40 | 107.30 |
| 24 | d | 403 | CLA | C2A-C1A-CHA | -2.33 | 119.82 | 123.87 |
| 24 | C | 504 | CLA | CMC-C2C-C1C | 2.33 | 128.68 | 125.03 |
| 31 | D | 404 | PL9 | C25-C24-C26 | 2.33 | 119.27 | 115.23 |
| 26 | D | 403 | BCR | C30-C25-C24 | 2.33 | 121.97 | 115.65 |
| 27 | A | 416 | SQD | C3-C4-C5 | 2.33 | 114.45 | 110.23 |
| 24 | C | 508 | CLA | O2A-CGA-O1A | -2.33 | 117.81 | 123.63 |
| 37 | e | 101 | LHG | O8-C23-C24 | 2.33 | 118.93 | 111.83 |
| 34 | z | 101 | LMG | C8-O7-C10 | -2.33 | 112.23 | 117.80 |
| 24 | b | 613 | CLA | C3B-C4B-NB | 2.33 | 112.61 | 110.53 |
| 24 | a | 407 | CLA | OBD-CAD-C3D | -2.32 | 122.98 | 128.42 |
| 24 | b | 619 | CLA | O2A-CGA-CBA | 2.32 | 118.92 | 111.83 |
| 24 | C | 507 | CLA | C2A-C1A-CHA | -2.32 | 119.83 | 123.87 |
| 37 | l | 101 | LHG | C6-C5-C4 | -2.32 | 106.37 | 111.78 |
| 24 | C | 504 | CLA | O2A-CGA-CBA | 2.32 | 118.91 | 111.83 |
| 26 | d | 404 | BCR | C37-C22-C23 | 2.32 | 121.63 | 118.09 |
| 24 | b | 606 | CLA | C2A-C1A-CHA | -2.32 | 119.84 | 123.87 |
| 24 | A | 407 | CLA | O2D-CGD-O1D | -2.32 | 119.34 | 123.85 |
| 36 | D | 405 | DGD | O6D-C5D-C6D | 2.32 | 111.29 | 106.69 |
| 38 | E | 103 | HEM | C4B-C3B-C2B | -2.32 | 105.15 | 107.28 |
| 24 | A | 407 | CLA | O2A-CGA-O1A | -2.31 | 117.84 | 123.63 |
| 26 | B | 618 | BCR | C37-C22-C23 | 2.31 | 121.62 | 118.09 |
| 24 | d | 401 | CLA | CAA-CBA-CGA | 2.31 | 119.78 | 113.21 |
| 24 | d | 403 | CLA | C4-C3-C5 | 2.31 | 119.24 | 115.23 |
| 27 | A | 416 | SQD | O5-C5-C4 | 2.31 | 113.86 | 109.70 |
| 24 | c | 905 | CLA | CAA-C2A-C3A | -2.31 | 106.75 | 113.00 |
| 24 | A | 410 | CLA | C4C-C3C-C2C | -2.31 | 103.53 | 106.89 |
| 24 | b | 608 | CLA | O2A-CGA-O1A | -2.31 | 117.85 | 123.63 |
| 24 | B | 617 | CLA | OBD-CAD-C3D | -2.31 | 123.02 | 128.42 |
| 24 | b | 620 | CLA | C4-C3-C5 | 2.31 | 119.24 | 115.23 |
| 24 | a | 407 | CLA | C1-O2A-CGA | 2.31 | 122.24 | 116.65 |
| 24 | b | 606 | CLA | CMA-C3A-C2A | -2.31 | 105.07 | 113.98 |
| 24 | B | 611 | CLA | CAA-CBA-CGA | -2.31 | 106.66 | 113.21 |
| 24 | A | 406 | CLA | CAC-C3C-C4C | 2.31 | 127.79 | 124.79 |
| 24 | C | 502 | CLA | C4-C3-C5 | 2.31 | 119.23 | 115.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 609 | CLA | C1-C2-C3 | -2.30 | 122.42 | 126.20 |
| 24 | B | 602 | CLA | C2A-C1A-CHA | -2.30 | 119.87 | 123.87 |
| 24 | B | 612 | CLA | CBC-CAC-C3C | -2.30 | 106.19 | 112.42 |
| 24 | d | 401 | CLA | O2A-CGA-CBA | 2.30 | 118.84 | 111.83 |
| 24 | A | 410 | CLA | CAC-C3C-C4C | 2.30 | 127.78 | 124.79 |
| 26 | C | 516 | BCR | C3-C4-C5 | -2.29 | 109.97 | 114.06 |
| 24 | B | 605 | CLA | C2A-C1A-CHA | -2.29 | 119.90 | 123.87 |
| 24 | B | 617 | CLA | CBC-CAC-C3C | -2.29 | 106.22 | 112.42 |
| 26 | d | 404 | BCR | C35-C13-C12 | 2.29 | 121.58 | 118.09 |
| 24 | c | 902 | CLA | C2A-C1A-CHA | -2.29 | 119.90 | 123.87 |
| 26 | k | 102 | BCR | C29-C30-C25 | 2.29 | 113.76 | 110.44 |
| 24 | b | 617 | CLA | C2A-C1A-CHA | -2.28 | 119.90 | 123.87 |
| 24 | A | 410 | CLA | O2A-CGA-O1A | -2.28 | 117.91 | 123.63 |
| 24 | B | 610 | CLA | C1-O2A-CGA | 2.28 | 122.17 | 116.65 |
| 24 | C | 509 | CLA | CMC-C2C-C1C | 2.28 | 128.60 | 125.03 |
| 24 | b | 617 | CLA | C6-C7-C8 | -2.28 | 108.39 | 115.97 |
| 24 | C | 508 | CLA | C1-C2-C3 | -2.28 | 122.46 | 126.20 |
| 24 | A | 407 | CLA | C1-O2A-CGA | 2.28 | 122.17 | 116.65 |
| 24 | C | 509 | CLA | CAA-C2A-C3A | -2.28 | 106.84 | 113.00 |
| 24 | c | 913 | CLA | C1-O2A-CGA | 2.28 | 122.16 | 116.65 |
| 35 | b | 626 | HTG | C1-C2-C3 | 2.28 | 115.00 | 110.55 |
| 24 | B | 615 | CLA | CAC-C3C-C4C | 2.28 | 127.75 | 124.79 |
| 24 | D | 401 | CLA | CMC-C2C-C1C | 2.28 | 128.59 | 125.03 |
| 24 | B | 606 | CLA | CAA-C2A-C3A | -2.28 | 106.85 | 113.00 |
| 24 | b | 610 | CLA | C2A-C1A-CHA | -2.27 | 119.92 | 123.87 |
| 24 | c | 912 | CLA | O2A-CGA-O1A | -2.27 | 117.94 | 123.63 |
| 24 | B | 607 | CLA | CMD-C2D-C3D | -2.27 | 122.47 | 127.69 |
| 24 | B | 616 | CLA | C2A-C1A-CHA | -2.27 | 119.92 | 123.87 |
| 24 | C | 510 | CLA | C2A-C1A-CHA | -2.27 | 119.92 | 123.87 |
| 26 | y | 101 | BCR | C38-C26-C25 | -2.27 | 122.00 | 124.48 |
| 26 | B | 619 | BCR | C15-C16-C17 | -2.27 | 118.87 | 123.52 |
| 35 | B | 625 | HTG | C1-C2-C3 | 2.27 | 114.99 | 110.55 |
| 24 | C | 506 | CLA | C1-O2A-CGA | 2.27 | 122.15 | 116.65 |
| 24 | B | 614 | CLA | CHD-C4C-NC | 2.27 | 127.75 | 124.23 |
| 24 | b | 612 | CLA | CMB-C2B-C1B | 2.27 | 128.87 | 125.42 |
| 24 | C | 513 | CLA | CHB-C4A-NA | 2.27 | 127.67 | 124.40 |
| 34 | c | 920 | LMG | O7-C10-O9 | -2.27 | 118.41 | 123.70 |
| 24 | B | 615 | CLA | O2A-CGA-O1A | -2.26 | 117.96 | 123.63 |
| 24 | C | 507 | CLA | O2A-CGA-CBA | 2.26 | 118.74 | 111.83 |
| 24 | c | 911 | CLA | CMA-C3A-C4A | -2.26 | 105.69 | 111.77 |
| 26 | B | 618 | BCR | C21-C20-C19 | -2.26 | 116.65 | 123.20 |
| 24 | B | 616 | CLA | CHA-C1A-NA | -2.26 | 121.27 | 126.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | b | 614 | CLA | CHB-C4A-NA | 2.26 | 127.66 | 124.40 |
| 26 | B | 620 | BCR | C3-C4-C5 | -2.26 | 110.03 | 114.06 |
| 24 | B | 613 | CLA | CMB-C2B-C1B | 2.26 | 128.86 | 125.42 |
| 24 | b | 619 | CLA | O2A-CGA-O1A | -2.26 | 117.98 | 123.63 |
| 24 | a | 407 | CLA | C4B-C3B-C2B | -2.26 | 104.49 | 107.30 |
| 24 | C | 511 | CLA | C6-C7-C8 | -2.26 | 108.46 | 115.97 |
| 37 | d | 407 | LHG | O8-C23-O10 | -2.26 | 117.98 | 123.63 |
| 31 | A | 419 | PL9 | C40-C39-C41 | 2.26 | 119.15 | 115.23 |
| 24 | C | 510 | CLA | CBC-CAC-C3C | -2.26 | 106.30 | 112.42 |
| 24 | a | 406 | CLA | C4C-C3C-C2C | -2.26 | 103.61 | 106.89 |
| 24 | C | 502 | CLA | C1-O2A-CGA | 2.26 | 122.12 | 116.65 |
| 24 | B | 615 | CLA | C1-O2A-CGA | 2.26 | 122.11 | 116.65 |
| 34 | b | 624 | LMG | O8-C28-O10 | -2.26 | 117.99 | 123.63 |
| 26 | T | 102 | BCR | C37-C22-C23 | 2.25 | 121.53 | 118.09 |
| 24 | b | 611 | CLA | C1-O2A-CGA | 2.25 | 122.10 | 116.65 |
| 26 | b | 623 | BCR | C7-C8-C9 | -2.25 | 122.90 | 126.23 |
| 24 | D | 401 | CLA | C2A-C1A-CHA | -2.25 | 119.96 | 123.87 |
| 24 | D | 402 | CLA | O2A-CGA-CBA | 2.25 | 118.70 | 111.83 |
| 36 | C | 518 | DGD | O6E-C5E-C6E | 2.25 | 112.02 | 106.44 |
| 34 | a | 412 | LMG | O7-C10-O9 | -2.25 | 118.45 | 123.70 |
| 25 | a | 408 | PHO | O2D-CGD-O1D | -2.24 | 119.48 | 123.85 |
| 24 | C | 511 | CLA | CAC-C3C-C4C | 2.24 | 127.71 | 124.79 |
| 24 | b | 616 | CLA | CHD-C4C-NC | 2.24 | 127.71 | 124.23 |
| 24 | B | 607 | CLA | O2D-CGD-O1D | -2.24 | 119.49 | 123.85 |
| 27 | a | 402 | SQD | O6-C1-C2 | 2.24 | 111.67 | 108.27 |
| 24 | b | 614 | CLA | C2A-C1A-CHA | -2.24 | 119.98 | 123.87 |
| 40 | V | 201 | HEC | CBC-CAC-C3C | -2.24 | 122.96 | 127.43 |
| 24 | a | 407 | CLA | CHB-C1B-C2B | -2.24 | 120.93 | 127.43 |
| 26 | t | 101 | BCR | C31-C1-C6 | 2.24 | 113.75 | 110.24 |
| 27 | A | 412 | SQD | O9-S-C6 | 2.24 | 110.09 | 106.76 |
| 26 | B | 619 | BCR | C37-C22-C21 | -2.23 | 119.20 | 122.82 |
| 24 | B | 616 | CLA | CED-O2D-CGD | 2.23 | 120.98 | 115.92 |
| 24 | b | 612 | CLA | C11-C10-C8 | -2.23 | 108.54 | 115.97 |
| 24 | b | 614 | CLA | C11-C12-C13 | -2.23 | 108.54 | 115.97 |
| 24 | C | 506 | CLA | CHD-C4C-NC | 2.23 | 127.69 | 124.23 |
| 24 | c | 905 | CLA | O2A-CGA-O1A | -2.23 | 118.04 | 123.63 |
| 37 | D | 407 | LHG | O8-C23-O10 | -2.23 | 118.04 | 123.63 |
| 36 | C | 518 | DGD | C6D-C5D-C4D | 2.23 | 116.75 | 112.07 |
| 24 | B | 616 | CLA | C1-O2A-CGA | 2.23 | 122.05 | 116.65 |
| 24 | C | 504 | CLA | O2A-CGA-O1A | -2.23 | 118.05 | 123.63 |
| 36 | C | 517 | DGD | C2G-O2G-C1B | -2.23 | 112.46 | 117.80 |
| 29 | a | 401 | LMT | C1'-O5'-C5' | 2.23 | 118.08 | 113.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 510 | CLA | C16-C15-C13 | -2.23 | 108.56 | 115.97 |
| 26 | A | 411 | BCR | C8-C7-C6 | -2.23 | 121.05 | 127.00 |
| 24 | c | 911 | CLA | CMB-C2B-C1B | 2.23 | 128.81 | 125.42 |
| 24 | b | 607 | CLA | CHD-C4C-NC | 2.23 | 127.68 | 124.23 |
| 24 | a | 407 | CLA | C4-C3-C5 | 2.23 | 119.09 | 115.23 |
| 24 | C | 512 | CLA | CED-O2D-CGD | 2.23 | 120.97 | 115.92 |
| 25 | A | 409 | PHO | O2A-CGA-CBA | 2.23 | 118.62 | 111.83 |
| 40 | v | 202 | HEC | CBC-CAC-C3C | -2.23 | 122.98 | 127.43 |
| 24 | c | 914 | CLA | O2A-CGA-O1A | -2.23 | 118.06 | 123.63 |
| 26 | y | 101 | BCR | C37-C22-C23 | 2.23 | 121.49 | 118.09 |
| 24 | C | 514 | CLA | CAA-C2A-C3A | -2.22 | 106.99 | 113.00 |
| 24 | d | 403 | CLA | O2A-CGA-O1A | -2.22 | 118.07 | 123.63 |
| 26 | K | 102 | BCR | C37-C22-C23 | 2.22 | 121.48 | 118.09 |
| 38 | E | 103 | HEM | CHA-C4D-ND | 2.22 | 127.11 | 124.37 |
| 27 | f | 102 | SQD | C3-C4-C5 | 2.22 | 114.26 | 110.23 |
| 40 | v | 202 | HEC | C4C-NC-C1C | 2.22 | 109.44 | 105.82 |
| 26 | K | 102 | BCR | C15-C14-C13 | -2.22 | 124.16 | 127.28 |
| 24 | C | 513 | CLA | CAA-C2A-C1A | 2.22 | 119.25 | 111.97 |
| 24 | c | 908 | CLA | CBC-CAC-C3C | -2.22 | 106.41 | 112.42 |
| 24 | b | 617 | CLA | O2D-CGD-O1D | -2.22 | 119.53 | 123.85 |
| 29 | M | 101 | LMT | O5B-C5B-C6B | 2.22 | 111.93 | 106.44 |
| 26 | h | 101 | BCR | C7-C6-C5 | 2.22 | 126.66 | 121.56 |
| 40 | V | 201 | HEC | CHD-C1D-ND | 2.22 | 127.88 | 123.86 |
| 29 | C | 522 | LMT | O5'-C5'-C4' | 2.22 | 114.31 | 109.72 |
| 24 | B | 611 | CLA | CMA-C3A-C4A | -2.22 | 105.82 | 111.77 |
| 24 | B | 612 | CLA | CHB-C4A-NA | 2.21 | 127.60 | 124.40 |
| 26 | D | 403 | BCR | C37-C22-C23 | 2.21 | 121.47 | 118.09 |
| 25 | A | 408 | PHO | O2D-CGD-O1D | -2.21 | 119.54 | 123.85 |
| 31 | A | 419 | PL9 | C17-C18-C19 | -2.21 | 122.56 | 127.62 |
| 24 | C | 514 | CLA | CBC-CAC-C3C | -2.21 | 106.43 | 112.42 |
| 37 | d | 407 | LHG | O7-C7-O9 | -2.21 | 118.54 | 123.70 |
| 24 | B | 604 | CLA | C5-C3-C2 | -2.21 | 116.21 | 121.17 |
| 24 | B | 602 | CLA | CMC-C2C-C1C | 2.21 | 128.49 | 125.03 |
| 27 | B | 621 | SQD | O47-C7-O49 | -2.21 | 118.54 | 123.70 |
| 24 | A | 410 | CLA | CHB-C4A-NA | 2.21 | 127.59 | 124.40 |
| 31 | D | 404 | PL9 | C51-C49-C50 | 2.21 | 119.67 | 114.59 |
| 26 | k | 101 | BCR | C16-C17-C18 | -2.21 | 124.18 | 127.28 |
| 24 | b | 618 | CLA | C4-C3-C5 | 2.21 | 119.06 | 115.23 |
| 24 | c | 911 | CLA | C2A-C1A-CHA | -2.21 | 120.04 | 123.87 |
| 24 | c | 914 | CLA | CED-O2D-CGD | 2.21 | 120.92 | 115.92 |
| 37 | D | 408 | LHG | O4-P-O5 | 2.21 | 122.71 | 112.44 |
| 24 | C | 506 | CLA | O2A-CGA-O1A | -2.21 | 118.11 | 123.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 607 | CLA | O2A-CGA-O1A | -2.20 | 118.11 | 123.63 |
| 34 | Z | 101 | LMG | C1-O6-C5 | 2.20 | 118.02 | 113.72 |
| 24 | B | 614 | CLA | CMB-C2B-C1B | 2.20 | 128.77 | 125.42 |
| 27 | L | 102 | SQD | C44-O6-C1 | -2.20 | 109.07 | 113.80 |
| 24 | C | 509 | CLA | CMB-C2B-C1B | 2.20 | 128.77 | 125.42 |
| 24 | b | 611 | CLA | CMB-C2B-C1B | 2.20 | 128.77 | 125.42 |
| 34 | C | 521 | LMG | O7-C10-O9 | -2.20 | 118.56 | 123.70 |
| 24 | c | 910 | CLA | OBD-CAD-C3D | -2.20 | 123.27 | 128.42 |
| 24 | C | 512 | CLA | CMC-C2C-C1C | 2.20 | 128.47 | 125.03 |
| 26 | H | 101 | BCR | C20-C21-C22 | -2.20 | 124.19 | 127.28 |
| 24 | C | 505 | CLA | C1-O2A-CGA | 2.20 | 121.97 | 116.65 |
| 24 | c | 905 | CLA | CBC-CAC-C3C | -2.20 | 106.46 | 112.42 |
| 24 | d | 403 | CLA | C1-C2-C3 | -2.20 | 122.60 | 126.20 |
| 34 | Z | 101 | LMG | C9-O8-C28 | 2.20 | 122.50 | 117.08 |
| 27 | L | 102 | SQD | C45-O47-C7 | -2.20 | 112.54 | 117.80 |
| 24 | D | 401 | CLA | CED-O2D-CGD | 2.19 | 120.89 | 115.92 |
| 38 | e | 102 | HEM | O2D-CGD-CBD | 2.19 | 120.93 | 114.00 |
| 24 | B | 603 | CLA | O2A-CGA-O1A | -2.19 | 118.14 | 123.63 |
| 24 | b | 619 | CLA | CHA-C1A-NA | -2.19 | 121.42 | 126.39 |
| 24 | c | 903 | CLA | C4B-C3B-C2B | -2.19 | 104.58 | 107.30 |
| 26 | A | 411 | BCR | C16-C17-C18 | -2.19 | 124.20 | 127.28 |
| 24 | C | 507 | CLA | CGD-CBD-CAD | -2.19 | 103.75 | 110.85 |
| 25 | a | 420 | PHO | OBD-CAD-C3D | -2.19 | 124.47 | 127.89 |
| 36 | C | 519 | DGD | O1G-C1A-O1A | -2.19 | 118.15 | 123.63 |
| 31 | a | 417 | PL9 | C7-C3-C2 | -2.19 | 120.81 | 123.39 |
| 37 | d | 408 | LHG | O8-C23-C24 | 2.19 | 118.51 | 111.83 |
| 27 | a | 411 | SQD | C1-C2-C3 | -2.19 | 105.41 | 110.01 |
| 26 | H | 101 | BCR | C29-C30-C25 | 2.19 | 113.62 | 110.44 |
| 24 | b | 613 | CLA | CMB-C2B-C1B | 2.19 | 128.75 | 125.42 |
| 27 | a | 402 | SQD | O48-C23-O10 | -2.19 | 118.16 | 123.63 |
| 34 | C | 501 | LMG | O8-C28-C29 | 2.19 | 118.50 | 111.83 |
| 27 | B | 621 | SQD | C3-C4-C5 | 2.19 | 114.20 | 110.23 |
| 36 | c | 918 | DGD | O2G-C1B-O1B | -2.19 | 118.59 | 123.70 |
| 40 | V | 201 | HEC | O2D-CGD-CBD | 2.19 | 120.91 | 114.00 |
| 24 | B | 614 | CLA | C2A-C1A-CHA | -2.19 | 120.08 | 123.87 |
| 24 | C | 514 | CLA | CMB-C2B-C1B | 2.18 | 128.75 | 125.42 |
| 24 | B | 612 | CLA | O2D-CGD-O1D | -2.18 | 119.60 | 123.85 |
| 24 | b | 607 | CLA | CMA-C3A-C2A | -2.18 | 105.54 | 113.98 |
| 24 | c | 908 | CLA | CHB-C4A-NA | 2.18 | 127.55 | 124.40 |
| 24 | d | 403 | CLA | CAA-C2A-C3A | -2.18 | 107.10 | 113.00 |
| 24 | B | 603 | CLA | CAC-C3C-C4C | 2.18 | 127.63 | 124.79 |
| 29 | c | 921 | LMT | C1B-O1B-C4' | -2.18 | 112.81 | 117.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | E | 101 | LHG | C5-O7-C7 | -2.18 | 112.58 | 117.80 |
| 24 | A | 406 | CLA | O2A-CGA-CBA | 2.18 | 118.47 | 111.83 |
| 29 | B | 623 | LMT | C1-O1'-C1' | -2.18 | 109.96 | 113.68 |
| 24 | c | 909 | CLA | O2A-CGA-CBA | 2.18 | 118.47 | 111.83 |
| 24 | A | 406 | CLA | O1D-CGD-CBD | -2.17 | 120.23 | 124.52 |
| 24 | D | 402 | CLA | O2D-CGD-O1D | -2.17 | 119.62 | 123.85 |
| 26 | K | 103 | BCR | C2-C1-C6 | 2.17 | 113.60 | 110.44 |
| 35 | C | 523 | HTG | C1-O5-C5 | 2.17 | 116.46 | 112.56 |
| 24 | a | 409 | CLA | OBD-CAD-C3D | -2.17 | 123.34 | 128.42 |
| 24 | A | 406 | CLA | C1-C2-C3 | -2.17 | 122.64 | 126.20 |
| 31 | D | 404 | PL9 | C7-C3-C2 | -2.17 | 120.83 | 123.39 |
| 24 | C | 512 | CLA | C11-C10-C8 | -2.17 | 108.77 | 115.97 |
| 24 | C | 510 | CLA | C11-C12-C13 | -2.16 | 108.77 | 115.97 |
| 24 | C | 512 | CLA | CBC-CAC-C3C | -2.16 | 106.56 | 112.42 |
| 24 | b | 618 | CLA | C4D-CHA-C1A | -2.16 | 118.67 | 121.24 |
| 24 | B | 603 | CLA | CMC-C2C-C1C | 2.16 | 128.41 | 125.03 |
| 24 | C | 507 | CLA | CMA-C3A-C2A | -2.16 | 105.62 | 113.98 |
| 24 | b | 607 | CLA | CHB-C4A-NA | 2.16 | 127.51 | 124.40 |
| 36 | h | 102 | DGD | C3B-C2B-C1B | -2.16 | 105.79 | 113.69 |
| 38 | e | 102 | HEM | C2A-C1A-NA | -2.16 | 107.76 | 110.15 |
| 24 | b | 620 | CLA | OBD-CAD-C3D | -2.16 | 123.38 | 128.42 |
| 24 | c | 907 | CLA | CAA-CBA-CGA | 2.16 | 119.33 | 113.21 |
| 26 | T | 102 | BCR | C15-C16-C17 | -2.16 | 119.11 | 123.52 |
| 26 | T | 102 | BCR | C29-C28-C27 | -2.15 | 106.55 | 111.28 |
| 24 | b | 611 | CLA | C2A-C1A-CHA | -2.15 | 120.13 | 123.87 |
| 24 | b | 607 | CLA | OBD-CAD-C3D | -2.15 | 123.39 | 128.42 |
| 26 | c | 915 | BCR | C39-C30-C25 | -2.15 | 106.87 | 110.24 |
| 36 | c | 916 | DGD | O2G-C1B-O1B | -2.15 | 118.68 | 123.70 |
| 24 | B | 608 | CLA | C1-C2-C3 | -2.15 | 122.67 | 126.20 |
| 29 | f | 103 | LMT | O1B-C1B-C2B | 2.15 | 113.38 | 108.09 |
| 24 | d | 403 | CLA | O2A-CGA-CBA | 2.14 | 118.37 | 111.83 |
| 24 | a | 406 | CLA | CBC-CAC-C3C | -2.14 | 106.61 | 112.42 |
| 24 | B | 606 | CLA | CMC-C2C-C1C | 2.14 | 128.38 | 125.03 |
| 34 | c | 920 | LMG | O8-C28-O10 | -2.14 | 118.27 | 123.63 |
| 38 | E | 103 | HEM | CHA-C1A-NA | 2.14 | 127.74 | 123.86 |
| 34 | C | 501 | LMG | C8-O7-C10 | -2.14 | 112.67 | 117.80 |
| 24 | b | 614 | CLA | O1D-CGD-CBD | -2.14 | 120.30 | 124.52 |
| 24 | d | 401 | CLA | CED-O2D-CGD | 2.14 | 120.77 | 115.92 |
| 24 | B | 611 | CLA | CHC-C1C-NC | 2.14 | 127.53 | 124.31 |
| 24 | d | 403 | CLA | CBC-CAC-C3C | -2.14 | 106.62 | 112.42 |
| 26 | y | 101 | BCR | C35-C13-C14 | -2.14 | 119.35 | 122.82 |
| 36 | C | 517 | DGD | O1G-C1A-O1A | -2.14 | 118.28 | 123.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 905 | CLA | O2A-CGA-CBA | 2.14 | 118.35 | 111.83 |
| 26 | d | 404 | BCR | C10-C11-C12 | -2.14 | 117.01 | 123.20 |
| 24 | b | 619 | CLA | CMC-C2C-C1C | 2.14 | 128.37 | 125.03 |
| 36 | c | 916 | DGD | O6E-C5E-C4E | 2.14 | 113.55 | 109.70 |
| 24 | c | 908 | CLA | O2A-CGA-O1A | -2.14 | 118.29 | 123.63 |
| 24 | B | 617 | CLA | C4-C3-C5 | 2.13 | 118.93 | 115.23 |
| 24 | B | 611 | CLA | O2A-CGA-O1A | -2.13 | 118.29 | 123.63 |
| 40 | v | 202 | HEC | O2A-CGA-O1A | -2.13 | 117.85 | 123.33 |
| 24 | b | 609 | CLA | CAC-C3C-C4C | 2.13 | 127.56 | 124.79 |
| 26 | T | 102 | BCR | C2-C1-C6 | 2.13 | 113.53 | 110.44 |
| 26 | b | 622 | BCR | C11-C10-C9 | -2.13 | 124.29 | 127.28 |
| 24 | c | 911 | CLA | CBC-CAC-C3C | -2.13 | 106.64 | 112.42 |
| 24 | b | 617 | CLA | CBC-CAC-C3C | -2.13 | 106.65 | 112.42 |
| 24 | C | 508 | CLA | C4B-C3B-C2B | -2.13 | 104.66 | 107.30 |
| 24 | b | 613 | CLA | C7-C6-C5 | -2.13 | 107.59 | 113.26 |
| 24 | c | 910 | CLA | CBC-CAC-C3C | -2.13 | 106.65 | 112.42 |
| 36 | C | 519 | DGD | C4D-C3D-C2D | -2.13 | 107.10 | 110.83 |
| 26 | H | 101 | BCR | C24-C23-C22 | -2.13 | 123.09 | 126.23 |
| 38 | e | 102 | HEM | C4D-ND-C1D | 2.13 | 107.72 | 105.21 |
| 24 | c | 904 | CLA | OBD-CAD-C3D | -2.13 | 123.45 | 128.42 |
| 24 | b | 620 | CLA | C2A-C1A-CHA | -2.12 | 120.18 | 123.87 |
| 24 | D | 402 | CLA | CAA-C2A-C3A | -2.12 | 107.26 | 113.00 |
| 31 | A | 419 | PL9 | C37-C36-C34 | -2.12 | 106.15 | 113.19 |
| 24 | a | 409 | CLA | O2A-CGA-O1A | -2.12 | 118.32 | 123.63 |
| 24 | B | 609 | CLA | C2A-C1A-CHA | -2.12 | 120.19 | 123.87 |
| 36 | C | 518 | DGD | C2G-O2G-C1B | -2.12 | 112.72 | 117.80 |
| 24 | c | 902 | CLA | O2A-CGA-CBA | 2.12 | 118.30 | 111.83 |
| 24 | C | 510 | CLA | OBD-CAD-C3D | -2.12 | 123.46 | 128.42 |
| 24 | c | 913 | CLA | CAC-C3C-C4C | 2.12 | 127.55 | 124.79 |
| 27 | a | 402 | SQD | C3-C4-C5 | 2.12 | 114.08 | 110.23 |
| 24 | B | 609 | CLA | CMB-C2B-C3B | 2.12 | 131.54 | 126.55 |
| 24 | A | 406 | CLA | C4C-C3C-C2C | -2.12 | 103.81 | 106.89 |
| 24 | B | 602 | CLA | O1D-CGD-CBD | -2.12 | 120.34 | 124.52 |
| 24 | B | 610 | CLA | C7-C6-C5 | -2.12 | 107.61 | 113.26 |
| 24 | b | 614 | CLA | CED-O2D-CGD | 2.12 | 120.72 | 115.92 |
| 24 | a | 409 | CLA | CED-O2D-CGD | 2.12 | 120.72 | 115.92 |
| 31 | A | 419 | PL9 | C7-C3-C2 | -2.12 | 120.89 | 123.39 |
| 24 | c | 907 | CLA | OBD-CAD-C3D | -2.12 | 123.47 | 128.42 |
| 35 | c | 923 | HTG | C4-C3-C2 | -2.12 | 107.12 | 110.83 |
| 26 | B | 618 | BCR | C37-C22-C21 | -2.11 | 119.39 | 122.82 |
| 24 | c | 904 | CLA | C2A-C1A-CHA | -2.11 | 120.20 | 123.87 |
| 24 | c | 914 | CLA | CBC-CAC-C3C | -2.11 | 106.69 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | C | 501 | LMG | O6-C5-C4 | 2.11 | 113.51 | 109.70 |
| 26 | T | 102 | BCR | C7-C8-C9 | -2.11 | 123.11 | 126.23 |
| 26 | k | 101 | BCR | C11-C10-C9 | -2.11 | 124.31 | 127.28 |
| 26 | C | 516 | BCR | C2-C1-C6 | 2.11 | 113.51 | 110.44 |
| 40 | v | 202 | HEC | O2D-CGD-CBD | 2.11 | 120.67 | 114.00 |
| 24 | C | 510 | CLA | O2A-CGA-O1A | -2.11 | 118.35 | 123.63 |
| 35 | b | 626 | HTG | O5-C1-C2 | 2.11 | 113.23 | 110.32 |
| 24 | b | 617 | CLA | CED-O2D-CGD | 2.11 | 120.70 | 115.92 |
| 24 | B | 610 | CLA | C6-C5-C3 | 2.11 | 118.61 | 113.47 |
| 24 | C | 508 | CLA | C4-C3-C5 | 2.11 | 118.89 | 115.23 |
| 26 | y | 101 | BCR | C8-C7-C6 | -2.11 | 121.37 | 127.00 |
| 34 | j | 101 | LMG | O8-C28-C29 | 2.11 | 118.26 | 111.83 |
| 26 | a | 410 | BCR | C38-C26-C25 | -2.11 | 122.18 | 124.48 |
| 24 | B | 616 | CLA | O2A-CGA-CBA | 2.11 | 118.26 | 111.83 |
| 24 | c | 908 | CLA | CAA-C2A-C1A | 2.11 | 118.88 | 111.97 |
| 24 | b | 618 | CLA | CHB-C4A-NA | 2.11 | 127.44 | 124.40 |
| 27 | B | 621 | SQD | C25-C24-C23 | -2.11 | 105.98 | 113.69 |
| 24 | c | 905 | CLA | O1D-CGD-CBD | -2.10 | 120.37 | 124.52 |
| 26 | k | 101 | BCR | C35-C13-C14 | -2.10 | 119.41 | 122.82 |
| 24 | A | 405 | CLA | CMA-C3A-C2A | -2.10 | 105.85 | 113.98 |
| 24 | b | 607 | CLA | CBC-CAC-C3C | -2.10 | 106.72 | 112.42 |
| 31 | A | 419 | PL9 | C12-C13-C14 | -2.10 | 122.82 | 127.62 |
| 24 | B | 602 | CLA | CAA-C2A-C3A | -2.10 | 107.33 | 113.00 |
| 24 | C | 510 | CLA | O2A-CGA-CBA | 2.10 | 118.23 | 111.83 |
| 26 | a | 410 | BCR | C16-C17-C18 | -2.10 | 124.34 | 127.28 |
| 26 | b | 622 | BCR | C20-C21-C22 | -2.10 | 124.34 | 127.28 |
| 24 | b | 611 | CLA | CMA-C3A-C2A | -2.10 | 105.88 | 113.98 |
| 36 | c | 916 | DGD | C3G-C2G-C1G | -2.10 | 106.90 | 111.78 |
| 24 | c | 908 | CLA | C1-C2-C3 | -2.10 | 122.76 | 126.20 |
| 24 | C | 509 | CLA | C7-C6-C5 | -2.09 | 107.68 | 113.26 |
| 26 | K | 103 | BCR | C33-C5-C6 | -2.09 | 122.20 | 124.48 |
| 24 | c | 912 | CLA | CED-O2D-CGD | 2.09 | 120.66 | 115.92 |
| 37 | d | 409 | LHG | O8-C23-O10 | -2.09 | 118.39 | 123.63 |
| 34 | C | 521 | LMG | O8-C28-C29 | 2.09 | 118.21 | 111.83 |
| 24 | b | 611 | CLA | O2A-CGA-O1A | -2.09 | 118.40 | 123.63 |
| 24 | c | 908 | CLA | C4-C3-C5 | 2.09 | 118.86 | 115.23 |
| 24 | c | 913 | CLA | CMA-C3A-C4A | -2.09 | 106.16 | 111.77 |
| 25 | A | 409 | PHO | CMC-C2C-C1C | 2.09 | 128.49 | 124.73 |
| 26 | T | 102 | BCR | C3-C4-C5 | -2.09 | 110.33 | 114.06 |
| 26 | A | 411 | BCR | C11-C10-C9 | -2.09 | 124.35 | 127.28 |
| 24 | b | 614 | CLA | CAA-CBA-CGA | -2.09 | 107.28 | 113.21 |
| 24 | B | 611 | CLA | CHA-C1A-NA | -2.09 | 121.66 | 126.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 502 | CLA | CMB-C2B-C1B | 2.09 | 128.60 | 125.42 |
| 24 | C | 506 | CLA | CHA-C1A-NA | -2.09 | 121.67 | 126.39 |
| 25 | a | 420 | PHO | C4-C3-C2 | -2.09 | 118.27 | 123.63 |
| 24 | c | 909 | CLA | CHD-C4C-NC | 2.08 | 127.46 | 124.23 |
| 29 | f | 103 | LMT | O5'-C5'-C4' | 2.08 | 114.03 | 109.72 |
| 24 | B | 603 | CLA | CHB-C4A-NA | 2.08 | 127.41 | 124.40 |
| 36 | c | 917 | DGD | O2G-C1B-O1B | -2.08 | 118.84 | 123.70 |
| 24 | c | 907 | CLA | CED-O2D-CGD | 2.08 | 120.64 | 115.92 |
| 24 | C | 513 | CLA | CHA-C1A-NA | -2.08 | 121.68 | 126.39 |
| 24 | c | 906 | CLA | CHB-C1B-NB | -2.08 | 120.93 | 124.05 |
| 36 | C | 517 | DGD | O1G-C1A-C2A | 2.08 | 118.17 | 111.83 |
| 24 | a | 406 | CLA | C11-C10-C8 | -2.08 | 109.05 | 115.97 |
| 25 | A | 409 | PHO | C4D-CHA-CBD | 2.08 | 109.45 | 108.45 |
| 24 | C | 505 | CLA | CAA-CBA-CGA | 2.08 | 119.11 | 113.21 |
| 31 | A | 419 | PL9 | C2-C1-C6 | 2.08 | 121.47 | 119.00 |
| 24 | a | 406 | CLA | C11-C12-C13 | -2.07 | 109.07 | 115.97 |
| 24 | D | 401 | CLA | CAA-C2A-C3A | -2.07 | 107.39 | 113.00 |
| 25 | a | 420 | PHO | CAC-C3C-C4C | 2.07 | 129.35 | 124.03 |
| 27 | A | 412 | SQD | C3-C4-C5 | 2.07 | 113.99 | 110.23 |
| 26 | A | 411 | BCR | C21-C20-C19 | -2.07 | 117.20 | 123.20 |
| 34 | j | 101 | LMG | O7-C10-C11 | 2.07 | 115.96 | 111.48 |
| 26 | B | 618 | BCR | C16-C17-C18 | -2.07 | 124.38 | 127.28 |
| 24 | b | 615 | CLA | C7-C6-C5 | -2.07 | 107.75 | 113.26 |
| 24 | B | 603 | CLA | O1D-CGD-CBD | -2.07 | 120.44 | 124.52 |
| 26 | K | 103 | BCR | C10-C11-C12 | -2.07 | 117.21 | 123.20 |
| 26 | d | 404 | BCR | C27-C26-C25 | -2.07 | 119.91 | 122.70 |
| 36 | D | 405 | DGD | C1E-O6E-C5E | 2.07 | 117.75 | 113.72 |
| 24 | a | 406 | CLA | CHD-C4C-NC | 2.07 | 127.43 | 124.23 |
| 24 | B | 608 | CLA | OBD-CAD-C3D | -2.07 | 123.59 | 128.42 |
| 38 | E | 103 | HEM | C4D-ND-C1D | 2.06 | 107.65 | 105.21 |
| 36 | d | 406 | DGD | O2G-C1B-O1B | -2.06 | 118.88 | 123.70 |
| 31 | d | 405 | PL9 | C12-C13-C14 | -2.06 | 122.90 | 127.62 |
| 24 | B | 614 | CLA | CMC-C2C-C1C | 2.06 | 128.26 | 125.03 |
| 24 | D | 401 | CLA | C4-C3-C5 | 2.06 | 118.81 | 115.23 |
| 27 | f | 102 | SQD | O48-C23-O10 | -2.06 | 118.47 | 123.63 |
| 24 | C | 513 | CLA | O1D-CGD-CBD | -2.06 | 120.45 | 124.52 |
| 24 | B | 606 | CLA | OBD-CAD-C3D | -2.06 | 123.61 | 128.42 |
| 34 | b | 624 | LMG | O7-C10-O9 | -2.06 | 118.90 | 123.70 |
| 24 | B | 605 | CLA | C4-C3-C5 | 2.05 | 118.80 | 115.23 |
| 24 | d | 403 | CLA | CMA-C3A-C2A | -2.05 | 106.04 | 113.98 |
| 26 | c | 915 | BCR | C20-C21-C22 | -2.05 | 124.40 | 127.28 |
| 27 | L | 102 | SQD | O48-C23-O10 | -2.05 | 118.49 | 123.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | c | 910 | CLA | O2A-CGA-O1A | -2.05 | 118.49 | 123.63 |
| 29 | m | 102 | LMT | C6'-C5'-C4' | -2.05 | 107.61 | 113.38 |
| 24 | b | 619 | CLA | CHD-C4C-NC | 2.05 | 127.42 | 124.23 |
| 24 | B | 609 | CLA | CHB-C1B-C2B | -2.05 | 121.47 | 127.43 |
| 24 | b | 610 | CLA | C1-C2-C3 | -2.05 | 122.83 | 126.20 |
| 37 | L | 101 | LHG | C6-C5-C4 | -2.05 | 107.00 | 111.78 |
| 34 | C | 520 | LMG | O6-C5-C6 | 2.05 | 111.52 | 106.44 |
| 36 | H | 102 | DGD | O6E-C5E-C6E | 2.05 | 111.52 | 106.44 |
| 26 | B | 618 | BCR | C34-C9-C10 | -2.05 | 119.49 | 122.82 |
| 36 | C | 518 | DGD | O6D-C1D-O3G | -2.05 | 105.20 | 110.04 |
| 24 | c | 914 | CLA | CHB-C4A-NA | 2.05 | 127.36 | 124.40 |
| 24 | A | 407 | CLA | O2A-CGA-CBA | 2.05 | 118.09 | 111.83 |
| 38 | e | 102 | HEM | CMD-C2D-C1D | 2.05 | 128.24 | 125.03 |
| 24 | c | 902 | CLA | O2A-CGA-O1A | -2.05 | 118.51 | 123.63 |
| 26 | B | 620 | BCR | C10-C11-C12 | -2.05 | 117.27 | 123.20 |
| 24 | b | 612 | CLA | CAA-C2A-C3A | -2.04 | 107.47 | 113.00 |
| 31 | D | 404 | PL9 | C2-C1-C6 | 2.04 | 121.43 | 119.00 |
| 26 | k | 101 | BCR | C20-C21-C22 | -2.04 | 124.41 | 127.28 |
| 26 | t | 101 | BCR | C7-C8-C9 | -2.04 | 123.21 | 126.23 |
| 24 | b | 611 | CLA | CED-O2D-CGD | 2.04 | 120.54 | 115.92 |
| 38 | e | 102 | HEM | C4C-CHD-C1D | -2.04 | 121.69 | 126.02 |
| 26 | C | 516 | BCR | C11-C10-C9 | -2.04 | 124.42 | 127.28 |
| 24 | b | 614 | CLA | CMC-C2C-C1C | 2.03 | 128.21 | 125.03 |
| 36 | c | 917 | DGD | C2G-O2G-C1B | -2.03 | 112.93 | 117.80 |
| 24 | b | 610 | CLA | C11-C10-C8 | -2.03 | 109.21 | 115.97 |
| 36 | h | 102 | DGD | O4E-C4E-C5E | 2.03 | 114.33 | 109.32 |
| 26 | b | 621 | BCR | C21-C20-C19 | -2.03 | 117.32 | 123.20 |
| 24 | c | 911 | CLA | C4-C3-C2 | -2.03 | 118.42 | 123.63 |
| 24 | a | 406 | CLA | CMA-C3A-C4A | -2.03 | 106.32 | 111.77 |
| 34 | j | 101 | LMG | O6-C5-C4 | 2.03 | 113.35 | 109.70 |
| 27 | F | 101 | SQD | O9-S-C6 | 2.03 | 109.78 | 106.76 |
| 24 | b | 613 | CLA | CED-O2D-CGD | 2.02 | 120.50 | 115.92 |
| 26 | D | 403 | BCR | C11-C10-C9 | -2.02 | 124.44 | 127.28 |
| 24 | B | 615 | CLA | OBD-CAD-C3D | -2.02 | 123.70 | 128.42 |
| 24 | B | 603 | CLA | CHB-C1B-C2B | -2.02 | 121.57 | 127.43 |
| 38 | e | 102 | HEM | C4C-NC-C1C | 2.02 | 109.11 | 105.82 |
| 24 | c | 906 | CLA | CHD-C4C-NC | 2.02 | 127.36 | 124.23 |
| 34 | C | 501 | LMG | O7-C10-O9 | -2.02 | 118.99 | 123.70 |
| 24 | A | 407 | CLA | CHB-C1B-C2B | -2.02 | 121.57 | 127.43 |
| 36 | h | 102 | DGD | C3E-C4E-C5E | -2.02 | 106.58 | 110.23 |
| 24 | b | 605 | CLA | CAC-C3C-C2C | 2.02 | 131.26 | 127.56 |
| 24 | B | 610 | CLA | CMA-C3A-C2A | -2.01 | 106.19 | 113.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | C | 513 | CLA | CBA-CAA-C2A | -2.01 | 107.80 | 113.79 |
| 27 | B | 621 | SQD | O48-C23-O10 | -2.01 | 118.59 | 123.63 |
| 26 | t | 101 | BCR | C11-C10-C9 | -2.01 | 124.46 | 127.28 |
| 24 | b | 605 | CLA | CMB-C2B-C1B | 2.01 | 128.48 | 125.42 |
| 24 | c | 906 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.40 |
| 29 | M | 101 | LMT | O5'-C1'-O1' | -2.01 | 105.30 | 110.04 |
| 24 | C | 513 | CLA | OBD-CAD-C3D | -2.01 | 123.72 | 128.42 |
| 24 | c | 913 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.40 |
| 24 | B | 608 | CLA | CHB-C1B-C2B | -2.01 | 121.59 | 127.43 |
| 24 | A | 406 | CLA | CHA-C1A-NA | -2.01 | 121.85 | 126.39 |
| 26 | C | 516 | BCR | C32-C1-C6 | -2.01 | 107.10 | 110.24 |
| 24 | B | 608 | CLA | CBC-CAC-C3C | -2.01 | 106.98 | 112.42 |
| 24 | C | 511 | CLA | CMB-C2B-C1B | 2.01 | 128.47 | 125.42 |
| 31 | a | 417 | PL9 | C45-C44-C46 | 2.00 | 118.71 | 115.23 |
| 24 | B | 613 | CLA | CMA-C3A-C2A | -2.00 | 106.23 | 113.98 |
| 24 | C | 506 | CLA | C2A-C1A-CHA | -2.00 | 120.39 | 123.87 |
| 29 | m | 103 | LMT | O5B-C5B-C6B | 2.00 | 111.40 | 106.44 |
| 24 | a | 406 | CLA | CMC-C2C-C1C | 2.00 | 128.16 | 125.03 |
| 34 | Z | 101 | LMG | O7-C10-O9 | -2.00 | 119.03 | 123.70 |
| 24 | b | 612 | CLA | C4-C3-C5 | 2.00 | 118.70 | 115.23 |
| 24 | c | 911 | CLA | O2D-CGD-O1D | -2.00 | 119.95 | 123.85 |

All (61) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 24 | A | 405 | CLA | ND |
| 24 | A | 406 | CLA | ND |
| 24 | B | 602 | CLA | ND |
| 24 | B | 603 | CLA | ND |
| 24 | B | 604 | CLA | ND |
| 24 | B | 605 | CLA | ND |
| 24 | B | 606 | CLA | ND |
| 24 | B | 607 | CLA | ND |
| 24 | B | 608 | CLA | ND |
| 24 | B | 610 | CLA | ND |
| 24 | B | 611 | CLA | ND |
| 24 | B | 612 | CLA | ND |
| 24 | B | 613 | CLA | ND |
| 24 | B | 614 | CLA | ND |
| 24 | B | 615 | CLA | ND |
| 24 | B | 616 | CLA | ND |
| 24 | B | 617 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 24 | C | 502 | CLA | ND |
| 24 | C | 504 | CLA | ND |
| 24 | C | 505 | CLA | ND |
| 24 | C | 506 | CLA | ND |
| 24 | C | 507 | CLA | ND |
| 24 | C | 508 | CLA | ND |
| 24 | C | 510 | CLA | ND |
| 24 | C | 511 | CLA | ND |
| 24 | C | 512 | CLA | ND |
| 24 | C | 513 | CLA | ND |
| 24 | D | 401 | CLA | ND |
| 24 | D | 402 | CLA | ND |
| 24 | a | 406 | CLA | ND |
| 24 | a | 409 | CLA | ND |
| 24 | b | 605 | CLA | ND |
| 24 | b | 606 | CLA | ND |
| 24 | b | 607 | CLA | ND |
| 24 | b | 608 | CLA | ND |
| 24 | b | 609 | CLA | ND |
| 24 | b | 610 | CLA | ND |
| 24 | b | 611 | CLA | ND |
| 24 | b | 613 | CLA | ND |
| 24 | b | 614 | CLA | ND |
| 24 | b | 615 | CLA | ND |
| 24 | b | 616 | CLA | ND |
| 24 | b | 617 | CLA | ND |
| 24 | b | 618 | CLA | ND |
| 24 | b | 619 | CLA | ND |
| 24 | b | 620 | CLA | ND |
| 24 | c | 902 | CLA | ND |
| 24 | c | 903 | CLA | ND |
| 24 | c | 904 | CLA | ND |
| 24 | c | 905 | CLA | ND |
| 24 | c | 906 | CLA | ND |
| 24 | c | 907 | CLA | ND |
| 24 | c | 908 | CLA | ND |
| 24 | c | 909 | CLA | ND |
| 24 | c | 910 | CLA | ND |
| 24 | c | 911 | CLA | ND |
| 24 | c | 912 | CLA | ND |
| 24 | c | 913 | CLA | ND |
| 24 | c | 914 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 24 | d | 401 | CLA | ND |
| 24 | d | 402 | CLA | ND |

All (1215) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | A | 410 | CLA | C4-C3-C5-C6 |
| 24 | B | 615 | CLA | CAD-CBD-CGD-O1D |
| 24 | B | 615 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 503 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 506 | CLA | C2B-C3B-CAB-CBB |
| 24 | C | 506 | CLA | C4B-C3B-CAB-CBB |
| 24 | C | 508 | CLA | CHA-CBD-CGD-O1D |
| 24 | C | 508 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 510 | CLA | CHA-CBD-CGD-O1D |
| 24 | C | 510 | CLA | CHA-CBD-CGD-O2D |
| 24 | b | 610 | CLA | C2B-C3B-CAB-CBB |
| 24 | b | 610 | CLA | C4B-C3B-CAB-CBB |
| 24 | b | 618 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 618 | CLA | CAD-CBD-CGD-O2D |
| 24 | c | 908 | CLA | CHA-CBD-CGD-O1D |
| 24 | c | 908 | CLA | CHA-CBD-CGD-O2D |
| 24 | c | 910 | CLA | CHA-CBD-CGD-O1D |
| 24 | c | 910 | CLA | CHA-CBD-CGD-O2D |
| 24 | c | 914 | CLA | C2B-C3B-CAB-CBB |
| 24 | c | 914 | CLA | C4B-C3B-CAB-CBB |
| 26 | D | 403 | BCR | C21-C22-C23-C24 |
| 26 | D | 403 | BCR | C37-C22-C23-C24 |
| 26 | H | 101 | BCR | C7-C8-C9-C10 |
| 26 | K | 102 | BCR | C5-C6-C7-C8 |
| 26 | K | 102 | BCR | C21-C22-C23-C24 |
| 26 | d | 404 | BCR | C21-C22-C23-C24 |
| 26 | y | 101 | BCR | C1-C6-C7-C8 |
| 26 | y | 101 | BCR | C5-C6-C7-C8 |
| 27 | A | 416 | SQD | O6-C44-C45-O47 |
| 27 | B | 621 | SQD | O49-C7-O47-C45 |
| 27 | B | 621 | SQD | C8-C7-O47-C45 |
| 27 | F | 101 | SQD | O49-C7-O47-C45 |
| 27 | F | 101 | SQD | C8-C7-O47-C45 |
| 27 | L | 102 | SQD | O5-C1-O6-C44 |
| 27 | L | 102 | SQD | O49-C7-O47-C45 |
| 27 | L | 102 | SQD | C5-C6-S-O7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | L | 102 | SQD | C5-C6-S-O8 |
| 27 | L | 102 | SQD | C5-C6-S-O9 |
| 27 | a | 402 | SQD | O6-C44-C45-O47 |
| 27 | f | 102 | SQD | O49-C7-O47-C45 |
| 27 | f | 102 | SQD | C8-C7-O47-C45 |
| 27 | f | 102 | SQD | C5-C6-S-O7 |
| 27 | f | 102 | SQD | C5-C6-S-O8 |
| 27 | f | 102 | SQD | C5-C6-S-O9 |
| 28 | A | 414 | GOL | C1-C2-C3-O3 |
| 28 | A | 414 | GOL | O2-C2-C3-O3 |
| 28 | A | 415 | GOL | O1-C1-C2-C3 |
| 28 | B | 629 | GOL | O1-C1-C2-C3 |
| 28 | B | 631 | GOL | O1-C1-C2-C3 |
| 28 | B | 637 | GOL | O1-C1-C2-C3 |
| 28 | F | 103 | GOL | O1-C1-C2-C3 |
| 28 | O | 302 | GOL | O1-C1-C2-C3 |
| 28 | T | 103 | GOL | O1-C1-C2-C3 |
| 28 | V | 203 | GOL | O1-C1-C2-C3 |
| 28 | V | 203 | GOL | C1-C2-C3-O3 |
| 28 | a | 415 | GOL | O1-C1-C2-C3 |
| 28 | b | 631 | GOL | O1-C1-C2-C3 |
| 28 | b | 633 | GOL | O1-C1-C2-O2 |
| 28 | f | 101 | GOL | O1-C1-C2-C3 |
| 28 | v | 203 | GOL | O1-C1-C2-C3 |
| 28 | v | 205 | GOL | O1-C1-C2-C3 |
| 29 | b | 601 | LMT | C2'-C1'-O1'-C1 |
| 29 | b | 601 | LMT | O5'-C1'-O1'-C1 |
| 29 | m | 102 | LMT | O5'-C1'-O1'-C1 |
| 29 | m | 102 | LMT | C2-C1-O1'-C1' |
| 34 | Z | 101 | LMG | O6-C1-O1-C7 |
| 34 | Z | 101 | LMG | O9-C10-O7-C8 |
| 34 | Z | 101 | LMG | C11-C10-O7-C8 |
| 34 | z | 101 | LMG | O9-C10-O7-C8 |
| 34 | z | 101 | LMG | C11-C10-O7-C8 |
| 35 | B | 625 | HTG | C2'-C1'-S1-C1 |
| 35 | V | 202 | HTG | O5-C1-S1-C1' |
| 36 | D | 405 | DGD | C2B-C1B-O2G-C2G |
| 36 | D | 405 | DGD | O6E-C1E-O5D-C6D |
| 36 | d | 406 | DGD | C2B-C1B-O2G-C2G |
| 36 | d | 406 | DGD | O1B-C1B-O2G-C2G |
| 36 | d | 406 | DGD | C2E-C1E-O5D-C6D |
| 36 | d | 406 | DGD | O6E-C1E-O5D-C6D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | D | 407 | LHG | C3-O3-P-O4 |
| 37 | D | 407 | LHG | C3-O3-P-O6 |
| 37 | E | 101 | LHG | C4-O6-P-O3 |
| 37 | E | 101 | LHG | C24-C23-O8-C6 |
| 37 | L | 101 | LHG | C4-O6-P-O3 |
| 37 | L | 101 | LHG | C4-O6-P-O4 |
| 37 | L | 101 | LHG | C4-O6-P-O5 |
| 37 | d | 408 | LHG | C3-O3-P-O4 |
| 37 | d | 408 | LHG | C3-O3-P-O6 |
| 37 | d | 408 | LHG | C4-O6-P-O3 |
| 37 | d | 408 | LHG | C4-O6-P-O4 |
| 37 | e | 101 | LHG | C3-O3-P-O6 |
| 37 | l | 101 | LHG | C4-O6-P-O3 |
| 37 | l | 101 | LHG | C4-O6-P-O4 |
| 37 | l | 101 | LHG | C4-O6-P-O5 |
| 40 | V | 201 | HEC | C2B-C3B-CAB-CBB |
| 40 | V | 201 | HEC | C4B-C3B-CAB-CBB |
| 40 | V | 201 | HEC | C2C-C3C-CAC-CBC |
| 40 | V | 201 | HEC | C4C-C3C-CAC-CBC |
| 40 | v | 202 | HEC | C2B-C3B-CAB-CBB |
| 40 | v | 202 | HEC | C4B-C3B-CAB-CBB |
| 40 | v | 202 | HEC | C2C-C3C-CAC-CBC |
| 40 | v | 202 | HEC | C4C-C3C-CAC-CBC |
| 29 | B | 623 | LMT | C3'-C4'-O1B-C1B |
| 29 | C | 522 | LMT | C3'-C4'-O1B-C1B |
| 37 | E | 101 | LHG | O10-C23-O8-C6 |
| 37 | e | 101 | LHG | O10-C23-O8-C6 |
| 37 | e | 101 | LHG | C24-C23-O8-C6 |
| 36 | D | 405 | DGD | O1B-C1B-O2G-C2G |
| 24 | B | 605 | CLA | C3-C5-C6-C7 |
| 27 | L | 102 | SQD | C8-C7-O47-C45 |
| 24 | C | 508 | CLA | C4-C3-C5-C6 |
| 24 | b | 607 | CLA | C4-C3-C5-C6 |
| 24 | b | 609 | CLA | C4-C3-C5-C6 |
| 24 | b | 618 | CLA | C4-C3-C5-C6 |
| 31 | a | 417 | PL9 | C15-C14-C16-C17 |
| 24 | A | 410 | CLA | C2-C3-C5-C6 |
| 24 | C | 508 | CLA | C2-C3-C5-C6 |
| 24 | b | 607 | CLA | C2-C3-C5-C6 |
| 24 | b | 609 | CLA | C2-C3-C5-C6 |
| 24 | b | 618 | CLA | C2-C3-C5-C6 |
| 31 | a | 417 | PL9 | C13-C14-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | B | 615 | CLA | C3-C5-C6-C7 |
| 24 | b | 618 | CLA | C3-C5-C6-C7 |
| 24 | c | 902 | CLA | CBD-CGD-O2D-CED |
| 37 | E | 101 | LHG | C8-C7-O7-C5 |
| 29 | B | 623 | LMT | O5B-C5B-C6B-O6B |
| 24 | B | 617 | CLA | C3-C5-C6-C7 |
| 24 | B | 604 | CLA | C4-C3-C5-C6 |
| 24 | B | 615 | CLA | C4-C3-C5-C6 |
| 24 | B | 615 | CLA | C2-C3-C5-C6 |
| 29 | f | 103 | LMT | O5'-C5'-C6'-O6' |
| 31 | a | 417 | PL9 | C9-C11-C12-C13 |
| 29 | B | 636 | LMT | O5'-C1'-O1'-C1 |
| 29 | C | 522 | LMT | O5'-C1'-O1'-C1 |
| 29 | E | 102 | LMT | O5'-C1'-O1'-C1 |
| 29 | b | 625 | LMT | O5'-C1'-O1'-C1 |
| 36 | D | 405 | DGD | O6D-C1D-O3G-C3G |
| 35 | B | 633 | HTG | O5-C5-C6-O6 |
| 24 | d | 401 | CLA | CBD-CGD-O2D-CED |
| 35 | V | 202 | HTG | C4-C5-C6-O6 |
| 29 | m | 102 | LMT | C4'-C5'-C6'-O6' |
| 24 | C | 510 | CLA | C3-C5-C6-C7 |
| 34 | C | 521 | LMG | O6-C5-C6-O5 |
| 31 | A | 419 | PL9 | C25-C24-C26-C27 |
| 24 | B | 604 | CLA | C2-C3-C5-C6 |
| 31 | A | 419 | PL9 | C23-C24-C26-C27 |
| 24 | d | 403 | CLA | C3-C5-C6-C7 |
| 24 | B | 617 | CLA | C6-C7-C8-C9 |
| 24 | C | 502 | CLA | C11-C12-C13-C14 |
| 24 | C | 513 | CLA | C6-C7-C8-C9 |
| 24 | a | 407 | CLA | C14-C13-C15-C16 |
| 24 | c | 907 | CLA | C6-C7-C8-C9 |
| 24 | c | 911 | CLA | C11-C12-C13-C14 |
| 29 | B | 623 | LMT | C4B-C5B-C6B-O6B |
| 29 | B | 636 | LMT | C2'-C1'-O1'-C1 |
| 29 | C | 522 | LMT | C2'-C1'-O1'-C1 |
| 29 | E | 102 | LMT | C2'-C1'-O1'-C1 |
| 29 | b | 625 | LMT | C2'-C1'-O1'-C1 |
| 34 | Z | 101 | LMG | C2-C1-O1-C7 |
| 36 | D | 405 | DGD | C2D-C1D-O3G-C3G |
| 26 | K | 102 | BCR | C37-C22-C23-C24 |
| 26 | d | 404 | BCR | C37-C22-C23-C24 |
| 35 | B | 633 | HTG | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | B | 621 | SQD | C7-C8-C9-C10 |
| 27 | F | 101 | SQD | C7-C8-C9-C10 |
| 37 | E | 101 | LHG | O6-C4-C5-O7 |
| 24 | a | 409 | CLA | C5-C6-C7-C8 |
| 28 | B | 629 | GOL | O1-C1-C2-O2 |
| 28 | B | 631 | GOL | O1-C1-C2-O2 |
| 28 | T | 103 | GOL | O1-C1-C2-O2 |
| 28 | b | 632 | GOL | O2-C2-C3-O3 |
| 28 | v | 203 | GOL | O1-C1-C2-O2 |
| 24 | C | 510 | CLA | C8-C10-C11-C12 |
| 35 | V | 202 | HTG | O5-C5-C6-O6 |
| 24 | A | 410 | CLA | C12-C13-C15-C16 |
| 24 | B | 615 | CLA | C11-C10-C8-C7 |
| 24 | b | 610 | CLA | C12-C13-C15-C16 |
| 24 | D | 402 | CLA | C4-C3-C5-C6 |
| 37 | E | 101 | LHG | O9-C7-O7-C5 |
| 35 | B | 626 | HTG | O5-C5-C6-O6 |
| 24 | B | 604 | CLA | C5-C6-C7-C8 |
| 29 | m | 103 | LMT | O5'-C5'-C6'-O6' |
| 29 | m | 104 | LMT | O5'-C5'-C6'-O6' |
| 27 | A | 416 | SQD | C23-C24-C25-C26 |
| 34 | C | 521 | LMG | C11-C10-O7-C8 |
| 24 | B | 615 | CLA | C5-C6-C7-C8 |
| 24 | C | 509 | CLA | C10-C11-C12-C13 |
| 24 | a | 409 | CLA | C8-C10-C11-C12 |
| 24 | b | 620 | CLA | C15-C16-C17-C18 |
| 24 | c | 907 | CLA | C10-C11-C12-C13 |
| 24 | c | 911 | CLA | C8-C10-C11-C12 |
| 29 | f | 103 | LMT | C4'-C5'-C6'-O6' |
| 24 | B | 607 | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 610 | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 610 | CLA | C10-C11-C12-C13 |
| 29 | f | 103 | LMT | O5'-C1'-O1'-C1 |
| 24 | B | 602 | CLA | C5-C6-C7-C8 |
| 24 | b | 607 | CLA | C5-C6-C7-C8 |
| 24 | b | 618 | CLA | C15-C16-C17-C18 |
| 24 | a | 409 | CLA | C15-C16-C17-C18 |
| 24 | c | 907 | CLA | C3-C5-C6-C7 |
| 29 | m | 102 | LMT | O5'-C5'-C6'-O6' |
| 34 | C | 520 | LMG | C28-C29-C30-C31 |
| 29 | C | 522 | LMT | O5B-C5B-C6B-O6B |
| 24 | B | 617 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | C | 507 | CLA | C13-C15-C16-C17 |
| 24 | D | 402 | CLA | C5-C6-C7-C8 |
| 24 | b | 618 | CLA | C10-C11-C12-C13 |
| 29 | a | 401 | LMT | C3-C4-C5-C6 |
| 35 | C | 524 | HTG | O5-C5-C6-O6 |
| 37 | d | 409 | LHG | C30-C31-C32-C33 |
| 34 | C | 521 | LMG | O9-C10-O7-C8 |
| 24 | C | 508 | CLA | C2A-CAA-CBA-CGA |
| 24 | c | 907 | CLA | C15-C16-C17-C18 |
| 24 | b | 610 | CLA | CBD-CGD-O2D-CED |
| 24 | b | 605 | CLA | CBA-CGA-O2A-C1 |
| 27 | F | 101 | SQD | C23-C24-C25-C26 |
| 24 | b | 605 | CLA | C8-C10-C11-C12 |
| 24 | B | 602 | CLA | C3-C5-C6-C7 |
| 34 | C | 501 | LMG | C11-C10-O7-C8 |
| 34 | b | 624 | LMG | C30-C31-C32-C33 |
| 34 | C | 501 | LMG | O9-C10-O7-C8 |
| 34 | c | 919 | LMG | O9-C10-O7-C8 |
| 29 | a | 401 | LMT | C2'-C1'-O1'-C1 |
| 29 | c | 921 | LMT | C2'-C1'-O1'-C1 |
| 29 | f | 103 | LMT | C2'-C1'-O1'-C1 |
| 29 | m | 102 | LMT | C2'-C1'-O1'-C1 |
| 36 | d | 406 | DGD | C2D-C1D-O3G-C3G |
| 24 | B | 615 | CLA | C10-C11-C12-C13 |
| 26 | D | 403 | BCR | C7-C8-C9-C34 |
| 26 | H | 101 | BCR | C7-C8-C9-C34 |
| 26 | b | 623 | BCR | C37-C22-C23-C24 |
| 26 | b | 623 | BCR | C21-C22-C23-C24 |
| 36 | c | 916 | DGD | O6D-C5D-C6D-O5D |
| 28 | B | 627 | GOL | O1-C1-C2-C3 |
| 28 | B | 632 | GOL | O1-C1-C2-C3 |
| 28 | T | 103 | GOL | C1-C2-C3-O3 |
| 28 | V | 204 | GOL | O1-C1-C2-C3 |
| 28 | V | 205 | GOL | O1-C1-C2-C3 |
| 28 | b | 628 | GOL | C1-C2-C3-O3 |
| 28 | b | 632 | GOL | C1-C2-C3-O3 |
| 28 | b | 633 | GOL | O1-C1-C2-C3 |
| 28 | f | 101 | GOL | C1-C2-C3-O3 |
| 28 | o | 302 | GOL | O1-C1-C2-C3 |
| 24 | a | 409 | CLA | C16-C17-C18-C19 |
| 24 | C | 513 | CLA | C3-C5-C6-C7 |
| 24 | b | 605 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | M | 101 | LMT | O5'-C5'-C6'-O6' |
| 29 | a | 401 | LMT | C4B-C5B-C6B-O6B |
| 29 | a | 401 | LMT | O5'-C1'-O1'-C1 |
| 29 | c | 921 | LMT | O5'-C1'-O1'-C1 |
| 36 | d | 406 | DGD | O6D-C1D-O3G-C3G |
| 34 | c | 919 | LMG | C11-C10-O7-C8 |
| 36 | d | 406 | DGD | C4E-C5E-C6E-O5E |
| 36 | c | 917 | DGD | C3B-C4B-C5B-C6B |
| 24 | B | 602 | CLA | CBA-CGA-O2A-C1 |
| 24 | B | 617 | CLA | C2-C1-O2A-CGA |
| 24 | C | 510 | CLA | C2-C1-O2A-CGA |
| 24 | b | 605 | CLA | C2-C1-O2A-CGA |
| 24 | C | 507 | CLA | C16-C17-C18-C20 |
| 24 | c | 903 | CLA | C16-C17-C18-C20 |
| 27 | L | 102 | SQD | C30-C31-C32-C33 |
| 29 | b | 601 | LMT | C3-C4-C5-C6 |
| 37 | d | 407 | LHG | C27-C28-C29-C30 |
| 27 | L | 102 | SQD | C14-C15-C16-C17 |
| 34 | J | 101 | LMG | C20-C21-C22-C23 |
| 36 | H | 102 | DGD | C7A-C8A-C9A-CAA |
| 36 | D | 405 | DGD | C1A-C2A-C3A-C4A |
| 35 | b | 627 | HTG | O5-C5-C6-O6 |
| 24 | C | 502 | CLA | C15-C16-C17-C18 |
| 27 | a | 411 | SQD | C25-C26-C27-C28 |
| 37 | D | 407 | LHG | C32-C33-C34-C35 |
| 37 | d | 407 | LHG | C32-C33-C34-C35 |
| 36 | C | 517 | DGD | O6D-C5D-C6D-O5D |
| 27 | a | 402 | SQD | C10-C11-C12-C13 |
| 27 | a | 411 | SQD | C34-C35-C36-C37 |
| 34 | B | 622 | LMG | C31-C32-C33-C34 |
| 34 | Z | 101 | LMG | C19-C20-C21-C22 |
| 35 | B | 625 | HTG | C2'-C3'-C4'-C5' |
| 36 | C | 517 | DGD | C3B-C4B-C5B-C6B |
| 37 | L | 101 | LHG | C12-C13-C14-C15 |
| 28 | A | 415 | GOL | O1-C1-C2-O2 |
| 28 | B | 637 | GOL | O1-C1-C2-O2 |
| 28 | F | 103 | GOL | O1-C1-C2-O2 |
| 28 | O | 302 | GOL | O1-C1-C2-O2 |
| 28 | T | 103 | GOL | O2-C2-C3-O3 |
| 28 | a | 415 | GOL | O1-C1-C2-O2 |
| 28 | f | 101 | GOL | O2-C2-C3-O3 |
| 28 | v | 205 | GOL | O1-C1-C2-O2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | f | 102 | SQD | C29-C30-C31-C32 |
| 36 | C | 519 | DGD | C2A-C3A-C4A-C5A |
| 36 | c | 918 | DGD | C5A-C6A-C7A-C8A |
| 24 | c | 902 | CLA | O1D-CGD-O2D-CED |
| 24 | D | 401 | CLA | C4B-C3B-CAB-CBB |
| 36 | c | 918 | DGD | C1A-C2A-C3A-C4A |
| 34 | J | 101 | LMG | O6-C5-C6-O5 |
| 34 | j | 101 | LMG | O6-C5-C6-O5 |
| 27 | a | 411 | SQD | C9-C10-C11-C12 |
| 37 | D | 408 | LHG | C29-C30-C31-C32 |
| 27 | A | 412 | SQD | C9-C10-C11-C12 |
| 27 | a | 411 | SQD | C30-C31-C32-C33 |
| 34 | C | 520 | LMG | C17-C18-C19-C20 |
| 24 | B | 616 | CLA | C11-C12-C13-C15 |
| 24 | b | 608 | CLA | C11-C12-C13-C15 |
| 34 | C | 501 | LMG | C37-C38-C39-C40 |
| 36 | c | 918 | DGD | C2B-C3B-C4B-C5B |
| 24 | B | 614 | CLA | C13-C15-C16-C17 |
| 27 | A | 412 | SQD | C32-C33-C34-C35 |
| 29 | C | 522 | LMT | C4-C5-C6-C7 |
| 34 | j | 101 | LMG | C17-C18-C19-C20 |
| 36 | H | 102 | DGD | CCB-CDB-CEB-CFB |
| 24 | b | 608 | CLA | C3-C5-C6-C7 |
| 27 | L | 102 | SQD | C26-C27-C28-C29 |
| 24 | B | 606 | CLA | C2-C3-C5-C6 |
| 24 | D | 402 | CLA | C2-C3-C5-C6 |
| 24 | b | 612 | CLA | C13-C15-C16-C17 |
| 24 | c | 910 | CLA | C13-C15-C16-C17 |
| 29 | m | 102 | LMT | O1'-C1-C2-C3 |
| 34 | C | 520 | LMG | C12-C13-C14-C15 |
| 27 | B | 621 | SQD | C31-C32-C33-C34 |
| 36 | c | 918 | DGD | C3B-C4B-C5B-C6B |
| 27 | B | 621 | SQD | C24-C23-O48-C46 |
| 34 | b | 624 | LMG | C38-C39-C40-C41 |
| 36 | C | 517 | DGD | C4B-C5B-C6B-C7B |
| 36 | D | 405 | DGD | C1B-C2B-C3B-C4B |
| 36 | H | 102 | DGD | CBA-CCA-CDA-CEA |
| 36 | c | 917 | DGD | C9B-CAB-CBB-CCB |
| 36 | d | 406 | DGD | C2A-C3A-C4A-C5A |
| 24 | b | 605 | CLA | O1A-CGA-O2A-C1 |
| 27 | f | 102 | SQD | C26-C27-C28-C29 |
| 34 | B | 622 | LMG | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 36 | c | 918 | DGD | C2A-C3A-C4A-C5A |
| 37 | L | 101 | LHG | C14-C15-C16-C17 |
| 37 | e | 101 | LHG | C9-C10-C11-C12 |
| 24 | d | 401 | CLA | O1D-CGD-O2D-CED |
| 35 | C | 524 | HTG | S1-C1'-C2'-C3' |
| 37 | d | 409 | LHG | C15-C16-C17-C18 |
| 24 | B | 602 | CLA | O1A-CGA-O2A-C1 |
| 24 | c | 913 | CLA | C2B-C3B-CAB-CBB |
| 26 | K | 102 | BCR | C1-C6-C7-C8 |
| 27 | L | 102 | SQD | C34-C35-C36-C37 |
| 34 | C | 501 | LMG | C11-C12-C13-C14 |
| 36 | c | 918 | DGD | CBA-CCA-CDA-CEA |
| 37 | l | 101 | LHG | C25-C26-C27-C28 |
| 34 | c | 919 | LMG | C13-C14-C15-C16 |
| 34 | J | 101 | LMG | C14-C15-C16-C17 |
| 24 | B | 606 | CLA | C4-C3-C5-C6 |
| 27 | f | 102 | SQD | C25-C26-C27-C28 |
| 29 | B | 636 | LMT | C3-C4-C5-C6 |
| 36 | d | 406 | DGD | C8B-C9B-CAB-CBB |
| 37 | L | 101 | LHG | C13-C14-C15-C16 |
| 37 | d | 409 | LHG | C29-C30-C31-C32 |
| 34 | C | 501 | LMG | C12-C13-C14-C15 |
| 37 | E | 101 | LHG | C23-C24-C25-C26 |
| 27 | B | 621 | SQD | C11-C10-C9-C8 |
| 27 | a | 402 | SQD | C16-C17-C18-C19 |
| 34 | z | 101 | LMG | C12-C13-C14-C15 |
| 34 | z | 101 | LMG | C15-C16-C17-C18 |
| 36 | h | 102 | DGD | CBB-CCB-CDB-CEB |
| 37 | D | 408 | LHG | C13-C14-C15-C16 |
| 37 | E | 101 | LHG | C10-C11-C12-C13 |
| 35 | c | 922 | HTG | S1-C1'-C2'-C3' |
| 24 | C | 502 | CLA | C13-C15-C16-C17 |
| 24 | b | 610 | CLA | C13-C15-C16-C17 |
| 36 | D | 405 | DGD | C2A-C3A-C4A-C5A |
| 36 | d | 406 | DGD | C9B-CAB-CBB-CCB |
| 37 | l | 101 | LHG | C13-C14-C15-C16 |
| 27 | L | 102 | SQD | C28-C29-C30-C31 |
| 36 | D | 405 | DGD | C2E-C1E-O5D-C6D |
| 24 | c | 913 | CLA | CBD-CGD-O2D-CED |
| 36 | C | 518 | DGD | CAB-CBB-CCB-CDB |
| 37 | E | 101 | LHG | C25-C26-C27-C28 |
| 34 | C | 501 | LMG | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | a | 411 | SQD | C16-C17-C18-C19 |
| 36 | H | 102 | DGD | CAB-CBB-CCB-CDB |
| 37 | E | 101 | LHG | C24-C25-C26-C27 |
| 24 | B | 607 | CLA | C10-C11-C12-C13 |
| 24 | C | 507 | CLA | C16-C17-C18-C19 |
| 24 | a | 409 | CLA | C16-C17-C18-C20 |
| 37 | D | 406 | LHG | C28-C29-C30-C31 |
| 27 | a | 411 | SQD | C10-C11-C12-C13 |
| 34 | J | 101 | LMG | C35-C36-C37-C38 |
| 35 | B | 626 | HTG | C3'-C4'-C5'-C6' |
| 36 | d | 406 | DGD | CAA-CBA-CCA-CDA |
| 24 | A | 405 | CLA | C2C-C3C-CAC-CBC |
| 26 | K | 103 | BCR | C7-C8-C9-C34 |
| 34 | C | 520 | LMG | C11-C12-C13-C14 |
| 24 | b | 620 | CLA | C3-C5-C6-C7 |
| 34 | C | 521 | LMG | C8-C7-O1-C1 |
| 36 | c | 917 | DGD | C2G-C3G-O3G-C1D |
| 24 | c | 903 | CLA | C16-C17-C18-C19 |
| 29 | B | 636 | LMT | C6-C7-C8-C9 |
| 36 | c | 917 | DGD | C2B-C3B-C4B-C5B |
| 36 | h | 102 | DGD | C5B-C6B-C7B-C8B |
| 38 | e | 102 | HEM | C2B-C3B-CAB-CBB |
| 29 | M | 101 | LMT | C4B-C5B-C6B-O6B |
| 36 | C | 517 | DGD | C7A-C8A-C9A-CAA |
| 36 | C | 518 | DGD | CAA-CBA-CCA-CDA |
| 37 | l | 101 | LHG | C33-C34-C35-C36 |
| 24 | b | 619 | CLA | C10-C11-C12-C13 |
| 36 | c | 918 | DGD | C6A-C7A-C8A-C9A |
| 27 | F | 101 | SQD | C32-C33-C34-C35 |
| 34 | c | 919 | LMG | C20-C21-C22-C23 |
| 37 | l | 101 | LHG | C14-C15-C16-C17 |
| 24 | a | 406 | CLA | C2C-C3C-CAC-CBC |
| 37 | d | 407 | LHG | C28-C29-C30-C31 |
| 35 | B | 625 | HTG | C1'-C2'-C3'-C4' |
| 34 | J | 101 | LMG | C16-C17-C18-C19 |
| 34 | Z | 101 | LMG | C10-C11-C12-C13 |
| 29 | E | 102 | LMT | C4'-C5'-C6'-O6' |
| 34 | J | 101 | LMG | C11-C12-C13-C14 |
| 34 | Z | 101 | LMG | O6-C5-C6-O5 |
| 34 | C | 521 | LMG | C11-C12-C13-C14 |
| 36 | C | 517 | DGD | C4D-C5D-C6D-O5D |
| 29 | M | 101 | LMT | O5B-C5B-C6B-O6B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 34 | j | 101 | LMG | C16-C17-C18-C19 |
| 36 | d | 406 | DGD | O6D-C5D-C6D-O5D |
| 24 | d | 403 | CLA | C4-C3-C5-C6 |
| 24 | B | 607 | CLA | C13-C15-C16-C17 |
| 27 | L | 102 | SQD | C12-C13-C14-C15 |
| 35 | V | 202 | HTG | C2'-C3'-C4'-C5' |
| 36 | C | 517 | DGD | O6E-C5E-C6E-O5E |
| 27 | a | 402 | SQD | C31-C32-C33-C34 |
| 36 | d | 406 | DGD | C3A-C4A-C5A-C6A |
| 24 | b | 620 | CLA | C10-C11-C12-C13 |
| 34 | j | 101 | LMG | C32-C33-C34-C35 |
| 29 | a | 401 | LMT | C1-C2-C3-C4 |
| 28 | V | 203 | GOL | O1-C1-C2-O2 |
| 28 | V | 203 | GOL | O2-C2-C3-O3 |
| 28 | b | 628 | GOL | O2-C2-C3-O3 |
| 28 | b | 631 | GOL | O1-C1-C2-O2 |
| 28 | f | 101 | GOL | O1-C1-C2-O2 |
| 28 | o | 302 | GOL | O1-C1-C2-O2 |
| 27 | B | 621 | SQD | O10-C23-O48-C46 |
| 27 | L | 102 | SQD | C15-C16-C17-C18 |
| 36 | h | 102 | DGD | CAA-CBA-CCA-CDA |
| 36 | D | 405 | DGD | C4A-C5A-C6A-C7A |
| 29 | A | 417 | LMT | O1'-C1-C2-C3 |
| 29 | f | 103 | LMT | C5-C6-C7-C8 |
| 24 | C | 502 | CLA | C12-C13-C15-C16 |
| 24 | C | 507 | CLA | C6-C7-C8-C10 |
| 24 | C | 513 | CLA | C11-C10-C8-C7 |
| 24 | b | 618 | CLA | C6-C7-C8-C10 |
| 24 | b | 620 | CLA | C11-C12-C13-C15 |
| 24 | c | 910 | CLA | C12-C13-C15-C16 |
| 27 | F | 101 | SQD | C31-C32-C33-C34 |
| 24 | b | 618 | CLA | C16-C17-C18-C20 |
| 24 | b | 619 | CLA | C5-C6-C7-C8 |
| 36 | d | 406 | DGD | C7A-C8A-C9A-CAA |
| 27 | B | 621 | SQD | C35-C36-C37-C38 |
| 24 | c | 904 | CLA | C8-C10-C11-C12 |
| 24 | c | 911 | CLA | C4-C3-C5-C6 |
| 31 | A | 419 | PL9 | C28-C29-C31-C32 |
| 37 | L | 101 | LHG | C32-C33-C34-C35 |
| 24 | C | 507 | CLA | C6-C7-C8-C9 |
| 24 | b | 608 | CLA | C11-C12-C13-C14 |
| 24 | b | 618 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | B | 616 | CLA | C16-C17-C18-C20 |
| 29 | a | 401 | LMT | C7-C8-C9-C10 |
| 34 | C | 520 | LMG | C16-C17-C18-C19 |
| 36 | H | 102 | DGD | C9B-CAB-CBB-CCB |
| 36 | C | 519 | DGD | C2A-C1A-O1G-C1G |
| 27 | F | 101 | SQD | C30-C31-C32-C33 |
| 34 | j | 101 | LMG | C14-C15-C16-C17 |
| 37 | l | 101 | LHG | C12-C13-C14-C15 |
| 34 | c | 919 | LMG | C7-C8-C9-O8 |
| 36 | D | 405 | DGD | O1G-C1G-C2G-C3G |
| 36 | c | 916 | DGD | O6E-C5E-C6E-O5E |
| 36 | h | 102 | DGD | CCA-CDA-CEA-CFA |
| 24 | c | 905 | CLA | C8-C10-C11-C12 |
| 29 | b | 601 | LMT | C4-C5-C6-C7 |
| 24 | A | 410 | CLA | C3-C5-C6-C7 |
| 34 | C | 520 | LMG | C21-C22-C23-C24 |
| 34 | C | 521 | LMG | C16-C17-C18-C19 |
| 29 | C | 522 | LMT | O5'-C5'-C6'-O6' |
| 37 | d | 407 | LHG | C30-C31-C32-C33 |
| 31 | A | 419 | PL9 | C30-C29-C31-C32 |
| 36 | c | 916 | DGD | CAA-CBA-CCA-CDA |
| 26 | c | 915 | BCR | C7-C8-C9-C34 |
| 36 | H | 102 | DGD | C5B-C6B-C7B-C8B |
| 36 | c | 917 | DGD | C1A-C2A-C3A-C4A |
| 36 | h | 102 | DGD | C8A-C9A-CAA-CBA |
| 26 | K | 103 | BCR | C7-C8-C9-C10 |
| 24 | B | 603 | CLA | C15-C16-C17-C18 |
| 24 | b | 614 | CLA | C15-C16-C17-C18 |
| 34 | a | 412 | LMG | C29-C30-C31-C32 |
| 36 | c | 916 | DGD | C4D-C5D-C6D-O5D |
| 34 | Z | 101 | LMG | C29-C28-O8-C9 |
| 27 | a | 402 | SQD | C25-C26-C27-C28 |
| 37 | d | 409 | LHG | C32-C33-C34-C35 |
| 24 | C | 508 | CLA | C5-C6-C7-C8 |
| 24 | b | 618 | CLA | C13-C15-C16-C17 |
| 29 | B | 623 | LMT | C5-C6-C7-C8 |
| 29 | b | 601 | LMT | C2-C3-C4-C5 |
| 37 | l | 101 | LHG | C31-C32-C33-C34 |
| 24 | B | 616 | CLA | C16-C17-C18-C19 |
| 29 | m | 104 | LMT | C2-C3-C4-C5 |
| 34 | b | 624 | LMG | C17-C18-C19-C20 |
| 36 | c | 917 | DGD | CAA-CBA-CCA-CDA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 34 | C | 521 | LMG | C17-C18-C19-C20 |
| 36 | C | 517 | DGD | C5B-C6B-C7B-C8B |
| 36 | d | 406 | DGD | C2A-C1A-O1G-C1G |
| 34 | a | 412 | LMG | C35-C36-C37-C38 |
| 35 | O | 303 | HTG | C3'-C4'-C5'-C6' |
| 36 | C | 519 | DGD | CBA-CCA-CDA-CEA |
| 24 | C | 511 | CLA | C2-C3-C5-C6 |
| 24 | c | 911 | CLA | C2-C3-C5-C6 |
| 36 | H | 102 | DGD | CDB-CEB-CFB-CGB |
| 27 | B | 621 | SQD | C34-C35-C36-C37 |
| 29 | B | 636 | LMT | C5-C6-C7-C8 |
| 34 | a | 412 | LMG | C28-C29-C30-C31 |
| 24 | c | 911 | CLA | CBA-CGA-O2A-C1 |
| 35 | B | 633 | HTG | C4'-C5'-C6'-C7' |
| 36 | c | 918 | DGD | C7A-C8A-C9A-CAA |
| 27 | A | 416 | SQD | C26-C27-C28-C29 |
| 29 | c | 921 | LMT | C6-C7-C8-C9 |
| 24 | b | 618 | CLA | C16-C17-C18-C19 |
| 34 | C | 520 | LMG | C22-C23-C24-C25 |
| 36 | C | 519 | DGD | O1A-C1A-O1G-C1G |
| 29 | m | 103 | LMT | C4'-C5'-C6'-O6' |
| 27 | f | 102 | SQD | C32-C33-C34-C35 |
| 24 | A | 410 | CLA | CBA-CGA-O2A-C1 |
| 35 | b | 626 | HTG | C2'-C1'-S1-C1 |
| 29 | b | 601 | LMT | C7-C8-C9-C10 |
| 34 | a | 412 | LMG | C21-C22-C23-C24 |
| 24 | C | 510 | CLA | C10-C11-C12-C13 |
| 24 | b | 605 | CLA | C5-C6-C7-C8 |
| 34 | b | 624 | LMG | C15-C16-C17-C18 |
| 24 | B | 616 | CLA | C4-C3-C5-C6 |
| 24 | C | 511 | CLA | C4-C3-C5-C6 |
| 24 | B | 616 | CLA | C2-C3-C5-C6 |
| 34 | B | 622 | LMG | C34-C35-C36-C37 |
| 34 | C | 501 | LMG | C13-C14-C15-C16 |
| 29 | b | 625 | LMT | C3'-C4'-O1B-C1B |
| 27 | a | 411 | SQD | C31-C32-C33-C34 |
| 24 | B | 602 | CLA | C11-C10-C8-C9 |
| 24 | B | 611 | CLA | C14-C13-C15-C16 |
| 24 | B | 615 | CLA | C11-C10-C8-C9 |
| 24 | C | 502 | CLA | C14-C13-C15-C16 |
| 24 | C | 513 | CLA | C11-C10-C8-C9 |
| 24 | a | 407 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | b | 609 | CLA | C11-C10-C8-C9 |
| 24 | b | 620 | CLA | C11-C12-C13-C14 |
| 24 | c | 910 | CLA | C14-C13-C15-C16 |
| 37 | D | 406 | LHG | C25-C26-C27-C28 |
| 24 | C | 510 | CLA | C15-C16-C17-C18 |
| 24 | B | 603 | CLA | C4B-C3B-CAB-CBB |
| 24 | C | 503 | CLA | C4B-C3B-CAB-CBB |
| 24 | b | 611 | CLA | C4B-C3B-CAB-CBB |
| 24 | c | 903 | CLA | C4B-C3B-CAB-CBB |
| 24 | c | 906 | CLA | C4B-C3B-CAB-CBB |
| 24 | c | 913 | CLA | C4B-C3B-CAB-CBB |
| 34 | C | 521 | LMG | C15-C16-C17-C18 |
| 36 | H | 102 | DGD | O2G-C1B-C2B-C3B |
| 24 | b | 610 | CLA | C15-C16-C17-C18 |
| 37 | E | 101 | LHG | O6-C4-C5-C6 |
| 37 | l | 101 | LHG | O6-C4-C5-C6 |
| 36 | c | 916 | DGD | C5A-C6A-C7A-C8A |
| 37 | L | 101 | LHG | C24-C25-C26-C27 |
| 24 | B | 602 | CLA | CAA-CBA-CGA-O2A |
| 29 | c | 921 | LMT | C7-C8-C9-C10 |
| 24 | B | 611 | CLA | C12-C13-C15-C16 |
| 24 | B | 615 | CLA | C11-C12-C13-C15 |
| 24 | C | 506 | CLA | C11-C12-C13-C15 |
| 24 | D | 402 | CLA | C11-C10-C8-C7 |
| 24 | c | 905 | CLA | C12-C13-C15-C16 |
| 24 | B | 616 | CLA | C10-C11-C12-C13 |
| 24 | C | 514 | CLA | C3A-C2A-CAA-CBA |
| 24 | b | 605 | CLA | C4-C3-C5-C6 |
| 24 | B | 614 | CLA | C10-C11-C12-C13 |
| 24 | B | 616 | CLA | C13-C15-C16-C17 |
| 24 | b | 605 | CLA | C2-C3-C5-C6 |
| 29 | f | 103 | LMT | C2B-C1B-O1B-C4' |
| 24 | c | 912 | CLA | CBA-CGA-O2A-C1 |
| 27 | a | 402 | SQD | C24-C23-O48-C46 |
| 27 | A | 412 | SQD | C15-C16-C17-C18 |
| 26 | h | 101 | BCR | C9-C10-C11-C12 |
| 29 | b | 601 | LMT | O1'-C1-C2-C3 |
| 24 | c | 911 | CLA | O1A-CGA-O2A-C1 |
| 34 | a | 412 | LMG | C33-C34-C35-C36 |
| 37 | D | 406 | LHG | C34-C35-C36-C37 |
| 37 | E | 101 | LHG | C7-C8-C9-C10 |
| 37 | d | 408 | LHG | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | L | 101 | LHG | C26-C27-C28-C29 |
| 27 | A | 416 | SQD | O6-C44-C45-C46 |
| 27 | a | 402 | SQD | O6-C44-C45-C46 |
| 27 | f | 102 | SQD | C44-C45-C46-O48 |
| 36 | d | 406 | DGD | O1G-C1G-C2G-C3G |
| 37 | E | 101 | LHG | C4-C5-C6-O8 |
| 37 | e | 101 | LHG | C4-C5-C6-O8 |
| 24 | d | 401 | CLA | C15-C16-C17-C18 |
| 36 | C | 517 | DGD | C6A-C7A-C8A-C9A |
| 29 | a | 401 | LMT | O5B-C5B-C6B-O6B |
| 25 | A | 408 | PHO | C4-C3-C5-C6 |
| 27 | F | 101 | SQD | C34-C35-C36-C37 |
| 25 | A | 408 | PHO | C2-C3-C5-C6 |
| 27 | A | 412 | SQD | C13-C14-C15-C16 |
| 27 | F | 101 | SQD | C29-C30-C31-C32 |
| 29 | a | 401 | LMT | C2-C3-C4-C5 |
| 26 | B | 618 | BCR | C1-C6-C7-C8 |
| 26 | H | 101 | BCR | C5-C6-C7-C8 |
| 26 | b | 621 | BCR | C1-C6-C7-C8 |
| 36 | d | 406 | DGD | C4D-C5D-C6D-O5D |
| 29 | A | 417 | LMT | C4B-C5B-C6B-O6B |
| 27 | F | 101 | SQD | C24-C25-C26-C27 |
| 27 | A | 412 | SQD | O6-C44-C45-O47 |
| 27 | B | 621 | SQD | O47-C45-C46-O48 |
| 27 | F | 101 | SQD | O47-C45-C46-O48 |
| 27 | L | 102 | SQD | O47-C45-C46-O48 |
| 34 | C | 501 | LMG | O1-C7-C8-O7 |
| 34 | c | 919 | LMG | O1-C7-C8-O7 |
| 34 | c | 919 | LMG | O7-C8-C9-O8 |
| 34 | z | 101 | LMG | O1-C7-C8-O7 |
| 36 | D | 405 | DGD | O2G-C2G-C3G-O3G |
| 31 | A | 419 | PL9 | C4-C3-C7-C8 |
| 31 | a | 417 | PL9 | C4-C3-C7-C8 |
| 36 | C | 519 | DGD | C9B-CAB-CBB-CCB |
| 27 | f | 102 | SQD | C23-C24-C25-C26 |
| 37 | D | 408 | LHG | C28-C29-C30-C31 |
| 24 | B | 607 | CLA | C11-C10-C8-C9 |
| 24 | B | 615 | CLA | C6-C7-C8-C9 |
| 24 | C | 509 | CLA | C11-C10-C8-C9 |
| 24 | c | 905 | CLA | C14-C13-C15-C16 |
| 36 | h | 102 | DGD | C6A-C7A-C8A-C9A |
| 35 | c | 922 | HTG | C3'-C4'-C5'-C6' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | C | 506 | CLA | C10-C11-C12-C13 |
| 34 | J | 101 | LMG | C13-C14-C15-C16 |
| 36 | C | 517 | DGD | O6E-C1E-O5D-C6D |
| 34 | c | 919 | LMG | C10-C11-C12-C13 |
| 36 | d | 406 | DGD | O1A-C1A-O1G-C1G |
| 29 | E | 102 | LMT | C2-C3-C4-C5 |
| 34 | a | 412 | LMG | C22-C23-C24-C25 |
| 27 | a | 402 | SQD | C27-C28-C29-C30 |
| 34 | C | 501 | LMG | C38-C39-C40-C41 |
| 24 | b | 609 | CLA | C10-C11-C12-C13 |
| 31 | a | 417 | PL9 | C14-C16-C17-C18 |
| 34 | C | 501 | LMG | C16-C17-C18-C19 |
| 24 | B | 612 | CLA | C8-C10-C11-C12 |
| 36 | h | 102 | DGD | CDA-CEA-CFA-CGA |
| 28 | B | 628 | GOL | O1-C1-C2-O2 |
| 28 | B | 632 | GOL | O1-C1-C2-O2 |
| 28 | v | 204 | GOL | O1-C1-C2-O2 |
| 24 | B | 614 | CLA | C15-C16-C17-C18 |
| 24 | b | 610 | CLA | C8-C10-C11-C12 |
| 24 | b | 617 | CLA | C5-C6-C7-C8 |
| 34 | B | 622 | LMG | C36-C37-C38-C39 |
| 34 | c | 919 | LMG | C39-C40-C41-C42 |
| 24 | c | 912 | CLA | O1A-CGA-O2A-C1 |
| 24 | B | 607 | CLA | C11-C10-C8-C7 |
| 24 | B | 615 | CLA | C12-C13-C15-C16 |
| 24 | B | 617 | CLA | C12-C13-C15-C16 |
| 24 | C | 505 | CLA | C12-C13-C15-C16 |
| 24 | C | 509 | CLA | C11-C10-C8-C7 |
| 24 | a | 407 | CLA | C11-C12-C13-C15 |
| 27 | a | 402 | SQD | C23-C24-C25-C26 |
| 34 | J | 101 | LMG | C10-C11-C12-C13 |
| 35 | B | 624 | HTG | S1-C1'-C2'-C3' |
| 36 | D | 405 | DGD | CDA-CEA-CFA-CGA |
| 34 | b | 624 | LMG | C32-C33-C34-C35 |
| 36 | c | 916 | DGD | C8A-C9A-CAA-CBA |
| 37 | d | 408 | LHG | C34-C35-C36-C37 |
| 26 | D | 403 | BCR | C7-C8-C9-C10 |
| 26 | c | 915 | BCR | C7-C8-C9-C10 |
| 24 | C | 512 | CLA | CBA-CGA-O2A-C1 |
| 37 | l | 101 | LHG | C30-C31-C32-C33 |
| 24 | A | 410 | CLA | O1A-CGA-O2A-C1 |
| 24 | C | 512 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 36 | C | 518 | DGD | C5D-C6D-O5D-C1E |
| 36 | c | 917 | DGD | C5D-C6D-O5D-C1E |
| 27 | L | 102 | SQD | C9-C10-C11-C12 |
| 36 | D | 405 | DGD | C8B-C9B-CAB-CBB |
| 36 | c | 917 | DGD | C7A-C8A-C9A-CAA |
| 37 | d | 407 | LHG | C25-C26-C27-C28 |
| 38 | E | 103 | HEM | C2C-C3C-CAC-CBC |
| 37 | L | 101 | LHG | C11-C12-C13-C14 |
| 28 | A | 413 | GOL | O1-C1-C2-C3 |
| 24 | c | 913 | CLA | O1D-CGD-O2D-CED |
| 27 | B | 621 | SQD | C46-C45-O47-C7 |
| 27 | L | 102 | SQD | C46-C45-O47-C7 |
| 24 | C | 507 | CLA | C8-C10-C11-C12 |
| 34 | J | 101 | LMG | C15-C16-C17-C18 |
| 29 | m | 104 | LMT | C9-C10-C11-C12 |
| 27 | a | 402 | SQD | O10-C23-O48-C46 |
| 37 | l | 101 | LHG | O6-C4-C5-O7 |
| 34 | z | 101 | LMG | C16-C17-C18-C19 |
| 36 | C | 518 | DGD | O6E-C1E-O5D-C6D |
| 36 | c | 917 | DGD | O6E-C1E-O5D-C6D |
| 27 | B | 621 | SQD | C44-C45-C46-O48 |
| 27 | L | 102 | SQD | C44-C45-C46-O48 |
| 34 | c | 919 | LMG | O1-C7-C8-C9 |
| 34 | z | 101 | LMG | O1-C7-C8-C9 |
| 25 | a | 420 | PHO | C2C-C3C-CAC-CBC |
| 37 | L | 101 | LHG | C7-C8-C9-C10 |
| 24 | d | 401 | CLA | C2C-C3C-CAC-CBC |
| 24 | c | 913 | CLA | C15-C16-C17-C18 |
| 38 | e | 102 | HEM | C4B-C3B-CAB-CBB |
| 24 | A | 405 | CLA | C4C-C3C-CAC-CBC |
| 24 | d | 403 | CLA | C2-C3-C5-C6 |
| 36 | C | 518 | DGD | C8A-C9A-CAA-CBA |
| 35 | V | 202 | HTG | C2-C1-S1-C1' |
| 31 | A | 419 | PL9 | C2-C3-C7-C8 |
| 36 | d | 406 | DGD | C5A-C6A-C7A-C8A |
| 34 | C | 521 | LMG | C4-C5-C6-O5 |
| 34 | b | 624 | LMG | C36-C37-C38-C39 |
| 27 | f | 102 | SQD | O47-C45-C46-O48 |
| 36 | d | 406 | DGD | O1G-C1G-C2G-O2G |
| 37 | E | 101 | LHG | O7-C5-C6-O8 |
| 24 | B | 617 | CLA | C14-C13-C15-C16 |
| 24 | c | 914 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 36 | c | 918 | DGD | CAB-CBB-CCB-CDB |
| 29 | B | 636 | LMT | C4'-C5'-C6'-O6' |
| 35 | B | 634 | HTG | C4-C5-C6-O6 |
| 34 | C | 501 | LMG | C17-C18-C19-C20 |
| 27 | L | 102 | SQD | C27-C28-C29-C30 |
| 27 | a | 411 | SQD | C26-C27-C28-C29 |
| 34 | j | 101 | LMG | C18-C19-C20-C21 |
| 36 | C | 517 | DGD | C5A-C6A-C7A-C8A |
| 27 | L | 102 | SQD | C31-C32-C33-C34 |
| 36 | h | 102 | DGD | CDB-CEB-CFB-CGB |
| 29 | A | 417 | LMT | C7-C8-C9-C10 |
| 27 | F | 101 | SQD | C2-C1-O6-C44 |
| 34 | C | 501 | LMG | C2-C1-O1-C7 |
| 29 | b | 625 | LMT | C4'-C5'-C6'-O6' |
| 27 | L | 102 | SQD | C13-C14-C15-C16 |
| 29 | E | 102 | LMT | C5-C6-C7-C8 |
| 37 | d | 409 | LHG | C9-C10-C11-C12 |
| 37 | d | 407 | LHG | C23-C24-C25-C26 |
| 37 | d | 408 | LHG | O2-C2-C3-O3 |
| 36 | d | 406 | DGD | C2B-C3B-C4B-C5B |
| 24 | B | 611 | CLA | C16-C17-C18-C20 |
| 36 | c | 918 | DGD | C4B-C5B-C6B-C7B |
| 37 | l | 101 | LHG | C35-C36-C37-C38 |
| 28 | A | 413 | GOL | O1-C1-C2-O2 |
| 29 | m | 104 | LMT | C11-C10-C9-C8 |
| 27 | A | 416 | SQD | C19-C20-C21-C22 |
| 27 | A | 416 | SQD | C17-C18-C19-C20 |
| 24 | D | 402 | CLA | C4B-C3B-CAB-CBB |
| 29 | b | 601 | LMT | C11-C10-C9-C8 |
| 34 | B | 622 | LMG | C10-C11-C12-C13 |
| 29 | m | 104 | LMT | C6-C7-C8-C9 |
| 37 | d | 409 | LHG | C17-C18-C19-C20 |
| 24 | B | 615 | CLA | C16-C17-C18-C20 |
| 34 | B | 622 | LMG | O9-C10-O7-C8 |
| 34 | B | 622 | LMG | C32-C33-C34-C35 |
| 34 | j | 101 | LMG | C19-C20-C21-C22 |
| 27 | B | 621 | SQD | C5-C6-S-O7 |
| 27 | B | 621 | SQD | C9-C10-C11-C12 |
| 24 | B | 602 | CLA | C12-C13-C15-C16 |
| 24 | B | 616 | CLA | C12-C13-C15-C16 |
| 24 | B | 617 | CLA | C6-C7-C8-C10 |
| 24 | C | 502 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | C | 506 | CLA | C12-C13-C15-C16 |
| 24 | D | 402 | CLA | C12-C13-C15-C16 |
| 24 | c | 907 | CLA | C6-C7-C8-C10 |
| 36 | C | 518 | DGD | C9A-CAA-CBA-CCA |
| 24 | b | 615 | CLA | C16-C17-C18-C19 |
| 34 | C | 520 | LMG | C37-C38-C39-C40 |
| 37 | e | 101 | LHG | C11-C12-C13-C14 |
| 29 | a | 401 | LMT | O1'-C1-C2-C3 |
| 37 | D | 406 | LHG | C27-C28-C29-C30 |
| 24 | B | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 408 | PHO | C8-C10-C11-C12 |
| 34 | B | 622 | LMG | C37-C38-C39-C40 |
| 37 | D | 407 | LHG | C33-C34-C35-C36 |
| 24 | b | 615 | CLA | C16-C17-C18-C20 |
| 37 | D | 408 | LHG | C12-C13-C14-C15 |
| 34 | B | 622 | LMG | C11-C10-O7-C8 |
| 24 | B | 615 | CLA | C14-C13-C15-C16 |
| 24 | B | 616 | CLA | C14-C13-C15-C16 |
| 24 | C | 505 | CLA | C14-C13-C15-C16 |
| 24 | C | 506 | CLA | C11-C12-C13-C14 |
| 36 | h | 102 | DGD | O2G-C1B-C2B-C3B |
| 29 | a | 401 | LMT | C6-C7-C8-C9 |
| 36 | C | 519 | DGD | C6B-C7B-C8B-C9B |
| 36 | c | 918 | DGD | C1B-C2B-C3B-C4B |
| 34 | J | 101 | LMG | C36-C37-C38-C39 |
| 34 | Z | 101 | LMG | O1-C7-C8-O7 |
| 37 | e | 101 | LHG | O7-C5-C6-O8 |
| 35 | B | 634 | HTG | C4'-C5'-C6'-C7' |
| 24 | A | 406 | CLA | C15-C16-C17-C18 |
| 24 | B | 606 | CLA | C8-C10-C11-C12 |
| 27 | B | 621 | SQD | C32-C33-C34-C35 |
| 34 | C | 501 | LMG | O1-C7-C8-C9 |
| 36 | h | 102 | DGD | O1G-C1G-C2G-C3G |
| 29 | f | 103 | LMT | O5B-C1B-O1B-C4' |
| 37 | d | 407 | LHG | C33-C34-C35-C36 |
| 24 | B | 602 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 507 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 605 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 609 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 611 | CLA | CAD-CBD-CGD-O2D |
| 24 | c | 903 | CLA | CAD-CBD-CGD-O2D |
| 24 | c | 905 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | a | 402 | SQD | C19-C20-C21-C22 |
| 36 | d | 406 | DGD | C1A-C2A-C3A-C4A |
| 24 | C | 511 | CLA | O1A-CGA-O2A-C1 |
| 36 | C | 518 | DGD | C3A-C4A-C5A-C6A |
| 27 | a | 411 | SQD | C15-C16-C17-C18 |
| 34 | C | 521 | LMG | C18-C19-C20-C21 |
| 36 | C | 519 | DGD | C2B-C3B-C4B-C5B |
| 24 | B | 602 | CLA | CAD-CBD-CGD-O1D |
| 24 | B | 606 | CLA | CAD-CBD-CGD-O1D |
| 24 | B | 617 | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 617 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 503 | CLA | CAD-CBD-CGD-O1D |
| 24 | C | 505 | CLA | CAD-CBD-CGD-O1D |
| 24 | C | 507 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 605 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 609 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 611 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 614 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 614 | CLA | CHA-CBD-CGD-O2D |
| 24 | c | 903 | CLA | CAD-CBD-CGD-O1D |
| 37 | E | 101 | LHG | C4-O6-P-O5 |
| 37 | d | 408 | LHG | C4-O6-P-O5 |
| 37 | e | 101 | LHG | C3-O3-P-O5 |
| 24 | b | 619 | CLA | C16-C17-C18-C19 |
| 27 | a | 402 | SQD | C34-C35-C36-C37 |
| 37 | d | 409 | LHG | O10-C23-O8-C6 |
| 24 | D | 401 | CLA | C2B-C3B-CAB-CBB |
| 24 | D | 402 | CLA | C2B-C3B-CAB-CBB |
| 26 | h | 101 | BCR | C23-C24-C25-C30 |
| 27 | A | 416 | SQD | C18-C19-C20-C21 |
| 26 | y | 101 | BCR | C36-C18-C19-C20 |
| 37 | D | 408 | LHG | C2-C3-O3-P |
| 37 | d | 409 | LHG | C2-C3-O3-P |
| 24 | B | 611 | CLA | C16-C17-C18-C19 |
| 34 | a | 412 | LMG | C10-C11-C12-C13 |
| 27 | A | 416 | SQD | O10-C23-O48-C46 |
| 37 | D | 408 | LHG | O10-C23-O8-C6 |
| 35 | D | 411 | HTG | O5-C5-C6-O6 |
| 27 | A | 416 | SQD | C24-C23-O48-C46 |
| 28 | V | 204 | GOL | O1-C1-C2-O2 |
| 27 | B | 621 | SQD | C27-C28-C29-C30 |
| 28 | B | 631 | GOL | C1-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 28 | v | 204 | GOL | C1-C2-C3-O3 |
| 34 | C | 501 | LMG | C10-C11-C12-C13 |
| 34 | B | 622 | LMG | C16-C17-C18-C19 |
| 24 | D | 402 | CLA | C8-C10-C11-C12 |
| 36 | c | 918 | DGD | C4A-C5A-C6A-C7A |
| 27 | B | 621 | SQD | C12-C13-C14-C15 |
| 31 | a | 417 | PL9 | C2-C3-C7-C8 |
| 27 | F | 101 | SQD | C11-C10-C9-C8 |
| 27 | A | 416 | SQD | C15-C16-C17-C18 |
| 24 | b | 616 | CLA | C3-C5-C6-C7 |
| 24 | C | 507 | CLA | C5-C6-C7-C8 |
| 24 | B | 615 | CLA | C11-C12-C13-C14 |
| 24 | D | 402 | CLA | C11-C10-C8-C9 |
| 24 | A | 407 | CLA | C12-C13-C15-C16 |
| 27 | L | 102 | SQD | C18-C19-C20-C21 |
| 34 | c | 919 | LMG | O6-C1-O1-C7 |
| 24 | C | 511 | CLA | CBA-CGA-O2A-C1 |
| 36 | c | 918 | DGD | CCB-CDB-CEB-CFB |
| 36 | d | 406 | DGD | CAB-CBB-CCB-CDB |
| 34 | c | 919 | LMG | C2-C1-O1-C7 |
| 36 | C | 517 | DGD | C2E-C1E-O5D-C6D |
| 36 | C | 518 | DGD | C2E-C1E-O5D-C6D |
| 36 | c | 917 | DGD | C2E-C1E-O5D-C6D |
| 24 | b | 607 | CLA | CBD-CGD-O2D-CED |
| 24 | b | 609 | CLA | CBD-CGD-O2D-CED |
| 34 | c | 920 | LMG | O7-C8-C9-O8 |
| 36 | D | 405 | DGD | O1G-C1G-C2G-O2G |
| 36 | C | 517 | DGD | CDB-CEB-CFB-CGB |
| 34 | Z | 101 | LMG | O10-C28-O8-C9 |
| 37 | D | 408 | LHG | C24-C23-O8-C6 |
| 34 | a | 412 | LMG | C13-C14-C15-C16 |
| 35 | B | 626 | HTG | C4-C5-C6-O6 |
| 29 | B | 636 | LMT | C11-C10-C9-C8 |
| 27 | A | 412 | SQD | C8-C7-O47-C45 |
| 34 | J | 101 | LMG | C34-C35-C36-C37 |
| 24 | a | 406 | CLA | C4C-C3C-CAC-CBC |
| 24 | b | 610 | CLA | O1D-CGD-O2D-CED |
| 37 | d | 407 | LHG | C26-C27-C28-C29 |
| 27 | L | 102 | SQD | C35-C36-C37-C38 |
| 27 | a | 402 | SQD | C18-C19-C20-C21 |
| 36 | C | 518 | DGD | C2G-C3G-O3G-C1D |
| 24 | C | 511 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | c | 907 | CLA | C13-C15-C16-C17 |
| 24 | B | 602 | CLA | C2A-CAA-CBA-CGA |
| 26 | t | 101 | BCR | C13-C14-C15-C16 |
| 24 | c | 910 | CLA | C16-C17-C18-C19 |
| 34 | C | 501 | LMG | O6-C1-O1-C7 |
| 24 | a | 409 | CLA | C4-C3-C5-C6 |
| 31 | a | 417 | PL9 | C45-C44-C46-C47 |
| 27 | A | 412 | SQD | O49-C7-O47-C45 |
| 24 | B | 604 | CLA | C16-C17-C18-C20 |
| 27 | A | 416 | SQD | C24-C25-C26-C27 |
| 37 | d | 409 | LHG | C24-C23-O8-C6 |
| 34 | j | 101 | LMG | C13-C14-C15-C16 |
| 24 | b | 609 | CLA | O1D-CGD-O2D-CED |
| 24 | b | 608 | CLA | C4B-C3B-CAB-CBB |
| 24 | d | 402 | CLA | C4B-C3B-CAB-CBB |
| 34 | c | 920 | LMG | C28-C29-C30-C31 |
| 29 | M | 101 | LMT | C4'-C5'-C6'-O6' |
| 24 | A | 406 | CLA | C2C-C3C-CAC-CBC |
| 24 | C | 513 | CLA | CBA-CGA-O2A-C1 |
| 34 | C | 520 | LMG | C29-C28-O8-C9 |
| 34 | b | 624 | LMG | C29-C28-O8-C9 |
| 35 | B | 626 | HTG | C2'-C3'-C4'-C5' |
| 36 | c | 917 | DGD | C4B-C5B-C6B-C7B |
| 34 | C | 520 | LMG | O10-C28-O8-C9 |
| 31 | D | 404 | PL9 | C39-C41-C42-C43 |
| 24 | b | 619 | CLA | C16-C17-C18-C20 |
| 36 | c | 916 | DGD | C4B-C5B-C6B-C7B |
| 27 | B | 621 | SQD | C19-C20-C21-C22 |
| 24 | B | 617 | CLA | C11-C12-C13-C15 |
| 35 | b | 627 | HTG | C1'-C2'-C3'-C4' |
| 24 | C | 507 | CLA | C10-C11-C12-C13 |
| 36 | C | 517 | DGD | C1B-C2B-C3B-C4B |
| 24 | C | 513 | CLA | O1A-CGA-O2A-C1 |
| 27 | A | 412 | SQD | C34-C35-C36-C37 |
| 36 | D | 405 | DGD | C7B-C8B-C9B-CAB |
| 24 | B | 602 | CLA | C3A-C2A-CAA-CBA |
| 31 | a | 417 | PL9 | C20-C19-C21-C22 |
| 29 | B | 623 | LMT | C4-C5-C6-C7 |
| 36 | h | 102 | DGD | C7A-C8A-C9A-CAA |
| 24 | B | 612 | CLA | C15-C16-C17-C18 |
| 24 | B | 614 | CLA | C2-C1-O2A-CGA |
| 24 | c | 912 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | B | 623 | LMT | C3-C4-C5-C6 |
| 36 | c | 916 | DGD | C5B-C6B-C7B-C8B |
| 24 | c | 914 | CLA | C4-C3-C5-C6 |
| 40 | v | 202 | HEC | CAD-CBD-CGD-O1D |
| 34 | B | 622 | LMG | C20-C21-C22-C23 |
| 37 | L | 101 | LHG | C31-C32-C33-C34 |
| 29 | B | 636 | LMT | O5'-C5'-C6'-O6' |
| 24 | C | 506 | CLA | C14-C13-C15-C16 |
| 24 | C | 511 | CLA | C6-C7-C8-C9 |
| 24 | c | 907 | CLA | C11-C10-C8-C9 |
| 28 | B | 628 | GOL | O1-C1-C2-C3 |
| 24 | B | 614 | CLA | CBD-CGD-O2D-CED |
| 24 | C | 502 | CLA | CBD-CGD-O2D-CED |
| 36 | C | 517 | DGD | CBA-CCA-CDA-CEA |
| 24 | B | 617 | CLA | C8-C10-C11-C12 |
| 25 | a | 420 | PHO | C8-C10-C11-C12 |
| 36 | d | 406 | DGD | C6A-C7A-C8A-C9A |
| 34 | J | 101 | LMG | C30-C31-C32-C33 |
| 24 | a | 409 | CLA | C2-C3-C5-C6 |
| 24 | c | 914 | CLA | C2-C3-C5-C6 |
| 24 | b | 614 | CLA | C2A-CAA-CBA-CGA |
| 24 | c | 902 | CLA | C2A-CAA-CBA-CGA |
| 24 | B | 602 | CLA | CAA-CBA-CGA-O1A |
| 24 | C | 514 | CLA | C1A-C2A-CAA-CBA |
| 40 | V | 201 | HEC | CAD-CBD-CGD-O1D |
| 36 | C | 518 | DGD | C4E-C5E-C6E-O5E |
| 36 | d | 406 | DGD | CCA-CDA-CEA-CFA |
| 24 | B | 603 | CLA | C2B-C3B-CAB-CBB |
| 24 | C | 503 | CLA | C2B-C3B-CAB-CBB |
| 24 | C | 504 | CLA | C2B-C3B-CAB-CBB |
| 24 | C | 513 | CLA | C2B-C3B-CAB-CBB |
| 24 | c | 903 | CLA | C2B-C3B-CAB-CBB |
| 24 | c | 904 | CLA | C2B-C3B-CAB-CBB |
| 26 | B | 618 | BCR | C5-C6-C7-C8 |
| 26 | D | 403 | BCR | C23-C24-C25-C30 |
| 26 | b | 621 | BCR | C5-C6-C7-C8 |
| 26 | d | 404 | BCR | C23-C24-C25-C30 |
| 26 | h | 101 | BCR | C23-C24-C25-C26 |
| 37 | d | 409 | LHG | C33-C34-C35-C36 |
| 40 | V | 201 | HEC | CAD-CBD-CGD-O2D |
| 36 | c | 918 | DGD | C2A-C1A-O1G-C1G |
| 27 | a | 411 | SQD | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | D | 406 | LHG | C33-C34-C35-C36 |
| 36 | c | 918 | DGD | C8B-C9B-CAB-CBB |
| 31 | a | 417 | PL9 | C12-C11-C9-C10 |
| 34 | a | 412 | LMG | C15-C16-C17-C18 |
| 29 | C | 522 | LMT | C1-C2-C3-C4 |
| 24 | a | 407 | CLA | C12-C13-C15-C16 |
| 24 | b | 610 | CLA | C11-C12-C13-C15 |
| 34 | C | 501 | LMG | C21-C22-C23-C24 |
| 24 | B | 603 | CLA | C2A-CAA-CBA-CGA |
| 24 | B | 611 | CLA | C2A-CAA-CBA-CGA |
| 27 | a | 411 | SQD | O6-C44-C45-O47 |
| 24 | B | 614 | CLA | O1D-CGD-O2D-CED |
| 27 | B | 621 | SQD | C17-C18-C19-C20 |
| 34 | c | 920 | LMG | C29-C30-C31-C32 |
| 37 | d | 407 | LHG | C11-C10-C9-C8 |
| 38 | e | 102 | HEM | CAA-CBA-CGA-O1A |
| 40 | v | 202 | HEC | CAD-CBD-CGD-O2D |
| 24 | B | 615 | CLA | C16-C17-C18-C19 |
| 29 | m | 104 | LMT | C1-C2-C3-C4 |
| 24 | b | 620 | CLA | C4-C3-C5-C6 |
| 31 | D | 404 | PL9 | C40-C39-C41-C42 |
| 36 | c | 917 | DGD | CBB-CCB-CDB-CEB |
| 24 | b | 605 | CLA | CAA-CBA-CGA-O2A |
| 31 | a | 417 | PL9 | C18-C19-C21-C22 |
| 31 | a | 417 | PL9 | C43-C44-C46-C47 |
| 29 | A | 417 | LMT | O5B-C5B-C6B-O6B |
| 37 | L | 101 | LHG | C25-C26-C27-C28 |
| 37 | D | 408 | LHG | C30-C31-C32-C33 |
| 24 | A | 410 | CLA | C6-C7-C8-C9 |
| 24 | d | 403 | CLA | C14-C13-C15-C16 |
| 24 | C | 504 | CLA | C5-C6-C7-C8 |
| 34 | c | 919 | LMG | C36-C37-C38-C39 |
| 37 | D | 408 | LHG | C10-C11-C12-C13 |
| 29 | B | 623 | LMT | C6-C7-C8-C9 |
| 36 | d | 406 | DGD | C4A-C5A-C6A-C7A |
| 24 | b | 612 | CLA | C4-C3-C5-C6 |
| 34 | C | 501 | LMG | C15-C16-C17-C18 |
| 29 | A | 417 | LMT | C1-C2-C3-C4 |
| 27 | L | 102 | SQD | C11-C10-C9-C8 |
| 34 | Z | 101 | LMG | C11-C12-C13-C14 |
| 34 | j | 101 | LMG | C29-C30-C31-C32 |
| 35 | C | 523 | HTG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | B | 603 | CLA | C13-C15-C16-C17 |
| 34 | b | 624 | LMG | C40-C41-C42-C43 |
| 36 | c | 917 | DGD | C1B-C2B-C3B-C4B |
| 31 | d | 405 | PL9 | C39-C41-C42-C43 |
| 34 | C | 521 | LMG | O1-C7-C8-C9 |
| 29 | a | 401 | LMT | C9-C10-C11-C12 |
| 34 | b | 624 | LMG | C18-C19-C20-C21 |
| 34 | b | 624 | LMG | O10-C28-O8-C9 |
| 36 | c | 918 | DGD | O1A-C1A-O1G-C1G |
| 34 | b | 624 | LMG | C10-C11-C12-C13 |
| 29 | C | 522 | LMT | C5-C6-C7-C8 |
| 38 | e | 102 | HEM | CAA-CBA-CGA-O2A |
| 34 | c | 919 | LMG | C21-C22-C23-C24 |
| 27 | A | 412 | SQD | C12-C13-C14-C15 |
| 28 | B | 631 | GOL | O2-C2-C3-O3 |
| 36 | D | 405 | DGD | CAA-CBA-CCA-CDA |
| 37 | E | 101 | LHG | C17-C18-C19-C20 |
| 24 | C | 513 | CLA | C4B-C3B-CAB-CBB |
| 24 | c | 904 | CLA | C4B-C3B-CAB-CBB |
| 24 | c | 908 | CLA | C4B-C3B-CAB-CBB |
| 24 | d | 401 | CLA | C4C-C3C-CAC-CBC |
| 35 | b | 602 | HTG | C4'-C5'-C6'-C7' |
| 24 | C | 504 | CLA | C8-C10-C11-C12 |
| 25 | A | 408 | PHO | C8-C10-C11-C12 |
| 38 | E | 103 | HEM | CAD-CBD-CGD-O1D |
| 34 | c | 919 | LMG | C32-C33-C34-C35 |
| 25 | A | 408 | PHO | CHA-CBD-CGD-O1D |
| 36 | H | 102 | DGD | O1B-C1B-C2B-C3B |
| 24 | A | 410 | CLA | C6-C7-C8-C10 |
| 34 | j | 101 | LMG | C36-C37-C38-C39 |
| 36 | D | 405 | DGD | CBA-CCA-CDA-CEA |
| 29 | f | 103 | LMT | C4-C5-C6-C7 |
| 34 | C | 501 | LMG | C18-C19-C20-C21 |
| 24 | A | 410 | CLA | C14-C13-C15-C16 |
| 24 | b | 608 | CLA | C11-C10-C8-C9 |
| 24 | b | 610 | CLA | C11-C10-C8-C9 |
| 27 | B | 621 | SQD | C5-C6-S-O8 |
| 34 | z | 101 | LMG | C8-C7-O1-C1 |
| 36 | C | 517 | DGD | C5D-C6D-O5D-C1E |
| 36 | D | 405 | DGD | C2G-C3G-O3G-C1D |
| 24 | c | 914 | CLA | C2-C1-O2A-CGA |
| 24 | B | 608 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | B | 610 | CLA | C3A-C2A-CAA-CBA |
| 37 | d | 408 | LHG | O10-C23-O8-C6 |
| 24 | b | 620 | CLA | C2-C3-C5-C6 |
| 34 | C | 520 | LMG | C29-C30-C31-C32 |
| 34 | j | 101 | LMG | C21-C22-C23-C24 |
| 36 | D | 405 | DGD | CAB-CBB-CCB-CDB |
| 36 | c | 916 | DGD | C7A-C8A-C9A-CAA |
| 29 | E | 102 | LMT | C2B-C1B-O1B-C4' |
| 27 | A | 416 | SQD | C16-C17-C18-C19 |
| 36 | C | 518 | DGD | CCB-CDB-CEB-CFB |
| 27 | B | 621 | SQD | C30-C31-C32-C33 |
| 29 | m | 104 | LMT | C3-C4-C5-C6 |
| 37 | d | 409 | LHG | C25-C26-C27-C28 |
| 24 | B | 611 | CLA | C15-C16-C17-C18 |
| 27 | F | 101 | SQD | C44-C45-C46-O48 |
| 34 | Z | 101 | LMG | O1-C7-C8-C9 |
| 36 | D | 405 | DGD | C1G-C2G-C3G-O3G |
| 37 | d | 409 | LHG | C28-C29-C30-C31 |
| 24 | B | 602 | CLA | C15-C16-C17-C18 |
| 24 | b | 618 | CLA | C8-C10-C11-C12 |
| 38 | E | 103 | HEM | C4C-C3C-CAC-CBC |
| 28 | a | 414 | GOL | O2-C2-C3-O3 |
| 28 | v | 203 | GOL | O2-C2-C3-O3 |
| 27 | B | 621 | SQD | C18-C19-C20-C21 |
| 29 | f | 103 | LMT | C9-C10-C11-C12 |
| 34 | c | 919 | LMG | C37-C38-C39-C40 |
| 24 | c | 914 | CLA | O1A-CGA-O2A-C1 |
| 37 | D | 408 | LHG | C24-C25-C26-C27 |
| 37 | E | 101 | LHG | C18-C19-C20-C21 |
| 29 | E | 102 | LMT | O5'-C5'-C6'-O6' |
| 24 | B | 602 | CLA | C14-C13-C15-C16 |
| 24 | B | 605 | CLA | C6-C7-C8-C9 |
| 24 | D | 402 | CLA | C14-C13-C15-C16 |
| 24 | c | 912 | CLA | C6-C7-C8-C9 |
| 34 | c | 920 | LMG | C30-C31-C32-C33 |
| 27 | A | 412 | SQD | C14-C15-C16-C17 |
| 36 | c | 918 | DGD | CBB-CCB-CDB-CEB |
| 34 | z | 101 | LMG | O7-C10-C11-C12 |
| 24 | C | 502 | CLA | C2A-CAA-CBA-CGA |
| 24 | C | 511 | CLA | C6-C7-C8-C10 |
| 24 | c | 907 | CLA | C11-C10-C8-C7 |
| 24 | c | 911 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | c | 914 | CLA | C12-C13-C15-C16 |
| 24 | d | 403 | CLA | C12-C13-C15-C16 |
| 24 | b | 608 | CLA | C2B-C3B-CAB-CBB |
| 24 | b | 611 | CLA | C2B-C3B-CAB-CBB |
| 24 | b | 620 | CLA | C2B-C3B-CAB-CBB |
| 24 | c | 906 | CLA | C2B-C3B-CAB-CBB |
| 24 | c | 908 | CLA | C2B-C3B-CAB-CBB |
| 24 | d | 402 | CLA | C2B-C3B-CAB-CBB |
| 26 | D | 403 | BCR | C23-C24-C25-C26 |
| 26 | c | 915 | BCR | C1-C6-C7-C8 |
| 26 | c | 915 | BCR | C5-C6-C7-C8 |
| 26 | d | 404 | BCR | C23-C24-C25-C26 |
| 37 | D | 407 | LHG | C17-C18-C19-C20 |
| 37 | d | 408 | LHG | C13-C14-C15-C16 |
| 34 | B | 622 | LMG | O8-C28-C29-C30 |
| 24 | c | 909 | CLA | C13-C15-C16-C17 |
| 27 | A | 416 | SQD | C25-C26-C27-C28 |
| 24 | C | 504 | CLA | C4-C3-C5-C6 |
| 24 | b | 615 | CLA | C2-C3-C5-C6 |
| 31 | d | 405 | PL9 | C13-C14-C16-C17 |
| 38 | E | 103 | HEM | CAD-CBD-CGD-O2D |
| 35 | c | 922 | HTG | C2'-C1'-S1-C1 |
| 37 | l | 101 | LHG | C11-C12-C13-C14 |
| 24 | C | 513 | CLA | CAA-CBA-CGA-O2A |
| 29 | C | 522 | LMT | O1'-C1-C2-C3 |
| 37 | L | 101 | LHG | C23-C24-C25-C26 |
| 24 | c | 913 | CLA | CAA-CBA-CGA-O2A |
| 36 | d | 406 | DGD | O2G-C1B-C2B-C3B |
| 37 | D | 408 | LHG | C9-C10-C11-C12 |
| 24 | A | 407 | CLA | C14-C13-C15-C16 |
| 24 | C | 505 | CLA | C11-C12-C13-C14 |
| 24 | c | 910 | CLA | C11-C10-C8-C9 |
| 35 | c | 922 | HTG | C2'-C3'-C4'-C5' |
| 24 | B | 614 | CLA | CAA-CBA-CGA-O2A |
| 37 | L | 101 | LHG | C16-C17-C18-C19 |
| 24 | B | 613 | CLA | O1A-CGA-O2A-C1 |
| 31 | a | 417 | PL9 | C39-C41-C42-C43 |
| 24 | B | 604 | CLA | C16-C17-C18-C19 |
| 24 | B | 616 | CLA | C4B-C3B-CAB-CBB |
| 24 | C | 504 | CLA | C4B-C3B-CAB-CBB |
| 24 | C | 509 | CLA | C1A-C2A-CAA-CBA |
| 27 | L | 102 | SQD | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 34 | C | 501 | LMG | C36-C37-C38-C39 |
| 31 | D | 404 | PL9 | C35-C34-C36-C37 |
| 29 | M | 101 | LMT | O5'-C1'-O1'-C1 |
| 36 | h | 102 | DGD | O1G-C1G-C2G-O2G |
| 26 | T | 102 | BCR | C13-C14-C15-C16 |
| 24 | B | 606 | CLA | C16-C17-C18-C19 |
| 24 | C | 511 | CLA | C16-C17-C18-C19 |
| 24 | b | 610 | CLA | C16-C17-C18-C19 |
| 24 | B | 613 | CLA | CBA-CGA-O2A-C1 |
| 37 | d | 408 | LHG | C24-C23-O8-C6 |
| 27 | f | 102 | SQD | O47-C7-C8-C9 |
| 37 | E | 101 | LHG | O8-C23-C24-C25 |
| 36 | C | 518 | DGD | CDA-CEA-CFA-CGA |
| 27 | f | 102 | SQD | C34-C35-C36-C37 |
| 29 | M | 101 | LMT | C7-C8-C9-C10 |
| 27 | A | 416 | SQD | C5-C6-S-O7 |
| 27 | B | 621 | SQD | C5-C6-S-O9 |
| 24 | b | 617 | CLA | C2-C1-O2A-CGA |
| 24 | B | 613 | CLA | CAA-CBA-CGA-O2A |
| 24 | C | 513 | CLA | C6-C7-C8-C10 |
| 24 | b | 610 | CLA | C11-C10-C8-C7 |
| 24 | b | 612 | CLA | C11-C10-C8-C7 |
| 24 | c | 914 | CLA | C10-C11-C12-C13 |
| 27 | B | 621 | SQD | C28-C29-C30-C31 |
| 36 | h | 102 | DGD | C5A-C6A-C7A-C8A |
| 24 | B | 606 | CLA | O1D-CGD-O2D-CED |
| 24 | C | 503 | CLA | C13-C15-C16-C17 |
| 24 | d | 403 | CLA | C10-C11-C12-C13 |
| 36 | c | 917 | DGD | C9A-CAA-CBA-CCA |
| 24 | c | 911 | CLA | CAA-CBA-CGA-O2A |
| 37 | e | 101 | LHG | O8-C23-C24-C25 |
| 24 | C | 505 | CLA | C4-C3-C5-C6 |
| 36 | D | 405 | DGD | O1G-C1A-C2A-C3A |
| 24 | C | 504 | CLA | C15-C16-C17-C18 |
| 34 | J | 101 | LMG | C32-C33-C34-C35 |
| 36 | C | 518 | DGD | CBB-CCB-CDB-CEB |
| 24 | C | 506 | CLA | CAA-CBA-CGA-O2A |
| 24 | b | 617 | CLA | CAA-CBA-CGA-O2A |
| 24 | b | 606 | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 610 | CLA | C11-C12-C13-C14 |
| 24 | b | 610 | CLA | C14-C13-C15-C16 |
| 36 | C | 518 | DGD | C5A-C6A-C7A-C8A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | l | 101 | LHG | O7-C7-C8-C9 |
| 34 | z | 101 | LMG | O9-C10-C11-C12 |
| 34 | C | 521 | LMG | C39-C40-C41-C42 |
| 34 | b | 624 | LMG | C39-C40-C41-C42 |
| 24 | b | 615 | CLA | C4-C3-C5-C6 |
| 27 | f | 102 | SQD | O49-C7-C8-C9 |
| 36 | c | 916 | DGD | C2A-C3A-C4A-C5A |
| 24 | C | 511 | CLA | CAA-CBA-CGA-O2A |
| 27 | B | 621 | SQD | O5-C5-C6-S |
| 24 | c | 913 | CLA | CAA-CBA-CGA-O1A |
| 24 | b | 615 | CLA | C8-C10-C11-C12 |
| 28 | V | 206 | GOL | O2-C2-C3-O3 |
| 36 | C | 517 | DGD | C2A-C3A-C4A-C5A |
| 36 | d | 406 | DGD | O1B-C1B-C2B-C3B |
| 37 | D | 406 | LHG | C11-C12-C13-C14 |
| 24 | C | 509 | CLA | C5-C6-C7-C8 |
| 27 | a | 411 | SQD | C45-C44-O6-C1 |
| 36 | H | 102 | DGD | C2G-C3G-O3G-C1D |
| 36 | h | 102 | DGD | C2G-C3G-O3G-C1D |
| 34 | b | 624 | LMG | O8-C28-C29-C30 |
| 27 | A | 412 | SQD | O6-C44-C45-C46 |
| 31 | A | 419 | PL9 | C19-C21-C22-C23 |
| 24 | B | 613 | CLA | CAA-CBA-CGA-O1A |
| 24 | C | 513 | CLA | CAA-CBA-CGA-O1A |
| 36 | C | 519 | DGD | C8A-C9A-CAA-CBA |
| 38 | e | 102 | HEM | C2C-C3C-CAC-CBC |
| 24 | c | 914 | CLA | CBA-CGA-O2A-C1 |
| 24 | B | 606 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 502 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 505 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 614 | CLA | CAD-CBD-CGD-O2D |
| 37 | E | 101 | LHG | O7-C7-C8-C9 |
| 29 | C | 522 | LMT | C3-C4-C5-C6 |
| 24 | A | 410 | CLA | C8-C10-C11-C12 |
| 37 | E | 101 | LHG | O10-C23-C24-C25 |
| 37 | e | 101 | LHG | O10-C23-C24-C25 |
| 24 | c | 906 | CLA | CAA-CBA-CGA-O2A |
| 34 | c | 919 | LMG | C34-C35-C36-C37 |
| 34 | C | 501 | LMG | O8-C28-C29-C30 |
| 34 | b | 624 | LMG | C31-C32-C33-C34 |
| 37 | l | 101 | LHG | C17-C18-C19-C20 |
| 27 | L | 102 | SQD | O48-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | C | 511 | CLA | CAA-CBA-CGA-O1A |
| 24 | b | 617 | CLA | CAA-CBA-CGA-O1A |
| 27 | a | 402 | SQD | C13-C14-C15-C16 |

