



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 10:01 PM BST

PDB ID : 5E79
Title : Macromolecular diffractive imaging using imperfect crystals
Authors : Ayer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.13 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.13 |

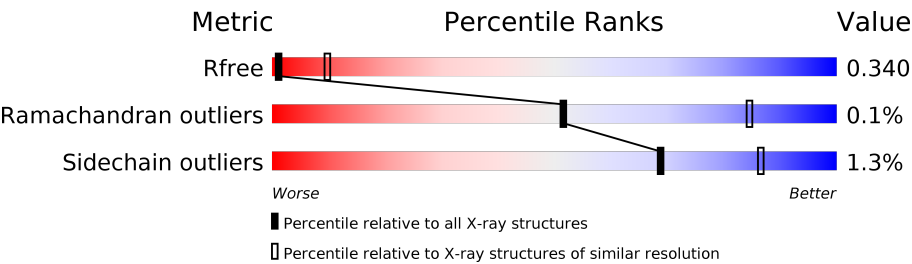
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



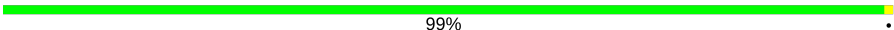

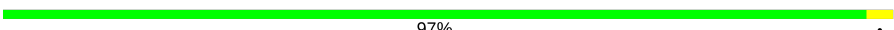
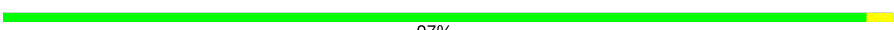











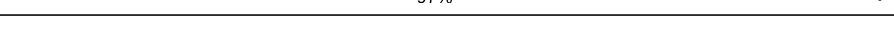
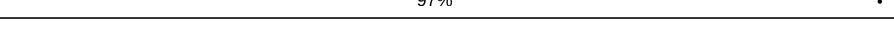
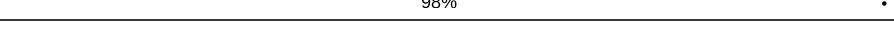
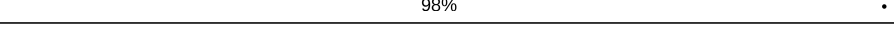
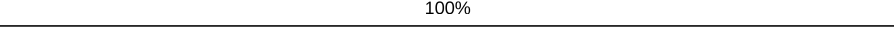
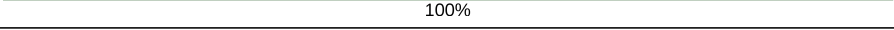
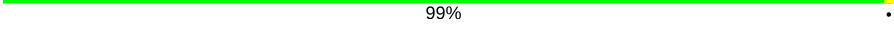
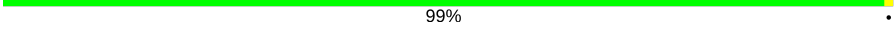
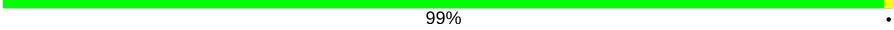
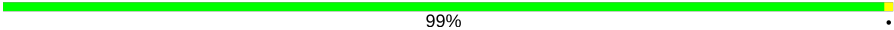
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R _{free} | 130704 | 1659 (3.60-3.40) |
| Ramachandran outliers | 138981 | 1005 (3.58-3.42) |
| Sidechain outliers | 138945 | 1006 (3.58-3.42) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 334 | 100% |
| 1 | a | 334 | 100% |
| 2 | B | 504 | 99% |
| 2 | b | 504 | 99% |
| 3 | C | 451 | 99% |
| 3 | c | 451 | 99% |
| 4 | D | 342 | 99% |
| 4 | d | 342 | 99% |

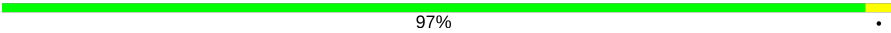
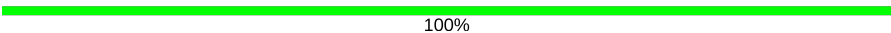

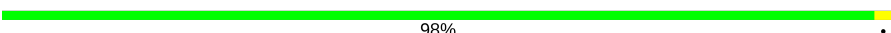
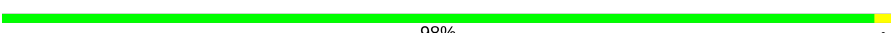
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | E | 81 |  99% . |
| 5 | e | 81 |  99% . |
| 6 | F | 34 |  97% . |
| 6 | f | 34 |  97% . |
| 7 | H | 65 |  95% 5% |
| 7 | h | 65 |  95% 5% |
| 8 | I | 38 |  100% |
| 8 | i | 38 |  100% |
| 9 | J | 38 |  100% |
| 9 | j | 38 |  100% |
| 10 | K | 37 |  95% 5% |
| 10 | k | 37 |  92% 8% |
| 11 | L | 37 |  97% . |
| 11 | l | 37 |  97% . |
| 12 | M | 34 |  97% . |
| 12 | m | 34 |  97% . |
| 13 | O | 243 |  98% . |
| 13 | o | 243 |  98% . |
| 14 | T | 30 |  100% |
| 14 | t | 30 |  100% |
| 15 | U | 97 |  99% . |
| 15 | u | 97 |  99% . |
| 16 | V | 137 |  99% . |
| 16 | v | 137 |  99% . |
| 17 | Y | 29 |  97% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 17 | y | 29 |  97% |
| 18 | X | 39 |  100% |
| 18 | x | 39 |  100% |
| 19 | Z | 62 |  98% |
| 19 | z | 62 |  98% |

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 |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 24 | CLA | A | 606 | X | - | - | - |
| 24 | CLA | A | 607 | X | - | - | - |
| 24 | CLA | A | 609 | 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[A] | X | - | - | - |
| 24 | CLA | B | 607[B] | X | - | - | - |
| 24 | CLA | B | 608 | X | - | - | - |
| 24 | CLA | B | 609 | 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 | 501 | X | - | - | - |
| 24 | CLA | C | 502 | X | - | - | - |
| 24 | CLA | C | 503 | X | - | - | - |
| 24 | CLA | C | 504 | X | - | - | - |
| 24 | CLA | C | 505 | X | - | - | - |
| 24 | CLA | C | 506 | X | - | - | - |
| 24 | CLA | C | 507 | X | - | - | - |
| 24 | CLA | C | 508 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 24 | CLA | C | 509 | X | - | - | - |
| 24 | CLA | C | 510 | X | - | - | - |
| 24 | CLA | C | 511 | X | - | - | - |
| 24 | CLA | C | 512 | X | - | - | - |
| 24 | CLA | C | 513 | X | - | - | - |
| 24 | CLA | D | 402 | X | - | - | - |
| 24 | CLA | D | 403 | X | - | - | - |
| 24 | CLA | D | 404 | X | - | - | - |
| 24 | CLA | a | 606 | X | - | - | - |
| 24 | CLA | a | 607 | X | - | - | - |
| 24 | CLA | a | 609 | X | - | - | - |
| 24 | CLA | a | 615 | 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[A] | X | - | - | - |
| 24 | CLA | b | 608[B] | X | - | - | - |
| 24 | CLA | b | 609 | 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 | b | 618 | X | - | - | - |
| 24 | CLA | c | 501 | X | - | - | - |
| 24 | CLA | c | 502 | X | - | - | - |
| 24 | CLA | c | 503 | X | - | - | - |
| 24 | CLA | c | 504 | X | - | - | - |
| 24 | CLA | c | 505 | X | - | - | - |
| 24 | CLA | c | 506 | X | - | - | - |
| 24 | CLA | c | 507 | X | - | - | - |
| 24 | CLA | c | 508 | X | - | - | - |
| 24 | CLA | c | 509 | X | - | - | - |
| 24 | CLA | c | 510 | X | - | - | - |
| 24 | CLA | c | 511 | X | - | - | - |
| 24 | CLA | c | 512 | X | - | - | - |
| 24 | CLA | c | 513 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | d | 402 | X | - | - | - |
| 24 | CLA | d | 403 | X | - | - | - |
| 26 | BCR | A | 610 | - | X | - | - |
| 26 | BCR | B | 618 | - | X | - | - |
| 26 | BCR | B | 619 | - | X | - | - |
| 26 | BCR | B | 620 | - | X | - | - |
| 26 | BCR | C | 514 | - | X | - | - |
| 26 | BCR | F | 101 | - | X | - | - |
| 26 | BCR | H | 101 | - | X | - | - |
| 26 | BCR | I | 101 | - | X | - | - |
| 26 | BCR | K | 101 | - | X | - | - |
| 26 | BCR | K | 102 | - | X | - | - |
| 26 | BCR | T | 101 | - | X | - | - |
| 26 | BCR | a | 610 | - | X | - | - |
| 26 | BCR | b | 619 | - | X | - | - |
| 26 | BCR | b | 620 | - | X | - | - |
| 26 | BCR | b | 621 | - | X | - | - |
| 26 | BCR | c | 514 | - | X | - | - |
| 26 | BCR | c | 515 | - | X | - | - |
| 26 | BCR | c | 521 | - | X | - | - |
| 26 | BCR | f | 101 | - | X | - | - |
| 26 | BCR | h | 101 | - | X | - | - |
| 26 | BCR | k | 101 | - | X | - | - |
| 26 | BCR | t | 101 | - | X | - | - |
| 27 | PL9 | D | 405 | - | X | - | - |
| 27 | PL9 | d | 404 | - | X | - | - |

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 50074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 334 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 2637 | 1730 | 432 | 460 | 15 | | | |
| 1 | a | 334 | Total | C | N | O | S | 3 | 4 | 0 |
| | | | 2637 | 1730 | 432 | 460 | 15 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 286 | ALA | THR | conflict | UNP P0A444 |
| a | 286 | ALA | THR | conflict | UNP P0A444 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 504 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 4024 | 2641 | 668 | 702 | 13 | | | |
| 2 | b | 504 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 4024 | 2641 | 668 | 702 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 451 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 3506 | 2296 | 584 | 613 | 13 | | | |
| 3 | c | 451 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 3506 | 2296 | 584 | 613 | 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 | 0 | 0 |
| | | | 2726 | 1805 | 445 | 464 | 12 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | d | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2726 | 1805 | 445 | 464 | 12 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 5 | E | 81 | Total | C | N | O | | 0 | 2 | 0 |
| | | | 668 | 436 | 107 | 125 | | | | |
| 5 | e | 81 | Total | C | N | O | | 0 | 2 | 0 |
| | | | 668 | 436 | 107 | 125 | | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | H | 65 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 525 | 351 | 86 | 86 | 2 | | | |
| 7 | h | 65 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 525 | 351 | 86 | 86 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | I | 38 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 320 | 215 | 49 | 54 | 2 | | | |
| 8 | i | 38 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 320 | 215 | 49 | 54 | 2 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11 | L | 37 | Total | C | N | O | S | 5 | 1 | 0 |
| | | | 309 | 207 | 48 | 53 | 1 | | | |
| 11 | l | 37 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 309 | 207 | 48 | 53 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | M | 34 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 272 | 183 | 40 | 48 | 1 | | | |
| 12 | m | 34 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 272 | 183 | 40 | 48 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | O | 243 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 1883 | 1178 | 315 | 385 | 5 | | | |
| 13 | o | 243 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 1883 | 1178 | 315 | 385 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | T | 30 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 270 | 189 | 37 | 41 | 3 | | | |
| 14 | t | 30 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 270 | 189 | 37 | 41 | 3 | | | |

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

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

- 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 | 1 | 0 |
| | | | 1072 | 680 | 180 | 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 | | | |

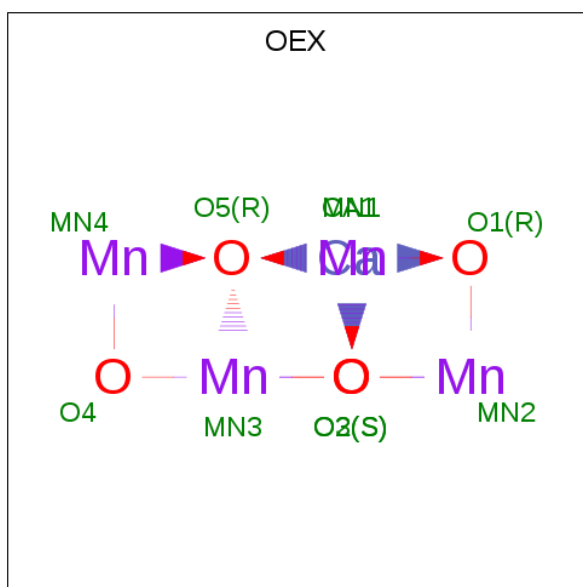
- Molecule 18 is a protein called Photosystem II reaction center X protein.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | X | 39 | Total | C | N | O | 0 | 1 | 0 |
| | | | 292 | 196 | 46 | 50 | | | |
| 18 | x | 39 | Total | C | N | O | 0 | 1 | 0 |
| | | | 292 | 196 | 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 CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20 | A | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |
| 20 | a | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |

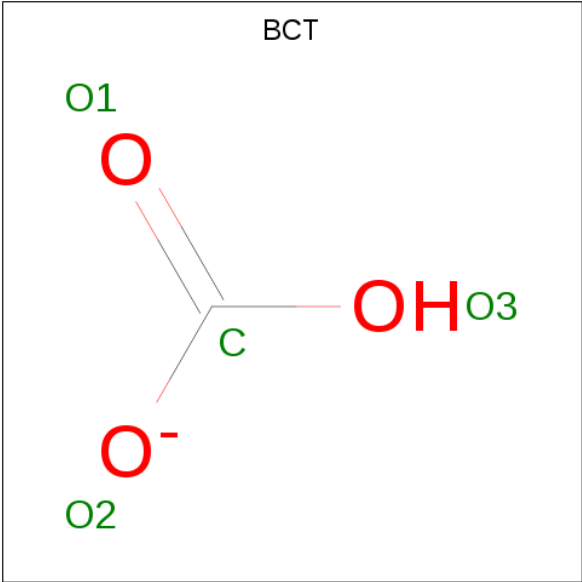
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

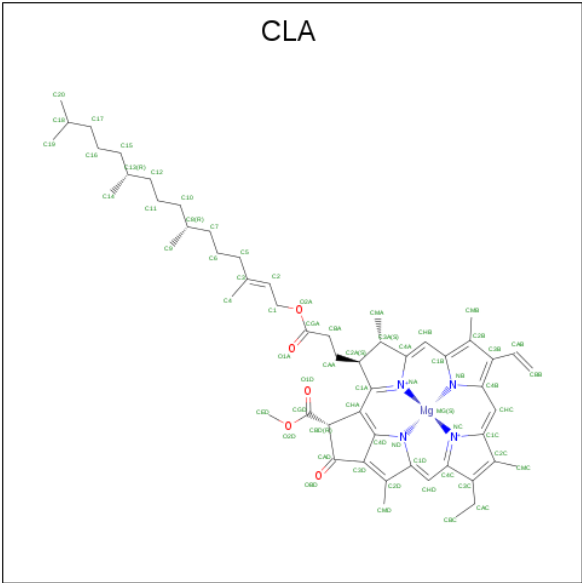
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 22 | u | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | a | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 22 | U | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| 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 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|---------|
| 24 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 130 | C 110 | Mg 2 | N 8 | O 10 | 0 | 1 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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

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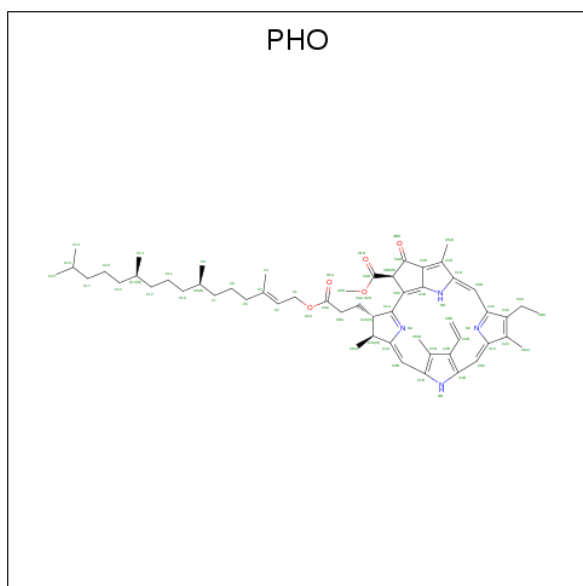
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|---------|
| 24 | b | 1 | Total 130 | C 110 | Mg 2 | N 8 | O 10 | 0 | 1 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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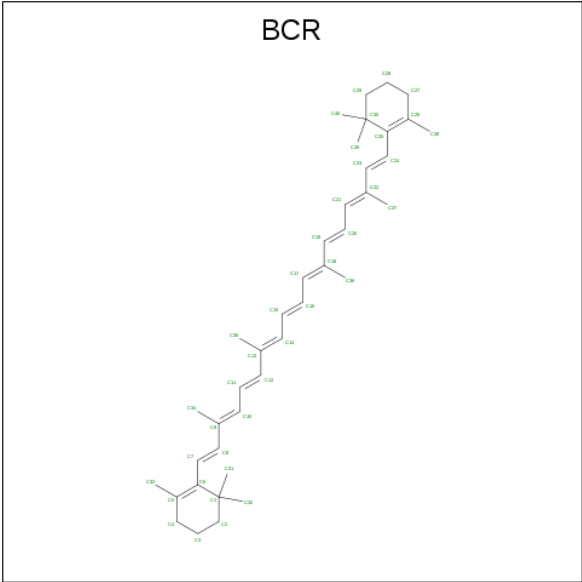
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | 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 (three-letter code: 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 | D | 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 | d | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



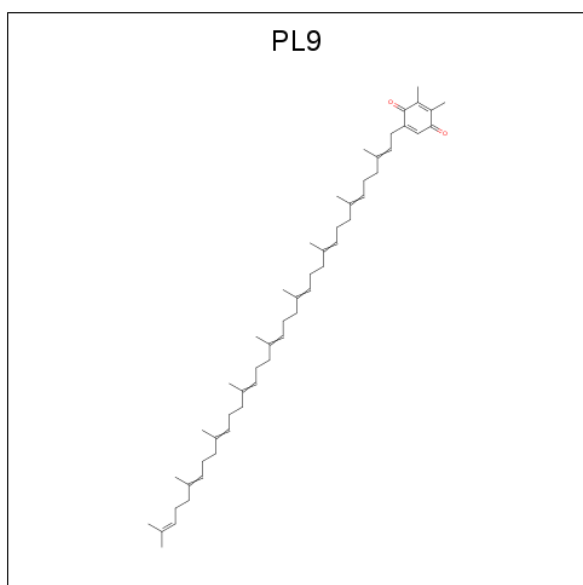
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26 | A | 1 | Total C 40 40 | 0 | 0 |
| 26 | B | 1 | Total C 40 40 | 0 | 0 |
| 26 | B | 1 | Total C 40 40 | 0 | 0 |
| 26 | B | 1 | Total C 40 40 | 0 | 0 |
| 26 | C | 1 | Total C 40 40 | 0 | 0 |
| 26 | F | 1 | Total C 40 40 | 0 | 0 |
| 26 | H | 1 | Total C 40 40 | 0 | 0 |
| 26 | I | 1 | Total C 40 40 | 0 | 0 |
| 26 | K | 1 | Total C 40 40 | 0 | 0 |
| 26 | K | 1 | Total C 40 40 | 0 | 0 |
| 26 | T | 1 | Total C 40 40 | 0 | 0 |
| 26 | a | 1 | Total C 40 40 | 0 | 0 |
| 26 | b | 1 | Total C 40 40 | 0 | 0 |
| 26 | b | 1 | Total C 40 40 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26 | b | 1 | Total C 40 40 | 0 | 0 |
| 26 | c | 1 | Total C 40 40 | 0 | 0 |
| 26 | c | 1 | Total C 40 40 | 0 | 0 |
| 26 | c | 1 | Total C 40 40 | 0 | 0 |
| 26 | f | 1 | Total C 40 40 | 0 | 0 |
| 26 | h | 1 | Total C 40 40 | 0 | 0 |
| 26 | k | 1 | Total C 40 40 | 0 | 0 |
| 26 | t | 1 | Total C 40 40 | 0 | 0 |

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



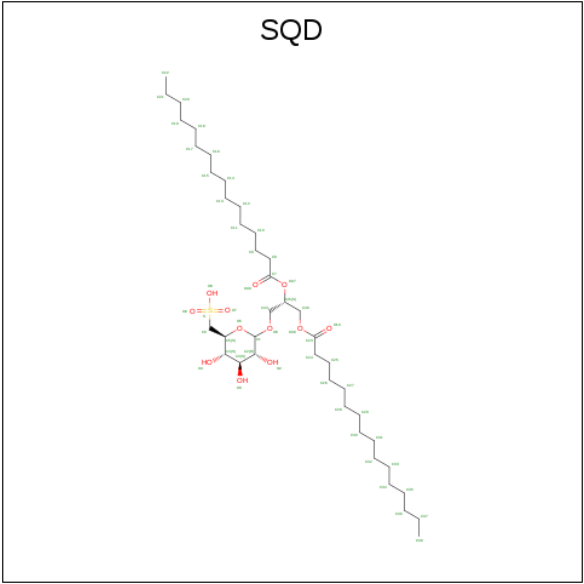
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 27 | A | 1 | Total C O 55 53 2 | 0 | 0 |
| 27 | D | 1 | Total C O 55 53 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 27 | a | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 27 | d | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |

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



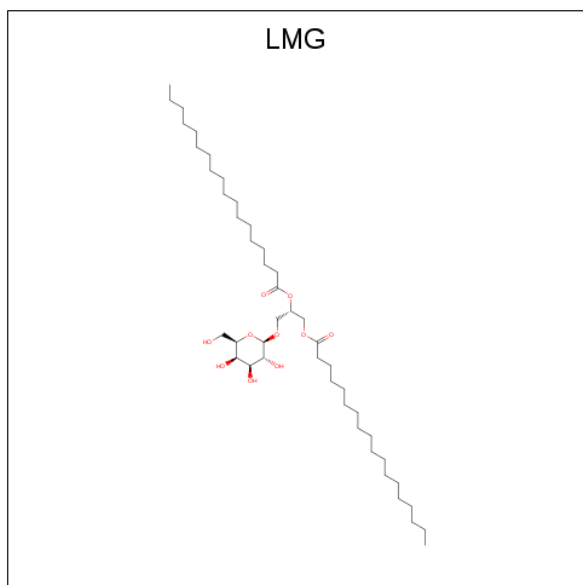
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 28 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 28 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 28 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 28 | L | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 28 | X | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 28 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 28 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 28 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 28 | l | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 28 | x | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



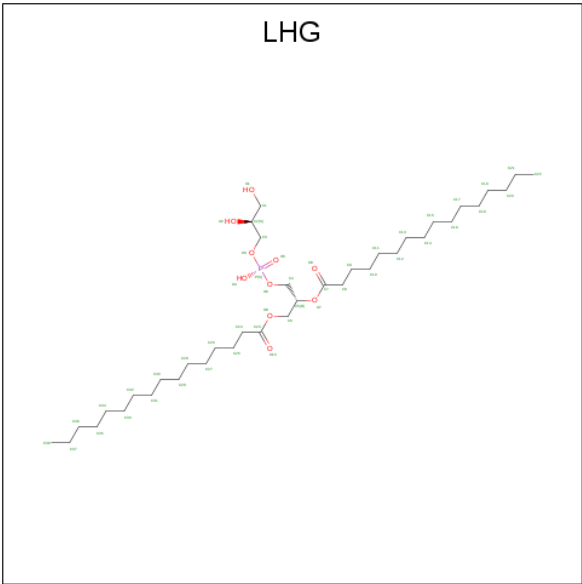
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|--|---------|---------|
| 29 | A | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | B | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | C | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | C | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | D | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | Z | 1 | Total | C | O | | 0 | 0 |
| | | | 37 | 27 | 10 | | | |
| 29 | a | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | b | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | c | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |
| 29 | c | 1 | Total | C | O | | 0 | 0 |
| | | | 51 | 41 | 10 | | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29 | j | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 29 | z | 1 | Total | C | O | 0 | 0 |
| | | | 37 | 27 | 10 | | |

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 30 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 30 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 30 | E | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |
| 30 | L | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 30 | a | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 30 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 30 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 30 | e | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |

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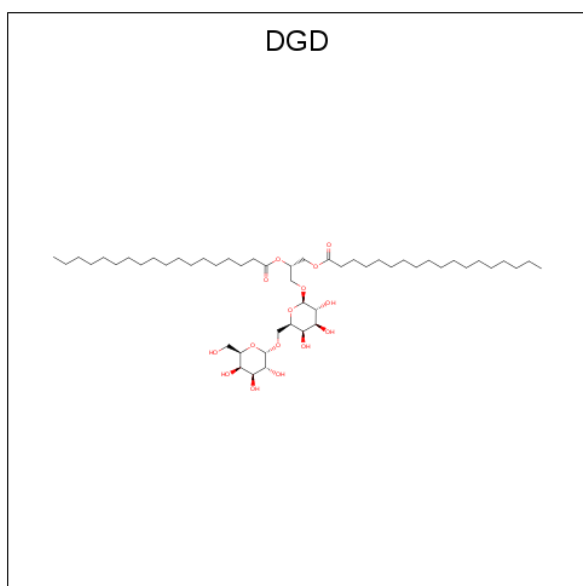
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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30 | l | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |

- Molecule 31 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 31 | B | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 31 | F | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 31 | o | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 31 | O | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 31 | b | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 31 | f | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



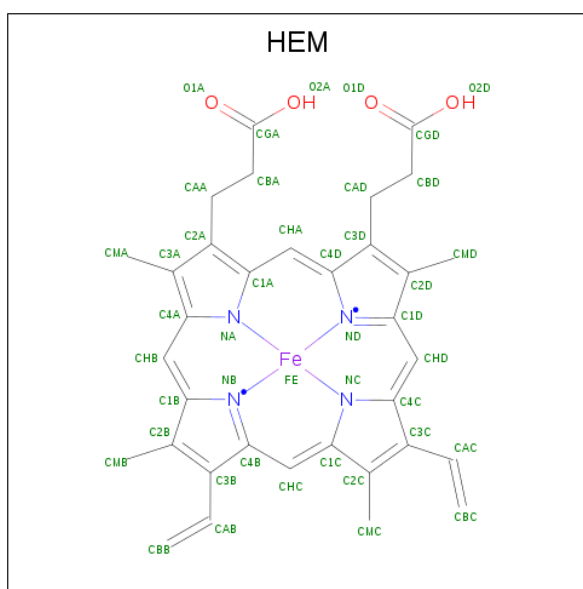
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 32 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 32 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 32 | C | 1 | Total C O 62 47 15 | 0 | 0 |
| 32 | E | 1 | Total C O 62 47 15 | 0 | 0 |
| 32 | H | 1 | Total C O 62 47 15 | 0 | 0 |
| 32 | c | 1 | Total C O 62 47 15 | 0 | 0 |
| 32 | c | 1 | Total C O 62 47 15 | 0 | 0 |
| 32 | c | 1 | Total C O 62 47 15 | 0 | 0 |
| 32 | d | 1 | Total C O 62 47 15 | 0 | 0 |
| 32 | h | 1 | Total C O 62 47 15 | 0 | 0 |

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 33 | E | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 33 | V | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 33 | e | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 33 | v | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 34 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 34 | j | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1 1

Chain A:  100%



- Molecule 1: Photosystem II protein D1 1

Chain a:  100%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



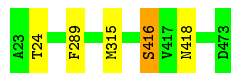
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  99%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  99%



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  99%



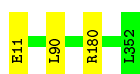
- Molecule 4: Photosystem II D2 protein

Chain D:  99%



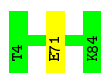
- Molecule 4: Photosystem II D2 protein

Chain d:  99%



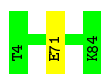
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  99%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  99%



- Molecule 6: Cytochrome b559 subunit beta

Chain F:  97%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  97%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  95%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 95% 5%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein I

Chain i: 100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J

Chain J: 100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J

Chain j: 100%

There are no outlier residues recorded for this chain.

- Molecule 10: Photosystem II reaction center protein K

Chain K: 95% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 92% 8%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 97% 3%



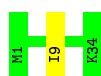
- Molecule 11: Photosystem II reaction center protein L

Chain l: 97%



- Molecule 12: Photosystem II reaction center protein M

Chain M: 97%



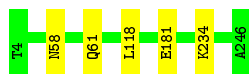
- Molecule 12: Photosystem II reaction center protein M

Chain m: 97%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 98%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 98%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 100%

There are no outlier residues recorded for this chain.

- Molecule 14: Photosystem II reaction center protein T

Chain t: 100%

There are no outlier residues recorded for this chain.

- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  99%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  99%



- Molecule 16: Cytochrome c-550

Chain V:  99%



- Molecule 16: Cytochrome c-550

Chain v:  99%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  97%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  97%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Photosystem II reaction center X protein

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  98% .



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  98% .



4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 250.80 Å 250.80 Å 250.80 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.98 – 3.50 250.80 – 3.28 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (29.98-3.50) 100.0 (250.80-3.28) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ | - | Xtrriage |
| Refinement program | PHENIX 1.9 _1692 | Depositor |
| R, R_{free} | 0.324 , 0.331 0.343 , 0.340 | Depositor DCC |
| R_{free} test set | 45921 reflections (4.90%) | wwPDB-VP |
| Wilson B-factor (Å ²) | (Not available) | Xtrriage |
| Anisotropy | (Not available) | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 27.3 | EDS |
| L-test for twinning ¹ | $\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available) | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.84 | EDS |
| Total number of atoms | 50074 | wwPDB-VP |
| Average B, all atoms (Å ²) | 83.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.56 | 0/2734 | 0.68 | 0/3727 |
| 1 | a | 0.49 | 0/2734 | 0.64 | 0/3727 |
| 2 | B | 0.51 | 0/4194 | 0.65 | 1/5713 (0.0%) |
| 2 | b | 0.48 | 0/4194 | 0.63 | 1/5713 (0.0%) |
| 3 | C | 0.51 | 0/3634 | 0.64 | 0/4947 |
| 3 | c | 0.47 | 0/3634 | 0.60 | 0/4947 |
| 4 | D | 0.53 | 0/2821 | 0.65 | 0/3844 |
| 4 | d | 0.48 | 0/2821 | 0.60 | 0/3844 |
| 5 | E | 0.46 | 0/693 | 0.63 | 0/944 |
| 5 | e | 0.43 | 0/693 | 0.58 | 0/944 |
| 6 | F | 0.51 | 0/284 | 0.61 | 0/387 |
| 6 | f | 0.41 | 0/284 | 0.56 | 0/387 |
| 7 | H | 0.47 | 0/544 | 0.64 | 0/739 |
| 7 | h | 0.46 | 0/544 | 0.66 | 0/739 |
| 8 | I | 0.52 | 0/327 | 0.68 | 0/439 |
| 8 | i | 0.46 | 0/327 | 0.60 | 0/439 |
| 9 | J | 0.46 | 0/278 | 0.59 | 0/376 |
| 9 | j | 0.43 | 0/278 | 0.53 | 0/376 |
| 10 | K | 0.48 | 0/303 | 0.70 | 0/416 |
| 10 | k | 0.55 | 0/303 | 0.79 | 0/416 |
| 11 | L | 0.55 | 0/319 | 0.70 | 0/433 |
| 11 | l | 0.48 | 0/319 | 0.62 | 0/433 |
| 12 | M | 0.52 | 0/278 | 0.74 | 0/378 |
| 12 | m | 0.49 | 0/278 | 0.69 | 0/378 |
| 13 | O | 0.46 | 0/1926 | 0.65 | 0/2611 |
| 13 | o | 0.41 | 0/1926 | 0.61 | 0/2611 |
| 14 | T | 0.60 | 0/282 | 0.68 | 0/382 |
| 14 | t | 0.49 | 0/282 | 0.60 | 0/382 |
| 15 | U | 0.48 | 0/785 | 0.64 | 0/1064 |
| 15 | u | 0.46 | 0/785 | 0.63 | 0/1064 |
| 16 | V | 0.52 | 1/1096 (0.1%) | 0.66 | 0/1487 |
| 16 | v | 0.42 | 0/1096 | 0.62 | 0/1487 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | Y | 0.44 | 0/216 | 0.61 | 0/289 |
| 17 | y | 0.44 | 0/216 | 0.59 | 0/289 |
| 18 | X | 0.43 | 0/298 | 0.53 | 0/403 |
| 18 | x | 0.44 | 0/298 | 0.54 | 0/403 |
| 19 | Z | 0.44 | 0/490 | 0.58 | 0/669 |
| 19 | z | 0.46 | 0/490 | 0.56 | 0/669 |
| All | All | 0.49 | 1/43004 (0.0%) | 0.63 | 2/58496 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 16 | V | 37 | CYS | CB-SG | -5.25 | 1.73 | 1.81 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | b | 127 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 2 | B | 39 | LEU | CA-CB-CG | -5.25 | 103.23 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|----------------|-----------|---------|----------|-------------|
| 1 | A | 336/334 (101%) | 332 (99%) | 3 (1%) | 1 (0%) | 41 75 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | a | 336/334 (101%) | 331 (98%) | 4 (1%) | 1 (0%) | 41 | 75 |
| 2 | B | 512/504 (102%) | 506 (99%) | 6 (1%) | 0 | 100 | 100 |
| 2 | b | 512/504 (102%) | 505 (99%) | 7 (1%) | 0 | 100 | 100 |
| 3 | C | 454/451 (101%) | 444 (98%) | 8 (2%) | 2 (0%) | 34 | 72 |
| 3 | c | 454/451 (101%) | 444 (98%) | 8 (2%) | 2 (0%) | 34 | 72 |
| 4 | D | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 4 | d | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 5 | E | 81/81 (100%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | e | 81/81 (100%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | F | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 65/65 (100%) | 60 (92%) | 5 (8%) | 0 | 100 | 100 |
| 7 | h | 65/65 (100%) | 60 (92%) | 5 (8%) | 0 | 100 | 100 |
| 8 | I | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | i | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 9 | J | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 9 | j | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 10 | k | 35/37 (95%) | 30 (86%) | 4 (11%) | 1 (3%) | 4 | 31 |
| 11 | L | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 33/34 (97%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 33/34 (97%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 13 | O | 245/243 (101%) | 237 (97%) | 7 (3%) | 1 (0%) | 34 | 72 |
| 13 | o | 245/243 (101%) | 237 (97%) | 7 (3%) | 1 (0%) | 34 | 72 |
| 14 | T | 29/30 (97%) | 28 (97%) | 1 (3%) | 0 | 100 | 100 |
| 14 | t | 29/30 (97%) | 28 (97%) | 1 (3%) | 0 | 100 | 100 |
| 15 | U | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | u | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | V | 136/137 (99%) | 132 (97%) | 4 (3%) | 0 | 100 | 100 |
| 16 | v | 136/137 (99%) | 132 (97%) | 4 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 17 | Y | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 17 | y | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 18 | X | 38/39 (97%) | 37 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | x | 38/39 (97%) | 37 (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 |
| All | All | 5252/5264 (100%) | 5139 (98%) | 104 (2%) | 9 (0%) | 51 | 81 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 13 | O | 58 | ASN |
| 13 | o | 58 | ASN |
| 3 | C | 416[A] | SER |
| 3 | C | 416[B] | SER |
| 3 | c | 416[A] | SER |
| 3 | c | 416[B] | SER |
| 10 | k | 11 | LEU |
| 1 | A | 259 | ILE |
| 1 | a | 259 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 273/269 (102%) | 273 (100%) | 0 | 100 | 100 |
| 1 | a | 273/269 (102%) | 273 (100%) | 0 | 100 | 100 |
| 2 | B | 412/402 (102%) | 408 (99%) | 4 (1%) | 76 | 88 |
| 2 | b | 412/402 (102%) | 410 (100%) | 2 (0%) | 88 | 94 |
| 3 | C | 357/352 (101%) | 351 (98%) | 6 (2%) | 60 | 82 |
| 3 | c | 357/352 (101%) | 353 (99%) | 4 (1%) | 73 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4 | D | 277/277 (100%) | 274 (99%) | 3 (1%) | 73 | 88 |
| 4 | d | 277/277 (100%) | 274 (99%) | 3 (1%) | 73 | 88 |
| 5 | E | 74/72 (103%) | 73 (99%) | 1 (1%) | 67 | 85 |
| 5 | e | 74/72 (103%) | 73 (99%) | 1 (1%) | 67 | 85 |
| 6 | F | 28/28 (100%) | 27 (96%) | 1 (4%) | 35 | 66 |
| 6 | f | 28/28 (100%) | 27 (96%) | 1 (4%) | 35 | 66 |
| 7 | H | 56/54 (104%) | 52 (93%) | 4 (7%) | 14 | 46 |
| 7 | h | 56/54 (104%) | 52 (93%) | 4 (7%) | 14 | 46 |
| 8 | I | 36/35 (103%) | 36 (100%) | 0 | 100 | 100 |
| 8 | i | 36/35 (103%) | 36 (100%) | 0 | 100 | 100 |
| 9 | J | 26/26 (100%) | 26 (100%) | 0 | 100 | 100 |
| 9 | j | 26/26 (100%) | 26 (100%) | 0 | 100 | 100 |
| 10 | K | 30/30 (100%) | 28 (93%) | 2 (7%) | 16 | 48 |
| 10 | k | 30/30 (100%) | 28 (93%) | 2 (7%) | 16 | 48 |
| 11 | L | 36/35 (103%) | 35 (97%) | 1 (3%) | 43 | 72 |
| 11 | l | 36/35 (103%) | 35 (97%) | 1 (3%) | 43 | 72 |
| 12 | M | 32/31 (103%) | 31 (97%) | 1 (3%) | 40 | 70 |
| 12 | m | 32/31 (103%) | 31 (97%) | 1 (3%) | 40 | 70 |
| 13 | O | 210/206 (102%) | 206 (98%) | 4 (2%) | 57 | 80 |
| 13 | o | 210/206 (102%) | 206 (98%) | 4 (2%) | 57 | 80 |
| 14 | T | 29/27 (107%) | 29 (100%) | 0 | 100 | 100 |
| 14 | t | 29/27 (107%) | 29 (100%) | 0 | 100 | 100 |
| 15 | U | 84/84 (100%) | 83 (99%) | 1 (1%) | 71 | 87 |
| 15 | u | 84/84 (100%) | 83 (99%) | 1 (1%) | 71 | 87 |
| 16 | V | 118/117 (101%) | 117 (99%) | 1 (1%) | 81 | 91 |
| 16 | v | 118/117 (101%) | 117 (99%) | 1 (1%) | 81 | 91 |
| 17 | Y | 22/22 (100%) | 21 (96%) | 1 (4%) | 27 | 61 |
| 17 | y | 22/22 (100%) | 21 (96%) | 1 (4%) | 27 | 61 |
| 18 | X | 33/32 (103%) | 33 (100%) | 0 | 100 | 100 |
| 18 | x | 33/32 (103%) | 33 (100%) | 0 | 100 | 100 |
| 19 | Z | 52/52 (100%) | 51 (98%) | 1 (2%) | 57 | 80 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 19 | z | 52/52 (100%) | 51 (98%) | 1 (2%) | 57 | 80 |
| All | All | 4370/4302 (102%) | 4312 (99%) | 58 (1%) | 69 | 86 |

All (58) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 2 | B | 76[A] | SER |
| 2 | B | 76[B] | SER |
| 2 | B | 246 | PHE |
| 2 | B | 472 | ARG |
| 3 | C | 24 | THR |
| 3 | C | 289 | PHE |
| 3 | C | 315 | MET |
| 3 | C | 416[A] | SER |
| 3 | C | 416[B] | SER |
| 3 | C | 418 | ASN |
| 4 | D | 11 | GLU |
| 4 | D | 90 | LEU |
| 4 | D | 180 | ARG |
| 5 | E | 71 | GLU |
| 6 | F | 44 | GLN |
| 7 | H | 12[A] | ARG |
| 7 | H | 12[B] | ARG |
| 7 | H | 49 | TYR |
| 7 | H | 65 | LEU |
| 10 | K | 13 | GLU |
| 10 | K | 17 | ILE |
| 11 | L | 1 | MET |
| 12 | M | 9 | ILE |
| 13 | O | 61 | GLN |
| 13 | O | 118 | LEU |
| 13 | O | 181 | GLU |
| 13 | O | 234 | LYS |
| 15 | U | 70 | ARG |
| 16 | V | 30 | LYS |
| 17 | Y | 27 | MET |
| 19 | Z | 31 | GLN |
| 2 | b | 246 | PHE |
| 2 | b | 472 | ARG |
| 3 | c | 24 | THR |
| 3 | c | 289 | PHE |
| 3 | c | 315 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 3 | c | 418 | ASN |
| 4 | d | 11 | GLU |
| 4 | d | 90 | LEU |
| 4 | d | 180 | ARG |
| 5 | e | 71 | GLU |
| 6 | f | 44 | GLN |
| 7 | h | 12[A] | ARG |
| 7 | h | 12[B] | ARG |
| 7 | h | 49 | TYR |
| 7 | h | 65 | LEU |
| 10 | k | 13 | GLU |
| 10 | k | 17 | ILE |
| 11 | l | 1 | MET |
| 12 | m | 9 | ILE |
| 13 | o | 61 | GLN |
| 13 | o | 118 | LEU |
| 13 | o | 181 | GLU |
| 13 | o | 234 | LYS |
| 15 | u | 70 | ARG |
| 16 | v | 30 | LYS |
| 17 | y | 27 | MET |
| 19 | z | 31 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 216 | HIS |
| 2 | B | 409 | GLN |
| 4 | d | 197 | HIS |
| 15 | u | 78 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 168 ligands modelled in this entry, 16 are monoatomic - leaving 152 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 |
| 30 | LHG | D | 407 | - | 48,48,48 | 1.11 | 3 (6%) | 51,54,54 | 0.89 | 3 (5%) |
| 28 | SQD | x | 101 | - | 42,43,54 | 1.20 | 4 (9%) | 51,54,65 | 1.46 | 7 (13%) |
| 26 | BCR | B | 620 | - | 41,41,41 | 9.12 | 29 (70%) | 56,56,56 | 5.77 | 33 (58%) |
| 24 | CLA | C | 508 | - | 59,73,73 | 3.46 | 25 (42%) | 67,113,113 | 2.07 | 15 (22%) |
| 24 | CLA | b | 607 | - | 59,73,73 | 3.40 | 24 (40%) | 67,113,113 | 1.96 | 13 (19%) |
| 26 | BCR | I | 101 | - | 41,41,41 | 9.05 | 31 (75%) | 56,56,56 | 5.91 | 30 (53%) |
| 26 | BCR | c | 515 | - | 41,41,41 | 9.15 | 31 (75%) | 56,56,56 | 5.57 | 27 (48%) |
| 32 | DGD | C | 516 | - | 63,63,67 | 1.67 | 15 (23%) | 77,77,81 | 1.21 | 10 (12%) |
| 26 | BCR | h | 101 | - | 41,41,41 | 9.16 | 30 (73%) | 56,56,56 | 5.68 | 33 (58%) |
| 24 | CLA | c | 511 | 3 | 59,73,73 | 3.42 | 23 (38%) | 67,113,113 | 1.96 | 16 (23%) |
| 24 | CLA | c | 504 | - | 59,73,73 | 3.46 | 25 (42%) | 67,113,113 | 2.09 | 19 (28%) |
| 24 | CLA | B | 617 | - | 59,73,73 | 3.42 | 23 (38%) | 67,113,113 | 2.08 | 17 (25%) |
| 32 | DGD | C | 515 | - | 63,63,67 | 1.70 | 15 (23%) | 77,77,81 | 1.03 | 5 (6%) |
| 28 | SQD | l | 101 | - | 53,54,54 | 1.04 | 4 (7%) | 62,65,65 | 1.36 | 8 (12%) |
| 24 | CLA | C | 504 | - | 59,73,73 | 3.40 | 25 (42%) | 67,113,113 | 2.12 | 17 (25%) |
| 29 | LMG | Z | 101 | - | 37,37,55 | 1.44 | 4 (10%) | 45,45,63 | 1.34 | 6 (13%) |
| 24 | CLA | a | 609 | - | 59,73,73 | 3.42 | 23 (38%) | 67,113,113 | 1.97 | 16 (23%) |
| 26 | BCR | B | 619 | - | 41,41,41 | 8.94 | 30 (73%) | 56,56,56 | 5.62 | 29 (51%) |
| 24 | CLA | d | 402 | - | 59,73,73 | 3.41 | 25 (42%) | 67,113,113 | 2.02 | 17 (25%) |
| 26 | BCR | H | 101 | - | 41,41,41 | 9.06 | 30 (73%) | 56,56,56 | 5.72 | 30 (53%) |
| 24 | CLA | a | 606 | - | 59,73,73 | 3.40 | 23 (38%) | 67,113,113 | 2.07 | 17 (25%) |
| 29 | LMG | C | 518 | - | 51,51,55 | 1.42 | 6 (11%) | 59,59,63 | 1.29 | 10 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | B | 607[A] | - | 59,73,73 | 3.41 | 23 (38%) | 67,113,113 | 2.07 | 18 (26%) |
| 24 | CLA | B | 607[B] | - | 59,73,73 | 3.40 | 24 (40%) | 67,113,113 | 2.03 | 17 (25%) |
| 26 | BCR | c | 514 | - | 41,41,41 | 8.98 | 30 (73%) | 56,56,56 | 5.91 | 34 (60%) |
| 24 | CLA | B | 605 | - | 59,73,73 | 3.40 | 22 (37%) | 67,113,113 | 2.19 | 17 (25%) |
| 30 | LHG | A | 615 | - | 48,48,48 | 1.11 | 3 (6%) | 51,54,54 | 1.30 | 5 (9%) |
| 24 | CLA | C | 512 | - | 59,73,73 | 3.37 | 25 (42%) | 67,113,113 | 2.08 | 20 (29%) |
| 20 | OEX | A | 601 | 1,3 | 0,15,15 | 0.00 | - | - | | |
| 24 | CLA | c | 513 | - | 59,73,73 | 3.35 | 25 (42%) | 67,113,113 | 2.01 | 16 (23%) |
| 24 | CLA | C | 501 | - | 59,73,73 | 3.35 | 24 (40%) | 67,113,113 | 2.16 | 20 (29%) |
| 23 | BCT | a | 605 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 26 | BCR | K | 101 | - | 41,41,41 | 9.12 | 31 (75%) | 56,56,56 | 5.42 | 29 (51%) |
| 26 | BCR | T | 101 | - | 41,41,41 | 9.04 | 30 (73%) | 56,56,56 | 6.12 | 32 (57%) |
| 24 | CLA | b | 605 | - | 59,73,73 | 3.50 | 24 (40%) | 67,113,113 | 2.11 | 19 (28%) |
| 33 | HEM | E | 103 | 5,6 | 27,50,50 | 2.24 | 7 (25%) | 17,82,82 | 1.92 | 3 (17%) |
| 26 | BCR | c | 521 | - | 41,41,41 | 9.34 | 29 (70%) | 56,56,56 | 5.62 | 26 (46%) |
| 26 | BCR | F | 101 | - | 41,41,41 | 9.04 | 26 (63%) | 56,56,56 | 6.08 | 27 (48%) |
| 27 | PL9 | A | 611 | - | 55,55,55 | 4.17 | 20 (36%) | 68,69,69 | 3.92 | 34 (50%) |
| 26 | BCR | k | 101 | - | 41,41,41 | 9.22 | 31 (75%) | 56,56,56 | 5.67 | 28 (50%) |
| 24 | CLA | B | 613 | - | 59,73,73 | 3.42 | 24 (40%) | 67,113,113 | 2.21 | 19 (28%) |
| 24 | CLA | c | 503 | - | 59,73,73 | 3.43 | 24 (40%) | 67,113,113 | 1.85 | 12 (17%) |
| 24 | CLA | b | 603 | - | 59,73,73 | 3.43 | 22 (37%) | 67,113,113 | 1.93 | 15 (22%) |
| 24 | CLA | c | 507 | - | 59,73,73 | 3.34 | 23 (38%) | 67,113,113 | 2.21 | 15 (22%) |
| 29 | LMG | c | 519 | - | 51,51,55 | 1.38 | 5 (9%) | 59,59,63 | 1.06 | 5 (8%) |
| 24 | CLA | C | 505 | - | 59,73,73 | 3.36 | 22 (37%) | 67,113,113 | 2.12 | 14 (20%) |
| 24 | CLA | b | 616 | - | 59,73,73 | 3.33 | 24 (40%) | 67,113,113 | 2.05 | 16 (23%) |
| 33 | HEM | e | 102 | 5,6 | 27,50,50 | 2.12 | 6 (22%) | 17,82,82 | 1.91 | 4 (23%) |
| 24 | CLA | b | 606 | - | 59,73,73 | 3.41 | 22 (37%) | 67,113,113 | 2.17 | 17 (25%) |
| 24 | CLA | A | 606 | - | 59,73,73 | 3.47 | 24 (40%) | 67,113,113 | 2.13 | 16 (23%) |
| 24 | CLA | C | 511 | 3 | 59,73,73 | 3.43 | 24 (40%) | 67,113,113 | 2.08 | 20 (29%) |
| 24 | CLA | c | 501 | - | 59,73,73 | 3.39 | 24 (40%) | 67,113,113 | 2.05 | 19 (28%) |
| 32 | DGD | c | 518 | - | 63,63,67 | 1.68 | 15 (23%) | 77,77,81 | 1.25 | 8 (10%) |
| 24 | CLA | C | 510 | - | 59,73,73 | 3.37 | 25 (42%) | 67,113,113 | 2.03 | 15 (22%) |
| 24 | CLA | D | 403 | - | 59,73,73 | 3.45 | 24 (40%) | 67,113,113 | 1.89 | 19 (28%) |
| 32 | DGD | c | 516 | - | 63,63,67 | 1.70 | 15 (23%) | 77,77,81 | 1.09 | 7 (9%) |
| 26 | BCR | A | 610 | - | 41,41,41 | 9.17 | 30 (73%) | 56,56,56 | 5.54 | 27 (48%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | BCR | K | 102 | - | 41,41,41 | 9.13 | 29 (70%) | 56,56,56 | 5.63 | 25 (44%) |
| 26 | BCR | B | 618 | - | 41,41,41 | 8.92 | 29 (70%) | 56,56,56 | 5.95 | 31 (55%) |
| 24 | CLA | B | 610 | - | 59,73,73 | 3.45 | 23 (38%) | 67,113,113 | 2.05 | 20 (29%) |
| 30 | LHG | D | 406 | - | 48,48,48 | 1.13 | 2 (4%) | 51,54,54 | 0.97 | 4 (7%) |
| 24 | CLA | c | 502 | - | 59,73,73 | 3.41 | 24 (40%) | 67,113,113 | 2.01 | 15 (22%) |
| 29 | LMG | A | 613 | - | 51,51,55 | 1.33 | 4 (7%) | 59,59,63 | 0.91 | 4 (6%) |
| 32 | DGD | d | 405 | - | 63,63,67 | 1.71 | 16 (25%) | 77,77,81 | 1.16 | 9 (11%) |
| 24 | CLA | b | 609 | - | 59,73,73 | 3.42 | 24 (40%) | 67,113,113 | 1.96 | 16 (23%) |
| 29 | LMG | b | 622 | - | 51,51,55 | 1.32 | 4 (7%) | 59,59,63 | 1.06 | 5 (8%) |
| 26 | BCR | b | 619 | - | 41,41,41 | 9.23 | 29 (70%) | 56,56,56 | 5.80 | 28 (50%) |
| 24 | CLA | c | 508 | - | 59,73,73 | 3.41 | 24 (40%) | 67,113,113 | 2.26 | 17 (25%) |
| 25 | PHO | a | 608 | - | 67,69,69 | 1.23 | 9 (13%) | 85,99,99 | 1.05 | 6 (7%) |
| 24 | CLA | C | 506 | - | 59,73,73 | 3.31 | 23 (38%) | 67,113,113 | 2.08 | 15 (22%) |
| 29 | LMG | j | 101 | 34 | 51,51,55 | 1.31 | 5 (9%) | 59,59,63 | 0.87 | 4 (6%) |
| 24 | CLA | C | 513 | - | 59,73,73 | 3.28 | 22 (37%) | 67,113,113 | 2.11 | 19 (28%) |
| 30 | LHG | a | 616 | - | 48,48,48 | 1.10 | 2 (4%) | 51,54,54 | 1.17 | 6 (11%) |
| 24 | CLA | C | 507 | - | 59,73,73 | 3.29 | 24 (40%) | 67,113,113 | 2.14 | 16 (23%) |
| 29 | LMG | D | 408 | - | 51,51,55 | 1.34 | 5 (9%) | 59,59,63 | 1.10 | 7 (11%) |
| 24 | CLA | B | 606 | - | 59,73,73 | 3.38 | 23 (38%) | 67,113,113 | 1.87 | 15 (22%) |
| 25 | PHO | A | 608 | - | 67,69,69 | 1.24 | 9 (13%) | 85,99,99 | 1.05 | 5 (5%) |
| 26 | BCR | t | 101 | - | 41,41,41 | 9.01 | 30 (73%) | 56,56,56 | 5.95 | 34 (60%) |
| 24 | CLA | B | 614 | - | 59,73,73 | 3.47 | 24 (40%) | 67,113,113 | 1.88 | 14 (20%) |
| 33 | HEM | v | 201 | 16 | 27,50,50 | 2.22 | 5 (18%) | 17,82,82 | 1.69 | 4 (23%) |
| 24 | CLA | a | 607 | - | 59,73,73 | 3.40 | 23 (38%) | 67,113,113 | 1.97 | 16 (23%) |
| 28 | SQD | a | 614 | - | 53,54,54 | 1.04 | 3 (5%) | 62,65,65 | 1.22 | 6 (9%) |
| 29 | LMG | z | 101 | - | 37,37,55 | 1.40 | 4 (10%) | 45,45,63 | 1.22 | 4 (8%) |
| 28 | SQD | X | 101 | - | 42,43,54 | 1.21 | 4 (9%) | 51,54,65 | 1.45 | 7 (13%) |
| 27 | PL9 | a | 611 | - | 55,55,55 | 4.18 | 21 (38%) | 68,69,69 | 3.89 | 34 (50%) |
| 26 | BCR | b | 620 | - | 41,41,41 | 8.87 | 29 (70%) | 56,56,56 | 5.73 | 31 (55%) |
| 24 | CLA | D | 404 | - | 59,73,73 | 3.40 | 25 (42%) | 67,113,113 | 2.19 | 17 (25%) |
| 25 | PHO | D | 401 | - | 67,69,69 | 1.29 | 11 (16%) | 85,99,99 | 1.11 | 5 (5%) |
| 24 | CLA | d | 403 | - | 59,73,73 | 3.40 | 25 (42%) | 67,113,113 | 2.05 | 17 (25%) |
| 30 | LHG | d | 406 | - | 48,48,48 | 1.11 | 2 (4%) | 51,54,54 | 1.02 | 3 (5%) |
| 20 | OEX | a | 601 | 1,3 | 0,15,15 | 0.00 | - | - | - | - |
| 24 | CLA | b | 615 | - | 59,73,73 | 3.47 | 23 (38%) | 67,113,113 | 1.94 | 15 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 28 | SQD | b | 601 | - | 53,54,54 | 1.08 | 4 (7%) | 62,65,65 | 1.44 | 9 (14%) |
| 28 | SQD | B | 622 | - | 53,54,54 | 1.07 | 4 (7%) | 62,65,65 | 1.44 | 9 (14%) |
| 32 | DGD | C | 517 | - | 63,63,67 | 1.66 | 15 (23%) | 77,77,81 | 1.14 | 6 (7%) |
| 24 | CLA | B | 609 | - | 59,73,73 | 3.34 | 23 (38%) | 67,113,113 | 2.22 | 23 (34%) |
| 26 | BCR | a | 610 | - | 41,41,41 | 8.98 | 30 (73%) | 56,56,56 | 5.53 | 24 (42%) |
| 30 | LHG | e | 101 | - | 41,41,48 | 1.23 | 3 (7%) | 44,47,54 | 1.05 | 2 (4%) |
| 30 | LHG | L | 101 | - | 48,48,48 | 1.10 | 2 (4%) | 51,54,54 | 0.90 | 3 (5%) |
| 32 | DGD | h | 102 | - | 63,63,67 | 1.68 | 15 (23%) | 77,77,81 | 1.21 | 8 (10%) |
| 24 | CLA | b | 612 | - | 59,73,73 | 3.40 | 23 (38%) | 67,113,113 | 2.10 | 18 (26%) |
| 30 | LHG | l | 102 | - | 48,48,48 | 1.18 | 2 (4%) | 51,54,54 | 0.92 | 2 (3%) |
| 27 | PL9 | D | 405 | - | 55,55,55 | 4.19 | 20 (36%) | 68,69,69 | 3.80 | 36 (52%) |
| 27 | PL9 | d | 404 | - | 55,55,55 | 4.15 | 20 (36%) | 68,69,69 | 3.85 | 34 (50%) |
| 24 | CLA | D | 402 | - | 59,73,73 | 3.48 | 27 (45%) | 67,113,113 | 2.02 | 18 (26%) |
| 24 | CLA | B | 603 | - | 59,73,73 | 3.42 | 25 (42%) | 67,113,113 | 2.07 | 19 (28%) |
| 32 | DGD | c | 517 | - | 63,63,67 | 1.62 | 16 (25%) | 77,77,81 | 1.11 | 9 (11%) |
| 24 | CLA | b | 608[A] | - | 59,73,73 | 3.39 | 24 (40%) | 67,113,113 | 2.03 | 17 (25%) |
| 28 | SQD | A | 614 | - | 53,54,54 | 1.04 | 3 (5%) | 62,65,65 | 1.22 | 6 (9%) |
| 26 | BCR | C | 514 | - | 41,41,41 | 8.98 | 30 (73%) | 56,56,56 | 5.93 | 33 (58%) |
| 33 | HEM | V | 201 | 16 | 27,50,50 | 2.21 | 6 (22%) | 17,82,82 | 1.88 | 3 (17%) |
| 29 | LMG | C | 519 | - | 51,51,55 | 1.33 | 5 (9%) | 59,59,63 | 1.02 | 4 (6%) |
| 24 | CLA | c | 505 | - | 59,73,73 | 3.40 | 23 (38%) | 67,113,113 | 2.05 | 15 (22%) |
| 24 | CLA | A | 607 | - | 59,73,73 | 3.37 | 24 (40%) | 67,113,113 | 2.04 | 17 (25%) |
| 24 | CLA | B | 604 | - | 59,73,73 | 3.34 | 25 (42%) | 67,113,113 | 2.03 | 18 (26%) |
| 24 | CLA | B | 616 | - | 59,73,73 | 3.39 | 24 (40%) | 67,113,113 | 1.88 | 17 (25%) |
| 24 | CLA | C | 509 | - | 59,73,73 | 3.37 | 24 (40%) | 67,113,113 | 2.06 | 15 (22%) |
| 29 | LMG | B | 621 | - | 51,51,55 | 1.29 | 4 (7%) | 59,59,63 | 1.01 | 3 (5%) |
| 24 | CLA | b | 608[B] | - | 59,73,73 | 3.39 | 24 (40%) | 67,113,113 | 1.99 | 18 (26%) |
| 28 | SQD | a | 612 | - | 53,54,54 | 0.99 | 3 (5%) | 62,65,65 | 1.53 | 11 (17%) |
| 32 | DGD | E | 101 | - | 63,63,67 | 1.73 | 15 (23%) | 77,77,81 | 1.23 | 10 (12%) |
| 24 | CLA | A | 609 | - | 59,73,73 | 3.42 | 25 (42%) | 67,113,113 | 2.00 | 18 (26%) |
| 26 | BCR | f | 101 | - | 41,41,41 | 8.99 | 29 (70%) | 56,56,56 | 5.59 | 26 (46%) |
| 24 | CLA | b | 604 | - | 59,73,73 | 3.41 | 23 (38%) | 67,113,113 | 2.15 | 16 (23%) |
| 24 | CLA | c | 510 | - | 59,73,73 | 3.44 | 24 (40%) | 67,113,113 | 1.92 | 16 (23%) |
| 24 | CLA | b | 613 | - | 59,73,73 | 3.48 | 24 (40%) | 67,113,113 | 2.11 | 18 (26%) |
| 24 | CLA | C | 503 | - | 59,73,73 | 3.42 | 24 (40%) | 67,113,113 | 1.78 | 12 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | BCR | b | 621 | - | 41,41,41 | 9.05 | 31 (75%) | 56,56,56 | 6.43 | 31 (55%) |
| 30 | LHG | E | 102 | - | 41,41,48 | 1.22 | 3 (7%) | 44,47,54 | 0.99 | 3 (6%) |
| 24 | CLA | B | 615 | - | 59,73,73 | 3.37 | 24 (40%) | 67,113,113 | 1.97 | 14 (20%) |
| 24 | CLA | b | 614 | - | 59,73,73 | 3.48 | 24 (40%) | 67,113,113 | 2.03 | 18 (26%) |
| 29 | LMG | a | 613 | - | 51,51,55 | 1.33 | 5 (9%) | 59,59,63 | 0.99 | 3 (5%) |
| 24 | CLA | c | 512 | - | 59,73,73 | 3.45 | 25 (42%) | 67,113,113 | 2.01 | 17 (25%) |
| 24 | CLA | B | 612 | - | 59,73,73 | 3.42 | 24 (40%) | 67,113,113 | 2.09 | 18 (26%) |
| 23 | BCT | A | 605 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 25 | PHO | d | 401 | - | 67,69,69 | 1.28 | 7 (10%) | 85,99,99 | 1.08 | 5 (5%) |
| 24 | CLA | b | 618 | - | 59,73,73 | 3.42 | 23 (38%) | 67,113,113 | 2.04 | 18 (26%) |
| 24 | CLA | a | 615 | - | 59,73,73 | 3.43 | 25 (42%) | 67,113,113 | 2.07 | 19 (28%) |
| 24 | CLA | b | 617 | - | 59,73,73 | 3.40 | 24 (40%) | 67,113,113 | 1.96 | 15 (22%) |
| 24 | CLA | c | 506 | - | 59,73,73 | 3.37 | 22 (37%) | 67,113,113 | 2.07 | 14 (20%) |
| 24 | CLA | B | 611 | - | 59,73,73 | 3.37 | 25 (42%) | 67,113,113 | 2.03 | 18 (26%) |
| 30 | LHG | d | 407 | - | 48,48,48 | 1.15 | 3 (6%) | 51,54,54 | 1.09 | 3 (5%) |
| 28 | SQD | L | 102 | - | 53,54,54 | 1.04 | 4 (7%) | 62,65,65 | 1.36 | 9 (14%) |
| 29 | LMG | c | 520 | - | 51,51,55 | 1.37 | 5 (9%) | 59,59,63 | 1.12 | 4 (6%) |
| 28 | SQD | A | 612 | - | 53,54,54 | 0.98 | 3 (5%) | 62,65,65 | 1.53 | 11 (17%) |
| 24 | CLA | c | 509 | - | 59,73,73 | 3.39 | 25 (42%) | 67,113,113 | 2.00 | 15 (22%) |
| 24 | CLA | B | 608 | - | 59,73,73 | 3.45 | 24 (40%) | 67,113,113 | 2.03 | 17 (25%) |
| 24 | CLA | B | 602 | - | 59,73,73 | 3.40 | 23 (38%) | 67,113,113 | 1.87 | 13 (19%) |
| 24 | CLA | b | 610 | - | 59,73,73 | 3.35 | 24 (40%) | 67,113,113 | 2.08 | 16 (23%) |
| 24 | CLA | b | 611 | - | 59,73,73 | 3.38 | 21 (35%) | 67,113,113 | 1.98 | 17 (25%) |
| 24 | CLA | C | 502 | - | 59,73,73 | 3.41 | 22 (37%) | 67,113,113 | 2.08 | 15 (22%) |
| 32 | DGD | H | 102 | - | 63,63,67 | 1.69 | 14 (22%) | 77,77,81 | 1.02 | 4 (5%) |

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 |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 30 | LHG | D | 407 | - | - | 19/53/53/53 | - |
| 28 | SQD | x | 101 | - | - | 16/38/58/69 | 0/1/1/1 |
| 26 | BCR | B | 620 | - | - | 19/29/63/63 | 0/2/2/2 |
| 24 | CLA | C | 508 | - | 3/3/20/25 | 6/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 24 | CLA | b | 607 | - | 3/3/20/25 | 6/37/135/135 | - |
| 26 | BCR | I | 101 | - | - | 21/29/63/63 | 0/2/2/2 |
| 26 | BCR | c | 515 | - | - | 20/29/63/63 | 0/2/2/2 |
| 32 | DGD | C | 516 | - | - | 31/51/91/95 | 0/2/2/2 |
| 26 | BCR | h | 101 | - | - | 25/29/63/63 | 0/2/2/2 |
| 24 | CLA | c | 511 | 3 | 3/3/20/25 | 4/37/135/135 | - |
| 24 | CLA | c | 504 | - | 3/3/20/25 | 11/37/135/135 | - |
| 24 | CLA | B | 617 | - | 2/2/20/25 | 14/37/135/135 | - |
| 32 | DGD | C | 515 | - | - | 23/51/91/95 | 0/2/2/2 |
| 28 | SQD | l | 101 | - | - | 28/49/69/69 | 0/1/1/1 |
| 24 | CLA | C | 504 | - | 3/3/20/25 | 12/37/135/135 | - |
| 29 | LMG | Z | 101 | - | - | 17/31/51/70 | 0/1/1/1 |
| 24 | CLA | a | 609 | - | 3/3/20/25 | 14/37/135/135 | - |
| 26 | BCR | B | 619 | - | - | 23/29/63/63 | 0/2/2/2 |
| 24 | CLA | d | 402 | - | 3/3/20/25 | 3/37/135/135 | - |
| 26 | BCR | H | 101 | - | - | 21/29/63/63 | 0/2/2/2 |
| 24 | CLA | a | 606 | - | 3/3/20/25 | 3/37/135/135 | - |
| 29 | LMG | C | 518 | - | - | 22/46/66/70 | 0/1/1/1 |
| 24 | CLA | B | 607[A] | - | 3/3/20/25 | 9/37/135/135 | - |
| 24 | CLA | B | 607[B] | - | 3/3/20/25 | 10/37/135/135 | - |
| 26 | BCR | c | 514 | - | - | 24/29/63/63 | 0/2/2/2 |
| 24 | CLA | B | 605 | - | 3/3/20/25 | 9/37/135/135 | - |
| 30 | LHG | A | 615 | - | - | 16/53/53/53 | - |
| 24 | CLA | C | 512 | - | 2/2/20/25 | 9/37/135/135 | - |
| 24 | CLA | c | 513 | - | 3/3/20/25 | 10/37/135/135 | - |
| 24 | CLA | C | 501 | - | 3/3/20/25 | 12/37/135/135 | - |
| 24 | CLA | c | 507 | - | 3/3/20/25 | 9/37/135/135 | - |
| 26 | BCR | K | 101 | - | - | 19/29/63/63 | 0/2/2/2 |
| 26 | BCR | T | 101 | - | - | 25/29/63/63 | 0/2/2/2 |
| 24 | CLA | b | 605 | - | 3/3/20/25 | 7/37/135/135 | - |
| 33 | HEM | E | 103 | 5,6 | - | 0/6/54/54 | - |
| 26 | BCR | c | 521 | - | - | 22/29/63/63 | 0/2/2/2 |
| 26 | BCR | F | 101 | - | - | 21/29/63/63 | 0/2/2/2 |
| 27 | PL9 | A | 611 | - | - | 25/53/73/73 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 26 | BCR | k | 101 | - | - | 20/29/63/63 | 0/2/2/2 |
| 24 | CLA | B | 613 | - | 2/2/20/25 | 7/37/135/135 | - |
| 24 | CLA | c | 503 | - | 3/3/20/25 | 3/37/135/135 | - |
| 24 | CLA | b | 603 | - | 3/3/20/25 | 19/37/135/135 | - |
| 26 | BCR | a | 610 | - | - | 22/29/63/63 | 0/2/2/2 |
| 29 | LMG | c | 519 | - | - | 21/46/66/70 | 0/1/1/1 |
| 24 | CLA | C | 505 | - | 3/3/20/25 | 7/37/135/135 | - |
| 24 | CLA | b | 616 | - | 3/3/20/25 | 13/37/135/135 | - |
| 33 | HEM | e | 102 | 5,6 | - | 0/6/54/54 | - |
| 24 | CLA | b | 606 | - | 3/3/20/25 | 10/37/135/135 | - |
| 24 | CLA | A | 606 | - | 3/3/20/25 | 1/37/135/135 | - |
| 24 | CLA | C | 511 | 3 | 2/2/20/25 | 6/37/135/135 | - |
| 28 | SQD | a | 612 | - | - | 16/49/69/69 | 0/1/1/1 |
| 24 | CLA | c | 501 | - | 2/2/20/25 | 11/37/135/135 | - |
| 32 | DGD | c | 518 | - | - | 21/51/91/95 | 0/2/2/2 |
| 24 | CLA | C | 510 | - | 2/2/20/25 | 12/37/135/135 | - |
| 24 | CLA | D | 403 | - | 3/3/20/25 | 6/37/135/135 | - |
| 32 | DGD | c | 516 | - | - | 22/51/91/95 | 0/2/2/2 |
| 26 | BCR | A | 610 | - | - | 23/29/63/63 | 0/2/2/2 |
| 26 | BCR | K | 102 | - | - | 20/29/63/63 | 0/2/2/2 |
| 26 | BCR | B | 618 | - | - | 23/29/63/63 | 0/2/2/2 |
| 24 | CLA | B | 610 | - | 3/3/20/25 | 6/37/135/135 | - |
| 30 | LHG | D | 406 | - | - | 19/53/53/53 | - |
| 24 | CLA | c | 502 | - | 3/3/20/25 | 10/37/135/135 | - |
| 29 | LMG | A | 613 | - | - | 32/46/66/70 | 0/1/1/1 |
| 32 | DGD | d | 405 | - | - | 34/51/91/95 | 0/2/2/2 |
| 24 | CLA | b | 609 | - | 3/3/20/25 | 4/37/135/135 | - |
| 29 | LMG | b | 622 | - | - | 19/46/66/70 | 0/1/1/1 |
| 26 | BCR | b | 619 | - | - | 21/29/63/63 | 0/2/2/2 |
| 24 | CLA | c | 508 | - | 3/3/20/25 | 4/37/135/135 | - |
| 25 | PHO | a | 608 | - | - | 3/53/103/103 | 0/5/6/6 |
| 24 | CLA | C | 506 | - | 3/3/20/25 | 17/37/135/135 | - |
| 29 | LMG | j | 101 | 34 | - | 17/46/66/70 | 0/1/1/1 |
| 24 | CLA | C | 513 | - | 2/2/20/25 | 12/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 30 | LHG | a | 616 | - | - | 17/53/53/53 | - |
| 24 | CLA | C | 507 | - | 3/3/20/25 | 9/37/135/135 | - |
| 29 | LMG | D | 408 | - | - | 20/46/66/70 | 0/1/1/1 |
| 24 | CLA | B | 606 | - | 3/3/20/25 | 7/37/135/135 | - |
| 25 | PHO | A | 608 | - | - | 6/53/103/103 | 0/5/6/6 |
| 26 | BCR | t | 101 | - | - | 26/29/63/63 | 0/2/2/2 |
| 24 | CLA | B | 614 | - | 3/3/20/25 | 3/37/135/135 | - |
| 33 | HEM | v | 201 | 16 | - | 2/6/54/54 | - |
| 24 | CLA | a | 607 | - | 3/3/20/25 | 11/37/135/135 | - |
| 28 | SQD | a | 614 | - | - | 23/49/69/69 | 0/1/1/1 |
| 29 | LMG | z | 101 | - | - | 18/31/51/70 | 0/1/1/1 |
| 28 | SQD | X | 101 | - | - | 16/38/58/69 | 0/1/1/1 |
| 27 | PL9 | a | 611 | - | - | 24/53/73/73 | 0/1/1/1 |
| 26 | BCR | b | 620 | - | - | 19/29/63/63 | 0/2/2/2 |
| 24 | CLA | D | 404 | - | 3/3/20/25 | 13/37/135/135 | - |
| 25 | PHO | D | 401 | - | - | 3/53/103/103 | 0/5/6/6 |
| 24 | CLA | d | 403 | - | 3/3/20/25 | 14/37/135/135 | - |
| 30 | LHG | d | 406 | - | - | 15/53/53/53 | - |
| 27 | PL9 | D | 405 | - | - | 26/53/73/73 | 0/1/1/1 |
| 24 | CLA | b | 615 | - | 3/3/20/25 | 5/37/135/135 | - |
| 28 | SQD | b | 601 | - | - | 29/49/69/69 | 0/1/1/1 |
| 28 | SQD | B | 622 | - | - | 29/49/69/69 | 0/1/1/1 |
| 32 | DGD | C | 517 | - | - | 17/51/91/95 | 0/2/2/2 |
| 24 | CLA | B | 609 | - | 3/3/20/25 | 4/37/135/135 | - |
| 30 | LHG | e | 101 | - | - | 24/46/46/53 | - |
| 30 | LHG | L | 101 | - | - | 19/53/53/53 | - |
| 32 | DGD | h | 102 | - | - | 17/51/91/95 | 0/2/2/2 |
| 24 | CLA | b | 612 | - | 3/3/20/25 | 10/37/135/135 | - |
| 30 | LHG | l | 102 | - | - | 23/53/53/53 | - |
| 27 | PL9 | d | 404 | - | - | 26/53/73/73 | 0/1/1/1 |
| 24 | CLA | D | 402 | - | 3/3/20/25 | 6/37/135/135 | - |
| 24 | CLA | B | 603 | - | 3/3/20/25 | 4/37/135/135 | - |
| 32 | DGD | c | 517 | - | - | 26/51/91/95 | 0/2/2/2 |
| 24 | CLA | b | 608[A] | - | 3/3/20/25 | 8/37/135/135 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 28 | SQD | A | 614 | - | - | 23/49/69/69 | 0/1/1/1 |
| 26 | BCR | C | 514 | - | - | 25/29/63/63 | 0/2/2/2 |
| 33 | HEM | V | 201 | 16 | - | 2/6/54/54 | - |
| 29 | LMG | C | 519 | - | - | 20/46/66/70 | 0/1/1/1 |
| 24 | CLA | c | 505 | - | 3/3/20/25 | 8/37/135/135 | - |
| 24 | CLA | A | 607 | - | 3/3/20/25 | 11/37/135/135 | - |
| 24 | CLA | B | 604 | - | 2/2/20/25 | 6/37/135/135 | - |
| 24 | CLA | B | 616 | - | 3/3/20/25 | 13/37/135/135 | - |
| 24 | CLA | C | 509 | - | 3/3/20/25 | 7/37/135/135 | - |
| 29 | LMG | B | 621 | - | - | 21/46/66/70 | 0/1/1/1 |
| 24 | CLA | b | 608[B] | - | 3/3/20/25 | 10/37/135/135 | - |
| 24 | CLA | B | 615 | - | 3/3/20/25 | 15/37/135/135 | - |
| 32 | DGD | E | 101 | - | - | 35/51/91/95 | 0/2/2/2 |
| 24 | CLA | A | 609 | - | 3/3/20/25 | 19/37/135/135 | - |
| 26 | BCR | f | 101 | - | - | 18/29/63/63 | 0/2/2/2 |
| 24 | CLA | b | 604 | - | 3/3/20/25 | 5/37/135/135 | - |
| 24 | CLA | c | 510 | - | 3/3/20/25 | 11/37/135/135 | - |
| 24 | CLA | b | 613 | - | 3/3/20/25 | 4/37/135/135 | - |
| 24 | CLA | C | 503 | - | 3/3/20/25 | 6/37/135/135 | - |
| 26 | BCR | b | 621 | - | - | 20/29/63/63 | 0/2/2/2 |
| 30 | LHG | E | 102 | - | - | 26/46/46/53 | - |
| 24 | CLA | b | 614 | - | 3/3/20/25 | 7/37/135/135 | - |
| 29 | LMG | a | 613 | - | - | 30/46/66/70 | 0/1/1/1 |
| 24 | CLA | c | 512 | - | 2/2/20/25 | 7/37/135/135 | - |
| 24 | CLA | B | 612 | - | 3/3/20/25 | 5/37/135/135 | - |
| 25 | PHO | d | 401 | - | - | 2/53/103/103 | 0/5/6/6 |
| 24 | CLA | b | 618 | - | 2/2/20/25 | 14/37/135/135 | - |
| 24 | CLA | a | 615 | - | 3/3/20/25 | 7/37/135/135 | - |
| 24 | CLA | b | 617 | - | 2/2/20/25 | 11/37/135/135 | - |
| 24 | CLA | c | 506 | - | 3/3/20/25 | 13/37/135/135 | - |
| 24 | CLA | B | 611 | - | 3/3/20/25 | 9/37/135/135 | - |
| 30 | LHG | d | 407 | - | - | 18/53/53/53 | - |
| 28 | SQD | L | 102 | - | - | 28/49/69/69 | 0/1/1/1 |
| 29 | LMG | c | 520 | - | - | 22/46/66/70 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 28 | SQD | A | 612 | - | - | 16/49/69/69 | 0/1/1/1 |
| 24 | CLA | c | 509 | - | 3/3/20/25 | 11/37/135/135 | - |
| 24 | CLA | B | 608 | - | 3/3/20/25 | 7/37/135/135 | - |
| 24 | CLA | B | 602 | - | 3/3/20/25 | 21/37/135/135 | - |
| 24 | CLA | b | 610 | - | 3/3/20/25 | 5/37/135/135 | - |
| 24 | CLA | b | 611 | - | 3/3/20/25 | 5/37/135/135 | - |
| 24 | CLA | C | 502 | - | 3/3/20/25 | 9/37/135/135 | - |
| 32 | DGD | H | 102 | - | - | 20/51/91/95 | 0/2/2/2 |