There are no ring outliers.

157 monomers are involved in 303 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | B | 606 | CLA | 1 | 0 |
| 26 | a | 410 | BCR | 3 | 0 |
| 28 | b | 633 | GOL | 1 | 0 |
| 35 | c | 922 | HTG | 1 | 0 |
| 28 | A | 414 | GOL | 1 | 0 |
| 28 | v | 203 | GOL | 2 | 0 |
| 24 | b | 616 | CLA | 2 | 0 |
| 28 | b | 631 | GOL | 1 | 0 |
| 24 | c | 912 | CLA | 2 | 0 |
| 35 | C | 524 | HTG | 1 | 0 |
| 24 | c | 914 | CLA | 3 | 0 |
| 34 | j | 101 | LMG | 5 | 0 |
| 24 | B | 608 | CLA | 1 | 0 |
| 35 | B | 625 | HTG | 1 | 0 |
| 24 | D | 401 | CLA | 1 | 0 |
| 24 | B | 603 | CLA | 2 | 0 |
| 29 | E | 102 | LMT | 1 | 0 |
| 34 | C | 501 | LMG | 2 | 0 |
| 26 | T | 102 | BCR | 4 | 0 |
| 35 | B | 633 | HTG | 2 | 0 |
| 36 | d | 406 | DGD | 6 | 0 |
| 24 | b | 615 | CLA | 1 | 0 |
| 34 | c | 920 | LMG | 2 | 0 |
| 38 | e | 102 | HEM | 2 | 0 |
| 35 | O | 303 | HTG | 1 | 0 |
| 24 | c | 903 | CLA | 3 | 0 |
| 24 | d | 401 | CLA | 1 | 0 |
| 24 | C | 510 | CLA | 3 | 0 |
| 37 | D | 408 | LHG | 7 | 0 |
| 24 | C | 505 | CLA | 1 | 0 |
| 37 | l | 101 | LHG | 2 | 0 |
| 24 | A | 405 | CLA | 2 | 0 |
| 24 | B | 613 | CLA | 1 | 0 |
| 24 | B | 604 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | b | 619 | CLA | 3 | 0 |
| 24 | b | 610 | CLA | 1 | 0 |
| 24 | b | 609 | CLA | 2 | 0 |
| 24 | B | 607 | CLA | 2 | 0 |
| 26 | C | 515 | BCR | 1 | 0 |
| 24 | c | 902 | CLA | 2 | 0 |
| 24 | B | 612 | CLA | 1 | 0 |
| 26 | H | 101 | BCR | 3 | 0 |
| 28 | T | 103 | GOL | 3 | 0 |
| 24 | A | 406 | CLA | 4 | 0 |
| 29 | C | 522 | LMT | 2 | 0 |
| 26 | t | 101 | BCR | 7 | 0 |
| 29 | b | 601 | LMT | 2 | 0 |
| 24 | c | 905 | CLA | 1 | 0 |
| 28 | B | 631 | GOL | 1 | 0 |
| 27 | a | 402 | SQD | 1 | 0 |
| 26 | b | 621 | BCR | 2 | 0 |
| 37 | e | 101 | LHG | 1 | 0 |
| 34 | z | 101 | LMG | 2 | 0 |
| 24 | C | 506 | CLA | 4 | 0 |
| 24 | b | 618 | CLA | 1 | 0 |
| 28 | B | 637 | GOL | 3 | 0 |
| 36 | D | 405 | DGD | 5 | 0 |
| 24 | c | 913 | CLA | 3 | 0 |
| 28 | T | 101 | GOL | 1 | 0 |
| 24 | a | 406 | CLA | 4 | 0 |
| 37 | d | 408 | LHG | 1 | 0 |
| 29 | M | 101 | LMT | 3 | 0 |
| 24 | c | 909 | CLA | 4 | 0 |
| 24 | c | 908 | CLA | 2 | 0 |
| 24 | C | 507 | CLA | 6 | 0 |
| 24 | A | 410 | CLA | 3 | 0 |
| 26 | B | 618 | BCR | 1 | 0 |
| 24 | B | 614 | CLA | 3 | 0 |
| 24 | B | 609 | CLA | 2 | 0 |
| 24 | B | 610 | CLA | 2 | 0 |
| 35 | B | 634 | HTG | 1 | 0 |
| 28 | c | 925 | GOL | 2 | 0 |
| 27 | L | 102 | SQD | 2 | 0 |
| 24 | C | 509 | CLA | 3 | 0 |
| 24 | c | 911 | CLA | 2 | 0 |
| 24 | b | 605 | CLA | 4 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | c | 910 | CLA | 2 | 0 |
| 28 | a | 414 | GOL | 2 | 0 |
| 37 | L | 101 | LHG | 1 | 0 |
| 28 | C | 525 | GOL | 2 | 0 |
| 26 | c | 915 | BCR | 2 | 0 |
| 26 | B | 620 | BCR | 2 | 0 |
| 24 | B | 616 | CLA | 2 | 0 |
| 24 | b | 608 | CLA | 2 | 0 |
| 36 | C | 518 | DGD | 2 | 0 |
| 24 | b | 607 | CLA | 1 | 0 |
| 26 | B | 619 | BCR | 4 | 0 |
| 24 | c | 906 | CLA | 2 | 0 |
| 34 | b | 624 | LMG | 2 | 0 |
| 26 | k | 102 | BCR | 1 | 0 |
| 26 | b | 622 | BCR | 2 | 0 |
| 24 | c | 907 | CLA | 3 | 0 |
| 27 | A | 412 | SQD | 5 | 0 |
| 29 | m | 104 | LMT | 3 | 0 |
| 24 | d | 403 | CLA | 1 | 0 |
| 26 | y | 101 | BCR | 2 | 0 |
| 28 | f | 101 | GOL | 1 | 0 |
| 24 | C | 502 | CLA | 1 | 0 |
| 34 | C | 520 | LMG | 2 | 0 |
| 24 | a | 409 | CLA | 1 | 0 |
| 37 | D | 406 | LHG | 2 | 0 |
| 24 | D | 402 | CLA | 2 | 0 |
| 24 | C | 508 | CLA | 4 | 0 |
| 36 | c | 916 | DGD | 1 | 0 |
| 37 | E | 101 | LHG | 2 | 0 |
| 24 | C | 503 | CLA | 2 | 0 |
| 24 | B | 602 | CLA | 4 | 0 |
| 36 | c | 917 | DGD | 4 | 0 |
| 34 | J | 101 | LMG | 3 | 0 |
| 25 | a | 420 | PHO | 1 | 0 |
| 29 | f | 103 | LMT | 1 | 0 |
| 31 | D | 404 | PL9 | 1 | 0 |
| 24 | C | 513 | CLA | 3 | 0 |
| 34 | C | 521 | LMG | 3 | 0 |
| 34 | a | 412 | LMG | 3 | 0 |
| 29 | b | 625 | LMT | 2 | 0 |
| 28 | b | 632 | GOL | 2 | 0 |
| 27 | F | 101 | SQD | 3 | 0 |

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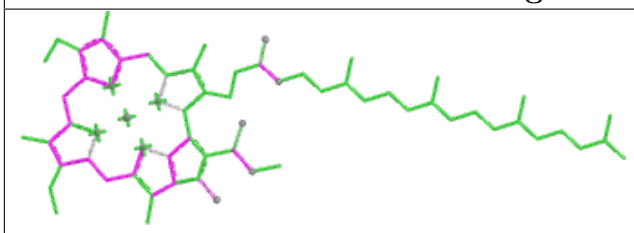
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 27 | A | 416 | SQD | 2 | 0 |
| 35 | D | 411 | HTG | 3 | 0 |
| 24 | d | 402 | CLA | 3 | 0 |
| 25 | A | 409 | PHO | 1 | 0 |
| 26 | K | 102 | BCR | 1 | 0 |
| 24 | B | 605 | CLA | 2 | 0 |
| 24 | C | 512 | CLA | 1 | 0 |
| 31 | a | 417 | PL9 | 5 | 0 |
| 29 | B | 636 | LMT | 1 | 0 |
| 27 | a | 411 | SQD | 3 | 0 |
| 29 | c | 921 | LMT | 1 | 0 |
| 29 | m | 102 | LMT | 4 | 0 |
| 36 | C | 517 | DGD | 4 | 0 |
| 34 | B | 622 | LMG | 2 | 0 |
| 24 | b | 612 | CLA | 1 | 0 |
| 24 | B | 617 | CLA | 5 | 0 |
| 27 | B | 621 | SQD | 3 | 0 |
| 31 | A | 419 | PL9 | 5 | 0 |
| 24 | b | 613 | CLA | 3 | 0 |
| 26 | h | 101 | BCR | 2 | 0 |
| 26 | b | 623 | BCR | 2 | 0 |
| 24 | c | 904 | CLA | 2 | 0 |
| 24 | C | 511 | CLA | 3 | 0 |
| 29 | a | 401 | LMT | 2 | 0 |
| 29 | B | 623 | LMT | 1 | 0 |
| 37 | d | 409 | LHG | 7 | 0 |
| 34 | Z | 101 | LMG | 3 | 0 |
| 24 | C | 514 | CLA | 4 | 0 |
| 26 | k | 101 | BCR | 5 | 0 |
| 24 | b | 606 | CLA | 2 | 0 |
| 26 | K | 103 | BCR | 3 | 0 |
| 26 | A | 411 | BCR | 1 | 0 |
| 36 | H | 102 | DGD | 1 | 0 |
| 36 | C | 519 | DGD | 2 | 0 |
| 26 | d | 404 | BCR | 4 | 0 |
| 31 | d | 405 | PL9 | 1 | 0 |
| 35 | d | 412 | HTG | 2 | 0 |
| 26 | D | 403 | BCR | 2 | 0 |
| 24 | b | 620 | CLA | 2 | 0 |

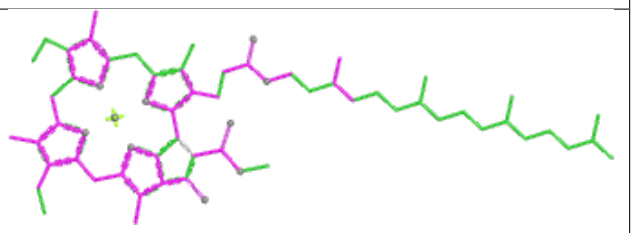
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

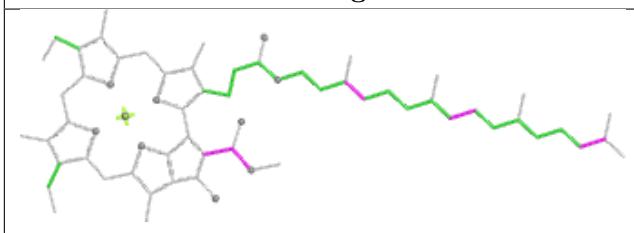
**Ligand CLA B 606**



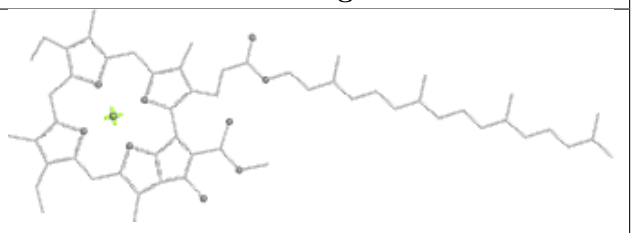
**Bond lengths**



**Bond angles**

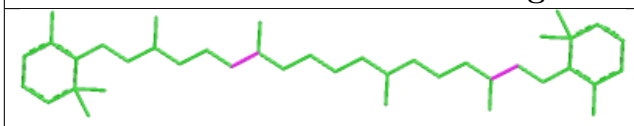


**Torsions**

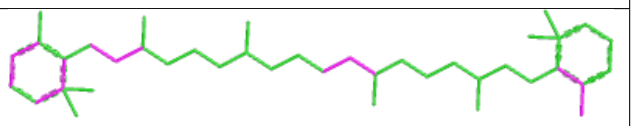


**Rings**

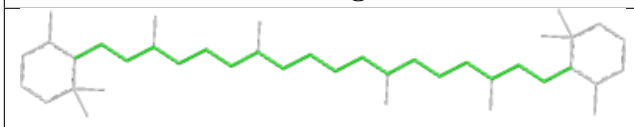
**Ligand BCR a 410**



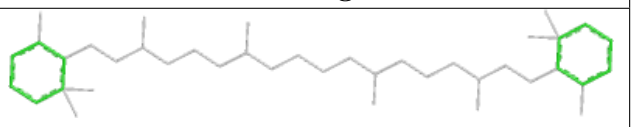
**Bond lengths**



**Bond angles**

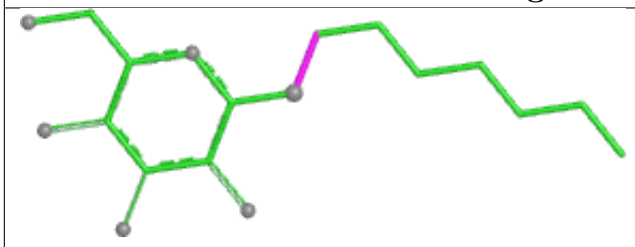


**Torsions**

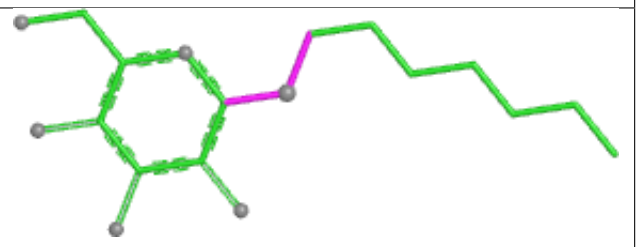


**Rings**

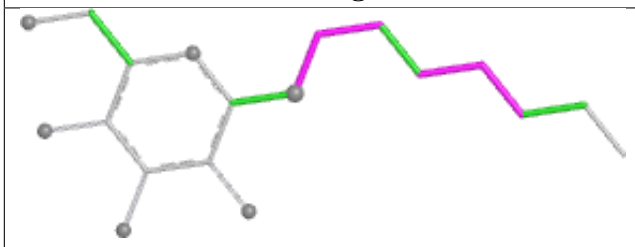
### Ligand HTG c 922



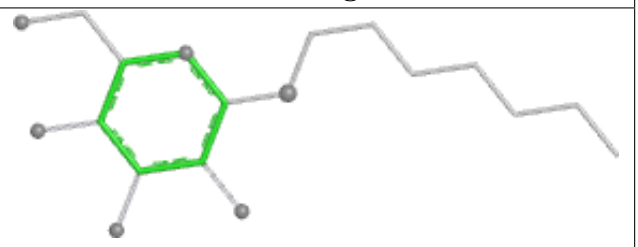
Bond lengths



Bond angles

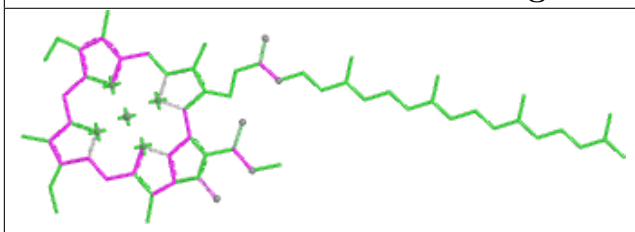


Torsions

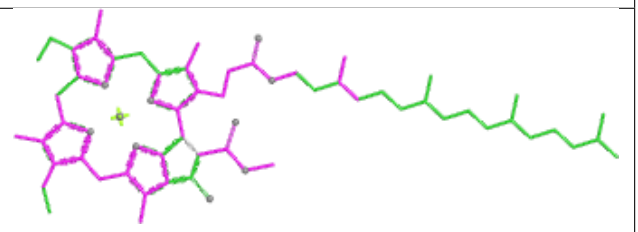


Rings

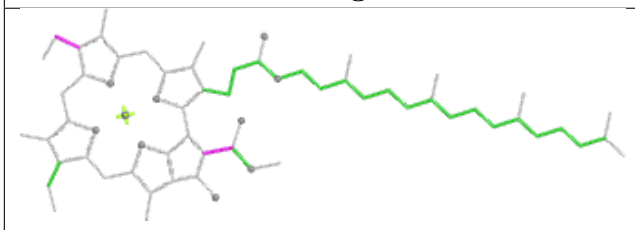
### Ligand CLA b 611



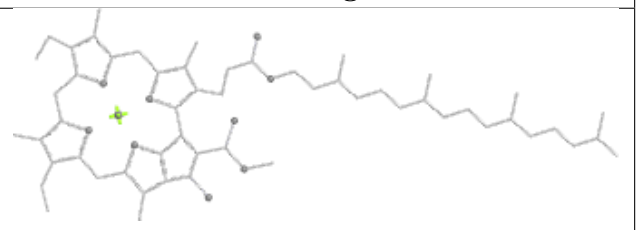
Bond lengths



Bond angles

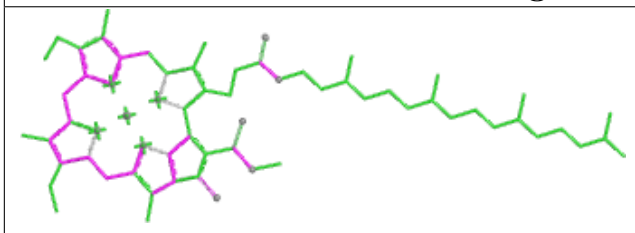


Torsions

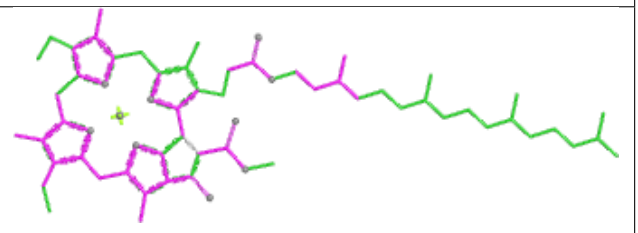


Rings

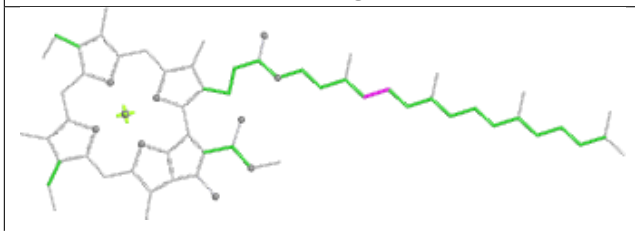
### Ligand CLA b 616



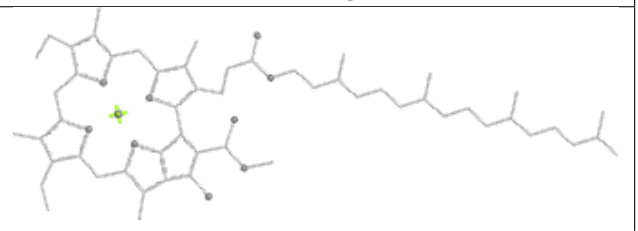
Bond lengths



Bond angles

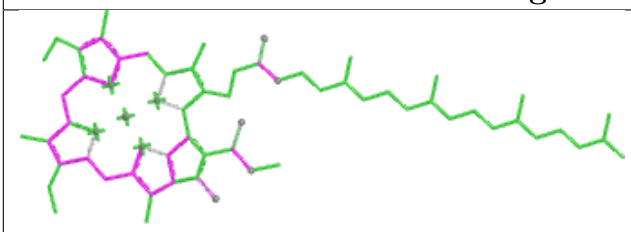


Torsions

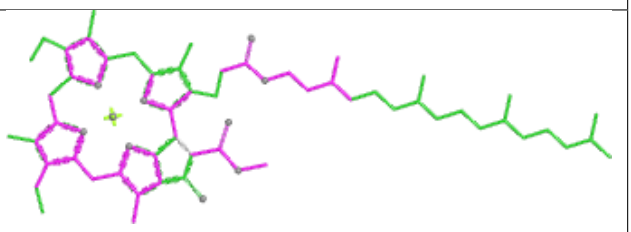


Rings

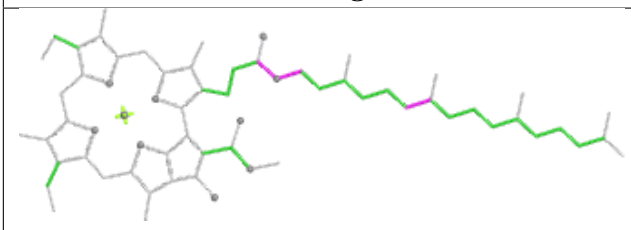
## Ligand CLA c 912



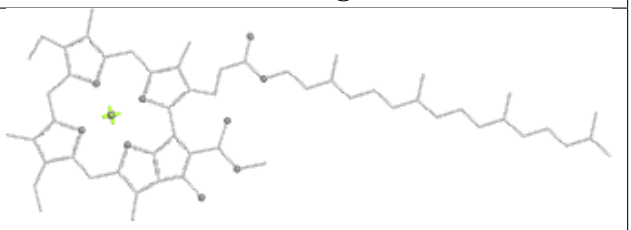
Bond lengths



Bond angles

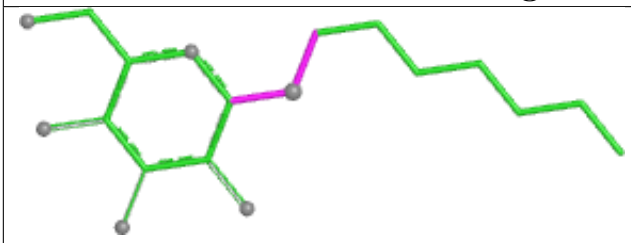


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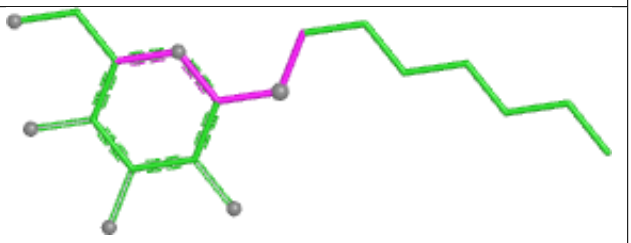


Rings

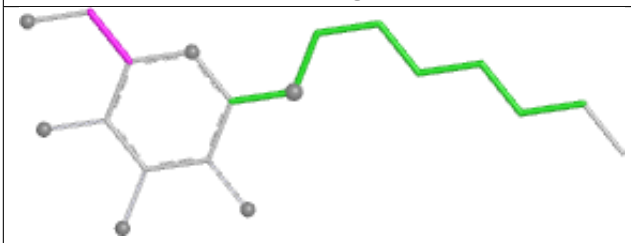
## Ligand HTG C 523



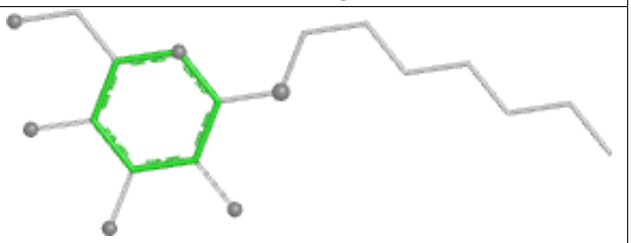
Bond lengths



Bond angles

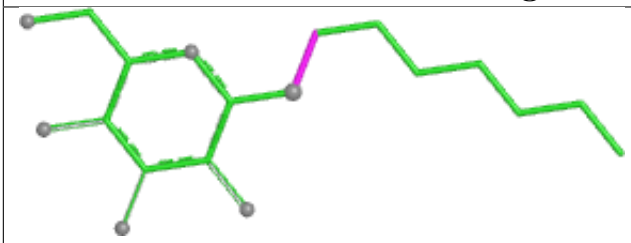


Torsions

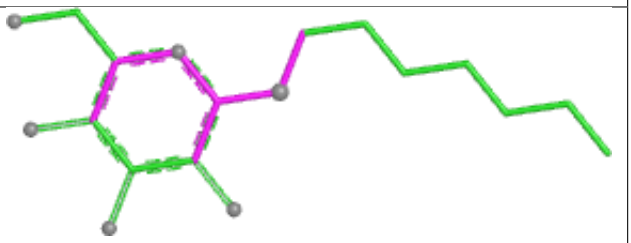


Rings

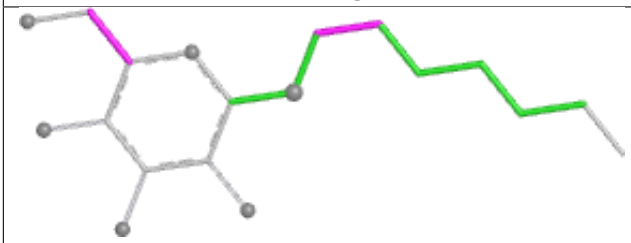
## Ligand HTG C 524



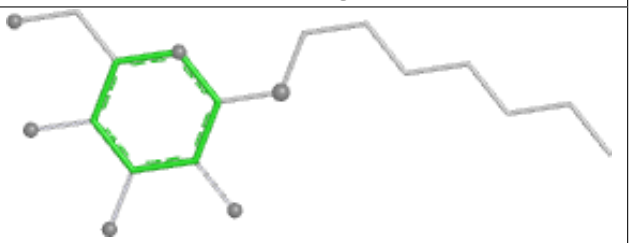
Bond lengths



Bond angles

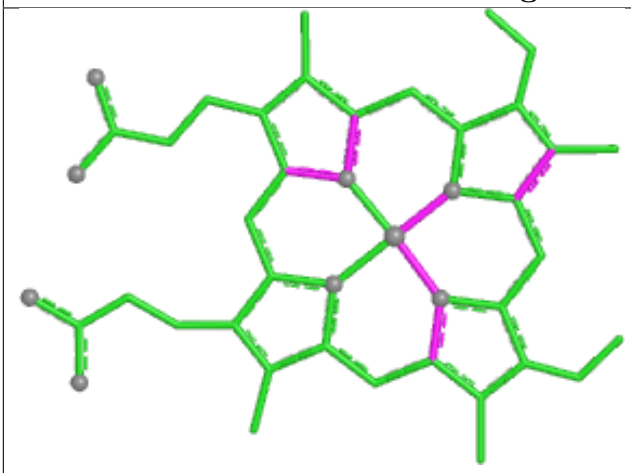


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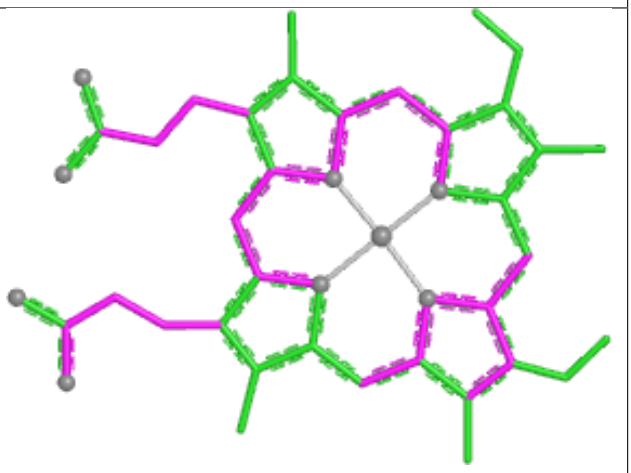


Rings

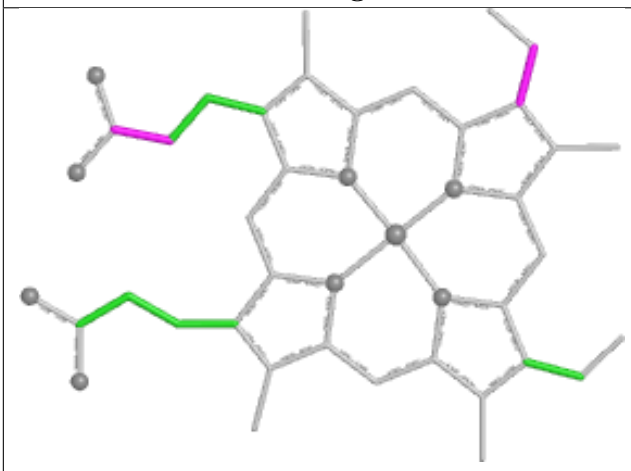
## Ligand HEM E 103



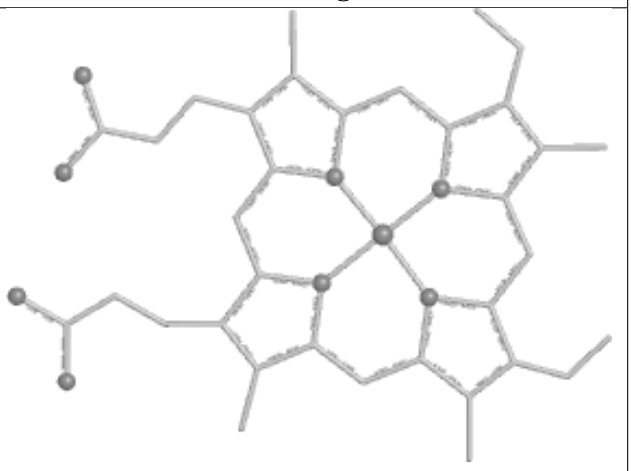
Bond lengths



Bond angles

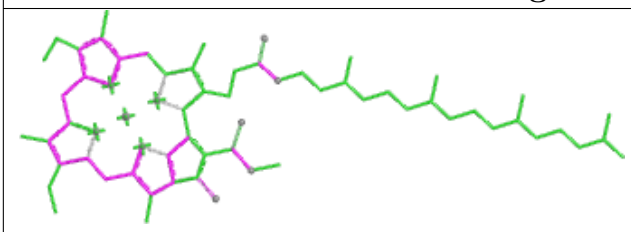


Torsions

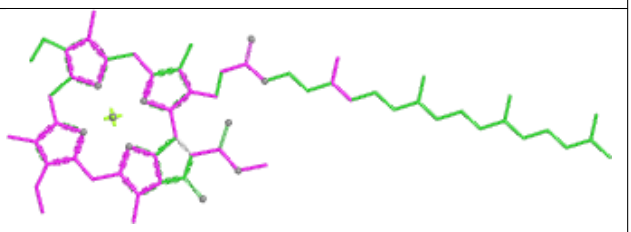


Rings

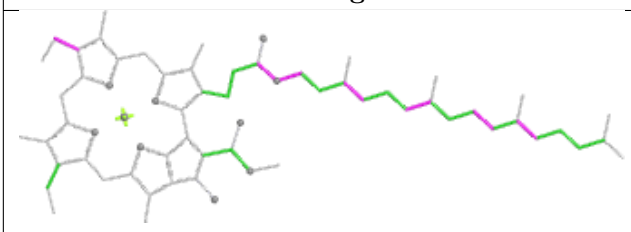
## Ligand CLA c 914



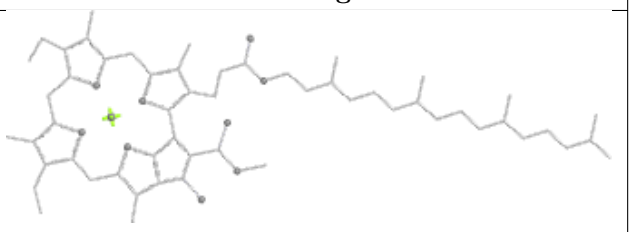
Bond lengths



Bond angles

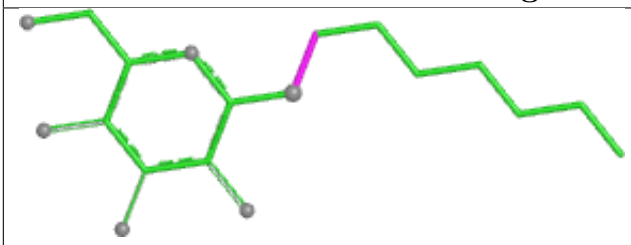


Torsions

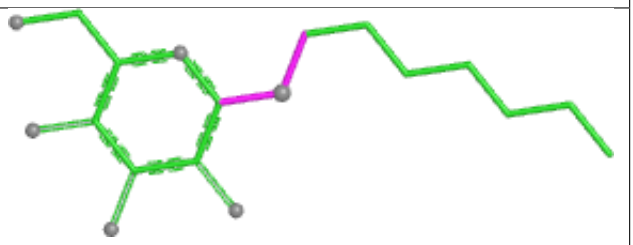


Rings

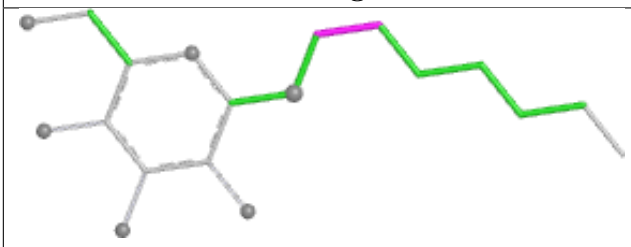
### Ligand HTG B 624



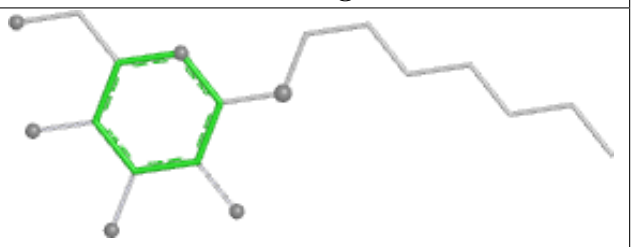
Bond lengths



Bond angles

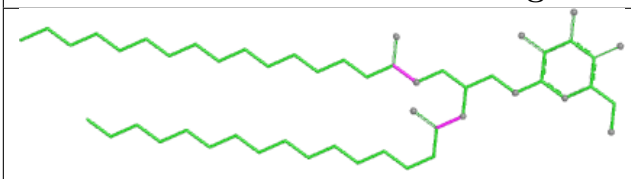


Torsions

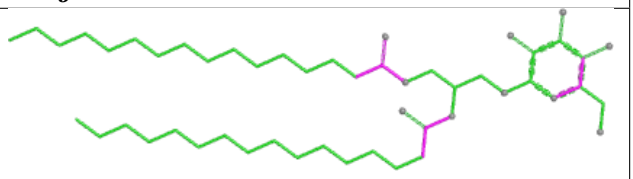


Rings

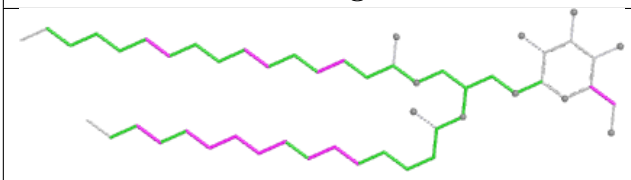
### Ligand LMG j 101



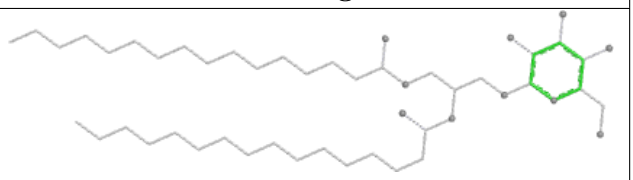
Bond lengths



Bond angles

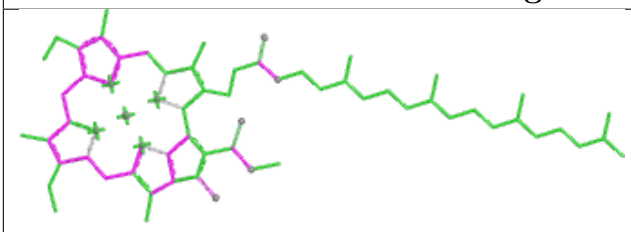


Torsions

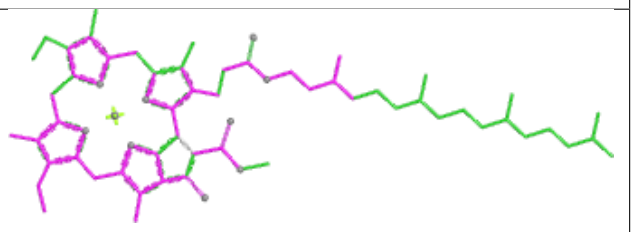


Rings

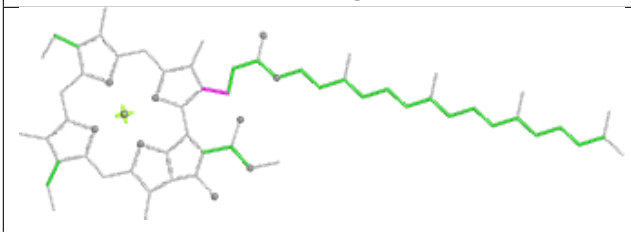
### Ligand CLA B 608



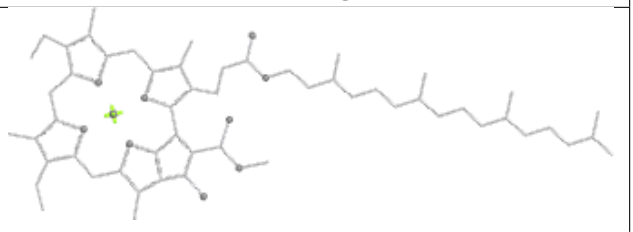
Bond lengths



Bond angles

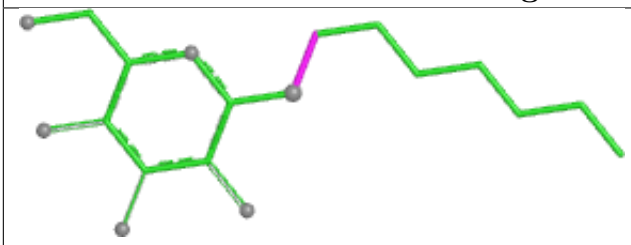


Torsions

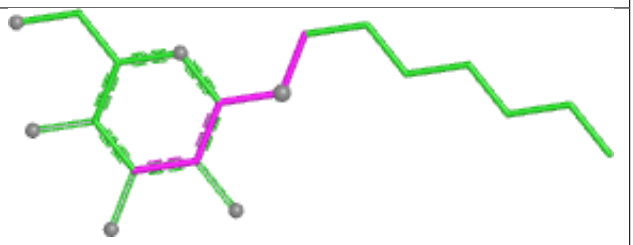


Rings

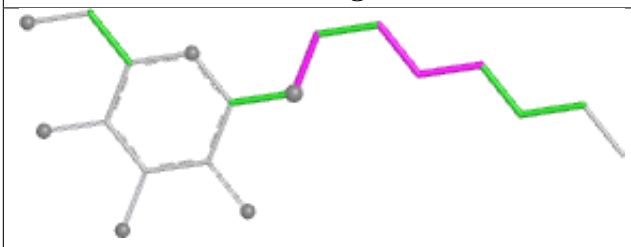
**Ligand HTG B 625**



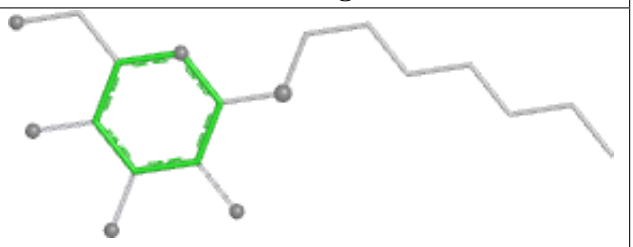
Bond lengths



Bond angles

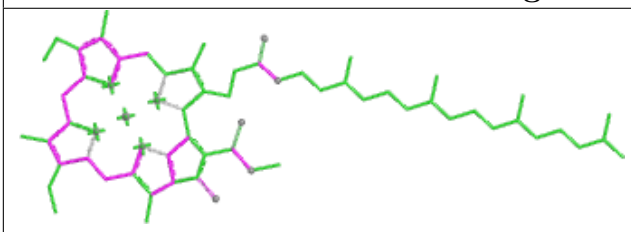


Torsions

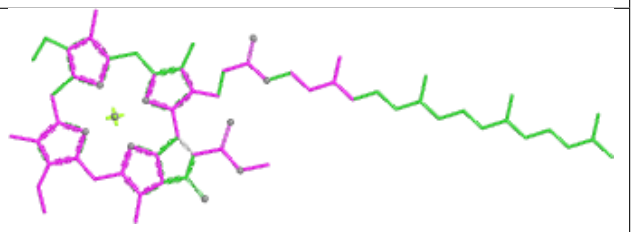


Rings

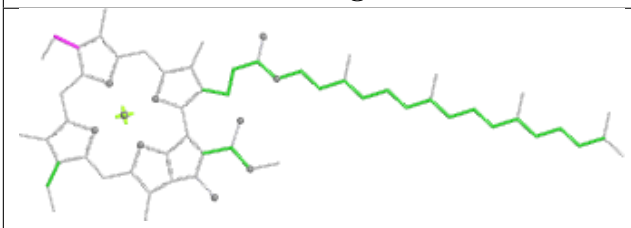
**Ligand CLA D 401**



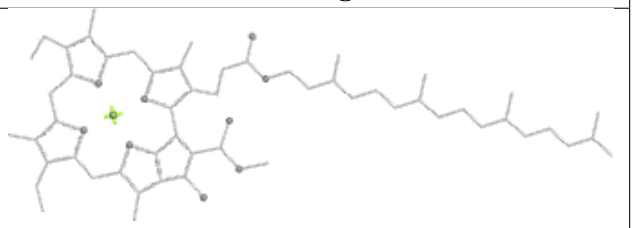
Bond lengths



Bond angles

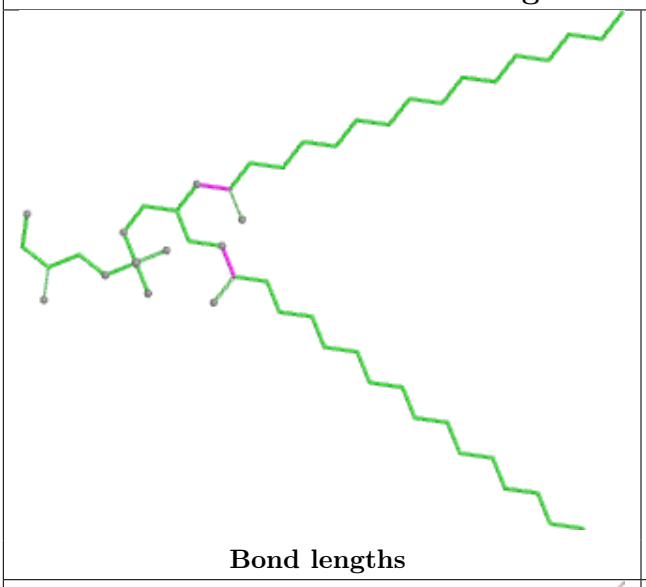


Torsions

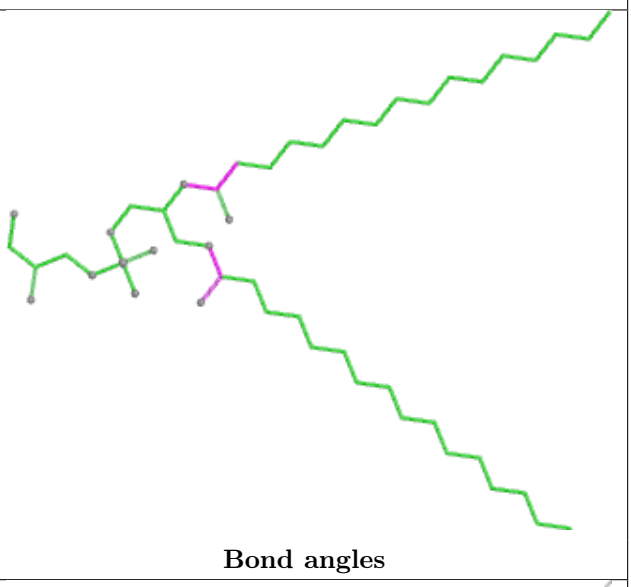


Rings

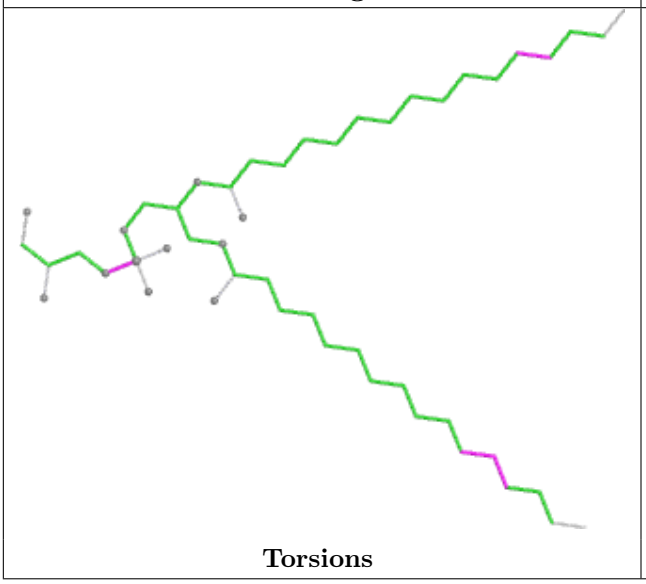
## Ligand LHG D 407



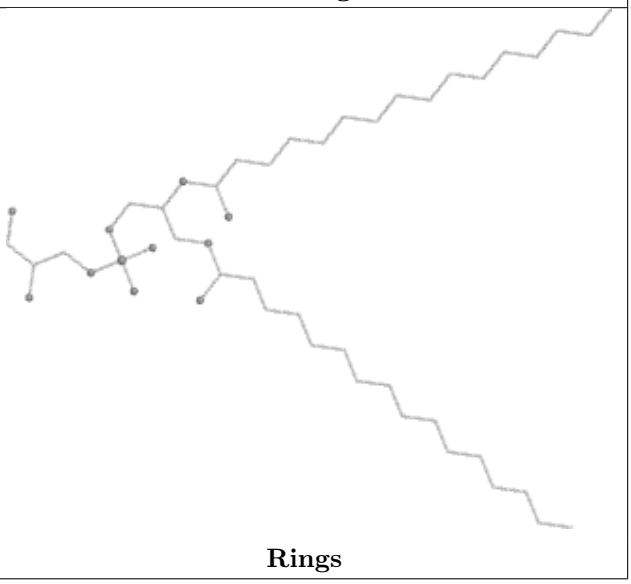
Bond lengths



Bond angles

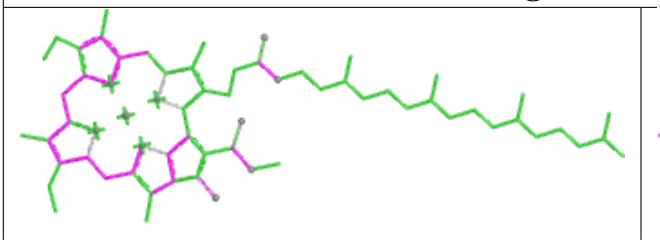


Torsions

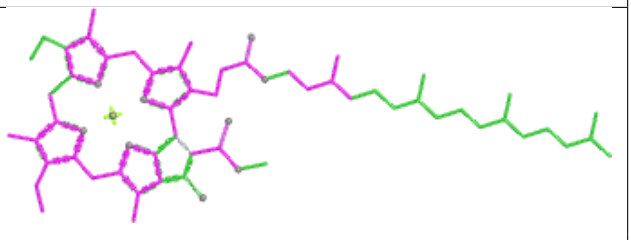


Rings

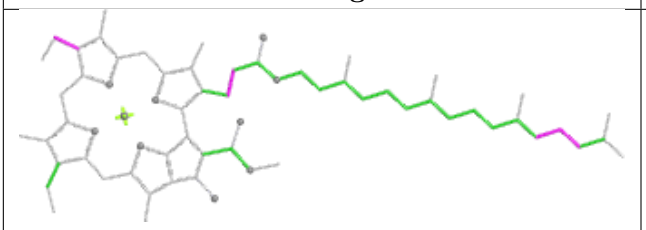
## Ligand CLA B 603



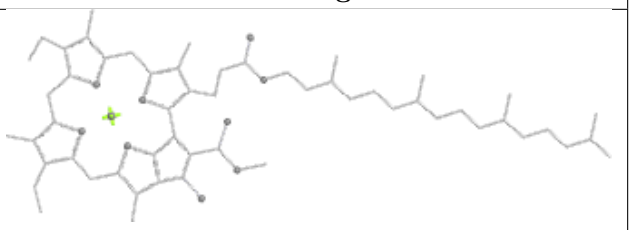
Bond lengths



Bond angles

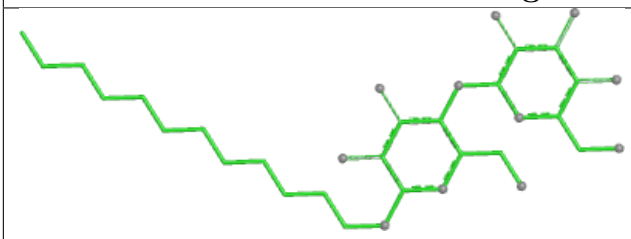


Torsions

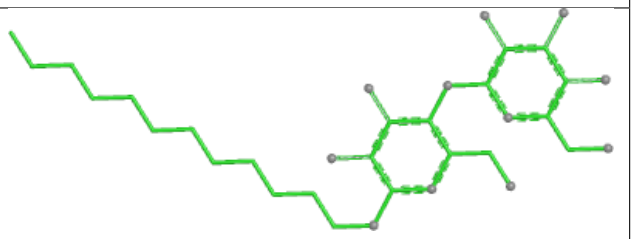


Rings

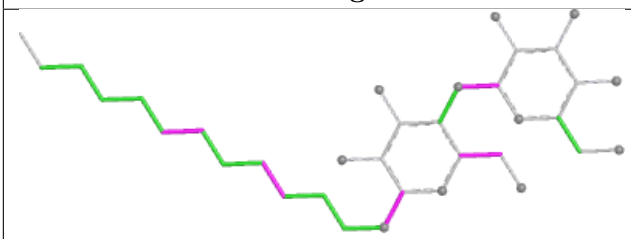
## Ligand LMT E 102



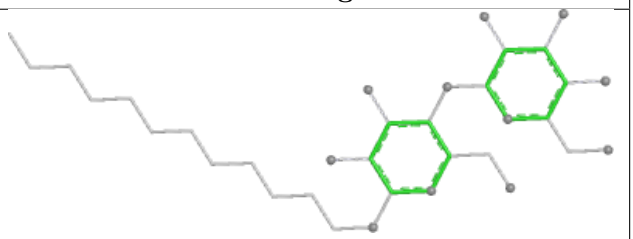
Bond lengths



Bond angles

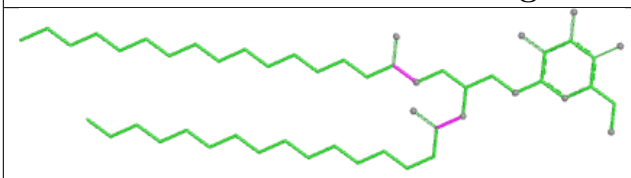


Torsions

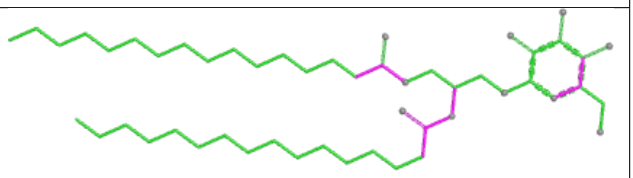


Rings

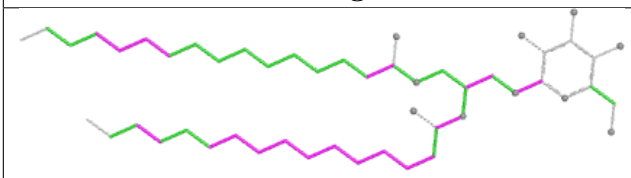
## Ligand LMG C 501



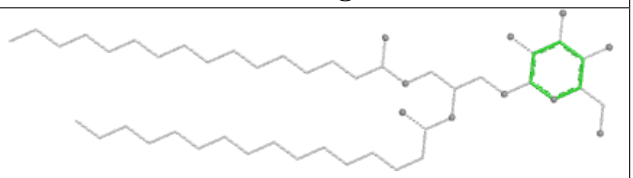
Bond lengths



Bond angles

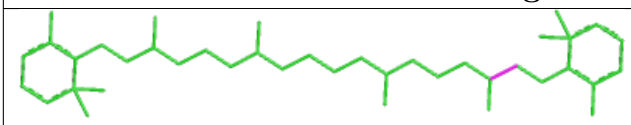


Torsions

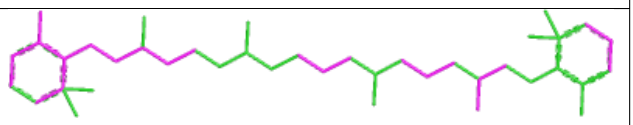


Rings

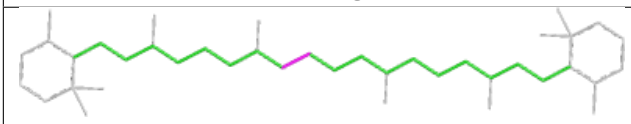
## Ligand BCR T 102



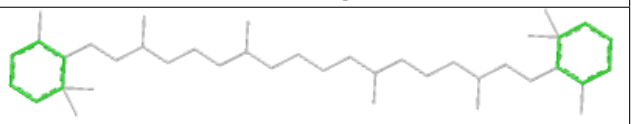
Bond lengths



Bond angles

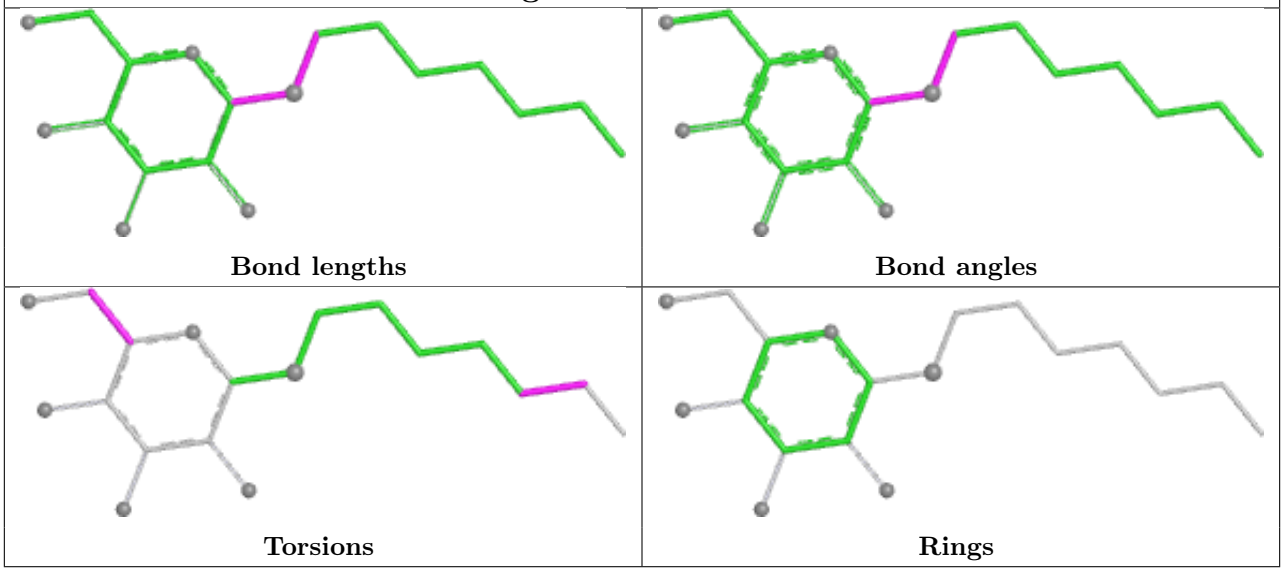


Torsions

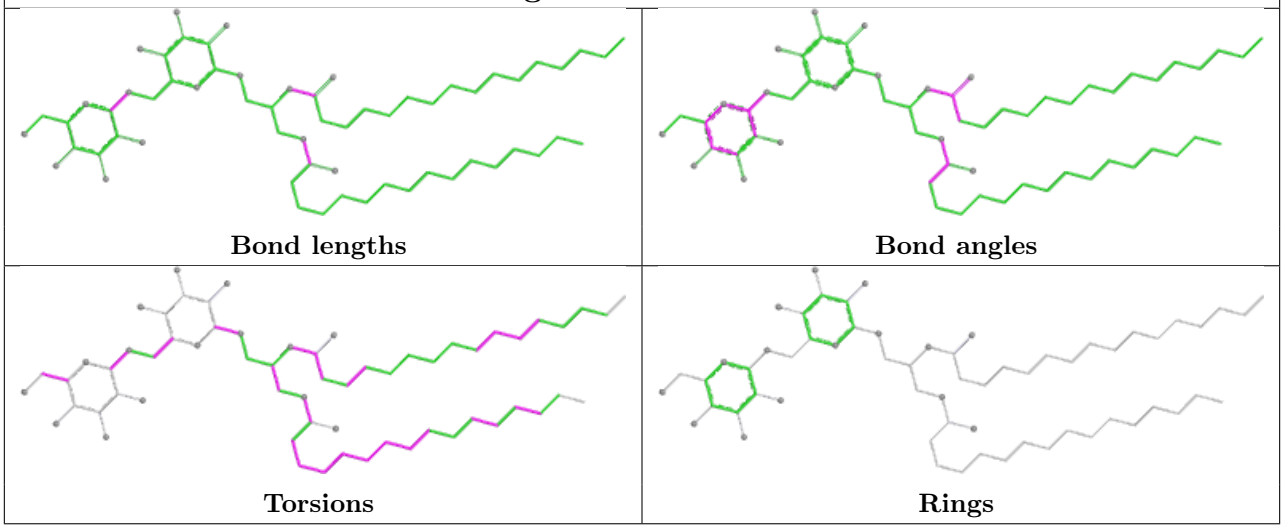


Rings

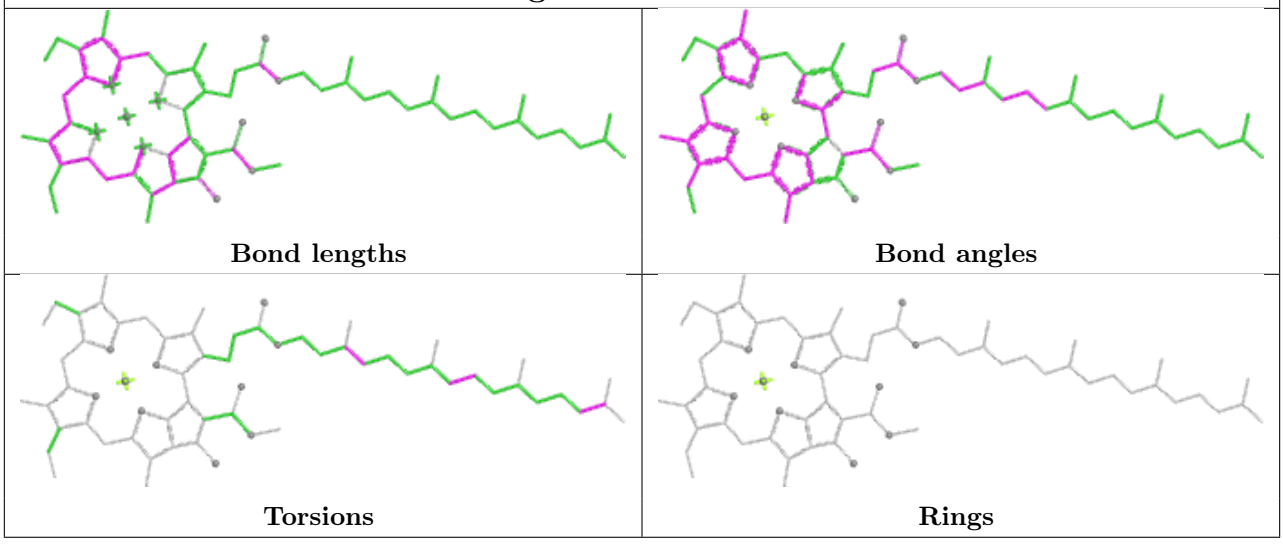
## Ligand HTG B 633



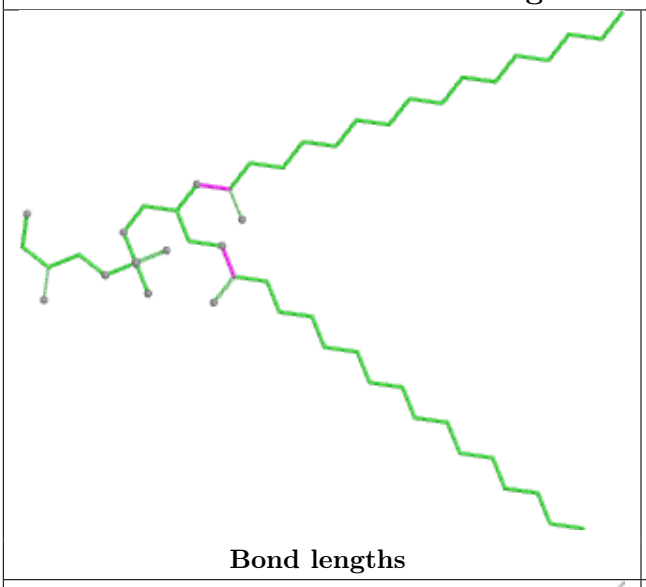

## Ligand DGD d 406



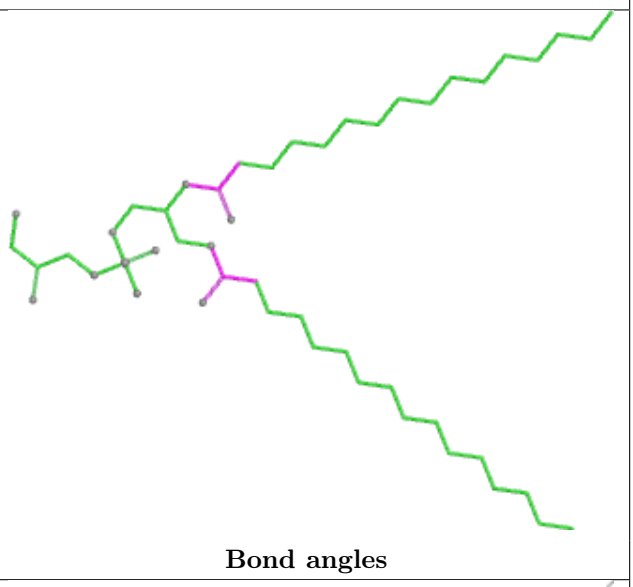

## Ligand CLA b 615



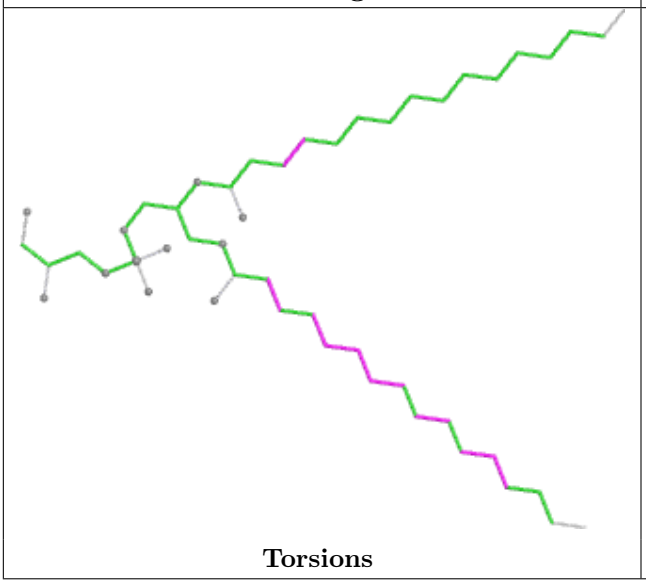
**Ligand LHG d 407**



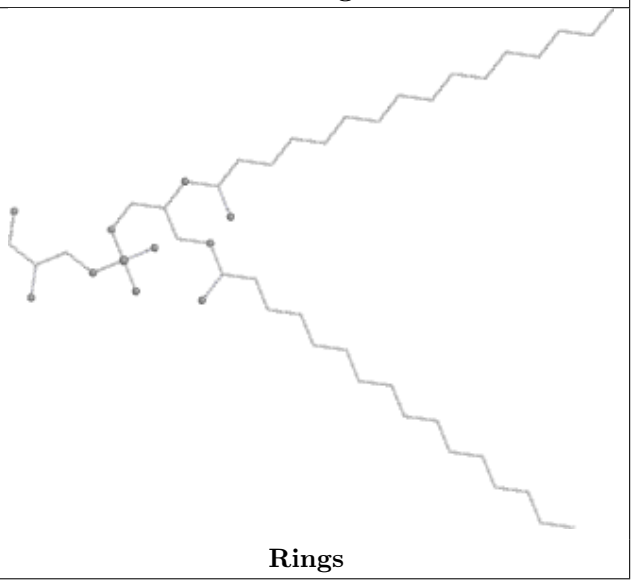
Bond lengths



Bond angles

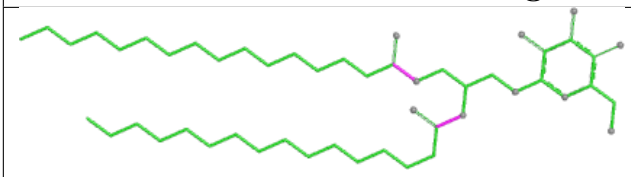


Torsions

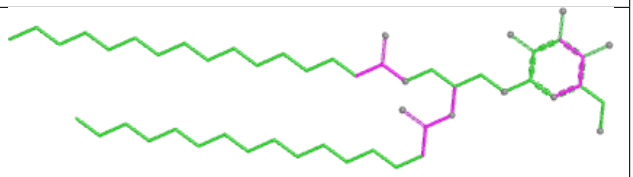


Rings

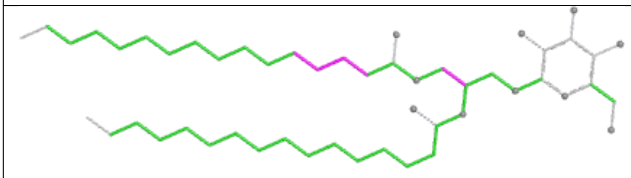
**Ligand LMG c 920**



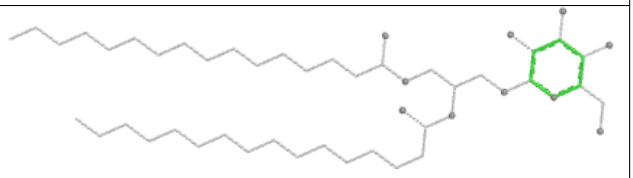
Bond lengths



Bond angles

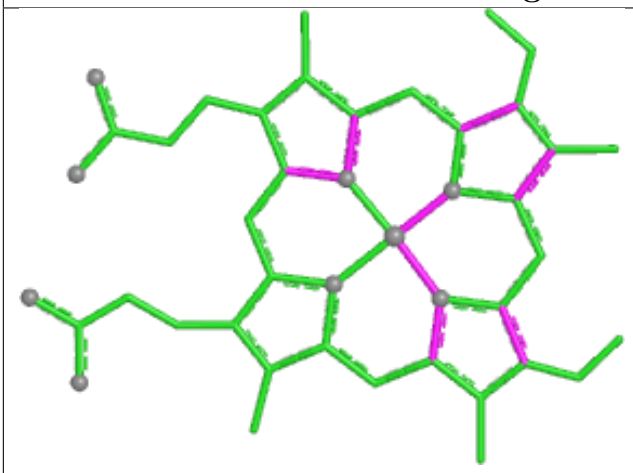


Torsions

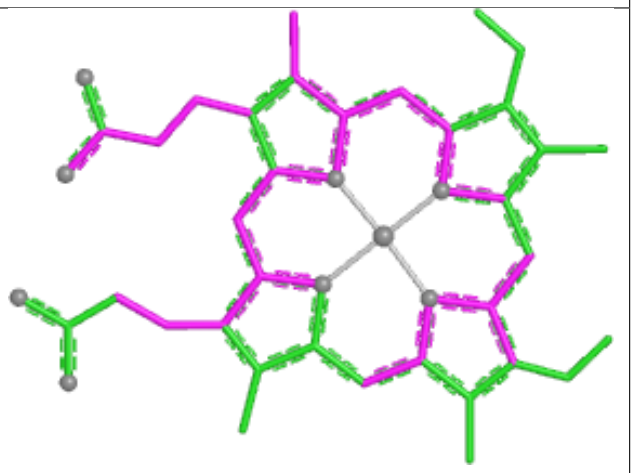


Rings

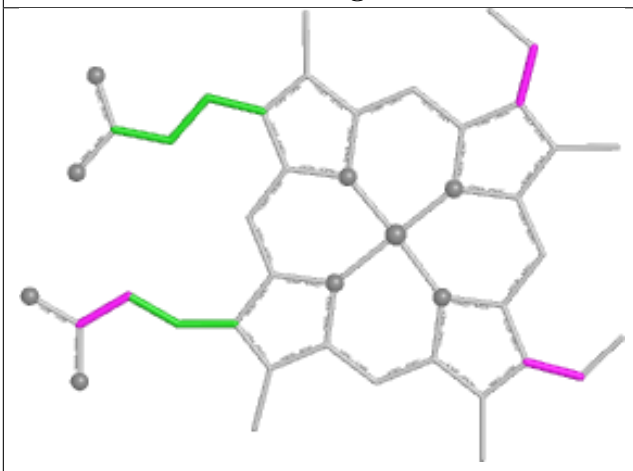
**Ligand HEM e 102**



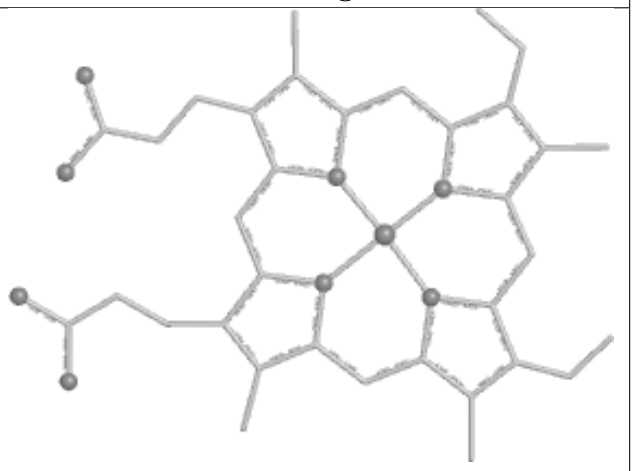
Bond lengths



Bond angles

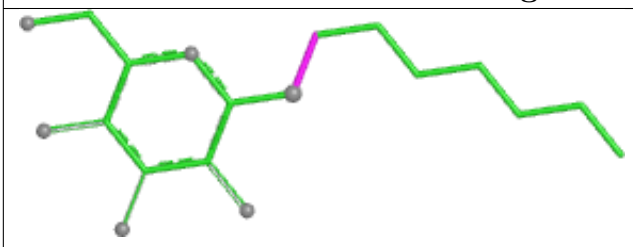


Torsions

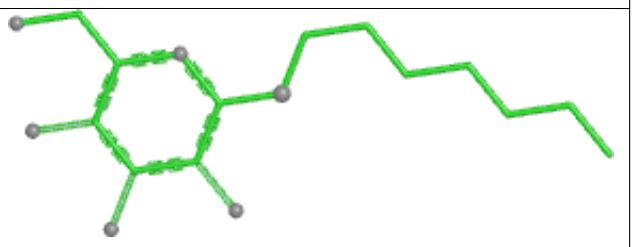


Rings

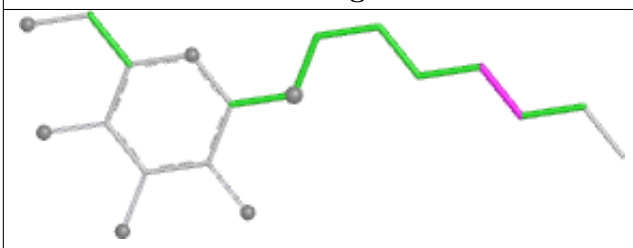
**Ligand HTG O 303**



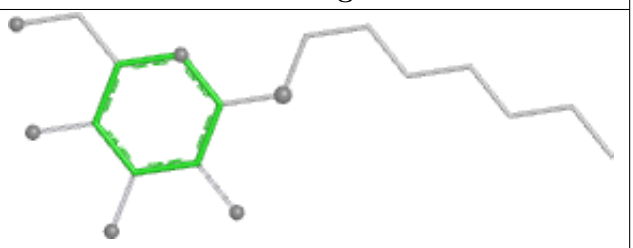
Bond lengths



Bond angles

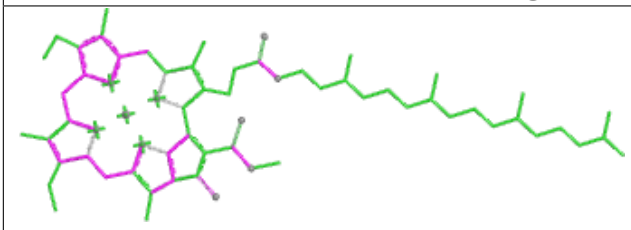


Torsions

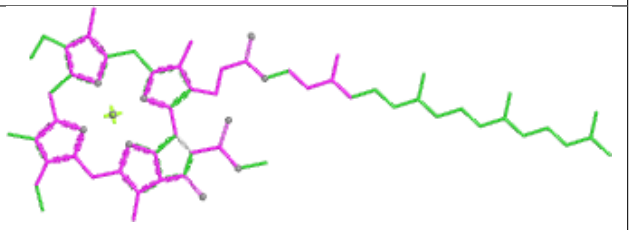


Rings

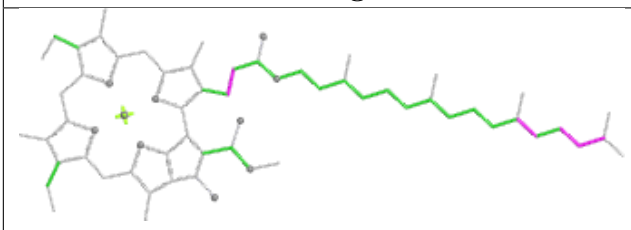
### Ligand CLA B 611



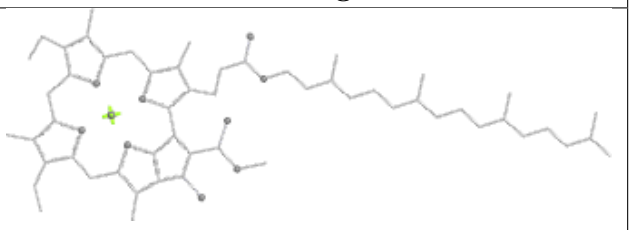
Bond lengths



Bond angles

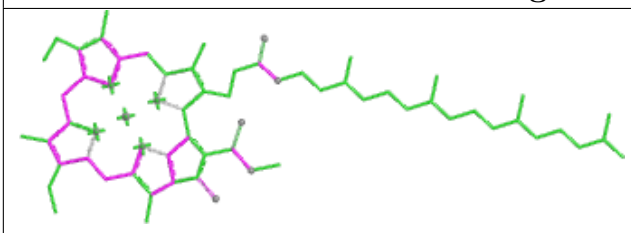


Torsions

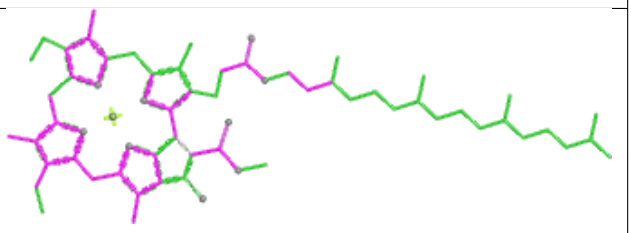


Rings

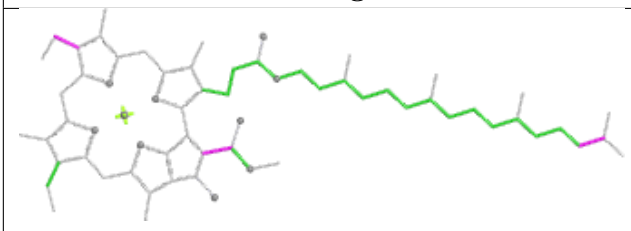
### Ligand CLA c 903



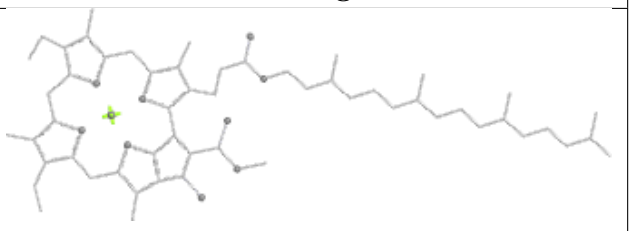
Bond lengths



Bond angles

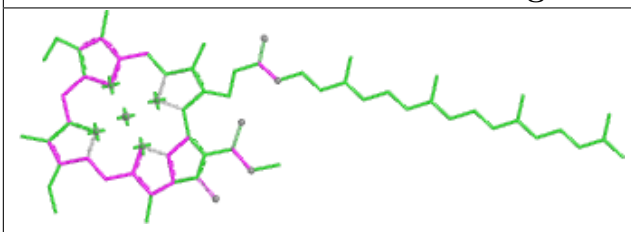


Torsions

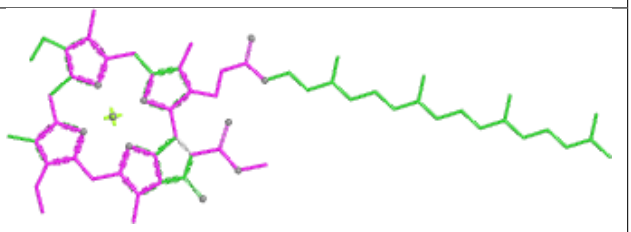


Rings

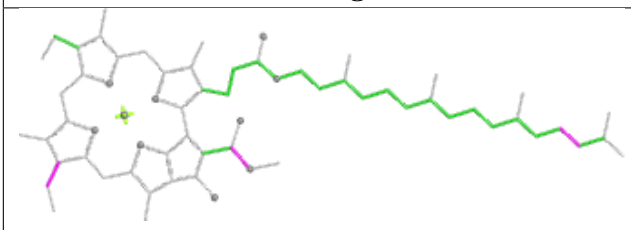
### Ligand CLA d 401



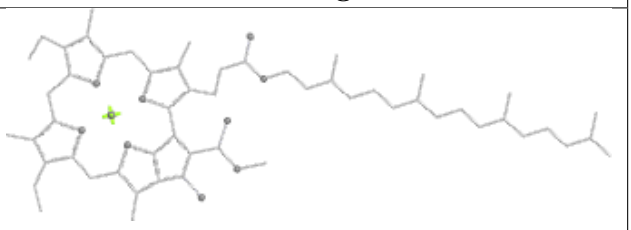
Bond lengths



Bond angles

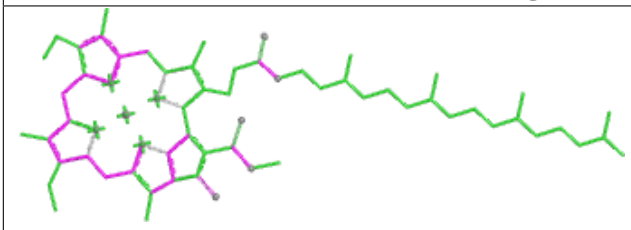


Torsions

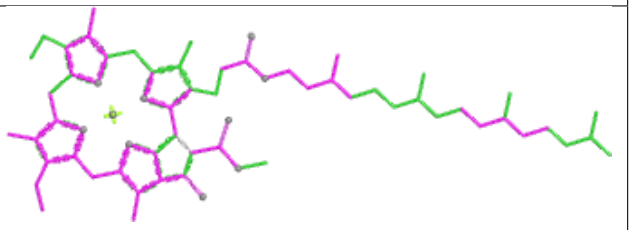


Rings

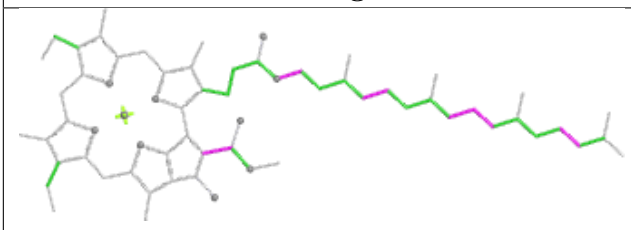
## Ligand CLA C 510



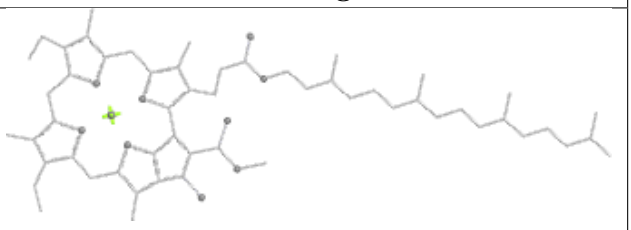
Bond lengths



Bond angles

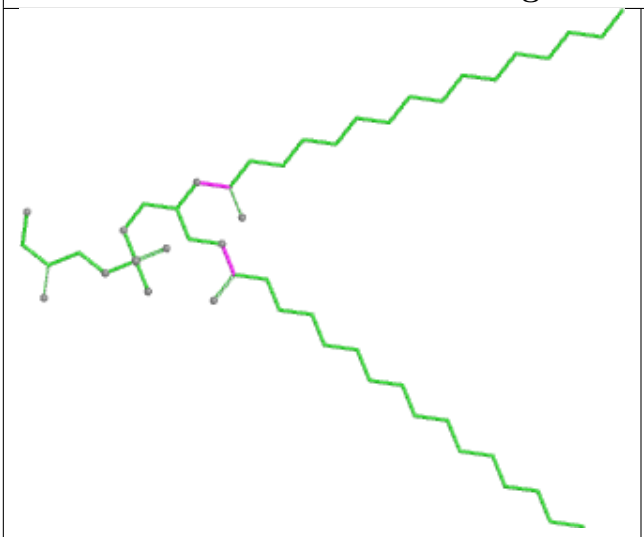


Torsions

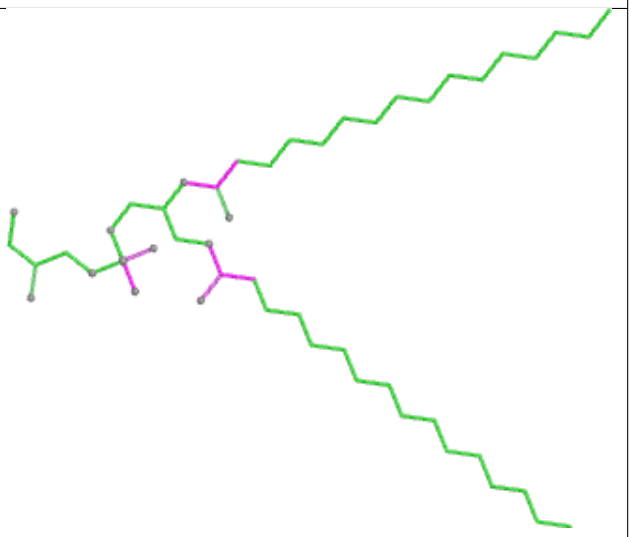


Rings

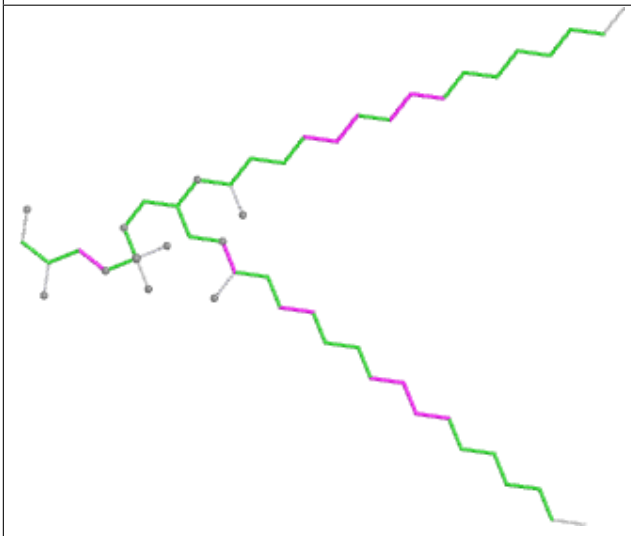
## Ligand LHG D 408



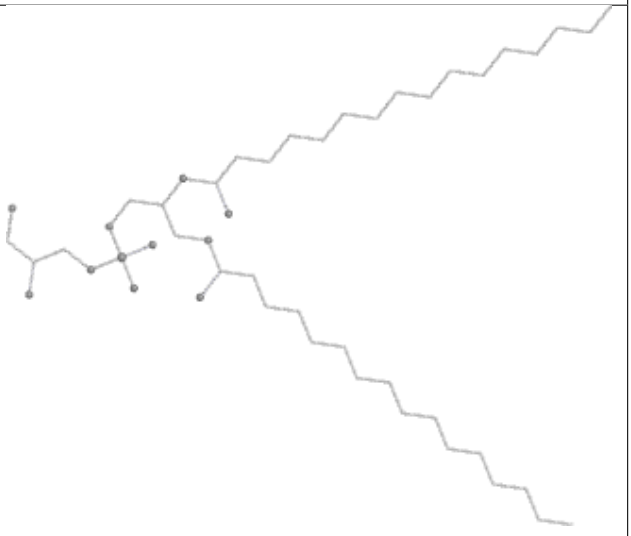
Bond lengths



Bond angles

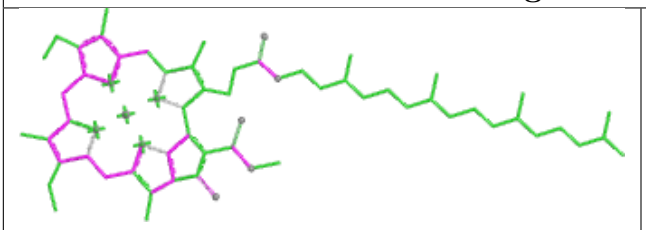


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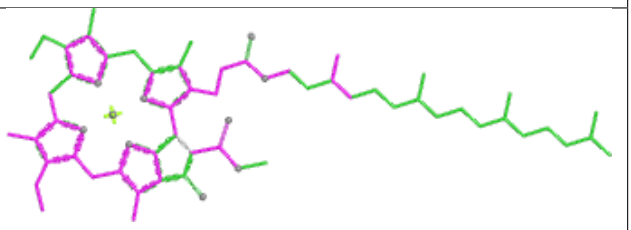


Rings

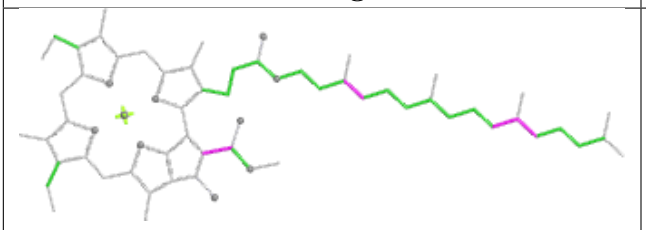
## Ligand CLA C 505



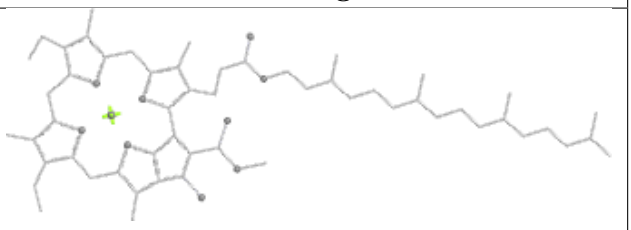
Bond lengths



Bond angles

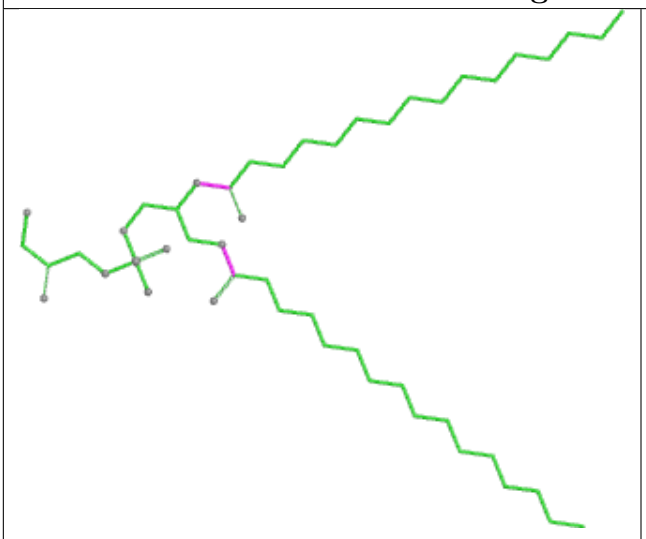


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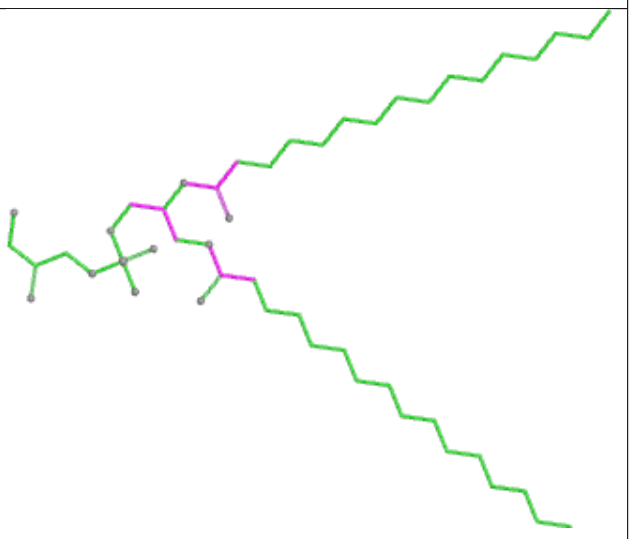


Rings

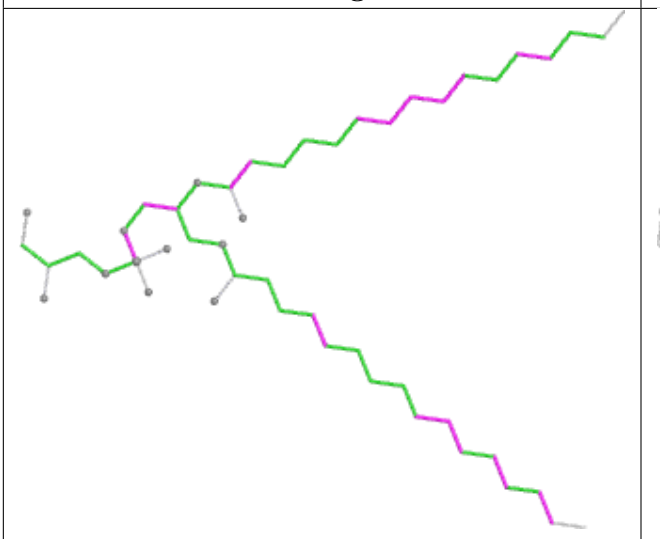
## Ligand LHG l 101



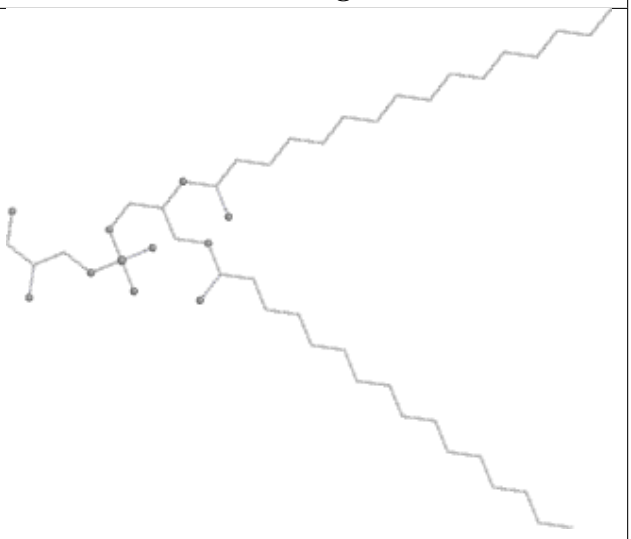
Bond lengths



Bond angles

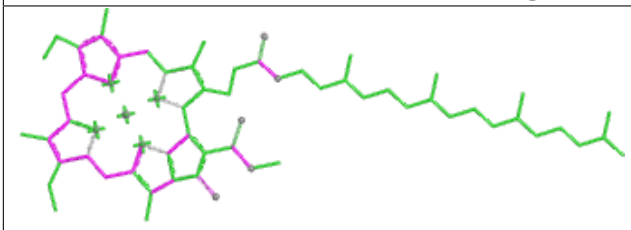


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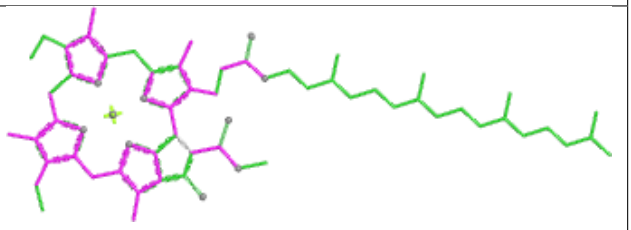


Rings

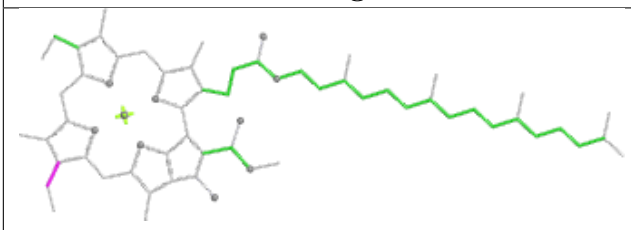
### Ligand CLA A 405



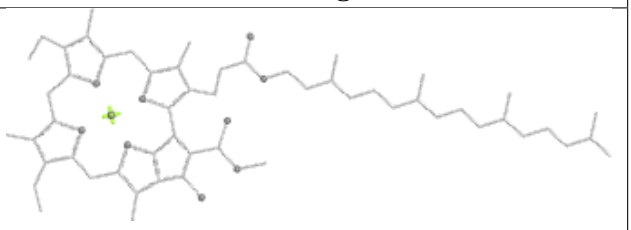
Bond lengths



Bond angles

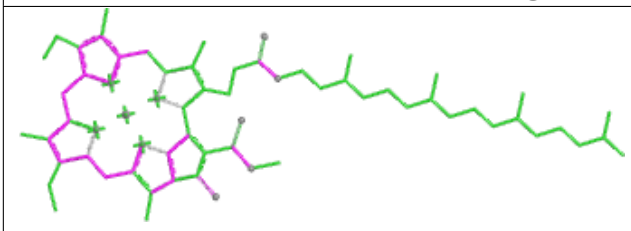


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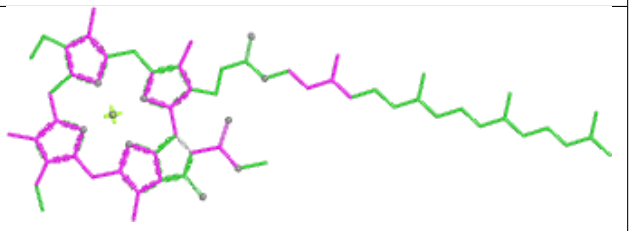


Rings

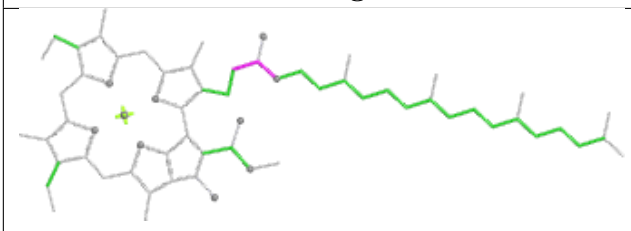
### Ligand CLA B 613



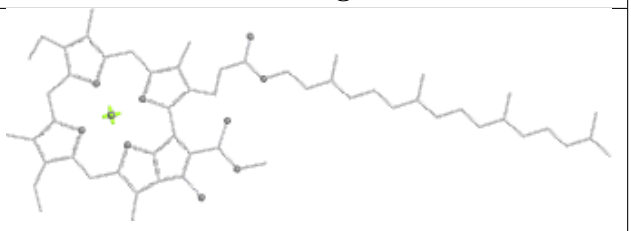
Bond lengths



Bond angles

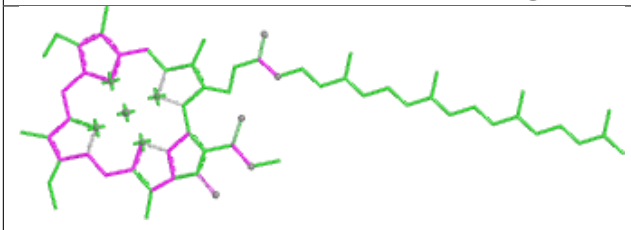


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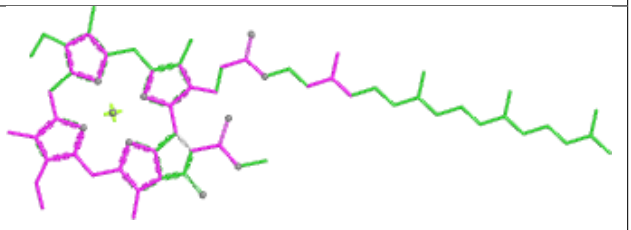


Rings

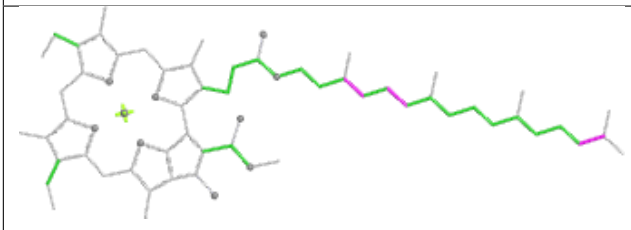
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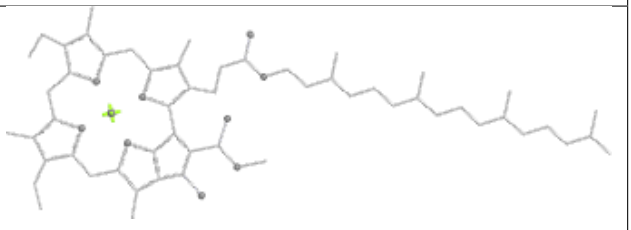
Bond lengths



Bond angles

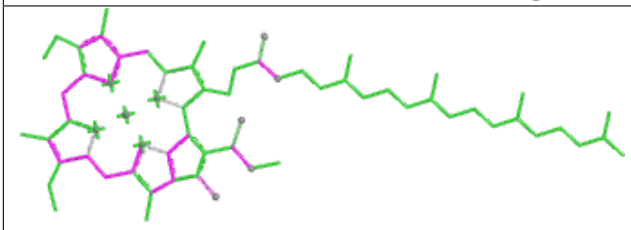


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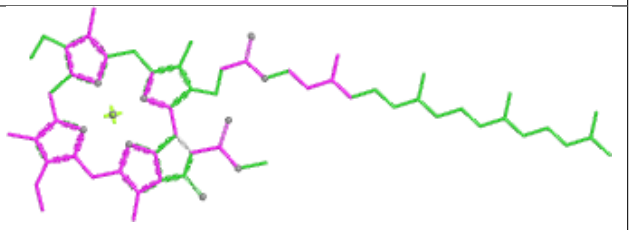


Rings

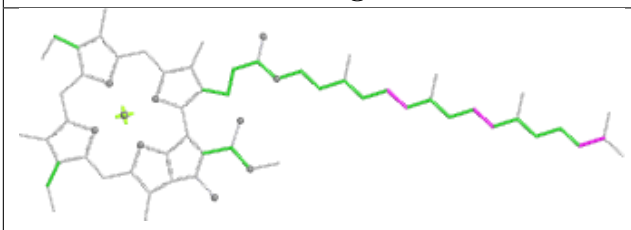
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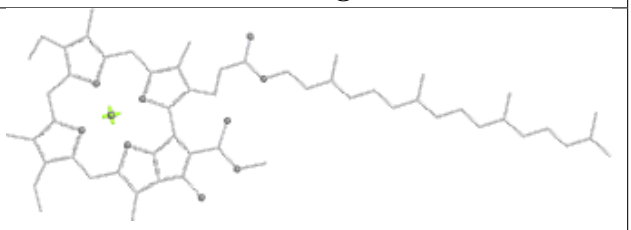
Bond lengths



Bond angles

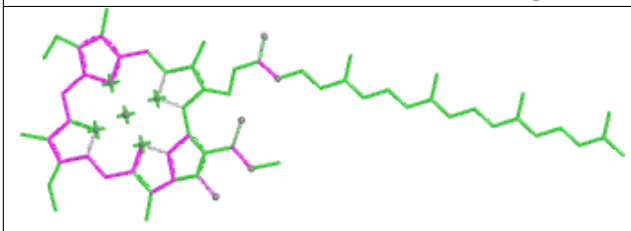


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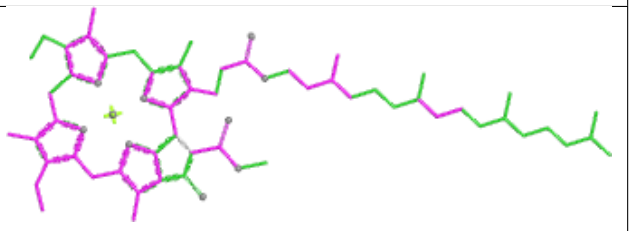


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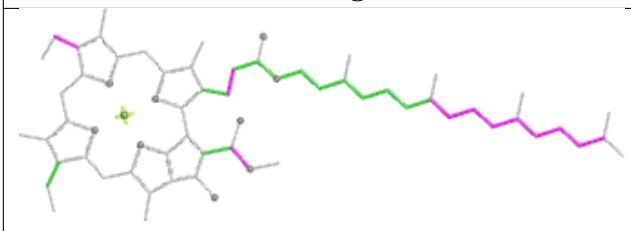
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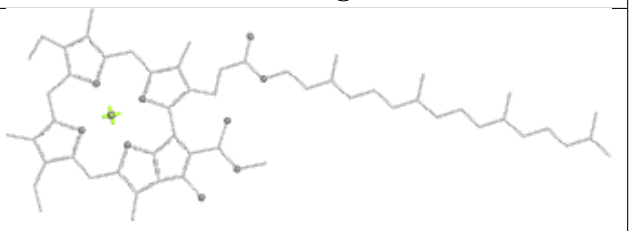
Bond lengths



Bond angles

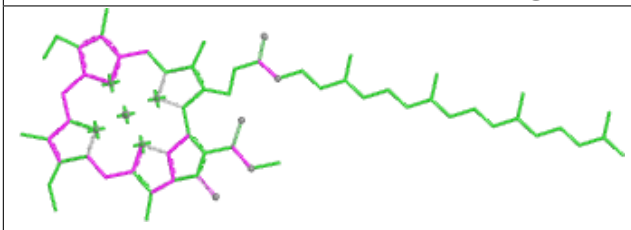


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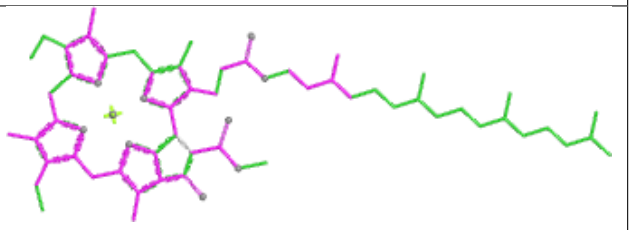


Rings

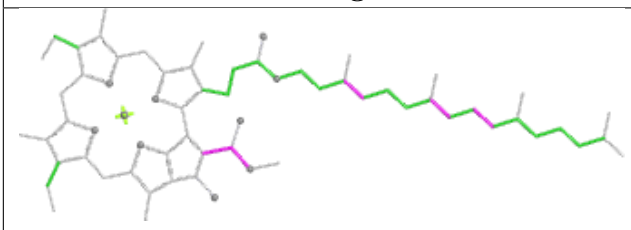
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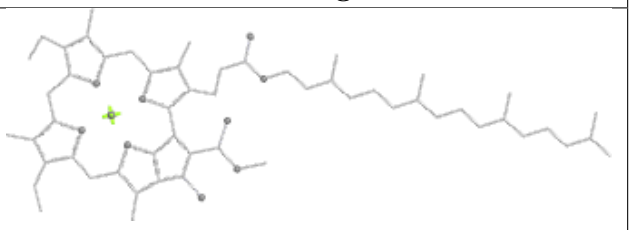
Bond lengths



Bond angles

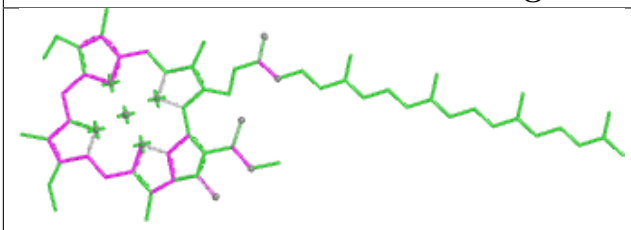


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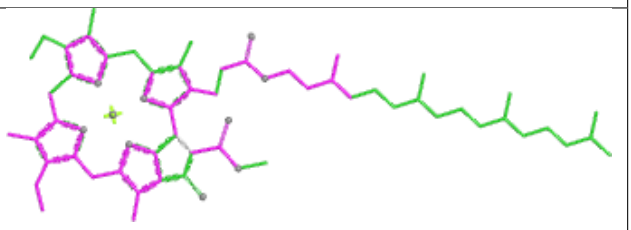


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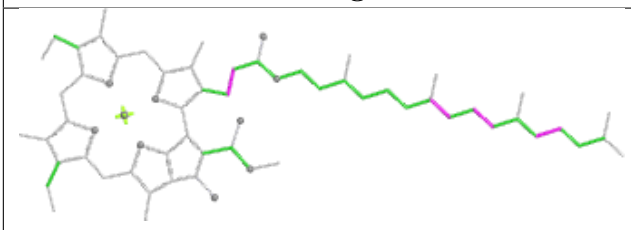
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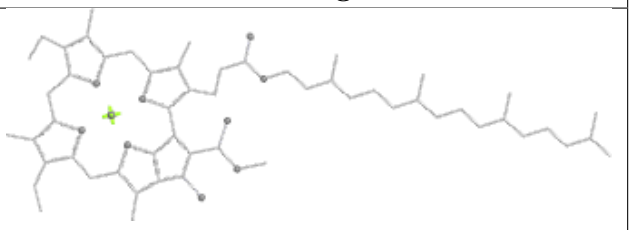
Bond lengths



Bond angles

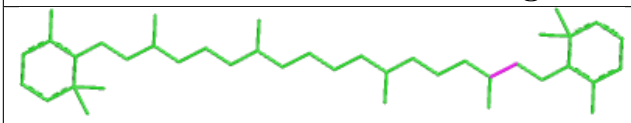


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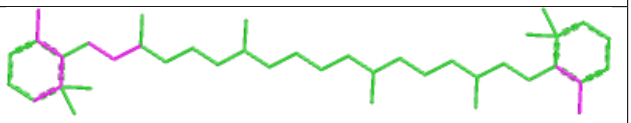


Rings

### Ligand BCR C 515



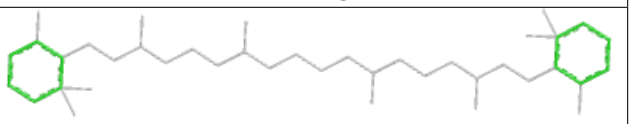
Bond lengths



Bond angles

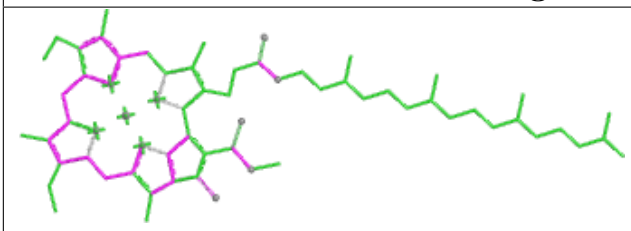


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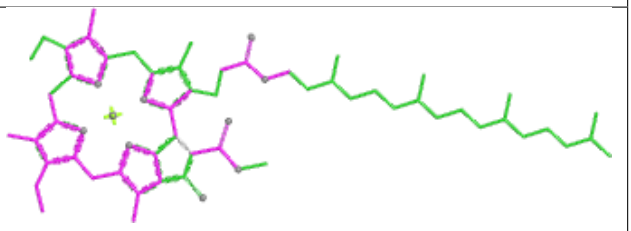


Rings

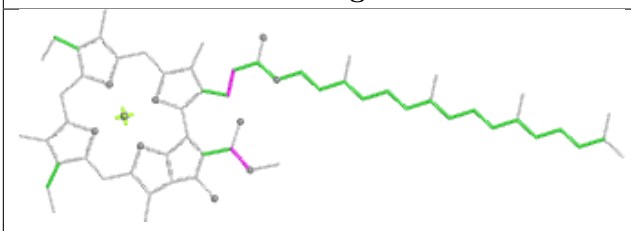
### Ligand CLA c 902



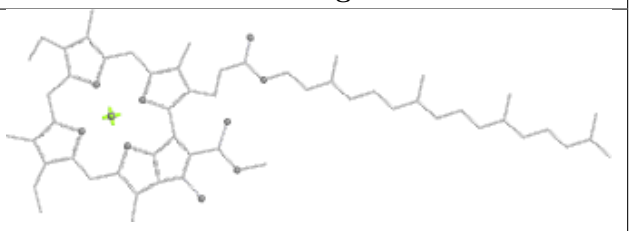
Bond lengths



Bond angles

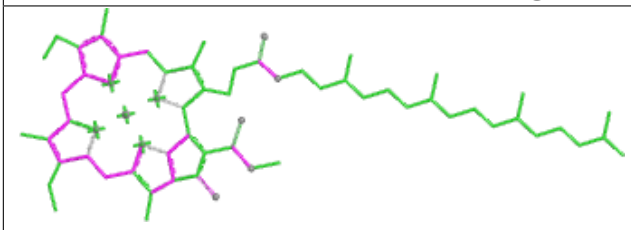


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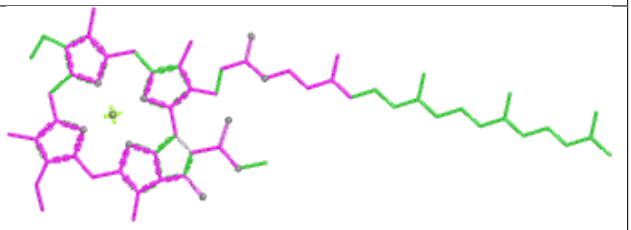


Rings

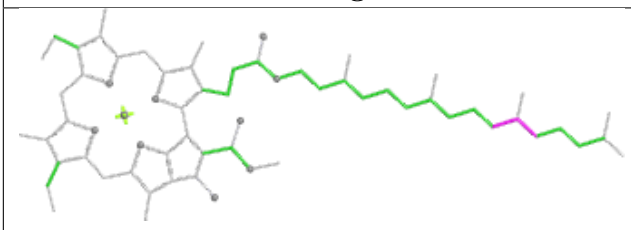
### Ligand CLA a 407



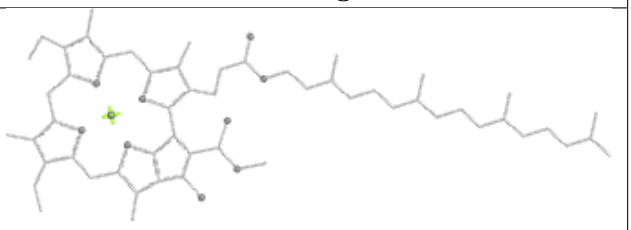
Bond lengths



Bond angles

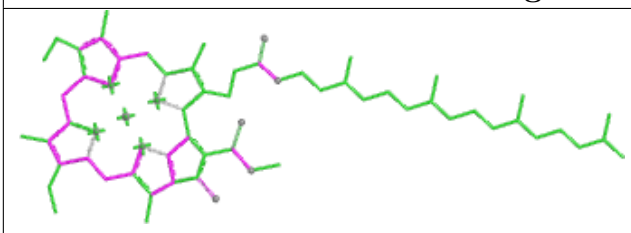


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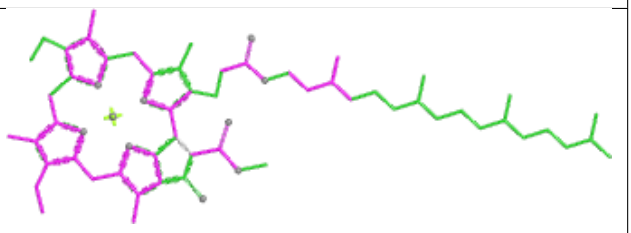


Rings

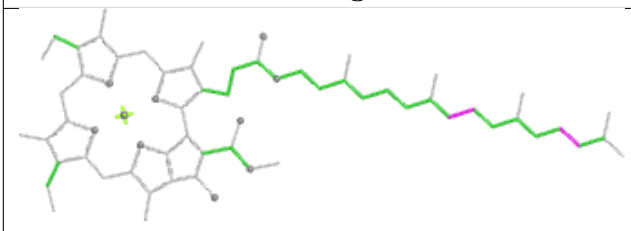
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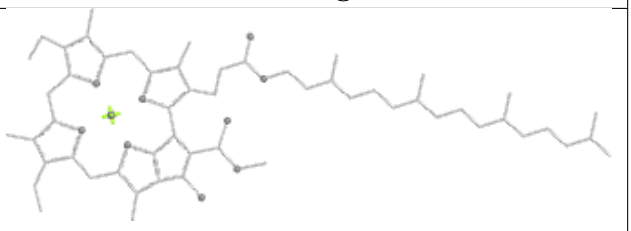
Bond lengths



Bond angles

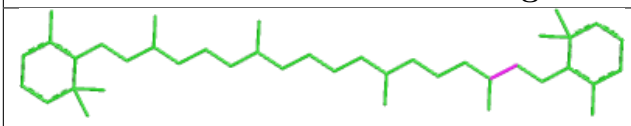


Torsions

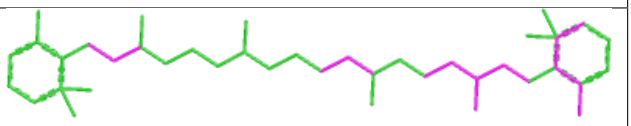


Rings

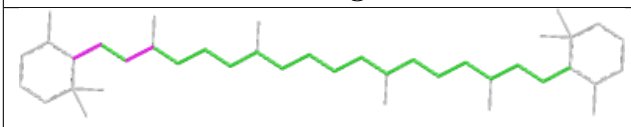
### Ligand BCR H 101



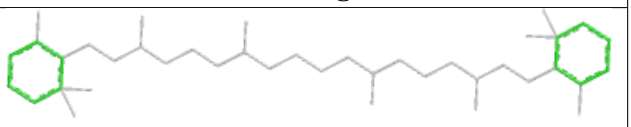
Bond lengths



Bond angles

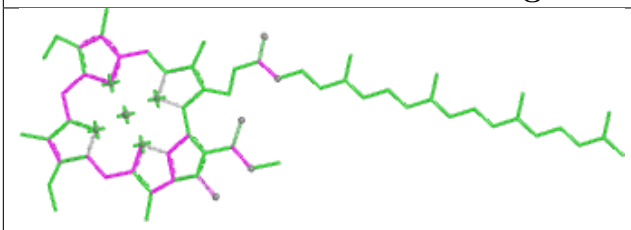


Torsions

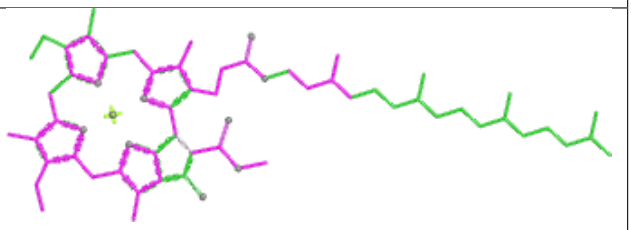


Rings

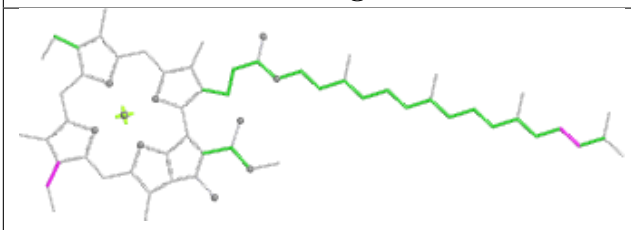
## Ligand CLA A 406



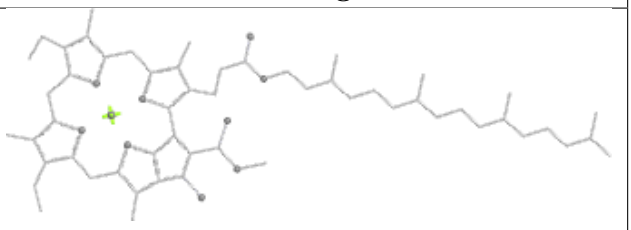
Bond lengths



Bond angles

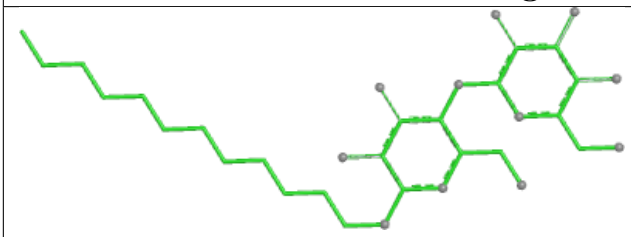


Torsions

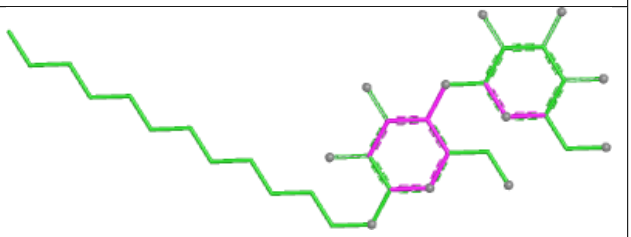


Rings

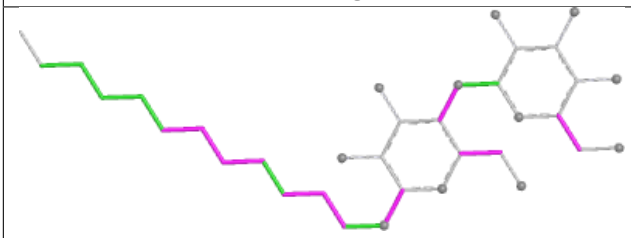
## Ligand LMT C 522



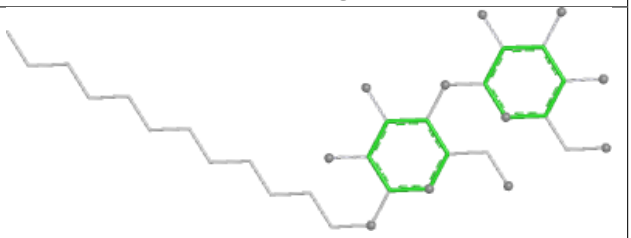
Bond lengths



Bond angles



Torsions

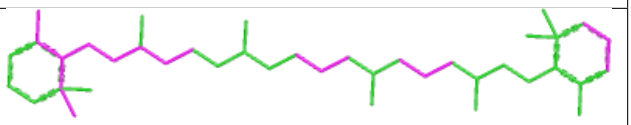


Rings

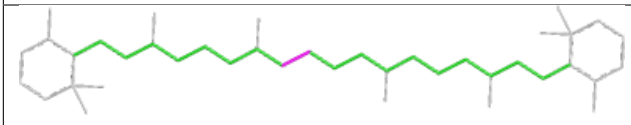
## Ligand BCR t 101



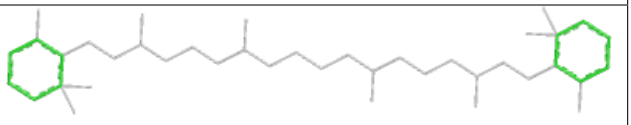
Bond lengths



Bond angles

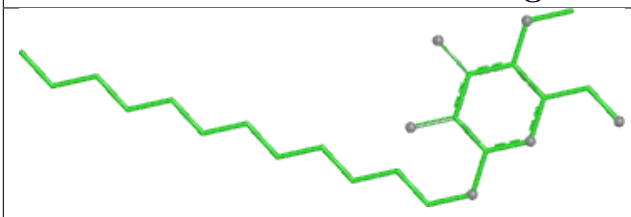


Torsions

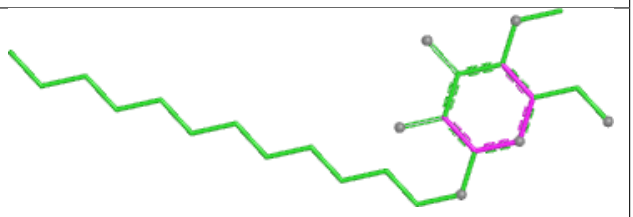


Rings

**Ligand LMT b 601**



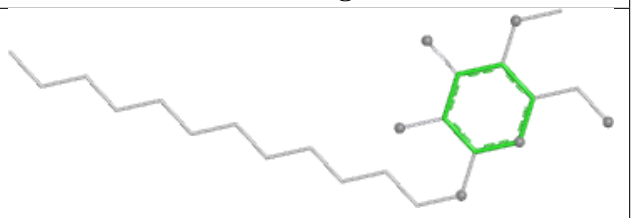
Bond lengths



Bond angles

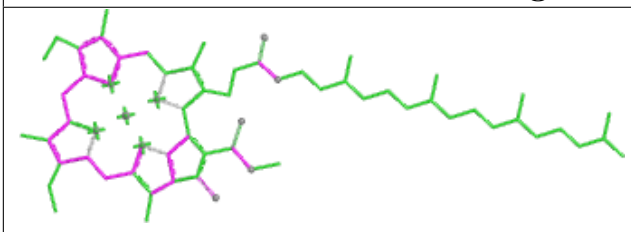


Torsions

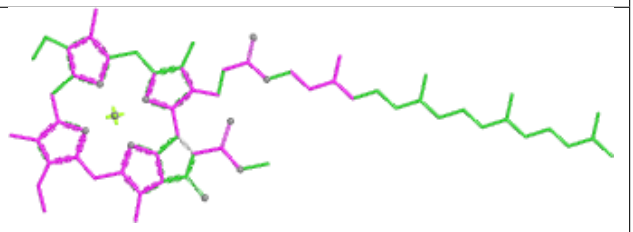


Rings

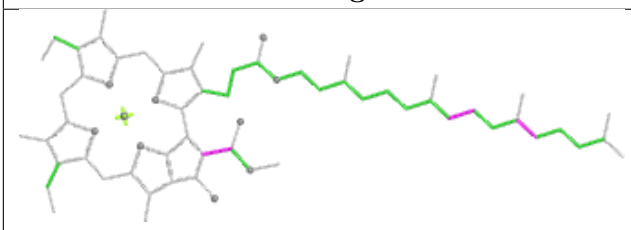
**Ligand CLA c 905**



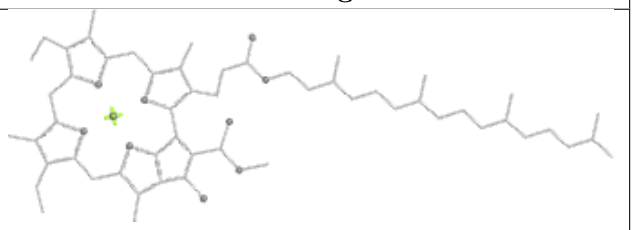
Bond lengths



Bond angles

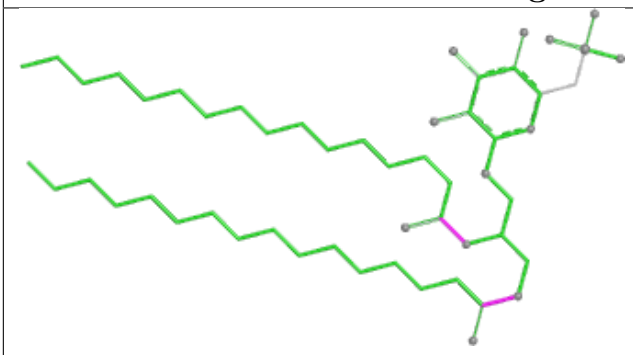


Torsions

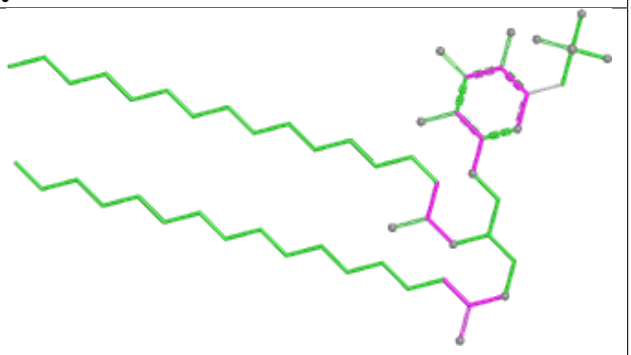


Rings

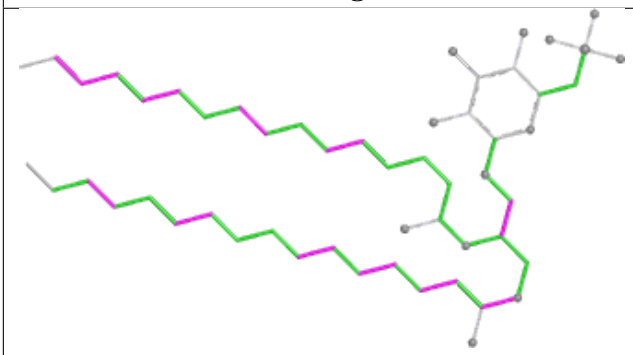
## Ligand SQD a 402



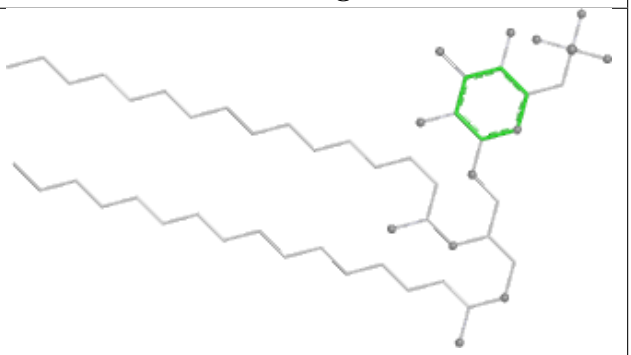
Bond lengths



Bond angles



Torsions

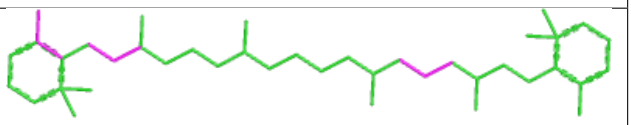


Rings

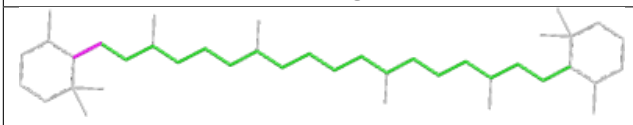
## Ligand BCR b 621



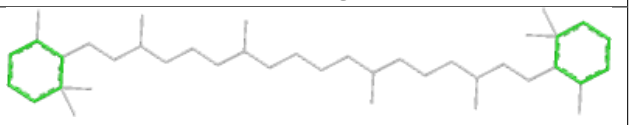
Bond lengths



Bond angles

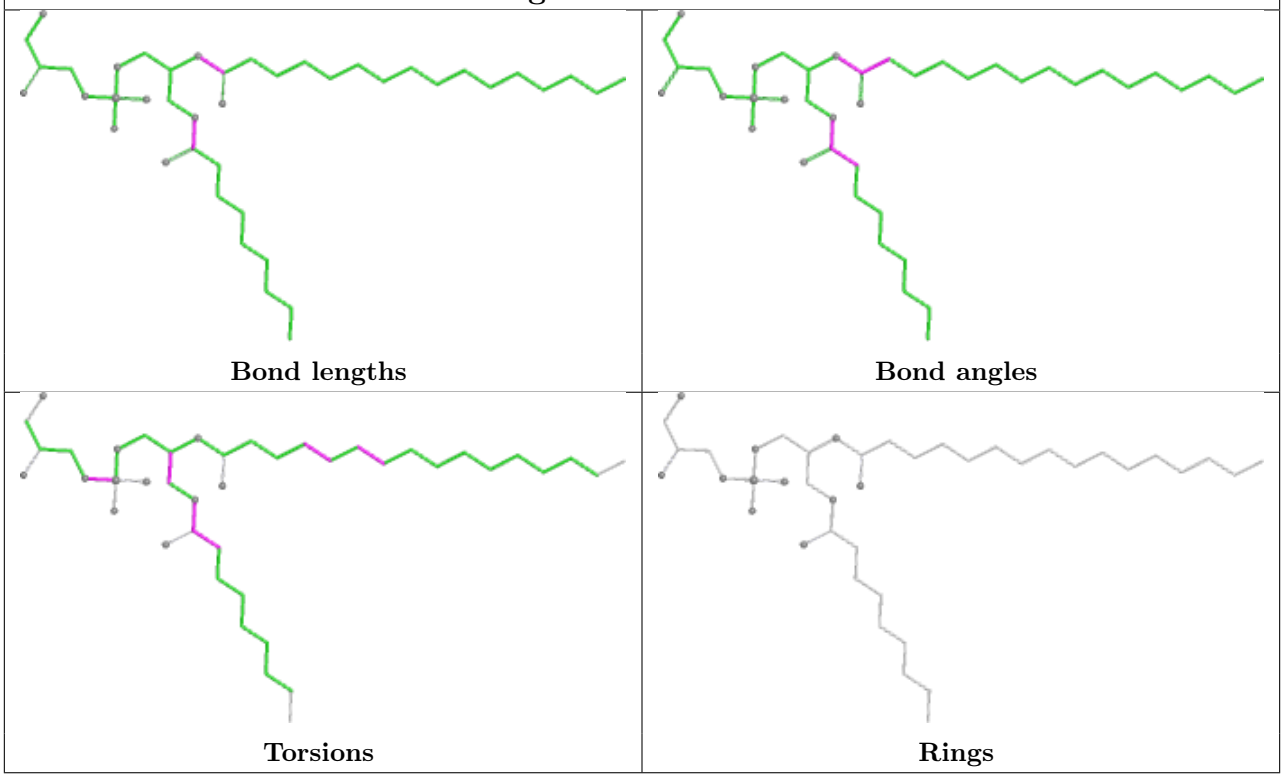


Torsions

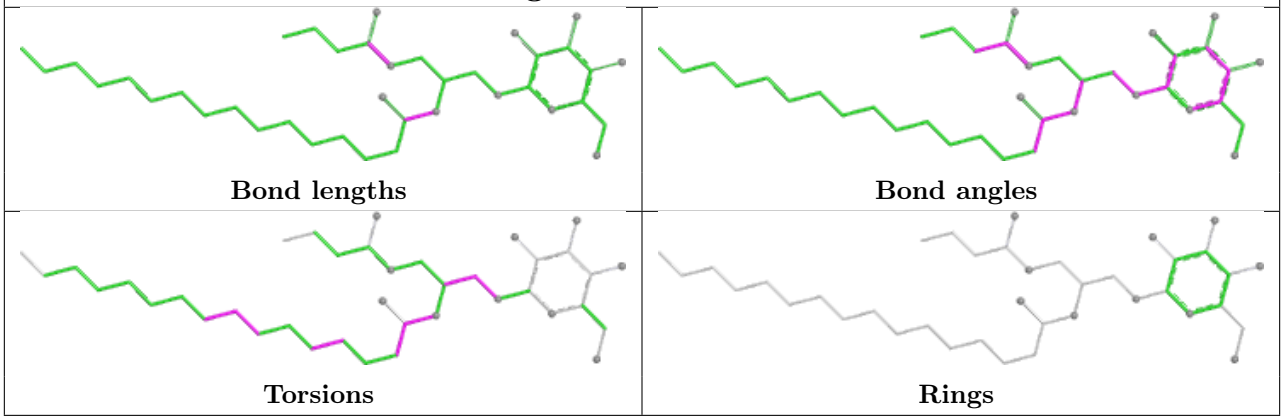


Rings

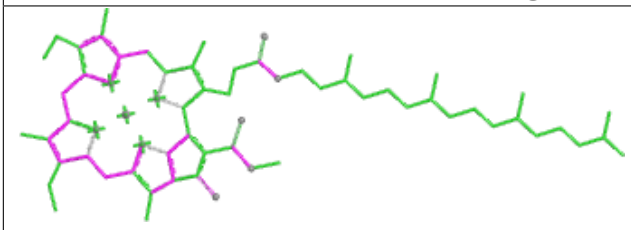
### Ligand LHG e 101



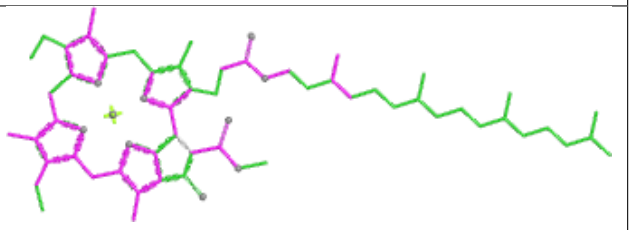

### Ligand LMG z 101



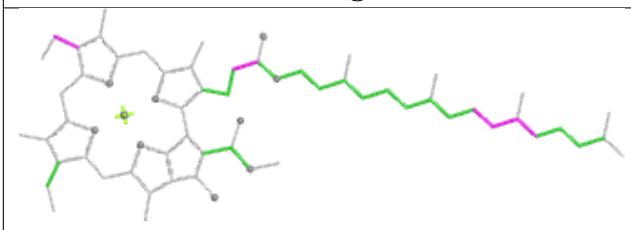
## Ligand CLA C 506



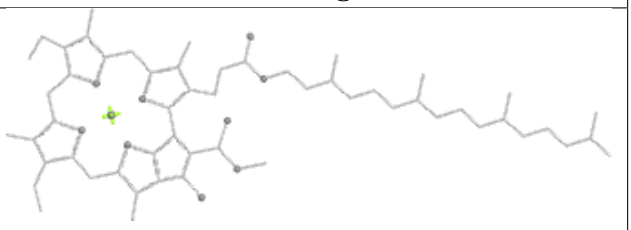
Bond lengths



Bond angles

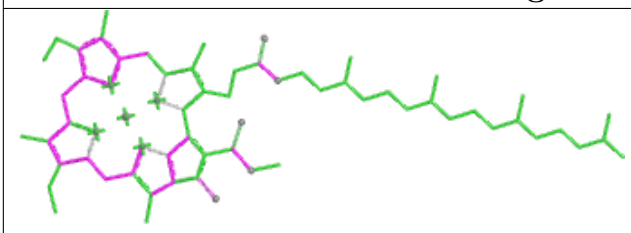


Torsions

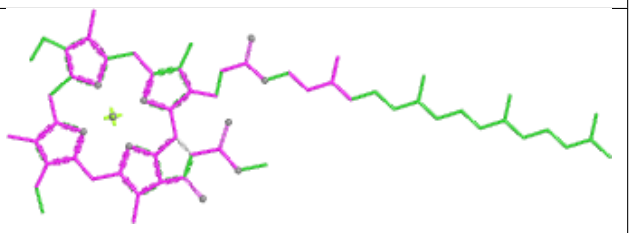


Rings

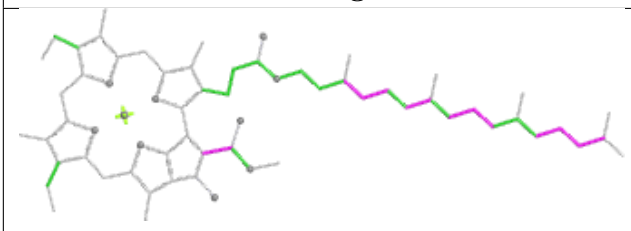
## Ligand CLA b 618



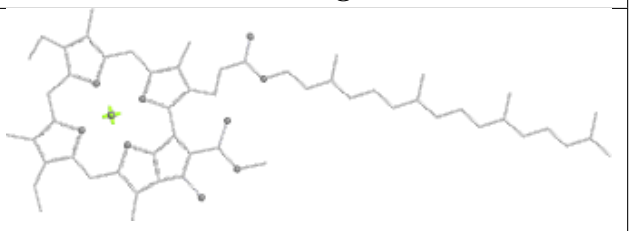
Bond lengths



Bond angles

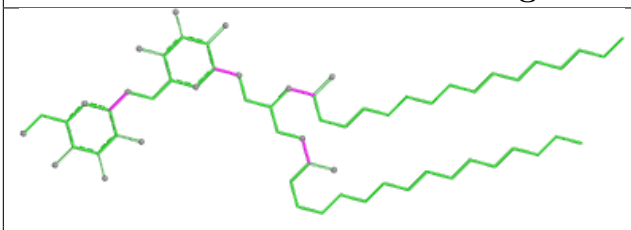


Torsions

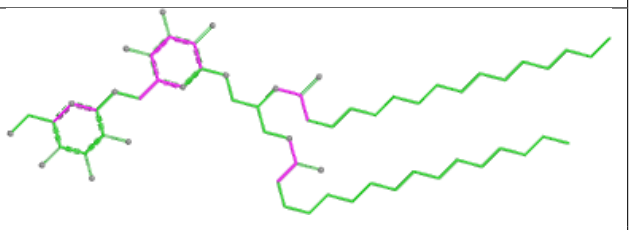


Rings

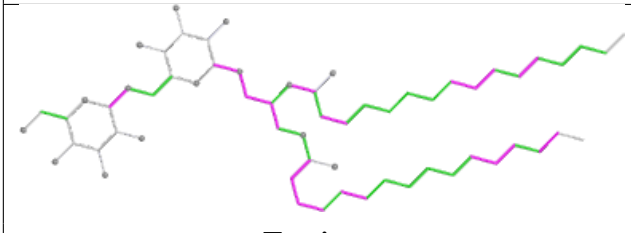
## Ligand DGD D 405



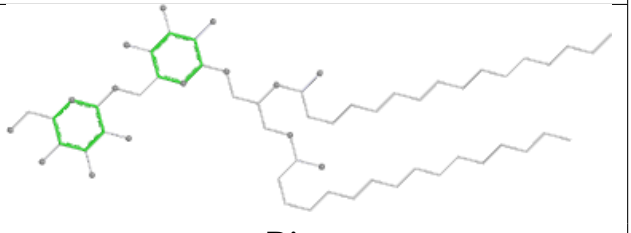
Bond lengths



Bond angles

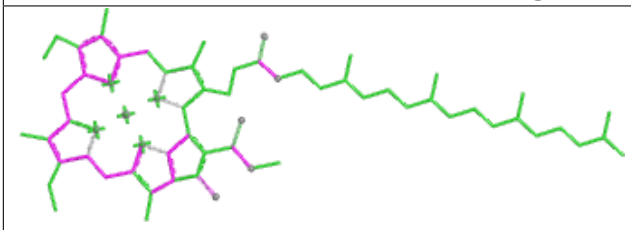


Torsions

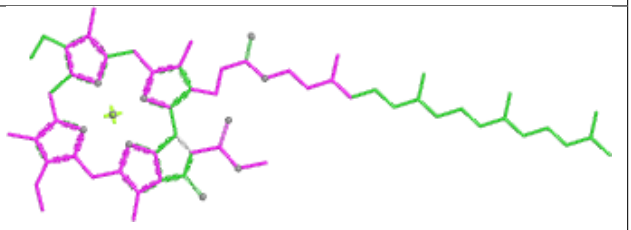


Rings

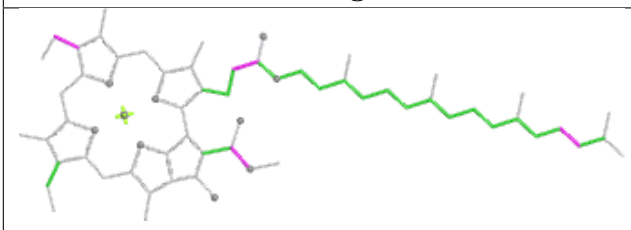
### Ligand CLA c 913



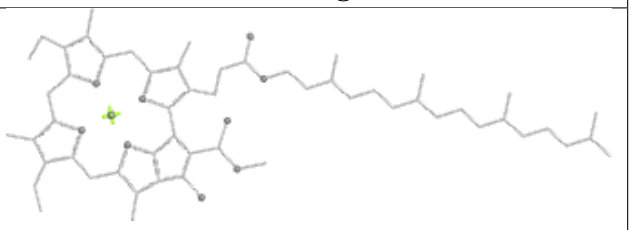
Bond lengths



Bond angles

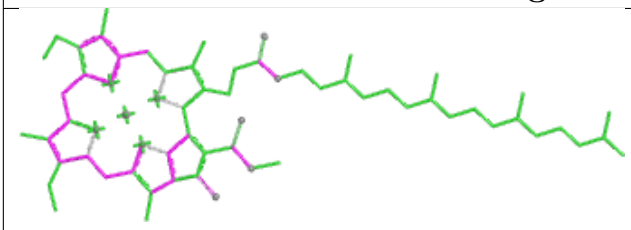


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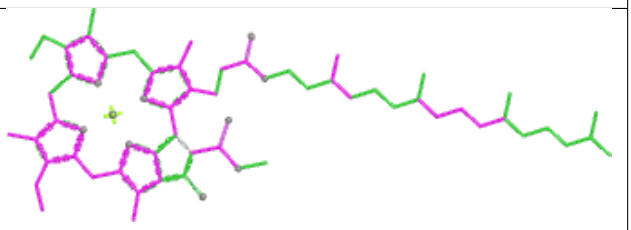


Rings

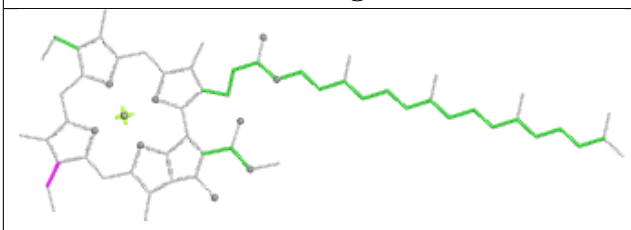
### Ligand CLA a 406



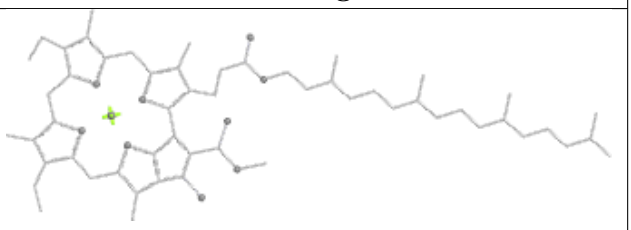
Bond lengths



Bond angles

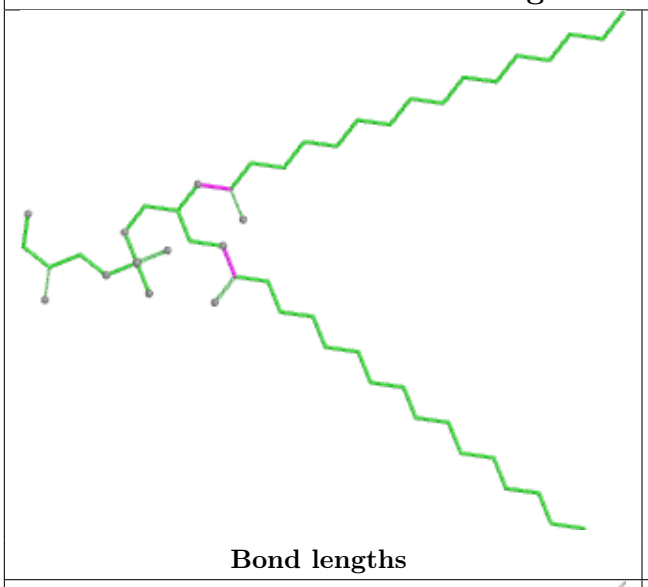


Torsions

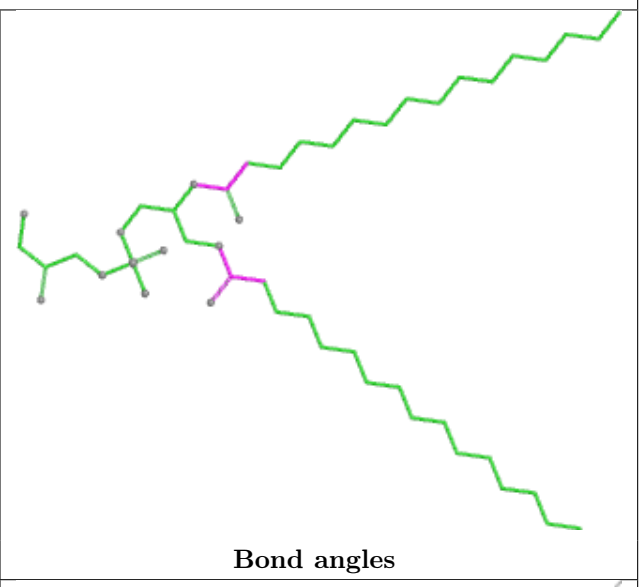


Rings

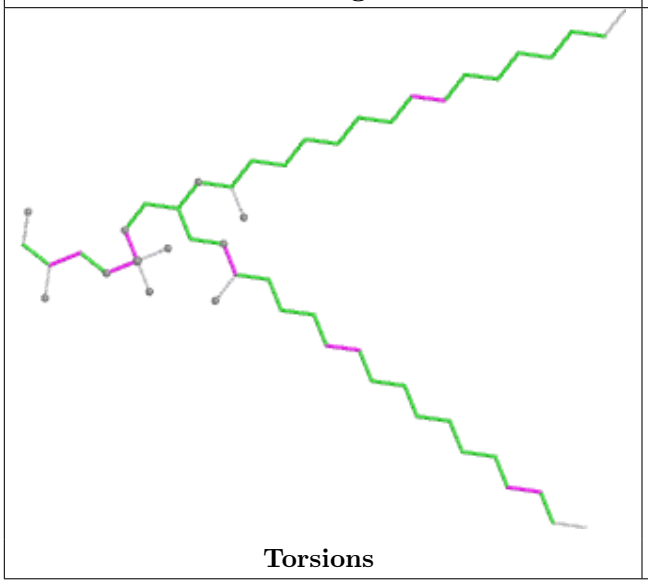
**Ligand LHG d 408**



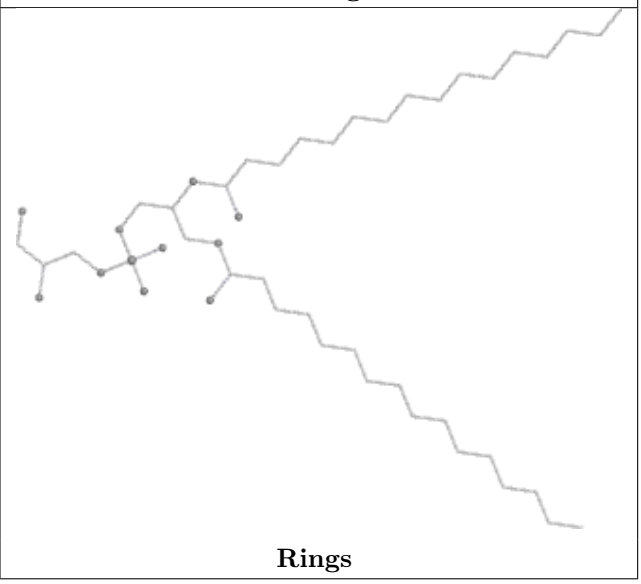
Bond lengths



Bond angles

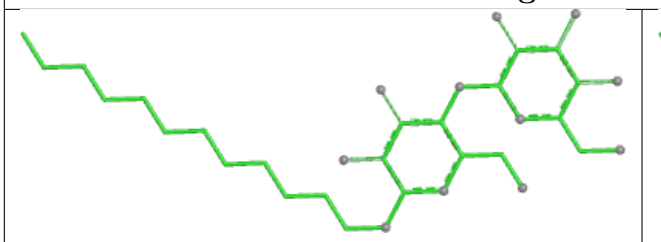


Torsions

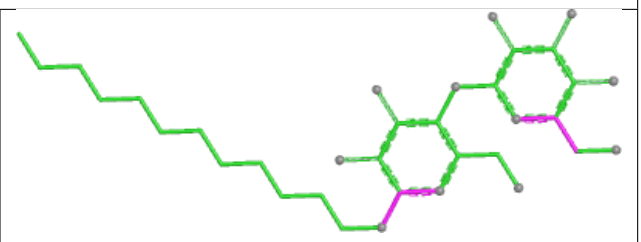


Rings

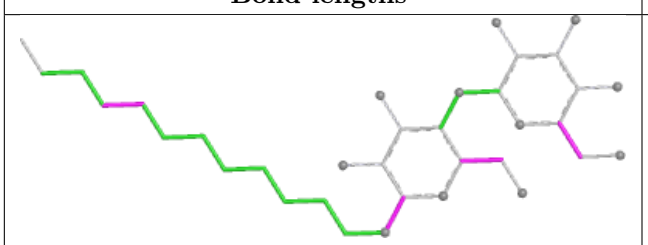
**Ligand LMT M 101**



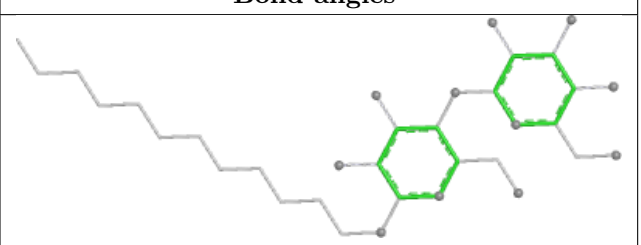
Bond lengths



Bond angles

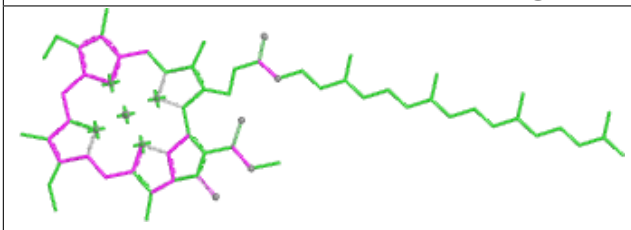


Torsions

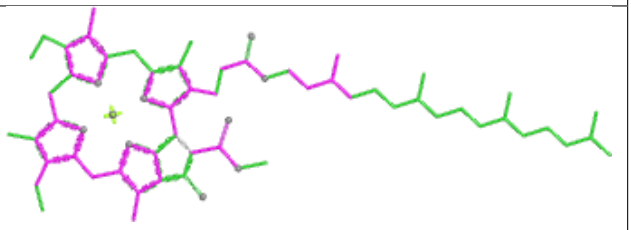


Rings

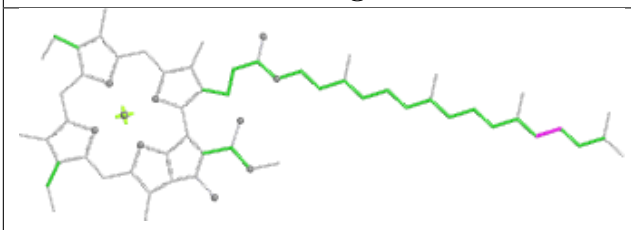
### Ligand CLA c 909



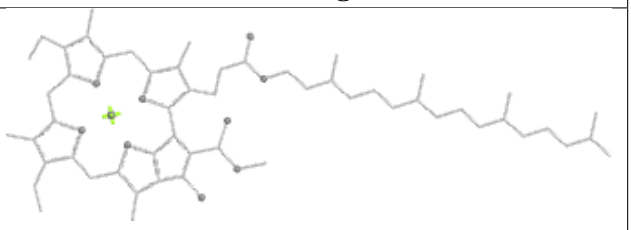
Bond lengths



Bond angles

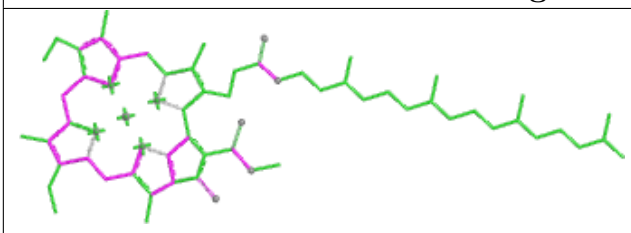


Torsions

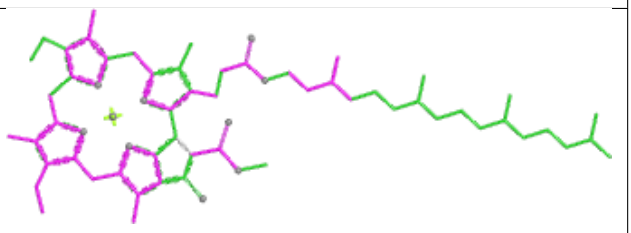


Rings

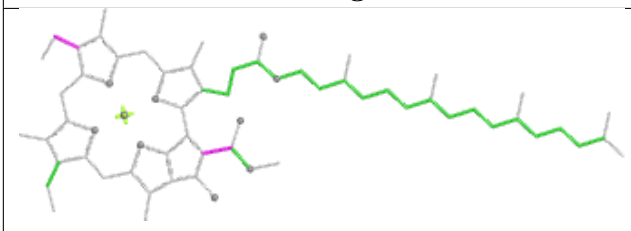
### Ligand CLA c 908



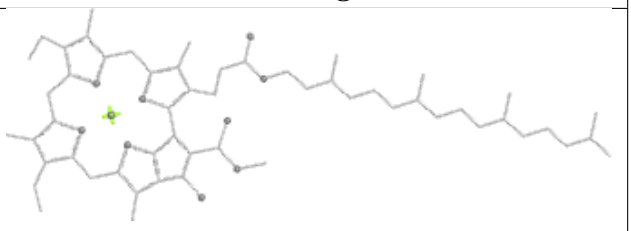
Bond lengths



Bond angles

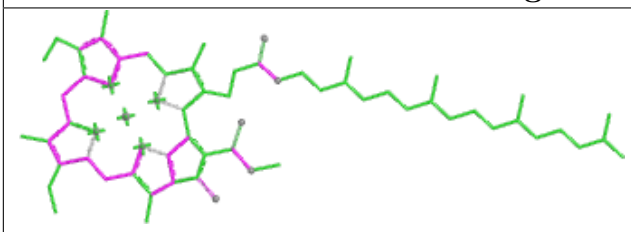


Torsions

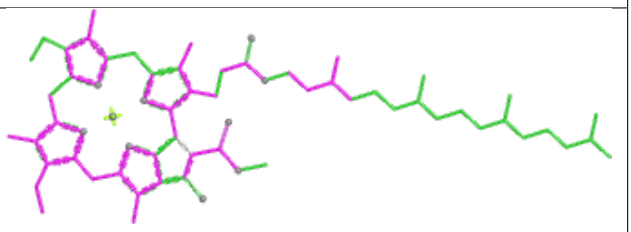


Rings

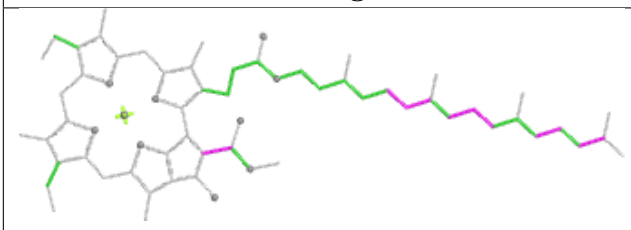
### Ligand CLA C 507



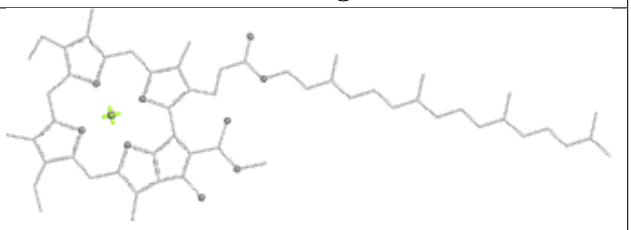
Bond lengths



Bond angles

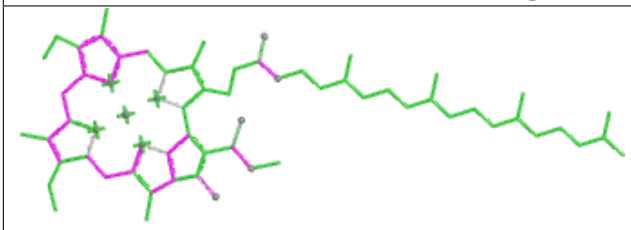


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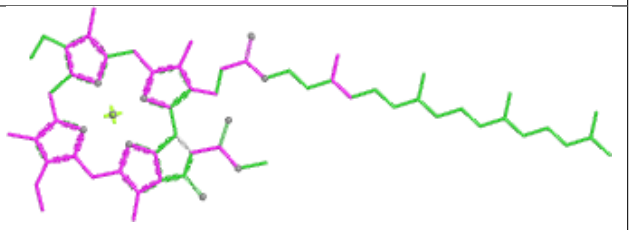


Rings

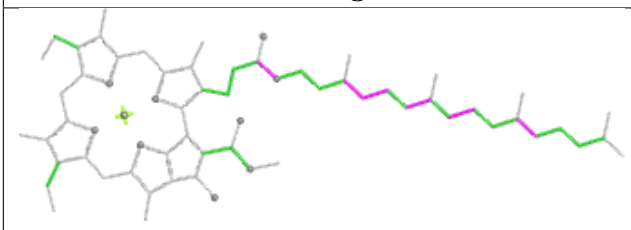
### Ligand CLA A 410



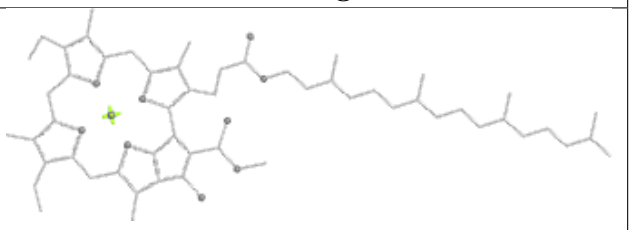
Bond lengths



Bond angles



Torsions

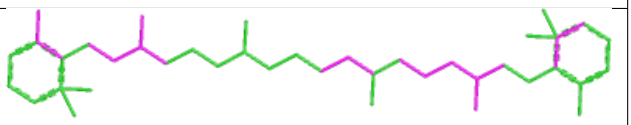


Rings

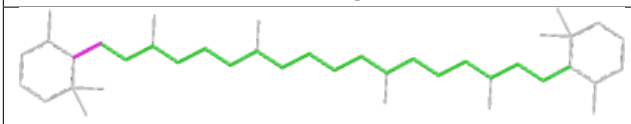
### Ligand BCR B 618



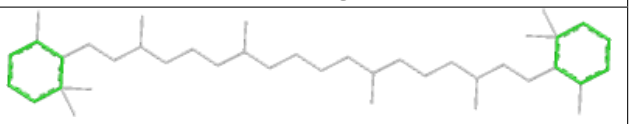
Bond lengths



Bond angles

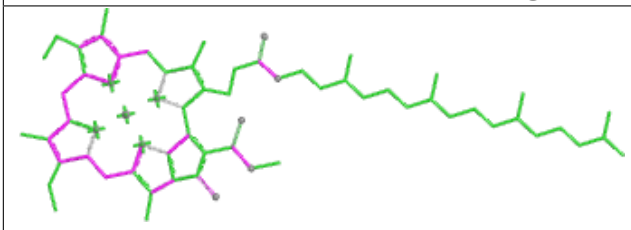


Torsions

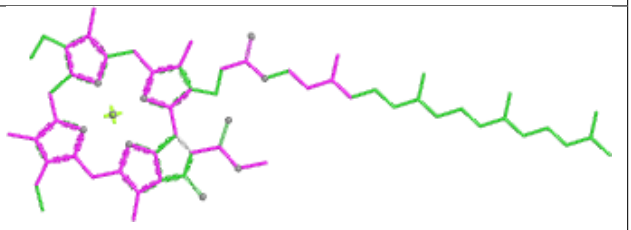


Rings

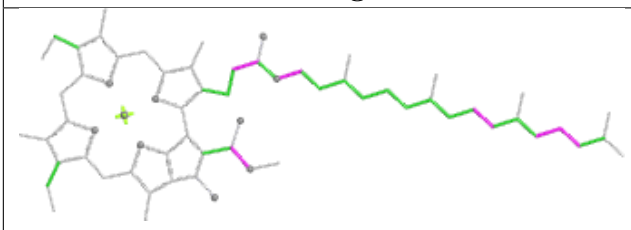
### Ligand CLA B 614



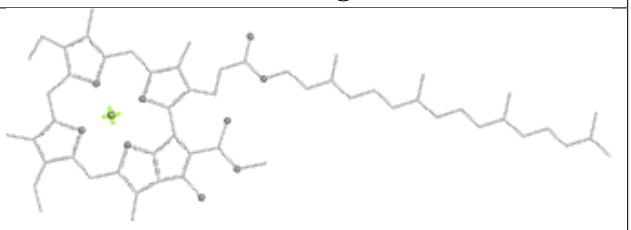
Bond lengths



Bond angles

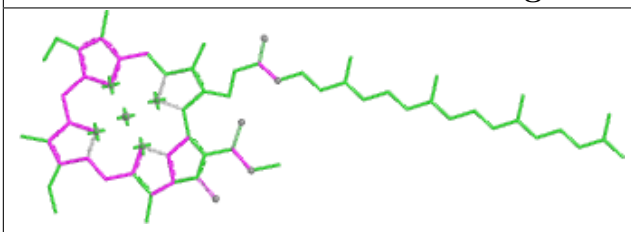


Torsions

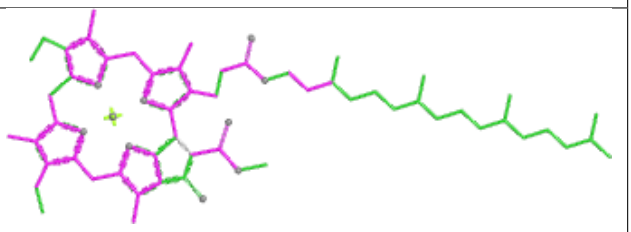


Rings

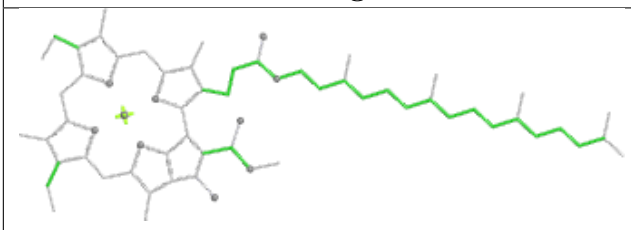
## Ligand CLA B 609



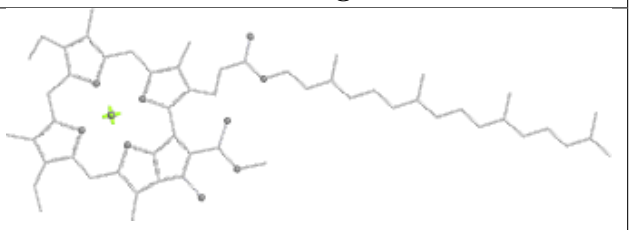
Bond lengths



Bond angles

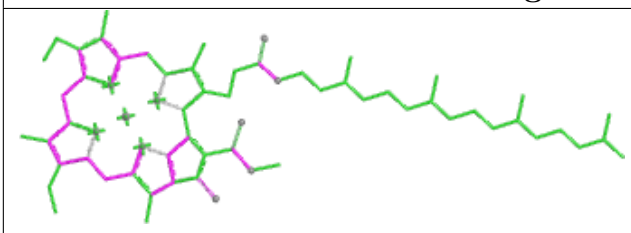


Torsions

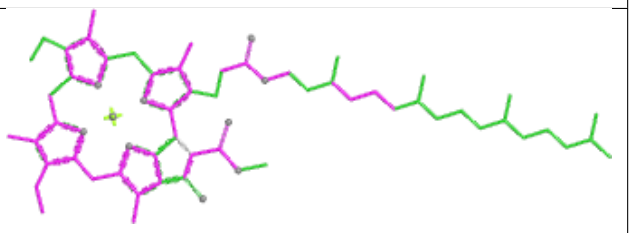


Rings

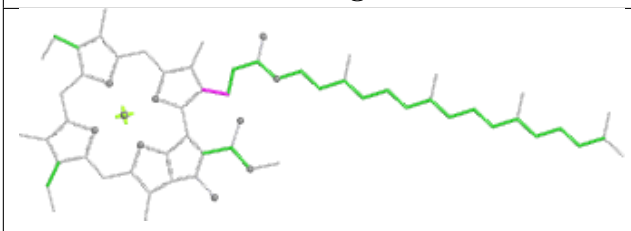
## Ligand CLA B 610



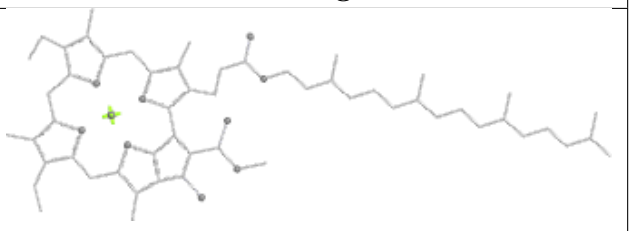
Bond lengths



Bond angles

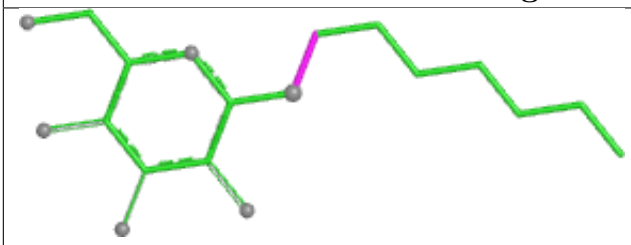


Torsions

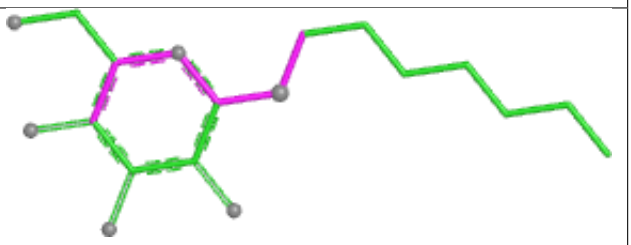


Rings

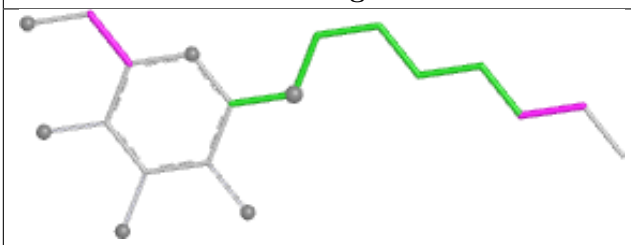
## Ligand HTG B 634



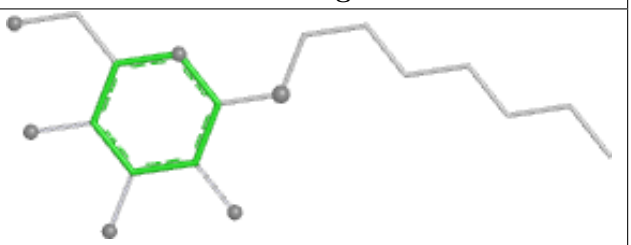
Bond lengths



Bond angles

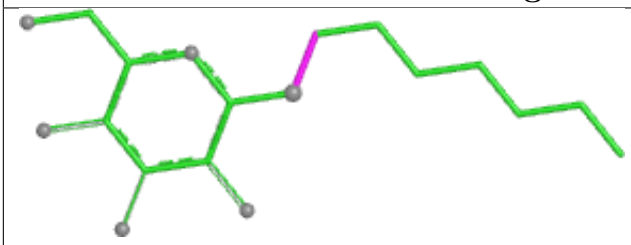


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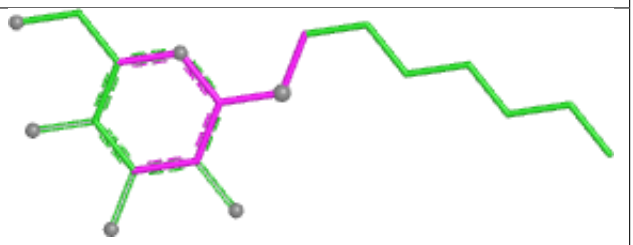