All (2776) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 26 | b | 619 | BCR | C14-C13 | 28.80 | 1.74 | 1.35 |
| 26 | F | 101 | BCR | C14-C13 | 27.15 | 1.71 | 1.35 |
| 26 | c | 515 | BCR | C14-C13 | 27.13 | 1.71 | 1.35 |
| 26 | K | 102 | BCR | C14-C13 | 26.70 | 1.71 | 1.35 |
| 26 | B | 620 | BCR | C14-C13 | 26.66 | 1.71 | 1.35 |
| 26 | A | 610 | BCR | C14-C13 | 26.48 | 1.70 | 1.35 |
| 26 | k | 101 | BCR | C14-C13 | 26.33 | 1.70 | 1.35 |
| 26 | I | 101 | BCR | C14-C13 | 26.33 | 1.70 | 1.35 |
| 26 | f | 101 | BCR | C14-C13 | 26.28 | 1.70 | 1.35 |
| 26 | B | 618 | BCR | C14-C13 | 26.13 | 1.70 | 1.35 |
| 26 | H | 101 | BCR | C14-C13 | 26.09 | 1.70 | 1.35 |
| 26 | K | 101 | BCR | C14-C13 | 26.04 | 1.70 | 1.35 |
| 26 | B | 619 | BCR | C14-C13 | 25.81 | 1.70 | 1.35 |
| 26 | h | 101 | BCR | C14-C13 | 25.67 | 1.69 | 1.35 |
| 26 | a | 610 | BCR | C14-C13 | 25.65 | 1.69 | 1.35 |
| 26 | b | 621 | BCR | C14-C13 | 25.45 | 1.69 | 1.35 |
| 26 | t | 101 | BCR | C14-C13 | 25.38 | 1.69 | 1.35 |
| 26 | c | 521 | BCR | C14-C13 | 25.31 | 1.69 | 1.35 |
| 26 | C | 514 | BCR | C14-C13 | 24.44 | 1.68 | 1.35 |
| 26 | c | 514 | BCR | C14-C13 | 24.44 | 1.68 | 1.35 |
| 26 | T | 101 | BCR | C14-C13 | 24.31 | 1.68 | 1.35 |
| 26 | b | 620 | BCR | C14-C13 | 24.21 | 1.67 | 1.35 |
| 26 | b | 620 | BCR | C21-C22 | -22.39 | 1.06 | 1.35 |
| 26 | T | 101 | BCR | C21-C22 | -22.21 | 1.06 | 1.35 |
| 26 | H | 101 | BCR | C21-C22 | -21.75 | 1.06 | 1.35 |
| 26 | h | 101 | BCR | C21-C22 | -21.74 | 1.07 | 1.35 |
| 26 | h | 101 | BCR | C10-C9 | 21.48 | 1.64 | 1.35 |
| 26 | b | 619 | BCR | C21-C22 | -21.35 | 1.07 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 26 | a | 610 | BCR | C10-C9 | 21.31 | 1.64 | 1.35 |
| 26 | c | 514 | BCR | C21-C22 | -21.25 | 1.07 | 1.35 |
| 26 | c | 515 | BCR | C10-C9 | 21.20 | 1.63 | 1.35 |
| 26 | k | 101 | BCR | C10-C9 | 21.19 | 1.63 | 1.35 |
| 26 | H | 101 | BCR | C10-C9 | 21.17 | 1.63 | 1.35 |
| 26 | A | 610 | BCR | C21-C22 | -21.11 | 1.07 | 1.35 |
| 26 | B | 620 | BCR | C21-C22 | -21.08 | 1.07 | 1.35 |
| 26 | k | 101 | BCR | C21-C22 | -21.05 | 1.07 | 1.35 |
| 26 | I | 101 | BCR | C10-C9 | 21.03 | 1.63 | 1.35 |
| 26 | b | 621 | BCR | C10-C9 | 21.02 | 1.63 | 1.35 |
| 26 | T | 101 | BCR | C10-C9 | 20.99 | 1.63 | 1.35 |
| 26 | K | 101 | BCR | C21-C22 | -20.99 | 1.08 | 1.35 |
| 26 | A | 610 | BCR | C10-C9 | 20.87 | 1.63 | 1.35 |
| 26 | t | 101 | BCR | C21-C22 | -20.84 | 1.08 | 1.35 |
| 26 | t | 101 | BCR | C10-C9 | 20.70 | 1.63 | 1.35 |
| 26 | F | 101 | BCR | C10-C9 | 20.69 | 1.63 | 1.35 |
| 26 | I | 101 | BCR | C21-C22 | -20.65 | 1.08 | 1.35 |
| 26 | K | 102 | BCR | C10-C9 | 20.65 | 1.63 | 1.35 |
| 26 | c | 521 | BCR | C10-C9 | 20.61 | 1.63 | 1.35 |
| 26 | f | 101 | BCR | C10-C9 | 20.55 | 1.63 | 1.35 |
| 26 | B | 618 | BCR | C10-C9 | 20.54 | 1.63 | 1.35 |
| 26 | K | 102 | BCR | C21-C22 | -20.44 | 1.08 | 1.35 |
| 26 | a | 610 | BCR | C21-C22 | -20.34 | 1.08 | 1.35 |
| 26 | C | 514 | BCR | C10-C9 | 20.33 | 1.62 | 1.35 |
| 26 | B | 620 | BCR | C10-C9 | 20.33 | 1.62 | 1.35 |
| 26 | c | 514 | BCR | C10-C9 | 20.28 | 1.62 | 1.35 |
| 26 | B | 619 | BCR | C10-C9 | 20.20 | 1.62 | 1.35 |
| 26 | K | 101 | BCR | C10-C9 | 20.10 | 1.62 | 1.35 |
| 26 | B | 618 | BCR | C21-C22 | -20.10 | 1.09 | 1.35 |
| 26 | c | 515 | BCR | C21-C22 | -20.08 | 1.09 | 1.35 |
| 26 | f | 101 | BCR | C21-C22 | -19.90 | 1.09 | 1.35 |
| 26 | c | 521 | BCR | C21-C22 | -19.84 | 1.09 | 1.35 |
| 26 | b | 619 | BCR | C10-C9 | 19.75 | 1.62 | 1.35 |
| 26 | b | 620 | BCR | C10-C9 | 19.53 | 1.61 | 1.35 |
| 26 | C | 514 | BCR | C21-C22 | -19.53 | 1.09 | 1.35 |
| 26 | B | 619 | BCR | C21-C22 | -19.49 | 1.09 | 1.35 |
| 26 | F | 101 | BCR | C21-C22 | -19.13 | 1.10 | 1.35 |
| 26 | b | 621 | BCR | C20-C19 | 18.76 | 1.82 | 1.34 |
| 24 | c | 510 | CLA | C4B-NB | 18.31 | 1.51 | 1.35 |
| 24 | C | 505 | CLA | C4B-NB | 18.27 | 1.51 | 1.35 |
| 24 | C | 502 | CLA | C4B-NB | 18.27 | 1.51 | 1.35 |
| 24 | B | 602 | CLA | C4B-NB | 18.22 | 1.51 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | a | 609 | CLA | C4B-NB | 18.20 | 1.51 | 1.35 |
| 24 | c | 512 | CLA | C4B-NB | 18.18 | 1.51 | 1.35 |
| 24 | b | 603 | CLA | C4B-NB | 18.17 | 1.51 | 1.35 |
| 24 | B | 616 | CLA | C4B-NB | 18.14 | 1.51 | 1.35 |
| 24 | b | 615 | CLA | C4B-NB | 18.14 | 1.51 | 1.35 |
| 24 | c | 503 | CLA | C4B-NB | 18.13 | 1.51 | 1.35 |
| 24 | c | 505 | CLA | C4B-NB | 18.06 | 1.51 | 1.35 |
| 24 | c | 508 | CLA | C4B-NB | 18.04 | 1.51 | 1.35 |
| 24 | B | 617 | CLA | C4B-NB | 18.01 | 1.51 | 1.35 |
| 24 | B | 609 | CLA | C4B-NB | 17.98 | 1.51 | 1.35 |
| 24 | B | 610 | CLA | C4B-NB | 17.96 | 1.51 | 1.35 |
| 24 | b | 612 | CLA | C4B-NB | 17.96 | 1.51 | 1.35 |
| 24 | b | 605 | CLA | C4B-NB | 17.92 | 1.51 | 1.35 |
| 24 | B | 606 | CLA | C4B-NB | 17.85 | 1.51 | 1.35 |
| 24 | c | 502 | CLA | C4B-NB | 17.82 | 1.51 | 1.35 |
| 24 | b | 611 | CLA | C4B-NB | 17.82 | 1.51 | 1.35 |
| 24 | B | 611 | CLA | C4B-NB | 17.81 | 1.51 | 1.35 |
| 24 | b | 617 | CLA | C4B-NB | 17.80 | 1.51 | 1.35 |
| 24 | b | 613 | CLA | C4B-NB | 17.80 | 1.51 | 1.35 |
| 24 | B | 603 | CLA | C4B-NB | 17.80 | 1.51 | 1.35 |
| 24 | c | 501 | CLA | C4B-NB | 17.79 | 1.51 | 1.35 |
| 24 | c | 511 | CLA | C4B-NB | 17.77 | 1.51 | 1.35 |
| 24 | C | 511 | CLA | C4B-NB | 17.76 | 1.51 | 1.35 |
| 24 | c | 513 | CLA | C4B-NB | 17.76 | 1.51 | 1.35 |
| 26 | c | 521 | BCR | C20-C19 | 17.73 | 1.80 | 1.34 |
| 24 | b | 608[A] | CLA | C4B-NB | 17.72 | 1.51 | 1.35 |
| 24 | B | 607[A] | CLA | C4B-NB | 17.68 | 1.51 | 1.35 |
| 24 | D | 402 | CLA | C4B-NB | 17.66 | 1.51 | 1.35 |
| 24 | c | 506 | CLA | C4B-NB | 17.61 | 1.50 | 1.35 |
| 24 | b | 608[B] | CLA | C4B-NB | 17.59 | 1.50 | 1.35 |
| 24 | a | 607 | CLA | C4B-NB | 17.57 | 1.50 | 1.35 |
| 24 | c | 507 | CLA | C4B-NB | 17.54 | 1.50 | 1.35 |
| 24 | b | 618 | CLA | C4B-NB | 17.54 | 1.50 | 1.35 |
| 24 | c | 504 | CLA | C4B-NB | 17.47 | 1.50 | 1.35 |
| 24 | B | 607[B] | CLA | C4B-NB | 17.46 | 1.50 | 1.35 |
| 24 | B | 608 | CLA | C4B-NB | 17.46 | 1.50 | 1.35 |
| 24 | B | 614 | CLA | C4B-NB | 17.40 | 1.50 | 1.35 |
| 24 | b | 610 | CLA | C4B-NB | 17.39 | 1.50 | 1.35 |
| 24 | b | 606 | CLA | C4B-NB | 17.33 | 1.50 | 1.35 |
| 24 | C | 503 | CLA | C4B-NB | 17.32 | 1.50 | 1.35 |
| 24 | b | 614 | CLA | C4B-NB | 17.31 | 1.50 | 1.35 |
| 24 | c | 509 | CLA | C4B-NB | 17.29 | 1.50 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 24 | C | 508 | CLA | C4B-NB | 17.29 | 1.50 | 1.35 |
| 24 | d | 403 | CLA | C4B-NB | 17.27 | 1.50 | 1.35 |
| 24 | C | 504 | CLA | C4B-NB | 17.22 | 1.50 | 1.35 |
| 24 | B | 612 | CLA | C4B-NB | 17.20 | 1.50 | 1.35 |
| 24 | C | 501 | CLA | C4B-NB | 17.18 | 1.50 | 1.35 |
| 24 | A | 606 | CLA | C4B-NB | 17.18 | 1.50 | 1.35 |
| 24 | B | 605 | CLA | C4B-NB | 17.14 | 1.50 | 1.35 |
| 24 | b | 607 | CLA | C4B-NB | 17.14 | 1.50 | 1.35 |
| 24 | C | 512 | CLA | C4B-NB | 17.10 | 1.50 | 1.35 |
| 24 | b | 609 | CLA | C4B-NB | 17.06 | 1.50 | 1.35 |
| 24 | D | 404 | CLA | C4B-NB | 17.05 | 1.50 | 1.35 |
| 24 | B | 615 | CLA | C4B-NB | 17.03 | 1.50 | 1.35 |
| 24 | b | 604 | CLA | C4B-NB | 17.01 | 1.50 | 1.35 |
| 24 | C | 506 | CLA | C4B-NB | 16.94 | 1.50 | 1.35 |
| 24 | C | 513 | CLA | C4B-NB | 16.72 | 1.50 | 1.35 |
| 24 | A | 609 | CLA | C4B-NB | 16.70 | 1.50 | 1.35 |
| 24 | C | 507 | CLA | C4B-NB | 16.70 | 1.50 | 1.35 |
| 24 | d | 402 | CLA | C4B-NB | 16.61 | 1.50 | 1.35 |
| 24 | a | 615 | CLA | C4B-NB | 16.58 | 1.50 | 1.35 |
| 24 | C | 509 | CLA | C4B-NB | 16.54 | 1.50 | 1.35 |
| 26 | b | 621 | BCR | C21-C22 | -16.52 | 1.13 | 1.35 |
| 24 | A | 607 | CLA | C4B-NB | 16.51 | 1.49 | 1.35 |
| 24 | B | 613 | CLA | C4B-NB | 16.48 | 1.49 | 1.35 |
| 24 | B | 604 | CLA | C4B-NB | 16.44 | 1.49 | 1.35 |
| 24 | a | 606 | CLA | C4B-NB | 16.39 | 1.49 | 1.35 |
| 24 | b | 616 | CLA | C4B-NB | 16.22 | 1.49 | 1.35 |
| 26 | t | 101 | BCR | C20-C19 | 16.18 | 1.76 | 1.34 |
| 24 | C | 510 | CLA | C4B-NB | 16.13 | 1.49 | 1.35 |
| 26 | B | 619 | BCR | C20-C19 | 16.10 | 1.76 | 1.34 |
| 26 | T | 101 | BCR | C20-C19 | 15.98 | 1.75 | 1.34 |
| 26 | b | 619 | BCR | C20-C19 | 15.92 | 1.75 | 1.34 |
| 26 | B | 618 | BCR | C20-C19 | 15.85 | 1.75 | 1.34 |
| 26 | h | 101 | BCR | C20-C19 | 15.82 | 1.75 | 1.34 |
| 24 | D | 403 | CLA | C4B-NB | 15.82 | 1.49 | 1.35 |
| 26 | F | 101 | BCR | C20-C19 | 15.66 | 1.74 | 1.34 |
| 26 | c | 515 | BCR | C20-C19 | 15.59 | 1.74 | 1.34 |
| 26 | c | 521 | BCR | C37-C22 | 15.56 | 1.83 | 1.50 |
| 26 | c | 514 | BCR | C20-C19 | 15.48 | 1.74 | 1.34 |
| 26 | A | 610 | BCR | C20-C19 | 15.42 | 1.74 | 1.34 |
| 26 | B | 620 | BCR | C20-C19 | 15.35 | 1.74 | 1.34 |
| 26 | K | 102 | BCR | C20-C19 | 15.34 | 1.74 | 1.34 |
| 26 | b | 620 | BCR | C20-C19 | 15.28 | 1.74 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | c | 521 | BCR | C36-C18 | 15.27 | 1.82 | 1.50 |
| 26 | k | 101 | BCR | C20-C19 | 15.16 | 1.73 | 1.34 |
| 26 | a | 610 | BCR | C20-C19 | 15.12 | 1.73 | 1.34 |
| 26 | b | 621 | BCR | C20-C21 | 15.11 | 1.90 | 1.43 |
| 26 | f | 101 | BCR | C20-C19 | 15.05 | 1.73 | 1.34 |
| 26 | C | 514 | BCR | C20-C19 | 14.97 | 1.73 | 1.34 |
| 26 | K | 101 | BCR | C20-C19 | 14.93 | 1.73 | 1.34 |
| 26 | I | 101 | BCR | C20-C19 | 14.87 | 1.72 | 1.34 |
| 26 | c | 514 | BCR | C5-C6 | 14.78 | 1.60 | 1.34 |
| 26 | h | 101 | BCR | C36-C18 | 14.59 | 1.81 | 1.50 |
| 26 | T | 101 | BCR | C5-C6 | 14.51 | 1.59 | 1.34 |
| 26 | c | 514 | BCR | C36-C18 | 14.45 | 1.80 | 1.50 |
| 26 | c | 515 | BCR | C5-C6 | 14.45 | 1.59 | 1.34 |
| 26 | C | 514 | BCR | C5-C6 | 14.45 | 1.59 | 1.34 |
| 26 | b | 621 | BCR | C5-C6 | 14.40 | 1.59 | 1.34 |
| 26 | B | 620 | BCR | C36-C18 | 14.32 | 1.80 | 1.50 |
| 26 | c | 521 | BCR | C5-C6 | 14.31 | 1.59 | 1.34 |
| 26 | K | 102 | BCR | C36-C18 | 14.28 | 1.80 | 1.50 |
| 26 | H | 101 | BCR | C20-C19 | 14.28 | 1.71 | 1.34 |
| 26 | c | 515 | BCR | C36-C18 | 14.28 | 1.80 | 1.50 |
| 26 | k | 101 | BCR | C5-C6 | 14.25 | 1.59 | 1.34 |
| 26 | C | 514 | BCR | C36-C18 | 14.21 | 1.80 | 1.50 |
| 26 | T | 101 | BCR | C16-C15 | 14.14 | 1.72 | 1.36 |
| 26 | K | 101 | BCR | C16-C15 | 14.11 | 1.72 | 1.36 |
| 26 | t | 101 | BCR | C16-C15 | 14.08 | 1.72 | 1.36 |
| 26 | k | 101 | BCR | C36-C18 | 14.07 | 1.80 | 1.50 |
| 26 | H | 101 | BCR | C36-C18 | 14.05 | 1.79 | 1.50 |
| 26 | K | 101 | BCR | C5-C6 | 14.05 | 1.58 | 1.34 |
| 26 | B | 620 | BCR | C16-C15 | 14.00 | 1.72 | 1.36 |
| 26 | k | 101 | BCR | C16-C15 | 13.98 | 1.72 | 1.36 |
| 26 | I | 101 | BCR | C36-C18 | 13.97 | 1.79 | 1.50 |
| 26 | K | 102 | BCR | C5-C6 | 13.95 | 1.58 | 1.34 |
| 26 | B | 620 | BCR | C5-C6 | 13.90 | 1.58 | 1.34 |
| 26 | C | 514 | BCR | C16-C15 | 13.89 | 1.72 | 1.36 |
| 26 | t | 101 | BCR | C5-C6 | 13.83 | 1.58 | 1.34 |
| 26 | F | 101 | BCR | C16-C15 | 13.79 | 1.71 | 1.36 |
| 26 | b | 620 | BCR | C36-C18 | 13.77 | 1.79 | 1.50 |
| 26 | a | 610 | BCR | C16-C15 | 13.74 | 1.71 | 1.36 |
| 26 | I | 101 | BCR | C5-C6 | 13.74 | 1.58 | 1.34 |
| 26 | A | 610 | BCR | C36-C18 | 13.71 | 1.79 | 1.50 |
| 26 | b | 619 | BCR | C36-C18 | 13.70 | 1.79 | 1.50 |
| 26 | b | 619 | BCR | C16-C15 | 13.70 | 1.71 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 26 | T | 101 | BCR | C36-C18 | 13.70 | 1.79 | 1.50 |
| 26 | A | 610 | BCR | C16-C15 | 13.68 | 1.71 | 1.36 |
| 26 | K | 102 | BCR | C16-C15 | 13.66 | 1.71 | 1.36 |
| 26 | A | 610 | BCR | C5-C6 | 13.60 | 1.58 | 1.34 |
| 26 | H | 101 | BCR | C16-C15 | 13.58 | 1.71 | 1.36 |
| 26 | c | 514 | BCR | C16-C15 | 13.54 | 1.71 | 1.36 |
| 26 | h | 101 | BCR | C16-C15 | 13.48 | 1.71 | 1.36 |
| 26 | a | 610 | BCR | C36-C18 | 13.48 | 1.78 | 1.50 |
| 26 | b | 620 | BCR | C16-C15 | 13.47 | 1.71 | 1.36 |
| 26 | F | 101 | BCR | C5-C6 | 13.47 | 1.57 | 1.34 |
| 26 | K | 101 | BCR | C36-C18 | 13.45 | 1.78 | 1.50 |
| 26 | a | 610 | BCR | C5-C6 | 13.43 | 1.57 | 1.34 |
| 26 | f | 101 | BCR | C5-C6 | 13.42 | 1.57 | 1.34 |
| 26 | t | 101 | BCR | C36-C18 | 13.30 | 1.78 | 1.50 |
| 26 | f | 101 | BCR | C36-C18 | 13.24 | 1.78 | 1.50 |
| 26 | b | 621 | BCR | C36-C18 | 13.20 | 1.78 | 1.50 |
| 26 | h | 101 | BCR | C5-C6 | 13.18 | 1.57 | 1.34 |
| 26 | K | 101 | BCR | C19-C18 | -13.18 | 1.17 | 1.45 |
| 26 | b | 621 | BCR | C16-C15 | 13.13 | 1.70 | 1.36 |
| 26 | I | 101 | BCR | C16-C15 | 13.12 | 1.70 | 1.36 |
| 26 | c | 515 | BCR | C16-C15 | 13.07 | 1.70 | 1.36 |
| 26 | c | 521 | BCR | C20-C21 | 13.06 | 1.83 | 1.43 |
| 26 | f | 101 | BCR | C16-C15 | 13.06 | 1.70 | 1.36 |
| 26 | b | 621 | BCR | C37-C22 | 13.03 | 1.77 | 1.50 |
| 26 | B | 618 | BCR | C36-C18 | 13.00 | 1.77 | 1.50 |
| 26 | B | 619 | BCR | C16-C15 | 13.00 | 1.69 | 1.36 |
| 26 | B | 618 | BCR | C19-C18 | -12.93 | 1.18 | 1.45 |
| 26 | B | 619 | BCR | C5-C6 | 12.86 | 1.56 | 1.34 |
| 26 | b | 619 | BCR | C5-C6 | 12.82 | 1.56 | 1.34 |
| 26 | F | 101 | BCR | C36-C18 | 12.78 | 1.77 | 1.50 |
| 26 | B | 618 | BCR | C5-C6 | 12.78 | 1.56 | 1.34 |
| 26 | H | 101 | BCR | C5-C6 | 12.52 | 1.56 | 1.34 |
| 26 | k | 101 | BCR | C19-C18 | -12.46 | 1.19 | 1.45 |
| 26 | a | 610 | BCR | C19-C18 | -12.44 | 1.19 | 1.45 |
| 26 | B | 620 | BCR | C37-C22 | 12.43 | 1.76 | 1.50 |
| 26 | B | 618 | BCR | C16-C15 | 12.36 | 1.68 | 1.36 |
| 26 | C | 514 | BCR | C37-C22 | 12.36 | 1.76 | 1.50 |
| 26 | b | 620 | BCR | C5-C6 | 12.34 | 1.55 | 1.34 |
| 26 | B | 619 | BCR | C36-C18 | 12.34 | 1.76 | 1.50 |
| 26 | H | 101 | BCR | C19-C18 | -12.27 | 1.19 | 1.45 |
| 26 | c | 515 | BCR | C19-C18 | -12.22 | 1.19 | 1.45 |
| 26 | K | 102 | BCR | C37-C22 | 12.22 | 1.76 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 26 | c | 521 | BCR | C16-C15 | 12.12 | 1.67 | 1.36 |
| 26 | K | 102 | BCR | C19-C18 | -12.10 | 1.19 | 1.45 |
| 26 | A | 610 | BCR | C37-C22 | 12.09 | 1.75 | 1.50 |
| 26 | a | 610 | BCR | C37-C22 | 12.06 | 1.75 | 1.50 |
| 26 | B | 619 | BCR | C20-C21 | 12.01 | 1.80 | 1.43 |
| 26 | C | 514 | BCR | C19-C18 | -11.98 | 1.20 | 1.45 |
| 26 | F | 101 | BCR | C20-C21 | 11.96 | 1.80 | 1.43 |
| 26 | A | 610 | BCR | C19-C18 | -11.90 | 1.20 | 1.45 |
| 26 | t | 101 | BCR | C37-C22 | 11.87 | 1.75 | 1.50 |
| 26 | b | 619 | BCR | C19-C18 | -11.87 | 1.20 | 1.45 |
| 26 | K | 101 | BCR | C37-C22 | 11.85 | 1.75 | 1.50 |
| 26 | B | 618 | BCR | C20-C21 | 11.84 | 1.80 | 1.43 |
| 26 | f | 101 | BCR | C19-C18 | -11.79 | 1.20 | 1.45 |
| 26 | f | 101 | BCR | C37-C22 | 11.79 | 1.75 | 1.50 |
| 26 | K | 102 | BCR | C20-C21 | 11.77 | 1.79 | 1.43 |
| 26 | I | 101 | BCR | C19-C18 | -11.76 | 1.20 | 1.45 |
| 26 | b | 619 | BCR | C20-C21 | 11.74 | 1.79 | 1.43 |
| 26 | c | 514 | BCR | C19-C18 | -11.74 | 1.20 | 1.45 |
| 26 | B | 618 | BCR | C37-C22 | 11.74 | 1.75 | 1.50 |
| 26 | k | 101 | BCR | C37-C22 | 11.70 | 1.75 | 1.50 |
| 26 | B | 620 | BCR | C19-C18 | -11.68 | 1.20 | 1.45 |
| 26 | b | 619 | BCR | C37-C22 | 11.65 | 1.75 | 1.50 |
| 26 | b | 620 | BCR | C19-C18 | -11.65 | 1.20 | 1.45 |
| 26 | B | 619 | BCR | C19-C18 | -11.54 | 1.21 | 1.45 |
| 26 | h | 101 | BCR | C19-C18 | -11.53 | 1.21 | 1.45 |
| 26 | k | 101 | BCR | C8-C7 | 11.53 | 1.67 | 1.33 |
| 26 | t | 101 | BCR | C20-C21 | 11.49 | 1.79 | 1.43 |
| 26 | t | 101 | BCR | C19-C18 | -11.47 | 1.21 | 1.45 |
| 26 | T | 101 | BCR | C37-C22 | 11.44 | 1.74 | 1.50 |
| 26 | c | 515 | BCR | C20-C21 | 11.44 | 1.78 | 1.43 |
| 26 | K | 101 | BCR | C20-C21 | 11.43 | 1.78 | 1.43 |
| 26 | K | 101 | BCR | C8-C7 | 11.42 | 1.67 | 1.33 |
| 26 | k | 101 | BCR | C20-C21 | 11.41 | 1.78 | 1.43 |
| 26 | B | 620 | BCR | C20-C21 | 11.40 | 1.78 | 1.43 |
| 26 | f | 101 | BCR | C20-C21 | 11.40 | 1.78 | 1.43 |
| 26 | B | 619 | BCR | C37-C22 | 11.37 | 1.74 | 1.50 |
| 26 | h | 101 | BCR | C20-C21 | 11.37 | 1.78 | 1.43 |
| 26 | c | 514 | BCR | C37-C22 | 11.35 | 1.74 | 1.50 |
| 26 | c | 521 | BCR | C19-C18 | -11.34 | 1.21 | 1.45 |
| 26 | c | 515 | BCR | C37-C22 | 11.34 | 1.74 | 1.50 |
| 26 | c | 521 | BCR | C8-C7 | 11.33 | 1.67 | 1.33 |
| 26 | F | 101 | BCR | C19-C18 | -11.30 | 1.21 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 26 | T | 101 | BCR | C20-C21 | 11.29 | 1.78 | 1.43 |
| 26 | C | 514 | BCR | C20-C21 | 11.29 | 1.78 | 1.43 |
| 26 | T | 101 | BCR | C19-C18 | -11.29 | 1.21 | 1.45 |
| 26 | c | 514 | BCR | C8-C7 | 11.22 | 1.67 | 1.33 |
| 26 | F | 101 | BCR | C37-C22 | 11.20 | 1.74 | 1.50 |
| 26 | I | 101 | BCR | C20-C21 | 11.17 | 1.78 | 1.43 |
| 26 | b | 620 | BCR | C37-C22 | 11.12 | 1.73 | 1.50 |
| 26 | I | 101 | BCR | C37-C22 | 11.11 | 1.73 | 1.50 |
| 26 | A | 610 | BCR | C20-C21 | 11.09 | 1.77 | 1.43 |
| 26 | C | 514 | BCR | C8-C7 | 11.06 | 1.66 | 1.33 |
| 26 | h | 101 | BCR | C37-C22 | 11.05 | 1.73 | 1.50 |
| 26 | b | 621 | BCR | C8-C7 | 11.03 | 1.66 | 1.33 |
| 26 | A | 610 | BCR | C8-C7 | 11.03 | 1.66 | 1.33 |
| 26 | H | 101 | BCR | C8-C7 | 11.00 | 1.66 | 1.33 |
| 26 | b | 620 | BCR | C20-C21 | 10.95 | 1.77 | 1.43 |
| 26 | a | 610 | BCR | C8-C7 | 10.92 | 1.66 | 1.33 |
| 26 | f | 101 | BCR | C8-C7 | 10.89 | 1.66 | 1.33 |
| 26 | T | 101 | BCR | C8-C7 | 10.88 | 1.66 | 1.33 |
| 26 | c | 515 | BCR | C8-C7 | 10.87 | 1.66 | 1.33 |
| 26 | I | 101 | BCR | C8-C7 | 10.86 | 1.65 | 1.33 |
| 26 | K | 102 | BCR | C8-C7 | 10.86 | 1.65 | 1.33 |
| 26 | b | 619 | BCR | C8-C7 | 10.86 | 1.65 | 1.33 |
| 26 | t | 101 | BCR | C8-C7 | 10.84 | 1.65 | 1.33 |
| 26 | F | 101 | BCR | C8-C7 | 10.83 | 1.65 | 1.33 |
| 26 | a | 610 | BCR | C20-C21 | 10.82 | 1.77 | 1.43 |
| 26 | h | 101 | BCR | C8-C7 | 10.79 | 1.65 | 1.33 |
| 26 | B | 618 | BCR | C8-C7 | 10.76 | 1.65 | 1.33 |
| 26 | B | 619 | BCR | C8-C7 | 10.72 | 1.65 | 1.33 |
| 26 | c | 514 | BCR | C20-C21 | 10.71 | 1.76 | 1.43 |
| 26 | b | 620 | BCR | C8-C7 | 10.68 | 1.65 | 1.33 |
| 26 | H | 101 | BCR | C20-C21 | 10.59 | 1.76 | 1.43 |
| 27 | a | 611 | PL9 | C18-C19 | 10.55 | 1.58 | 1.33 |
| 27 | A | 611 | PL9 | C18-C19 | 10.54 | 1.58 | 1.33 |
| 27 | D | 405 | PL9 | C18-C19 | 10.50 | 1.58 | 1.33 |
| 26 | B | 620 | BCR | C8-C7 | 10.39 | 1.64 | 1.33 |
| 27 | d | 404 | PL9 | C18-C19 | 10.38 | 1.57 | 1.33 |
| 27 | D | 405 | PL9 | C38-C39 | 9.94 | 1.56 | 1.33 |
| 26 | C | 514 | BCR | C16-C17 | 9.90 | 1.74 | 1.43 |
| 27 | d | 404 | PL9 | C38-C39 | 9.83 | 1.56 | 1.33 |
| 27 | a | 611 | PL9 | C38-C39 | 9.82 | 1.56 | 1.33 |
| 27 | D | 405 | PL9 | C23-C24 | 9.78 | 1.56 | 1.33 |
| 26 | T | 101 | BCR | C16-C17 | 9.70 | 1.73 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | B | 619 | BCR | C26-C25 | 9.69 | 1.51 | 1.34 |
| 26 | H | 101 | BCR | C16-C17 | 9.68 | 1.73 | 1.43 |
| 26 | K | 101 | BCR | C16-C17 | 9.68 | 1.73 | 1.43 |
| 27 | A | 611 | PL9 | C23-C24 | 9.68 | 1.56 | 1.33 |
| 26 | t | 101 | BCR | C16-C17 | 9.63 | 1.73 | 1.43 |
| 26 | f | 101 | BCR | C26-C25 | 9.58 | 1.51 | 1.34 |
| 26 | h | 101 | BCR | C16-C17 | 9.53 | 1.73 | 1.43 |
| 27 | a | 611 | PL9 | C23-C24 | 9.53 | 1.55 | 1.33 |
| 26 | k | 101 | BCR | C16-C17 | 9.51 | 1.72 | 1.43 |
| 26 | b | 621 | BCR | C19-C18 | -9.51 | 1.25 | 1.45 |
| 26 | b | 620 | BCR | C26-C25 | 9.50 | 1.50 | 1.34 |
| 26 | F | 101 | BCR | C26-C25 | 9.49 | 1.50 | 1.34 |
| 27 | A | 611 | PL9 | C38-C39 | 9.48 | 1.55 | 1.33 |
| 26 | K | 102 | BCR | C16-C17 | 9.46 | 1.72 | 1.43 |
| 26 | c | 514 | BCR | C16-C17 | 9.46 | 1.72 | 1.43 |
| 26 | B | 620 | BCR | C16-C17 | 9.45 | 1.72 | 1.43 |
| 27 | d | 404 | PL9 | C23-C24 | 9.45 | 1.55 | 1.33 |
| 26 | H | 101 | BCR | C37-C22 | 9.44 | 1.70 | 1.50 |
| 26 | b | 619 | BCR | C16-C17 | 9.44 | 1.72 | 1.43 |
| 26 | A | 610 | BCR | C16-C17 | 9.31 | 1.72 | 1.43 |
| 26 | b | 621 | BCR | C16-C17 | 9.23 | 1.72 | 1.43 |
| 26 | I | 101 | BCR | C16-C17 | 9.20 | 1.71 | 1.43 |
| 26 | F | 101 | BCR | C16-C17 | 9.13 | 1.71 | 1.43 |
| 26 | a | 610 | BCR | C16-C17 | 9.10 | 1.71 | 1.43 |
| 26 | b | 620 | BCR | C16-C17 | 9.04 | 1.71 | 1.43 |
| 26 | c | 521 | BCR | C16-C17 | 8.97 | 1.71 | 1.43 |
| 27 | d | 404 | PL9 | C28-C29 | 8.97 | 1.54 | 1.33 |
| 26 | f | 101 | BCR | C16-C17 | 8.93 | 1.71 | 1.43 |
| 26 | c | 515 | BCR | C16-C17 | 8.85 | 1.70 | 1.43 |
| 27 | a | 611 | PL9 | C48-C49 | 8.83 | 1.57 | 1.32 |
| 27 | D | 405 | PL9 | C28-C29 | 8.81 | 1.54 | 1.33 |
| 26 | B | 619 | BCR | C16-C17 | 8.78 | 1.70 | 1.43 |
| 27 | A | 611 | PL9 | C48-C49 | 8.77 | 1.57 | 1.32 |
| 27 | d | 404 | PL9 | C13-C14 | 8.75 | 1.54 | 1.33 |
| 27 | D | 405 | PL9 | C13-C14 | 8.75 | 1.54 | 1.33 |
| 26 | B | 618 | BCR | C16-C17 | 8.70 | 1.70 | 1.43 |
| 26 | A | 610 | BCR | C26-C25 | 8.65 | 1.49 | 1.34 |
| 26 | h | 101 | BCR | C26-C25 | 8.64 | 1.49 | 1.34 |
| 26 | H | 101 | BCR | C26-C25 | 8.58 | 1.49 | 1.34 |
| 27 | a | 611 | PL9 | C28-C29 | 8.52 | 1.53 | 1.33 |
| 27 | D | 405 | PL9 | C48-C49 | 8.50 | 1.56 | 1.32 |
| 27 | A | 611 | PL9 | C13-C14 | 8.50 | 1.53 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27 | D | 405 | PL9 | C43-C44 | 8.50 | 1.53 | 1.33 |
| 27 | d | 404 | PL9 | C48-C49 | 8.47 | 1.56 | 1.32 |
| 27 | A | 611 | PL9 | C28-C29 | 8.44 | 1.53 | 1.33 |
| 26 | I | 101 | BCR | C26-C25 | 8.42 | 1.49 | 1.34 |
| 27 | a | 611 | PL9 | C8-C9 | 8.41 | 1.53 | 1.33 |
| 26 | b | 619 | BCR | C26-C25 | 8.39 | 1.49 | 1.34 |
| 24 | D | 403 | CLA | C1B-NB | -8.38 | 1.27 | 1.35 |
| 27 | d | 404 | PL9 | C43-C44 | 8.34 | 1.53 | 1.33 |
| 27 | D | 405 | PL9 | C8-C9 | 8.30 | 1.52 | 1.33 |
| 27 | A | 611 | PL9 | C8-C9 | 8.29 | 1.52 | 1.33 |
| 27 | a | 611 | PL9 | C13-C14 | 8.29 | 1.52 | 1.33 |
| 26 | k | 101 | BCR | C26-C25 | 8.26 | 1.48 | 1.34 |
| 27 | A | 611 | PL9 | C43-C44 | 8.23 | 1.52 | 1.33 |
| 27 | a | 611 | PL9 | C43-C44 | 8.21 | 1.52 | 1.33 |
| 26 | A | 610 | BCR | C8-C9 | 8.13 | 1.63 | 1.45 |
| 27 | d | 404 | PL9 | O1-C4 | 8.12 | 1.41 | 1.23 |
| 27 | d | 404 | PL9 | C8-C9 | 8.08 | 1.52 | 1.33 |
| 26 | k | 101 | BCR | C8-C9 | 8.07 | 1.63 | 1.45 |
| 27 | a | 611 | PL9 | C33-C34 | 8.06 | 1.52 | 1.33 |
| 27 | A | 611 | PL9 | C33-C34 | 7.93 | 1.52 | 1.33 |
| 26 | K | 102 | BCR | C26-C25 | 7.89 | 1.48 | 1.34 |
| 26 | c | 515 | BCR | C26-C25 | 7.89 | 1.48 | 1.34 |
| 26 | K | 101 | BCR | C8-C9 | 7.88 | 1.62 | 1.45 |
| 24 | A | 606 | CLA | C3A-C2A | -7.88 | 1.32 | 1.54 |
| 26 | K | 101 | BCR | C26-C25 | 7.86 | 1.48 | 1.34 |
| 26 | C | 514 | BCR | C26-C25 | 7.84 | 1.48 | 1.34 |
| 27 | A | 611 | PL9 | O1-C4 | 7.81 | 1.40 | 1.23 |
| 24 | a | 606 | CLA | C3A-C2A | -7.79 | 1.32 | 1.54 |
| 26 | c | 521 | BCR | C8-C9 | 7.78 | 1.62 | 1.45 |
| 26 | c | 514 | BCR | C8-C9 | 7.75 | 1.62 | 1.45 |
| 26 | c | 521 | BCR | C26-C25 | 7.74 | 1.47 | 1.34 |
| 26 | c | 521 | BCR | C17-C18 | 7.74 | 1.46 | 1.35 |
| 27 | D | 405 | PL9 | C33-C34 | 7.70 | 1.51 | 1.33 |
| 26 | C | 514 | BCR | C8-C9 | 7.70 | 1.62 | 1.45 |
| 26 | a | 610 | BCR | C8-C9 | 7.69 | 1.62 | 1.45 |
| 24 | B | 613 | CLA | C1B-NB | -7.68 | 1.28 | 1.35 |
| 27 | d | 404 | PL9 | C33-C34 | 7.67 | 1.51 | 1.33 |
| 24 | B | 613 | CLA | C3A-C2A | -7.66 | 1.33 | 1.54 |
| 24 | D | 402 | CLA | C3A-C2A | -7.62 | 1.33 | 1.54 |
| 26 | I | 101 | BCR | C8-C9 | 7.62 | 1.62 | 1.45 |
| 24 | b | 614 | CLA | C3A-C2A | -7.62 | 1.33 | 1.54 |
| 24 | B | 608 | CLA | C3A-C2A | -7.62 | 1.33 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | D | 403 | CLA | C3A-C2A | -7.60 | 1.33 | 1.54 |
| 24 | b | 610 | CLA | C3A-C2A | -7.60 | 1.33 | 1.54 |
| 24 | C | 509 | CLA | C1B-NB | -7.60 | 1.28 | 1.35 |
| 24 | B | 604 | CLA | C1B-NB | -7.58 | 1.28 | 1.35 |
| 24 | b | 605 | CLA | C3A-C2A | -7.57 | 1.33 | 1.54 |
| 26 | c | 515 | BCR | C8-C9 | 7.55 | 1.62 | 1.45 |
| 24 | b | 618 | CLA | C3A-C2A | -7.55 | 1.33 | 1.54 |
| 24 | b | 604 | CLA | C3A-C2A | -7.53 | 1.33 | 1.54 |
| 24 | B | 607[A] | CLA | C3A-C2A | -7.53 | 1.33 | 1.54 |
| 24 | B | 607[B] | CLA | C3A-C2A | -7.53 | 1.33 | 1.54 |
| 24 | B | 609 | CLA | C3A-C2A | -7.52 | 1.33 | 1.54 |
| 24 | D | 404 | CLA | C3A-C2A | -7.52 | 1.33 | 1.54 |
| 24 | C | 510 | CLA | C3A-C2A | -7.51 | 1.33 | 1.54 |
| 24 | c | 506 | CLA | C3A-C2A | -7.51 | 1.33 | 1.54 |
| 26 | B | 618 | BCR | C26-C25 | 7.51 | 1.47 | 1.34 |
| 24 | b | 608[A] | CLA | C3A-C2A | -7.51 | 1.33 | 1.54 |
| 24 | b | 608[B] | CLA | C3A-C2A | -7.50 | 1.33 | 1.54 |
| 24 | B | 612 | CLA | C1B-NB | -7.49 | 1.28 | 1.35 |
| 24 | b | 609 | CLA | C3A-C2A | -7.49 | 1.33 | 1.54 |
| 26 | b | 621 | BCR | C8-C9 | 7.48 | 1.62 | 1.45 |
| 24 | b | 614 | CLA | C1B-NB | -7.47 | 1.28 | 1.35 |
| 24 | b | 612 | CLA | C3A-C2A | -7.46 | 1.33 | 1.54 |
| 24 | C | 504 | CLA | C3A-C2A | -7.46 | 1.33 | 1.54 |
| 24 | C | 501 | CLA | C3A-C2A | -7.44 | 1.33 | 1.54 |
| 24 | B | 614 | CLA | C3A-C2A | -7.44 | 1.33 | 1.54 |
| 24 | B | 615 | CLA | C3A-C2A | -7.44 | 1.33 | 1.54 |
| 26 | t | 101 | BCR | C8-C9 | 7.43 | 1.61 | 1.45 |
| 24 | C | 509 | CLA | C3A-C2A | -7.41 | 1.33 | 1.54 |
| 24 | a | 609 | CLA | C3A-C2A | -7.41 | 1.33 | 1.54 |
| 26 | B | 620 | BCR | C26-C25 | 7.40 | 1.47 | 1.34 |
| 24 | A | 609 | CLA | C3A-C2A | -7.40 | 1.33 | 1.54 |
| 24 | c | 512 | CLA | C3A-C2A | -7.39 | 1.33 | 1.54 |
| 27 | D | 405 | PL9 | O1-C4 | 7.38 | 1.39 | 1.23 |
| 26 | b | 621 | BCR | C26-C25 | 7.38 | 1.47 | 1.34 |
| 26 | H | 101 | BCR | C8-C9 | 7.37 | 1.61 | 1.45 |
| 26 | f | 101 | BCR | C8-C9 | 7.37 | 1.61 | 1.45 |
| 24 | c | 511 | CLA | C3A-C2A | -7.37 | 1.33 | 1.54 |
| 27 | a | 611 | PL9 | O1-C4 | 7.37 | 1.39 | 1.23 |
| 24 | b | 615 | CLA | C3A-C2A | -7.35 | 1.33 | 1.54 |
| 26 | T | 101 | BCR | C8-C9 | 7.35 | 1.61 | 1.45 |
| 24 | B | 603 | CLA | C3A-C2A | -7.34 | 1.34 | 1.54 |
| 24 | a | 615 | CLA | C3A-C2A | -7.34 | 1.34 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | C | 511 | CLA | C3A-C2A | -7.33 | 1.34 | 1.54 |
| 24 | c | 504 | CLA | C3A-C2A | -7.32 | 1.34 | 1.54 |
| 24 | C | 512 | CLA | C3A-C2A | -7.31 | 1.34 | 1.54 |
| 24 | C | 502 | CLA | C3A-C2A | -7.30 | 1.34 | 1.54 |
| 24 | c | 509 | CLA | C3A-C2A | -7.30 | 1.34 | 1.54 |
| 24 | C | 508 | CLA | C3A-C2A | -7.30 | 1.34 | 1.54 |
| 24 | b | 607 | CLA | C3A-C2A | -7.30 | 1.34 | 1.54 |
| 24 | c | 502 | CLA | C3A-C2A | -7.29 | 1.34 | 1.54 |
| 24 | b | 613 | CLA | C3A-C2A | -7.29 | 1.34 | 1.54 |
| 24 | d | 402 | CLA | C3A-C2A | -7.27 | 1.34 | 1.54 |
| 26 | c | 514 | BCR | C26-C25 | 7.27 | 1.47 | 1.34 |
| 26 | h | 101 | BCR | C8-C9 | 7.26 | 1.61 | 1.45 |
| 26 | b | 619 | BCR | C8-C9 | 7.25 | 1.61 | 1.45 |
| 24 | b | 606 | CLA | C3A-C2A | -7.25 | 1.34 | 1.54 |
| 24 | c | 510 | CLA | C3A-C2A | -7.25 | 1.34 | 1.54 |
| 24 | C | 510 | CLA | C1B-NB | -7.25 | 1.28 | 1.35 |
| 24 | d | 403 | CLA | C3A-C2A | -7.23 | 1.34 | 1.54 |
| 24 | b | 617 | CLA | C3A-C2A | -7.22 | 1.34 | 1.54 |
| 26 | f | 101 | BCR | C38-C26 | 7.22 | 1.62 | 1.50 |
| 24 | b | 616 | CLA | C3A-C2A | -7.22 | 1.34 | 1.54 |
| 24 | B | 610 | CLA | C3A-C2A | -7.22 | 1.34 | 1.54 |
| 24 | b | 611 | CLA | C3A-C2A | -7.21 | 1.34 | 1.54 |
| 24 | a | 606 | CLA | C1B-NB | -7.21 | 1.28 | 1.35 |
| 26 | a | 610 | BCR | C26-C25 | 7.21 | 1.46 | 1.34 |
| 24 | C | 503 | CLA | C3A-C2A | -7.20 | 1.34 | 1.54 |
| 26 | b | 620 | BCR | C8-C9 | 7.20 | 1.61 | 1.45 |
| 24 | d | 402 | CLA | C1B-NB | -7.19 | 1.28 | 1.35 |
| 24 | A | 607 | CLA | C3A-C2A | -7.17 | 1.34 | 1.54 |
| 24 | c | 508 | CLA | C3A-C2A | -7.16 | 1.34 | 1.54 |
| 24 | B | 612 | CLA | C3A-C2A | -7.16 | 1.34 | 1.54 |
| 24 | C | 505 | CLA | C3A-C2A | -7.15 | 1.34 | 1.54 |
| 26 | K | 102 | BCR | C8-C9 | 7.15 | 1.61 | 1.45 |
| 24 | c | 505 | CLA | C3A-C2A | -7.13 | 1.34 | 1.54 |
| 24 | B | 605 | CLA | C3A-C2A | -7.12 | 1.34 | 1.54 |
| 24 | B | 617 | CLA | C3A-C2A | -7.12 | 1.34 | 1.54 |
| 24 | C | 506 | CLA | C3A-C2A | -7.10 | 1.34 | 1.54 |
| 24 | c | 503 | CLA | C3A-C2A | -7.10 | 1.34 | 1.54 |
| 24 | a | 607 | CLA | C3A-C2A | -7.10 | 1.34 | 1.54 |
| 24 | C | 507 | CLA | C3A-C2A | -7.08 | 1.34 | 1.54 |
| 24 | c | 501 | CLA | C3A-C2A | -7.08 | 1.34 | 1.54 |
| 26 | B | 619 | BCR | C8-C9 | 7.05 | 1.61 | 1.45 |
| 24 | B | 616 | CLA | C3A-C2A | -7.03 | 1.34 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | c | 513 | CLA | C3A-C2A | -7.03 | 1.34 | 1.54 |
| 24 | B | 604 | CLA | C3A-C2A | -7.02 | 1.34 | 1.54 |
| 24 | B | 611 | CLA | C3A-C2A | -7.00 | 1.34 | 1.54 |
| 24 | a | 615 | CLA | C1B-NB | -7.00 | 1.29 | 1.35 |
| 26 | B | 618 | BCR | C8-C9 | 6.99 | 1.61 | 1.45 |
| 24 | c | 504 | CLA | C1B-NB | -6.98 | 1.29 | 1.35 |
| 24 | B | 606 | CLA | C3A-C2A | -6.97 | 1.35 | 1.54 |
| 24 | b | 603 | CLA | C3A-C2A | -6.96 | 1.35 | 1.54 |
| 24 | c | 507 | CLA | C3A-C2A | -6.95 | 1.35 | 1.54 |
| 24 | B | 602 | CLA | C3A-C2A | -6.90 | 1.35 | 1.54 |
| 26 | t | 101 | BCR | C26-C25 | 6.86 | 1.46 | 1.34 |
| 24 | C | 513 | CLA | C3A-C2A | -6.85 | 1.35 | 1.54 |
| 26 | F | 101 | BCR | C8-C9 | 6.84 | 1.60 | 1.45 |
| 24 | b | 605 | CLA | C1B-NB | -6.84 | 1.29 | 1.35 |
| 24 | C | 508 | CLA | C1B-NB | -6.80 | 1.29 | 1.35 |
| 24 | B | 605 | CLA | C1B-NB | -6.79 | 1.29 | 1.35 |
| 26 | K | 101 | BCR | C34-C9 | -6.79 | 1.36 | 1.50 |
| 24 | A | 606 | CLA | C1B-NB | -6.78 | 1.29 | 1.35 |
| 24 | b | 613 | CLA | C1B-NB | -6.76 | 1.29 | 1.35 |
| 26 | B | 619 | BCR | C34-C9 | -6.73 | 1.37 | 1.50 |
| 26 | T | 101 | BCR | C26-C25 | 6.71 | 1.46 | 1.34 |
| 26 | h | 101 | BCR | C38-C26 | 6.70 | 1.61 | 1.50 |
| 26 | F | 101 | BCR | C38-C26 | 6.70 | 1.61 | 1.50 |
| 27 | a | 611 | PL9 | O2-C1 | 6.68 | 1.42 | 1.24 |
| 24 | C | 504 | CLA | C1B-NB | -6.68 | 1.29 | 1.35 |
| 26 | B | 620 | BCR | C8-C9 | 6.67 | 1.60 | 1.45 |
| 26 | b | 620 | BCR | C38-C26 | 6.65 | 1.61 | 1.50 |
| 26 | H | 101 | BCR | C38-C26 | 6.63 | 1.61 | 1.50 |
| 24 | D | 404 | CLA | C1B-NB | -6.62 | 1.29 | 1.35 |
| 26 | b | 619 | BCR | C34-C9 | -6.55 | 1.37 | 1.50 |
| 27 | A | 611 | PL9 | O2-C1 | 6.55 | 1.42 | 1.24 |
| 24 | B | 614 | CLA | C1B-NB | -6.54 | 1.29 | 1.35 |
| 26 | B | 618 | BCR | C34-C9 | -6.53 | 1.37 | 1.50 |
| 26 | b | 621 | BCR | C34-C9 | -6.52 | 1.37 | 1.50 |
| 26 | I | 101 | BCR | C34-C9 | -6.50 | 1.37 | 1.50 |
| 26 | C | 514 | BCR | C34-C9 | -6.49 | 1.37 | 1.50 |
| 24 | C | 506 | CLA | C1B-NB | -6.47 | 1.29 | 1.35 |
| 24 | D | 403 | CLA | C3D-C2D | -6.46 | 1.27 | 1.39 |
| 24 | b | 618 | CLA | C1B-NB | -6.46 | 1.29 | 1.35 |
| 26 | C | 514 | BCR | C17-C18 | 6.45 | 1.44 | 1.35 |
| 24 | b | 606 | CLA | C1B-NB | -6.44 | 1.29 | 1.35 |
| 24 | b | 615 | CLA | C1B-NB | -6.44 | 1.29 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 616 | CLA | C1B-NB | -6.44 | 1.29 | 1.35 |
| 24 | c | 506 | CLA | C1B-NB | -6.43 | 1.29 | 1.35 |
| 26 | c | 514 | BCR | C34-C9 | -6.42 | 1.37 | 1.50 |
| 26 | F | 101 | BCR | C34-C9 | -6.42 | 1.37 | 1.50 |
| 24 | c | 501 | CLA | C1B-NB | -6.41 | 1.29 | 1.35 |
| 26 | b | 620 | BCR | C34-C9 | -6.41 | 1.37 | 1.50 |
| 24 | b | 604 | CLA | C1B-NB | -6.40 | 1.29 | 1.35 |
| 26 | c | 515 | BCR | C34-C9 | -6.35 | 1.37 | 1.50 |
| 24 | C | 512 | CLA | C1B-NB | -6.34 | 1.29 | 1.35 |
| 24 | A | 607 | CLA | C1B-NB | -6.34 | 1.29 | 1.35 |
| 24 | A | 609 | CLA | C1B-NB | -6.33 | 1.29 | 1.35 |
| 26 | t | 101 | BCR | C34-C9 | -6.32 | 1.37 | 1.50 |
| 26 | I | 101 | BCR | C38-C26 | 6.31 | 1.61 | 1.50 |
| 24 | B | 606 | CLA | C3D-C2D | -6.30 | 1.28 | 1.39 |
| 24 | C | 503 | CLA | C1B-NB | -6.29 | 1.29 | 1.35 |
| 24 | B | 615 | CLA | C1B-NB | -6.28 | 1.29 | 1.35 |
| 24 | b | 609 | CLA | C1B-NB | -6.27 | 1.29 | 1.35 |
| 24 | D | 402 | CLA | C1B-NB | -6.26 | 1.29 | 1.35 |
| 26 | c | 521 | BCR | C34-C9 | -6.26 | 1.37 | 1.50 |
| 26 | A | 610 | BCR | C38-C26 | 6.24 | 1.61 | 1.50 |
| 26 | B | 620 | BCR | C34-C9 | -6.24 | 1.38 | 1.50 |
| 27 | d | 404 | PL9 | O2-C1 | 6.23 | 1.41 | 1.24 |
| 27 | D | 405 | PL9 | O2-C1 | 6.23 | 1.41 | 1.24 |
| 24 | b | 614 | CLA | C3D-C2D | -6.23 | 1.28 | 1.39 |
| 26 | f | 101 | BCR | C34-C9 | -6.23 | 1.38 | 1.50 |
| 26 | B | 619 | BCR | C24-C23 | 6.22 | 1.51 | 1.33 |
| 26 | B | 619 | BCR | C38-C26 | 6.21 | 1.61 | 1.50 |
| 24 | B | 615 | CLA | C3D-C2D | -6.21 | 1.28 | 1.39 |
| 24 | B | 614 | CLA | C3D-C2D | -6.21 | 1.28 | 1.39 |
| 24 | b | 607 | CLA | C1B-NB | -6.18 | 1.29 | 1.35 |
| 26 | c | 521 | BCR | C38-C26 | 6.17 | 1.61 | 1.50 |
| 26 | K | 102 | BCR | C38-C26 | 6.16 | 1.61 | 1.50 |
| 26 | c | 521 | BCR | C11-C12 | 6.14 | 1.50 | 1.34 |
| 26 | H | 101 | BCR | C34-C9 | -6.13 | 1.38 | 1.50 |
| 26 | K | 102 | BCR | C34-C9 | -6.13 | 1.38 | 1.50 |
| 24 | C | 503 | CLA | C3D-C2D | -6.13 | 1.28 | 1.39 |
| 26 | c | 514 | BCR | C38-C26 | 6.13 | 1.61 | 1.50 |
| 24 | b | 608[B] | CLA | C1B-NB | -6.11 | 1.29 | 1.35 |
| 24 | B | 617 | CLA | C1B-NB | -6.11 | 1.29 | 1.35 |
| 26 | A | 610 | BCR | C34-C9 | -6.10 | 1.38 | 1.50 |
| 26 | k | 101 | BCR | C38-C26 | 6.10 | 1.60 | 1.50 |
| 26 | k | 101 | BCR | C34-C9 | -6.09 | 1.38 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 513 | CLA | C1B-NB | -6.08 | 1.29 | 1.35 |
| 24 | C | 511 | CLA | C3D-C2D | -6.08 | 1.28 | 1.39 |
| 24 | a | 606 | CLA | C3D-C2D | -6.08 | 1.28 | 1.39 |
| 26 | B | 620 | BCR | C38-C26 | 6.07 | 1.60 | 1.50 |
| 26 | T | 101 | BCR | C34-C9 | -6.07 | 1.38 | 1.50 |
| 26 | F | 101 | BCR | C23-C22 | 6.07 | 1.59 | 1.45 |
| 24 | c | 502 | CLA | C1B-NB | -6.06 | 1.29 | 1.35 |
| 24 | B | 603 | CLA | C1B-NB | -6.05 | 1.29 | 1.35 |
| 26 | b | 621 | BCR | C38-C26 | 6.04 | 1.60 | 1.50 |
| 26 | F | 101 | BCR | C24-C23 | 6.04 | 1.51 | 1.33 |
| 26 | I | 101 | BCR | C11-C12 | 6.04 | 1.50 | 1.34 |
| 24 | b | 609 | CLA | C3D-C2D | -6.03 | 1.28 | 1.39 |
| 26 | h | 101 | BCR | C34-C9 | -6.03 | 1.38 | 1.50 |
| 24 | b | 613 | CLA | C3D-C2D | -6.02 | 1.28 | 1.39 |
| 24 | b | 606 | CLA | C3D-C2D | -6.02 | 1.28 | 1.39 |
| 24 | a | 615 | CLA | C3D-C2D | -6.00 | 1.28 | 1.39 |
| 24 | c | 509 | CLA | C1B-NB | -6.00 | 1.29 | 1.35 |
| 26 | I | 101 | BCR | C17-C18 | 5.98 | 1.43 | 1.35 |
| 24 | D | 402 | CLA | C3D-C2D | -5.98 | 1.28 | 1.39 |
| 24 | b | 608[A] | CLA | C1B-NB | -5.95 | 1.29 | 1.35 |
| 24 | B | 607[B] | CLA | C1B-NB | -5.94 | 1.29 | 1.35 |
| 26 | b | 619 | BCR | C38-C26 | 5.93 | 1.60 | 1.50 |
| 26 | B | 618 | BCR | C38-C26 | 5.92 | 1.60 | 1.50 |
| 26 | c | 515 | BCR | C38-C26 | 5.92 | 1.60 | 1.50 |
| 24 | B | 608 | CLA | C1B-NB | -5.92 | 1.29 | 1.35 |
| 24 | C | 508 | CLA | C3D-C2D | -5.90 | 1.28 | 1.39 |
| 26 | a | 610 | BCR | C34-C9 | -5.90 | 1.38 | 1.50 |
| 26 | A | 610 | BCR | C11-C12 | 5.90 | 1.49 | 1.34 |
| 24 | c | 504 | CLA | C3D-C2D | -5.88 | 1.28 | 1.39 |
| 24 | C | 502 | CLA | C1B-NB | -5.88 | 1.30 | 1.35 |
| 24 | a | 607 | CLA | C1B-NB | -5.86 | 1.30 | 1.35 |
| 26 | b | 621 | BCR | C11-C12 | 5.85 | 1.49 | 1.34 |
| 26 | C | 514 | BCR | C38-C26 | 5.84 | 1.60 | 1.50 |
| 24 | b | 612 | CLA | C1B-NB | -5.83 | 1.30 | 1.35 |
| 24 | b | 610 | CLA | C1B-NB | -5.81 | 1.30 | 1.35 |
| 24 | b | 605 | CLA | C3D-C2D | -5.81 | 1.29 | 1.39 |
| 26 | K | 101 | BCR | C38-C26 | 5.81 | 1.60 | 1.50 |
| 26 | B | 619 | BCR | C23-C22 | 5.81 | 1.58 | 1.45 |
| 24 | c | 507 | CLA | C1B-NB | -5.80 | 1.30 | 1.35 |
| 24 | A | 609 | CLA | C3D-C2D | -5.80 | 1.29 | 1.39 |
| 24 | d | 403 | CLA | C1B-NB | -5.80 | 1.30 | 1.35 |
| 24 | a | 607 | CLA | C3D-C2D | -5.79 | 1.29 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | c | 508 | CLA | C1B-NB | -5.79 | 1.30 | 1.35 |
| 24 | C | 507 | CLA | C1B-NB | -5.79 | 1.30 | 1.35 |
| 26 | h | 101 | BCR | C11-C12 | 5.79 | 1.49 | 1.34 |
| 26 | t | 101 | BCR | C38-C26 | 5.79 | 1.60 | 1.50 |
| 24 | B | 608 | CLA | C3D-C2D | -5.78 | 1.29 | 1.39 |
| 26 | K | 102 | BCR | C11-C12 | 5.77 | 1.49 | 1.34 |
| 24 | C | 510 | CLA | C3D-C2D | -5.77 | 1.29 | 1.39 |
| 26 | c | 515 | BCR | C11-C12 | 5.75 | 1.49 | 1.34 |
| 24 | B | 607[A] | CLA | C1B-NB | -5.75 | 1.30 | 1.35 |
| 24 | b | 603 | CLA | C3D-C2D | -5.74 | 1.29 | 1.39 |
| 26 | H | 101 | BCR | C24-C23 | 5.74 | 1.50 | 1.33 |
| 26 | B | 619 | BCR | C11-C12 | 5.74 | 1.49 | 1.34 |
| 26 | H | 101 | BCR | C11-C12 | 5.73 | 1.49 | 1.34 |
| 24 | c | 512 | CLA | C1B-NB | -5.73 | 1.30 | 1.35 |
| 26 | B | 618 | BCR | C23-C22 | 5.72 | 1.58 | 1.45 |
| 24 | c | 510 | CLA | C3D-C2D | -5.71 | 1.29 | 1.39 |
| 26 | b | 621 | BCR | C17-C18 | 5.70 | 1.43 | 1.35 |
| 26 | C | 514 | BCR | C11-C12 | 5.70 | 1.49 | 1.34 |
| 24 | c | 503 | CLA | C3D-C2D | -5.69 | 1.29 | 1.39 |
| 26 | t | 101 | BCR | C11-C12 | 5.69 | 1.49 | 1.34 |
| 24 | b | 604 | CLA | C3D-C2D | -5.69 | 1.29 | 1.39 |
| 26 | T | 101 | BCR | C11-C12 | 5.67 | 1.49 | 1.34 |
| 24 | b | 608[B] | CLA | C3D-C2D | -5.67 | 1.29 | 1.39 |
| 24 | a | 609 | CLA | C3D-C2D | -5.66 | 1.29 | 1.39 |
| 24 | d | 402 | CLA | C3D-C2D | -5.66 | 1.29 | 1.39 |
| 24 | c | 505 | CLA | C3D-C2D | -5.65 | 1.29 | 1.39 |
| 24 | b | 608[A] | CLA | C3D-C2D | -5.64 | 1.29 | 1.39 |
| 24 | c | 511 | CLA | C3D-C2D | -5.62 | 1.29 | 1.39 |
| 24 | C | 509 | CLA | C3D-C2D | -5.62 | 1.29 | 1.39 |
| 26 | t | 101 | BCR | C23-C22 | 5.61 | 1.58 | 1.45 |
| 26 | H | 101 | BCR | C17-C18 | 5.61 | 1.43 | 1.35 |
| 24 | c | 505 | CLA | C1B-NB | -5.61 | 1.30 | 1.35 |
| 26 | a | 610 | BCR | C11-C12 | 5.60 | 1.49 | 1.34 |
| 26 | c | 521 | BCR | C23-C22 | 5.60 | 1.58 | 1.45 |
| 26 | c | 514 | BCR | C11-C12 | 5.60 | 1.49 | 1.34 |
| 24 | c | 513 | CLA | C1B-NB | -5.60 | 1.30 | 1.35 |
| 24 | B | 604 | CLA | C3D-C2D | -5.60 | 1.29 | 1.39 |
| 24 | b | 607 | CLA | C3D-C2D | -5.60 | 1.29 | 1.39 |
| 26 | C | 514 | BCR | C23-C22 | 5.59 | 1.58 | 1.45 |
| 26 | A | 610 | BCR | C24-C23 | 5.57 | 1.49 | 1.33 |
| 24 | C | 506 | CLA | C3D-C2D | -5.57 | 1.29 | 1.39 |
| 26 | a | 610 | BCR | C38-C26 | 5.57 | 1.60 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | A | 607 | CLA | C3D-C2D | -5.56 | 1.29 | 1.39 |
| 24 | C | 501 | CLA | C1B-NB | -5.56 | 1.30 | 1.35 |
| 33 | v | 201 | HEM | C3D-C2D | 5.56 | 1.54 | 1.37 |
| 26 | a | 610 | BCR | C23-C22 | 5.55 | 1.57 | 1.45 |
| 24 | B | 610 | CLA | C1B-NB | -5.54 | 1.30 | 1.35 |
| 26 | k | 101 | BCR | C11-C12 | 5.53 | 1.48 | 1.34 |
| 26 | K | 101 | BCR | C17-C18 | 5.53 | 1.43 | 1.35 |
| 24 | B | 616 | CLA | C1B-NB | -5.50 | 1.30 | 1.35 |
| 26 | b | 620 | BCR | C24-C23 | 5.50 | 1.49 | 1.33 |
| 24 | b | 617 | CLA | C3D-C2D | -5.49 | 1.29 | 1.39 |
| 24 | B | 607[B] | CLA | C3D-C2D | -5.49 | 1.29 | 1.39 |
| 26 | T | 101 | BCR | C23-C22 | 5.47 | 1.57 | 1.45 |
| 27 | D | 405 | PL9 | C3-C4 | -5.47 | 1.40 | 1.49 |
| 26 | A | 610 | BCR | C23-C22 | 5.46 | 1.57 | 1.45 |
| 26 | f | 101 | BCR | C24-C23 | 5.45 | 1.49 | 1.33 |
| 24 | B | 603 | CLA | CHC-C1C | 5.44 | 1.48 | 1.35 |
| 26 | B | 619 | BCR | C24-C25 | 5.44 | 1.64 | 1.45 |
| 24 | D | 404 | CLA | C3D-C2D | -5.44 | 1.29 | 1.39 |
| 24 | B | 607[A] | CLA | C3D-C2D | -5.42 | 1.29 | 1.39 |
| 24 | b | 616 | CLA | C3D-C2D | -5.40 | 1.29 | 1.39 |
| 26 | B | 620 | BCR | C11-C12 | 5.38 | 1.48 | 1.34 |
| 26 | h | 101 | BCR | C24-C23 | 5.37 | 1.49 | 1.33 |
| 24 | c | 502 | CLA | C3D-C2D | -5.37 | 1.29 | 1.39 |
| 26 | B | 618 | BCR | C11-C12 | 5.36 | 1.48 | 1.34 |
| 24 | B | 602 | CLA | C3D-C2D | -5.36 | 1.29 | 1.39 |
| 24 | C | 511 | CLA | C1B-NB | -5.36 | 1.30 | 1.35 |
| 24 | B | 610 | CLA | C3D-C2D | -5.35 | 1.29 | 1.39 |
| 24 | b | 617 | CLA | C1B-NB | -5.34 | 1.30 | 1.35 |
| 24 | B | 612 | CLA | C3D-C2D | -5.34 | 1.29 | 1.39 |
| 24 | B | 603 | CLA | C3D-C2D | -5.34 | 1.29 | 1.39 |
| 26 | T | 101 | BCR | C38-C26 | 5.33 | 1.59 | 1.50 |
| 24 | D | 403 | CLA | C4B-CHC | -5.33 | 1.26 | 1.41 |
| 24 | B | 611 | CLA | C1B-NB | -5.32 | 1.30 | 1.35 |
| 24 | A | 606 | CLA | C3D-C2D | -5.31 | 1.29 | 1.39 |
| 24 | C | 507 | CLA | C3D-C2D | -5.31 | 1.29 | 1.39 |
| 26 | f | 101 | BCR | C23-C22 | 5.31 | 1.57 | 1.45 |
| 26 | F | 101 | BCR | C11-C12 | 5.30 | 1.48 | 1.34 |
| 26 | H | 101 | BCR | C23-C22 | 5.29 | 1.57 | 1.45 |
| 24 | c | 510 | CLA | C1B-NB | -5.29 | 1.30 | 1.35 |
| 26 | h | 101 | BCR | C17-C18 | 5.27 | 1.42 | 1.35 |
| 26 | B | 618 | BCR | C24-C23 | 5.27 | 1.49 | 1.33 |
| 26 | a | 610 | BCR | C24-C23 | 5.26 | 1.49 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | c | 503 | CLA | C1B-NB | -5.26 | 1.30 | 1.35 |
| 26 | b | 619 | BCR | C23-C22 | 5.22 | 1.57 | 1.45 |
| 24 | C | 505 | CLA | C1B-NB | -5.20 | 1.30 | 1.35 |
| 24 | b | 606 | CLA | CHC-C1C | 5.19 | 1.48 | 1.35 |
| 24 | C | 501 | CLA | CHC-C1C | 5.19 | 1.48 | 1.35 |
| 24 | c | 506 | CLA | C3D-C2D | -5.19 | 1.30 | 1.39 |
| 26 | B | 620 | BCR | C17-C18 | 5.18 | 1.42 | 1.35 |
| 24 | B | 613 | CLA | C3D-C2D | -5.18 | 1.30 | 1.39 |
| 26 | K | 101 | BCR | C24-C23 | 5.17 | 1.48 | 1.33 |
| 33 | V | 201 | HEM | C3D-C2D | 5.17 | 1.53 | 1.37 |
| 24 | b | 615 | CLA | C3D-C2D | -5.17 | 1.30 | 1.39 |
| 24 | B | 614 | CLA | C4B-CHC | -5.16 | 1.26 | 1.41 |
| 24 | C | 503 | CLA | CHC-C1C | 5.15 | 1.48 | 1.35 |
| 24 | c | 508 | CLA | C3D-C2D | -5.15 | 1.30 | 1.39 |
| 33 | e | 102 | HEM | C3D-C2D | 5.14 | 1.52 | 1.37 |
| 26 | b | 620 | BCR | C11-C12 | 5.14 | 1.47 | 1.34 |
| 26 | c | 515 | BCR | C24-C23 | 5.14 | 1.48 | 1.33 |
| 24 | B | 617 | CLA | C4B-CHC | -5.14 | 1.26 | 1.41 |
| 24 | b | 604 | CLA | CHC-C1C | 5.12 | 1.48 | 1.35 |
| 26 | b | 619 | BCR | C11-C12 | 5.10 | 1.47 | 1.34 |
| 24 | B | 605 | CLA | C3D-C2D | -5.10 | 1.30 | 1.39 |
| 26 | f | 101 | BCR | C11-C12 | 5.10 | 1.47 | 1.34 |
| 24 | c | 512 | CLA | C3D-C2D | -5.10 | 1.30 | 1.39 |
| 24 | b | 618 | CLA | C3D-C2D | -5.10 | 1.30 | 1.39 |
| 24 | c | 501 | CLA | C3D-C2D | -5.09 | 1.30 | 1.39 |
| 24 | B | 604 | CLA | C4B-CHC | -5.08 | 1.26 | 1.41 |
| 24 | a | 607 | CLA | CHC-C1C | 5.07 | 1.48 | 1.35 |
| 24 | B | 606 | CLA | C1B-NB | -5.06 | 1.30 | 1.35 |
| 24 | a | 615 | CLA | C4B-CHC | -5.06 | 1.26 | 1.41 |
| 30 | l | 102 | LHG | O8-C23 | 5.05 | 1.48 | 1.33 |
| 24 | b | 611 | CLA | C1B-NB | -5.04 | 1.30 | 1.35 |
| 24 | C | 510 | CLA | C4B-CHC | -5.04 | 1.27 | 1.41 |
| 24 | b | 618 | CLA | C4B-CHC | -5.04 | 1.27 | 1.41 |
| 26 | C | 514 | BCR | C24-C23 | 5.03 | 1.48 | 1.33 |
| 24 | B | 611 | CLA | C3D-C2D | -5.03 | 1.30 | 1.39 |
| 26 | b | 619 | BCR | C24-C23 | 5.02 | 1.48 | 1.33 |
| 24 | C | 512 | CLA | C4B-CHC | -5.00 | 1.27 | 1.41 |
| 24 | b | 605 | CLA | C4B-CHC | -5.00 | 1.27 | 1.41 |
| 24 | c | 511 | CLA | C1B-NB | -5.00 | 1.30 | 1.35 |
| 29 | c | 520 | LMG | O7-C10 | 5.00 | 1.48 | 1.34 |
| 24 | c | 503 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 24 | b | 610 | CLA | C3D-C2D | -4.99 | 1.30 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | B | 620 | BCR | C23-C22 | 4.99 | 1.56 | 1.45 |
| 24 | b | 616 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 24 | C | 513 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 24 | b | 609 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 24 | B | 602 | CLA | C1B-NB | -4.99 | 1.30 | 1.35 |
| 24 | c | 501 | CLA | CHC-C1C | 4.98 | 1.47 | 1.35 |
| 24 | B | 616 | CLA | CHC-C1C | 4.98 | 1.47 | 1.35 |
| 24 | B | 609 | CLA | C3D-C2D | -4.98 | 1.30 | 1.39 |
| 24 | b | 613 | CLA | C4B-CHC | -4.98 | 1.27 | 1.41 |
| 29 | C | 518 | LMG | O7-C10 | 4.97 | 1.48 | 1.34 |
| 24 | B | 609 | CLA | C1B-NB | -4.97 | 1.30 | 1.35 |
| 24 | c | 504 | CLA | CHC-C1C | 4.97 | 1.47 | 1.35 |
| 33 | E | 103 | HEM | C3D-C2D | 4.96 | 1.52 | 1.37 |
| 26 | K | 101 | BCR | C11-C12 | 4.96 | 1.47 | 1.34 |
| 24 | d | 403 | CLA | C3D-C2D | -4.96 | 1.30 | 1.39 |
| 24 | b | 611 | CLA | C3D-C2D | -4.96 | 1.30 | 1.39 |
| 24 | b | 617 | CLA | C4C-C3C | -4.95 | 1.36 | 1.45 |
| 24 | c | 511 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 26 | A | 610 | BCR | C24-C25 | 4.95 | 1.62 | 1.45 |
| 26 | F | 101 | BCR | C24-C25 | 4.94 | 1.62 | 1.45 |
| 29 | a | 613 | LMG | O7-C10 | 4.93 | 1.48 | 1.34 |
| 24 | D | 404 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 24 | C | 505 | CLA | C3D-C2D | -4.93 | 1.30 | 1.39 |
| 24 | c | 508 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 26 | c | 514 | BCR | C24-C23 | 4.93 | 1.48 | 1.33 |
| 26 | c | 515 | BCR | C23-C22 | 4.92 | 1.56 | 1.45 |
| 24 | c | 510 | CLA | CHC-C1C | 4.92 | 1.47 | 1.35 |
| 26 | K | 101 | BCR | C23-C22 | 4.92 | 1.56 | 1.45 |
| 26 | k | 101 | BCR | C24-C23 | 4.92 | 1.47 | 1.33 |
| 24 | D | 403 | CLA | C4C-C3C | -4.92 | 1.36 | 1.45 |
| 24 | c | 509 | CLA | C3D-C2D | -4.91 | 1.30 | 1.39 |
| 24 | b | 611 | CLA | CHC-C1C | 4.91 | 1.47 | 1.35 |
| 24 | B | 613 | CLA | C4B-CHC | -4.89 | 1.27 | 1.41 |
| 24 | B | 605 | CLA | C4B-CHC | -4.89 | 1.27 | 1.41 |
| 24 | C | 513 | CLA | C3D-C2D | -4.88 | 1.30 | 1.39 |
| 26 | b | 620 | BCR | C24-C25 | 4.88 | 1.62 | 1.45 |
| 24 | C | 508 | CLA | C4B-CHC | -4.88 | 1.27 | 1.41 |
| 24 | b | 603 | CLA | C4C-C3C | -4.88 | 1.36 | 1.45 |
| 24 | C | 502 | CLA | C3D-C2D | -4.87 | 1.30 | 1.39 |
| 26 | t | 101 | BCR | C24-C23 | 4.87 | 1.47 | 1.33 |
| 24 | d | 403 | CLA | C4C-C3C | -4.87 | 1.36 | 1.45 |
| 26 | T | 101 | BCR | C24-C23 | 4.86 | 1.47 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 26 | f | 101 | BCR | C24-C25 | 4.86 | 1.62 | 1.45 |
| 24 | a | 606 | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 24 | c | 512 | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 24 | b | 608[B] | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 24 | A | 607 | CLA | CHC-C1C | 4.84 | 1.47 | 1.35 |
| 24 | b | 607 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 24 | b | 612 | CLA | C3D-C2D | -4.83 | 1.30 | 1.39 |
| 24 | c | 509 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 24 | a | 609 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 26 | k | 101 | BCR | C17-C18 | 4.83 | 1.42 | 1.35 |
| 24 | a | 606 | CLA | C4B-CHC | -4.83 | 1.27 | 1.41 |
| 24 | b | 603 | CLA | CHD-C4C | -4.82 | 1.27 | 1.41 |
| 24 | c | 506 | CLA | CHC-C1C | 4.82 | 1.47 | 1.35 |
| 30 | d | 407 | LHG | O8-C23 | 4.82 | 1.47 | 1.33 |
| 24 | b | 614 | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 24 | B | 606 | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 24 | c | 513 | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 24 | b | 608[A] | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 24 | C | 509 | CLA | C4B-CHC | -4.80 | 1.27 | 1.41 |
| 24 | C | 511 | CLA | CHC-C1C | 4.79 | 1.47 | 1.35 |
| 24 | C | 510 | CLA | C1C-NC | -4.79 | 1.30 | 1.37 |
| 24 | d | 403 | CLA | CHC-C1C | 4.79 | 1.47 | 1.35 |
| 24 | B | 609 | CLA | C4B-CHC | -4.78 | 1.27 | 1.41 |
| 29 | c | 519 | LMG | O7-C10 | 4.78 | 1.47 | 1.34 |
| 24 | B | 607[B] | CLA | CHC-C1C | 4.77 | 1.47 | 1.35 |
| 24 | B | 611 | CLA | CHC-C1C | 4.77 | 1.47 | 1.35 |
| 24 | c | 502 | CLA | CHC-C1C | 4.77 | 1.47 | 1.35 |
| 26 | c | 515 | BCR | C17-C18 | 4.77 | 1.42 | 1.35 |
| 26 | B | 620 | BCR | C24-C23 | 4.77 | 1.47 | 1.33 |
| 24 | B | 616 | CLA | C3D-C2D | -4.77 | 1.30 | 1.39 |
| 26 | b | 619 | BCR | C17-C18 | 4.76 | 1.42 | 1.35 |
| 30 | D | 406 | LHG | O8-C23 | 4.76 | 1.47 | 1.33 |
| 26 | c | 514 | BCR | C17-C18 | 4.76 | 1.42 | 1.35 |
| 24 | C | 504 | CLA | C3D-C2D | -4.76 | 1.30 | 1.39 |
| 24 | c | 507 | CLA | C3D-C2D | -4.75 | 1.30 | 1.39 |
| 26 | b | 620 | BCR | C23-C22 | 4.75 | 1.56 | 1.45 |
| 24 | B | 608 | CLA | CHC-C1C | 4.74 | 1.47 | 1.35 |
| 24 | D | 404 | CLA | C4B-CHC | -4.74 | 1.27 | 1.41 |
| 24 | C | 506 | CLA | C4B-CHC | -4.74 | 1.27 | 1.41 |
| 26 | h | 101 | BCR | C23-C22 | 4.74 | 1.56 | 1.45 |
| 24 | b | 607 | CLA | C4C-C3C | -4.74 | 1.36 | 1.45 |
| 26 | K | 102 | BCR | C23-C22 | 4.74 | 1.56 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | A | 609 | CLA | C4C-C3C | -4.73 | 1.36 | 1.45 |
| 24 | C | 507 | CLA | CHC-C1C | 4.73 | 1.47 | 1.35 |
| 24 | d | 402 | CLA | CHC-C1C | 4.73 | 1.47 | 1.35 |
| 24 | B | 614 | CLA | C4C-C3C | -4.72 | 1.36 | 1.45 |
| 26 | I | 101 | BCR | C23-C22 | 4.72 | 1.56 | 1.45 |
| 24 | C | 508 | CLA | CHC-C1C | 4.72 | 1.47 | 1.35 |
| 24 | b | 615 | CLA | CHC-C1C | 4.71 | 1.47 | 1.35 |
| 24 | c | 504 | CLA | C4B-CHC | -4.71 | 1.27 | 1.41 |
| 24 | B | 610 | CLA | CHC-C1C | 4.70 | 1.47 | 1.35 |
| 24 | A | 606 | CLA | CHC-C1C | 4.70 | 1.47 | 1.35 |
| 24 | A | 607 | CLA | C4B-CHC | -4.70 | 1.27 | 1.41 |
| 29 | C | 519 | LMG | O7-C10 | 4.70 | 1.47 | 1.34 |
| 24 | b | 614 | CLA | C4B-CHC | -4.70 | 1.27 | 1.41 |
| 26 | I | 101 | BCR | C24-C23 | 4.69 | 1.47 | 1.33 |
| 26 | B | 619 | BCR | C17-C18 | 4.69 | 1.42 | 1.35 |
| 24 | b | 617 | CLA | CHC-C1C | 4.69 | 1.47 | 1.35 |
| 24 | B | 607[A] | CLA | CHC-C1C | 4.68 | 1.47 | 1.35 |
| 24 | A | 606 | CLA | C4B-CHC | -4.68 | 1.28 | 1.41 |
| 24 | B | 602 | CLA | CHC-C1C | 4.68 | 1.47 | 1.35 |
| 24 | b | 606 | CLA | C4B-CHC | -4.68 | 1.28 | 1.41 |
| 24 | C | 501 | CLA | C3D-C2D | -4.67 | 1.31 | 1.39 |
| 24 | C | 512 | CLA | CHC-C1C | 4.67 | 1.46 | 1.35 |
| 24 | C | 506 | CLA | CHC-C1C | 4.67 | 1.46 | 1.35 |
| 24 | B | 615 | CLA | CHC-C1C | 4.67 | 1.46 | 1.35 |
| 24 | a | 609 | CLA | C1B-NB | -4.66 | 1.31 | 1.35 |
| 24 | c | 512 | CLA | C4B-CHC | -4.66 | 1.28 | 1.41 |
| 24 | b | 616 | CLA | C4C-C3C | -4.66 | 1.37 | 1.45 |
| 24 | c | 505 | CLA | C4B-CHC | -4.66 | 1.28 | 1.41 |
| 24 | A | 607 | CLA | C1C-NC | -4.66 | 1.30 | 1.37 |
| 24 | c | 513 | CLA | C3D-C2D | -4.65 | 1.31 | 1.39 |
| 24 | c | 505 | CLA | CHC-C1C | 4.65 | 1.46 | 1.35 |
| 24 | a | 615 | CLA | C1C-NC | -4.65 | 1.30 | 1.37 |
| 24 | A | 609 | CLA | CHC-C1C | 4.65 | 1.46 | 1.35 |
| 24 | C | 502 | CLA | CHC-C1C | 4.65 | 1.46 | 1.35 |
| 26 | K | 102 | BCR | C24-C23 | 4.65 | 1.47 | 1.33 |
| 24 | C | 504 | CLA | C4B-CHC | -4.64 | 1.28 | 1.41 |
| 24 | d | 403 | CLA | C4B-CHC | -4.64 | 1.28 | 1.41 |
| 24 | b | 615 | CLA | C4C-C3C | -4.63 | 1.37 | 1.45 |
| 24 | B | 605 | CLA | CHC-C1C | 4.63 | 1.46 | 1.35 |
| 24 | b | 603 | CLA | C4B-CHC | -4.63 | 1.28 | 1.41 |
| 32 | E | 101 | DGD | O2G-C1B | 4.63 | 1.47 | 1.34 |
| 24 | D | 402 | CLA | CHC-C1C | 4.62 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 505 | CLA | C4B-CHC | -4.62 | 1.28 | 1.41 |
| 24 | C | 512 | CLA | C3D-C2D | -4.62 | 1.31 | 1.39 |
| 27 | a | 611 | PL9 | C3-C4 | -4.61 | 1.41 | 1.49 |
| 24 | A | 609 | CLA | C1C-NC | -4.61 | 1.30 | 1.37 |
| 24 | b | 607 | CLA | C4B-CHC | -4.61 | 1.28 | 1.41 |
| 27 | d | 404 | PL9 | C3-C4 | -4.60 | 1.41 | 1.49 |
| 26 | c | 514 | BCR | C23-C22 | 4.60 | 1.55 | 1.45 |
| 24 | A | 606 | CLA | CHD-C4C | -4.60 | 1.27 | 1.41 |
| 24 | b | 615 | CLA | C4B-CHC | -4.60 | 1.28 | 1.41 |
| 29 | z | 101 | LMG | O7-C10 | 4.60 | 1.47 | 1.34 |
| 26 | K | 101 | BCR | C24-C25 | 4.59 | 1.61 | 1.45 |
| 24 | c | 507 | CLA | C4B-CHC | -4.58 | 1.28 | 1.41 |
| 24 | b | 610 | CLA | C4B-CHC | -4.58 | 1.28 | 1.41 |
| 24 | b | 609 | CLA | C4C-C3C | -4.58 | 1.37 | 1.45 |
| 24 | C | 502 | CLA | C4B-CHC | -4.58 | 1.28 | 1.41 |
| 24 | b | 603 | CLA | C1C-NC | -4.58 | 1.31 | 1.37 |
| 24 | d | 402 | CLA | C4B-CHC | -4.57 | 1.28 | 1.41 |
| 24 | b | 617 | CLA | C4B-CHC | -4.57 | 1.28 | 1.41 |
| 32 | d | 405 | DGD | O2G-C1B | 4.57 | 1.47 | 1.34 |
| 24 | c | 506 | CLA | C4B-CHC | -4.57 | 1.28 | 1.41 |
| 28 | X | 101 | SQD | O48-C23 | 4.57 | 1.46 | 1.33 |
| 24 | b | 603 | CLA | CHC-C1C | 4.56 | 1.46 | 1.35 |
| 24 | b | 610 | CLA | CHC-C1C | 4.56 | 1.46 | 1.35 |
| 24 | D | 402 | CLA | CMA-C3A | -4.56 | 1.43 | 1.53 |
| 24 | c | 509 | CLA | C4B-CHC | -4.55 | 1.28 | 1.41 |
| 29 | A | 613 | LMG | O7-C10 | 4.55 | 1.47 | 1.34 |
| 24 | B | 613 | CLA | CHC-C1C | 4.55 | 1.46 | 1.35 |
| 24 | b | 612 | CLA | C4B-CHC | -4.55 | 1.28 | 1.41 |
| 24 | B | 612 | CLA | CHC-C1C | 4.55 | 1.46 | 1.35 |
| 24 | c | 510 | CLA | C4B-CHC | -4.55 | 1.28 | 1.41 |
| 24 | B | 608 | CLA | C4B-CHC | -4.55 | 1.28 | 1.41 |
| 24 | c | 502 | CLA | C4B-CHC | -4.54 | 1.28 | 1.41 |
| 26 | c | 521 | BCR | C24-C23 | 4.54 | 1.46 | 1.33 |
| 24 | a | 606 | CLA | CHD-C4C | -4.54 | 1.27 | 1.41 |
| 24 | C | 504 | CLA | C4C-C3C | -4.54 | 1.37 | 1.45 |
| 24 | c | 511 | CLA | C1C-NC | -4.53 | 1.31 | 1.37 |
| 24 | B | 610 | CLA | C4B-CHC | -4.53 | 1.28 | 1.41 |
| 27 | a | 611 | PL9 | C7-C3 | 4.53 | 1.55 | 1.51 |
| 30 | L | 101 | LHG | O8-C23 | 4.53 | 1.46 | 1.33 |
| 24 | C | 507 | CLA | C4B-CHC | -4.53 | 1.28 | 1.41 |
| 24 | C | 512 | CLA | C4C-C3C | -4.53 | 1.37 | 1.45 |
| 24 | B | 607[B] | CLA | C4B-CHC | -4.53 | 1.28 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 511 | CLA | C4B-CHC | -4.52 | 1.28 | 1.41 |
| 24 | C | 505 | CLA | CHC-C1C | 4.52 | 1.46 | 1.35 |
| 28 | x | 101 | SQD | O48-C23 | 4.52 | 1.46 | 1.33 |
| 24 | D | 402 | CLA | C4B-CHC | -4.51 | 1.28 | 1.41 |
| 26 | K | 102 | BCR | C17-C18 | 4.50 | 1.41 | 1.35 |
| 26 | H | 101 | BCR | C24-C25 | 4.50 | 1.61 | 1.45 |
| 30 | E | 102 | LHG | O7-C7 | 4.50 | 1.47 | 1.34 |
| 24 | A | 607 | CLA | CHD-C4C | -4.49 | 1.28 | 1.41 |
| 24 | B | 606 | CLA | C4B-CHC | -4.49 | 1.28 | 1.41 |
| 24 | d | 403 | CLA | C1C-NC | -4.49 | 1.31 | 1.37 |
| 24 | B | 608 | CLA | CHD-C4C | -4.49 | 1.28 | 1.41 |