Rings

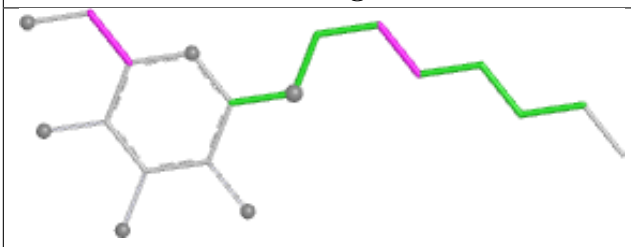
**Ligand HTG b 627**



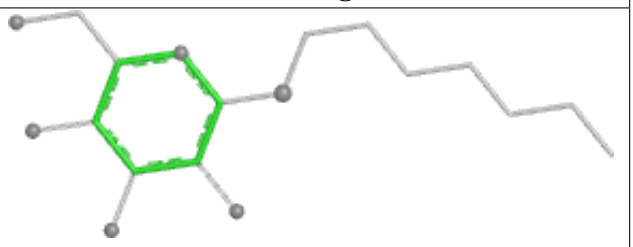
Bond lengths



Bond angles

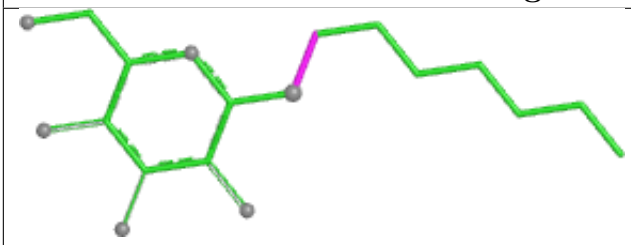


Torsions

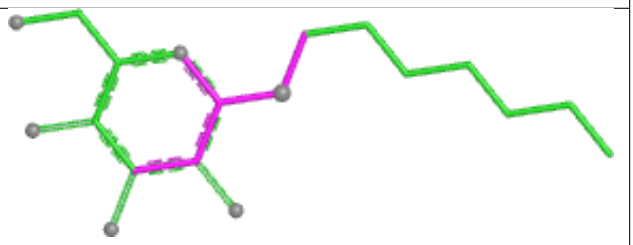


Rings

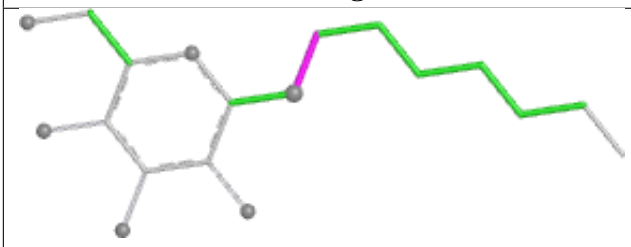
**Ligand HTG b 626**



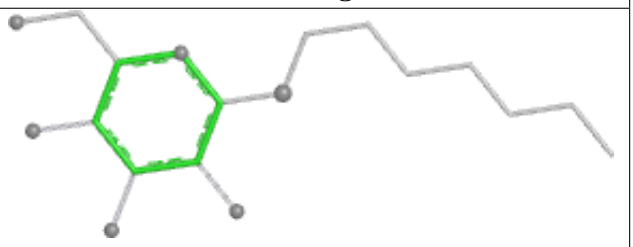
Bond lengths



Bond angles

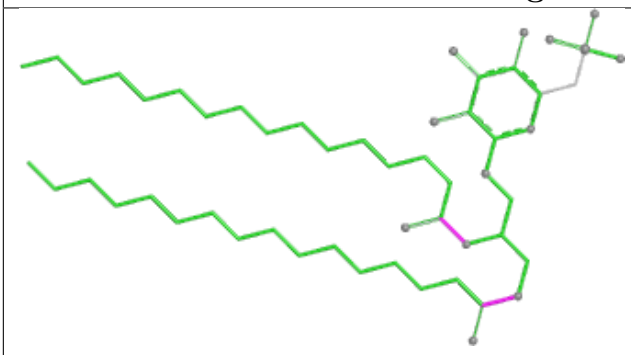


Torsions

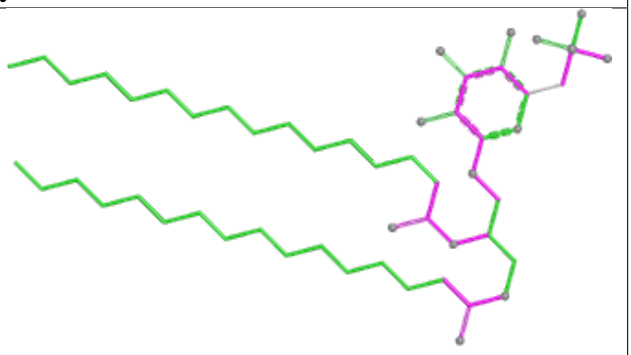


Rings

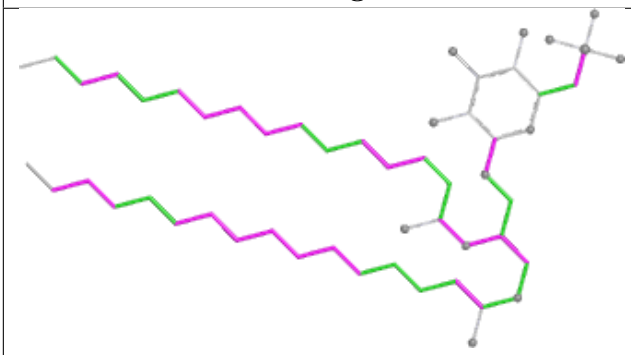
### Ligand SQD L 102



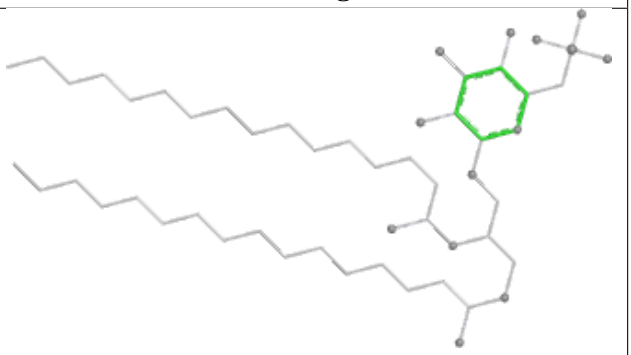
Bond lengths



Bond angles

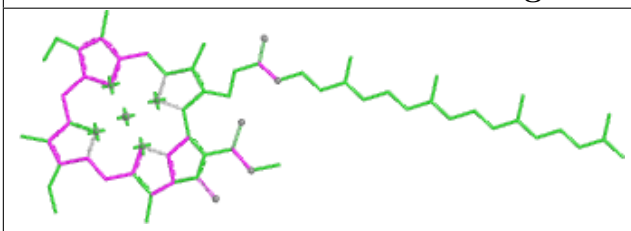


Torsions

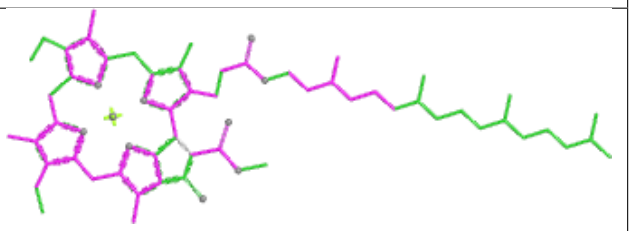


Rings

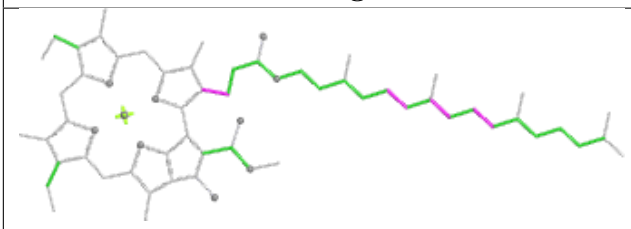
### Ligand CLA C 509



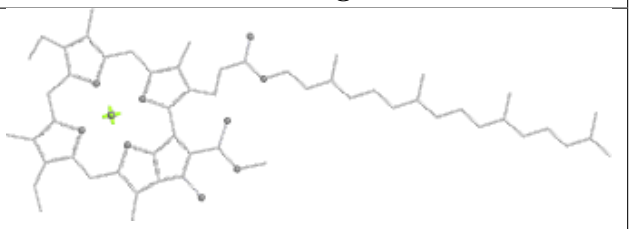
Bond lengths



Bond angles

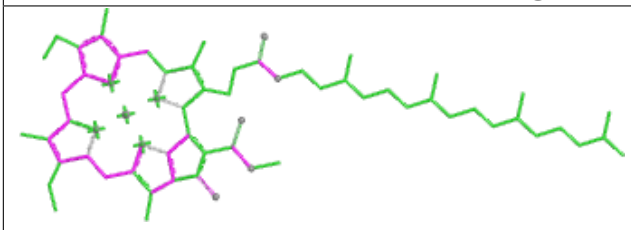


Torsions

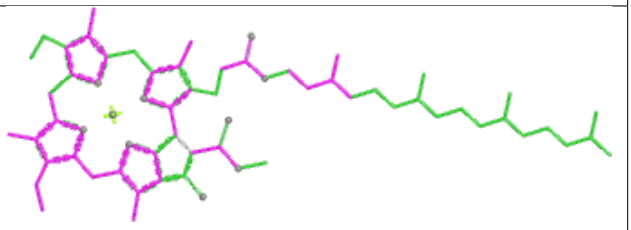


Rings

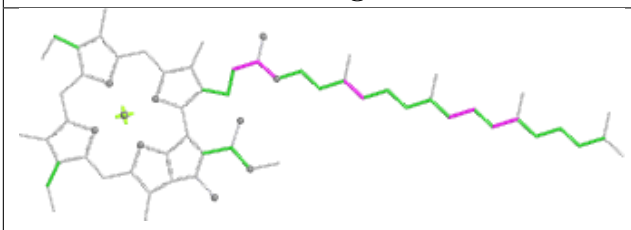
### Ligand CLA c 911



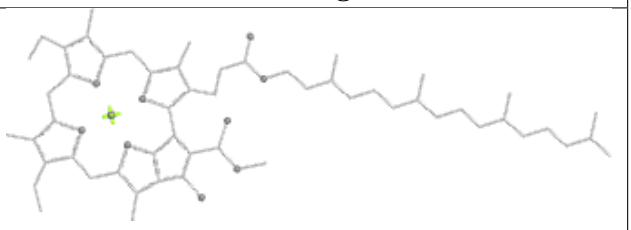
Bond lengths



Bond angles

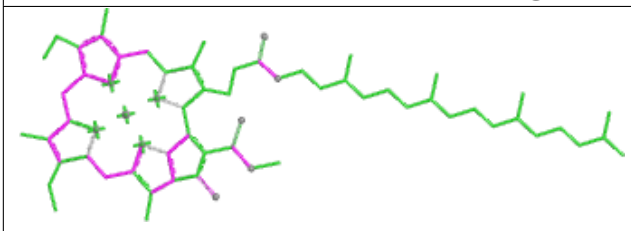


Torsions

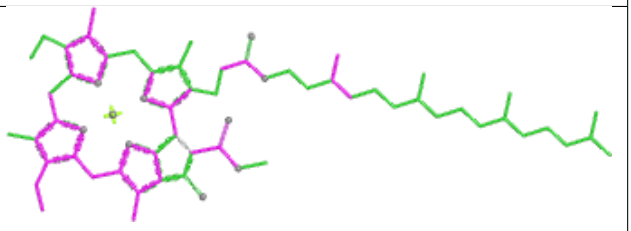


Rings

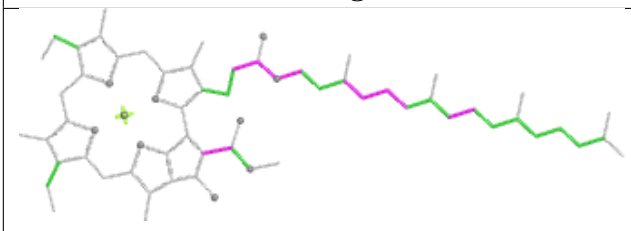
### Ligand CLA b 605



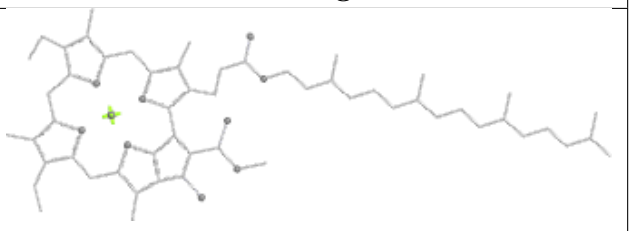
Bond lengths



Bond angles

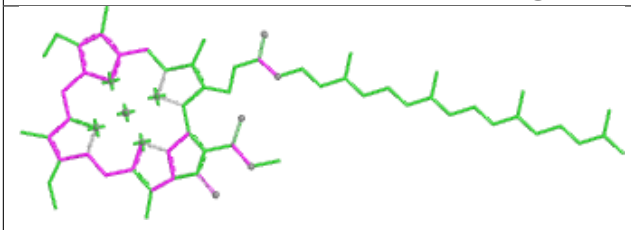


Torsions

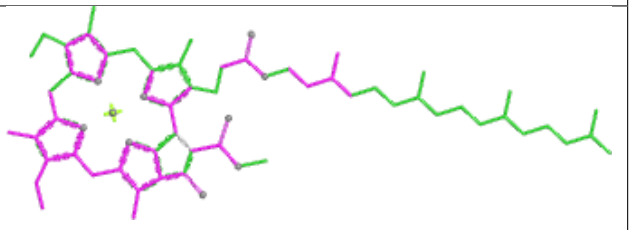


Rings

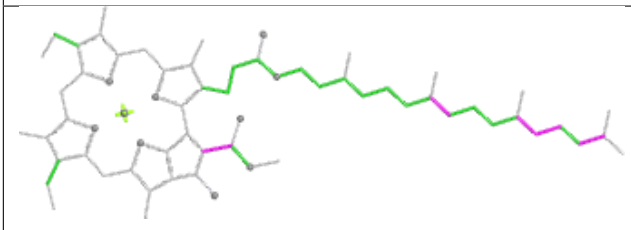
### Ligand CLA c 910



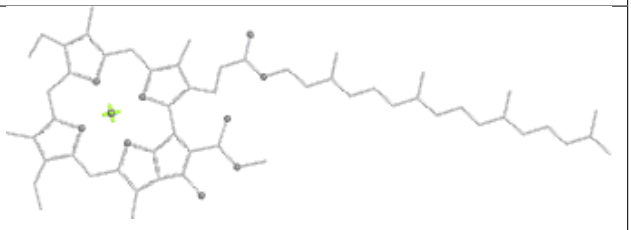
Bond lengths



Bond angles

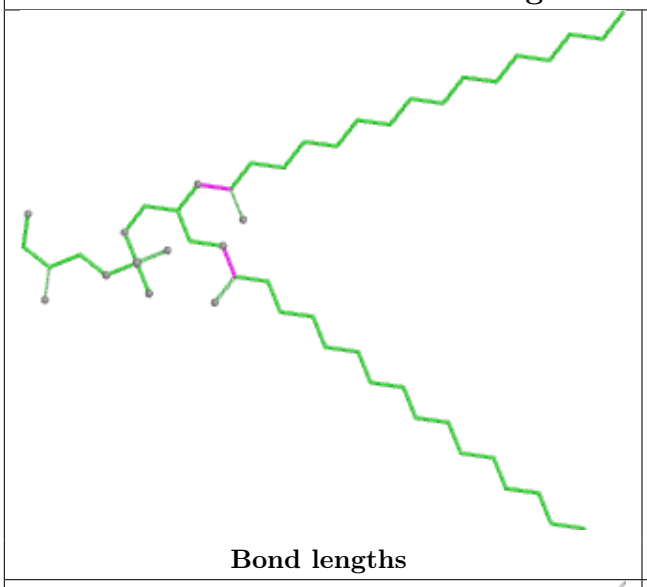


Torsions

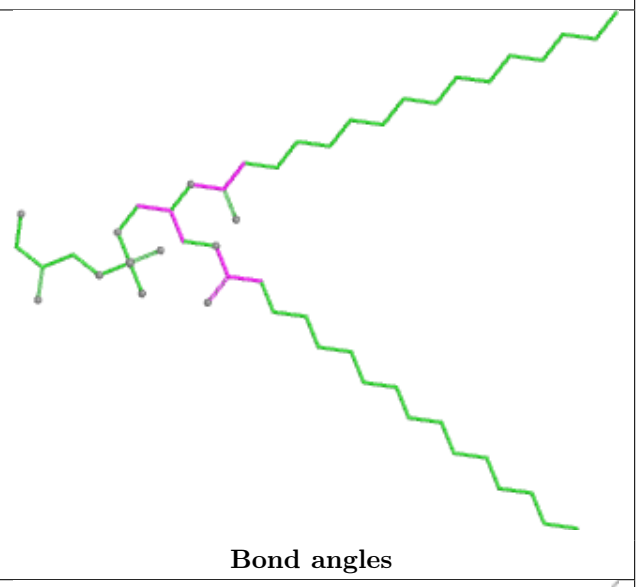


Rings

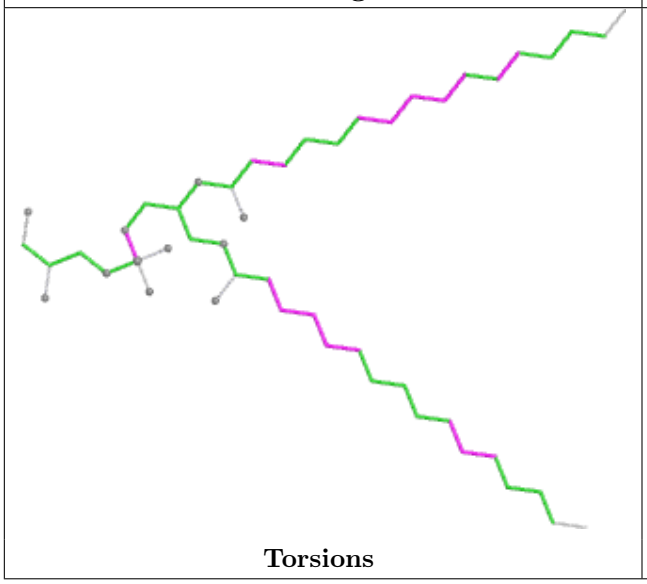
## Ligand LHG L 101



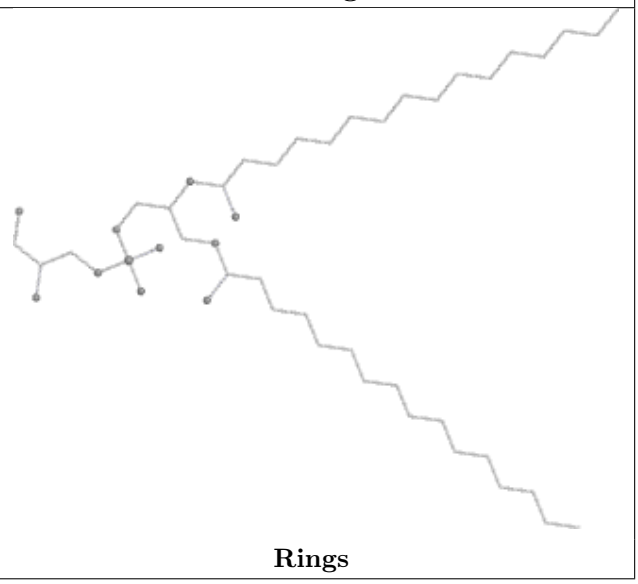
Bond lengths



Bond angles



Torsions

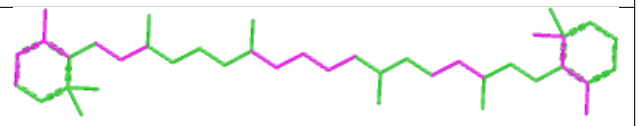


Rings

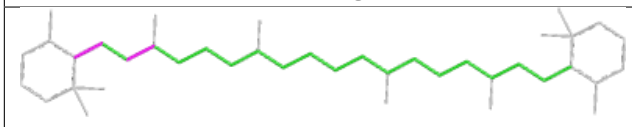
## Ligand BCR c 915



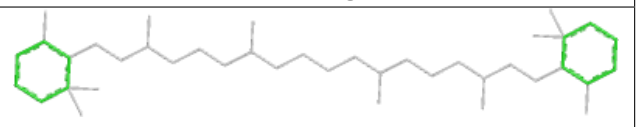
Bond lengths



Bond angles

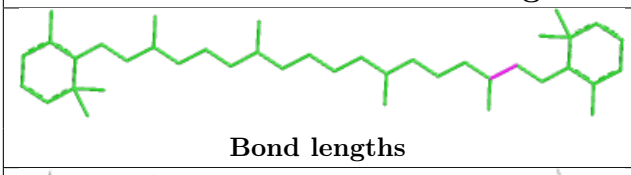


Torsions

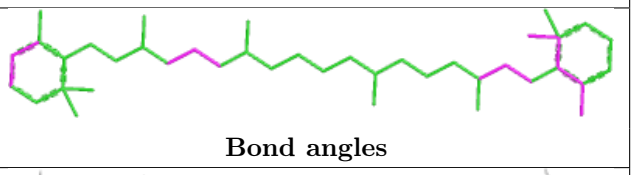


Rings

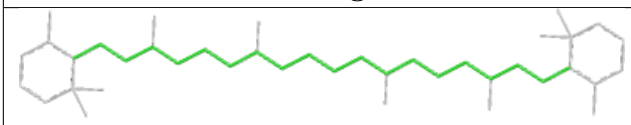
### Ligand BCR B 620



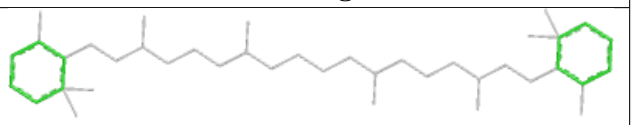
Bond lengths



Bond angles

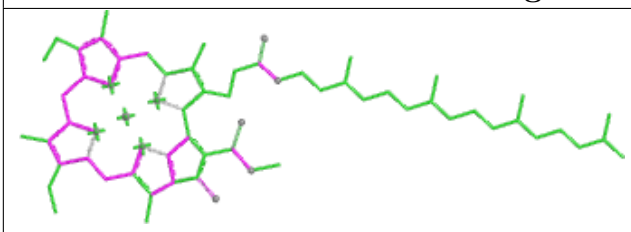


Torsions

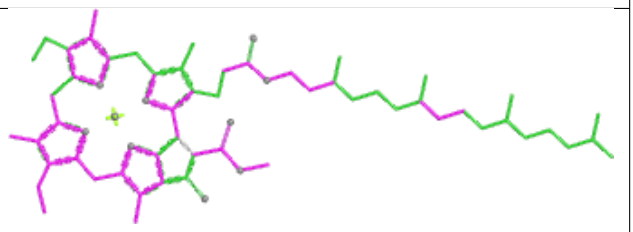


Rings

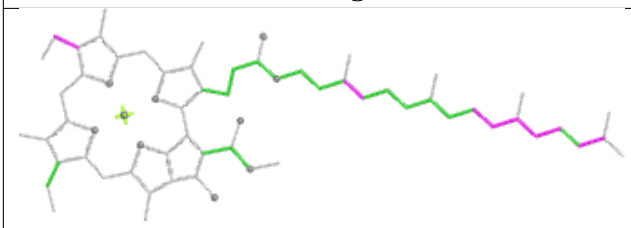
### Ligand CLA B 616



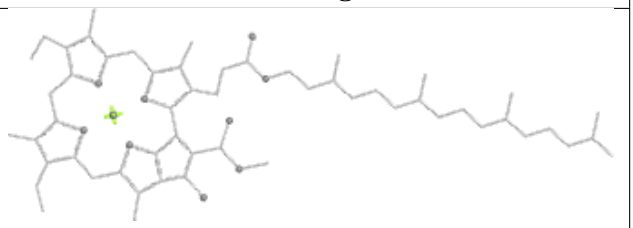
Bond lengths



Bond angles

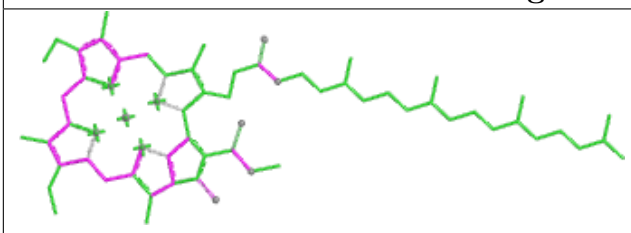


Torsions

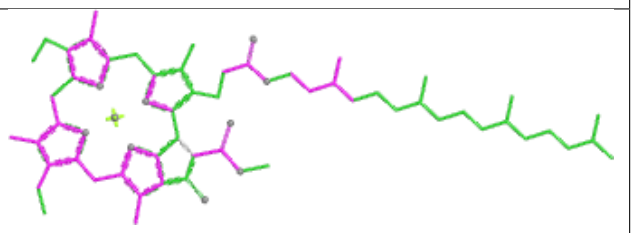


Rings

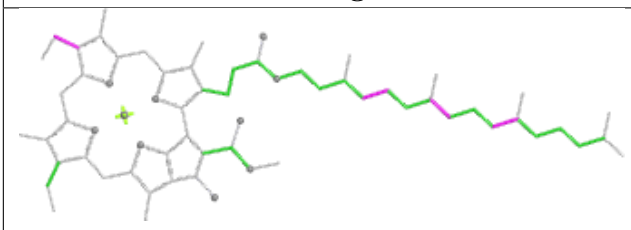
### Ligand CLA b 608



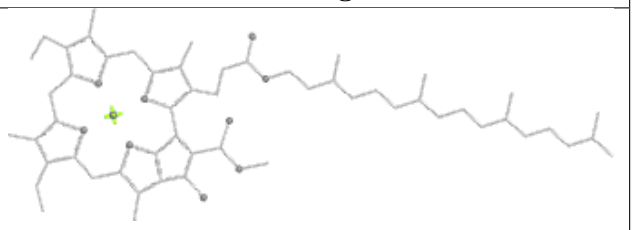
Bond lengths



Bond angles

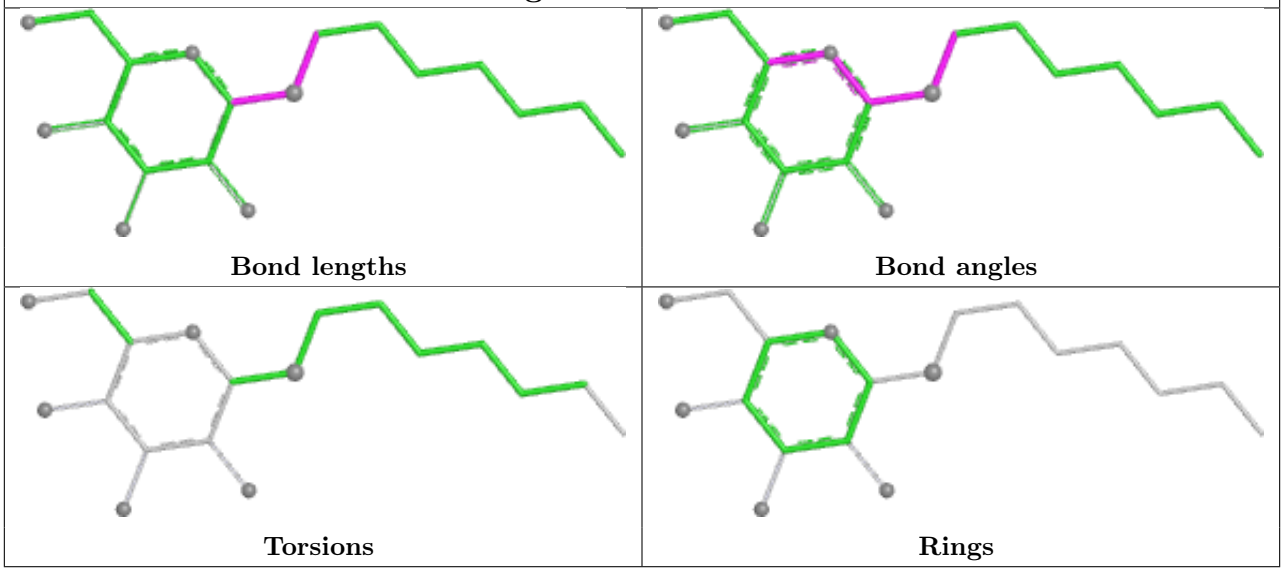


Torsions

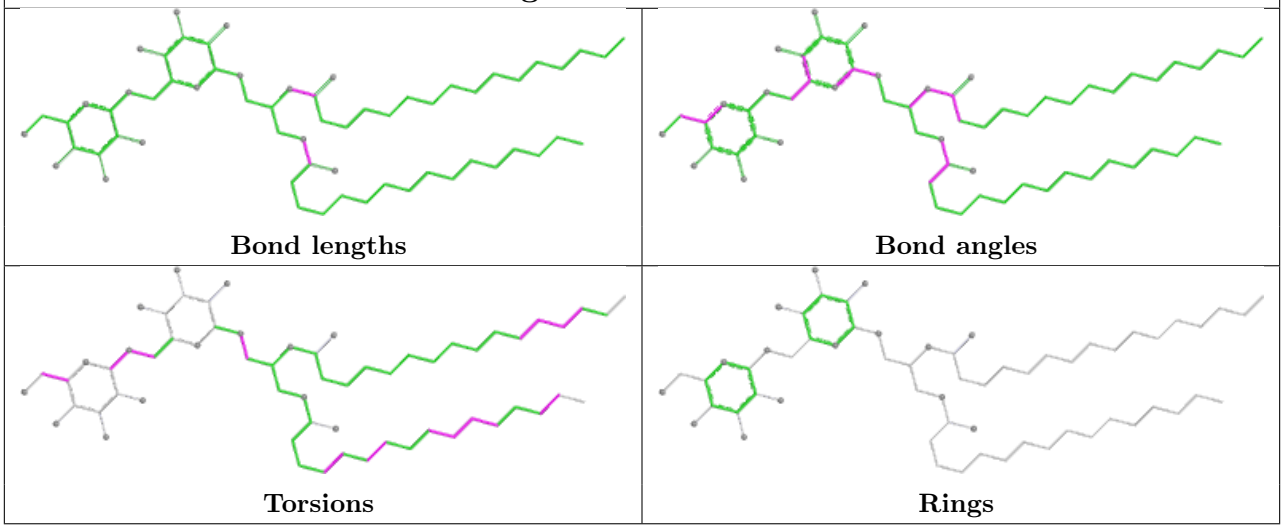


Rings

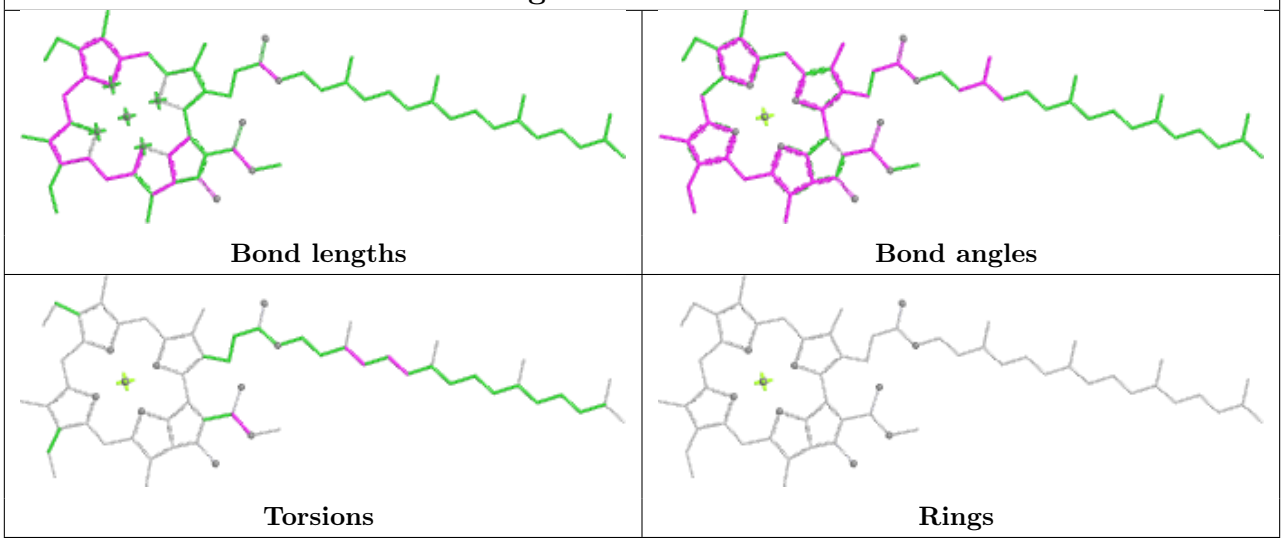
## Ligand HTG b 603



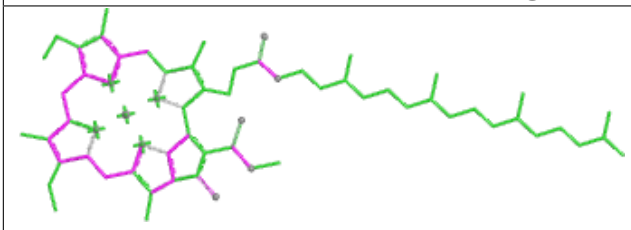

## Ligand DGD C 518



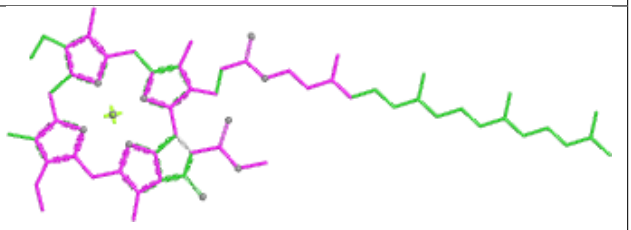

## Ligand CLA b 607



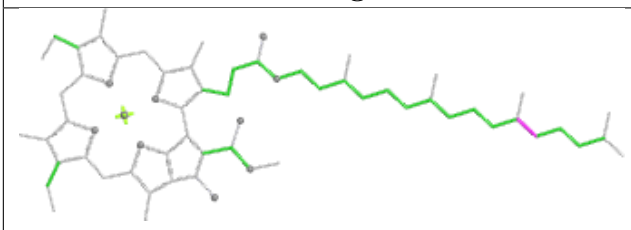
## Ligand CLA A 407



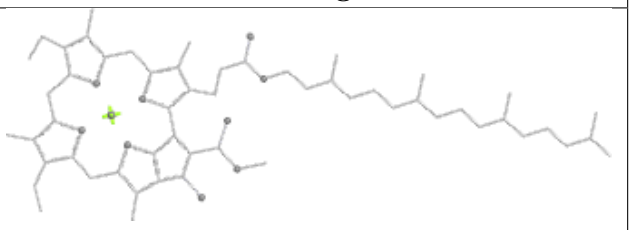
Bond lengths



Bond angles

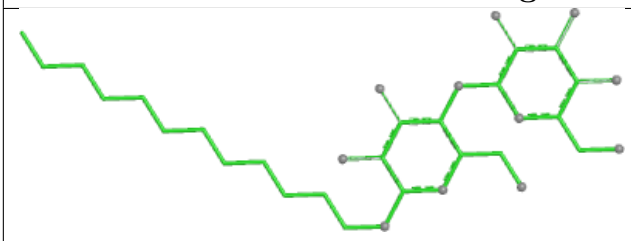


Torsions

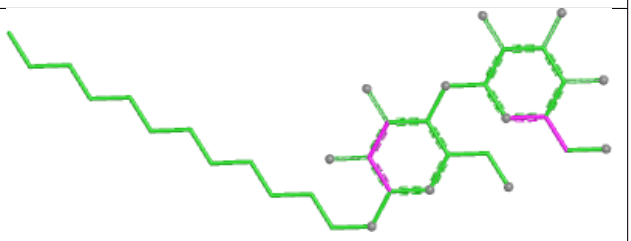


Rings

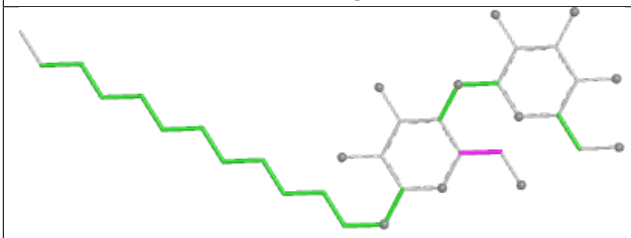
## Ligand LMT m 103



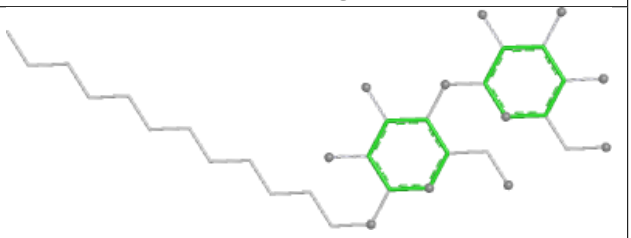
Bond lengths



Bond angles



Torsions

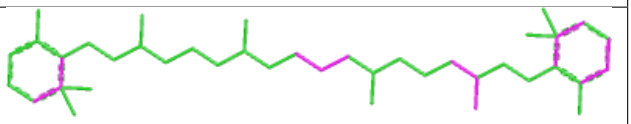


Rings

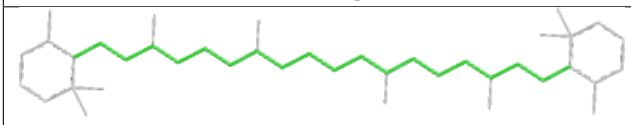
## Ligand BCR B 619



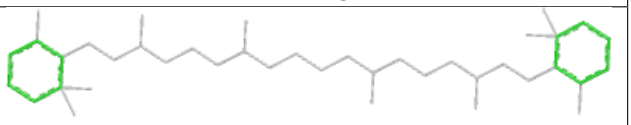
Bond lengths



Bond angles

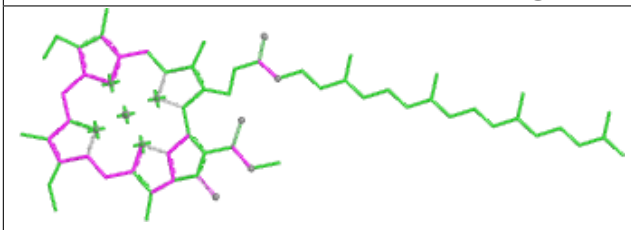


Torsions

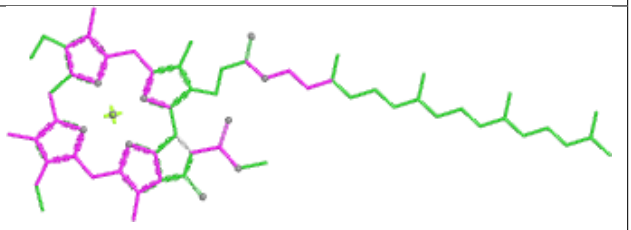


Rings

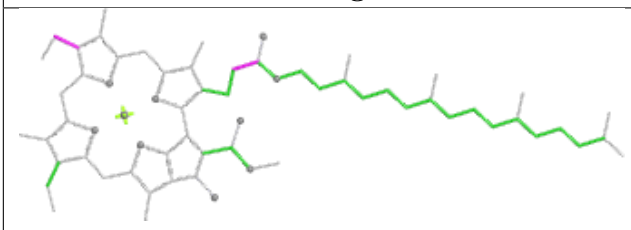
## Ligand CLA c 906



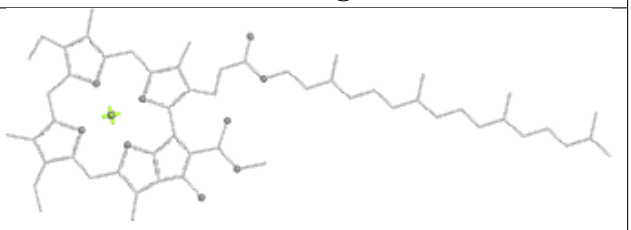
Bond lengths



Bond angles

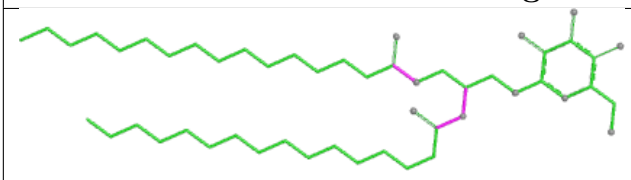


Torsions

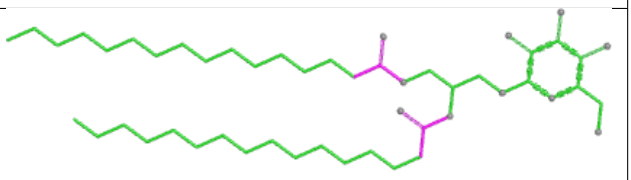


Rings

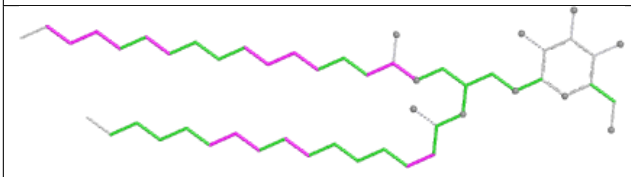
## Ligand LMG b 624



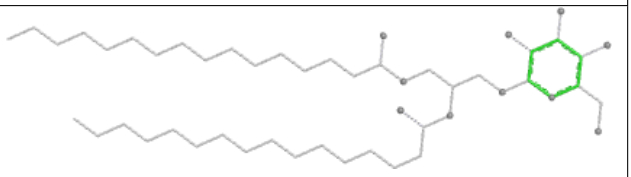
Bond lengths



Bond angles

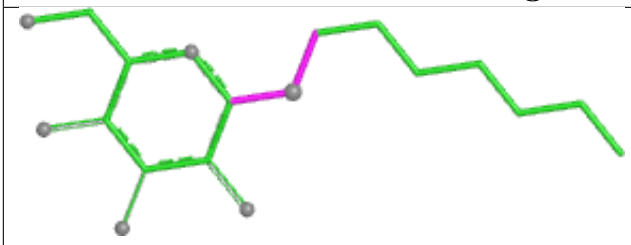


Torsions

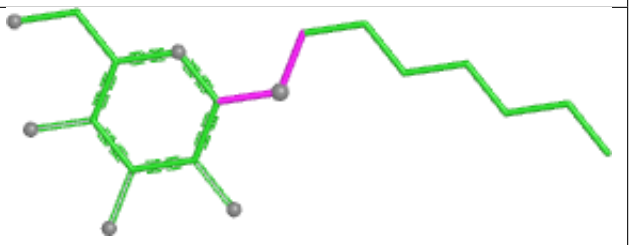


Rings

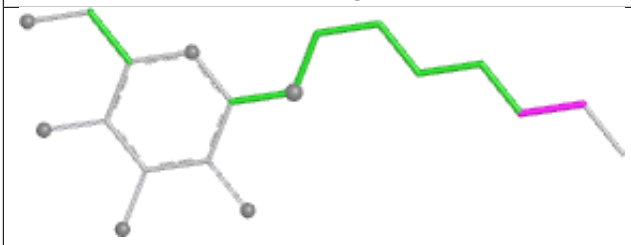
## Ligand HTG b 602



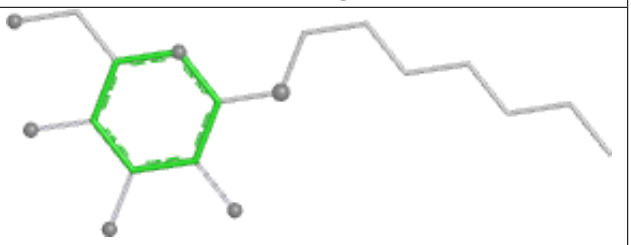
Bond lengths



Bond angles

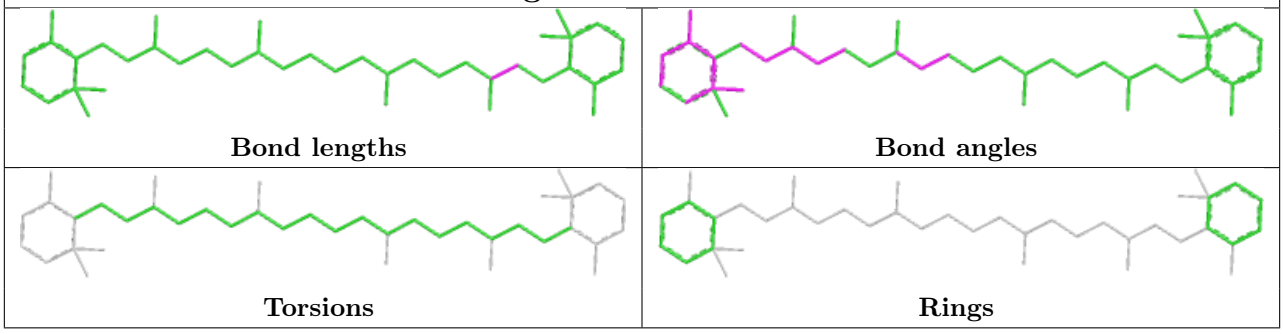


Torsions

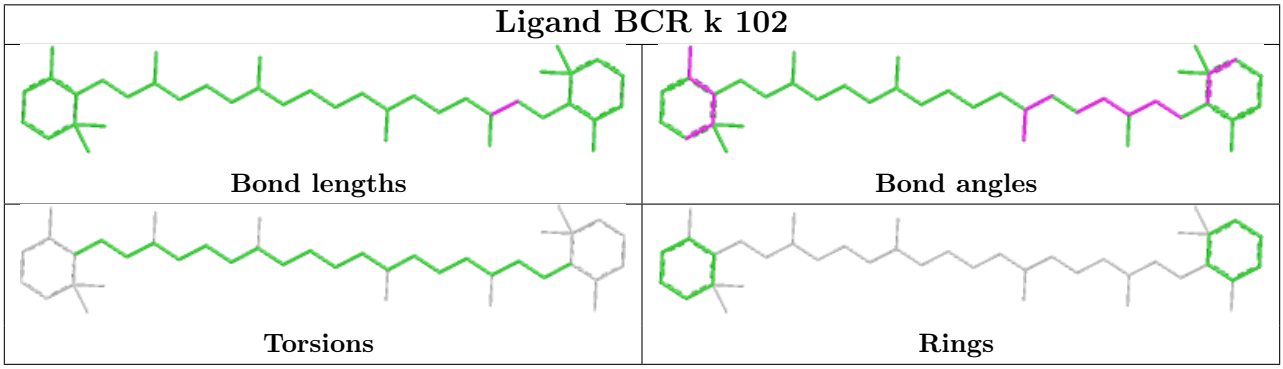


Rings

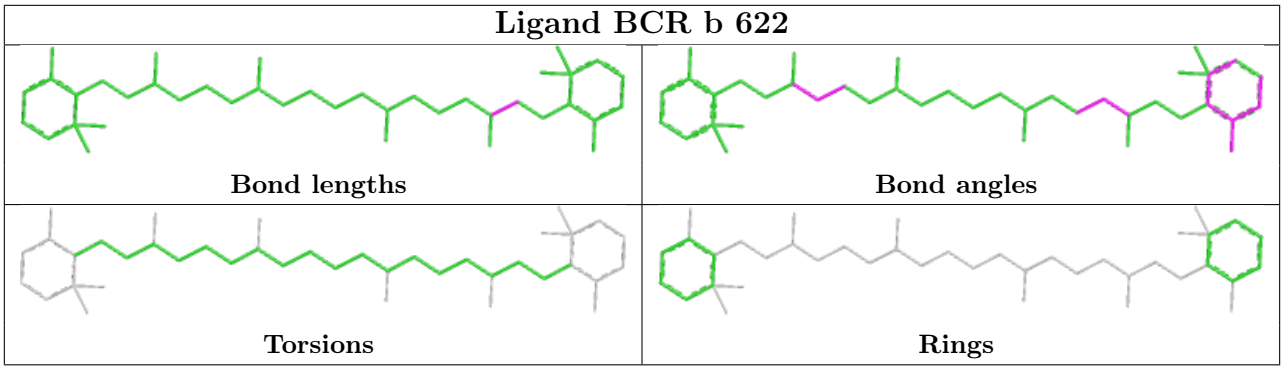
## Ligand BCR C 516



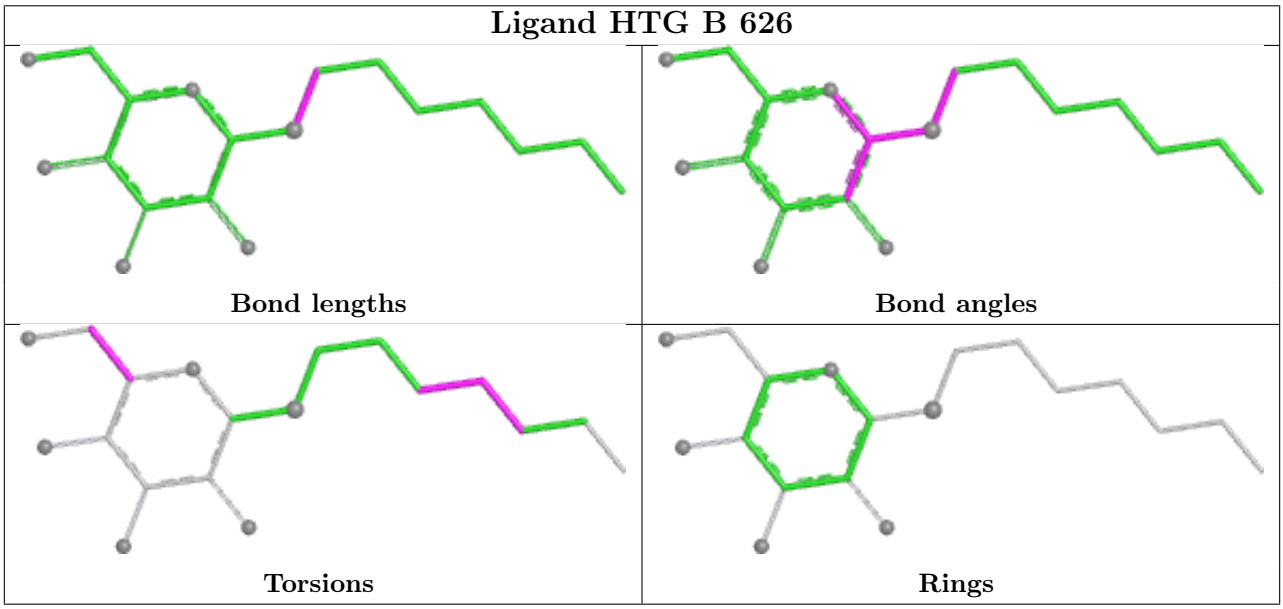

## Ligand BCR k 102



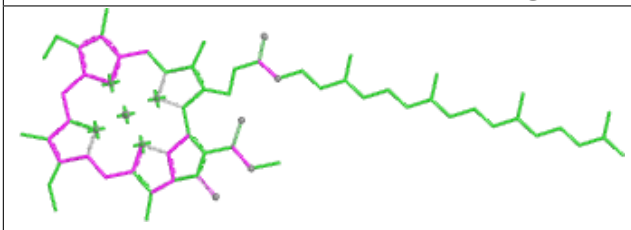

## Ligand BCR b 622



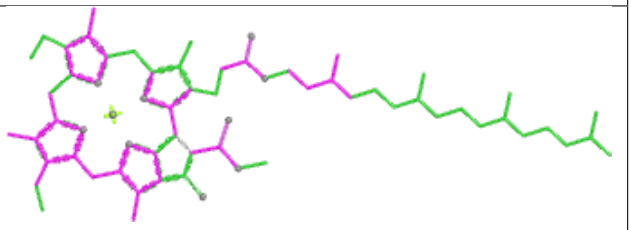

## Ligand HTG B 626



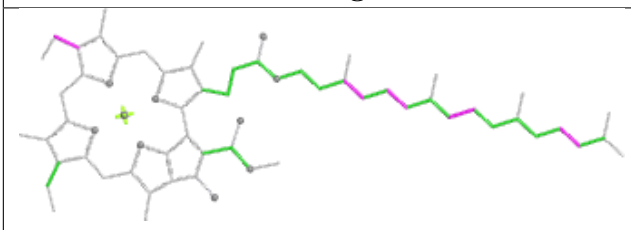
### Ligand CLA C 504



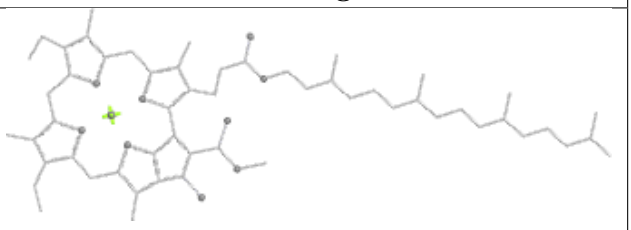
Bond lengths



Bond angles

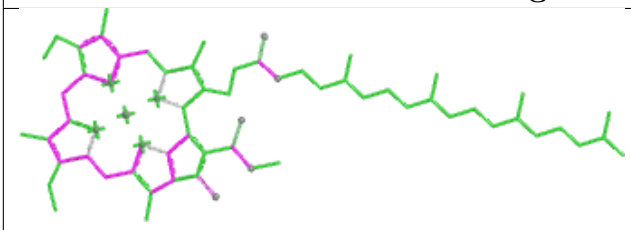


Torsions

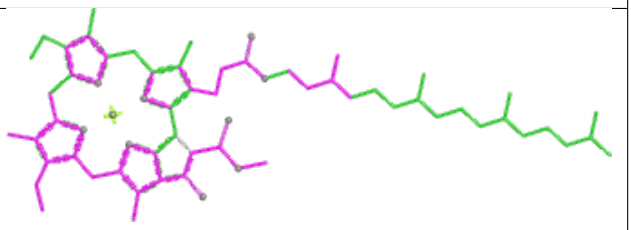


Rings

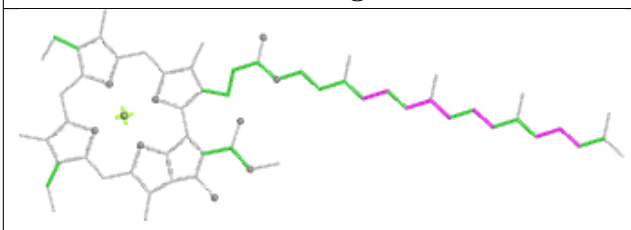
### Ligand CLA c 907



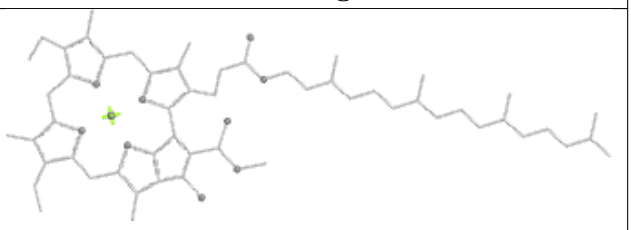
Bond lengths



Bond angles

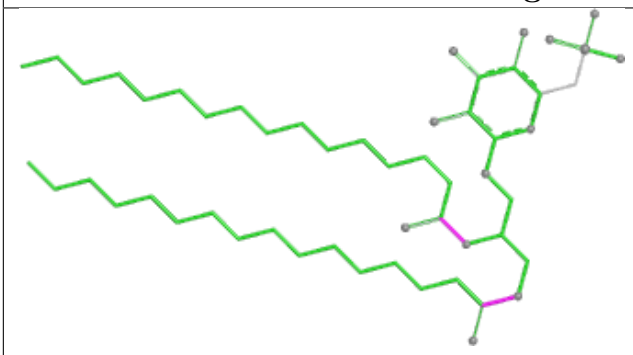


Torsions

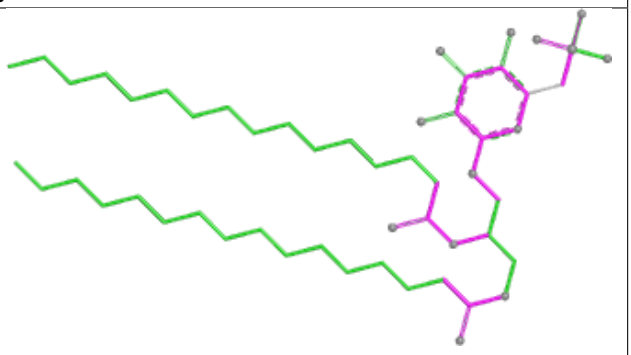


Rings

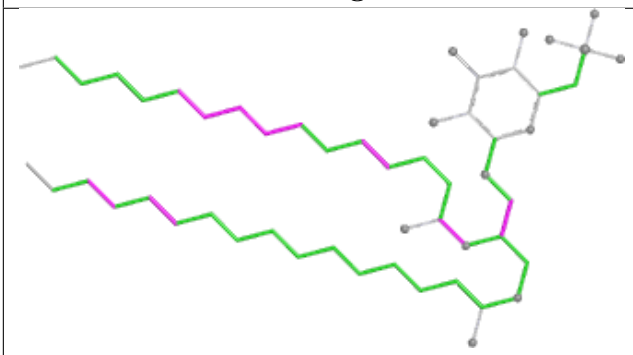
### Ligand SQD A 412



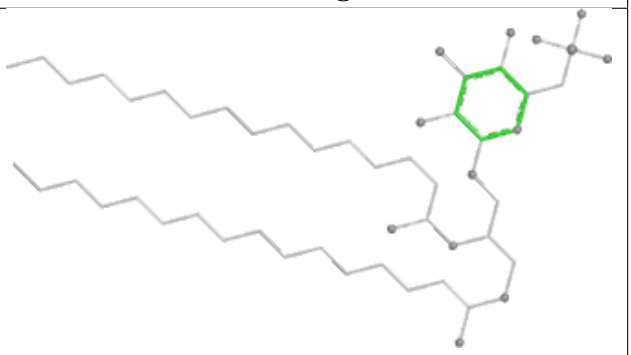
Bond lengths



Bond angles

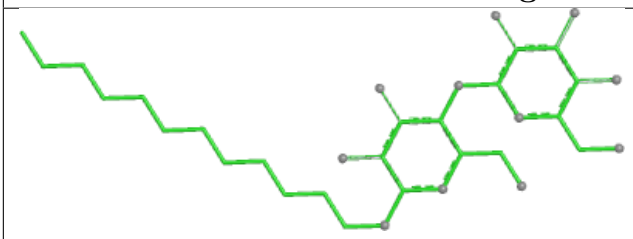


Torsions

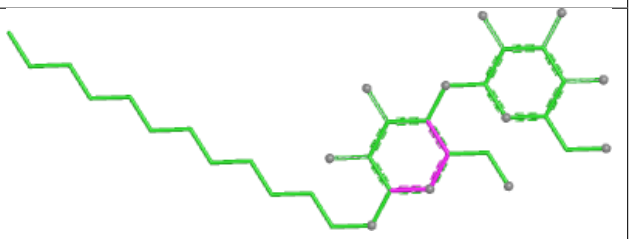


Rings

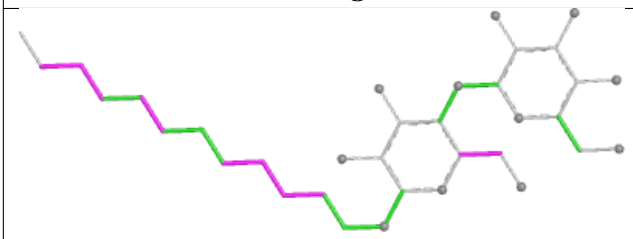
### Ligand LMT m 104



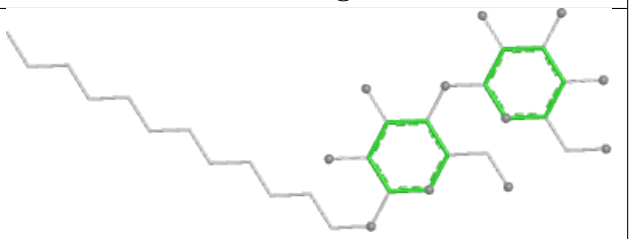
Bond lengths



Bond angles

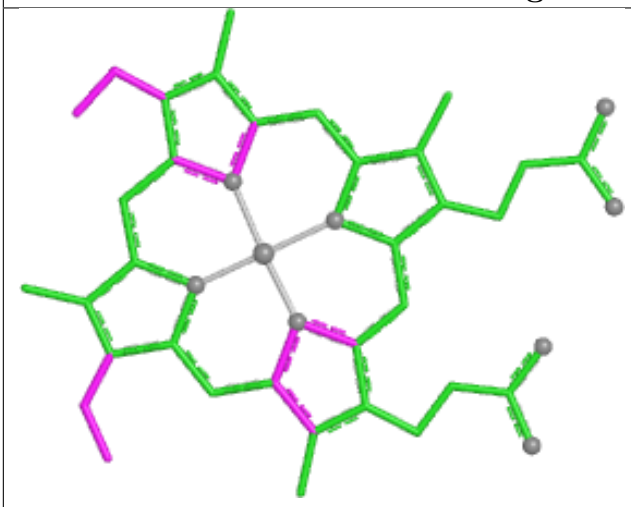


Torsions

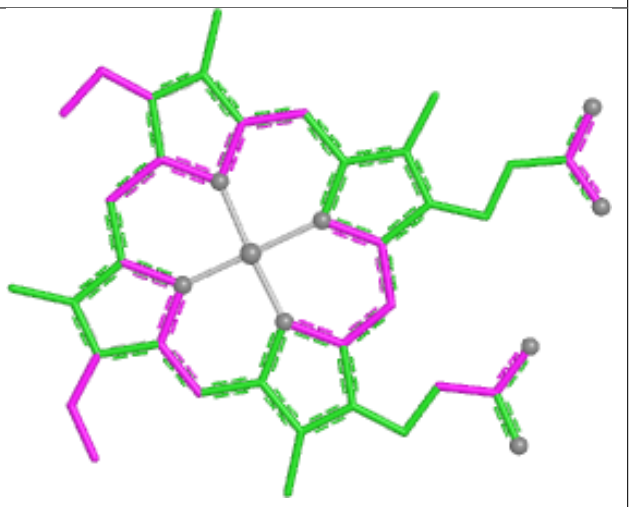


Rings

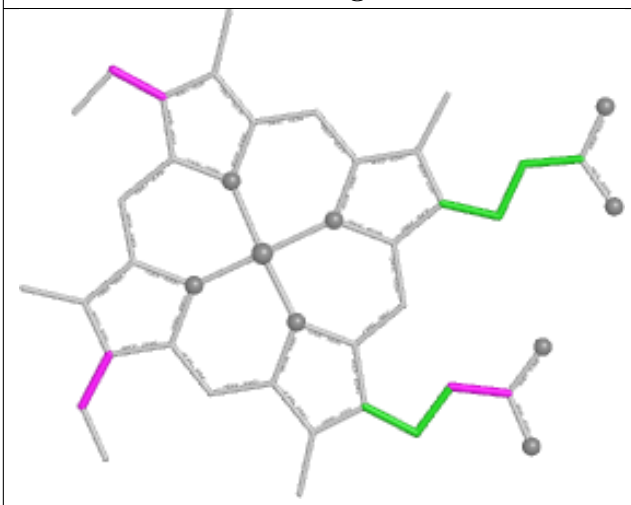
## Ligand HEC v 202



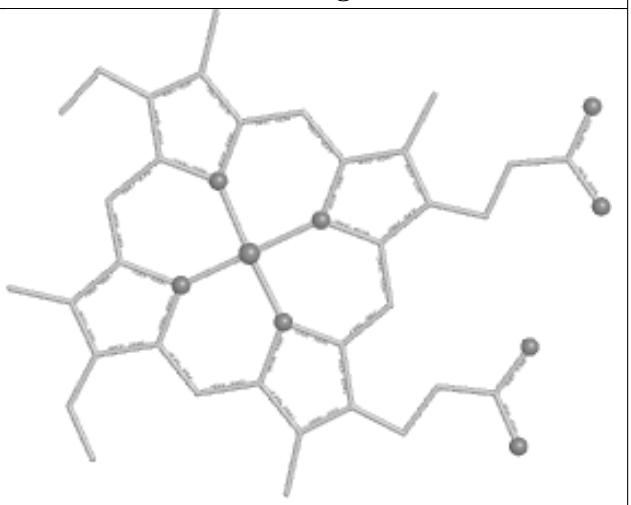
Bond lengths



Bond angles

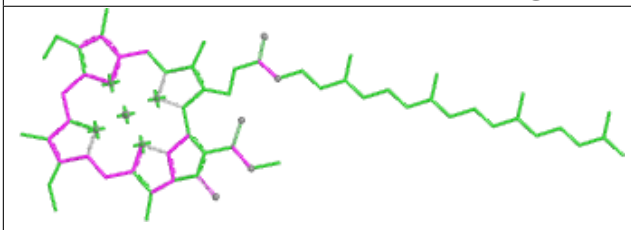


Torsions

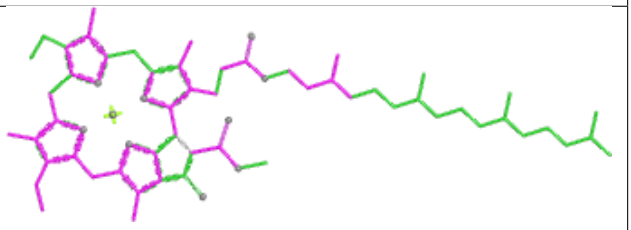


Rings

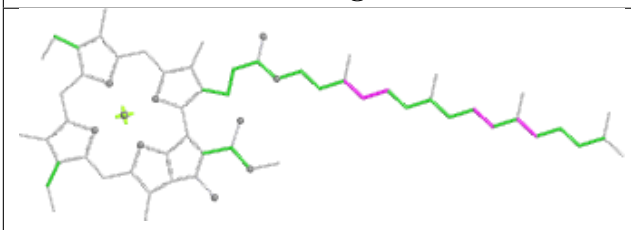
## Ligand CLA d 403



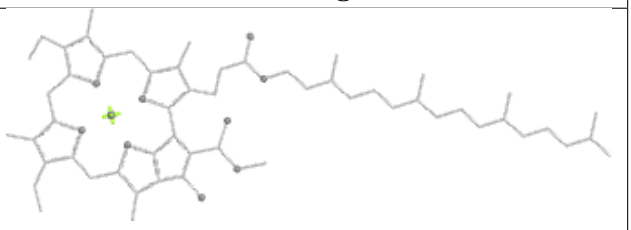
Bond lengths



Bond angles

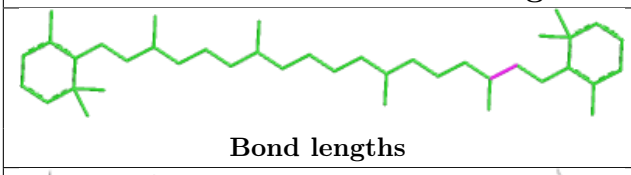


Torsions

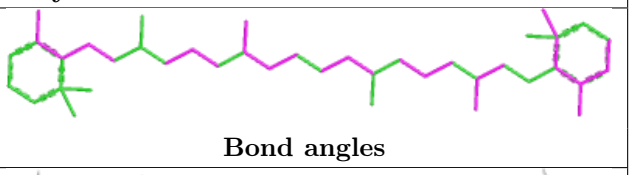


Rings

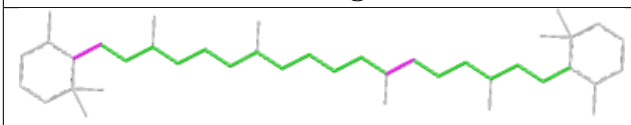
## Ligand BCR y 101



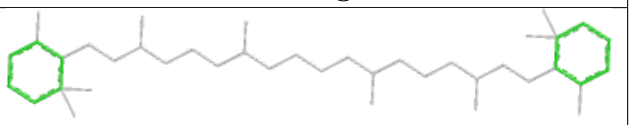
Bond lengths



Bond angles

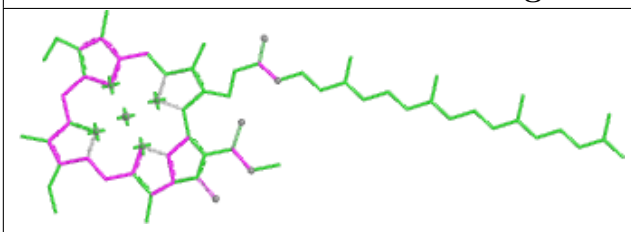


Torsions

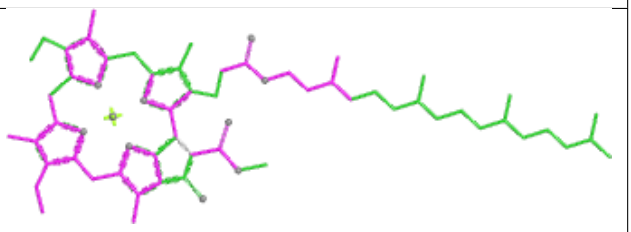


Rings

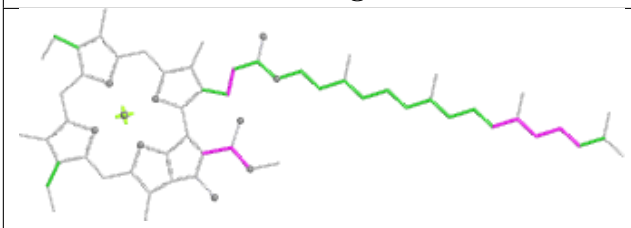
## Ligand CLA C 502



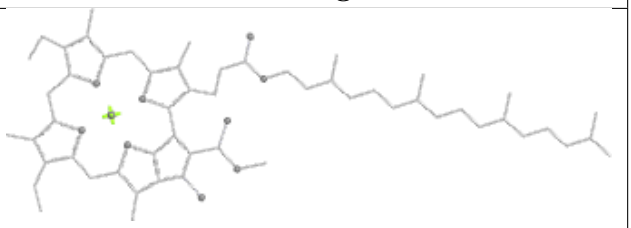
Bond lengths



Bond angles

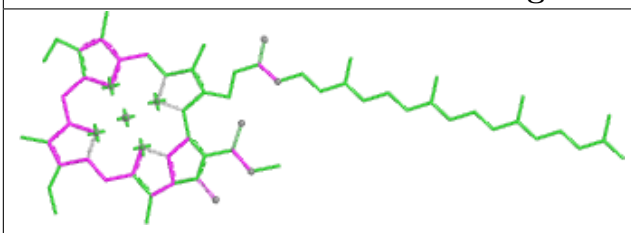


Torsions

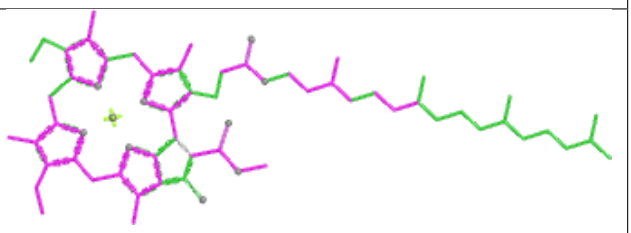


Rings

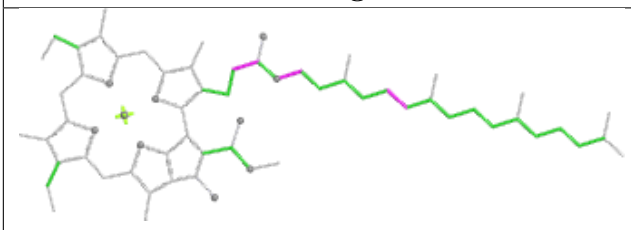
## Ligand CLA b 617



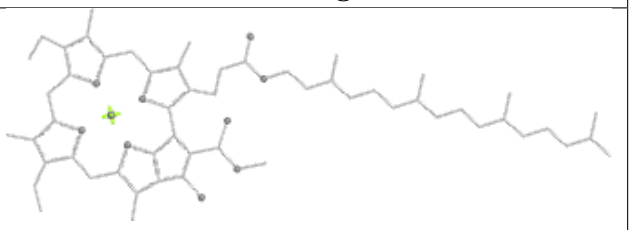
Bond lengths



Bond angles

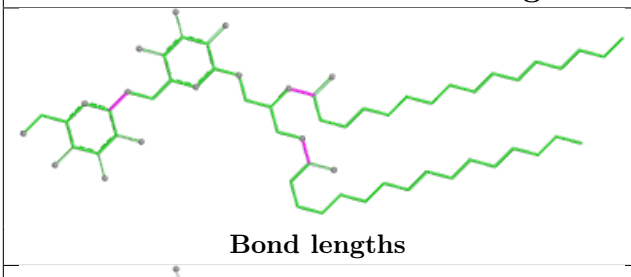


Torsions

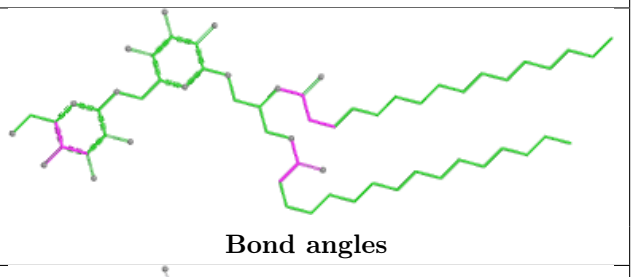


Rings

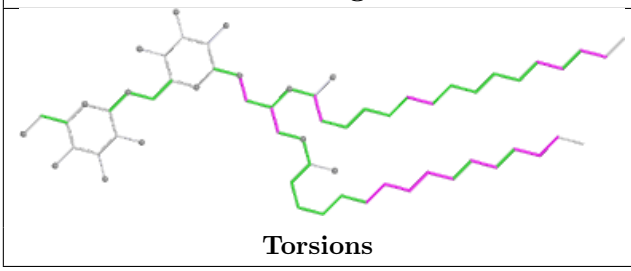
## Ligand DGD h 102



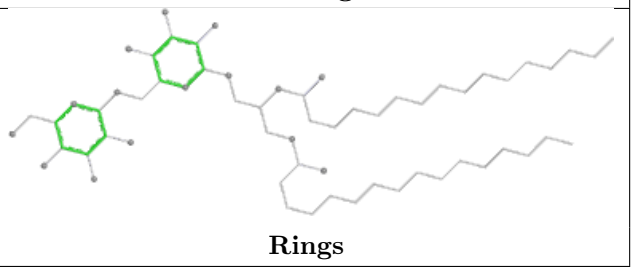
Bond lengths



Bond angles

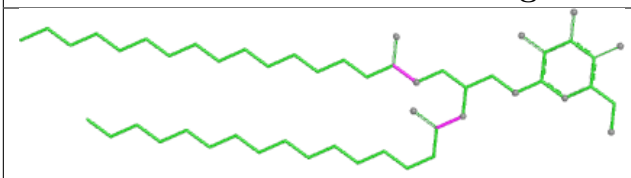


Torsions

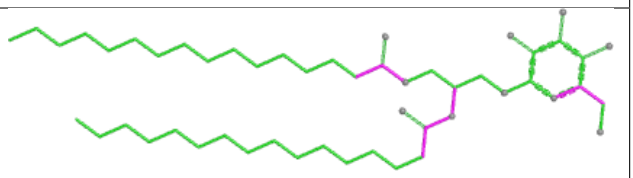


Rings

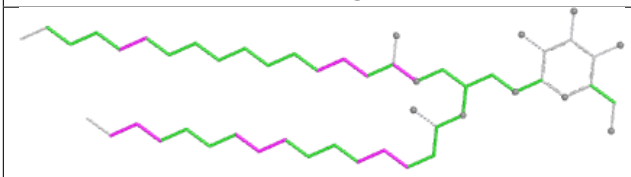
## Ligand LMG C 520



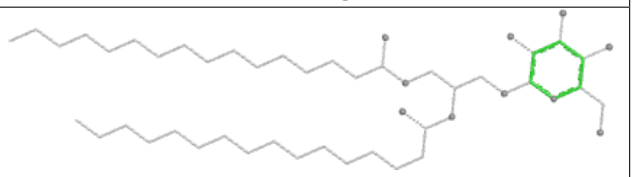
Bond lengths



Bond angles

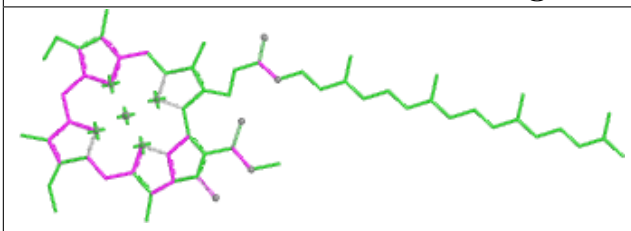


Torsions

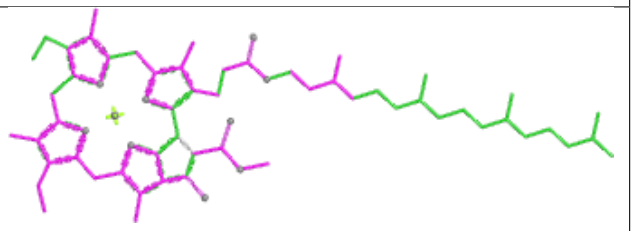


Rings

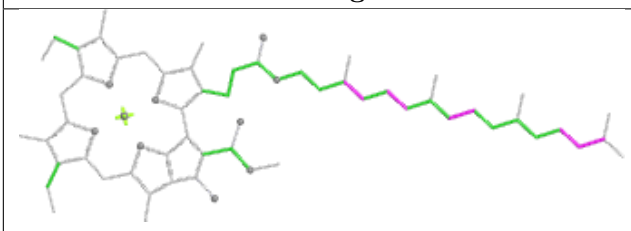
## Ligand CLA a 409



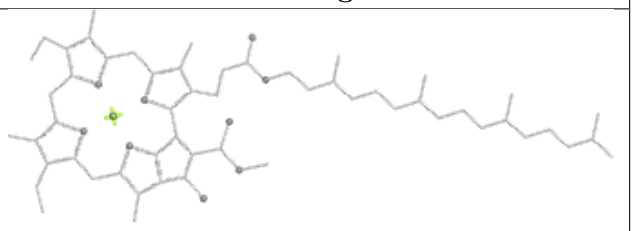
Bond lengths



Bond angles

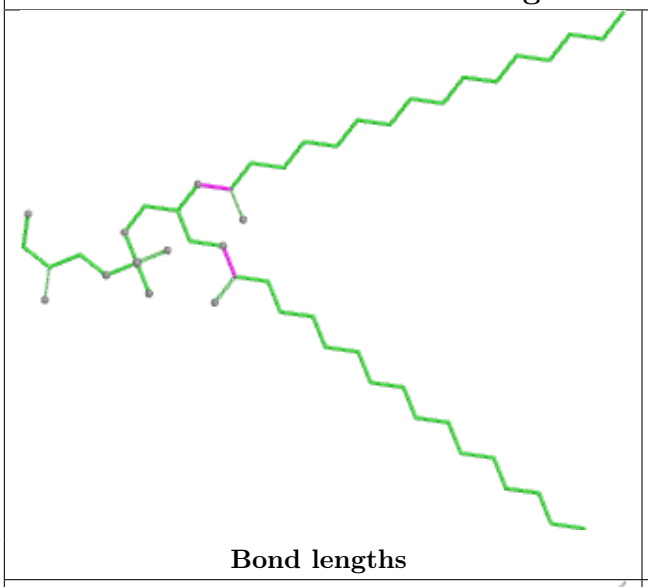


Torsions

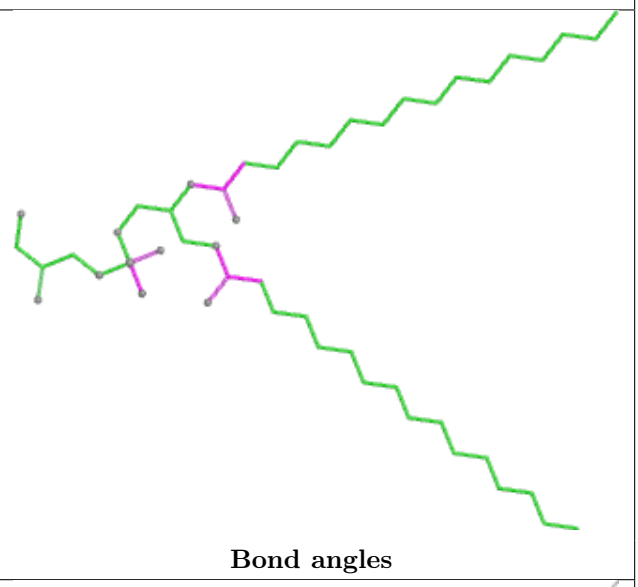


Rings

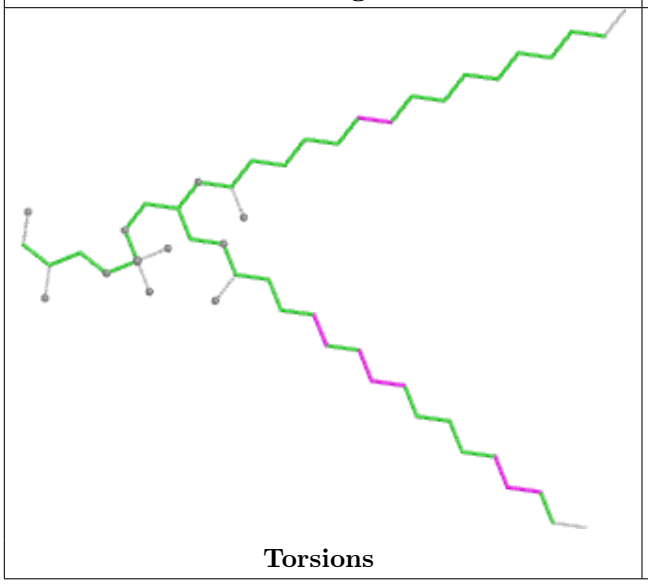
## Ligand LHG D 406



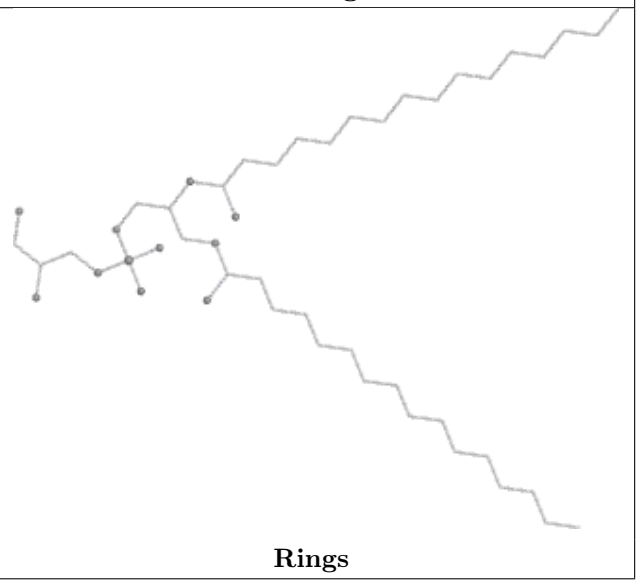
Bond lengths



Bond angles

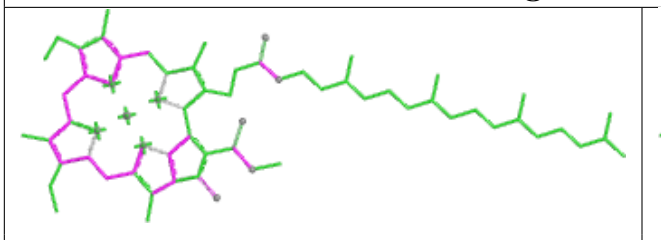


Torsions

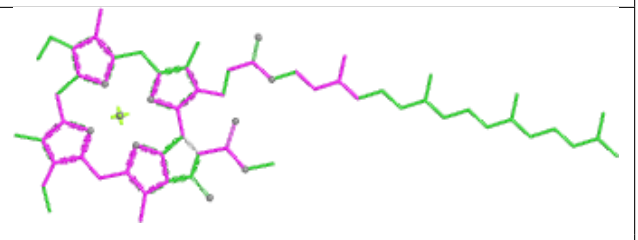


Rings

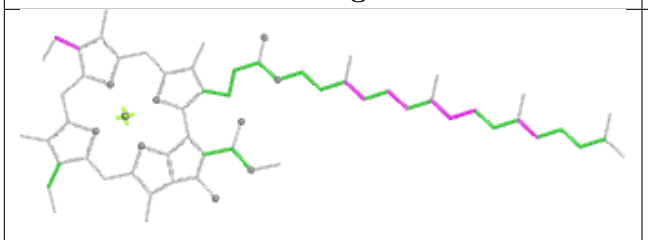
## Ligand CLA D 402



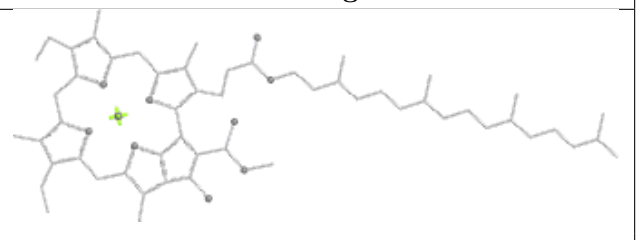
Bond lengths



Bond angles

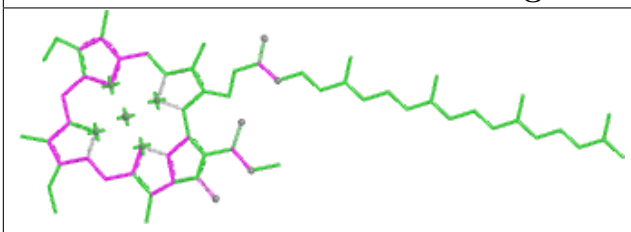


Torsions

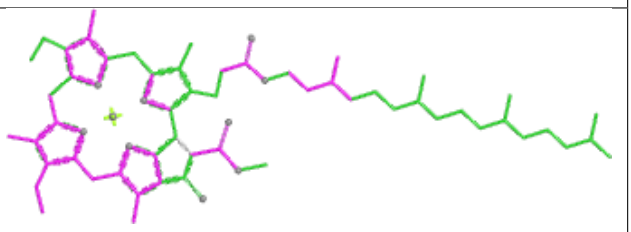


Rings

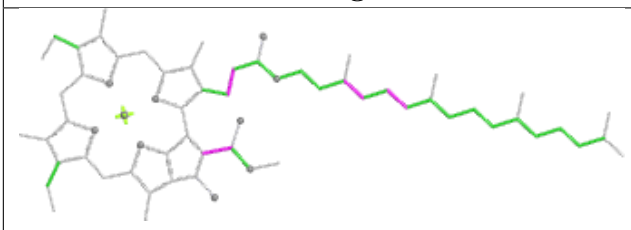
### Ligand CLA C 508



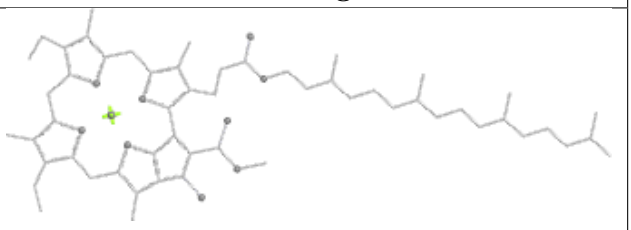
Bond lengths



Bond angles

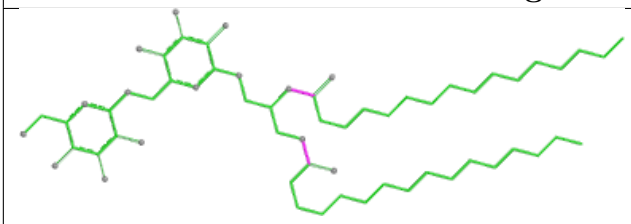


Torsions

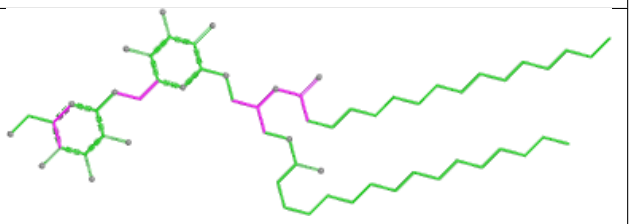


Rings

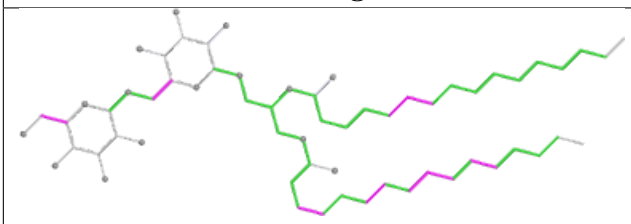
### Ligand DGD c 916



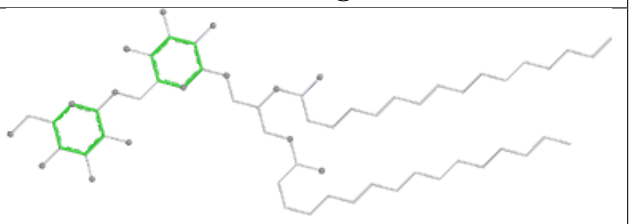
Bond lengths



Bond angles

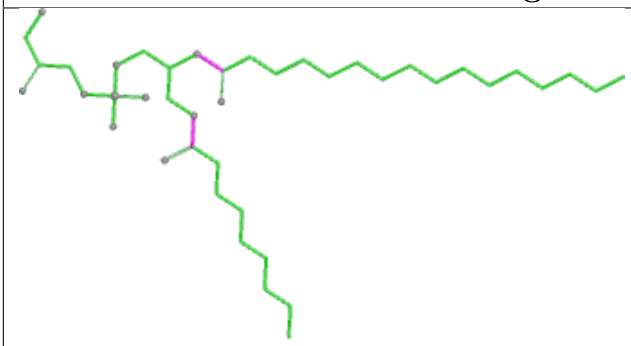


Torsions

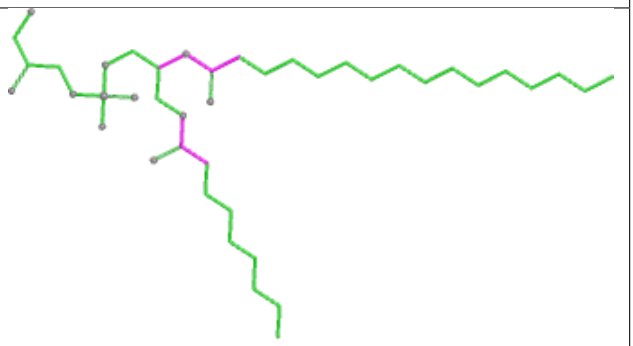


Rings

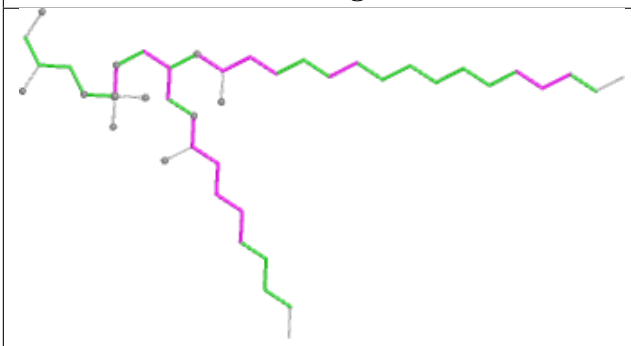
## Ligand LHG E 101



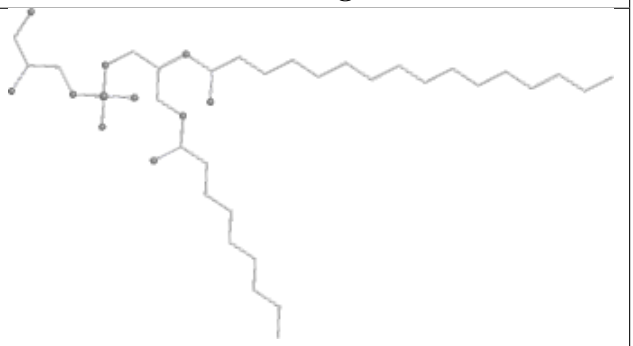
Bond lengths



Bond angles

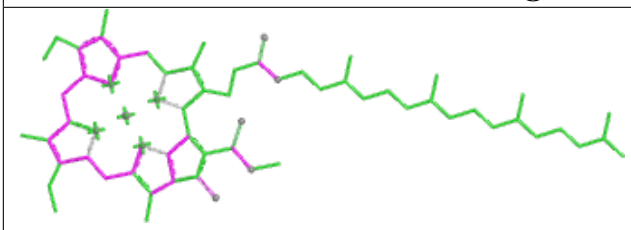


Torsions

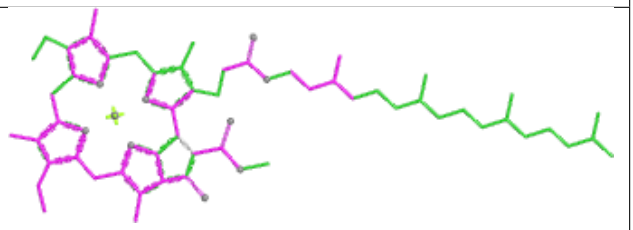


Rings

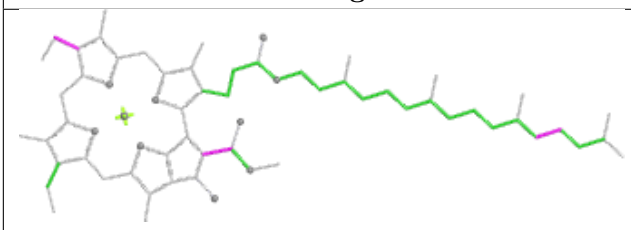
## Ligand CLA C 503



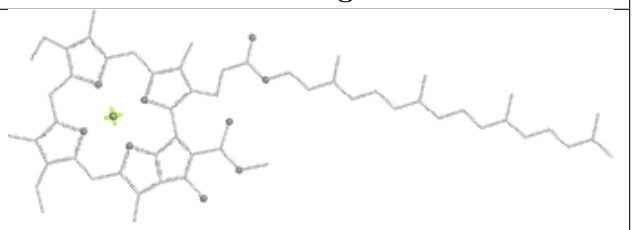
Bond lengths



Bond angles

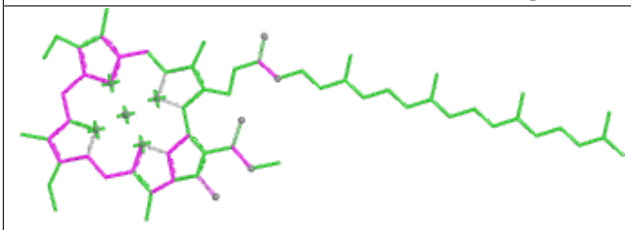


Torsions

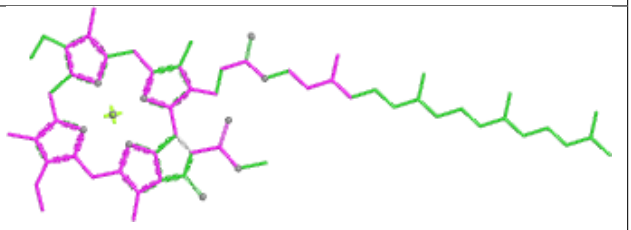


Rings

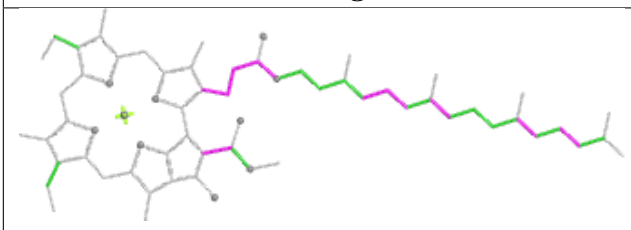
## Ligand CLA B 602



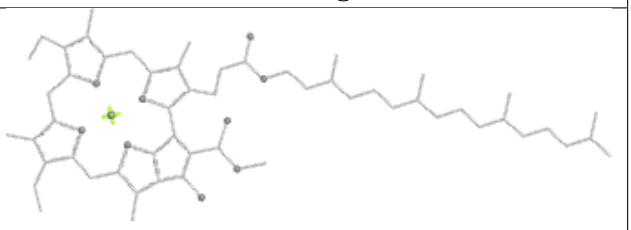
Bond lengths



Bond angles

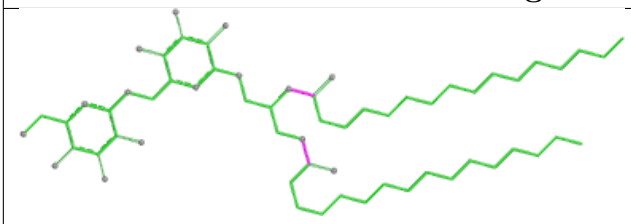


Torsions

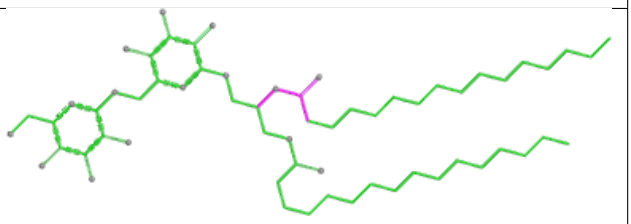


Rings

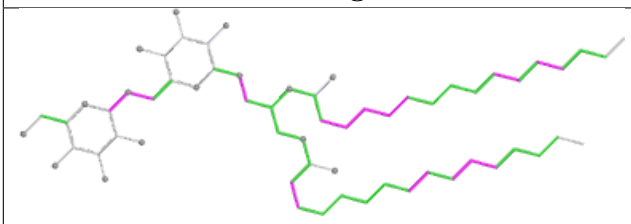
## Ligand DGD c 917



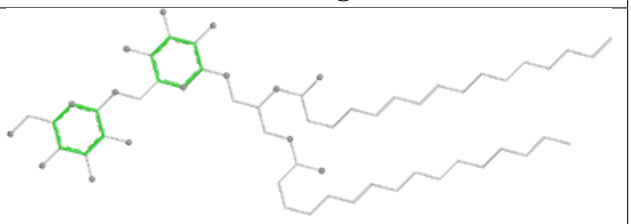
Bond lengths



Bond angles

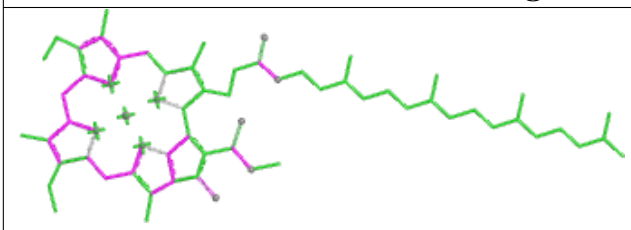


Torsions

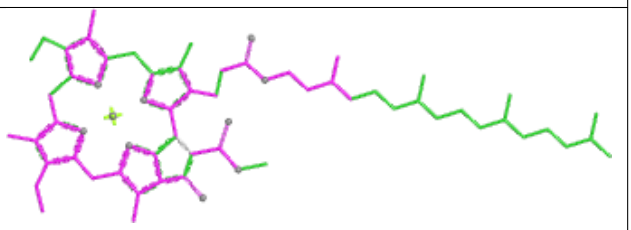


Rings

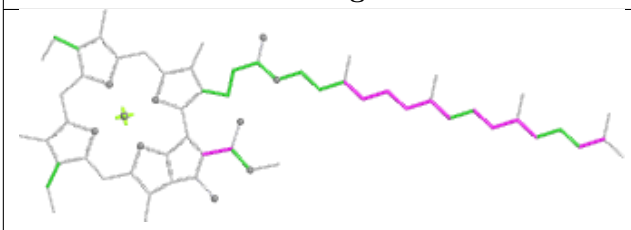
## Ligand CLA B 615



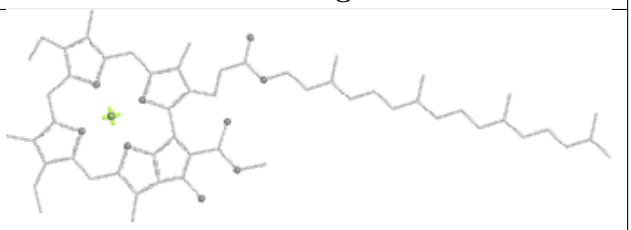
Bond lengths



Bond angles

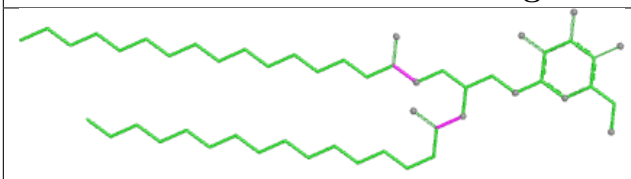


Torsions

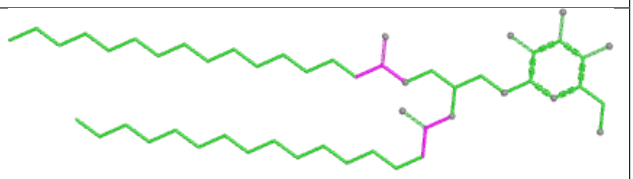


Rings

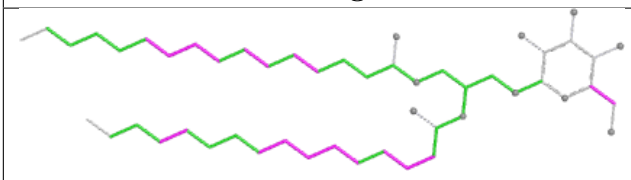
## Ligand LMG J 101



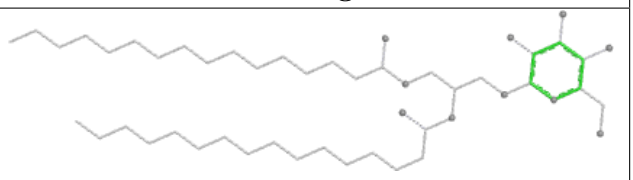
Bond lengths



Bond angles

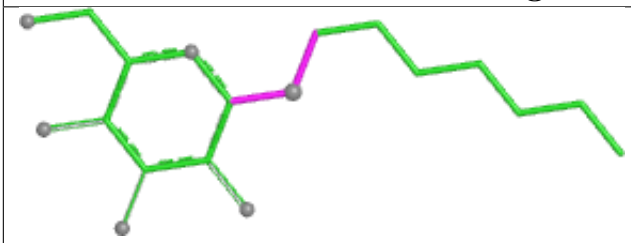


Torsions

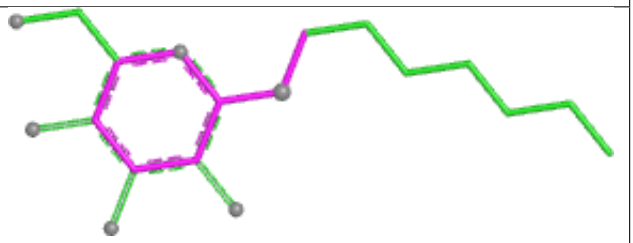


Rings

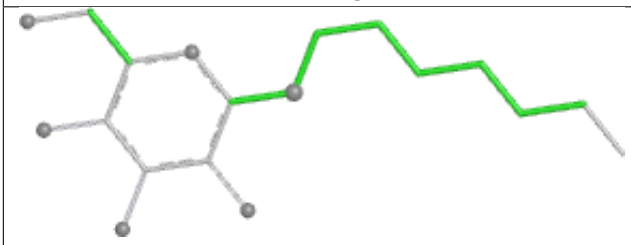
## Ligand HTG c 923



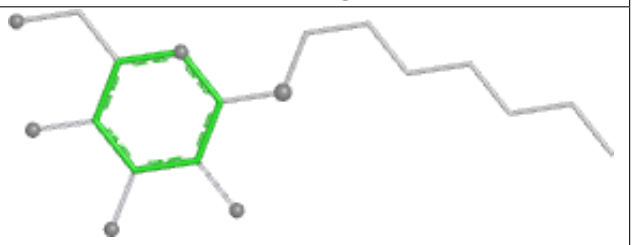
Bond lengths



Bond angles

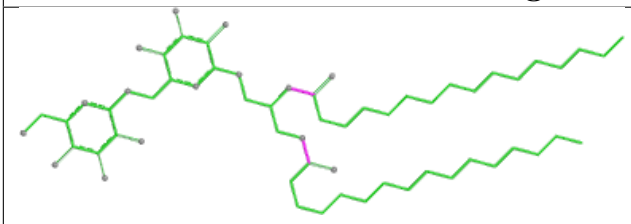


Torsions

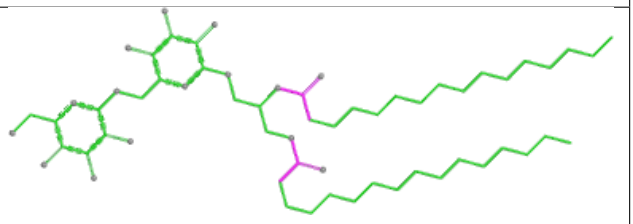


Rings

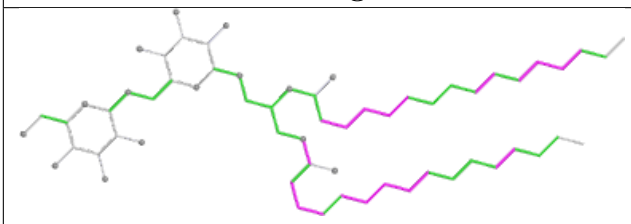
## Ligand DGD c 918



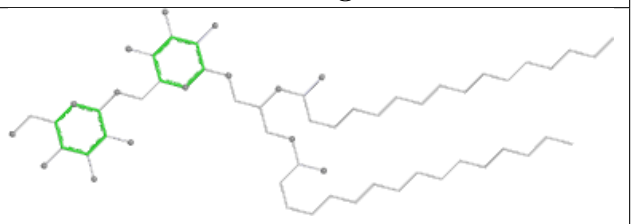
Bond lengths



Bond angles

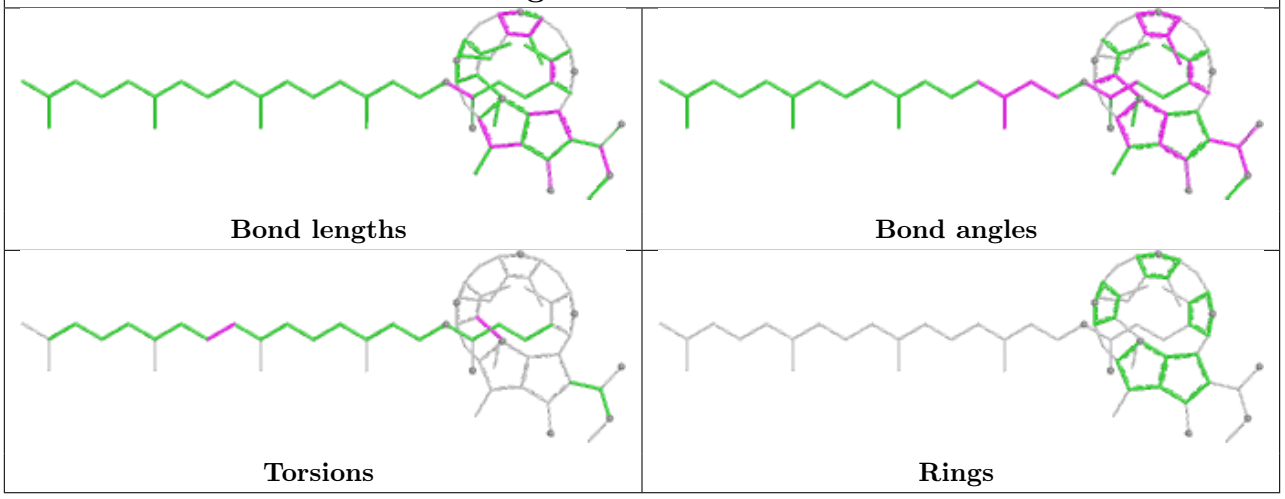


Torsions

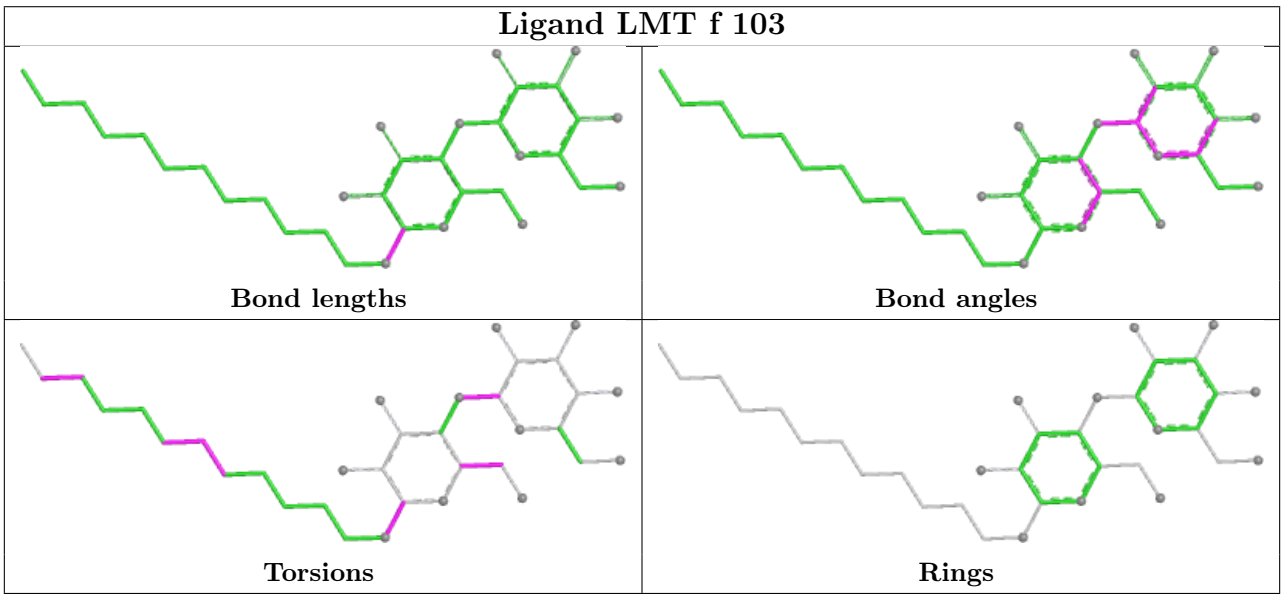


Rings

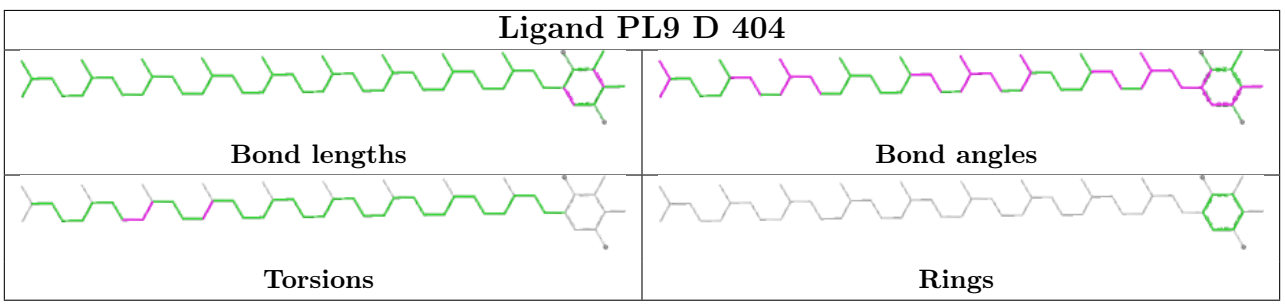
## Ligand PHO a 420



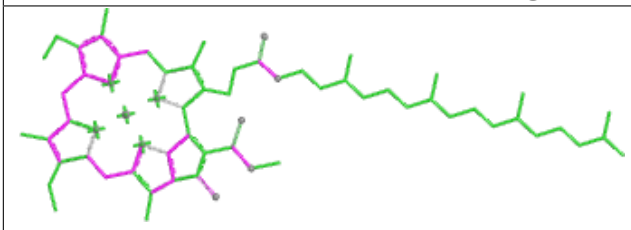

## Ligand LMT f 103



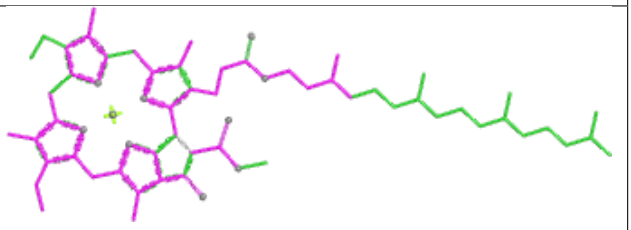

## Ligand PL9 D 404



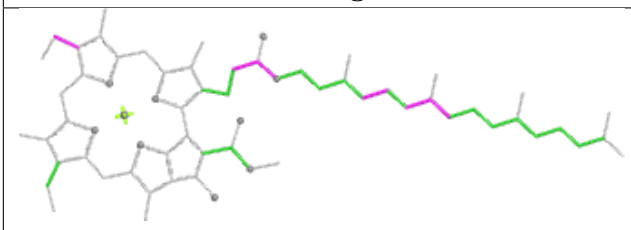
### Ligand CLA C 513



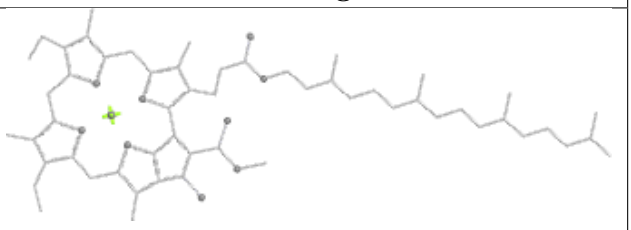
Bond lengths



Bond angles

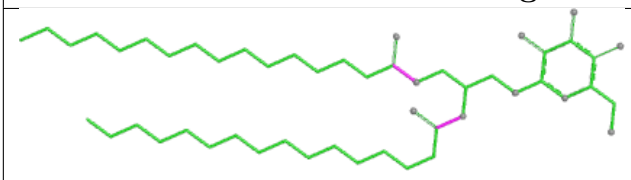


Torsions

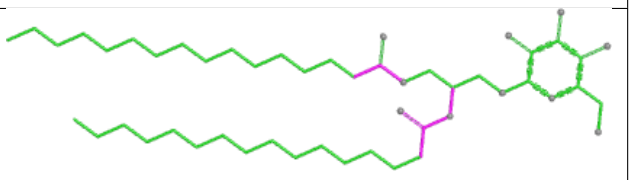


Rings

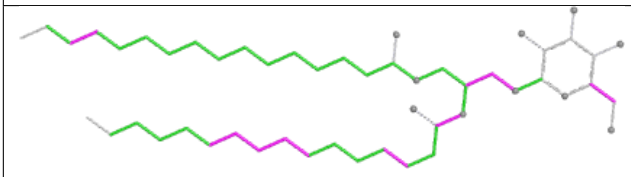
### Ligand LMG C 521



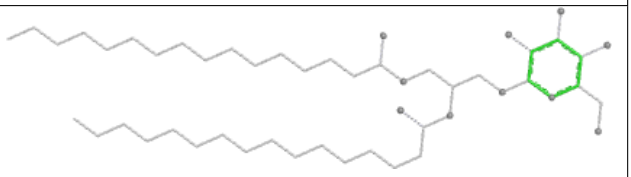
Bond lengths



Bond angles

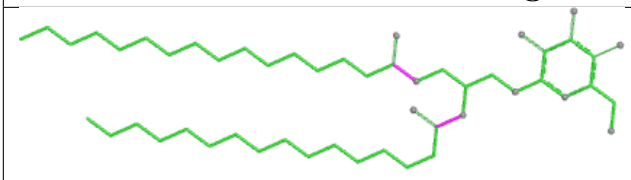


Torsions

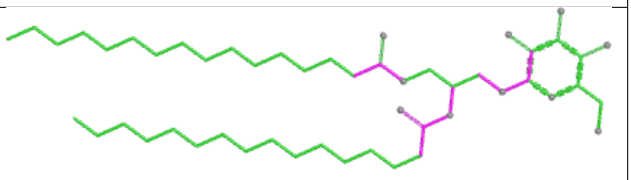


Rings

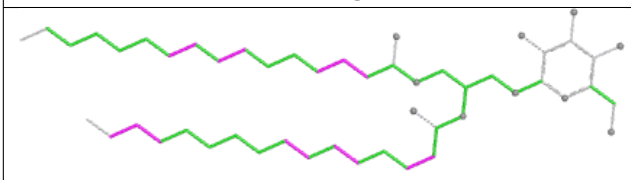
### Ligand LMG a 412



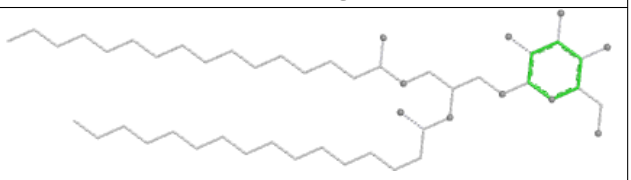
Bond lengths



Bond angles

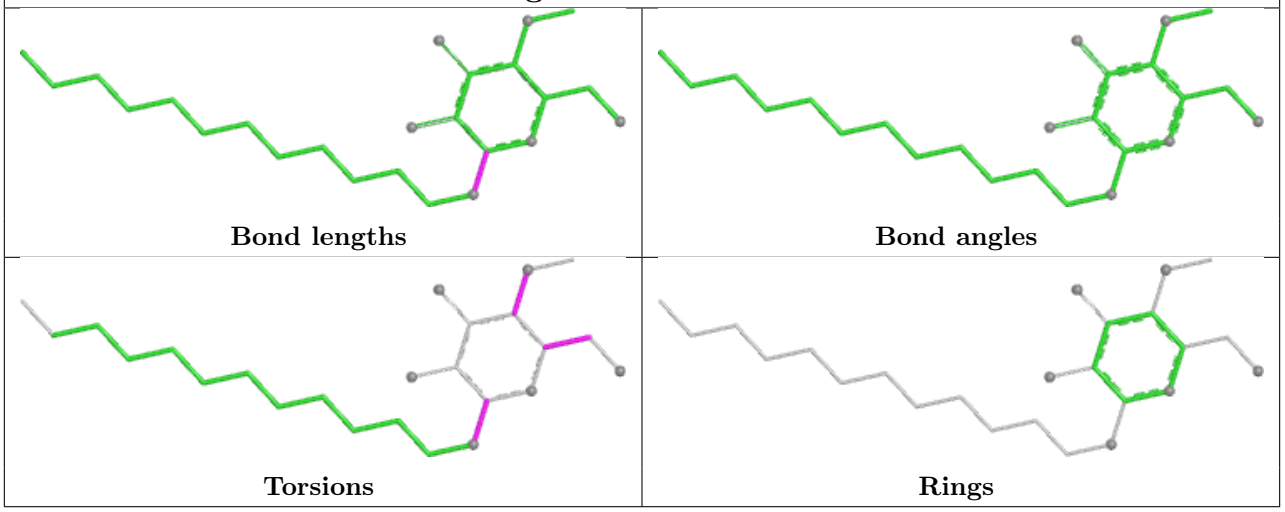


Torsions

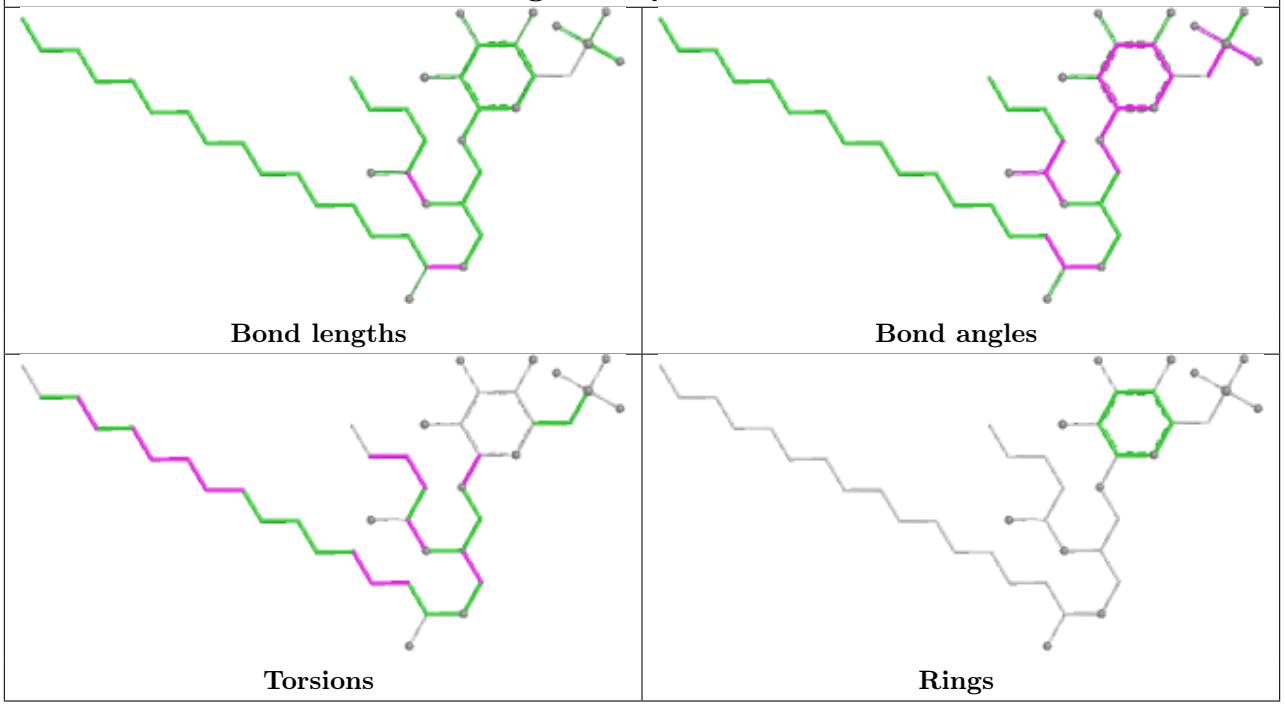


Rings

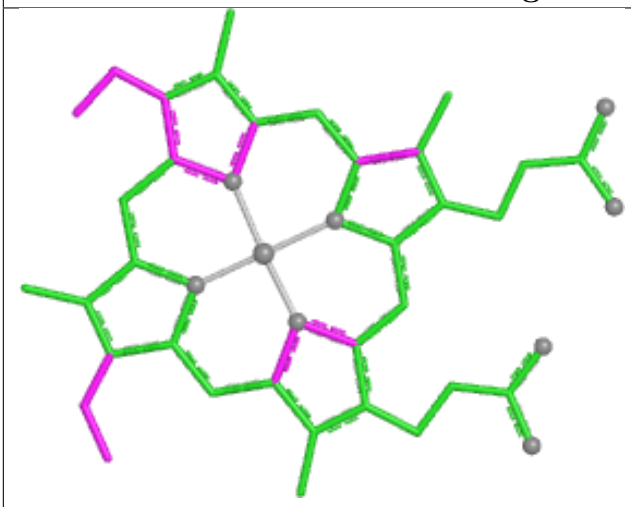
**Ligand LMT b 625**



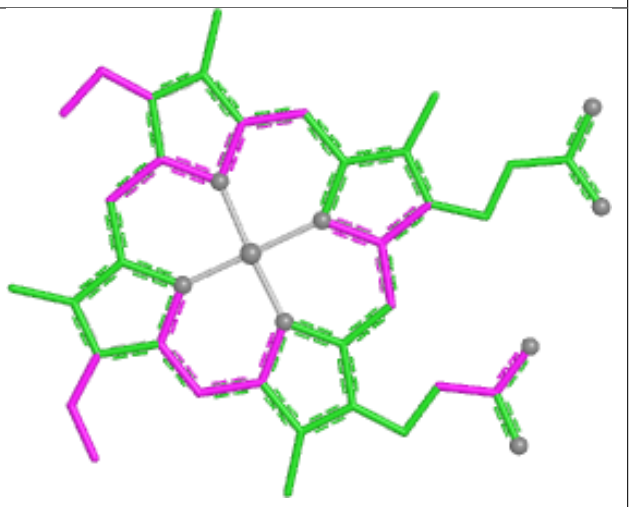

**Ligand SQD F 101**



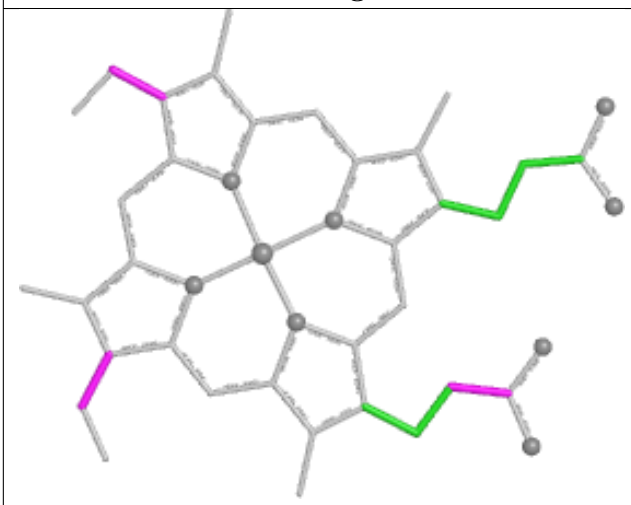
**Ligand HEC V 201**



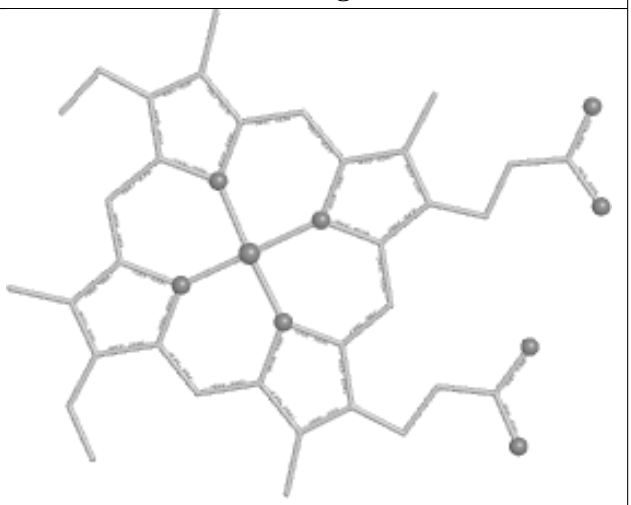
**Bond lengths**



**Bond angles**

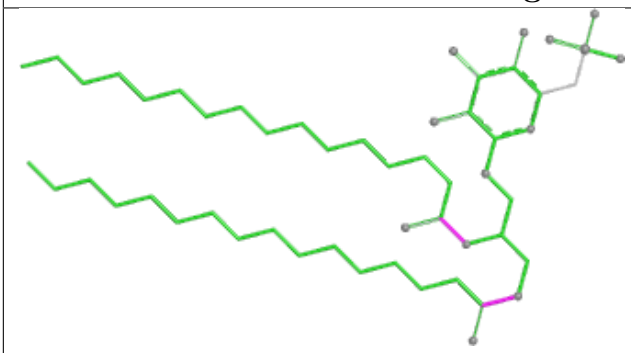


**Torsions**

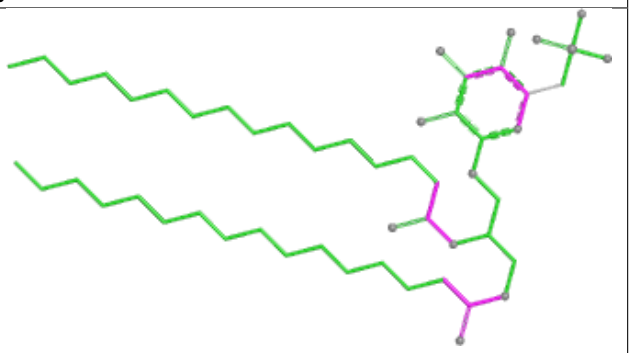


**Rings**

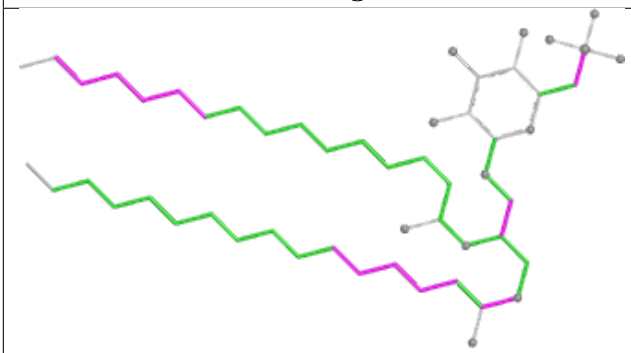
**Ligand SQD A 416**



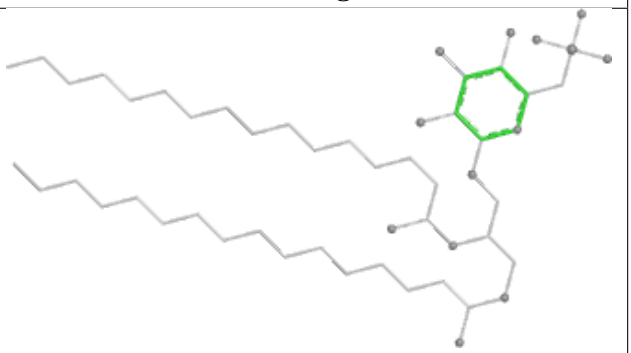
Bond lengths



Bond angles

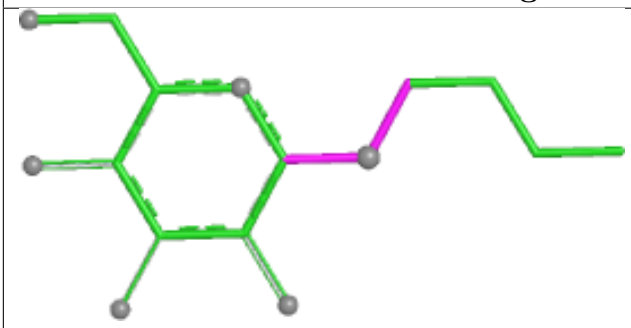


Torsions

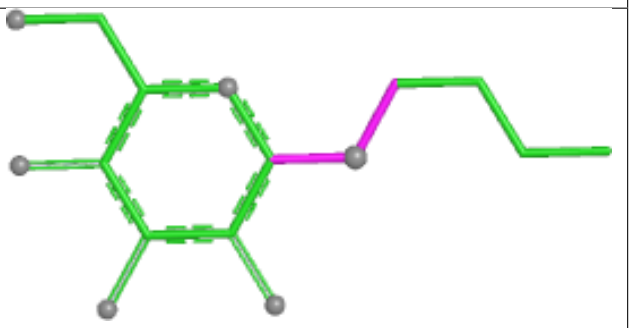


Rings

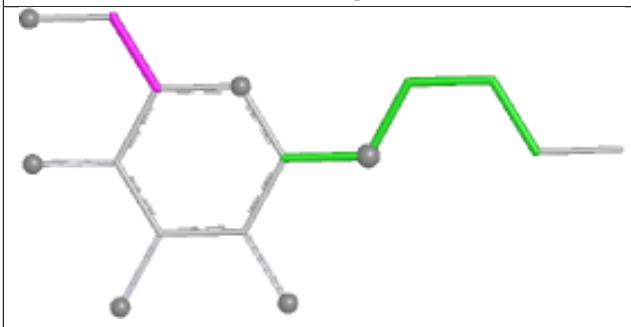
**Ligand HTG D 411**



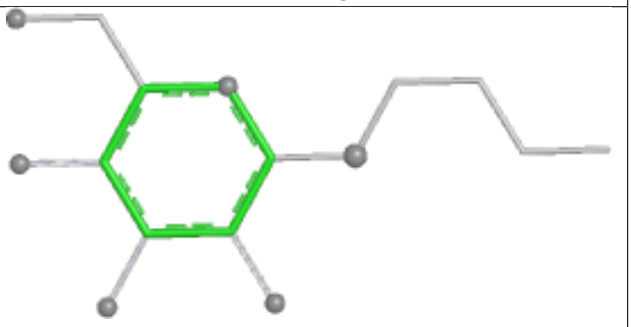
Bond lengths



Bond angles

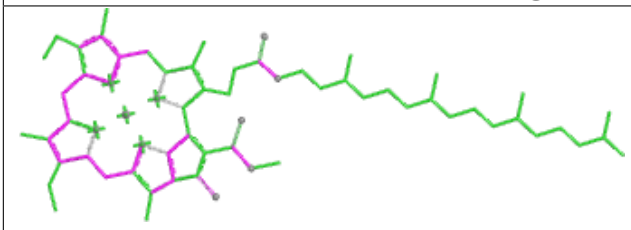


Torsions

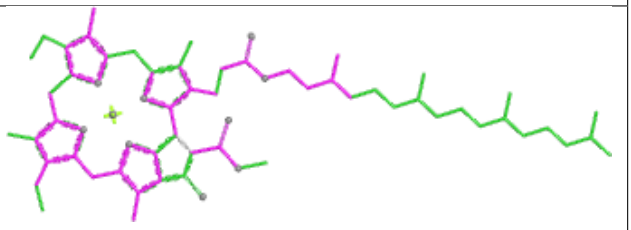


Rings

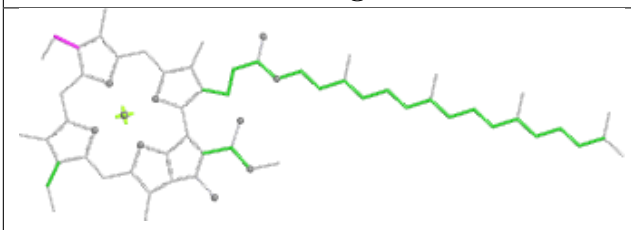
## Ligand CLA d 402



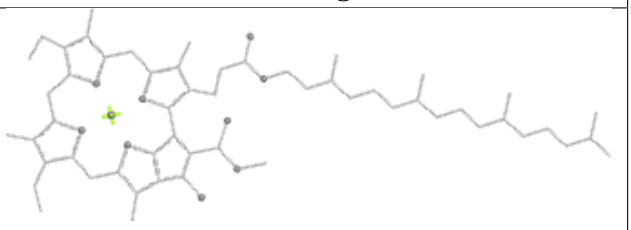
Bond lengths



Bond angles



Torsions

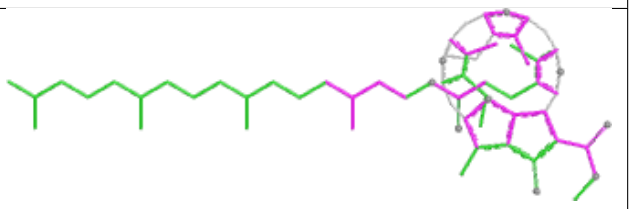


Rings

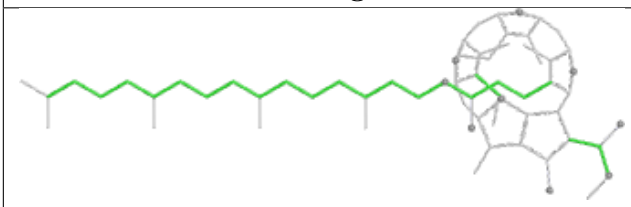
## Ligand PHO A 409



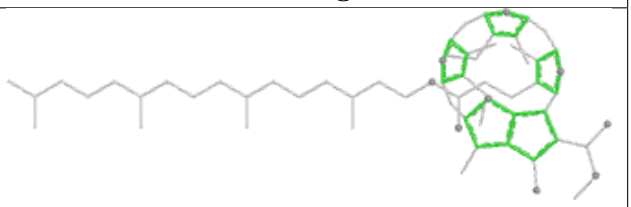
Bond lengths



Bond angles

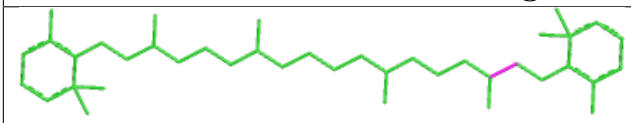


Torsions

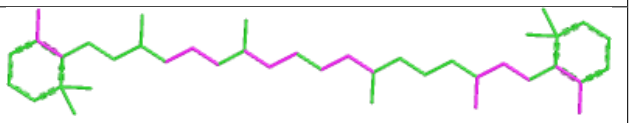


Rings

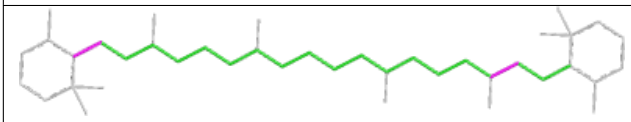
## Ligand BCR K 102



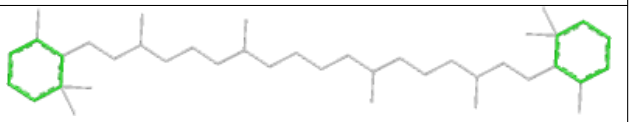
Bond lengths



Bond angles

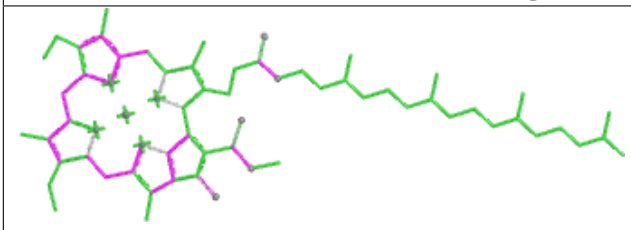


Torsions

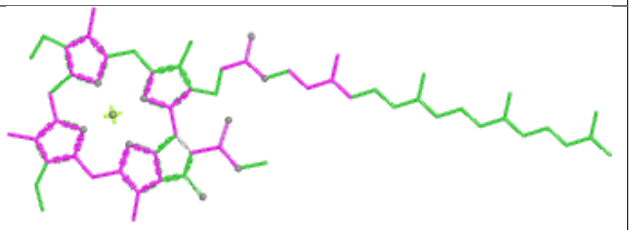


Rings

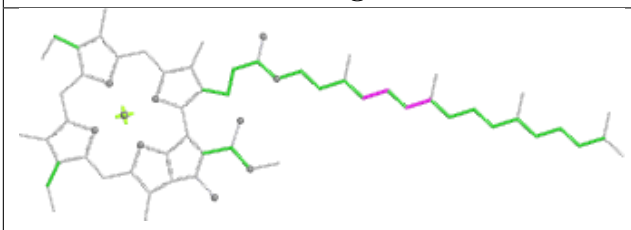
## Ligand CLA B 605



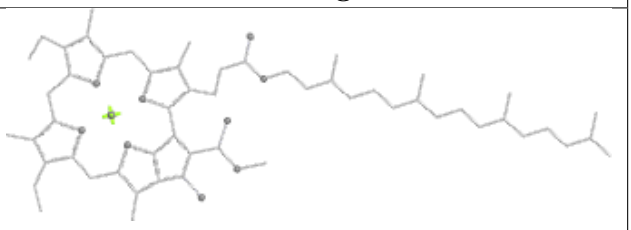
Bond lengths



Bond angles

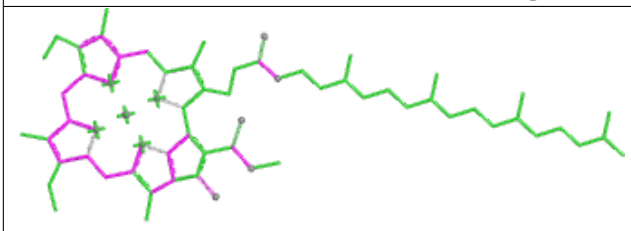


Torsions

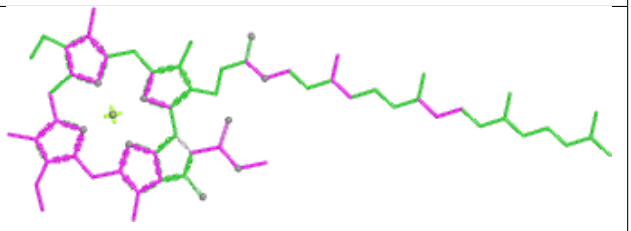


Rings

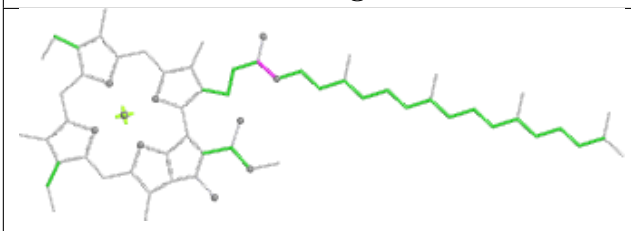
## Ligand CLA C 512



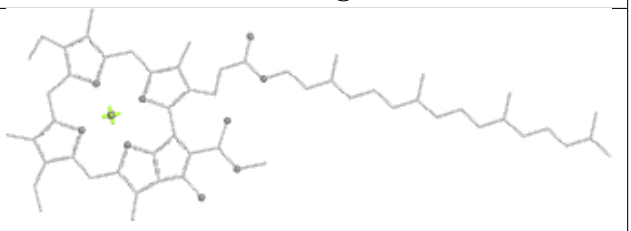
Bond lengths



Bond angles

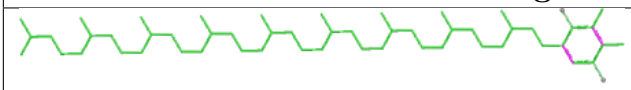


Torsions

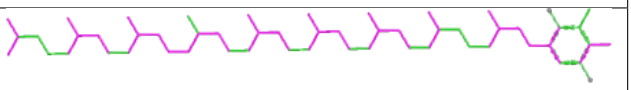


Rings

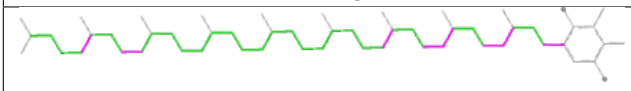
## Ligand PL9 a 417



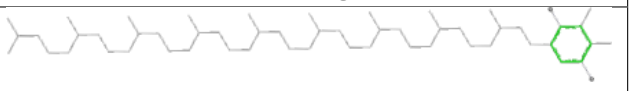
Bond lengths



Bond angles

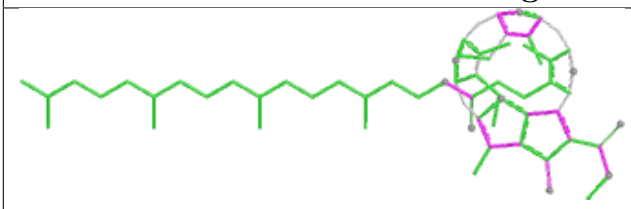


Torsions

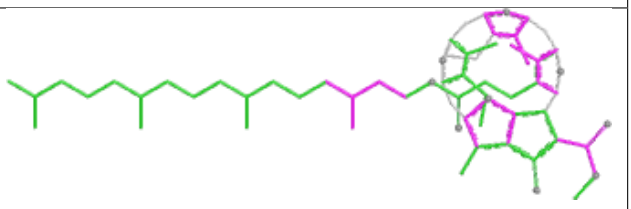


Rings

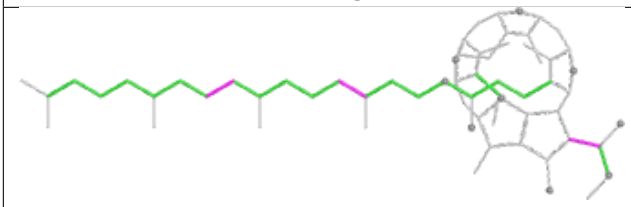
## Ligand PHO A 408



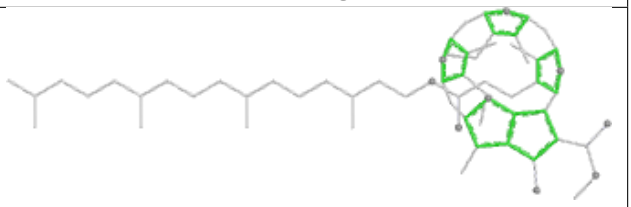
Bond lengths



Bond angles



Torsions

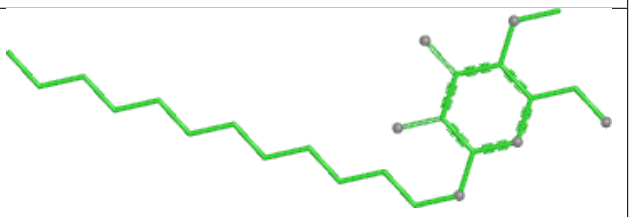


Rings

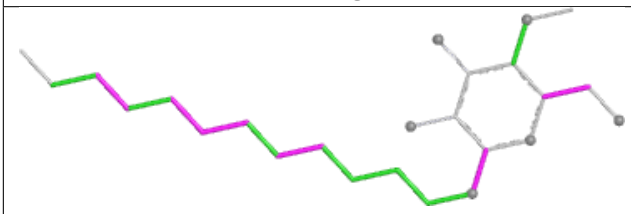
## Ligand LMT B 636



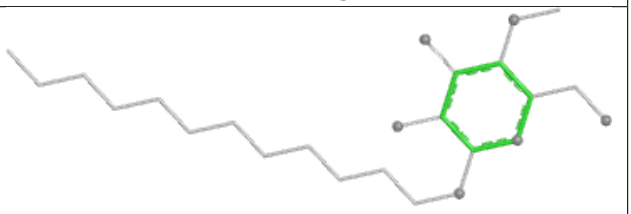
Bond lengths



Bond angles

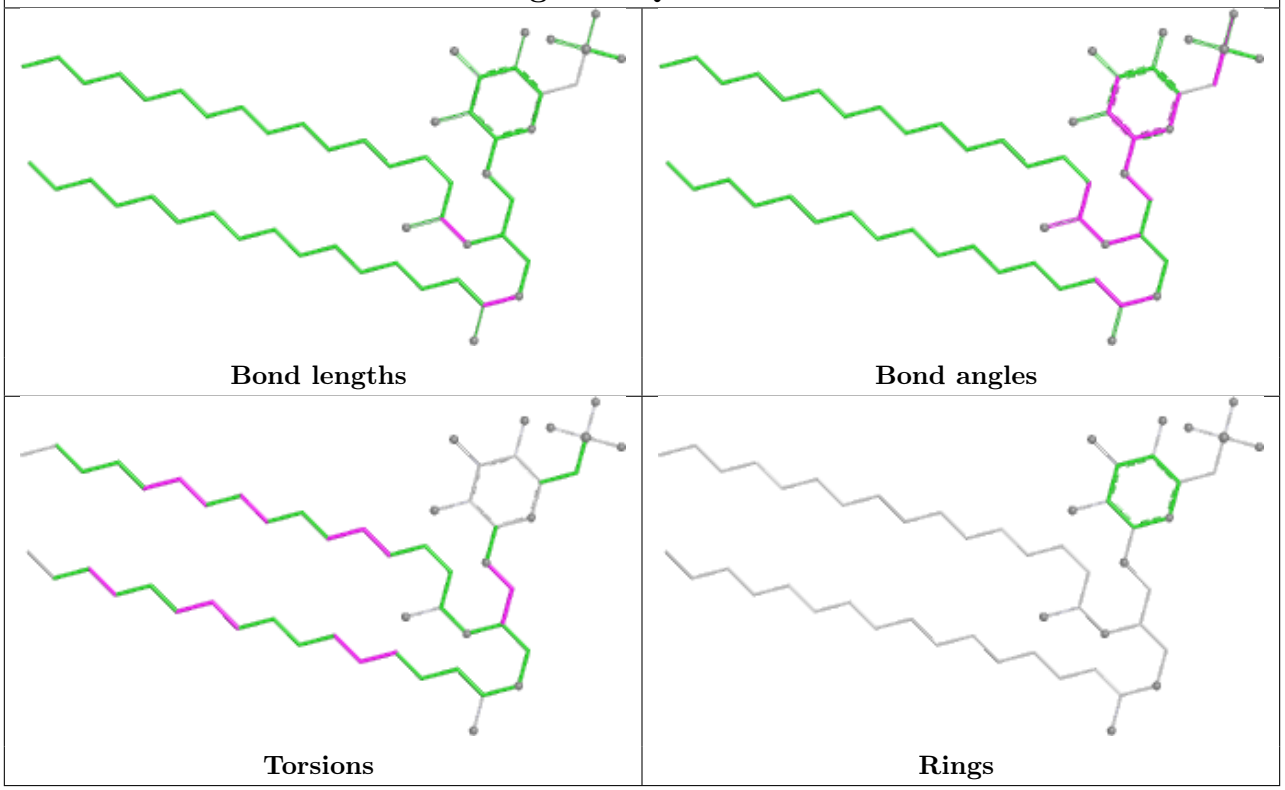


Torsions

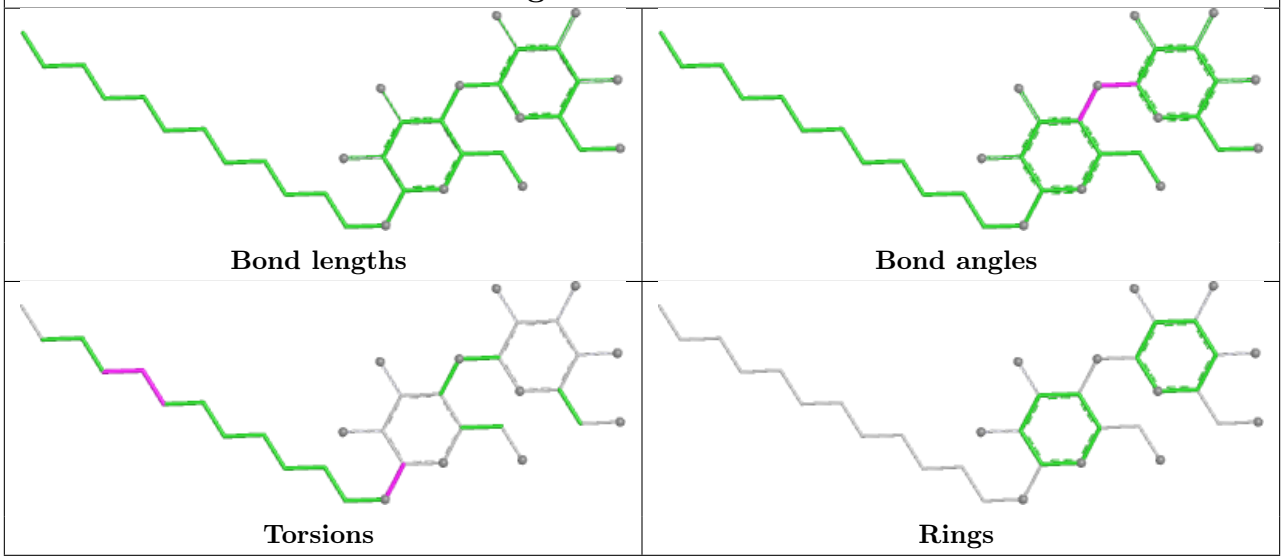


Rings

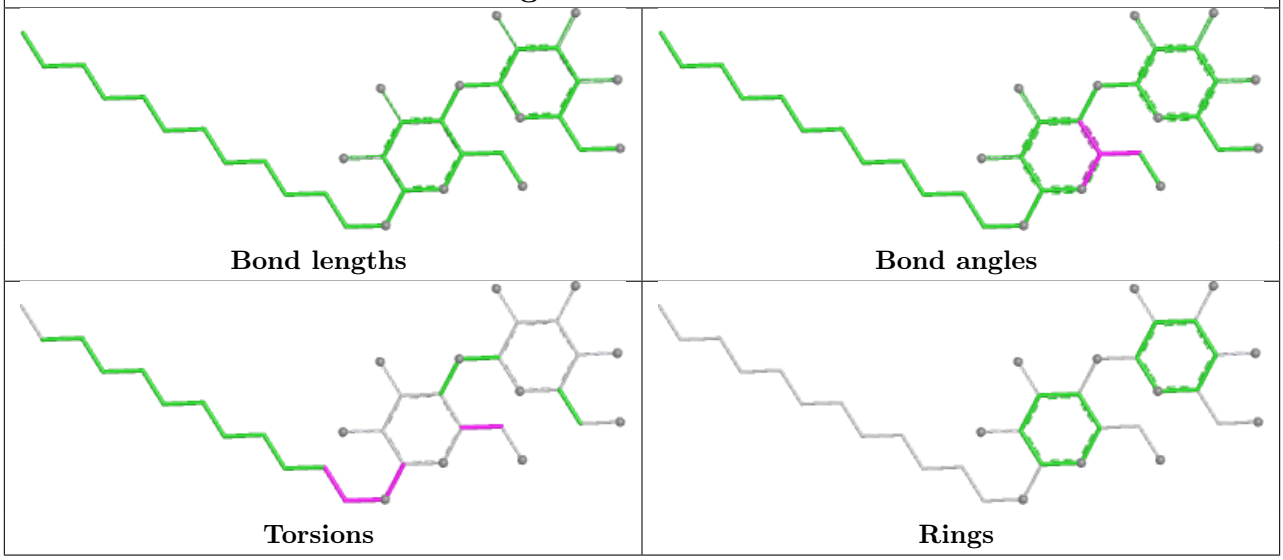
### Ligand SQD a 411



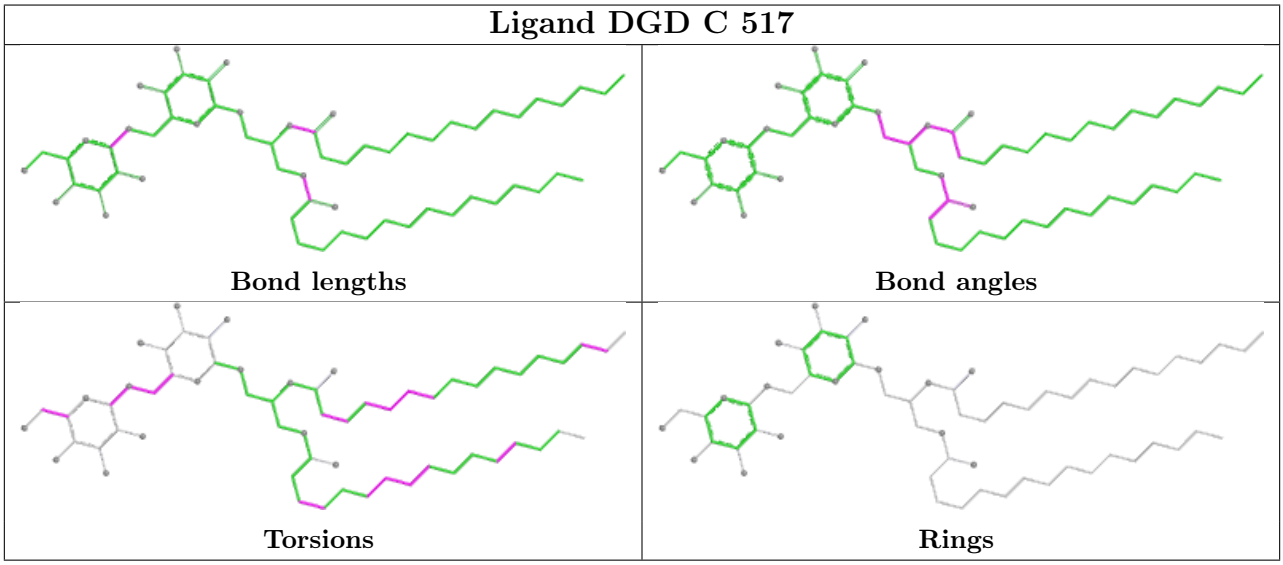

### Ligand LMT c 921



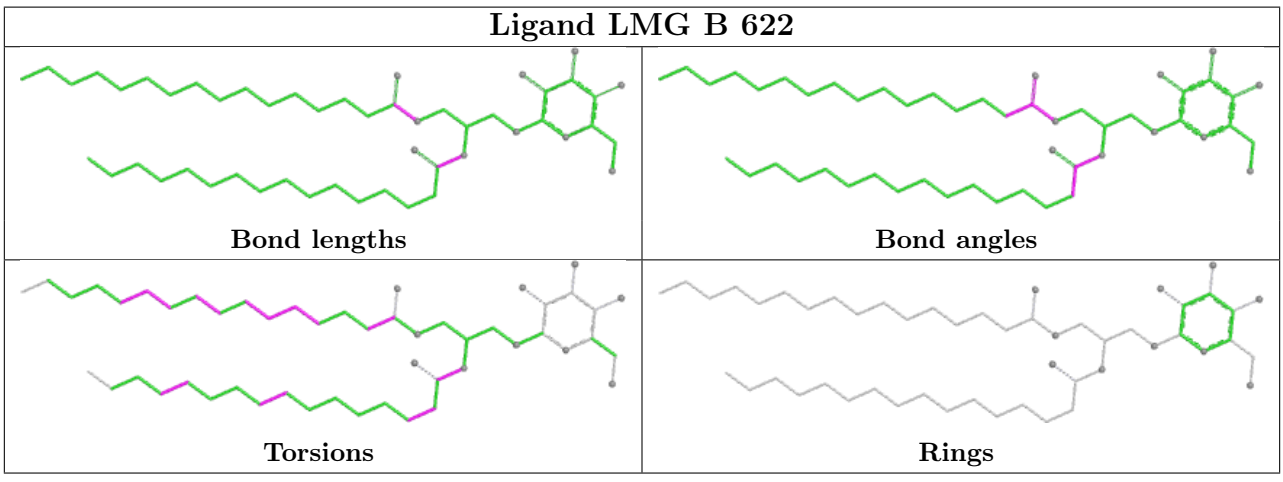
## Ligand LMT m 102



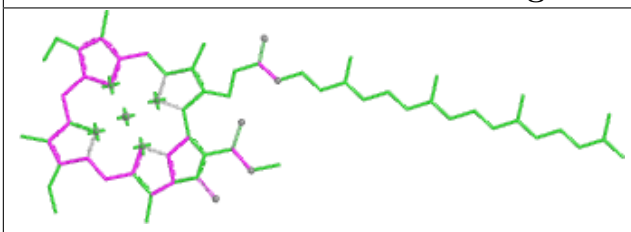

## Ligand DGD C 517



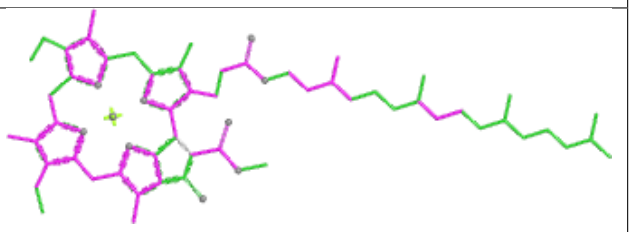

## Ligand LMG B 622



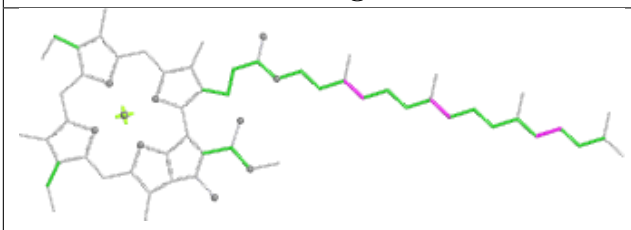
## Ligand CLA b 612



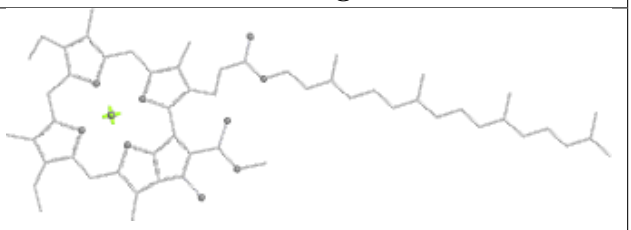
Bond lengths



Bond angles



Torsions



Rings

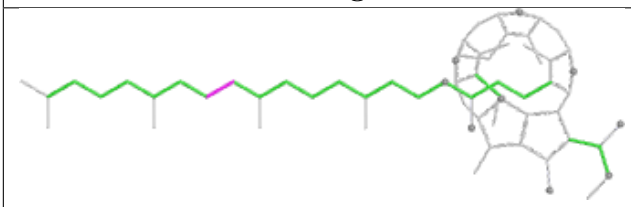
## Ligand PHO a 408



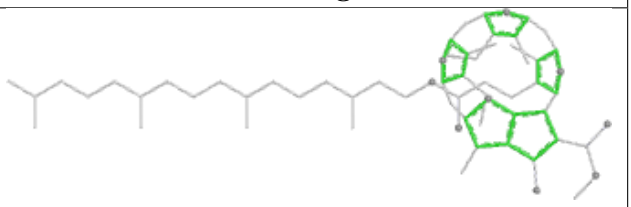
Bond lengths



Bond angles

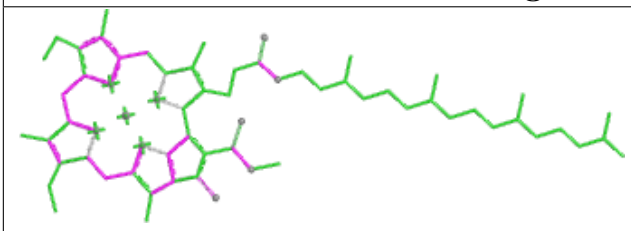


Torsions

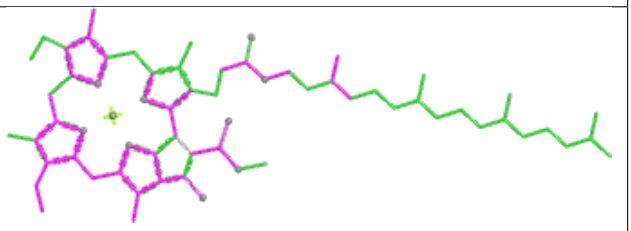


Rings

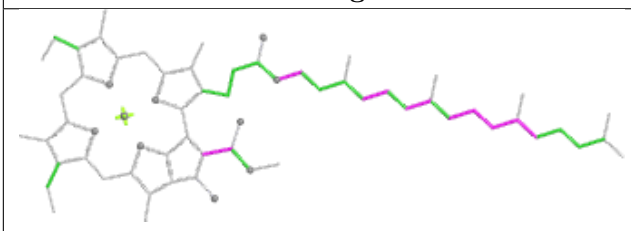
## Ligand CLA B 617



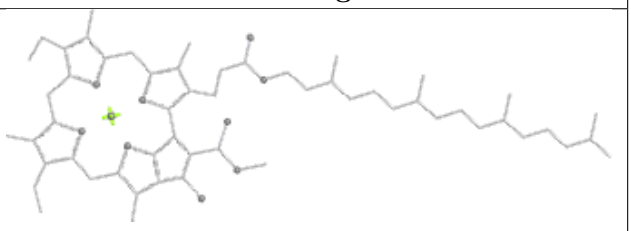
Bond lengths



Bond angles

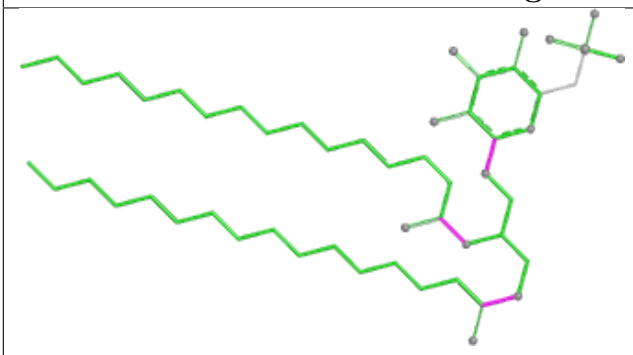


Torsions

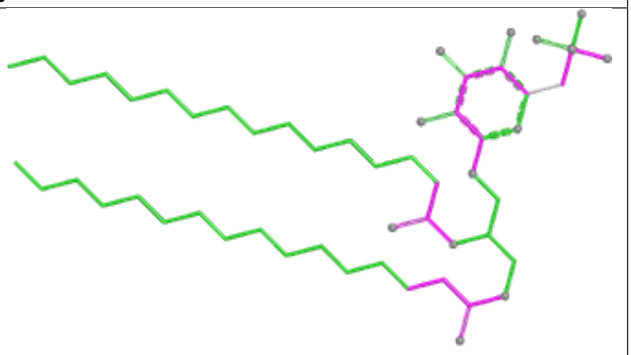


Rings

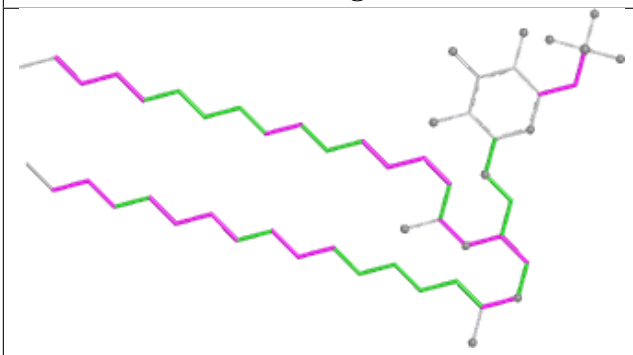
## Ligand SQD B 621



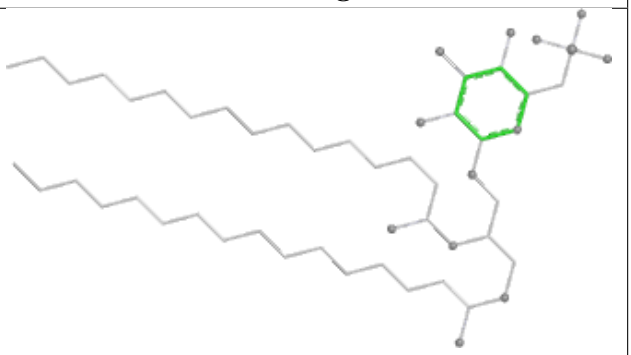
Bond lengths



Bond angles



Torsions

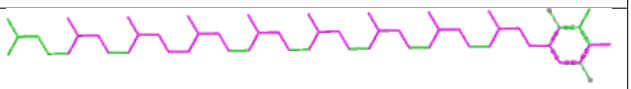


Rings

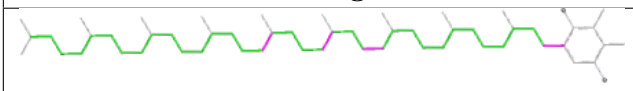
## Ligand PL9 A 419



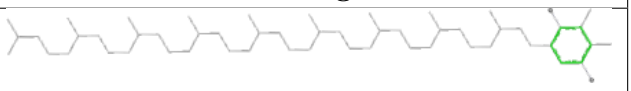
Bond lengths



Bond angles

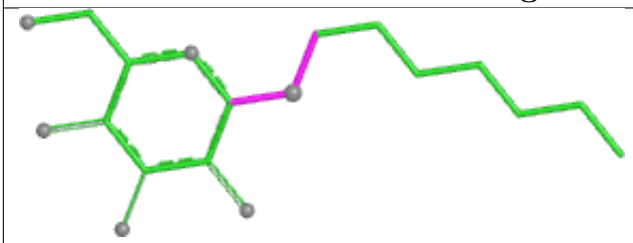


Torsions

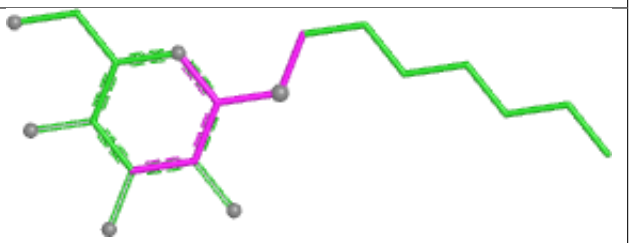


Rings

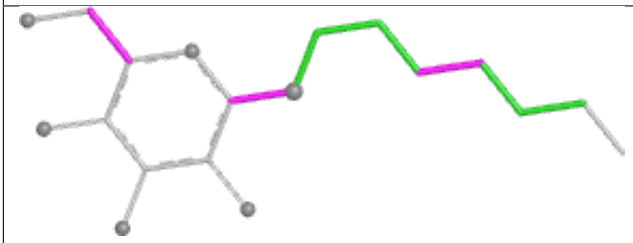
## Ligand HTG V 202



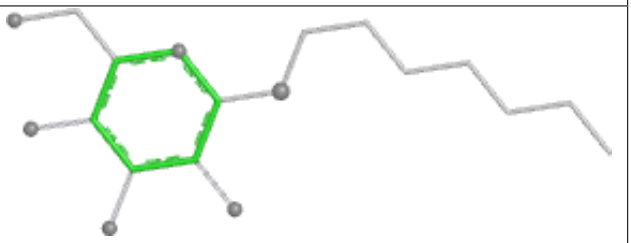
Bond lengths



Bond angles

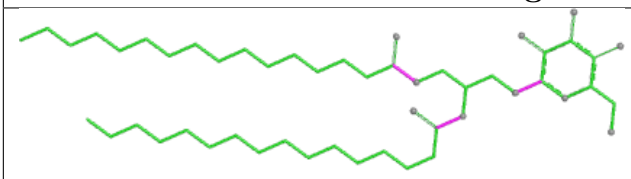


Torsions

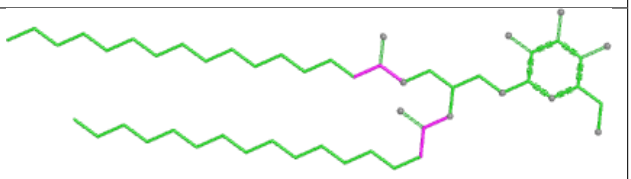


Rings

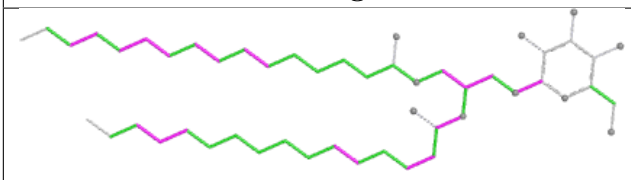
## Ligand LMG c 919



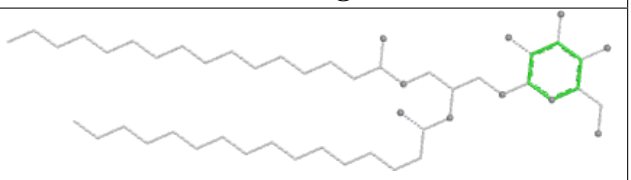
Bond lengths



Bond angles

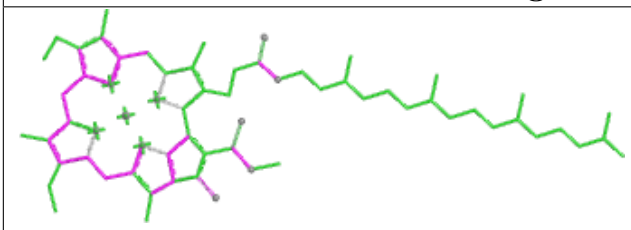


Torsions

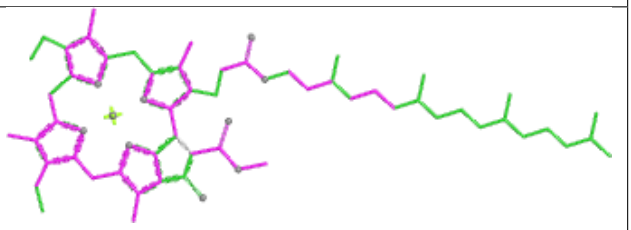


Rings

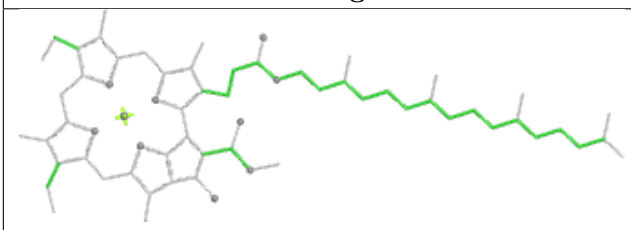
## Ligand CLA b 613



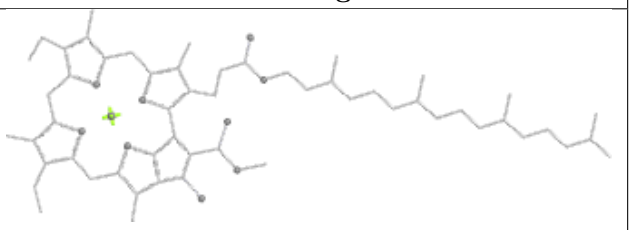
Bond lengths



Bond angles



Torsions



Rings

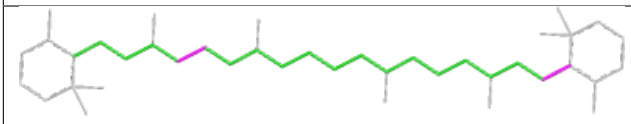
## Ligand BCR h 101



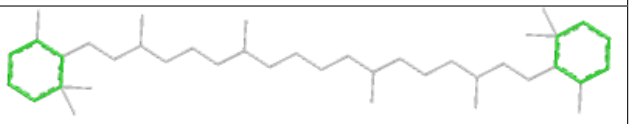
Bond lengths



Bond angles

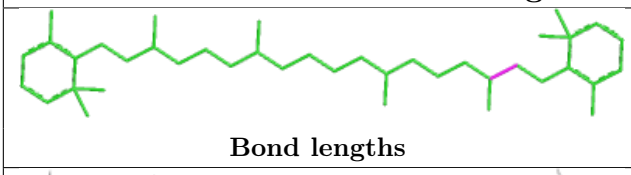


Torsions

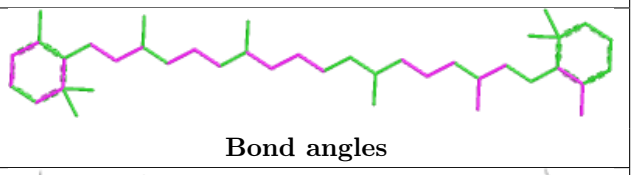


Rings

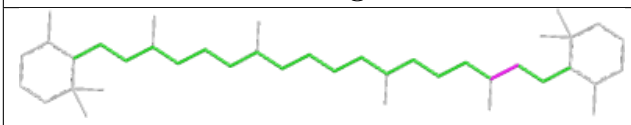
### Ligand BCR b 623



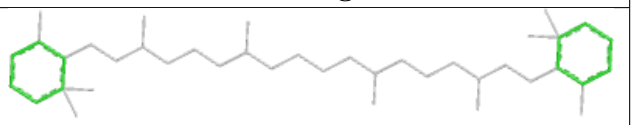
Bond lengths



Bond angles

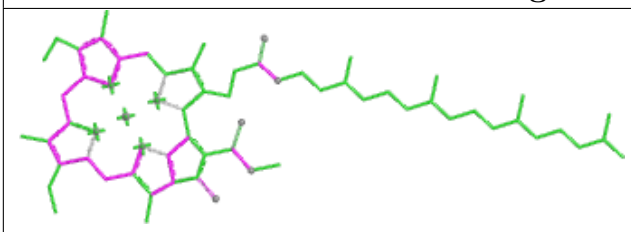


Torsions

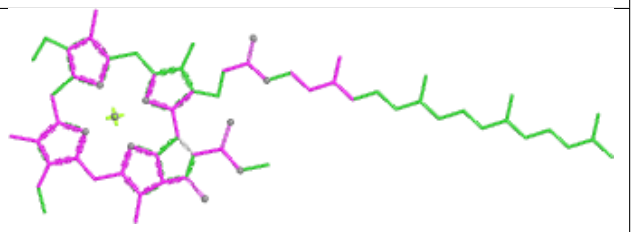


Rings

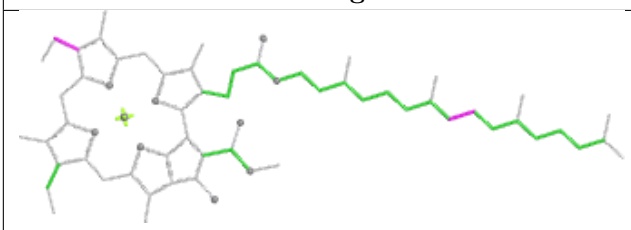
### Ligand CLA c 904



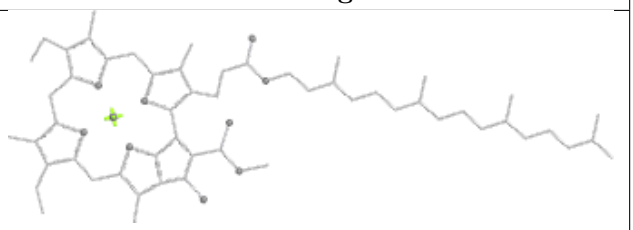
Bond lengths



Bond angles

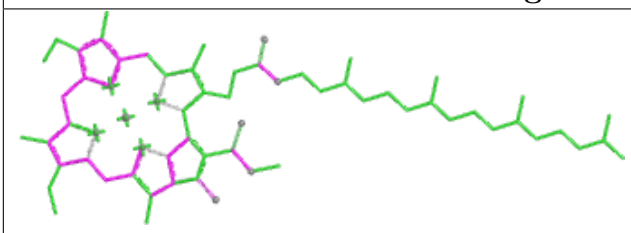


Torsions

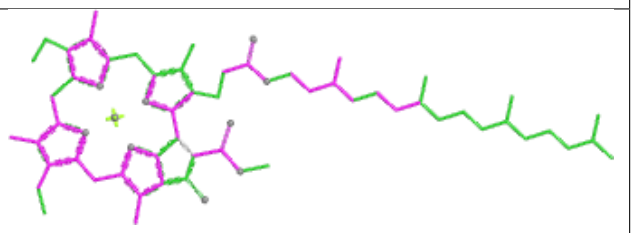


Rings

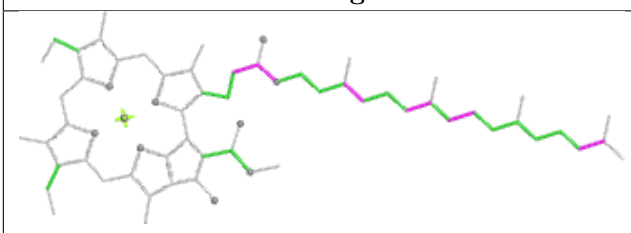
### Ligand CLA C 511



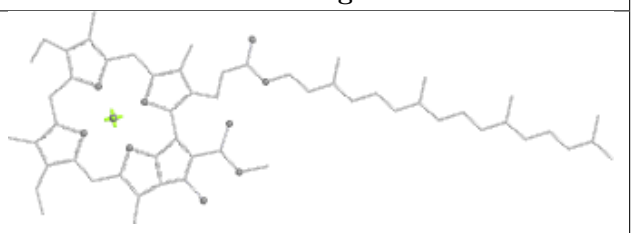
Bond lengths



Bond angles

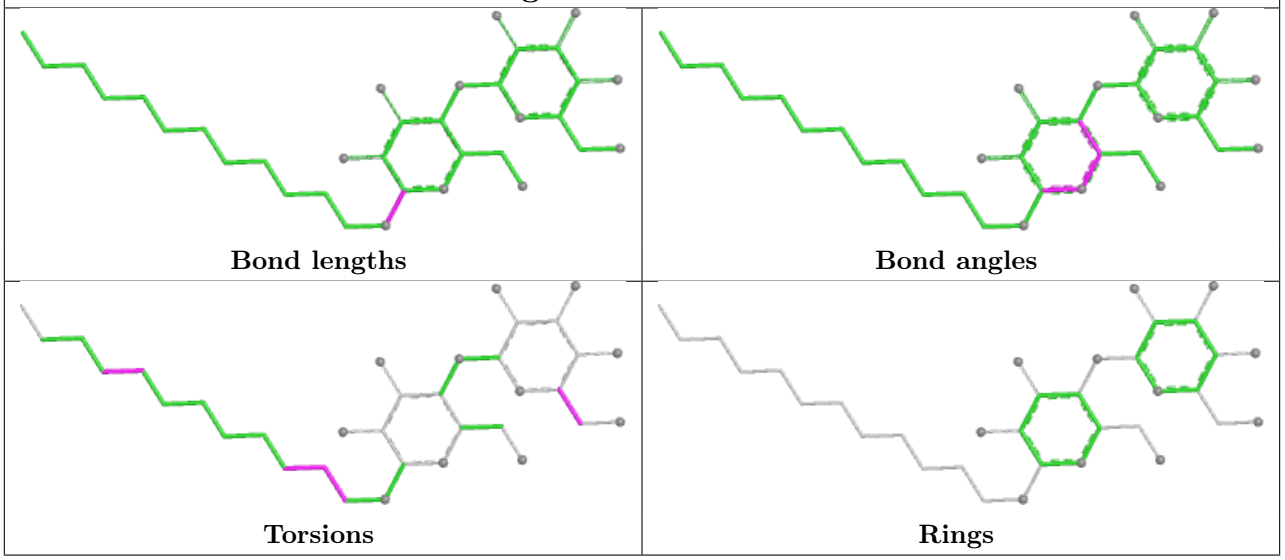


Torsions

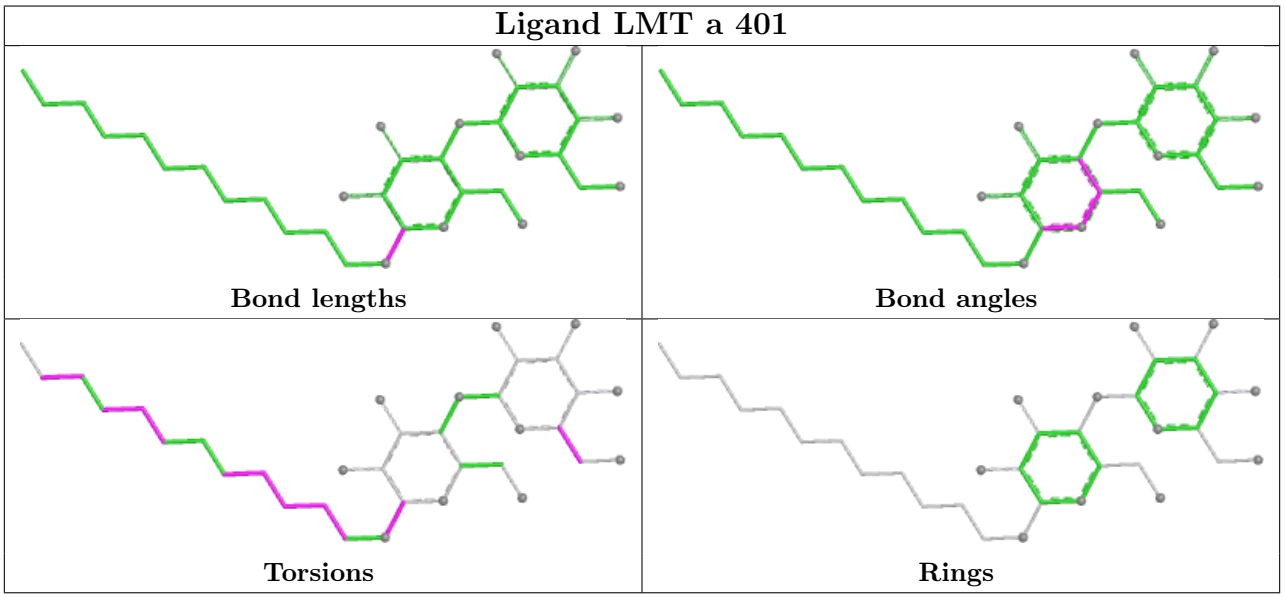


Rings

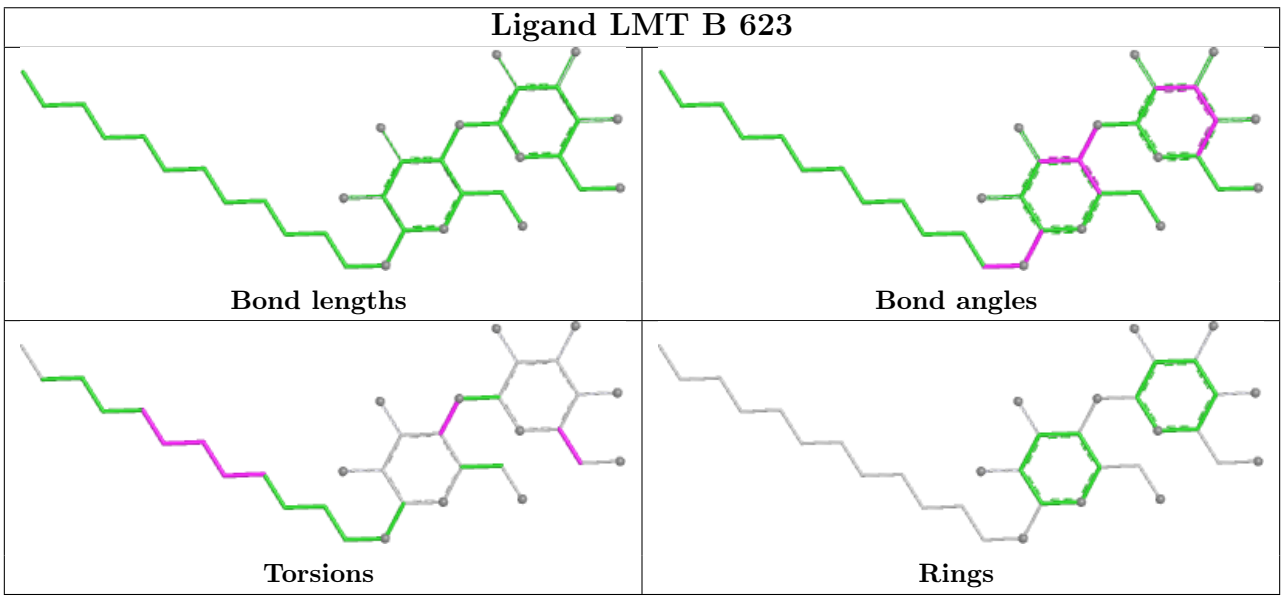
## Ligand LMT A 417



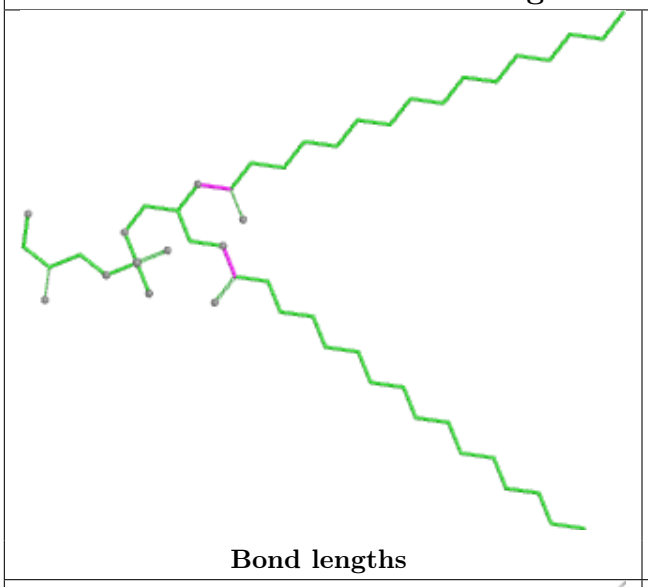

## Ligand LMT a 401



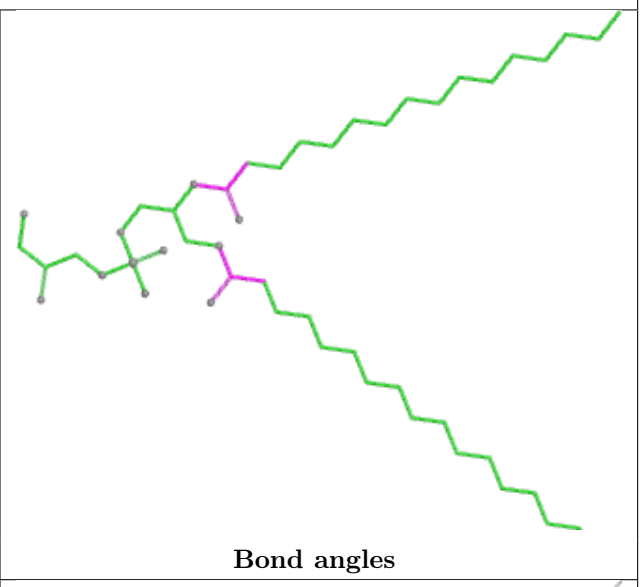

## Ligand LMT B 623



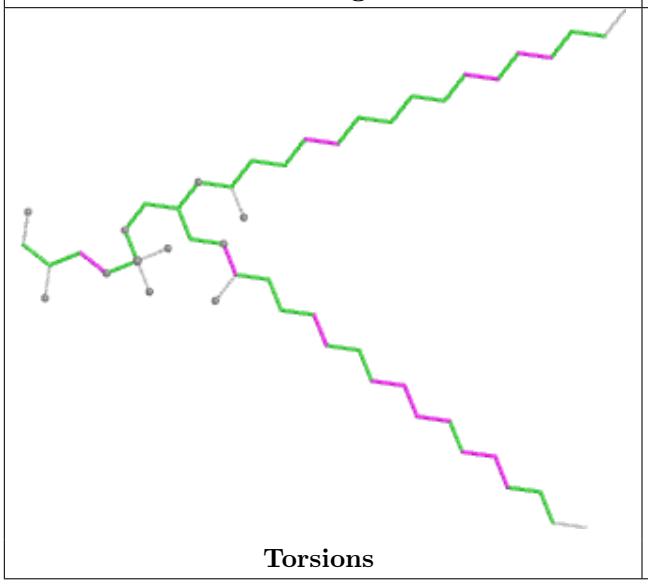
**Ligand LHG d 409**



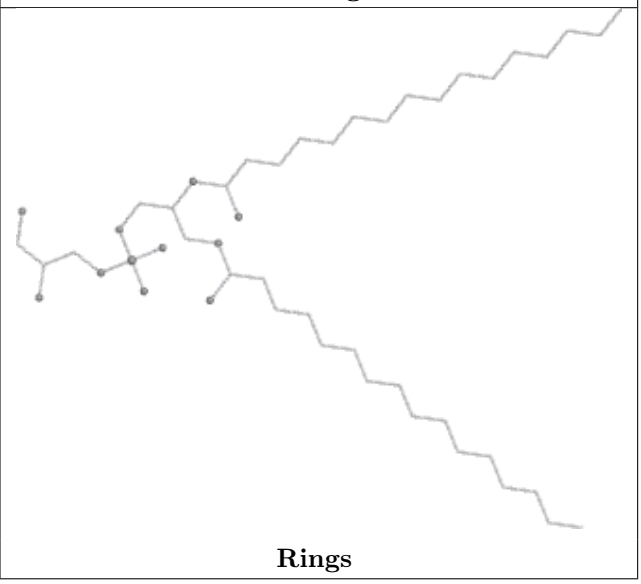
Bond lengths



Bond angles

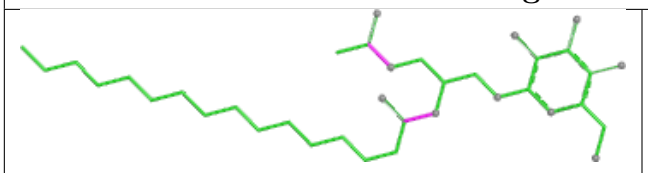


Torsions

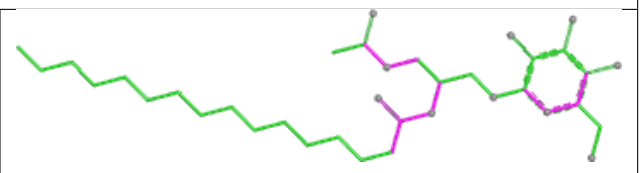


Rings

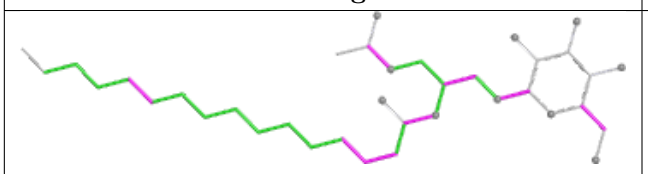
**Ligand LMG Z 101**



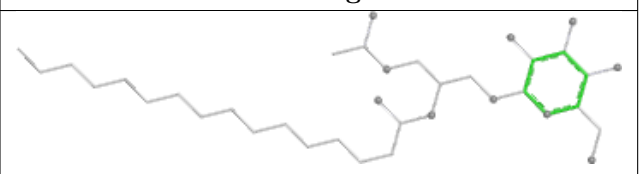
Bond lengths



Bond angles

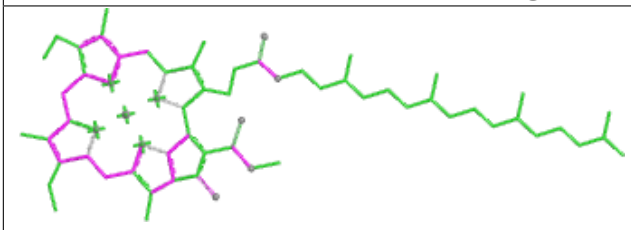


Torsions

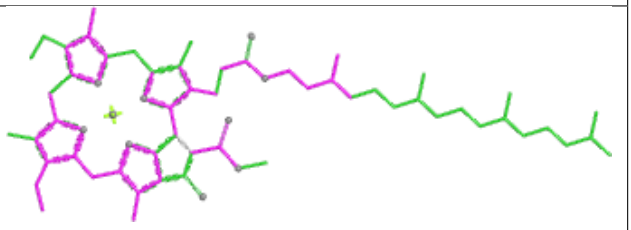


Rings

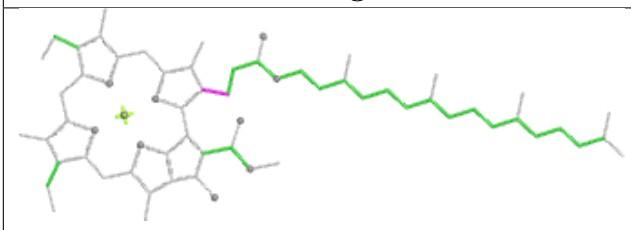
## Ligand CLA C 514



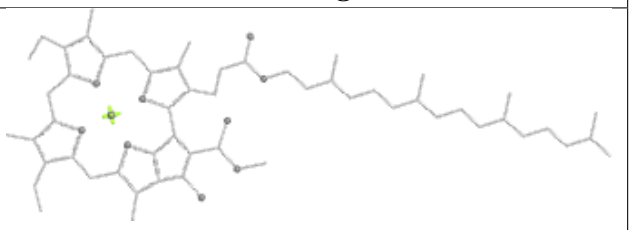
Bond lengths



Bond angles



Torsions

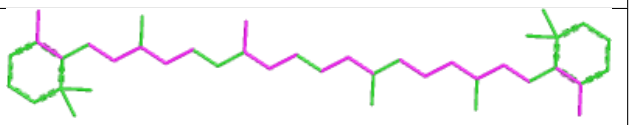


Rings

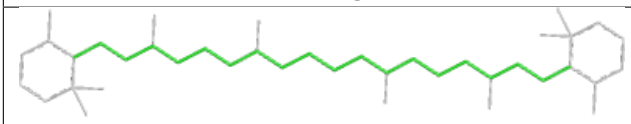
## Ligand BCR k 101



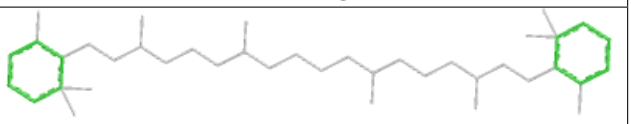
Bond lengths



Bond angles

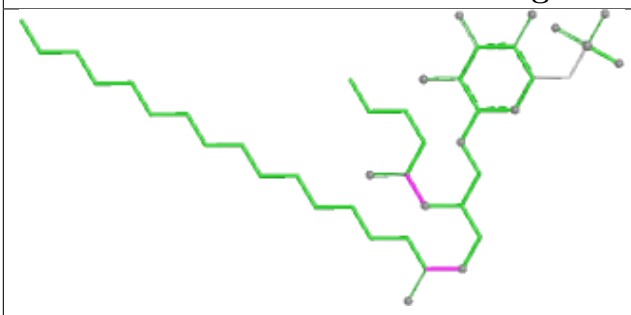


Torsions

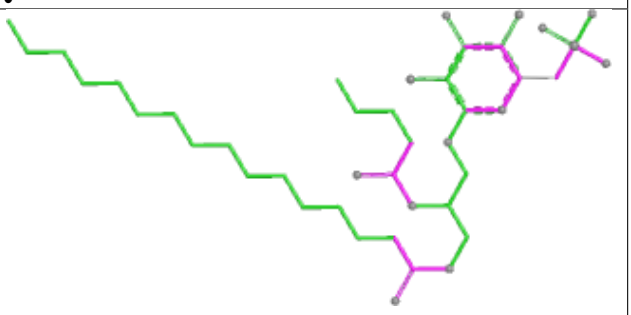


Rings

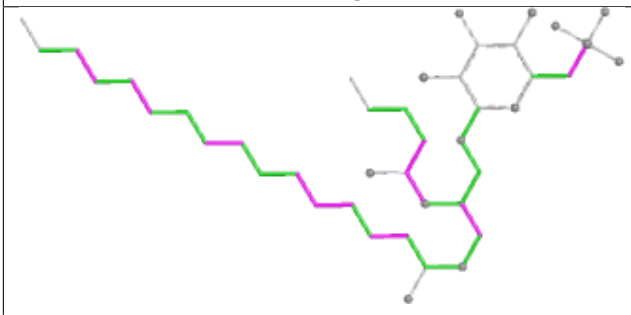
## Ligand SQD f 102



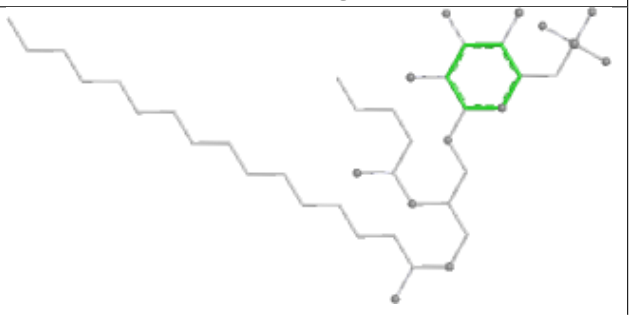
Bond lengths



Bond angles

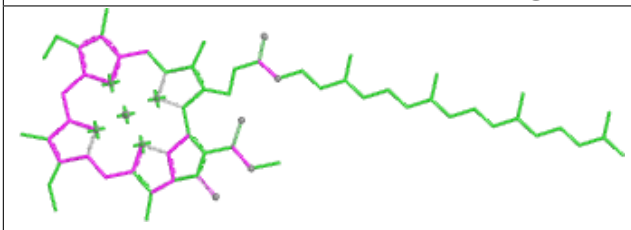


Torsions

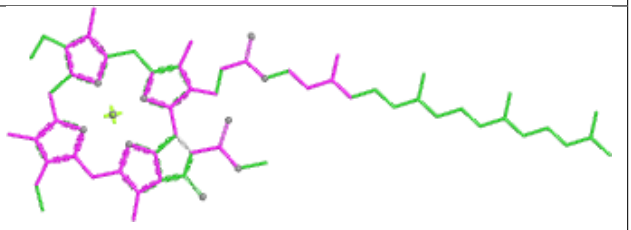


Rings

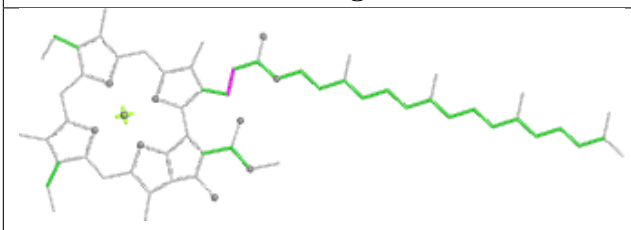
### Ligand CLA b 606



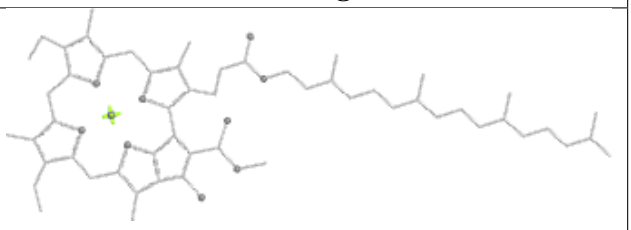
Bond lengths



Bond angles



Torsions

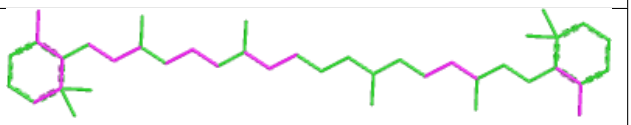


Rings

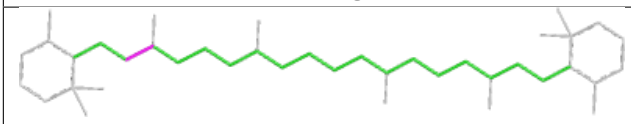
### Ligand BCR K 103



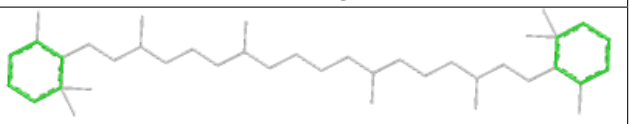
Bond lengths



Bond angles

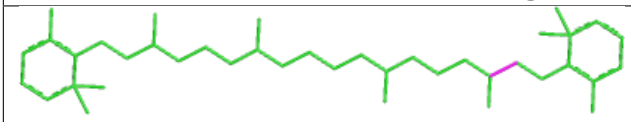


Torsions

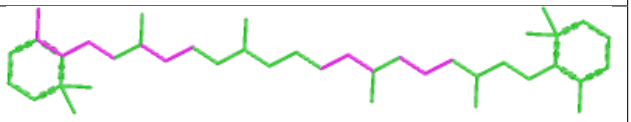


Rings

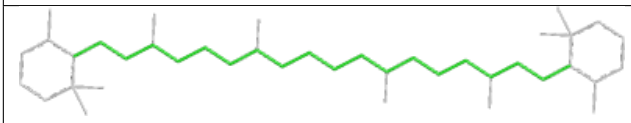
### Ligand BCR A 411



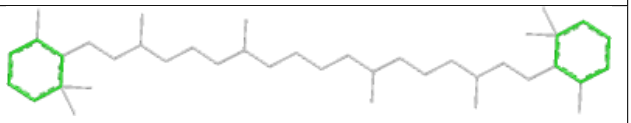
Bond lengths



Bond angles

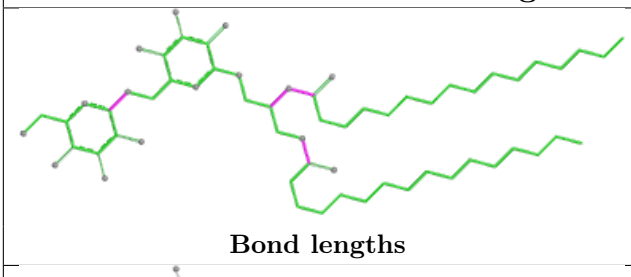


Torsions

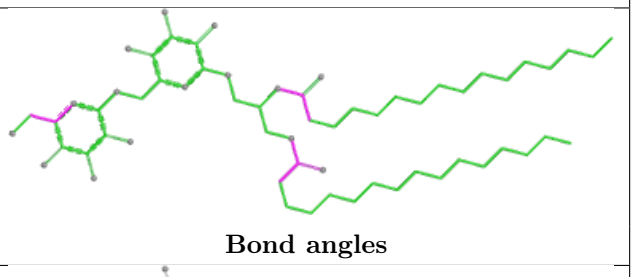


Rings

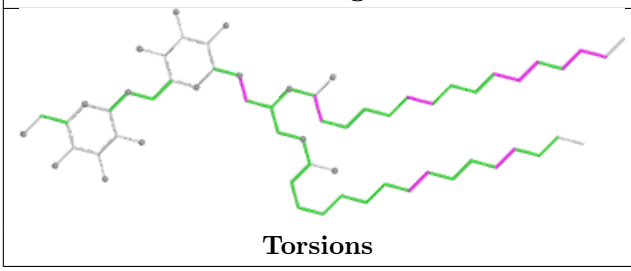
## Ligand DGD H 102



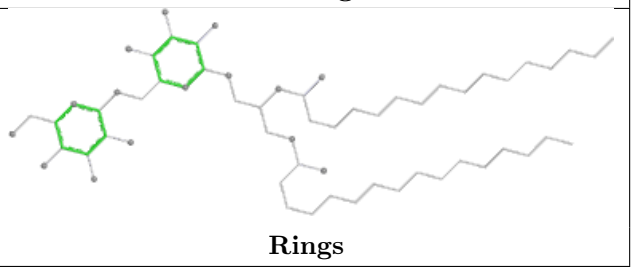
Bond lengths



Bond angles

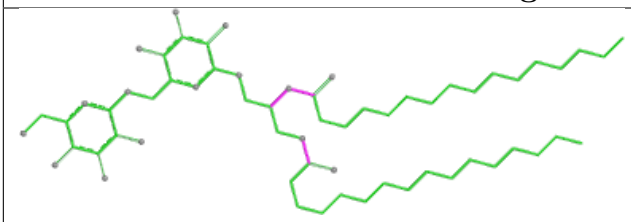


Torsions

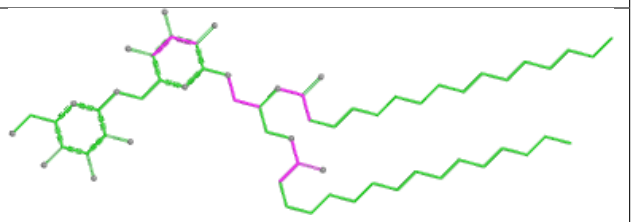


Rings

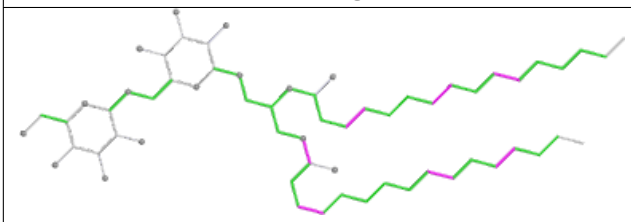
## Ligand DGD C 519



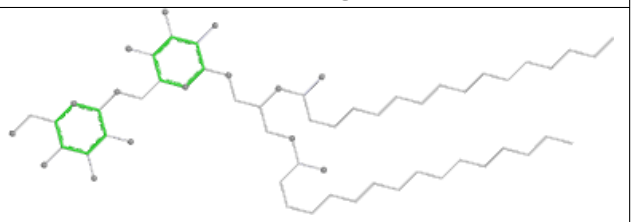
Bond lengths



Bond angles

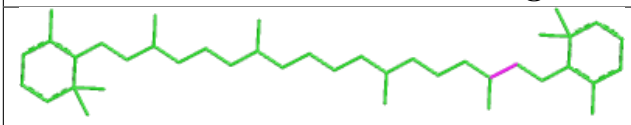


Torsions

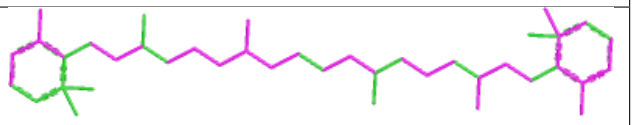


Rings

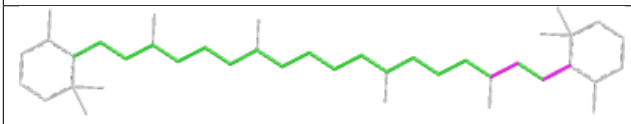
## Ligand BCR d 404



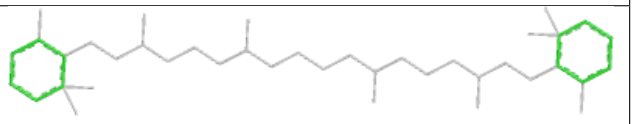
Bond lengths



Bond angles

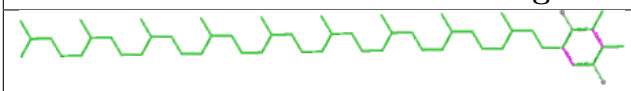


Torsions

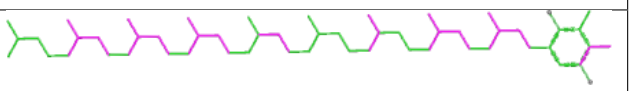


Rings

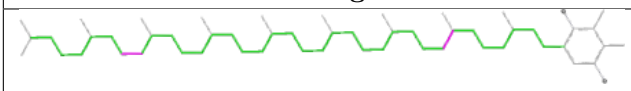
### Ligand PL9 d 405



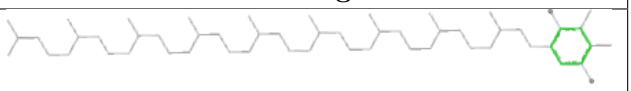
Bond lengths



Bond angles

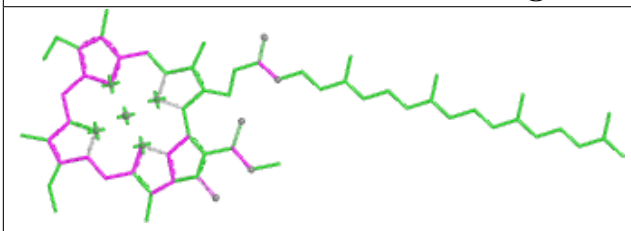


Torsions

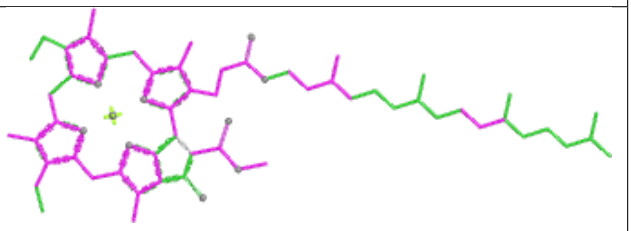


Rings

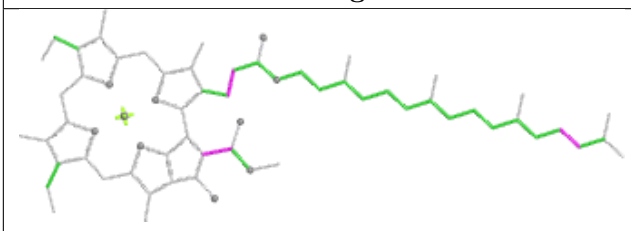
### Ligand CLA b 614



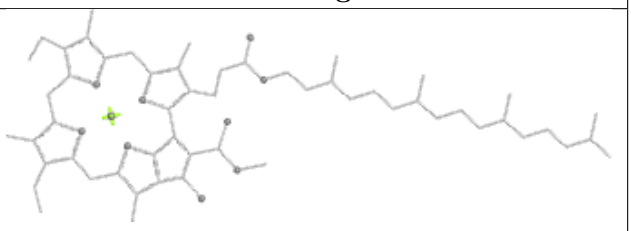
Bond lengths



Bond angles

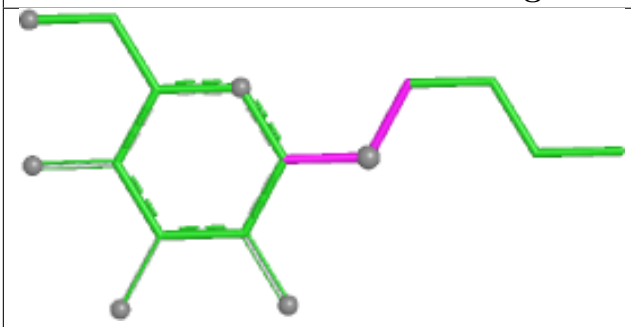


Torsions

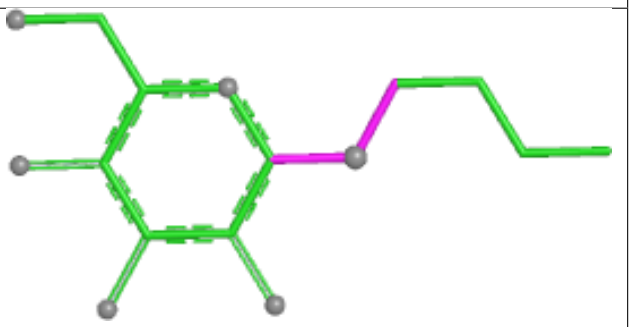


Rings

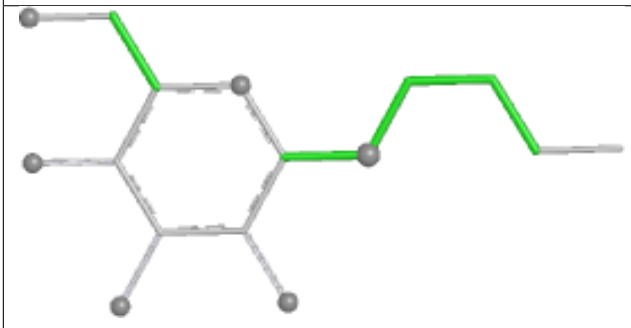
### Ligand HTG d 412



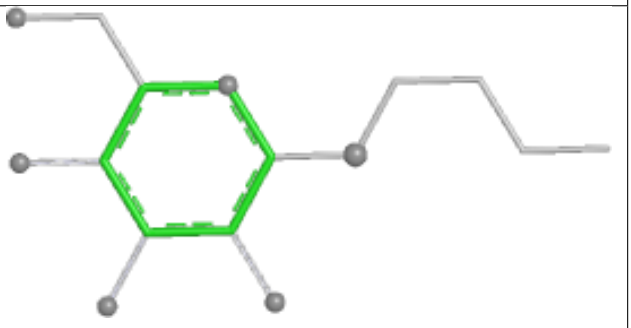
Bond lengths



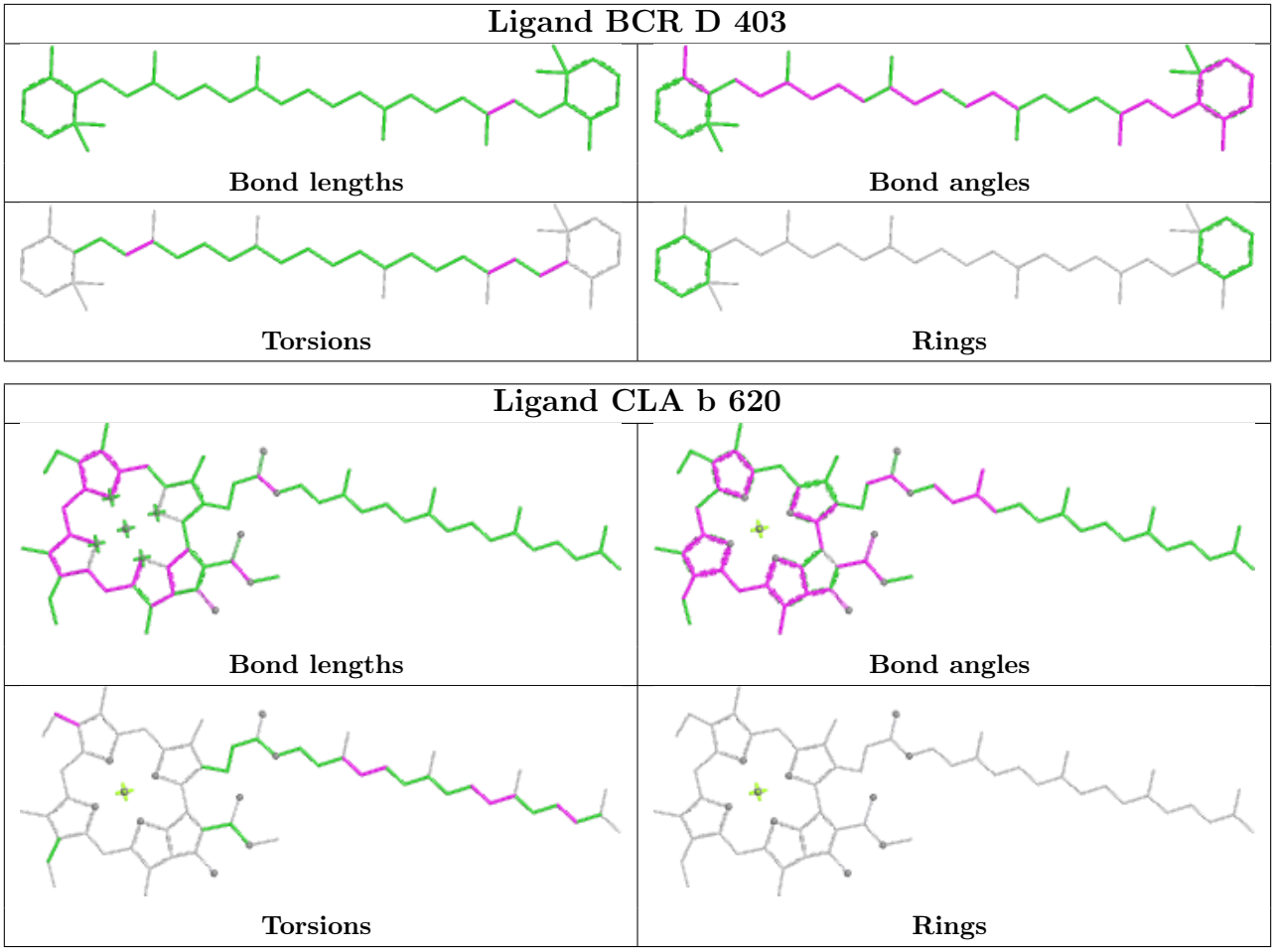
Bond angles



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 | 334/344 (97%) | -0.08 | 6 (1%) 67 75 | 13, 21, 37, 73 | 3 (0%) |
| 1 | a | 334/344 (97%) | 0.05 | 9 (2%) 56 62 | 15, 23, 47, 90 | 6 (1%) |
| 2 | B | 504/505 (99%) | 0.20 | 19 (3%) 44 50 | 14, 25, 48, 78 | 11 (2%) |
| 2 | b | 504/505 (99%) | 0.28 | 31 (6%) 26 31 | 16, 27, 58, 92 | 12 (2%) |
| 3 | C | 451/455 (99%) | 0.34 | 19 (4%) 40 47 | 17, 30, 46, 73 | 4 (0%) |
| 3 | c | 455/455 (100%) | 0.42 | 17 (3%) 45 52 | 16, 33, 49, 92 | 6 (1%) |
| 4 | D | 342/342 (100%) | -0.09 | 5 (1%) 72 78 | 11, 22, 37, 97 | 1 (0%) |
| 4 | d | 341/342 (99%) | -0.03 | 2 (0%) 85 89 | 12, 25, 39, 90 | 1 (0%) |
| 5 | E | 81/84 (96%) | 0.98 | 8 (9%) 13 14 | 20, 37, 66, 92 | 2 (2%) |
| 5 | e | 81/84 (96%) | 1.29 | 17 (20%) 2 2 | 23, 41, 71, 92 | 2 (2%) |
| 6 | F | 34/44 (77%) | 0.57 | 4 (11%) 9 10 | 23, 30, 50, 61 | 0 |
| 6 | f | 32/44 (72%) | 0.84 | 3 (9%) 14 16 | 30, 34, 79, 84 | 0 |
| 7 | H | 65/65 (100%) | 0.66 | 4 (6%) 26 31 | 18, 31, 46, 110 | 1 (1%) |
| 7 | h | 65/65 (100%) | 0.91 | 7 (10%) 11 12 | 27, 35, 52, 105 | 0 |
| 8 | I | 37/38 (97%) | 1.13 | 6 (16%) 4 5 | 26, 33, 88, 108 | 0 |
| 8 | i | 37/38 (97%) | 0.92 | 6 (16%) 4 5 | 27, 33, 73, 102 | 0 |
| 9 | J | 38/39 (97%) | 1.07 | 6 (15%) 5 5 | 24, 35, 84, 98 | 0 |
| 9 | j | 39/39 (100%) | 1.10 | 7 (17%) 3 3 | 29, 38, 84, 96 | 0 |
| 10 | K | 37/37 (100%) | 0.79 | 3 (8%) 18 21 | 27, 35, 54, 65 | 0 |
| 10 | k | 37/37 (100%) | 1.07 | 5 (13%) 7 7 | 30, 38, 55, 68 | 0 |
| 11 | L | 37/37 (100%) | 0.04 | 3 (8%) 18 21 | 11, 19, 56, 82 | 1 (2%) |
| 11 | l | 37/37 (100%) | 0.18 | 2 (5%) 31 37 | 11, 20, 58, 83 | 1 (2%) |
| 12 | M | 33/36 (91%) | 0.27 | 3 (9%) 15 17 | 13, 21, 45, 89 | 1 (3%) |
| 12 | m | 33/36 (91%) | 0.16 | 2 (6%) 27 31 | 16, 21, 41, 88 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | O | 243/244 (99%) | 0.48 | 17 (6%) 22 26 | 16, 31, 66, 110 | 8 (3%) |
| 13 | o | 243/244 (99%) | 0.64 | 31 (12%) 7 9 | 15, 33, 71, 125 | 5 (2%) |
| 14 | T | 29/32 (90%) | 0.21 | 2 (6%) 23 26 | 16, 20, 43, 89 | 1 (3%) |
| 14 | t | 29/32 (90%) | 0.29 | 2 (6%) 23 26 | 16, 20, 46, 89 | 1 (3%) |
| 15 | U | 97/104 (93%) | 0.47 | 4 (4%) 41 48 | 21, 31, 54, 84 | 0 |
| 15 | u | 97/104 (93%) | 0.33 | 2 (2%) 63 70 | 23, 33, 51, 84 | 0 |
| 16 | V | 137/137 (100%) | 0.42 | 5 (3%) 46 53 | 16, 31, 51, 69 | 1 (0%) |
| 16 | v | 137/137 (100%) | 0.52 | 5 (3%) 46 53 | 24, 36, 57, 70 | 0 |
| 17 | Y | 29/30 (96%) | 2.02 | 10 (34%) 1 0 | 35, 47, 82, 101 | 0 |
| 17 | y | 29/30 (96%) | 2.00 | 14 (48%) 0 0 | 38, 50, 83, 100 | 0 |
| 18 | X | 39/40 (97%) | 1.40 | 8 (20%) 2 2 | 31, 38, 75, 102 | 0 |
| 18 | x | 39/40 (97%) | 1.20 | 7 (17%) 3 3 | 33, 41, 83, 102 | 0 |
| 19 | Z | 62/62 (100%) | 1.84 | 21 (33%) 1 0 | 36, 47, 83, 96 | 0 |
| 19 | z | 62/62 (100%) | 2.12 | 28 (45%) 0 0 | 42, 49, 82, 96 | 0 |
| 20 | R | 34/34 (100%) | 3.20 | 27 (79%) 0 0 | 54, 75, 98, 106 | 0 |
| All | All | 5294/5384 (98%) | 0.41 | 377 (7%) 22 25 | 11, 29, 61, 125 | 68 (1%) |

All (377) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 19 | z | 62 | VAL | 10.5 |
| 7 | H | 65 | LEU | 9.2 |
| 17 | Y | 18 | VAL | 8.2 |
| 7 | h | 65 | LEU | 7.4 |
| 20 | R | 24 | LEU | 7.3 |
| 19 | Z | 62 | VAL | 6.9 |
| 8 | i | 37 | LEU | 6.6 |
| 9 | j | 1 | MET | 6.4 |
| 19 | Z | 7 | LEU | 6.2 |
| 8 | I | 37 | LEU | 6.1 |
| 19 | z | 3 | ILE | 6.1 |
| 17 | Y | 19 | ILE | 6.0 |
| 1 | a | 11 | ALA | 5.9 |
| 20 | R | 28 | VAL | 5.9 |
| 14 | T | 30 | THR | 5.5 |
| 7 | H | 64 | ALA | 5.4 |
| 18 | X | 2 | THR | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | J | 4 | GLY | 5.4 |
| 9 | J | 2 | SER | 5.4 |
| 19 | Z | 3 | ILE | 5.3 |
| 2 | b | 495 | PHE | 5.3 |
| 5 | e | 5 | THR | 5.3 |
| 7 | h | 64 | ALA | 5.1 |
| 17 | y | 18 | VAL | 5.0 |
| 19 | Z | 1 | MET | 4.9 |
| 13 | o | 58 | ASN | 4.9 |
| 13 | O | 56 | PRO | 4.8 |
| 20 | R | 31 | VAL | 4.8 |
| 18 | x | 2 | THR | 4.8 |
| 14 | t | 30 | THR | 4.7 |
| 7 | h | 66 | GLY | 4.7 |
| 13 | O | 58 | ASN | 4.7 |
| 2 | b | 86[A] | ILE | 4.6 |
| 2 | b | 491 | VAL | 4.6 |
| 17 | y | 19 | ILE | 4.6 |
| 2 | b | 502 | VAL | 4.5 |
| 19 | z | 4 | LEU | 4.5 |
| 13 | O | 4 | THR | 4.5 |
| 2 | B | 479 | PHE | 4.5 |
| 2 | b | 486 | LEU | 4.5 |
| 20 | R | 23 | ILE | 4.5 |
| 8 | I | 38 | GLU | 4.5 |
| 2 | b | 493 | TRP | 4.4 |
| 18 | X | 40 | SER | 4.4 |
| 5 | e | 4 | THR | 4.4 |
| 13 | o | 63 | ALA | 4.4 |
| 11 | l | 1 | MET | 4.4 |
| 2 | B | 127 | ARG | 4.4 |
| 2 | B | 486 | LEU | 4.3 |
| 2 | b | 488 | PRO | 4.3 |
| 17 | Y | 22 | LEU | 4.3 |
| 20 | R | 10 | LEU | 4.3 |
| 2 | b | 84 | THR | 4.3 |
| 17 | y | 25 | ILE | 4.3 |
| 12 | M | 34 | LYS | 4.3 |
| 2 | B | 86 | ILE | 4.3 |
| 20 | R | 19 | ALA | 4.3 |
| 20 | R | 3 | TRP | 4.3 |
| 6 | f | 16 | PHE | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 20 | R | 20 | VAL | 4.2 |
| 13 | o | 37 | THR | 4.2 |
| 20 | R | 6 | LEU | 4.2 |
| 19 | Z | 4 | LEU | 4.2 |
| 20 | R | 27 | ALA | 4.1 |
| 19 | z | 30 | PRO | 4.1 |
| 17 | Y | 25 | ILE | 4.1 |
| 19 | Z | 61 | VAL | 4.1 |
| 19 | Z | 60 | PHE | 4.0 |
| 19 | z | 41 | PHE | 4.0 |
| 18 | X | 31 | ILE | 4.0 |
| 20 | R | 18 | TRP | 4.0 |
| 3 | c | 19 | ASN | 4.0 |
| 2 | b | 293 | ALA | 3.9 |
| 3 | C | 23 | ALA | 3.9 |
| 13 | o | 4 | THR | 3.9 |
| 2 | b | 496 | TYR | 3.9 |
| 19 | Z | 41 | PHE | 3.8 |
| 19 | z | 60 | PHE | 3.8 |
| 5 | E | 84 | LYS | 3.8 |
| 5 | E | 61 | ARG | 3.8 |
| 7 | H | 66 | GLY | 3.8 |
| 19 | Z | 30 | PRO | 3.8 |
| 12 | M | 33 | GLN | 3.8 |
| 17 | y | 20 | ALA | 3.8 |
| 9 | J | 3 | GLU | 3.8 |
| 13 | o | 59 | LYS | 3.8 |
| 2 | b | 479 | PHE | 3.8 |
| 19 | z | 5 | PHE | 3.8 |
| 5 | E | 4 | THR | 3.7 |
| 13 | O | 246 | ALA | 3.7 |
| 6 | f | 15 | ILE | 3.7 |
| 14 | t | 29 | ILE | 3.7 |
| 17 | Y | 21 | GLN | 3.7 |
| 15 | U | 67 | LEU | 3.7 |
| 20 | R | 9 | LEU | 3.6 |
| 12 | m | 33 | GLN | 3.6 |
| 2 | B | 505 | ARG | 3.6 |
| 20 | R | 26 | TYR | 3.6 |
| 2 | b | 85 | GLY | 3.6 |
| 3 | c | 134 | ILE | 3.6 |
| 1 | a | 230 | THR | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | f | 14 | PRO | 3.6 |
| 20 | R | 35 | LEU | 3.6 |
| 13 | o | 246 | ALA | 3.6 |
| 10 | K | 17 | ILE | 3.6 |
| 19 | z | 1 | MET | 3.6 |
| 18 | x | 40 | SER | 3.5 |
| 13 | O | 62 | GLU | 3.5 |
| 10 | k | 18 | PHE | 3.5 |
| 19 | z | 61 | VAL | 3.5 |
| 17 | Y | 20 | ALA | 3.5 |
| 16 | V | 106 | ASN | 3.4 |
| 16 | v | 106 | ASN | 3.4 |
| 11 | L | 1 | MET | 3.4 |
| 19 | z | 33 | TRP | 3.4 |
| 5 | e | 61 | ARG | 3.4 |
| 20 | R | 15 | ALA | 3.3 |
| 1 | A | 13 | LEU | 3.3 |
| 2 | B | 84 | THR | 3.3 |
| 12 | m | 34 | LYS | 3.3 |
| 13 | O | 61 | GLN | 3.3 |
| 9 | j | 3 | GLU | 3.3 |
| 20 | R | 13 | LEU | 3.3 |
| 18 | x | 38 | GLN | 3.3 |
| 9 | J | 5 | GLY | 3.3 |
| 9 | j | 4 | GLY | 3.3 |
| 16 | V | 14 | SER | 3.3 |
| 14 | T | 29 | ILE | 3.3 |
| 18 | x | 34 | ILE | 3.3 |
| 19 | z | 7 | LEU | 3.3 |
| 3 | c | 143 | TYR | 3.2 |
| 19 | Z | 10 | ALA | 3.2 |
| 4 | D | 238 | THR | 3.2 |
| 18 | x | 37 | VAL | 3.2 |
| 2 | B | 494 | GLY | 3.2 |
| 13 | o | 56 | PRO | 3.2 |
| 3 | c | 151 | TRP | 3.1 |
| 5 | E | 60 | GLN | 3.1 |
| 19 | z | 42 | LEU | 3.1 |
| 2 | B | 495 | PHE | 3.1 |
| 8 | I | 33 | LYS | 3.1 |
| 20 | R | 25 | PRO | 3.1 |
| 2 | B | 85 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | e | 6 | GLY | 3.1 |
| 19 | z | 31 | GLN | 3.1 |
| 4 | D | 12 | ARG | 3.1 |
| 3 | C | 24 | THR | 3.1 |
| 1 | A | 11 | ALA | 3.1 |
| 3 | C | 246 | ALA | 3.1 |
| 9 | j | 5 | GLY | 3.1 |
| 19 | Z | 49 | ALA | 3.1 |
| 2 | B | 490 | GLN | 3.0 |
| 4 | d | 12 | ARG | 3.0 |
| 15 | U | 73 | GLN | 3.0 |
| 5 | e | 13 | ILE | 3.0 |
| 18 | X | 34 | ILE | 3.0 |
| 8 | I | 36 | ASP | 3.0 |
| 18 | X | 3 | ILE | 3.0 |
| 2 | b | 489 | GLU | 3.0 |
| 19 | Z | 31 | GLN | 3.0 |
| 3 | C | 260 | ALA | 3.0 |
| 1 | A | 235 | TYR | 2.9 |
| 1 | a | 262 | TYR | 2.9 |
| 19 | Z | 6 | GLN | 2.9 |
| 9 | J | 6 | ARG | 2.9 |
| 17 | Y | 23 | THR | 2.9 |
| 2 | b | 490 | GLN | 2.9 |
| 17 | y | 41 | VAL | 2.9 |
| 2 | b | 82 | GLY | 2.9 |
| 19 | Z | 53 | VAL | 2.9 |
| 5 | e | 14 | ILE | 2.9 |
| 20 | R | 5 | VAL | 2.8 |
| 13 | O | 60 | ARG | 2.8 |
| 2 | b | 487 | SER | 2.8 |
| 13 | o | 36 | GLN | 2.8 |
| 20 | R | 8 | VAL | 2.8 |
| 1 | a | 235 | TYR | 2.8 |
| 10 | K | 16 | ALA | 2.8 |
| 17 | Y | 27 | MET | 2.8 |
| 3 | C | 155 | ASN | 2.8 |
| 13 | O | 206 | GLY | 2.8 |
| 3 | C | 134 | ILE | 2.8 |
| 13 | o | 25 | THR | 2.8 |
| 2 | B | 485 | GLU | 2.8 |
| 2 | B | 492 | GLU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 17 | y | 43 | ARG | 2.8 |
| 19 | Z | 2 | THR | 2.8 |
| 7 | h | 6 | TRP | 2.8 |
| 13 | O | 23 | ASP | 2.8 |
| 3 | c | 20 | SER | 2.7 |
| 1 | A | 12 | ASN | 2.7 |
| 8 | I | 34 | ARG | 2.7 |
| 20 | R | 32 | GLN | 2.7 |
| 3 | C | 257 | PHE | 2.7 |
| 2 | b | 494 | GLY | 2.7 |
| 8 | I | 2 | GLU | 2.7 |
| 17 | y | 22 | LEU | 2.7 |
| 3 | c | 21 | ILE | 2.7 |
| 20 | R | 11 | PRO | 2.7 |
| 10 | k | 13 | GLU | 2.7 |
| 13 | o | 57 | LYS | 2.7 |
| 19 | z | 8 | ALA | 2.7 |
| 6 | F | 16 | PHE | 2.7 |
| 19 | z | 2 | THR | 2.7 |
| 19 | z | 9 | LEU | 2.7 |
| 20 | R | 14 | LEU | 2.7 |
| 2 | b | 484 | PRO | 2.7 |
| 16 | v | 14 | SER | 2.7 |
| 17 | y | 27 | MET | 2.7 |
| 11 | l | 3 | PRO | 2.7 |
| 13 | O | 5 | LEU | 2.7 |
| 4 | D | 11 | GLU | 2.7 |
| 10 | k | 17 | ILE | 2.7 |
| 15 | u | 8 | GLU | 2.7 |
| 2 | b | 373 | LYS | 2.6 |
| 8 | i | 33 | LYS | 2.6 |
| 13 | o | 32 | ILE | 2.6 |
| 2 | B | 491 | VAL | 2.6 |
| 2 | b | 499 | VAL | 2.6 |
| 13 | o | 23 | ASP | 2.6 |
| 13 | o | 24 | ASP | 2.6 |
| 19 | z | 35 | ARG | 2.6 |
| 16 | V | 86 | GLN | 2.6 |
| 1 | a | 260 | PHE | 2.6 |
| 5 | e | 79 | PHE | 2.6 |
| 2 | B | 488 | PRO | 2.6 |
| 5 | E | 83 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | b | 295 | GLY | 2.6 |
| 13 | o | 55 | GLU | 2.6 |
| 10 | K | 10 | LYS | 2.6 |
| 13 | O | 59 | LYS | 2.6 |
| 3 | C | 255 | THR | 2.6 |
| 17 | y | 23 | THR | 2.6 |
| 2 | b | 223 | GLN | 2.6 |
| 1 | a | 248 | ILE | 2.6 |
| 8 | i | 36 | ASP | 2.6 |
| 13 | O | 55 | GLU | 2.6 |
| 19 | Z | 32 | ASP | 2.6 |
| 2 | b | 290 | ALA | 2.6 |
| 5 | E | 79 | PHE | 2.5 |
| 18 | x | 35 | ASP | 2.5 |
| 13 | o | 34 | SER | 2.5 |
| 20 | R | 7 | VAL | 2.5 |
| 2 | b | 505 | ARG | 2.5 |
| 13 | o | 60 | ARG | 2.5 |
| 2 | b | 126 | PRO | 2.5 |
| 3 | C | 462[A] | GLU | 2.5 |
| 10 | k | 12 | PRO | 2.5 |
| 7 | H | 63 | LYS | 2.5 |
| 19 | Z | 33 | TRP | 2.5 |
| 9 | j | 2 | SER | 2.5 |
| 1 | a | 263 | ALA | 2.5 |
| 17 | y | 26 | ALA | 2.5 |
| 1 | A | 230 | THR | 2.5 |
| 4 | D | 136 | VAL | 2.5 |
| 13 | o | 61 | GLN | 2.5 |
| 16 | v | 17 | LYS | 2.5 |
| 15 | U | 8 | GLU | 2.5 |
| 2 | b | 127 | ARG | 2.4 |
| 5 | e | 10 | PHE | 2.4 |
| 5 | e | 83 | LEU | 2.4 |
| 20 | R | 33 | LYS | 2.4 |
| 5 | e | 20 | TRP | 2.4 |
| 5 | e | 18 | ARG | 2.4 |
| 2 | B | 500 | GLY | 2.4 |
| 3 | c | 183 | GLY | 2.4 |
| 16 | v | 16 | GLY | 2.4 |
| 3 | C | 142 | GLU | 2.4 |
| 13 | o | 62 | GLU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | C | 75 | PHE | 2.4 |
| 5 | e | 84 | LYS | 2.4 |
| 3 | C | 245 | ILE | 2.4 |
| 5 | e | 25 | ILE | 2.4 |
| 19 | z | 10 | ALA | 2.4 |
| 4 | d | 24 | ARG | 2.4 |
| 2 | b | 492 | GLU | 2.4 |
| 19 | Z | 36 | SER | 2.4 |
| 19 | z | 50 | LEU | 2.4 |
| 9 | j | 7 | ILE | 2.4 |
| 13 | o | 135 | SER | 2.4 |
| 9 | j | 6 | ARG | 2.3 |
| 1 | A | 262 | TYR | 2.3 |
| 1 | a | 246 | TYR | 2.3 |
| 3 | c | 78 | GLU | 2.3 |
| 13 | o | 98 | GLU | 2.3 |
| 7 | h | 57 | GLY | 2.3 |
| 17 | y | 38 | LEU | 2.3 |
| 18 | X | 38 | GLN | 2.3 |
| 6 | F | 44 | GLN | 2.3 |
| 12 | M | 5 | GLN | 2.3 |
| 7 | h | 63 | LYS | 2.3 |
| 8 | i | 35 | LYS | 2.3 |
| 13 | o | 206 | GLY | 2.3 |
| 2 | B | 83 | GLU | 2.3 |
| 8 | i | 38 | GLU | 2.3 |
| 11 | L | 2 | GLU | 2.3 |
| 4 | D | 134 | ARG | 2.2 |
| 2 | b | 500 | GLY | 2.2 |
| 3 | C | 77 | PRO | 2.2 |
| 5 | e | 7 | GLU | 2.2 |
| 13 | o | 95 | PHE | 2.2 |
| 5 | e | 17 | VAL | 2.2 |
| 18 | X | 19 | VAL | 2.2 |
| 2 | b | 503 | THR | 2.2 |
| 13 | o | 137 | THR | 2.2 |
| 19 | z | 52 | LEU | 2.2 |
| 3 | c | 184 | GLY | 2.2 |
| 19 | z | 11 | ALA | 2.2 |
| 13 | o | 38 | TYR | 2.2 |
| 16 | v | 26 | TYR | 2.2 |
| 20 | R | 29 | LYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | C | 78 | GLU | 2.2 |
| 11 | L | 3 | PRO | 2.2 |
| 6 | F | 13 | TYR | 2.2 |
| 7 | h | 18 | TYR | 2.2 |
| 3 | C | 259 | TRP | 2.2 |
| 19 | Z | 35 | ARG | 2.2 |
| 19 | z | 18 | VAL | 2.2 |
| 13 | O | 25 | THR | 2.2 |
| 17 | y | 40 | ALA | 2.2 |
| 8 | i | 34 | ARG | 2.2 |
| 3 | C | 105 | VAL | 2.1 |
| 3 | c | 255 | THR | 2.1 |
| 9 | J | 15 | VAL | 2.1 |
| 13 | O | 87 | VAL | 2.1 |
| 16 | V | 18 | THR | 2.1 |
| 19 | Z | 56 | VAL | 2.1 |
| 13 | O | 89 | SER | 2.1 |
| 19 | z | 29 | SER | 2.1 |
| 16 | V | 6 | GLU | 2.1 |
| 13 | O | 63 | ALA | 2.1 |
| 6 | F | 17 | THR | 2.1 |
| 13 | o | 83 | GLY | 2.1 |
| 15 | U | 70 | ARG | 2.1 |
| 19 | z | 43 | GLY | 2.1 |
| 13 | o | 67 | PRO | 2.1 |
| 13 | o | 199 | LEU | 2.1 |
| 18 | X | 5 | PRO | 2.1 |
| 19 | Z | 42 | LEU | 2.1 |
| 17 | Y | 26 | ALA | 2.1 |
| 20 | R | 30 | GLN | 2.1 |
| 3 | c | 257 | PHE | 2.1 |
| 3 | C | 143 | TYR | 2.1 |
| 3 | c | 131 | TYR | 2.1 |
| 13 | o | 141 | ASP | 2.1 |
| 2 | B | 487 | SER | 2.1 |
| 3 | c | 145 | SER | 2.1 |
| 2 | B | 489 | GLU | 2.1 |
| 2 | b | 83 | GLU | 2.1 |
| 13 | o | 21 | THR | 2.1 |
| 3 | c | 155 | ASN | 2.1 |
| 19 | z | 23 | VAL | 2.1 |
| 5 | E | 82 | GLN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 18 | x | 15 | LEU | 2.1 |
| 2 | B | 290 | ALA | 2.1 |
| 19 | z | 28 | ALA | 2.1 |
| 20 | R | 16 | ALA | 2.1 |
| 13 | O | 141 | ASP | 2.1 |
| 2 | b | 485 | GLU | 2.0 |
| 3 | c | 146 | PHE | 2.0 |
| 1 | a | 264 | SER | 2.0 |
| 5 | E | 11 | SER | 2.0 |
| 5 | e | 32 | ILE | 2.0 |
| 13 | o | 181[A] | GLU | 2.0 |
| 15 | u | 66 | GLY | 2.0 |
| 5 | e | 82 | GLN | 2.0 |
| 19 | z | 39 | LEU | 2.0 |
| 3 | c | 246 | ALA | 2.0 |
| 17 | y | 24 | MET | 2.0 |
| 13 | o | 243 | ILE | 2.0 |
| 3 | C | 192 | GLY | 2.0 |
| 3 | C | 254 | THR | 2.0 |
| 17 | y | 44 | GLY | 2.0 |
| 3 | c | 106 | VAL | 2.0 |
| 10 | k | 27 | VAL | 2.0 |
| 17 | Y | 41 | VAL | 2.0 |
| 19 | z | 54 | VAL | 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 |
|---|---|---|---|---|---|---|---|---|
| 12 | FME | m | 1 | 10/11 | 0.92 | 0.15 | 13,32,67,68 | 0 |
| 14 | FME | t | 1 | 10/11 | 0.93 | 0.09 | 12,22,31,68 | 0 |
| 14 | FME | T | 1 | 10/11 | 0.95 | 0.09 | 18,26,40,49 | 0 |
| 12 | FME | M | 1 | 10/11 | 0.95 | 0.14 | 23,36,70,74 | 0 |
| 8 | FME | I | 1 | 10/11 | 0.96 | 0.08 | 22,34,38,38 | 0 |
| 8 | FME | i | 1 | 10/11 | 0.97 | 0.08 | 21,31,39,42 | 0 |

## 6.3 Carbohydrates (i)

There are no oligosaccharides 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 |
|---|---|---|---|---|---|---|---|---|
| 29 | LMT | f | 103 | 35/35 | 0.65 | 0.21 | 43,86,107,111 | 0 |
| 36 | DGD | D | 405 | 62/66 | 0.65 | 0.22 | 48,79,113,122 | 0 |
| 29 | LMT | E | 102 | 35/35 | 0.68 | 0.22 | 43,80,109,115 | 0 |
| 29 | LMT | C | 522 | 35/35 | 0.70 | 0.21 | 52,81,102,104 | 0 |
| 36 | DGD | d | 406 | 62/66 | 0.70 | 0.23 | 38,89,122,130 | 0 |
| 33 | CA | b | 604 | 1/1 | 0.71 | 0.19 | 117,117,117,117 | 0 |
| 28 | GOL | v | 203 | 6/6 | 0.72 | 0.22 | 39,74,86,87 | 0 |
| 34 | LMG | z | 101 | 39/55 | 0.72 | 0.24 | 45,82,99,107 | 0 |
| 29 | LMT | b | 625 | 25/35 | 0.72 | 0.20 | 44,67,109,119 | 0 |
| 28 | GOL | V | 203 | 6/6 | 0.72 | 0.23 | 50,64,71,72 | 0 |
| 37 | LHG | e | 101 | 42/49 | 0.72 | 0.22 | 52,89,118,129 | 0 |
| 28 | GOL | B | 637 | 6/6 | 0.73 | 0.23 | 51,72,83,86 | 0 |
| 32 | UNL | B | 635 | 33/- | 0.74 | 0.23 | 33,58,102,102 | 0 |
| 29 | LMT | m | 102 | 35/35 | 0.74 | 0.19 | 33,61,79,95 | 0 |
| 28 | GOL | O | 302 | 6/6 | 0.75 | 0.14 | 49,55,57,61 | 0 |
| 35 | HTG | B | 626 | 19/19 | 0.75 | 0.18 | 48,81,94,95 | 0 |
| 32 | UNL | b | 634 | 33/- | 0.75 | 0.23 | 29,62,111,117 | 0 |
| 32 | UNL | m | 101 | 10/- | 0.75 | 0.22 | 35,50,55,61 | 0 |
| 32 | UNL | A | 420 | 28/- | 0.75 | 0.22 | 50,71,78,86 | 0 |
| 35 | HTG | d | 412 | 16/19 | 0.76 | 0.19 | 38,78,97,98 | 0 |
| 35 | HTG | B | 634 | 19/19 | 0.76 | 0.17 | 32,76,109,127 | 0 |
| 35 | HTG | c | 923 | 19/19 | 0.77 | 0.16 | 45,80,94,97 | 0 |
| 32 | UNL | I | 101 | 40/- | 0.77 | 0.22 | 27,62,110,120 | 0 |
| 32 | UNL | K | 101 | 34/- | 0.77 | 0.19 | 37,61,83,88 | 0 |
| 35 | HTG | D | 411 | 16/19 | 0.77 | 0.20 | 38,102,111,112 | 0 |
| 35 | HTG | b | 627 | 19/19 | 0.77 | 0.17 | 49,86,110,116 | 0 |
| 32 | UNL | M | 102 | 10/- | 0.78 | 0.19 | 28,38,57,58 | 0 |
| 34 | LMG | C | 521 | 51/55 | 0.78 | 0.18 | 32,69,88,108 | 0 |
| 32 | UNL | c | 926 | 32/- | 0.78 | 0.23 | 39,79,98,105 | 0 |
| 32 | UNL | a | 418 | 30/- | 0.78 | 0.22 | 42,66,98,106 | 0 |
| 32 | UNL | i | 101 | 40/- | 0.79 | 0.21 | 28,62,105,117 | 0 |
| 29 | LMT | m | 104 | 35/35 | 0.79 | 0.18 | 29,59,85,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 35 | HTG | c | 922 | 19/19 | 0.80 | 0.17 | 43,67,84,95 | 0 |
| 28 | GOL | C | 525 | 6/6 | 0.80 | 0.16 | 32,41,61,69 | 0 |
| 32 | UNL | j | 102 | 10/- | 0.80 | 0.21 | 47,57,63,63 | 0 |
| 29 | LMT | c | 921 | 35/35 | 0.80 | 0.18 | 46,76,97,104 | 0 |
| 32 | UNL | J | 102 | 10/- | 0.80 | 0.23 | 39,51,64,67 | 0 |
| 27 | SQD | a | 402 | 54/54 | 0.80 | 0.16 | 29,55,76,90 | 0 |
| 35 | HTG | b | 603 | 19/19 | 0.81 | 0.18 | 46,84,110,111 | 0 |
| 29 | LMT | a | 401 | 35/35 | 0.81 | 0.18 | 21,53,74,80 | 0 |
| 29 | LMT | A | 417 | 35/35 | 0.81 | 0.17 | 22,57,79,97 | 0 |
| 34 | LMG | Z | 101 | 37/55 | 0.81 | 0.21 | 30,75,96,112 | 0 |
| 32 | UNL | d | 411 | 36/- | 0.81 | 0.19 | 32,56,104,111 | 0 |
| 27 | SQD | L | 102 | 54/54 | 0.81 | 0.19 | 24,52,86,91 | 0 |
| 28 | GOL | v | 204 | 6/6 | 0.81 | 0.17 | 54,66,71,80 | 0 |
| 32 | UNL | D | 410 | 40/- | 0.81 | 0.21 | 24,54,93,101 | 0 |
| 31 | PL9 | a | 417 | 55/55 | 0.82 | 0.22 | 41,73,92,99 | 0 |
| 28 | GOL | B | 628 | 6/6 | 0.82 | 0.17 | 33,42,54,72 | 0 |
| 37 | LHG | E | 101 | 42/49 | 0.82 | 0.17 | 22,63,78,93 | 0 |
| 29 | LMT | B | 623 | 35/35 | 0.82 | 0.17 | 26,74,96,101 | 0 |
| 29 | LMT | B | 636 | 25/35 | 0.83 | 0.21 | 24,61,106,122 | 0 |
| 27 | SQD | A | 416 | 54/54 | 0.83 | 0.17 | 26,51,78,85 | 0 |
| 35 | HTG | C | 524 | 19/19 | 0.83 | 0.15 | 41,69,99,100 | 0 |
| 28 | GOL | b | 632 | 6/6 | 0.83 | 0.19 | 38,52,59,59 | 0 |
| 35 | HTG | V | 202 | 19/19 | 0.83 | 0.18 | 40,59,77,163 | 0 |
| 34 | LMG | c | 920 | 51/55 | 0.83 | 0.17 | 33,74,88,93 | 0 |
| 28 | GOL | T | 103 | 6/6 | 0.83 | 0.22 | 52,68,70,79 | 0 |
| 27 | SQD | f | 102 | 43/54 | 0.84 | 0.18 | 41,75,103,108 | 0 |
| 34 | LMG | a | 412 | 51/55 | 0.84 | 0.18 | 33,62,84,90 | 0 |
| 28 | GOL | a | 415 | 6/6 | 0.85 | 0.16 | 48,62,65,66 | 0 |
| 28 | GOL | B | 631 | 6/6 | 0.85 | 0.19 | 30,48,62,65 | 0 |
| 34 | LMG | C | 501 | 51/55 | 0.85 | 0.15 | 34,56,76,85 | 0 |
| 28 | GOL | c | 925 | 6/6 | 0.85 | 0.19 | 34,52,63,66 | 0 |
| 31 | PL9 | A | 419 | 55/55 | 0.85 | 0.19 | 28,56,91,98 | 0 |
| 28 | GOL | t | 102 | 6/6 | 0.85 | 0.20 | 22,59,67,67 | 0 |
| 29 | LMT | M | 101 | 35/35 | 0.85 | 0.15 | 23,52,69,77 | 0 |
| 28 | GOL | T | 101 | 6/6 | 0.85 | 0.20 | 54,60,61,69 | 0 |
| 32 | UNL | d | 413 | 18/- | 0.85 | 0.18 | 30,52,81,84 | 0 |
| 28 | GOL | A | 414 | 6/6 | 0.85 | 0.15 | 30,40,43,49 | 0 |
| 27 | SQD | B | 621 | 54/54 | 0.85 | 0.16 | 26,55,94,104 | 0 |
| 28 | GOL | A | 415 | 6/6 | 0.86 | 0.17 | 36,49,64,64 | 0 |
| 32 | UNL | D | 409 | 17/- | 0.86 | 0.15 | 30,40,63,66 | 0 |
| 24 | CLA | c | 914 | 65/65 | 0.86 | 0.15 | 35,48,81,87 | 0 |
| 28 | GOL | V | 206 | 6/6 | 0.86 | 0.15 | 47,63,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 29 | LMT | m | 103 | 35/35 | 0.86 | 0.13 | 19,48,62,74 | 0 |
| 28 | GOL | a | 413 | 6/6 | 0.86 | 0.12 | 30,32,37,42 | 0 |
| 28 | GOL | B | 629 | 6/6 | 0.86 | 0.17 | 28,42,50,56 | 0 |
| 29 | LMT | b | 601 | 25/35 | 0.86 | 0.20 | 18,55,104,111 | 0 |
| 27 | SQD | F | 101 | 43/54 | 0.86 | 0.17 | 34,59,81,90 | 0 |
| 32 | UNL | d | 410 | 17/- | 0.87 | 0.16 | 34,48,82,82 | 0 |
| 28 | GOL | F | 103 | 6/6 | 0.87 | 0.15 | 60,65,71,71 | 0 |
| 33 | CA | B | 601 | 1/1 | 0.87 | 0.09 | 83,83,83,83 | 0 |
| 35 | HTG | C | 523 | 19/19 | 0.87 | 0.16 | 54,62,86,88 | 0 |
| 35 | HTG | b | 626 | 19/19 | 0.88 | 0.19 | 30,50,86,86 | 0 |
| 32 | UNL | X | 101 | 18/- | 0.88 | 0.16 | 29,44,62,79 | 0 |
| 34 | LMG | C | 520 | 51/55 | 0.88 | 0.16 | 22,52,72,90 | 0 |
| 24 | CLA | b | 605 | 65/65 | 0.89 | 0.14 | 29,48,89,102 | 0 |
| 34 | LMG | c | 919 | 51/55 | 0.89 | 0.16 | 29,57,78,81 | 0 |
| 28 | GOL | f | 101 | 6/6 | 0.89 | 0.14 | 44,50,62,64 | 0 |
| 26 | BCR | k | 101 | 40/40 | 0.89 | 0.13 | 34,45,63,75 | 0 |
| 35 | HTG | B | 633 | 19/19 | 0.90 | 0.12 | 28,54,70,76 | 0 |
| 35 | HTG | b | 602 | 19/19 | 0.90 | 0.13 | 29,45,65,68 | 0 |
| 27 | SQD | a | 411 | 54/54 | 0.90 | 0.15 | 32,52,73,81 | 0 |
| 28 | GOL | B | 632 | 6/6 | 0.90 | 0.14 | 24,40,53,57 | 0 |
| 35 | HTG | B | 625 | 19/19 | 0.90 | 0.17 | 28,43,74,86 | 0 |
| 28 | GOL | B | 627 | 6/6 | 0.90 | 0.17 | 23,36,45,72 | 0 |
| 33 | CA | f | 104 | 1/1 | 0.91 | 0.09 | 77,77,77,77 | 0 |
| 34 | LMG | B | 622 | 51/55 | 0.91 | 0.11 | 19,32,49,71 | 0 |
| 24 | CLA | c | 913 | 65/65 | 0.91 | 0.11 | 31,40,59,65 | 0 |
| 24 | CLA | C | 507 | 65/65 | 0.91 | 0.12 | 25,40,75,77 | 0 |
| 26 | BCR | C | 515 | 40/40 | 0.91 | 0.11 | 29,38,49,53 | 0 |
| 26 | BCR | K | 103 | 40/40 | 0.91 | 0.09 | 24,30,40,43 | 0 |
| 28 | GOL | b | 628 | 6/6 | 0.91 | 0.10 | 30,35,42,53 | 0 |
| 34 | LMG | b | 624 | 51/55 | 0.91 | 0.11 | 21,36,57,81 | 0 |
| 28 | GOL | b | 631 | 6/6 | 0.91 | 0.12 | 28,41,48,51 | 0 |
| 26 | BCR | c | 915 | 40/40 | 0.91 | 0.10 | 25,34,42,45 | 0 |
| 26 | BCR | d | 404 | 40/40 | 0.91 | 0.11 | 27,36,54,60 | 0 |
| 28 | GOL | A | 413 | 6/6 | 0.91 | 0.10 | 23,30,33,36 | 0 |
| 26 | BCR | h | 101 | 40/40 | 0.91 | 0.10 | 25,35,48,52 | 0 |
| 24 | CLA | C | 513 | 65/65 | 0.91 | 0.11 | 27,40,59,71 | 0 |
| 24 | CLA | B | 602 | 65/65 | 0.91 | 0.13 | 22,40,80,101 | 0 |
| 26 | BCR | k | 102 | 40/40 | 0.92 | 0.10 | 30,37,50,61 | 0 |
| 26 | BCR | y | 101 | 40/40 | 0.92 | 0.11 | 29,37,57,63 | 0 |
| 28 | GOL | b | 629 | 6/6 | 0.92 | 0.12 | 27,36,50,54 | 0 |
| 28 | GOL | b | 630 | 6/6 | 0.92 | 0.11 | 35,39,50,53 | 0 |
| 27 | SQD | A | 412 | 54/54 | 0.92 | 0.13 | 15,45,72,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 26 | BCR | K | 102 | 40/40 | 0.92 | 0.09 | 22,30,39,47 | 0 |
| 28 | GOL | b | 633 | 6/6 | 0.92 | 0.14 | 34,60,65,65 | 0 |
| 34 | LMG | j | 101 | 51/55 | 0.92 | 0.13 | 25,35,71,81 | 0 |
| 24 | CLA | C | 514 | 65/65 | 0.92 | 0.11 | 30,42,67,73 | 0 |
| 24 | CLA | c | 902 | 65/65 | 0.92 | 0.10 | 26,32,45,52 | 0 |
| 28 | GOL | o | 302 | 6/6 | 0.92 | 0.11 | 44,50,53,58 | 0 |
| 26 | BCR | B | 620 | 40/40 | 0.92 | 0.09 | 16,26,39,49 | 0 |
| 24 | CLA | c | 907 | 65/65 | 0.92 | 0.13 | 28,37,64,72 | 0 |
| 26 | BCR | H | 101 | 40/40 | 0.92 | 0.10 | 19,32,45,59 | 0 |
| 24 | CLA | c | 912 | 65/65 | 0.93 | 0.10 | 27,36,50,54 | 0 |
| 26 | BCR | T | 102 | 40/40 | 0.93 | 0.08 | 13,26,37,42 | 0 |
| 24 | CLA | b | 610 | 65/65 | 0.93 | 0.11 | 18,31,78,87 | 0 |
| 24 | CLA | C | 512 | 65/65 | 0.93 | 0.09 | 22,30,39,45 | 0 |
| 24 | CLA | d | 403 | 65/65 | 0.93 | 0.11 | 26,31,79,93 | 0 |
| 34 | LMG | J | 101 | 51/55 | 0.93 | 0.12 | 18,32,75,81 | 0 |
| 25 | PHO | a | 420 | 64/64 | 0.93 | 0.08 | 17,24,30,33 | 0 |
| 24 | CLA | c | 904 | 65/65 | 0.93 | 0.09 | 26,33,44,47 | 0 |
| 26 | BCR | t | 101 | 40/40 | 0.93 | 0.09 | 12,26,45,48 | 0 |
| 24 | CLA | c | 905 | 65/65 | 0.93 | 0.09 | 25,32,49,68 | 0 |
| 31 | PL9 | d | 405 | 55/55 | 0.93 | 0.08 | 13,19,33,44 | 0 |
| 26 | BCR | C | 516 | 40/40 | 0.93 | 0.09 | 23,32,42,43 | 0 |
| 28 | GOL | B | 630 | 6/6 | 0.93 | 0.10 | 26,32,40,42 | 0 |
| 36 | DGD | c | 916 | 62/66 | 0.93 | 0.11 | 22,31,64,82 | 0 |
| 36 | DGD | c | 917 | 62/66 | 0.93 | 0.11 | 26,35,61,87 | 0 |
| 26 | BCR | D | 403 | 40/40 | 0.93 | 0.10 | 19,30,58,70 | 0 |
| 36 | DGD | h | 102 | 62/66 | 0.93 | 0.10 | 19,31,48,60 | 0 |
| 24 | CLA | c | 906 | 65/65 | 0.93 | 0.10 | 21,28,44,56 | 0 |
| 37 | LHG | d | 407 | 49/49 | 0.93 | 0.11 | 15,31,44,53 | 0 |
| 37 | LHG | d | 409 | 49/49 | 0.93 | 0.14 | 21,32,85,88 | 0 |
| 24 | CLA | C | 504 | 65/65 | 0.93 | 0.08 | 22,28,40,45 | 0 |
| 37 | LHG | l | 101 | 49/49 | 0.93 | 0.10 | 15,27,39,56 | 0 |
| 22 | CL | U | 201 | 1/1 | 0.94 | 0.09 | 50,50,50,50 | 0 |
| 28 | GOL | V | 204 | 6/6 | 0.94 | 0.11 | 19,26,30,37 | 0 |
| 28 | GOL | V | 205 | 6/6 | 0.94 | 0.08 | 34,41,45,52 | 0 |
| 31 | PL9 | D | 404 | 55/55 | 0.94 | 0.08 | 11,18,31,41 | 0 |
| 24 | CLA | C | 508 | 65/65 | 0.94 | 0.09 | 23,35,47,54 | 0 |
| 24 | CLA | C | 510 | 65/65 | 0.94 | 0.09 | 23,30,45,62 | 0 |
| 28 | GOL | a | 414 | 6/6 | 0.94 | 0.12 | 25,34,43,53 | 0 |
| 24 | CLA | C | 511 | 65/65 | 0.94 | 0.09 | 21,29,38,45 | 0 |
| 24 | CLA | c | 908 | 65/65 | 0.94 | 0.09 | 26,33,49,60 | 0 |
| 24 | CLA | c | 910 | 65/65 | 0.94 | 0.09 | 27,34,47,53 | 0 |
| 24 | CLA | c | 911 | 65/65 | 0.94 | 0.09 | 24,31,43,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 24 | CLA | B | 615 | 65/65 | 0.94 | 0.10 | 12,21,66,79 | 0 |
| 24 | CLA | B | 617 | 65/65 | 0.94 | 0.12 | 16,28,79,88 | 0 |
| 24 | CLA | C | 502 | 65/65 | 0.94 | 0.09 | 22,30,42,54 | 0 |
| 24 | CLA | a | 407 | 65/65 | 0.94 | 0.11 | 18,23,72,84 | 0 |
| 23 | BCT | a | 419 | 4/4 | 0.94 | 0.12 | 21,32,41,50 | 0 |
| 26 | BCR | A | 411 | 40/40 | 0.94 | 0.08 | 15,22,29,31 | 0 |
| 26 | BCR | B | 619 | 40/40 | 0.94 | 0.08 | 15,23,46,49 | 0 |
| 24 | CLA | b | 606 | 65/65 | 0.94 | 0.08 | 22,28,38,48 | 0 |
| 24 | CLA | C | 505 | 65/65 | 0.94 | 0.09 | 18,27,47,61 | 0 |
| 24 | CLA | b | 613 | 65/65 | 0.94 | 0.08 | 23,29,42,48 | 0 |
| 24 | CLA | b | 614 | 65/65 | 0.94 | 0.08 | 20,29,39,42 | 0 |
| 36 | DGD | C | 517 | 62/66 | 0.94 | 0.10 | 19,28,60,72 | 0 |
| 36 | DGD | C | 518 | 62/66 | 0.94 | 0.11 | 19,29,78,90 | 0 |
| 24 | CLA | b | 615 | 65/65 | 0.94 | 0.08 | 17,22,38,46 | 0 |
| 36 | DGD | H | 102 | 62/66 | 0.94 | 0.09 | 16,28,46,59 | 0 |
| 24 | CLA | b | 618 | 65/65 | 0.94 | 0.11 | 14,24,78,80 | 0 |
| 24 | CLA | b | 619 | 65/65 | 0.94 | 0.09 | 20,30,49,51 | 0 |
| 36 | DGD | c | 918 | 62/66 | 0.94 | 0.10 | 25,31,52,70 | 0 |
| 24 | CLA | b | 620 | 65/65 | 0.94 | 0.12 | 19,33,77,78 | 0 |
| 26 | BCR | a | 410 | 40/40 | 0.94 | 0.07 | 15,23,28,32 | 0 |
| 37 | LHG | D | 406 | 49/49 | 0.94 | 0.10 | 14,26,38,52 | 0 |
| 37 | LHG | D | 408 | 49/49 | 0.94 | 0.15 | 17,29,88,100 | 0 |
| 26 | BCR | b | 621 | 40/40 | 0.94 | 0.07 | 14,24,33,38 | 0 |
| 26 | BCR | b | 622 | 40/40 | 0.94 | 0.08 | 14,24,43,51 | 0 |
| 26 | BCR | b | 623 | 40/40 | 0.94 | 0.09 | 18,31,42,48 | 0 |
| 24 | CLA | C | 506 | 65/65 | 0.94 | 0.09 | 18,27,47,54 | 0 |
| 24 | CLA | c | 903 | 65/65 | 0.94 | 0.09 | 24,30,41,51 | 0 |
| 28 | GOL | C | 526 | 6/6 | 0.95 | 0.07 | 17,21,26,26 | 0 |
| 24 | CLA | b | 609 | 65/65 | 0.95 | 0.08 | 16,24,37,44 | 0 |
| 24 | CLA | B | 608 | 65/65 | 0.95 | 0.07 | 11,19,28,40 | 0 |
| 24 | CLA | b | 611 | 65/65 | 0.95 | 0.07 | 13,20,31,34 | 0 |
| 35 | HTG | O | 303 | 19/19 | 0.95 | 0.11 | 23,32,46,55 | 0 |
| 24 | CLA | b | 612 | 65/65 | 0.95 | 0.07 | 21,28,40,43 | 0 |
| 24 | CLA | d | 402 | 65/65 | 0.95 | 0.08 | 16,20,36,46 | 0 |
| 24 | CLA | B | 609 | 65/65 | 0.95 | 0.07 | 15,24,30,36 | 0 |
| 25 | PHO | A | 408 | 64/64 | 0.95 | 0.07 | 12,16,23,24 | 0 |
| 25 | PHO | a | 408 | 64/64 | 0.95 | 0.07 | 15,18,27,30 | 0 |
| 33 | CA | F | 102 | 1/1 | 0.95 | 0.08 | 69,69,69,69 | 0 |
| 24 | CLA | B | 610 | 65/65 | 0.95 | 0.08 | 17,24,36,45 | 0 |
| 24 | CLA | C | 509 | 65/65 | 0.95 | 0.09 | 18,25,67,82 | 0 |
| 26 | BCR | B | 618 | 40/40 | 0.95 | 0.07 | 11,23,32,35 | 0 |
| 24 | CLA | b | 616 | 65/65 | 0.95 | 0.07 | 16,23,32,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 36 | DGD | C | 519 | 62/66 | 0.95 | 0.09 | 18,29,48,55 | 0 |
| 24 | CLA | b | 617 | 65/65 | 0.95 | 0.08 | 14,22,44,52 | 0 |
| 24 | CLA | B | 611 | 65/65 | 0.95 | 0.07 | 17,25,33,50 | 0 |
| 24 | CLA | B | 613 | 65/65 | 0.95 | 0.07 | 13,20,27,33 | 0 |
| 24 | CLA | B | 614 | 65/65 | 0.95 | 0.08 | 12,20,43,55 | 0 |
| 22 | CL | v | 201 | 1/1 | 0.95 | 0.07 | 62,62,62,62 | 0 |
| 23 | BCT | A | 404 | 4/4 | 0.95 | 0.13 | 21,24,36,47 | 0 |
| 24 | CLA | D | 402 | 65/65 | 0.95 | 0.10 | 18,27,68,84 | 0 |
| 24 | CLA | B | 603 | 65/65 | 0.95 | 0.07 | 17,24,36,47 | 0 |
| 24 | CLA | a | 409 | 65/65 | 0.95 | 0.12 | 18,26,79,83 | 0 |
| 24 | CLA | B | 606 | 65/65 | 0.95 | 0.07 | 13,20,31,41 | 0 |
| 35 | HTG | B | 624 | 19/19 | 0.95 | 0.09 | 20,32,43,46 | 0 |
| 24 | CLA | B | 607 | 65/65 | 0.95 | 0.10 | 16,25,70,76 | 0 |
| 24 | CLA | c | 909 | 65/65 | 0.95 | 0.10 | 23,28,67,91 | 0 |
| 24 | CLA | b | 607 | 65/65 | 0.95 | 0.08 | 21,28,38,50 | 0 |
| 38 | HEM | e | 102 | 43/43 | 0.95 | 0.13 | 37,46,76,95 | 0 |
| 24 | CLA | B | 604 | 65/65 | 0.96 | 0.07 | 16,25,32,38 | 0 |
| 24 | CLA | b | 608 | 65/65 | 0.96 | 0.08 | 15,23,51,62 | 0 |
| 24 | CLA | C | 503 | 65/65 | 0.96 | 0.07 | 20,25,39,63 | 0 |
| 24 | CLA | d | 401 | 65/65 | 0.96 | 0.07 | 14,18,27,47 | 0 |
| 24 | CLA | B | 605 | 65/65 | 0.96 | 0.08 | 13,19,44,57 | 0 |
| 28 | GOL | v | 205 | 6/6 | 0.96 | 0.12 | 23,35,46,50 | 0 |
| 24 | CLA | B | 612 | 65/65 | 0.96 | 0.06 | 12,18,30,37 | 0 |
| 24 | CLA | D | 401 | 65/65 | 0.96 | 0.06 | 12,16,32,36 | 0 |
| 25 | PHO | A | 409 | 64/64 | 0.96 | 0.06 | 13,20,29,35 | 0 |
| 37 | LHG | D | 407 | 49/49 | 0.96 | 0.08 | 13,22,44,57 | 0 |
| 24 | CLA | A | 407 | 65/65 | 0.96 | 0.09 | 13,20,71,73 | 0 |
| 24 | CLA | a | 406 | 65/65 | 0.96 | 0.07 | 15,17,32,38 | 0 |
| 37 | LHG | L | 101 | 49/49 | 0.96 | 0.08 | 12,26,38,46 | 0 |
| 24 | CLA | A | 410 | 65/65 | 0.96 | 0.10 | 17,26,80,89 | 0 |
| 37 | LHG | d | 408 | 49/49 | 0.96 | 0.08 | 15,23,41,54 | 0 |
| 24 | CLA | A | 405 | 65/65 | 0.96 | 0.07 | 13,17,27,52 | 0 |
| 24 | CLA | B | 616 | 65/65 | 0.96 | 0.08 | 16,23,42,45 | 0 |
| 33 | CA | O | 301 | 1/1 | 0.96 | 0.07 | 53,53,53,53 | 0 |
| 24 | CLA | A | 406 | 65/65 | 0.96 | 0.07 | 12,16,30,35 | 0 |
| 38 | HEM | E | 103 | 43/43 | 0.97 | 0.09 | 23,35,45,56 | 0 |
| 28 | GOL | c | 924 | 6/6 | 0.97 | 0.07 | 24,24,25,29 | 0 |
| 39 | MG | j | 103 | 1/1 | 0.97 | 0.09 | 33,33,33,33 | 0 |
| 40 | HEC | V | 201 | 43/43 | 0.97 | 0.08 | 22,25,32,39 | 0 |
| 40 | HEC | v | 202 | 43/43 | 0.97 | 0.08 | 28,31,40,46 | 0 |
| 33 | CA | c | 901 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 21 | FE2 | a | 403 | 1/1 | 0.99 | 0.04 | 28,28,28,28 | 0 |