| 26 | T | 101 | BCR | C17-C18 | 4.49 | 1.41 | 1.35 |
| 24 | C | 503 | CLA | C4C-C3C | -4.49 | 1.37 | 1.45 |
| 28 | X | 101 | SQD | O47-C7 | 4.48 | 1.46 | 1.34 |
| 26 | k | 101 | BCR | C24-C25 | 4.48 | 1.61 | 1.45 |
| 24 | c | 507 | CLA | CHC-C1C | 4.48 | 1.46 | 1.35 |
| 28 | a | 614 | SQD | O48-C23 | 4.48 | 1.46 | 1.33 |
| 24 | b | 616 | CLA | CHD-C4C | -4.47 | 1.28 | 1.41 |
| 28 | A | 614 | SQD | O48-C23 | 4.47 | 1.46 | 1.33 |
| 26 | k | 101 | BCR | C23-C22 | 4.47 | 1.55 | 1.45 |
| 30 | D | 407 | LHG | O7-C7 | 4.47 | 1.46 | 1.34 |
| 33 | v | 201 | HEM | C3B-CAB | 4.46 | 1.57 | 1.47 |
| 24 | b | 612 | CLA | CHC-C1C | 4.46 | 1.46 | 1.35 |
| 27 | A | 611 | PL9 | C3-C4 | -4.46 | 1.42 | 1.49 |
| 24 | b | 609 | CLA | C1C-NC | -4.46 | 1.31 | 1.37 |
| 24 | c | 511 | CLA | C4C-C3C | -4.46 | 1.37 | 1.45 |
| 24 | B | 612 | CLA | C4B-CHC | -4.45 | 1.28 | 1.41 |
| 24 | C | 503 | CLA | CHD-C4C | -4.45 | 1.28 | 1.41 |
| 24 | b | 608[B] | CLA | C4B-CHC | -4.45 | 1.28 | 1.41 |
| 28 | x | 101 | SQD | O47-C7 | 4.45 | 1.46 | 1.34 |
| 24 | b | 616 | CLA | C4B-CHC | -4.44 | 1.28 | 1.41 |
| 24 | b | 617 | CLA | CHD-C4C | -4.44 | 1.28 | 1.41 |
| 24 | B | 608 | CLA | C4C-C3C | -4.44 | 1.37 | 1.45 |
| 24 | c | 508 | CLA | C4B-CHC | -4.44 | 1.28 | 1.41 |
| 24 | b | 609 | CLA | C4B-CHC | -4.44 | 1.28 | 1.41 |
| 24 | B | 602 | CLA | C4B-CHC | -4.43 | 1.28 | 1.41 |
| 29 | Z | 101 | LMG | O7-C10 | 4.43 | 1.46 | 1.34 |
| 24 | B | 615 | CLA | C4B-CHC | -4.43 | 1.28 | 1.41 |
| 24 | c | 513 | CLA | C4B-CHC | -4.43 | 1.28 | 1.41 |
| 24 | b | 609 | CLA | CHD-C4C | -4.43 | 1.28 | 1.41 |
| 28 | b | 601 | SQD | O47-C7 | 4.43 | 1.46 | 1.34 |
| 24 | C | 504 | CLA | C1C-NC | -4.42 | 1.31 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 30 | e | 101 | LHG | O7-C7 | 4.42 | 1.46 | 1.34 |
| 24 | B | 607[A] | CLA | C4B-CHC | -4.41 | 1.28 | 1.41 |
| 28 | b | 601 | SQD | O48-C23 | 4.41 | 1.46 | 1.33 |
| 24 | C | 507 | CLA | CHD-C4C | -4.41 | 1.28 | 1.41 |
| 24 | A | 606 | CLA | C4C-C3C | -4.41 | 1.37 | 1.45 |
| 28 | l | 101 | SQD | O47-C7 | 4.41 | 1.46 | 1.34 |
| 24 | B | 617 | CLA | C3D-C2D | -4.41 | 1.31 | 1.39 |
| 28 | B | 622 | SQD | O48-C23 | 4.40 | 1.46 | 1.33 |
| 24 | A | 609 | CLA | CHD-C4C | -4.40 | 1.28 | 1.41 |
| 24 | d | 402 | CLA | C1C-NC | -4.40 | 1.31 | 1.37 |
| 28 | B | 622 | SQD | O47-C7 | 4.40 | 1.46 | 1.34 |
| 24 | B | 614 | CLA | CHC-C1C | 4.40 | 1.46 | 1.35 |
| 26 | B | 620 | BCR | C40-C30 | 4.40 | 1.62 | 1.53 |
| 24 | c | 511 | CLA | CHD-C4C | -4.40 | 1.28 | 1.41 |
| 24 | d | 403 | CLA | CHD-C4C | -4.39 | 1.28 | 1.41 |
| 30 | e | 101 | LHG | O8-C23 | 4.39 | 1.46 | 1.33 |
| 26 | K | 102 | BCR | C40-C30 | 4.39 | 1.62 | 1.53 |
| 24 | a | 607 | CLA | C4B-CHC | -4.39 | 1.28 | 1.41 |
| 24 | b | 607 | CLA | CHD-C4C | -4.39 | 1.28 | 1.41 |
| 24 | a | 609 | CLA | CHD-C4C | -4.39 | 1.28 | 1.41 |
| 24 | C | 503 | CLA | C4B-CHC | -4.39 | 1.28 | 1.41 |
| 24 | B | 609 | CLA | CHC-C1C | 4.38 | 1.46 | 1.35 |
| 28 | L | 102 | SQD | O47-C7 | 4.38 | 1.46 | 1.34 |
| 24 | B | 616 | CLA | C4C-C3C | -4.38 | 1.37 | 1.45 |
| 24 | C | 512 | CLA | CHD-C4C | -4.38 | 1.28 | 1.41 |
| 24 | C | 509 | CLA | CHC-C1C | 4.36 | 1.46 | 1.35 |
| 24 | B | 604 | CLA | CHC-C1C | 4.36 | 1.46 | 1.35 |
| 33 | V | 201 | HEM | C3C-CAC | 4.36 | 1.56 | 1.47 |
| 24 | b | 618 | CLA | CHC-C1C | 4.36 | 1.46 | 1.35 |
| 24 | c | 509 | CLA | C4C-C3C | -4.36 | 1.37 | 1.45 |
| 24 | B | 606 | CLA | C4C-C3C | -4.35 | 1.37 | 1.45 |
| 24 | c | 511 | CLA | C4B-CHC | -4.35 | 1.28 | 1.41 |
| 24 | b | 604 | CLA | C1C-NC | -4.35 | 1.31 | 1.37 |
| 30 | E | 102 | LHG | O8-C23 | 4.35 | 1.46 | 1.33 |
| 32 | C | 515 | DGD | O2G-C1B | 4.35 | 1.46 | 1.34 |
| 24 | D | 404 | CLA | CHD-C4C | -4.34 | 1.28 | 1.41 |
| 24 | B | 616 | CLA | CHD-C4C | -4.34 | 1.28 | 1.41 |
| 24 | a | 607 | CLA | C1C-NC | -4.34 | 1.31 | 1.37 |
| 24 | b | 606 | CLA | C1D-C2D | -4.34 | 1.32 | 1.42 |
| 24 | b | 603 | CLA | C1B-NB | -4.33 | 1.31 | 1.35 |
| 30 | a | 616 | LHG | O8-C23 | 4.33 | 1.46 | 1.33 |
| 29 | b | 622 | LMG | O7-C10 | 4.33 | 1.46 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 618 | CLA | C4C-C3C | -4.33 | 1.37 | 1.45 |
| 26 | I | 101 | BCR | C24-C25 | 4.32 | 1.60 | 1.45 |
| 24 | b | 615 | CLA | CHD-C4C | -4.32 | 1.28 | 1.41 |
| 24 | b | 608[A] | CLA | C4B-CHC | -4.32 | 1.29 | 1.41 |
| 24 | b | 611 | CLA | CHD-C4C | -4.32 | 1.28 | 1.41 |
| 24 | b | 613 | CLA | CHD-C4C | -4.32 | 1.28 | 1.41 |
| 24 | C | 509 | CLA | CHD-C4C | -4.31 | 1.28 | 1.41 |
| 29 | B | 621 | LMG | O7-C10 | 4.31 | 1.46 | 1.34 |
| 24 | D | 403 | CLA | CMA-C3A | -4.31 | 1.43 | 1.53 |
| 24 | c | 513 | CLA | C4C-C3C | -4.31 | 1.37 | 1.45 |
| 24 | B | 610 | CLA | CHD-C4C | -4.31 | 1.28 | 1.41 |
| 24 | C | 504 | CLA | CMA-C3A | -4.31 | 1.43 | 1.53 |
| 24 | a | 607 | CLA | CHD-C4C | -4.31 | 1.28 | 1.41 |
| 24 | b | 613 | CLA | CHC-C1C | 4.30 | 1.46 | 1.35 |
| 24 | b | 616 | CLA | C1C-NC | -4.30 | 1.31 | 1.37 |
| 26 | c | 521 | BCR | C40-C30 | 4.30 | 1.62 | 1.53 |
| 26 | b | 619 | BCR | C24-C25 | 4.29 | 1.60 | 1.45 |
| 28 | A | 614 | SQD | O47-C7 | 4.28 | 1.46 | 1.34 |
| 24 | b | 611 | CLA | C4B-CHC | -4.28 | 1.29 | 1.41 |
| 24 | B | 611 | CLA | C4B-CHC | -4.28 | 1.29 | 1.41 |
| 24 | B | 605 | CLA | C1C-NC | -4.28 | 1.31 | 1.37 |
| 24 | a | 615 | CLA | CHD-C4C | -4.28 | 1.28 | 1.41 |
| 28 | a | 614 | SQD | O47-C7 | 4.28 | 1.46 | 1.34 |
| 24 | c | 501 | CLA | C4B-CHC | -4.28 | 1.29 | 1.41 |
| 24 | D | 403 | CLA | CBD-CGD | -4.27 | 1.39 | 1.52 |
| 24 | b | 604 | CLA | C4B-CHC | -4.27 | 1.29 | 1.41 |
| 24 | b | 605 | CLA | CMA-C3A | -4.27 | 1.44 | 1.53 |
| 24 | B | 603 | CLA | C4B-CHC | -4.27 | 1.29 | 1.41 |
| 24 | B | 608 | CLA | CAA-C2A | -4.27 | 1.46 | 1.54 |
| 24 | C | 504 | CLA | CHC-C1C | 4.27 | 1.45 | 1.35 |
| 24 | A | 609 | CLA | C4B-CHC | -4.26 | 1.29 | 1.41 |
| 24 | a | 615 | CLA | CHC-C1C | 4.26 | 1.45 | 1.35 |
| 24 | b | 605 | CLA | CHC-C1C | 4.26 | 1.45 | 1.35 |
| 24 | C | 513 | CLA | C4B-CHC | -4.26 | 1.29 | 1.41 |
| 26 | c | 515 | BCR | C24-C25 | 4.26 | 1.60 | 1.45 |
| 24 | B | 607[B] | CLA | CMA-C3A | -4.26 | 1.44 | 1.53 |
| 24 | b | 607 | CLA | C1C-NC | -4.26 | 1.31 | 1.37 |
| 24 | D | 403 | CLA | CHD-C4C | -4.25 | 1.28 | 1.41 |
| 24 | c | 510 | CLA | CHD-C4C | -4.25 | 1.28 | 1.41 |
| 24 | C | 510 | CLA | CHC-C1C | 4.25 | 1.45 | 1.35 |
| 24 | B | 612 | CLA | CHD-C4C | -4.25 | 1.28 | 1.41 |
| 24 | B | 614 | CLA | CMA-C3A | -4.24 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 32 | h | 102 | DGD | O2G-C1B | 4.24 | 1.46 | 1.34 |
| 24 | B | 612 | CLA | C1C-NC | -4.24 | 1.31 | 1.37 |
| 24 | b | 616 | CLA | C1A-CHA | -4.24 | 1.25 | 1.43 |
| 24 | B | 606 | CLA | CHD-C4C | -4.24 | 1.28 | 1.41 |
| 26 | h | 101 | BCR | C24-C25 | 4.23 | 1.60 | 1.45 |
| 24 | D | 403 | CLA | CHC-C1C | 4.23 | 1.45 | 1.35 |
| 24 | B | 614 | CLA | CHD-C4C | -4.23 | 1.28 | 1.41 |
| 24 | B | 616 | CLA | C4B-CHC | -4.23 | 1.29 | 1.41 |
| 24 | C | 509 | CLA | C1C-NC | -4.23 | 1.31 | 1.37 |
| 33 | E | 103 | HEM | C3B-C2B | -4.23 | 1.34 | 1.40 |
| 24 | B | 608 | CLA | CMA-C3A | -4.23 | 1.44 | 1.53 |
| 24 | C | 513 | CLA | C4C-C3C | -4.22 | 1.37 | 1.45 |
| 24 | d | 403 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 33 | v | 201 | HEM | C3C-CAC | 4.22 | 1.56 | 1.47 |
| 26 | B | 618 | BCR | C24-C25 | 4.22 | 1.60 | 1.45 |
| 24 | B | 607[A] | CLA | CMA-C3A | -4.22 | 1.44 | 1.53 |
| 26 | B | 620 | BCR | C24-C25 | 4.22 | 1.60 | 1.45 |
| 24 | B | 602 | CLA | CHD-C4C | -4.22 | 1.28 | 1.41 |
| 30 | d | 407 | LHG | O7-C7 | 4.22 | 1.46 | 1.34 |
| 24 | B | 607[B] | CLA | C4C-C3C | -4.22 | 1.37 | 1.45 |
| 24 | c | 503 | CLA | C4B-CHC | -4.22 | 1.29 | 1.41 |
| 24 | b | 614 | CLA | CMA-C3A | -4.22 | 1.44 | 1.53 |
| 24 | B | 605 | CLA | CHD-C4C | -4.22 | 1.28 | 1.41 |
| 24 | b | 606 | CLA | CHD-C4C | -4.22 | 1.28 | 1.41 |
| 24 | D | 404 | CLA | CMA-C3A | -4.21 | 1.44 | 1.53 |
| 24 | c | 507 | CLA | CHD-C4C | -4.21 | 1.28 | 1.41 |
| 24 | B | 613 | CLA | CMA-C3A | -4.21 | 1.44 | 1.53 |
| 26 | a | 610 | BCR | C24-C25 | 4.21 | 1.60 | 1.45 |
| 24 | B | 613 | CLA | C1C-NC | -4.21 | 1.31 | 1.37 |
| 24 | c | 509 | CLA | CMA-C3A | -4.21 | 1.44 | 1.53 |
| 24 | B | 607[B] | CLA | CHD-C4C | -4.21 | 1.28 | 1.41 |
| 24 | a | 609 | CLA | C4B-CHC | -4.21 | 1.29 | 1.41 |
| 24 | c | 509 | CLA | CHD-C4C | -4.20 | 1.28 | 1.41 |
| 24 | A | 606 | CLA | CMA-C3A | -4.20 | 1.44 | 1.53 |
| 24 | b | 605 | CLA | CHD-C4C | -4.20 | 1.28 | 1.41 |
| 26 | A | 610 | BCR | C17-C18 | 4.20 | 1.41 | 1.35 |
| 24 | C | 511 | CLA | CHD-C4C | -4.19 | 1.28 | 1.41 |
| 24 | A | 606 | CLA | C1D-C2D | -4.19 | 1.33 | 1.42 |
| 24 | B | 602 | CLA | C4C-C3C | -4.19 | 1.37 | 1.45 |
| 24 | B | 613 | CLA | C1A-CHA | -4.19 | 1.25 | 1.43 |
| 32 | H | 102 | DGD | O1G-C1A | 4.19 | 1.45 | 1.33 |
| 24 | C | 502 | CLA | C4C-C3C | -4.19 | 1.37 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 33 | v | 201 | HEM | C3C-C2C | -4.18 | 1.34 | 1.40 |
| 30 | d | 406 | LHG | O8-C23 | 4.18 | 1.45 | 1.33 |
| 24 | C | 508 | CLA | CHD-C4C | -4.18 | 1.28 | 1.41 |
| 24 | B | 614 | CLA | C1C-NC | -4.18 | 1.31 | 1.37 |
| 24 | C | 501 | CLA | C4B-CHC | -4.18 | 1.29 | 1.41 |
| 32 | c | 517 | DGD | O2G-C2G | -4.18 | 1.36 | 1.46 |
| 24 | B | 607[A] | CLA | CHD-C4C | -4.17 | 1.28 | 1.41 |
| 24 | B | 617 | CLA | CHC-C1C | 4.17 | 1.45 | 1.35 |
| 32 | c | 518 | DGD | O2G-C2G | -4.17 | 1.36 | 1.46 |
| 24 | B | 617 | CLA | C1C-NC | -4.17 | 1.31 | 1.37 |
| 24 | C | 507 | CLA | C1C-NC | -4.17 | 1.31 | 1.37 |
| 24 | b | 617 | CLA | C1C-NC | -4.17 | 1.31 | 1.37 |
| 24 | B | 605 | CLA | CMA-C3A | -4.16 | 1.44 | 1.53 |
| 24 | C | 501 | CLA | CMA-C3A | -4.16 | 1.44 | 1.53 |
| 24 | b | 606 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 24 | D | 403 | CLA | C1C-NC | -4.16 | 1.31 | 1.37 |
| 24 | c | 503 | CLA | C4C-C3C | -4.16 | 1.37 | 1.45 |
| 24 | b | 618 | CLA | CHD-C4C | -4.16 | 1.29 | 1.41 |
| 24 | B | 611 | CLA | CMA-C3A | -4.16 | 1.44 | 1.53 |
| 24 | C | 506 | CLA | C1C-NC | -4.16 | 1.31 | 1.37 |
| 30 | l | 102 | LHG | O7-C7 | 4.16 | 1.46 | 1.34 |
| 24 | B | 607[A] | CLA | C4C-C3C | -4.16 | 1.37 | 1.45 |
| 24 | b | 614 | CLA | CHD-C4C | -4.15 | 1.29 | 1.41 |
| 24 | C | 511 | CLA | CMA-C3A | -4.15 | 1.44 | 1.53 |
| 32 | c | 518 | DGD | O2G-C1B | 4.15 | 1.46 | 1.34 |
| 24 | C | 502 | CLA | C1C-NC | -4.15 | 1.31 | 1.37 |
| 24 | b | 611 | CLA | C4C-C3C | -4.15 | 1.37 | 1.45 |
| 26 | b | 621 | BCR | C40-C30 | 4.14 | 1.61 | 1.53 |
| 24 | c | 502 | CLA | CMA-C3A | -4.14 | 1.44 | 1.53 |
| 26 | c | 521 | BCR | C24-C25 | 4.14 | 1.59 | 1.45 |
| 24 | b | 605 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 30 | d | 406 | LHG | O7-C7 | 4.14 | 1.46 | 1.34 |
| 28 | A | 612 | SQD | O47-C7 | 4.14 | 1.46 | 1.34 |
| 24 | c | 504 | CLA | CMA-C3A | -4.14 | 1.44 | 1.53 |
| 24 | d | 402 | CLA | CMA-C3A | -4.13 | 1.44 | 1.53 |
| 24 | C | 510 | CLA | CHD-C4C | -4.13 | 1.29 | 1.41 |
| 29 | c | 519 | LMG | O8-C28 | 4.13 | 1.45 | 1.33 |
| 24 | a | 615 | CLA | C4C-C3C | -4.13 | 1.37 | 1.45 |
| 24 | C | 510 | CLA | CMA-C3A | -4.13 | 1.44 | 1.53 |
| 28 | l | 101 | SQD | O48-C23 | 4.13 | 1.45 | 1.33 |
| 33 | E | 103 | HEM | C3C-CAC | 4.13 | 1.56 | 1.47 |
| 28 | a | 612 | SQD | O47-C7 | 4.13 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 30 | A | 615 | LHG | O7-C7 | 4.13 | 1.45 | 1.34 |
| 24 | b | 613 | CLA | C1C-NC | -4.13 | 1.31 | 1.37 |
| 32 | C | 516 | DGD | O1G-C1A | 4.13 | 1.45 | 1.33 |
| 24 | b | 608[A] | CLA | CMA-C3A | -4.13 | 1.44 | 1.53 |
| 26 | F | 101 | BCR | C2-C3 | 4.12 | 1.62 | 1.52 |
| 24 | c | 511 | CLA | CMA-C3A | -4.12 | 1.44 | 1.53 |
| 24 | b | 609 | CLA | CMA-C3A | -4.12 | 1.44 | 1.53 |
| 26 | C | 514 | BCR | C24-C25 | 4.12 | 1.59 | 1.45 |
| 24 | B | 617 | CLA | CHD-C4C | -4.12 | 1.29 | 1.41 |
| 29 | C | 518 | LMG | O6-C1 | 4.12 | 1.52 | 1.41 |
| 26 | k | 101 | BCR | C40-C30 | 4.12 | 1.61 | 1.53 |
| 24 | b | 608[B] | CLA | CMA-C3A | -4.12 | 1.44 | 1.53 |
| 24 | B | 615 | CLA | CHD-C4C | -4.12 | 1.29 | 1.41 |
| 24 | c | 512 | CLA | C4C-C3C | -4.12 | 1.37 | 1.45 |
| 24 | B | 617 | CLA | C4C-C3C | -4.12 | 1.37 | 1.45 |
| 28 | L | 102 | SQD | O48-C23 | 4.11 | 1.45 | 1.33 |
| 24 | A | 609 | CLA | CMA-C3A | -4.11 | 1.44 | 1.53 |
| 24 | c | 503 | CLA | CHD-C4C | -4.11 | 1.29 | 1.41 |
| 29 | j | 101 | LMG | O7-C10 | 4.11 | 1.45 | 1.34 |
| 24 | c | 507 | CLA | C1C-NC | -4.11 | 1.31 | 1.37 |
| 24 | a | 615 | CLA | CMA-C3A | -4.11 | 1.44 | 1.53 |
| 24 | C | 502 | CLA | CMA-C3A | -4.11 | 1.44 | 1.53 |
| 24 | c | 506 | CLA | CMA-C3A | -4.11 | 1.44 | 1.53 |
| 32 | c | 516 | DGD | O2G-C2G | -4.10 | 1.36 | 1.46 |
| 32 | c | 516 | DGD | O2G-C1B | 4.10 | 1.45 | 1.34 |
| 24 | B | 605 | CLA | C4C-C3C | -4.10 | 1.38 | 1.45 |
| 32 | C | 516 | DGD | O2G-C1B | 4.10 | 1.45 | 1.34 |
| 24 | d | 402 | CLA | C4C-C3C | -4.10 | 1.38 | 1.45 |
| 27 | A | 611 | PL9 | C7-C3 | 4.10 | 1.55 | 1.51 |
| 24 | c | 512 | CLA | CHD-C4C | -4.09 | 1.29 | 1.41 |
| 24 | C | 508 | CLA | C4C-C3C | -4.09 | 1.38 | 1.45 |
| 24 | a | 606 | CLA | C4C-C3C | -4.09 | 1.38 | 1.45 |
| 24 | a | 609 | CLA | C1C-NC | -4.09 | 1.31 | 1.37 |
| 33 | V | 201 | HEM | C3B-CAB | 4.09 | 1.56 | 1.47 |
| 30 | A | 615 | LHG | O8-C23 | 4.08 | 1.45 | 1.33 |
| 24 | B | 612 | CLA | C4C-C3C | -4.08 | 1.38 | 1.45 |
| 32 | c | 517 | DGD | O1G-C1A | 4.08 | 1.45 | 1.33 |
| 24 | C | 506 | CLA | CHD-C4C | -4.08 | 1.29 | 1.41 |
| 24 | d | 402 | CLA | CHD-C4C | -4.08 | 1.29 | 1.41 |
| 30 | D | 407 | LHG | O8-C23 | 4.08 | 1.45 | 1.33 |
| 24 | b | 607 | CLA | CMA-C3A | -4.08 | 1.44 | 1.53 |
| 26 | b | 621 | BCR | C24-C25 | 4.08 | 1.59 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | B | 613 | CLA | CHD-C4C | -4.07 | 1.29 | 1.41 |
| 32 | C | 517 | DGD | O2G-C2G | -4.07 | 1.36 | 1.46 |
| 24 | B | 602 | CLA | C1C-NC | -4.07 | 1.31 | 1.37 |
| 32 | E | 101 | DGD | O1G-C1A | 4.07 | 1.45 | 1.33 |
| 29 | C | 518 | LMG | O8-C28 | 4.07 | 1.45 | 1.33 |
| 24 | a | 609 | CLA | O2A-CGA | 4.07 | 1.45 | 1.33 |
| 24 | b | 604 | CLA | CHD-C4C | -4.06 | 1.29 | 1.41 |
| 24 | B | 604 | CLA | C1C-NC | -4.06 | 1.31 | 1.37 |
| 24 | D | 404 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 24 | B | 615 | CLA | C4C-C3C | -4.06 | 1.38 | 1.45 |
| 24 | B | 603 | CLA | CHD-C4C | -4.06 | 1.29 | 1.41 |
| 24 | b | 615 | CLA | C1C-NC | -4.05 | 1.31 | 1.37 |
| 32 | H | 102 | DGD | O2G-C2G | -4.05 | 1.36 | 1.46 |
| 24 | B | 605 | CLA | C1D-C2D | -4.05 | 1.33 | 1.42 |
| 26 | K | 102 | BCR | C24-C25 | 4.05 | 1.59 | 1.45 |
| 24 | b | 610 | CLA | CMA-C3A | -4.05 | 1.44 | 1.53 |
| 24 | B | 608 | CLA | C1C-NC | -4.05 | 1.31 | 1.37 |
| 24 | C | 510 | CLA | C4C-C3C | -4.05 | 1.38 | 1.45 |
| 24 | B | 611 | CLA | C1C-NC | -4.05 | 1.31 | 1.37 |
| 24 | c | 504 | CLA | C4C-C3C | -4.05 | 1.38 | 1.45 |
| 28 | a | 612 | SQD | O48-C23 | 4.04 | 1.45 | 1.33 |
| 24 | B | 611 | CLA | CHD-C4C | -4.04 | 1.29 | 1.41 |
| 26 | f | 101 | BCR | C27-C26 | 4.04 | 1.59 | 1.51 |
| 32 | c | 516 | DGD | O1G-C1A | 4.04 | 1.45 | 1.33 |
| 24 | B | 604 | CLA | C1D-C2D | -4.04 | 1.33 | 1.42 |
| 32 | d | 405 | DGD | O1G-C1A | 4.04 | 1.45 | 1.33 |
| 24 | B | 604 | CLA | CHD-C4C | -4.04 | 1.29 | 1.41 |
| 24 | b | 604 | CLA | C4C-C3C | -4.03 | 1.38 | 1.45 |
| 26 | a | 610 | BCR | C17-C18 | 4.03 | 1.41 | 1.35 |
| 24 | a | 609 | CLA | CMA-C3A | -4.03 | 1.44 | 1.53 |
| 24 | C | 501 | CLA | C1A-CHA | -4.03 | 1.26 | 1.43 |
| 24 | B | 609 | CLA | CMA-C3A | -4.03 | 1.44 | 1.53 |
| 24 | b | 605 | CLA | C4C-C3C | -4.03 | 1.38 | 1.45 |
| 24 | C | 511 | CLA | C4C-C3C | -4.03 | 1.38 | 1.45 |
| 24 | B | 615 | CLA | C1C-NC | -4.03 | 1.31 | 1.37 |
| 24 | b | 613 | CLA | C4C-C3C | -4.03 | 1.38 | 1.45 |
| 26 | H | 101 | BCR | C40-C30 | 4.02 | 1.61 | 1.53 |
| 24 | c | 504 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 30 | L | 101 | LHG | O7-C7 | 4.02 | 1.45 | 1.34 |
| 27 | D | 405 | PL9 | C6-C1 | -4.02 | 1.41 | 1.48 |
| 29 | c | 520 | LMG | O8-C28 | 4.02 | 1.45 | 1.33 |
| 32 | C | 517 | DGD | O1G-C1A | 4.02 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | c | 512 | CLA | C1C-NC | -4.02 | 1.31 | 1.37 |
| 24 | b | 604 | CLA | CMA-C3A | -4.01 | 1.44 | 1.53 |
| 24 | a | 609 | CLA | C4C-C3C | -4.01 | 1.38 | 1.45 |
| 24 | B | 612 | CLA | CMA-C3A | -4.01 | 1.44 | 1.53 |
| 30 | a | 616 | LHG | O7-C7 | 4.01 | 1.45 | 1.34 |
| 25 | d | 401 | PHO | C3B-C4B | 4.00 | 1.51 | 1.43 |
| 26 | c | 521 | BCR | C12-C13 | 4.00 | 1.54 | 1.45 |
| 24 | B | 610 | CLA | CMA-C3A | -4.00 | 1.44 | 1.53 |
| 29 | D | 408 | LMG | O7-C10 | 4.00 | 1.45 | 1.34 |
| 32 | C | 517 | DGD | O2G-C1B | 4.00 | 1.45 | 1.34 |
| 33 | E | 103 | HEM | C3C-C2C | -4.00 | 1.34 | 1.40 |
| 24 | B | 613 | CLA | C1D-C2D | -4.00 | 1.33 | 1.42 |
| 24 | a | 606 | CLA | CMA-C3A | -4.00 | 1.44 | 1.53 |
| 24 | B | 612 | CLA | C1A-CHA | -4.00 | 1.26 | 1.43 |
| 24 | c | 509 | CLA | C1C-NC | -3.99 | 1.31 | 1.37 |
| 24 | b | 608[B] | CLA | CHD-C4C | -3.99 | 1.29 | 1.41 |
| 24 | C | 509 | CLA | C4C-C3C | -3.99 | 1.38 | 1.45 |
| 24 | c | 508 | CLA | C1C-NC | -3.98 | 1.31 | 1.37 |
| 24 | B | 608 | CLA | C1D-C2D | -3.98 | 1.33 | 1.42 |
| 24 | c | 504 | CLA | CHD-C4C | -3.98 | 1.29 | 1.41 |
| 33 | E | 103 | HEM | C3B-CAB | 3.98 | 1.56 | 1.47 |
| 28 | A | 612 | SQD | O48-C23 | 3.97 | 1.44 | 1.33 |
| 24 | D | 402 | CLA | C1C-NC | -3.97 | 1.31 | 1.37 |
| 24 | C | 507 | CLA | O2A-CGA | 3.97 | 1.44 | 1.33 |
| 24 | b | 606 | CLA | CMA-C3A | -3.97 | 1.44 | 1.53 |
| 24 | b | 611 | CLA | C1C-NC | -3.97 | 1.31 | 1.37 |
| 24 | b | 613 | CLA | CMA-C3A | -3.97 | 1.44 | 1.53 |
| 24 | c | 510 | CLA | C4C-C3C | -3.97 | 1.38 | 1.45 |
| 24 | c | 502 | CLA | C1C-NC | -3.97 | 1.31 | 1.37 |
| 24 | b | 605 | CLA | C1D-C2D | -3.97 | 1.33 | 1.42 |
| 24 | B | 615 | CLA | CMA-C3A | -3.97 | 1.44 | 1.53 |
| 24 | C | 504 | CLA | CHD-C4C | -3.97 | 1.29 | 1.41 |
| 24 | a | 606 | CLA | C1D-C2D | -3.96 | 1.33 | 1.42 |
| 24 | c | 507 | CLA | O2A-CGA | 3.96 | 1.44 | 1.33 |
| 24 | A | 606 | CLA | C1C-NC | -3.96 | 1.31 | 1.37 |
| 24 | b | 612 | CLA | CMA-C3A | -3.96 | 1.44 | 1.53 |
| 24 | C | 508 | CLA | C1D-C2D | -3.96 | 1.33 | 1.42 |
| 24 | C | 513 | CLA | CHD-C4C | -3.96 | 1.29 | 1.41 |
| 24 | b | 611 | CLA | CMA-C3A | -3.96 | 1.44 | 1.53 |
| 24 | C | 505 | CLA | CMA-C3A | -3.95 | 1.44 | 1.53 |
| 24 | C | 509 | CLA | CMA-C3A | -3.95 | 1.44 | 1.53 |
| 24 | b | 615 | CLA | CMA-C3A | -3.95 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 512 | CLA | C1C-NC | -3.95 | 1.31 | 1.37 |
| 24 | c | 507 | CLA | C4C-C3C | -3.95 | 1.38 | 1.45 |
| 24 | c | 501 | CLA | CHD-C4C | -3.95 | 1.29 | 1.41 |
| 24 | C | 502 | CLA | CHD-C4C | -3.95 | 1.29 | 1.41 |
| 26 | c | 514 | BCR | C24-C25 | 3.94 | 1.59 | 1.45 |
| 26 | B | 618 | BCR | C2-C3 | 3.94 | 1.62 | 1.52 |
| 32 | c | 518 | DGD | O6E-C5E | 3.94 | 1.53 | 1.44 |
| 26 | T | 101 | BCR | C2-C3 | 3.94 | 1.62 | 1.52 |
| 24 | A | 606 | CLA | C1A-CHA | -3.94 | 1.26 | 1.43 |
| 24 | c | 512 | CLA | CMA-C3A | -3.94 | 1.44 | 1.53 |
| 33 | e | 102 | HEM | C3C-CAC | 3.94 | 1.55 | 1.47 |
| 24 | b | 605 | CLA | C1C-NC | -3.94 | 1.31 | 1.37 |
| 24 | C | 508 | CLA | C1C-NC | -3.93 | 1.31 | 1.37 |
| 24 | b | 606 | CLA | C1C-NC | -3.93 | 1.31 | 1.37 |
| 24 | b | 614 | CLA | C1A-CHA | -3.93 | 1.26 | 1.43 |
| 24 | A | 609 | CLA | C1A-CHA | -3.93 | 1.26 | 1.43 |
| 24 | d | 403 | CLA | CMA-C3A | -3.93 | 1.44 | 1.53 |
| 24 | C | 502 | CLA | O2A-CGA | 3.93 | 1.44 | 1.33 |
| 24 | b | 616 | CLA | CMA-C3A | -3.93 | 1.44 | 1.53 |
| 24 | b | 617 | CLA | CMA-C3A | -3.93 | 1.44 | 1.53 |
| 32 | c | 518 | DGD | O1G-C1A | 3.93 | 1.44 | 1.33 |
| 32 | C | 516 | DGD | O2G-C2G | -3.93 | 1.36 | 1.46 |
| 29 | D | 408 | LMG | O6-C1 | 3.93 | 1.51 | 1.41 |
| 32 | h | 102 | DGD | O1G-C1A | 3.92 | 1.44 | 1.33 |
| 24 | D | 404 | CLA | C1C-NC | -3.92 | 1.31 | 1.37 |
| 24 | c | 508 | CLA | CHD-C4C | -3.92 | 1.29 | 1.41 |
| 24 | c | 506 | CLA | CHD-C4C | -3.92 | 1.29 | 1.41 |
| 24 | B | 607[B] | CLA | C1C-NC | -3.92 | 1.32 | 1.37 |
| 24 | b | 610 | CLA | C1C-NC | -3.92 | 1.32 | 1.37 |
| 24 | B | 610 | CLA | C1D-C2D | -3.92 | 1.33 | 1.42 |
| 33 | e | 102 | HEM | C3B-CAB | 3.91 | 1.55 | 1.47 |
| 24 | B | 602 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 24 | B | 610 | CLA | C1C-NC | -3.91 | 1.32 | 1.37 |
| 24 | c | 508 | CLA | C4C-C3C | -3.91 | 1.38 | 1.45 |
| 24 | b | 610 | CLA | CHD-C4C | -3.91 | 1.29 | 1.41 |
| 24 | c | 502 | CLA | CHD-C4C | -3.91 | 1.29 | 1.41 |
| 24 | D | 402 | CLA | CBD-CGD | -3.91 | 1.40 | 1.52 |
| 24 | C | 508 | CLA | CMA-C3A | -3.91 | 1.44 | 1.53 |
| 24 | B | 607[A] | CLA | C1C-NC | -3.91 | 1.32 | 1.37 |
| 24 | b | 612 | CLA | C1C-NC | -3.91 | 1.32 | 1.37 |
| 24 | c | 510 | CLA | CMA-C3A | -3.90 | 1.44 | 1.53 |
| 24 | B | 606 | CLA | CMA-C3A | -3.90 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 32 | E | 101 | DGD | O6E-C5E | 3.90 | 1.53 | 1.44 |
| 30 | D | 406 | LHG | O7-C7 | 3.90 | 1.45 | 1.34 |
| 24 | b | 608[A] | CLA | CHD-C4C | -3.90 | 1.29 | 1.41 |
| 32 | C | 515 | DGD | O1G-C1A | 3.90 | 1.44 | 1.33 |
| 26 | t | 101 | BCR | C24-C25 | 3.90 | 1.58 | 1.45 |
| 24 | D | 402 | CLA | C1A-CHA | -3.90 | 1.26 | 1.43 |
| 24 | A | 607 | CLA | O2A-CGA | 3.90 | 1.44 | 1.33 |
| 24 | B | 617 | CLA | O2A-CGA | 3.90 | 1.44 | 1.33 |
| 24 | B | 610 | CLA | C1A-CHA | -3.90 | 1.26 | 1.43 |
| 24 | c | 501 | CLA | CMA-C3A | -3.89 | 1.44 | 1.53 |
| 24 | c | 510 | CLA | CAA-C2A | -3.89 | 1.46 | 1.54 |
| 24 | C | 501 | CLA | CHD-C4C | -3.89 | 1.29 | 1.41 |
| 24 | c | 505 | CLA | CMA-C3A | -3.89 | 1.44 | 1.53 |
| 24 | a | 615 | CLA | C1A-CHA | -3.89 | 1.27 | 1.43 |
| 24 | b | 612 | CLA | CHD-C4C | -3.89 | 1.29 | 1.41 |
| 24 | b | 604 | CLA | CAA-C2A | -3.88 | 1.46 | 1.54 |
| 33 | V | 201 | HEM | C3B-C2B | -3.88 | 1.35 | 1.40 |
| 24 | c | 508 | CLA | CMA-C3A | -3.88 | 1.44 | 1.53 |
| 32 | h | 102 | DGD | O2G-C2G | -3.88 | 1.36 | 1.46 |
| 24 | b | 613 | CLA | C1D-C2D | -3.88 | 1.33 | 1.42 |
| 24 | C | 511 | CLA | C1D-C2D | -3.88 | 1.33 | 1.42 |
| 27 | d | 404 | PL9 | C6-C1 | -3.88 | 1.41 | 1.48 |
| 24 | C | 506 | CLA | C1D-C2D | -3.88 | 1.33 | 1.42 |
| 29 | A | 613 | LMG | O8-C28 | 3.87 | 1.44 | 1.33 |
| 24 | b | 613 | CLA | CBD-CGD | -3.87 | 1.40 | 1.52 |
| 29 | j | 101 | LMG | O6-C1 | 3.86 | 1.51 | 1.41 |
| 24 | c | 502 | CLA | C4C-C3C | -3.86 | 1.38 | 1.45 |
| 24 | a | 606 | CLA | C1C-NC | -3.86 | 1.32 | 1.37 |
| 24 | C | 503 | CLA | C1C-NC | -3.86 | 1.32 | 1.37 |
| 24 | C | 508 | CLA | C1A-CHA | -3.86 | 1.27 | 1.43 |
| 24 | c | 506 | CLA | C1C-NC | -3.86 | 1.32 | 1.37 |
| 24 | c | 503 | CLA | CMA-C3A | -3.86 | 1.44 | 1.53 |
| 24 | C | 513 | CLA | C1C-NC | -3.85 | 1.32 | 1.37 |
| 24 | B | 606 | CLA | C1C-NC | -3.85 | 1.32 | 1.37 |
| 24 | b | 609 | CLA | C1A-CHA | -3.85 | 1.27 | 1.43 |
| 29 | a | 613 | LMG | O8-C28 | 3.85 | 1.44 | 1.33 |
| 24 | A | 609 | CLA | CBD-CGD | -3.85 | 1.40 | 1.52 |
| 26 | c | 515 | BCR | C12-C13 | 3.85 | 1.54 | 1.45 |
| 29 | b | 622 | LMG | O6-C1 | 3.85 | 1.51 | 1.41 |
| 24 | c | 513 | CLA | CHD-C4C | -3.85 | 1.29 | 1.41 |
| 32 | h | 102 | DGD | O6E-C5E | 3.84 | 1.53 | 1.44 |
| 26 | b | 619 | BCR | C40-C30 | 3.84 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 614 | CLA | CAA-C2A | -3.84 | 1.47 | 1.54 |
| 26 | T | 101 | BCR | C24-C25 | 3.84 | 1.58 | 1.45 |
| 24 | c | 504 | CLA | C1D-C2D | -3.83 | 1.33 | 1.42 |
| 26 | I | 101 | BCR | C12-C13 | 3.83 | 1.54 | 1.45 |
| 24 | B | 603 | CLA | C4C-C3C | -3.83 | 1.38 | 1.45 |
| 26 | f | 101 | BCR | C2-C3 | 3.83 | 1.62 | 1.52 |
| 24 | c | 505 | CLA | CHD-C4C | -3.83 | 1.29 | 1.41 |
| 24 | C | 506 | CLA | C4C-C3C | -3.83 | 1.38 | 1.45 |
| 32 | H | 102 | DGD | O2G-C1B | 3.83 | 1.45 | 1.34 |
| 32 | C | 516 | DGD | O6E-C5E | 3.83 | 1.53 | 1.44 |
| 24 | A | 607 | CLA | C4C-C3C | -3.82 | 1.38 | 1.45 |
| 24 | b | 606 | CLA | C4C-C3C | -3.82 | 1.38 | 1.45 |
| 24 | c | 505 | CLA | C1D-C2D | -3.82 | 1.33 | 1.42 |
| 26 | B | 619 | BCR | C2-C3 | 3.82 | 1.62 | 1.52 |
| 26 | c | 521 | BCR | C2-C3 | 3.81 | 1.62 | 1.52 |
| 24 | B | 611 | CLA | C1D-C2D | -3.81 | 1.33 | 1.42 |
| 24 | b | 608[B] | CLA | C4C-C3C | -3.81 | 1.38 | 1.45 |
| 24 | b | 611 | CLA | O2D-CGD | 3.81 | 1.42 | 1.33 |
| 24 | B | 608 | CLA | C1A-CHA | -3.81 | 1.27 | 1.43 |
| 24 | C | 501 | CLA | O2A-CGA | 3.81 | 1.44 | 1.33 |
| 24 | b | 618 | CLA | CAA-C2A | -3.80 | 1.47 | 1.54 |
| 24 | B | 603 | CLA | CMA-C3A | -3.80 | 1.45 | 1.53 |
| 24 | c | 504 | CLA | C1C-NC | -3.80 | 1.32 | 1.37 |
| 24 | b | 616 | CLA | C1D-C2D | -3.80 | 1.34 | 1.42 |
| 24 | b | 618 | CLA | C1C-NC | -3.80 | 1.32 | 1.37 |
| 24 | B | 602 | CLA | CMA-C3A | -3.80 | 1.45 | 1.53 |
| 24 | C | 507 | CLA | C4C-C3C | -3.80 | 1.38 | 1.45 |
| 24 | C | 504 | CLA | C1A-CHA | -3.80 | 1.27 | 1.43 |
| 24 | B | 604 | CLA | O2A-CGA | 3.80 | 1.44 | 1.33 |
| 24 | D | 402 | CLA | CHD-C4C | -3.79 | 1.30 | 1.41 |
| 24 | c | 505 | CLA | C1C-NC | -3.79 | 1.32 | 1.37 |
| 24 | c | 507 | CLA | CMA-C3A | -3.79 | 1.45 | 1.53 |
| 26 | c | 514 | BCR | C40-C30 | 3.79 | 1.61 | 1.53 |
| 32 | C | 515 | DGD | O6E-C5E | 3.79 | 1.53 | 1.44 |
| 24 | a | 607 | CLA | C4C-C3C | -3.78 | 1.38 | 1.45 |
| 24 | C | 506 | CLA | O2D-CGD | 3.78 | 1.42 | 1.33 |
| 24 | a | 607 | CLA | CMA-C3A | -3.78 | 1.45 | 1.53 |
| 24 | c | 513 | CLA | CMA-C3A | -3.78 | 1.45 | 1.53 |
| 24 | D | 404 | CLA | C4C-C3C | -3.77 | 1.38 | 1.45 |
| 24 | B | 612 | CLA | C1D-C2D | -3.77 | 1.34 | 1.42 |
| 26 | t | 101 | BCR | C17-C18 | 3.77 | 1.40 | 1.35 |
| 29 | c | 519 | LMG | O6-C1 | 3.77 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | a | 615 | CLA | C1D-C2D | -3.77 | 1.34 | 1.42 |
| 24 | b | 614 | CLA | C1C-NC | -3.77 | 1.32 | 1.37 |
| 24 | b | 618 | CLA | CMA-C3A | -3.77 | 1.45 | 1.53 |
| 24 | A | 609 | CLA | C1D-C2D | -3.77 | 1.34 | 1.42 |
| 24 | B | 613 | CLA | CAA-C2A | -3.76 | 1.47 | 1.54 |
| 32 | c | 517 | DGD | O2G-C1B | 3.76 | 1.44 | 1.34 |
| 24 | C | 505 | CLA | CAA-C2A | -3.76 | 1.47 | 1.54 |
| 26 | c | 515 | BCR | C40-C30 | 3.76 | 1.61 | 1.53 |
| 24 | d | 402 | CLA | C1D-C2D | -3.76 | 1.34 | 1.42 |
| 24 | C | 513 | CLA | O2A-CGA | 3.76 | 1.44 | 1.33 |
| 32 | C | 515 | DGD | O2G-C2G | -3.76 | 1.37 | 1.46 |
| 26 | C | 514 | BCR | C40-C30 | 3.76 | 1.61 | 1.53 |
| 29 | B | 621 | LMG | O8-C28 | 3.76 | 1.44 | 1.33 |
| 24 | b | 610 | CLA | C4C-C3C | -3.75 | 1.38 | 1.45 |
| 24 | b | 615 | CLA | CAA-C2A | -3.75 | 1.47 | 1.54 |
| 24 | B | 603 | CLA | C1C-NC | -3.75 | 1.32 | 1.37 |
| 24 | B | 604 | CLA | C4C-C3C | -3.75 | 1.38 | 1.45 |
| 24 | c | 512 | CLA | O2A-CGA | 3.75 | 1.44 | 1.33 |
| 33 | e | 102 | HEM | C3B-C2B | -3.75 | 1.35 | 1.40 |
| 26 | F | 101 | BCR | C40-C30 | 3.75 | 1.61 | 1.53 |
| 24 | c | 506 | CLA | O2A-CGA | 3.75 | 1.44 | 1.33 |
| 29 | b | 622 | LMG | O8-C28 | 3.75 | 1.44 | 1.33 |
| 24 | c | 509 | CLA | O2A-CGA | 3.74 | 1.44 | 1.33 |
| 24 | c | 513 | CLA | C1C-NC | -3.74 | 1.32 | 1.37 |
| 24 | b | 604 | CLA | C1D-C2D | -3.74 | 1.34 | 1.42 |
| 32 | d | 405 | DGD | O6E-C5E | 3.73 | 1.53 | 1.44 |
| 26 | B | 620 | BCR | C2-C3 | 3.73 | 1.61 | 1.52 |
| 24 | B | 610 | CLA | O2A-CGA | 3.72 | 1.44 | 1.33 |
| 24 | c | 511 | CLA | O2A-CGA | 3.72 | 1.44 | 1.33 |
| 24 | A | 607 | CLA | C1A-CHA | -3.72 | 1.27 | 1.43 |
| 24 | b | 604 | CLA | C1A-CHA | -3.72 | 1.27 | 1.43 |
| 24 | a | 609 | CLA | C1D-C2D | -3.72 | 1.34 | 1.42 |
| 24 | c | 503 | CLA | CBD-CGD | -3.72 | 1.40 | 1.52 |
| 24 | C | 507 | CLA | C1D-C2D | -3.72 | 1.34 | 1.42 |
| 24 | C | 511 | CLA | O2A-CGA | 3.72 | 1.44 | 1.33 |
| 29 | D | 408 | LMG | O8-C28 | 3.72 | 1.44 | 1.33 |
| 24 | B | 616 | CLA | C1C-NC | -3.71 | 1.32 | 1.37 |
| 27 | A | 611 | PL9 | C6-C1 | -3.71 | 1.42 | 1.48 |
| 24 | c | 502 | CLA | O2A-CGA | 3.70 | 1.44 | 1.33 |
| 24 | B | 610 | CLA | C4C-C3C | -3.70 | 1.38 | 1.45 |
| 29 | C | 519 | LMG | O8-C28 | 3.70 | 1.44 | 1.33 |
| 32 | H | 102 | DGD | O6E-C5E | 3.70 | 1.53 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 507 | CLA | CMA-C3A | -3.70 | 1.45 | 1.53 |
| 24 | b | 608[A] | CLA | O2A-CGA | 3.70 | 1.44 | 1.33 |
| 24 | c | 503 | CLA | O2A-CGA | 3.69 | 1.44 | 1.33 |
| 26 | K | 102 | BCR | C2-C3 | 3.69 | 1.61 | 1.52 |
| 24 | B | 607[B] | CLA | C1D-C2D | -3.69 | 1.34 | 1.42 |
| 24 | b | 614 | CLA | C4C-C3C | -3.69 | 1.38 | 1.45 |
| 24 | B | 609 | CLA | C1C-NC | -3.69 | 1.32 | 1.37 |
| 24 | b | 608[A] | CLA | C4C-C3C | -3.68 | 1.38 | 1.45 |
| 26 | B | 618 | BCR | C40-C30 | 3.68 | 1.61 | 1.53 |
| 24 | b | 609 | CLA | CAA-C2A | -3.68 | 1.47 | 1.54 |
| 24 | a | 615 | CLA | CBD-CGD | -3.68 | 1.40 | 1.52 |
| 32 | C | 517 | DGD | O6E-C5E | 3.68 | 1.53 | 1.44 |
| 24 | c | 513 | CLA | C3D-CAD | 3.68 | 1.55 | 1.46 |
| 24 | A | 606 | CLA | CAA-C2A | -3.68 | 1.47 | 1.54 |
| 26 | c | 515 | BCR | C2-C3 | 3.68 | 1.61 | 1.52 |
| 24 | c | 501 | CLA | C1C-NC | -3.68 | 1.32 | 1.37 |
| 24 | C | 503 | CLA | CMA-C3A | -3.68 | 1.45 | 1.53 |
| 27 | a | 611 | PL9 | C36-C34 | 3.67 | 1.58 | 1.51 |
| 33 | e | 102 | HEM | C3C-C2C | -3.67 | 1.35 | 1.40 |
| 24 | B | 614 | CLA | C1A-CHA | -3.67 | 1.27 | 1.43 |
| 24 | b | 612 | CLA | C1A-CHA | -3.67 | 1.27 | 1.43 |
| 24 | C | 512 | CLA | C1D-C2D | -3.67 | 1.34 | 1.42 |
| 24 | b | 611 | CLA | CAA-C2A | -3.67 | 1.47 | 1.54 |
| 24 | B | 614 | CLA | CBD-CGD | -3.66 | 1.40 | 1.52 |
| 24 | D | 404 | CLA | CBD-CGD | -3.66 | 1.41 | 1.52 |
| 24 | C | 513 | CLA | C1A-CHA | -3.66 | 1.27 | 1.43 |
| 26 | K | 102 | BCR | C12-C13 | 3.66 | 1.53 | 1.45 |
| 24 | B | 613 | CLA | MG-NA | -3.66 | 1.97 | 2.06 |
| 24 | B | 605 | CLA | C1A-CHA | -3.66 | 1.27 | 1.43 |
| 24 | D | 403 | CLA | C1D-C2D | -3.66 | 1.34 | 1.42 |
| 24 | C | 513 | CLA | CMA-C3A | -3.66 | 1.45 | 1.53 |
| 24 | A | 607 | CLA | CMA-C3A | -3.66 | 1.45 | 1.53 |
| 26 | I | 101 | BCR | C40-C30 | 3.66 | 1.61 | 1.53 |
| 24 | C | 511 | CLA | C1C-NC | -3.66 | 1.32 | 1.37 |
| 24 | d | 403 | CLA | CBD-CGD | -3.66 | 1.41 | 1.52 |
| 24 | b | 608[A] | CLA | CBD-CGD | -3.66 | 1.41 | 1.52 |
| 24 | c | 508 | CLA | C1D-C2D | -3.65 | 1.34 | 1.42 |
| 24 | b | 608[B] | CLA | C1A-CHA | -3.65 | 1.28 | 1.43 |
| 24 | C | 503 | CLA | CBD-CGD | -3.65 | 1.41 | 1.52 |
| 26 | B | 619 | BCR | C27-C26 | 3.65 | 1.58 | 1.51 |
| 24 | d | 402 | CLA | C1A-CHA | -3.65 | 1.28 | 1.43 |
| 24 | b | 618 | CLA | O2A-CGA | 3.65 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | c | 505 | CLA | C4C-C3C | -3.65 | 1.38 | 1.45 |
| 24 | b | 612 | CLA | O2A-CGA | 3.65 | 1.44 | 1.33 |
| 24 | C | 509 | CLA | CBD-CGD | -3.65 | 1.41 | 1.52 |
| 29 | Z | 101 | LMG | O6-C1 | 3.65 | 1.51 | 1.41 |
| 24 | b | 608[B] | CLA | O2A-CGA | 3.64 | 1.44 | 1.33 |
| 24 | C | 511 | CLA | C1B-CHB | 3.64 | 1.51 | 1.41 |
| 24 | a | 615 | CLA | MG-NA | -3.64 | 1.97 | 2.06 |
| 24 | b | 603 | CLA | CMA-C3A | -3.64 | 1.45 | 1.53 |
| 24 | B | 617 | CLA | C1B-CHB | 3.64 | 1.51 | 1.41 |
| 26 | A | 610 | BCR | C12-C13 | 3.64 | 1.53 | 1.45 |
| 24 | B | 614 | CLA | CAA-C2A | -3.64 | 1.47 | 1.54 |
| 24 | a | 606 | CLA | C1A-CHA | -3.64 | 1.28 | 1.43 |
| 24 | a | 615 | CLA | CAA-C2A | -3.64 | 1.47 | 1.54 |
| 24 | B | 604 | CLA | C1A-CHA | -3.63 | 1.28 | 1.43 |
| 24 | C | 506 | CLA | CMA-C3A | -3.63 | 1.45 | 1.53 |
| 24 | C | 510 | CLA | C1A-CHA | -3.63 | 1.28 | 1.43 |
| 24 | C | 501 | CLA | C3D-CAD | 3.62 | 1.55 | 1.46 |
| 24 | b | 603 | CLA | C1D-C2D | -3.62 | 1.34 | 1.42 |
| 24 | C | 512 | CLA | CMA-C3A | -3.62 | 1.45 | 1.53 |
| 24 | b | 608[B] | CLA | CBD-CGD | -3.62 | 1.41 | 1.52 |
| 27 | a | 611 | PL9 | C6-C1 | -3.61 | 1.42 | 1.48 |
| 24 | A | 606 | CLA | C3D-CAD | 3.61 | 1.55 | 1.46 |
| 24 | b | 608[B] | CLA | C1C-NC | -3.61 | 1.32 | 1.37 |
| 26 | a | 610 | BCR | C2-C3 | 3.61 | 1.61 | 1.52 |
| 24 | c | 503 | CLA | C1C-NC | -3.61 | 1.32 | 1.37 |
| 24 | b | 613 | CLA | O2A-CGA | 3.61 | 1.43 | 1.33 |
| 24 | B | 602 | CLA | CBD-CGD | -3.61 | 1.41 | 1.52 |
| 24 | B | 607[A] | CLA | O2A-CGA | 3.61 | 1.43 | 1.33 |
| 24 | B | 617 | CLA | C3D-CAD | 3.61 | 1.55 | 1.46 |
| 24 | C | 502 | CLA | C3D-CAD | 3.61 | 1.55 | 1.46 |
| 29 | C | 519 | LMG | O6-C1 | 3.61 | 1.51 | 1.41 |
| 24 | B | 616 | CLA | CMA-C3A | -3.61 | 1.45 | 1.53 |
| 24 | A | 607 | CLA | MG-NA | -3.61 | 1.97 | 2.06 |
| 29 | z | 101 | LMG | O6-C1 | 3.61 | 1.51 | 1.41 |
| 32 | d | 405 | DGD | O2G-C2G | -3.60 | 1.37 | 1.46 |
| 24 | b | 610 | CLA | CAA-C2A | -3.60 | 1.47 | 1.54 |
| 32 | c | 517 | DGD | O6E-C5E | 3.60 | 1.53 | 1.44 |
| 26 | B | 618 | BCR | C1-C6 | -3.60 | 1.48 | 1.53 |
| 24 | b | 618 | CLA | C1D-C2D | -3.60 | 1.34 | 1.42 |
| 26 | b | 620 | BCR | C2-C3 | 3.60 | 1.61 | 1.52 |
| 26 | b | 621 | BCR | C2-C3 | 3.60 | 1.61 | 1.52 |
| 24 | b | 614 | CLA | C1D-C2D | -3.60 | 1.34 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | A | 607 | CLA | CBD-CGD | -3.60 | 1.41 | 1.52 |
| 24 | C | 511 | CLA | O2D-CGD | 3.60 | 1.42 | 1.33 |
| 24 | D | 402 | CLA | C1D-C2D | -3.60 | 1.34 | 1.42 |
| 24 | b | 603 | CLA | O2A-CGA | 3.60 | 1.43 | 1.33 |
| 24 | b | 608[A] | CLA | C1A-CHA | -3.60 | 1.28 | 1.43 |
| 24 | c | 512 | CLA | C1A-CHA | -3.60 | 1.28 | 1.43 |
| 24 | B | 603 | CLA | C1A-CHA | -3.60 | 1.28 | 1.43 |
| 27 | A | 611 | PL9 | C36-C34 | 3.60 | 1.58 | 1.51 |
| 26 | b | 621 | BCR | C24-C23 | 3.59 | 1.43 | 1.33 |
| 24 | c | 501 | CLA | O2A-CGA | 3.59 | 1.43 | 1.33 |
| 26 | h | 101 | BCR | C2-C3 | 3.59 | 1.61 | 1.52 |
| 24 | b | 604 | CLA | O2D-CGD | 3.59 | 1.42 | 1.33 |
| 24 | D | 404 | CLA | C1A-CHA | -3.59 | 1.28 | 1.43 |
| 24 | c | 508 | CLA | CAA-C2A | -3.59 | 1.47 | 1.54 |
| 24 | C | 503 | CLA | C1D-C2D | -3.59 | 1.34 | 1.42 |
| 24 | d | 403 | CLA | C1A-CHA | -3.58 | 1.28 | 1.43 |
| 26 | c | 514 | BCR | C2-C3 | 3.58 | 1.61 | 1.52 |
| 24 | b | 618 | CLA | C1A-CHA | -3.58 | 1.28 | 1.43 |
| 29 | c | 520 | LMG | O6-C1 | 3.58 | 1.51 | 1.41 |
| 24 | C | 505 | CLA | C1C-NC | -3.57 | 1.32 | 1.37 |
| 32 | C | 515 | DGD | O6D-C5D | 3.57 | 1.53 | 1.44 |
| 24 | C | 508 | CLA | O2A-CGA | 3.57 | 1.43 | 1.33 |
| 24 | b | 603 | CLA | C1B-CHB | 3.57 | 1.50 | 1.41 |
| 24 | B | 607[A] | CLA | C1D-C2D | -3.57 | 1.34 | 1.42 |
| 24 | B | 606 | CLA | O2A-CGA | 3.57 | 1.43 | 1.33 |
| 24 | B | 603 | CLA | C1D-C2D | -3.57 | 1.34 | 1.42 |
| 24 | A | 609 | CLA | C3B-CAB | 3.57 | 1.55 | 1.47 |
| 24 | b | 613 | CLA | C1A-CHA | -3.57 | 1.28 | 1.43 |
| 24 | B | 607[A] | CLA | C1A-CHA | -3.57 | 1.28 | 1.43 |
| 24 | c | 505 | CLA | C1B-CHB | 3.57 | 1.50 | 1.41 |
| 26 | b | 619 | BCR | C2-C3 | 3.56 | 1.61 | 1.52 |
| 24 | B | 607[B] | CLA | C1A-CHA | -3.56 | 1.28 | 1.43 |
| 26 | C | 514 | BCR | C4-C5 | 3.56 | 1.58 | 1.51 |
| 26 | A | 610 | BCR | C2-C3 | 3.56 | 1.61 | 1.52 |
| 24 | D | 402 | CLA | O2A-CGA | 3.56 | 1.43 | 1.33 |
| 26 | K | 101 | BCR | C40-C30 | 3.56 | 1.60 | 1.53 |
| 24 | a | 606 | CLA | CAA-C2A | -3.56 | 1.47 | 1.54 |
| 24 | D | 402 | CLA | C4C-C3C | -3.56 | 1.38 | 1.45 |
| 24 | d | 402 | CLA | MG-NA | -3.55 | 1.97 | 2.06 |
| 26 | a | 610 | BCR | C40-C30 | 3.55 | 1.60 | 1.53 |
| 24 | B | 606 | CLA | C1D-C2D | -3.55 | 1.34 | 1.42 |
| 24 | b | 610 | CLA | C3D-CAD | 3.55 | 1.55 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | c | 510 | CLA | C1C-NC | -3.55 | 1.32 | 1.37 |
| 24 | B | 607[B] | CLA | CAA-C2A | -3.55 | 1.47 | 1.54 |
| 24 | C | 511 | CLA | C1A-CHA | -3.55 | 1.28 | 1.43 |
| 24 | A | 606 | CLA | O2A-CGA | 3.54 | 1.43 | 1.33 |
| 26 | F | 101 | BCR | C27-C26 | 3.54 | 1.58 | 1.51 |
| 26 | t | 101 | BCR | C2-C3 | 3.54 | 1.61 | 1.52 |
| 24 | c | 504 | CLA | C1A-CHA | -3.54 | 1.28 | 1.43 |
| 24 | b | 607 | CLA | CAA-C2A | -3.54 | 1.47 | 1.54 |
| 24 | B | 606 | CLA | O2D-CGD | 3.54 | 1.41 | 1.33 |
| 24 | b | 610 | CLA | C1A-CHA | -3.54 | 1.28 | 1.43 |
| 24 | B | 610 | CLA | CAA-C2A | -3.54 | 1.47 | 1.54 |
| 24 | c | 501 | CLA | C4C-C3C | -3.53 | 1.38 | 1.45 |
| 24 | b | 618 | CLA | C1B-CHB | 3.53 | 1.50 | 1.41 |
| 24 | b | 607 | CLA | O2A-CGA | 3.53 | 1.43 | 1.33 |
| 24 | A | 607 | CLA | CAA-C2A | -3.53 | 1.47 | 1.54 |
| 24 | B | 607[B] | CLA | O2A-CGA | 3.53 | 1.43 | 1.33 |
| 26 | T | 101 | BCR | C40-C30 | 3.53 | 1.60 | 1.53 |
| 24 | b | 611 | CLA | C1D-C2D | -3.53 | 1.34 | 1.42 |
| 24 | D | 403 | CLA | C1A-CHA | -3.53 | 1.28 | 1.43 |
| 24 | a | 607 | CLA | C1A-CHA | -3.53 | 1.28 | 1.43 |
| 24 | C | 501 | CLA | C1C-NC | -3.53 | 1.32 | 1.37 |
| 24 | c | 507 | CLA | C1D-C2D | -3.52 | 1.34 | 1.42 |
| 24 | a | 607 | CLA | CBD-CGD | -3.52 | 1.41 | 1.52 |
| 24 | a | 607 | CLA | O2A-CGA | 3.52 | 1.43 | 1.33 |
| 24 | C | 510 | CLA | CAA-C2A | -3.52 | 1.47 | 1.54 |
| 32 | E | 101 | DGD | O2G-C2G | -3.51 | 1.37 | 1.46 |
| 24 | c | 506 | CLA | C4C-C3C | -3.51 | 1.39 | 1.45 |
| 33 | V | 201 | HEM | C3C-C2C | -3.51 | 1.35 | 1.40 |
| 24 | B | 615 | CLA | C1D-C2D | -3.51 | 1.34 | 1.42 |
| 24 | c | 508 | CLA | C3D-CAD | 3.51 | 1.55 | 1.46 |
| 26 | H | 101 | BCR | C2-C3 | 3.51 | 1.61 | 1.52 |
| 24 | B | 616 | CLA | C1A-CHA | -3.51 | 1.28 | 1.43 |
| 24 | b | 608[B] | CLA | C1D-C2D | -3.50 | 1.34 | 1.42 |
| 24 | C | 509 | CLA | C1D-C2D | -3.50 | 1.34 | 1.42 |
| 24 | b | 608[A] | CLA | C1C-NC | -3.50 | 1.32 | 1.37 |
| 24 | B | 614 | CLA | C1B-CHB | 3.50 | 1.50 | 1.41 |
| 24 | C | 505 | CLA | CHD-C4C | -3.50 | 1.30 | 1.41 |
| 26 | f | 101 | BCR | C40-C30 | 3.50 | 1.60 | 1.53 |
| 26 | C | 514 | BCR | C2-C3 | 3.50 | 1.61 | 1.52 |
| 26 | A | 610 | BCR | C27-C26 | 3.50 | 1.57 | 1.51 |
| 24 | C | 510 | CLA | MG-NA | -3.49 | 1.98 | 2.06 |
| 24 | D | 402 | CLA | MG-NA | -3.49 | 1.98 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | d | 403 | CLA | C1B-CHB | 3.49 | 1.50 | 1.41 |
| 24 | B | 611 | CLA | O2A-CGA | 3.49 | 1.43 | 1.33 |
| 24 | a | 606 | CLA | O2A-CGA | 3.49 | 1.43 | 1.33 |
| 24 | c | 501 | CLA | O2D-CGD | 3.49 | 1.41 | 1.33 |
| 24 | B | 609 | CLA | C1B-CHB | 3.49 | 1.50 | 1.41 |
| 24 | b | 611 | CLA | C3D-CAD | 3.49 | 1.54 | 1.46 |
| 26 | h | 101 | BCR | C40-C30 | 3.49 | 1.60 | 1.53 |
| 24 | B | 617 | CLA | CAA-C2A | -3.49 | 1.47 | 1.54 |
| 24 | B | 603 | CLA | O2A-CGA | 3.48 | 1.43 | 1.33 |
| 24 | B | 617 | CLA | CMA-C3A | -3.48 | 1.45 | 1.53 |
| 24 | b | 605 | CLA | CBD-CGD | -3.48 | 1.41 | 1.52 |
| 24 | A | 609 | CLA | O2A-CGA | 3.48 | 1.43 | 1.33 |
| 24 | b | 606 | CLA | C1A-CHA | -3.48 | 1.28 | 1.43 |
| 24 | b | 617 | CLA | O2A-CGA | 3.48 | 1.43 | 1.33 |
| 24 | d | 402 | CLA | CAA-C2A | -3.47 | 1.47 | 1.54 |
| 24 | B | 609 | CLA | CHD-C4C | -3.47 | 1.31 | 1.41 |
| 26 | b | 620 | BCR | C27-C26 | 3.47 | 1.57 | 1.51 |
| 24 | B | 616 | CLA | CBD-CGD | -3.47 | 1.41 | 1.52 |
| 24 | C | 504 | CLA | C3D-CAD | 3.47 | 1.54 | 1.46 |
| 24 | C | 512 | CLA | CAA-C2A | -3.47 | 1.47 | 1.54 |
| 24 | B | 616 | CLA | O2A-CGA | 3.47 | 1.43 | 1.33 |
| 26 | F | 101 | BCR | C12-C13 | 3.46 | 1.53 | 1.45 |
| 24 | b | 609 | CLA | CBD-CGD | -3.46 | 1.41 | 1.52 |
| 24 | c | 508 | CLA | C1A-CHA | -3.46 | 1.28 | 1.43 |
| 24 | C | 513 | CLA | C1D-C2D | -3.46 | 1.34 | 1.42 |
| 24 | a | 609 | CLA | C1B-CHB | 3.46 | 1.50 | 1.41 |
| 24 | C | 513 | CLA | O2D-CGD | 3.45 | 1.41 | 1.33 |
| 24 | b | 607 | CLA | C1D-C2D | -3.45 | 1.34 | 1.42 |
| 24 | C | 502 | CLA | C1A-CHA | -3.45 | 1.28 | 1.43 |
| 24 | C | 508 | CLA | CAA-C2A | -3.45 | 1.47 | 1.54 |
| 32 | c | 518 | DGD | C3D-C2D | -3.45 | 1.43 | 1.52 |
| 24 | c | 501 | CLA | C3D-CAD | 3.45 | 1.54 | 1.46 |
| 24 | C | 512 | CLA | O2A-CGA | 3.44 | 1.43 | 1.33 |
| 29 | B | 621 | LMG | O6-C1 | 3.44 | 1.50 | 1.41 |
| 24 | c | 509 | CLA | CAA-C2A | -3.44 | 1.47 | 1.54 |
| 32 | c | 516 | DGD | O6E-C5E | 3.44 | 1.52 | 1.44 |
| 24 | B | 611 | CLA | CBD-CGD | -3.44 | 1.41 | 1.52 |
| 32 | c | 516 | DGD | C3D-C2D | -3.44 | 1.43 | 1.52 |
| 24 | c | 509 | CLA | C1A-CHA | -3.43 | 1.28 | 1.43 |
| 25 | A | 608 | PHO | C3B-C4B | 3.43 | 1.50 | 1.43 |
| 26 | I | 101 | BCR | C2-C3 | 3.43 | 1.61 | 1.52 |
| 24 | B | 609 | CLA | C1A-CHA | -3.43 | 1.28 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 607 | CLA | C1A-CHA | -3.43 | 1.28 | 1.43 |
| 24 | B | 617 | CLA | CBD-CGD | -3.43 | 1.41 | 1.52 |
| 24 | b | 606 | CLA | O2D-CGD | 3.42 | 1.41 | 1.33 |
| 24 | B | 607[A] | CLA | CAA-C2A | -3.42 | 1.47 | 1.54 |
| 32 | C | 515 | DGD | C3D-C2D | -3.42 | 1.43 | 1.52 |
| 24 | B | 615 | CLA | C1A-CHA | -3.42 | 1.28 | 1.43 |
| 26 | f | 101 | BCR | C4-C5 | 3.41 | 1.57 | 1.51 |
| 24 | c | 507 | CLA | C3D-CAD | 3.41 | 1.54 | 1.46 |
| 26 | t | 101 | BCR | C40-C30 | 3.41 | 1.60 | 1.53 |
| 27 | A | 611 | PL9 | C21-C19 | 3.41 | 1.58 | 1.51 |
| 24 | B | 612 | CLA | CBD-CGD | -3.41 | 1.41 | 1.52 |
| 24 | b | 615 | CLA | C3D-CAD | 3.41 | 1.54 | 1.46 |
| 24 | c | 507 | CLA | C1A-CHA | -3.41 | 1.29 | 1.43 |
| 24 | c | 506 | CLA | CAA-C2A | -3.41 | 1.47 | 1.54 |
| 24 | b | 611 | CLA | O2A-CGA | 3.41 | 1.43 | 1.33 |
| 24 | C | 505 | CLA | C3D-CAD | 3.41 | 1.54 | 1.46 |
| 26 | k | 101 | BCR | C4-C5 | 3.41 | 1.57 | 1.51 |
| 24 | d | 402 | CLA | CBD-CGD | -3.40 | 1.41 | 1.52 |
| 24 | a | 606 | CLA | CBD-CGD | -3.40 | 1.41 | 1.52 |
| 24 | c | 511 | CLA | C1B-CHB | 3.40 | 1.50 | 1.41 |
| 32 | H | 102 | DGD | C3D-C2D | -3.40 | 1.43 | 1.52 |
| 24 | b | 618 | CLA | O2D-CGD | 3.40 | 1.41 | 1.33 |
| 24 | b | 617 | CLA | C1D-C2D | -3.40 | 1.34 | 1.42 |
| 24 | b | 615 | CLA | C1A-CHA | -3.40 | 1.29 | 1.43 |
| 24 | C | 504 | CLA | CAA-C2A | -3.39 | 1.47 | 1.54 |
| 24 | b | 616 | CLA | CAA-C2A | -3.39 | 1.47 | 1.54 |
| 24 | d | 402 | CLA | O2A-CGA | 3.39 | 1.43 | 1.33 |
| 24 | c | 509 | CLA | C3D-CAD | 3.39 | 1.54 | 1.46 |
| 24 | b | 614 | CLA | O2A-CGA | 3.39 | 1.43 | 1.33 |
| 24 | B | 617 | CLA | C1A-CHA | -3.39 | 1.29 | 1.43 |
| 24 | b | 608[A] | CLA | C1D-C2D | -3.39 | 1.34 | 1.42 |
| 24 | c | 510 | CLA | C1B-CHB | 3.39 | 1.50 | 1.41 |
| 24 | B | 605 | CLA | O2A-CGA | 3.39 | 1.43 | 1.33 |
| 24 | b | 618 | CLA | C3D-CAD | 3.38 | 1.54 | 1.46 |
| 24 | C | 503 | CLA | O2A-CGA | 3.38 | 1.43 | 1.33 |
| 24 | B | 604 | CLA | CMA-C3A | -3.38 | 1.45 | 1.53 |
| 24 | b | 616 | CLA | CBD-CGD | -3.38 | 1.41 | 1.52 |
| 26 | K | 101 | BCR | C2-C3 | 3.38 | 1.60 | 1.52 |
| 24 | C | 513 | CLA | C3D-CAD | 3.38 | 1.54 | 1.46 |
| 33 | E | 103 | HEM | CAA-C2A | 3.38 | 1.57 | 1.52 |
| 24 | c | 503 | CLA | C1A-CHA | -3.38 | 1.29 | 1.43 |
| 32 | C | 517 | DGD | O6D-C5D | 3.38 | 1.52 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | A | 613 | LMG | O6-C1 | 3.37 | 1.50 | 1.41 |
| 24 | c | 501 | CLA | C1D-C2D | -3.37 | 1.34 | 1.42 |
| 24 | B | 609 | CLA | CAA-C2A | -3.37 | 1.47 | 1.54 |
| 24 | c | 509 | CLA | O2D-CGD | 3.37 | 1.41 | 1.33 |
| 24 | C | 503 | CLA | C1A-CHA | -3.37 | 1.29 | 1.43 |
| 26 | H | 101 | BCR | C27-C26 | 3.37 | 1.57 | 1.51 |
| 24 | B | 613 | CLA | C3D-CAD | 3.37 | 1.54 | 1.46 |
| 24 | D | 403 | CLA | O2A-CGA | 3.37 | 1.43 | 1.33 |
| 24 | c | 511 | CLA | C1A-CHA | -3.37 | 1.29 | 1.43 |
| 24 | C | 512 | CLA | C3D-CAD | 3.37 | 1.54 | 1.46 |
| 24 | c | 509 | CLA | C1D-C2D | -3.36 | 1.34 | 1.42 |
| 24 | c | 512 | CLA | C1B-CHB | 3.36 | 1.50 | 1.41 |
| 24 | B | 616 | CLA | C1D-C2D | -3.36 | 1.35 | 1.42 |
| 24 | c | 503 | CLA | C1D-C2D | -3.36 | 1.35 | 1.42 |
| 24 | c | 502 | CLA | C1A-CHA | -3.36 | 1.29 | 1.43 |
| 24 | c | 501 | CLA | C1A-CHA | -3.36 | 1.29 | 1.43 |
| 24 | B | 615 | CLA | CBD-CGD | -3.35 | 1.41 | 1.52 |
| 24 | c | 505 | CLA | C1A-CHA | -3.35 | 1.29 | 1.43 |
| 24 | C | 504 | CLA | CBD-CGD | -3.35 | 1.41 | 1.52 |
| 24 | B | 604 | CLA | CBD-CGD | -3.35 | 1.41 | 1.52 |
| 24 | D | 404 | CLA | C1D-C2D | -3.35 | 1.35 | 1.42 |
| 24 | c | 505 | CLA | CAA-C2A | -3.35 | 1.47 | 1.54 |
| 24 | C | 505 | CLA | C1B-CHB | 3.35 | 1.50 | 1.41 |
| 24 | C | 510 | CLA | CBD-CGD | -3.35 | 1.41 | 1.52 |
| 24 | B | 608 | CLA | O2A-CGA | 3.34 | 1.43 | 1.33 |
| 24 | c | 508 | CLA | O2D-CGD | 3.34 | 1.41 | 1.33 |
| 26 | B | 620 | BCR | C1-C6 | -3.34 | 1.49 | 1.53 |
| 24 | b | 617 | CLA | CAA-C2A | -3.34 | 1.47 | 1.54 |
| 27 | d | 404 | PL9 | C36-C34 | 3.34 | 1.58 | 1.51 |
| 24 | c | 506 | CLA | C1D-C2D | -3.34 | 1.35 | 1.42 |
| 24 | B | 605 | CLA | CBD-CGD | -3.33 | 1.42 | 1.52 |
| 24 | b | 610 | CLA | O2D-CGD | 3.33 | 1.41 | 1.33 |
| 29 | j | 101 | LMG | O8-C28 | 3.33 | 1.43 | 1.33 |
| 24 | c | 512 | CLA | CBD-CGD | -3.33 | 1.42 | 1.52 |
| 26 | b | 621 | BCR | C23-C22 | 3.33 | 1.53 | 1.45 |
| 24 | b | 604 | CLA | O2A-CGA | 3.33 | 1.43 | 1.33 |
| 24 | d | 403 | CLA | C3D-CAD | 3.33 | 1.54 | 1.46 |
| 24 | b | 605 | CLA | C1B-CHB | 3.33 | 1.50 | 1.41 |
| 24 | c | 513 | CLA | C1A-CHA | -3.32 | 1.29 | 1.43 |
| 24 | B | 615 | CLA | CAA-C2A | -3.32 | 1.47 | 1.54 |
| 26 | b | 621 | BCR | C4-C5 | 3.32 | 1.57 | 1.51 |
| 24 | b | 612 | CLA | CAA-C2A | -3.32 | 1.47 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | C | 508 | CLA | CBD-CGD | -3.32 | 1.42 | 1.52 |
| 25 | D | 401 | PHO | C3B-C4B | 3.32 | 1.50 | 1.43 |
| 27 | D | 405 | PL9 | C21-C19 | 3.32 | 1.58 | 1.51 |
| 24 | c | 513 | CLA | O2D-CGD | 3.32 | 1.41 | 1.33 |
| 24 | C | 512 | CLA | C1A-CHA | -3.32 | 1.29 | 1.43 |
| 32 | d | 405 | DGD | O6D-C5D | 3.32 | 1.52 | 1.44 |
| 24 | D | 402 | CLA | CAA-C2A | -3.32 | 1.47 | 1.54 |
| 24 | a | 615 | CLA | O2A-CGA | 3.31 | 1.43 | 1.33 |
| 24 | C | 504 | CLA | O2A-CGA | 3.31 | 1.43 | 1.33 |
| 24 | C | 509 | CLA | O2A-CGA | 3.31 | 1.43 | 1.33 |
| 24 | B | 613 | CLA | C4C-C3C | -3.31 | 1.39 | 1.45 |
| 24 | b | 615 | CLA | CBD-CGD | -3.31 | 1.42 | 1.52 |
| 24 | C | 505 | CLA | C1D-C2D | -3.31 | 1.35 | 1.42 |
| 24 | B | 613 | CLA | O2A-CGA | 3.31 | 1.43 | 1.33 |
| 24 | C | 501 | CLA | C1D-C2D | -3.30 | 1.35 | 1.42 |
| 24 | C | 502 | CLA | C1B-CHB | 3.30 | 1.50 | 1.41 |
| 24 | b | 603 | CLA | O2D-CGD | 3.30 | 1.41 | 1.33 |
| 24 | A | 607 | CLA | C3D-CAD | 3.30 | 1.54 | 1.46 |
| 24 | C | 505 | CLA | C1A-CHA | -3.30 | 1.29 | 1.43 |
| 24 | D | 403 | CLA | CAA-C2A | -3.30 | 1.48 | 1.54 |
| 24 | c | 504 | CLA | CAA-C2A | -3.29 | 1.48 | 1.54 |
| 24 | C | 508 | CLA | O2D-CGD | 3.29 | 1.41 | 1.33 |
| 24 | B | 602 | CLA | C3D-CAD | 3.29 | 1.54 | 1.46 |
| 29 | b | 622 | LMG | O7-C8 | -3.29 | 1.38 | 1.46 |
| 24 | b | 609 | CLA | C1D-C2D | -3.29 | 1.35 | 1.42 |
| 24 | c | 513 | CLA | O2A-CGA | 3.29 | 1.42 | 1.33 |
| 24 | B | 609 | CLA | C3D-CAD | 3.29 | 1.54 | 1.46 |
| 24 | C | 507 | CLA | C3D-CAD | 3.29 | 1.54 | 1.46 |
| 24 | b | 615 | CLA | C1D-C2D | -3.29 | 1.35 | 1.42 |
| 24 | B | 610 | CLA | C3D-CAD | 3.28 | 1.54 | 1.46 |
| 24 | c | 509 | CLA | CBD-CGD | -3.28 | 1.42 | 1.52 |
| 24 | b | 611 | CLA | C1A-CHA | -3.28 | 1.29 | 1.43 |
| 24 | B | 609 | CLA | O2D-CGD | 3.28 | 1.41 | 1.33 |
| 24 | b | 605 | CLA | C1A-CHA | -3.28 | 1.29 | 1.43 |
| 24 | c | 505 | CLA | O2D-CGD | 3.28 | 1.41 | 1.33 |
| 24 | d | 402 | CLA | C3B-CAB | 3.28 | 1.54 | 1.47 |
| 24 | B | 612 | CLA | CAA-C2A | -3.28 | 1.48 | 1.54 |
| 26 | K | 101 | BCR | C4-C5 | 3.28 | 1.57 | 1.51 |
| 24 | b | 607 | CLA | CBD-CGD | -3.28 | 1.42 | 1.52 |
| 26 | b | 621 | BCR | C12-C13 | 3.27 | 1.53 | 1.45 |
| 24 | b | 613 | CLA | C1B-CHB | 3.27 | 1.50 | 1.41 |
| 24 | b | 614 | CLA | MG-NA | -3.27 | 1.98 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | B | 610 | CLA | C1B-CHB | 3.27 | 1.50 | 1.41 |
| 24 | b | 610 | CLA | C1D-C2D | -3.27 | 1.35 | 1.42 |
| 32 | h | 102 | DGD | C3D-C2D | -3.27 | 1.44 | 1.52 |
| 24 | B | 614 | CLA | C1D-C2D | -3.27 | 1.35 | 1.42 |
| 32 | E | 101 | DGD | O6D-C5D | 3.27 | 1.52 | 1.44 |
| 24 | c | 510 | CLA | C1D-C2D | -3.27 | 1.35 | 1.42 |
| 25 | D | 401 | PHO | C4C-NC | 3.26 | 1.44 | 1.36 |
| 26 | A | 610 | BCR | C40-C30 | 3.26 | 1.60 | 1.53 |
| 24 | b | 612 | CLA | C1B-CHB | 3.26 | 1.50 | 1.41 |
| 24 | B | 607[A] | CLA | O2D-CGD | 3.25 | 1.41 | 1.33 |
| 24 | c | 502 | CLA | C3D-CAD | 3.25 | 1.54 | 1.46 |
| 24 | B | 616 | CLA | C3D-CAD | 3.25 | 1.54 | 1.46 |
| 24 | B | 603 | CLA | C3D-CAD | 3.25 | 1.54 | 1.46 |
| 24 | C | 501 | CLA | CAA-C2A | -3.25 | 1.48 | 1.54 |
| 24 | c | 502 | CLA | CBD-CGD | -3.25 | 1.42 | 1.52 |
| 24 | C | 509 | CLA | C1A-CHA | -3.25 | 1.29 | 1.43 |
| 24 | c | 512 | CLA | C1D-C2D | -3.25 | 1.35 | 1.42 |
| 26 | H | 101 | BCR | C12-C13 | 3.25 | 1.52 | 1.45 |
| 24 | C | 512 | CLA | CBD-CGD | -3.25 | 1.42 | 1.52 |
| 26 | b | 620 | BCR | C17-C18 | 3.24 | 1.40 | 1.35 |
| 24 | C | 505 | CLA | C4C-C3C | -3.24 | 1.39 | 1.45 |
| 24 | b | 616 | CLA | MG-NA | -3.24 | 1.98 | 2.06 |
| 24 | B | 612 | CLA | C3D-CAD | 3.24 | 1.54 | 1.46 |
| 24 | c | 511 | CLA | C1D-C2D | -3.24 | 1.35 | 1.42 |
| 24 | c | 503 | CLA | C1B-CHB | 3.24 | 1.50 | 1.41 |
| 24 | b | 612 | CLA | CBD-CGD | -3.24 | 1.42 | 1.52 |
| 24 | C | 506 | CLA | CAA-C2A | -3.24 | 1.48 | 1.54 |
| 24 | B | 615 | CLA | O2A-CGA | 3.24 | 1.42 | 1.33 |
| 24 | C | 510 | CLA | O2A-CGA | 3.23 | 1.42 | 1.33 |
| 24 | B | 613 | CLA | CBD-CGD | -3.23 | 1.42 | 1.52 |
| 24 | c | 501 | CLA | C1B-CHB | 3.23 | 1.50 | 1.41 |
| 24 | B | 611 | CLA | C3D-CAD | 3.23 | 1.54 | 1.46 |
| 24 | c | 513 | CLA | C1D-C2D | -3.23 | 1.35 | 1.42 |
| 24 | B | 614 | CLA | O2A-CGA | 3.22 | 1.42 | 1.33 |
| 24 | c | 511 | CLA | O2D-CGD | 3.22 | 1.41 | 1.33 |
| 24 | C | 507 | CLA | C1A-CHA | -3.22 | 1.29 | 1.43 |
| 26 | k | 101 | BCR | C2-C3 | 3.22 | 1.60 | 1.52 |
| 24 | B | 607[B] | CLA | O2D-CGD | 3.22 | 1.41 | 1.33 |
| 24 | b | 603 | CLA | C1A-CHA | -3.22 | 1.29 | 1.43 |
| 24 | c | 502 | CLA | O2D-CGD | 3.22 | 1.41 | 1.33 |
| 24 | B | 610 | CLA | O2D-CGD | 3.21 | 1.41 | 1.33 |
| 24 | C | 511 | CLA | MG-NA | -3.21 | 1.98 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 29 | D | 408 | LMG | O7-C8 | -3.21 | 1.38 | 1.46 |
| 24 | B | 605 | CLA | O2D-CGD | 3.21 | 1.41 | 1.33 |
| 24 | c | 510 | CLA | O2A-CGA | 3.21 | 1.42 | 1.33 |
| 32 | c | 518 | DGD | O6D-C5D | 3.21 | 1.52 | 1.44 |
| 24 | b | 608[B] | CLA | CAA-C2A | -3.21 | 1.48 | 1.54 |
| 24 | C | 501 | CLA | O2D-CGD | 3.20 | 1.41 | 1.33 |
| 24 | a | 607 | CLA | C3B-CAB | 3.20 | 1.54 | 1.47 |
| 26 | c | 515 | BCR | C4-C5 | 3.20 | 1.57 | 1.51 |
| 27 | a | 611 | PL9 | C21-C19 | 3.20 | 1.57 | 1.51 |
| 33 | v | 201 | HEM | C3B-C2B | -3.20 | 1.35 | 1.40 |
| 24 | b | 612 | CLA | C3D-CAD | 3.20 | 1.54 | 1.46 |
| 26 | h | 101 | BCR | C27-C26 | 3.20 | 1.57 | 1.51 |
| 24 | B | 612 | CLA | O2D-CGD | 3.19 | 1.41 | 1.33 |
| 24 | B | 612 | CLA | O2A-CGA | 3.19 | 1.42 | 1.33 |
| 24 | a | 609 | CLA | C1A-CHA | -3.19 | 1.29 | 1.43 |
| 24 | C | 509 | CLA | C3D-CAD | 3.19 | 1.54 | 1.46 |
| 24 | c | 510 | CLA | O2D-CGD | 3.18 | 1.41 | 1.33 |
| 25 | d | 401 | PHO | CHC-C1C | 3.18 | 1.44 | 1.38 |
| 24 | B | 608 | CLA | CBD-CGD | -3.18 | 1.42 | 1.52 |
| 24 | C | 512 | CLA | C1B-CHB | 3.18 | 1.49 | 1.41 |
| 24 | b | 605 | CLA | CAA-C2A | -3.18 | 1.48 | 1.54 |
| 24 | c | 501 | CLA | CAA-C2A | -3.17 | 1.48 | 1.54 |
| 24 | A | 607 | CLA | C1D-C2D | -3.17 | 1.35 | 1.42 |
| 26 | c | 514 | BCR | C4-C5 | 3.17 | 1.57 | 1.51 |
| 24 | b | 613 | CLA | C3B-CAB | 3.17 | 1.54 | 1.47 |
| 26 | h | 101 | BCR | C12-C13 | 3.17 | 1.52 | 1.45 |
| 24 | b | 605 | CLA | O2D-CGD | 3.17 | 1.40 | 1.33 |
| 24 | B | 611 | CLA | C1A-CHA | -3.17 | 1.30 | 1.43 |
| 24 | B | 607[A] | CLA | CBD-CGD | -3.17 | 1.42 | 1.52 |
| 24 | C | 505 | CLA | O2D-CGD | 3.17 | 1.40 | 1.33 |
| 24 | B | 611 | CLA | C4C-C3C | -3.17 | 1.39 | 1.45 |
| 24 | B | 609 | CLA | C1D-C2D | -3.17 | 1.35 | 1.42 |
| 24 | b | 615 | CLA | C1B-CHB | 3.16 | 1.49 | 1.41 |
| 24 | c | 507 | CLA | C1B-CHB | 3.16 | 1.49 | 1.41 |
| 24 | c | 505 | CLA | O2A-CGA | 3.16 | 1.42 | 1.33 |
| 24 | c | 502 | CLA | C1D-C2D | -3.16 | 1.35 | 1.42 |
| 24 | b | 604 | CLA | MG-NA | -3.16 | 1.98 | 2.06 |
| 25 | D | 401 | PHO | CHC-C1C | 3.16 | 1.44 | 1.38 |
| 26 | B | 619 | BCR | C12-C13 | 3.16 | 1.52 | 1.45 |
| 24 | b | 617 | CLA | O2D-CGD | 3.16 | 1.40 | 1.33 |
| 24 | B | 612 | CLA | MG-NA | -3.16 | 1.98 | 2.06 |
| 24 | B | 602 | CLA | C1D-C2D | -3.15 | 1.35 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 507 | CLA | O2D-CGD | 3.15 | 1.40 | 1.33 |
| 24 | B | 607[A] | CLA | C3D-CAD | 3.15 | 1.54 | 1.46 |
| 24 | B | 609 | CLA | CBD-CGD | -3.15 | 1.42 | 1.52 |
| 24 | c | 511 | CLA | CAA-C2A | -3.15 | 1.48 | 1.54 |
| 32 | C | 517 | DGD | C3D-C2D | -3.15 | 1.44 | 1.52 |
| 24 | c | 506 | CLA | C3D-CAD | 3.15 | 1.54 | 1.46 |
| 24 | b | 611 | CLA | C1B-CHB | 3.15 | 1.49 | 1.41 |
| 32 | h | 102 | DGD | O6D-C5D | 3.15 | 1.52 | 1.44 |
| 27 | D | 405 | PL9 | C36-C34 | 3.14 | 1.57 | 1.51 |
| 24 | C | 513 | CLA | C1B-CHB | 3.14 | 1.49 | 1.41 |
| 24 | C | 505 | CLA | O2A-CGA | 3.14 | 1.42 | 1.33 |