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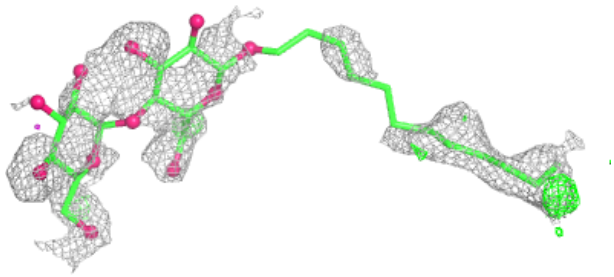
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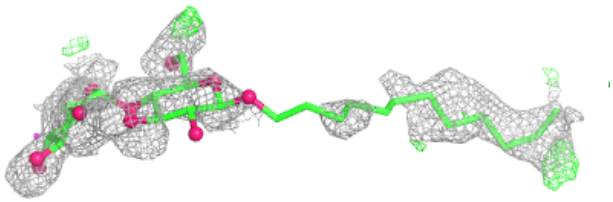
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 33 | CA | o | 301 | 1/1 | 0.99 | 0.04 | 54,54,54,54 | 0 |
| 30 | OEX | A | 418 | 10/10 | 0.99 | 0.04 | 15,20,24,28 | 0 |
| 30 | OEX | a | 416 | 10/10 | 0.99 | 0.04 | 18,21,24,34 | 0 |
| 39 | MG | J | 103 | 1/1 | 0.99 | 0.07 | 27,27,27,27 | 0 |
| 22 | CL | a | 404 | 1/1 | 0.99 | 0.04 | 20,20,20,20 | 0 |
| 22 | CL | a | 405 | 1/1 | 0.99 | 0.03 | 26,26,26,26 | 0 |
| 22 | CL | A | 402 | 1/1 | 0.99 | 0.03 | 18,18,18,18 | 0 |
| 22 | CL | A | 403 | 1/1 | 1.00 | 0.03 | 19,19,19,19 | 0 |
| 21 | FE2 | A | 401 | 1/1 | 1.00 | 0.02 | 24,24,24,24 | 0 |

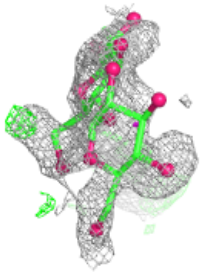
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT f 103:**

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

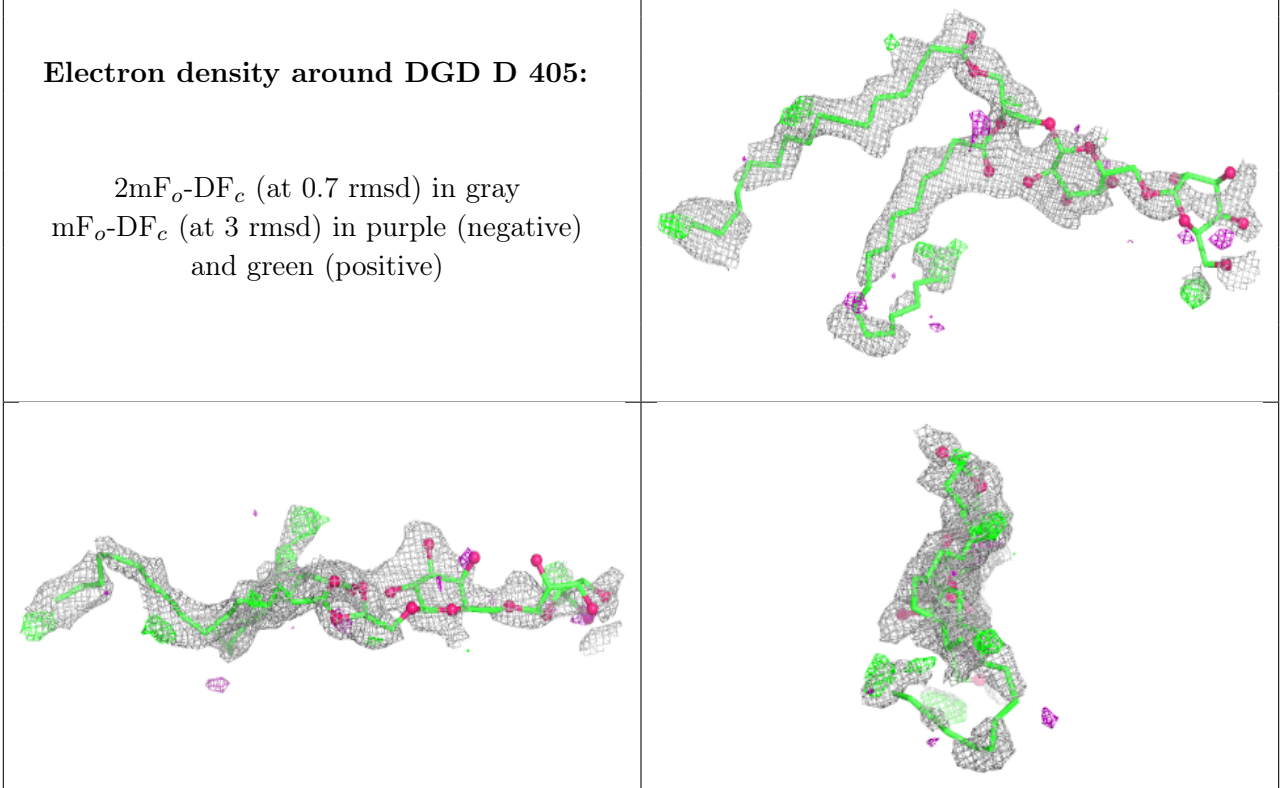






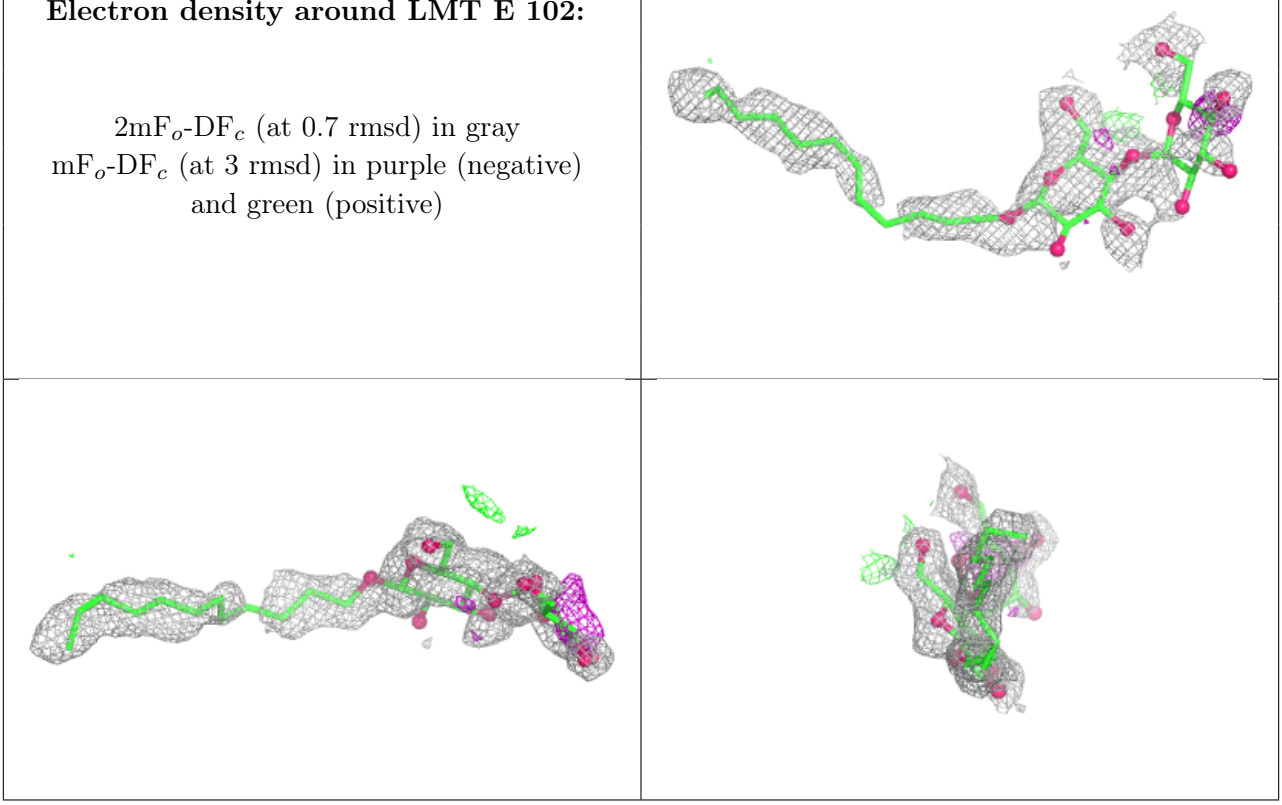
**Electron density around DGD D 405:**

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



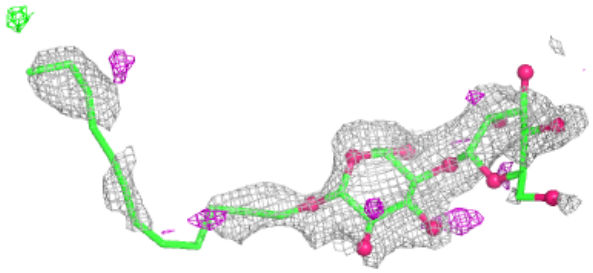
**Electron density around LMT E 102:**

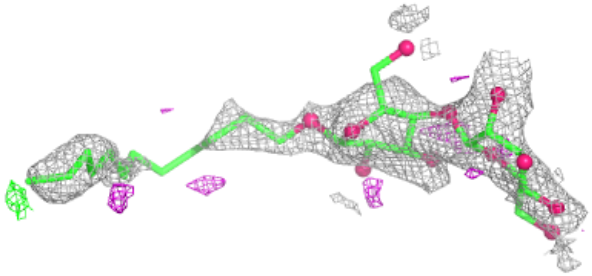
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

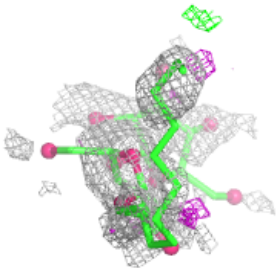


**Electron density around LMT C 522:**

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

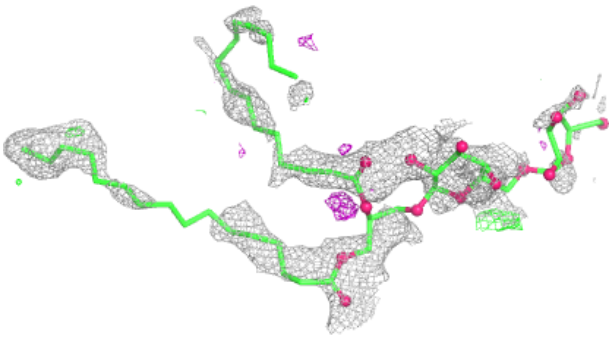


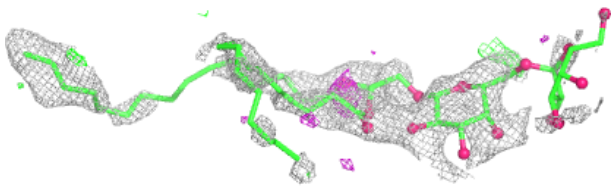


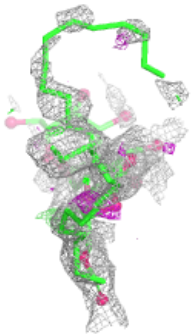


**Electron density around DGD d 406:**

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

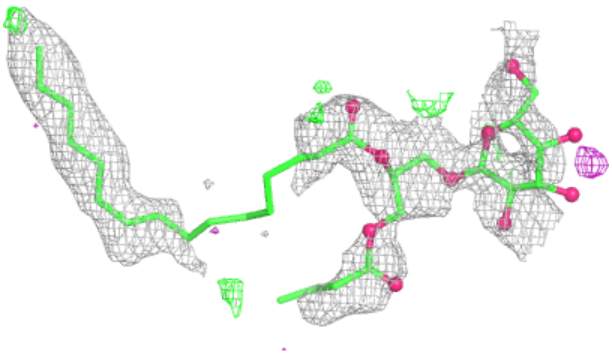


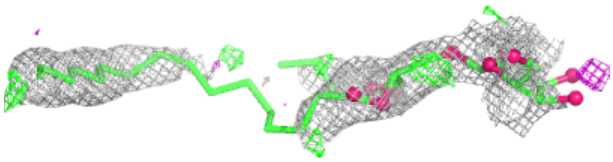


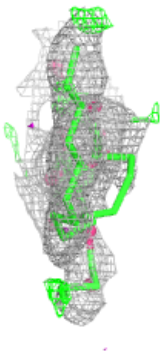


**Electron density around LMG z 101:**

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

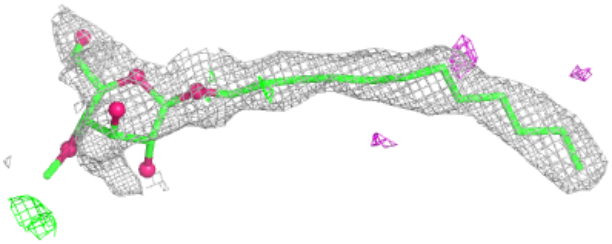


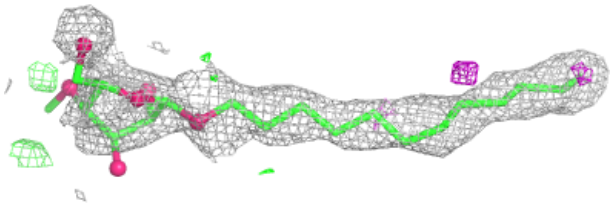


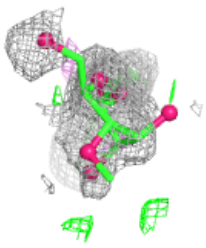


**Electron density around LMT b 625:**

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

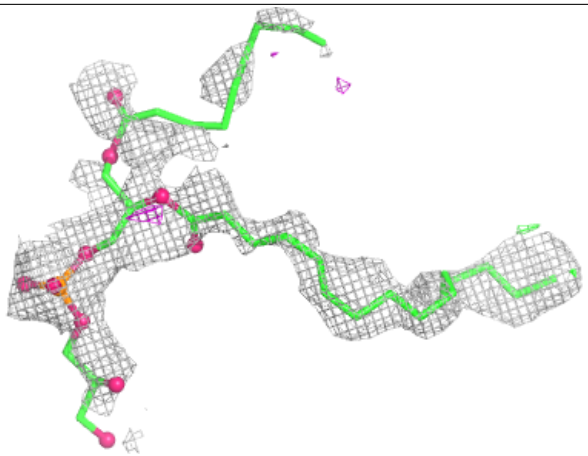


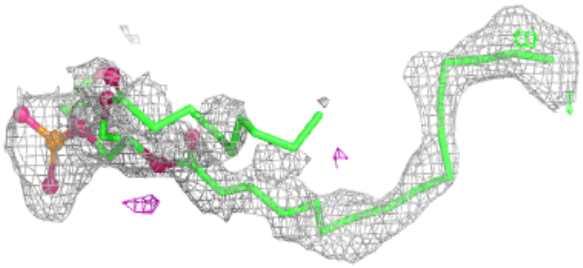


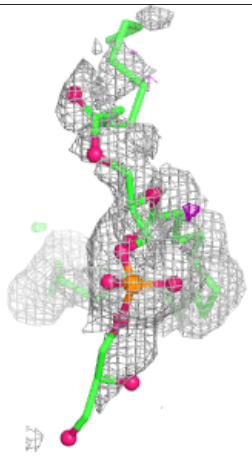


**Electron density around LHG e 101:**

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

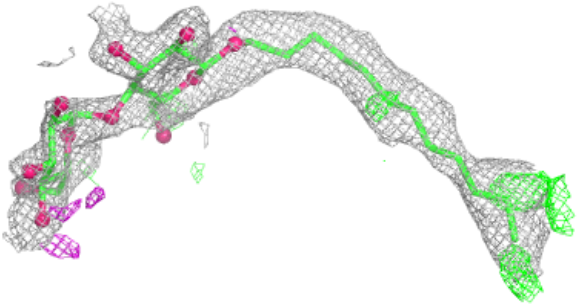


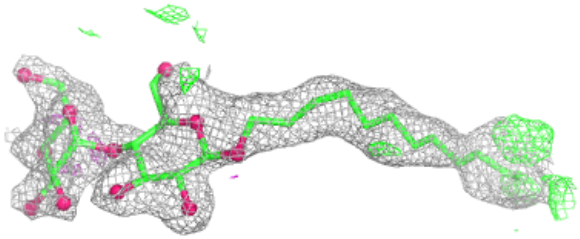


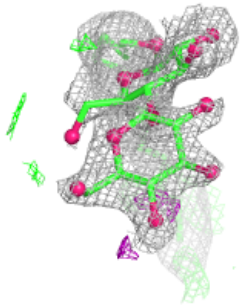


**Electron density around LMT m 102:**

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

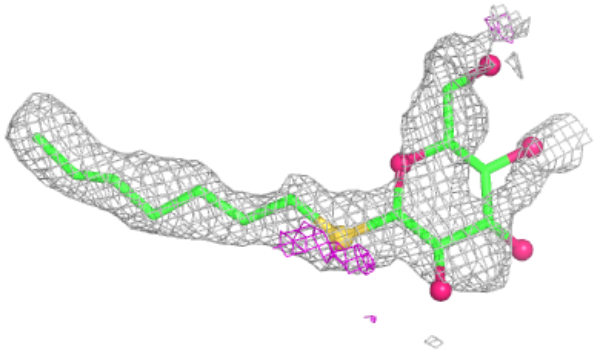


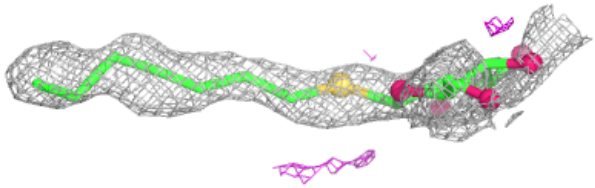


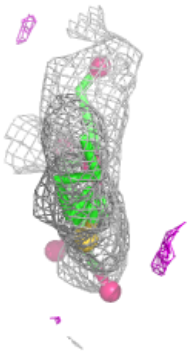


**Electron density around HTG B 626:**

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

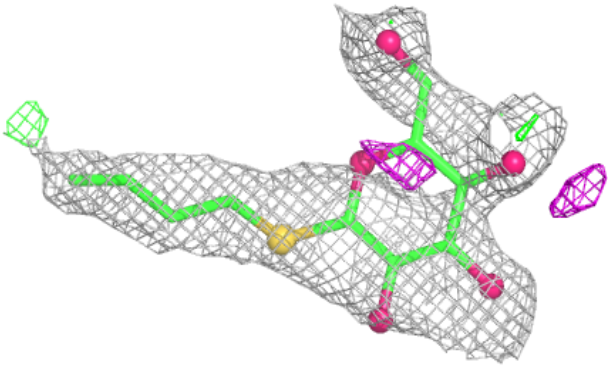


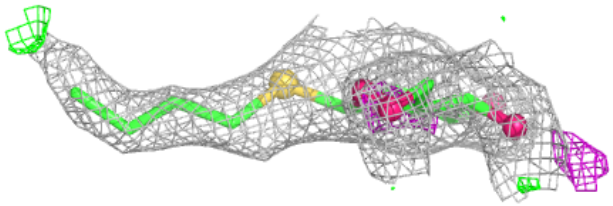


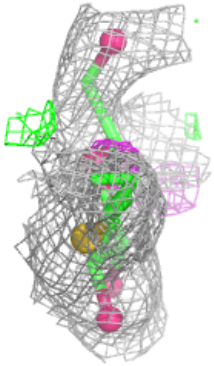


**Electron density around HTG d 412:**

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

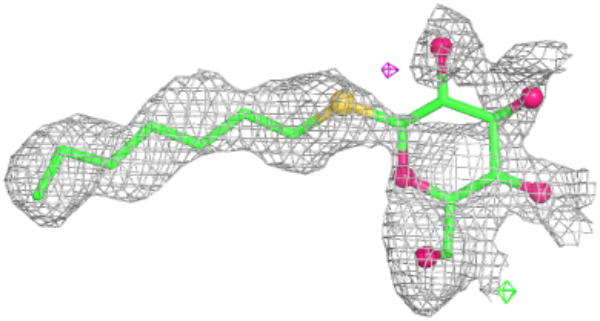


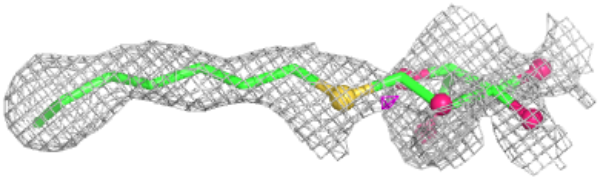


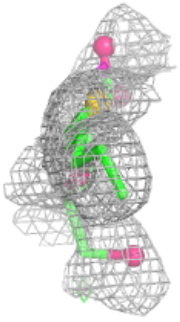


**Electron density around HTG B 634:**

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

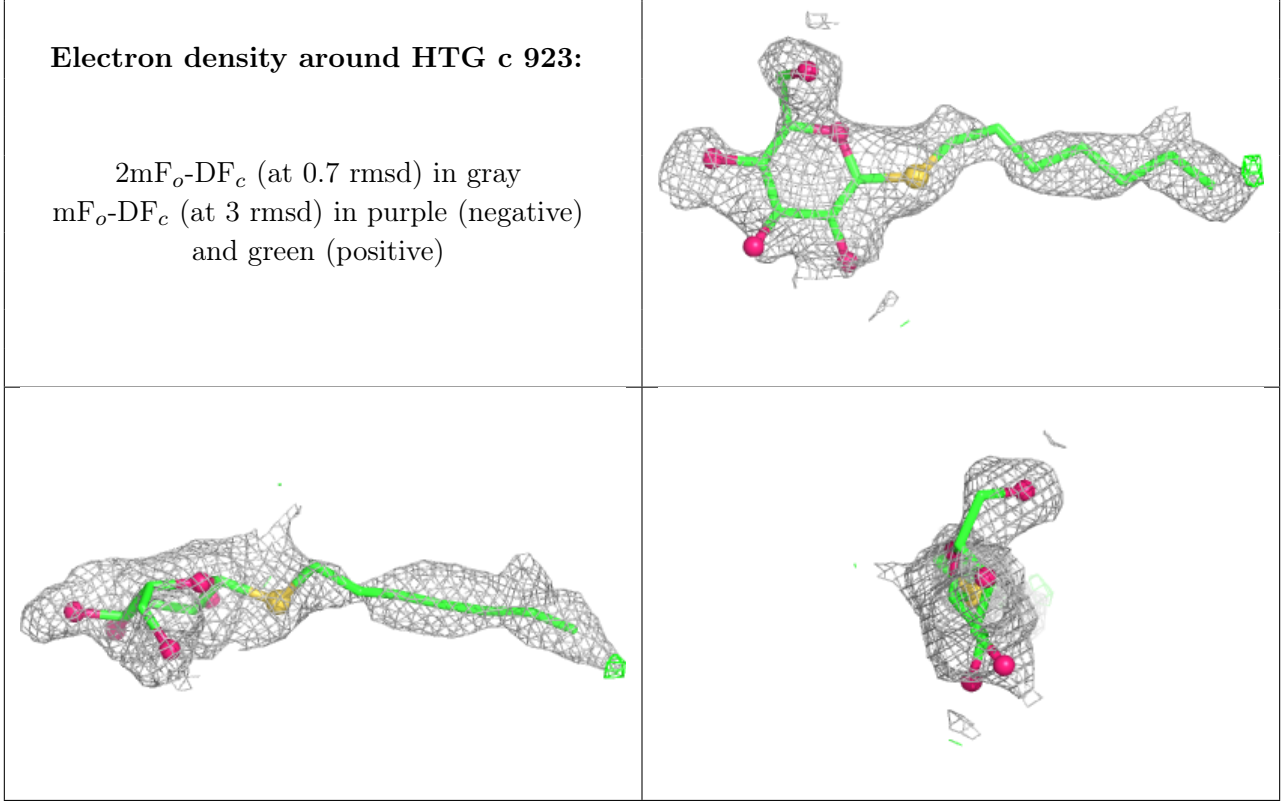






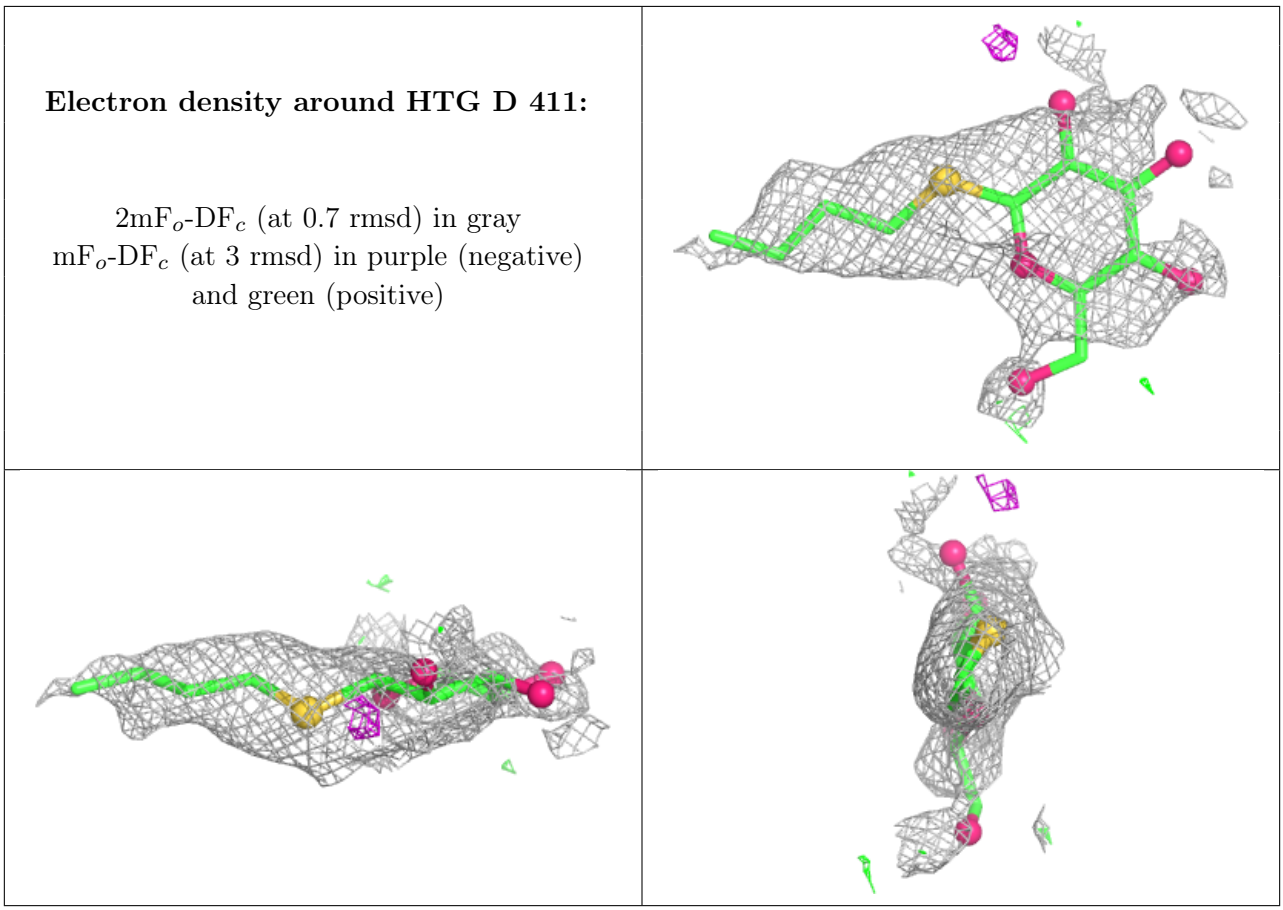
**Electron density around HTG c 923:**

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



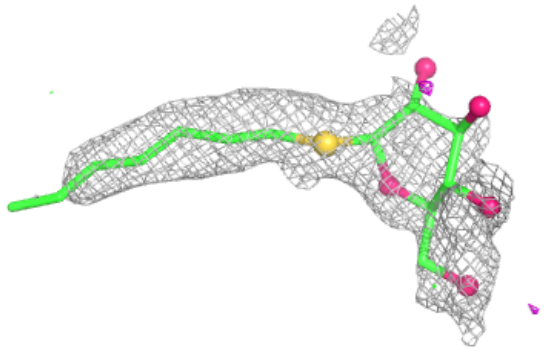
**Electron density around HTG D 411:**

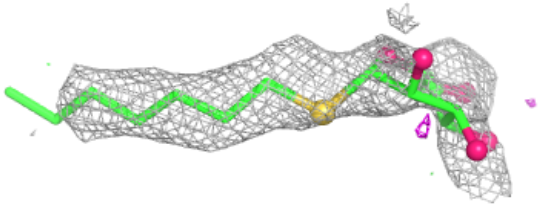
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

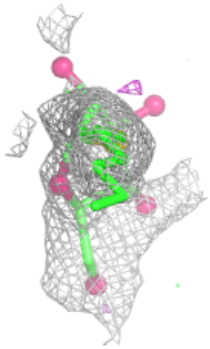


**Electron density around HTG b 627:**

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

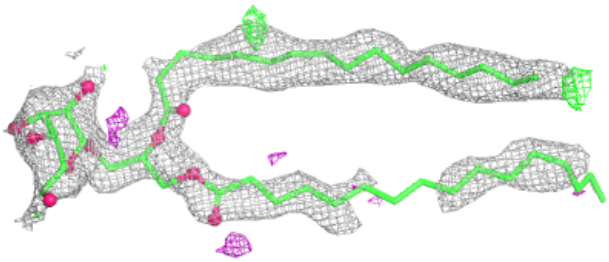


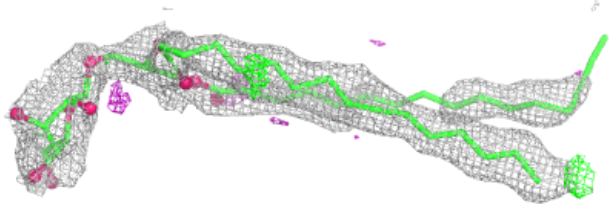


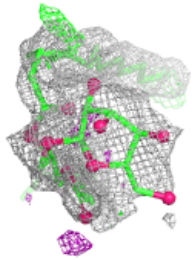


**Electron density around LMG C 521:**

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

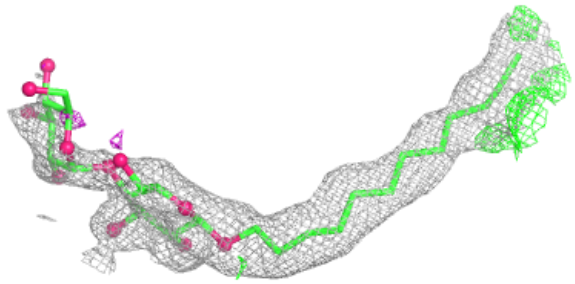


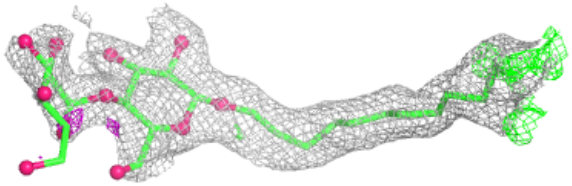


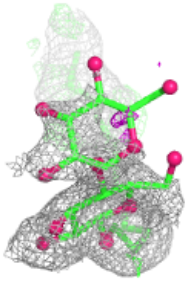


**Electron density around LMT m 104:**

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

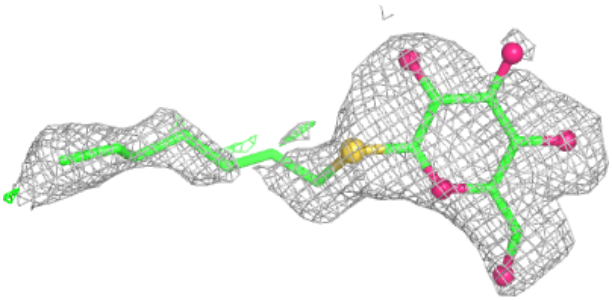


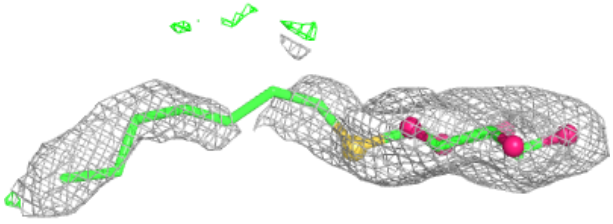


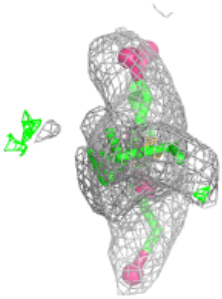


**Electron density around HTG c 922:**

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

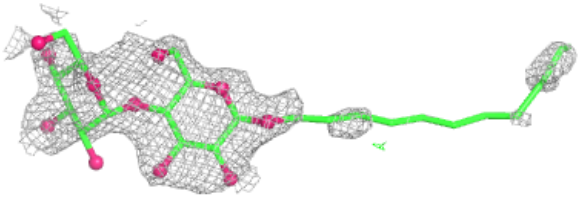


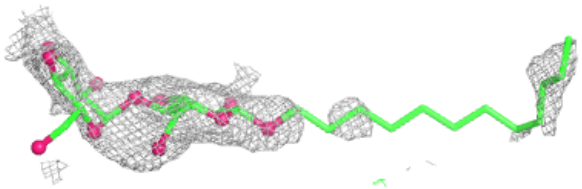


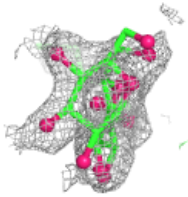


**Electron density around LMT c 921:**

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

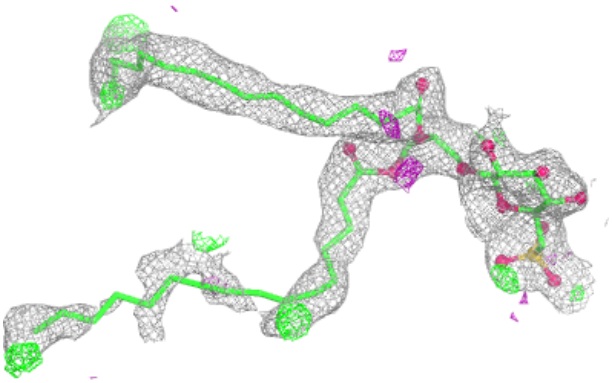


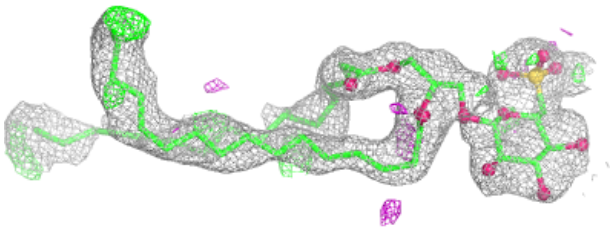


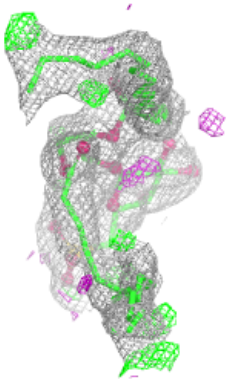


**Electron density around SQD a 402:**

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

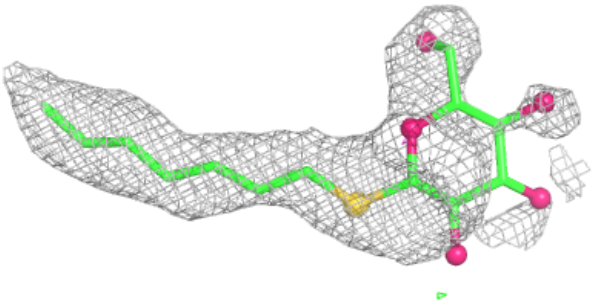


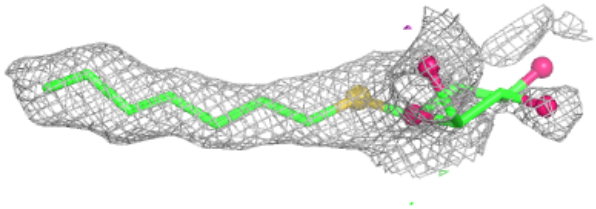


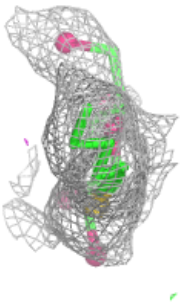


**Electron density around HTG b 603:**

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

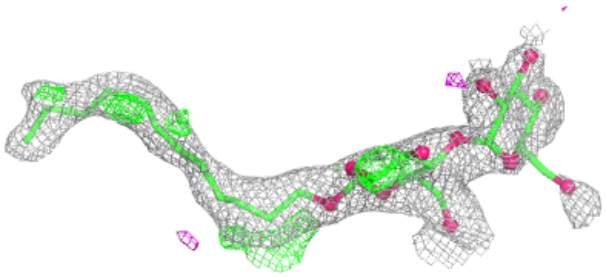


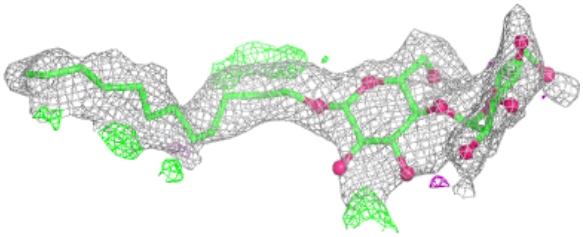


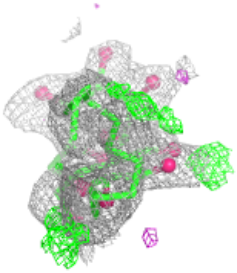


**Electron density around LMT a 401:**

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

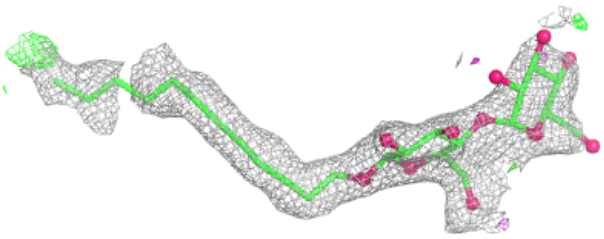


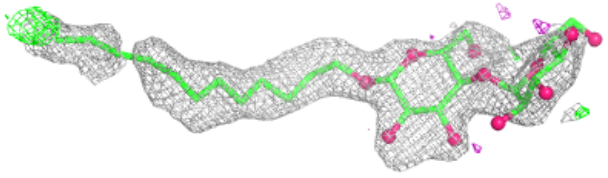


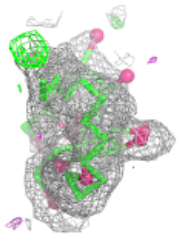


**Electron density around LMT A 417:**

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

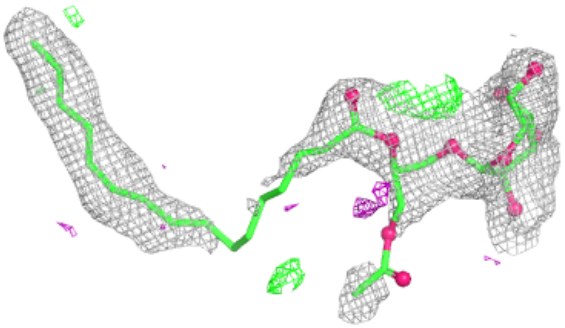


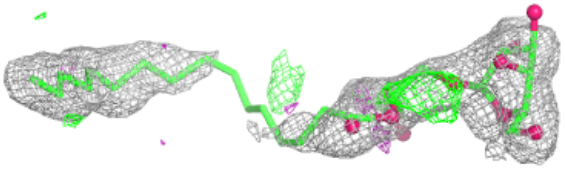


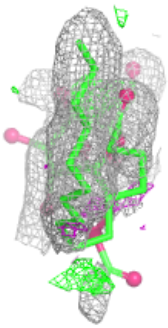


**Electron density around LMG Z 101:**

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

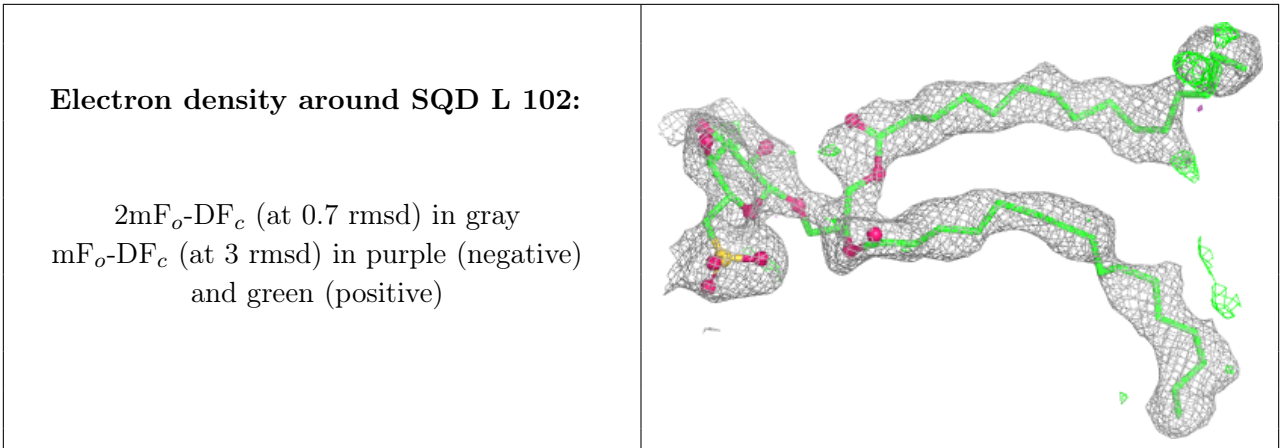






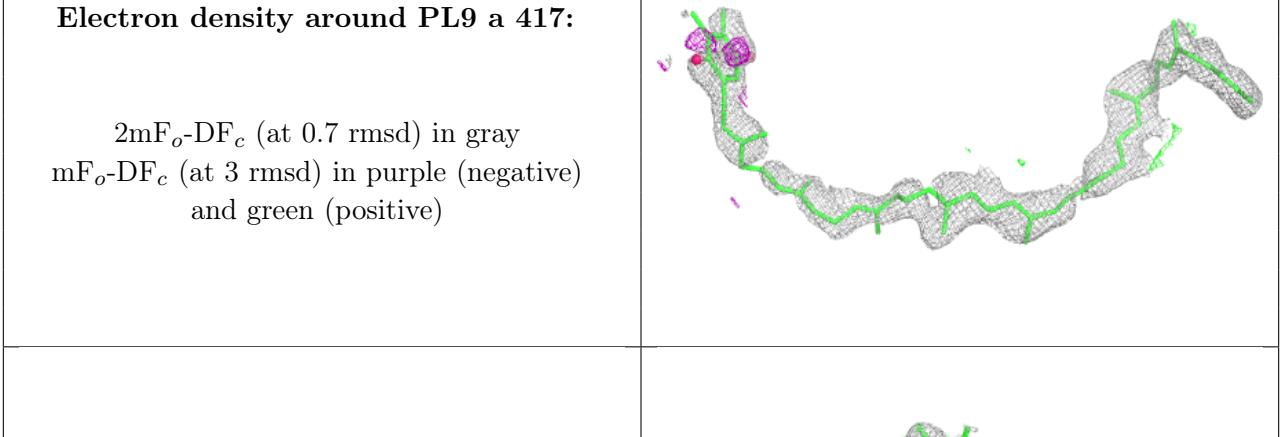
**Electron density around SQD L 102:**

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



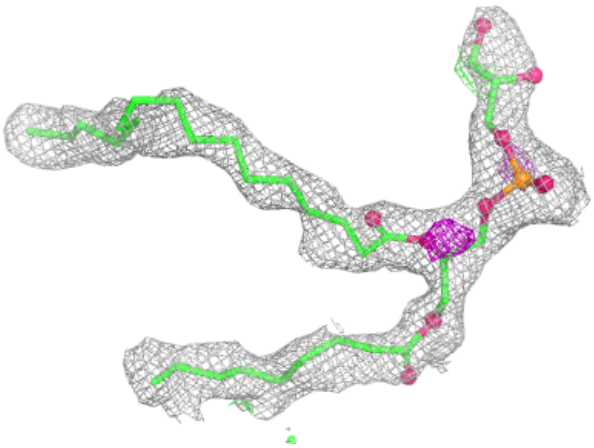
**Electron density around PL9 a 417:**

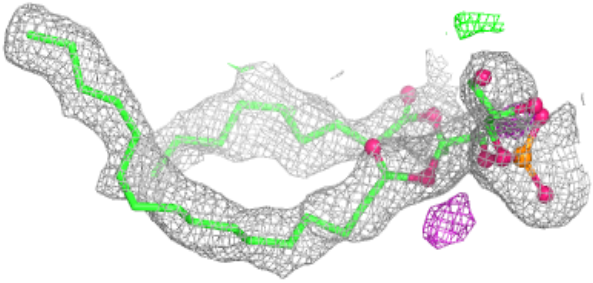
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

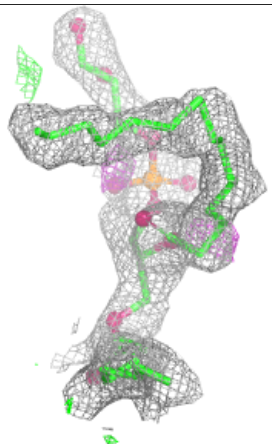


**Electron density around LHG E 101:**

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

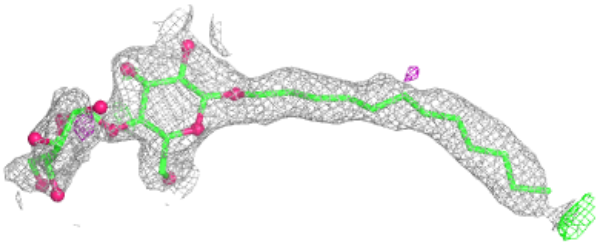


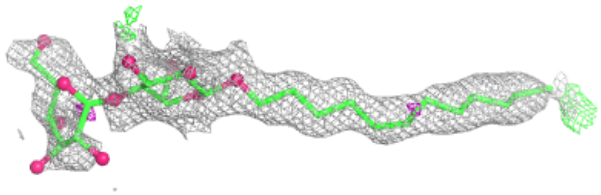


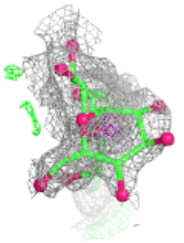


**Electron density around LMT B 623:**

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

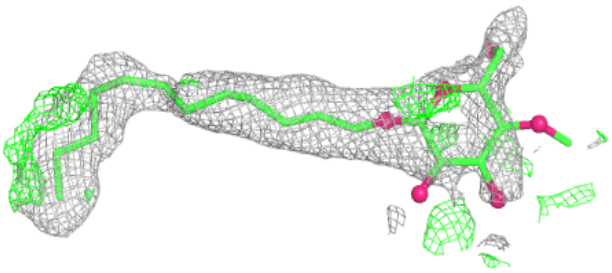


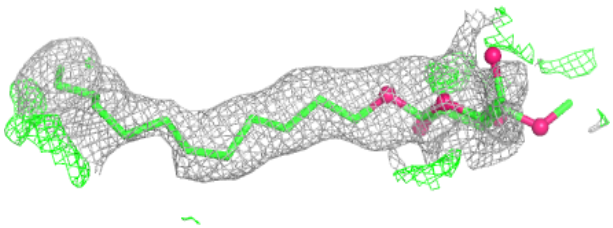


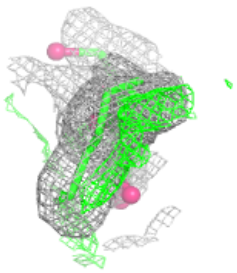


**Electron density around LMT B 636:**

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

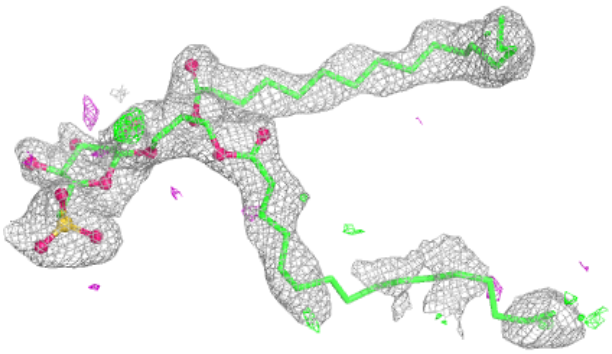


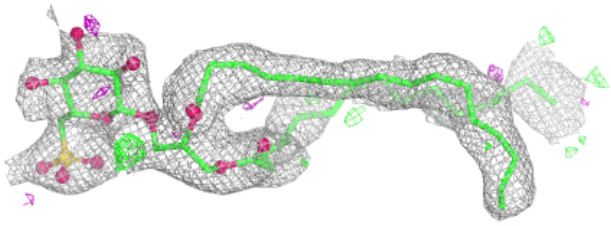


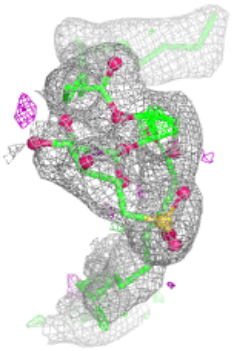


**Electron density around SQD A 416:**

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

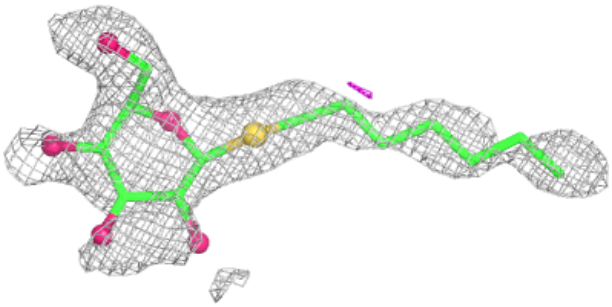


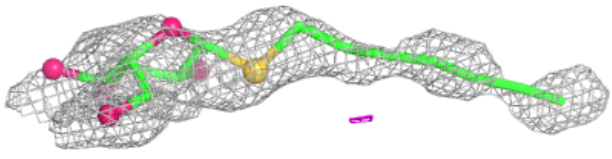


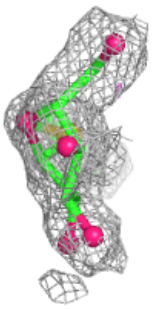


**Electron density around HTG C 524:**

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

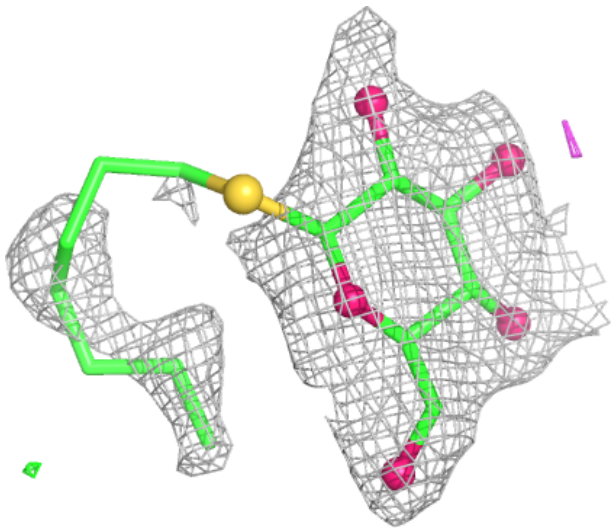


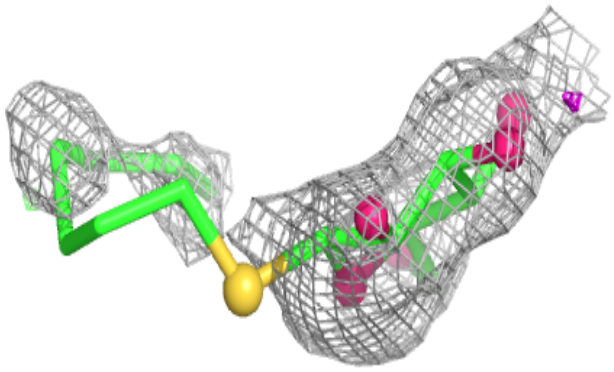


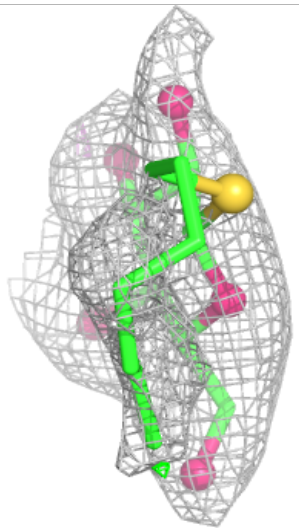


**Electron density around HTG V 202:**

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

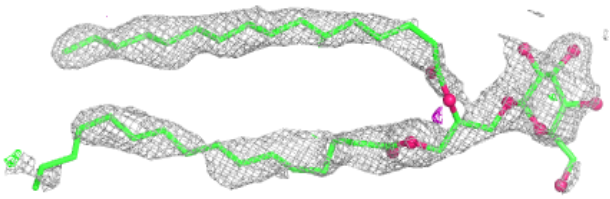


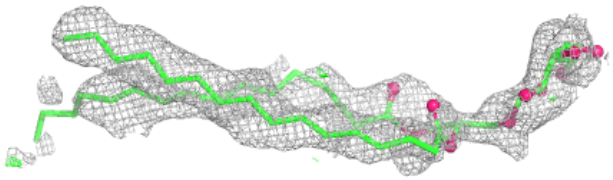


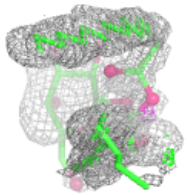


**Electron density around LMG c 920:**

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

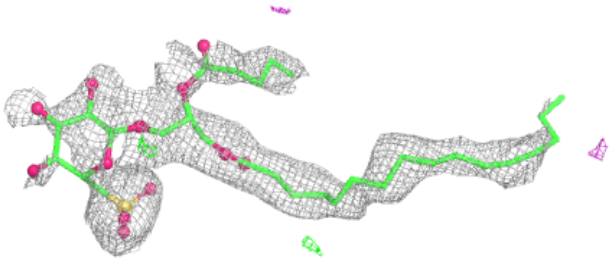


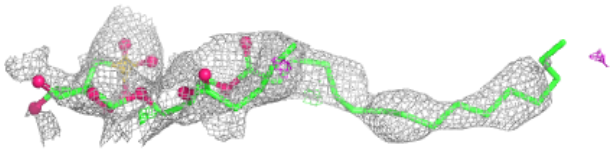


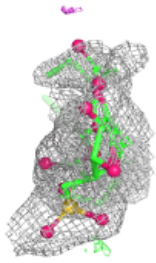


**Electron density around SQD f 102:**

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

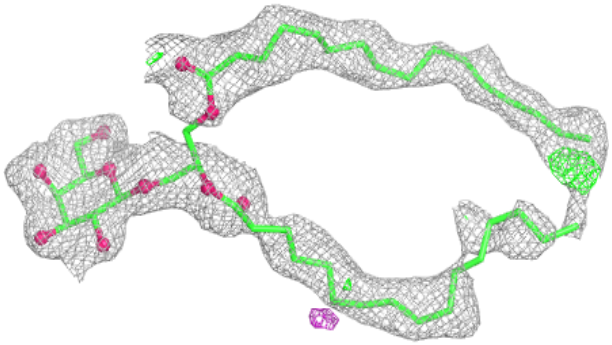


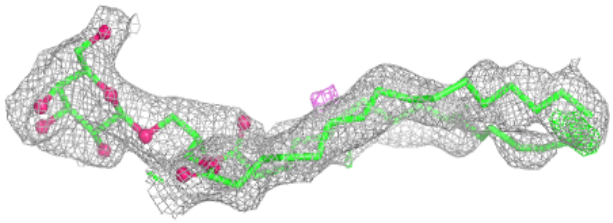


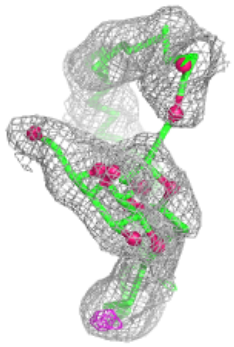


**Electron density around LMG a 412:**

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

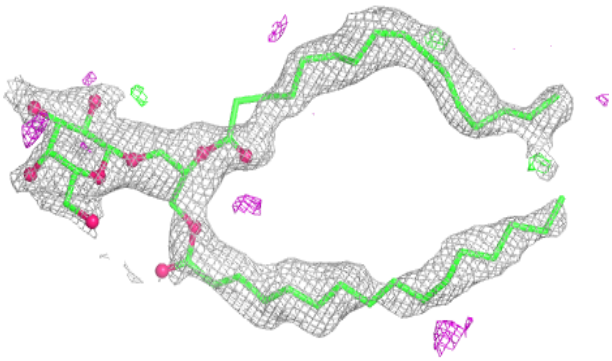


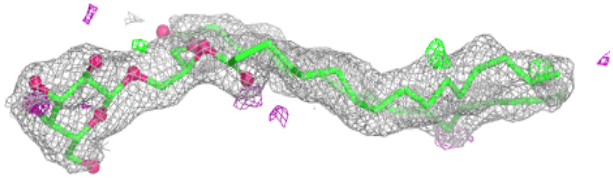


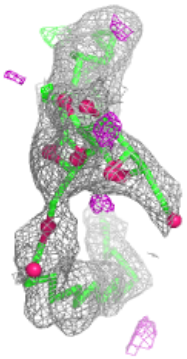


**Electron density around LMG C 501:**

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

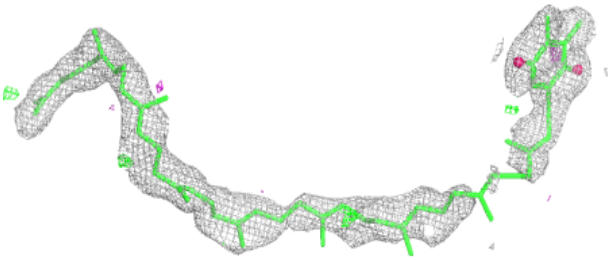


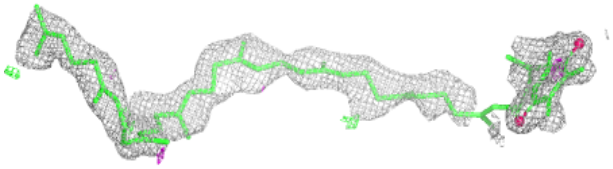


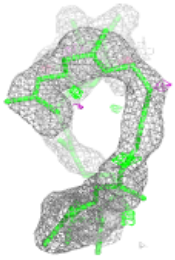


**Electron density around PL9 A 419:**

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

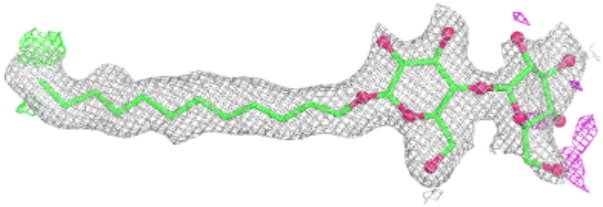


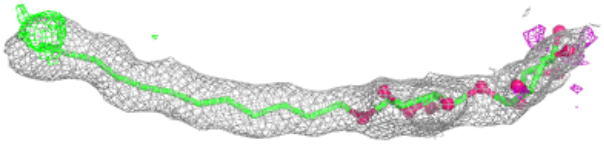


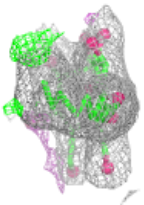


**Electron density around LMT M 101:**

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

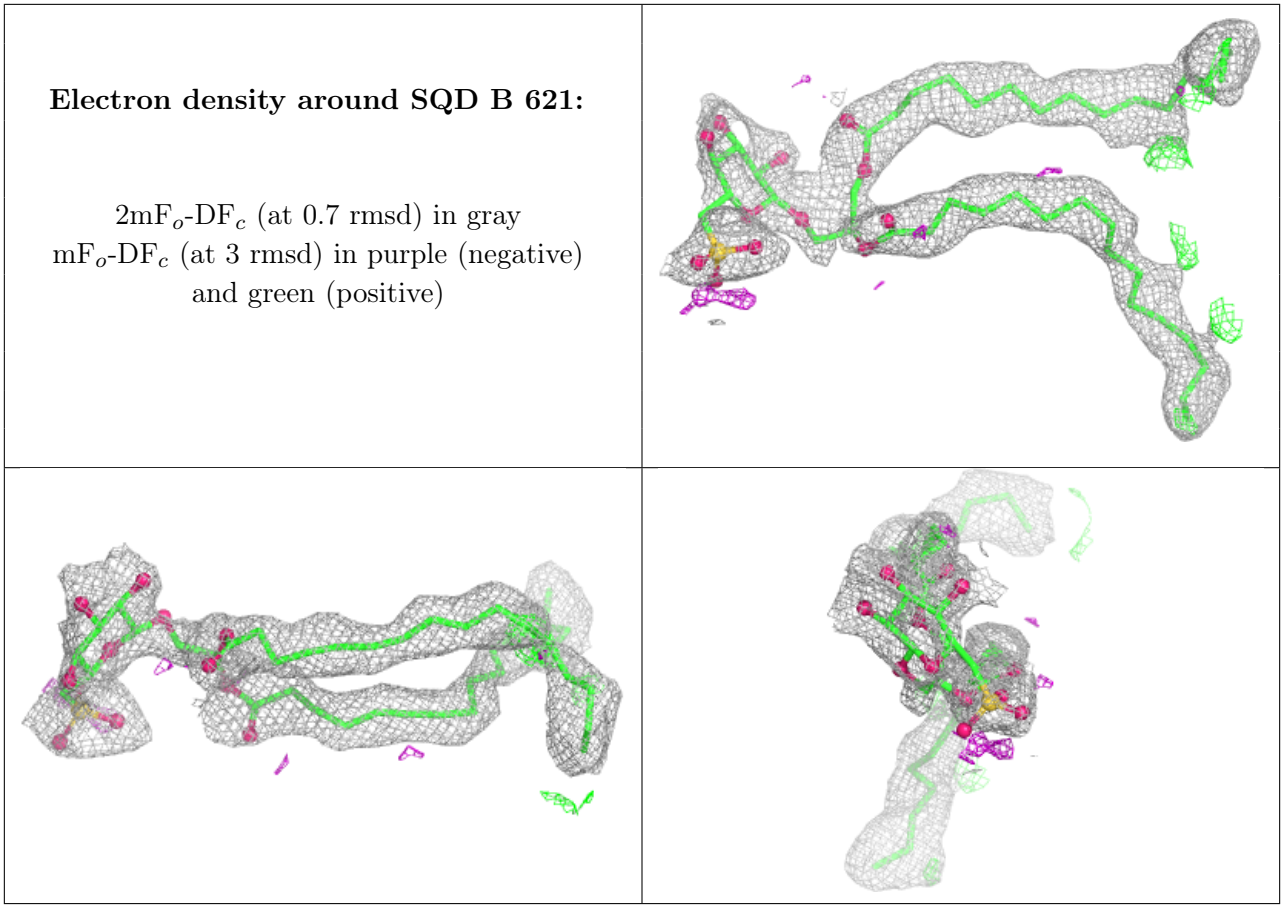






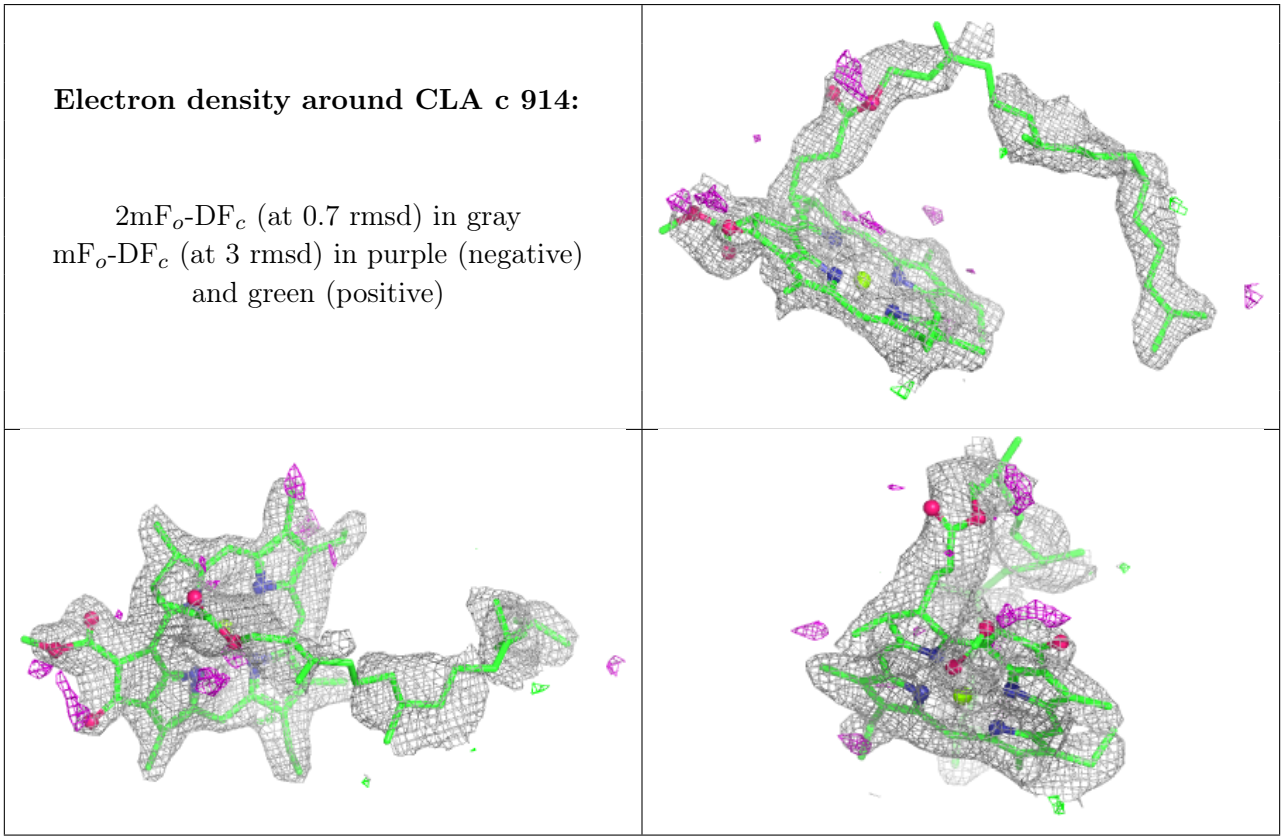
**Electron density around SQD B 621:**

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



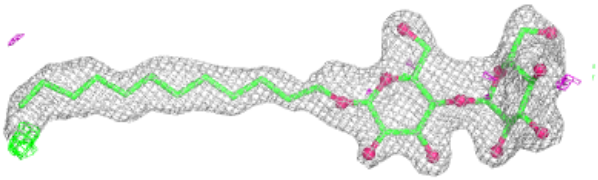
**Electron density around CLA c 914:**

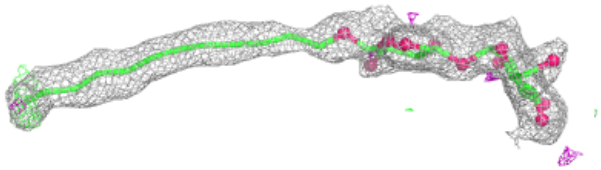
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

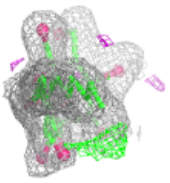


**Electron density around LMT m 103:**

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

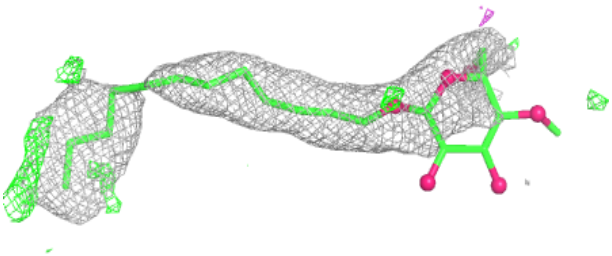


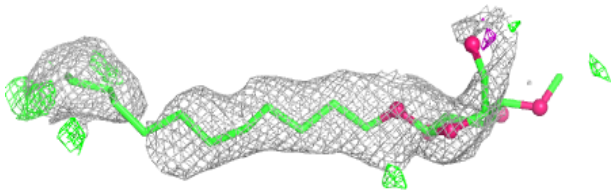


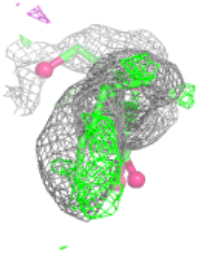


**Electron density around LMT b 601:**

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

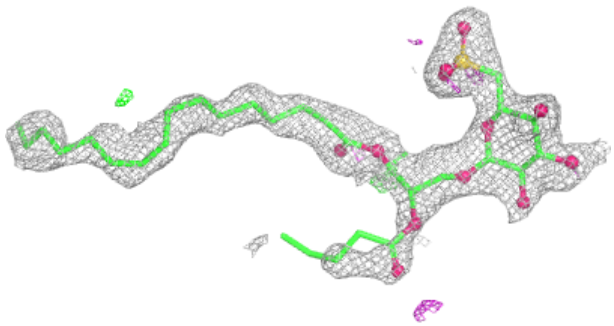


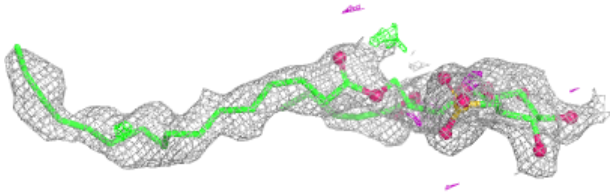


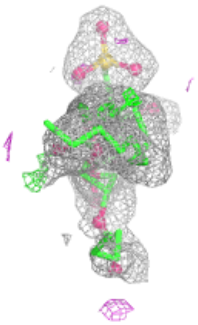


**Electron density around SQD F 101:**

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

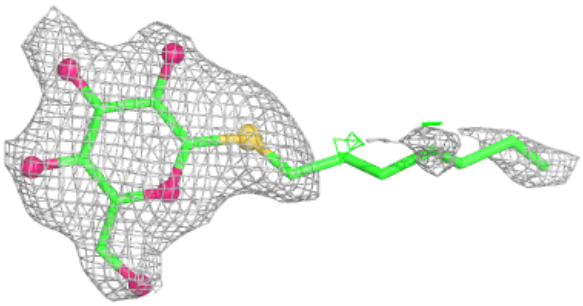


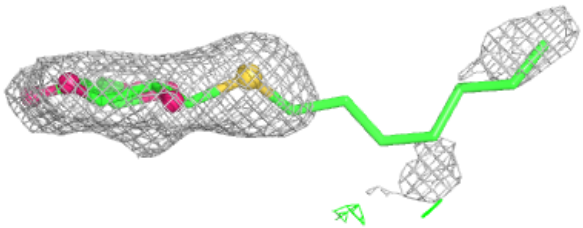


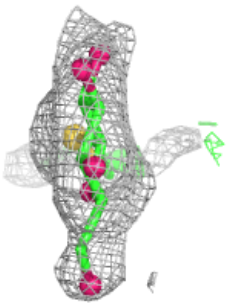


**Electron density around HTG C 523:**

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

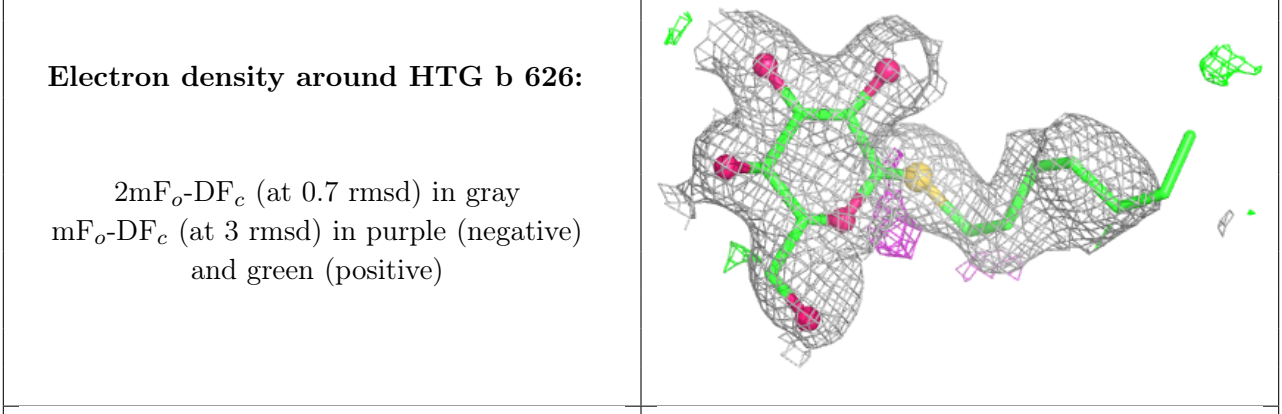






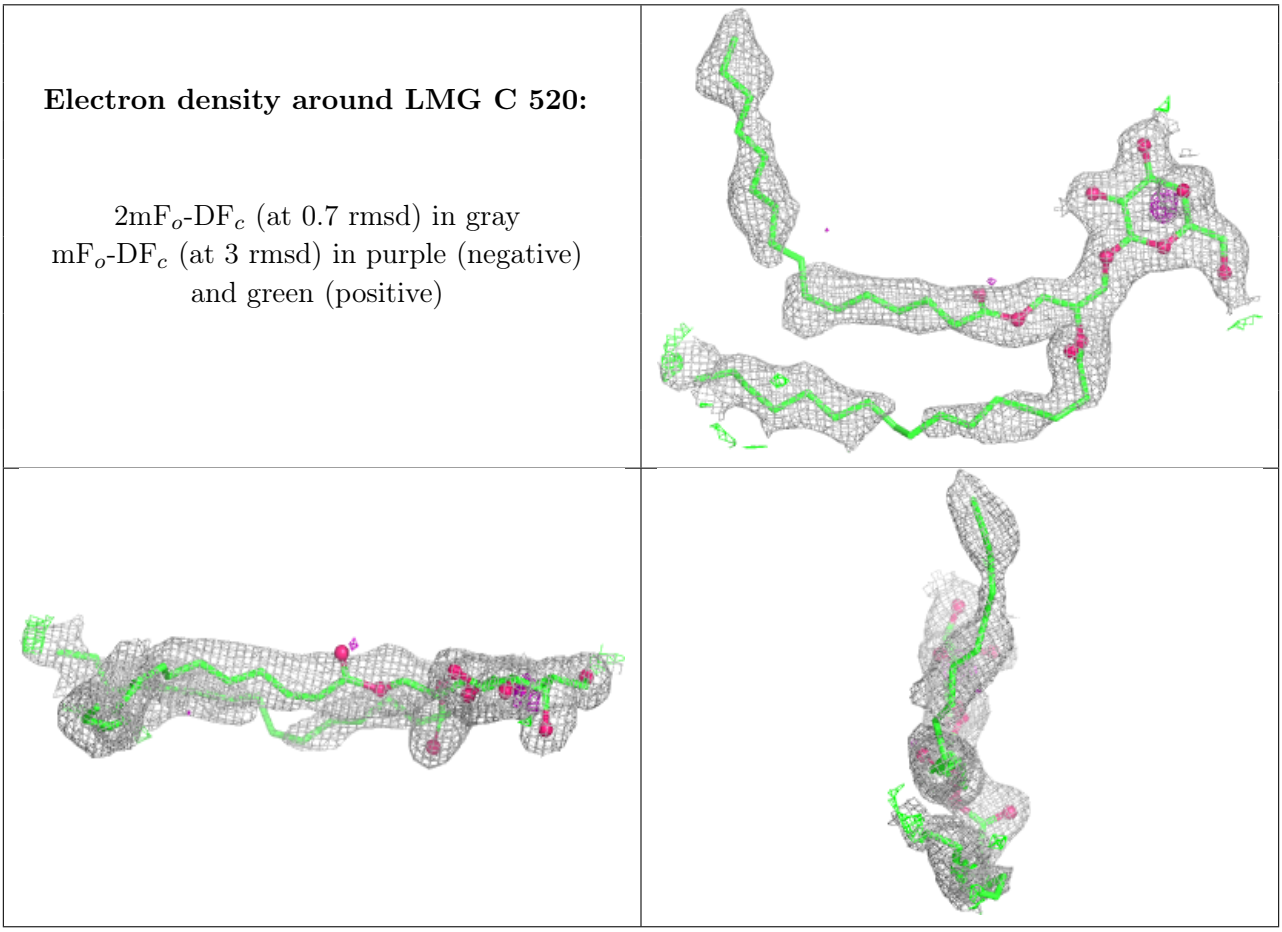
**Electron density around HTG b 626:**

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



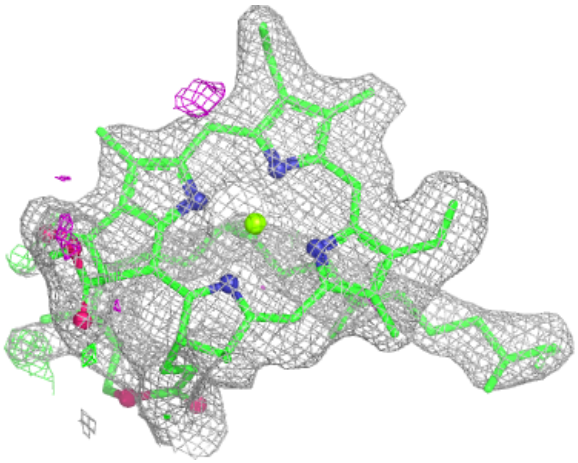
**Electron density around LMG C 520:**

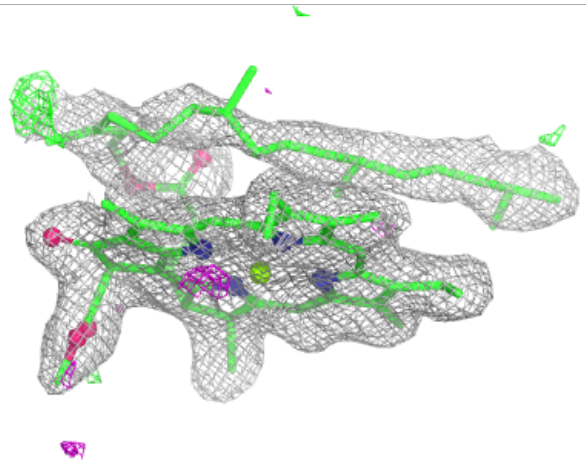
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

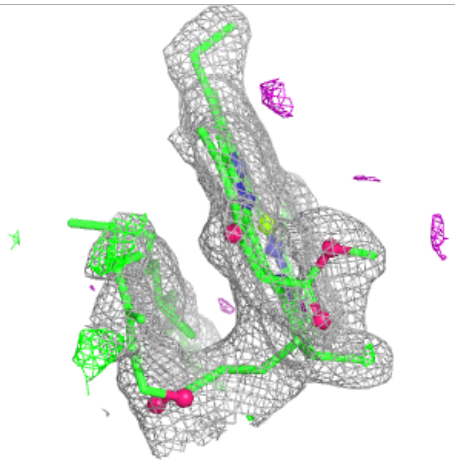


**Electron density around CLA b 605:**

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

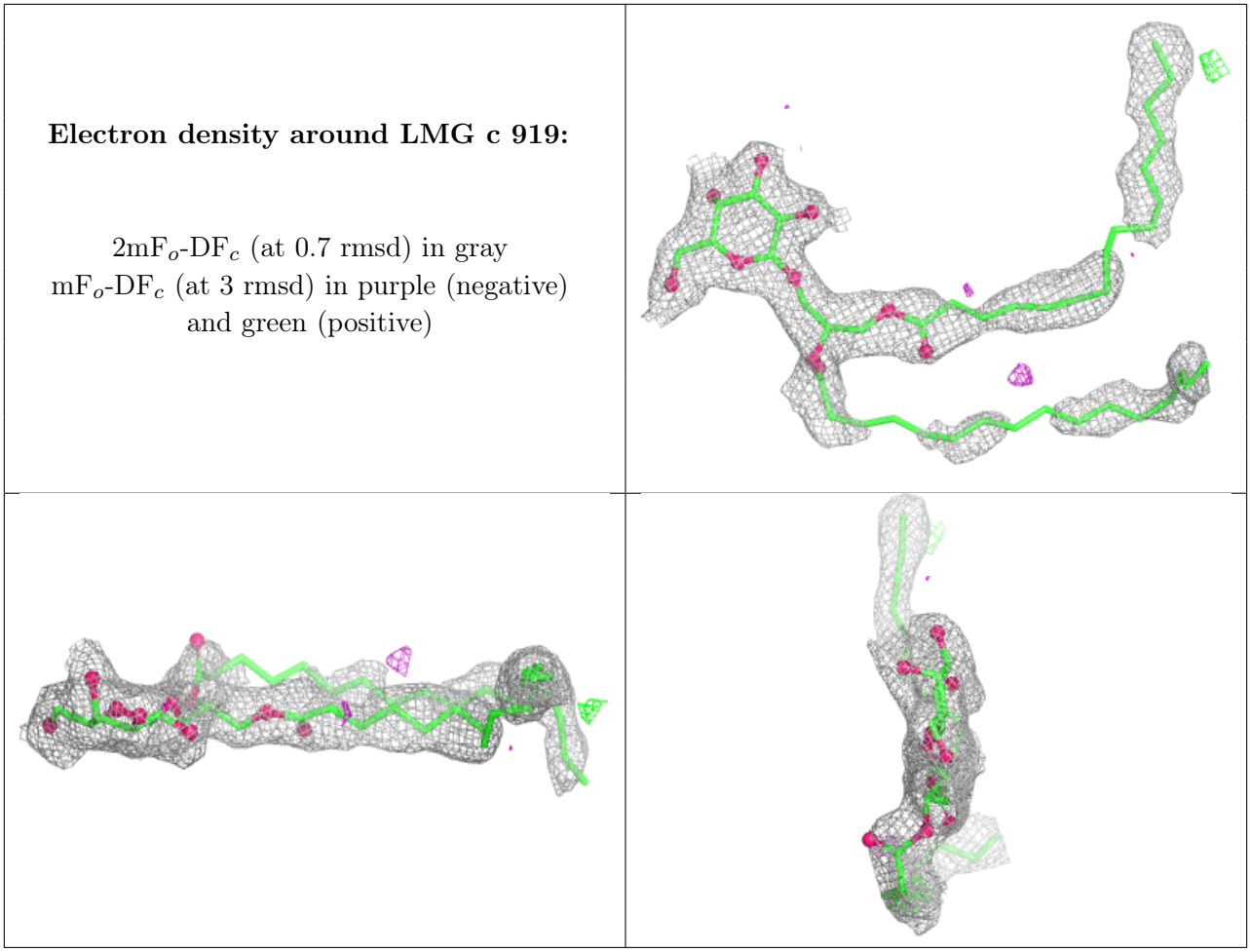






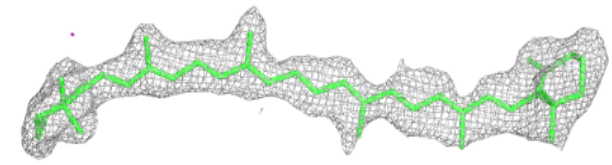
**Electron density around LMG c 919:**

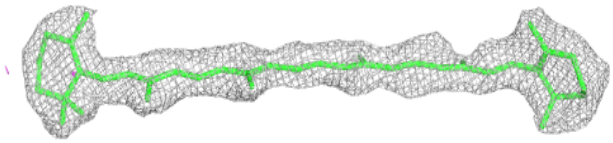
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

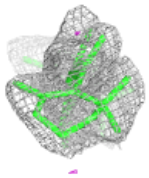


**Electron density around BCR k 101:**

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

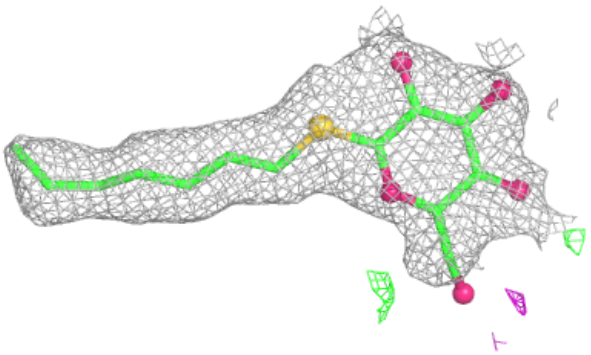


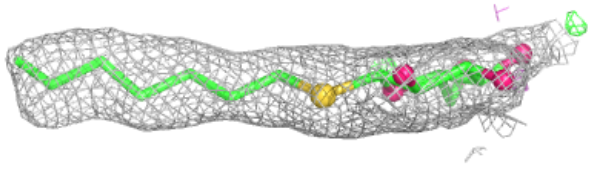


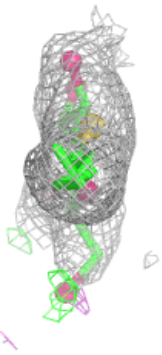


**Electron density around HTG B 633:**

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

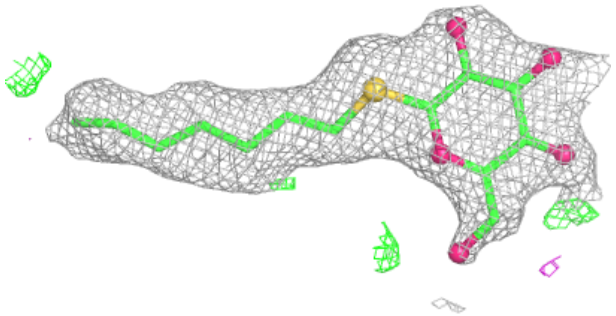


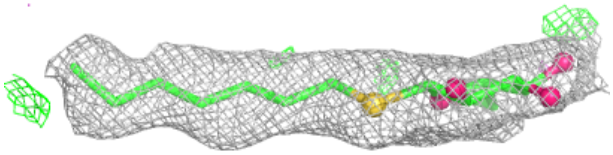


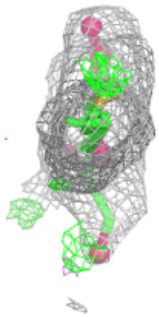


**Electron density around HTG b 602:**

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

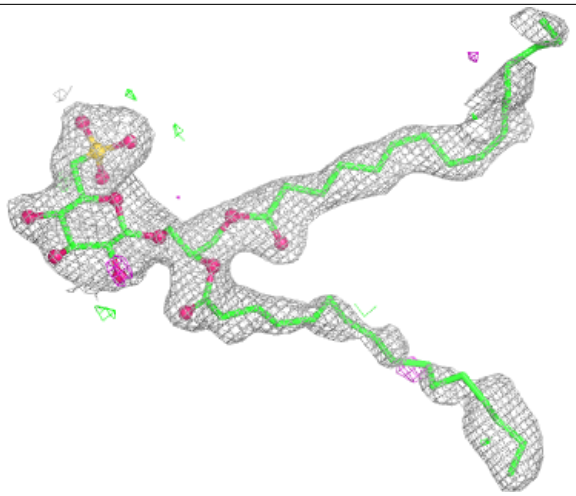


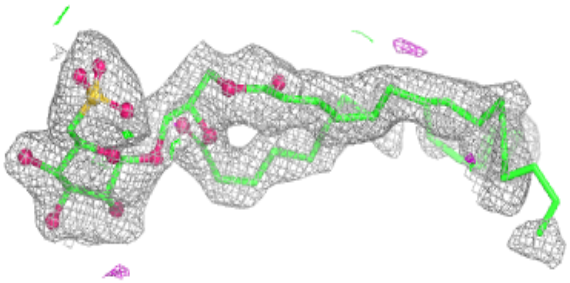


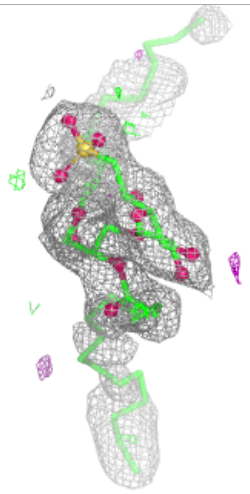


**Electron density around SQD a 411:**

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

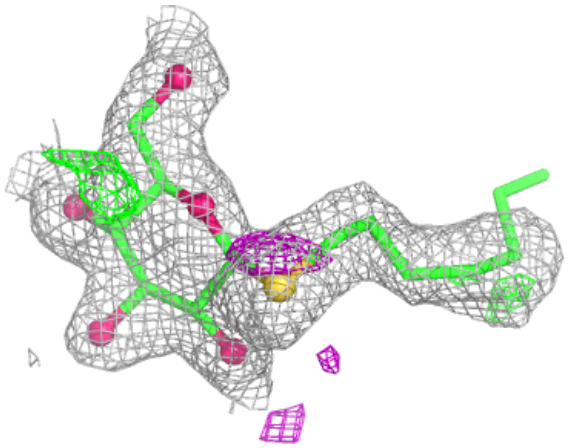


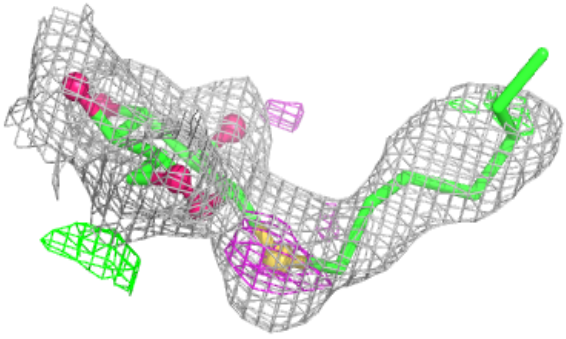


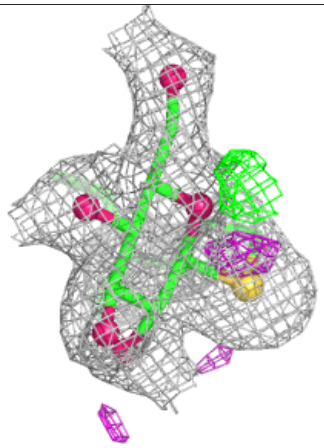


**Electron density around HTG B 625:**

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

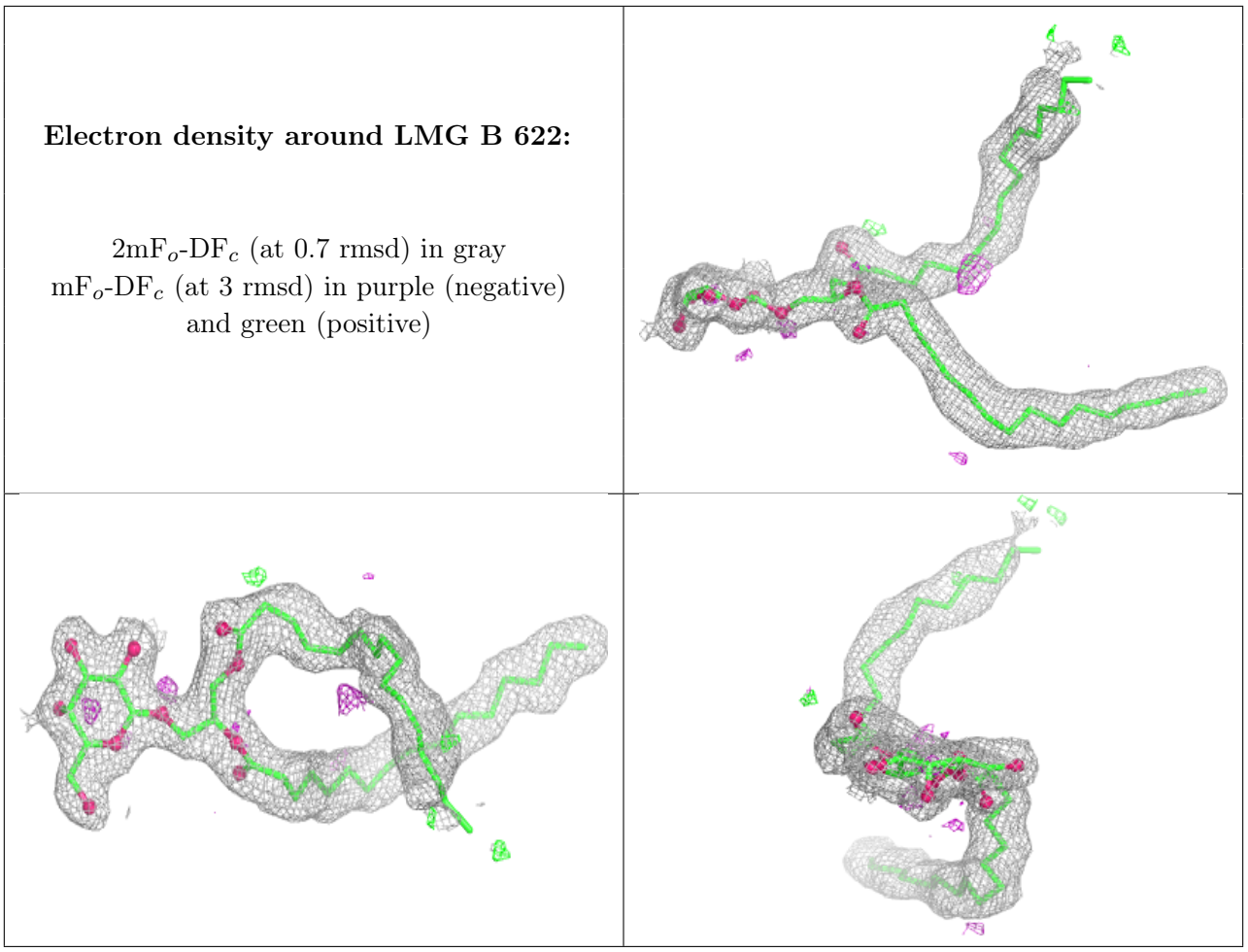






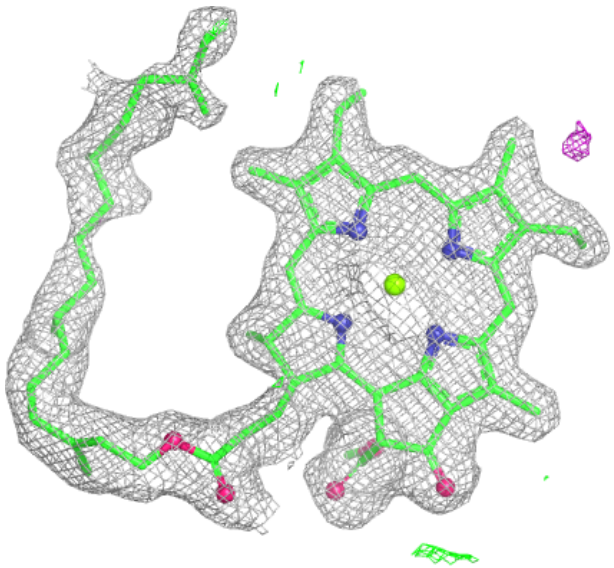
**Electron density around LMG B 622:**

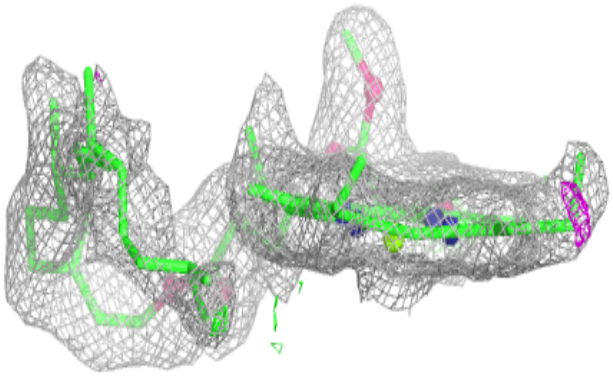
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

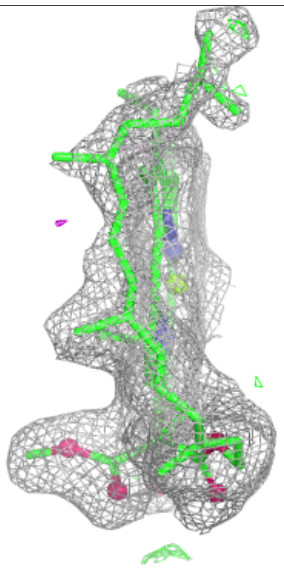


**Electron density around CLA c 913:**

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

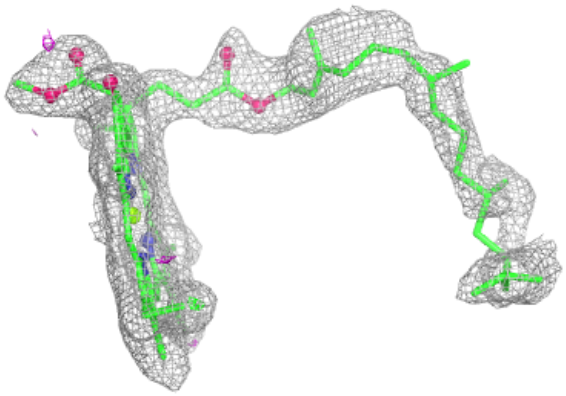


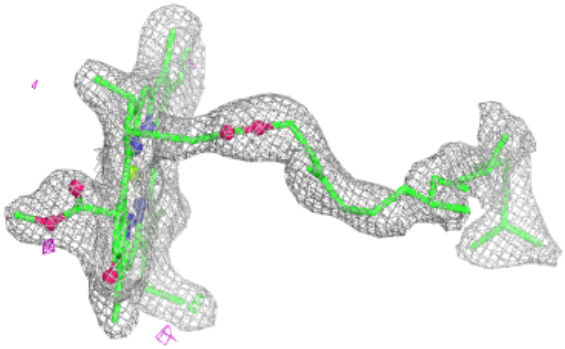


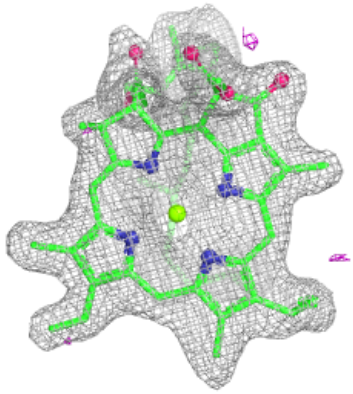


**Electron density around CLA C 507:**

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

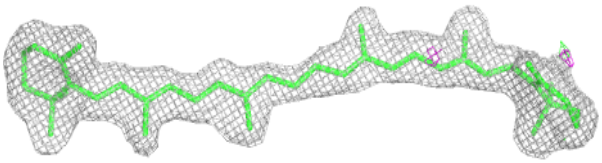


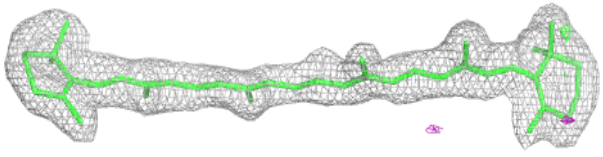


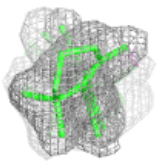


**Electron density around BCR C 515:**

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

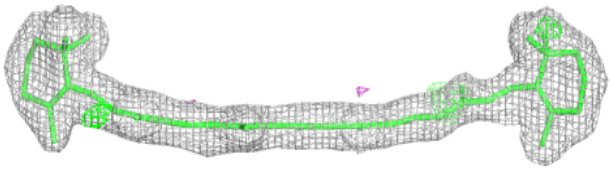


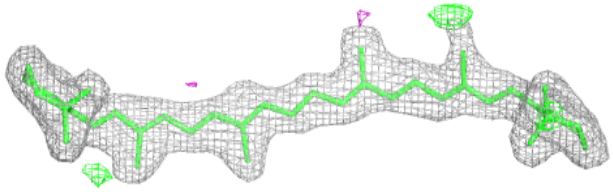


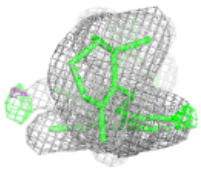


**Electron density around BCR K 103:**

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

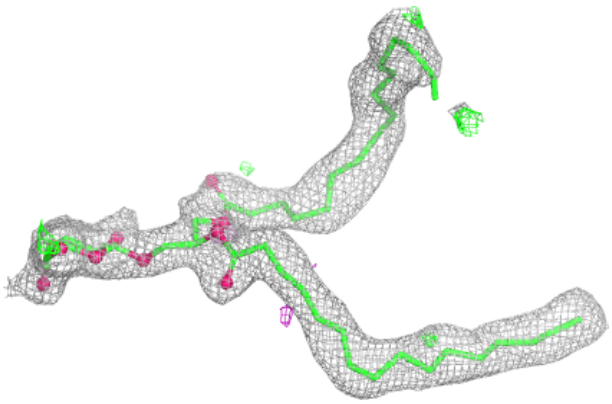


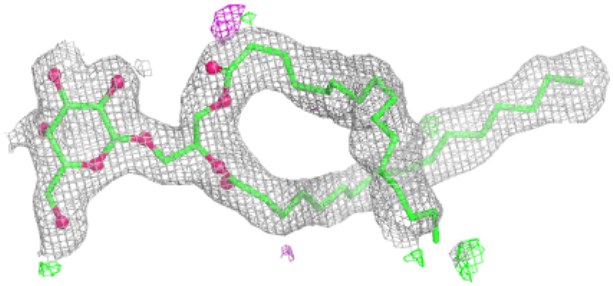


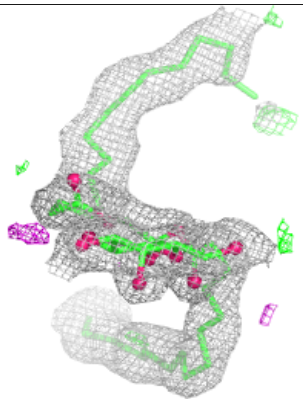


**Electron density around LMG b 624:**

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

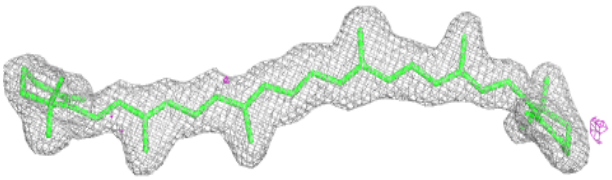


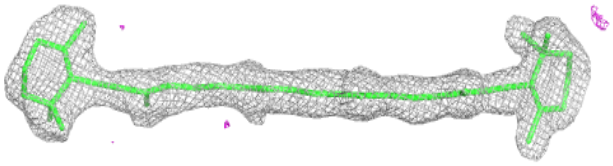


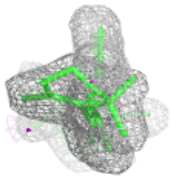


**Electron density around BCR c 915:**

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

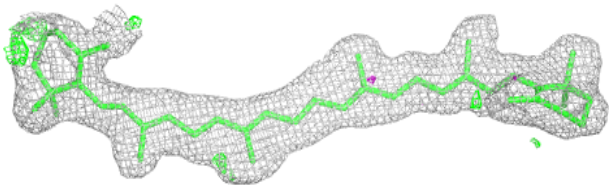


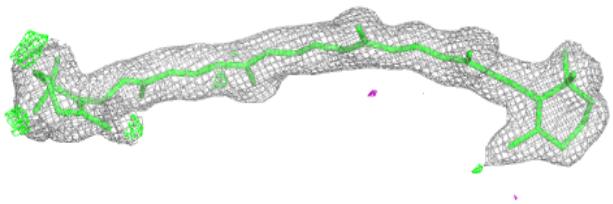


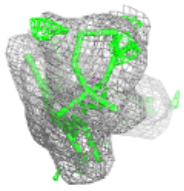


**Electron density around BCR d 404:**

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

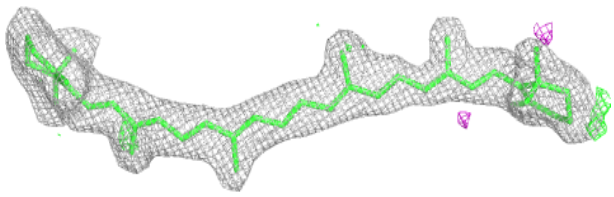


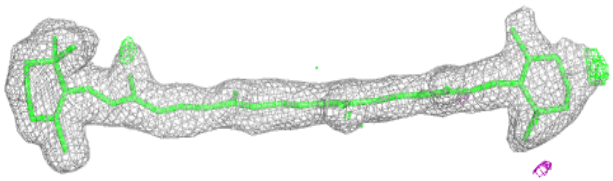


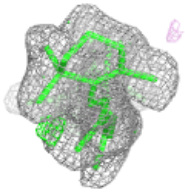


**Electron density around BCR h 101:**

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

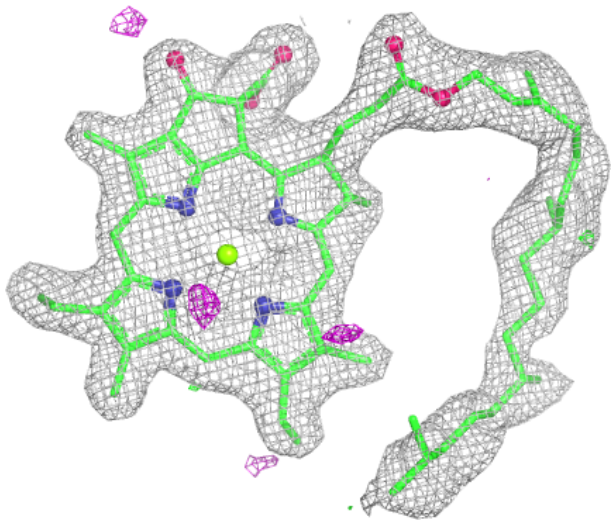


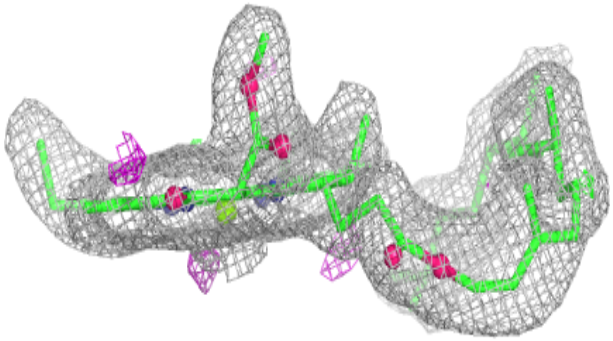


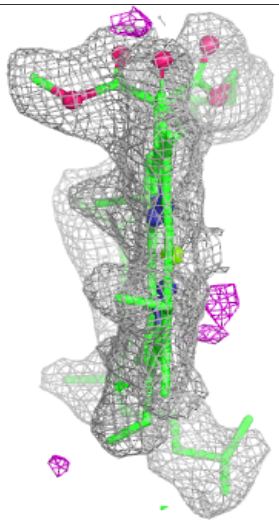


**Electron density around CLA C 513:**

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

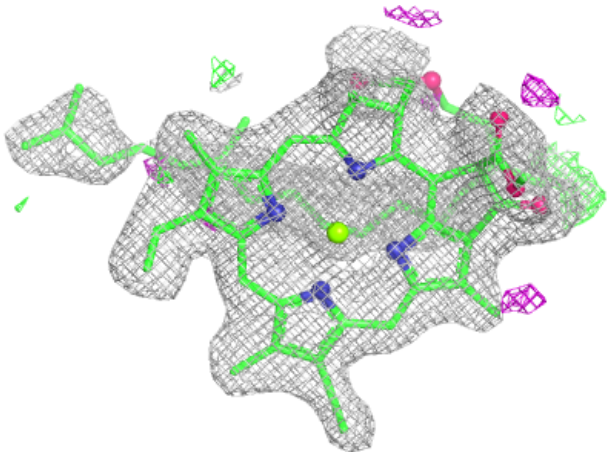


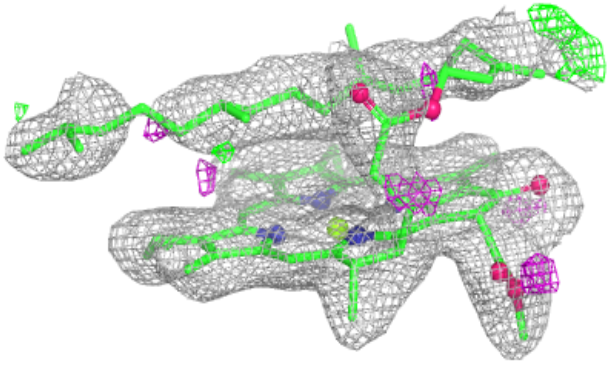


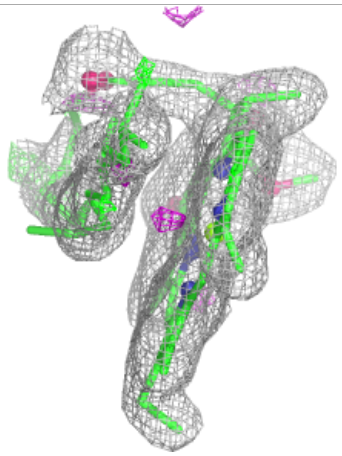


**Electron density around CLA B 602:**

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

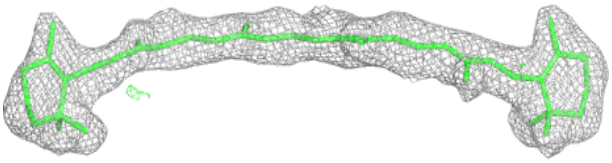


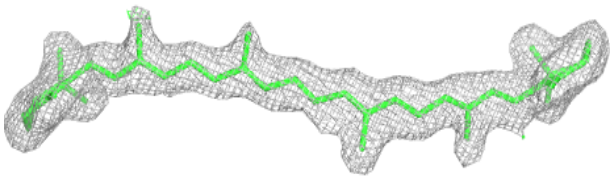


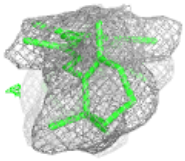


**Electron density around BCR k 102:**

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

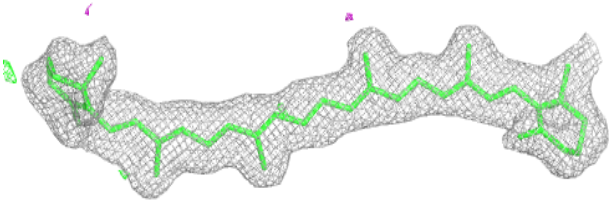


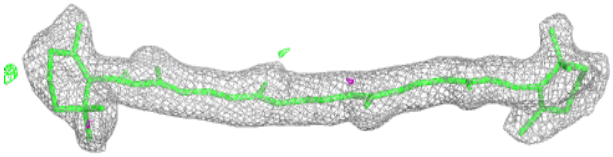


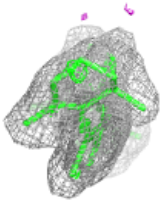


**Electron density around BCR y 101:**

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

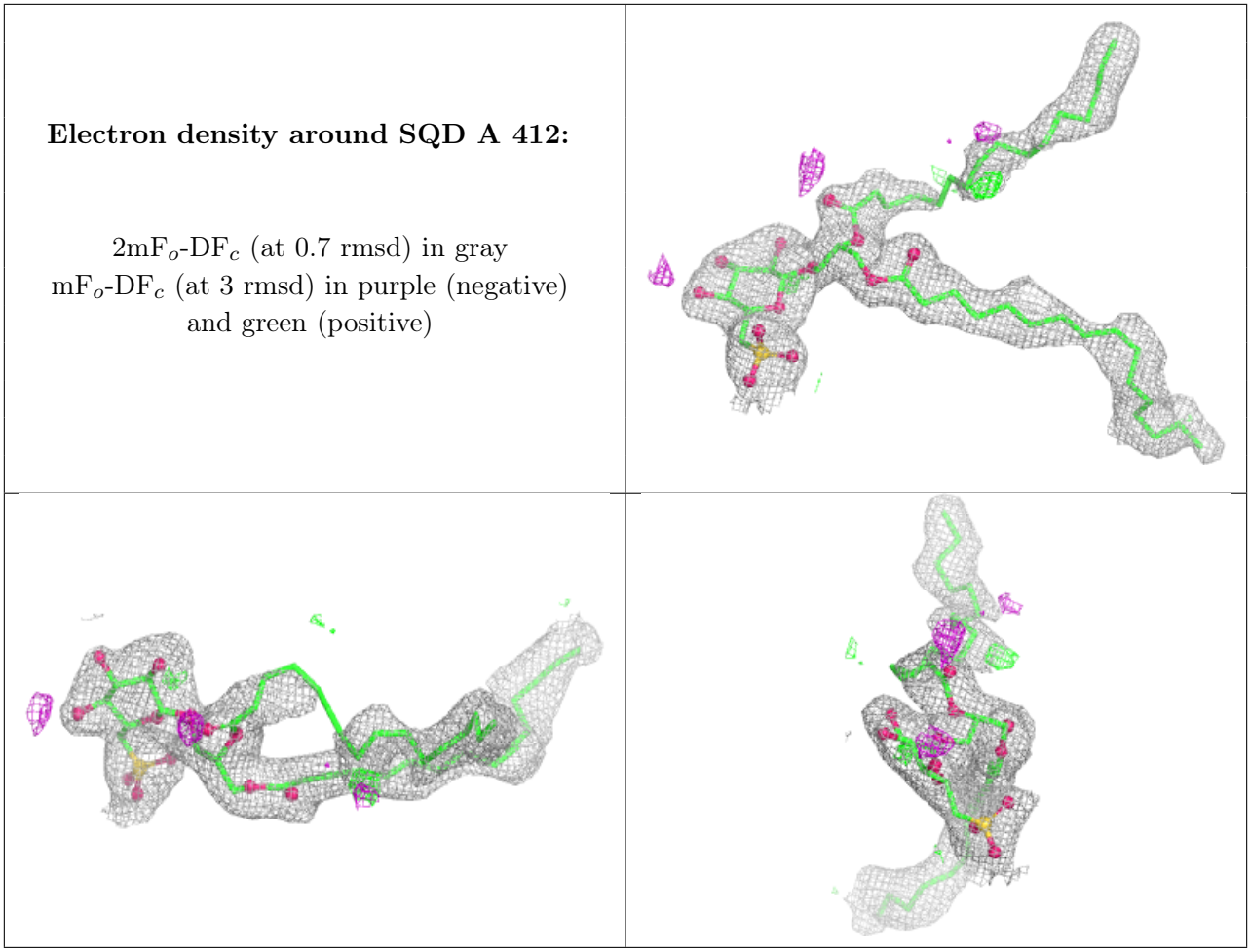






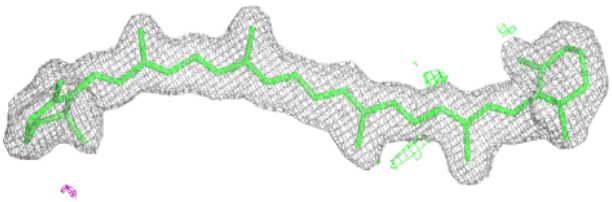
**Electron density around SQD A 412:**

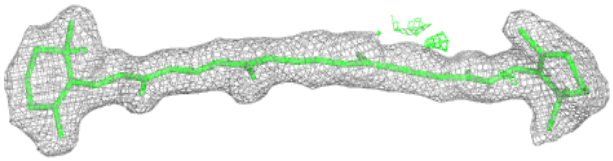
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

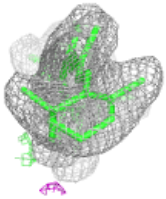


**Electron density around BCR K 102:**

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

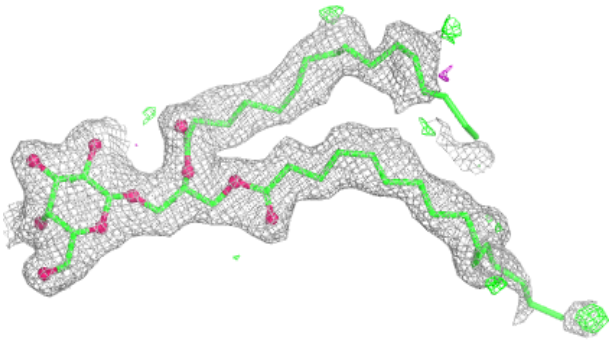


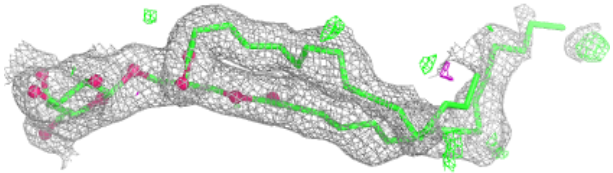


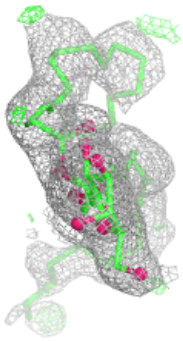


**Electron density around LMG j 101:**

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

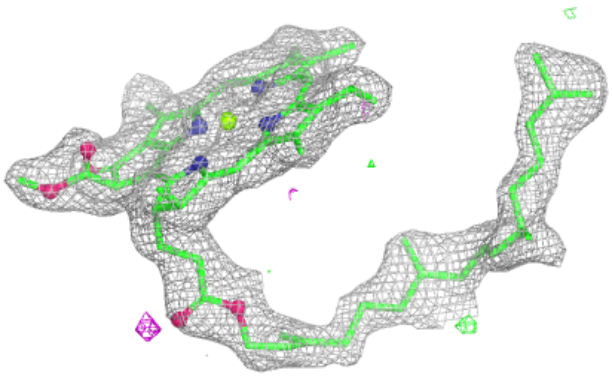


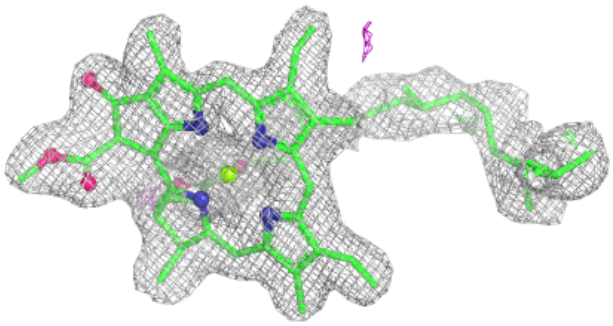


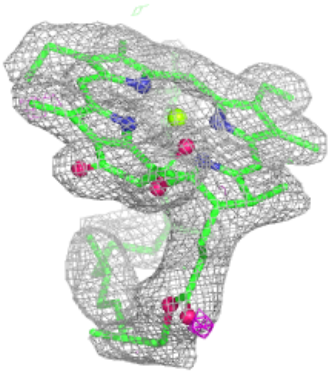


**Electron density around CLA C 514:**

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

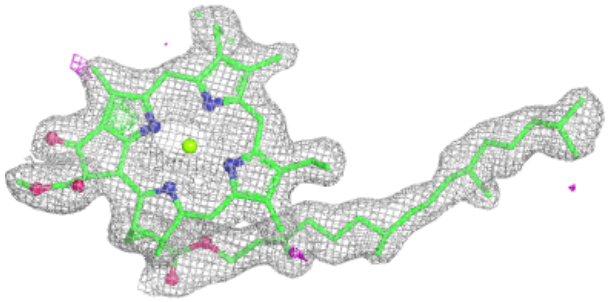


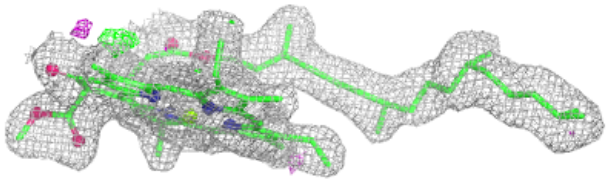


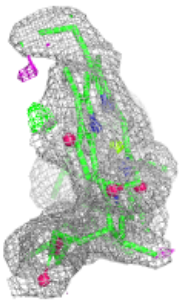


**Electron density around CLA c 902:**

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

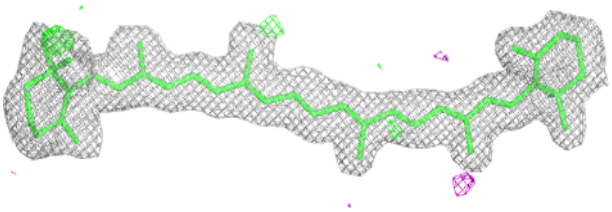


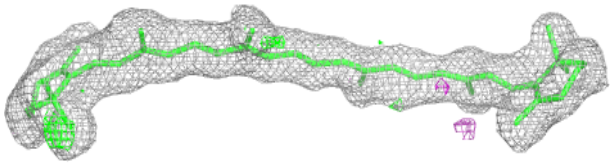


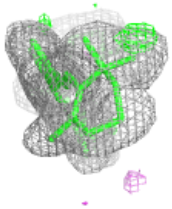


**Electron density around BCR B 620:**

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

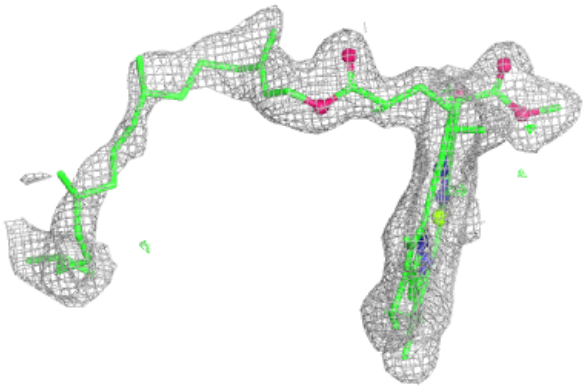


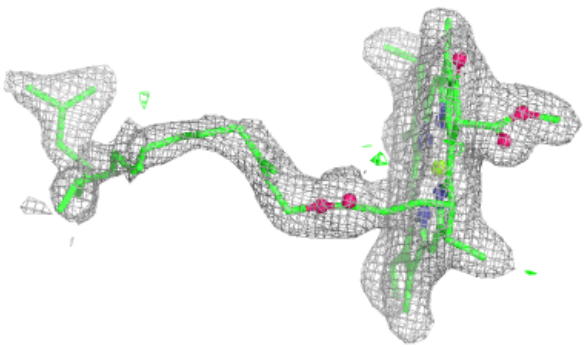


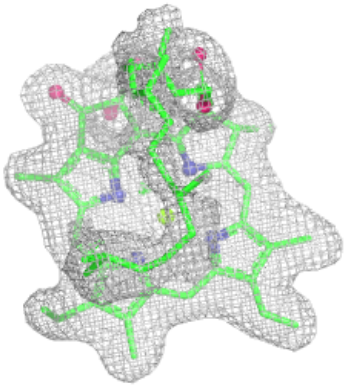


**Electron density around CLA c 907:**

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

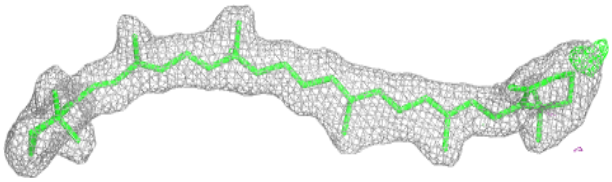


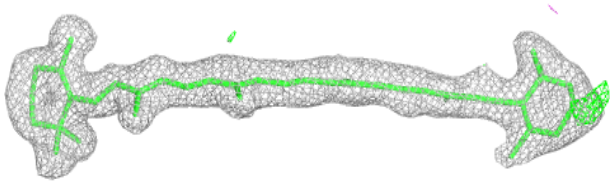


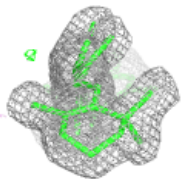


**Electron density around BCR H 101:**

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

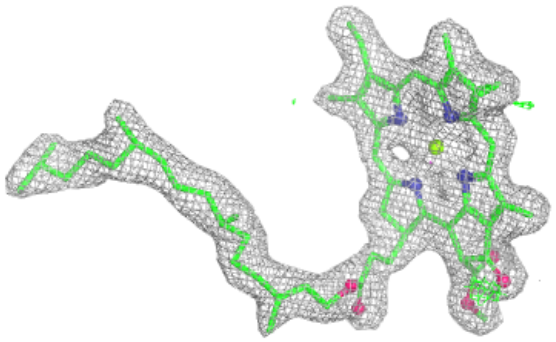


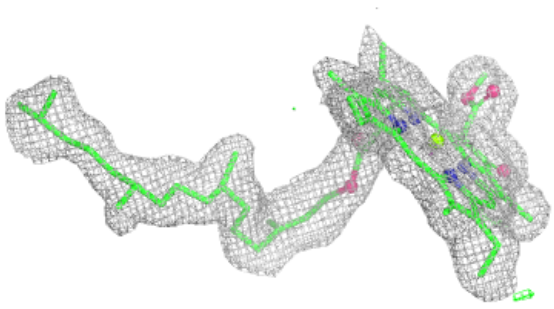


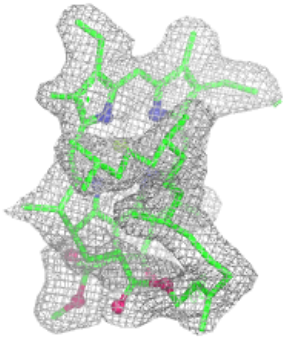


**Electron density around CLA c 912:**

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

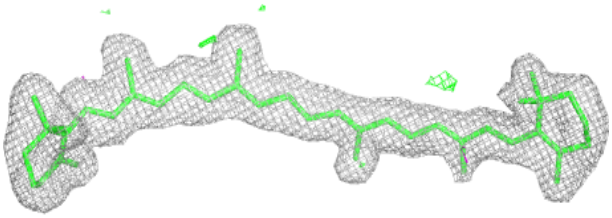


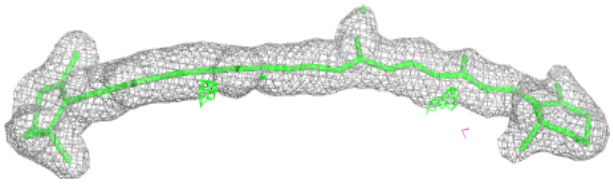


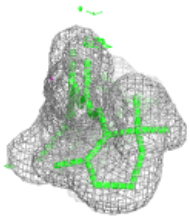


**Electron density around BCR T 102:**

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

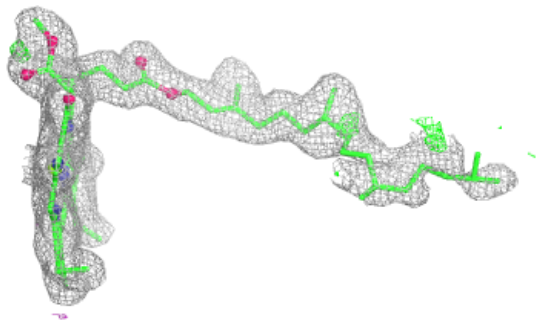


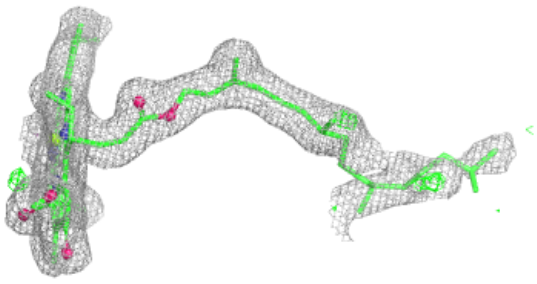


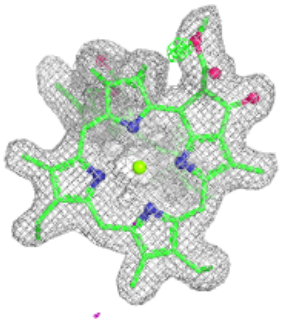


**Electron density around CLA b 610:**

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

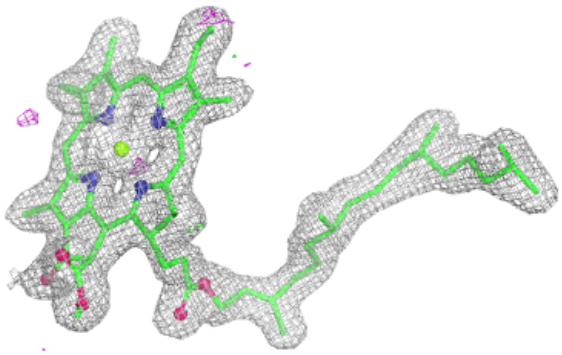


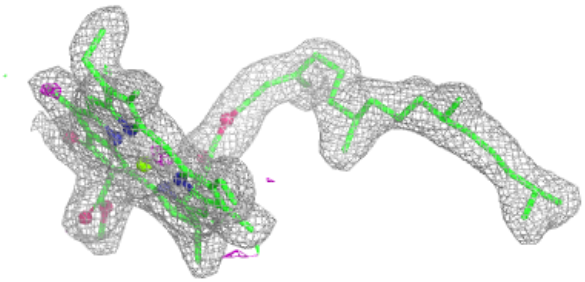


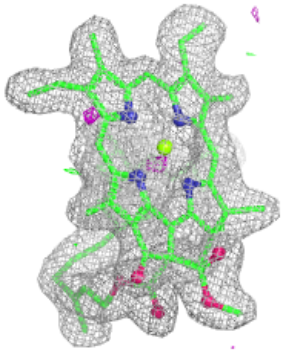


**Electron density around CLA C 512:**

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

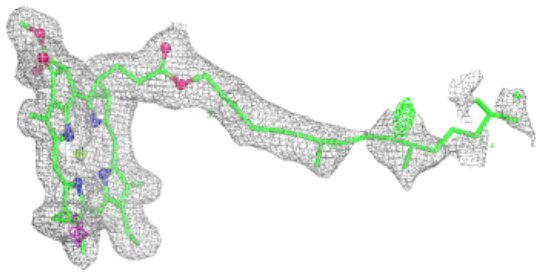


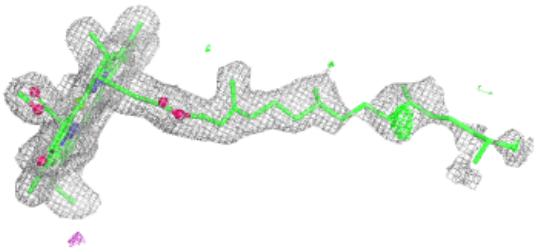


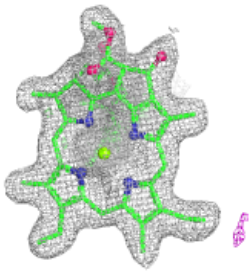


**Electron density around CLA d 403:**

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

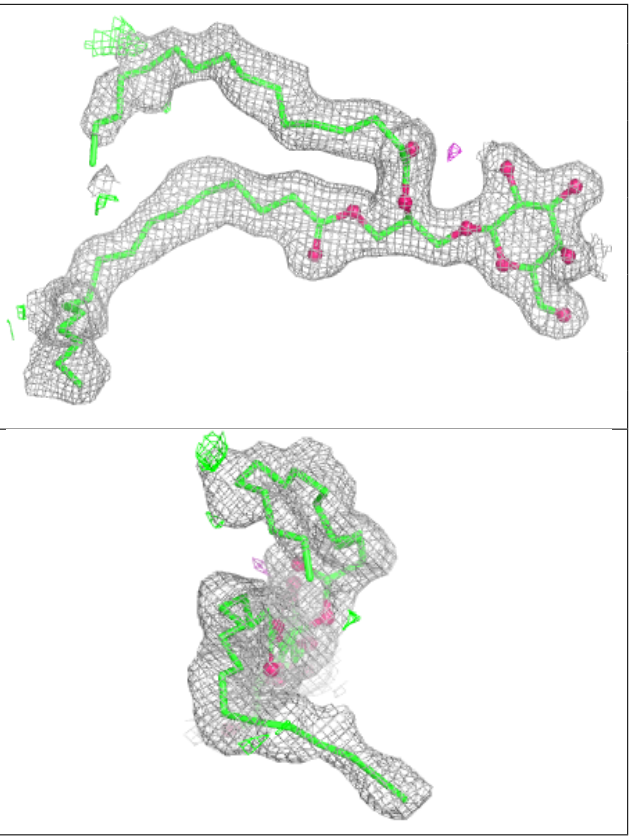






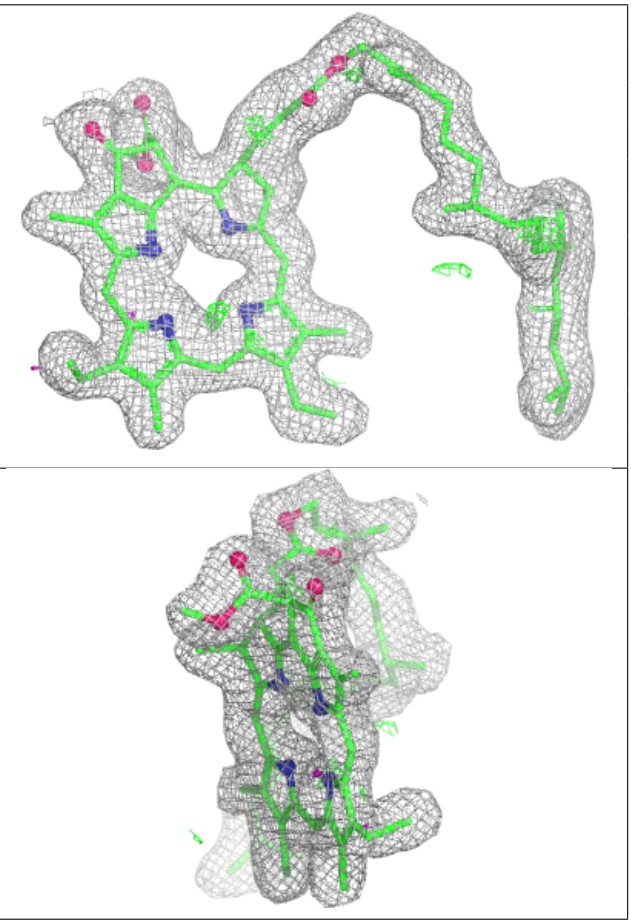
**Electron density around LMG J 101:**

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



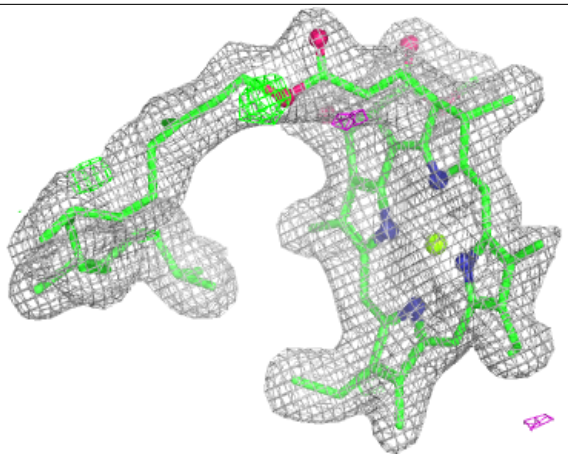
**Electron density around PHO a 420:**

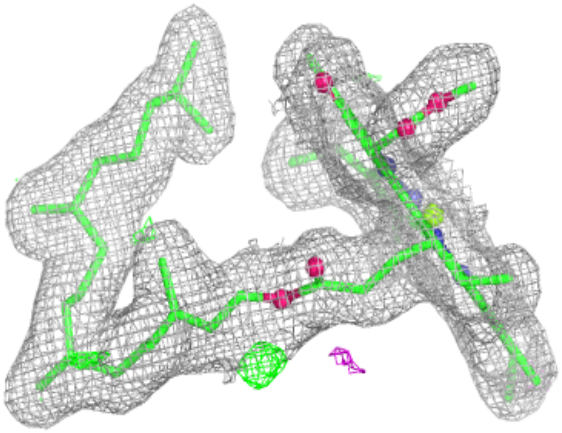
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

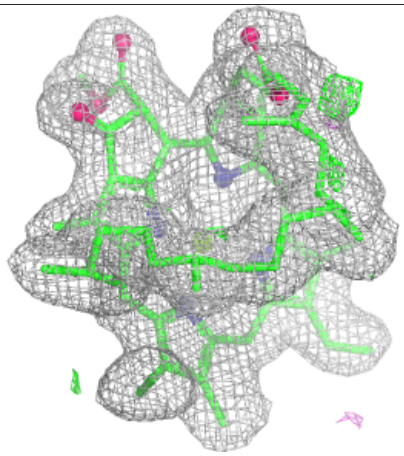


**Electron density around CLA c 904:**

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

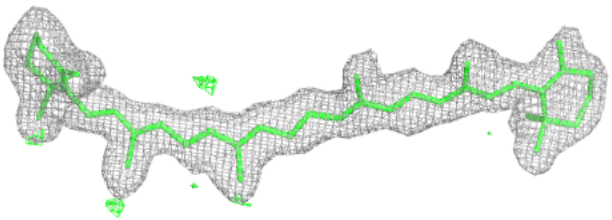


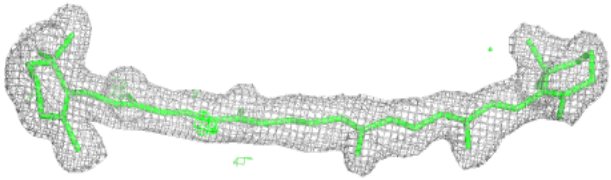


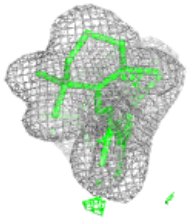


**Electron density around BCR t 101:**

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

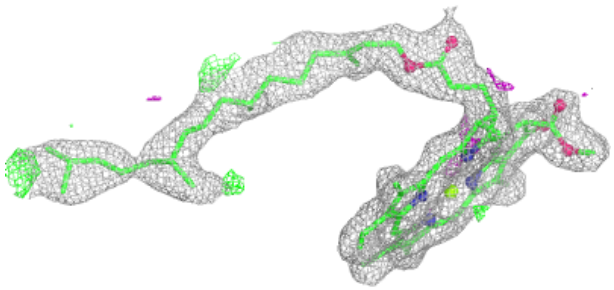


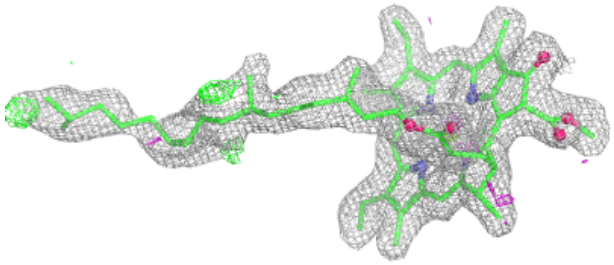


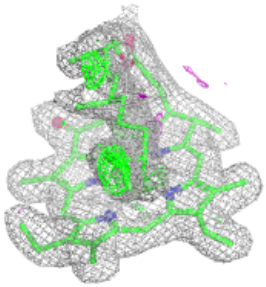


**Electron density around CLA c 905:**

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

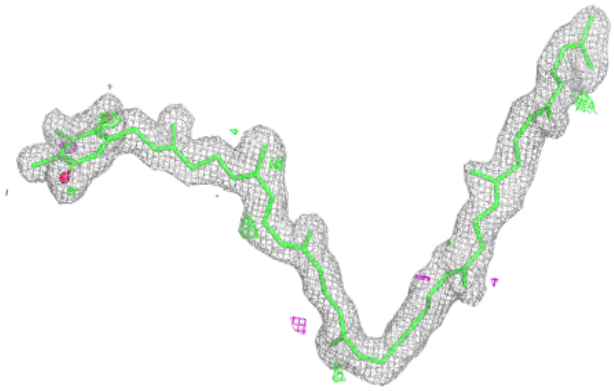


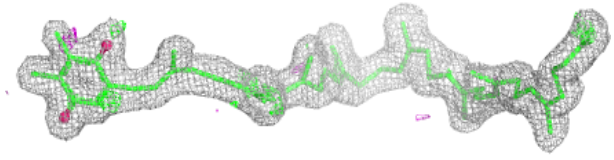


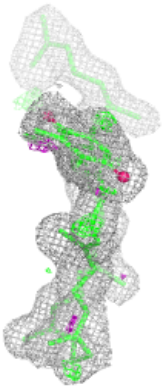


**Electron density around PL9 d 405:**

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

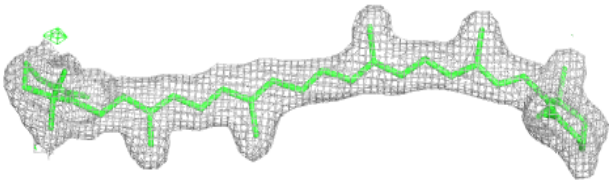


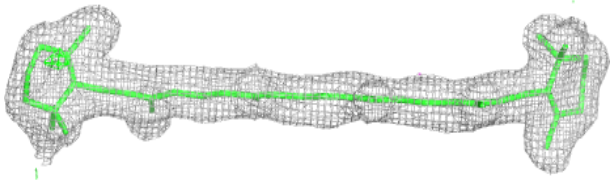


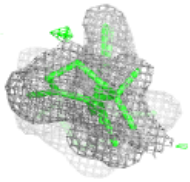


**Electron density around BCR C 516:**

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

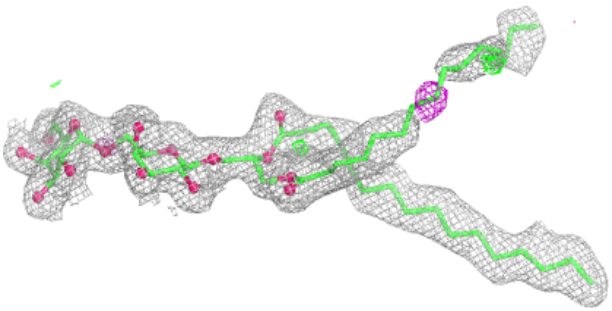


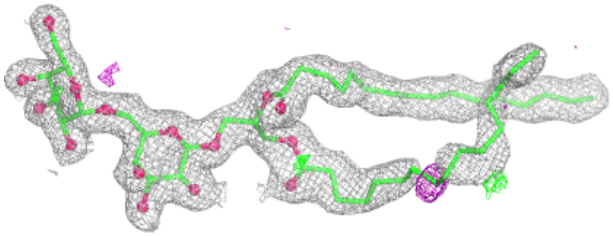


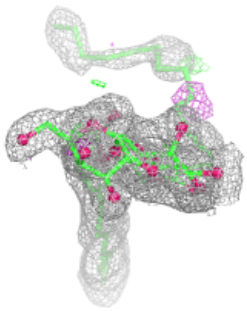


**Electron density around DGD c 916:**

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

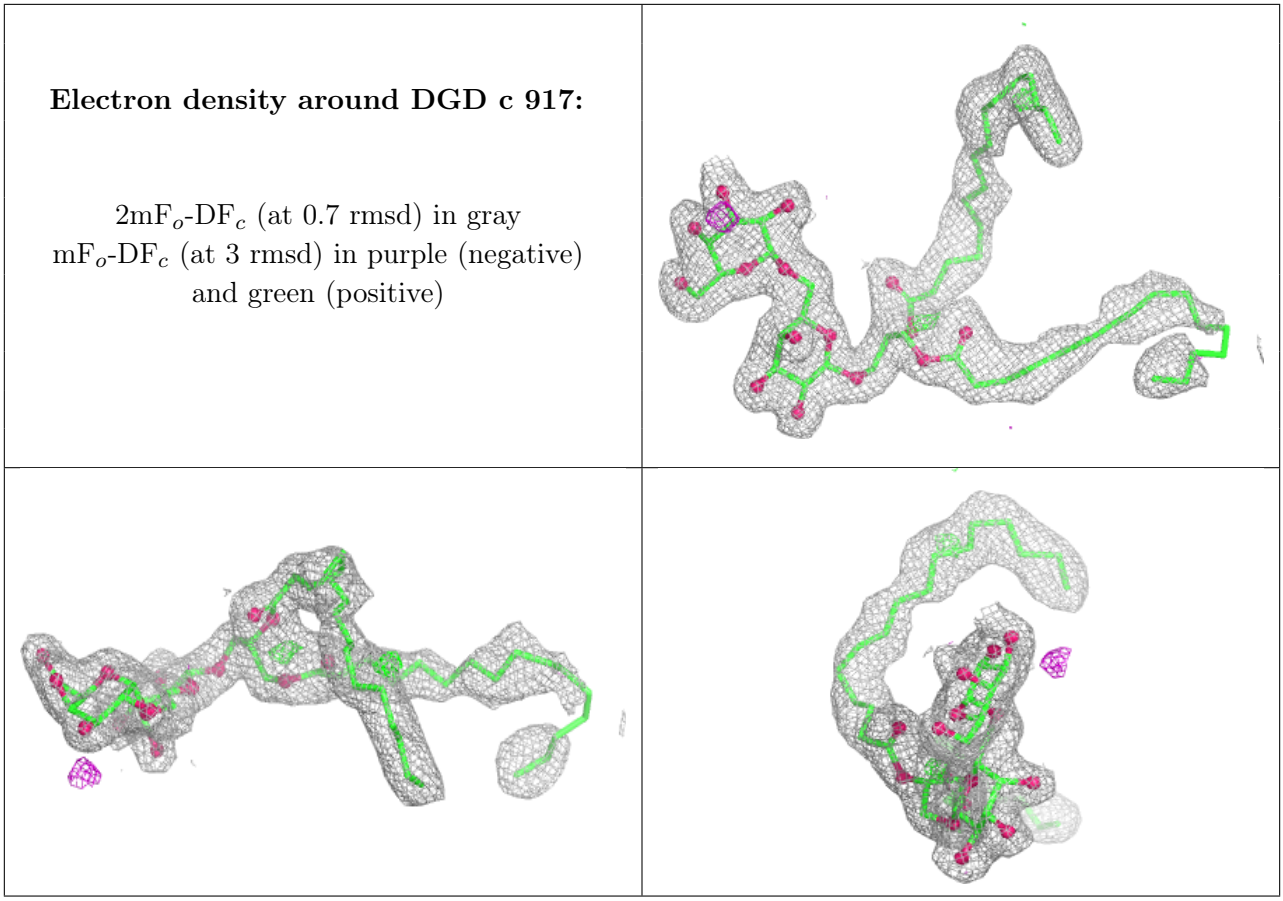






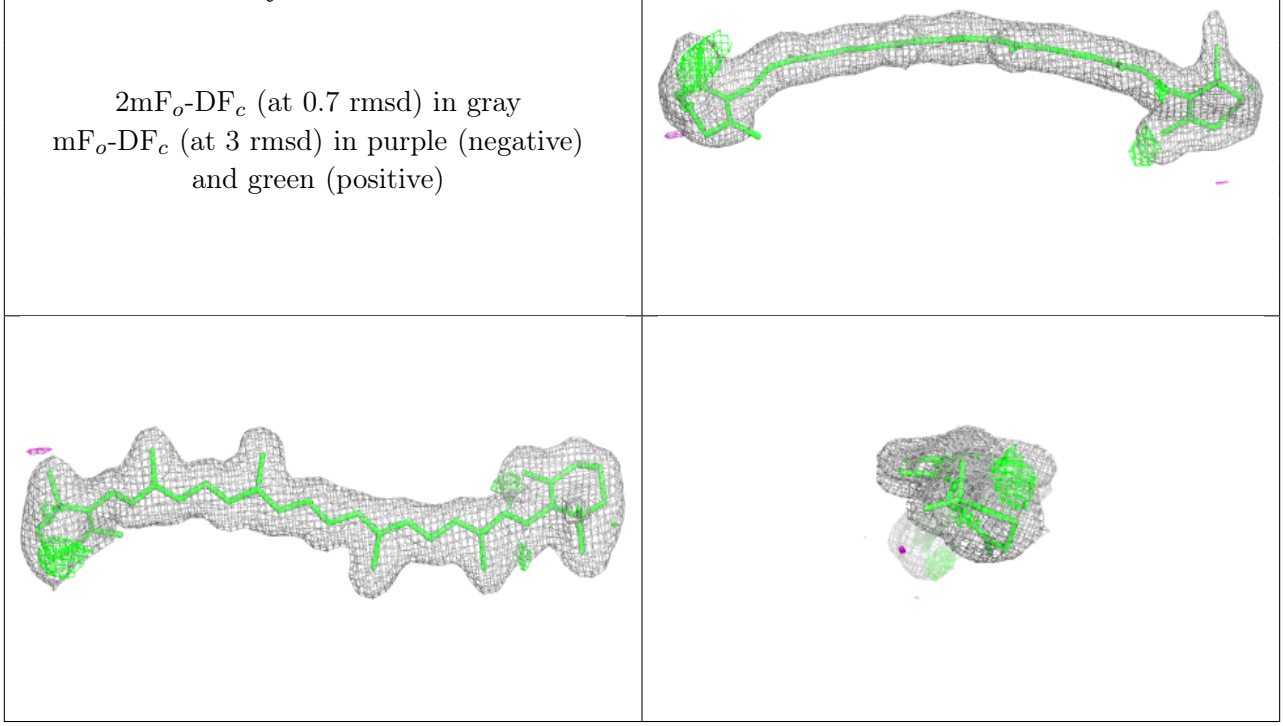
**Electron density around DGD c 917:**

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



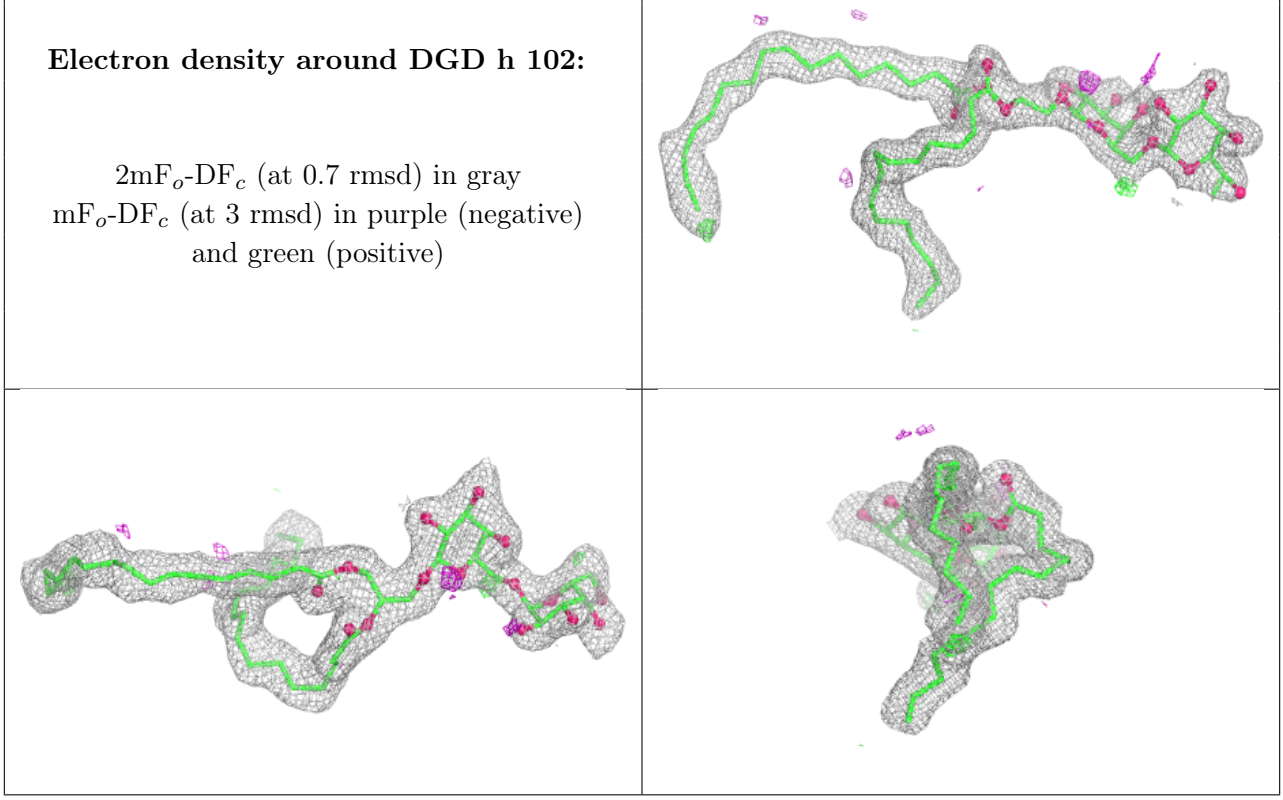
**Electron density around BCR D 403:**

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



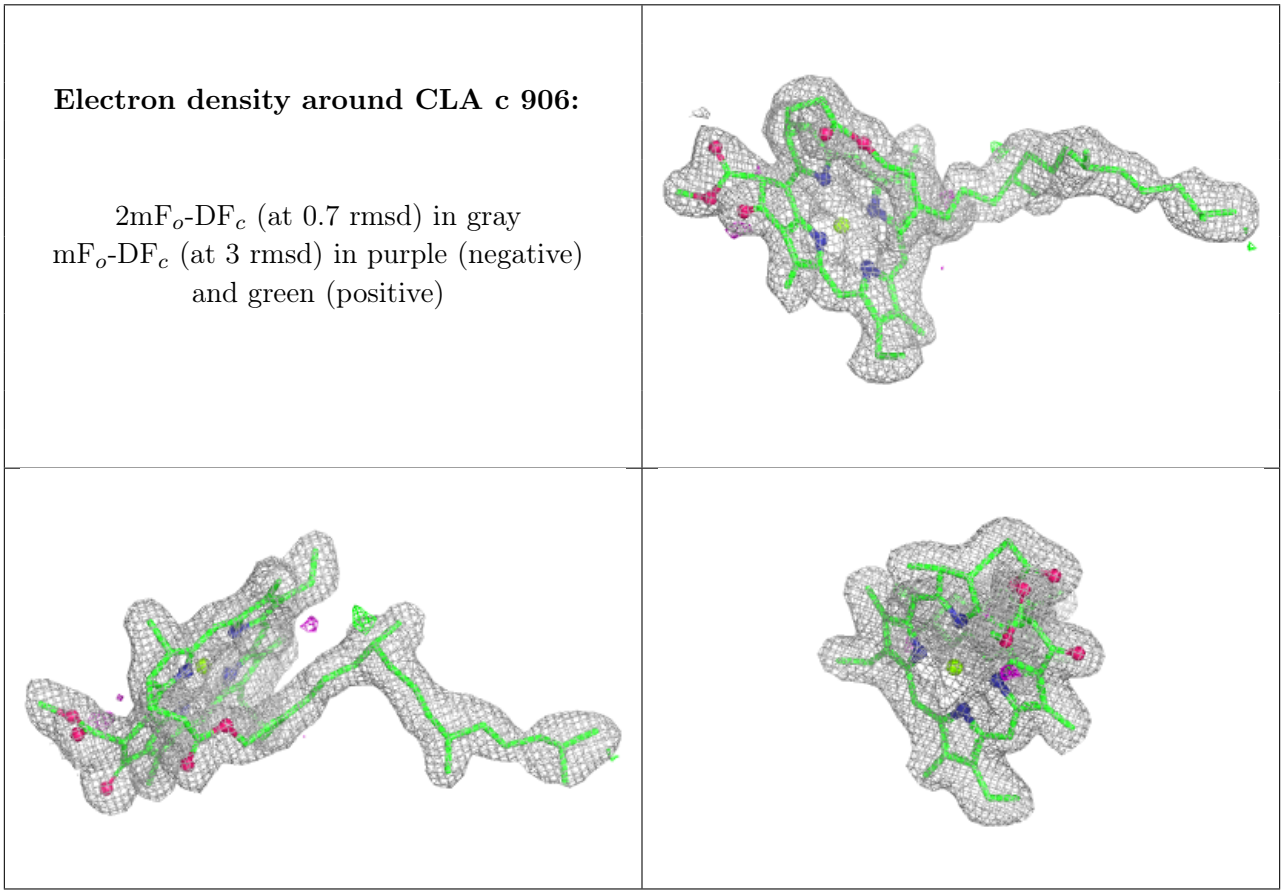
**Electron density around DGD h 102:**

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



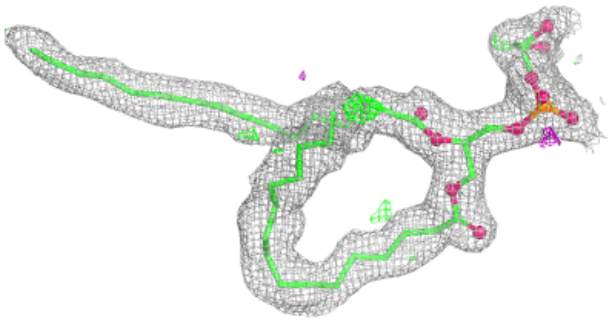
**Electron density around CLA c 906:**

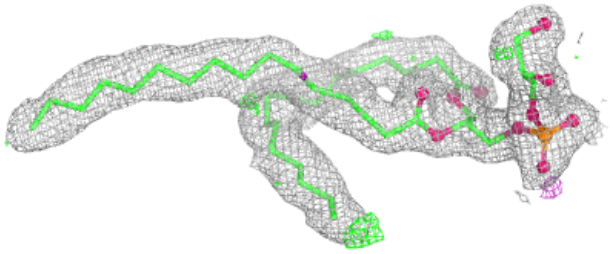
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

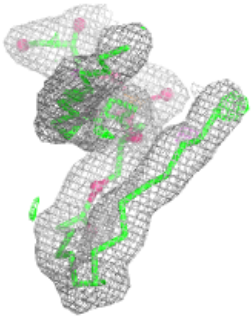


**Electron density around LHG d 407:**

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

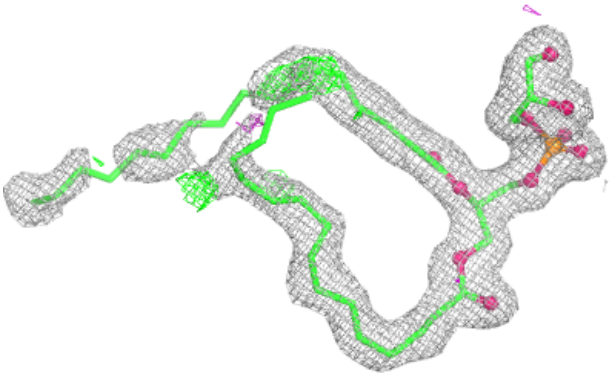


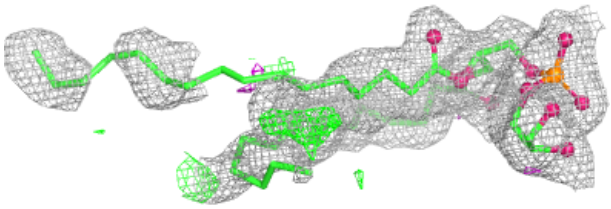


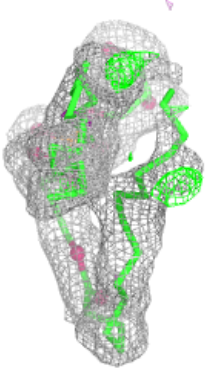


**Electron density around LHG d 409:**

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

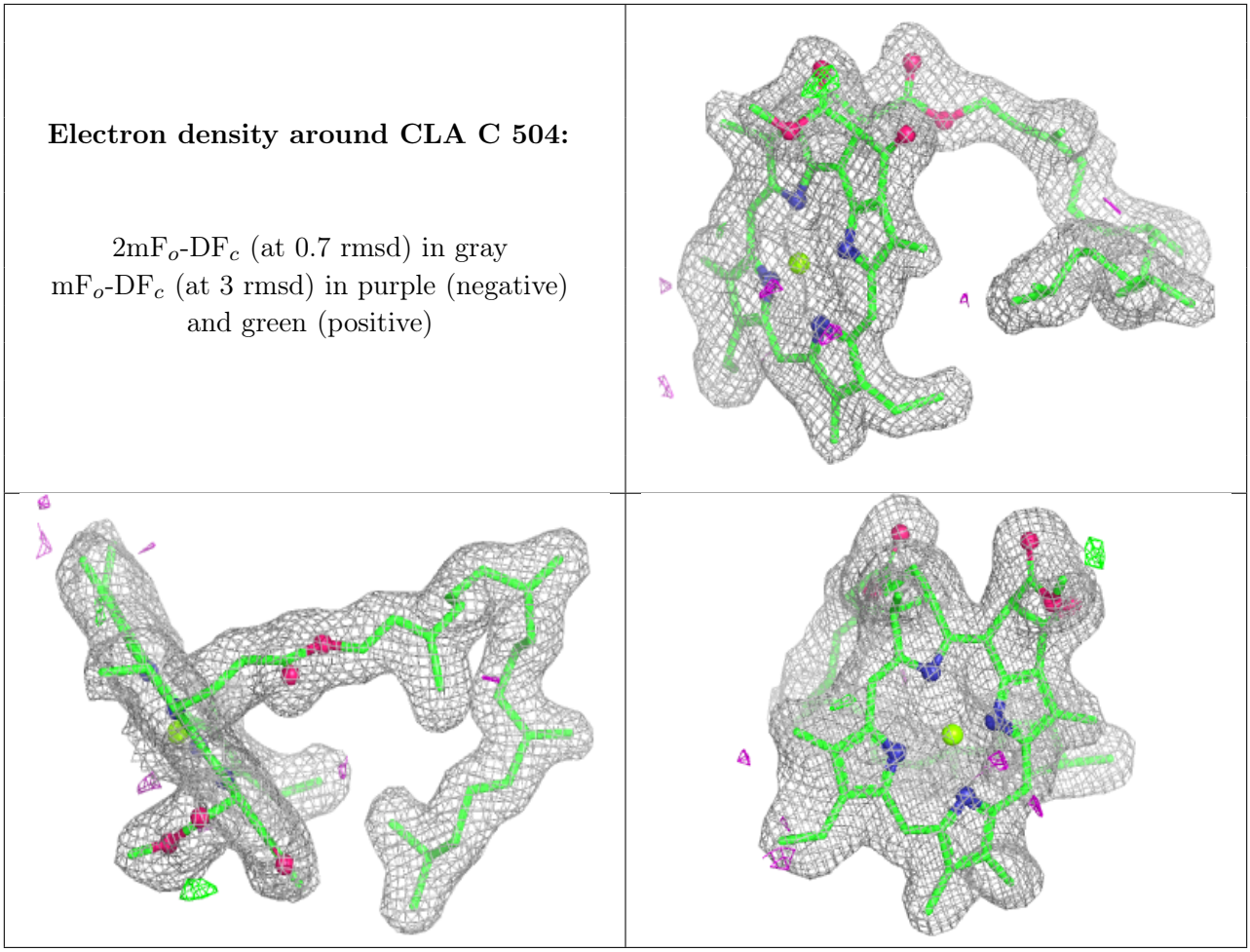






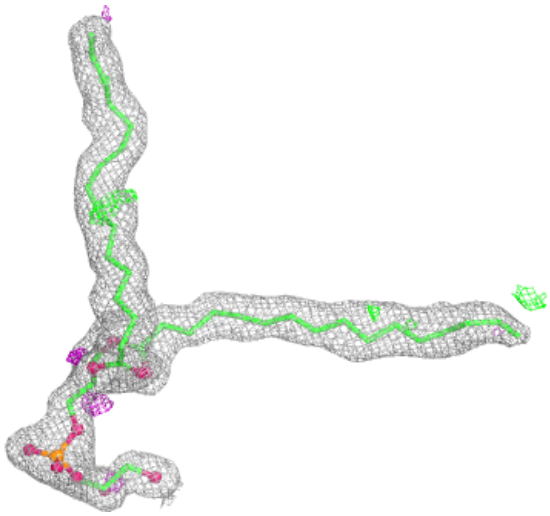
**Electron density around CLA C 504:**

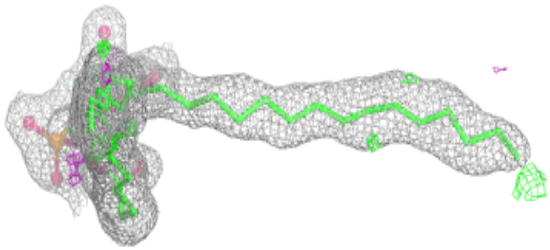
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

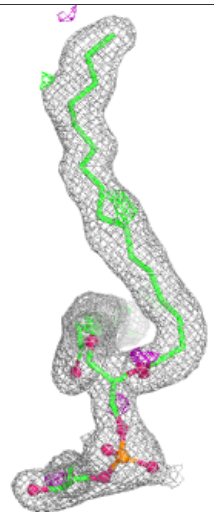


**Electron density around LHG l 101:**

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

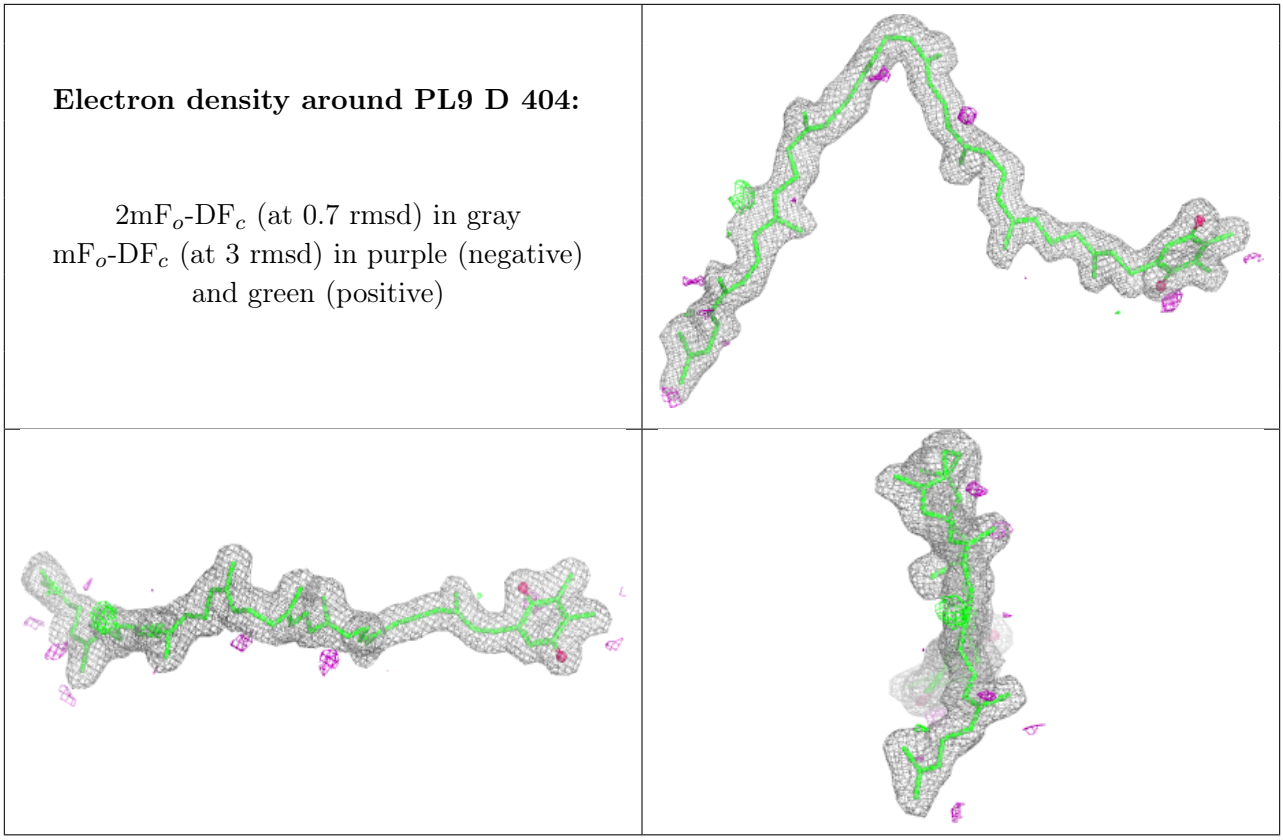






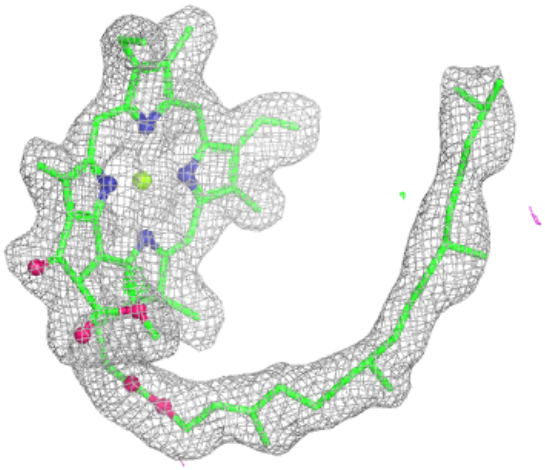
**Electron density around PL9 D 404:**

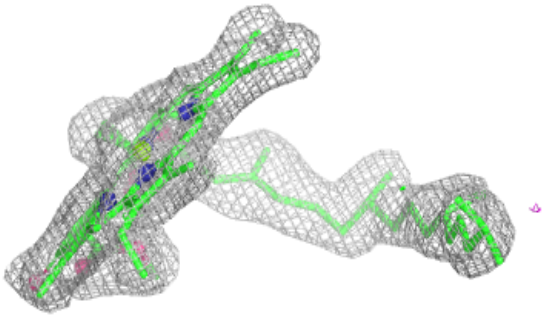
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

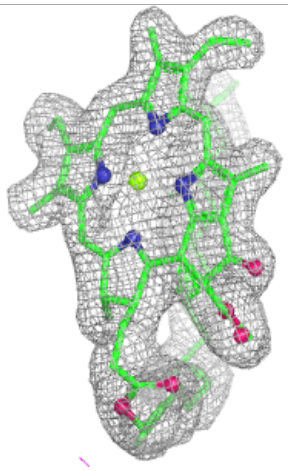


**Electron density around CLA C 508:**

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

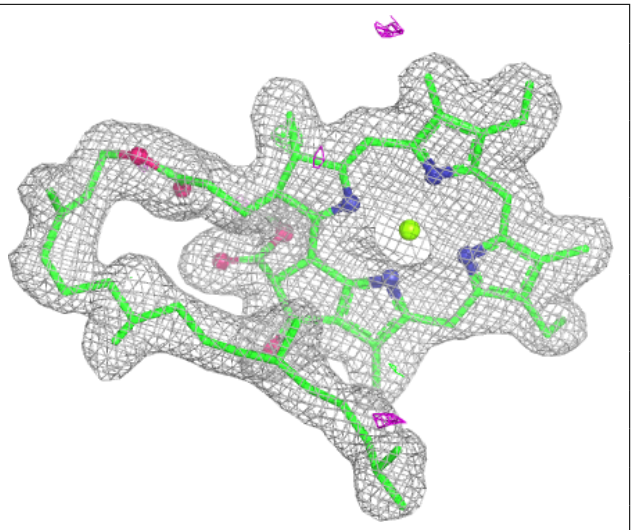


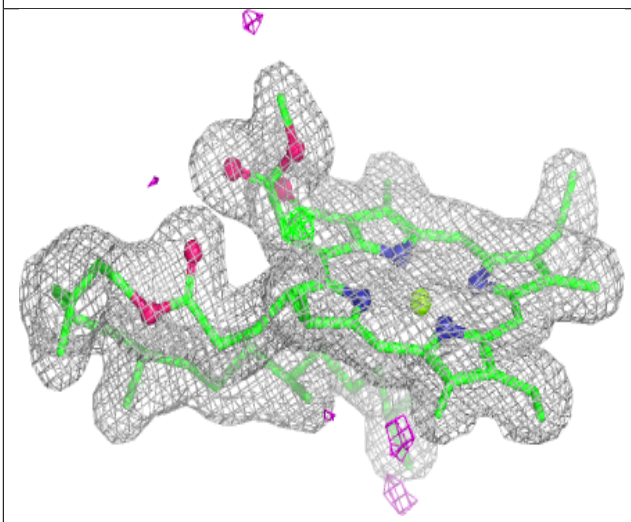


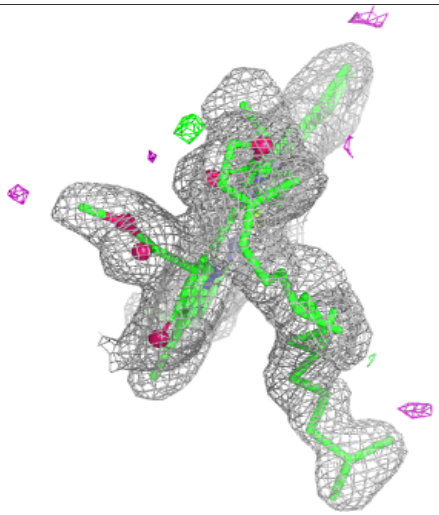


**Electron density around CLA C 510:**

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

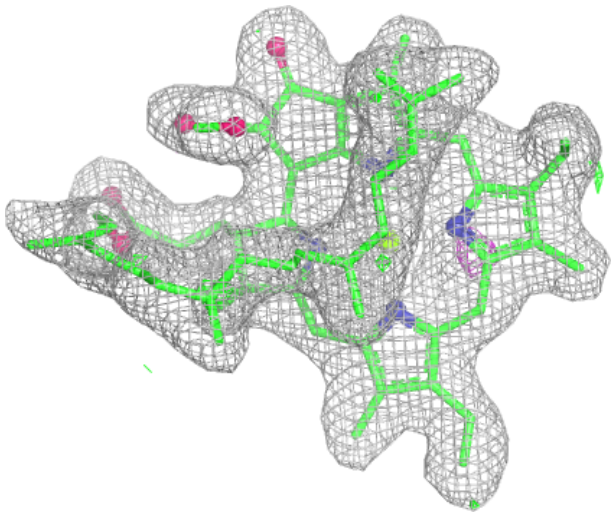


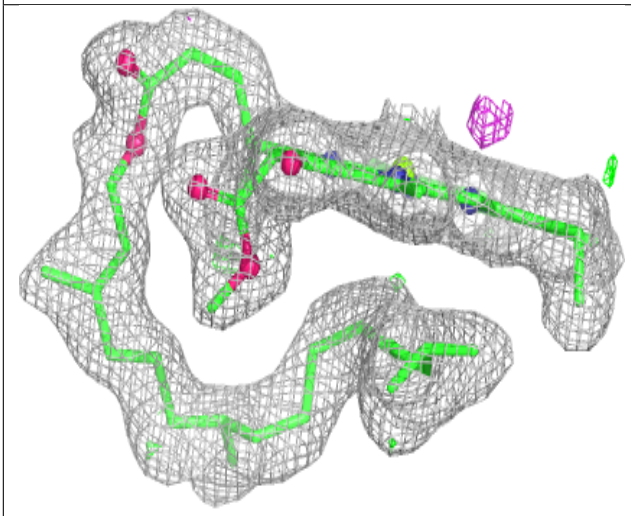


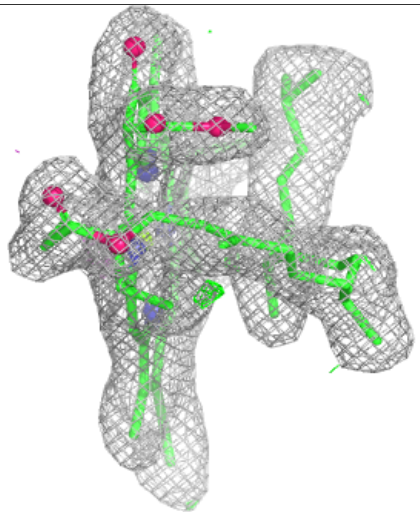


**Electron density around CLA C 511:**

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

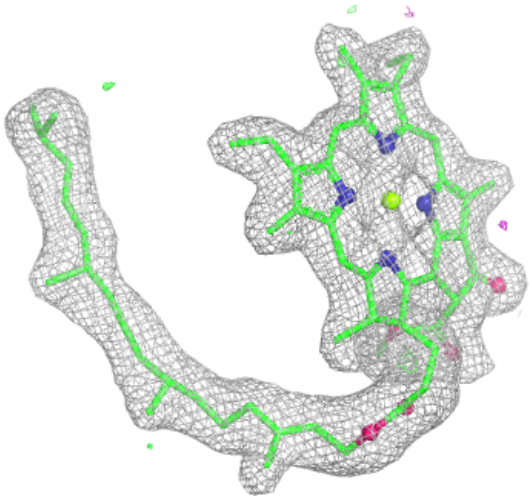


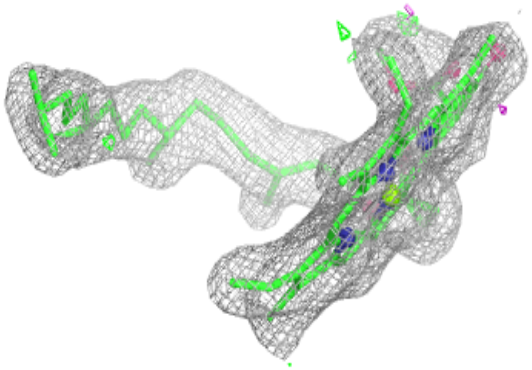




**Electron density around CLA c 908:**

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

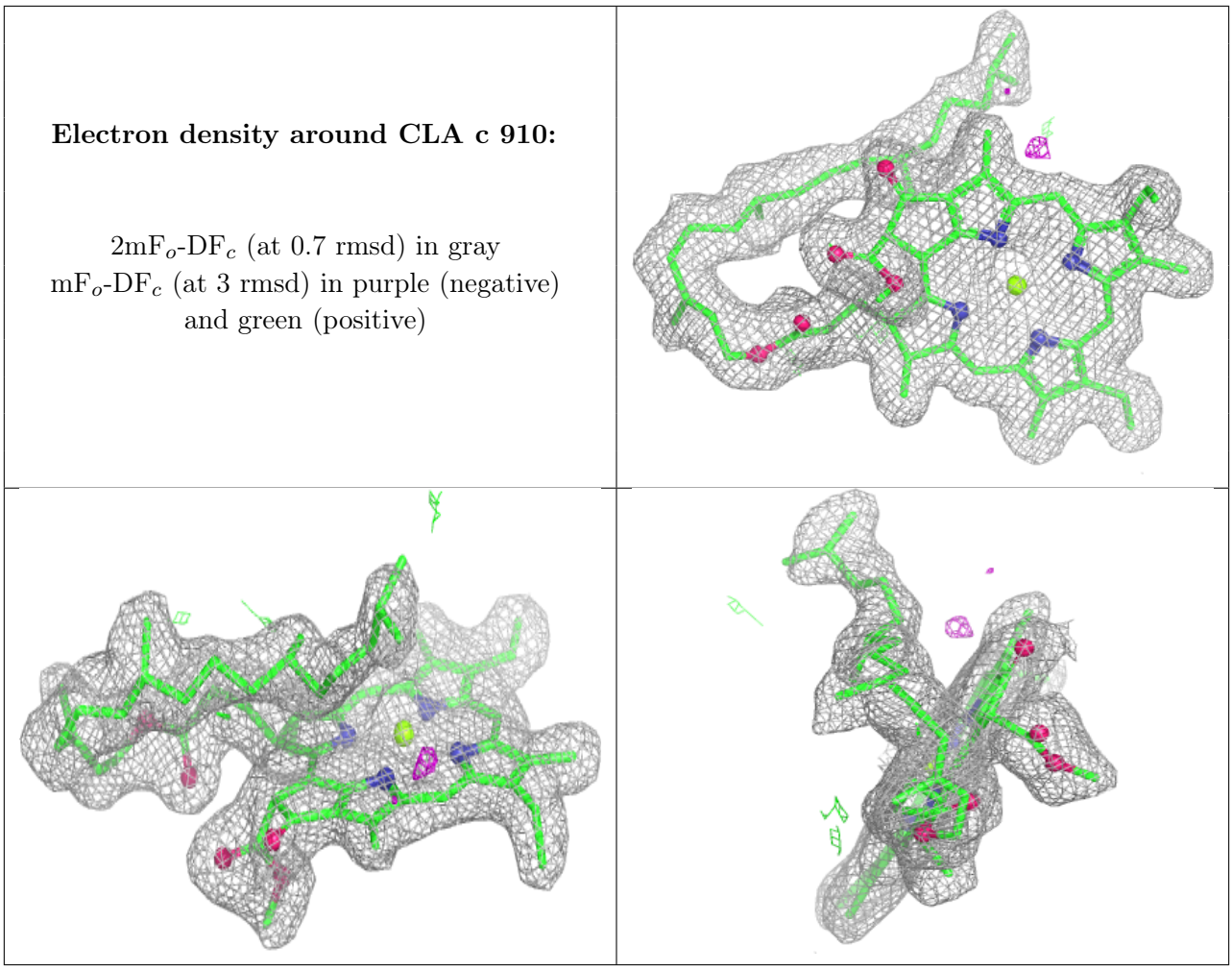






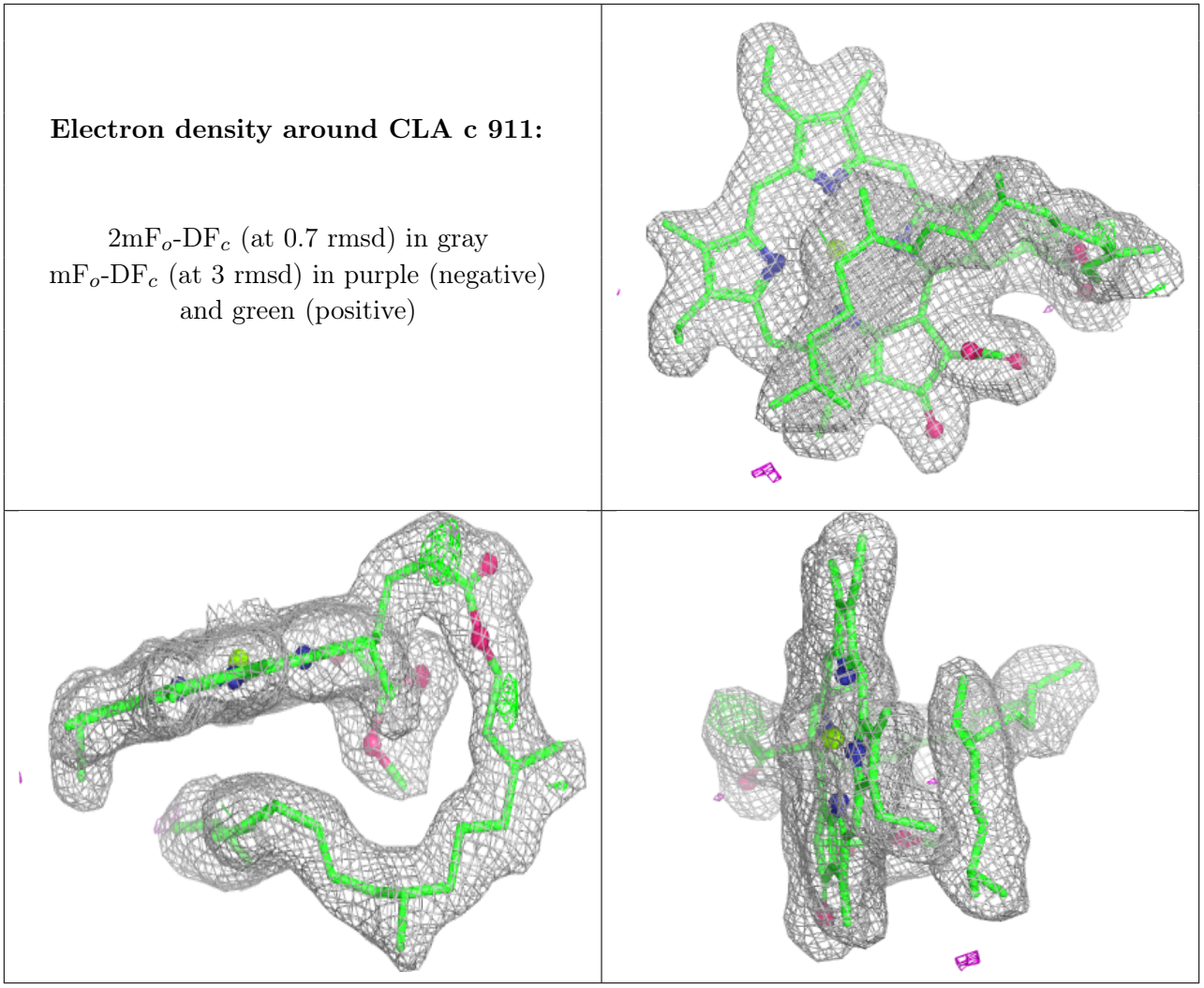
**Electron density around CLA c 910:**

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



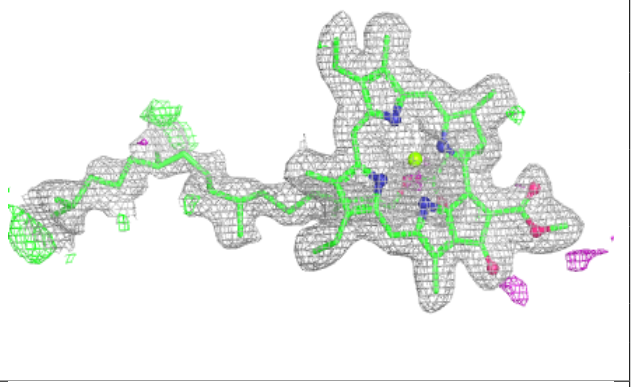
**Electron density around CLA c 911:**

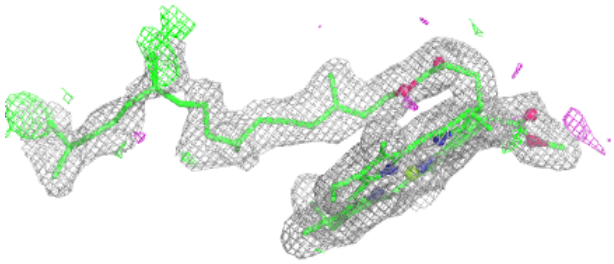
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

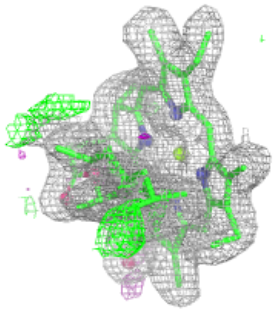


**Electron density around CLA B 615:**

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

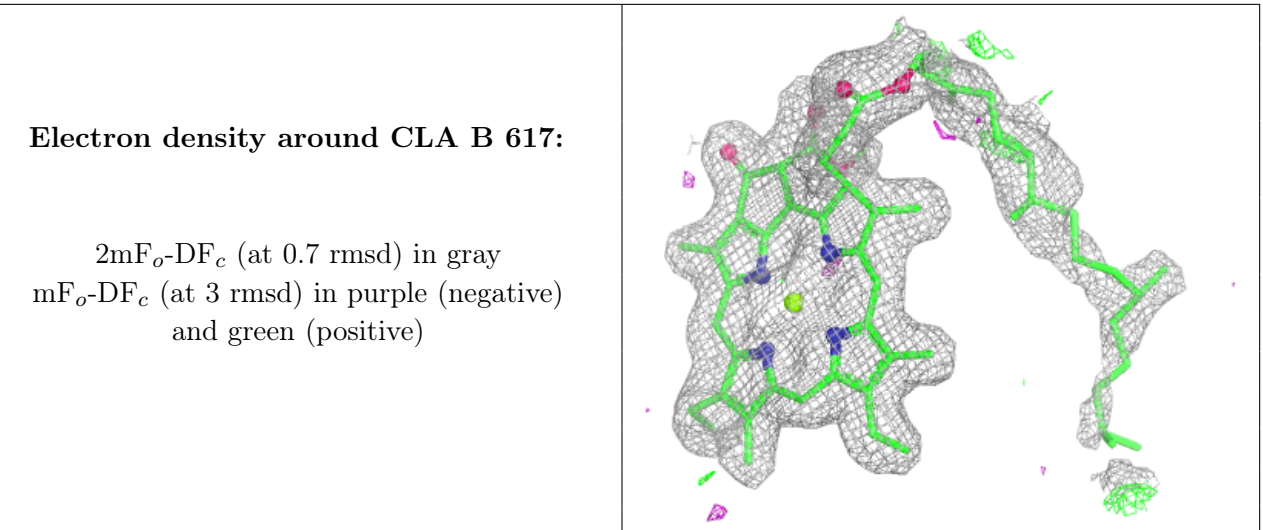


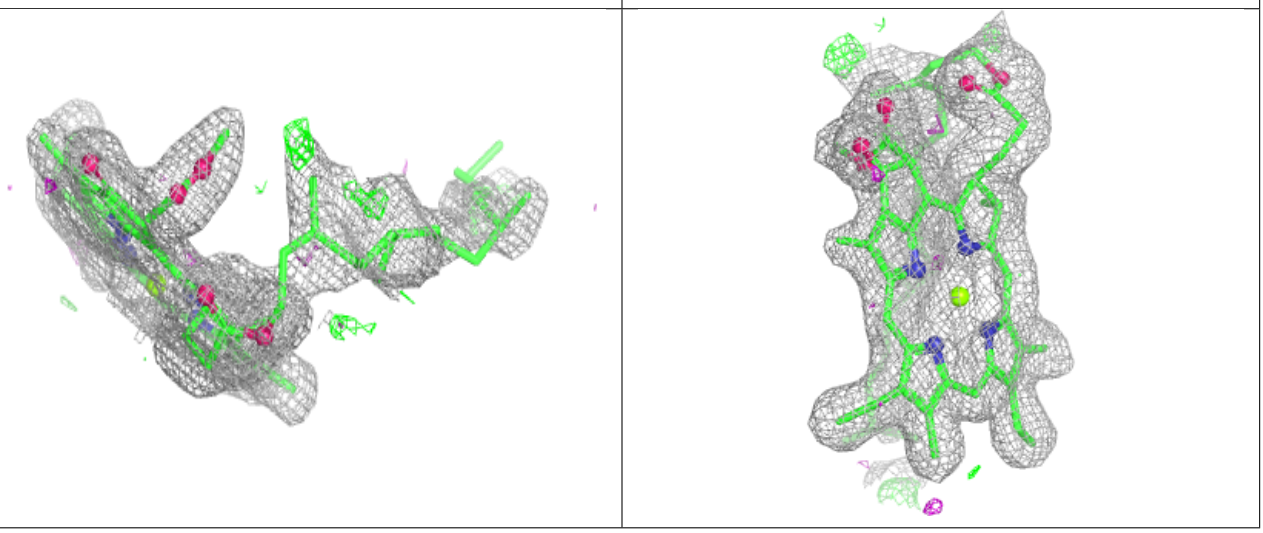




**Electron density around CLA B 617:**

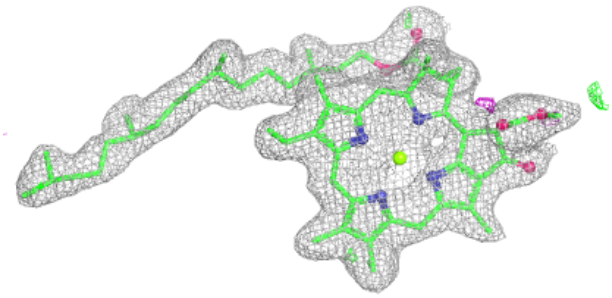
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

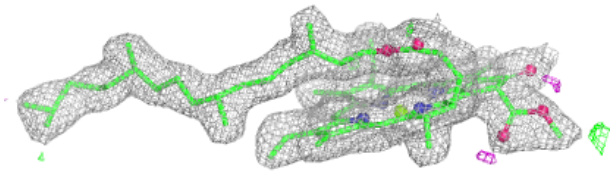


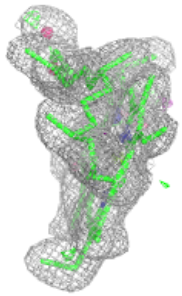


**Electron density around CLA C 502:**

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

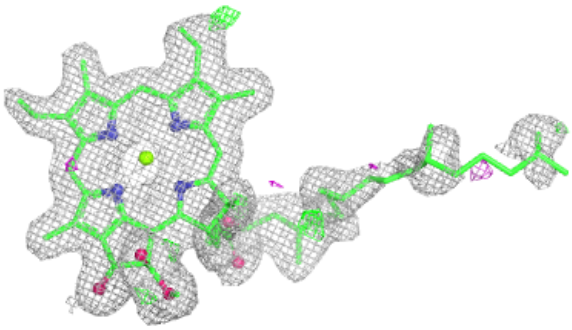


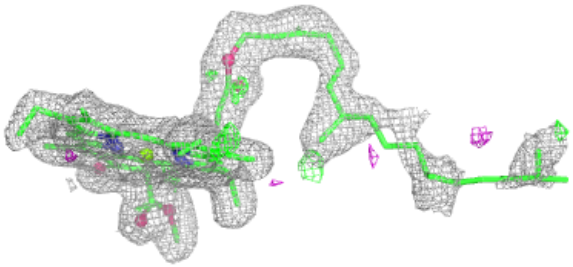


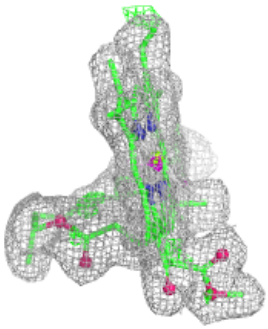


**Electron density around CLA a 407:**

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

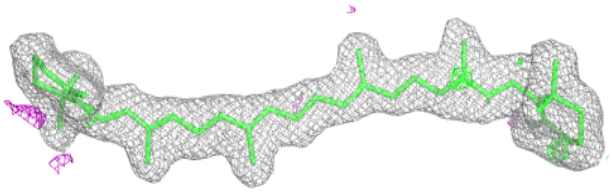


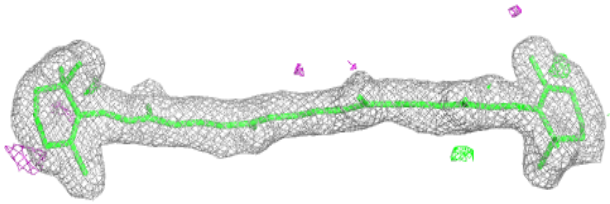


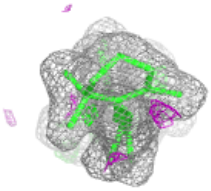


**Electron density around BCR A 411:**

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

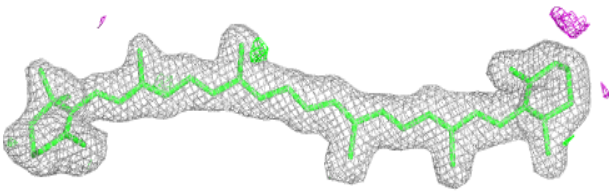


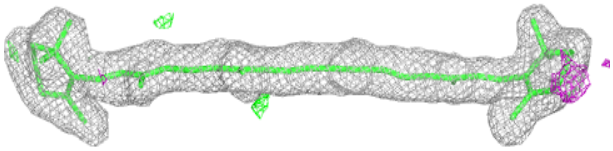


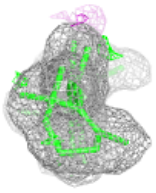


**Electron density around BCR B 619:**

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

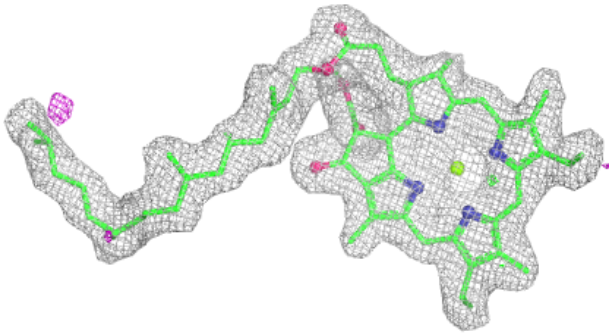


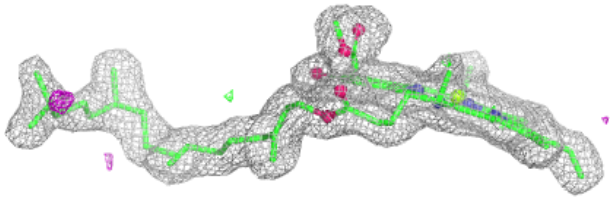


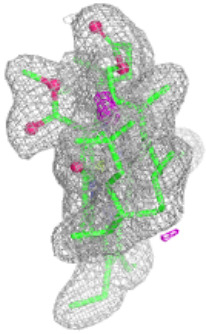


**Electron density around CLA b 606:**

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

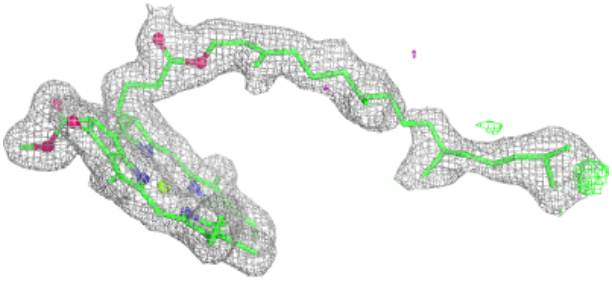


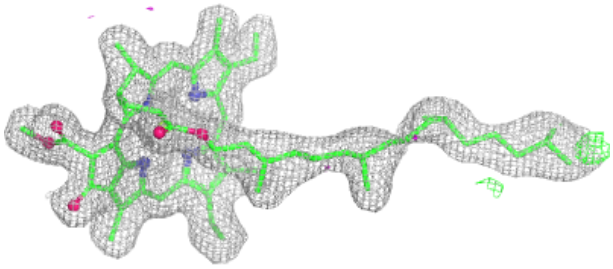


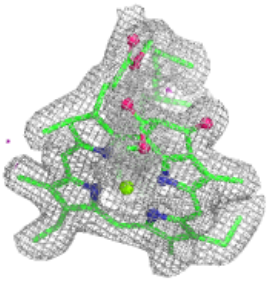


**Electron density around CLA C 505:**

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

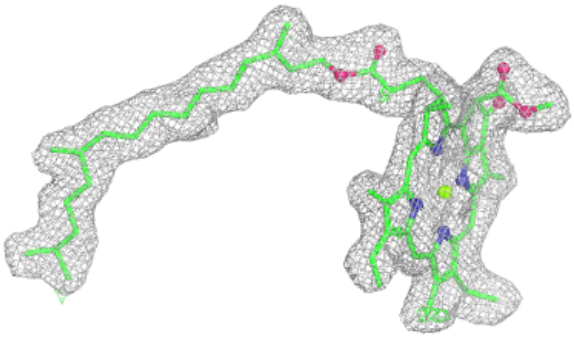


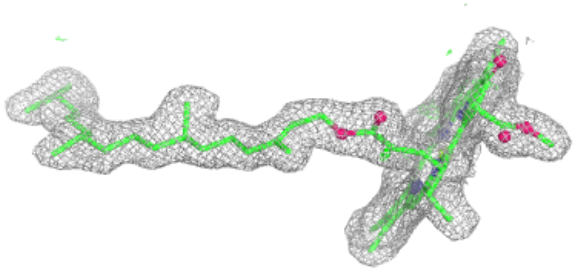


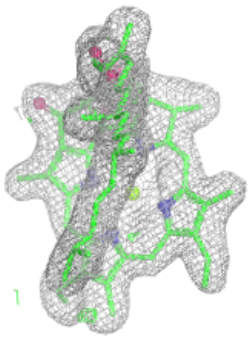


**Electron density around CLA b 613:**

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

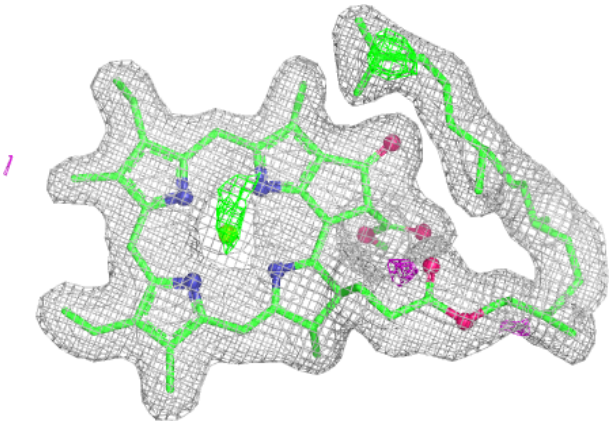


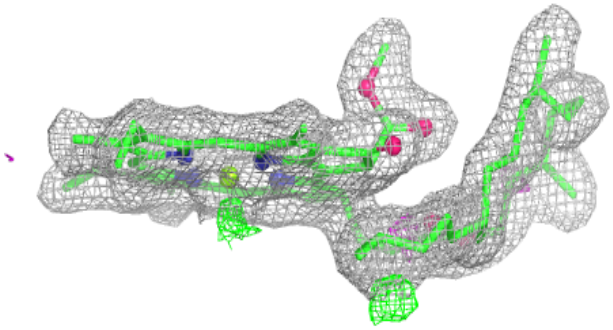


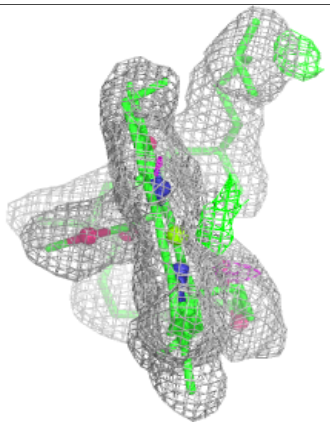


**Electron density around CLA b 614:**

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

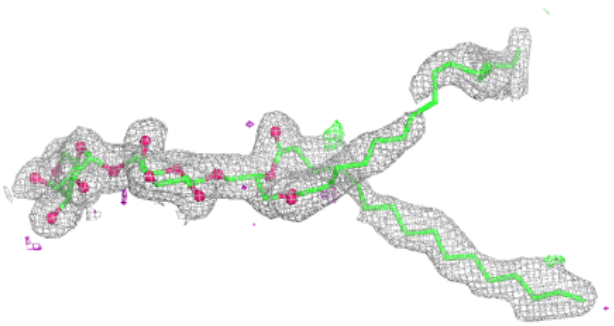


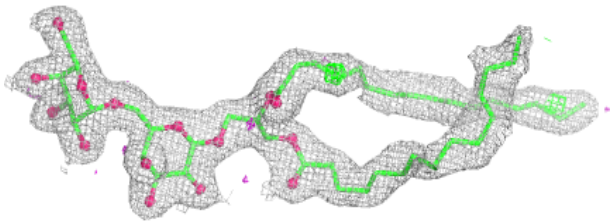


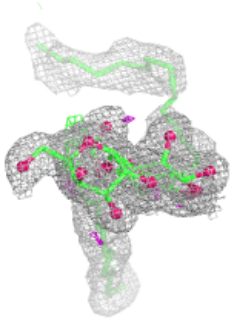


**Electron density around DGD C 517:**

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

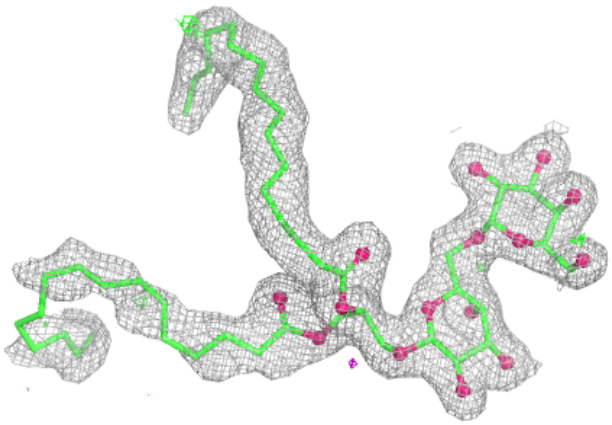


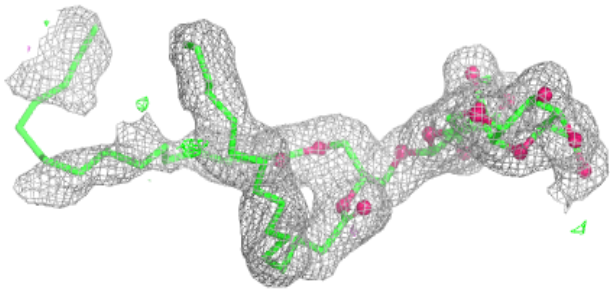


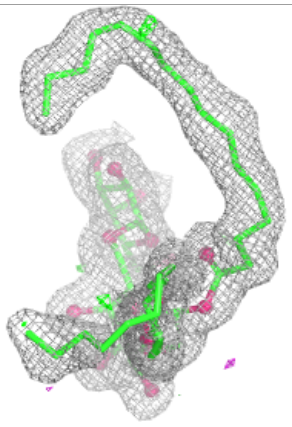


**Electron density around DGD C 518:**

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

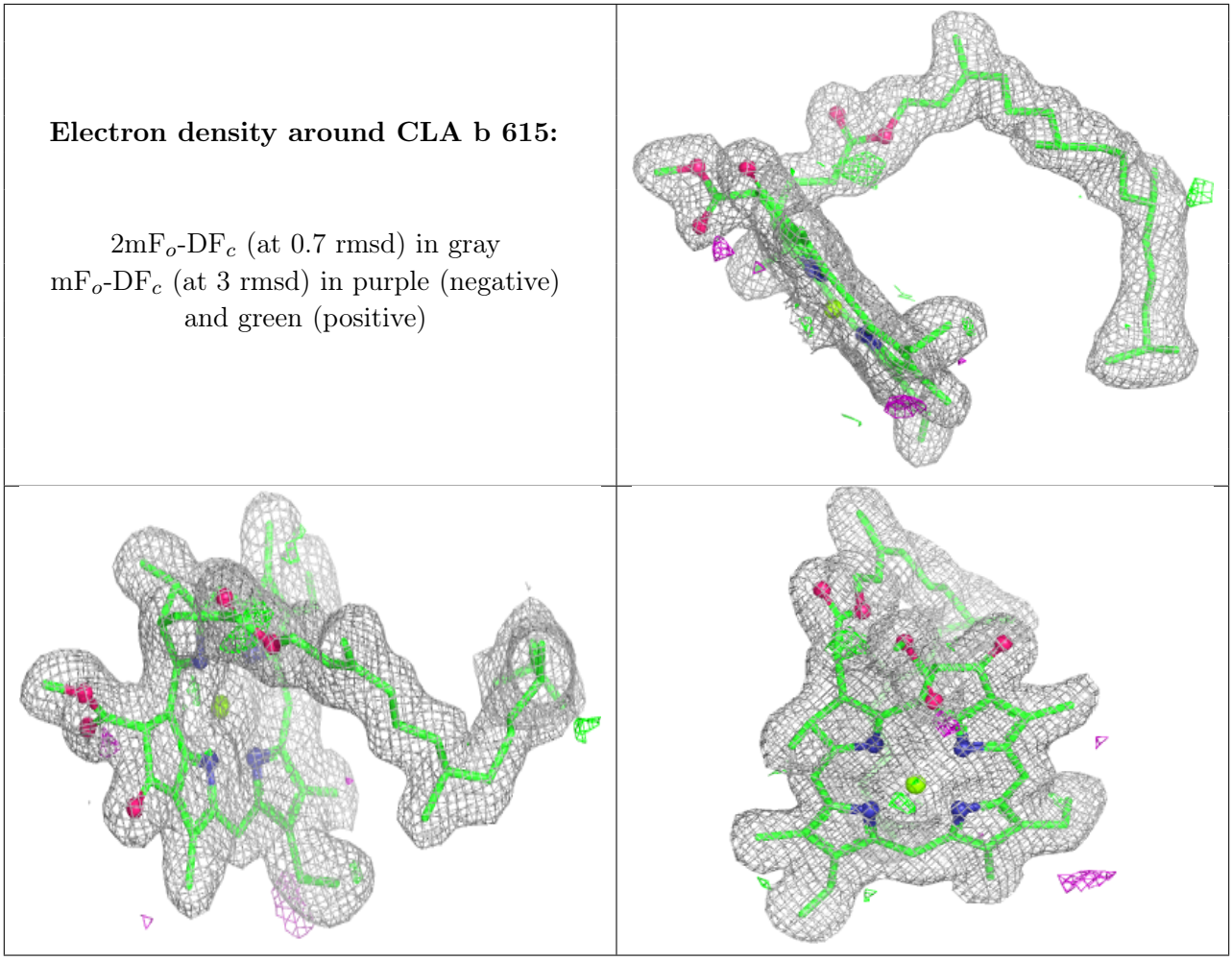






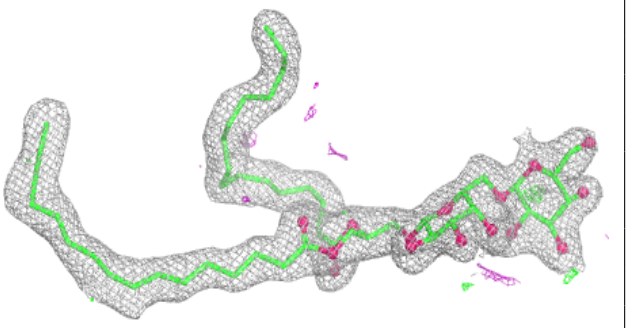
**Electron density around CLA b 615:**

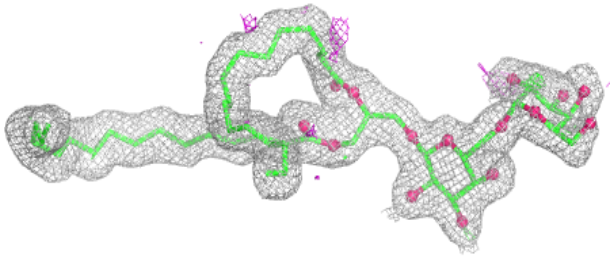
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