| 24 | b | 612 | CLA | O2D-CGD | 3.14 | 1.40 | 1.33 |
| 26 | k | 101 | BCR | C12-C13 | 3.14 | 1.52 | 1.45 |
| 24 | C | 513 | CLA | MG-NA | -3.13 | 1.98 | 2.06 |
| 26 | B | 620 | BCR | C4-C5 | 3.13 | 1.57 | 1.51 |
| 24 | a | 607 | CLA | O2D-CGD | 3.13 | 1.40 | 1.33 |
| 24 | c | 501 | CLA | C3B-CAB | 3.13 | 1.54 | 1.47 |
| 26 | T | 101 | BCR | C4-C5 | 3.13 | 1.57 | 1.51 |
| 25 | a | 608 | PHO | CHC-C1C | 3.13 | 1.44 | 1.38 |
| 26 | b | 619 | BCR | C1-C6 | -3.13 | 1.49 | 1.53 |
| 24 | c | 510 | CLA | C1A-CHA | -3.13 | 1.30 | 1.43 |
| 24 | C | 507 | CLA | CAA-C2A | -3.13 | 1.48 | 1.54 |
| 24 | B | 605 | CLA | CAA-C2A | -3.12 | 1.48 | 1.54 |
| 24 | B | 606 | CLA | CAA-C2A | -3.12 | 1.48 | 1.54 |
| 24 | A | 606 | CLA | MG-NA | -3.12 | 1.98 | 2.06 |
| 24 | B | 613 | CLA | C2A-C1A | -3.12 | 1.45 | 1.52 |
| 24 | b | 612 | CLA | C1D-C2D | -3.12 | 1.35 | 1.42 |
| 24 | B | 607[B] | CLA | CBD-CGD | -3.12 | 1.42 | 1.52 |
| 24 | C | 506 | CLA | O2A-CGA | 3.12 | 1.42 | 1.33 |
| 24 | B | 609 | CLA | O2A-CGA | 3.11 | 1.42 | 1.33 |
| 24 | C | 501 | CLA | C4C-C3C | -3.11 | 1.39 | 1.45 |
| 24 | B | 603 | CLA | O2D-CGD | 3.11 | 1.40 | 1.33 |
| 24 | d | 403 | CLA | C1D-C2D | -3.11 | 1.35 | 1.42 |
| 24 | a | 607 | CLA | MG-NA | -3.11 | 1.98 | 2.06 |
| 26 | b | 620 | BCR | C1-C6 | -3.11 | 1.49 | 1.53 |
| 26 | k | 101 | BCR | C27-C26 | 3.11 | 1.57 | 1.51 |
| 24 | a | 607 | CLA | C3D-CAD | 3.11 | 1.54 | 1.46 |
| 24 | c | 512 | CLA | C3D-CAD | 3.11 | 1.54 | 1.46 |
| 24 | b | 612 | CLA | C4C-C3C | -3.10 | 1.39 | 1.45 |
| 26 | h | 101 | BCR | C4-C5 | 3.10 | 1.57 | 1.51 |
| 24 | B | 617 | CLA | C1D-C2D | -3.10 | 1.35 | 1.42 |
| 24 | b | 617 | CLA | C1A-CHA | -3.10 | 1.30 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 609 | CLA | O2D-CGD | 3.10 | 1.40 | 1.33 |
| 24 | c | 513 | CLA | CAA-C2A | -3.09 | 1.48 | 1.54 |
| 24 | b | 615 | CLA | O2A-CGA | 3.09 | 1.42 | 1.33 |
| 24 | B | 607[B] | CLA | C3D-CAD | 3.09 | 1.53 | 1.46 |
| 32 | E | 101 | DGD | C3D-C2D | -3.09 | 1.44 | 1.52 |
| 24 | B | 608 | CLA | C1B-CHB | 3.09 | 1.49 | 1.41 |
| 24 | C | 506 | CLA | C3D-CAD | 3.09 | 1.53 | 1.46 |
| 24 | C | 504 | CLA | C3B-CAB | 3.09 | 1.54 | 1.47 |
| 24 | A | 606 | CLA | O2D-CGD | 3.09 | 1.40 | 1.33 |
| 24 | a | 607 | CLA | C1D-C2D | -3.09 | 1.35 | 1.42 |
| 24 | c | 509 | CLA | C1B-CHB | 3.08 | 1.49 | 1.41 |
| 24 | B | 606 | CLA | C1B-CHB | 3.08 | 1.49 | 1.41 |
| 24 | a | 606 | CLA | C1B-CHB | 3.08 | 1.49 | 1.41 |
| 29 | a | 613 | LMG | O6-C1 | 3.08 | 1.49 | 1.41 |
| 24 | B | 610 | CLA | MG-NA | -3.08 | 1.99 | 2.06 |
| 24 | b | 614 | CLA | C1B-CHB | 3.08 | 1.49 | 1.41 |
| 24 | B | 615 | CLA | O2D-CGD | 3.07 | 1.40 | 1.33 |
| 24 | c | 507 | CLA | CBD-CGD | -3.07 | 1.42 | 1.52 |
| 24 | A | 609 | CLA | C1B-CHB | 3.07 | 1.49 | 1.41 |
| 24 | B | 617 | CLA | O2D-CGD | 3.06 | 1.40 | 1.33 |
| 24 | A | 609 | CLA | OBD-CAD | -3.06 | 1.18 | 1.22 |
| 32 | E | 101 | DGD | O5D-C1E | 3.06 | 1.45 | 1.40 |
| 24 | b | 608[A] | CLA | CAA-C2A | -3.06 | 1.48 | 1.54 |
| 24 | A | 606 | CLA | C1B-CHB | 3.05 | 1.49 | 1.41 |
| 24 | d | 402 | CLA | C3D-CAD | 3.05 | 1.53 | 1.46 |
| 24 | b | 614 | CLA | C2A-C1A | -3.05 | 1.45 | 1.52 |
| 24 | C | 510 | CLA | C1D-C2D | -3.04 | 1.35 | 1.42 |
| 24 | D | 402 | CLA | OBD-CAD | -3.04 | 1.18 | 1.22 |
| 24 | C | 508 | CLA | MG-NA | -3.04 | 1.99 | 2.06 |
| 24 | D | 403 | CLA | C3B-CAB | 3.04 | 1.54 | 1.47 |
| 32 | H | 102 | DGD | C6E-C5E | -3.04 | 1.41 | 1.51 |
| 26 | C | 514 | BCR | C27-C26 | 3.04 | 1.57 | 1.51 |
| 24 | c | 510 | CLA | C3D-CAD | 3.04 | 1.53 | 1.46 |
| 24 | b | 605 | CLA | C3B-CAB | 3.03 | 1.54 | 1.47 |
| 24 | D | 404 | CLA | C3D-CAD | 3.03 | 1.53 | 1.46 |
| 32 | E | 101 | DGD | O6E-C1E | 3.03 | 1.49 | 1.41 |
| 24 | B | 606 | CLA | C1A-CHA | -3.03 | 1.30 | 1.43 |
| 24 | c | 504 | CLA | C3B-CAB | 3.03 | 1.54 | 1.47 |
| 24 | C | 501 | CLA | CBD-CGD | -3.03 | 1.42 | 1.52 |
| 24 | C | 510 | CLA | C2A-C1A | -3.03 | 1.45 | 1.52 |
| 32 | c | 517 | DGD | C3D-C2D | -3.02 | 1.44 | 1.52 |
| 24 | B | 604 | CLA | O2D-CGD | 3.02 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | B | 614 | CLA | OBD-CAD | -3.02 | 1.18 | 1.22 |
| 24 | c | 512 | CLA | C3B-CAB | 3.02 | 1.54 | 1.47 |
| 26 | a | 610 | BCR | C35-C13 | -3.02 | 1.44 | 1.50 |
| 24 | c | 510 | CLA | CBD-CGD | -3.02 | 1.43 | 1.52 |
| 24 | B | 602 | CLA | C1A-CHA | -3.02 | 1.30 | 1.43 |
| 24 | B | 607[B] | CLA | C1B-CHB | 3.02 | 1.49 | 1.41 |
| 24 | b | 608[B] | CLA | C1B-CHB | 3.01 | 1.49 | 1.41 |
| 24 | c | 504 | CLA | MG-NA | -3.01 | 1.99 | 2.06 |
| 24 | a | 609 | CLA | O2D-CGD | 3.01 | 1.40 | 1.33 |
| 26 | c | 521 | BCR | C4-C5 | 3.01 | 1.56 | 1.51 |
| 24 | b | 616 | CLA | C1B-CHB | 3.00 | 1.49 | 1.41 |
| 24 | b | 610 | CLA | C1B-CHB | 3.00 | 1.49 | 1.41 |
| 24 | b | 609 | CLA | MG-NA | -3.00 | 1.99 | 2.06 |
| 24 | b | 608[A] | CLA | C1B-CHB | 3.00 | 1.49 | 1.41 |
| 24 | B | 616 | CLA | O2D-CGD | 2.99 | 1.40 | 1.33 |
| 24 | b | 603 | CLA | C3D-CAD | 2.99 | 1.53 | 1.46 |
| 26 | b | 619 | BCR | C12-C13 | 2.99 | 1.52 | 1.45 |
| 24 | C | 503 | CLA | C1B-CHB | 2.99 | 1.49 | 1.41 |
| 24 | c | 511 | CLA | C3D-CAD | 2.99 | 1.53 | 1.46 |
| 24 | c | 503 | CLA | C3B-CAB | 2.99 | 1.54 | 1.47 |
| 29 | Z | 101 | LMG | O7-C8 | -2.99 | 1.39 | 1.46 |
| 25 | a | 608 | PHO | C3B-C4B | 2.99 | 1.49 | 1.43 |
| 24 | c | 504 | CLA | CBD-CGD | -2.99 | 1.43 | 1.52 |
| 24 | b | 607 | CLA | MG-NA | -2.98 | 1.99 | 2.06 |
| 26 | t | 101 | BCR | C4-C5 | 2.98 | 1.56 | 1.51 |
| 32 | H | 102 | DGD | O6D-C5D | 2.98 | 1.51 | 1.44 |
| 24 | A | 607 | CLA | C1B-CHB | 2.98 | 1.49 | 1.41 |
| 27 | d | 404 | PL9 | C41-C39 | 2.98 | 1.57 | 1.51 |
| 26 | B | 618 | BCR | C12-C13 | 2.98 | 1.52 | 1.45 |
| 24 | a | 609 | CLA | C3D-CAD | 2.98 | 1.53 | 1.46 |
| 24 | c | 504 | CLA | C3D-CAD | 2.98 | 1.53 | 1.46 |
| 24 | b | 607 | CLA | O2D-CGD | 2.98 | 1.40 | 1.33 |
| 24 | b | 603 | CLA | CBD-CGD | -2.97 | 1.43 | 1.52 |
| 24 | b | 611 | CLA | MG-NA | -2.97 | 1.99 | 2.06 |
| 24 | c | 502 | CLA | C1B-CHB | 2.97 | 1.49 | 1.41 |
| 24 | B | 604 | CLA | C1B-CHB | 2.97 | 1.49 | 1.41 |
| 24 | C | 502 | CLA | CBD-CGD | -2.97 | 1.43 | 1.52 |
| 24 | C | 501 | CLA | C1B-CHB | 2.97 | 1.49 | 1.41 |
| 29 | j | 101 | LMG | O7-C8 | -2.97 | 1.39 | 1.46 |
| 24 | c | 506 | CLA | C1B-CHB | 2.96 | 1.49 | 1.41 |
| 24 | B | 603 | CLA | MG-NA | -2.96 | 1.99 | 2.06 |
| 24 | C | 509 | CLA | O2D-CGD | 2.96 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 33 | e | 102 | HEM | CAA-C2A | 2.96 | 1.56 | 1.52 |
| 24 | C | 504 | CLA | C1D-C2D | -2.96 | 1.35 | 1.42 |
| 24 | C | 503 | CLA | OBD-CAD | -2.95 | 1.18 | 1.22 |
| 24 | C | 508 | CLA | C3D-CAD | 2.95 | 1.53 | 1.46 |
| 24 | D | 404 | CLA | C1B-CHB | 2.95 | 1.49 | 1.41 |
| 24 | c | 508 | CLA | O2A-CGA | 2.95 | 1.42 | 1.33 |
| 24 | B | 602 | CLA | C1B-CHB | 2.95 | 1.49 | 1.41 |
| 24 | C | 510 | CLA | C3D-CAD | 2.95 | 1.53 | 1.46 |
| 24 | B | 615 | CLA | MG-NA | -2.95 | 1.99 | 2.06 |
| 24 | B | 607[A] | CLA | C1B-CHB | 2.95 | 1.49 | 1.41 |
| 24 | A | 609 | CLA | CAA-C2A | -2.94 | 1.48 | 1.54 |
| 24 | b | 617 | CLA | C3B-CAB | 2.94 | 1.53 | 1.47 |
| 24 | C | 509 | CLA | CAA-C2A | -2.94 | 1.48 | 1.54 |
| 32 | d | 405 | DGD | C3D-C2D | -2.94 | 1.44 | 1.52 |
| 24 | d | 402 | CLA | C2A-C1A | -2.94 | 1.45 | 1.52 |
| 26 | K | 101 | BCR | C12-C13 | 2.94 | 1.52 | 1.45 |
| 24 | b | 606 | CLA | C1B-CHB | 2.93 | 1.49 | 1.41 |
| 24 | C | 508 | CLA | MG-NC | -2.93 | 1.99 | 2.06 |
| 24 | C | 508 | CLA | C1B-CHB | 2.93 | 1.49 | 1.41 |
| 24 | b | 617 | CLA | C1B-CHB | 2.93 | 1.49 | 1.41 |
| 24 | b | 614 | CLA | O2D-CGD | 2.93 | 1.40 | 1.33 |
| 24 | B | 603 | CLA | CAA-C2A | -2.93 | 1.48 | 1.54 |
| 24 | b | 610 | CLA | O2A-CGA | 2.93 | 1.41 | 1.33 |
| 24 | B | 602 | CLA | C3B-CAB | 2.93 | 1.53 | 1.47 |
| 24 | B | 605 | CLA | C3D-CAD | 2.92 | 1.53 | 1.46 |
| 24 | B | 604 | CLA | MG-NA | -2.92 | 1.99 | 2.06 |
| 24 | B | 604 | CLA | CAA-C2A | -2.92 | 1.48 | 1.54 |
| 32 | C | 516 | DGD | O6E-C1E | 2.92 | 1.49 | 1.41 |
| 24 | b | 609 | CLA | O2A-CGA | 2.92 | 1.41 | 1.33 |
| 24 | a | 606 | CLA | O2D-CGD | 2.92 | 1.40 | 1.33 |
| 24 | B | 616 | CLA | C1B-CHB | 2.92 | 1.49 | 1.41 |
| 26 | B | 619 | BCR | C40-C30 | 2.92 | 1.59 | 1.53 |
| 32 | C | 517 | DGD | C3E-C2E | -2.92 | 1.44 | 1.52 |
| 24 | b | 604 | CLA | OBD-CAD | -2.92 | 1.18 | 1.22 |
| 24 | b | 604 | CLA | C2A-C1A | -2.91 | 1.45 | 1.52 |
| 24 | b | 609 | CLA | C2A-C1A | -2.91 | 1.45 | 1.52 |
| 24 | B | 613 | CLA | O2D-CGD | 2.91 | 1.40 | 1.33 |
| 26 | H | 101 | BCR | C4-C5 | 2.91 | 1.56 | 1.51 |
| 24 | D | 403 | CLA | OBD-CAD | -2.91 | 1.18 | 1.22 |
| 24 | C | 506 | CLA | C1A-CHA | -2.91 | 1.31 | 1.43 |
| 24 | a | 607 | CLA | C1B-CHB | 2.91 | 1.49 | 1.41 |
| 24 | C | 511 | CLA | CBD-CGD | -2.91 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 507 | CLA | MG-NA | -2.91 | 1.99 | 2.06 |
| 26 | K | 101 | BCR | C27-C26 | 2.91 | 1.56 | 1.51 |
| 24 | C | 503 | CLA | C3B-CAB | 2.90 | 1.53 | 1.47 |
| 24 | c | 506 | CLA | C1A-CHA | -2.90 | 1.31 | 1.43 |
| 24 | a | 615 | CLA | O2D-CGD | 2.90 | 1.40 | 1.33 |
| 24 | c | 508 | CLA | MG-NA | -2.90 | 1.99 | 2.06 |
| 26 | T | 101 | BCR | C35-C13 | -2.90 | 1.44 | 1.50 |
| 26 | c | 514 | BCR | C27-C26 | 2.90 | 1.56 | 1.51 |
| 24 | b | 613 | CLA | MG-NA | -2.90 | 1.99 | 2.06 |
| 26 | C | 514 | BCR | C31-C1 | -2.89 | 1.48 | 1.53 |
| 26 | c | 514 | BCR | C35-C13 | -2.89 | 1.44 | 1.50 |
| 24 | B | 605 | CLA | C1B-CHB | 2.89 | 1.49 | 1.41 |
| 24 | c | 506 | CLA | O2D-CGD | 2.89 | 1.40 | 1.33 |
| 24 | a | 609 | CLA | CBD-CGD | -2.89 | 1.43 | 1.52 |
| 24 | b | 604 | CLA | CBD-CGD | -2.89 | 1.43 | 1.52 |
| 24 | C | 503 | CLA | CAA-C2A | -2.88 | 1.48 | 1.54 |
| 26 | B | 620 | BCR | C27-C26 | 2.88 | 1.56 | 1.51 |
| 24 | B | 610 | CLA | C3B-CAB | 2.88 | 1.53 | 1.47 |
| 24 | C | 509 | CLA | MG-NA | -2.88 | 1.99 | 2.06 |
| 24 | b | 606 | CLA | CBD-CGD | -2.88 | 1.43 | 1.52 |
| 24 | b | 615 | CLA | O2D-CGD | 2.88 | 1.40 | 1.33 |
| 24 | B | 609 | CLA | C4C-C3C | -2.88 | 1.40 | 1.45 |
| 24 | b | 616 | CLA | C3D-CAD | 2.87 | 1.53 | 1.46 |
| 24 | D | 404 | CLA | O2D-CED | -2.87 | 1.38 | 1.45 |
| 24 | C | 512 | CLA | O2D-CGD | 2.87 | 1.40 | 1.33 |
| 24 | b | 608[A] | CLA | C3D-CAD | 2.87 | 1.53 | 1.46 |
| 24 | C | 507 | CLA | C1B-CHB | 2.87 | 1.49 | 1.41 |
| 32 | C | 516 | DGD | O2D-C2D | 2.87 | 1.49 | 1.43 |
| 24 | C | 510 | CLA | O2D-CGD | 2.87 | 1.40 | 1.33 |
| 24 | C | 506 | CLA | C1B-CHB | 2.86 | 1.49 | 1.41 |
| 24 | c | 504 | CLA | O2D-CGD | 2.86 | 1.40 | 1.33 |
| 27 | d | 404 | PL9 | C21-C19 | 2.86 | 1.57 | 1.51 |
| 26 | b | 621 | BCR | C31-C1 | -2.86 | 1.48 | 1.53 |
| 24 | c | 503 | CLA | C3D-CAD | 2.86 | 1.53 | 1.46 |
| 26 | f | 101 | BCR | C12-C13 | 2.86 | 1.52 | 1.45 |
| 24 | a | 606 | CLA | O2D-CED | -2.86 | 1.38 | 1.45 |
| 26 | K | 102 | BCR | C27-C26 | 2.86 | 1.56 | 1.51 |
| 24 | b | 614 | CLA | C3D-CAD | 2.86 | 1.53 | 1.46 |
| 24 | C | 508 | CLA | OBD-CAD | -2.86 | 1.18 | 1.22 |
| 26 | c | 514 | BCR | C31-C1 | -2.85 | 1.48 | 1.53 |
| 24 | c | 502 | CLA | CAA-C2A | -2.85 | 1.48 | 1.54 |
| 24 | c | 503 | CLA | CAA-C2A | -2.85 | 1.48 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | c | 512 | CLA | CAA-C2A | -2.85 | 1.48 | 1.54 |
| 29 | C | 518 | LMG | O7-C8 | -2.85 | 1.39 | 1.46 |
| 24 | D | 403 | CLA | C1B-CHB | 2.85 | 1.48 | 1.41 |
| 24 | b | 614 | CLA | C3B-CAB | 2.85 | 1.53 | 1.47 |
| 24 | a | 606 | CLA | MG-NA | -2.85 | 1.99 | 2.06 |
| 24 | b | 608[B] | CLA | C3D-CAD | 2.84 | 1.53 | 1.46 |
| 24 | b | 607 | CLA | C3D-CAD | 2.84 | 1.53 | 1.46 |
| 24 | c | 507 | CLA | O2D-CGD | 2.84 | 1.40 | 1.33 |
| 24 | C | 501 | CLA | C3B-CAB | 2.84 | 1.53 | 1.47 |
| 24 | B | 602 | CLA | O2D-CGD | 2.84 | 1.40 | 1.33 |
| 26 | b | 620 | BCR | C40-C30 | 2.84 | 1.59 | 1.53 |
| 26 | K | 102 | BCR | C4-C5 | 2.84 | 1.56 | 1.51 |
| 24 | B | 615 | CLA | C1B-CHB | 2.84 | 1.48 | 1.41 |
| 24 | C | 509 | CLA | C1B-CHB | 2.84 | 1.48 | 1.41 |
| 24 | c | 510 | CLA | MG-NA | -2.83 | 1.99 | 2.06 |
| 24 | C | 512 | CLA | C3B-CAB | 2.83 | 1.53 | 1.47 |
| 24 | B | 611 | CLA | MG-NA | -2.83 | 1.99 | 2.06 |
| 24 | c | 503 | CLA | O2D-CED | -2.83 | 1.38 | 1.45 |
| 24 | B | 605 | CLA | MG-NA | -2.83 | 1.99 | 2.06 |
| 24 | B | 608 | CLA | O2D-CGD | 2.83 | 1.40 | 1.33 |
| 24 | A | 606 | CLA | MG-NC | -2.83 | 1.99 | 2.06 |
| 24 | B | 611 | CLA | O2D-CGD | 2.83 | 1.40 | 1.33 |
| 26 | B | 620 | BCR | C31-C1 | -2.83 | 1.48 | 1.53 |
| 24 | c | 504 | CLA | C1B-CHB | 2.82 | 1.48 | 1.41 |
| 24 | a | 606 | CLA | C3D-CAD | 2.82 | 1.53 | 1.46 |
| 24 | b | 605 | CLA | C3D-CAD | 2.82 | 1.53 | 1.46 |
| 24 | B | 608 | CLA | C2A-C1A | -2.82 | 1.45 | 1.52 |
| 24 | c | 513 | CLA | C1B-CHB | 2.82 | 1.48 | 1.41 |
| 24 | b | 612 | CLA | OBD-CAD | -2.82 | 1.18 | 1.22 |
| 24 | c | 513 | CLA | C3B-CAB | 2.82 | 1.53 | 1.47 |
| 24 | C | 513 | CLA | CAA-C2A | -2.82 | 1.48 | 1.54 |
| 25 | d | 401 | PHO | C4C-NC | 2.81 | 1.43 | 1.36 |
| 26 | h | 101 | BCR | C31-C1 | -2.81 | 1.48 | 1.53 |
| 24 | a | 615 | CLA | C1B-CHB | 2.81 | 1.48 | 1.41 |
| 29 | c | 519 | LMG | O7-C8 | -2.81 | 1.39 | 1.46 |
| 26 | f | 101 | BCR | C17-C18 | 2.81 | 1.39 | 1.35 |
| 24 | c | 505 | CLA | C3D-CAD | 2.81 | 1.53 | 1.46 |
| 24 | C | 504 | CLA | O2D-CGD | 2.81 | 1.40 | 1.33 |
| 24 | D | 404 | CLA | C3B-CAB | 2.81 | 1.53 | 1.47 |
| 32 | c | 516 | DGD | O6D-C5D | 2.80 | 1.51 | 1.44 |
| 26 | c | 514 | BCR | C12-C13 | 2.80 | 1.52 | 1.45 |
| 24 | b | 616 | CLA | C2A-C1A | -2.80 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 611 | CLA | C3B-CAB | 2.80 | 1.53 | 1.47 |
| 24 | B | 613 | CLA | C1B-CHB | 2.80 | 1.48 | 1.41 |
| 26 | t | 101 | BCR | C12-C13 | 2.80 | 1.51 | 1.45 |
| 26 | H | 101 | BCR | C1-C6 | -2.79 | 1.49 | 1.53 |
| 24 | c | 508 | CLA | C1B-CHB | 2.79 | 1.48 | 1.41 |
| 28 | A | 612 | SQD | C6-S | -2.79 | 1.67 | 1.77 |
| 24 | B | 610 | CLA | CBD-CGD | -2.79 | 1.43 | 1.52 |
| 24 | B | 616 | CLA | C3B-CAB | 2.79 | 1.53 | 1.47 |
| 32 | c | 516 | DGD | C6E-C5E | -2.79 | 1.42 | 1.51 |
| 24 | B | 611 | CLA | O2D-CED | -2.79 | 1.38 | 1.45 |
| 32 | H | 102 | DGD | O5D-C1E | 2.78 | 1.44 | 1.40 |
| 24 | c | 506 | CLA | CBD-CGD | -2.78 | 1.43 | 1.52 |
| 32 | c | 518 | DGD | O5D-C1E | 2.78 | 1.44 | 1.40 |
| 24 | B | 605 | CLA | OBD-CAD | -2.78 | 1.18 | 1.22 |
| 24 | C | 510 | CLA | C3B-CAB | 2.78 | 1.53 | 1.47 |
| 29 | A | 613 | LMG | O7-C8 | -2.78 | 1.39 | 1.46 |
| 29 | B | 621 | LMG | O7-C8 | -2.78 | 1.39 | 1.46 |
| 32 | c | 516 | DGD | O6E-C1E | 2.77 | 1.48 | 1.41 |
| 28 | a | 612 | SQD | C6-S | -2.77 | 1.67 | 1.77 |
| 26 | a | 610 | BCR | C4-C5 | 2.77 | 1.56 | 1.51 |
| 26 | k | 101 | BCR | C31-C1 | -2.77 | 1.48 | 1.53 |
| 24 | c | 510 | CLA | C3B-CAB | 2.77 | 1.53 | 1.47 |
| 27 | D | 405 | PL9 | C41-C39 | 2.77 | 1.57 | 1.51 |
| 26 | F | 101 | BCR | C4-C5 | 2.77 | 1.56 | 1.51 |
| 24 | b | 608[A] | CLA | O2D-CGD | 2.77 | 1.40 | 1.33 |
| 24 | A | 607 | CLA | C3B-CAB | 2.76 | 1.53 | 1.47 |
| 24 | C | 505 | CLA | CBD-CGD | -2.76 | 1.43 | 1.52 |
| 24 | c | 502 | CLA | MG-NA | -2.76 | 1.99 | 2.06 |
| 26 | b | 620 | BCR | C4-C5 | 2.76 | 1.56 | 1.51 |
| 24 | B | 606 | CLA | CBD-CGD | -2.76 | 1.43 | 1.52 |
| 24 | C | 504 | CLA | C1B-CHB | 2.76 | 1.48 | 1.41 |
| 32 | d | 405 | DGD | O3G-C1D | 2.76 | 1.44 | 1.40 |
| 24 | b | 606 | CLA | C3B-CAB | 2.76 | 1.53 | 1.47 |
| 24 | B | 610 | CLA | C2A-C1A | -2.75 | 1.46 | 1.52 |
| 24 | b | 613 | CLA | C3D-CAD | 2.75 | 1.53 | 1.46 |
| 24 | b | 617 | CLA | C3D-CAD | 2.75 | 1.53 | 1.46 |
| 24 | b | 613 | CLA | O2D-CGD | 2.75 | 1.39 | 1.33 |
| 24 | B | 606 | CLA | C3B-CAB | 2.75 | 1.53 | 1.47 |
| 32 | d | 405 | DGD | O6E-C1E | 2.75 | 1.48 | 1.41 |
| 24 | A | 607 | CLA | MG-NC | -2.75 | 1.99 | 2.06 |
| 24 | b | 613 | CLA | CAA-C2A | -2.75 | 1.49 | 1.54 |
| 26 | B | 619 | BCR | C4-C5 | 2.75 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | C | 504 | CLA | MG-NA | -2.75 | 1.99 | 2.06 |
| 26 | A | 610 | BCR | C4-C5 | 2.75 | 1.56 | 1.51 |
| 25 | A | 608 | PHO | C1C-NC | -2.75 | 1.32 | 1.38 |
| 32 | h | 102 | DGD | C6E-C5E | -2.74 | 1.42 | 1.51 |
| 26 | k | 101 | BCR | C7-C6 | 2.74 | 1.54 | 1.45 |
| 24 | b | 609 | CLA | C1B-CHB | 2.74 | 1.48 | 1.41 |
| 24 | c | 511 | CLA | CBD-CGD | -2.74 | 1.43 | 1.52 |
| 24 | B | 608 | CLA | MG-NA | -2.74 | 1.99 | 2.06 |
| 32 | c | 516 | DGD | C3E-C2E | -2.74 | 1.45 | 1.52 |
| 24 | c | 511 | CLA | C3B-CAB | 2.74 | 1.53 | 1.47 |
| 24 | A | 606 | CLA | O2D-CED | -2.73 | 1.38 | 1.45 |
| 26 | C | 514 | BCR | C12-C13 | 2.73 | 1.51 | 1.45 |
| 24 | b | 607 | CLA | C1B-CHB | 2.73 | 1.48 | 1.41 |
| 24 | A | 606 | CLA | C2A-C1A | -2.73 | 1.46 | 1.52 |
| 24 | D | 402 | CLA | C3B-CAB | 2.73 | 1.53 | 1.47 |
| 26 | K | 102 | BCR | C31-C1 | -2.73 | 1.48 | 1.53 |
| 24 | C | 502 | CLA | CAA-C2A | -2.73 | 1.49 | 1.54 |
| 24 | c | 505 | CLA | CBD-CGD | -2.73 | 1.43 | 1.52 |
| 24 | D | 404 | CLA | O2D-CGD | 2.73 | 1.39 | 1.33 |
| 24 | C | 502 | CLA | O2D-CGD | 2.73 | 1.39 | 1.33 |
| 26 | I | 101 | BCR | C27-C26 | 2.73 | 1.56 | 1.51 |
| 24 | D | 402 | CLA | O2D-CED | -2.73 | 1.38 | 1.45 |
| 32 | H | 102 | DGD | O6E-C1E | 2.73 | 1.48 | 1.41 |
| 24 | B | 615 | CLA | C3D-CAD | 2.72 | 1.53 | 1.46 |
| 24 | C | 503 | CLA | C3D-CAD | 2.72 | 1.53 | 1.46 |
| 26 | B | 619 | BCR | C35-C13 | -2.72 | 1.45 | 1.50 |
| 32 | C | 516 | DGD | O5D-C1E | 2.72 | 1.44 | 1.40 |
| 24 | C | 511 | CLA | CAA-C2A | -2.71 | 1.49 | 1.54 |
| 26 | b | 619 | BCR | C27-C26 | 2.71 | 1.56 | 1.51 |
| 24 | D | 403 | CLA | MG-NA | -2.71 | 1.99 | 2.06 |
| 24 | B | 603 | CLA | C1B-CHB | 2.71 | 1.48 | 1.41 |
| 32 | C | 515 | DGD | C1D-C2D | -2.70 | 1.44 | 1.52 |
| 24 | b | 608[B] | CLA | O2D-CGD | 2.70 | 1.39 | 1.33 |
| 24 | B | 608 | CLA | C3D-CAD | 2.70 | 1.52 | 1.46 |
| 24 | c | 505 | CLA | C3B-CAB | 2.70 | 1.53 | 1.47 |
| 24 | C | 501 | CLA | C2A-C1A | -2.69 | 1.46 | 1.52 |
| 24 | C | 504 | CLA | C2A-C1A | -2.69 | 1.46 | 1.52 |
| 26 | B | 620 | BCR | C12-C13 | 2.69 | 1.51 | 1.45 |
| 24 | B | 613 | CLA | C3B-CAB | 2.69 | 1.53 | 1.47 |
| 24 | c | 508 | CLA | C3B-CAB | 2.69 | 1.53 | 1.47 |
| 24 | d | 403 | CLA | O2D-CED | -2.69 | 1.39 | 1.45 |
| 24 | B | 616 | CLA | CAA-C2A | -2.69 | 1.49 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | c | 509 | CLA | MG-NA | -2.69 | 1.99 | 2.06 |
| 32 | c | 517 | DGD | O6D-C5D | 2.69 | 1.50 | 1.44 |
| 28 | A | 614 | SQD | C6-S | -2.68 | 1.67 | 1.77 |
| 24 | B | 606 | CLA | C3D-CAD | 2.68 | 1.52 | 1.46 |
| 24 | d | 402 | CLA | OBD-CAD | -2.68 | 1.18 | 1.22 |
| 28 | a | 614 | SQD | C6-S | -2.68 | 1.67 | 1.77 |
| 24 | D | 403 | CLA | O2D-CED | -2.68 | 1.39 | 1.45 |
| 26 | t | 101 | BCR | C27-C26 | 2.68 | 1.56 | 1.51 |
| 26 | c | 521 | BCR | C7-C6 | 2.68 | 1.54 | 1.45 |
| 24 | a | 615 | CLA | C3D-CAD | 2.68 | 1.52 | 1.46 |
| 24 | c | 507 | CLA | CAA-C2A | -2.67 | 1.49 | 1.54 |
| 24 | d | 403 | CLA | C3B-CAB | 2.67 | 1.53 | 1.47 |
| 24 | B | 603 | CLA | CBD-CGD | -2.67 | 1.44 | 1.52 |
| 32 | h | 102 | DGD | C3E-C2E | -2.67 | 1.45 | 1.52 |
| 24 | b | 614 | CLA | CBD-CGD | -2.67 | 1.44 | 1.52 |
| 24 | C | 505 | CLA | MG-NA | -2.67 | 1.99 | 2.06 |
| 26 | K | 101 | BCR | C31-C1 | -2.67 | 1.48 | 1.53 |
| 26 | b | 619 | BCR | C4-C5 | 2.66 | 1.56 | 1.51 |
| 24 | A | 609 | CLA | C3D-CAD | 2.66 | 1.52 | 1.46 |
| 25 | D | 401 | PHO | C4C-C3C | 2.66 | 1.50 | 1.45 |
| 32 | C | 516 | DGD | C3D-C2D | -2.66 | 1.45 | 1.52 |
| 24 | C | 509 | CLA | OBD-CAD | -2.66 | 1.18 | 1.22 |
| 25 | d | 401 | PHO | C1C-NC | -2.66 | 1.32 | 1.38 |
| 32 | c | 517 | DGD | C6E-C5E | -2.66 | 1.42 | 1.51 |
| 24 | b | 617 | CLA | CBD-CGD | -2.66 | 1.44 | 1.52 |
| 24 | B | 604 | CLA | C3D-CAD | 2.66 | 1.52 | 1.46 |
| 24 | b | 603 | CLA | C3B-CAB | 2.65 | 1.53 | 1.47 |
| 24 | c | 506 | CLA | C3B-CAB | 2.65 | 1.53 | 1.47 |
| 32 | C | 515 | DGD | C6E-C5E | -2.65 | 1.43 | 1.51 |
| 24 | B | 612 | CLA | C2A-C1A | -2.65 | 1.46 | 1.52 |
| 24 | a | 607 | CLA | CAA-C2A | -2.65 | 1.49 | 1.54 |
| 24 | D | 402 | CLA | C1B-CHB | 2.65 | 1.48 | 1.41 |
| 32 | C | 517 | DGD | O2D-C2D | 2.65 | 1.49 | 1.43 |
| 29 | z | 101 | LMG | O7-C8 | -2.65 | 1.40 | 1.46 |
| 24 | A | 607 | CLA | O2D-CGD | 2.65 | 1.39 | 1.33 |
| 24 | C | 503 | CLA | O2D-CED | -2.65 | 1.39 | 1.45 |
| 24 | b | 604 | CLA | C3D-CAD | 2.64 | 1.52 | 1.46 |
| 26 | b | 620 | BCR | C31-C1 | -2.64 | 1.48 | 1.53 |
| 24 | A | 609 | CLA | O2D-CGD | 2.64 | 1.39 | 1.33 |
| 32 | c | 518 | DGD | C6E-C5E | -2.64 | 1.43 | 1.51 |
| 24 | B | 611 | CLA | OBD-CAD | -2.64 | 1.18 | 1.22 |
| 24 | c | 503 | CLA | OBD-CAD | -2.64 | 1.18 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | d | 403 | CLA | O2D-CGD | 2.64 | 1.39 | 1.33 |
| 26 | b | 621 | BCR | C27-C26 | 2.64 | 1.56 | 1.51 |
| 24 | B | 614 | CLA | O2D-CED | -2.64 | 1.39 | 1.45 |
| 24 | a | 615 | CLA | C2A-C1A | -2.63 | 1.46 | 1.52 |
| 32 | c | 518 | DGD | O2D-C2D | 2.63 | 1.49 | 1.43 |
| 24 | B | 614 | CLA | MG-NC | -2.63 | 2.00 | 2.06 |
| 24 | c | 512 | CLA | O2D-CGD | 2.63 | 1.39 | 1.33 |
| 24 | B | 607[A] | CLA | MG-NA | -2.63 | 2.00 | 2.06 |
| 28 | X | 101 | SQD | C6-S | -2.63 | 1.67 | 1.77 |
| 24 | a | 609 | CLA | CAA-C2A | -2.63 | 1.49 | 1.54 |
| 24 | C | 503 | CLA | MG-NA | -2.63 | 2.00 | 2.06 |
| 24 | b | 606 | CLA | C3D-CAD | 2.63 | 1.52 | 1.46 |
| 24 | a | 609 | CLA | O2D-CED | -2.63 | 1.39 | 1.45 |
| 24 | b | 610 | CLA | C2A-C1A | -2.63 | 1.46 | 1.52 |
| 24 | a | 615 | CLA | MG-NC | -2.63 | 2.00 | 2.06 |
| 24 | D | 402 | CLA | C3D-CAD | 2.62 | 1.52 | 1.46 |
| 24 | a | 609 | CLA | C3B-CAB | 2.62 | 1.53 | 1.47 |
| 24 | B | 612 | CLA | C1B-CHB | 2.62 | 1.48 | 1.41 |
| 28 | x | 101 | SQD | C6-S | -2.62 | 1.67 | 1.77 |
| 24 | B | 607[B] | CLA | C2A-C1A | -2.62 | 1.46 | 1.52 |
| 32 | C | 517 | DGD | C6E-C5E | -2.62 | 1.43 | 1.51 |
| 24 | C | 508 | CLA | C2A-C1A | -2.62 | 1.46 | 1.52 |
| 25 | d | 401 | PHO | C4C-C3C | 2.61 | 1.49 | 1.45 |
| 24 | b | 604 | CLA | C3B-CAB | 2.61 | 1.53 | 1.47 |
| 24 | b | 615 | CLA | MG-NA | -2.61 | 2.00 | 2.06 |
| 24 | B | 604 | CLA | C3B-CAB | 2.61 | 1.53 | 1.47 |
| 24 | C | 502 | CLA | C1D-C2D | -2.61 | 1.36 | 1.42 |
| 24 | C | 502 | CLA | O2D-CED | -2.61 | 1.39 | 1.45 |
| 24 | b | 616 | CLA | O2A-CGA | 2.61 | 1.41 | 1.33 |
| 26 | c | 515 | BCR | C27-C26 | 2.61 | 1.56 | 1.51 |
| 24 | B | 615 | CLA | C3B-CAB | 2.61 | 1.53 | 1.47 |
| 26 | c | 521 | BCR | C27-C26 | 2.60 | 1.56 | 1.51 |
| 24 | C | 501 | CLA | CMC-C2C | 2.60 | 1.56 | 1.50 |
| 24 | B | 611 | CLA | C3B-CAB | 2.60 | 1.53 | 1.47 |
| 26 | T | 101 | BCR | C27-C26 | 2.60 | 1.56 | 1.51 |
| 25 | A | 608 | PHO | C4C-NC | 2.60 | 1.42 | 1.36 |
| 26 | h | 101 | BCR | C35-C13 | -2.60 | 1.45 | 1.50 |
| 32 | d | 405 | DGD | C6E-C5E | -2.60 | 1.43 | 1.51 |
| 24 | a | 615 | CLA | C3B-CAB | 2.59 | 1.53 | 1.47 |
| 26 | b | 620 | BCR | C12-C13 | 2.59 | 1.51 | 1.45 |
| 24 | D | 402 | CLA | O2D-CGD | 2.59 | 1.39 | 1.33 |
| 24 | A | 606 | CLA | CBD-CGD | -2.59 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | D | 403 | CLA | MG-NC | -2.59 | 2.00 | 2.06 |
| 24 | b | 603 | CLA | CAA-C2A | -2.59 | 1.49 | 1.54 |
| 24 | C | 505 | CLA | C2A-C1A | -2.59 | 1.46 | 1.52 |
| 26 | k | 101 | BCR | C1-C6 | -2.59 | 1.50 | 1.53 |
| 24 | C | 513 | CLA | CBD-CGD | -2.59 | 1.44 | 1.52 |
| 24 | B | 614 | CLA | MG-NA | -2.58 | 2.00 | 2.06 |
| 24 | b | 616 | CLA | O2D-CGD | 2.58 | 1.39 | 1.33 |
| 24 | c | 505 | CLA | C2A-C1A | -2.58 | 1.46 | 1.52 |
| 25 | A | 608 | PHO | C4C-C3C | 2.58 | 1.49 | 1.45 |
| 24 | B | 603 | CLA | C3B-CAB | 2.57 | 1.53 | 1.47 |
| 24 | C | 502 | CLA | C3B-CAB | 2.57 | 1.53 | 1.47 |
| 24 | d | 402 | CLA | O2D-CGD | 2.57 | 1.39 | 1.33 |
| 24 | C | 506 | CLA | MG-NA | -2.57 | 2.00 | 2.06 |
| 24 | D | 402 | CLA | C2A-C1A | -2.57 | 1.46 | 1.52 |
| 24 | C | 508 | CLA | C3B-CAB | 2.57 | 1.53 | 1.47 |
| 24 | B | 607[A] | CLA | C2A-C1A | -2.57 | 1.46 | 1.52 |
| 24 | b | 608[B] | CLA | O2D-CED | -2.56 | 1.39 | 1.45 |
| 24 | b | 616 | CLA | OBD-CAD | -2.56 | 1.18 | 1.22 |
| 24 | b | 618 | CLA | MG-NA | -2.56 | 2.00 | 2.06 |
| 27 | D | 405 | PL9 | C26-C24 | 2.56 | 1.56 | 1.51 |
| 32 | c | 516 | DGD | O2D-C2D | 2.56 | 1.49 | 1.43 |
| 24 | b | 607 | CLA | C2A-C1A | -2.56 | 1.46 | 1.52 |
| 24 | b | 606 | CLA | MG-NA | -2.55 | 2.00 | 2.06 |
| 24 | b | 615 | CLA | OBD-CAD | -2.55 | 1.18 | 1.22 |
| 24 | b | 609 | CLA | C3D-CAD | 2.55 | 1.52 | 1.46 |
| 24 | B | 611 | CLA | C1B-CHB | 2.55 | 1.48 | 1.41 |
| 24 | b | 606 | CLA | OBD-CAD | -2.55 | 1.18 | 1.22 |
| 32 | h | 102 | DGD | C1D-C2D | -2.55 | 1.45 | 1.52 |
| 28 | b | 601 | SQD | C6-S | -2.55 | 1.68 | 1.77 |
| 24 | B | 611 | CLA | CAA-C2A | -2.55 | 1.49 | 1.54 |
| 24 | b | 613 | CLA | OBD-CAD | -2.55 | 1.18 | 1.22 |
| 24 | A | 609 | CLA | MG-NA | -2.55 | 2.00 | 2.06 |
| 24 | C | 503 | CLA | CMC-C2C | 2.55 | 1.56 | 1.50 |
| 24 | b | 609 | CLA | C3B-CAB | 2.54 | 1.53 | 1.47 |
| 24 | b | 615 | CLA | C3B-CAB | 2.54 | 1.53 | 1.47 |
| 24 | C | 506 | CLA | C3B-CAB | 2.54 | 1.53 | 1.47 |
| 24 | B | 606 | CLA | MG-NA | -2.54 | 2.00 | 2.06 |
| 32 | C | 516 | DGD | C6D-C5D | -2.54 | 1.43 | 1.51 |
| 24 | c | 513 | CLA | MG-NA | -2.54 | 2.00 | 2.06 |
| 24 | d | 403 | CLA | CAA-C2A | -2.53 | 1.49 | 1.54 |
| 24 | C | 511 | CLA | C3D-CAD | 2.53 | 1.52 | 1.46 |
| 24 | C | 509 | CLA | C3B-CAB | 2.53 | 1.53 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 32 | C | 515 | DGD | C3E-C2E | -2.53 | 1.45 | 1.52 |
| 24 | B | 612 | CLA | C3B-CAB | 2.53 | 1.53 | 1.47 |
| 24 | c | 501 | CLA | CBD-CGD | -2.53 | 1.44 | 1.52 |
| 26 | f | 101 | BCR | C35-C13 | -2.53 | 1.45 | 1.50 |
| 29 | C | 519 | LMG | O7-C8 | -2.53 | 1.40 | 1.46 |
| 24 | B | 604 | CLA | OBD-CAD | -2.53 | 1.18 | 1.22 |
| 24 | c | 503 | CLA | O2D-CGD | 2.53 | 1.39 | 1.33 |
| 32 | E | 101 | DGD | O3G-C1D | 2.52 | 1.44 | 1.40 |
| 24 | b | 606 | CLA | CAA-C2A | -2.52 | 1.49 | 1.54 |
| 26 | B | 618 | BCR | C27-C26 | 2.52 | 1.56 | 1.51 |
| 32 | h | 102 | DGD | O6E-C1E | 2.52 | 1.48 | 1.41 |
| 26 | t | 101 | BCR | C35-C13 | -2.52 | 1.45 | 1.50 |
| 24 | c | 504 | CLA | OBD-CAD | -2.52 | 1.18 | 1.22 |
| 32 | d | 405 | DGD | O6D-C1D | 2.52 | 1.48 | 1.41 |
| 24 | b | 613 | CLA | MG-NC | -2.52 | 2.00 | 2.06 |
| 24 | A | 609 | CLA | O2D-CED | -2.52 | 1.39 | 1.45 |
| 24 | c | 507 | CLA | MG-NA | -2.52 | 2.00 | 2.06 |
| 24 | B | 605 | CLA | C3B-CAB | 2.51 | 1.53 | 1.47 |
| 26 | H | 101 | BCR | C31-C1 | -2.51 | 1.48 | 1.53 |
| 32 | d | 405 | DGD | O5D-C1E | 2.51 | 1.44 | 1.40 |
| 24 | c | 501 | CLA | MG-NA | -2.51 | 2.00 | 2.06 |
| 24 | c | 504 | CLA | CMC-C2C | 2.51 | 1.56 | 1.50 |
| 28 | B | 622 | SQD | C6-S | -2.51 | 1.68 | 1.77 |
| 24 | c | 504 | CLA | MG-NC | -2.51 | 2.00 | 2.06 |
| 24 | C | 511 | CLA | OBD-CAD | -2.51 | 1.18 | 1.22 |
| 32 | H | 102 | DGD | O2D-C2D | 2.50 | 1.48 | 1.43 |
| 24 | A | 607 | CLA | O2D-CED | -2.50 | 1.39 | 1.45 |
| 24 | c | 506 | CLA | O2D-CED | -2.50 | 1.39 | 1.45 |
| 25 | a | 608 | PHO | C4C-NC | 2.50 | 1.42 | 1.36 |
| 24 | B | 614 | CLA | C3D-CAD | 2.50 | 1.52 | 1.46 |
| 24 | D | 404 | CLA | CAA-C2A | -2.50 | 1.49 | 1.54 |
| 24 | c | 511 | CLA | O2D-CED | -2.50 | 1.39 | 1.45 |
| 24 | c | 511 | CLA | MG-NA | -2.50 | 2.00 | 2.06 |
| 26 | a | 610 | BCR | C12-C13 | 2.50 | 1.51 | 1.45 |
| 26 | b | 621 | BCR | C35-C13 | -2.50 | 1.45 | 1.50 |
| 24 | C | 507 | CLA | CBD-CGD | -2.50 | 1.44 | 1.52 |
| 24 | d | 402 | CLA | O2D-CED | -2.49 | 1.39 | 1.45 |
| 24 | b | 612 | CLA | MG-NA | -2.49 | 2.00 | 2.06 |
| 26 | C | 514 | BCR | C33-C5 | 2.49 | 1.55 | 1.50 |
| 24 | b | 608[A] | CLA | OBD-CAD | -2.49 | 1.18 | 1.22 |
| 24 | c | 508 | CLA | C2A-C1A | -2.49 | 1.46 | 1.52 |
| 24 | b | 608[A] | CLA | O2D-CED | -2.49 | 1.39 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 618 | CLA | CBD-CGD | -2.49 | 1.44 | 1.52 |
| 32 | d | 405 | DGD | O2D-C2D | 2.48 | 1.48 | 1.43 |
| 24 | C | 510 | CLA | C1B-CHB | 2.48 | 1.47 | 1.41 |
| 24 | B | 603 | CLA | C2A-C1A | -2.48 | 1.46 | 1.52 |
| 24 | b | 610 | CLA | CBD-CGD | -2.48 | 1.44 | 1.52 |
| 32 | c | 517 | DGD | O6E-C1E | 2.48 | 1.48 | 1.41 |
| 24 | b | 610 | CLA | MG-NA | -2.48 | 2.00 | 2.06 |
| 24 | B | 603 | CLA | OBD-CAD | -2.48 | 1.18 | 1.22 |
| 24 | B | 608 | CLA | O2D-CED | -2.48 | 1.39 | 1.45 |
| 24 | c | 503 | CLA | CMC-C2C | 2.47 | 1.56 | 1.50 |
| 24 | B | 607[B] | CLA | MG-NA | -2.47 | 2.00 | 2.06 |
| 24 | D | 403 | CLA | O2D-CGD | 2.47 | 1.39 | 1.33 |
| 26 | B | 618 | BCR | C31-C1 | -2.47 | 1.48 | 1.53 |
| 32 | c | 516 | DGD | O5D-C1E | 2.47 | 1.44 | 1.40 |
| 24 | b | 611 | CLA | C2A-C1A | -2.47 | 1.46 | 1.52 |
| 24 | c | 512 | CLA | O2D-CED | -2.47 | 1.39 | 1.45 |
| 26 | K | 101 | BCR | C7-C6 | 2.47 | 1.53 | 1.45 |
| 24 | B | 614 | CLA | C2A-C1A | -2.47 | 1.46 | 1.52 |
| 28 | l | 101 | SQD | C6-S | -2.47 | 1.68 | 1.77 |
| 26 | K | 101 | BCR | C1-C6 | -2.47 | 1.50 | 1.53 |
| 24 | b | 617 | CLA | OBD-CAD | -2.46 | 1.18 | 1.22 |
| 24 | c | 507 | CLA | C3B-CAB | 2.46 | 1.53 | 1.47 |
| 24 | B | 616 | CLA | O2D-CED | -2.46 | 1.39 | 1.45 |
| 24 | c | 502 | CLA | C3B-CAB | 2.46 | 1.53 | 1.47 |
| 24 | B | 602 | CLA | O2D-CED | -2.46 | 1.39 | 1.45 |
| 24 | c | 509 | CLA | C3B-CAB | 2.46 | 1.52 | 1.47 |
| 24 | B | 617 | CLA | C3B-CAB | 2.46 | 1.52 | 1.47 |
| 24 | c | 501 | CLA | CMC-C2C | 2.46 | 1.56 | 1.50 |
| 24 | C | 501 | CLA | MG-NA | -2.46 | 2.00 | 2.06 |
| 24 | C | 511 | CLA | C3B-CAB | 2.46 | 1.52 | 1.47 |
| 32 | C | 515 | DGD | O6E-C1E | 2.46 | 1.48 | 1.41 |
| 32 | E | 101 | DGD | O3D-C3D | 2.45 | 1.48 | 1.43 |
| 24 | b | 607 | CLA | OBD-CAD | -2.45 | 1.18 | 1.22 |
| 24 | A | 607 | CLA | C2A-C1A | -2.45 | 1.46 | 1.52 |
| 24 | C | 509 | CLA | MG-NC | -2.45 | 2.00 | 2.06 |
| 32 | C | 516 | DGD | O6D-C5D | 2.45 | 1.50 | 1.44 |
| 24 | C | 513 | CLA | OBD-CAD | -2.45 | 1.18 | 1.22 |
| 25 | D | 401 | PHO | CHC-C4B | -2.45 | 1.34 | 1.40 |
| 26 | C | 514 | BCR | C35-C13 | -2.45 | 1.45 | 1.50 |
| 24 | b | 604 | CLA | C1B-CHB | 2.45 | 1.47 | 1.41 |
| 24 | B | 617 | CLA | O2D-CED | -2.45 | 1.39 | 1.45 |
| 24 | c | 505 | CLA | MG-NA | -2.45 | 2.00 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | a | 610 | BCR | C31-C1 | -2.45 | 1.48 | 1.53 |
| 24 | C | 509 | CLA | O2D-CED | -2.45 | 1.39 | 1.45 |
| 28 | L | 102 | SQD | C6-S | -2.44 | 1.68 | 1.77 |
| 24 | B | 605 | CLA | C2A-C1A | -2.44 | 1.46 | 1.52 |
| 26 | A | 610 | BCR | C7-C6 | 2.44 | 1.53 | 1.45 |
| 32 | c | 518 | DGD | O6E-C1E | 2.44 | 1.48 | 1.41 |
| 24 | c | 509 | CLA | C2A-C1A | -2.44 | 1.46 | 1.52 |
| 24 | b | 615 | CLA | O2D-CED | -2.44 | 1.39 | 1.45 |
| 24 | b | 607 | CLA | C3B-CAB | 2.44 | 1.52 | 1.47 |
| 24 | c | 513 | CLA | CBD-CGD | -2.44 | 1.44 | 1.52 |
| 26 | k | 101 | BCR | C35-C13 | -2.44 | 1.45 | 1.50 |
| 24 | C | 513 | CLA | C2A-C1A | -2.44 | 1.46 | 1.52 |
| 24 | D | 403 | CLA | C2A-C1A | -2.44 | 1.46 | 1.52 |
| 24 | B | 615 | CLA | OBD-CAD | -2.44 | 1.18 | 1.22 |
| 24 | d | 403 | CLA | MG-NA | -2.43 | 2.00 | 2.06 |
| 29 | a | 613 | LMG | O7-C8 | -2.43 | 1.40 | 1.46 |
| 24 | C | 505 | CLA | C3B-CAB | 2.43 | 1.52 | 1.47 |
| 26 | B | 619 | BCR | C1-C6 | -2.43 | 1.50 | 1.53 |
| 29 | c | 520 | LMG | O7-C8 | -2.42 | 1.40 | 1.46 |
| 26 | I | 101 | BCR | C35-C13 | -2.42 | 1.45 | 1.50 |
| 26 | K | 101 | BCR | C35-C13 | -2.42 | 1.45 | 1.50 |
| 26 | c | 521 | BCR | C31-C1 | -2.42 | 1.49 | 1.53 |
| 26 | B | 619 | BCR | C30-C25 | 2.42 | 1.57 | 1.53 |
| 24 | C | 504 | CLA | O2D-CED | -2.42 | 1.39 | 1.45 |
| 25 | A | 608 | PHO | CHC-C1C | 2.42 | 1.43 | 1.38 |
| 32 | C | 517 | DGD | O3D-C3D | 2.42 | 1.48 | 1.43 |
| 26 | a | 610 | BCR | C7-C6 | 2.41 | 1.53 | 1.45 |
| 24 | b | 609 | CLA | MG-NC | -2.41 | 2.00 | 2.06 |
| 24 | C | 503 | CLA | O2D-CGD | 2.41 | 1.39 | 1.33 |
| 32 | h | 102 | DGD | O2D-C2D | 2.41 | 1.48 | 1.43 |
| 26 | K | 102 | BCR | C7-C6 | 2.41 | 1.53 | 1.45 |
| 24 | c | 504 | CLA | O2D-CED | -2.41 | 1.39 | 1.45 |
| 27 | d | 404 | PL9 | C7-C3 | 2.41 | 1.53 | 1.51 |
| 24 | d | 403 | CLA | MG-NC | -2.40 | 2.00 | 2.06 |
| 32 | E | 101 | DGD | O6D-C1D | 2.40 | 1.48 | 1.41 |
| 32 | h | 102 | DGD | O5D-C1E | 2.40 | 1.44 | 1.40 |
| 24 | b | 605 | CLA | MG-NA | -2.40 | 2.00 | 2.06 |
| 24 | a | 615 | CLA | O2D-CED | -2.40 | 1.39 | 1.45 |
| 26 | t | 101 | BCR | C7-C6 | 2.40 | 1.53 | 1.45 |
| 24 | c | 507 | CLA | O2D-CED | -2.40 | 1.39 | 1.45 |
| 26 | B | 618 | BCR | C4-C5 | 2.39 | 1.55 | 1.51 |
| 25 | a | 608 | PHO | C1A-NA | 2.39 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 608[A] | CLA | MG-NA | -2.39 | 2.00 | 2.06 |
| 32 | c | 516 | DGD | C6D-C5D | -2.39 | 1.44 | 1.51 |
| 24 | C | 510 | CLA | O2D-CED | -2.39 | 1.39 | 1.45 |
| 24 | c | 513 | CLA | C2A-C1A | -2.39 | 1.46 | 1.52 |
| 32 | c | 518 | DGD | O3D-C3D | 2.39 | 1.48 | 1.43 |
| 24 | C | 510 | CLA | OBD-CAD | -2.39 | 1.19 | 1.22 |
| 26 | b | 621 | BCR | C1-C6 | -2.38 | 1.50 | 1.53 |
| 32 | E | 101 | DGD | C6E-C5E | -2.38 | 1.43 | 1.51 |
| 24 | b | 610 | CLA | O2D-CED | -2.38 | 1.39 | 1.45 |
| 24 | C | 503 | CLA | MG-NC | -2.38 | 2.00 | 2.06 |
| 29 | C | 518 | LMG | O6-C5 | 2.38 | 1.50 | 1.44 |
| 26 | I | 101 | BCR | C4-C5 | 2.38 | 1.55 | 1.51 |
| 24 | B | 612 | CLA | OBD-CAD | -2.37 | 1.19 | 1.22 |
| 24 | B | 609 | CLA | O2D-CED | -2.37 | 1.39 | 1.45 |
| 26 | H | 101 | BCR | C7-C6 | 2.37 | 1.53 | 1.45 |
| 24 | C | 512 | CLA | CMC-C2C | 2.37 | 1.55 | 1.50 |
| 24 | B | 608 | CLA | CMC-C2C | 2.37 | 1.55 | 1.50 |
| 24 | A | 606 | CLA | C3B-CAB | 2.37 | 1.52 | 1.47 |
| 32 | C | 515 | DGD | O2D-C2D | 2.37 | 1.48 | 1.43 |
| 32 | C | 517 | DGD | C1E-C2E | -2.37 | 1.45 | 1.52 |
| 26 | f | 101 | BCR | C7-C6 | 2.37 | 1.53 | 1.45 |
| 26 | c | 515 | BCR | C7-C6 | 2.37 | 1.53 | 1.45 |
| 26 | T | 101 | BCR | C12-C13 | 2.37 | 1.51 | 1.45 |
| 32 | C | 515 | DGD | O6D-C1D | 2.37 | 1.47 | 1.41 |
| 32 | c | 516 | DGD | O6D-C1D | 2.37 | 1.47 | 1.41 |
| 26 | T | 101 | BCR | C7-C6 | 2.36 | 1.53 | 1.45 |
| 24 | B | 608 | CLA | C3B-CAB | 2.36 | 1.52 | 1.47 |
| 32 | c | 517 | DGD | O2D-C2D | 2.36 | 1.48 | 1.43 |
| 24 | B | 610 | CLA | O2D-CED | -2.36 | 1.39 | 1.45 |
| 32 | H | 102 | DGD | O3D-C3D | 2.36 | 1.48 | 1.43 |
| 24 | d | 402 | CLA | C3A-C4A | -2.35 | 1.44 | 1.51 |
| 26 | c | 515 | BCR | C35-C13 | -2.35 | 1.46 | 1.50 |
| 24 | D | 404 | CLA | MG-NA | -2.35 | 2.00 | 2.06 |
| 24 | b | 612 | CLA | O2D-CED | -2.35 | 1.39 | 1.45 |
| 24 | B | 603 | CLA | O2D-CED | -2.35 | 1.39 | 1.45 |
| 24 | b | 617 | CLA | O2D-CED | -2.35 | 1.39 | 1.45 |
| 32 | C | 516 | DGD | C6E-C5E | -2.35 | 1.44 | 1.51 |
| 29 | z | 101 | LMG | O8-C28 | 2.34 | 1.45 | 1.33 |
| 24 | c | 504 | CLA | C2A-C1A | -2.34 | 1.46 | 1.52 |
| 26 | t | 101 | BCR | C31-C1 | -2.34 | 1.49 | 1.53 |
| 24 | C | 512 | CLA | MG-NC | -2.34 | 2.00 | 2.06 |
| 24 | C | 507 | CLA | CMC-C2C | 2.34 | 1.55 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 618 | CLA | C2A-C1A | -2.34 | 1.47 | 1.52 |
| 26 | c | 514 | BCR | C7-C6 | 2.34 | 1.53 | 1.45 |
| 24 | c | 511 | CLA | MG-NC | -2.34 | 2.00 | 2.06 |
| 29 | Z | 101 | LMG | O8-C28 | 2.33 | 1.44 | 1.33 |
| 24 | B | 607[B] | CLA | O2D-CED | -2.33 | 1.39 | 1.45 |
| 32 | d | 405 | DGD | O3D-C3D | 2.33 | 1.48 | 1.43 |
| 24 | C | 504 | CLA | MG-NC | -2.33 | 2.00 | 2.06 |
| 24 | B | 602 | CLA | CMC-C2C | 2.33 | 1.55 | 1.50 |
| 26 | a | 610 | BCR | C27-C26 | 2.33 | 1.55 | 1.51 |
| 24 | b | 608[B] | CLA | MG-NA | -2.33 | 2.00 | 2.06 |
| 24 | B | 607[A] | CLA | O2D-CED | -2.33 | 1.39 | 1.45 |
| 24 | c | 509 | CLA | MG-NC | -2.33 | 2.00 | 2.06 |
| 24 | a | 607 | CLA | CMC-C2C | 2.33 | 1.55 | 1.50 |
| 24 | C | 511 | CLA | O2D-CED | -2.33 | 1.39 | 1.45 |
| 24 | B | 603 | CLA | MG-NC | -2.32 | 2.00 | 2.06 |
| 24 | C | 501 | CLA | OBD-CAD | -2.32 | 1.19 | 1.22 |
| 26 | b | 619 | BCR | C31-C1 | -2.32 | 1.49 | 1.53 |
| 24 | b | 616 | CLA | O2D-CED | -2.32 | 1.39 | 1.45 |
| 24 | c | 510 | CLA | O2D-CED | -2.32 | 1.39 | 1.45 |
| 24 | d | 402 | CLA | C1B-CHB | 2.32 | 1.47 | 1.41 |
| 24 | b | 603 | CLA | MG-NC | -2.32 | 2.00 | 2.06 |
| 24 | B | 613 | CLA | OBD-CAD | -2.32 | 1.19 | 1.22 |
| 24 | b | 614 | CLA | O2D-CED | -2.32 | 1.39 | 1.45 |
| 30 | e | 101 | LHG | C8-C7 | 2.32 | 1.57 | 1.50 |
| 26 | b | 621 | BCR | C7-C6 | 2.32 | 1.53 | 1.45 |
| 24 | b | 609 | CLA | OBD-CAD | -2.32 | 1.19 | 1.22 |
| 24 | c | 505 | CLA | OBD-CAD | -2.31 | 1.19 | 1.22 |
| 24 | B | 617 | CLA | MG-NC | -2.31 | 2.00 | 2.06 |
| 26 | b | 620 | BCR | C35-C13 | -2.31 | 1.46 | 1.50 |
| 24 | B | 617 | CLA | C2A-C1A | -2.31 | 1.47 | 1.52 |
| 32 | E | 101 | DGD | O2D-C2D | 2.31 | 1.48 | 1.43 |
| 24 | a | 607 | CLA | O2D-CED | -2.31 | 1.39 | 1.45 |
| 26 | h | 101 | BCR | C7-C6 | 2.31 | 1.53 | 1.45 |
| 26 | B | 620 | BCR | C33-C5 | 2.31 | 1.54 | 1.50 |
| 24 | B | 615 | CLA | CMC-C2C | 2.31 | 1.55 | 1.50 |
| 24 | C | 505 | CLA | O2D-CED | -2.31 | 1.39 | 1.45 |
| 24 | B | 602 | CLA | CAA-C2A | -2.31 | 1.49 | 1.54 |
| 24 | C | 506 | CLA | OBD-CAD | -2.30 | 1.19 | 1.22 |
| 24 | d | 402 | CLA | MG-NC | -2.30 | 2.00 | 2.06 |
| 24 | b | 617 | CLA | C2A-C1A | -2.30 | 1.47 | 1.52 |
| 24 | B | 607[A] | CLA | OBD-CAD | -2.30 | 1.19 | 1.22 |
| 24 | D | 404 | CLA | CMC-C2C | 2.30 | 1.55 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | B | 613 | CLA | O2D-CED | -2.30 | 1.39 | 1.45 |
| 24 | b | 614 | CLA | OBD-CAD | -2.29 | 1.19 | 1.22 |
| 26 | A | 610 | BCR | C31-C1 | -2.29 | 1.49 | 1.53 |
| 24 | b | 615 | CLA | C2A-C1A | -2.29 | 1.47 | 1.52 |
| 24 | D | 402 | CLA | C3A-C4A | -2.29 | 1.44 | 1.51 |
| 24 | b | 607 | CLA | O2D-CED | -2.29 | 1.39 | 1.45 |
| 26 | K | 101 | BCR | C33-C5 | 2.29 | 1.54 | 1.50 |
| 24 | b | 605 | CLA | O2D-CED | -2.29 | 1.39 | 1.45 |
| 24 | b | 608[B] | CLA | C2A-C1A | -2.29 | 1.47 | 1.52 |
| 27 | a | 611 | PL9 | C41-C39 | 2.29 | 1.56 | 1.51 |
| 24 | b | 605 | CLA | OBD-CAD | -2.29 | 1.19 | 1.22 |
| 24 | b | 603 | CLA | O2D-CED | -2.28 | 1.39 | 1.45 |
| 24 | A | 609 | CLA | MG-NC | -2.28 | 2.00 | 2.06 |
| 32 | c | 517 | DGD | O5D-C1E | 2.28 | 1.44 | 1.40 |
| 32 | C | 517 | DGD | O6E-C1E | 2.28 | 1.47 | 1.41 |
| 24 | d | 403 | CLA | C2A-C1A | -2.28 | 1.47 | 1.52 |
| 32 | C | 515 | DGD | O5D-C1E | 2.28 | 1.44 | 1.40 |
| 24 | B | 608 | CLA | OBD-CAD | -2.28 | 1.19 | 1.22 |
| 32 | C | 515 | DGD | C1E-C2E | -2.28 | 1.45 | 1.52 |
| 24 | a | 615 | CLA | OBD-CAD | -2.28 | 1.19 | 1.22 |
| 26 | c | 514 | BCR | C33-C5 | 2.28 | 1.54 | 1.50 |
| 24 | b | 605 | CLA | MG-NC | -2.28 | 2.00 | 2.06 |
| 24 | b | 613 | CLA | O2D-CED | -2.28 | 1.40 | 1.45 |
| 24 | c | 502 | CLA | OBD-CAD | -2.27 | 1.19 | 1.22 |
| 26 | f | 101 | BCR | C1-C6 | -2.27 | 1.50 | 1.53 |
| 24 | c | 512 | CLA | CMC-C2C | 2.27 | 1.55 | 1.50 |
| 24 | C | 511 | CLA | CBA-CGA | 2.27 | 1.57 | 1.50 |
| 32 | C | 516 | DGD | O3D-C3D | 2.26 | 1.48 | 1.43 |
| 24 | B | 604 | CLA | O2D-CED | -2.26 | 1.40 | 1.45 |
| 24 | B | 606 | CLA | O2D-CED | -2.26 | 1.40 | 1.45 |
| 29 | C | 518 | LMG | C11-C10 | 2.26 | 1.57 | 1.50 |
| 24 | b | 610 | CLA | C3B-CAB | 2.26 | 1.52 | 1.47 |
| 32 | c | 516 | DGD | O3D-C3D | 2.26 | 1.48 | 1.43 |
| 26 | c | 515 | BCR | C31-C1 | -2.26 | 1.49 | 1.53 |
| 24 | A | 607 | CLA | CMC-C2C | 2.25 | 1.55 | 1.50 |
| 25 | D | 401 | PHO | C1B-C2B | 2.25 | 1.50 | 1.45 |
| 24 | c | 508 | CLA | OBD-CAD | -2.25 | 1.19 | 1.22 |
| 24 | c | 510 | CLA | C2A-C1A | -2.25 | 1.47 | 1.52 |
| 24 | b | 612 | CLA | C2A-C1A | -2.25 | 1.47 | 1.52 |
| 24 | c | 508 | CLA | CBD-CGD | -2.25 | 1.45 | 1.52 |
| 24 | c | 510 | CLA | CMC-C2C | 2.25 | 1.55 | 1.50 |
| 24 | C | 510 | CLA | MG-NC | -2.25 | 2.00 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | a | 609 | CLA | CBA-CGA | 2.25 | 1.57 | 1.50 |
| 32 | d | 405 | DGD | C6D-C5D | -2.25 | 1.44 | 1.51 |
| 24 | B | 610 | CLA | OBD-CAD | -2.25 | 1.19 | 1.22 |
| 24 | c | 512 | CLA | C2A-C1A | -2.25 | 1.47 | 1.52 |
| 24 | b | 618 | CLA | O2D-CED | -2.25 | 1.40 | 1.45 |
| 24 | b | 603 | CLA | MG-NA | -2.25 | 2.00 | 2.06 |
| 24 | B | 616 | CLA | MG-NA | -2.25 | 2.00 | 2.06 |
| 32 | C | 516 | DGD | C3E-C2E | -2.24 | 1.46 | 1.52 |
| 26 | A | 610 | BCR | C1-C6 | -2.24 | 1.50 | 1.53 |
| 32 | C | 517 | DGD | C1D-C2D | -2.24 | 1.46 | 1.52 |
| 24 | C | 512 | CLA | MG-NA | -2.24 | 2.00 | 2.06 |
| 29 | c | 520 | LMG | C7-C8 | 2.24 | 1.57 | 1.50 |
| 25 | A | 608 | PHO | C1A-NA | 2.24 | 1.41 | 1.37 |
| 26 | c | 521 | BCR | C35-C13 | -2.24 | 1.46 | 1.50 |
| 24 | C | 506 | CLA | MG-NC | -2.24 | 2.01 | 2.06 |
| 24 | c | 511 | CLA | OBD-CAD | -2.24 | 1.19 | 1.22 |
| 25 | A | 608 | PHO | CHC-C4B | -2.23 | 1.35 | 1.40 |
| 24 | C | 510 | CLA | CMC-C2C | 2.23 | 1.55 | 1.50 |
| 24 | a | 606 | CLA | C2A-C1A | -2.23 | 1.47 | 1.52 |
| 24 | b | 611 | CLA | OBD-CAD | -2.23 | 1.19 | 1.22 |
| 24 | C | 512 | CLA | O2D-CED | -2.23 | 1.40 | 1.45 |
| 24 | c | 507 | CLA | OBD-CAD | -2.23 | 1.19 | 1.22 |
| 24 | c | 512 | CLA | MG-NA | -2.23 | 2.01 | 2.06 |
| 24 | B | 617 | CLA | OBD-CAD | -2.23 | 1.19 | 1.22 |
| 24 | B | 602 | CLA | MG-NA | -2.23 | 2.01 | 2.06 |
| 26 | b | 619 | BCR | C7-C6 | 2.23 | 1.53 | 1.45 |
| 32 | H | 102 | DGD | C3E-C2E | -2.23 | 1.46 | 1.52 |
| 24 | B | 609 | CLA | OBD-CAD | -2.23 | 1.19 | 1.22 |
| 24 | c | 502 | CLA | C2A-C1A | -2.23 | 1.47 | 1.52 |
| 24 | B | 609 | CLA | C3B-CAB | 2.22 | 1.52 | 1.47 |
| 26 | b | 621 | BCR | C33-C5 | 2.22 | 1.54 | 1.50 |
| 24 | c | 508 | CLA | O2D-CED | -2.22 | 1.40 | 1.45 |
| 30 | E | 102 | LHG | C8-C7 | 2.22 | 1.57 | 1.50 |
| 25 | D | 401 | PHO | CAA-C2A | -2.22 | 1.50 | 1.54 |
| 24 | c | 509 | CLA | O2D-CED | -2.22 | 1.40 | 1.45 |
| 24 | b | 618 | CLA | OBD-CAD | -2.22 | 1.19 | 1.22 |
| 25 | D | 401 | PHO | C1C-NC | -2.22 | 1.33 | 1.38 |
| 26 | I | 101 | BCR | C1-C6 | -2.21 | 1.50 | 1.53 |
| 32 | H | 102 | DGD | C6D-C5D | -2.21 | 1.44 | 1.51 |
| 24 | c | 509 | CLA | OBD-CAD | -2.21 | 1.19 | 1.22 |
| 27 | D | 405 | PL9 | C22-C23 | 2.21 | 1.57 | 1.50 |
| 24 | A | 609 | CLA | C2A-C1A | -2.21 | 1.47 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 29 | c | 519 | LMG | C11-C10 | 2.21 | 1.57 | 1.50 |
| 24 | b | 605 | CLA | CMC-C2C | 2.21 | 1.55 | 1.50 |
| 24 | B | 615 | CLA | O2D-CED | -2.21 | 1.40 | 1.45 |
| 26 | I | 101 | BCR | C7-C6 | 2.20 | 1.52 | 1.45 |
| 24 | c | 512 | CLA | OBD-CAD | -2.20 | 1.19 | 1.22 |
| 26 | T | 101 | BCR | C32-C1 | 2.20 | 1.58 | 1.53 |
| 24 | B | 604 | CLA | CMC-C2C | 2.20 | 1.55 | 1.50 |
| 24 | c | 513 | CLA | OBD-CAD | -2.20 | 1.19 | 1.22 |
| 25 | D | 401 | PHO | CHD-C1D | 2.20 | 1.43 | 1.38 |
| 24 | c | 506 | CLA | MG-NA | -2.20 | 2.01 | 2.06 |
| 24 | C | 509 | CLA | CMC-C2C | 2.20 | 1.55 | 1.50 |
| 24 | b | 608[B] | CLA | CMC-C2C | 2.20 | 1.55 | 1.50 |
| 24 | c | 513 | CLA | CMC-C2C | 2.19 | 1.55 | 1.50 |
| 24 | C | 508 | CLA | O2D-CED | -2.19 | 1.40 | 1.45 |
| 24 | c | 505 | CLA | O2D-CED | -2.19 | 1.40 | 1.45 |
| 32 | c | 518 | DGD | C1D-C2D | -2.19 | 1.46 | 1.52 |
| 24 | b | 608[B] | CLA | OBD-CAD | -2.19 | 1.19 | 1.22 |
| 27 | A | 611 | PL9 | C41-C39 | 2.19 | 1.55 | 1.51 |
| 24 | B | 606 | CLA | CMC-C2C | 2.19 | 1.55 | 1.50 |
| 24 | c | 502 | CLA | O2D-CED | -2.19 | 1.40 | 1.45 |
| 24 | D | 404 | CLA | CBA-CGA | 2.19 | 1.57 | 1.50 |
| 24 | B | 612 | CLA | MG-NC | -2.18 | 2.01 | 2.06 |
| 24 | B | 611 | CLA | C3A-C4A | -2.18 | 1.44 | 1.51 |
| 24 | b | 618 | CLA | MG-NC | -2.18 | 2.01 | 2.06 |
| 24 | B | 614 | CLA | C3B-CAB | 2.18 | 1.52 | 1.47 |
| 26 | H | 101 | BCR | C35-C13 | -2.18 | 1.46 | 1.50 |
| 25 | d | 401 | PHO | CHD-C1D | 2.18 | 1.42 | 1.38 |
| 24 | C | 507 | CLA | O2D-CED | -2.18 | 1.40 | 1.45 |
| 29 | C | 519 | LMG | C7-C8 | 2.18 | 1.57 | 1.50 |
| 26 | a | 610 | BCR | C1-C6 | -2.18 | 1.50 | 1.53 |
| 24 | C | 506 | CLA | CBD-CGD | -2.18 | 1.45 | 1.52 |
| 27 | a | 611 | PL9 | C2-C3 | 2.18 | 1.40 | 1.34 |
| 32 | E | 101 | DGD | C3G-C2G | 2.17 | 1.57 | 1.50 |
| 24 | B | 604 | CLA | C2A-C1A | -2.17 | 1.47 | 1.52 |
| 24 | B | 612 | CLA | O2D-CED | -2.17 | 1.40 | 1.45 |
| 32 | c | 517 | DGD | C1E-C2E | -2.17 | 1.46 | 1.52 |
| 24 | B | 606 | CLA | MG-NC | -2.17 | 2.01 | 2.06 |
| 32 | c | 518 | DGD | C3E-C2E | -2.17 | 1.46 | 1.52 |
| 24 | b | 609 | CLA | O2D-CED | -2.17 | 1.40 | 1.45 |
| 24 | b | 617 | CLA | MG-NA | -2.16 | 2.01 | 2.06 |
| 26 | C | 514 | BCR | C7-C6 | 2.16 | 1.52 | 1.45 |
| 24 | b | 608[B] | CLA | C3B-CAB | 2.16 | 1.52 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 608[A] | CLA | C2A-C1A | -2.16 | 1.47 | 1.52 |
| 26 | c | 515 | BCR | C1-C6 | -2.16 | 1.50 | 1.53 |
| 24 | c | 513 | CLA | O2D-CED | -2.16 | 1.40 | 1.45 |
| 24 | c | 503 | CLA | MG-NC | -2.16 | 2.01 | 2.06 |
| 26 | K | 102 | BCR | C1-C6 | -2.16 | 1.50 | 1.53 |
| 24 | C | 502 | CLA | MG-NA | -2.16 | 2.01 | 2.06 |
| 24 | b | 608[A] | CLA | C3B-CAB | 2.16 | 1.52 | 1.47 |
| 27 | A | 611 | PL9 | C22-C23 | 2.15 | 1.57 | 1.50 |
| 32 | c | 516 | DGD | C1D-C2D | -2.15 | 1.46 | 1.52 |
| 25 | a | 608 | PHO | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 28 | B | 622 | SQD | O6-C1 | 2.15 | 1.43 | 1.40 |
| 24 | B | 607[B] | CLA | OBD-CAD | -2.15 | 1.19 | 1.22 |
| 24 | c | 512 | CLA | CBA-CGA | 2.15 | 1.57 | 1.50 |
| 28 | L | 102 | SQD | O6-C1 | 2.15 | 1.43 | 1.40 |
| 24 | B | 614 | CLA | O2D-CGD | 2.14 | 1.38 | 1.33 |
| 27 | D | 405 | PL9 | C37-C38 | 2.14 | 1.57 | 1.50 |
| 24 | C | 511 | CLA | C2A-C1A | -2.14 | 1.47 | 1.52 |
| 24 | C | 502 | CLA | C2A-C1A | -2.14 | 1.47 | 1.52 |
| 26 | c | 515 | BCR | C33-C5 | 2.14 | 1.54 | 1.50 |
| 24 | D | 402 | CLA | MG-NC | -2.13 | 2.01 | 2.06 |
| 24 | C | 513 | CLA | O2D-CED | -2.13 | 1.40 | 1.45 |
| 24 | B | 607[B] | CLA | C3B-CAB | 2.13 | 1.52 | 1.47 |
| 24 | B | 604 | CLA | MG-NC | -2.13 | 2.01 | 2.06 |
| 24 | b | 616 | CLA | MG-NC | -2.13 | 2.01 | 2.06 |
| 32 | C | 516 | DGD | O6D-C1D | 2.13 | 1.47 | 1.41 |
| 32 | H | 102 | DGD | O6D-C1D | 2.13 | 1.47 | 1.41 |
| 26 | B | 618 | BCR | C17-C18 | 2.13 | 1.38 | 1.35 |
| 24 | a | 609 | CLA | OBD-CAD | -2.13 | 1.19 | 1.22 |
| 26 | B | 618 | BCR | C35-C13 | -2.13 | 1.46 | 1.50 |
| 27 | d | 404 | PL9 | C37-C38 | 2.13 | 1.57 | 1.50 |
| 28 | b | 601 | SQD | O6-C1 | 2.12 | 1.43 | 1.40 |
| 24 | C | 512 | CLA | OBD-CAD | -2.12 | 1.19 | 1.22 |
| 29 | D | 408 | LMG | O6-C5 | 2.12 | 1.49 | 1.44 |
| 24 | B | 607[B] | CLA | MG-NC | -2.12 | 2.01 | 2.06 |
| 24 | b | 607 | CLA | MG-NC | -2.12 | 2.01 | 2.06 |
| 24 | b | 617 | CLA | MG-NC | -2.12 | 2.01 | 2.06 |
| 24 | d | 403 | CLA | CBA-CGA | 2.12 | 1.56 | 1.50 |
| 32 | E | 101 | DGD | C6D-C5D | -2.12 | 1.45 | 1.51 |
| 24 | b | 612 | CLA | CMC-C2C | 2.12 | 1.55 | 1.50 |
| 32 | c | 518 | DGD | O6D-C1D | 2.12 | 1.47 | 1.41 |
| 24 | B | 609 | CLA | C2A-C1A | -2.12 | 1.47 | 1.52 |
| 25 | A | 608 | PHO | C1B-C2B | 2.11 | 1.50 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | b | 614 | CLA | CMC-C2C | 2.11 | 1.55 | 1.50 |
| 32 | C | 517 | DGD | O6D-C1D | 2.11 | 1.47 | 1.41 |
| 32 | c | 517 | DGD | C6D-C5D | -2.11 | 1.45 | 1.51 |
| 24 | c | 503 | CLA | MG-NA | -2.11 | 2.01 | 2.06 |
| 24 | c | 508 | CLA | MG-NC | -2.11 | 2.01 | 2.06 |
| 25 | a | 608 | PHO | C1C-NC | -2.11 | 1.34 | 1.38 |
| 24 | a | 606 | CLA | CMC-C2C | 2.11 | 1.55 | 1.50 |
| 24 | c | 506 | CLA | OBD-CAD | -2.11 | 1.19 | 1.22 |
| 32 | d | 405 | DGD | C3G-C2G | 2.11 | 1.57 | 1.50 |
| 24 | B | 602 | CLA | CBA-CGA | 2.10 | 1.56 | 1.50 |
| 27 | A | 611 | PL9 | C2-C3 | 2.10 | 1.40 | 1.34 |
| 27 | d | 404 | PL9 | C26-C24 | 2.10 | 1.55 | 1.51 |
| 24 | B | 611 | CLA | CMC-C2C | 2.10 | 1.55 | 1.50 |
| 32 | h | 102 | DGD | O3D-C3D | 2.10 | 1.47 | 1.43 |
| 25 | D | 401 | PHO | C1C-C2C | 2.10 | 1.50 | 1.45 |
| 24 | a | 609 | CLA | CMC-C2C | 2.10 | 1.55 | 1.50 |
| 24 | c | 501 | CLA | C2A-C1A | -2.10 | 1.47 | 1.52 |
| 32 | c | 517 | DGD | C3E-C2E | -2.10 | 1.47 | 1.52 |
| 32 | h | 102 | DGD | C6D-C5D | -2.10 | 1.45 | 1.51 |
| 24 | a | 615 | CLA | C3A-C4A | -2.09 | 1.45 | 1.51 |
| 24 | C | 504 | CLA | OBD-CAD | -2.09 | 1.19 | 1.22 |
| 24 | b | 608[A] | CLA | CMC-C2C | 2.09 | 1.55 | 1.50 |
| 28 | l | 101 | SQD | O6-C1 | 2.09 | 1.43 | 1.40 |
| 24 | b | 610 | CLA | OBD-CAD | -2.09 | 1.19 | 1.22 |
| 32 | h | 102 | DGD | O6D-C1D | 2.09 | 1.47 | 1.41 |
| 26 | T | 101 | BCR | C31-C1 | -2.09 | 1.49 | 1.53 |
| 24 | C | 501 | CLA | O2D-CED | -2.09 | 1.40 | 1.45 |
| 24 | b | 610 | CLA | CMC-C2C | 2.09 | 1.55 | 1.50 |
| 24 | C | 512 | CLA | C2A-C1A | -2.09 | 1.47 | 1.52 |
| 24 | D | 404 | CLA | OBD-CAD | -2.09 | 1.19 | 1.22 |
| 32 | C | 515 | DGD | O3D-C3D | 2.09 | 1.47 | 1.43 |
| 26 | A | 610 | BCR | C35-C13 | -2.08 | 1.46 | 1.50 |
| 25 | d | 401 | PHO | C1C-C2C | 2.08 | 1.50 | 1.45 |
| 24 | a | 606 | CLA | C3B-CAB | 2.08 | 1.52 | 1.47 |
| 24 | c | 502 | CLA | CBA-CGA | 2.08 | 1.56 | 1.50 |
| 24 | D | 403 | CLA | C3D-CAD | 2.08 | 1.51 | 1.46 |
| 25 | A | 608 | PHO | CHD-C4C | -2.08 | 1.35 | 1.40 |
| 24 | b | 616 | CLA | CBD-CHA | -2.08 | 1.42 | 1.52 |
| 32 | c | 517 | DGD | C1D-C2D | -2.08 | 1.46 | 1.52 |
| 26 | F | 101 | BCR | C7-C6 | 2.08 | 1.52 | 1.45 |
| 24 | B | 603 | CLA | CMC-C2C | 2.08 | 1.55 | 1.50 |
| 30 | A | 615 | LHG | C8-C7 | 2.08 | 1.56 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 24 | B | 613 | CLA | CMC-C2C | 2.07 | 1.55 | 1.50 |
| 24 | C | 504 | CLA | CMC-C2C | 2.07 | 1.55 | 1.50 |
| 24 | C | 506 | CLA | O2D-CED | -2.07 | 1.40 | 1.45 |
| 24 | d | 403 | CLA | OBD-CAD | -2.07 | 1.19 | 1.22 |
| 24 | a | 607 | CLA | OBD-CAD | -2.07 | 1.19 | 1.22 |
| 24 | C | 507 | CLA | MG-NC | -2.07 | 2.01 | 2.06 |
| 27 | a | 611 | PL9 | C37-C38 | 2.07 | 1.57 | 1.50 |
| 24 | c | 509 | CLA | CMC-C2C | 2.07 | 1.55 | 1.50 |
| 24 | A | 606 | CLA | CMC-C2C | 2.06 | 1.55 | 1.50 |
| 24 | D | 402 | CLA | CMC-C2C | 2.06 | 1.55 | 1.50 |
| 27 | D | 405 | PL9 | C17-C18 | 2.06 | 1.57 | 1.50 |
| 24 | B | 615 | CLA | MG-NC | -2.06 | 2.01 | 2.06 |
| 26 | k | 101 | BCR | C33-C5 | 2.06 | 1.54 | 1.50 |
| 24 | c | 501 | CLA | O2D-CED | -2.06 | 1.40 | 1.45 |
| 25 | a | 608 | PHO | C4C-C3C | 2.06 | 1.49 | 1.45 |
| 24 | c | 501 | CLA | MG-NC | -2.06 | 2.01 | 2.06 |
| 32 | c | 517 | DGD | O3G-C1D | 2.06 | 1.43 | 1.40 |
| 27 | d | 404 | PL9 | C22-C23 | 2.05 | 1.57 | 1.50 |
| 24 | b | 604 | CLA | C3A-C4A | -2.05 | 1.45 | 1.51 |
| 24 | C | 507 | CLA | OBD-CAD | -2.05 | 1.19 | 1.22 |
| 24 | B | 609 | CLA | CMC-C2C | 2.05 | 1.55 | 1.50 |
| 33 | E | 103 | HEM | C1D-CHD | -2.05 | 1.35 | 1.41 |
| 27 | a | 611 | PL9 | C17-C18 | 2.05 | 1.57 | 1.50 |
| 29 | a | 613 | LMG | C7-C8 | 2.04 | 1.57 | 1.50 |
| 24 | B | 607[A] | CLA | C3B-CAB | 2.04 | 1.52 | 1.47 |
| 27 | a | 611 | PL9 | C22-C23 | 2.04 | 1.57 | 1.50 |
| 24 | D | 404 | CLA | MG-NC | -2.04 | 2.01 | 2.06 |
| 30 | D | 407 | LHG | C8-C7 | 2.04 | 1.56 | 1.50 |
| 24 | c | 513 | CLA | MG-NC | -2.04 | 2.01 | 2.06 |
| 24 | b | 613 | CLA | C2A-C1A | -2.04 | 1.47 | 1.52 |
| 24 | D | 402 | CLA | CBD-CHA | -2.04 | 1.42 | 1.52 |
| 24 | c | 507 | CLA | CMC-C2C | 2.04 | 1.55 | 1.50 |
| 28 | X | 101 | SQD | O6-C1 | 2.04 | 1.43 | 1.40 |
| 29 | j | 101 | LMG | O8-C9 | -2.03 | 1.40 | 1.45 |
| 33 | V | 201 | HEM | CMC-C2C | 2.03 | 1.56 | 1.51 |
| 24 | A | 609 | CLA | CBD-CHA | -2.03 | 1.42 | 1.52 |
| 24 | c | 510 | CLA | OBD-CAD | -2.03 | 1.19 | 1.22 |
| 24 | B | 616 | CLA | MG-NC | -2.03 | 2.01 | 2.06 |
| 26 | I | 101 | BCR | C32-C1 | 2.03 | 1.57 | 1.53 |
| 26 | B | 619 | BCR | C31-C1 | -2.03 | 1.49 | 1.53 |
| 30 | d | 407 | LHG | C8-C7 | 2.03 | 1.56 | 1.50 |
| 24 | B | 611 | CLA | CBA-CGA | 2.03 | 1.56 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | h | 101 | BCR | C1-C6 | -2.02 | 1.51 | 1.53 |
| 26 | t | 101 | BCR | C39-C30 | -2.02 | 1.49 | 1.53 |
| 32 | C | 517 | DGD | O3G-C3G | -2.02 | 1.40 | 1.43 |
| 25 | a | 608 | PHO | C1C-C2C | 2.02 | 1.50 | 1.45 |
| 32 | d | 405 | DGD | C3E-C2E | -2.02 | 1.47 | 1.52 |
| 24 | B | 616 | CLA | C2A-C1A | -2.01 | 1.47 | 1.52 |
| 26 | I | 101 | BCR | C31-C1 | -2.01 | 1.49 | 1.53 |
| 28 | x | 101 | SQD | O6-C1 | 2.01 | 1.43 | 1.40 |
| 24 | C | 508 | CLA | CMC-C2C | 2.01 | 1.55 | 1.50 |
| 24 | C | 507 | CLA | C3B-CAB | 2.01 | 1.52 | 1.47 |
| 24 | B | 616 | CLA | OBD-CAD | -2.01 | 1.19 | 1.22 |
| 27 | A | 611 | PL9 | C17-C18 | 2.01 | 1.57 | 1.50 |
| 32 | c | 518 | DGD | O3G-C3G | -2.01 | 1.40 | 1.43 |
| 32 | c | 517 | DGD | O6D-C1D | 2.01 | 1.47 | 1.41 |
| 24 | b | 606 | CLA | O2D-CED | -2.00 | 1.40 | 1.45 |
| 25 | D | 401 | PHO | O2D-CGD | 2.00 | 1.38 | 1.33 |
| 25 | a | 608 | PHO | C1B-C2B | 2.00 | 1.50 | 1.45 |
| 32 | C | 516 | DGD | C1D-C2D | -2.00 | 1.46 | 1.52 |

All (2275) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | b | 621 | BCR | C15-C16-C17 | 25.00 | 174.68 | 123.47 |
| 26 | k | 101 | BCR | C15-C16-C17 | 24.97 | 174.62 | 123.47 |
| 26 | T | 101 | BCR | C15-C16-C17 | 24.91 | 174.50 | 123.47 |
| 26 | t | 101 | BCR | C15-C16-C17 | 24.76 | 174.19 | 123.47 |
| 26 | A | 610 | BCR | C15-C16-C17 | 23.82 | 172.26 | 123.47 |
| 26 | B | 620 | BCR | C15-C16-C17 | 23.09 | 170.76 | 123.47 |
| 26 | I | 101 | BCR | C15-C16-C17 | 23.08 | 170.75 | 123.47 |
| 26 | F | 101 | BCR | C15-C16-C17 | 23.06 | 170.72 | 123.47 |
| 26 | C | 514 | BCR | C15-C16-C17 | 22.99 | 170.57 | 123.47 |
| 26 | B | 618 | BCR | C15-C16-C17 | 22.79 | 170.16 | 123.47 |
| 26 | c | 521 | BCR | C15-C16-C17 | 22.79 | 170.15 | 123.47 |
| 26 | H | 101 | BCR | C15-C16-C17 | 22.69 | 169.95 | 123.47 |
| 26 | c | 515 | BCR | C15-C16-C17 | 22.57 | 169.72 | 123.47 |
| 26 | K | 102 | BCR | C15-C16-C17 | 22.45 | 169.46 | 123.47 |
| 26 | b | 620 | BCR | C15-C16-C17 | 22.32 | 169.19 | 123.47 |
| 26 | B | 619 | BCR | C15-C16-C17 | 22.09 | 168.72 | 123.47 |
| 26 | f | 101 | BCR | C15-C16-C17 | 21.73 | 167.99 | 123.47 |
| 26 | h | 101 | BCR | C15-C16-C17 | 21.61 | 167.74 | 123.47 |
| 26 | c | 514 | BCR | C15-C16-C17 | 21.60 | 167.72 | 123.47 |
| 26 | b | 619 | BCR | C15-C16-C17 | 21.27 | 167.04 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 26 | K | 101 | BCR | C15-C16-C17 | 21.21 | 166.92 | 123.47 |
| 26 | a | 610 | BCR | C15-C16-C17 | 20.30 | 165.06 | 123.47 |
| 26 | b | 619 | BCR | C21-C20-C19 | 18.01 | 179.43 | 123.22 |
| 26 | T | 101 | BCR | C21-C20-C19 | 17.74 | 178.57 | 123.22 |
| 26 | a | 610 | BCR | C21-C20-C19 | 17.43 | 177.61 | 123.22 |
| 26 | c | 514 | BCR | C21-C20-C19 | 17.42 | 177.57 | 123.22 |
| 26 | I | 101 | BCR | C21-C20-C19 | 17.33 | 177.31 | 123.22 |
| 26 | c | 515 | BCR | C21-C20-C19 | 17.25 | 177.04 | 123.22 |
| 26 | K | 102 | BCR | C21-C20-C19 | 17.18 | 176.83 | 123.22 |
| 26 | h | 101 | BCR | C21-C20-C19 | 17.14 | 176.72 | 123.22 |
| 26 | t | 101 | BCR | C21-C20-C19 | 17.11 | 176.60 | 123.22 |
| 26 | A | 610 | BCR | C21-C20-C19 | 17.08 | 176.52 | 123.22 |
| 26 | b | 621 | BCR | C21-C20-C19 | 16.91 | 175.99 | 123.22 |
| 26 | b | 620 | BCR | C21-C20-C19 | 16.82 | 175.72 | 123.22 |
| 26 | F | 101 | BCR | C21-C20-C19 | 16.80 | 175.63 | 123.22 |
| 26 | B | 618 | BCR | C21-C20-C19 | 16.78 | 175.59 | 123.22 |
| 26 | C | 514 | BCR | C21-C20-C19 | 16.69 | 175.30 | 123.22 |
| 26 | c | 521 | BCR | C21-C20-C19 | 16.52 | 174.78 | 123.22 |
| 26 | B | 619 | BCR | C21-C20-C19 | 16.31 | 174.13 | 123.22 |
| 26 | k | 101 | BCR | C21-C20-C19 | 16.06 | 173.33 | 123.22 |
| 26 | f | 101 | BCR | C21-C20-C19 | 15.91 | 172.85 | 123.22 |
| 26 | K | 101 | BCR | C21-C20-C19 | 15.82 | 172.58 | 123.22 |
| 26 | B | 620 | BCR | C21-C20-C19 | 15.49 | 171.57 | 123.22 |
| 26 | F | 101 | BCR | C33-C5-C6 | -15.38 | 107.26 | 124.53 |
| 26 | B | 618 | BCR | C33-C5-C6 | -15.09 | 107.59 | 124.53 |
| 26 | T | 101 | BCR | C38-C26-C25 | -14.94 | 107.75 | 124.53 |
| 26 | B | 618 | BCR | C38-C26-C25 | -14.58 | 108.15 | 124.53 |
| 26 | b | 619 | BCR | C33-C5-C6 | -14.40 | 108.36 | 124.53 |
| 26 | f | 101 | BCR | C33-C5-C6 | -14.22 | 108.56 | 124.53 |
| 26 | H | 101 | BCR | C21-C20-C19 | 14.16 | 167.40 | 123.22 |
| 26 | b | 621 | BCR | C38-C26-C25 | -14.09 | 108.71 | 124.53 |
| 26 | H | 101 | BCR | C33-C5-C6 | -13.87 | 108.95 | 124.53 |
| 26 | b | 620 | BCR | C33-C5-C6 | -13.84 | 108.98 | 124.53 |
| 26 | B | 620 | BCR | C38-C26-C25 | -13.71 | 109.14 | 124.53 |
| 26 | C | 514 | BCR | C38-C26-C25 | -13.66 | 109.18 | 124.53 |
| 26 | K | 101 | BCR | C38-C26-C25 | -13.55 | 109.31 | 124.53 |
| 26 | k | 101 | BCR | C33-C5-C6 | -13.45 | 109.42 | 124.53 |
| 26 | B | 619 | BCR | C33-C5-C6 | -13.32 | 109.57 | 124.53 |
| 26 | t | 101 | BCR | C38-C26-C25 | -13.30 | 109.59 | 124.53 |
| 26 | c | 515 | BCR | C38-C26-C25 | -13.23 | 109.68 | 124.53 |
| 26 | b | 621 | BCR | C15-C14-C13 | -13.22 | 108.44 | 127.31 |
| 26 | K | 101 | BCR | C33-C5-C6 | -13.09 | 109.83 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 26 | a | 610 | BCR | C33-C5-C6 | -13.06 | 109.86 | 124.53 |
| 26 | A | 610 | BCR | C33-C5-C6 | -13.03 | 109.90 | 124.53 |
| 26 | I | 101 | BCR | C38-C26-C25 | -13.02 | 109.91 | 124.53 |
| 26 | c | 514 | BCR | C38-C26-C25 | -12.94 | 110.00 | 124.53 |
| 26 | k | 101 | BCR | C38-C26-C25 | -12.82 | 110.13 | 124.53 |
| 26 | a | 610 | BCR | C38-C26-C25 | -12.66 | 110.31 | 124.53 |
| 26 | b | 619 | BCR | C38-C26-C25 | -12.64 | 110.33 | 124.53 |
| 26 | K | 102 | BCR | C33-C5-C6 | -12.54 | 110.45 | 124.53 |
| 26 | A | 610 | BCR | C38-C26-C25 | -12.37 | 110.63 | 124.53 |
| 26 | T | 101 | BCR | C33-C5-C6 | -12.35 | 110.66 | 124.53 |
| 26 | t | 101 | BCR | C33-C5-C6 | -12.25 | 110.78 | 124.53 |
| 26 | h | 101 | BCR | C33-C5-C6 | -11.94 | 111.12 | 124.53 |
| 26 | b | 620 | BCR | C24-C23-C22 | -11.64 | 108.64 | 126.23 |
| 26 | F | 101 | BCR | C16-C17-C18 | -11.63 | 110.72 | 127.31 |
| 26 | b | 621 | BCR | C16-C17-C18 | -11.59 | 110.77 | 127.31 |
| 26 | H | 101 | BCR | C38-C26-C25 | -11.50 | 111.62 | 124.53 |
| 27 | D | 405 | PL9 | C7-C8-C9 | -11.45 | 107.74 | 126.79 |
| 26 | c | 521 | BCR | C33-C5-C6 | -11.44 | 111.69 | 124.53 |
| 26 | C | 514 | BCR | C33-C5-C6 | -11.44 | 111.69 | 124.53 |
| 26 | K | 102 | BCR | C16-C17-C18 | -11.36 | 111.09 | 127.31 |
| 26 | h | 101 | BCR | C38-C26-C25 | -11.36 | 111.78 | 124.53 |
| 26 | b | 619 | BCR | C16-C17-C18 | -11.34 | 111.13 | 127.31 |
| 27 | d | 404 | PL9 | C7-C8-C9 | -11.29 | 108.00 | 126.79 |
| 26 | b | 621 | BCR | C33-C5-C6 | -11.27 | 111.88 | 124.53 |
| 26 | c | 514 | BCR | C16-C17-C18 | -11.24 | 111.27 | 127.31 |
| 26 | c | 521 | BCR | C38-C26-C25 | -11.20 | 111.95 | 124.53 |
| 26 | c | 521 | BCR | C20-C21-C22 | -11.09 | 111.48 | 127.31 |
| 26 | f | 101 | BCR | C16-C17-C18 | -11.08 | 111.49 | 127.31 |
| 26 | B | 620 | BCR | C33-C5-C6 | -11.07 | 112.10 | 124.53 |
| 26 | b | 621 | BCR | C24-C23-C22 | -10.99 | 109.62 | 126.23 |
| 26 | c | 514 | BCR | C33-C5-C6 | -10.81 | 112.39 | 124.53 |
| 26 | b | 621 | BCR | C20-C21-C22 | -10.77 | 111.94 | 127.31 |
| 26 | c | 521 | BCR | C24-C23-C22 | -10.57 | 110.26 | 126.23 |
| 26 | B | 620 | BCR | C16-C17-C18 | -10.55 | 112.26 | 127.31 |
| 26 | h | 101 | BCR | C15-C14-C13 | -10.25 | 112.69 | 127.31 |
| 26 | c | 514 | BCR | C24-C23-C22 | -10.24 | 110.77 | 126.23 |
| 26 | F | 101 | BCR | C7-C8-C9 | -10.18 | 110.85 | 126.23 |
| 26 | I | 101 | BCR | C4-C5-C6 | -10.16 | 107.98 | 122.73 |
| 26 | F | 101 | BCR | C11-C10-C9 | -10.16 | 112.81 | 127.31 |
| 26 | t | 101 | BCR | C24-C23-C22 | -10.15 | 110.89 | 126.23 |
| 26 | c | 521 | BCR | C16-C17-C18 | -10.13 | 112.85 | 127.31 |
| 26 | c | 515 | BCR | C33-C5-C6 | -10.00 | 113.30 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | a | 610 | BCR | C16-C17-C18 | -9.95 | 113.11 | 127.31 |
| 26 | B | 619 | BCR | C11-C10-C9 | -9.82 | 113.30 | 127.31 |
| 26 | h | 101 | BCR | C16-C17-C18 | -9.81 | 113.31 | 127.31 |
| 26 | B | 619 | BCR | C16-C17-C18 | -9.75 | 113.40 | 127.31 |
| 26 | K | 102 | BCR | C38-C26-C25 | -9.72 | 113.61 | 124.53 |
| 26 | T | 101 | BCR | C24-C23-C22 | -9.72 | 111.55 | 126.23 |
| 26 | F | 101 | BCR | C36-C18-C17 | -9.54 | 109.56 | 122.92 |
| 26 | I | 101 | BCR | C33-C5-C6 | -9.46 | 113.91 | 124.53 |
| 26 | I | 101 | BCR | C24-C23-C22 | -9.45 | 111.95 | 126.23 |
| 26 | f | 101 | BCR | C30-C25-C26 | -9.34 | 109.45 | 122.61 |
| 26 | C | 514 | BCR | C11-C10-C9 | -9.29 | 114.05 | 127.31 |
| 26 | I | 101 | BCR | C11-C10-C9 | -9.22 | 114.15 | 127.31 |
| 26 | B | 620 | BCR | C8-C7-C6 | -9.20 | 101.36 | 127.20 |
| 26 | H | 101 | BCR | C37-C22-C21 | -9.18 | 110.06 | 122.92 |
| 26 | B | 618 | BCR | C16-C17-C18 | -9.12 | 114.30 | 127.31 |
| 26 | H | 101 | BCR | C15-C14-C13 | -9.09 | 114.33 | 127.31 |
| 26 | K | 102 | BCR | C24-C23-C22 | -9.04 | 112.57 | 126.23 |
| 24 | c | 508 | CLA | C4D-C3D-CAD | -9.02 | 103.44 | 108.47 |
| 26 | A | 610 | BCR | C16-C17-C18 | -8.98 | 114.50 | 127.31 |
| 26 | t | 101 | BCR | C30-C25-C26 | -8.97 | 109.97 | 122.61 |
| 26 | b | 620 | BCR | C38-C26-C25 | -8.89 | 114.55 | 124.53 |
| 26 | f | 101 | BCR | C4-C5-C6 | -8.84 | 109.90 | 122.73 |
| 26 | c | 515 | BCR | C11-C10-C9 | -8.83 | 114.71 | 127.31 |
| 26 | I | 101 | BCR | C16-C17-C18 | -8.81 | 114.74 | 127.31 |
| 26 | F | 101 | BCR | C24-C23-C22 | -8.80 | 112.94 | 126.23 |
| 26 | T | 101 | BCR | C16-C17-C18 | -8.74 | 114.84 | 127.31 |
| 26 | T | 101 | BCR | C30-C25-C26 | -8.64 | 110.44 | 122.61 |
| 26 | b | 619 | BCR | C11-C10-C9 | -8.62 | 115.01 | 127.31 |
| 26 | I | 101 | BCR | C7-C8-C9 | -8.58 | 113.27 | 126.23 |
| 26 | b | 619 | BCR | C4-C5-C6 | -8.58 | 110.28 | 122.73 |
| 26 | b | 620 | BCR | C8-C7-C6 | -8.57 | 103.13 | 127.20 |
| 26 | B | 619 | BCR | C38-C26-C25 | -8.52 | 114.97 | 124.53 |
| 26 | F | 101 | BCR | C38-C26-C25 | -8.51 | 114.97 | 124.53 |
| 26 | k | 101 | BCR | C16-C17-C18 | -8.50 | 115.18 | 127.31 |
| 26 | b | 620 | BCR | C11-C10-C9 | -8.44 | 115.27 | 127.31 |
| 26 | F | 101 | BCR | C4-C5-C6 | -8.43 | 110.50 | 122.73 |
| 24 | B | 605 | CLA | C4D-C3D-CAD | -8.35 | 103.81 | 108.47 |
| 24 | A | 606 | CLA | C4A-NA-C1A | -8.34 | 102.96 | 106.71 |
| 26 | K | 101 | BCR | C30-C25-C26 | -8.32 | 110.90 | 122.61 |
| 26 | B | 619 | BCR | C7-C8-C9 | -8.28 | 113.73 | 126.23 |
| 26 | F | 101 | BCR | C30-C25-C26 | -8.27 | 110.96 | 122.61 |
| 24 | C | 510 | CLA | C4A-NA-C1A | -8.27 | 102.99 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | b | 619 | BCR | C7-C8-C9 | -8.22 | 113.82 | 126.23 |
| 26 | K | 102 | BCR | C20-C21-C22 | -8.17 | 115.66 | 127.31 |
| 26 | C | 514 | BCR | C7-C8-C9 | -8.16 | 113.90 | 126.23 |
| 26 | t | 101 | BCR | C27-C26-C25 | -8.16 | 110.88 | 122.73 |
| 26 | b | 620 | BCR | C15-C14-C13 | -8.15 | 115.68 | 127.31 |
| 26 | a | 610 | BCR | C27-C26-C25 | -8.14 | 110.91 | 122.73 |
| 26 | T | 101 | BCR | C27-C26-C25 | -8.11 | 110.96 | 122.73 |
| 24 | B | 617 | CLA | C4D-C3D-CAD | -8.06 | 103.98 | 108.47 |
| 26 | B | 618 | BCR | C7-C8-C9 | -8.06 | 114.06 | 126.23 |
| 26 | T | 101 | BCR | C15-C14-C13 | -8.05 | 115.83 | 127.31 |
| 26 | H | 101 | BCR | C16-C17-C18 | -8.05 | 115.83 | 127.31 |
| 27 | A | 611 | PL9 | C37-C38-C39 | -8.03 | 108.31 | 127.66 |
| 26 | C | 514 | BCR | C16-C17-C18 | -8.01 | 115.88 | 127.31 |
| 26 | c | 515 | BCR | C24-C23-C22 | -7.98 | 114.18 | 126.23 |
| 26 | c | 515 | BCR | C4-C5-C6 | -7.96 | 111.17 | 122.73 |
| 26 | c | 514 | BCR | C11-C10-C9 | -7.95 | 115.97 | 127.31 |
| 26 | a | 610 | BCR | C4-C5-C6 | -7.95 | 111.19 | 122.73 |
| 27 | A | 611 | PL9 | C42-C43-C44 | -7.91 | 108.62 | 127.66 |
| 26 | H | 101 | BCR | C24-C23-C22 | -7.84 | 114.38 | 126.23 |
| 26 | C | 514 | BCR | C20-C21-C22 | -7.81 | 116.17 | 127.31 |
| 26 | f | 101 | BCR | C38-C26-C25 | -7.79 | 115.78 | 124.53 |
| 26 | C | 514 | BCR | C24-C23-C22 | -7.76 | 114.50 | 126.23 |
| 26 | B | 619 | BCR | C8-C7-C6 | -7.76 | 105.41 | 127.20 |
| 27 | a | 611 | PL9 | C7-C8-C9 | -7.73 | 113.93 | 126.79 |
| 24 | C | 508 | CLA | C4D-C3D-CAD | -7.72 | 104.16 | 108.47 |
| 27 | a | 611 | PL9 | C37-C38-C39 | -7.70 | 109.11 | 127.66 |
| 27 | A | 611 | PL9 | C7-C8-C9 | -7.70 | 113.98 | 126.79 |
| 26 | K | 101 | BCR | C11-C10-C9 | -7.70 | 116.33 | 127.31 |
| 26 | B | 620 | BCR | C27-C26-C25 | -7.69 | 111.56 | 122.73 |
| 24 | C | 501 | CLA | C4D-C3D-CAD | -7.68 | 104.19 | 108.47 |
| 26 | I | 101 | BCR | C27-C26-C25 | -7.66 | 111.61 | 122.73 |
| 26 | C | 514 | BCR | C15-C14-C13 | -7.63 | 116.41 | 127.31 |
| 26 | c | 514 | BCR | C15-C14-C13 | -7.62 | 116.44 | 127.31 |
| 26 | B | 618 | BCR | C11-C10-C9 | -7.58 | 116.49 | 127.31 |
| 26 | f | 101 | BCR | C11-C10-C9 | -7.57 | 116.51 | 127.31 |
| 27 | d | 404 | PL9 | C12-C13-C14 | -7.57 | 109.44 | 127.66 |
| 27 | a | 611 | PL9 | C16-C14-C13 | -7.55 | 105.84 | 121.12 |
| 27 | D | 405 | PL9 | C32-C33-C34 | -7.54 | 109.51 | 127.66 |
| 26 | t | 101 | BCR | C7-C6-C5 | -7.54 | 103.20 | 121.46 |
| 26 | T | 101 | BCR | C7-C8-C9 | -7.53 | 114.86 | 126.23 |
| 26 | H | 101 | BCR | C8-C7-C6 | -7.50 | 106.14 | 127.20 |
| 26 | b | 621 | BCR | C36-C18-C19 | -7.49 | 106.28 | 118.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | f | 101 | BCR | C24-C23-C22 | -7.48 | 114.93 | 126.23 |
| 27 | D | 405 | PL9 | C22-C23-C24 | -7.47 | 109.67 | 127.66 |
| 26 | B | 618 | BCR | C4-C5-C6 | -7.45 | 111.92 | 122.73 |
| 26 | A | 610 | BCR | C4-C5-C6 | -7.41 | 111.97 | 122.73 |
| 24 | B | 613 | CLA | C4D-C3D-CAD | -7.40 | 104.34 | 108.47 |
| 27 | A | 611 | PL9 | C16-C14-C13 | -7.37 | 106.19 | 121.12 |
| 26 | b | 620 | BCR | C4-C5-C6 | -7.37 | 112.03 | 122.73 |
| 24 | C | 513 | CLA | C4D-C3D-CAD | -7.36 | 104.37 | 108.47 |
| 26 | I | 101 | BCR | C1-C6-C5 | -7.35 | 112.26 | 122.61 |
| 24 | d | 403 | CLA | C4D-C3D-CAD | -7.33 | 104.38 | 108.47 |
| 26 | b | 621 | BCR | C8-C7-C6 | -7.30 | 106.71 | 127.20 |
| 26 | k | 101 | BCR | C24-C23-C22 | -7.30 | 115.21 | 126.23 |
| 26 | a | 610 | BCR | C30-C25-C26 | -7.29 | 112.35 | 122.61 |
| 26 | H | 101 | BCR | C4-C5-C6 | -7.29 | 112.15 | 122.73 |
| 26 | c | 514 | BCR | C30-C25-C26 | -7.29 | 112.35 | 122.61 |
| 24 | C | 505 | CLA | C4D-C3D-CAD | -7.27 | 104.42 | 108.47 |
| 27 | a | 611 | PL9 | C27-C28-C29 | -7.24 | 110.22 | 127.66 |
| 24 | C | 505 | CLA | C3A-C2A-C1A | 7.23 | 112.17 | 101.34 |
| 27 | a | 611 | PL9 | C42-C43-C44 | -7.22 | 110.26 | 127.66 |
| 27 | a | 611 | PL9 | C22-C23-C24 | -7.22 | 110.29 | 127.66 |
| 26 | t | 101 | BCR | C11-C10-C9 | -7.21 | 117.02 | 127.31 |
| 26 | f | 101 | BCR | C7-C8-C9 | -7.19 | 115.37 | 126.23 |
| 24 | B | 611 | CLA | C4D-C3D-CAD | -7.19 | 104.46 | 108.47 |
| 27 | D | 405 | PL9 | C27-C28-C29 | -7.17 | 110.39 | 127.66 |
| 27 | A | 611 | PL9 | C27-C28-C29 | -7.17 | 110.39 | 127.66 |
| 26 | f | 101 | BCR | C1-C6-C5 | -7.17 | 112.51 | 122.61 |
| 26 | K | 102 | BCR | C30-C25-C26 | -7.16 | 112.52 | 122.61 |
| 26 | c | 515 | BCR | C7-C8-C9 | -7.15 | 115.42 | 126.23 |
| 27 | d | 404 | PL9 | C32-C33-C34 | -7.14 | 110.47 | 127.66 |
| 24 | B | 610 | CLA | C4D-C3D-CAD | -7.12 | 104.50 | 108.47 |
| 26 | c | 515 | BCR | C27-C26-C25 | -7.09 | 112.44 | 122.73 |
| 24 | C | 504 | CLA | C4D-C3D-CAD | -7.04 | 104.55 | 108.47 |
| 27 | d | 404 | PL9 | C22-C23-C24 | -7.02 | 110.75 | 127.66 |
| 26 | B | 620 | BCR | C30-C25-C26 | -7.02 | 112.72 | 122.61 |
| 24 | c | 513 | CLA | C4D-C3D-CAD | -7.00 | 104.57 | 108.47 |
| 24 | b | 606 | CLA | C4D-C3D-CAD | -6.99 | 104.57 | 108.47 |
| 26 | k | 101 | BCR | C30-C25-C26 | -6.99 | 112.77 | 122.61 |
| 24 | C | 509 | CLA | C4D-C3D-CAD | -6.97 | 104.58 | 108.47 |
| 24 | B | 612 | CLA | C4D-C3D-CAD | -6.97 | 104.58 | 108.47 |
| 26 | b | 620 | BCR | C16-C17-C18 | -6.96 | 117.37 | 127.31 |
| 24 | b | 604 | CLA | C4D-C3D-CAD | -6.96 | 104.59 | 108.47 |
| 26 | b | 619 | BCR | C1-C6-C5 | -6.96 | 112.82 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | D | 404 | CLA | C4A-NA-C1A | -6.95 | 103.58 | 106.71 |
| 26 | b | 621 | BCR | C11-C10-C9 | -6.93 | 117.42 | 127.31 |
| 27 | A | 611 | PL9 | C41-C39-C38 | -6.93 | 107.10 | 121.12 |
| 26 | T | 101 | BCR | C7-C6-C5 | -6.91 | 104.73 | 121.46 |
| 27 | D | 405 | PL9 | C16-C14-C13 | -6.90 | 107.15 | 121.12 |
| 26 | B | 618 | BCR | C1-C6-C5 | -6.90 | 112.89 | 122.61 |
| 24 | b | 618 | CLA | C4D-C3D-CAD | -6.88 | 104.63 | 108.47 |
| 24 | b | 610 | CLA | C4D-C3D-CAD | -6.86 | 104.65 | 108.47 |
| 26 | c | 514 | BCR | C20-C21-C22 | -6.86 | 117.52 | 127.31 |
| 26 | c | 514 | BCR | C27-C26-C25 | -6.85 | 112.79 | 122.73 |
| 26 | c | 515 | BCR | C1-C6-C5 | -6.83 | 112.99 | 122.61 |
| 24 | C | 507 | CLA | O2D-CGD-CBD | 6.83 | 123.40 | 111.27 |
| 26 | a | 610 | BCR | C1-C6-C5 | -6.79 | 113.05 | 122.61 |
| 26 | c | 514 | BCR | C34-C9-C10 | -6.76 | 113.46 | 122.92 |
| 27 | d | 404 | PL9 | C46-C44-C43 | -6.75 | 107.47 | 121.12 |
| 24 | c | 502 | CLA | C4D-C3D-CAD | -6.73 | 104.72 | 108.47 |
| 26 | c | 515 | BCR | C15-C14-C13 | -6.72 | 117.72 | 127.31 |
| 26 | K | 102 | BCR | C27-C26-C25 | -6.72 | 112.97 | 122.73 |
| 24 | C | 502 | CLA | C4D-C3D-CAD | -6.72 | 104.72 | 108.47 |
| 26 | B | 619 | BCR | C7-C6-C5 | -6.71 | 105.20 | 121.46 |
| 27 | A | 611 | PL9 | C17-C18-C19 | -6.71 | 111.51 | 127.66 |
| 24 | c | 509 | CLA | C4D-C3D-CAD | -6.70 | 104.73 | 108.47 |
| 26 | h | 101 | BCR | C36-C18-C17 | -6.68 | 113.56 | 122.92 |
| 27 | a | 611 | PL9 | C17-C18-C19 | -6.63 | 111.70 | 127.66 |
| 24 | c | 505 | CLA | C3A-C2A-C1A | 6.63 | 111.27 | 101.34 |
| 26 | c | 521 | BCR | C30-C25-C26 | -6.62 | 113.29 | 122.61 |
| 26 | t | 101 | BCR | C15-C14-C13 | -6.61 | 117.88 | 127.31 |
| 24 | c | 504 | CLA | C4D-C3D-CAD | -6.60 | 104.79 | 108.47 |
| 26 | c | 515 | BCR | C16-C17-C18 | -6.60 | 117.89 | 127.31 |
| 24 | b | 605 | CLA | C4D-C3D-CAD | -6.59 | 104.79 | 108.47 |
| 26 | B | 619 | BCR | C19-C18-C17 | 6.59 | 129.06 | 118.94 |
| 24 | C | 512 | CLA | C3A-C2A-C1A | 6.58 | 111.20 | 101.34 |
| 24 | b | 604 | CLA | O2D-CGD-CBD | 6.58 | 122.97 | 111.27 |
| 26 | B | 620 | BCR | C4-C5-C6 | -6.57 | 113.19 | 122.73 |
| 24 | b | 614 | CLA | O2D-CGD-CBD | 6.56 | 122.92 | 111.27 |
| 24 | B | 604 | CLA | C4D-C3D-CAD | -6.53 | 104.83 | 108.47 |
| 24 | a | 606 | CLA | C4A-NA-C1A | -6.53 | 103.77 | 106.71 |
| 27 | a | 611 | PL9 | C32-C33-C34 | -6.53 | 111.94 | 127.66 |
| 27 | d | 404 | PL9 | C16-C14-C13 | -6.52 | 107.93 | 121.12 |
| 24 | c | 507 | CLA | C4D-C3D-CAD | -6.50 | 104.84 | 108.47 |
| 26 | f | 101 | BCR | C27-C26-C25 | -6.50 | 113.30 | 122.73 |
| 26 | f | 101 | BCR | C36-C18-C17 | -6.49 | 113.83 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 609 | CLA | C4D-C3D-CAD | -6.49 | 104.85 | 108.47 |
| 24 | D | 402 | CLA | C4D-C3D-CAD | -6.48 | 104.86 | 108.47 |
| 24 | A | 609 | CLA | C4D-C3D-CAD | -6.45 | 104.87 | 108.47 |
| 26 | A | 610 | BCR | C15-C14-C13 | -6.45 | 118.11 | 127.31 |
| 24 | C | 506 | CLA | C3A-C2A-C1A | 6.43 | 110.97 | 101.34 |
| 24 | B | 603 | CLA | C4D-C3D-CAD | -6.42 | 104.89 | 108.47 |
| 26 | a | 610 | BCR | C24-C23-C22 | -6.42 | 116.53 | 126.23 |
| 24 | b | 616 | CLA | C4D-C3D-CAD | -6.42 | 104.89 | 108.47 |
| 26 | B | 618 | BCR | C20-C21-C22 | -6.42 | 118.15 | 127.31 |
| 24 | b | 615 | CLA | C4D-C3D-CAD | -6.41 | 104.89 | 108.47 |
| 24 | C | 505 | CLA | O2D-CGD-CBD | 6.41 | 122.66 | 111.27 |
| 27 | d | 404 | PL9 | C21-C19-C18 | -6.41 | 108.14 | 121.12 |
| 26 | K | 101 | BCR | C8-C7-C6 | -6.41 | 109.21 | 127.20 |
| 26 | K | 101 | BCR | C27-C26-C25 | -6.40 | 113.44 | 122.73 |
| 24 | c | 506 | CLA | C4D-C3D-CAD | -6.40 | 104.90 | 108.47 |
| 24 | c | 507 | CLA | C4A-NA-C1A | -6.39 | 103.83 | 106.71 |
| 24 | B | 603 | CLA | O2D-CGD-CBD | 6.39 | 122.62 | 111.27 |
| 27 | A | 611 | PL9 | C22-C23-C24 | -6.38 | 112.31 | 127.66 |
| 27 | A | 611 | PL9 | C26-C24-C23 | -6.37 | 108.22 | 121.12 |
| 26 | b | 621 | BCR | C27-C26-C25 | -6.36 | 113.50 | 122.73 |
| 26 | b | 619 | BCR | C36-C18-C17 | -6.36 | 114.01 | 122.92 |
| 26 | k | 101 | BCR | C27-C26-C25 | -6.36 | 113.50 | 122.73 |
| 26 | h | 101 | BCR | C24-C23-C22 | -6.36 | 116.63 | 126.23 |
| 26 | c | 514 | BCR | C8-C7-C6 | -6.35 | 109.38 | 127.20 |
| 26 | f | 101 | BCR | C15-C14-C13 | -6.34 | 118.27 | 127.31 |
| 24 | b | 612 | CLA | C4D-C3D-CAD | -6.33 | 104.94 | 108.47 |
| 24 | b | 617 | CLA | C4D-C3D-CAD | -6.31 | 104.95 | 108.47 |
| 26 | F | 101 | BCR | C27-C26-C25 | -6.30 | 113.59 | 122.73 |
| 27 | d | 404 | PL9 | C11-C9-C8 | -6.29 | 108.39 | 121.12 |
| 26 | k | 101 | BCR | C8-C7-C6 | -6.29 | 109.55 | 127.20 |
| 24 | D | 404 | CLA | C4D-C3D-CAD | -6.28 | 104.97 | 108.47 |
| 24 | c | 511 | CLA | C3A-C2A-C1A | 6.28 | 110.74 | 101.34 |
| 26 | t | 101 | BCR | C16-C17-C18 | -6.27 | 118.37 | 127.31 |
| 26 | b | 620 | BCR | C12-C13-C14 | -6.24 | 109.37 | 118.94 |
| 26 | A | 610 | BCR | C11-C10-C9 | -6.23 | 118.41 | 127.31 |
| 27 | a | 611 | PL9 | C40-C39-C38 | -6.22 | 107.73 | 123.68 |
| 27 | d | 404 | PL9 | C17-C18-C19 | -6.21 | 112.70 | 127.66 |
| 26 | B | 619 | BCR | C15-C14-C13 | -6.20 | 118.46 | 127.31 |
| 26 | F | 101 | BCR | C23-C22-C21 | 6.20 | 128.45 | 118.94 |
| 27 | a | 611 | PL9 | C12-C13-C14 | -6.19 | 112.76 | 127.66 |
| 26 | H | 101 | BCR | C1-C6-C5 | -6.17 | 113.92 | 122.61 |
| 24 | c | 510 | CLA | C3A-C2A-C1A | 6.17 | 110.58 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | A | 611 | PL9 | C12-C13-C14 | -6.16 | 112.83 | 127.66 |
| 26 | I | 101 | BCR | C37-C22-C21 | -6.14 | 114.32 | 122.92 |
| 27 | d | 404 | PL9 | C27-C28-C29 | -6.14 | 112.87 | 127.66 |
| 27 | A | 611 | PL9 | C40-C39-C38 | -6.13 | 107.95 | 123.68 |
| 27 | A | 611 | PL9 | C32-C33-C34 | -6.13 | 112.90 | 127.66 |
| 26 | C | 514 | BCR | C23-C24-C25 | -6.12 | 110.00 | 127.20 |
| 26 | B | 620 | BCR | C24-C23-C22 | -6.12 | 116.98 | 126.23 |
| 24 | c | 501 | CLA | C4D-C3D-CAD | -6.12 | 105.06 | 108.47 |
| 26 | C | 514 | BCR | C8-C7-C6 | -6.09 | 110.08 | 127.20 |
| 26 | A | 610 | BCR | C1-C6-C5 | -6.08 | 114.04 | 122.61 |
| 27 | a | 611 | PL9 | C45-C44-C43 | -6.07 | 108.11 | 123.68 |
| 26 | B | 620 | BCR | C15-C14-C13 | -6.05 | 118.67 | 127.31 |
| 24 | b | 617 | CLA | C3A-C2A-C1A | 6.05 | 110.41 | 101.34 |
| 26 | B | 619 | BCR | C24-C23-C22 | -6.05 | 117.09 | 126.23 |
| 24 | c | 506 | CLA | C3A-C2A-C1A | 6.05 | 110.40 | 101.34 |
| 26 | B | 620 | BCR | C36-C18-C17 | -6.04 | 114.46 | 122.92 |
| 24 | c | 507 | CLA | O2D-CGD-CBD | 6.04 | 122.00 | 111.27 |
| 24 | B | 609 | CLA | C3A-C2A-C1A | 6.03 | 110.38 | 101.34 |
| 24 | C | 512 | CLA | C4D-C3D-CAD | -6.02 | 105.11 | 108.47 |
| 26 | h | 101 | BCR | C1-C6-C5 | -6.02 | 114.14 | 122.61 |
| 27 | d | 404 | PL9 | C37-C38-C39 | -6.01 | 113.19 | 127.66 |
| 24 | b | 610 | CLA | C3A-C2A-C1A | 6.00 | 110.33 | 101.34 |
| 26 | b | 620 | BCR | C1-C6-C5 | -6.00 | 114.16 | 122.61 |
| 26 | C | 514 | BCR | C30-C25-C26 | -5.99 | 114.17 | 122.61 |
| 24 | c | 501 | CLA | C3A-C2A-C1A | 5.99 | 110.31 | 101.34 |
| 27 | A | 611 | PL9 | C10-C9-C8 | -5.98 | 108.33 | 123.68 |
| 24 | c | 508 | CLA | C3A-C2A-C1A | 5.98 | 110.30 | 101.34 |
| 27 | d | 404 | PL9 | C42-C43-C44 | -5.98 | 113.26 | 127.66 |
| 26 | k | 101 | BCR | C34-C9-C10 | -5.98 | 114.55 | 122.92 |
| 24 | c | 505 | CLA | C4D-C3D-CAD | -5.96 | 105.15 | 108.47 |
| 27 | A | 611 | PL9 | C45-C44-C43 | -5.96 | 108.40 | 123.68 |
| 26 | B | 620 | BCR | C11-C10-C9 | -5.95 | 118.81 | 127.31 |
| 24 | b | 616 | CLA | C3A-C2A-C1A | 5.95 | 110.25 | 101.34 |
| 27 | a | 611 | PL9 | C11-C9-C8 | -5.95 | 109.08 | 121.12 |
| 24 | C | 509 | CLA | C4A-NA-C1A | -5.93 | 104.04 | 106.71 |
| 24 | b | 612 | CLA | C4A-NA-C1A | -5.93 | 104.04 | 106.71 |
| 26 | H | 101 | BCR | C36-C18-C17 | -5.93 | 114.62 | 122.92 |
| 24 | b | 613 | CLA | C4D-C3D-CAD | -5.92 | 105.17 | 108.47 |
| 24 | b | 611 | CLA | C4D-C3D-CAD | -5.92 | 105.17 | 108.47 |
| 24 | C | 506 | CLA | C4D-C3D-CAD | -5.91 | 105.18 | 108.47 |
| 26 | H | 101 | BCR | C31-C1-C6 | -5.90 | 100.72 | 110.30 |
| 24 | B | 610 | CLA | C3A-C2A-C1A | 5.90 | 110.18 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | b | 615 | CLA | C3A-C2A-C1A | 5.90 | 110.18 | 101.34 |
| 26 | c | 521 | BCR | C11-C10-C9 | -5.90 | 118.89 | 127.31 |
| 24 | b | 618 | CLA | C3A-C2A-C1A | 5.89 | 110.17 | 101.34 |
| 24 | C | 511 | CLA | C3A-C2A-C1A | 5.89 | 110.16 | 101.34 |
| 27 | A | 611 | PL9 | C11-C9-C8 | -5.89 | 109.21 | 121.12 |
| 24 | b | 607 | CLA | C3A-C2A-C1A | 5.88 | 110.15 | 101.34 |
| 24 | C | 502 | CLA | C4A-NA-C1A | -5.88 | 104.06 | 106.71 |
| 26 | h | 101 | BCR | C20-C21-C22 | -5.88 | 118.92 | 127.31 |
| 26 | b | 620 | BCR | C7-C6-C5 | -5.88 | 107.23 | 121.46 |
| 24 | c | 512 | CLA | C4D-C3D-CAD | -5.87 | 105.20 | 108.47 |
| 26 | K | 101 | BCR | C34-C9-C10 | -5.86 | 114.71 | 122.92 |
| 24 | b | 613 | CLA | O2D-CGD-CBD | 5.86 | 121.68 | 111.27 |
| 24 | b | 606 | CLA | C4A-NA-C1A | -5.86 | 104.07 | 106.71 |
| 26 | b | 621 | BCR | C4-C5-C6 | -5.86 | 114.23 | 122.73 |
| 26 | c | 514 | BCR | C24-C25-C26 | -5.85 | 107.28 | 121.46 |
| 26 | k | 101 | BCR | C1-C6-C5 | -5.85 | 114.38 | 122.61 |
| 24 | b | 611 | CLA | C3A-C2A-C1A | 5.84 | 110.09 | 101.34 |
| 24 | d | 402 | CLA | C4D-C3D-CAD | -5.83 | 105.22 | 108.47 |
| 26 | A | 610 | BCR | C30-C25-C26 | -5.82 | 114.42 | 122.61 |
| 24 | b | 608[B] | CLA | C2A-C3A-C4A | 5.81 | 111.25 | 101.87 |
| 26 | c | 515 | BCR | C30-C25-C26 | -5.81 | 114.44 | 122.61 |
| 24 | B | 606 | CLA | C3A-C2A-C1A | 5.80 | 110.02 | 101.34 |
| 26 | K | 101 | BCR | C7-C8-C9 | -5.79 | 117.49 | 126.23 |
| 24 | B | 615 | CLA | C3A-C2A-C1A | 5.79 | 110.01 | 101.34 |
| 24 | b | 618 | CLA | O2D-CGD-CBD | 5.79 | 121.55 | 111.27 |
| 26 | c | 521 | BCR | C27-C26-C25 | -5.79 | 114.33 | 122.73 |
| 27 | A | 611 | PL9 | C46-C44-C43 | -5.78 | 109.43 | 121.12 |
| 24 | b | 604 | CLA | C3A-C2A-C1A | 5.77 | 109.99 | 101.34 |
| 24 | B | 613 | CLA | C2A-C3A-C4A | 5.77 | 111.19 | 101.87 |
| 27 | D | 405 | PL9 | C17-C18-C19 | -5.77 | 113.77 | 127.66 |
| 26 | a | 610 | BCR | C20-C21-C22 | -5.76 | 119.09 | 127.31 |
| 27 | a | 611 | PL9 | C10-C9-C8 | -5.76 | 108.91 | 123.68 |
| 24 | b | 607 | CLA | C4D-C3D-CAD | -5.75 | 105.26 | 108.47 |
| 27 | d | 404 | PL9 | C35-C34-C33 | -5.75 | 108.93 | 123.68 |
| 27 | D | 405 | PL9 | C11-C9-C8 | -5.74 | 109.50 | 121.12 |
| 26 | B | 618 | BCR | C27-C26-C25 | -5.74 | 114.40 | 122.73 |
| 26 | b | 620 | BCR | C20-C21-C22 | -5.73 | 119.13 | 127.31 |
| 26 | b | 619 | BCR | C38-C26-C27 | -5.72 | 102.62 | 113.62 |
| 27 | D | 405 | PL9 | C21-C19-C18 | -5.72 | 109.54 | 121.12 |
| 27 | a | 611 | PL9 | C40-C39-C41 | -5.72 | 105.65 | 115.27 |
| 24 | C | 503 | CLA | C3A-C2A-C1A | 5.72 | 109.90 | 101.34 |
| 24 | B | 613 | CLA | C4A-NA-C1A | -5.71 | 104.14 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | k | 101 | BCR | C15-C14-C13 | -5.71 | 119.16 | 127.31 |
| 26 | a | 610 | BCR | C7-C8-C9 | -5.70 | 117.62 | 126.23 |
| 26 | F | 101 | BCR | C7-C6-C5 | -5.70 | 107.66 | 121.46 |
| 27 | a | 611 | PL9 | C26-C24-C23 | -5.70 | 109.59 | 121.12 |
| 24 | C | 501 | CLA | C2A-C3A-C4A | 5.69 | 111.07 | 101.87 |
| 24 | C | 510 | CLA | C4D-C3D-CAD | -5.69 | 105.30 | 108.47 |
| 26 | K | 102 | BCR | C15-C14-C13 | -5.69 | 119.19 | 127.31 |
| 24 | b | 608[A] | CLA | C2A-C3A-C4A | 5.69 | 111.06 | 101.87 |
| 24 | c | 503 | CLA | C4D-C3D-CAD | -5.68 | 105.30 | 108.47 |
| 24 | b | 608[A] | CLA | C4D-C3D-CAD | -5.68 | 105.30 | 108.47 |
| 24 | C | 501 | CLA | O2D-CGD-CBD | 5.68 | 121.36 | 111.27 |
| 26 | h | 101 | BCR | C7-C6-C5 | -5.67 | 107.72 | 121.46 |
| 26 | a | 610 | BCR | C15-C14-C13 | -5.67 | 119.22 | 127.31 |
| 24 | B | 616 | CLA | C4D-C3D-CAD | -5.67 | 105.31 | 108.47 |
| 24 | B | 616 | CLA | C2A-C3A-C4A | 5.65 | 111.00 | 101.87 |
| 33 | e | 102 | HEM | CBD-CAD-C3D | -5.65 | 102.08 | 112.48 |
| 24 | b | 617 | CLA | C2A-C3A-C4A | 5.65 | 110.99 | 101.87 |
| 26 | B | 618 | BCR | C8-C7-C6 | -5.64 | 111.35 | 127.20 |
| 24 | c | 512 | CLA | O2D-CGD-CBD | 5.64 | 121.30 | 111.27 |
| 26 | b | 619 | BCR | C20-C21-C22 | -5.64 | 119.26 | 127.31 |
| 24 | c | 509 | CLA | C2A-C3A-C4A | 5.63 | 110.96 | 101.87 |
| 24 | c | 502 | CLA | C3A-C2A-C1A | 5.62 | 109.76 | 101.34 |
| 24 | c | 513 | CLA | C3A-C2A-C1A | 5.62 | 109.76 | 101.34 |
| 26 | t | 101 | BCR | C7-C8-C9 | -5.62 | 117.74 | 126.23 |
| 24 | b | 611 | CLA | C2A-C3A-C4A | 5.62 | 110.94 | 101.87 |
| 26 | a | 610 | BCR | C11-C10-C9 | -5.61 | 119.30 | 127.31 |
| 24 | b | 605 | CLA | C2A-C3A-C4A | 5.61 | 110.93 | 101.87 |
| 26 | I | 101 | BCR | C20-C21-C22 | -5.61 | 119.31 | 127.31 |
| 24 | B | 617 | CLA | C3A-C2A-C1A | 5.60 | 109.73 | 101.34 |
| 26 | c | 521 | BCR | C4-C5-C6 | -5.60 | 114.60 | 122.73 |
| 26 | B | 619 | BCR | C4-C5-C6 | -5.59 | 114.62 | 122.73 |
| 24 | B | 607[B] | CLA | C2A-C3A-C4A | 5.59 | 110.89 | 101.87 |
| 24 | A | 607 | CLA | O2D-CGD-CBD | 5.59 | 121.19 | 111.27 |
| 27 | a | 611 | PL9 | C35-C34-C33 | -5.58 | 109.36 | 123.68 |
| 26 | K | 102 | BCR | C7-C6-C5 | -5.58 | 107.95 | 121.46 |
| 24 | B | 608 | CLA | C4D-C3D-CAD | -5.58 | 105.36 | 108.47 |
| 26 | K | 102 | BCR | C11-C10-C9 | -5.57 | 119.36 | 127.31 |
| 24 | C | 508 | CLA | C3A-C2A-C1A | 5.57 | 109.69 | 101.34 |
| 24 | B | 607[A] | CLA | C4D-C3D-CAD | -5.57 | 105.36 | 108.47 |
| 24 | C | 512 | CLA | O2D-CGD-CBD | 5.57 | 121.17 | 111.27 |
| 26 | B | 618 | BCR | C15-C14-C13 | -5.57 | 119.36 | 127.31 |
| 27 | a | 611 | PL9 | C15-C14-C13 | -5.57 | 109.39 | 123.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 30 | A | 615 | LHG | O7-C7-C8 | 5.57 | 123.50 | 111.50 |
| 24 | B | 608 | CLA | C2A-C3A-C4A | 5.57 | 110.86 | 101.87 |
| 24 | C | 507 | CLA | C4D-C3D-CAD | -5.55 | 105.38 | 108.47 |
| 26 | B | 618 | BCR | C37-C22-C21 | -5.55 | 115.15 | 122.92 |
| 24 | b | 603 | CLA | C3A-C2A-C1A | 5.54 | 109.64 | 101.34 |
| 24 | B | 608 | CLA | C3A-C2A-C1A | 5.54 | 109.64 | 101.34 |
| 26 | h | 101 | BCR | C2-C1-C6 | 5.54 | 119.00 | 110.48 |
| 24 | B | 612 | CLA | O2D-CGD-CBD | 5.53 | 121.09 | 111.27 |
| 24 | c | 509 | CLA | C3A-C2A-C1A | 5.53 | 109.61 | 101.34 |
| 26 | c | 514 | BCR | C7-C6-C5 | -5.52 | 108.09 | 121.46 |
| 24 | b | 613 | CLA | C3A-C2A-C1A | 5.52 | 109.60 | 101.34 |
| 24 | c | 505 | CLA | O2D-CGD-CBD | 5.52 | 121.07 | 111.27 |
| 26 | B | 618 | BCR | C24-C23-C22 | -5.51 | 117.90 | 126.23 |
| 24 | B | 602 | CLA | C3A-C2A-C1A | 5.50 | 109.58 | 101.34 |
| 26 | C | 514 | BCR | C7-C6-C5 | -5.50 | 108.14 | 121.46 |
| 24 | C | 507 | CLA | C3A-C2A-C1A | 5.50 | 109.58 | 101.34 |
| 26 | b | 619 | BCR | C24-C23-C22 | -5.49 | 117.93 | 126.23 |
| 27 | D | 405 | PL9 | C42-C43-C44 | -5.49 | 114.45 | 127.66 |
| 24 | B | 614 | CLA | C3A-C2A-C1A | 5.48 | 109.55 | 101.34 |
| 24 | b | 614 | CLA | C2A-C3A-C4A | 5.47 | 110.71 | 101.87 |
| 26 | H | 101 | BCR | C29-C30-C25 | 5.47 | 118.90 | 110.48 |
| 24 | B | 607[B] | CLA | C3A-C2A-C1A | 5.47 | 109.53 | 101.34 |
| 24 | B | 617 | CLA | C4A-NA-C1A | -5.45 | 104.25 | 106.71 |
| 24 | B | 607[A] | CLA | C2A-C3A-C4A | 5.45 | 110.67 | 101.87 |
| 33 | E | 103 | HEM | CBD-CAD-C3D | -5.44 | 102.45 | 112.48 |
| 24 | b | 605 | CLA | C2A-C1A-CHA | 5.44 | 133.37 | 123.86 |
| 27 | D | 405 | PL9 | C46-C44-C43 | -5.44 | 110.11 | 121.12 |
| 24 | C | 504 | CLA | C2A-C3A-C4A | 5.43 | 110.65 | 101.87 |
| 24 | c | 503 | CLA | C3A-C2A-C1A | 5.43 | 109.47 | 101.34 |
| 26 | T | 101 | BCR | C11-C10-C9 | -5.42 | 119.57 | 127.31 |
| 24 | C | 509 | CLA | C2A-C3A-C4A | 5.41 | 110.61 | 101.87 |
| 24 | c | 507 | CLA | C2A-C3A-C4A | 5.41 | 110.61 | 101.87 |
| 24 | B | 610 | CLA | C2A-C3A-C4A | 5.41 | 110.60 | 101.87 |
| 24 | b | 606 | CLA | C3A-C2A-C1A | 5.40 | 109.43 | 101.34 |
| 24 | C | 507 | CLA | C2A-C3A-C4A | 5.40 | 110.59 | 101.87 |
| 26 | C | 514 | BCR | C16-C15-C14 | -5.40 | 112.42 | 123.47 |
| 26 | C | 514 | BCR | C2-C1-C6 | 5.40 | 118.79 | 110.48 |
| 26 | h | 101 | BCR | C4-C5-C6 | -5.39 | 114.90 | 122.73 |
| 24 | b | 605 | CLA | C3A-C2A-C1A | 5.39 | 109.42 | 101.34 |
| 24 | a | 606 | CLA | C4D-C3D-CAD | -5.39 | 105.47 | 108.47 |
| 26 | K | 102 | BCR | C8-C7-C6 | -5.38 | 112.10 | 127.20 |
| 24 | B | 607[A] | CLA | C3A-C2A-C1A | 5.38 | 109.39 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 27 | D | 405 | PL9 | C30-C29-C28 | -5.37 | 109.90 | 123.68 |
| 24 | C | 506 | CLA | C2A-C1A-CHA | 5.37 | 133.24 | 123.86 |
| 24 | b | 609 | CLA | C2A-C3A-C4A | 5.36 | 110.53 | 101.87 |
| 24 | c | 508 | CLA | O2D-CGD-CBD | 5.36 | 120.80 | 111.27 |
| 26 | K | 101 | BCR | C7-C6-C5 | -5.36 | 108.47 | 121.46 |
| 27 | D | 405 | PL9 | C37-C38-C39 | -5.36 | 114.76 | 127.66 |
| 26 | c | 521 | BCR | C8-C7-C6 | -5.36 | 112.16 | 127.20 |
| 24 | C | 504 | CLA | C4A-NA-C1A | -5.35 | 104.30 | 106.71 |
| 24 | c | 501 | CLA | O2D-CGD-CBD | 5.35 | 120.78 | 111.27 |
| 26 | F | 101 | BCR | C1-C6-C5 | -5.35 | 115.08 | 122.61 |
| 27 | A | 611 | PL9 | C15-C14-C13 | -5.34 | 109.97 | 123.68 |
| 24 | b | 612 | CLA | O2D-CGD-CBD | 5.33 | 120.73 | 111.27 |
| 24 | B | 614 | CLA | C2A-C3A-C4A | 5.33 | 110.47 | 101.87 |
| 26 | c | 521 | BCR | C7-C6-C5 | -5.32 | 108.57 | 121.46 |
| 26 | B | 619 | BCR | C34-C9-C10 | -5.32 | 115.47 | 122.92 |
| 24 | C | 511 | CLA | O2D-CGD-CBD | 5.30 | 120.69 | 111.27 |
| 24 | c | 506 | CLA | C2A-C1A-CHA | 5.30 | 133.13 | 123.86 |
| 24 | B | 606 | CLA | C2A-C3A-C4A | 5.30 | 110.43 | 101.87 |
| 24 | a | 609 | CLA | C3A-C2A-C1A | 5.29 | 109.27 | 101.34 |
| 24 | b | 607 | CLA | C2A-C3A-C4A | 5.29 | 110.41 | 101.87 |
| 24 | b | 609 | CLA | C3A-C2A-C1A | 5.29 | 109.25 | 101.34 |
| 24 | C | 502 | CLA | C2A-C3A-C4A | 5.28 | 110.40 | 101.87 |
| 26 | B | 620 | BCR | C7-C6-C5 | -5.27 | 108.69 | 121.46 |
| 24 | B | 612 | CLA | C3A-C2A-C1A | 5.26 | 109.22 | 101.34 |
| 24 | b | 609 | CLA | C4A-NA-C1A | -5.26 | 104.34 | 106.71 |
| 24 | B | 605 | CLA | C2A-C3A-C4A | 5.26 | 110.36 | 101.87 |
| 26 | b | 621 | BCR | C30-C25-C26 | -5.26 | 115.21 | 122.61 |
| 24 | B | 610 | CLA | O2D-CGD-CBD | 5.26 | 120.61 | 111.27 |
| 24 | B | 612 | CLA | C2A-C3A-C4A | 5.25 | 110.36 | 101.87 |
| 24 | B | 606 | CLA | C2A-C1A-CHA | 5.25 | 133.04 | 123.86 |
| 24 | c | 512 | CLA | C3A-C2A-C1A | 5.25 | 109.21 | 101.34 |
| 27 | D | 405 | PL9 | C25-C24-C23 | -5.25 | 110.22 | 123.68 |
| 24 | A | 607 | CLA | C3A-C2A-C1A | 5.24 | 109.19 | 101.34 |
| 26 | K | 102 | BCR | C36-C18-C17 | -5.24 | 115.58 | 122.92 |
| 26 | B | 619 | BCR | C38-C26-C27 | -5.24 | 103.55 | 113.62 |
| 27 | D | 405 | PL9 | C10-C9-C8 | -5.24 | 110.23 | 123.68 |
| 26 | I | 101 | BCR | C16-C15-C14 | -5.24 | 112.75 | 123.47 |
| 26 | C | 514 | BCR | C27-C26-C25 | -5.23 | 115.13 | 122.73 |
| 24 | b | 608[B] | CLA | C3A-C2A-C1A | 5.23 | 109.18 | 101.34 |
| 24 | a | 615 | CLA | O2D-CGD-CBD | 5.23 | 120.56 | 111.27 |
| 27 | A | 611 | PL9 | C21-C19-C18 | -5.23 | 110.53 | 121.12 |
| 27 | d | 404 | PL9 | C25-C24-C23 | -5.23 | 110.26 | 123.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | A | 606 | CLA | C4D-C3D-CAD | -5.23 | 105.55 | 108.47 |
| 26 | b | 621 | BCR | C35-C13-C14 | -5.23 | 115.60 | 122.92 |
| 26 | C | 514 | BCR | C24-C25-C26 | -5.23 | 108.80 | 121.46 |
| 24 | A | 609 | CLA | C3A-C2A-C1A | 5.22 | 109.16 | 101.34 |
| 27 | D | 405 | PL9 | C45-C44-C43 | -5.22 | 110.30 | 123.68 |
| 26 | K | 101 | BCR | C16-C17-C18 | -5.22 | 119.87 | 127.31 |
| 24 | B | 602 | CLA | C2A-C3A-C4A | 5.22 | 110.29 | 101.87 |
| 27 | a | 611 | PL9 | C46-C44-C43 | -5.20 | 110.59 | 121.12 |
| 24 | C | 511 | CLA | C2A-C1A-CHA | 5.20 | 132.95 | 123.86 |
| 24 | d | 403 | CLA | C2A-C3A-C4A | 5.20 | 110.27 | 101.87 |
| 26 | h | 101 | BCR | C27-C26-C25 | -5.20 | 115.19 | 122.73 |
| 26 | H | 101 | BCR | C27-C26-C25 | -5.20 | 115.19 | 122.73 |
| 24 | B | 605 | CLA | C3A-C2A-C1A | 5.19 | 109.11 | 101.34 |
| 27 | D | 405 | PL9 | C15-C14-C13 | -5.17 | 110.41 | 123.68 |
| 24 | b | 603 | CLA | C2A-C1A-CHA | 5.17 | 132.90 | 123.86 |
| 24 | a | 607 | CLA | C2A-C1A-CHA | 5.17 | 132.90 | 123.86 |
| 26 | I | 101 | BCR | C34-C9-C10 | -5.16 | 115.69 | 122.92 |
| 24 | c | 504 | CLA | C2A-C3A-C4A | 5.16 | 110.20 | 101.87 |
| 24 | B | 614 | CLA | O2D-CGD-CBD | 5.16 | 120.43 | 111.27 |
| 24 | b | 608[A] | CLA | C3A-C2A-C1A | 5.15 | 109.05 | 101.34 |
| 24 | B | 607[B] | CLA | C4D-C3D-CAD | -5.14 | 105.60 | 108.47 |
| 27 | a | 611 | PL9 | C25-C24-C23 | -5.14 | 110.49 | 123.68 |
| 27 | d | 404 | PL9 | C15-C14-C13 | -5.14 | 110.50 | 123.68 |
| 26 | B | 620 | BCR | C7-C8-C9 | -5.13 | 118.48 | 126.23 |
| 24 | a | 607 | CLA | C4D-C3D-CAD | -5.13 | 105.61 | 108.47 |
| 26 | B | 618 | BCR | C30-C25-C26 | -5.13 | 115.38 | 122.61 |
| 26 | T | 101 | BCR | C23-C24-C25 | -5.13 | 112.80 | 127.20 |
| 24 | b | 614 | CLA | C3A-C2A-C1A | 5.12 | 109.01 | 101.34 |
| 24 | a | 615 | CLA | C4D-C3D-CAD | -5.11 | 105.62 | 108.47 |
| 26 | t | 101 | BCR | C35-C13-C12 | -5.11 | 110.02 | 118.08 |
| 24 | c | 502 | CLA | C2A-C3A-C4A | 5.11 | 110.12 | 101.87 |
| 26 | b | 621 | BCR | C37-C22-C23 | 5.11 | 126.13 | 118.08 |
| 24 | b | 617 | CLA | O2D-CGD-CBD | 5.11 | 120.34 | 111.27 |
| 24 | d | 402 | CLA | C1B-CHB-C4A | -5.10 | 120.01 | 130.12 |
| 24 | B | 604 | CLA | C3A-C2A-C1A | 5.10 | 108.98 | 101.34 |
| 24 | d | 402 | CLA | C3A-C2A-C1A | 5.10 | 108.97 | 101.34 |
| 26 | h | 101 | BCR | C7-C8-C9 | -5.09 | 118.54 | 126.23 |
| 24 | C | 511 | CLA | C4D-C3D-CAD | -5.09 | 105.63 | 108.47 |
| 24 | D | 404 | CLA | C2A-C1A-CHA | 5.09 | 132.76 | 123.86 |
| 24 | B | 616 | CLA | C3A-C2A-C1A | 5.08 | 108.95 | 101.34 |
| 24 | C | 509 | CLA | C3A-C2A-C1A | 5.08 | 108.94 | 101.34 |
| 27 | A | 611 | PL9 | C35-C34-C33 | -5.07 | 110.67 | 123.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 27 | D | 405 | PL9 | C20-C19-C18 | -5.07 | 110.67 | 123.68 |
| 24 | B | 615 | CLA | C2A-C1A-CHA | 5.07 | 132.72 | 123.86 |
| 24 | C | 513 | CLA | C3A-C2A-C1A | 5.07 | 108.93 | 101.34 |
| 24 | c | 503 | CLA | C2A-C3A-C4A | 5.06 | 110.05 | 101.87 |
| 24 | a | 615 | CLA | C3A-C2A-C1A | 5.06 | 108.92 | 101.34 |
| 27 | d | 404 | PL9 | C26-C24-C23 | -5.06 | 110.88 | 121.12 |
| 26 | B | 620 | BCR | C20-C19-C18 | -5.05 | 112.22 | 126.42 |
| 26 | B | 619 | BCR | C1-C6-C5 | -5.05 | 115.50 | 122.61 |
| 24 | B | 609 | CLA | O2D-CGD-CBD | 5.05 | 120.23 | 111.27 |
| 24 | B | 605 | CLA | O1D-CGD-CBD | -5.04 | 114.17 | 124.48 |
| 27 | d | 404 | PL9 | C10-C9-C8 | -5.04 | 110.75 | 123.68 |
| 24 | D | 403 | CLA | C2A-C3A-C4A | 5.04 | 110.00 | 101.87 |
| 24 | C | 502 | CLA | C3A-C2A-C1A | 5.03 | 108.87 | 101.34 |
| 24 | d | 402 | CLA | O2D-CGD-CBD | 5.03 | 120.20 | 111.27 |
| 27 | D | 405 | PL9 | C40-C39-C38 | -5.03 | 110.78 | 123.68 |
| 26 | c | 514 | BCR | C7-C8-C9 | -5.03 | 118.64 | 126.23 |
| 24 | B | 609 | CLA | C2A-C1A-CHA | 5.02 | 132.65 | 123.86 |
| 24 | b | 603 | CLA | C2A-C3A-C4A | 5.02 | 109.98 | 101.87 |
| 26 | K | 101 | BCR | C38-C26-C27 | -5.02 | 103.97 | 113.62 |
| 24 | C | 501 | CLA | C3A-C2A-C1A | 5.01 | 108.85 | 101.34 |
| 27 | a | 611 | PL9 | C41-C39-C38 | -5.01 | 110.98 | 121.12 |
| 24 | a | 607 | CLA | C3A-C2A-C1A | 5.00 | 108.83 | 101.34 |
| 24 | B | 611 | CLA | C2A-C3A-C4A | 5.00 | 109.94 | 101.87 |
| 24 | a | 609 | CLA | C4D-C3D-CAD | -4.99 | 105.69 | 108.47 |
| 27 | d | 404 | PL9 | C45-C44-C43 | -4.99 | 110.88 | 123.68 |
| 26 | t | 101 | BCR | C4-C5-C6 | -4.99 | 115.49 | 122.73 |
| 26 | c | 514 | BCR | C4-C5-C6 | -4.98 | 115.50 | 122.73 |
| 24 | b | 608[B] | CLA | C4D-C3D-CAD | -4.98 | 105.69 | 108.47 |
| 26 | T | 101 | BCR | C8-C7-C6 | -4.98 | 113.23 | 127.20 |
| 27 | D | 405 | PL9 | C47-C48-C49 | -4.97 | 110.76 | 127.75 |
| 26 | c | 514 | BCR | C23-C24-C25 | -4.97 | 113.24 | 127.20 |
| 27 | a | 611 | PL9 | C30-C29-C28 | -4.97 | 110.93 | 123.68 |
| 24 | c | 506 | CLA | C2A-C3A-C4A | 4.97 | 109.89 | 101.87 |
| 24 | b | 612 | CLA | C3A-C2A-C1A | 4.96 | 108.77 | 101.34 |
| 24 | c | 510 | CLA | C2A-C1A-CHA | 4.95 | 132.52 | 123.86 |
| 24 | B | 607[A] | CLA | O2D-CGD-CBD | 4.95 | 120.07 | 111.27 |
| 24 | c | 510 | CLA | O2D-CGD-CBD | 4.95 | 120.07 | 111.27 |
| 24 | C | 503 | CLA | C2A-C3A-C4A | 4.95 | 109.86 | 101.87 |
| 24 | c | 511 | CLA | C2A-C1A-CHA | 4.94 | 132.50 | 123.86 |
| 24 | b | 608[A] | CLA | C2A-C1A-CHA | 4.94 | 132.50 | 123.86 |
| 26 | b | 619 | BCR | C23-C24-C25 | -4.94 | 113.33 | 127.20 |
| 24 | A | 609 | CLA | C2A-C3A-C4A | 4.94 | 109.85 | 101.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | B | 611 | CLA | C3A-C2A-C1A | 4.94 | 108.73 | 101.34 |
| 33 | V | 201 | HEM | CBA-CAA-C2A | -4.94 | 103.38 | 112.49 |
| 24 | D | 404 | CLA | C2A-C3A-C4A | 4.92 | 109.82 | 101.87 |
| 24 | B | 604 | CLA | C2A-C3A-C4A | 4.92 | 109.82 | 101.87 |
| 24 | B | 613 | CLA | O2D-CGD-CBD | 4.92 | 120.01 | 111.27 |
| 26 | h | 101 | BCR | C29-C30-C25 | 4.92 | 118.05 | 110.48 |
| 26 | t | 101 | BCR | C8-C7-C6 | -4.91 | 113.40 | 127.20 |
| 24 | b | 610 | CLA | O2D-CGD-CBD | 4.91 | 119.99 | 111.27 |
| 24 | c | 512 | CLA | C4A-NA-C1A | -4.90 | 104.50 | 106.71 |
| 24 | B | 607[B] | CLA | O2D-CGD-CBD | 4.90 | 119.98 | 111.27 |
| 26 | H | 101 | BCR | C2-C1-C6 | 4.90 | 118.02 | 110.48 |
| 26 | b | 619 | BCR | C34-C9-C10 | -4.90 | 116.07 | 122.92 |
| 26 | h | 101 | BCR | C8-C7-C6 | -4.89 | 113.46 | 127.20 |
| 24 | c | 506 | CLA | O2D-CGD-CBD | 4.89 | 119.96 | 111.27 |
| 26 | A | 610 | BCR | C24-C23-C22 | -4.89 | 118.84 | 126.23 |
| 30 | a | 616 | LHG | O7-C7-C8 | 4.89 | 122.04 | 111.50 |
| 24 | C | 513 | CLA | C2A-C3A-C4A | 4.89 | 109.77 | 101.87 |
| 24 | A | 607 | CLA | C2A-C3A-C4A | 4.89 | 109.77 | 101.87 |
| 24 | c | 501 | CLA | C2A-C3A-C4A | 4.89 | 109.76 | 101.87 |
| 24 | b | 606 | CLA | C2A-C1A-CHA | 4.89 | 132.40 | 123.86 |
| 30 | d | 407 | LHG | O7-C7-C8 | 4.88 | 122.03 | 111.50 |
| 26 | I | 101 | BCR | C36-C18-C17 | -4.88 | 116.09 | 122.92 |
| 24 | b | 615 | CLA | C2A-C3A-C4A | 4.88 | 109.75 | 101.87 |
| 26 | H | 101 | BCR | C24-C25-C26 | -4.87 | 109.65 | 121.46 |
| 24 | c | 511 | CLA | O2D-CGD-CBD | 4.87 | 119.92 | 111.27 |
| 24 | b | 606 | CLA | C2A-C3A-C4A | 4.87 | 109.73 | 101.87 |
| 26 | K | 101 | BCR | C1-C6-C5 | -4.87 | 115.76 | 122.61 |
| 26 | T | 101 | BCR | C35-C13-C12 | -4.87 | 110.41 | 118.08 |
| 26 | h | 101 | BCR | C35-C13-C14 | -4.86 | 116.12 | 122.92 |
| 24 | B | 602 | CLA | C4A-NA-C1A | -4.86 | 104.52 | 106.71 |
| 24 | b | 613 | CLA | C2A-C3A-C4A | 4.85 | 109.71 | 101.87 |
| 26 | b | 621 | BCR | C24-C25-C26 | -4.85 | 109.72 | 121.46 |
| 27 | D | 405 | PL9 | C35-C34-C33 | -4.84 | 111.25 | 123.68 |
| 26 | B | 618 | BCR | C7-C6-C5 | -4.84 | 109.74 | 121.46 |
| 24 | B | 611 | CLA | C2A-C1A-CHA | 4.83 | 132.30 | 123.86 |
| 24 | B | 602 | CLA | C4D-C3D-CAD | -4.82 | 105.78 | 108.47 |
| 24 | d | 403 | CLA | C2A-C1A-CHA | 4.82 | 132.29 | 123.86 |
| 26 | C | 514 | BCR | C4-C5-C6 | -4.82 | 115.73 | 122.73 |
| 26 | B | 618 | BCR | C24-C25-C26 | -4.82 | 109.78 | 121.46 |
| 24 | a | 609 | CLA | C2A-C1A-CHA | 4.82 | 132.29 | 123.86 |
| 24 | c | 513 | CLA | O2D-CGD-CBD | 4.82 | 119.83 | 111.27 |
| 27 | D | 405 | PL9 | C12-C13-C14 | -4.82 | 116.06 | 127.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | k | 101 | BCR | C11-C10-C9 | -4.81 | 120.45 | 127.31 |
| 24 | a | 606 | CLA | C2A-C1A-CHA | 4.81 | 132.27 | 123.86 |
| 27 | d | 404 | PL9 | C30-C29-C28 | -4.80 | 111.35 | 123.68 |
| 24 | b | 614 | CLA | C4D-C3D-CAD | -4.80 | 105.79 | 108.47 |
| 24 | C | 502 | CLA | O2D-CGD-CBD | 4.80 | 119.79 | 111.27 |
| 24 | B | 615 | CLA | C4A-NA-C1A | -4.79 | 104.55 | 106.71 |
| 24 | c | 513 | CLA | C2A-C3A-C4A | 4.78 | 109.60 | 101.87 |
| 24 | D | 402 | CLA | C3A-C2A-C1A | 4.77 | 108.49 | 101.34 |
| 26 | B | 620 | BCR | C20-C21-C22 | -4.77 | 120.50 | 127.31 |
| 26 | b | 620 | BCR | C7-C8-C9 | -4.77 | 119.03 | 126.23 |
| 26 | K | 101 | BCR | C15-C14-C13 | -4.76 | 120.51 | 127.31 |
| 24 | c | 504 | CLA | C3A-C2A-C1A | 4.75 | 108.46 | 101.34 |
| 24 | c | 504 | CLA | C4A-NA-C1A | -4.75 | 104.57 | 106.71 |
| 26 | C | 514 | BCR | C31-C1-C6 | -4.75 | 102.59 | 110.30 |
| 24 | c | 507 | CLA | C3A-C2A-C1A | 4.75 | 108.45 | 101.34 |
| 24 | B | 603 | CLA | C2A-C1A-CHA | 4.75 | 132.16 | 123.86 |
| 26 | k | 101 | BCR | C7-C6-C5 | -4.74 | 109.98 | 121.46 |
| 24 | b | 608[B] | CLA | C2A-C1A-CHA | 4.74 | 132.15 | 123.86 |
| 30 | e | 101 | LHG | O7-C7-C8 | 4.74 | 121.71 | 111.50 |
| 26 | K | 102 | BCR | C7-C8-C9 | -4.74 | 119.08 | 126.23 |
| 27 | A | 611 | PL9 | C30-C29-C28 | -4.74 | 111.53 | 123.68 |
| 24 | B | 608 | CLA | C2A-C1A-CHA | 4.73 | 132.14 | 123.86 |
| 24 | b | 604 | CLA | C1B-CHB-C4A | -4.73 | 120.75 | 130.12 |
| 24 | b | 606 | CLA | O2D-CGD-CBD | 4.73 | 119.67 | 111.27 |
| 26 | b | 621 | BCR | C31-C1-C6 | -4.73 | 102.64 | 110.30 |
| 24 | B | 605 | CLA | C2A-C1A-CHA | 4.72 | 132.12 | 123.86 |
| 24 | C | 508 | CLA | C2A-C3A-C4A | 4.72 | 109.49 | 101.87 |
| 24 | d | 403 | CLA | C3A-C2A-C1A | 4.72 | 108.41 | 101.34 |
| 27 | d | 404 | PL9 | C47-C48-C49 | -4.72 | 111.63 | 127.75 |
| 27 | d | 404 | PL9 | C40-C39-C38 | -4.72 | 111.58 | 123.68 |
| 24 | C | 507 | CLA | C2A-C1A-CHA | 4.71 | 132.10 | 123.86 |
| 26 | c | 515 | BCR | C38-C26-C27 | -4.71 | 104.56 | 113.62 |
| 24 | b | 615 | CLA | C2A-C1A-CHA | 4.71 | 132.10 | 123.86 |
| 24 | c | 503 | CLA | C4A-NA-C1A | -4.71 | 104.59 | 106.71 |
| 24 | b | 607 | CLA | O2D-CGD-CBD | 4.70 | 119.62 | 111.27 |
| 24 | A | 607 | CLA | C2A-C1A-CHA | 4.70 | 132.07 | 123.86 |
| 32 | c | 518 | DGD | O2G-C1B-C2B | 4.69 | 121.62 | 111.50 |
| 24 | B | 602 | CLA | C2A-C1A-CHA | 4.69 | 132.05 | 123.86 |
| 26 | K | 102 | BCR | C1-C6-C5 | -4.69 | 116.01 | 122.61 |
| 28 | A | 612 | SQD | O6-C1-C2 | 4.68 | 115.62 | 108.30 |
| 26 | b | 621 | BCR | C7-C6-C5 | -4.68 | 110.12 | 121.46 |
| 24 | B | 615 | CLA | C4D-C3D-CAD | -4.68 | 105.86 | 108.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | I | 101 | BCR | C33-C5-C4 | -4.68 | 104.62 | 113.62 |
| 26 | h | 101 | BCR | C23-C24-C25 | -4.68 | 114.06 | 127.20 |
| 24 | C | 513 | CLA | O2D-CGD-CBD | 4.68 | 119.58 | 111.27 |
| 24 | D | 404 | CLA | C3A-C2A-C1A | 4.68 | 108.35 | 101.34 |
| 24 | a | 606 | CLA | C3A-C2A-C1A | 4.68 | 108.34 | 101.34 |
| 28 | a | 612 | SQD | O6-C1-C2 | 4.67 | 115.59 | 108.30 |
| 24 | B | 611 | CLA | C1B-CHB-C4A | -4.66 | 120.88 | 130.12 |
| 27 | A | 611 | PL9 | C20-C19-C18 | -4.66 | 111.72 | 123.68 |
| 24 | C | 507 | CLA | C4A-NA-C1A | -4.66 | 104.61 | 106.71 |
| 26 | H | 101 | BCR | C7-C6-C5 | -4.65 | 110.20 | 121.46 |
| 24 | b | 604 | CLA | C2A-C3A-C4A | 4.65 | 109.38 | 101.87 |
| 26 | t | 101 | BCR | C24-C25-C26 | -4.64 | 110.21 | 121.46 |
| 24 | B | 605 | CLA | O2D-CGD-O1D | -4.64 | 114.76 | 123.84 |
| 26 | H | 101 | BCR | C38-C26-C27 | -4.64 | 104.70 | 113.62 |
| 24 | b | 612 | CLA | C2A-C3A-C4A | 4.64 | 109.36 | 101.87 |
| 24 | B | 609 | CLA | C2A-C3A-C4A | 4.64 | 109.36 | 101.87 |
| 26 | T | 101 | BCR | C11-C12-C13 | -4.63 | 113.42 | 126.42 |
| 24 | b | 603 | CLA | C4D-C3D-CAD | -4.63 | 105.89 | 108.47 |
| 26 | K | 101 | BCR | C24-C23-C22 | -4.63 | 119.25 | 126.23 |
| 26 | c | 514 | BCR | C36-C18-C17 | -4.62 | 116.45 | 122.92 |
| 24 | C | 503 | CLA | C4D-C3D-CAD | -4.62 | 105.89 | 108.47 |
| 26 | t | 101 | BCR | C11-C12-C13 | -4.62 | 113.44 | 126.42 |
| 24 | C | 510 | CLA | C3A-C2A-C1A | 4.62 | 108.25 | 101.34 |
| 27 | A | 611 | PL9 | C40-C39-C41 | -4.62 | 107.51 | 115.27 |
| 26 | c | 521 | BCR | C38-C26-C27 | -4.61 | 104.75 | 113.62 |
| 24 | a | 609 | CLA | C2A-C3A-C4A | 4.61 | 109.32 | 101.87 |
| 24 | C | 510 | CLA | C2A-C3A-C4A | 4.61 | 109.32 | 101.87 |
| 24 | B | 606 | CLA | O2D-CGD-CBD | 4.61 | 119.46 | 111.27 |
| 28 | l | 101 | SQD | O6-C1-C2 | 4.60 | 115.49 | 108.30 |
| 28 | L | 102 | SQD | O6-C1-C2 | 4.60 | 115.49 | 108.30 |
| 24 | c | 508 | CLA | C2A-C3A-C4A | 4.60 | 109.30 | 101.87 |
| 24 | c | 512 | CLA | C2A-C3A-C4A | 4.59 | 109.28 | 101.87 |
| 26 | K | 101 | BCR | C4-C5-C6 | -4.59 | 116.07 | 122.73 |
| 24 | a | 615 | CLA | C1B-CHB-C4A | -4.59 | 121.04 | 130.12 |
| 24 | a | 609 | CLA | O2D-CGD-CBD | 4.58 | 119.42 | 111.27 |
| 32 | h | 102 | DGD | O2G-C1B-C2B | 4.58 | 121.38 | 111.50 |
| 26 | a | 610 | BCR | C7-C6-C5 | -4.58 | 110.37 | 121.46 |
| 26 | F | 101 | BCR | C15-C14-C13 | -4.57 | 120.78 | 127.31 |
| 24 | C | 508 | CLA | C2A-C1A-CHA | 4.57 | 131.86 | 123.86 |
| 26 | B | 618 | BCR | C34-C9-C10 | -4.57 | 116.52 | 122.92 |
| 26 | F | 101 | BCR | C8-C7-C6 | -4.57 | 114.36 | 127.20 |
| 27 | D | 405 | PL9 | C45-C44-C46 | -4.57 | 107.58 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | B | 620 | BCR | C31-C1-C6 | -4.57 | 102.89 | 110.30 |
| 26 | h | 101 | BCR | C38-C26-C27 | -4.57 | 104.84 | 113.62 |
| 24 | b | 610 | CLA | C2A-C3A-C4A | 4.56 | 109.24 | 101.87 |
| 24 | c | 502 | CLA | O2D-CGD-CBD | 4.56 | 119.37 | 111.27 |
| 24 | c | 504 | CLA | C2A-C1A-CHA | 4.56 | 131.83 | 123.86 |
| 24 | c | 504 | CLA | O2D-CGD-CBD | 4.56 | 119.37 | 111.27 |
| 24 | B | 607[A] | CLA | C4A-NA-C1A | -4.56 | 104.66 | 106.71 |
| 24 | C | 512 | CLA | C4A-NA-C1A | -4.55 | 104.66 | 106.71 |
| 24 | C | 506 | CLA | O2D-CGD-CBD | 4.55 | 119.35 | 111.27 |
| 24 | d | 402 | CLA | C2A-C3A-C4A | 4.54 | 109.21 | 101.87 |
| 24 | b | 616 | CLA | C2A-C3A-C4A | 4.54 | 109.20 | 101.87 |
| 24 | C | 511 | CLA | C2A-C3A-C4A | 4.53 | 109.19 | 101.87 |
| 26 | K | 102 | BCR | C4-C5-C6 | -4.52 | 116.17 | 122.73 |
| 24 | D | 403 | CLA | C3A-C2A-C1A | 4.52 | 108.11 | 101.34 |
| 24 | B | 614 | CLA | C4D-C3D-CAD | -4.52 | 105.95 | 108.47 |
| 26 | c | 515 | BCR | C8-C7-C6 | -4.52 | 114.51 | 127.20 |
| 24 | b | 611 | CLA | O2D-CGD-CBD | 4.51 | 119.29 | 111.27 |
| 24 | b | 603 | CLA | C4A-NA-C1A | -4.51 | 104.68 | 106.71 |
| 26 | A | 610 | BCR | C7-C8-C9 | -4.51 | 119.42 | 126.23 |
| 24 | C | 511 | CLA | C4A-NA-C1A | -4.51 | 104.68 | 106.71 |
| 24 | c | 511 | CLA | C4D-C3D-CAD | -4.51 | 105.96 | 108.47 |
| 27 | a | 611 | PL9 | C21-C19-C18 | -4.50 | 112.01 | 121.12 |
| 24 | b | 613 | CLA | C2A-C1A-CHA | 4.49 | 131.71 | 123.86 |
| 24 | c | 509 | CLA | C2A-C1A-CHA | 4.49 | 131.71 | 123.86 |
| 27 | A | 611 | PL9 | C25-C24-C23 | -4.49 | 112.17 | 123.68 |
| 26 | B | 619 | BCR | C30-C25-C26 | -4.48 | 116.30 | 122.61 |
| 24 | B | 617 | CLA | CHC-C1C-NC | 4.48 | 131.00 | 124.20 |
| 24 | B | 613 | CLA | C3A-C2A-C1A | 4.47 | 108.04 | 101.34 |
| 24 | C | 512 | CLA | C2A-C3A-C4A | 4.46 | 109.08 | 101.87 |
| 26 | a | 610 | BCR | C38-C26-C27 | -4.46 | 105.05 | 113.62 |
| 26 | c | 514 | BCR | C2-C1-C6 | 4.46 | 117.34 | 110.48 |
| 24 | A | 609 | CLA | O2D-CGD-CBD | 4.46 | 119.19 | 111.27 |
| 24 | B | 615 | CLA | C2A-C3A-C4A | 4.46 | 109.07 | 101.87 |
| 24 | C | 504 | CLA | O2D-CGD-CBD | 4.45 | 119.18 | 111.27 |
| 24 | b | 612 | CLA | C2A-C1A-CHA | 4.45 | 131.65 | 123.86 |
| 24 | c | 511 | CLA | C4A-NA-C1A | -4.45 | 104.70 | 106.71 |
| 24 | c | 505 | CLA | C2A-C1A-CHA | 4.45 | 131.63 | 123.86 |
| 24 | B | 603 | CLA | C1B-CHB-C4A | -4.45 | 121.31 | 130.12 |
| 24 | c | 502 | CLA | C2A-C1A-CHA | 4.44 | 131.63 | 123.86 |
| 26 | b | 619 | BCR | C7-C6-C5 | -4.44 | 110.70 | 121.46 |
| 24 | A | 606 | CLA | C2A-C1A-CHA | 4.44 | 131.63 | 123.86 |
| 29 | c | 520 | LMG | O7-C10-C11 | 4.44 | 121.07 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | D | 402 | CLA | C2A-C3A-C4A | 4.44 | 109.04 | 101.87 |
| 26 | c | 521 | BCR | C1-C6-C5 | -4.44 | 116.36 | 122.61 |
| 26 | K | 102 | BCR | C38-C26-C27 | -4.43 | 105.10 | 113.62 |
| 24 | C | 504 | CLA | C3A-C2A-C1A | 4.42 | 107.96 | 101.34 |
| 24 | c | 511 | CLA | C2A-C3A-C4A | 4.42 | 109.00 | 101.87 |
| 24 | C | 506 | CLA | C1B-CHB-C4A | -4.41 | 121.38 | 130.12 |
| 26 | T | 101 | BCR | C4-C5-C6 | -4.41 | 116.33 | 122.73 |
| 27 | a | 611 | PL9 | C20-C19-C18 | -4.41 | 112.37 | 123.68 |
| 26 | T | 101 | BCR | C35-C13-C14 | -4.41 | 116.75 | 122.92 |
| 27 | A | 611 | PL9 | C36-C34-C33 | -4.40 | 112.20 | 121.12 |
| 24 | B | 614 | CLA | C2A-C1A-CHA | 4.39 | 131.53 | 123.86 |
| 24 | B | 605 | CLA | O2D-CGD-CBD | 4.38 | 119.04 | 111.27 |
| 24 | b | 610 | CLA | C2A-C1A-CHA | 4.37 | 131.51 | 123.86 |
| 24 | b | 607 | CLA | C2A-C1A-CHA | 4.37 | 131.51 | 123.86 |
| 24 | c | 510 | CLA | C2A-C3A-C4A | 4.37 | 108.93 | 101.87 |
| 26 | c | 521 | BCR | C15-C14-C13 | -4.37 | 121.07 | 127.31 |
| 26 | H | 101 | BCR | C30-C25-C26 | -4.37 | 116.46 | 122.61 |
| 26 | k | 101 | BCR | C38-C26-C27 | -4.37 | 105.22 | 113.62 |
| 24 | a | 606 | CLA | C2A-C3A-C4A | 4.37 | 108.92 | 101.87 |
| 24 | b | 618 | CLA | C2A-C3A-C4A | 4.37 | 108.92 | 101.87 |
| 24 | A | 606 | CLA | O2D-CGD-CBD | 4.36 | 119.02 | 111.27 |
| 24 | D | 402 | CLA | C1B-CHB-C4A | -4.36 | 121.48 | 130.12 |
| 24 | B | 607[A] | CLA | C2A-C1A-CHA | 4.36 | 131.48 | 123.86 |
| 28 | a | 612 | SQD | O9-S-C6 | 4.35 | 112.11 | 106.94 |
| 24 | c | 505 | CLA | C2A-C3A-C4A | 4.34 | 108.88 | 101.87 |
| 24 | c | 508 | CLA | C2A-C1A-CHA | 4.33 | 131.44 | 123.86 |
| 24 | C | 501 | CLA | C4A-NA-C1A | -4.33 | 104.76 | 106.71 |
| 24 | b | 615 | CLA | O2D-CGD-CBD | 4.33 | 118.96 | 111.27 |
| 24 | a | 607 | CLA | C2A-C3A-C4A | 4.33 | 108.86 | 101.87 |
| 26 | h | 101 | BCR | C24-C25-C26 | -4.33 | 110.98 | 121.46 |
| 28 | a | 612 | SQD | O47-C7-C8 | 4.32 | 120.82 | 111.50 |
| 26 | I | 101 | BCR | C30-C25-C26 | -4.32 | 116.52 | 122.61 |
| 24 | D | 402 | CLA | CHA-C1A-NA | -4.32 | 116.50 | 126.40 |
| 26 | T | 101 | BCR | C24-C25-C26 | -4.32 | 111.00 | 121.46 |
| 28 | A | 612 | SQD | O47-C7-C8 | 4.31 | 120.80 | 111.50 |
| 28 | A | 612 | SQD | O9-S-C6 | 4.31 | 112.06 | 106.94 |
| 24 | c | 507 | CLA | C2A-C1A-CHA | 4.31 | 131.39 | 123.86 |
| 26 | b | 620 | BCR | C38-C26-C27 | -4.30 | 105.35 | 113.62 |
| 30 | d | 406 | LHG | O7-C7-C8 | 4.30 | 120.77 | 111.50 |
| 24 | C | 502 | CLA | C2A-C1A-CHA | 4.30 | 131.38 | 123.86 |
| 24 | B | 617 | CLA | C2A-C3A-C4A | 4.30 | 108.81 | 101.87 |
| 26 | b | 619 | BCR | C37-C22-C21 | -4.30 | 116.90 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | B | 619 | BCR | C36-C18-C19 | -4.29 | 111.32 | 118.08 |
| 26 | T | 101 | BCR | C20-C21-C22 | -4.28 | 121.20 | 127.31 |
| 24 | C | 504 | CLA | C1B-CHB-C4A | -4.27 | 121.66 | 130.12 |
| 26 | f | 101 | BCR | C8-C7-C6 | -4.27 | 115.20 | 127.20 |
| 24 | b | 616 | CLA | O2D-CGD-CBD | 4.27 | 118.86 | 111.27 |
| 24 | D | 403 | CLA | C4D-C3D-CAD | -4.27 | 106.09 | 108.47 |
| 24 | C | 505 | CLA | C2A-C1A-CHA | 4.27 | 131.32 | 123.86 |
| 26 | b | 621 | BCR | C37-C22-C21 | -4.26 | 116.95 | 122.92 |
| 24 | C | 506 | CLA | C2A-C3A-C4A | 4.26 | 108.75 | 101.87 |
| 24 | c | 509 | CLA | O2D-CGD-CBD | 4.26 | 118.83 | 111.27 |
| 24 | b | 608[A] | CLA | O2D-CGD-CBD | 4.25 | 118.83 | 111.27 |
| 26 | H | 101 | BCR | C23-C24-C25 | -4.25 | 115.26 | 127.20 |
| 24 | B | 604 | CLA | O2D-CGD-CBD | 4.25 | 118.82 | 111.27 |
| 24 | d | 403 | CLA | C1-O2A-CGA | 4.25 | 127.59 | 116.44 |
| 33 | V | 201 | HEM | C1D-C2D-C3D | -4.25 | 104.04 | 107.00 |
| 26 | B | 620 | BCR | C23-C22-C21 | -4.24 | 112.43 | 118.94 |
| 26 | C | 514 | BCR | C20-C19-C18 | -4.24 | 114.50 | 126.42 |
| 24 | b | 608[A] | CLA | C4A-NA-C1A | -4.24 | 104.80 | 106.71 |
| 26 | A | 610 | BCR | C7-C6-C5 | -4.23 | 111.21 | 121.46 |
| 24 | C | 513 | CLA | C4A-NA-C1A | -4.23 | 104.80 | 106.71 |
| 24 | C | 508 | CLA | O2D-CGD-CBD | 4.23 | 118.78 | 111.27 |
| 28 | B | 622 | SQD | O6-C1-C2 | 4.22 | 114.90 | 108.30 |
| 28 | b | 601 | SQD | O6-C1-C2 | 4.22 | 114.89 | 108.30 |
| 32 | c | 516 | DGD | O2G-C1B-C2B | 4.22 | 120.60 | 111.50 |
| 24 | B | 616 | CLA | C2A-C1A-CHA | 4.22 | 131.24 | 123.86 |
| 26 | t | 101 | BCR | C23-C24-C25 | -4.22 | 115.36 | 127.20 |
| 24 | b | 608[B] | CLA | O2D-CGD-CBD | 4.21 | 118.75 | 111.27 |
| 24 | C | 504 | CLA | C2A-C1A-CHA | 4.21 | 131.22 | 123.86 |
| 24 | c | 513 | CLA | C2A-C1A-CHA | 4.20 | 131.21 | 123.86 |
| 26 | f | 101 | BCR | C7-C6-C5 | -4.20 | 111.28 | 121.46 |
| 24 | A | 607 | CLA | C1B-CHB-C4A | -4.20 | 121.80 | 130.12 |
| 24 | b | 616 | CLA | C4A-NA-C1A | -4.20 | 104.82 | 106.71 |
| 27 | d | 404 | PL9 | C20-C19-C18 | -4.19 | 112.92 | 123.68 |
| 24 | B | 608 | CLA | C4A-NA-C1A | -4.19 | 104.82 | 106.71 |
| 24 | b | 610 | CLA | C1B-CHB-C4A | -4.18 | 121.83 | 130.12 |
| 26 | C | 514 | BCR | C36-C18-C17 | -4.18 | 117.07 | 122.92 |
| 24 | B | 615 | CLA | O2D-CGD-CBD | 4.18 | 118.70 | 111.27 |
| 30 | E | 102 | LHG | O7-C7-C8 | 4.18 | 120.50 | 111.50 |
| 27 | d | 404 | PL9 | C31-C29-C28 | -4.17 | 112.67 | 121.12 |
| 24 | C | 505 | CLA | C2A-C3A-C4A | 4.17 | 108.61 | 101.87 |
| 24 | c | 503 | CLA | C2A-C1A-CHA | 4.17 | 131.15 | 123.86 |
| 26 | B | 619 | BCR | C20-C19-C18 | -4.17 | 114.70 | 126.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | b | 616 | CLA | C2A-C1A-CHA | 4.17 | 131.15 | 123.86 |
| 24 | B | 607[B] | CLA | C2A-C1A-CHA | 4.16 | 131.14 | 123.86 |
| 24 | c | 501 | CLA | C2A-C1A-CHA | 4.16 | 131.13 | 123.86 |
| 24 | c | 510 | CLA | C4D-C3D-CAD | -4.16 | 106.15 | 108.47 |
| 26 | c | 521 | BCR | C35-C13-C14 | -4.16 | 117.10 | 122.92 |
| 26 | b | 621 | BCR | C38-C26-C27 | -4.15 | 105.64 | 113.62 |
| 24 | c | 513 | CLA | C1B-CHB-C4A | -4.15 | 121.91 | 130.12 |
| 24 | a | 607 | CLA | C4A-NA-C1A | -4.14 | 104.84 | 106.71 |
| 26 | A | 610 | BCR | C39-C30-C25 | 4.14 | 117.01 | 110.30 |
| 24 | d | 403 | CLA | C4A-NA-C1A | -4.13 | 104.85 | 106.71 |
| 27 | d | 404 | PL9 | C36-C34-C33 | -4.13 | 112.76 | 121.12 |
| 24 | C | 513 | CLA | CMB-C2B-C1B | -4.13 | 122.12 | 128.46 |
| 32 | d | 405 | DGD | O2G-C1B-C2B | 4.12 | 120.39 | 111.50 |
| 24 | D | 402 | CLA | O1D-CGD-CBD | -4.12 | 116.05 | 124.48 |
| 24 | b | 609 | CLA | O2D-CGD-CBD | 4.12 | 118.58 | 111.27 |
| 24 | B | 603 | CLA | C2A-C3A-C4A | 4.12 | 108.52 | 101.87 |
| 28 | X | 101 | SQD | O6-C1-C2 | 4.12 | 114.73 | 108.30 |
| 27 | A | 611 | PL9 | C47-C48-C49 | -4.11 | 113.70 | 127.75 |
| 26 | a | 610 | BCR | C24-C25-C26 | -4.11 | 111.51 | 121.46 |
| 24 | C | 510 | CLA | O2D-CGD-CBD | 4.11 | 118.57 | 111.27 |
| 26 | C | 514 | BCR | C38-C26-C27 | -4.11 | 105.72 | 113.62 |
| 26 | B | 618 | BCR | C36-C18-C17 | -4.11 | 117.17 | 122.92 |
| 28 | x | 101 | SQD | O6-C1-C2 | 4.10 | 114.71 | 108.30 |
| 26 | a | 610 | BCR | C36-C18-C17 | -4.10 | 117.19 | 122.92 |
| 24 | B | 614 | CLA | CHC-C1C-NC | 4.09 | 130.41 | 124.20 |
| 26 | k | 101 | BCR | C23-C24-C25 | -4.09 | 115.71 | 127.20 |
| 26 | c | 514 | BCR | C16-C15-C14 | -4.09 | 115.10 | 123.47 |
| 24 | C | 513 | CLA | C1B-CHB-C4A | -4.08 | 122.03 | 130.12 |
| 24 | b | 611 | CLA | C1B-CHB-C4A | -4.08 | 122.03 | 130.12 |
| 26 | B | 618 | BCR | C23-C24-C25 | -4.08 | 115.73 | 127.20 |
| 29 | C | 518 | LMG | O7-C10-C11 | 4.08 | 120.30 | 111.50 |
| 26 | K | 101 | BCR | C23-C22-C21 | -4.08 | 112.68 | 118.94 |
| 26 | B | 619 | BCR | C11-C12-C13 | -4.07 | 114.99 | 126.42 |
| 27 | D | 405 | PL9 | C7-C3-C4 | 4.07 | 120.18 | 116.88 |
| 24 | C | 512 | CLA | CHC-C1C-NC | 4.06 | 130.36 | 124.20 |
| 26 | F | 101 | BCR | C37-C22-C21 | -4.06 | 117.24 | 122.92 |
| 27 | a | 611 | PL9 | C47-C48-C49 | -4.06 | 113.88 | 127.75 |
| 24 | B | 613 | CLA | C1B-CHB-C4A | -4.05 | 122.09 | 130.12 |
| 26 | A | 610 | BCR | C34-C9-C10 | -4.05 | 117.25 | 122.92 |
| 26 | K | 102 | BCR | C23-C24-C25 | -4.04 | 115.85 | 127.20 |
| 24 | B | 603 | CLA | CHC-C1C-NC | 4.04 | 130.34 | 124.20 |
| 26 | k | 101 | BCR | C4-C5-C6 | -4.04 | 116.87 | 122.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27 | a | 611 | PL9 | C31-C29-C28 | -4.03 | 112.95 | 121.12 |
| 27 | A | 611 | PL9 | C31-C29-C28 | -4.03 | 112.96 | 121.12 |
| 24 | a | 615 | CLA | C2A-C3A-C4A | 4.03 | 108.38 | 101.87 |
| 32 | C | 515 | DGD | O2G-C1B-C2B | 4.03 | 120.18 | 111.50 |
| 26 | a | 610 | BCR | C8-C7-C6 | -4.03 | 115.89 | 127.20 |
| 26 | F | 101 | BCR | C36-C18-C19 | 4.02 | 124.41 | 118.08 |
| 24 | b | 613 | CLA | C4A-NA-C1A | -4.02 | 104.90 | 106.71 |
| 24 | D | 402 | CLA | C2A-C1A-CHA | 4.01 | 130.87 | 123.86 |
| 24 | B | 609 | CLA | CAC-C3C-C4C | 4.00 | 130.00 | 124.81 |
| 24 | A | 609 | CLA | C2A-C1A-CHA | 4.00 | 130.85 | 123.86 |
| 26 | B | 619 | BCR | C35-C13-C14 | -3.99 | 117.33 | 122.92 |
| 26 | I | 101 | BCR | C38-C26-C27 | -3.99 | 105.96 | 113.62 |
| 24 | D | 404 | CLA | C1-O2A-CGA | 3.99 | 126.91 | 116.44 |
| 24 | A | 607 | CLA | C4D-C3D-CAD | -3.99 | 106.25 | 108.47 |
| 24 | a | 607 | CLA | O1D-CGD-CBD | -3.98 | 116.33 | 124.48 |
| 24 | a | 609 | CLA | CHA-C1A-NA | -3.98 | 117.29 | 126.40 |
| 26 | c | 515 | BCR | C20-C21-C22 | -3.97 | 121.64 | 127.31 |
| 27 | D | 405 | PL9 | C51-C49-C48 | -3.97 | 111.17 | 122.65 |
| 24 | c | 508 | CLA | O2D-CGD-O1D | -3.97 | 116.08 | 123.84 |
| 28 | b | 601 | SQD | O47-C7-C8 | 3.97 | 120.06 | 111.50 |
| 28 | B | 622 | SQD | O47-C7-C8 | 3.97 | 120.05 | 111.50 |
| 32 | E | 101 | DGD | O2G-C1B-C2B | 3.97 | 120.05 | 111.50 |
| 24 | a | 607 | CLA | C1B-CHB-C4A | -3.96 | 122.27 | 130.12 |
| 26 | B | 618 | BCR | C33-C5-C4 | -3.96 | 106.00 | 113.62 |
| 26 | b | 620 | BCR | C37-C22-C21 | -3.96 | 117.38 | 122.92 |
| 24 | c | 503 | CLA | O2D-CGD-CBD | 3.96 | 118.30 | 111.27 |
| 32 | C | 517 | DGD | O2G-C1B-C2B | 3.95 | 120.02 | 111.50 |
| 24 | b | 618 | CLA | CHC-C1C-NC | 3.94 | 130.19 | 124.20 |
| 24 | B | 612 | CLA | C1B-CHB-C4A | -3.94 | 122.31 | 130.12 |
| 24 | c | 510 | CLA | CHC-C1C-NC | 3.94 | 130.18 | 124.20 |
| 24 | c | 508 | CLA | C1B-CHB-C4A | -3.93 | 122.33 | 130.12 |
| 24 | b | 611 | CLA | C2A-C1A-CHA | 3.93 | 130.73 | 123.86 |
| 24 | B | 606 | CLA | C4-C3-C5 | 3.93 | 121.88 | 115.27 |
| 24 | C | 508 | CLA | CHC-C1C-NC | 3.92 | 130.15 | 124.20 |
| 28 | b | 601 | SQD | O7-S-C6 | 3.92 | 111.60 | 106.94 |
| 24 | a | 615 | CLA | CHC-C1C-NC | 3.91 | 130.13 | 124.20 |
| 24 | B | 617 | CLA | O2D-CGD-CBD | 3.90 | 118.21 | 111.27 |
| 24 | c | 505 | CLA | CMB-C2B-C1B | -3.90 | 122.47 | 128.46 |
| 24 | b | 607 | CLA | C4-C3-C5 | 3.90 | 121.83 | 115.27 |
| 24 | c | 504 | CLA | C1B-CHB-C4A | -3.90 | 122.39 | 130.12 |
| 24 | D | 404 | CLA | CMB-C2B-C1B | -3.90 | 122.48 | 128.46 |
| 28 | B | 622 | SQD | O7-S-C6 | 3.89 | 111.56 | 106.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25 | D | 401 | PHO | O2D-CGD-O1D | -3.89 | 116.23 | 123.84 |
| 26 | b | 619 | BCR | C30-C25-C26 | -3.88 | 117.15 | 122.61 |
| 30 | l | 102 | LHG | O7-C7-C8 | 3.88 | 119.86 | 111.50 |
| 24 | b | 603 | CLA | O2D-CGD-CBD | 3.88 | 118.16 | 111.27 |
| 26 | b | 621 | BCR | C19-C18-C17 | 3.87 | 124.88 | 118.94 |
| 27 | D | 405 | PL9 | C41-C39-C38 | -3.87 | 113.29 | 121.12 |
| 26 | b | 620 | BCR | C30-C25-C26 | -3.87 | 117.17 | 122.61 |
| 24 | A | 607 | CLA | CHC-C1C-NC | 3.86 | 130.06 | 124.20 |
| 26 | h | 101 | BCR | C31-C1-C6 | -3.86 | 104.04 | 110.30 |
| 24 | c | 502 | CLA | C4A-NA-C1A | -3.86 | 104.97 | 106.71 |
| 29 | C | 519 | LMG | O7-C10-C11 | 3.86 | 119.82 | 111.50 |
| 26 | f | 101 | BCR | C37-C22-C23 | -3.86 | 112.00 | 118.08 |
| 24 | A | 606 | CLA | CHC-C1C-NC | 3.85 | 130.05 | 124.20 |
| 27 | d | 404 | PL9 | C50-C49-C48 | -3.85 | 111.52 | 122.65 |
| 24 | b | 613 | CLA | CMB-C2B-C1B | -3.85 | 122.55 | 128.46 |
| 24 | b | 614 | CLA | O2D-CGD-O1D | -3.85 | 116.32 | 123.84 |
| 24 | B | 612 | CLA | C4A-NA-C1A | -3.84 | 104.98 | 106.71 |
| 26 | K | 101 | BCR | C35-C13-C14 | -3.84 | 117.54 | 122.92 |
| 24 | b | 613 | CLA | CHC-C1C-NC | 3.84 | 130.03 | 124.20 |
| 27 | A | 611 | PL9 | C50-C49-C48 | -3.84 | 111.55 | 122.65 |
| 26 | A | 610 | BCR | C23-C22-C21 | -3.84 | 113.05 | 118.94 |
| 24 | B | 607[B] | CLA | CHC-C1C-NC | 3.84 | 130.02 | 124.20 |
| 24 | D | 404 | CLA | C1B-CHB-C4A | -3.83 | 122.52 | 130.12 |
| 24 | C | 503 | CLA | C2A-C1A-CHA | 3.83 | 130.56 | 123.86 |
| 28 | B | 622 | SQD | C3-C4-C5 | 3.83 | 117.07 | 110.24 |
| 24 | B | 615 | CLA | C1B-CHB-C4A | -3.82 | 122.55 | 130.12 |
| 28 | b | 601 | SQD | C3-C4-C5 | 3.82 | 117.05 | 110.24 |
| 27 | d | 404 | PL9 | C41-C39-C38 | -3.82 | 113.39 | 121.12 |
| 26 | h | 101 | BCR | C40-C30-C25 | -3.82 | 104.11 | 110.30 |
| 24 | C | 506 | CLA | CED-O2D-CGD | 3.81 | 124.56 | 115.94 |
| 24 | b | 609 | CLA | C4D-C3D-CAD | -3.81 | 106.35 | 108.47 |
| 26 | A | 610 | BCR | C8-C7-C6 | -3.81 | 116.52 | 127.20 |
| 24 | b | 612 | CLA | C1B-CHB-C4A | -3.80 | 122.60 | 130.12 |
| 27 | A | 611 | PL9 | C7-C3-C4 | 3.79 | 119.96 | 116.88 |
| 24 | b | 610 | CLA | CMB-C2B-C1B | -3.79 | 122.64 | 128.46 |
| 24 | b | 603 | CLA | CHC-C1C-NC | 3.79 | 129.95 | 124.20 |
| 26 | b | 621 | BCR | C2-C1-C6 | 3.78 | 116.30 | 110.48 |
| 26 | B | 618 | BCR | C38-C26-C27 | -3.78 | 106.36 | 113.62 |
| 26 | c | 521 | BCR | C24-C25-C26 | -3.78 | 112.31 | 121.46 |
| 24 | b | 605 | CLA | CHB-C4A-NA | -3.78 | 119.29 | 124.51 |
| 26 | b | 619 | BCR | C8-C7-C6 | -3.77 | 116.60 | 127.20 |
| 28 | X | 101 | SQD | O47-C7-C8 | 3.77 | 119.63 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 29 | Z | 101 | LMG | O1-C1-C2 | 3.77 | 114.19 | 108.30 |
| 24 | C | 503 | CLA | C4A-NA-C1A | -3.77 | 105.01 | 106.71 |
| 32 | c | 518 | DGD | O3G-C3G-C2G | -3.77 | 101.80 | 110.90 |
| 28 | x | 101 | SQD | O47-C7-C8 | 3.77 | 119.62 | 111.50 |
| 27 | D | 405 | PL9 | C10-C9-C11 | -3.77 | 108.93 | 115.27 |
| 26 | A | 610 | BCR | C36-C18-C17 | -3.77 | 117.64 | 122.92 |
| 24 | b | 604 | CLA | O1D-CGD-CBD | -3.77 | 116.78 | 124.48 |
| 33 | E | 103 | HEM | C1D-C2D-C3D | -3.77 | 104.38 | 107.00 |
| 24 | a | 615 | CLA | O2A-CGA-CBA | 3.76 | 123.72 | 111.91 |
| 24 | B | 607[A] | CLA | CHC-C1C-NC | 3.76 | 129.91 | 124.20 |
| 24 | C | 505 | CLA | C1B-CHB-C4A | -3.76 | 122.67 | 130.12 |
| 24 | b | 605 | CLA | O1D-CGD-CBD | -3.76 | 116.80 | 124.48 |
| 26 | C | 514 | BCR | C34-C9-C10 | -3.75 | 117.66 | 122.92 |
| 29 | a | 613 | LMG | O7-C10-C11 | 3.75 | 119.59 | 111.50 |
| 24 | C | 511 | CLA | CHC-C1C-NC | 3.74 | 129.87 | 124.20 |
| 24 | b | 607 | CLA | C1-O2A-CGA | 3.73 | 126.24 | 116.44 |
| 27 | a | 611 | PL9 | C7-C3-C4 | 3.73 | 119.91 | 116.88 |
| 24 | d | 403 | CLA | CHC-C1C-NC | 3.73 | 129.86 | 124.20 |
| 26 | B | 620 | BCR | C38-C26-C27 | -3.73 | 106.45 | 113.62 |
| 24 | C | 501 | CLA | C2A-C1A-CHA | 3.73 | 130.37 | 123.86 |
| 28 | L | 102 | SQD | O47-C7-C8 | 3.72 | 119.52 | 111.50 |
| 26 | B | 620 | BCR | C24-C25-C26 | -3.71 | 112.47 | 121.46 |
| 26 | h | 101 | BCR | C33-C5-C4 | -3.71 | 106.49 | 113.62 |
| 24 | A | 606 | CLA | C1B-CHB-C4A | -3.71 | 122.78 | 130.12 |
| 26 | c | 514 | BCR | C20-C19-C18 | -3.71 | 116.00 | 126.42 |
| 24 | B | 604 | CLA | C2A-C1A-CHA | 3.70 | 130.34 | 123.86 |
| 32 | C | 517 | DGD | O3G-C3G-C2G | -3.70 | 101.96 | 110.90 |
| 24 | b | 609 | CLA | C1B-CHB-C4A | -3.70 | 122.79 | 130.12 |
| 24 | D | 404 | CLA | O2D-CGD-CBD | 3.70 | 117.84 | 111.27 |
| 24 | c | 502 | CLA | C1B-CHB-C4A | -3.70 | 122.79 | 130.12 |
| 26 | B | 619 | BCR | C37-C22-C21 | -3.69 | 117.75 | 122.92 |
| 24 | B | 612 | CLA | CMB-C2B-C1B | -3.69 | 122.79 | 128.46 |
| 24 | c | 503 | CLA | C1B-CHB-C4A | -3.69 | 122.82 | 130.12 |
| 24 | b | 616 | CLA | C1B-CHB-C4A | -3.68 | 122.83 | 130.12 |
| 28 | L | 102 | SQD | O7-S-C6 | 3.68 | 111.31 | 106.94 |
| 26 | B | 620 | BCR | C16-C15-C14 | -3.67 | 115.95 | 123.47 |
| 24 | c | 507 | CLA | CHC-C1C-NC | 3.67 | 129.78 | 124.20 |
| 28 | l | 101 | SQD | O7-S-C6 | 3.67 | 111.31 | 106.94 |
| 28 | l | 101 | SQD | O47-C7-C8 | 3.67 | 119.42 | 111.50 |
| 27 | a | 611 | PL9 | C45-C44-C46 | -3.66 | 109.11 | 115.27 |
| 24 | c | 501 | CLA | C1B-CHB-C4A | -3.66 | 122.87 | 130.12 |
| 24 | A | 609 | CLA | C1B-CHB-C4A | -3.65 | 122.88 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | A | 607 | CLA | C4A-NA-C1A | -3.65 | 105.06 | 106.71 |
| 24 | a | 615 | CLA | C2A-C1A-CHA | 3.65 | 130.24 | 123.86 |
| 24 | C | 508 | CLA | CMB-C2B-C1B | -3.65 | 122.85 | 128.46 |
| 24 | a | 606 | CLA | CHC-C1C-NC | 3.65 | 129.74 | 124.20 |
| 26 | I | 101 | BCR | C8-C7-C6 | -3.65 | 116.96 | 127.20 |
| 24 | C | 506 | CLA | CMB-C2B-C1B | -3.64 | 122.86 | 128.46 |
| 24 | c | 506 | CLA | C1B-CHB-C4A | -3.64 | 122.90 | 130.12 |
| 24 | B | 610 | CLA | C1B-CHB-C4A | -3.64 | 122.91 | 130.12 |
| 24 | c | 505 | CLA | C1B-CHB-C4A | -3.63 | 122.93 | 130.12 |
| 24 | B | 607[B] | CLA | C4A-NA-C1A | -3.63 | 105.08 | 106.71 |
| 27 | d | 404 | PL9 | C51-C49-C48 | -3.62 | 112.17 | 122.65 |
| 24 | B | 604 | CLA | CHB-C4A-NA | -3.62 | 119.50 | 124.51 |
| 24 | B | 616 | CLA | O2D-CGD-CBD | 3.61 | 117.69 | 111.27 |
| 26 | c | 515 | BCR | C23-C24-C25 | -3.61 | 117.06 | 127.20 |
| 26 | c | 515 | BCR | C34-C9-C10 | -3.61 | 117.86 | 122.92 |
| 24 | b | 615 | CLA | CHC-C1C-NC | 3.61 | 129.68 | 124.20 |
| 24 | b | 616 | CLA | CMB-C2B-C1B | -3.61 | 122.92 | 128.46 |
| 26 | I | 101 | BCR | C20-C19-C18 | -3.61 | 116.28 | 126.42 |
| 26 | h | 101 | BCR | C30-C25-C26 | -3.61 | 117.53 | 122.61 |
| 24 | B | 603 | CLA | C4A-NA-C1A | -3.61 | 105.08 | 106.71 |
| 29 | z | 101 | LMG | O7-C10-C11 | 3.60 | 119.25 | 111.50 |
| 27 | D | 405 | PL9 | C50-C49-C48 | -3.59 | 112.26 | 122.65 |
| 27 | a | 611 | PL9 | C50-C49-C48 | -3.59 | 112.26 | 122.65 |
| 24 | b | 609 | CLA | CMB-C2B-C1B | -3.59 | 122.95 | 128.46 |
| 24 | a | 609 | CLA | C4-C3-C5 | 3.59 | 121.30 | 115.27 |
| 26 | I | 101 | BCR | C7-C6-C5 | -3.59 | 112.78 | 121.46 |
| 26 | c | 515 | BCR | C7-C6-C5 | -3.58 | 112.79 | 121.46 |
| 24 | c | 508 | CLA | CMB-C2B-C1B | -3.58 | 122.96 | 128.46 |
| 24 | A | 609 | CLA | C4-C3-C5 | 3.58 | 121.29 | 115.27 |
| 29 | Z | 101 | LMG | O7-C10-C11 | 3.57 | 119.20 | 111.50 |
| 26 | t | 101 | BCR | C34-C9-C10 | -3.57 | 117.93 | 122.92 |
| 24 | C | 502 | CLA | C1-O2A-CGA | 3.56 | 125.79 | 116.44 |
| 24 | a | 607 | CLA | CHA-C1A-NA | -3.56 | 118.24 | 126.40 |
| 24 | d | 402 | CLA | C2A-C1A-CHA | 3.56 | 130.09 | 123.86 |
| 24 | a | 615 | CLA | CHA-C1A-NA | -3.56 | 118.25 | 126.40 |
| 26 | K | 102 | BCR | C33-C5-C4 | -3.56 | 106.78 | 113.62 |
| 24 | a | 615 | CLA | CMB-C2B-C1B | -3.55 | 123.00 | 128.46 |
| 24 | D | 403 | CLA | C4A-NA-C1A | -3.55 | 105.11 | 106.71 |
| 24 | B | 602 | CLA | C1B-CHB-C4A | -3.55 | 123.09 | 130.12 |
| 24 | C | 503 | CLA | O2D-CGD-CBD | 3.54 | 117.56 | 111.27 |
| 24 | C | 507 | CLA | C1B-CHB-C4A | -3.54 | 123.11 | 130.12 |
| 26 | k | 101 | BCR | C24-C25-C26 | -3.54 | 112.89 | 121.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | C | 510 | CLA | C1B-CHB-C4A | -3.54 | 123.11 | 130.12 |
| 30 | D | 407 | LHG | O7-C7-C8 | 3.53 | 119.12 | 111.50 |
| 29 | c | 519 | LMG | O7-C10-C11 | 3.53 | 119.11 | 111.50 |
| 26 | c | 515 | BCR | C33-C5-C4 | -3.53 | 106.83 | 113.62 |
| 26 | a | 610 | BCR | C34-C9-C10 | -3.53 | 117.98 | 122.92 |
| 24 | b | 617 | CLA | CHC-C1C-NC | 3.52 | 129.55 | 124.20 |
| 26 | A | 610 | BCR | C33-C5-C4 | -3.52 | 106.85 | 113.62 |
| 24 | D | 403 | CLA | C1B-CHB-C4A | -3.52 | 123.15 | 130.12 |
| 24 | c | 510 | CLA | C4A-NA-C1A | -3.52 | 105.12 | 106.71 |
| 24 | B | 613 | CLA | CHB-C4A-NA | -3.52 | 119.65 | 124.51 |
| 29 | D | 408 | LMG | O6-C5-C4 | 3.52 | 116.08 | 109.69 |
| 24 | c | 509 | CLA | CHC-C1C-NC | 3.51 | 129.53 | 124.20 |
| 24 | b | 605 | CLA | CHC-C1C-NC | 3.51 | 129.53 | 124.20 |
| 26 | k | 101 | BCR | C20-C21-C22 | -3.51 | 122.31 | 127.31 |
| 27 | A | 611 | PL9 | C15-C14-C16 | -3.50 | 109.38 | 115.27 |
| 24 | b | 613 | CLA | O1D-CGD-CBD | -3.50 | 117.32 | 124.48 |
| 24 | B | 605 | CLA | CHC-C1C-NC | 3.50 | 129.51 | 124.20 |
| 24 | B | 610 | CLA | CHC-C1C-NC | 3.50 | 129.51 | 124.20 |
| 24 | b | 608[B] | CLA | C4A-NA-C1A | -3.49 | 105.14 | 106.71 |
| 26 | K | 102 | BCR | C24-C25-C26 | -3.49 | 113.00 | 121.46 |
| 27 | A | 611 | PL9 | C45-C44-C46 | -3.49 | 109.40 | 115.27 |
| 24 | A | 607 | CLA | O2A-CGA-CBA | 3.49 | 122.86 | 111.91 |
| 24 | B | 616 | CLA | CHC-C1C-NC | 3.49 | 129.50 | 124.20 |
| 24 | c | 511 | CLA | C1B-CHB-C4A | -3.49 | 123.21 | 130.12 |
| 24 | b | 611 | CLA | O2D-CGD-O1D | -3.49 | 117.02 | 123.84 |
| 27 | a | 611 | PL9 | C36-C34-C33 | -3.48 | 114.08 | 121.12 |
| 26 | A | 610 | BCR | C16-C15-C14 | -3.48 | 116.35 | 123.47 |
| 24 | c | 501 | CLA | CMB-C2B-C1B | -3.47 | 123.12 | 128.46 |
| 24 | B | 606 | CLA | C1B-CHB-C4A | -3.47 | 123.24 | 130.12 |
| 24 | d | 403 | CLA | O2D-CGD-CBD | 3.47 | 117.44 | 111.27 |
| 24 | B | 604 | CLA | O1D-CGD-CBD | -3.47 | 117.39 | 124.48 |
| 24 | D | 404 | CLA | CHA-C1A-NA | -3.46 | 118.47 | 126.40 |
| 24 | B | 610 | CLA | C2A-C1A-CHA | 3.46 | 129.91 | 123.86 |
| 24 | c | 508 | CLA | CHC-C1C-NC | 3.46 | 129.45 | 124.20 |
| 26 | I | 101 | BCR | C30-C25-C24 | -3.46 | 106.00 | 115.78 |
| 28 | A | 614 | SQD | O9-S-C6 | 3.46 | 111.05 | 106.94 |
| 24 | a | 606 | CLA | CMB-C2B-C1B | -3.46 | 123.15 | 128.46 |
| 24 | C | 503 | CLA | C1B-CHB-C4A | -3.45 | 123.28 | 130.12 |
| 24 | b | 616 | CLA | C4-C3-C5 | 3.45 | 121.08 | 115.27 |
| 24 | c | 508 | CLA | C4A-NA-C1A | -3.45 | 105.16 | 106.71 |
| 26 | K | 102 | BCR | C40-C30-C25 | 3.45 | 115.89 | 110.30 |
| 24 | C | 508 | CLA | C1B-CHB-C4A | -3.44 | 123.30 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | B | 615 | CLA | C4-C3-C5 | 3.44 | 121.06 | 115.27 |
| 24 | b | 616 | CLA | O2D-CGD-O1D | -3.44 | 117.11 | 123.84 |
| 26 | b | 619 | BCR | C24-C25-C26 | -3.44 | 113.13 | 121.46 |
| 24 | C | 507 | CLA | O2D-CGD-O1D | -3.44 | 117.11 | 123.84 |
| 24 | C | 509 | CLA | C2A-C1A-CHA | 3.44 | 129.87 | 123.86 |
| 24 | c | 505 | CLA | C4A-NA-C1A | -3.44 | 105.16 | 106.71 |
| 26 | b | 620 | BCR | C16-C15-C14 | -3.44 | 116.44 | 123.47 |
| 24 | B | 609 | CLA | CHC-C1C-NC | 3.44 | 129.41 | 124.20 |
| 24 | c | 506 | CLA | CMB-C2B-C1B | -3.43 | 123.19 | 128.46 |
| 26 | b | 620 | BCR | C27-C26-C25 | -3.43 | 117.75 | 122.73 |
| 24 | A | 606 | CLA | C3A-C2A-C1A | 3.42 | 106.47 | 101.34 |
| 24 | A | 606 | CLA | C2A-C3A-C4A | 3.42 | 107.40 | 101.87 |
| 24 | c | 506 | CLA | CHB-C4A-NA | -3.42 | 119.78 | 124.51 |
| 30 | L | 101 | LHG | O7-C7-C8 | 3.42 | 118.87 | 111.50 |
| 24 | B | 602 | CLA | O2D-CGD-CBD | 3.41 | 117.34 | 111.27 |
| 24 | B | 603 | CLA | O2D-CGD-O1D | -3.41 | 117.17 | 123.84 |
| 28 | a | 614 | SQD | O9-S-C6 | 3.41 | 110.99 | 106.94 |
| 26 | t | 101 | BCR | C1-C6-C5 | -3.40 | 117.82 | 122.61 |
| 24 | B | 607[B] | CLA | C1B-CHB-C4A | -3.40 | 123.39 | 130.12 |
| 24 | b | 610 | CLA | O2D-CGD-O1D | -3.40 | 117.20 | 123.84 |
| 24 | C | 511 | CLA | C1B-CHB-C4A | -3.40 | 123.39 | 130.12 |
| 27 | a | 611 | PL9 | C15-C14-C16 | -3.39 | 109.56 | 115.27 |