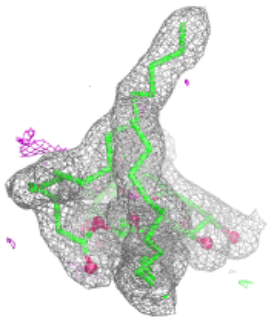


**Electron density around DGD H 102:**

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

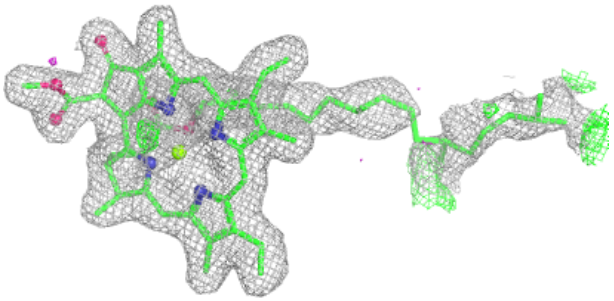


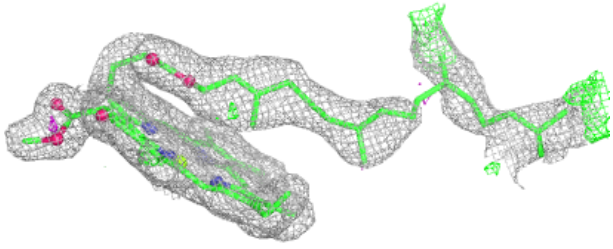


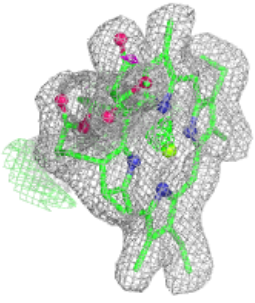


**Electron density around CLA b 618:**

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

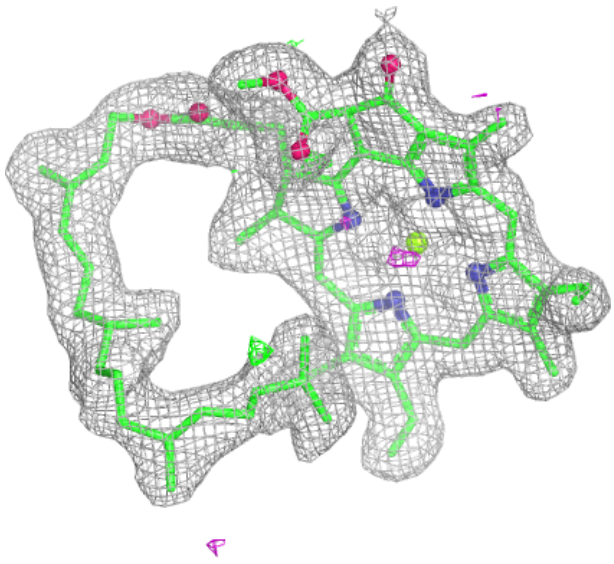


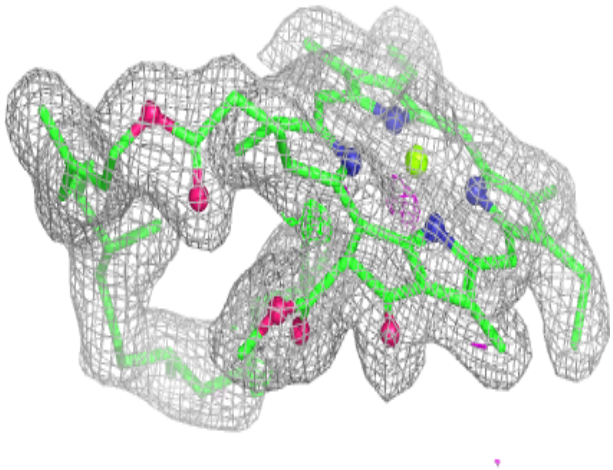




**Electron density around CLA b 619:**

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

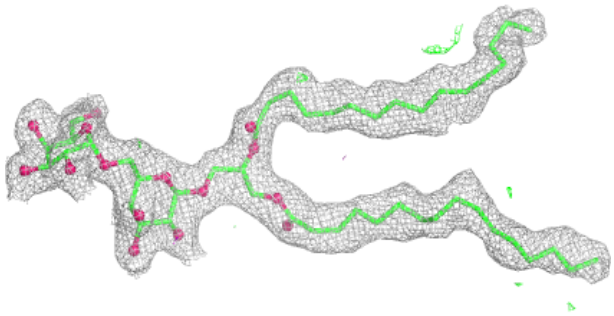


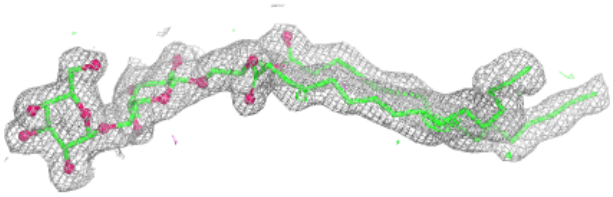


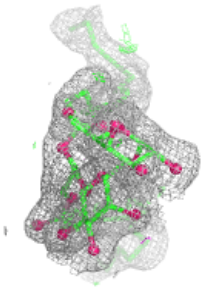


**Electron density around DGD c 918:**

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

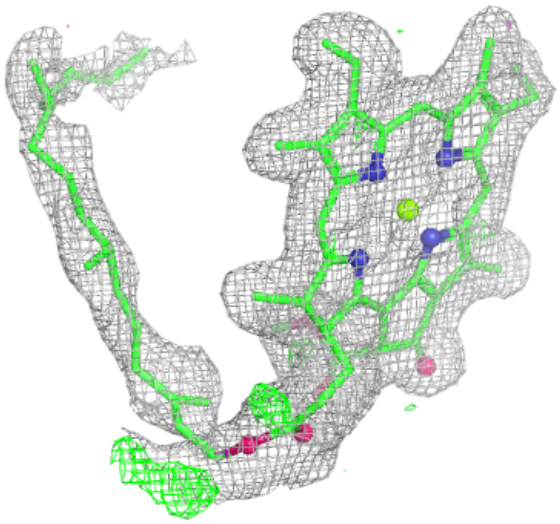


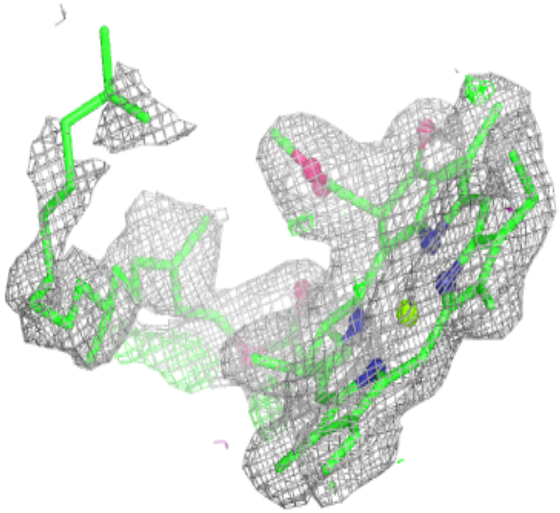


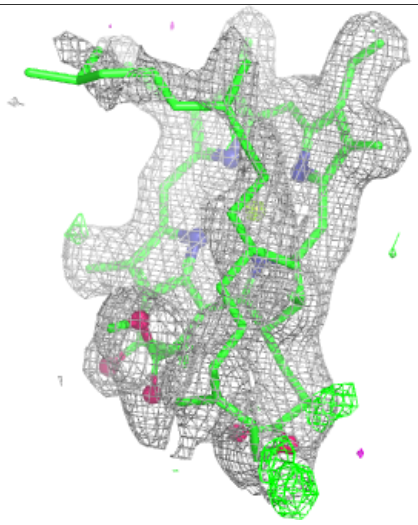


**Electron density around CLA b 620:**

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

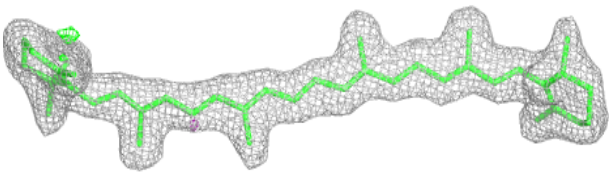


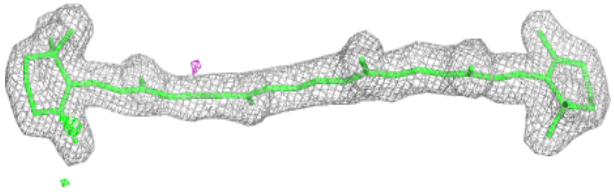


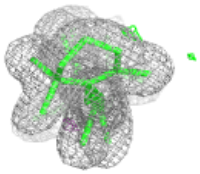


**Electron density around BCR a 410:**

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

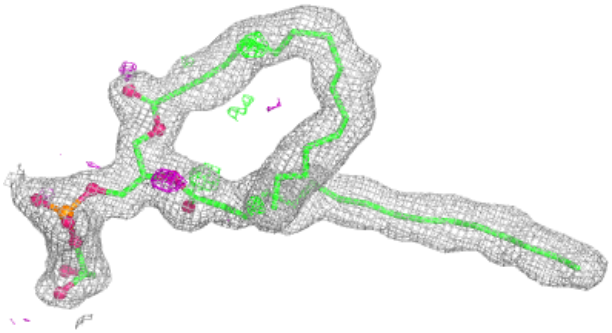


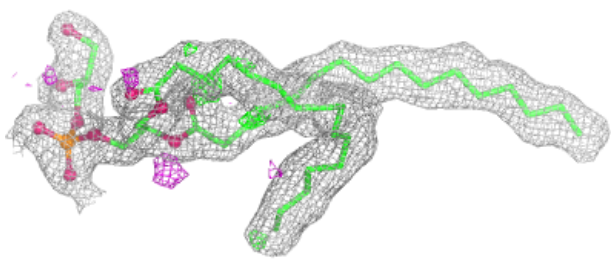




**Electron density around LHG D 406:**

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

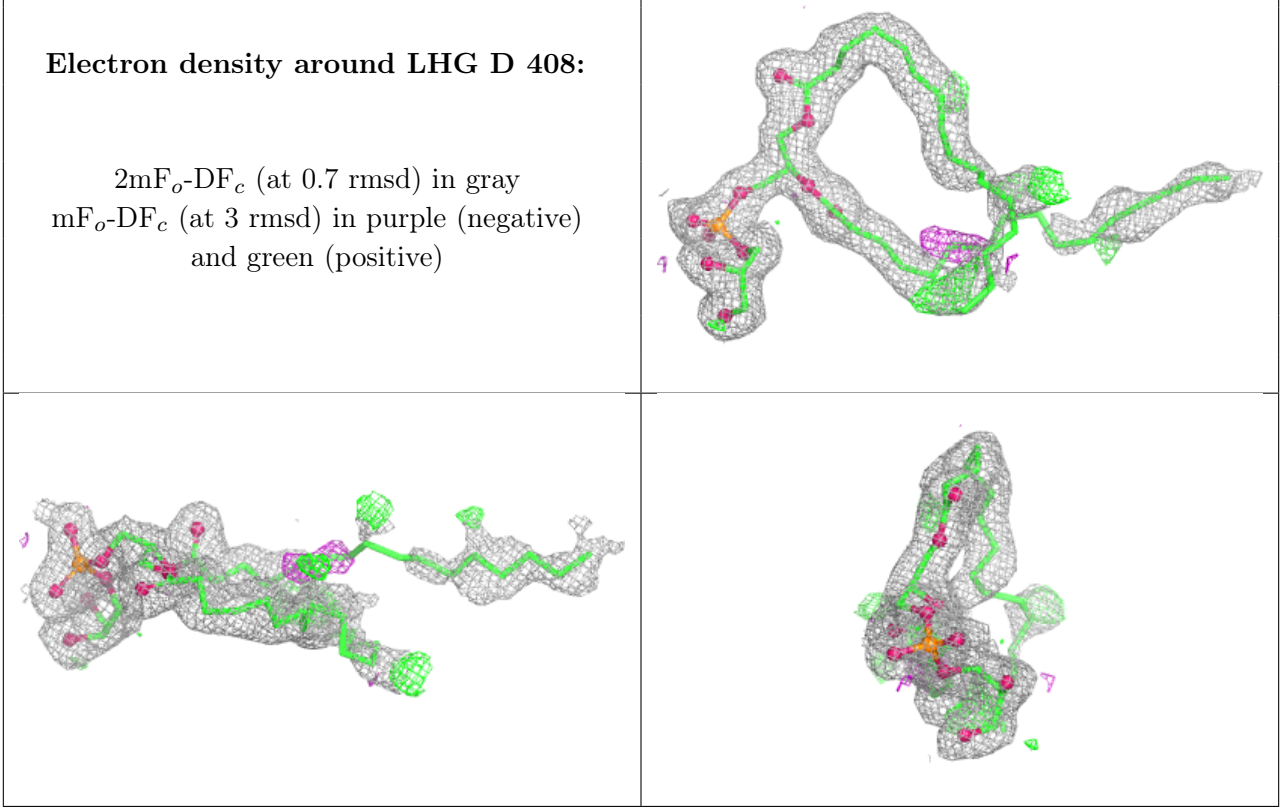






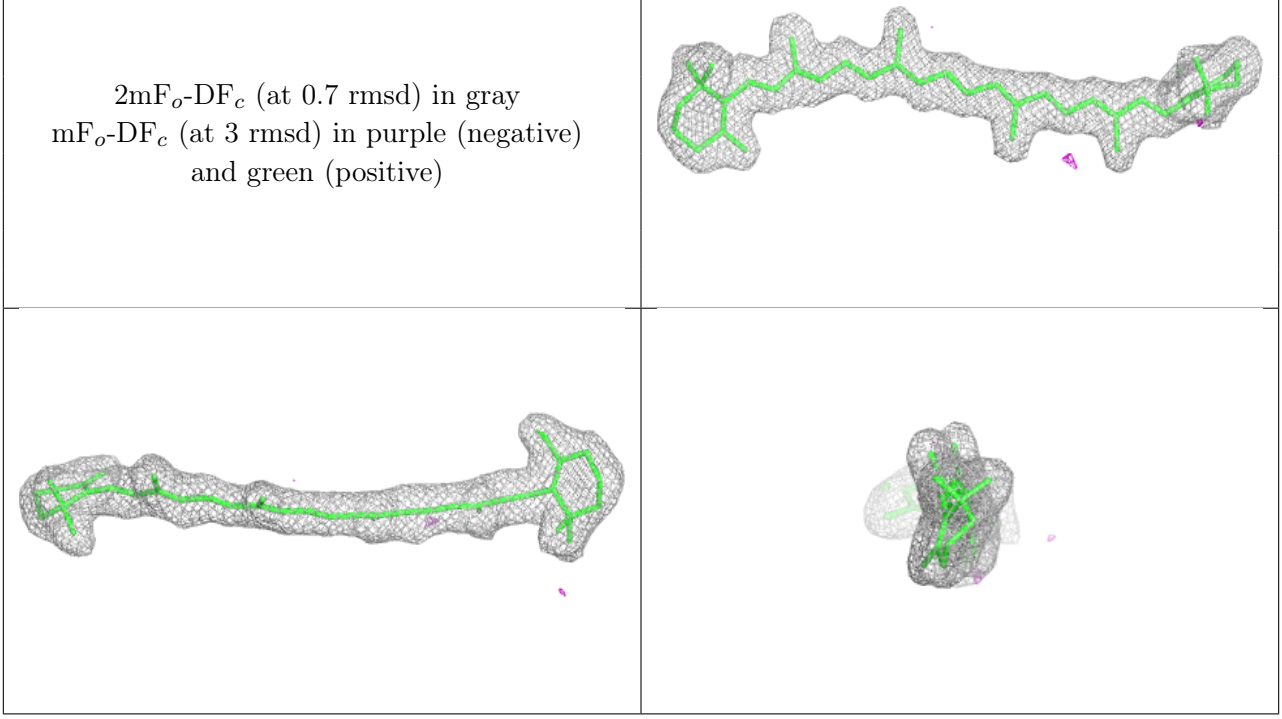
**Electron density around LHG D 408:**

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



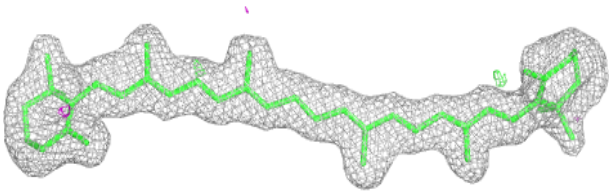
**Electron density around BCR b 621:**

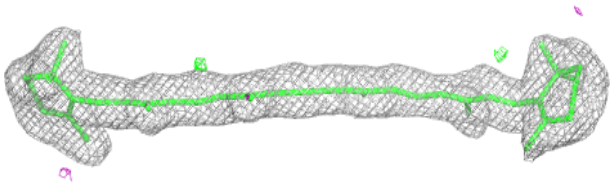
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

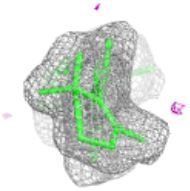


**Electron density around BCR b 622:**

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

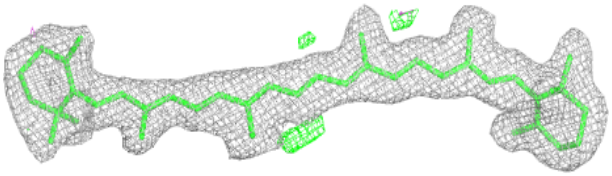


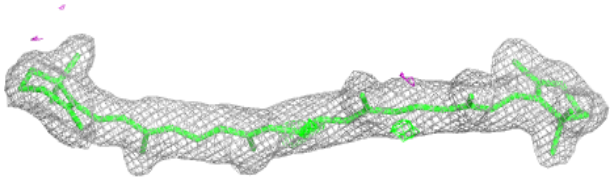


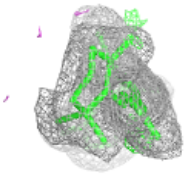


**Electron density around BCR b 623:**

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

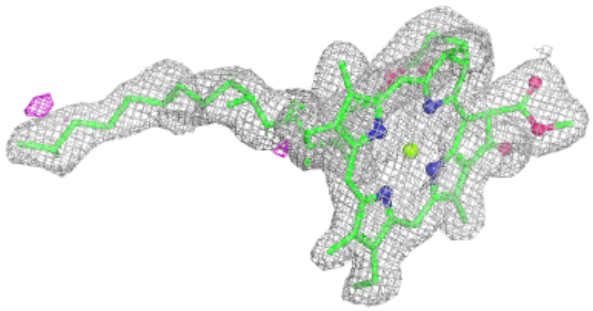


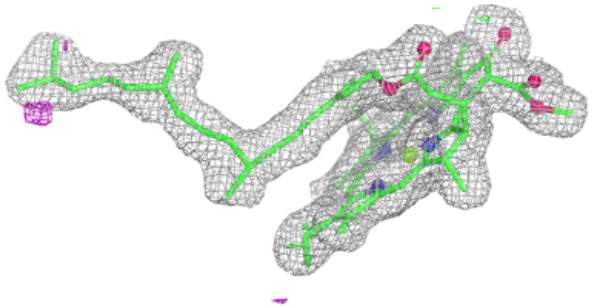


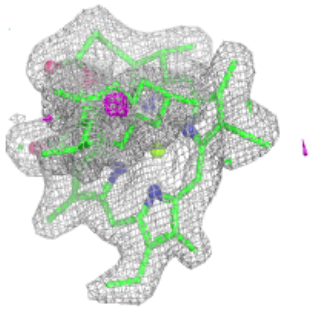


**Electron density around CLA C 506:**

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

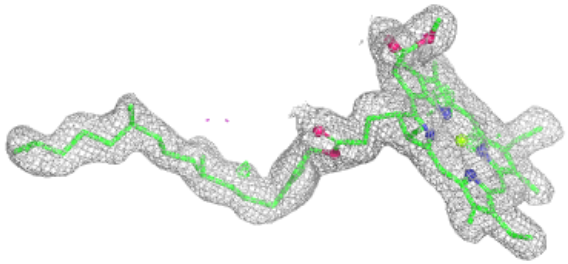


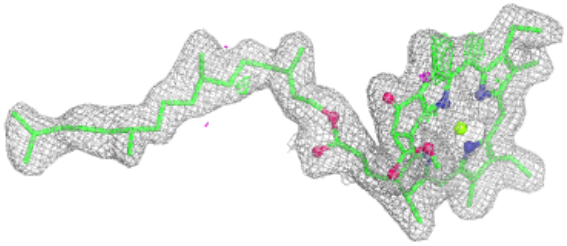


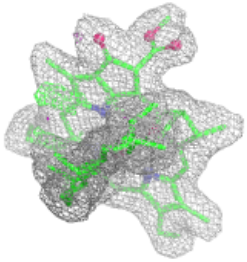


**Electron density around CLA c 903:**

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

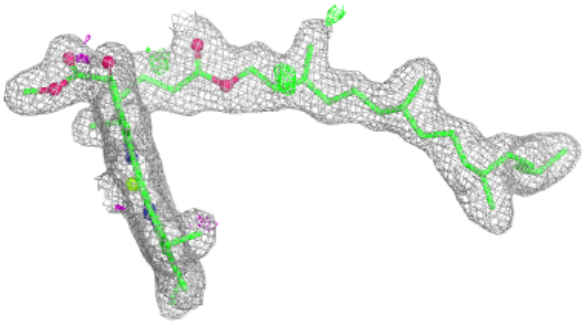


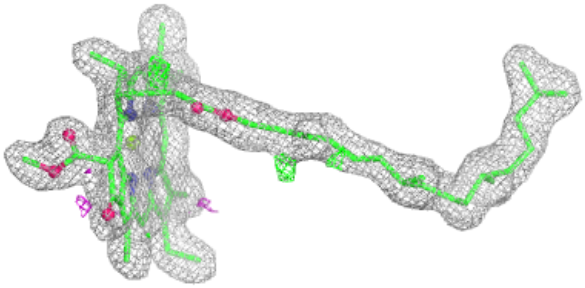


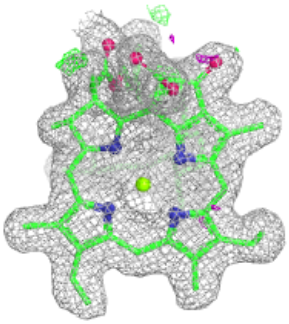


**Electron density around CLA b 609:**

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

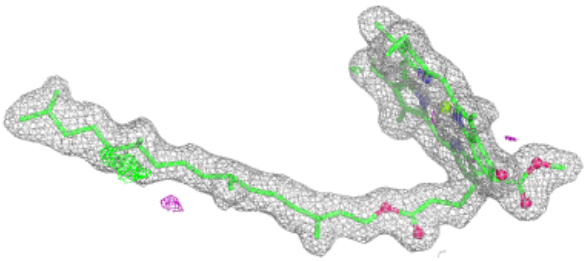


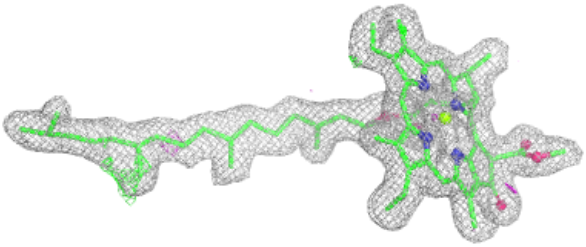


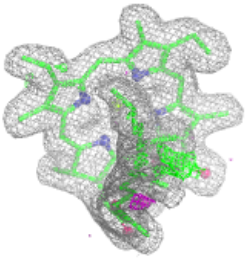


**Electron density around CLA B 608:**

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

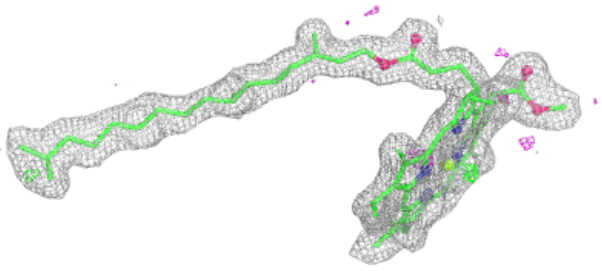


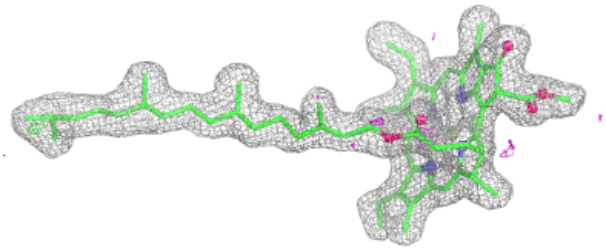


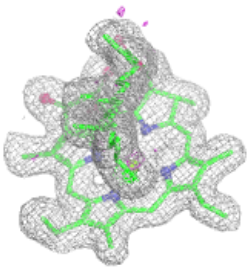


**Electron density around CLA b 611:**

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

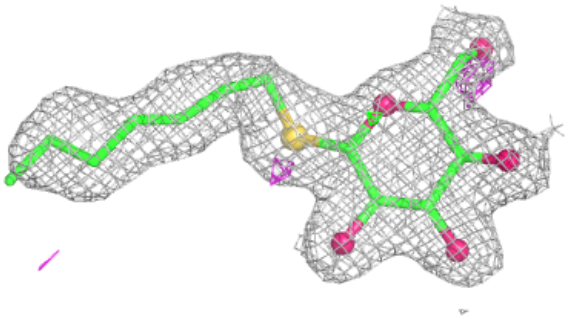


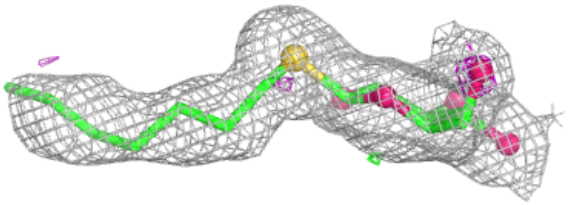


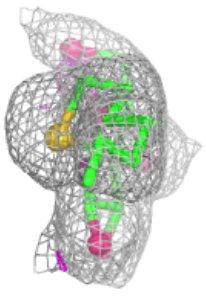


**Electron density around HTG O 303:**

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

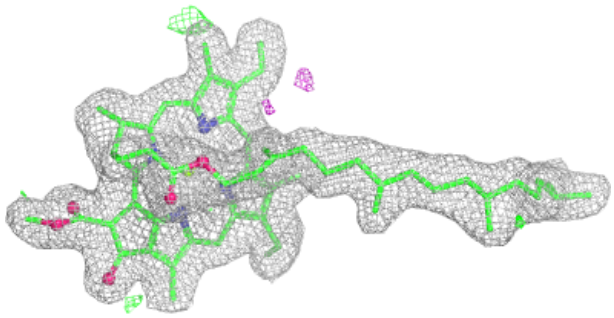


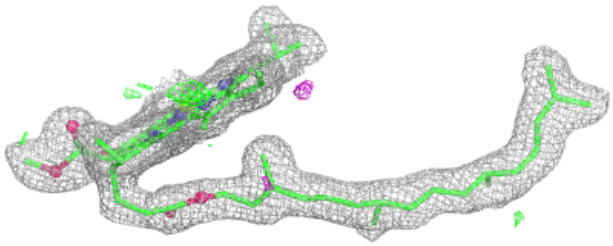


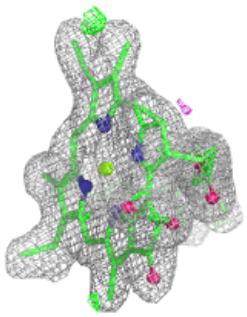


**Electron density around CLA b 612:**

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

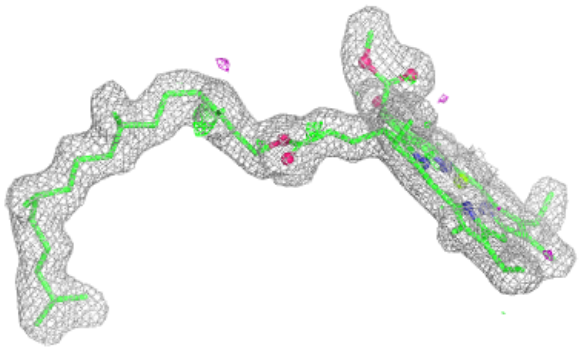


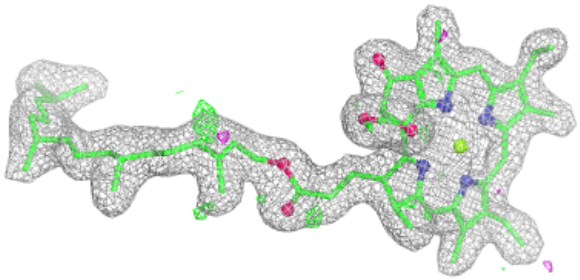


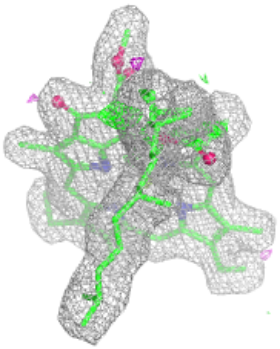


**Electron density around CLA d 402:**

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

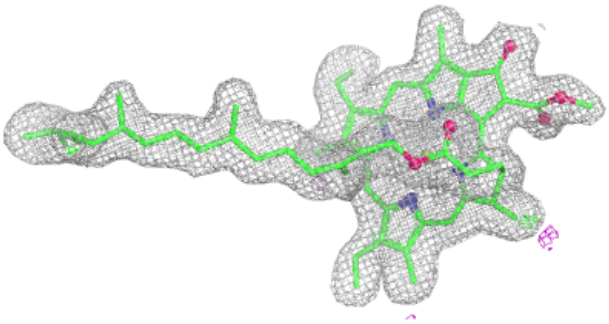


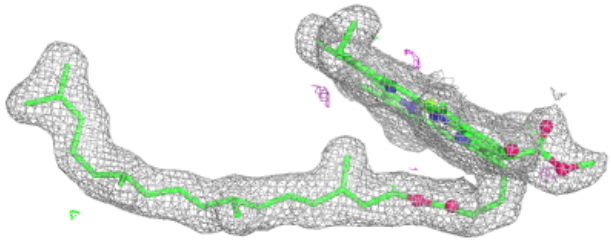




**Electron density around CLA B 609:**

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

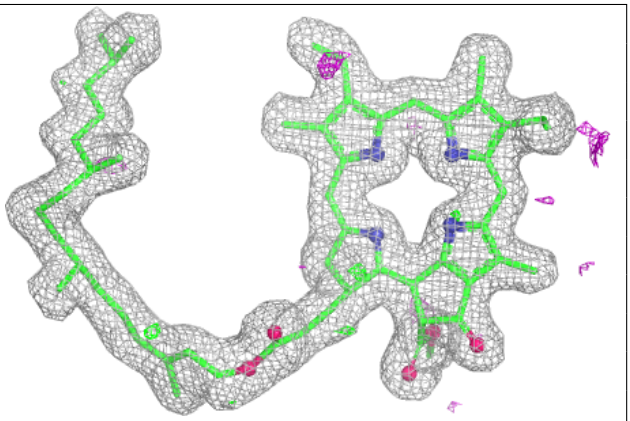


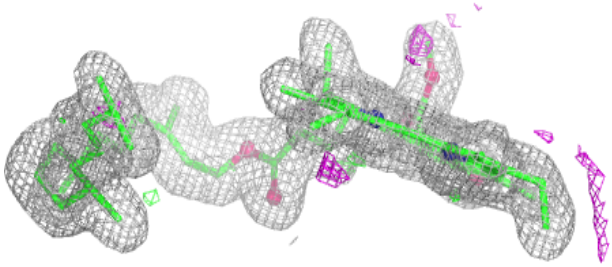


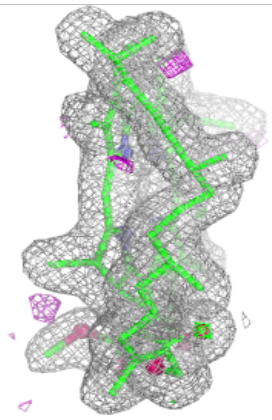


**Electron density around PHO A 408:**

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

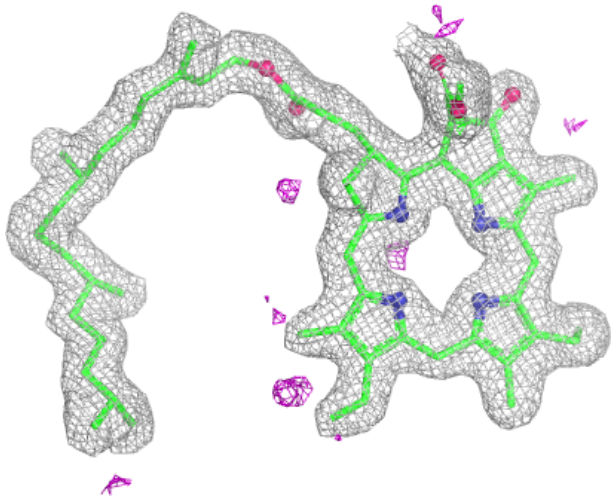


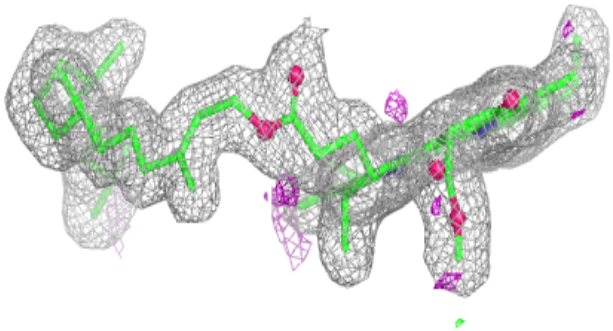


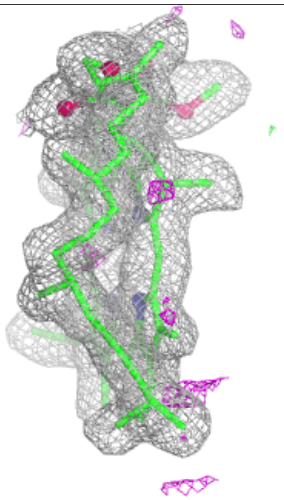


**Electron density around PHO a 408:**

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

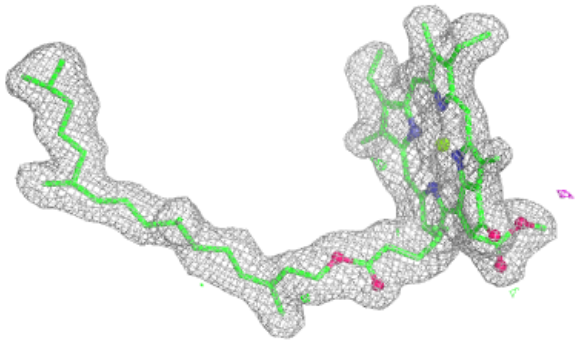


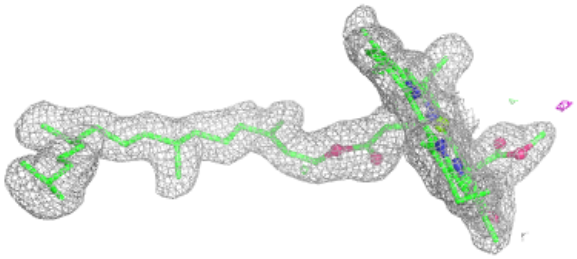




**Electron density around CLA B 610:**

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

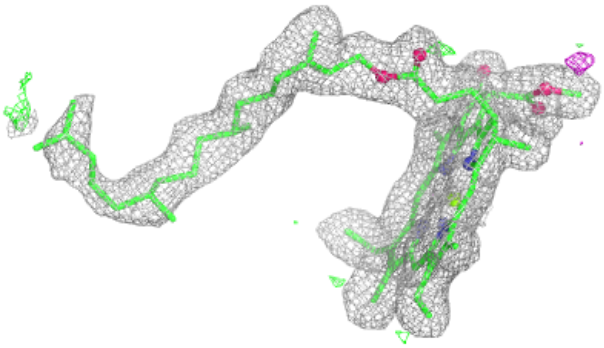


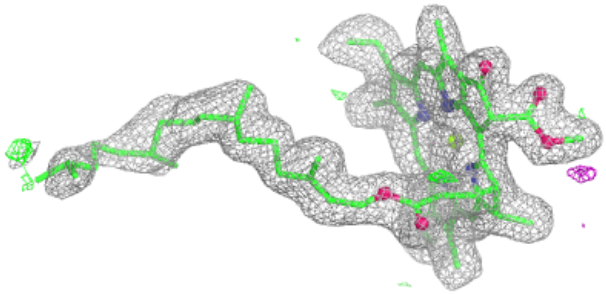


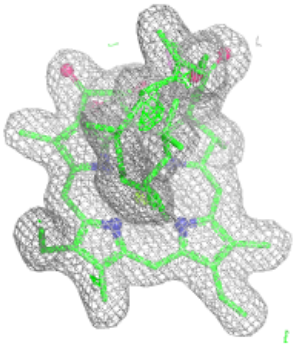


**Electron density around CLA C 509:**

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

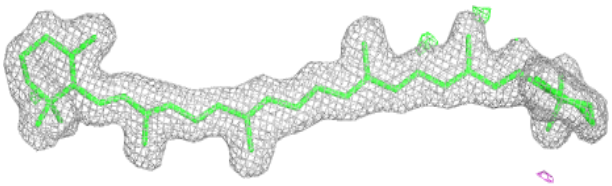


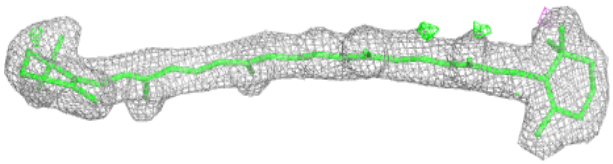


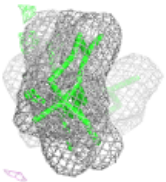


**Electron density around BCR B 618:**

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

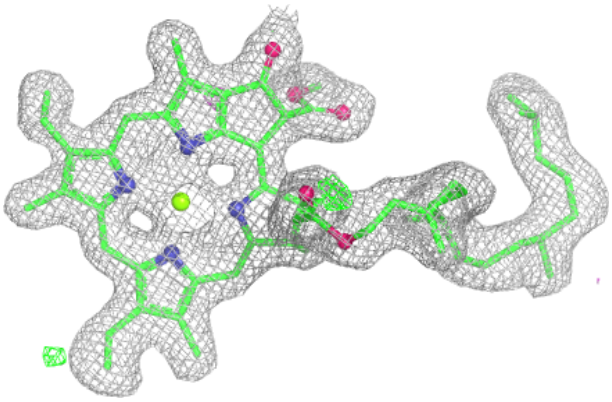


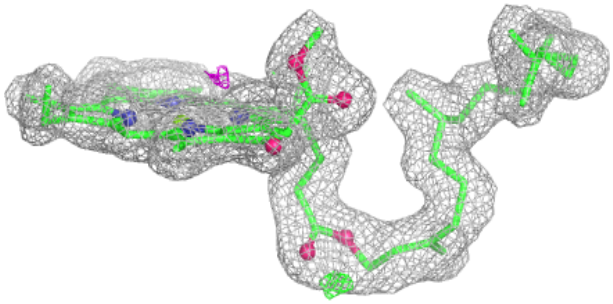


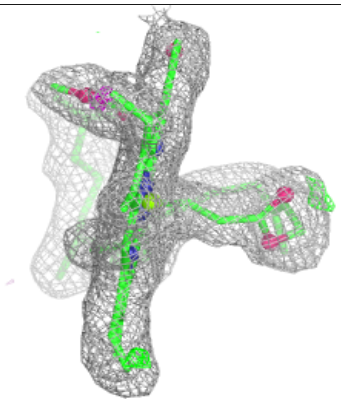


**Electron density around CLA b 616:**

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

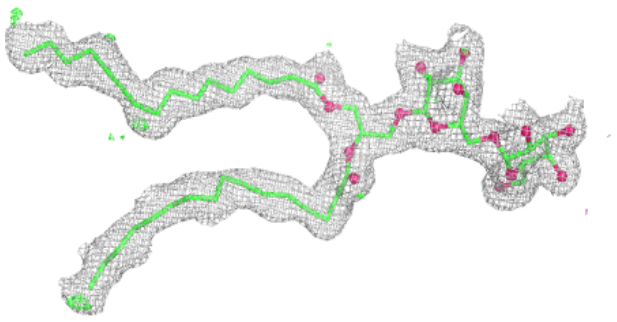


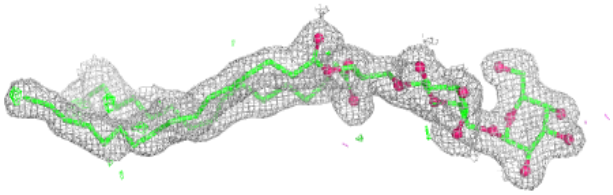


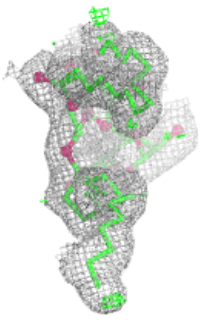


**Electron density around DGD C 519:**

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

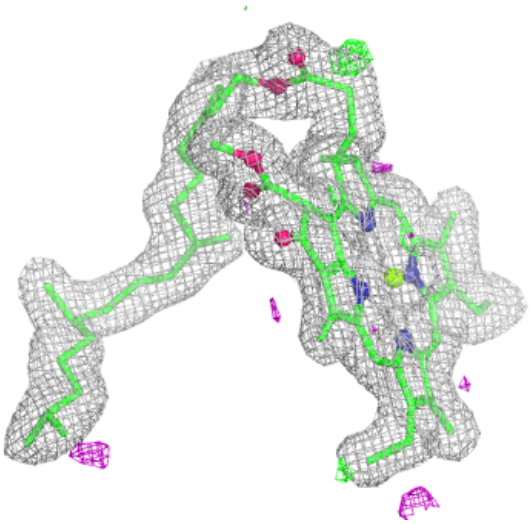


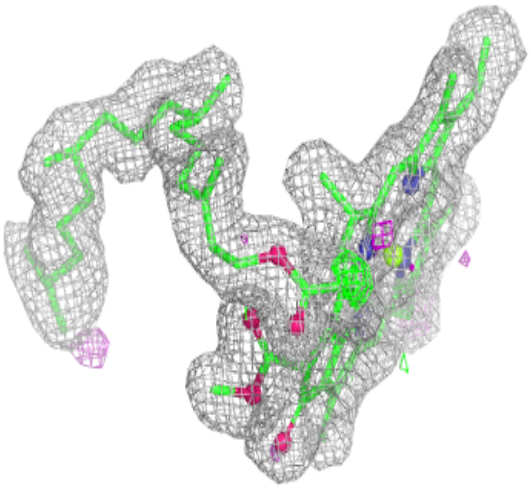


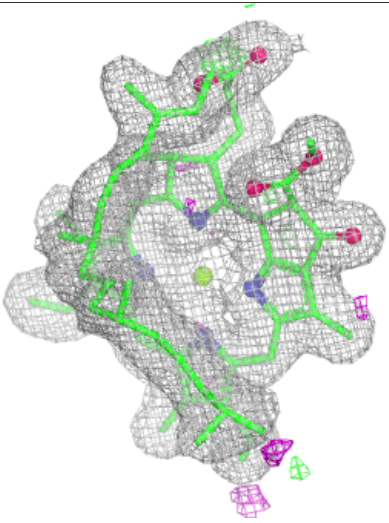


**Electron density around CLA b 617:**

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

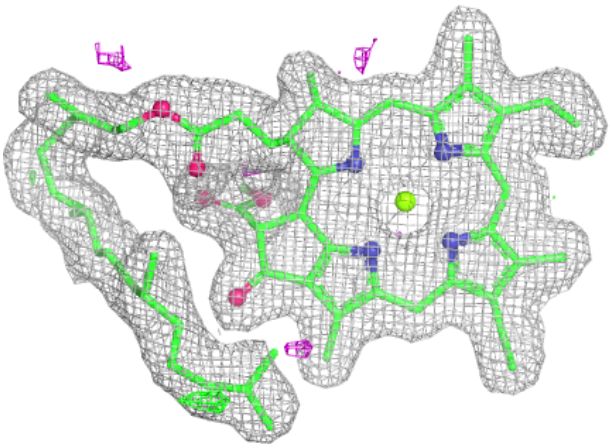


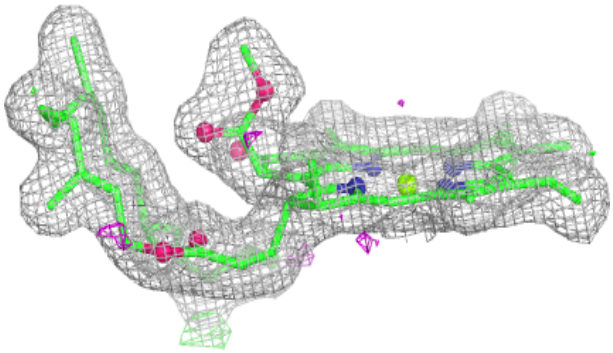


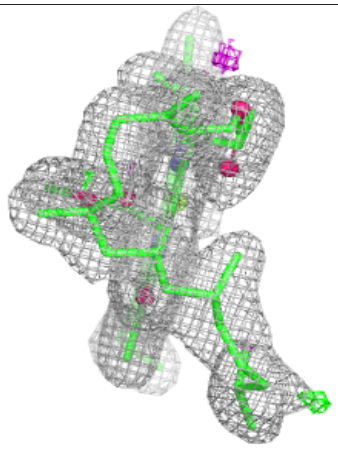


**Electron density around CLA B 611:**

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

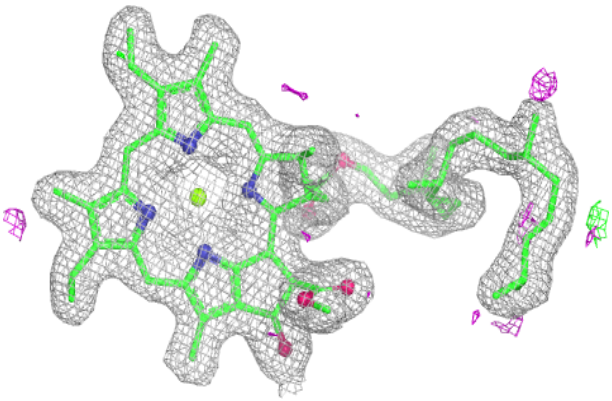


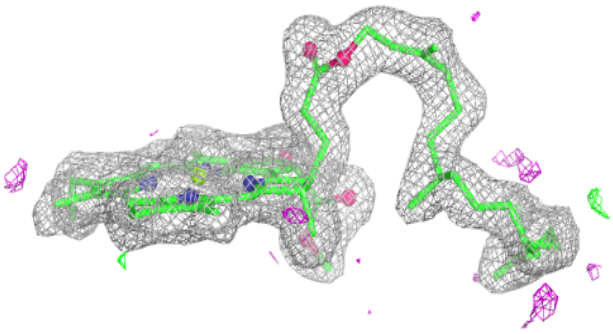


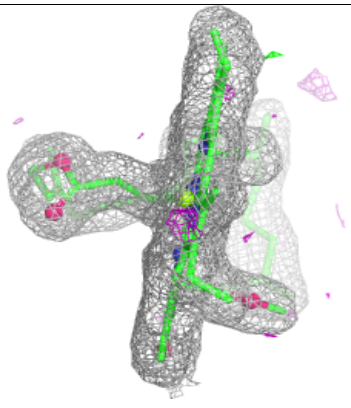


**Electron density around CLA B 613:**

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

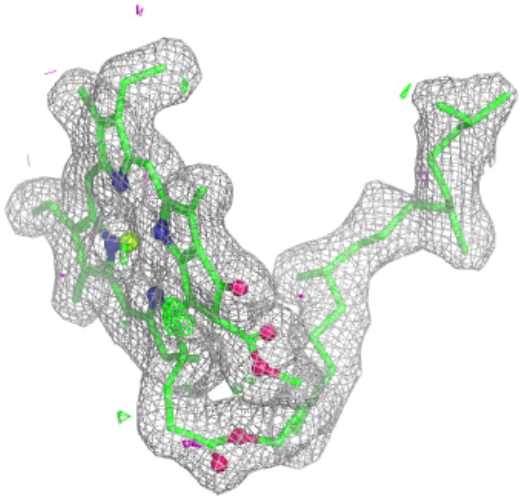


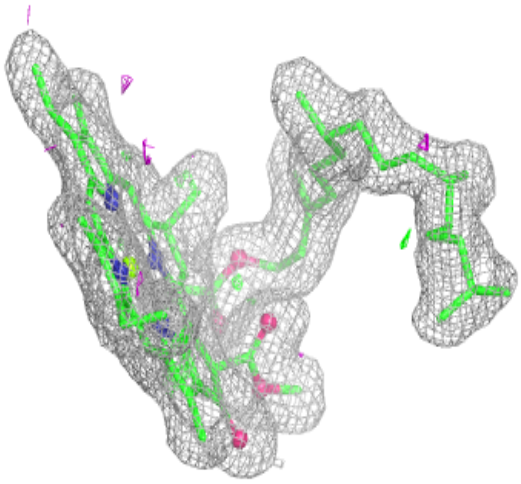


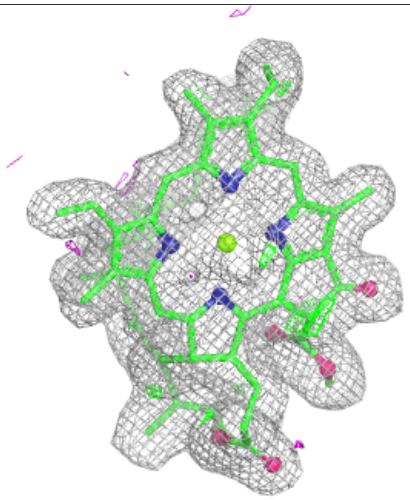


**Electron density around CLA B 614:**

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

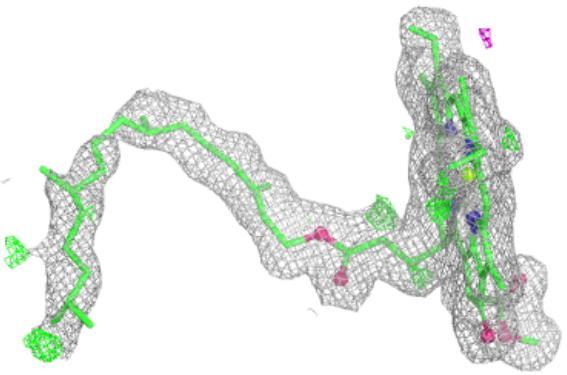


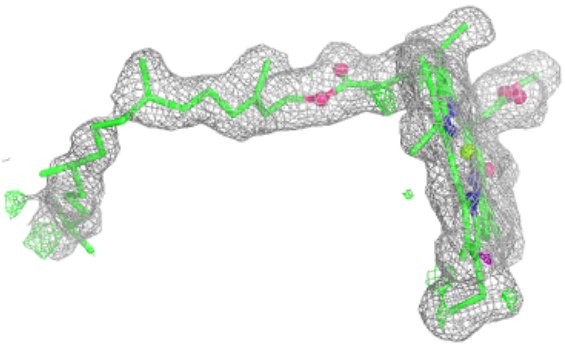


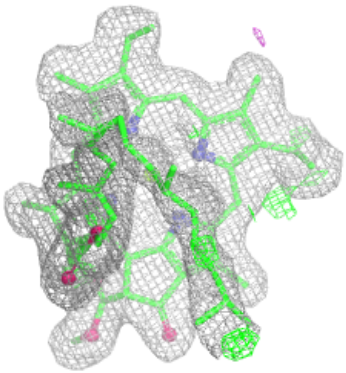


**Electron density around CLA D 402:**

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

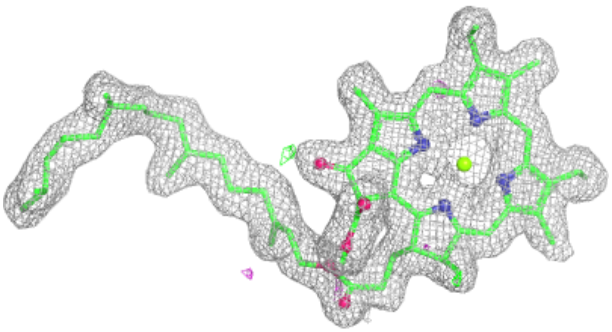


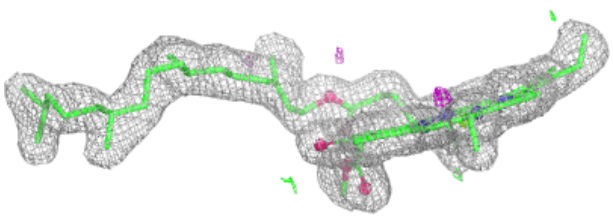


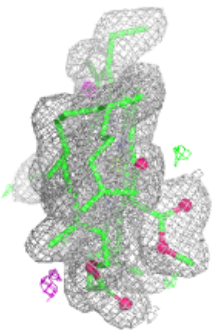


**Electron density around CLA B 603:**

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

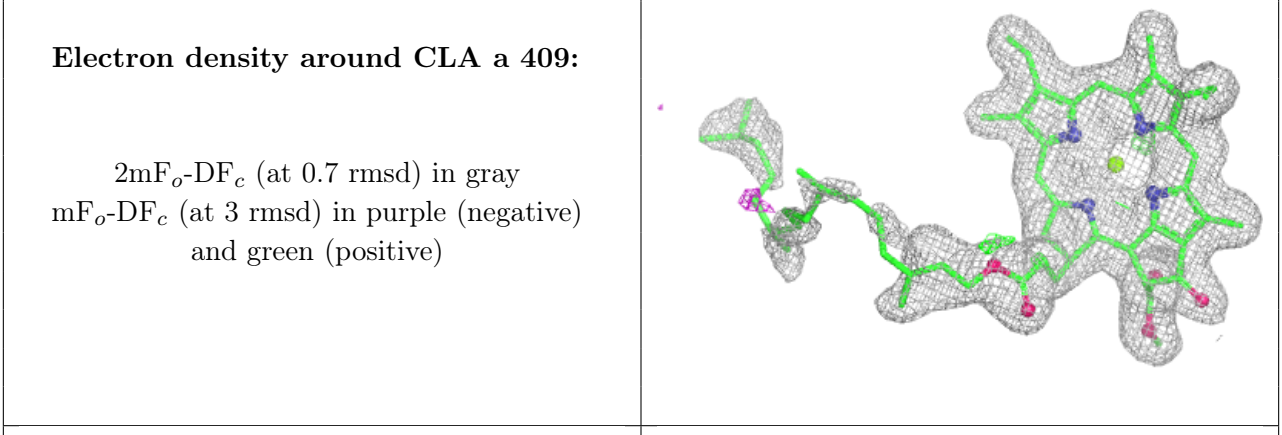






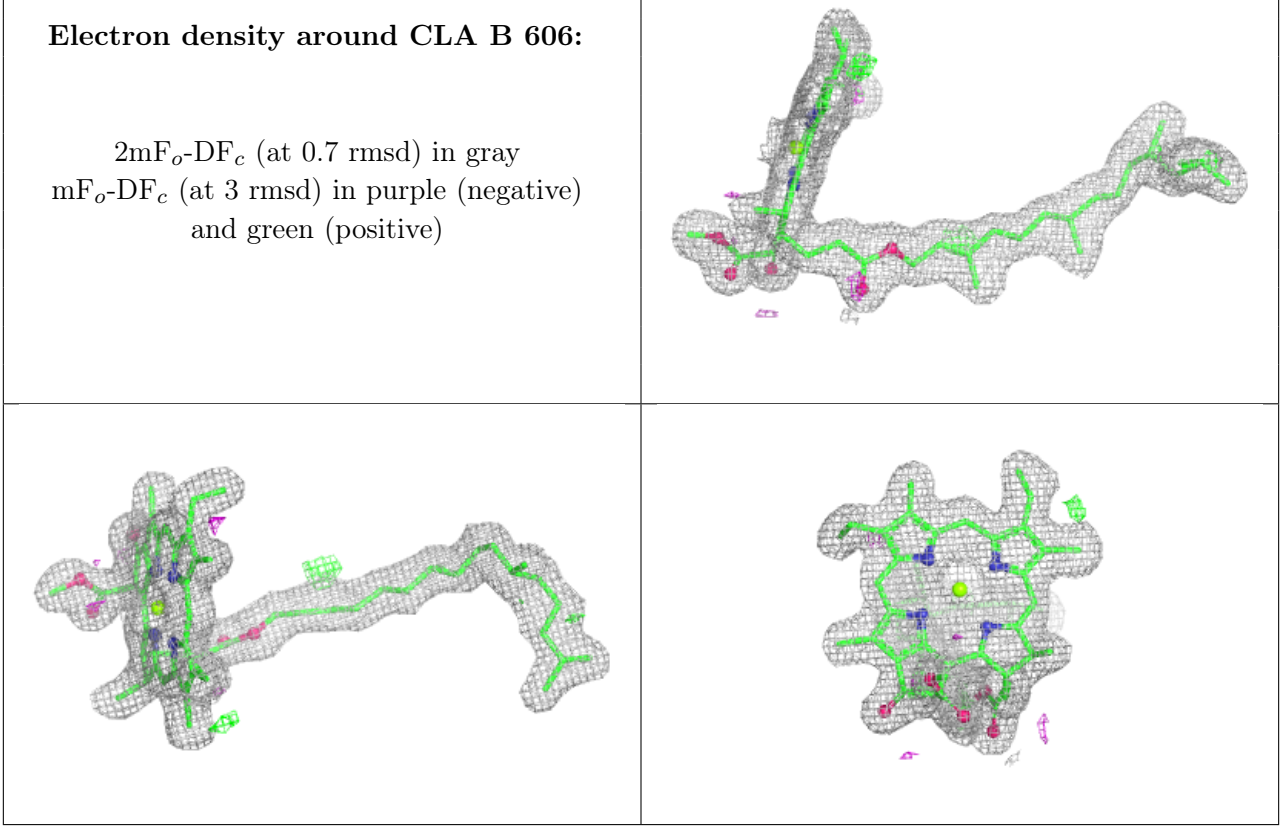
**Electron density around CLA a 409:**

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



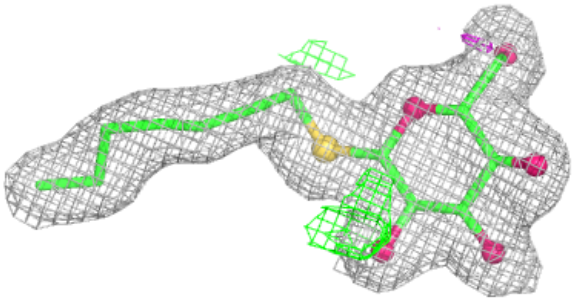
**Electron density around CLA B 606:**

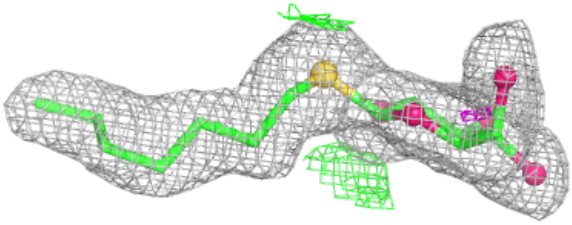
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

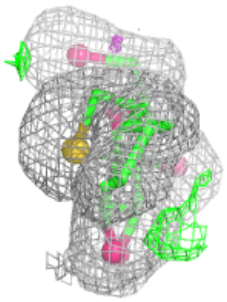


**Electron density around HTG B 624:**

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

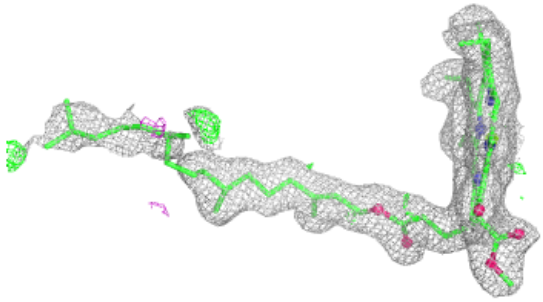


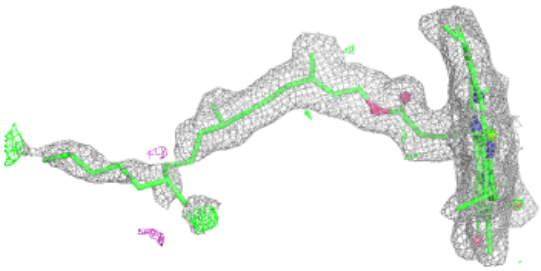


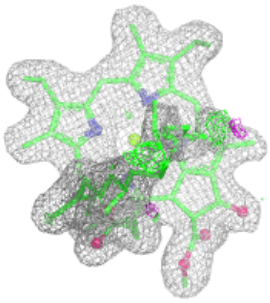


**Electron density around CLA B 607:**

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

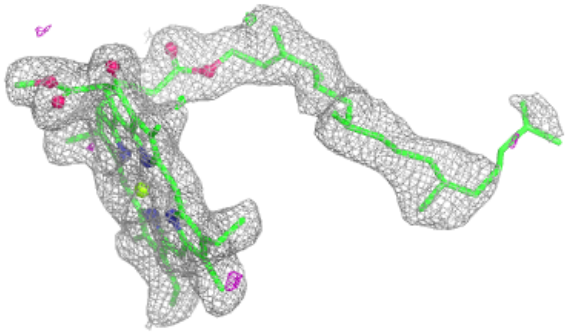


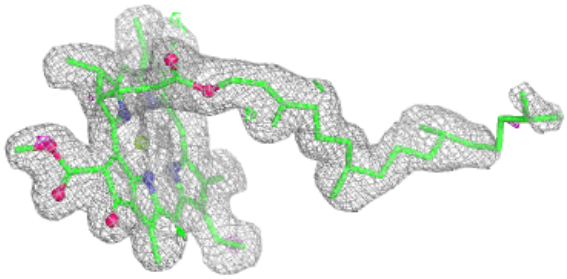


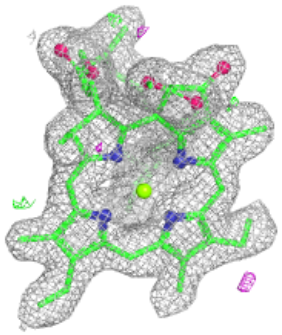


**Electron density around CLA c 909:**

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

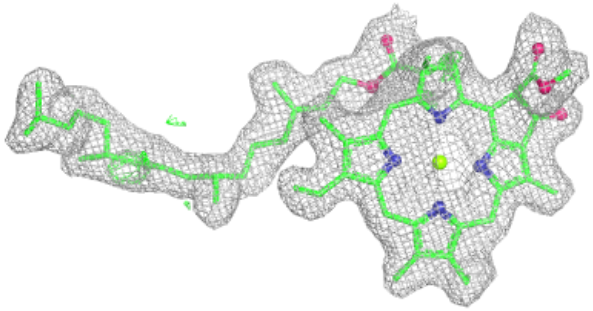


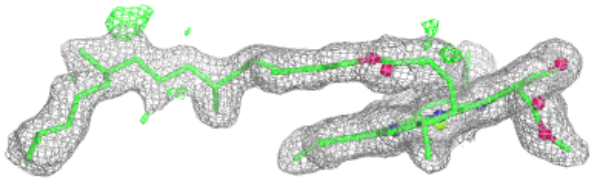


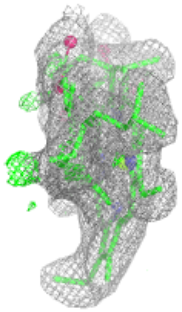


**Electron density around CLA b 607:**

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

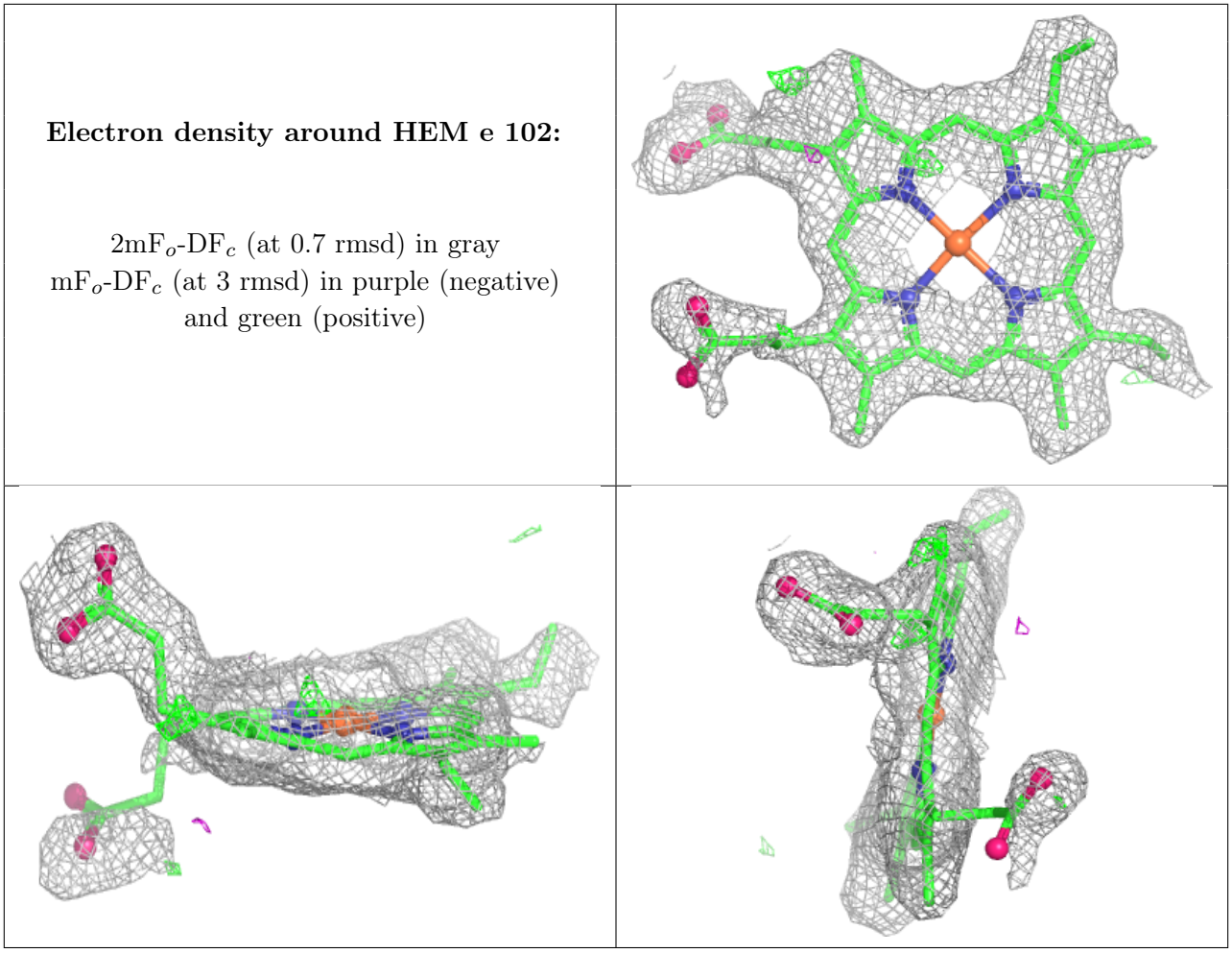






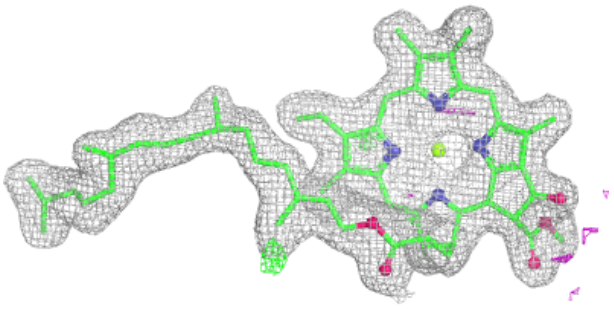
**Electron density around HEM e 102:**

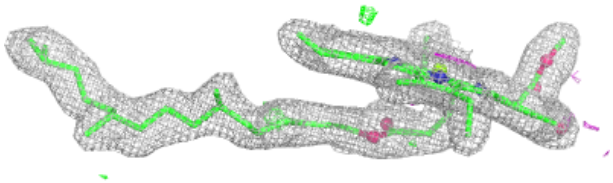
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

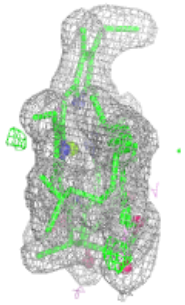


**Electron density around CLA B 604:**

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

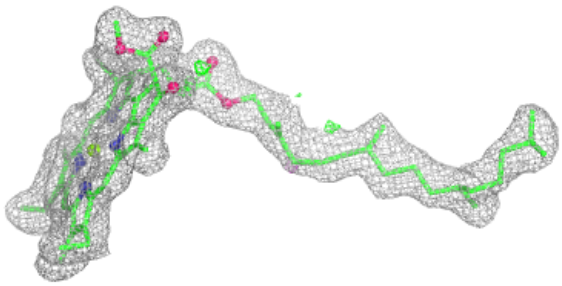


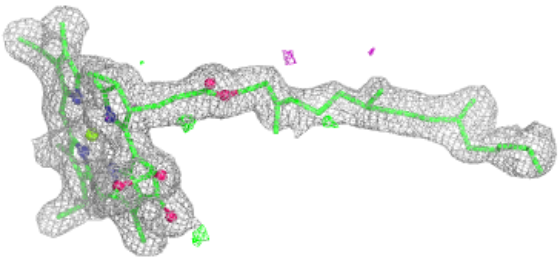


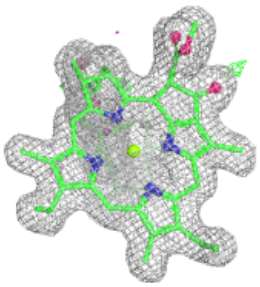


**Electron density around CLA b 608:**

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

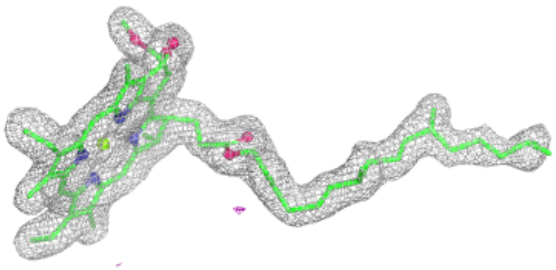


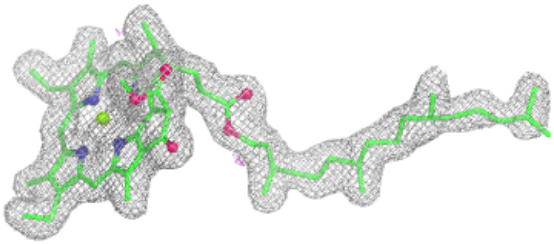


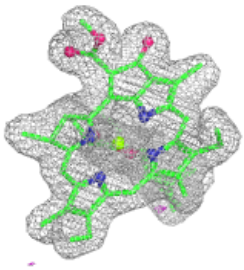


**Electron density around CLA C 503:**

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

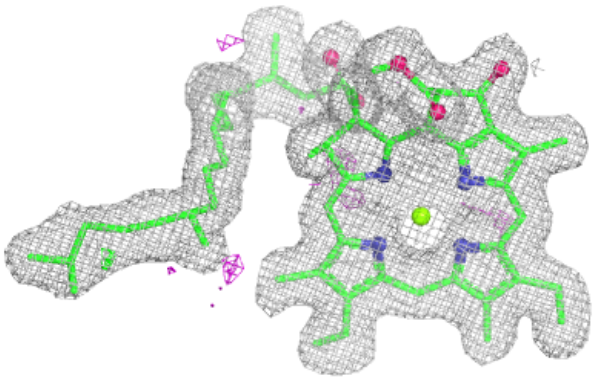


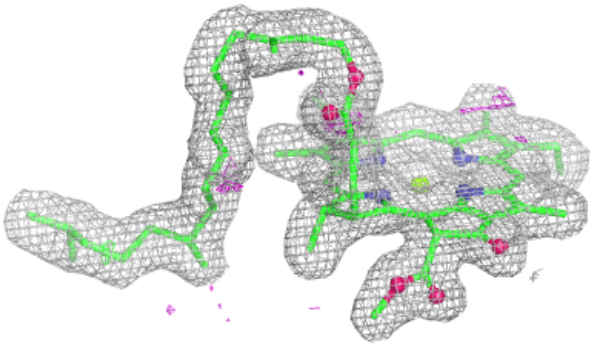


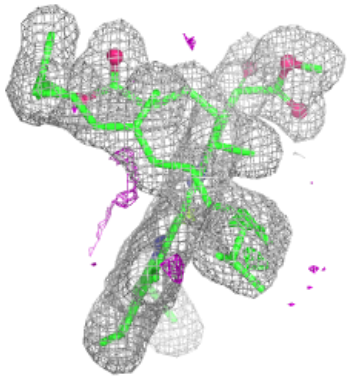


**Electron density around CLA d 401:**

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

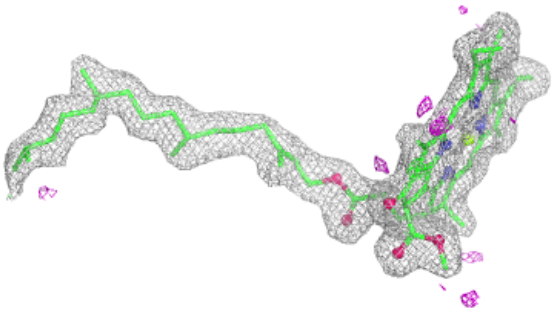


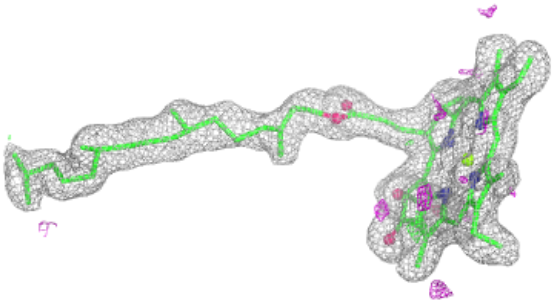


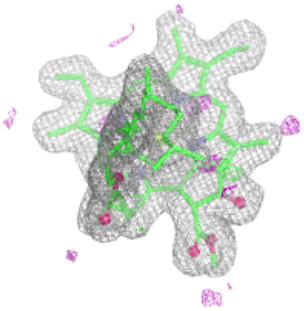


**Electron density around CLA B 605:**

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

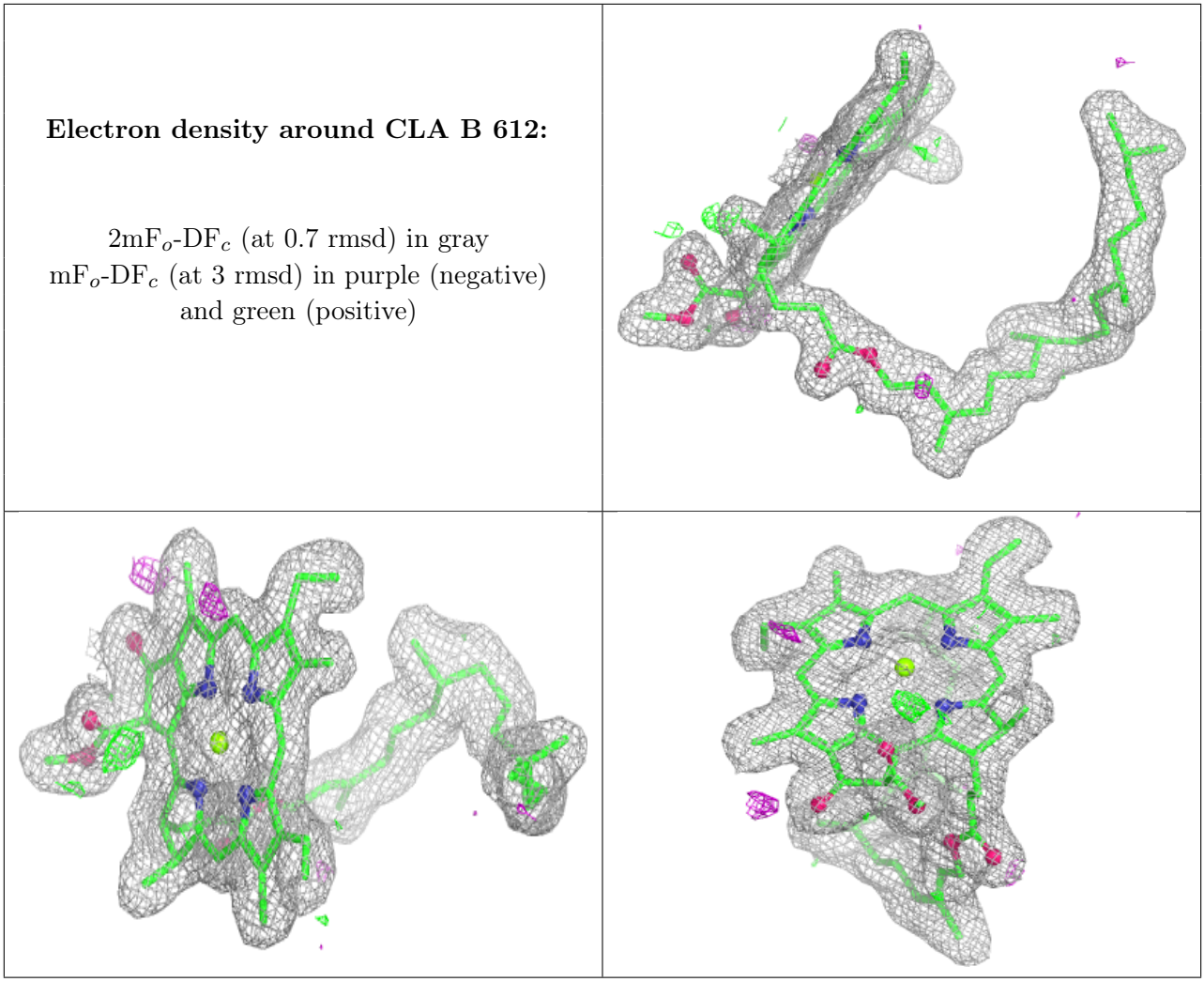






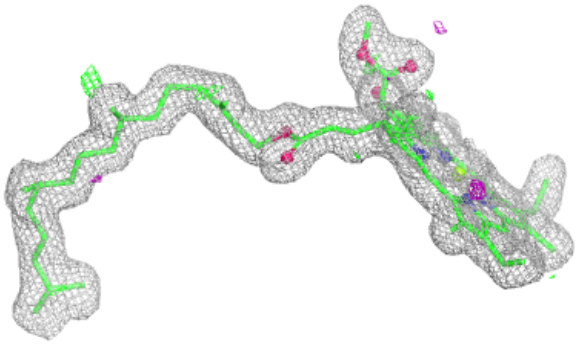
**Electron density around CLA B 612:**

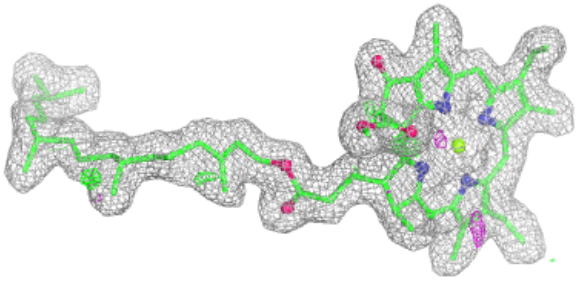
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

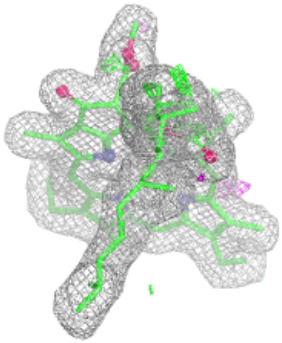


**Electron density around CLA D 401:**

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

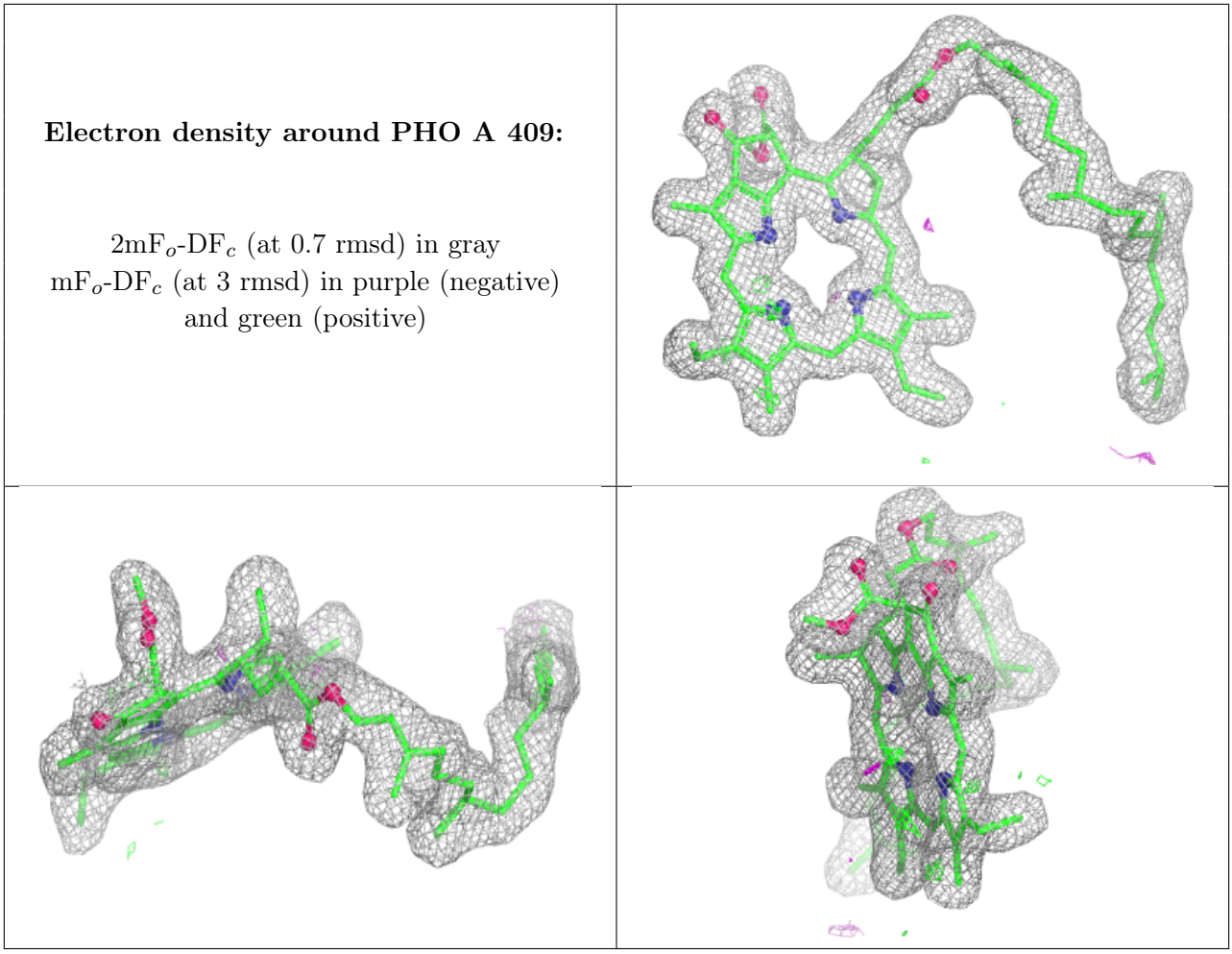






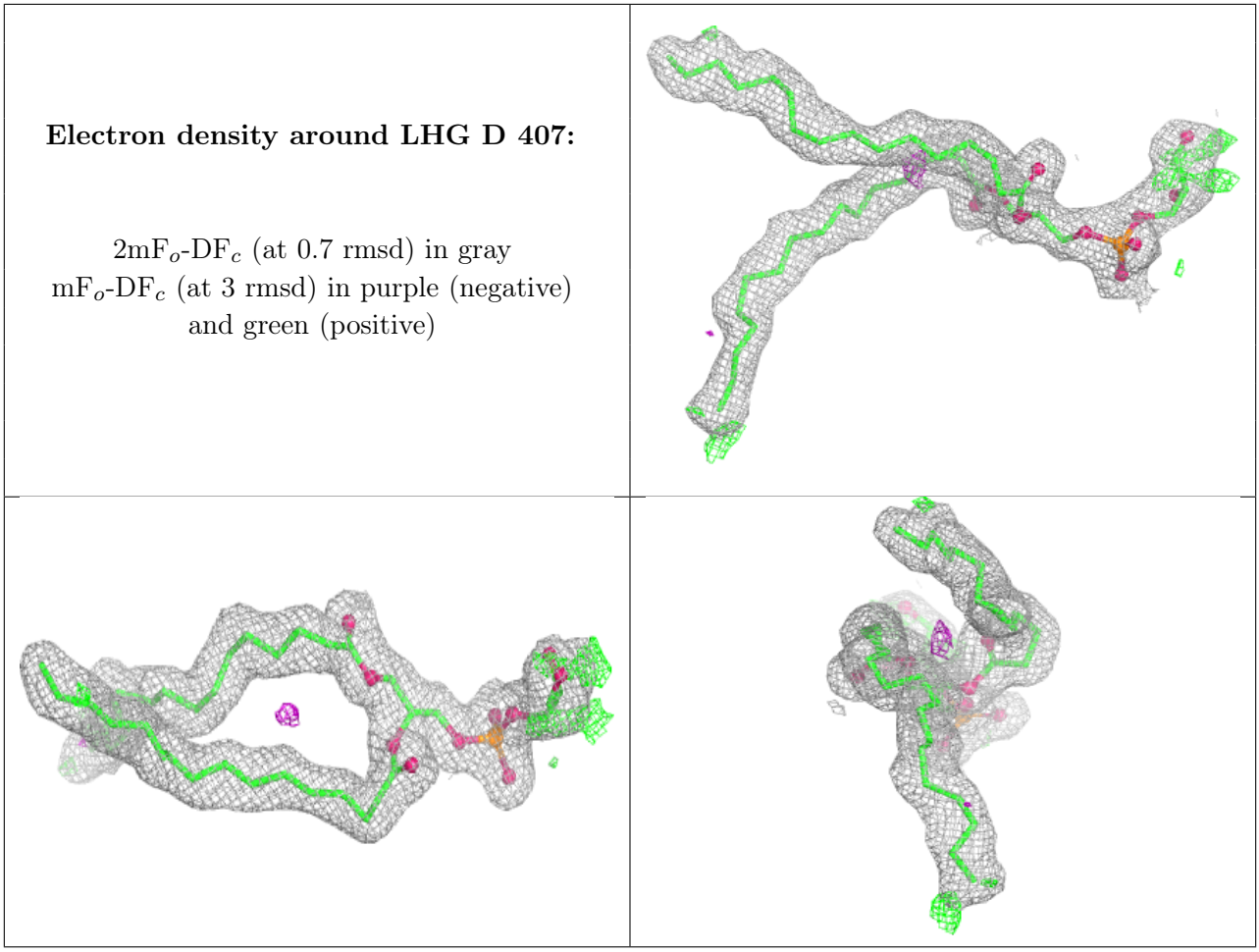
**Electron density around PHO A 409:**

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



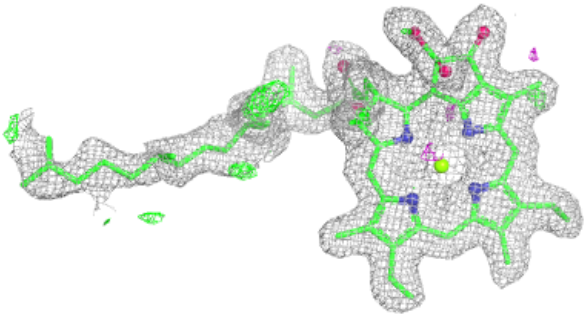
**Electron density around LHG D 407:**

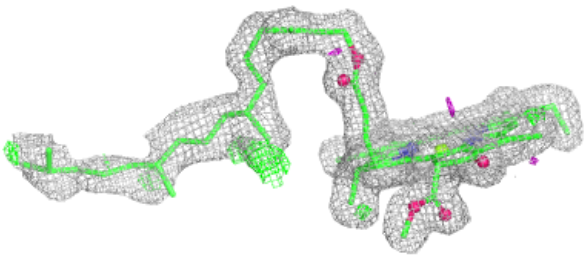
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

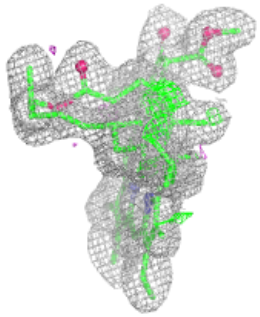


**Electron density around CLA A 407:**

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

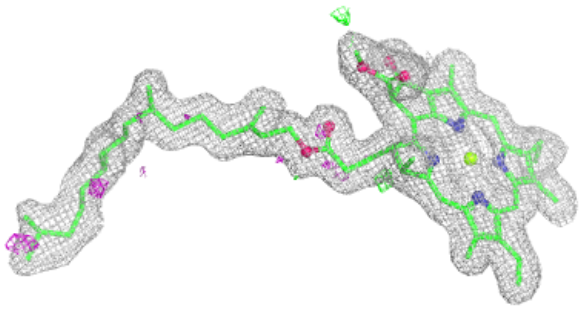


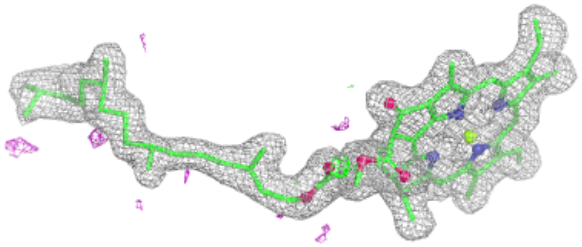


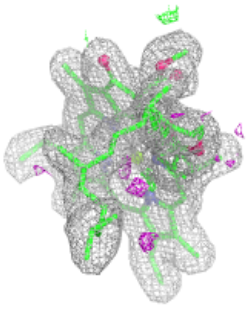


**Electron density around CLA a 406:**

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

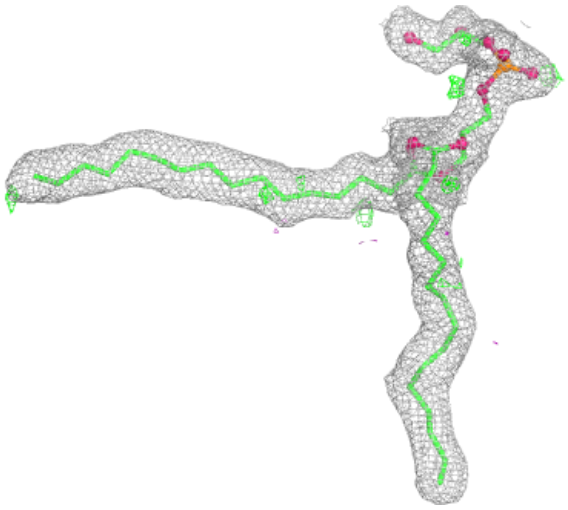


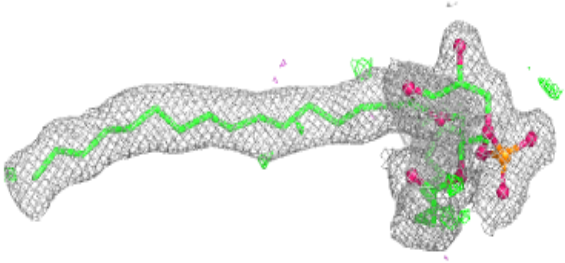


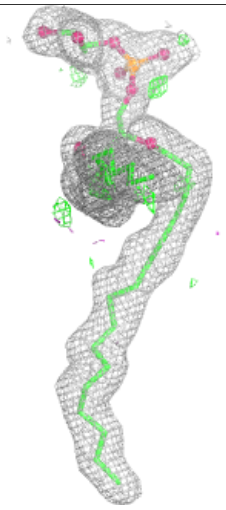


**Electron density around LHG L 101:**

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

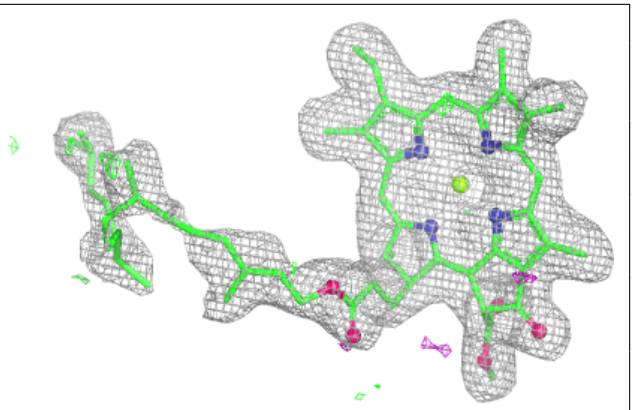


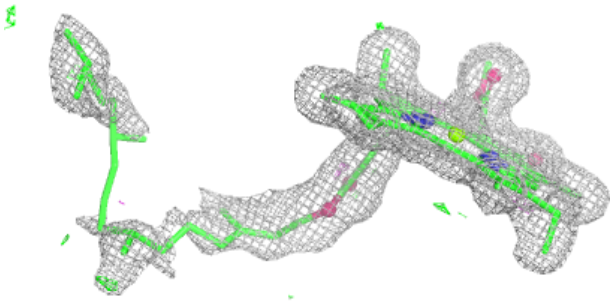


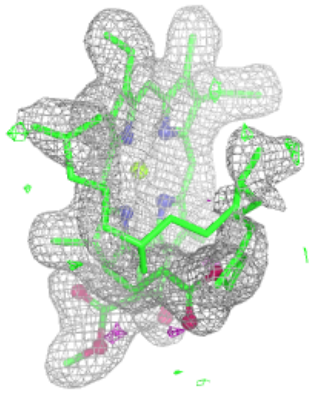


**Electron density around CLA A 410:**

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

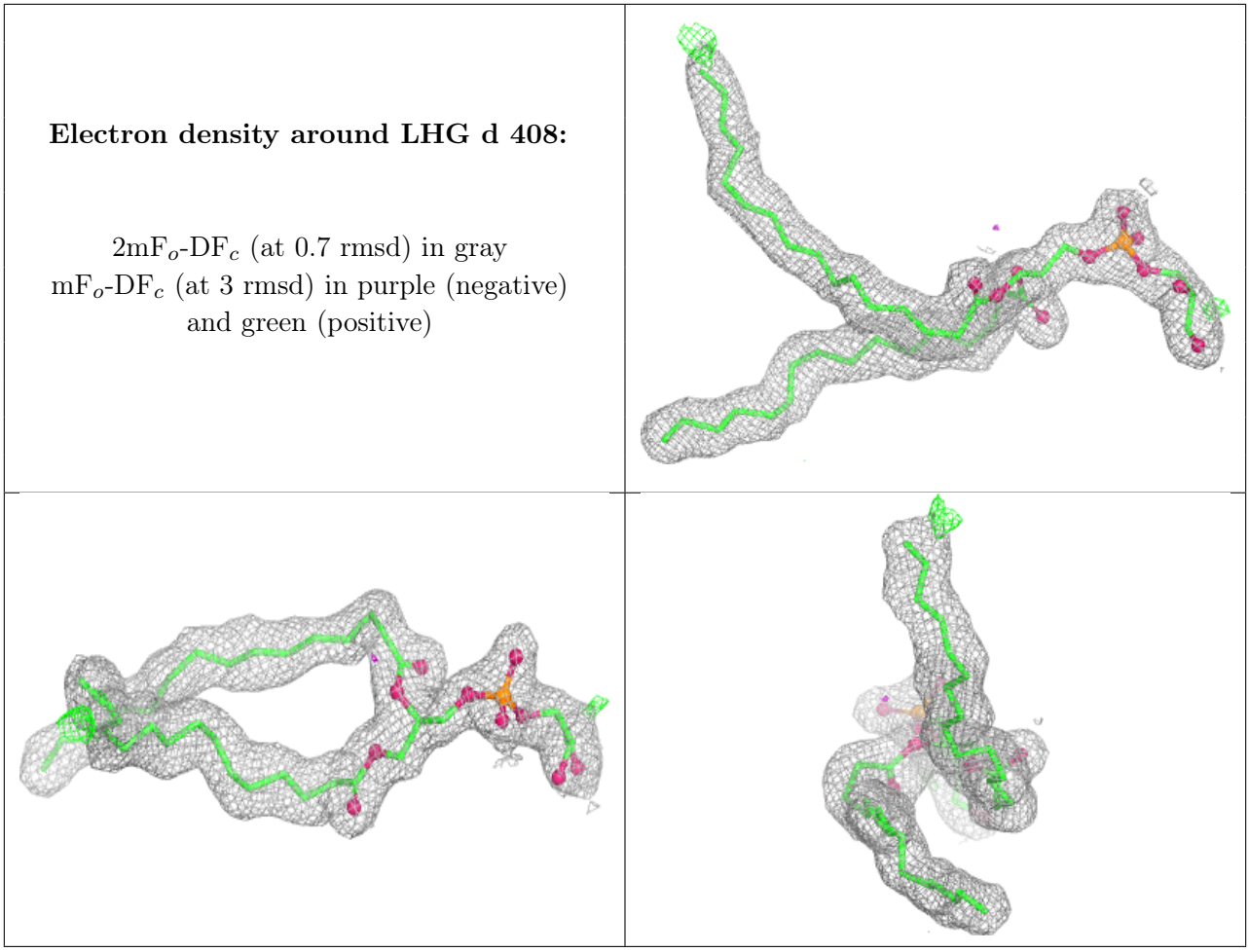






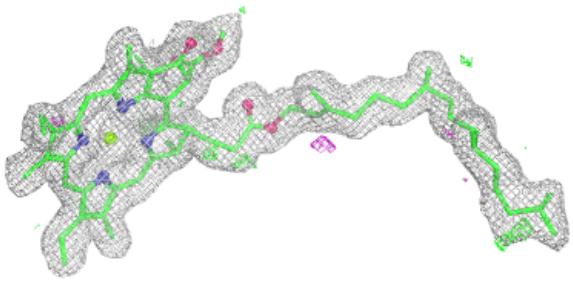
**Electron density around LHG d 408:**

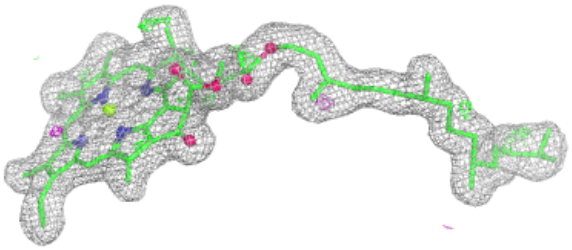
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

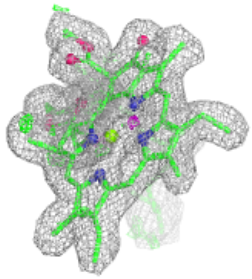


**Electron density around CLA A 405:**

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

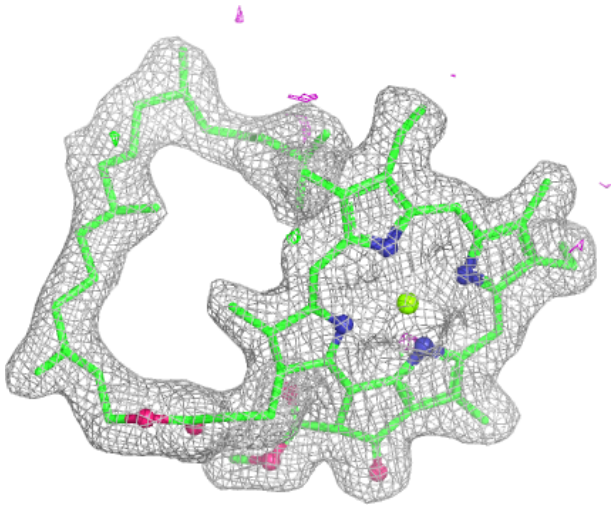


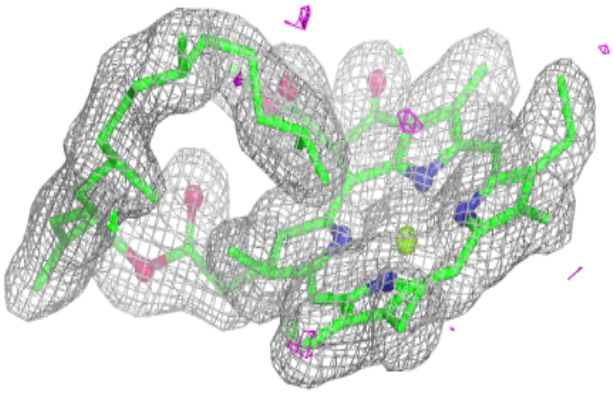


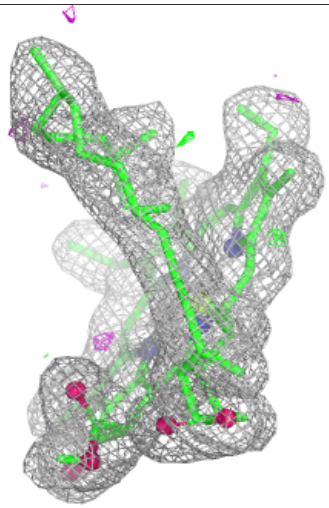


**Electron density around CLA B 616:**

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

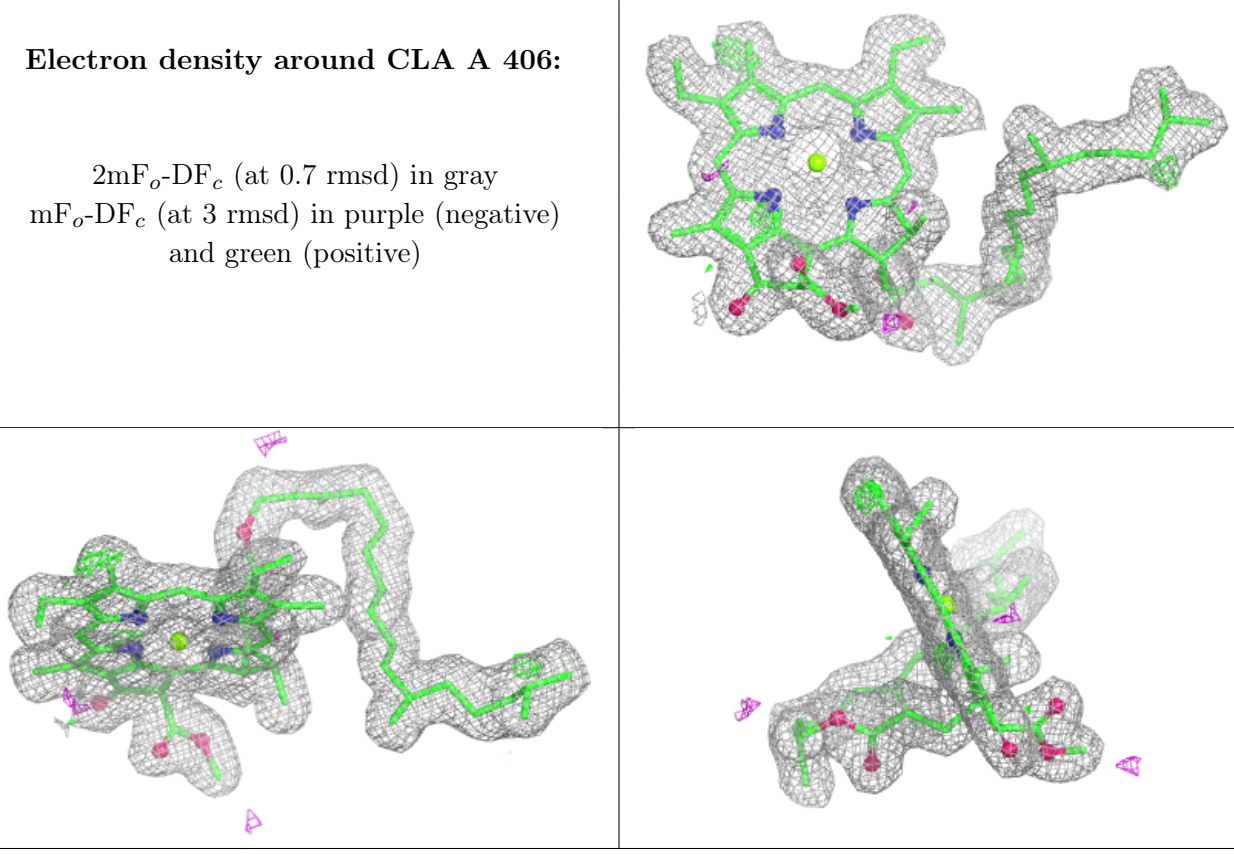






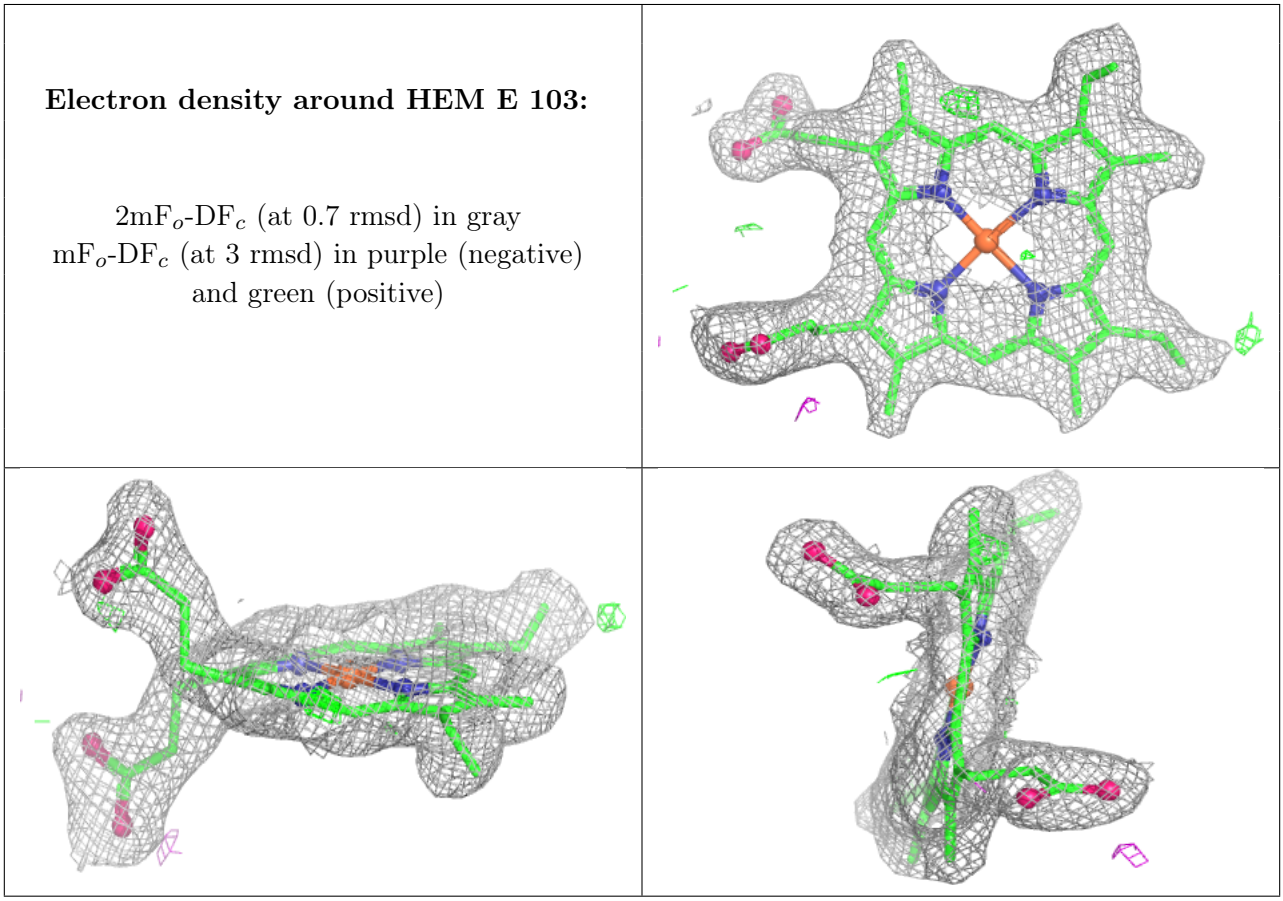
**Electron density around CLA A 406:**

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



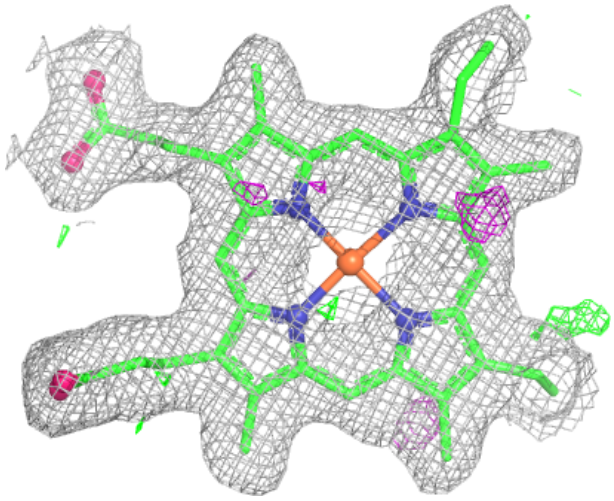
**Electron density around HEM E 103:**

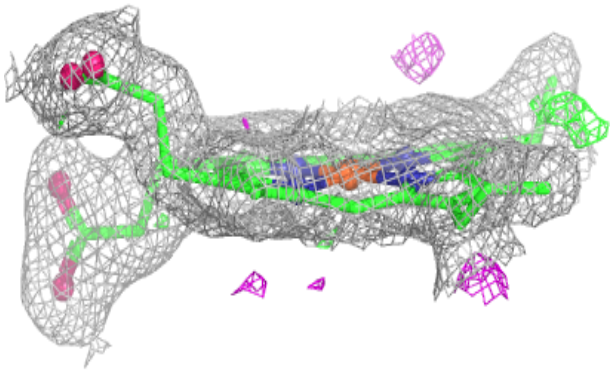
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



**Electron density around HEC V 201:**

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

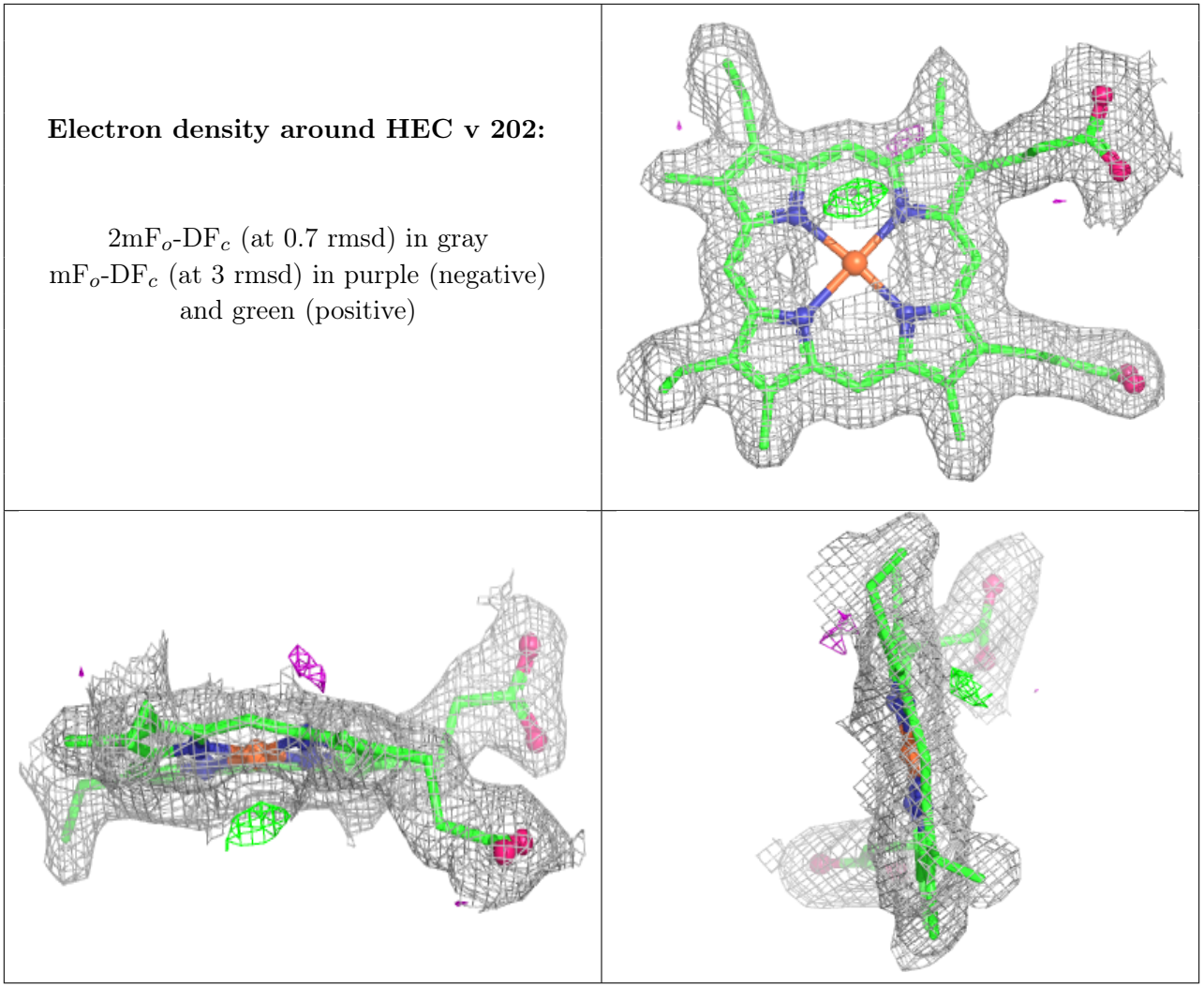






**Electron density around HEC v 202:**

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



## 6.5 Other polymers (i)

There are no such residues in this entry.