| 24 | c | 507 | CLA | C1-O2A-CGA | 3.39 | 125.35 | 116.44 |
| 24 | b | 606 | CLA | C1-O2A-CGA | 3.39 | 125.34 | 116.44 |
| 24 | a | 607 | CLA | C1-O2A-CGA | 3.39 | 125.33 | 116.44 |
| 28 | A | 614 | SQD | O47-C7-C8 | 3.37 | 118.77 | 111.50 |
| 28 | a | 614 | SQD | O47-C7-C8 | 3.37 | 118.77 | 111.50 |
| 24 | b | 605 | CLA | O2A-C1-C2 | 3.37 | 117.50 | 108.64 |
| 24 | A | 609 | CLA | CHA-C1A-NA | -3.36 | 118.70 | 126.40 |
| 24 | B | 606 | CLA | C4D-C3D-CAD | -3.36 | 106.59 | 108.47 |
| 24 | B | 605 | CLA | C1B-CHB-C4A | -3.36 | 123.47 | 130.12 |
| 29 | C | 518 | LMG | O8-C28-C29 | 3.36 | 122.44 | 111.91 |
| 24 | b | 604 | CLA | C2A-C1A-CHA | 3.36 | 129.73 | 123.86 |
| 26 | b | 621 | BCR | C1-C6-C5 | -3.35 | 117.89 | 122.61 |
| 29 | D | 408 | LMG | O7-C10-C11 | 3.35 | 118.73 | 111.50 |
| 24 | C | 512 | CLA | CMB-C2B-C1B | -3.35 | 123.31 | 128.46 |
| 28 | A | 612 | SQD | O8-S-C6 | 3.35 | 111.08 | 105.74 |
| 24 | b | 605 | CLA | O2D-CGD-CBD | 3.34 | 117.20 | 111.27 |
| 27 | A | 611 | PL9 | C51-C49-C48 | -3.34 | 113.00 | 122.65 |
| 24 | b | 617 | CLA | O2D-CGD-O1D | -3.34 | 117.31 | 123.84 |
| 24 | a | 607 | CLA | CHC-C1C-NC | 3.33 | 129.26 | 124.20 |
| 24 | B | 616 | CLA | C1B-CHB-C4A | -3.33 | 123.52 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 28 | a | 612 | SQD | C1-C2-C3 | -3.33 | 103.06 | 110.00 |
| 32 | c | 517 | DGD | O2G-C1B-C2B | 3.33 | 118.67 | 111.50 |
| 24 | b | 606 | CLA | C1B-CHB-C4A | -3.32 | 123.54 | 130.12 |
| 24 | d | 402 | CLA | CMB-C2B-C1B | -3.32 | 123.36 | 128.46 |
| 24 | C | 509 | CLA | C1B-CHB-C4A | -3.32 | 123.55 | 130.12 |
| 24 | A | 607 | CLA | O1D-CGD-CBD | -3.32 | 117.70 | 124.48 |
| 28 | a | 612 | SQD | O8-S-C6 | 3.31 | 111.02 | 105.74 |
| 28 | A | 612 | SQD | C1-C2-C3 | -3.31 | 103.10 | 110.00 |
| 32 | E | 101 | DGD | C4E-C3E-C2E | 3.31 | 116.60 | 110.82 |
| 24 | c | 507 | CLA | C1B-CHB-C4A | -3.31 | 123.56 | 130.12 |
| 24 | b | 609 | CLA | C2A-C1A-CHA | 3.31 | 129.64 | 123.86 |
| 26 | t | 101 | BCR | C35-C13-C14 | -3.30 | 118.30 | 122.92 |
| 24 | C | 512 | CLA | C4-C3-C5 | 3.30 | 120.82 | 115.27 |
| 27 | D | 405 | PL9 | C15-C14-C16 | -3.30 | 109.72 | 115.27 |
| 24 | c | 512 | CLA | CHC-C1C-NC | 3.29 | 129.20 | 124.20 |
| 24 | c | 504 | CLA | CHC-C1C-NC | 3.29 | 129.20 | 124.20 |
| 26 | B | 620 | BCR | C37-C22-C21 | -3.29 | 118.31 | 122.92 |
| 24 | c | 505 | CLA | O2D-CGD-O1D | -3.29 | 117.41 | 123.84 |
| 24 | a | 607 | CLA | CMB-C2B-C1B | -3.29 | 123.41 | 128.46 |
| 26 | c | 521 | BCR | C34-C9-C10 | -3.28 | 118.32 | 122.92 |
| 24 | C | 507 | CLA | CHC-C1C-NC | 3.28 | 129.19 | 124.20 |
| 24 | c | 512 | CLA | C4-C3-C5 | 3.28 | 120.80 | 115.27 |
| 24 | C | 509 | CLA | CHC-C1C-NC | 3.28 | 129.18 | 124.20 |
| 24 | b | 608[B] | CLA | CHC-C1C-NC | 3.28 | 129.18 | 124.20 |
| 32 | C | 516 | DGD | O1G-C1A-C2A | 3.28 | 122.20 | 111.91 |
| 24 | B | 604 | CLA | C1B-CHB-C4A | -3.28 | 123.62 | 130.12 |
| 24 | c | 512 | CLA | CMB-C2B-C1B | -3.28 | 123.42 | 128.46 |
| 24 | D | 402 | CLA | CHC-C1C-NC | 3.28 | 129.18 | 124.20 |
| 24 | C | 501 | CLA | C1B-CHB-C4A | -3.28 | 123.63 | 130.12 |
| 24 | C | 505 | CLA | O2D-CGD-O1D | -3.28 | 117.43 | 123.84 |
| 26 | B | 620 | BCR | C12-C13-C14 | -3.27 | 113.92 | 118.94 |
| 26 | T | 101 | BCR | C37-C22-C21 | -3.27 | 118.34 | 122.92 |
| 26 | F | 101 | BCR | C20-C21-C22 | -3.27 | 122.64 | 127.31 |
| 24 | c | 501 | CLA | CHC-C1C-NC | 3.27 | 129.16 | 124.20 |
| 24 | c | 511 | CLA | CHC-C1C-NC | 3.27 | 129.16 | 124.20 |
| 26 | k | 101 | BCR | C23-C22-C21 | -3.26 | 113.94 | 118.94 |
| 26 | K | 101 | BCR | C11-C12-C13 | -3.26 | 117.27 | 126.42 |
| 24 | C | 502 | CLA | CHC-C1C-NC | 3.25 | 129.14 | 124.20 |
| 24 | c | 509 | CLA | O1D-CGD-CBD | -3.25 | 117.83 | 124.48 |
| 24 | b | 614 | CLA | C4-C3-C5 | 3.25 | 120.74 | 115.27 |
| 24 | a | 606 | CLA | O2D-CGD-CBD | 3.25 | 117.04 | 111.27 |
| 24 | b | 604 | CLA | CHC-C1C-NC | 3.25 | 129.13 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | h | 101 | BCR | C20-C19-C18 | -3.25 | 117.30 | 126.42 |
| 24 | b | 614 | CLA | CHC-C1C-NC | 3.25 | 129.13 | 124.20 |
| 24 | B | 611 | CLA | C4A-NA-C1A | -3.25 | 105.25 | 106.71 |
| 26 | h | 101 | BCR | C37-C22-C21 | -3.24 | 118.38 | 122.92 |
| 24 | B | 614 | CLA | O2D-CGD-O1D | -3.24 | 117.50 | 123.84 |
| 24 | b | 604 | CLA | O2D-CGD-O1D | -3.24 | 117.50 | 123.84 |
| 26 | K | 101 | BCR | C23-C24-C25 | -3.24 | 118.10 | 127.20 |
| 24 | a | 609 | CLA | C1B-CHB-C4A | -3.24 | 123.70 | 130.12 |
| 24 | c | 509 | CLA | C1B-CHB-C4A | -3.24 | 123.71 | 130.12 |
| 24 | C | 501 | CLA | O2A-CGA-CBA | 3.24 | 122.06 | 111.91 |
| 26 | t | 101 | BCR | C16-C15-C14 | -3.24 | 116.85 | 123.47 |
| 24 | B | 604 | CLA | CMB-C2B-C1B | -3.24 | 123.49 | 128.46 |
| 26 | T | 101 | BCR | C16-C15-C14 | -3.23 | 116.85 | 123.47 |
| 24 | B | 603 | CLA | C3A-C2A-C1A | 3.23 | 106.18 | 101.34 |
| 26 | t | 101 | BCR | C38-C26-C27 | -3.23 | 107.42 | 113.62 |
| 26 | K | 101 | BCR | C37-C22-C21 | -3.22 | 118.41 | 122.92 |
| 26 | T | 101 | BCR | C33-C5-C4 | -3.22 | 107.43 | 113.62 |
| 24 | c | 502 | CLA | CHC-C1C-NC | 3.22 | 129.09 | 124.20 |
| 26 | K | 101 | BCR | C33-C5-C4 | -3.22 | 107.44 | 113.62 |
| 24 | B | 607[A] | CLA | C1B-CHB-C4A | -3.22 | 123.75 | 130.12 |
| 28 | x | 101 | SQD | O7-S-C6 | 3.22 | 110.76 | 106.94 |
| 24 | b | 606 | CLA | O1D-CGD-CBD | -3.21 | 117.91 | 124.48 |
| 24 | B | 613 | CLA | C4-C3-C5 | 3.21 | 120.68 | 115.27 |
| 27 | D | 405 | PL9 | C7-C3-C2 | -3.21 | 119.08 | 123.30 |
| 27 | D | 405 | PL9 | C31-C29-C28 | -3.21 | 114.62 | 121.12 |
| 24 | B | 608 | CLA | CHB-C4A-NA | -3.21 | 120.08 | 124.51 |
| 24 | b | 617 | CLA | C1B-CHB-C4A | -3.21 | 123.77 | 130.12 |
| 24 | B | 613 | CLA | CBA-CAA-C2A | -3.21 | 104.40 | 113.86 |
| 24 | C | 509 | CLA | O2D-CGD-CBD | 3.20 | 116.96 | 111.27 |
| 24 | b | 615 | CLA | C4A-NA-C1A | -3.20 | 105.27 | 106.71 |
| 24 | C | 502 | CLA | C1B-CHB-C4A | -3.20 | 123.78 | 130.12 |
| 24 | c | 512 | CLA | C1-O2A-CGA | 3.20 | 124.83 | 116.44 |
| 26 | b | 621 | BCR | C20-C19-C18 | -3.20 | 117.44 | 126.42 |
| 26 | b | 619 | BCR | C27-C26-C25 | -3.20 | 118.09 | 122.73 |
| 24 | B | 603 | CLA | C4-C3-C5 | 3.19 | 120.64 | 115.27 |
| 25 | D | 401 | PHO | CBA-CAA-C2A | -3.19 | 104.44 | 113.86 |
| 26 | k | 101 | BCR | C33-C5-C4 | -3.19 | 107.48 | 113.62 |
| 26 | b | 621 | BCR | C7-C8-C9 | -3.19 | 121.41 | 126.23 |
| 26 | k | 101 | BCR | C37-C22-C21 | -3.19 | 118.46 | 122.92 |
| 24 | B | 613 | CLA | CMB-C2B-C1B | -3.18 | 123.57 | 128.46 |
| 24 | B | 609 | CLA | C1B-CHB-C4A | -3.18 | 123.81 | 130.12 |
| 26 | b | 619 | BCR | C30-C25-C24 | -3.18 | 106.78 | 115.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | C | 510 | CLA | O2D-CGD-O1D | -3.18 | 117.63 | 123.84 |
| 24 | b | 614 | CLA | C4A-NA-C1A | -3.17 | 105.28 | 106.71 |
| 24 | B | 602 | CLA | O2A-CGA-CBA | 3.17 | 121.86 | 111.91 |
| 28 | X | 101 | SQD | O7-S-C6 | 3.17 | 110.71 | 106.94 |
| 24 | d | 402 | CLA | CHC-C1C-NC | 3.17 | 129.01 | 124.20 |
| 24 | b | 606 | CLA | CHC-C1C-NC | 3.17 | 129.01 | 124.20 |
| 24 | D | 403 | CLA | CHC-C1C-NC | 3.17 | 129.01 | 124.20 |
| 24 | C | 510 | CLA | CHC-C1C-NC | 3.16 | 129.00 | 124.20 |
| 24 | c | 504 | CLA | C1-O2A-CGA | 3.16 | 124.74 | 116.44 |
| 26 | T | 101 | BCR | C38-C26-C27 | -3.16 | 107.54 | 113.62 |
| 32 | C | 516 | DGD | O6D-C5D-C4D | -3.16 | 103.96 | 109.69 |
| 24 | B | 609 | CLA | CHD-C4C-C3C | 3.16 | 129.48 | 124.84 |
| 24 | b | 604 | CLA | C4-C3-C5 | 3.16 | 120.58 | 115.27 |
| 32 | d | 405 | DGD | C4E-C3E-C2E | 3.16 | 116.33 | 110.82 |
| 26 | a | 610 | BCR | C11-C12-C13 | -3.15 | 117.57 | 126.42 |
| 24 | a | 607 | CLA | C4-C3-C5 | 3.15 | 120.57 | 115.27 |
| 32 | C | 516 | DGD | C3E-C4E-C5E | 3.15 | 115.86 | 110.24 |
| 27 | d | 404 | PL9 | C7-C3-C2 | -3.15 | 119.16 | 123.30 |
| 24 | a | 609 | CLA | C4A-NA-C1A | -3.15 | 105.29 | 106.71 |
| 26 | b | 620 | BCR | C20-C19-C18 | -3.15 | 117.58 | 126.42 |
| 24 | C | 510 | CLA | CMB-C2B-C1B | -3.15 | 123.63 | 128.46 |
| 24 | B | 607[A] | CLA | C1-O2A-CGA | 3.14 | 124.69 | 116.44 |
| 24 | b | 604 | CLA | CHB-C4A-NA | -3.14 | 120.17 | 124.51 |
| 26 | A | 610 | BCR | C38-C26-C27 | -3.14 | 107.58 | 113.62 |
| 24 | c | 513 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 24 | D | 404 | CLA | O1D-CGD-CBD | -3.13 | 118.07 | 124.48 |
| 24 | A | 607 | CLA | C4-C3-C5 | 3.13 | 120.54 | 115.27 |
| 24 | B | 606 | CLA | CHC-C1C-NC | 3.13 | 128.95 | 124.20 |
| 26 | B | 619 | BCR | C27-C26-C25 | -3.13 | 118.19 | 122.73 |
| 24 | C | 513 | CLA | C2A-C1A-CHA | 3.13 | 129.33 | 123.86 |
| 30 | d | 406 | LHG | C5-O7-C7 | -3.13 | 110.10 | 117.79 |
| 28 | a | 614 | SQD | O6-C1-C2 | 3.13 | 113.18 | 108.30 |
| 29 | A | 613 | LMG | O7-C10-C11 | 3.12 | 118.23 | 111.50 |
| 24 | B | 608 | CLA | CHC-C1C-NC | 3.12 | 128.94 | 124.20 |
| 24 | c | 507 | CLA | C4-C3-C5 | 3.12 | 120.52 | 115.27 |
| 27 | D | 405 | PL9 | C26-C24-C23 | -3.12 | 114.80 | 121.12 |
| 24 | D | 404 | CLA | CHC-C1C-NC | 3.12 | 128.94 | 124.20 |
| 32 | C | 516 | DGD | O2G-C1B-C2B | 3.12 | 118.22 | 111.50 |
| 24 | C | 506 | CLA | C4-C3-C5 | 3.12 | 120.52 | 115.27 |
| 24 | D | 403 | CLA | CMC-C2C-C1C | 3.12 | 129.79 | 125.04 |
| 24 | b | 603 | CLA | C1B-CHB-C4A | -3.12 | 123.94 | 130.12 |
| 24 | b | 612 | CLA | O2D-CGD-O1D | -3.11 | 117.75 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 29 | B | 621 | LMG | C6-C5-C4 | -3.11 | 105.72 | 113.00 |
| 28 | X | 101 | SQD | O9-S-C6 | 3.10 | 110.63 | 106.94 |
| 24 | b | 608[A] | CLA | CHC-C1C-NC | 3.10 | 128.91 | 124.20 |
| 24 | B | 609 | CLA | O1D-CGD-CBD | -3.10 | 118.14 | 124.48 |
| 24 | b | 607 | CLA | C1B-CHB-C4A | -3.10 | 123.98 | 130.12 |
| 24 | c | 501 | CLA | C4A-NA-C1A | -3.10 | 105.31 | 106.71 |
| 26 | H | 101 | BCR | C8-C9-C10 | -3.10 | 114.19 | 118.94 |
| 24 | B | 613 | CLA | C2A-C1A-CHA | 3.09 | 129.27 | 123.86 |
| 29 | b | 622 | LMG | O7-C10-C11 | 3.09 | 118.17 | 111.50 |
| 24 | c | 506 | CLA | C4-C3-C5 | 3.09 | 120.47 | 115.27 |
| 24 | C | 504 | CLA | CMB-C2B-C1B | -3.09 | 123.72 | 128.46 |
| 24 | d | 403 | CLA | CHA-C1A-NA | -3.09 | 119.33 | 126.40 |
| 24 | b | 607 | CLA | CHC-C1C-NC | 3.08 | 128.88 | 124.20 |
| 26 | f | 101 | BCR | C36-C18-C19 | 3.08 | 122.93 | 118.08 |
| 28 | x | 101 | SQD | O9-S-C6 | 3.08 | 110.60 | 106.94 |
| 26 | H | 101 | BCR | C35-C13-C14 | -3.08 | 118.61 | 122.92 |
| 24 | B | 612 | CLA | C2A-C1A-CHA | 3.08 | 129.24 | 123.86 |
| 24 | A | 606 | CLA | O2A-CGA-CBA | 3.08 | 121.56 | 111.91 |
| 26 | f | 101 | BCR | C34-C9-C10 | -3.08 | 118.61 | 122.92 |
| 24 | C | 507 | CLA | O2A-CGA-CBA | 3.08 | 121.56 | 111.91 |
| 27 | a | 611 | PL9 | C53-C6-C1 | 3.08 | 121.28 | 114.99 |
| 24 | B | 608 | CLA | O2D-CGD-CBD | 3.07 | 116.73 | 111.27 |
| 27 | d | 404 | PL9 | C7-C3-C4 | 3.07 | 119.37 | 116.88 |
| 26 | I | 101 | BCR | C15-C14-C13 | -3.07 | 122.93 | 127.31 |
| 24 | b | 617 | CLA | C2A-C1A-CHA | 3.07 | 129.22 | 123.86 |
| 24 | b | 614 | CLA | CHA-C1A-NA | -3.07 | 119.37 | 126.40 |
| 24 | c | 510 | CLA | C1B-CHB-C4A | -3.07 | 124.04 | 130.12 |
| 24 | B | 604 | CLA | O2D-CGD-O1D | -3.07 | 117.84 | 123.84 |
| 28 | A | 614 | SQD | O6-C1-C2 | 3.06 | 113.09 | 108.30 |
| 29 | b | 622 | LMG | C6-C5-C4 | -3.06 | 105.83 | 113.00 |
| 24 | b | 610 | CLA | C4A-NA-C1A | -3.06 | 105.33 | 106.71 |
| 24 | a | 615 | CLA | O1D-CGD-CBD | -3.06 | 118.22 | 124.48 |
| 24 | B | 612 | CLA | CHA-C1A-NA | -3.06 | 119.39 | 126.40 |
| 26 | H | 101 | BCR | C10-C11-C12 | -3.06 | 113.67 | 123.22 |
| 32 | E | 101 | DGD | C3E-C4E-C5E | 3.06 | 115.69 | 110.24 |
| 24 | A | 606 | CLA | CMB-C2B-C1B | -3.06 | 123.77 | 128.46 |
| 24 | C | 513 | CLA | CMB-C2B-C3B | 3.05 | 130.39 | 124.68 |
| 27 | D | 405 | PL9 | C36-C34-C33 | -3.05 | 114.94 | 121.12 |
| 24 | b | 613 | CLA | C1-O2A-CGA | 3.05 | 124.45 | 116.44 |
| 24 | B | 617 | CLA | O2A-CGA-CBA | 3.05 | 121.48 | 111.91 |
| 24 | c | 507 | CLA | O2D-CGD-O1D | -3.05 | 117.88 | 123.84 |
| 24 | B | 604 | CLA | CHC-C1C-NC | 3.05 | 128.83 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 606 | CLA | CMB-C2B-C1B | -3.05 | 123.78 | 128.46 |
| 26 | b | 620 | BCR | C34-C9-C10 | -3.05 | 118.65 | 122.92 |
| 26 | B | 620 | BCR | C23-C24-C25 | -3.05 | 118.65 | 127.20 |
| 24 | B | 611 | CLA | CHC-C1C-NC | 3.05 | 128.82 | 124.20 |
| 24 | C | 507 | CLA | C4-C3-C5 | 3.04 | 120.39 | 115.27 |
| 24 | B | 612 | CLA | O1D-CGD-CBD | -3.04 | 118.26 | 124.48 |
| 24 | C | 504 | CLA | C4-C3-C5 | 3.04 | 120.38 | 115.27 |
| 26 | A | 610 | BCR | C27-C26-C25 | -3.04 | 118.32 | 122.73 |
| 26 | F | 101 | BCR | C12-C13-C14 | -3.03 | 114.29 | 118.94 |
| 32 | c | 517 | DGD | O6D-C5D-C4D | -3.03 | 104.19 | 109.69 |
| 24 | a | 606 | CLA | C1B-CHB-C4A | -3.03 | 124.12 | 130.12 |
| 24 | B | 609 | CLA | CMB-C2B-C1B | -3.03 | 123.81 | 128.46 |
| 27 | a | 611 | PL9 | C51-C49-C48 | -3.03 | 113.90 | 122.65 |
| 24 | b | 603 | CLA | CHA-C1A-NA | -3.03 | 119.47 | 126.40 |
| 24 | B | 604 | CLA | C4-C3-C5 | 3.03 | 120.36 | 115.27 |
| 24 | A | 609 | CLA | C4A-NA-C1A | -3.03 | 105.35 | 106.71 |
| 24 | b | 605 | CLA | C4-C3-C5 | 3.02 | 120.36 | 115.27 |
| 26 | c | 515 | BCR | C36-C18-C17 | -3.02 | 118.69 | 122.92 |
| 26 | c | 521 | BCR | C33-C5-C4 | -3.02 | 107.81 | 113.62 |
| 26 | c | 514 | BCR | C3-C4-C5 | -3.02 | 108.69 | 114.08 |
| 24 | B | 611 | CLA | O2A-CGA-CBA | 3.02 | 121.38 | 111.91 |
| 24 | b | 618 | CLA | C2A-C1A-CHA | 3.02 | 129.13 | 123.86 |
| 24 | B | 609 | CLA | CAC-C3C-C2C | -3.01 | 122.37 | 127.53 |
| 24 | a | 609 | CLA | C1-O2A-CGA | 3.01 | 124.35 | 116.44 |
| 24 | b | 612 | CLA | O2A-CGA-CBA | 3.01 | 121.36 | 111.91 |
| 32 | c | 517 | DGD | O1G-C1A-C2A | 3.01 | 121.34 | 111.91 |
| 24 | c | 504 | CLA | C4-C3-C5 | 3.00 | 120.33 | 115.27 |
| 30 | A | 615 | LHG | O8-C23-O10 | -3.00 | 116.01 | 123.59 |
| 24 | C | 503 | CLA | CHC-C1C-NC | 3.00 | 128.76 | 124.20 |
| 33 | e | 102 | HEM | C1D-C2D-C3D | -3.00 | 104.91 | 107.00 |
| 24 | c | 506 | CLA | C4A-NA-C1A | -2.99 | 105.36 | 106.71 |
| 24 | B | 611 | CLA | O2D-CGD-CBD | 2.99 | 116.58 | 111.27 |
| 24 | B | 617 | CLA | CHC-C1C-C2C | -2.99 | 118.45 | 126.72 |
| 29 | Z | 101 | LMG | O2-C2-C3 | -2.99 | 103.44 | 110.35 |
| 24 | C | 510 | CLA | CHA-C1A-NA | -2.99 | 119.56 | 126.40 |
| 26 | t | 101 | BCR | C20-C21-C22 | -2.99 | 123.05 | 127.31 |
| 24 | C | 505 | CLA | CHC-C1C-NC | 2.99 | 128.73 | 124.20 |
| 26 | c | 515 | BCR | C24-C25-C26 | -2.99 | 114.23 | 121.46 |
| 24 | C | 511 | CLA | C1-O2A-CGA | 2.98 | 124.27 | 116.44 |
| 30 | A | 615 | LHG | C5-O7-C7 | -2.98 | 110.45 | 117.79 |
| 24 | c | 502 | CLA | O1D-CGD-CBD | -2.98 | 118.39 | 124.48 |
| 24 | B | 612 | CLA | CHC-C1C-NC | 2.98 | 128.72 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | b | 608[A] | CLA | C1B-CHB-C4A | -2.98 | 124.22 | 130.12 |
| 26 | a | 610 | BCR | C33-C5-C4 | -2.98 | 107.90 | 113.62 |
| 26 | c | 514 | BCR | C31-C1-C6 | -2.97 | 105.48 | 110.30 |
| 25 | A | 608 | PHO | CMD-C2D-C1D | 2.97 | 129.64 | 125.06 |
| 24 | c | 505 | CLA | O2A-C1-C2 | 2.97 | 116.44 | 108.64 |
| 24 | C | 506 | CLA | CHC-C1C-NC | 2.96 | 128.70 | 124.20 |
| 24 | C | 504 | CLA | CHC-C1C-NC | 2.96 | 128.70 | 124.20 |
| 24 | d | 402 | CLA | C3C-C4C-NC | -2.96 | 107.25 | 110.57 |
| 26 | t | 101 | BCR | C2-C1-C6 | 2.96 | 115.04 | 110.48 |
| 24 | D | 403 | CLA | O2A-CGA-CBA | 2.96 | 121.19 | 111.91 |
| 24 | b | 613 | CLA | CHA-C1A-NA | -2.96 | 119.63 | 126.40 |
| 24 | b | 608[B] | CLA | C1B-CHB-C4A | -2.96 | 124.26 | 130.12 |
| 26 | b | 620 | BCR | C35-C13-C14 | -2.96 | 118.78 | 122.92 |
| 24 | d | 403 | CLA | C1B-CHB-C4A | -2.96 | 124.26 | 130.12 |
| 24 | B | 607[B] | CLA | C1-O2A-CGA | 2.96 | 124.20 | 116.44 |
| 24 | a | 615 | CLA | CHC-C1C-C2C | -2.95 | 118.55 | 126.72 |
| 30 | D | 406 | LHG | O7-C7-C8 | 2.95 | 117.86 | 111.50 |
| 26 | t | 101 | BCR | C36-C18-C17 | -2.95 | 118.79 | 122.92 |
| 24 | A | 607 | CLA | CHA-C1A-NA | -2.95 | 119.64 | 126.40 |
| 24 | a | 606 | CLA | CHA-C1A-NA | -2.95 | 119.65 | 126.40 |
| 26 | B | 620 | BCR | C1-C6-C7 | -2.95 | 107.44 | 115.78 |
| 24 | b | 605 | CLA | CHA-C1A-NA | -2.95 | 119.65 | 126.40 |
| 24 | B | 608 | CLA | C1-C2-C3 | -2.94 | 120.95 | 126.04 |
| 24 | A | 609 | CLA | CMB-C2B-C1B | -2.94 | 123.94 | 128.46 |
| 28 | a | 614 | SQD | O48-C23-C24 | 2.94 | 121.13 | 111.91 |
| 24 | B | 607[B] | CLA | C4-C3-C5 | 2.94 | 120.21 | 115.27 |
| 28 | X | 101 | SQD | O48-C23-C24 | 2.94 | 121.12 | 111.91 |
| 24 | b | 610 | CLA | CHC-C1C-NC | 2.94 | 128.66 | 124.20 |
| 26 | H | 101 | BCR | C33-C5-C4 | -2.94 | 107.98 | 113.62 |
| 24 | B | 613 | CLA | CMD-C2D-C3D | 2.93 | 130.17 | 124.68 |
| 28 | x | 101 | SQD | O48-C23-C24 | 2.93 | 121.11 | 111.91 |
| 25 | d | 401 | PHO | CMB-C2B-C1B | -2.93 | 120.55 | 125.06 |
| 24 | b | 608[B] | CLA | C4-C3-C5 | 2.93 | 120.20 | 115.27 |
| 29 | C | 518 | LMG | C4-C3-C2 | 2.93 | 115.94 | 110.82 |
| 32 | C | 516 | DGD | C1D-O6D-C5D | -2.92 | 107.95 | 113.69 |
| 24 | B | 613 | CLA | CHC-C1C-NC | 2.92 | 128.64 | 124.20 |
| 27 | a | 611 | PL9 | C25-C24-C26 | -2.92 | 110.36 | 115.27 |
| 25 | D | 401 | PHO | C1-C2-C3 | -2.92 | 120.99 | 126.04 |
| 28 | A | 614 | SQD | O48-C23-C24 | 2.92 | 121.08 | 111.91 |
| 24 | B | 607[A] | CLA | C4-C3-C5 | 2.92 | 120.18 | 115.27 |
| 32 | C | 516 | DGD | C4E-C3E-C2E | 2.92 | 115.92 | 110.82 |
| 24 | A | 609 | CLA | O1D-CGD-CBD | -2.92 | 118.51 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | a | 610 | BCR | C23-C24-C25 | -2.92 | 119.01 | 127.20 |
| 26 | F | 101 | BCR | C37-C22-C23 | -2.91 | 113.49 | 118.08 |
| 24 | B | 608 | CLA | C1B-CHB-C4A | -2.91 | 124.35 | 130.12 |
| 33 | v | 201 | HEM | C1D-C2D-C3D | -2.91 | 104.97 | 107.00 |
| 24 | c | 502 | CLA | CED-O2D-CGD | 2.91 | 122.52 | 115.94 |
| 32 | C | 516 | DGD | O6E-C5E-C6E | 2.91 | 113.67 | 106.44 |
| 32 | c | 516 | DGD | O6D-C5D-C4D | -2.91 | 104.41 | 109.69 |
| 24 | C | 505 | CLA | O1D-CGD-CBD | -2.91 | 118.53 | 124.48 |
| 24 | b | 609 | CLA | CHC-C1C-NC | 2.91 | 128.62 | 124.20 |
| 26 | H | 101 | BCR | C34-C9-C8 | 2.91 | 122.66 | 118.08 |
| 24 | b | 616 | CLA | CHC-C1C-NC | 2.91 | 128.61 | 124.20 |
| 26 | A | 610 | BCR | C20-C19-C18 | -2.91 | 118.25 | 126.42 |
| 27 | d | 404 | PL9 | C45-C44-C46 | -2.91 | 110.38 | 115.27 |
| 24 | a | 609 | CLA | CMB-C2B-C1B | -2.90 | 124.00 | 128.46 |
| 24 | b | 609 | CLA | C1-C2-C3 | -2.90 | 121.02 | 126.04 |
| 24 | c | 507 | CLA | O2A-CGA-CBA | 2.90 | 121.02 | 111.91 |
| 24 | B | 616 | CLA | O2A-CGA-CBA | 2.90 | 121.02 | 111.91 |
| 24 | B | 611 | CLA | CMD-C2D-C3D | 2.90 | 130.10 | 124.68 |
| 24 | b | 608[A] | CLA | C1-O2A-CGA | 2.90 | 124.05 | 116.44 |
| 25 | d | 401 | PHO | C1-C2-C3 | -2.90 | 121.03 | 126.04 |
| 26 | c | 514 | BCR | C19-C18-C17 | 2.89 | 123.38 | 118.94 |
| 29 | C | 518 | LMG | O6-C5-C4 | 2.89 | 114.93 | 109.69 |
| 24 | b | 608[A] | CLA | O1D-CGD-CBD | -2.88 | 118.58 | 124.48 |
| 26 | K | 101 | BCR | C24-C25-C26 | -2.88 | 114.48 | 121.46 |
| 24 | B | 611 | CLA | CED-O2D-CGD | 2.88 | 122.45 | 115.94 |
| 24 | b | 608[A] | CLA | C4-C3-C5 | 2.88 | 120.11 | 115.27 |
| 24 | c | 506 | CLA | CHC-C1C-NC | 2.88 | 128.57 | 124.20 |
| 24 | a | 615 | CLA | C4-C3-C5 | 2.87 | 120.11 | 115.27 |
| 24 | D | 403 | CLA | O2D-CGD-CBD | 2.87 | 116.37 | 111.27 |
| 24 | B | 612 | CLA | C1-C2-C3 | -2.87 | 121.08 | 126.04 |
| 24 | D | 402 | CLA | C4A-NA-C1A | -2.87 | 105.42 | 106.71 |
| 24 | B | 617 | CLA | C2A-C1A-CHA | 2.87 | 128.88 | 123.86 |
| 24 | b | 614 | CLA | O2A-CGA-CBA | 2.87 | 120.90 | 111.91 |
| 24 | c | 512 | CLA | O2D-CGD-O1D | -2.87 | 118.24 | 123.84 |
| 24 | b | 606 | CLA | CHA-C1A-NA | -2.86 | 119.84 | 126.40 |
| 24 | A | 607 | CLA | CMB-C2B-C1B | -2.86 | 124.06 | 128.46 |
| 28 | A | 612 | SQD | C45-O47-C7 | -2.86 | 110.75 | 117.79 |
| 24 | A | 606 | CLA | CHA-C1A-NA | -2.86 | 119.84 | 126.40 |
| 24 | C | 505 | CLA | C1-O2A-CGA | 2.86 | 123.95 | 116.44 |
| 28 | a | 612 | SQD | C45-O47-C7 | -2.86 | 110.76 | 117.79 |
| 29 | c | 519 | LMG | O8-C28-C29 | 2.85 | 120.86 | 111.91 |
| 26 | B | 618 | BCR | C29-C30-C25 | 2.85 | 114.86 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 608 | CLA | C4-C3-C5 | 2.85 | 120.06 | 115.27 |
| 24 | b | 613 | CLA | C1-C2-C3 | -2.85 | 121.12 | 126.04 |
| 29 | c | 520 | LMG | O8-C28-C29 | 2.84 | 120.83 | 111.91 |
| 24 | b | 605 | CLA | C1B-CHB-C4A | -2.84 | 124.48 | 130.12 |
| 24 | a | 606 | CLA | CHB-C4A-NA | -2.84 | 120.58 | 124.51 |
| 24 | D | 402 | CLA | C4-C3-C5 | 2.84 | 120.05 | 115.27 |
| 26 | c | 514 | BCR | C10-C11-C12 | -2.84 | 114.35 | 123.22 |
| 24 | b | 612 | CLA | CHC-C1C-NC | 2.84 | 128.51 | 124.20 |
| 26 | B | 620 | BCR | C1-C6-C5 | -2.84 | 118.62 | 122.61 |
| 24 | b | 612 | CLA | O1D-CGD-CBD | -2.83 | 118.69 | 124.48 |
| 24 | B | 609 | CLA | C4A-NA-C1A | -2.83 | 105.43 | 106.71 |
| 26 | H | 101 | BCR | C20-C19-C18 | -2.83 | 118.46 | 126.42 |
| 24 | c | 501 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 26 | b | 619 | BCR | C2-C3-C4 | 2.83 | 117.70 | 111.38 |
| 24 | D | 403 | CLA | CHB-C4A-NA | -2.83 | 120.60 | 124.51 |
| 24 | b | 615 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 24 | b | 618 | CLA | CHC-C1C-C2C | -2.83 | 118.90 | 126.72 |
| 24 | c | 513 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 24 | c | 512 | CLA | O2A-CGA-CBA | 2.83 | 120.77 | 111.91 |
| 24 | a | 609 | CLA | CHC-C1C-NC | 2.82 | 128.49 | 124.20 |
| 24 | B | 614 | CLA | CHC-C1C-C2C | -2.82 | 118.91 | 126.72 |
| 24 | C | 502 | CLA | CMB-C2B-C1B | -2.82 | 124.13 | 128.46 |
| 32 | h | 102 | DGD | C4D-C3D-C2D | 2.82 | 115.75 | 110.82 |
| 24 | b | 609 | CLA | C4-C3-C5 | 2.82 | 120.02 | 115.27 |
| 33 | v | 201 | HEM | CBA-CAA-C2A | -2.82 | 107.28 | 112.49 |
| 32 | C | 517 | DGD | C3G-C2G-C1G | -2.82 | 105.12 | 111.79 |
| 24 | B | 611 | CLA | CMA-C3A-C4A | -2.81 | 104.22 | 111.77 |
| 32 | E | 101 | DGD | C1E-C2E-C3E | 2.81 | 115.84 | 110.00 |
| 24 | c | 505 | CLA | CHC-C1C-NC | 2.81 | 128.46 | 124.20 |
| 24 | d | 403 | CLA | O2A-CGA-CBA | 2.81 | 120.72 | 111.91 |
| 24 | b | 611 | CLA | CHC-C1C-NC | 2.81 | 128.46 | 124.20 |
| 24 | b | 613 | CLA | CHC-C1C-C2C | -2.80 | 118.96 | 126.72 |
| 24 | b | 611 | CLA | O2A-CGA-CBA | 2.80 | 120.70 | 111.91 |
| 26 | k | 101 | BCR | C35-C13-C14 | -2.80 | 119.00 | 122.92 |
| 24 | c | 501 | CLA | O2A-CGA-CBA | 2.80 | 120.70 | 111.91 |
| 28 | a | 612 | SQD | C44-O6-C1 | -2.80 | 108.27 | 113.74 |
| 26 | C | 514 | BCR | C37-C22-C21 | -2.80 | 119.00 | 122.92 |
| 24 | D | 402 | CLA | CMB-C2B-C1B | -2.80 | 124.17 | 128.46 |
| 24 | b | 615 | CLA | C1B-CHB-C4A | -2.80 | 124.58 | 130.12 |
| 26 | B | 618 | BCR | C30-C25-C24 | -2.79 | 107.88 | 115.78 |
| 28 | l | 101 | SQD | C1-O5-C5 | -2.79 | 108.21 | 113.69 |
| 24 | b | 606 | CLA | CED-O2D-CGD | 2.79 | 122.24 | 115.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | f | 101 | BCR | C19-C18-C17 | 2.78 | 123.21 | 118.94 |
| 28 | L | 102 | SQD | C1-O5-C5 | -2.78 | 108.22 | 113.69 |
| 26 | b | 621 | BCR | C23-C24-C25 | -2.78 | 119.39 | 127.20 |
| 28 | A | 612 | SQD | C44-O6-C1 | -2.78 | 108.31 | 113.74 |
| 27 | d | 404 | PL9 | C30-C29-C31 | -2.78 | 110.60 | 115.27 |
| 24 | b | 605 | CLA | C1-O2A-CGA | 2.78 | 123.73 | 116.44 |
| 24 | d | 402 | CLA | O2D-CGD-O1D | -2.78 | 118.41 | 123.84 |
| 26 | I | 101 | BCR | C1-C6-C7 | -2.78 | 107.93 | 115.78 |
| 24 | b | 605 | CLA | CED-O2D-CGD | 2.77 | 122.20 | 115.94 |
| 30 | D | 406 | LHG | O8-C23-C24 | 2.77 | 120.58 | 111.91 |
| 24 | b | 606 | CLA | C4-C3-C5 | 2.76 | 119.92 | 115.27 |
| 24 | B | 609 | CLA | C1D-CHD-C4C | 2.76 | 126.20 | 122.56 |
| 24 | C | 508 | CLA | C4-C3-C5 | 2.76 | 119.92 | 115.27 |
| 24 | c | 507 | CLA | CHC-C1C-C2C | -2.76 | 119.09 | 126.72 |
| 24 | c | 508 | CLA | C4-C3-C5 | 2.76 | 119.91 | 115.27 |
| 24 | b | 608[B] | CLA | C1-O2A-CGA | 2.76 | 123.68 | 116.44 |
| 24 | C | 512 | CLA | C1B-CHB-C4A | -2.76 | 124.66 | 130.12 |
| 24 | C | 511 | CLA | CMB-C2B-C1B | -2.75 | 124.23 | 128.46 |
| 25 | a | 608 | PHO | C1-C2-C3 | -2.75 | 121.29 | 126.04 |
| 24 | C | 513 | CLA | O2A-CGA-CBA | 2.75 | 120.53 | 111.91 |
| 24 | b | 611 | CLA | CED-O2D-CGD | 2.75 | 122.15 | 115.94 |
| 24 | b | 613 | CLA | C1B-CHB-C4A | -2.75 | 124.68 | 130.12 |
| 24 | C | 506 | CLA | CHB-C4A-NA | -2.75 | 120.72 | 124.51 |
| 24 | B | 614 | CLA | C4A-NA-C1A | -2.74 | 105.47 | 106.71 |
| 33 | v | 201 | HEM | CAA-CBA-CGA | -2.74 | 108.07 | 112.67 |
| 24 | B | 605 | CLA | C4-C3-C5 | 2.74 | 119.89 | 115.27 |
| 24 | c | 513 | CLA | CHC-C1C-NC | 2.74 | 128.36 | 124.20 |
| 27 | A | 611 | PL9 | C53-C6-C1 | 2.74 | 120.59 | 114.99 |
| 24 | B | 608 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 24 | c | 509 | CLA | CMB-C2B-C1B | -2.74 | 124.26 | 128.46 |
| 28 | B | 622 | SQD | O48-C23-C24 | 2.74 | 120.50 | 111.91 |
| 24 | C | 502 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 27 | D | 405 | PL9 | C40-C39-C41 | -2.73 | 110.68 | 115.27 |
| 26 | b | 620 | BCR | C10-C11-C12 | -2.73 | 114.71 | 123.22 |
| 24 | c | 513 | CLA | C4A-NA-C1A | -2.72 | 105.48 | 106.71 |
| 28 | b | 601 | SQD | O48-C23-C24 | 2.72 | 120.44 | 111.91 |
| 30 | E | 102 | LHG | O8-C23-C24 | 2.72 | 120.44 | 111.91 |
| 30 | I | 102 | LHG | O8-C23-C24 | 2.72 | 120.44 | 111.91 |
| 24 | C | 511 | CLA | O1D-CGD-CBD | -2.72 | 118.93 | 124.48 |
| 24 | b | 610 | CLA | CMB-C2B-C3B | 2.72 | 129.76 | 124.68 |
| 30 | D | 406 | LHG | C5-O7-C7 | -2.71 | 111.11 | 117.79 |
| 28 | L | 102 | SQD | O48-C23-C24 | 2.71 | 120.42 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | H | 101 | BCR | C19-C18-C17 | 2.71 | 123.10 | 118.94 |
| 26 | T | 101 | BCR | C1-C6-C5 | -2.71 | 118.80 | 122.61 |
| 28 | l | 101 | SQD | O48-C23-C24 | 2.71 | 120.41 | 111.91 |
| 24 | c | 509 | CLA | CED-O2D-CGD | 2.71 | 122.06 | 115.94 |
| 29 | b | 622 | LMG | O8-C28-C29 | 2.71 | 120.40 | 111.91 |
| 24 | C | 504 | CLA | CED-O2D-CGD | 2.71 | 122.06 | 115.94 |
| 24 | D | 403 | CLA | CMB-C2B-C1B | -2.71 | 124.31 | 128.46 |
| 26 | A | 610 | BCR | C24-C25-C26 | -2.70 | 114.91 | 121.46 |
| 26 | h | 101 | BCR | C11-C12-C13 | -2.70 | 118.82 | 126.42 |
| 24 | c | 504 | CLA | CMB-C2B-C1B | -2.70 | 124.31 | 128.46 |
| 24 | b | 612 | CLA | CHB-C4A-NA | -2.70 | 120.78 | 124.51 |
| 24 | b | 618 | CLA | CHA-C1A-NA | -2.70 | 120.21 | 126.40 |
| 24 | D | 403 | CLA | CHA-C1A-NA | -2.70 | 120.21 | 126.40 |
| 26 | b | 621 | BCR | C34-C9-C10 | -2.70 | 119.14 | 122.92 |
| 24 | C | 512 | CLA | O2A-CGA-CBA | 2.70 | 120.37 | 111.91 |
| 24 | c | 503 | CLA | C4-C3-C5 | 2.69 | 119.80 | 115.27 |
| 24 | D | 403 | CLA | C4-C3-C5 | 2.69 | 119.80 | 115.27 |
| 26 | I | 101 | BCR | C24-C25-C26 | -2.69 | 114.94 | 121.46 |
| 26 | B | 618 | BCR | C36-C18-C19 | 2.69 | 122.32 | 118.08 |
| 28 | L | 102 | SQD | O8-S-C6 | 2.69 | 110.03 | 105.74 |
| 28 | b | 601 | SQD | O9-S-C6 | 2.69 | 110.14 | 106.94 |
| 24 | D | 402 | CLA | O2D-CGD-O1D | -2.69 | 118.58 | 123.84 |
| 30 | e | 101 | LHG | O8-C23-C24 | 2.69 | 120.35 | 111.91 |
| 26 | K | 101 | BCR | C35-C13-C12 | 2.69 | 122.31 | 118.08 |
| 24 | c | 503 | CLA | CHC-C1C-NC | 2.69 | 128.28 | 124.20 |
| 24 | c | 512 | CLA | CHA-C1A-NA | -2.69 | 120.24 | 126.40 |
| 25 | d | 401 | PHO | O2D-CGD-O1D | -2.69 | 118.58 | 123.84 |
| 24 | a | 607 | CLA | O2D-CGD-CBD | 2.69 | 116.04 | 111.27 |
| 24 | a | 606 | CLA | O2A-CGA-CBA | 2.69 | 120.34 | 111.91 |
| 24 | b | 616 | CLA | CMB-C2B-C3B | 2.69 | 129.70 | 124.68 |
| 28 | b | 601 | SQD | C4-C3-C2 | 2.68 | 115.50 | 110.82 |
| 26 | K | 102 | BCR | C16-C15-C14 | -2.68 | 117.98 | 123.47 |
| 24 | b | 603 | CLA | O1D-CGD-CBD | -2.68 | 119.00 | 124.48 |
| 30 | d | 406 | LHG | O8-C23-C24 | 2.68 | 120.32 | 111.91 |
| 24 | c | 511 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 28 | B | 622 | SQD | O9-S-C6 | 2.68 | 110.12 | 106.94 |
| 32 | c | 518 | DGD | C3G-O3G-C1D | -2.68 | 108.51 | 113.74 |
| 29 | c | 520 | LMG | C3-C4-C5 | 2.67 | 115.01 | 110.24 |
| 28 | B | 622 | SQD | C4-C3-C2 | 2.67 | 115.49 | 110.82 |
| 24 | A | 606 | CLA | CHC-C1C-C2C | -2.67 | 119.33 | 126.72 |
| 24 | d | 402 | CLA | C4-C3-C5 | 2.67 | 119.76 | 115.27 |
| 24 | b | 607 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | C | 508 | CLA | CED-O2D-CGD | 2.67 | 121.97 | 115.94 |
| 24 | B | 607[A] | CLA | O1D-CGD-CBD | -2.67 | 119.03 | 124.48 |
| 24 | b | 618 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 24 | c | 511 | CLA | O2A-CGA-CBA | 2.67 | 120.28 | 111.91 |
| 24 | B | 608 | CLA | CMB-C2B-C1B | -2.67 | 124.37 | 128.46 |
| 24 | b | 603 | CLA | O2A-CGA-CBA | 2.66 | 120.27 | 111.91 |
| 28 | l | 101 | SQD | O8-S-C6 | 2.66 | 109.98 | 105.74 |
| 24 | C | 503 | CLA | C4-C3-C5 | 2.66 | 119.75 | 115.27 |
| 26 | c | 515 | BCR | C1-C6-C7 | -2.66 | 108.24 | 115.78 |
| 26 | I | 101 | BCR | C8-C9-C10 | 2.66 | 123.03 | 118.94 |
| 32 | c | 518 | DGD | C2G-O2G-C1B | -2.66 | 111.24 | 117.79 |
| 24 | b | 608[B] | CLA | C1-C2-C3 | -2.66 | 121.45 | 126.04 |
| 24 | A | 606 | CLA | O2D-CGD-O1D | -2.66 | 118.65 | 123.84 |
| 26 | b | 619 | BCR | C36-C18-C19 | 2.66 | 122.26 | 118.08 |
| 24 | c | 510 | CLA | CMB-C2B-C1B | -2.66 | 124.38 | 128.46 |
| 24 | C | 513 | CLA | CHA-C1A-NA | -2.65 | 120.32 | 126.40 |
| 32 | E | 101 | DGD | O1G-C1A-C2A | 2.65 | 120.23 | 111.91 |
| 24 | b | 608[B] | CLA | O1D-CGD-CBD | -2.65 | 119.06 | 124.48 |
| 25 | A | 608 | PHO | O2D-CGD-O1D | -2.65 | 118.66 | 123.84 |
| 24 | d | 402 | CLA | O2A-CGA-CBA | 2.65 | 120.21 | 111.91 |
| 24 | B | 607[B] | CLA | C1-C2-C3 | -2.65 | 121.47 | 126.04 |
| 26 | b | 619 | BCR | C33-C5-C4 | -2.65 | 108.53 | 113.62 |
| 26 | C | 514 | BCR | C12-C13-C14 | -2.65 | 114.88 | 118.94 |
| 30 | D | 407 | LHG | O8-C23-C24 | 2.64 | 120.20 | 111.91 |
| 24 | C | 509 | CLA | O1D-CGD-CBD | -2.64 | 119.08 | 124.48 |
| 27 | d | 404 | PL9 | C15-C14-C16 | -2.64 | 110.83 | 115.27 |
| 24 | B | 611 | CLA | O2A-CGA-O1A | -2.64 | 116.93 | 123.59 |
| 24 | c | 512 | CLA | C1B-CHB-C4A | -2.64 | 124.89 | 130.12 |
| 24 | a | 615 | CLA | CMB-C2B-C3B | 2.64 | 129.62 | 124.68 |
| 30 | d | 407 | LHG | C5-O7-C7 | -2.64 | 111.30 | 117.79 |
| 26 | c | 521 | BCR | C7-C8-C9 | -2.64 | 122.25 | 126.23 |
| 33 | v | 201 | HEM | CMB-C2B-C3B | 2.63 | 129.61 | 124.68 |
| 24 | C | 513 | CLA | CED-O2D-CGD | 2.63 | 121.89 | 115.94 |
| 24 | b | 608[A] | CLA | CHA-C1A-NA | -2.63 | 120.37 | 126.40 |
| 24 | c | 509 | CLA | O2A-CGA-CBA | 2.63 | 120.16 | 111.91 |
| 24 | B | 606 | CLA | CED-O2D-CGD | 2.63 | 121.88 | 115.94 |
| 26 | c | 514 | BCR | C29-C30-C25 | 2.63 | 114.53 | 110.48 |
| 24 | C | 513 | CLA | CHC-C1C-NC | 2.62 | 128.18 | 124.20 |
| 24 | C | 511 | CLA | CED-O2D-CGD | 2.62 | 121.87 | 115.94 |
| 26 | t | 101 | BCR | C30-C25-C24 | -2.62 | 108.36 | 115.78 |
| 24 | c | 502 | CLA | C4-C3-C5 | 2.62 | 119.68 | 115.27 |
| 24 | C | 508 | CLA | C4A-NA-C1A | -2.62 | 105.53 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | T | 101 | BCR | C20-C19-C18 | -2.62 | 119.06 | 126.42 |
| 24 | A | 607 | CLA | CHC-C1C-C2C | -2.62 | 119.48 | 126.72 |
| 32 | d | 405 | DGD | O1G-C1A-C2A | 2.62 | 120.13 | 111.91 |
| 26 | t | 101 | BCR | C29-C30-C25 | 2.62 | 114.51 | 110.48 |
| 26 | h | 101 | BCR | C30-C25-C24 | -2.62 | 108.37 | 115.78 |
| 24 | C | 509 | CLA | CHC-C1C-C2C | -2.62 | 119.48 | 126.72 |
| 24 | C | 501 | CLA | CHD-C4C-C3C | 2.61 | 128.68 | 124.84 |
| 24 | c | 506 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 24 | b | 615 | CLA | CHC-C1C-C2C | -2.61 | 119.50 | 126.72 |
| 24 | C | 511 | CLA | C4-C3-C5 | 2.61 | 119.66 | 115.27 |
| 26 | K | 101 | BCR | C16-C15-C14 | -2.61 | 118.13 | 123.47 |
| 32 | C | 517 | DGD | O2E-C2E-C3E | -2.61 | 104.31 | 110.35 |
| 24 | b | 605 | CLA | CHC-C1C-C2C | -2.61 | 119.50 | 126.72 |
| 25 | D | 401 | PHO | CMB-C2B-C1B | -2.61 | 121.05 | 125.06 |
| 24 | b | 609 | CLA | O1D-CGD-CBD | -2.61 | 119.15 | 124.48 |
| 27 | D | 405 | PL9 | C53-C6-C1 | 2.61 | 120.32 | 114.99 |
| 24 | b | 617 | CLA | C4-C3-C5 | 2.61 | 119.65 | 115.27 |
| 24 | a | 609 | CLA | O2A-CGA-CBA | 2.60 | 120.08 | 111.91 |
| 24 | C | 509 | CLA | CMB-C2B-C1B | -2.60 | 124.47 | 128.46 |
| 30 | D | 406 | LHG | O7-C7-O9 | -2.59 | 117.43 | 123.70 |
| 26 | B | 619 | BCR | C29-C30-C25 | 2.59 | 114.47 | 110.48 |
| 24 | B | 613 | CLA | O2A-CGA-CBA | 2.59 | 120.03 | 111.91 |
| 26 | t | 101 | BCR | C8-C9-C10 | -2.58 | 114.97 | 118.94 |
| 24 | B | 604 | CLA | O2A-CGA-CBA | 2.58 | 120.02 | 111.91 |
| 24 | c | 505 | CLA | O1D-CGD-CBD | -2.58 | 119.20 | 124.48 |
| 24 | B | 611 | CLA | O2A-C1-C2 | 2.58 | 115.42 | 108.64 |
| 26 | k | 101 | BCR | C36-C18-C17 | -2.58 | 119.31 | 122.92 |
| 24 | c | 511 | CLA | C4-C3-C5 | 2.58 | 119.61 | 115.27 |
| 24 | b | 618 | CLA | C1B-CHB-C4A | -2.58 | 125.00 | 130.12 |
| 24 | C | 502 | CLA | C4-C3-C5 | 2.58 | 119.61 | 115.27 |
| 24 | C | 509 | CLA | C1-O2A-CGA | 2.58 | 123.21 | 116.44 |
| 24 | B | 616 | CLA | C4-C3-C5 | 2.58 | 119.61 | 115.27 |
| 26 | c | 514 | BCR | C38-C26-C27 | -2.58 | 108.67 | 113.62 |
| 24 | C | 512 | CLA | CHC-C1C-C2C | -2.58 | 119.59 | 126.72 |
| 24 | c | 512 | CLA | C1-C2-C3 | -2.58 | 121.59 | 126.04 |
| 25 | a | 608 | PHO | O1D-CGD-CBD | 2.58 | 129.75 | 124.48 |
| 32 | h | 102 | DGD | O1G-C1A-C2A | 2.57 | 119.99 | 111.91 |
| 26 | B | 620 | BCR | C33-C5-C4 | -2.57 | 108.67 | 113.62 |
| 24 | B | 611 | CLA | C4-C3-C5 | 2.57 | 119.60 | 115.27 |
| 24 | B | 603 | CLA | C1-O2A-CGA | 2.57 | 123.19 | 116.44 |
| 24 | b | 615 | CLA | C4-C3-C5 | 2.57 | 119.60 | 115.27 |
| 26 | c | 521 | BCR | C19-C18-C17 | 2.57 | 122.88 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | a | 615 | CLA | O2A-CGA-O1A | -2.56 | 117.12 | 123.59 |
| 26 | F | 101 | BCR | C34-C9-C10 | -2.56 | 119.33 | 122.92 |
| 26 | B | 619 | BCR | C36-C18-C17 | -2.56 | 119.33 | 122.92 |
| 26 | c | 521 | BCR | C29-C28-C27 | 2.56 | 117.10 | 111.38 |
| 24 | b | 611 | CLA | CHB-C4A-NA | -2.56 | 120.97 | 124.51 |
| 24 | B | 610 | CLA | C1-O2A-CGA | 2.56 | 123.16 | 116.44 |
| 24 | B | 614 | CLA | C4-C3-C5 | 2.56 | 119.58 | 115.27 |
| 24 | c | 512 | CLA | C2A-C1A-CHA | 2.56 | 128.33 | 123.86 |
| 24 | B | 602 | CLA | O1D-CGD-CBD | -2.56 | 119.25 | 124.48 |
| 30 | a | 616 | LHG | O8-C23-C24 | 2.56 | 119.93 | 111.91 |
| 24 | b | 613 | CLA | CHB-C4A-NA | -2.56 | 120.98 | 124.51 |
| 24 | C | 502 | CLA | CHA-C1A-NA | -2.55 | 120.55 | 126.40 |
| 24 | b | 603 | CLA | CED-O2D-CGD | 2.55 | 121.71 | 115.94 |
| 24 | D | 403 | CLA | C2A-C1A-CHA | 2.55 | 128.32 | 123.86 |
| 32 | C | 515 | DGD | O6D-C5D-C6D | 2.55 | 111.81 | 106.67 |
| 26 | c | 515 | BCR | C30-C25-C24 | -2.55 | 108.57 | 115.78 |
| 28 | a | 614 | SQD | O8-S-C6 | 2.55 | 109.80 | 105.74 |
| 26 | c | 514 | BCR | C30-C25-C24 | -2.55 | 108.57 | 115.78 |
| 29 | c | 520 | LMG | O6-C5-C4 | 2.55 | 114.32 | 109.69 |
| 28 | A | 612 | SQD | C1-O5-C5 | -2.55 | 108.69 | 113.69 |
| 24 | D | 403 | CLA | OBD-CAD-CBD | 2.55 | 129.53 | 125.89 |
| 24 | c | 501 | CLA | CHA-C1A-NA | -2.54 | 120.57 | 126.40 |
| 24 | A | 609 | CLA | CED-O2D-CGD | 2.54 | 121.69 | 115.94 |
| 26 | C | 514 | BCR | C1-C6-C5 | -2.54 | 119.03 | 122.61 |
| 24 | D | 402 | CLA | O2A-CGA-CBA | 2.54 | 119.88 | 111.91 |
| 24 | C | 512 | CLA | C1-C2-C3 | -2.54 | 121.65 | 126.04 |
| 24 | b | 608[B] | CLA | CHA-C1A-NA | -2.54 | 120.58 | 126.40 |
| 24 | b | 618 | CLA | CHB-C4A-NA | -2.54 | 121.00 | 124.51 |
| 24 | b | 615 | CLA | O1D-CGD-CBD | -2.54 | 119.29 | 124.48 |
| 26 | a | 610 | BCR | C20-C19-C18 | -2.54 | 119.29 | 126.42 |
| 28 | A | 614 | SQD | O8-S-C6 | 2.53 | 109.78 | 105.74 |
| 32 | c | 517 | DGD | O3G-C1D-C2D | 2.53 | 112.26 | 108.30 |
| 24 | B | 602 | CLA | CHC-C1C-NC | 2.53 | 128.04 | 124.20 |
| 26 | B | 620 | BCR | C2-C1-C6 | 2.53 | 114.38 | 110.48 |
| 32 | c | 516 | DGD | C2G-O2G-C1B | -2.53 | 111.56 | 117.79 |
| 24 | C | 513 | CLA | C3C-C4C-NC | -2.53 | 107.73 | 110.57 |
| 33 | e | 102 | HEM | CMB-C2B-C3B | 2.53 | 129.41 | 124.68 |
| 32 | c | 517 | DGD | O6E-C5E-C6E | 2.53 | 112.72 | 106.44 |
| 29 | z | 101 | LMG | O2-C2-C3 | -2.53 | 104.51 | 110.35 |
| 24 | B | 609 | CLA | CHB-C4A-NA | -2.53 | 121.02 | 124.51 |
| 24 | C | 512 | CLA | O2D-CGD-O1D | -2.53 | 118.90 | 123.84 |
| 24 | d | 403 | CLA | C4-C3-C5 | 2.53 | 119.52 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | D | 404 | CLA | C4-C3-C5 | 2.52 | 119.52 | 115.27 |
| 24 | B | 615 | CLA | CHA-C1A-NA | -2.52 | 120.62 | 126.40 |
| 32 | c | 516 | DGD | O3G-C3G-C2G | -2.52 | 104.81 | 110.90 |
| 26 | T | 101 | BCR | C36-C18-C17 | -2.52 | 119.39 | 122.92 |
| 26 | t | 101 | BCR | C3-C4-C5 | -2.52 | 109.57 | 114.08 |
| 24 | b | 606 | CLA | O2A-CGA-CBA | 2.52 | 119.82 | 111.91 |
| 24 | B | 605 | CLA | C4A-NA-C1A | -2.52 | 105.57 | 106.71 |
| 24 | c | 510 | CLA | CHC-C1C-C2C | -2.52 | 119.76 | 126.72 |
| 24 | c | 502 | CLA | C1-O2A-CGA | 2.51 | 123.04 | 116.44 |
| 24 | C | 501 | CLA | O2D-CGD-O1D | -2.51 | 118.92 | 123.84 |
| 24 | B | 607[B] | CLA | CHC-C1C-C2C | -2.51 | 119.77 | 126.72 |
| 24 | c | 513 | CLA | CMD-C2D-C3D | 2.51 | 129.38 | 124.68 |
| 32 | E | 101 | DGD | C6D-C5D-C4D | -2.51 | 106.85 | 112.09 |
| 26 | I | 101 | BCR | C23-C22-C21 | -2.51 | 115.09 | 118.94 |
| 24 | c | 507 | CLA | CHA-C1A-NA | -2.51 | 120.66 | 126.40 |
| 24 | a | 606 | CLA | CHC-C1C-C2C | -2.50 | 119.80 | 126.72 |
| 24 | b | 612 | CLA | C4-C3-C5 | 2.50 | 119.48 | 115.27 |
| 32 | d | 405 | DGD | O2G-C1B-O1B | -2.50 | 117.66 | 123.70 |
| 28 | a | 612 | SQD | C1-O5-C5 | -2.50 | 108.78 | 113.69 |
| 24 | B | 616 | CLA | CHA-C1A-NA | -2.50 | 120.68 | 126.40 |
| 24 | c | 508 | CLA | CMD-C2D-C3D | 2.50 | 129.35 | 124.68 |
| 24 | b | 604 | CLA | CED-O2D-CGD | 2.50 | 121.58 | 115.94 |
| 24 | B | 607[B] | CLA | O1D-CGD-CBD | -2.50 | 119.38 | 124.48 |
| 24 | D | 402 | CLA | CHC-C1C-C2C | -2.49 | 119.82 | 126.72 |
| 24 | C | 511 | CLA | CHC-C1C-C2C | -2.49 | 119.82 | 126.72 |
| 24 | C | 504 | CLA | O1D-CGD-CBD | -2.49 | 119.38 | 124.48 |
| 24 | b | 612 | CLA | CHC-C1C-C2C | -2.49 | 119.83 | 126.72 |
| 24 | C | 501 | CLA | C1-O2A-CGA | 2.49 | 122.98 | 116.44 |
| 27 | A | 611 | PL9 | C7-C3-C2 | -2.49 | 120.02 | 123.30 |
| 30 | a | 616 | LHG | C5-O7-C7 | -2.49 | 111.67 | 117.79 |
| 26 | B | 618 | BCR | C2-C1-C6 | -2.49 | 106.66 | 110.48 |
| 26 | A | 610 | BCR | C40-C30-C25 | -2.48 | 106.27 | 110.30 |
| 26 | c | 515 | BCR | C8-C9-C10 | 2.48 | 122.74 | 118.94 |
| 24 | b | 605 | CLA | CMB-C2B-C1B | -2.47 | 124.66 | 128.46 |
| 25 | a | 608 | PHO | O2A-CGA-O1A | -2.47 | 117.35 | 123.59 |
| 24 | B | 613 | CLA | CAC-C3C-C4C | 2.47 | 128.02 | 124.81 |
| 24 | b | 611 | CLA | C1-C2-C3 | -2.47 | 121.77 | 126.04 |
| 24 | B | 617 | CLA | C1B-CHB-C4A | -2.47 | 125.23 | 130.12 |
| 24 | B | 604 | CLA | C4A-NA-C1A | -2.47 | 105.60 | 106.71 |
| 24 | B | 615 | CLA | CHC-C1C-NC | 2.47 | 127.94 | 124.20 |
| 24 | B | 612 | CLA | CED-O2D-CGD | 2.47 | 121.52 | 115.94 |
| 24 | C | 510 | CLA | C2A-C1A-CHA | 2.46 | 128.17 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 26 | C | 514 | BCR | C30-C25-C24 | -2.46 | 108.81 | 115.78 |
| 32 | h | 102 | DGD | O2G-C1B-O1B | -2.46 | 117.75 | 123.70 |
| 24 | B | 609 | CLA | CHC-C1C-C2C | -2.46 | 119.91 | 126.72 |
| 24 | b | 618 | CLA | CBA-CAA-C2A | -2.46 | 106.59 | 113.86 |
| 32 | E | 101 | DGD | O6D-C5D-C6D | 2.46 | 111.64 | 106.67 |
| 26 | b | 621 | BCR | C11-C12-C13 | -2.46 | 119.50 | 126.42 |
| 24 | b | 608[A] | CLA | C1-C2-C3 | -2.46 | 121.79 | 126.04 |
| 24 | D | 403 | CLA | O1D-CGD-CBD | -2.46 | 119.45 | 124.48 |
| 24 | C | 512 | CLA | O1D-CGD-CBD | -2.46 | 119.46 | 124.48 |
| 24 | B | 607[A] | CLA | CHC-C1C-C2C | -2.46 | 119.92 | 126.72 |
| 26 | c | 515 | BCR | C16-C15-C14 | -2.46 | 118.44 | 123.47 |
| 24 | b | 612 | CLA | CHA-C1A-NA | -2.46 | 120.78 | 126.40 |
| 24 | B | 609 | CLA | O2D-CGD-O1D | -2.45 | 119.04 | 123.84 |
| 24 | B | 609 | CLA | O2A-CGA-CBA | 2.45 | 119.60 | 111.91 |
| 24 | d | 403 | CLA | CMB-C2B-C1B | -2.45 | 124.70 | 128.46 |
| 24 | B | 615 | CLA | O1D-CGD-CBD | -2.45 | 119.47 | 124.48 |
| 32 | d | 405 | DGD | O6D-C5D-C6D | 2.45 | 111.60 | 106.67 |
| 24 | C | 508 | CLA | O1D-CGD-CBD | -2.45 | 119.48 | 124.48 |
| 32 | c | 518 | DGD | C3G-C2G-C1G | -2.45 | 106.00 | 111.79 |
| 24 | c | 504 | CLA | CHA-C1A-NA | -2.45 | 120.80 | 126.40 |
| 24 | b | 606 | CLA | O2D-CGD-O1D | -2.45 | 119.06 | 123.84 |
| 24 | C | 507 | CLA | O1D-CGD-CBD | -2.44 | 119.48 | 124.48 |
| 24 | b | 603 | CLA | CHC-C1C-C2C | -2.44 | 119.96 | 126.72 |
| 24 | b | 614 | CLA | CAC-C3C-C4C | 2.44 | 127.98 | 124.81 |
| 24 | B | 604 | CLA | CHA-C1A-NA | -2.44 | 120.81 | 126.40 |
| 29 | D | 408 | LMG | O7-C10-O9 | -2.44 | 117.80 | 123.70 |
| 24 | b | 604 | CLA | CHA-C1A-NA | -2.44 | 120.81 | 126.40 |
| 24 | c | 513 | CLA | C4-C3-C5 | 2.44 | 119.37 | 115.27 |
| 24 | C | 513 | CLA | C4-C3-C5 | 2.44 | 119.37 | 115.27 |
| 24 | C | 507 | CLA | CHC-C1C-C2C | -2.44 | 119.98 | 126.72 |
| 26 | A | 610 | BCR | C34-C9-C8 | 2.43 | 121.91 | 118.08 |
| 26 | c | 514 | BCR | C33-C5-C4 | -2.43 | 108.94 | 113.62 |
| 24 | B | 605 | CLA | CED-O2D-CGD | 2.43 | 121.44 | 115.94 |
| 26 | B | 619 | BCR | C24-C25-C26 | -2.43 | 115.57 | 121.46 |
| 26 | b | 619 | BCR | C19-C18-C17 | 2.43 | 122.67 | 118.94 |
| 24 | B | 605 | CLA | O2A-CGA-CBA | 2.43 | 119.53 | 111.91 |
| 24 | c | 513 | CLA | O2A-CGA-CBA | 2.43 | 119.53 | 111.91 |
| 24 | B | 607[A] | CLA | C1-C2-C3 | -2.43 | 121.84 | 126.04 |
| 24 | c | 504 | CLA | CHB-C4A-NA | -2.43 | 121.16 | 124.51 |
| 26 | B | 619 | BCR | C12-C13-C14 | 2.42 | 122.66 | 118.94 |
| 26 | T | 101 | BCR | C2-C1-C6 | 2.42 | 114.21 | 110.48 |
| 29 | D | 408 | LMG | O8-C28-O10 | -2.42 | 117.48 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | C | 511 | CLA | CHA-C1A-NA | -2.42 | 120.85 | 126.40 |
| 24 | a | 615 | CLA | C4A-NA-C1A | -2.42 | 105.62 | 106.71 |
| 32 | C | 517 | DGD | O6E-C5E-C6E | 2.42 | 112.45 | 106.44 |
| 24 | C | 512 | CLA | C1-O2A-CGA | 2.42 | 122.78 | 116.44 |
| 24 | B | 605 | CLA | CMD-C2D-C3D | 2.41 | 129.20 | 124.68 |
| 26 | b | 621 | BCR | C33-C5-C4 | -2.41 | 108.98 | 113.62 |
| 24 | B | 610 | CLA | C1-C2-C3 | -2.41 | 121.87 | 126.04 |
| 29 | a | 613 | LMG | O8-C28-C29 | 2.41 | 119.47 | 111.91 |
| 26 | K | 101 | BCR | C34-C9-C8 | 2.41 | 121.88 | 118.08 |
| 24 | C | 510 | CLA | O1D-CGD-CBD | -2.41 | 119.55 | 124.48 |
| 26 | b | 620 | BCR | C34-C9-C8 | 2.41 | 121.87 | 118.08 |
| 24 | B | 608 | CLA | CHC-C1C-C2C | -2.41 | 120.07 | 126.72 |
| 24 | C | 501 | CLA | CAC-C3C-C4C | 2.40 | 127.93 | 124.81 |
| 32 | C | 515 | DGD | O3G-C3G-C2G | -2.40 | 105.10 | 110.90 |
| 24 | c | 511 | CLA | CHA-C1A-NA | -2.40 | 120.90 | 126.40 |
| 24 | C | 503 | CLA | CHA-C1A-NA | -2.40 | 120.90 | 126.40 |
| 24 | C | 512 | CLA | CHA-C1A-NA | -2.40 | 120.90 | 126.40 |
| 24 | B | 603 | CLA | CMB-C2B-C1B | -2.40 | 124.78 | 128.46 |
| 24 | b | 611 | CLA | CBA-CAA-C2A | -2.40 | 106.79 | 113.86 |
| 26 | f | 101 | BCR | C30-C25-C24 | -2.39 | 109.00 | 115.78 |
| 32 | H | 102 | DGD | C1D-C2D-C3D | 2.39 | 114.98 | 110.00 |
| 26 | K | 101 | BCR | C1-C6-C7 | -2.39 | 109.01 | 115.78 |
| 24 | b | 618 | CLA | O2A-CGA-CBA | 2.39 | 119.42 | 111.91 |
| 26 | h | 101 | BCR | C10-C11-C12 | -2.39 | 115.76 | 123.22 |
| 24 | C | 504 | CLA | O2A-CGA-CBA | 2.39 | 119.40 | 111.91 |
| 26 | B | 619 | BCR | C40-C30-C25 | 2.39 | 114.17 | 110.30 |
| 24 | B | 612 | CLA | C1-O2A-CGA | 2.39 | 122.70 | 116.44 |
| 24 | B | 613 | CLA | CHA-C1A-NA | -2.39 | 120.93 | 126.40 |
| 29 | C | 518 | LMG | C1-C2-C3 | 2.38 | 114.96 | 110.00 |
| 24 | b | 609 | CLA | CMB-C2B-C3B | 2.38 | 129.14 | 124.68 |
| 24 | C | 501 | CLA | CHC-C1C-NC | 2.38 | 127.82 | 124.20 |
| 24 | B | 617 | CLA | CED-O2D-CGD | 2.38 | 121.32 | 115.94 |
| 26 | h | 101 | BCR | C11-C10-C9 | -2.38 | 123.91 | 127.31 |
| 24 | b | 611 | CLA | O1D-CGD-CBD | -2.38 | 119.62 | 124.48 |
| 24 | B | 603 | CLA | C1-C2-C3 | -2.38 | 121.93 | 126.04 |
| 27 | d | 404 | PL9 | C53-C6-C1 | 2.38 | 119.85 | 114.99 |
| 24 | B | 613 | CLA | O2D-CGD-O1D | -2.38 | 119.19 | 123.84 |
| 26 | B | 618 | BCR | C1-C6-C7 | -2.38 | 109.06 | 115.78 |
| 24 | c | 507 | CLA | O1D-CGD-CBD | -2.38 | 119.62 | 124.48 |
| 24 | b | 614 | CLA | CHC-C1C-C2C | -2.37 | 120.15 | 126.72 |
| 24 | b | 607 | CLA | O1D-CGD-CBD | -2.37 | 119.63 | 124.48 |
| 24 | B | 606 | CLA | C3D-CAD-CBD | -2.37 | 104.48 | 107.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | D | 402 | CLA | CHD-C4C-C3C | 2.37 | 128.33 | 124.84 |
| 24 | B | 616 | CLA | O1D-CGD-CBD | -2.37 | 119.63 | 124.48 |
| 24 | C | 501 | CLA | O1D-CGD-CBD | -2.37 | 119.63 | 124.48 |
| 25 | d | 401 | PHO | O1D-CGD-CBD | 2.37 | 129.33 | 124.48 |
| 25 | D | 401 | PHO | O1D-CGD-CBD | 2.37 | 129.33 | 124.48 |
| 24 | C | 509 | CLA | CHA-C1A-NA | -2.37 | 120.98 | 126.40 |
| 24 | b | 614 | CLA | CBA-CAA-C2A | -2.37 | 106.88 | 113.86 |
| 26 | B | 618 | BCR | C2-C3-C4 | 2.36 | 116.66 | 111.38 |
| 26 | k | 101 | BCR | C12-C13-C14 | -2.36 | 115.31 | 118.94 |
| 24 | c | 513 | CLA | C3C-C4C-NC | -2.36 | 107.92 | 110.57 |
| 24 | C | 506 | CLA | CMB-C2B-C3B | 2.36 | 129.10 | 124.68 |
| 24 | B | 602 | CLA | CMC-C2C-C1C | 2.36 | 128.63 | 125.04 |
| 24 | B | 604 | CLA | CHC-C1C-C2C | -2.36 | 120.19 | 126.72 |
| 25 | A | 608 | PHO | C1-C2-C3 | -2.36 | 121.97 | 126.04 |
| 24 | b | 612 | CLA | CED-O2D-CGD | 2.36 | 121.27 | 115.94 |
| 26 | c | 514 | BCR | C12-C13-C14 | -2.36 | 115.33 | 118.94 |
| 24 | C | 505 | CLA | CMD-C2D-C3D | 2.36 | 129.09 | 124.68 |
| 29 | B | 621 | LMG | C3-C4-C5 | 2.35 | 114.44 | 110.24 |
| 24 | B | 605 | CLA | CHC-C1C-C2C | -2.35 | 120.21 | 126.72 |
| 24 | B | 610 | CLA | O2A-CGA-CBA | 2.35 | 119.29 | 111.91 |
| 24 | C | 512 | CLA | CMD-C2D-C3D | 2.35 | 129.08 | 124.68 |
| 24 | C | 513 | CLA | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 24 | B | 610 | CLA | CHC-C1C-C2C | -2.35 | 120.22 | 126.72 |
| 30 | A | 615 | LHG | O7-C7-O9 | -2.35 | 118.02 | 123.70 |
| 24 | C | 508 | CLA | CHC-C1C-C2C | -2.35 | 120.22 | 126.72 |
| 26 | h | 101 | BCR | C1-C6-C7 | -2.35 | 109.13 | 115.78 |
| 24 | c | 504 | CLA | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 24 | C | 501 | CLA | CHA-C1A-NA | -2.35 | 121.02 | 126.40 |
| 24 | b | 615 | CLA | C1-O2A-CGA | 2.35 | 122.61 | 116.44 |
| 24 | C | 507 | CLA | OBD-CAD-C3D | -2.35 | 124.08 | 127.98 |
| 24 | B | 603 | CLA | O1D-CGD-CBD | -2.35 | 119.69 | 124.48 |
| 32 | c | 516 | DGD | O1G-C1A-O1A | -2.35 | 117.67 | 123.59 |
| 24 | a | 615 | CLA | CAA-CBA-CGA | -2.34 | 106.41 | 113.25 |
| 24 | B | 604 | CLA | CMD-C2D-C3D | 2.34 | 129.06 | 124.68 |
| 24 | c | 504 | CLA | CED-O2D-CGD | 2.34 | 121.23 | 115.94 |
| 26 | c | 521 | BCR | C16-C15-C14 | -2.34 | 118.68 | 123.47 |
| 24 | b | 605 | CLA | O2D-CGD-O1D | -2.34 | 119.26 | 123.84 |
| 24 | b | 604 | CLA | O2A-CGA-CBA | 2.34 | 119.25 | 111.91 |
| 29 | A | 613 | LMG | O1-C1-C2 | 2.34 | 111.95 | 108.30 |
| 24 | c | 503 | CLA | CMB-C2B-C1B | -2.34 | 124.87 | 128.46 |
| 24 | B | 602 | CLA | CHA-C1A-NA | -2.34 | 121.04 | 126.40 |
| 24 | c | 501 | CLA | C1-O2A-CGA | 2.34 | 122.57 | 116.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | b | 609 | CLA | CED-O2D-CGD | 2.34 | 121.22 | 115.94 |
| 24 | A | 606 | CLA | C1-O2A-CGA | 2.33 | 122.57 | 116.44 |
| 24 | b | 604 | CLA | C1-C2-C3 | -2.33 | 122.01 | 126.04 |
| 26 | T | 101 | BCR | C1-C6-C7 | -2.33 | 109.18 | 115.78 |
| 24 | c | 501 | CLA | CHC-C1C-C2C | -2.33 | 120.27 | 126.72 |
| 24 | b | 618 | CLA | O2A-CGA-O1A | -2.33 | 117.71 | 123.59 |
| 24 | B | 612 | CLA | CHC-C1C-C2C | -2.33 | 120.28 | 126.72 |
| 24 | A | 609 | CLA | C1-O2A-CGA | 2.33 | 122.55 | 116.44 |
| 29 | c | 519 | LMG | O7-C10-O9 | -2.33 | 118.08 | 123.70 |
| 32 | C | 517 | DGD | C2G-O2G-C1B | -2.33 | 112.06 | 117.79 |
| 26 | f | 101 | BCR | C16-C15-C14 | -2.32 | 118.71 | 123.47 |
| 24 | d | 403 | CLA | CHB-C4A-NA | -2.32 | 121.30 | 124.51 |
| 24 | a | 607 | CLA | O2D-CGD-O1D | -2.32 | 119.30 | 123.84 |
| 26 | F | 101 | BCR | C8-C9-C10 | 2.32 | 122.50 | 118.94 |
| 24 | B | 607[A] | CLA | O2A-CGA-CBA | 2.32 | 119.19 | 111.91 |
| 32 | h | 102 | DGD | O6D-C5D-C6D | 2.32 | 111.35 | 106.67 |
| 24 | B | 607[B] | CLA | CMB-C2B-C1B | -2.32 | 124.90 | 128.46 |
| 24 | b | 617 | CLA | O2A-CGA-CBA | 2.32 | 119.19 | 111.91 |
| 24 | c | 506 | CLA | CHA-C1A-NA | -2.32 | 121.09 | 126.40 |
| 32 | H | 102 | DGD | O5E-C6E-C5E | -2.32 | 103.34 | 111.29 |
| 24 | C | 511 | CLA | O2A-CGA-O1A | -2.32 | 117.75 | 123.59 |
| 24 | B | 616 | CLA | C4A-NA-C1A | -2.31 | 105.67 | 106.71 |
| 24 | D | 403 | CLA | CBC-CAC-C3C | -2.31 | 106.05 | 112.43 |
| 24 | B | 610 | CLA | CED-O2D-CGD | 2.31 | 121.16 | 115.94 |
| 24 | B | 616 | CLA | O2A-CGA-O1A | -2.31 | 117.77 | 123.59 |
| 24 | c | 510 | CLA | CHA-C1A-NA | -2.31 | 121.11 | 126.40 |
| 24 | C | 504 | CLA | C3C-C4C-NC | -2.31 | 107.98 | 110.57 |
| 28 | a | 614 | SQD | C3-C4-C5 | 2.31 | 114.36 | 110.24 |
| 24 | b | 616 | CLA | O1D-CGD-CBD | -2.31 | 119.76 | 124.48 |
| 24 | b | 618 | CLA | O1D-CGD-CBD | -2.31 | 119.76 | 124.48 |
| 24 | C | 511 | CLA | CHB-C4A-NA | -2.31 | 121.32 | 124.51 |
| 26 | B | 620 | BCR | C11-C12-C13 | -2.30 | 119.95 | 126.42 |
| 24 | B | 610 | CLA | CHA-C1A-NA | -2.30 | 121.13 | 126.40 |
| 24 | D | 402 | CLA | CMA-C3A-C4A | -2.30 | 105.59 | 111.77 |
| 26 | C | 514 | BCR | C11-C12-C13 | -2.30 | 119.95 | 126.42 |
| 29 | Z | 101 | LMG | O6-C5-C4 | 2.30 | 113.87 | 109.69 |
| 24 | B | 608 | CLA | CHA-C1A-NA | -2.30 | 121.13 | 126.40 |
| 24 | b | 608[B] | CLA | CHC-C1C-C2C | -2.30 | 120.36 | 126.72 |
| 24 | C | 503 | CLA | O2A-C1-C2 | 2.30 | 114.67 | 108.64 |
| 24 | c | 511 | CLA | CMB-C2B-C1B | -2.30 | 124.93 | 128.46 |
| 24 | B | 610 | CLA | O2D-CGD-O1D | -2.30 | 119.35 | 123.84 |
| 26 | c | 515 | BCR | C35-C13-C14 | -2.30 | 119.71 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 29 | D | 408 | LMG | O8-C28-C29 | 2.29 | 119.11 | 111.91 |
| 26 | t | 101 | BCR | C33-C5-C4 | -2.29 | 109.21 | 113.62 |
| 24 | b | 617 | CLA | OBD-CAD-C3D | -2.29 | 124.17 | 127.98 |
| 24 | C | 507 | CLA | C1-O2A-CGA | 2.29 | 122.46 | 116.44 |
| 24 | b | 610 | CLA | C4-C3-C5 | 2.29 | 119.12 | 115.27 |
| 24 | D | 404 | CLA | O2A-CGA-CBA | 2.29 | 119.09 | 111.91 |
| 32 | d | 405 | DGD | C1E-C2E-C3E | 2.29 | 114.77 | 110.00 |
| 24 | B | 607[A] | CLA | CHA-C1A-NA | -2.29 | 121.15 | 126.40 |
| 32 | c | 516 | DGD | O6D-C5D-C6D | 2.29 | 111.29 | 106.67 |
| 24 | b | 608[B] | CLA | CMB-C2B-C1B | -2.29 | 124.94 | 128.46 |
| 24 | C | 513 | CLA | C1-O2A-CGA | 2.29 | 122.45 | 116.44 |
| 24 | c | 508 | CLA | CMB-C2B-C3B | 2.29 | 128.96 | 124.68 |
| 24 | d | 402 | CLA | CMA-C3A-C4A | -2.29 | 105.63 | 111.77 |
| 24 | C | 507 | CLA | CHA-C1A-NA | -2.29 | 121.16 | 126.40 |
| 29 | c | 519 | LMG | O6-C5-C4 | 2.29 | 113.84 | 109.69 |
| 24 | C | 505 | CLA | CHD-C4C-C3C | 2.28 | 128.20 | 124.84 |
| 32 | E | 101 | DGD | O2G-C1B-O1B | -2.28 | 118.18 | 123.70 |
| 24 | B | 609 | CLA | C4-C3-C5 | 2.28 | 119.11 | 115.27 |
| 32 | C | 516 | DGD | O1G-C1A-O1A | -2.28 | 117.83 | 123.59 |
| 30 | d | 407 | LHG | O8-C23-C24 | 2.28 | 119.07 | 111.91 |
| 24 | B | 606 | CLA | O1D-CGD-CBD | -2.28 | 119.82 | 124.48 |
| 24 | b | 610 | CLA | C11-C12-C13 | -2.28 | 108.55 | 115.92 |
| 24 | A | 606 | CLA | C4-C3-C5 | 2.28 | 119.11 | 115.27 |
| 24 | A | 606 | CLA | C3C-C4C-NC | -2.28 | 108.01 | 110.57 |
| 26 | K | 102 | BCR | C39-C30-C25 | -2.28 | 106.61 | 110.30 |
| 24 | a | 609 | CLA | O2D-CGD-O1D | -2.28 | 119.39 | 123.84 |
| 24 | C | 501 | CLA | CMD-C2D-C3D | 2.27 | 128.93 | 124.68 |
| 26 | k | 101 | BCR | C11-C12-C13 | -2.27 | 120.04 | 126.42 |
| 27 | a | 611 | PL9 | C3-C4-C5 | 2.27 | 121.55 | 118.60 |
| 25 | a | 608 | PHO | CMB-C2B-C1B | -2.27 | 121.57 | 125.06 |
| 24 | d | 402 | CLA | O1D-CGD-CBD | -2.27 | 119.84 | 124.48 |
| 24 | C | 504 | CLA | CHC-C1C-C2C | -2.27 | 120.45 | 126.72 |
| 28 | A | 614 | SQD | C3-C4-C5 | 2.26 | 114.28 | 110.24 |
| 30 | A | 615 | LHG | O8-C23-C24 | 2.26 | 119.01 | 111.91 |
| 24 | A | 607 | CLA | O2D-CGD-O1D | -2.26 | 119.41 | 123.84 |
| 32 | d | 405 | DGD | C3E-C4E-C5E | 2.26 | 114.28 | 110.24 |
| 24 | a | 607 | CLA | CHC-C1C-C2C | -2.26 | 120.47 | 126.72 |
| 24 | B | 610 | CLA | CAC-C3C-C4C | 2.26 | 127.74 | 124.81 |
| 24 | d | 403 | CLA | O1D-CGD-CBD | -2.26 | 119.86 | 124.48 |
| 24 | b | 614 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 24 | B | 611 | CLA | CHA-C1A-NA | -2.26 | 121.22 | 126.40 |
| 32 | c | 518 | DGD | O4D-C4D-C3D | -2.26 | 105.13 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | a | 609 | CLA | CED-O2D-CGD | 2.26 | 121.05 | 115.94 |
| 24 | B | 605 | CLA | CHA-C1A-NA | -2.26 | 121.23 | 126.40 |
| 26 | F | 101 | BCR | C30-C25-C24 | -2.26 | 109.39 | 115.78 |
| 24 | C | 508 | CLA | CMB-C2B-C3B | 2.26 | 128.90 | 124.68 |
| 29 | C | 518 | LMG | O1-C7-C8 | -2.25 | 105.46 | 110.90 |
| 24 | B | 616 | CLA | CHC-C1C-C2C | -2.25 | 120.48 | 126.72 |
| 24 | A | 609 | CLA | CBC-CAC-C3C | -2.25 | 106.22 | 112.43 |
| 24 | c | 502 | CLA | CMB-C2B-C1B | -2.25 | 125.00 | 128.46 |
| 25 | a | 608 | PHO | O2D-CGD-O1D | -2.25 | 119.43 | 123.84 |
| 24 | B | 607[B] | CLA | C3C-C4C-NC | -2.25 | 108.05 | 110.57 |
| 24 | C | 512 | CLA | CMB-C2B-C3B | 2.25 | 128.89 | 124.68 |
| 24 | B | 604 | CLA | CHD-C4C-C3C | 2.25 | 128.15 | 124.84 |
| 24 | c | 504 | CLA | O1D-CGD-CBD | -2.25 | 119.88 | 124.48 |
| 24 | A | 609 | CLA | CHC-C1C-NC | 2.25 | 127.61 | 124.20 |
| 24 | c | 513 | CLA | CMB-C2B-C3B | 2.25 | 128.88 | 124.68 |
| 24 | B | 609 | CLA | C11-C12-C13 | -2.25 | 108.65 | 115.92 |
| 24 | c | 504 | CLA | C3C-C4C-NC | -2.25 | 108.05 | 110.57 |
| 24 | C | 513 | CLA | CMD-C2D-C3D | 2.25 | 128.88 | 124.68 |
| 29 | A | 613 | LMG | O8-C28-O10 | -2.25 | 117.92 | 123.59 |
| 24 | B | 613 | CLA | CHD-C4C-C3C | 2.24 | 128.14 | 124.84 |
| 24 | c | 513 | CLA | CHA-C1A-NA | -2.24 | 121.26 | 126.40 |
| 24 | B | 611 | CLA | CHC-C1C-C2C | -2.24 | 120.52 | 126.72 |
| 24 | C | 511 | CLA | O2A-CGA-CBA | 2.24 | 118.95 | 111.91 |
| 26 | k | 101 | BCR | C20-C19-C18 | -2.24 | 120.11 | 126.42 |
| 29 | j | 101 | LMG | O8-C28-O10 | -2.24 | 117.93 | 123.59 |
| 24 | a | 606 | CLA | C4-C3-C5 | 2.24 | 119.04 | 115.27 |
| 29 | D | 408 | LMG | C1-O6-C5 | 2.24 | 118.09 | 113.69 |
| 24 | D | 402 | CLA | C3C-C4C-NC | -2.24 | 108.06 | 110.57 |
| 24 | A | 609 | CLA | CHD-C4C-C3C | 2.24 | 128.13 | 124.84 |
| 24 | b | 614 | CLA | C2A-C1A-CHA | 2.24 | 127.78 | 123.86 |
| 24 | c | 510 | CLA | O1D-CGD-CBD | -2.24 | 119.90 | 124.48 |
| 32 | C | 515 | DGD | C3G-C2G-C1G | -2.24 | 106.49 | 111.79 |
| 26 | F | 101 | BCR | C38-C26-C27 | -2.24 | 109.32 | 113.62 |
| 24 | c | 503 | CLA | CHA-C1A-NA | -2.24 | 121.27 | 126.40 |
| 24 | b | 607 | CLA | CED-O2D-CGD | 2.24 | 121.00 | 115.94 |
| 24 | B | 610 | CLA | CHD-C4C-C3C | 2.24 | 128.13 | 124.84 |
| 24 | B | 608 | CLA | O2A-CGA-CBA | 2.24 | 118.92 | 111.91 |
| 32 | C | 516 | DGD | C1E-C2E-C3E | 2.23 | 114.65 | 110.00 |
| 24 | c | 502 | CLA | CHA-C1A-NA | -2.23 | 121.28 | 126.40 |
| 24 | b | 605 | CLA | CAA-C2A-C3A | -2.23 | 106.67 | 112.78 |
| 24 | c | 505 | CLA | CMD-C2D-C3D | 2.23 | 128.85 | 124.68 |
| 24 | A | 609 | CLA | O2A-CGA-CBA | 2.23 | 118.91 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | C | 512 | CLA | C2A-C1A-CHA | 2.23 | 127.76 | 123.86 |
| 24 | B | 610 | CLA | O1D-CGD-CBD | -2.23 | 119.93 | 124.48 |
| 29 | C | 518 | LMG | O4-C4-C5 | 2.23 | 114.83 | 109.30 |
| 24 | C | 502 | CLA | CHC-C1C-C2C | -2.22 | 120.57 | 126.72 |
| 24 | B | 616 | CLA | CED-O2D-CGD | 2.22 | 120.96 | 115.94 |
| 26 | f | 101 | BCR | C28-C27-C26 | -2.22 | 110.11 | 114.08 |
| 29 | a | 613 | LMG | O8-C28-O10 | -2.22 | 118.00 | 123.59 |
| 29 | B | 621 | LMG | O7-C10-C11 | 2.22 | 116.28 | 111.50 |
| 24 | b | 615 | CLA | C1-C2-C3 | -2.21 | 122.21 | 126.04 |
| 28 | A | 612 | SQD | O48-C23-C24 | 2.21 | 118.86 | 111.91 |
| 28 | x | 101 | SQD | O48-C23-O10 | -2.21 | 118.01 | 123.59 |
| 24 | D | 404 | CLA | CHC-C1C-C2C | -2.21 | 120.60 | 126.72 |
| 26 | B | 618 | BCR | C16-C15-C14 | -2.21 | 118.94 | 123.47 |
| 26 | A | 610 | BCR | C1-C6-C7 | -2.21 | 109.52 | 115.78 |
| 26 | C | 514 | BCR | C8-C9-C10 | 2.21 | 122.33 | 118.94 |
| 24 | b | 615 | CLA | CHA-C1A-NA | -2.21 | 121.33 | 126.40 |
| 29 | j | 101 | LMG | O7-C10-C11 | 2.21 | 116.26 | 111.50 |
| 26 | c | 514 | BCR | C37-C22-C21 | -2.21 | 119.83 | 122.92 |
| 32 | c | 517 | DGD | O2G-C1B-O1B | -2.21 | 118.37 | 123.70 |
| 28 | X | 101 | SQD | O48-C23-O10 | -2.21 | 118.03 | 123.59 |
| 24 | B | 607[B] | CLA | O2A-CGA-CBA | 2.20 | 118.83 | 111.91 |
| 24 | c | 509 | CLA | CHC-C1C-C2C | -2.20 | 120.62 | 126.72 |
| 32 | E | 101 | DGD | O6E-C5E-C6E | 2.20 | 111.91 | 106.44 |
| 24 | A | 607 | CLA | CHD-C4C-C3C | 2.20 | 128.08 | 124.84 |
| 24 | b | 616 | CLA | CMD-C2D-C3D | 2.20 | 128.80 | 124.68 |
| 24 | b | 608[A] | CLA | CHC-C1C-C2C | -2.20 | 120.63 | 126.72 |
| 24 | B | 603 | CLA | O2A-CGA-CBA | 2.20 | 118.81 | 111.91 |
| 24 | D | 403 | CLA | CED-O2D-CGD | 2.20 | 120.91 | 115.94 |
| 24 | B | 614 | CLA | C1-O2A-CGA | 2.20 | 122.22 | 116.44 |
| 24 | C | 501 | CLA | CMB-C2B-C1B | -2.20 | 125.08 | 128.46 |
| 28 | a | 612 | SQD | O48-C23-C24 | 2.20 | 118.81 | 111.91 |
| 26 | I | 101 | BCR | C23-C24-C25 | -2.20 | 121.03 | 127.20 |
| 26 | T | 101 | BCR | C30-C25-C24 | -2.20 | 109.56 | 115.78 |
| 29 | Z | 101 | LMG | O7-C10-O9 | -2.20 | 118.39 | 123.70 |
| 24 | B | 614 | CLA | C1-C2-C3 | -2.20 | 122.25 | 126.04 |
| 24 | d | 403 | CLA | CHC-C1C-C2C | -2.20 | 120.65 | 126.72 |
| 24 | B | 607[A] | CLA | C3C-C4C-NC | -2.20 | 108.11 | 110.57 |
| 26 | B | 620 | BCR | C3-C4-C5 | -2.19 | 110.16 | 114.08 |
| 24 | c | 501 | CLA | CHD-C4C-C3C | 2.19 | 128.06 | 124.84 |
| 24 | B | 602 | CLA | C1-O2A-CGA | 2.19 | 122.20 | 116.44 |
| 24 | c | 510 | CLA | CED-O2D-CGD | 2.19 | 120.89 | 115.94 |
| 26 | H | 101 | BCR | C11-C12-C13 | -2.19 | 120.26 | 126.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 29 | A | 613 | LMG | O8-C28-C29 | 2.19 | 118.78 | 111.91 |
| 24 | c | 503 | CLA | O2A-CGA-CBA | 2.19 | 118.78 | 111.91 |
| 29 | C | 518 | LMG | O8-C28-O10 | -2.19 | 118.07 | 123.59 |
| 24 | b | 609 | CLA | CHA-C1A-NA | -2.19 | 121.39 | 126.40 |
| 24 | C | 501 | CLA | C4-C3-C5 | 2.19 | 118.95 | 115.27 |
| 24 | c | 501 | CLA | CED-O2D-CGD | 2.18 | 120.88 | 115.94 |
| 24 | a | 609 | CLA | CHC-C1C-C2C | -2.18 | 120.69 | 126.72 |
| 26 | h | 101 | BCR | C2-C3-C4 | 2.18 | 116.25 | 111.38 |
| 26 | b | 620 | BCR | C29-C30-C25 | 2.18 | 113.84 | 110.48 |
| 28 | a | 612 | SQD | O48-C23-O10 | -2.18 | 118.09 | 123.59 |
| 32 | d | 405 | DGD | C6D-C5D-C4D | -2.18 | 107.54 | 112.09 |
| 24 | c | 506 | CLA | O2A-CGA-CBA | 2.18 | 118.75 | 111.91 |
| 26 | t | 101 | BCR | C39-C30-C25 | -2.18 | 106.76 | 110.30 |
| 24 | c | 501 | CLA | C4-C3-C5 | 2.18 | 118.94 | 115.27 |
| 24 | b | 617 | CLA | CHC-C1C-C2C | -2.18 | 120.69 | 126.72 |
| 24 | C | 511 | CLA | C3C-C4C-NC | -2.17 | 108.13 | 110.57 |
| 24 | b | 609 | CLA | O2A-CGA-O1A | -2.17 | 118.11 | 123.59 |
| 26 | I | 101 | BCR | C19-C18-C17 | 2.17 | 122.27 | 118.94 |
| 26 | B | 619 | BCR | C28-C27-C26 | 2.17 | 117.95 | 114.08 |
| 24 | c | 505 | CLA | CMB-C2B-C3B | 2.17 | 128.74 | 124.68 |
| 24 | C | 508 | CLA | CHA-C1A-NA | -2.17 | 121.42 | 126.40 |
| 24 | B | 617 | CLA | CMD-C2D-C3D | 2.17 | 128.74 | 124.68 |
| 26 | b | 620 | BCR | C28-C27-C26 | 2.17 | 117.95 | 114.08 |
| 28 | A | 612 | SQD | O48-C23-O10 | -2.17 | 118.12 | 123.59 |
| 24 | c | 512 | CLA | O2A-CGA-O1A | -2.17 | 118.12 | 123.59 |
| 26 | T | 101 | BCR | C3-C4-C5 | -2.17 | 110.21 | 114.08 |
| 26 | f | 101 | BCR | C20-C19-C18 | -2.17 | 120.33 | 126.42 |
| 24 | b | 608[B] | CLA | CHD-C4C-C3C | 2.17 | 128.02 | 124.84 |
| 26 | c | 514 | BCR | C35-C13-C12 | 2.17 | 121.49 | 118.08 |
| 24 | c | 508 | CLA | C3C-C4C-NC | -2.16 | 108.14 | 110.57 |
| 25 | d | 401 | PHO | CBC-CAC-C3C | 2.16 | 118.40 | 112.43 |
| 26 | t | 101 | BCR | C1-C6-C7 | -2.16 | 109.66 | 115.78 |
| 33 | V | 201 | HEM | CMB-C2B-C3B | 2.16 | 128.72 | 124.68 |
| 24 | B | 612 | CLA | CHD-C4C-C3C | 2.16 | 128.01 | 124.84 |
| 30 | D | 407 | LHG | O8-C23-O10 | -2.16 | 118.15 | 123.59 |
| 29 | D | 408 | LMG | C3-C4-C5 | 2.15 | 114.08 | 110.24 |
| 24 | B | 609 | CLA | CMB-C2B-C3B | 2.15 | 128.71 | 124.68 |
| 24 | b | 614 | CLA | CMB-C2B-C1B | -2.15 | 125.15 | 128.46 |
| 29 | C | 519 | LMG | O8-C28-C29 | 2.15 | 118.66 | 111.91 |
| 24 | B | 606 | CLA | CHA-C1A-NA | -2.15 | 121.47 | 126.40 |
| 24 | b | 618 | CLA | C4A-NA-C1A | -2.15 | 105.74 | 106.71 |
| 32 | d | 405 | DGD | O1G-C1A-O1A | -2.15 | 118.17 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | c | 508 | CLA | O2A-CGA-CBA | 2.15 | 118.65 | 111.91 |
| 24 | c | 511 | CLA | O1D-CGD-CBD | -2.15 | 120.09 | 124.48 |
| 24 | B | 614 | CLA | CHA-C1A-NA | -2.15 | 121.48 | 126.40 |
| 24 | b | 612 | CLA | CHD-C4C-C3C | 2.14 | 127.99 | 124.84 |
| 24 | a | 607 | CLA | CED-O2D-CGD | 2.14 | 120.78 | 115.94 |
| 24 | b | 614 | CLA | CAC-C3C-C2C | -2.14 | 123.87 | 127.53 |
| 28 | b | 601 | SQD | O47-C7-O49 | -2.14 | 118.53 | 123.70 |
| 24 | B | 610 | CLA | CMB-C2B-C1B | -2.14 | 125.17 | 128.46 |
| 26 | c | 521 | BCR | C23-C24-C25 | -2.14 | 121.19 | 127.20 |
| 24 | B | 617 | CLA | CAC-C3C-C4C | 2.14 | 127.59 | 124.81 |
| 24 | b | 608[A] | CLA | O2A-CGA-CBA | 2.14 | 118.62 | 111.91 |
| 24 | C | 506 | CLA | O1D-CGD-CBD | -2.14 | 120.11 | 124.48 |
| 26 | C | 514 | BCR | C1-C6-C7 | -2.14 | 109.73 | 115.78 |
| 29 | C | 519 | LMG | C3-C4-C5 | 2.14 | 114.05 | 110.24 |
| 24 | B | 612 | CLA | CMB-C2B-C3B | 2.14 | 128.68 | 124.68 |
| 24 | B | 613 | CLA | CHC-C1C-C2C | -2.14 | 120.81 | 126.72 |
| 24 | B | 607[B] | CLA | CHA-C1A-NA | -2.14 | 121.51 | 126.40 |
| 26 | C | 514 | BCR | C35-C13-C14 | -2.14 | 119.93 | 122.92 |
| 26 | T | 101 | BCR | C23-C22-C21 | 2.13 | 122.22 | 118.94 |
| 24 | B | 617 | CLA | CHA-C1A-NA | -2.13 | 121.51 | 126.40 |
| 24 | C | 505 | CLA | CHA-C1A-NA | -2.13 | 121.51 | 126.40 |
| 24 | B | 614 | CLA | C1B-CHB-C4A | -2.13 | 125.89 | 130.12 |
| 24 | B | 617 | CLA | O1D-CGD-CBD | -2.13 | 120.12 | 124.48 |
| 24 | b | 608[A] | CLA | CMB-C2B-C1B | -2.13 | 125.19 | 128.46 |
| 28 | B | 622 | SQD | O47-C7-O49 | -2.13 | 118.55 | 123.70 |
| 24 | c | 504 | CLA | C7-C6-C5 | -2.13 | 107.58 | 113.36 |
| 24 | B | 608 | CLA | O1D-CGD-CBD | -2.12 | 120.14 | 124.48 |
| 24 | A | 607 | CLA | CMB-C2B-C3B | 2.12 | 128.65 | 124.68 |
| 32 | c | 516 | DGD | O2G-C1B-O1B | -2.12 | 118.58 | 123.70 |
| 24 | b | 616 | CLA | CHA-C1A-NA | -2.12 | 121.55 | 126.40 |
| 24 | c | 509 | CLA | CHA-C1A-NA | -2.12 | 121.55 | 126.40 |
| 24 | C | 504 | CLA | C7-C6-C5 | -2.12 | 107.61 | 113.36 |
| 24 | B | 603 | CLA | CHC-C1C-C2C | -2.12 | 120.87 | 126.72 |
| 24 | C | 509 | CLA | O2A-CGA-CBA | 2.12 | 118.55 | 111.91 |
| 26 | K | 101 | BCR | C20-C21-C22 | -2.12 | 124.29 | 127.31 |
| 32 | C | 515 | DGD | O1G-C1A-O1A | -2.11 | 118.25 | 123.59 |
| 30 | L | 101 | LHG | O8-C23-C24 | 2.11 | 118.54 | 111.91 |
| 24 | C | 512 | CLA | CED-O2D-CGD | 2.11 | 120.72 | 115.94 |
| 28 | b | 601 | SQD | O5-C1-C2 | -2.11 | 105.88 | 110.35 |
| 24 | b | 617 | CLA | OBD-CAD-CBD | 2.11 | 128.91 | 125.89 |
| 24 | d | 402 | CLA | CHD-C4C-C3C | 2.11 | 127.94 | 124.84 |
| 24 | c | 505 | CLA | CHD-C4C-C3C | 2.11 | 127.94 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | c | 514 | BCR | C37-C22-C23 | -2.11 | 114.76 | 118.08 |
| 24 | C | 504 | CLA | CHA-C1A-NA | -2.11 | 121.57 | 126.40 |
| 24 | C | 510 | CLA | CHC-C1C-C2C | -2.11 | 120.89 | 126.72 |
| 24 | b | 611 | CLA | CMD-C2D-C3D | 2.11 | 128.62 | 124.68 |
| 24 | b | 618 | CLA | C4-C3-C5 | 2.10 | 118.81 | 115.27 |
| 24 | b | 603 | CLA | CHB-C4A-NA | -2.10 | 121.60 | 124.51 |
| 24 | c | 509 | CLA | C4-C3-C5 | 2.10 | 118.81 | 115.27 |
| 24 | c | 502 | CLA | CHC-C1C-C2C | -2.10 | 120.91 | 126.72 |
| 24 | B | 617 | CLA | C4-C3-C5 | 2.10 | 118.81 | 115.27 |
| 24 | B | 612 | CLA | CMD-C2D-C3D | 2.10 | 128.61 | 124.68 |
| 29 | z | 101 | LMG | O1-C1-C2 | 2.10 | 111.58 | 108.30 |
| 28 | B | 622 | SQD | O5-C1-C2 | -2.10 | 105.91 | 110.35 |
| 30 | L | 101 | LHG | O8-C23-O10 | -2.10 | 118.30 | 123.59 |
| 24 | b | 614 | CLA | O1D-CGD-CBD | -2.10 | 120.20 | 124.48 |
| 24 | C | 501 | CLA | C1-C2-C3 | -2.09 | 122.42 | 126.04 |
| 26 | C | 514 | BCR | C3-C4-C5 | -2.09 | 110.34 | 114.08 |
| 24 | C | 511 | CLA | OBD-CAD-C3D | -2.09 | 124.51 | 127.98 |
| 26 | t | 101 | BCR | C19-C18-C17 | 2.09 | 122.15 | 118.94 |
| 32 | c | 517 | DGD | C4E-C3E-C2E | 2.09 | 114.47 | 110.82 |
| 24 | B | 609 | CLA | C11-C10-C8 | -2.09 | 109.17 | 115.92 |
| 24 | b | 610 | CLA | C11-C10-C8 | -2.09 | 109.17 | 115.92 |
| 24 | c | 512 | CLA | CHC-C1C-C2C | -2.09 | 120.95 | 126.72 |
| 24 | D | 404 | CLA | CMB-C2B-C3B | 2.09 | 128.58 | 124.68 |
| 24 | a | 606 | CLA | CBA-CAA-C2A | -2.09 | 107.71 | 113.86 |
| 24 | b | 618 | CLA | CED-O2D-CGD | 2.09 | 120.65 | 115.94 |
| 24 | c | 501 | CLA | C1-C2-C3 | -2.08 | 122.44 | 126.04 |
| 24 | B | 611 | CLA | CHD-C4C-C3C | 2.08 | 127.90 | 124.84 |
| 24 | b | 617 | CLA | C11-C10-C8 | -2.08 | 109.18 | 115.92 |
| 24 | D | 403 | CLA | CHC-C1C-C2C | -2.08 | 120.96 | 126.72 |
| 24 | C | 509 | CLA | C4-C3-C5 | 2.08 | 118.77 | 115.27 |
| 24 | B | 603 | CLA | CHB-C4A-NA | -2.08 | 121.64 | 124.51 |
| 33 | E | 103 | HEM | CMA-C3A-C4A | -2.08 | 125.27 | 128.46 |
| 28 | X | 101 | SQD | C3-C4-C5 | 2.08 | 113.95 | 110.24 |
| 26 | b | 620 | BCR | C36-C18-C17 | -2.08 | 120.01 | 122.92 |
| 24 | B | 605 | CLA | C1-O2A-CGA | 2.08 | 121.90 | 116.44 |
| 25 | a | 608 | PHO | CBD-CHA-C1A | 2.08 | 131.22 | 126.40 |
| 24 | B | 615 | CLA | CED-O2D-CGD | 2.08 | 120.64 | 115.94 |
| 26 | b | 619 | BCR | C35-C13-C14 | 2.08 | 125.83 | 122.92 |
| 26 | B | 618 | BCR | C39-C30-C25 | -2.08 | 106.93 | 110.30 |
| 30 | a | 616 | LHG | C9-C8-C7 | -2.07 | 106.08 | 113.62 |
| 24 | b | 605 | CLA | O2A-CGA-CBA | 2.07 | 118.41 | 111.91 |
| 24 | B | 606 | CLA | OBD-CAD-CBD | 2.07 | 128.85 | 125.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | B | 616 | CLA | C11-C10-C8 | -2.07 | 109.23 | 115.92 |
| 32 | h | 102 | DGD | O3G-C3G-C2G | -2.07 | 105.90 | 110.90 |
| 29 | C | 519 | LMG | O6-C5-C4 | 2.07 | 113.45 | 109.69 |
| 26 | b | 620 | BCR | C32-C1-C6 | -2.07 | 106.94 | 110.30 |
| 24 | C | 501 | CLA | O2A-CGA-O1A | -2.07 | 118.37 | 123.59 |
| 26 | b | 620 | BCR | C11-C12-C13 | -2.07 | 120.60 | 126.42 |
| 24 | b | 608[B] | CLA | O2A-CGA-CBA | 2.07 | 118.40 | 111.91 |
| 24 | b | 608[B] | CLA | C3C-C4C-NC | -2.07 | 108.25 | 110.57 |
| 27 | D | 405 | PL9 | C20-C19-C21 | -2.07 | 111.79 | 115.27 |
| 27 | d | 404 | PL9 | C10-C9-C11 | -2.07 | 111.79 | 115.27 |
| 24 | C | 503 | CLA | O2A-CGA-CBA | 2.07 | 118.39 | 111.91 |
| 24 | B | 615 | CLA | CHC-C1C-C2C | -2.07 | 121.01 | 126.72 |
| 24 | B | 607[A] | CLA | CMB-C2B-C1B | -2.07 | 125.29 | 128.46 |
| 29 | b | 622 | LMG | O1-C7-C8 | -2.06 | 105.92 | 110.90 |
| 24 | b | 610 | CLA | CHB-C4A-NA | -2.06 | 121.66 | 124.51 |
| 24 | B | 606 | CLA | CBA-CAA-C2A | -2.06 | 107.77 | 113.86 |
| 26 | F | 101 | BCR | C28-C27-C26 | -2.06 | 110.39 | 114.08 |
| 25 | A | 608 | PHO | O2A-CGA-O1A | -2.06 | 118.39 | 123.59 |
| 26 | b | 620 | BCR | C35-C13-C12 | 2.06 | 121.32 | 118.08 |
| 32 | c | 518 | DGD | C3D-C4D-C5D | 2.06 | 113.91 | 110.24 |
| 24 | C | 510 | CLA | C4-C3-C5 | 2.06 | 118.73 | 115.27 |
| 24 | b | 611 | CLA | CHA-C1A-NA | -2.06 | 121.69 | 126.40 |
| 24 | C | 506 | CLA | C4A-NA-C1A | -2.06 | 105.78 | 106.71 |
| 29 | j | 101 | LMG | O7-C10-O9 | -2.05 | 118.74 | 123.70 |
| 24 | B | 603 | CLA | C3C-C4C-NC | -2.05 | 108.27 | 110.57 |
| 24 | a | 606 | CLA | O1D-CGD-CBD | -2.05 | 120.28 | 124.48 |
| 28 | A | 612 | SQD | O5-C1-C2 | -2.05 | 106.00 | 110.35 |
| 26 | b | 621 | BCR | C1-C6-C7 | -2.05 | 109.97 | 115.78 |
| 29 | j | 101 | LMG | O6-C5-C4 | 2.05 | 113.42 | 109.69 |
| 24 | b | 610 | CLA | CHC-C1C-C2C | -2.05 | 121.05 | 126.72 |
| 24 | b | 617 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 24 | B | 616 | CLA | C3C-C4C-NC | -2.05 | 108.27 | 110.57 |
| 26 | f | 101 | BCR | C12-C13-C14 | -2.05 | 115.80 | 118.94 |
| 30 | a | 616 | LHG | O7-C7-O9 | -2.05 | 118.75 | 123.70 |
| 24 | C | 502 | CLA | O2A-CGA-CBA | 2.05 | 118.34 | 111.91 |
| 26 | k | 101 | BCR | C8-C9-C10 | -2.05 | 115.80 | 118.94 |
| 28 | x | 101 | SQD | C3-C4-C5 | 2.05 | 113.89 | 110.24 |
| 24 | a | 615 | CLA | CMA-C3A-C4A | -2.05 | 106.27 | 111.77 |
| 24 | d | 402 | CLA | CHB-C4A-NA | -2.05 | 121.68 | 124.51 |
| 24 | d | 403 | CLA | C6-C7-C8 | -2.04 | 109.31 | 115.92 |
| 26 | c | 521 | BCR | C36-C18-C19 | -2.04 | 114.86 | 118.08 |
| 24 | D | 402 | CLA | O2D-CGD-CBD | 2.04 | 114.90 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 616 | CLA | C1-O2A-CGA | 2.04 | 121.80 | 116.44 |
| 26 | H | 101 | BCR | C35-C13-C12 | 2.04 | 121.29 | 118.08 |
| 29 | C | 518 | LMG | O6-C5-C6 | 2.04 | 111.51 | 106.44 |
| 32 | c | 518 | DGD | O2G-C1B-O1B | -2.04 | 118.77 | 123.70 |
| 24 | a | 615 | CLA | CHD-C4C-C3C | 2.04 | 127.84 | 124.84 |
| 28 | l | 101 | SQD | C4-C3-C2 | 2.04 | 114.38 | 110.82 |
| 32 | c | 517 | DGD | C1E-O6E-C5E | -2.04 | 109.69 | 113.69 |
| 24 | B | 603 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 24 | B | 610 | CLA | CMD-C2D-C3D | 2.04 | 128.49 | 124.68 |
| 24 | b | 612 | CLA | O2A-CGA-O1A | -2.04 | 118.45 | 123.59 |
| 27 | A | 611 | PL9 | C25-C24-C26 | -2.03 | 111.85 | 115.27 |
| 32 | c | 517 | DGD | O1G-C1A-O1A | -2.03 | 118.46 | 123.59 |
| 29 | b | 622 | LMG | C8-O7-C10 | -2.03 | 112.78 | 117.79 |
| 24 | c | 508 | CLA | CHC-C1C-C2C | -2.03 | 121.10 | 126.72 |
| 28 | L | 102 | SQD | C4-C3-C2 | 2.03 | 114.37 | 110.82 |
| 27 | D | 405 | PL9 | C3-C2-C1 | -2.03 | 118.70 | 122.52 |
| 24 | B | 610 | CLA | CHB-C4A-NA | -2.03 | 121.70 | 124.51 |
| 24 | b | 613 | CLA | O2D-CGD-O1D | -2.03 | 119.87 | 123.84 |
| 28 | a | 612 | SQD | O5-C1-C2 | -2.03 | 106.05 | 110.35 |
| 24 | c | 510 | CLA | C1-O2A-CGA | 2.03 | 121.76 | 116.44 |
| 24 | c | 510 | CLA | C4-C3-C5 | 2.03 | 118.68 | 115.27 |
| 33 | e | 102 | HEM | CMC-C2C-C3C | 2.03 | 128.47 | 124.68 |
| 24 | B | 609 | CLA | C3C-C4C-NC | -2.03 | 108.30 | 110.57 |
| 29 | C | 518 | LMG | O7-C10-O9 | -2.03 | 118.80 | 123.70 |
| 24 | c | 510 | CLA | OBD-CAD-CBD | 2.03 | 128.79 | 125.89 |
| 24 | C | 505 | CLA | CHC-C1C-C2C | -2.03 | 121.12 | 126.72 |
| 24 | B | 606 | CLA | CHC-C1C-C2C | -2.03 | 121.12 | 126.72 |
| 24 | C | 513 | CLA | CMC-C2C-C1C | 2.03 | 128.12 | 125.04 |
| 24 | D | 404 | CLA | C6-C7-C8 | -2.03 | 109.37 | 115.92 |
| 32 | E | 101 | DGD | O1B-C1B-C2B | -2.03 | 115.83 | 123.73 |
| 24 | c | 509 | CLA | CMD-C2D-C3D | 2.02 | 128.47 | 124.68 |
| 24 | b | 611 | CLA | CHC-C1C-C2C | -2.02 | 121.12 | 126.72 |
| 24 | c | 504 | CLA | CHC-C1C-C2C | -2.02 | 121.13 | 126.72 |
| 28 | L | 102 | SQD | O9-S-C6 | 2.02 | 109.34 | 106.94 |
| 32 | C | 516 | DGD | O2G-C1B-O1B | -2.02 | 118.82 | 123.70 |
| 32 | H | 102 | DGD | O6D-C1D-C2D | 2.02 | 114.63 | 110.35 |
| 26 | b | 619 | BCR | C39-C30-C25 | -2.02 | 107.02 | 110.30 |
| 26 | f | 101 | BCR | C28-C29-C30 | -2.02 | 107.38 | 114.60 |
| 26 | B | 620 | BCR | C10-C11-C12 | -2.02 | 116.91 | 123.22 |
| 28 | l | 101 | SQD | O9-S-C6 | 2.02 | 109.34 | 106.94 |
| 24 | c | 501 | CLA | CMB-C2B-C3B | 2.02 | 128.46 | 124.68 |
| 24 | b | 603 | CLA | O2D-CGD-O1D | -2.02 | 119.89 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 24 | A | 609 | CLA | CHC-C1C-C2C | -2.02 | 121.14 | 126.72 |
| 24 | a | 606 | CLA | CMB-C2B-C3B | 2.02 | 128.45 | 124.68 |
| 24 | b | 613 | CLA | CHD-C4C-C3C | 2.02 | 127.80 | 124.84 |
| 29 | c | 519 | LMG | O1-C7-C8 | -2.02 | 106.03 | 110.90 |
| 30 | E | 102 | LHG | O7-C7-O9 | -2.02 | 118.83 | 123.70 |
| 26 | K | 102 | BCR | C1-C6-C7 | -2.02 | 110.07 | 115.78 |
| 25 | A | 608 | PHO | O1D-CGD-CBD | 2.02 | 128.61 | 124.48 |
| 24 | b | 608[A] | CLA | CHD-C4C-C3C | 2.01 | 127.80 | 124.84 |
| 24 | c | 508 | CLA | CED-O2D-CGD | 2.01 | 120.49 | 115.94 |
| 24 | C | 506 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 24 | d | 402 | CLA | O2A-CGA-O1A | -2.01 | 118.52 | 123.59 |
| 24 | b | 606 | CLA | CMD-C2D-C3D | 2.01 | 128.44 | 124.68 |
| 24 | C | 510 | CLA | CMB-C2B-C3B | 2.01 | 128.44 | 124.68 |
| 29 | Z | 101 | LMG | C6-C5-C4 | -2.01 | 108.30 | 113.00 |
| 24 | b | 604 | CLA | CMB-C2B-C1B | -2.01 | 125.37 | 128.46 |
| 32 | h | 102 | DGD | C2G-O2G-C1B | -2.01 | 112.84 | 117.79 |
| 24 | b | 613 | CLA | O2A-CGA-CBA | 2.01 | 118.21 | 111.91 |
| 26 | B | 620 | BCR | C34-C9-C8 | 2.01 | 121.24 | 118.08 |
| 32 | H | 102 | DGD | O3D-C3D-C2D | -2.01 | 105.71 | 110.35 |
| 24 | B | 607[A] | CLA | CED-O2D-CGD | 2.01 | 120.48 | 115.94 |
| 24 | c | 511 | CLA | CHC-C1C-C2C | -2.01 | 121.17 | 126.72 |
| 29 | z | 101 | LMG | C4-C3-C2 | 2.01 | 114.33 | 110.82 |
| 24 | b | 607 | CLA | C4A-NA-C1A | -2.01 | 105.80 | 106.71 |
| 28 | L | 102 | SQD | O47-C7-O49 | -2.01 | 118.86 | 123.70 |
| 32 | h | 102 | DGD | O5D-C1E-C2E | 2.00 | 111.43 | 108.30 |
| 24 | B | 615 | CLA | C1-O2A-CGA | 2.00 | 121.70 | 116.44 |
| 30 | a | 616 | LHG | O8-C23-O10 | -2.00 | 118.54 | 123.59 |
| 24 | c | 511 | CLA | CHB-C4A-NA | -2.00 | 121.74 | 124.51 |
| 24 | B | 617 | CLA | CHB-C4A-NA | -2.00 | 121.75 | 124.51 |

All (205) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | C | 508 | CLA | NA |
| 24 | C | 508 | CLA | NC |
| 24 | C | 508 | CLA | ND |
| 24 | b | 607 | CLA | NA |
| 24 | b | 607 | CLA | NC |
| 24 | b | 607 | CLA | ND |
| 24 | c | 511 | CLA | NA |
| 24 | c | 511 | CLA | NC |
| 24 | c | 511 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|------------|--------------|------------|-------------|-------------|
| 24 | c | 504 | CLA | NC |
| 24 | c | 504 | CLA | ND |
| 24 | c | 504 | CLA | NA |
| 24 | B | 617 | CLA | NC |
| 24 | B | 617 | CLA | ND |
| 24 | C | 504 | CLA | NC |
| 24 | C | 504 | CLA | ND |
| 24 | C | 504 | CLA | NA |
| 24 | a | 609 | CLA | NC |
| 24 | a | 609 | CLA | ND |
| 24 | a | 609 | CLA | NA |
| 24 | d | 402 | CLA | NC |
| 24 | d | 402 | CLA | ND |
| 24 | d | 402 | CLA | NA |
| 24 | a | 606 | CLA | NA |
| 24 | a | 606 | CLA | NC |
| 24 | a | 606 | CLA | ND |
| 24 | B | 607[A] | CLA | NA |
| 24 | B | 607[A] | CLA | NC |
| 24 | B | 607[A] | CLA | ND |
| 24 | B | 607[B] | CLA | NA |
| 24 | B | 607[B] | CLA | NC |
| 24 | B | 607[B] | CLA | ND |
| 24 | B | 605 | CLA | NC |
| 24 | B | 605 | CLA | ND |
| 24 | B | 605 | CLA | NA |
| 24 | C | 512 | CLA | NC |
| 24 | C | 512 | CLA | ND |
| 24 | c | 513 | CLA | NA |
| 24 | c | 513 | CLA | NC |
| 24 | c | 513 | CLA | ND |
| 24 | C | 501 | CLA | NA |
| 24 | C | 501 | CLA | NC |
| 24 | C | 501 | CLA | ND |
| 24 | c | 507 | CLA | NC |
| 24 | c | 507 | CLA | ND |
| 24 | c | 507 | CLA | NA |
| 24 | b | 605 | CLA | NC |
| 24 | b | 605 | CLA | ND |
| 24 | b | 605 | CLA | NA |
| 24 | B | 613 | CLA | NC |
| 24 | B | 613 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | c | 503 | CLA | NC |
| 24 | c | 503 | CLA | ND |
| 24 | c | 503 | CLA | NA |
| 24 | b | 603 | CLA | NC |
| 24 | b | 603 | CLA | ND |
| 24 | b | 603 | CLA | NA |
| 24 | C | 505 | CLA | NC |
| 24 | C | 505 | CLA | ND |
| 24 | C | 505 | CLA | NA |
| 24 | b | 616 | CLA | NA |
| 24 | b | 616 | CLA | NC |
| 24 | b | 616 | CLA | ND |
| 24 | b | 606 | CLA | NA |
| 24 | b | 606 | CLA | NC |
| 24 | b | 606 | CLA | ND |
| 24 | A | 606 | CLA | NA |
| 24 | A | 606 | CLA | NC |
| 24 | A | 606 | CLA | ND |
| 24 | C | 511 | CLA | NC |
| 24 | C | 511 | CLA | ND |
| 24 | c | 501 | CLA | NC |
| 24 | c | 501 | CLA | ND |
| 24 | C | 510 | CLA | NC |
| 24 | C | 510 | CLA | ND |
| 24 | D | 403 | CLA | NA |
| 24 | D | 403 | CLA | NC |
| 24 | D | 403 | CLA | ND |
| 24 | B | 610 | CLA | NC |
| 24 | B | 610 | CLA | ND |
| 24 | B | 610 | CLA | NA |
| 24 | c | 502 | CLA | NA |
| 24 | c | 502 | CLA | NC |
| 24 | c | 502 | CLA | ND |
| 24 | b | 609 | CLA | NC |
| 24 | b | 609 | CLA | ND |
| 24 | b | 609 | CLA | NA |
| 24 | c | 508 | CLA | NA |
| 24 | c | 508 | CLA | NC |
| 24 | c | 508 | CLA | ND |
| 24 | C | 506 | CLA | NC |
| 24 | C | 506 | CLA | ND |
| 24 | C | 506 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|--------|------|------|
| 24 | C | 513 | CLA | NC |
| 24 | C | 513 | CLA | ND |
| 24 | C | 507 | CLA | NC |
| 24 | C | 507 | CLA | ND |
| 24 | C | 507 | CLA | NA |
| 24 | B | 606 | CLA | NC |
| 24 | B | 606 | CLA | ND |
| 24 | B | 606 | CLA | NA |
| 24 | B | 614 | CLA | NC |
| 24 | B | 614 | CLA | ND |
| 24 | B | 614 | CLA | NA |
| 24 | a | 607 | CLA | NC |
| 24 | a | 607 | CLA | ND |
| 24 | a | 607 | CLA | NA |
| 24 | D | 404 | CLA | NA |
| 24 | D | 404 | CLA | NC |
| 24 | D | 404 | CLA | ND |
| 24 | d | 403 | CLA | NA |
| 24 | d | 403 | CLA | NC |
| 24 | d | 403 | CLA | ND |
| 24 | b | 615 | CLA | NC |
| 24 | b | 615 | CLA | ND |
| 24 | b | 615 | CLA | NA |
| 24 | B | 609 | CLA | NC |
| 24 | B | 609 | CLA | ND |
| 24 | B | 609 | CLA | NA |
| 24 | b | 612 | CLA | NC |
| 24 | b | 612 | CLA | ND |
| 24 | b | 612 | CLA | NA |
| 24 | D | 402 | CLA | NC |
| 24 | D | 402 | CLA | ND |
| 24 | D | 402 | CLA | NA |
| 24 | B | 603 | CLA | NA |
| 24 | B | 603 | CLA | NC |
| 24 | B | 603 | CLA | ND |
| 24 | b | 608[A] | CLA | NA |
| 24 | b | 608[A] | CLA | NC |
| 24 | b | 608[A] | CLA | ND |
| 24 | c | 505 | CLA | NA |
| 24 | c | 505 | CLA | NC |
| 24 | c | 505 | CLA | ND |
| 24 | A | 607 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|--------|------|------|
| 24 | A | 607 | CLA | ND |
| 24 | A | 607 | CLA | NA |
| 24 | B | 604 | CLA | NC |
| 24 | B | 604 | CLA | ND |
| 24 | B | 616 | CLA | NC |
| 24 | B | 616 | CLA | ND |
| 24 | B | 616 | CLA | NA |
| 24 | C | 509 | CLA | NA |
| 24 | C | 509 | CLA | NC |
| 24 | C | 509 | CLA | ND |
| 24 | b | 608[B] | CLA | NA |
| 24 | b | 608[B] | CLA | NC |
| 24 | b | 608[B] | CLA | ND |
| 24 | B | 615 | CLA | NC |
| 24 | B | 615 | CLA | ND |
| 24 | B | 615 | CLA | NA |
| 24 | A | 609 | CLA | NC |
| 24 | A | 609 | CLA | ND |
| 24 | A | 609 | CLA | NA |
| 24 | b | 604 | CLA | NC |
| 24 | b | 604 | CLA | ND |
| 24 | b | 604 | CLA | NA |
| 24 | c | 510 | CLA | NC |
| 24 | c | 510 | CLA | ND |
| 24 | c | 510 | CLA | NA |
| 24 | b | 613 | CLA | NA |
| 24 | b | 613 | CLA | NC |
| 24 | b | 613 | CLA | ND |
| 24 | C | 503 | CLA | NC |
| 24 | C | 503 | CLA | ND |
| 24 | C | 503 | CLA | NA |
| 24 | b | 614 | CLA | NC |
| 24 | b | 614 | CLA | ND |
| 24 | b | 614 | CLA | NA |
| 24 | c | 512 | CLA | NC |
| 24 | c | 512 | CLA | ND |
| 24 | B | 612 | CLA | NA |
| 24 | B | 612 | CLA | NC |
| 24 | B | 612 | CLA | ND |
| 24 | b | 618 | CLA | NC |
| 24 | b | 618 | CLA | ND |
| 24 | a | 615 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | a | 615 | CLA | ND |
| 24 | a | 615 | CLA | NA |
| 24 | b | 617 | CLA | NC |
| 24 | b | 617 | CLA | ND |
| 24 | c | 506 | CLA | NC |
| 24 | c | 506 | CLA | ND |
| 24 | c | 506 | CLA | NA |
| 24 | B | 611 | CLA | NA |
| 24 | B | 611 | CLA | NC |
| 24 | B | 611 | CLA | ND |
| 24 | c | 509 | CLA | NC |
| 24 | c | 509 | CLA | ND |
| 24 | c | 509 | CLA | NA |
| 24 | B | 608 | CLA | NC |
| 24 | B | 608 | CLA | ND |
| 24 | B | 608 | CLA | NA |
| 24 | B | 602 | CLA | NC |
| 24 | B | 602 | CLA | ND |
| 24 | B | 602 | CLA | NA |
| 24 | b | 610 | CLA | NC |
| 24 | b | 610 | CLA | ND |
| 24 | b | 610 | CLA | NA |
| 24 | b | 611 | CLA | NC |
| 24 | b | 611 | CLA | ND |
| 24 | b | 611 | CLA | NA |
| 24 | C | 502 | CLA | NA |
| 24 | C | 502 | CLA | NC |
| 24 | C | 502 | CLA | ND |

All (2157) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 30 | D | 407 | LHG | O1-C1-C2-C3 |
| 30 | D | 407 | LHG | O2-C2-C3-O3 |
| 30 | D | 407 | LHG | C3-O3-P-O5 |
| 30 | D | 407 | LHG | C4-O6-P-O4 |
| 30 | D | 407 | LHG | C4-O6-P-O5 |
| 28 | x | 101 | SQD | C2-C1-O6-C44 |
| 28 | x | 101 | SQD | O5-C1-O6-C44 |
| 26 | B | 620 | BCR | C5-C6-C7-C8 |
| 26 | B | 620 | BCR | C11-C10-C9-C8 |
| 26 | B | 620 | BCR | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | B | 620 | BCR | C11-C12-C13-C14 |
| 26 | B | 620 | BCR | C14-C15-C16-C17 |
| 26 | B | 620 | BCR | C16-C17-C18-C19 |
| 26 | B | 620 | BCR | C16-C17-C18-C36 |
| 26 | B | 620 | BCR | C17-C18-C19-C20 |
| 26 | B | 620 | BCR | C36-C18-C19-C20 |
| 26 | B | 620 | BCR | C18-C19-C20-C21 |
| 26 | B | 620 | BCR | C19-C20-C21-C22 |
| 26 | B | 620 | BCR | C20-C21-C22-C23 |
| 26 | B | 620 | BCR | C20-C21-C22-C37 |
| 26 | B | 620 | BCR | C37-C22-C23-C24 |
| 24 | b | 607 | CLA | C2-C3-C5-C6 |
| 24 | b | 607 | CLA | C4-C3-C5-C6 |
| 26 | I | 101 | BCR | C6-C7-C8-C9 |
| 26 | I | 101 | BCR | C7-C8-C9-C34 |
| 26 | I | 101 | BCR | C11-C10-C9-C8 |
| 26 | I | 101 | BCR | C12-C13-C14-C15 |
| 26 | I | 101 | BCR | C35-C13-C14-C15 |
| 26 | I | 101 | BCR | C14-C15-C16-C17 |
| 26 | I | 101 | BCR | C36-C18-C19-C20 |
| 26 | I | 101 | BCR | C18-C19-C20-C21 |
| 26 | I | 101 | BCR | C20-C21-C22-C23 |
| 26 | c | 515 | BCR | C6-C7-C8-C9 |
| 26 | c | 515 | BCR | C12-C13-C14-C15 |
| 26 | c | 515 | BCR | C35-C13-C14-C15 |
| 26 | c | 515 | BCR | C14-C15-C16-C17 |
| 26 | c | 515 | BCR | C16-C17-C18-C36 |
| 26 | c | 515 | BCR | C36-C18-C19-C20 |
| 26 | c | 515 | BCR | C18-C19-C20-C21 |
| 26 | c | 515 | BCR | C20-C21-C22-C23 |
| 26 | c | 515 | BCR | C37-C22-C23-C24 |
| 26 | h | 101 | BCR | C6-C7-C8-C9 |
| 26 | h | 101 | BCR | C7-C8-C9-C34 |
| 26 | h | 101 | BCR | C11-C10-C9-C8 |
| 26 | h | 101 | BCR | C11-C10-C9-C34 |
| 26 | h | 101 | BCR | C10-C11-C12-C13 |
| 26 | h | 101 | BCR | C11-C12-C13-C14 |
| 26 | h | 101 | BCR | C12-C13-C14-C15 |
| 26 | h | 101 | BCR | C13-C14-C15-C16 |
| 26 | h | 101 | BCR | C14-C15-C16-C17 |
| 26 | h | 101 | BCR | C16-C17-C18-C19 |
| 26 | h | 101 | BCR | C16-C17-C18-C36 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | h | 101 | BCR | C36-C18-C19-C20 |
| 26 | h | 101 | BCR | C18-C19-C20-C21 |
| 26 | h | 101 | BCR | C20-C21-C22-C23 |
| 26 | h | 101 | BCR | C20-C21-C22-C37 |
| 26 | h | 101 | BCR | C21-C22-C23-C24 |
| 26 | c | 514 | BCR | C5-C6-C7-C8 |
| 26 | c | 514 | BCR | C6-C7-C8-C9 |
| 26 | c | 514 | BCR | C7-C8-C9-C10 |
| 26 | c | 514 | BCR | C11-C10-C9-C8 |
| 26 | c | 514 | BCR | C11-C10-C9-C34 |
| 26 | c | 514 | BCR | C10-C11-C12-C13 |
| 26 | c | 514 | BCR | C12-C13-C14-C15 |
| 26 | c | 514 | BCR | C35-C13-C14-C15 |
| 26 | c | 514 | BCR | C14-C15-C16-C17 |
| 26 | c | 514 | BCR | C15-C16-C17-C18 |
| 26 | c | 514 | BCR | C16-C17-C18-C19 |
| 26 | c | 514 | BCR | C16-C17-C18-C36 |
| 26 | c | 514 | BCR | C17-C18-C19-C20 |
| 26 | c | 514 | BCR | C36-C18-C19-C20 |
| 26 | c | 514 | BCR | C18-C19-C20-C21 |
| 26 | c | 514 | BCR | C20-C21-C22-C23 |
| 26 | c | 514 | BCR | C20-C21-C22-C37 |
| 26 | c | 514 | BCR | C21-C22-C23-C24 |
| 26 | c | 514 | BCR | C22-C23-C24-C25 |
| 26 | c | 514 | BCR | C23-C24-C25-C26 |
| 32 | C | 515 | DGD | O6D-C1D-O3G-C3G |
| 28 | l | 101 | SQD | C8-C7-O47-C45 |
| 28 | l | 101 | SQD | O5-C5-C6-S |
| 24 | C | 504 | CLA | CHA-CBD-CGD-O1D |
| 26 | B | 619 | BCR | C5-C6-C7-C8 |
| 26 | B | 619 | BCR | C7-C8-C9-C34 |
| 26 | B | 619 | BCR | C11-C10-C9-C8 |
| 26 | B | 619 | BCR | C11-C10-C9-C34 |
| 26 | B | 619 | BCR | C10-C11-C12-C13 |
| 26 | B | 619 | BCR | C14-C15-C16-C17 |
| 26 | B | 619 | BCR | C16-C17-C18-C19 |
| 26 | B | 619 | BCR | C16-C17-C18-C36 |
| 26 | B | 619 | BCR | C18-C19-C20-C21 |
| 26 | B | 619 | BCR | C20-C21-C22-C23 |
| 26 | B | 619 | BCR | C20-C21-C22-C37 |
| 26 | B | 619 | BCR | C21-C22-C23-C24 |
| 26 | H | 101 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 26 | H | 101 | BCR | C11-C10-C9-C8 |
| 26 | H | 101 | BCR | C11-C10-C9-C34 |
| 26 | H | 101 | BCR | C10-C11-C12-C13 |
| 26 | H | 101 | BCR | C11-C12-C13-C35 |
| 26 | H | 101 | BCR | C14-C15-C16-C17 |
| 26 | H | 101 | BCR | C15-C16-C17-C18 |
| 26 | H | 101 | BCR | C16-C17-C18-C19 |
| 26 | H | 101 | BCR | C16-C17-C18-C36 |
| 26 | H | 101 | BCR | C36-C18-C19-C20 |
| 26 | H | 101 | BCR | C18-C19-C20-C21 |
| 26 | H | 101 | BCR | C20-C21-C22-C23 |
| 26 | H | 101 | BCR | C20-C21-C22-C37 |
| 26 | H | 101 | BCR | C22-C23-C24-C25 |
| 24 | B | 607[A] | CLA | CHA-CBD-CGD-O2D |
| 24 | B | 607[B] | CLA | CHA-CBD-CGD-O2D |
| 26 | a | 610 | BCR | C7-C8-C9-C10 |
| 26 | a | 610 | BCR | C11-C10-C9-C34 |
| 26 | a | 610 | BCR | C11-C12-C13-C14 |
| 26 | a | 610 | BCR | C12-C13-C14-C15 |
| 26 | a | 610 | BCR | C35-C13-C14-C15 |
| 26 | a | 610 | BCR | C14-C15-C16-C17 |
| 26 | a | 610 | BCR | C15-C16-C17-C18 |
| 26 | a | 610 | BCR | C17-C18-C19-C20 |
| 26 | a | 610 | BCR | C18-C19-C20-C21 |
| 26 | a | 610 | BCR | C20-C21-C22-C23 |
| 26 | a | 610 | BCR | C20-C21-C22-C37 |
| 26 | a | 610 | BCR | C21-C22-C23-C24 |
| 24 | C | 512 | CLA | C1A-C2A-CAA-CBA |
| 26 | K | 101 | BCR | C7-C8-C9-C10 |
| 26 | K | 101 | BCR | C7-C8-C9-C34 |
| 26 | K | 101 | BCR | C10-C11-C12-C13 |
| 26 | K | 101 | BCR | C11-C12-C13-C35 |
| 26 | K | 101 | BCR | C12-C13-C14-C15 |
| 26 | K | 101 | BCR | C14-C15-C16-C17 |
| 26 | K | 101 | BCR | C16-C17-C18-C19 |
| 26 | K | 101 | BCR | C16-C17-C18-C36 |
| 26 | K | 101 | BCR | C17-C18-C19-C20 |
| 26 | K | 101 | BCR | C36-C18-C19-C20 |
| 26 | K | 101 | BCR | C20-C21-C22-C37 |
| 26 | T | 101 | BCR | C6-C7-C8-C9 |
| 26 | T | 101 | BCR | C11-C10-C9-C8 |
| 26 | T | 101 | BCR | C11-C10-C9-C34 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | T | 101 | BCR | C10-C11-C12-C13 |
| 26 | T | 101 | BCR | C11-C12-C13-C14 |
| 26 | T | 101 | BCR | C12-C13-C14-C15 |
| 26 | T | 101 | BCR | C14-C15-C16-C17 |
| 26 | T | 101 | BCR | C16-C17-C18-C19 |
| 26 | T | 101 | BCR | C16-C17-C18-C36 |
| 26 | T | 101 | BCR | C18-C19-C20-C21 |
| 26 | T | 101 | BCR | C37-C22-C23-C24 |
| 26 | T | 101 | BCR | C22-C23-C24-C25 |
| 26 | c | 521 | BCR | C6-C7-C8-C9 |
| 26 | c | 521 | BCR | C7-C8-C9-C34 |
| 26 | c | 521 | BCR | C11-C10-C9-C8 |
| 26 | c | 521 | BCR | C10-C11-C12-C13 |
| 26 | c | 521 | BCR | C12-C13-C14-C15 |
| 26 | c | 521 | BCR | C13-C14-C15-C16 |
| 26 | c | 521 | BCR | C14-C15-C16-C17 |
| 26 | c | 521 | BCR | C18-C19-C20-C21 |
| 26 | c | 521 | BCR | C20-C21-C22-C37 |
| 26 | c | 521 | BCR | C22-C23-C24-C25 |
| 26 | c | 521 | BCR | C23-C24-C25-C30 |
| 26 | F | 101 | BCR | C10-C11-C12-C13 |
| 26 | F | 101 | BCR | C11-C12-C13-C14 |
| 26 | F | 101 | BCR | C12-C13-C14-C15 |
| 26 | F | 101 | BCR | C35-C13-C14-C15 |
| 26 | F | 101 | BCR | C13-C14-C15-C16 |
| 26 | F | 101 | BCR | C14-C15-C16-C17 |
| 26 | F | 101 | BCR | C16-C17-C18-C19 |
| 26 | F | 101 | BCR | C16-C17-C18-C36 |
| 26 | F | 101 | BCR | C36-C18-C19-C20 |
| 26 | F | 101 | BCR | C18-C19-C20-C21 |
| 26 | F | 101 | BCR | C21-C22-C23-C24 |
| 26 | F | 101 | BCR | C37-C22-C23-C24 |
| 26 | F | 101 | BCR | C22-C23-C24-C25 |
| 27 | A | 611 | PL9 | C7-C8-C9-C10 |
| 27 | A | 611 | PL9 | C12-C11-C9-C10 |
| 27 | A | 611 | PL9 | C12-C13-C14-C15 |
| 27 | A | 611 | PL9 | C14-C16-C17-C18 |
| 27 | A | 611 | PL9 | C19-C21-C22-C23 |
| 27 | A | 611 | PL9 | C22-C23-C24-C25 |
| 27 | A | 611 | PL9 | C32-C33-C34-C35 |
| 27 | A | 611 | PL9 | C35-C34-C36-C37 |
| 29 | Z | 101 | LMG | O6-C1-O1-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | Z | 101 | LMG | O1-C7-C8-O7 |
| 29 | Z | 101 | LMG | O9-C10-O7-C8 |
| 29 | Z | 101 | LMG | C11-C10-O7-C8 |
| 26 | k | 101 | BCR | C7-C8-C9-C34 |
| 26 | k | 101 | BCR | C11-C10-C9-C8 |
| 26 | k | 101 | BCR | C10-C11-C12-C13 |
| 26 | k | 101 | BCR | C11-C12-C13-C35 |
| 26 | k | 101 | BCR | C12-C13-C14-C15 |
| 26 | k | 101 | BCR | C16-C17-C18-C19 |
| 26 | k | 101 | BCR | C16-C17-C18-C36 |
| 26 | k | 101 | BCR | C36-C18-C19-C20 |
| 26 | k | 101 | BCR | C20-C21-C22-C23 |
| 26 | k | 101 | BCR | C20-C21-C22-C37 |
| 24 | b | 603 | CLA | C1A-C2A-CAA-CBA |
| 24 | b | 603 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 603 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 505 | CLA | C1A-C2A-CAA-CBA |
| 24 | b | 616 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 616 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 616 | CLA | CAD-CBD-CGD-O2D |
| 26 | A | 610 | BCR | C11-C12-C13-C14 |
| 26 | A | 610 | BCR | C12-C13-C14-C15 |
| 26 | A | 610 | BCR | C35-C13-C14-C15 |
| 26 | A | 610 | BCR | C13-C14-C15-C16 |
| 26 | A | 610 | BCR | C14-C15-C16-C17 |
| 26 | A | 610 | BCR | C16-C17-C18-C19 |
| 26 | A | 610 | BCR | C16-C17-C18-C36 |
| 26 | A | 610 | BCR | C17-C18-C19-C20 |
| 26 | A | 610 | BCR | C18-C19-C20-C21 |
| 26 | A | 610 | BCR | C20-C21-C22-C37 |
| 26 | A | 610 | BCR | C23-C24-C25-C30 |
| 26 | K | 102 | BCR | C6-C7-C8-C9 |
| 26 | K | 102 | BCR | C7-C8-C9-C10 |
| 26 | K | 102 | BCR | C7-C8-C9-C34 |
| 26 | K | 102 | BCR | C10-C11-C12-C13 |
| 26 | K | 102 | BCR | C11-C12-C13-C14 |
| 26 | K | 102 | BCR | C13-C14-C15-C16 |
| 26 | K | 102 | BCR | C14-C15-C16-C17 |
| 26 | K | 102 | BCR | C17-C18-C19-C20 |
| 26 | K | 102 | BCR | C18-C19-C20-C21 |
| 26 | K | 102 | BCR | C20-C21-C22-C37 |
| 26 | K | 102 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | K | 102 | BCR | C37-C22-C23-C24 |
| 26 | K | 102 | BCR | C22-C23-C24-C25 |
| 26 | B | 618 | BCR | C1-C6-C7-C8 |
| 26 | B | 618 | BCR | C9-C10-C11-C12 |
| 26 | B | 618 | BCR | C10-C11-C12-C13 |
| 26 | B | 618 | BCR | C11-C12-C13-C14 |
| 26 | B | 618 | BCR | C11-C12-C13-C35 |
| 26 | B | 618 | BCR | C14-C15-C16-C17 |
| 26 | B | 618 | BCR | C15-C16-C17-C18 |
| 26 | B | 618 | BCR | C16-C17-C18-C19 |
| 26 | B | 618 | BCR | C16-C17-C18-C36 |
| 26 | B | 618 | BCR | C36-C18-C19-C20 |
| 26 | B | 618 | BCR | C20-C21-C22-C23 |
| 26 | B | 618 | BCR | C20-C21-C22-C37 |
| 26 | B | 618 | BCR | C21-C22-C23-C24 |
| 26 | B | 618 | BCR | C22-C23-C24-C25 |
| 26 | B | 618 | BCR | C23-C24-C25-C26 |
| 24 | c | 502 | CLA | CHA-CBD-CGD-O1D |
| 32 | d | 405 | DGD | C2B-C1B-O2G-C2G |
| 32 | d | 405 | DGD | O1B-C1B-O2G-C2G |
| 32 | d | 405 | DGD | C2E-C1E-O5D-C6D |
| 24 | b | 609 | CLA | C1A-C2A-CAA-CBA |
| 24 | b | 609 | CLA | C3A-C2A-CAA-CBA |
| 26 | b | 619 | BCR | C9-C10-C11-C12 |
| 26 | b | 619 | BCR | C10-C11-C12-C13 |
| 26 | b | 619 | BCR | C11-C12-C13-C14 |
| 26 | b | 619 | BCR | C11-C12-C13-C35 |
| 26 | b | 619 | BCR | C12-C13-C14-C15 |
| 26 | b | 619 | BCR | C35-C13-C14-C15 |
| 26 | b | 619 | BCR | C14-C15-C16-C17 |
| 26 | b | 619 | BCR | C15-C16-C17-C18 |
| 26 | b | 619 | BCR | C16-C17-C18-C19 |
| 26 | b | 619 | BCR | C16-C17-C18-C36 |
| 26 | b | 619 | BCR | C18-C19-C20-C21 |
| 26 | b | 619 | BCR | C19-C20-C21-C22 |
| 26 | b | 619 | BCR | C21-C22-C23-C24 |
| 26 | b | 619 | BCR | C22-C23-C24-C25 |
| 24 | c | 508 | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 606 | CLA | C2-C3-C5-C6 |
| 24 | B | 606 | CLA | C4-C3-C5-C6 |
| 26 | t | 101 | BCR | C7-C8-C9-C34 |
| 26 | t | 101 | BCR | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | t | 101 | BCR | C11-C12-C13-C14 |
| 26 | t | 101 | BCR | C12-C13-C14-C15 |
| 26 | t | 101 | BCR | C35-C13-C14-C15 |
| 26 | t | 101 | BCR | C14-C15-C16-C17 |
| 26 | t | 101 | BCR | C16-C17-C18-C19 |
| 26 | t | 101 | BCR | C16-C17-C18-C36 |
| 26 | t | 101 | BCR | C18-C19-C20-C21 |
| 26 | t | 101 | BCR | C21-C22-C23-C24 |
| 26 | t | 101 | BCR | C37-C22-C23-C24 |
| 26 | t | 101 | BCR | C22-C23-C24-C25 |
| 26 | t | 101 | BCR | C23-C24-C25-C30 |
| 33 | v | 201 | HEM | C2D-C3D-CAD-CBD |
| 28 | a | 614 | SQD | O6-C44-C45-O47 |
| 29 | z | 101 | LMG | O6-C1-O1-C7 |
| 29 | z | 101 | LMG | O1-C7-C8-O7 |
| 29 | z | 101 | LMG | O9-C10-O7-C8 |
| 29 | z | 101 | LMG | C11-C10-O7-C8 |
| 28 | X | 101 | SQD | C2-C1-O6-C44 |
| 28 | X | 101 | SQD | O5-C1-O6-C44 |
| 27 | a | 611 | PL9 | C12-C11-C9-C10 |
| 27 | a | 611 | PL9 | C12-C13-C14-C15 |
| 27 | a | 611 | PL9 | C14-C16-C17-C18 |
| 27 | a | 611 | PL9 | C18-C19-C21-C22 |
| 27 | a | 611 | PL9 | C19-C21-C22-C23 |
| 27 | a | 611 | PL9 | C22-C23-C24-C25 |
| 27 | a | 611 | PL9 | C25-C24-C26-C27 |
| 27 | a | 611 | PL9 | C24-C26-C27-C28 |
| 26 | b | 620 | BCR | C5-C6-C7-C8 |
| 26 | b | 620 | BCR | C11-C12-C13-C35 |
| 26 | b | 620 | BCR | C12-C13-C14-C15 |
| 26 | b | 620 | BCR | C14-C15-C16-C17 |
| 26 | b | 620 | BCR | C16-C17-C18-C19 |
| 26 | b | 620 | BCR | C16-C17-C18-C36 |
| 26 | b | 620 | BCR | C17-C18-C19-C20 |
| 26 | b | 620 | BCR | C36-C18-C19-C20 |
| 26 | b | 620 | BCR | C18-C19-C20-C21 |
| 26 | b | 620 | BCR | C20-C21-C22-C23 |
| 26 | b | 620 | BCR | C20-C21-C22-C37 |
| 26 | b | 620 | BCR | C21-C22-C23-C24 |
| 28 | b | 601 | SQD | O5-C1-O6-C44 |
| 28 | b | 601 | SQD | C8-C7-O47-C45 |
| 28 | b | 601 | SQD | O5-C5-C6-S |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 28 | B | 622 | SQD | O5-C1-O6-C44 |
| 28 | B | 622 | SQD | C8-C7-O47-C45 |
| 28 | B | 622 | SQD | O5-C5-C6-S |
| 30 | e | 101 | LHG | C8-C7-O7-C5 |
| 30 | e | 101 | LHG | C24-C23-O8-C6 |
| 30 | L | 101 | LHG | C4-O6-P-O4 |
| 30 | l | 102 | LHG | C4-O6-P-O4 |
| 27 | D | 405 | PL9 | C7-C8-C9-C10 |
| 27 | D | 405 | PL9 | C12-C13-C14-C15 |
| 27 | D | 405 | PL9 | C17-C18-C19-C20 |
| 27 | D | 405 | PL9 | C22-C23-C24-C25 |
| 27 | D | 405 | PL9 | C42-C43-C44-C46 |
| 27 | D | 405 | PL9 | C44-C46-C47-C48 |
| 27 | d | 404 | PL9 | C17-C18-C19-C20 |
| 27 | d | 404 | PL9 | C25-C24-C26-C27 |
| 27 | d | 404 | PL9 | C27-C28-C29-C30 |
| 27 | d | 404 | PL9 | C42-C43-C44-C46 |
| 24 | B | 603 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 608[A] | CLA | CHA-CBD-CGD-O2D |
| 28 | A | 614 | SQD | O6-C44-C45-O47 |
| 26 | C | 514 | BCR | C5-C6-C7-C8 |
| 26 | C | 514 | BCR | C11-C10-C9-C8 |
| 26 | C | 514 | BCR | C11-C10-C9-C34 |
| 26 | C | 514 | BCR | C10-C11-C12-C13 |
| 26 | C | 514 | BCR | C13-C14-C15-C16 |
| 26 | C | 514 | BCR | C14-C15-C16-C17 |
| 26 | C | 514 | BCR | C16-C17-C18-C19 |
| 26 | C | 514 | BCR | C16-C17-C18-C36 |
| 26 | C | 514 | BCR | C36-C18-C19-C20 |
| 26 | C | 514 | BCR | C18-C19-C20-C21 |
| 26 | C | 514 | BCR | C20-C21-C22-C23 |
| 26 | C | 514 | BCR | C20-C21-C22-C37 |
| 26 | C | 514 | BCR | C22-C23-C24-C25 |
| 26 | C | 514 | BCR | C23-C24-C25-C26 |
| 33 | V | 201 | HEM | C2D-C3D-CAD-CBD |
| 33 | V | 201 | HEM | C4D-C3D-CAD-CBD |
| 24 | A | 607 | CLA | CHA-CBD-CGD-O2D |
| 24 | b | 608[B] | CLA | CHA-CBD-CGD-O2D |
| 24 | B | 615 | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 615 | CLA | CAD-CBD-CGD-O2D |
| 32 | E | 101 | DGD | C2B-C1B-O2G-C2G |
| 24 | A | 609 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | f | 101 | BCR | C10-C11-C12-C13 |
| 26 | f | 101 | BCR | C11-C12-C13-C35 |
| 26 | f | 101 | BCR | C12-C13-C14-C15 |
| 26 | f | 101 | BCR | C35-C13-C14-C15 |
| 26 | f | 101 | BCR | C14-C15-C16-C17 |
| 26 | f | 101 | BCR | C16-C17-C18-C19 |
| 26 | f | 101 | BCR | C16-C17-C18-C36 |
| 26 | f | 101 | BCR | C18-C19-C20-C21 |
| 26 | f | 101 | BCR | C20-C21-C22-C37 |
| 26 | f | 101 | BCR | C22-C23-C24-C25 |
| 26 | f | 101 | BCR | C23-C24-C25-C26 |
| 26 | b | 621 | BCR | C5-C6-C7-C8 |
| 26 | b | 621 | BCR | C7-C8-C9-C34 |
| 26 | b | 621 | BCR | C11-C10-C9-C8 |
| 26 | b | 621 | BCR | C11-C10-C9-C34 |
| 26 | b | 621 | BCR | C12-C13-C14-C15 |
| 26 | b | 621 | BCR | C35-C13-C14-C15 |
| 26 | b | 621 | BCR | C14-C15-C16-C17 |
| 26 | b | 621 | BCR | C16-C17-C18-C19 |
| 26 | b | 621 | BCR | C16-C17-C18-C36 |
| 26 | b | 621 | BCR | C36-C18-C19-C20 |
| 26 | b | 621 | BCR | C18-C19-C20-C21 |
| 26 | b | 621 | BCR | C19-C20-C21-C22 |
| 26 | b | 621 | BCR | C20-C21-C22-C23 |
| 26 | b | 621 | BCR | C20-C21-C22-C37 |
| 24 | a | 615 | CLA | CHA-CBD-CGD-O1D |
| 24 | a | 615 | CLA | CHA-CBD-CGD-O2D |
| 30 | d | 407 | LHG | O1-C1-C2-C3 |
| 30 | d | 407 | LHG | C3-O3-P-O4 |
| 30 | d | 407 | LHG | C3-O3-P-O5 |
| 28 | L | 102 | SQD | C8-C7-O47-C45 |
| 28 | L | 102 | SQD | O5-C5-C6-S |
| 24 | B | 608 | CLA | C1A-C2A-CAA-CBA |
| 24 | B | 608 | CLA | C3A-C2A-CAA-CBA |
| 24 | B | 602 | CLA | C1A-C2A-CAA-CBA |
| 24 | B | 602 | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 602 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 611 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 502 | CLA | CHA-CBD-CGD-O1D |
| 29 | z | 101 | LMG | C29-C28-O8-C9 |
| 24 | b | 611 | CLA | CBD-CGD-O2D-CED |
| 28 | x | 101 | SQD | O10-C23-O48-C46 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 28 | X | 101 | SQD | O10-C23-O48-C46 |
| 30 | e | 101 | LHG | O10-C23-O8-C6 |
| 30 | E | 102 | LHG | O10-C23-O8-C6 |
| 24 | b | 611 | CLA | O1D-CGD-O2D-CED |
| 28 | x | 101 | SQD | C24-C23-O48-C46 |
| 28 | X | 101 | SQD | C24-C23-O48-C46 |
| 30 | E | 102 | LHG | C24-C23-O8-C6 |
| 29 | Z | 101 | LMG | C29-C28-O8-C9 |
| 24 | b | 606 | CLA | CBD-CGD-O2D-CED |
| 24 | C | 503 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 617 | CLA | O1A-CGA-O2A-C1 |
| 24 | b | 618 | CLA | O1A-CGA-O2A-C1 |
| 29 | Z | 101 | LMG | O10-C28-O8-C9 |
| 29 | z | 101 | LMG | O10-C28-O8-C9 |
| 24 | b | 612 | CLA | O1D-CGD-O2D-CED |
| 29 | A | 613 | LMG | O9-C10-O7-C8 |
| 28 | b | 601 | SQD | O49-C7-O47-C45 |
| 28 | B | 622 | SQD | O49-C7-O47-C45 |
| 32 | E | 101 | DGD | O1B-C1B-O2G-C2G |
| 24 | b | 616 | CLA | C3-C5-C6-C7 |
| 24 | B | 615 | CLA | C3-C5-C6-C7 |
| 24 | B | 609 | CLA | C2C-C3C-CAC-CBC |
| 30 | E | 102 | LHG | C8-C7-O7-C5 |
| 24 | c | 510 | CLA | CBD-CGD-O2D-CED |
| 29 | C | 519 | LMG | O6-C5-C6-O5 |
| 27 | A | 611 | PL9 | C25-C24-C26-C27 |
| 27 | A | 611 | PL9 | C18-C19-C21-C22 |
| 24 | b | 612 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 607[A] | CLA | C2A-CAA-CBA-CGA |
| 24 | B | 607[B] | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 608[A] | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 608[B] | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 603 | CLA | C3-C5-C6-C7 |
| 24 | B | 602 | CLA | C3-C5-C6-C7 |
| 24 | b | 618 | CLA | CBA-CGA-O2A-C1 |
| 27 | A | 611 | PL9 | C27-C28-C29-C30 |
| 27 | A | 611 | PL9 | C37-C38-C39-C40 |
| 27 | A | 611 | PL9 | C42-C43-C44-C45 |
| 27 | a | 611 | PL9 | C7-C8-C9-C10 |
| 27 | a | 611 | PL9 | C27-C28-C29-C30 |
| 27 | a | 611 | PL9 | C32-C33-C34-C35 |
| 27 | a | 611 | PL9 | C37-C38-C39-C40 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | a | 611 | PL9 | C42-C43-C44-C45 |
| 27 | D | 405 | PL9 | C32-C33-C34-C35 |
| 27 | D | 405 | PL9 | C37-C38-C39-C40 |
| 27 | d | 404 | PL9 | C7-C8-C9-C10 |
| 27 | d | 404 | PL9 | C12-C13-C14-C15 |
| 27 | d | 404 | PL9 | C22-C23-C24-C25 |
| 27 | d | 404 | PL9 | C32-C33-C34-C35 |
| 27 | d | 404 | PL9 | C37-C38-C39-C40 |
| 24 | b | 607 | CLA | O1D-CGD-O2D-CED |
| 24 | B | 602 | CLA | O1D-CGD-O2D-CED |
| 28 | l | 101 | SQD | O49-C7-O47-C45 |
| 30 | E | 102 | LHG | O9-C7-O7-C5 |
| 28 | L | 102 | SQD | O49-C7-O47-C45 |
| 26 | B | 620 | BCR | C13-C14-C15-C16 |
| 26 | I | 101 | BCR | C13-C14-C15-C16 |
| 26 | I | 101 | BCR | C19-C20-C21-C22 |
| 26 | h | 101 | BCR | C15-C16-C17-C18 |
| 26 | c | 514 | BCR | C19-C20-C21-C22 |
| 26 | B | 619 | BCR | C15-C16-C17-C18 |
| 26 | H | 101 | BCR | C19-C20-C21-C22 |
| 26 | T | 101 | BCR | C15-C16-C17-C18 |
| 26 | F | 101 | BCR | C15-C16-C17-C18 |
| 26 | k | 101 | BCR | C15-C16-C17-C18 |
| 26 | A | 610 | BCR | C9-C10-C11-C12 |
| 26 | C | 514 | BCR | C15-C16-C17-C18 |
| 26 | f | 101 | BCR | C13-C14-C15-C16 |
| 32 | H | 102 | DGD | O6E-C5E-C6E-O5E |
| 24 | b | 607 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 605 | CLA | CBD-CGD-O2D-CED |
| 24 | c | 503 | CLA | CBD-CGD-O2D-CED |
| 24 | b | 609 | CLA | CBD-CGD-O2D-CED |
| 24 | C | 513 | CLA | CBD-CGD-O2D-CED |
| 24 | A | 609 | CLA | CBD-CGD-O2D-CED |
| 30 | d | 407 | LHG | O2-C2-C3-O3 |
| 24 | B | 617 | CLA | CBA-CGA-O2A-C1 |
| 29 | j | 101 | LMG | O6-C5-C6-O5 |
| 24 | a | 606 | CLA | O1D-CGD-O2D-CED |
| 24 | b | 616 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 602 | CLA | CBD-CGD-O2D-CED |
| 29 | D | 408 | LMG | O6-C5-C6-O5 |
| 32 | c | 516 | DGD | C4D-C5D-C6D-O5D |
| 29 | c | 520 | LMG | O6-C5-C6-O5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | A | 611 | PL9 | C47-C48-C49-C51 |
| 27 | D | 405 | PL9 | C47-C48-C49-C50 |
| 27 | A | 611 | PL9 | C38-C39-C41-C42 |
| 27 | a | 611 | PL9 | C38-C39-C41-C42 |
| 30 | D | 407 | LHG | C14-C15-C16-C17 |
| 24 | c | 505 | CLA | O1A-CGA-O2A-C1 |
| 32 | H | 102 | DGD | O6E-C1E-O5D-C6D |
| 27 | A | 611 | PL9 | C24-C26-C27-C28 |
| 27 | d | 404 | PL9 | C29-C31-C32-C33 |
| 27 | d | 404 | PL9 | C44-C46-C47-C48 |
| 32 | H | 102 | DGD | C6B-C7B-C8B-C9B |
| 27 | A | 611 | PL9 | C17-C18-C19-C20 |
| 24 | B | 616 | CLA | O1D-CGD-O2D-CED |
| 30 | D | 407 | LHG | C1-C2-C3-O3 |
| 32 | c | 516 | DGD | O6E-C5E-C6E-O5E |
| 30 | d | 407 | LHG | C1-C2-C3-O3 |
| 29 | C | 519 | LMG | C4-C5-C6-O5 |
| 29 | c | 520 | LMG | C4-C5-C6-O5 |
| 24 | C | 509 | CLA | O1D-CGD-O2D-CED |
| 28 | l | 101 | SQD | C24-C23-O48-C46 |
| 32 | c | 518 | DGD | C2A-C1A-O1G-C1G |
| 28 | L | 102 | SQD | C24-C23-O48-C46 |
| 32 | h | 102 | DGD | O6E-C5E-C6E-O5E |
| 24 | a | 606 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 612 | CLA | CBD-CGD-O2D-CED |
| 32 | h | 102 | DGD | C6B-C7B-C8B-C9B |
| 26 | B | 620 | BCR | C15-C16-C17-C18 |
| 26 | h | 101 | BCR | C19-C20-C21-C22 |
| 26 | a | 610 | BCR | C13-C14-C15-C16 |
| 32 | H | 102 | DGD | C4E-C5E-C6E-O5E |
| 29 | Z | 101 | LMG | C2-C1-O1-C7 |
| 29 | z | 101 | LMG | C2-C1-O1-C7 |
| 32 | c | 518 | DGD | O1A-C1A-O1G-C1G |
| 24 | c | 504 | CLA | C11-C12-C13-C14 |
| 24 | C | 504 | CLA | C11-C12-C13-C14 |
| 24 | C | 501 | CLA | C11-C12-C13-C14 |
| 24 | b | 603 | CLA | C11-C10-C8-C9 |
| 24 | c | 501 | CLA | C11-C12-C13-C14 |
| 24 | c | 502 | CLA | C14-C13-C15-C16 |
| 24 | C | 509 | CLA | C6-C7-C8-C9 |
| 24 | c | 509 | CLA | C6-C7-C8-C9 |
| 24 | B | 602 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | C | 502 | CLA | C14-C13-C15-C16 |
| 26 | I | 101 | BCR | C37-C22-C23-C24 |
| 26 | c | 515 | BCR | C7-C8-C9-C34 |
| 26 | h | 101 | BCR | C11-C12-C13-C35 |
| 26 | c | 514 | BCR | C7-C8-C9-C34 |
| 26 | B | 619 | BCR | C36-C18-C19-C20 |
| 26 | T | 101 | BCR | C7-C8-C9-C34 |
| 26 | F | 101 | BCR | C11-C12-C13-C35 |
| 26 | A | 610 | BCR | C11-C12-C13-C35 |
| 26 | A | 610 | BCR | C36-C18-C19-C20 |
| 26 | A | 610 | BCR | C37-C22-C23-C24 |
| 26 | B | 618 | BCR | C37-C22-C23-C24 |
| 26 | b | 620 | BCR | C7-C8-C9-C34 |
| 26 | C | 514 | BCR | C37-C22-C23-C24 |
| 26 | f | 101 | BCR | C36-C18-C19-C20 |
| 26 | H | 101 | BCR | C17-C18-C19-C20 |
| 26 | t | 101 | BCR | C7-C8-C9-C10 |
| 26 | b | 620 | BCR | C7-C8-C9-C10 |
| 26 | C | 514 | BCR | C7-C8-C9-C10 |
| 26 | C | 514 | BCR | C17-C18-C19-C20 |
| 26 | C | 514 | BCR | C21-C22-C23-C24 |
| 26 | b | 621 | BCR | C7-C8-C9-C10 |
| 29 | A | 613 | LMG | O6-C5-C6-O5 |
| 29 | B | 621 | LMG | O9-C10-O7-C8 |
| 29 | a | 613 | LMG | O9-C10-O7-C8 |
| 24 | B | 609 | CLA | C4C-C3C-CAC-CBC |
| 32 | C | 516 | DGD | C4E-C5E-C6E-O5E |
| 29 | a | 613 | LMG | C28-C29-C30-C31 |
| 27 | a | 611 | PL9 | C47-C48-C49-C51 |
| 27 | d | 404 | PL9 | C47-C48-C49-C51 |
| 28 | l | 101 | SQD | O10-C23-O48-C46 |
| 29 | a | 613 | LMG | O10-C28-O8-C9 |
| 28 | L | 102 | SQD | O10-C23-O48-C46 |
| 24 | a | 609 | CLA | C10-C11-C12-C13 |
| 24 | B | 616 | CLA | C5-C6-C7-C8 |
| 24 | A | 609 | CLA | C10-C11-C12-C13 |
| 24 | b | 617 | CLA | C5-C6-C7-C8 |
| 24 | B | 616 | CLA | CBD-CGD-O2D-CED |
| 32 | C | 516 | DGD | O6E-C5E-C6E-O5E |
| 29 | D | 408 | LMG | C4-C5-C6-O5 |
| 24 | a | 609 | CLA | C13-C15-C16-C17 |
| 24 | b | 603 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | A | 609 | CLA | C13-C15-C16-C17 |
| 24 | B | 602 | CLA | C10-C11-C12-C13 |
| 32 | c | 516 | DGD | C2A-C3A-C4A-C5A |
| 32 | C | 516 | DGD | C1B-C2B-C3B-C4B |
| 32 | d | 405 | DGD | C1A-C2A-C3A-C4A |
| 24 | C | 511 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 608 | CLA | CBD-CGD-O2D-CED |
| 32 | c | 516 | DGD | O6D-C5D-C6D-O5D |
| 24 | b | 616 | CLA | C5-C6-C7-C8 |
| 24 | b | 616 | CLA | C10-C11-C12-C13 |
| 24 | C | 509 | CLA | C8-C10-C11-C12 |
| 24 | B | 615 | CLA | C5-C6-C7-C8 |
| 24 | B | 615 | CLA | C10-C11-C12-C13 |
| 24 | c | 509 | CLA | C8-C10-C11-C12 |
| 32 | h | 102 | DGD | C4E-C5E-C6E-O5E |
| 24 | c | 510 | CLA | O1D-CGD-O2D-CED |
| 30 | D | 407 | LHG | O1-C1-C2-O2 |
| 30 | d | 407 | LHG | O1-C1-C2-O2 |
| 27 | a | 611 | PL9 | C17-C18-C19-C20 |
| 29 | C | 518 | LMG | C28-C29-C30-C31 |
| 29 | Z | 101 | LMG | C10-C11-C12-C13 |
| 32 | d | 405 | DGD | C1B-C2B-C3B-C4B |
| 28 | b | 601 | SQD | C7-C8-C9-C10 |
| 28 | B | 622 | SQD | C7-C8-C9-C10 |
| 32 | c | 517 | DGD | C1A-C2A-C3A-C4A |
| 32 | c | 517 | DGD | C1B-C2B-C3B-C4B |
| 29 | B | 621 | LMG | C10-C11-C12-C13 |
| 32 | E | 101 | DGD | C1B-C2B-C3B-C4B |
| 29 | c | 520 | LMG | C28-C29-C30-C31 |
| 24 | B | 613 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 607[A] | CLA | C13-C15-C16-C17 |
| 24 | b | 608[A] | CLA | C13-C15-C16-C17 |
| 30 | e | 101 | LHG | O9-C7-O7-C5 |
| 24 | C | 506 | CLA | C5-C6-C7-C8 |
| 24 | D | 404 | CLA | C8-C10-C11-C12 |
| 24 | d | 403 | CLA | C8-C10-C11-C12 |
| 32 | C | 516 | DGD | C1A-C2A-C3A-C4A |
| 29 | A | 613 | LMG | C28-C29-C30-C31 |
| 28 | a | 614 | SQD | C23-C24-C25-C26 |
| 28 | A | 614 | SQD | C23-C24-C25-C26 |
| 29 | C | 519 | LMG | C28-C29-C30-C31 |
| 32 | E | 101 | DGD | C1A-C2A-C3A-C4A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | c | 506 | CLA | C5-C6-C7-C8 |
| 24 | C | 513 | CLA | O1D-CGD-O2D-CED |
| 26 | c | 514 | BCR | C13-C14-C15-C16 |
| 26 | a | 610 | BCR | C9-C10-C11-C12 |
| 26 | a | 610 | BCR | C19-C20-C21-C22 |
| 26 | c | 521 | BCR | C15-C16-C17-C18 |
| 26 | c | 521 | BCR | C19-C20-C21-C22 |
| 26 | b | 620 | BCR | C13-C14-C15-C16 |
| 26 | b | 621 | BCR | C9-C10-C11-C12 |
| 29 | z | 101 | LMG | C10-C11-C12-C13 |
| 24 | b | 604 | CLA | O1D-CGD-O2D-CED |
| 24 | B | 607[A] | CLA | C15-C16-C17-C18 |
| 24 | D | 404 | CLA | C10-C11-C12-C13 |
| 24 | d | 403 | CLA | C10-C11-C12-C13 |
| 24 | b | 608[A] | CLA | C15-C16-C17-C18 |
| 24 | C | 504 | CLA | O1A-CGA-O2A-C1 |
| 24 | C | 511 | CLA | O1A-CGA-O2A-C1 |
| 32 | d | 405 | DGD | O6E-C1E-O5D-C6D |
| 24 | a | 607 | CLA | C13-C15-C16-C17 |
| 24 | A | 607 | CLA | C13-C15-C16-C17 |
| 27 | A | 611 | PL9 | C9-C11-C12-C13 |
| 27 | D | 405 | PL9 | C9-C11-C12-C13 |
| 27 | D | 405 | PL9 | C14-C16-C17-C18 |
| 27 | D | 405 | PL9 | C29-C31-C32-C33 |
| 27 | d | 404 | PL9 | C9-C11-C12-C13 |
| 27 | d | 404 | PL9 | C39-C41-C42-C43 |
| 29 | C | 518 | LMG | C10-C11-C12-C13 |
| 29 | c | 519 | LMG | C28-C29-C30-C31 |
| 26 | I | 101 | BCR | C10-C11-C12-C13 |
| 26 | c | 515 | BCR | C10-C11-C12-C13 |
| 27 | d | 404 | PL9 | C47-C48-C49-C50 |
| 30 | l | 102 | LHG | O2-C2-C3-O3 |
| 29 | j | 101 | LMG | C4-C5-C6-O5 |
| 24 | C | 509 | CLA | C13-C15-C16-C17 |
| 24 | c | 509 | CLA | C13-C15-C16-C17 |
| 29 | z | 101 | LMG | C4-C5-C6-O5 |
| 24 | a | 609 | CLA | C15-C16-C17-C18 |
| 24 | A | 609 | CLA | C15-C16-C17-C18 |
| 24 | b | 613 | CLA | C15-C16-C17-C18 |
| 24 | B | 612 | CLA | C15-C16-C17-C18 |
| 29 | A | 613 | LMG | C11-C10-O7-C8 |
| 24 | B | 617 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | B | 607[B] | CLA | C10-C11-C12-C13 |
| 24 | C | 501 | CLA | C15-C16-C17-C18 |
| 24 | c | 501 | CLA | C15-C16-C17-C18 |
| 24 | C | 506 | CLA | C10-C11-C12-C13 |
| 24 | b | 608[B] | CLA | C10-C11-C12-C13 |
| 24 | b | 618 | CLA | C10-C11-C12-C13 |
| 24 | c | 506 | CLA | C10-C11-C12-C13 |
| 30 | D | 407 | LHG | C4-O6-P-O3 |
| 30 | L | 101 | LHG | C4-O6-P-O3 |
| 30 | l | 102 | LHG | C4-O6-P-O3 |
| 30 | d | 407 | LHG | C3-O3-P-O6 |
| 24 | c | 505 | CLA | CBA-CGA-O2A-C1 |
| 24 | a | 607 | CLA | C16-C17-C18-C20 |
| 24 | A | 607 | CLA | C16-C17-C18-C20 |
| 30 | A | 615 | LHG | C24-C23-O8-C6 |
| 29 | a | 613 | LMG | C29-C28-O8-C9 |
| 26 | k | 101 | BCR | C14-C15-C16-C17 |
| 26 | T | 101 | BCR | C19-C20-C21-C22 |
| 26 | B | 618 | BCR | C13-C14-C15-C16 |
| 26 | B | 618 | BCR | C19-C20-C21-C22 |
| 26 | b | 619 | BCR | C13-C14-C15-C16 |
| 26 | C | 514 | BCR | C19-C20-C21-C22 |
| 26 | f | 101 | BCR | C19-C20-C21-C22 |
| 29 | D | 408 | LMG | C16-C17-C18-C19 |
| 28 | X | 101 | SQD | C29-C30-C31-C32 |
| 32 | H | 102 | DGD | CBA-CCA-CDA-CEA |
| 24 | b | 603 | CLA | O1D-CGD-O2D-CED |
| 24 | c | 513 | CLA | CBD-CGD-O2D-CED |
| 29 | a | 613 | LMG | C11-C10-O7-C8 |
| 26 | B | 620 | BCR | C11-C10-C9-C34 |
| 26 | I | 101 | BCR | C16-C17-C18-C36 |
| 26 | c | 515 | BCR | C20-C21-C22-C37 |
| 26 | a | 610 | BCR | C16-C17-C18-C36 |
| 26 | A | 610 | BCR | C11-C10-C9-C34 |
| 26 | B | 618 | BCR | C35-C13-C14-C15 |
| 26 | t | 101 | BCR | C11-C10-C9-C34 |
| 28 | x | 101 | SQD | C26-C27-C28-C29 |
| 28 | x | 101 | SQD | C29-C30-C31-C32 |
| 28 | x | 101 | SQD | C34-C35-C36-C37 |
| 28 | l | 101 | SQD | C11-C10-C9-C8 |
| 28 | l | 101 | SQD | C10-C11-C12-C13 |
| 28 | l | 101 | SQD | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | a | 612 | SQD | C11-C12-C13-C14 |
| 29 | c | 519 | LMG | C15-C16-C17-C18 |
| 32 | c | 516 | DGD | C5B-C6B-C7B-C8B |
| 30 | D | 406 | LHG | C29-C30-C31-C32 |
| 32 | d | 405 | DGD | CCA-CDA-CEA-CFA |
| 29 | b | 622 | LMG | C32-C33-C34-C35 |
| 29 | b | 622 | LMG | C34-C35-C36-C37 |
| 28 | a | 614 | SQD | C15-C16-C17-C18 |
| 28 | X | 101 | SQD | C26-C27-C28-C29 |
| 28 | X | 101 | SQD | C34-C35-C36-C37 |
| 28 | A | 614 | SQD | C15-C16-C17-C18 |
| 32 | E | 101 | DGD | C7B-C8B-C9B-CAB |
| 30 | E | 102 | LHG | C15-C16-C17-C18 |
| 28 | L | 102 | SQD | C15-C16-C17-C18 |
| 29 | c | 520 | LMG | C29-C30-C31-C32 |
| 28 | A | 612 | SQD | C11-C12-C13-C14 |
| 32 | H | 102 | DGD | C7A-C8A-C9A-CAA |
| 24 | C | 506 | CLA | C16-C17-C18-C19 |
| 27 | D | 405 | PL9 | C47-C48-C49-C51 |
| 28 | a | 612 | SQD | C28-C29-C30-C31 |
| 29 | A | 613 | LMG | C18-C19-C20-C21 |
| 32 | d | 405 | DGD | C9B-CAB-CBB-CCB |
| 29 | b | 622 | LMG | C17-C18-C19-C20 |
| 29 | j | 101 | LMG | C14-C15-C16-C17 |
| 29 | D | 408 | LMG | C38-C39-C40-C41 |
| 30 | d | 406 | LHG | C32-C33-C34-C35 |
| 30 | l | 102 | LHG | C11-C12-C13-C14 |
| 30 | l | 102 | LHG | C31-C32-C33-C34 |
| 30 | E | 102 | LHG | C24-C25-C26-C27 |
| 28 | L | 102 | SQD | C11-C10-C9-C8 |
| 28 | L | 102 | SQD | C10-C11-C12-C13 |
| 28 | A | 612 | SQD | C28-C29-C30-C31 |
| 28 | l | 101 | SQD | C46-C45-O47-C7 |
| 28 | L | 102 | SQD | C46-C45-O47-C7 |
| 32 | c | 517 | DGD | C3A-C4A-C5A-C6A |
| 32 | c | 517 | DGD | C9A-CAA-CBA-CCA |
| 32 | c | 517 | DGD | C6B-C7B-C8B-C9B |
| 24 | c | 511 | CLA | O1A-CGA-O2A-C1 |
| 29 | z | 101 | LMG | O6-C5-C6-O5 |
| 32 | C | 516 | DGD | C6B-C7B-C8B-C9B |
| 32 | C | 516 | DGD | CAB-CBB-CCB-CDB |
| 28 | a | 612 | SQD | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | a | 612 | SQD | C15-C16-C17-C18 |
| 32 | c | 518 | DGD | C6A-C7A-C8A-C9A |
| 30 | e | 101 | LHG | C18-C19-C20-C21 |
| 30 | L | 101 | LHG | C33-C34-C35-C36 |
| 29 | C | 519 | LMG | C30-C31-C32-C33 |
| 29 | B | 621 | LMG | C12-C13-C14-C15 |
| 32 | E | 101 | DGD | C9A-CAA-CBA-CCA |
| 32 | E | 101 | DGD | C9B-CAB-CBB-CCB |
| 30 | E | 102 | LHG | C14-C15-C16-C17 |
| 28 | A | 612 | SQD | C12-C13-C14-C15 |
| 28 | A | 612 | SQD | C15-C16-C17-C18 |
| 28 | l | 101 | SQD | C12-C13-C14-C15 |
| 29 | j | 101 | LMG | C16-C17-C18-C19 |
| 29 | a | 613 | LMG | C13-C14-C15-C16 |
| 28 | L | 102 | SQD | C12-C13-C14-C15 |
| 30 | e | 101 | LHG | C7-C8-C9-C10 |
| 24 | C | 508 | CLA | O1D-CGD-O2D-CED |
| 26 | c | 515 | BCR | C16-C17-C18-C19 |
| 32 | C | 516 | DGD | C2E-C1E-O5D-C6D |
| 26 | B | 619 | BCR | C12-C13-C14-C15 |
| 26 | H | 101 | BCR | C12-C13-C14-C15 |
| 26 | a | 610 | BCR | C11-C10-C9-C8 |
| 26 | a | 610 | BCR | C16-C17-C18-C19 |
| 26 | K | 101 | BCR | C11-C10-C9-C8 |
| 26 | T | 101 | BCR | C20-C21-C22-C23 |
| 26 | c | 521 | BCR | C16-C17-C18-C19 |
| 26 | c | 521 | BCR | C20-C21-C22-C23 |
| 26 | F | 101 | BCR | C20-C21-C22-C23 |
| 26 | K | 102 | BCR | C12-C13-C14-C15 |
| 26 | K | 102 | BCR | C20-C21-C22-C23 |
| 26 | B | 618 | BCR | C11-C10-C9-C8 |
| 26 | B | 618 | BCR | C12-C13-C14-C15 |
| 32 | d | 405 | DGD | C2D-C1D-O3G-C3G |
| 26 | b | 619 | BCR | C20-C21-C22-C23 |
| 26 | t | 101 | BCR | C20-C21-C22-C23 |
| 26 | C | 514 | BCR | C12-C13-C14-C15 |
| 32 | E | 101 | DGD | C2D-C1D-O3G-C3G |
| 32 | E | 101 | DGD | C2E-C1E-O5D-C6D |
| 28 | l | 101 | SQD | C17-C18-C19-C20 |
| 28 | l | 101 | SQD | C18-C19-C20-C21 |
| 29 | C | 518 | LMG | C15-C16-C17-C18 |
| 30 | D | 406 | LHG | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | j | 101 | LMG | C12-C13-C14-C15 |
| 30 | e | 101 | LHG | C24-C25-C26-C27 |
| 30 | L | 101 | LHG | C34-C35-C36-C37 |
| 30 | l | 102 | LHG | C33-C34-C35-C36 |
| 32 | c | 517 | DGD | CAA-CBA-CCA-CDA |
| 32 | E | 101 | DGD | CCA-CDA-CEA-CFA |
| 28 | L | 102 | SQD | C17-C18-C19-C20 |
| 28 | L | 102 | SQD | C24-C25-C26-C27 |
| 24 | B | 614 | CLA | C15-C16-C17-C18 |
| 24 | b | 615 | CLA | C15-C16-C17-C18 |
| 24 | D | 404 | CLA | C16-C17-C18-C19 |
| 24 | d | 403 | CLA | C16-C17-C18-C19 |
| 24 | c | 506 | CLA | C16-C17-C18-C19 |
| 27 | D | 405 | PL9 | C27-C28-C29-C30 |
| 28 | l | 101 | SQD | C24-C25-C26-C27 |
| 32 | c | 518 | DGD | C9B-CAB-CBB-CCB |
| 32 | c | 516 | DGD | C4B-C5B-C6B-C7B |
| 29 | A | 613 | LMG | C14-C15-C16-C17 |
| 28 | X | 101 | SQD | C24-C25-C26-C27 |
| 29 | C | 519 | LMG | C31-C32-C33-C34 |
| 29 | B | 621 | LMG | C37-C38-C39-C40 |
| 28 | L | 102 | SQD | C18-C19-C20-C21 |
| 24 | b | 605 | CLA | C6-C7-C8-C9 |
| 24 | B | 604 | CLA | C6-C7-C8-C9 |
| 28 | x | 101 | SQD | C24-C25-C26-C27 |
| 28 | l | 101 | SQD | C29-C30-C31-C32 |
| 29 | A | 613 | LMG | C12-C13-C14-C15 |
| 32 | d | 405 | DGD | C2A-C3A-C4A-C5A |
| 32 | d | 405 | DGD | CBA-CCA-CDA-CEA |
| 29 | b | 622 | LMG | C37-C38-C39-C40 |
| 29 | D | 408 | LMG | C12-C13-C14-C15 |
| 29 | D | 408 | LMG | C15-C16-C17-C18 |
| 30 | d | 406 | LHG | C29-C30-C31-C32 |
| 28 | b | 601 | SQD | C34-C35-C36-C37 |
| 28 | B | 622 | SQD | C34-C35-C36-C37 |
| 30 | E | 102 | LHG | C25-C26-C27-C28 |
| 28 | L | 102 | SQD | C29-C30-C31-C32 |
| 29 | c | 520 | LMG | C31-C32-C33-C34 |
| 32 | H | 102 | DGD | CBB-CCB-CDB-CEB |
| 24 | B | 617 | CLA | C8-C10-C11-C12 |
| 24 | b | 618 | CLA | C8-C10-C11-C12 |
| 32 | c | 516 | DGD | C4E-C5E-C6E-O5E |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | c | 514 | BCR | C37-C22-C23-C24 |
| 26 | H | 101 | BCR | C37-C22-C23-C24 |
| 26 | b | 619 | BCR | C37-C22-C23-C24 |
| 26 | C | 514 | BCR | C7-C8-C9-C34 |
| 28 | a | 612 | SQD | C16-C17-C18-C19 |
| 32 | d | 405 | DGD | CCB-CDB-CEB-CFB |
| 29 | j | 101 | LMG | C30-C31-C32-C33 |
| 29 | j | 101 | LMG | C39-C40-C41-C42 |
| 28 | B | 622 | SQD | C31-C32-C33-C34 |
| 30 | L | 101 | LHG | C11-C12-C13-C14 |
| 29 | C | 519 | LMG | C29-C30-C31-C32 |
| 30 | E | 102 | LHG | C13-C14-C15-C16 |
| 28 | A | 612 | SQD | C16-C17-C18-C19 |
| 30 | D | 406 | LHG | O1-C1-C2-C3 |
| 30 | a | 616 | LHG | O1-C1-C2-C3 |
| 26 | I | 101 | BCR | C21-C22-C23-C24 |
| 26 | c | 515 | BCR | C17-C18-C19-C20 |
| 26 | h | 101 | BCR | C17-C18-C19-C20 |
| 26 | B | 619 | BCR | C7-C8-C9-C10 |
| 26 | B | 619 | BCR | C17-C18-C19-C20 |
| 26 | T | 101 | BCR | C7-C8-C9-C10 |
| 26 | T | 101 | BCR | C21-C22-C23-C24 |
| 26 | k | 101 | BCR | C7-C8-C9-C10 |
| 26 | k | 101 | BCR | C17-C18-C19-C20 |
| 26 | f | 101 | BCR | C11-C12-C13-C14 |
| 26 | f | 101 | BCR | C17-C18-C19-C20 |
| 24 | c | 503 | CLA | O1D-CGD-O2D-CED |
| 32 | C | 515 | DGD | C6B-C7B-C8B-C9B |
| 28 | l | 101 | SQD | C27-C28-C29-C30 |
| 29 | Z | 101 | LMG | C16-C17-C18-C19 |
| 29 | b | 622 | LMG | C14-C15-C16-C17 |
| 29 | j | 101 | LMG | C15-C16-C17-C18 |
| 30 | d | 406 | LHG | C25-C26-C27-C28 |
| 28 | b | 601 | SQD | C31-C32-C33-C34 |
| 28 | B | 622 | SQD | C11-C12-C13-C14 |
| 30 | e | 101 | LHG | C25-C26-C27-C28 |
| 30 | L | 101 | LHG | C13-C14-C15-C16 |
| 29 | B | 621 | LMG | C38-C39-C40-C41 |
| 29 | a | 613 | LMG | C34-C35-C36-C37 |
| 28 | L | 102 | SQD | C27-C28-C29-C30 |
| 24 | b | 610 | CLA | C2C-C3C-CAC-CBC |
| 29 | c | 519 | LMG | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 30 | E | 102 | LHG | C7-C8-C9-C10 |
| 32 | C | 516 | DGD | C3A-C4A-C5A-C6A |
| 32 | C | 515 | DGD | C6A-C7A-C8A-C9A |
| 28 | l | 101 | SQD | C14-C15-C16-C17 |
| 32 | d | 405 | DGD | C9A-CAA-CBA-CCA |
| 29 | j | 101 | LMG | C13-C14-C15-C16 |
| 29 | D | 408 | LMG | C14-C15-C16-C17 |
| 28 | a | 614 | SQD | C16-C17-C18-C19 |
| 29 | z | 101 | LMG | C12-C13-C14-C15 |
| 28 | b | 601 | SQD | C11-C10-C9-C8 |
| 28 | b | 601 | SQD | C11-C12-C13-C14 |
| 28 | B | 622 | SQD | C11-C10-C9-C8 |
| 32 | C | 517 | DGD | C6A-C7A-C8A-C9A |
| 30 | e | 101 | LHG | C14-C15-C16-C17 |
| 32 | h | 102 | DGD | CBA-CCA-CDA-CEA |
| 32 | c | 517 | DGD | C4A-C5A-C6A-C7A |
| 32 | c | 517 | DGD | CAB-CBB-CCB-CDB |
| 32 | c | 517 | DGD | CBB-CCB-CDB-CEB |
| 28 | A | 614 | SQD | C16-C17-C18-C19 |
| 29 | B | 621 | LMG | C16-C17-C18-C19 |
| 32 | E | 101 | DGD | C2A-C3A-C4A-C5A |
| 32 | E | 101 | DGD | C5B-C6B-C7B-C8B |
| 28 | L | 102 | SQD | C32-C33-C34-C35 |
| 29 | c | 520 | LMG | C17-C18-C19-C20 |
| 29 | c | 520 | LMG | C30-C31-C32-C33 |
| 32 | d | 405 | DGD | O6D-C1D-O3G-C3G |
| 32 | E | 101 | DGD | O6D-C1D-O3G-C3G |
| 32 | E | 101 | DGD | O6E-C1E-O5D-C6D |
| 32 | C | 516 | DGD | C9A-CAA-CBA-CCA |
| 32 | C | 515 | DGD | CAB-CBB-CCB-CDB |
| 28 | l | 101 | SQD | C32-C33-C34-C35 |
| 28 | a | 612 | SQD | C9-C10-C11-C12 |
| 29 | C | 518 | LMG | C16-C17-C18-C19 |
| 32 | d | 405 | DGD | C7B-C8B-C9B-CAB |
| 29 | j | 101 | LMG | C36-C37-C38-C39 |
| 28 | a | 614 | SQD | C26-C27-C28-C29 |
| 29 | z | 101 | LMG | C19-C20-C21-C22 |
| 28 | b | 601 | SQD | C24-C25-C26-C27 |
| 28 | B | 622 | SQD | C24-C25-C26-C27 |
| 32 | C | 517 | DGD | C2A-C3A-C4A-C5A |
| 32 | c | 517 | DGD | C9B-CAB-CBB-CCB |
| 28 | A | 614 | SQD | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | B | 621 | LMG | C14-C15-C16-C17 |
| 29 | a | 613 | LMG | C38-C39-C40-C41 |
| 28 | L | 102 | SQD | C14-C15-C16-C17 |
| 28 | A | 612 | SQD | C9-C10-C11-C12 |
| 24 | C | 505 | CLA | CBD-CGD-O2D-CED |
| 32 | C | 516 | DGD | CAA-CBA-CCA-CDA |
| 32 | C | 516 | DGD | C5B-C6B-C7B-C8B |
| 32 | C | 515 | DGD | C4B-C5B-C6B-C7B |
| 29 | c | 519 | LMG | C16-C17-C18-C19 |
| 32 | c | 516 | DGD | C6A-C7A-C8A-C9A |
| 32 | c | 516 | DGD | C6B-C7B-C8B-C9B |
| 29 | A | 613 | LMG | C36-C37-C38-C39 |
| 29 | z | 101 | LMG | C16-C17-C18-C19 |
| 30 | e | 101 | LHG | C13-C14-C15-C16 |
| 30 | L | 101 | LHG | C25-C26-C27-C28 |
| 28 | A | 614 | SQD | C28-C29-C30-C31 |
| 29 | B | 621 | LMG | C32-C33-C34-C35 |
| 32 | c | 518 | DGD | C2A-C3A-C4A-C5A |
| 30 | a | 616 | LHG | C15-C16-C17-C18 |
| 29 | D | 408 | LMG | C20-C21-C22-C23 |
| 28 | a | 614 | SQD | C28-C29-C30-C31 |
| 30 | l | 102 | LHG | C13-C14-C15-C16 |
| 30 | E | 102 | LHG | C27-C28-C29-C30 |
| 30 | a | 616 | LHG | C27-C28-C29-C30 |
| 30 | L | 101 | LHG | C12-C13-C14-C15 |
| 29 | c | 520 | LMG | C18-C19-C20-C21 |
| 24 | c | 504 | CLA | O1D-CGD-O2D-CED |
| 28 | x | 101 | SQD | C31-C32-C33-C34 |
| 32 | C | 515 | DGD | C5B-C6B-C7B-C8B |
| 28 | l | 101 | SQD | C16-C17-C18-C19 |
| 28 | l | 101 | SQD | C28-C29-C30-C31 |
| 30 | A | 615 | LHG | C15-C16-C17-C18 |
| 29 | c | 519 | LMG | C29-C30-C31-C32 |
| 29 | b | 622 | LMG | C31-C32-C33-C34 |
| 30 | a | 616 | LHG | C30-C31-C32-C33 |
| 28 | X | 101 | SQD | C31-C32-C33-C34 |
| 30 | d | 406 | LHG | C13-C14-C15-C16 |
| 29 | B | 621 | LMG | C17-C18-C19-C20 |
| 32 | E | 101 | DGD | CCB-CDB-CEB-CFB |
| 28 | L | 102 | SQD | C16-C17-C18-C19 |
| 24 | C | 510 | CLA | O1A-CGA-O2A-C1 |
| 29 | A | 613 | LMG | O10-C28-O8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 30 | d | 407 | LHG | O10-C23-O8-C6 |
| 32 | c | 518 | DGD | C8B-C9B-CAB-CBB |
| 29 | A | 613 | LMG | C31-C32-C33-C34 |
| 28 | b | 601 | SQD | C10-C11-C12-C13 |
| 28 | B | 622 | SQD | C10-C11-C12-C13 |
| 30 | L | 101 | LHG | C31-C32-C33-C34 |
| 32 | h | 102 | DGD | C7B-C8B-C9B-CAB |
| 29 | a | 613 | LMG | C14-C15-C16-C17 |
| 29 | a | 613 | LMG | C32-C33-C34-C35 |
| 24 | a | 615 | CLA | C2C-C3C-CAC-CBC |
| 28 | L | 102 | SQD | C28-C29-C30-C31 |
| 32 | H | 102 | DGD | CCA-CDA-CEA-CFA |
| 24 | D | 402 | CLA | O1D-CGD-O2D-CED |
| 32 | h | 102 | DGD | O1G-C1G-C2G-C3G |
| 29 | c | 519 | LMG | C19-C20-C21-C22 |
| 29 | c | 519 | LMG | C38-C39-C40-C41 |
| 29 | a | 613 | LMG | C12-C13-C14-C15 |
| 32 | C | 515 | DGD | O6D-C5D-C6D-O5D |
| 32 | E | 101 | DGD | O6D-C5D-C6D-O5D |
| 29 | b | 622 | LMG | C16-C17-C18-C19 |
| 29 | c | 520 | LMG | C33-C34-C35-C36 |
| 27 | D | 405 | PL9 | C45-C44-C46-C47 |
| 27 | d | 404 | PL9 | C30-C29-C31-C32 |
| 24 | c | 511 | CLA | CBA-CGA-O2A-C1 |
| 27 | D | 405 | PL9 | C28-C29-C31-C32 |
| 27 | D | 405 | PL9 | C43-C44-C46-C47 |
| 27 | d | 404 | PL9 | C28-C29-C31-C32 |
| 28 | x | 101 | SQD | C30-C31-C32-C33 |
| 30 | A | 615 | LHG | C12-C13-C14-C15 |
| 32 | c | 518 | DGD | C9A-CAA-CBA-CCA |
| 28 | X | 101 | SQD | C30-C31-C32-C33 |
| 32 | C | 516 | DGD | C3B-C4B-C5B-C6B |
| 32 | c | 516 | DGD | CAB-CBB-CCB-CDB |
| 29 | A | 613 | LMG | C30-C31-C32-C33 |
| 29 | b | 622 | LMG | C12-C13-C14-C15 |
| 32 | c | 517 | DGD | C8B-C9B-CAB-CBB |
| 30 | E | 102 | LHG | C18-C19-C20-C21 |
| 29 | a | 613 | LMG | C31-C32-C33-C34 |
| 24 | c | 507 | CLA | C16-C17-C18-C19 |
| 24 | C | 507 | CLA | C16-C17-C18-C19 |
| 29 | b | 622 | LMG | C36-C37-C38-C39 |
| 24 | B | 605 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | C | 518 | LMG | C13-C14-C15-C16 |
| 29 | Z | 101 | LMG | C19-C20-C21-C22 |
| 30 | l | 102 | LHG | C16-C17-C18-C19 |
| 32 | C | 516 | DGD | CBB-CCB-CDB-CEB |
| 28 | A | 612 | SQD | C32-C33-C34-C35 |
| 24 | b | 606 | CLA | C13-C15-C16-C17 |
| 30 | l | 102 | LHG | C1-C2-C3-O3 |
| 28 | a | 612 | SQD | C32-C33-C34-C35 |
| 30 | A | 615 | LHG | C10-C11-C12-C13 |
| 29 | b | 622 | LMG | C38-C39-C40-C41 |
| 32 | H | 102 | DGD | CCB-CDB-CEB-CFB |
| 32 | C | 515 | DGD | C7B-C8B-C9B-CAB |
| 29 | c | 519 | LMG | C32-C33-C34-C35 |
| 32 | c | 516 | DGD | C4A-C5A-C6A-C7A |
| 32 | c | 516 | DGD | CAA-CBA-CCA-CDA |
| 29 | j | 101 | LMG | C20-C21-C22-C23 |
| 30 | e | 101 | LHG | C12-C13-C14-C15 |
| 29 | C | 519 | LMG | C38-C39-C40-C41 |
| 29 | D | 408 | LMG | C39-C40-C41-C42 |
| 30 | d | 406 | LHG | C33-C34-C35-C36 |
| 30 | l | 102 | LHG | C12-C13-C14-C15 |
| 26 | B | 620 | BCR | C23-C24-C25-C30 |
| 26 | I | 101 | BCR | C5-C6-C7-C8 |
| 26 | I | 101 | BCR | C23-C24-C25-C26 |
| 26 | c | 515 | BCR | C5-C6-C7-C8 |
| 26 | c | 515 | BCR | C23-C24-C25-C26 |
| 26 | h | 101 | BCR | C5-C6-C7-C8 |
| 26 | h | 101 | BCR | C23-C24-C25-C26 |
| 26 | B | 619 | BCR | C23-C24-C25-C30 |
| 26 | H | 101 | BCR | C23-C24-C25-C26 |
| 26 | a | 610 | BCR | C1-C6-C7-C8 |
| 26 | a | 610 | BCR | C23-C24-C25-C26 |
| 26 | K | 101 | BCR | C5-C6-C7-C8 |
| 26 | K | 101 | BCR | C23-C24-C25-C26 |
| 26 | T | 101 | BCR | C1-C6-C7-C8 |
| 26 | T | 101 | BCR | C23-C24-C25-C26 |
| 26 | c | 521 | BCR | C5-C6-C7-C8 |
| 26 | F | 101 | BCR | C5-C6-C7-C8 |
| 26 | F | 101 | BCR | C23-C24-C25-C26 |
| 26 | k | 101 | BCR | C1-C6-C7-C8 |
| 26 | k | 101 | BCR | C5-C6-C7-C8 |
| 26 | A | 610 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | A | 610 | BCR | C23-C24-C25-C26 |
| 26 | K | 102 | BCR | C5-C6-C7-C8 |
| 26 | K | 102 | BCR | C23-C24-C25-C30 |
| 26 | b | 619 | BCR | C1-C6-C7-C8 |
| 26 | t | 101 | BCR | C1-C6-C7-C8 |
| 26 | t | 101 | BCR | C5-C6-C7-C8 |
| 26 | b | 620 | BCR | C23-C24-C25-C30 |
| 26 | f | 101 | BCR | C1-C6-C7-C8 |
| 26 | b | 621 | BCR | C23-C24-C25-C26 |
| 30 | D | 406 | LHG | C33-C34-C35-C36 |
| 29 | A | 613 | LMG | C13-C14-C15-C16 |
| 29 | a | 613 | LMG | C30-C31-C32-C33 |
| 30 | a | 616 | LHG | C24-C23-O8-C6 |
| 28 | a | 614 | SQD | C24-C23-O48-C46 |
| 28 | A | 614 | SQD | C24-C23-O48-C46 |
| 24 | C | 506 | CLA | C13-C15-C16-C17 |
| 24 | c | 506 | CLA | C13-C15-C16-C17 |
| 28 | x | 101 | SQD | C8-C7-O47-C45 |
| 28 | X | 101 | SQD | C8-C7-O47-C45 |
| 32 | C | 517 | DGD | C9B-CAB-CBB-CCB |
| 32 | d | 405 | DGD | O6E-C5E-C6E-O5E |
| 30 | D | 406 | LHG | C23-C24-C25-C26 |
| 32 | C | 515 | DGD | CAA-CBA-CCA-CDA |
| 32 | c | 516 | DGD | C8B-C9B-CAB-CBB |
| 28 | b | 601 | SQD | C32-C33-C34-C35 |
| 28 | B | 622 | SQD | C32-C33-C34-C35 |
| 27 | a | 611 | PL9 | C47-C48-C49-C50 |
| 29 | D | 408 | LMG | C13-C14-C15-C16 |
| 30 | d | 406 | LHG | C11-C10-C9-C8 |
| 30 | d | 406 | LHG | C31-C32-C33-C34 |
| 30 | e | 101 | LHG | C27-C28-C29-C30 |
| 24 | B | 606 | CLA | O1D-CGD-O2D-CED |
| 24 | c | 504 | CLA | C11-C12-C13-C15 |
| 24 | B | 617 | CLA | C6-C7-C8-C10 |
| 24 | C | 504 | CLA | C11-C12-C13-C15 |
| 24 | b | 605 | CLA | C6-C7-C8-C10 |
| 24 | C | 510 | CLA | C2-C3-C5-C6 |
| 24 | a | 607 | CLA | C6-C7-C8-C10 |
| 24 | b | 612 | CLA | C12-C13-C15-C16 |
| 24 | A | 607 | CLA | C6-C7-C8-C10 |
| 24 | B | 604 | CLA | C6-C7-C8-C10 |
| 24 | c | 510 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | b | 618 | CLA | C6-C7-C8-C10 |
| 24 | B | 611 | CLA | C12-C13-C15-C16 |
| 24 | A | 609 | CLA | O1A-CGA-O2A-C1 |
| 32 | d | 405 | DGD | C5B-C6B-C7B-C8B |
| 28 | b | 601 | SQD | C29-C30-C31-C32 |
| 28 | B | 622 | SQD | C29-C30-C31-C32 |
| 30 | e | 101 | LHG | C17-C18-C19-C20 |
| 24 | c | 504 | CLA | C13-C15-C16-C17 |
| 24 | C | 504 | CLA | C13-C15-C16-C17 |
| 26 | A | 610 | BCR | C19-C20-C21-C22 |
| 29 | c | 520 | LMG | O9-C10-O7-C8 |
| 28 | l | 101 | SQD | C7-C8-C9-C10 |
| 28 | L | 102 | SQD | C7-C8-C9-C10 |
| 24 | C | 504 | CLA | CBA-CGA-O2A-C1 |
| 29 | D | 408 | LMG | C29-C28-O8-C9 |
| 32 | C | 516 | DGD | C4A-C5A-C6A-C7A |
| 30 | L | 101 | LHG | C27-C28-C29-C30 |
| 24 | C | 503 | CLA | C2A-CAA-CBA-CGA |
| 24 | C | 503 | CLA | O1D-CGD-O2D-CED |
| 28 | b | 601 | SQD | C18-C19-C20-C21 |
| 32 | c | 517 | DGD | C3B-C4B-C5B-C6B |
| 25 | d | 401 | PHO | C2C-C3C-CAC-CBC |
| 28 | B | 622 | SQD | C18-C19-C20-C21 |
| 30 | d | 406 | LHG | C23-C24-C25-C26 |
| 30 | A | 615 | LHG | C29-C30-C31-C32 |
| 29 | C | 519 | LMG | C15-C16-C17-C18 |
| 32 | E | 101 | DGD | C8B-C9B-CAB-CBB |
| 30 | E | 102 | LHG | C11-C10-C9-C8 |
| 27 | D | 405 | PL9 | C42-C43-C44-C45 |
| 28 | a | 612 | SQD | C30-C31-C32-C33 |
| 29 | C | 518 | LMG | C32-C33-C34-C35 |
| 32 | c | 518 | DGD | C2B-C3B-C4B-C5B |
| 32 | C | 517 | DGD | C6B-C7B-C8B-C9B |
| 26 | h | 101 | BCR | C22-C23-C24-C25 |
| 26 | B | 619 | BCR | C6-C7-C8-C9 |
| 26 | C | 514 | BCR | C6-C7-C8-C9 |
| 32 | C | 516 | DGD | O6E-C1E-O5D-C6D |
| 32 | C | 515 | DGD | O6E-C1E-O5D-C6D |
| 32 | c | 517 | DGD | O6E-C1E-O5D-C6D |
| 24 | C | 501 | CLA | C13-C15-C16-C17 |
| 24 | c | 501 | CLA | C13-C15-C16-C17 |
| 27 | a | 611 | PL9 | C9-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 29 | A | 613 | LMG | C29-C30-C31-C32 |
| 32 | d | 405 | DGD | C5A-C6A-C7A-C8A |
| 29 | j | 101 | LMG | C38-C39-C40-C41 |
| 30 | l | 102 | LHG | C34-C35-C36-C37 |
| 32 | c | 517 | DGD | C7B-C8B-C9B-CAB |
| 28 | A | 612 | SQD | C30-C31-C32-C33 |
| 30 | D | 406 | LHG | C8-C7-O7-C5 |
| 29 | B | 621 | LMG | C11-C10-O7-C8 |
| 26 | t | 101 | BCR | C10-C11-C12-C13 |
| 30 | a | 616 | LHG | C29-C30-C31-C32 |
| 29 | C | 519 | LMG | C17-C18-C19-C20 |
| 24 | B | 607[A] | CLA | CBD-CGD-O2D-CED |
| 32 | d | 405 | DGD | C8B-C9B-CAB-CBB |
| 28 | x | 101 | SQD | O49-C7-O47-C45 |
| 28 | X | 101 | SQD | O49-C7-O47-C45 |
| 29 | j | 101 | LMG | C19-C20-C21-C22 |
| 32 | h | 102 | DGD | C7A-C8A-C9A-CAA |
| 32 | d | 405 | DGD | O1A-C1A-O1G-C1G |
| 32 | d | 405 | DGD | C3A-C4A-C5A-C6A |
| 32 | C | 517 | DGD | C9A-CAA-CBA-CCA |
| 24 | C | 510 | CLA | C4-C3-C5-C6 |
| 27 | D | 405 | PL9 | C30-C29-C31-C32 |
| 24 | c | 510 | CLA | C4-C3-C5-C6 |
| 29 | b | 622 | LMG | C10-C11-C12-C13 |
| 29 | b | 622 | LMG | C28-C29-C30-C31 |
| 27 | A | 611 | PL9 | C4-C3-C7-C8 |
| 27 | a | 611 | PL9 | C4-C3-C7-C8 |
| 29 | A | 613 | LMG | C34-C35-C36-C37 |
| 24 | B | 617 | CLA | C6-C7-C8-C9 |
| 24 | a | 607 | CLA | C6-C7-C8-C9 |
| 24 | D | 404 | CLA | C11-C10-C8-C9 |
| 24 | d | 403 | CLA | C11-C10-C8-C9 |
| 24 | b | 612 | CLA | C14-C13-C15-C16 |
| 24 | A | 607 | CLA | C6-C7-C8-C9 |
| 24 | B | 616 | CLA | C14-C13-C15-C16 |
| 24 | b | 618 | CLA | C6-C7-C8-C9 |
| 24 | b | 617 | CLA | C14-C13-C15-C16 |
| 24 | B | 611 | CLA | C14-C13-C15-C16 |
| 29 | C | 518 | LMG | C38-C39-C40-C41 |
| 30 | l | 102 | LHG | C32-C33-C34-C35 |
| 24 | b | 616 | CLA | C2A-CAA-CBA-CGA |
| 28 | a | 614 | SQD | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 28 | A | 614 | SQD | C18-C19-C20-C21 |
| 29 | a | 613 | LMG | C18-C19-C20-C21 |
| 26 | a | 610 | BCR | C36-C18-C19-C20 |
| 26 | c | 521 | BCR | C37-C22-C23-C24 |
| 26 | b | 619 | BCR | C36-C18-C19-C20 |
| 28 | X | 101 | SQD | C23-C24-C25-C26 |
| 32 | C | 517 | DGD | C3B-C4B-C5B-C6B |
| 28 | A | 612 | SQD | C34-C35-C36-C37 |
| 26 | T | 101 | BCR | C17-C18-C19-C20 |
| 26 | c | 521 | BCR | C11-C12-C13-C14 |
| 26 | c | 521 | BCR | C17-C18-C19-C20 |
| 28 | a | 614 | SQD | O10-C23-O48-C46 |
| 28 | A | 614 | SQD | O10-C23-O48-C46 |
| 24 | C | 506 | CLA | C1A-C2A-CAA-CBA |
| 24 | D | 402 | CLA | C1A-C2A-CAA-CBA |
| 24 | c | 512 | CLA | C1A-C2A-CAA-CBA |
| 24 | a | 615 | CLA | C1A-C2A-CAA-CBA |
| 24 | B | 605 | CLA | C16-C17-C18-C20 |
| 24 | b | 606 | CLA | C16-C17-C18-C20 |
| 24 | C | 506 | CLA | C16-C17-C18-C20 |
| 24 | D | 404 | CLA | C16-C17-C18-C20 |
| 24 | d | 403 | CLA | C16-C17-C18-C20 |
| 29 | b | 622 | LMG | O9-C10-O7-C8 |
| 28 | a | 612 | SQD | C34-C35-C36-C37 |
| 32 | c | 518 | DGD | C4A-C5A-C6A-C7A |
| 26 | I | 101 | BCR | C9-C10-C11-C12 |
| 26 | B | 619 | BCR | C13-C14-C15-C16 |
| 26 | f | 101 | BCR | C15-C16-C17-C18 |
| 26 | b | 621 | BCR | C15-C16-C17-C18 |
| 24 | B | 607[B] | CLA | C15-C16-C17-C18 |
| 24 | c | 507 | CLA | C5-C6-C7-C8 |
| 24 | C | 507 | CLA | C5-C6-C7-C8 |
| 24 | b | 608[B] | CLA | C15-C16-C17-C18 |
| 30 | D | 407 | LHG | C3-O3-P-O6 |
| 30 | e | 101 | LHG | C3-O3-P-O6 |
| 32 | C | 516 | DGD | C6A-C7A-C8A-C9A |
| 29 | c | 519 | LMG | C11-C12-C13-C14 |
| 30 | D | 406 | LHG | C25-C26-C27-C28 |
| 28 | x | 101 | SQD | C23-C24-C25-C26 |
| 29 | C | 518 | LMG | C17-C18-C19-C20 |
| 24 | D | 404 | CLA | C13-C15-C16-C17 |
| 24 | d | 403 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | C | 519 | LMG | C29-C28-O8-C9 |
| 29 | b | 622 | LMG | C33-C34-C35-C36 |
| 29 | c | 520 | LMG | C38-C39-C40-C41 |
| 32 | C | 515 | DGD | O6E-C5E-C6E-O5E |
| 24 | c | 507 | CLA | C16-C17-C18-C20 |
| 24 | C | 507 | CLA | C16-C17-C18-C20 |
| 24 | A | 609 | CLA | C16-C17-C18-C19 |
| 24 | c | 506 | CLA | C16-C17-C18-C20 |
| 32 | C | 515 | DGD | C4A-C5A-C6A-C7A |
| 28 | b | 601 | SQD | C27-C28-C29-C30 |
| 28 | B | 622 | SQD | C27-C28-C29-C30 |
| 30 | l | 102 | LHG | C27-C28-C29-C30 |
| 29 | C | 518 | LMG | C11-C12-C13-C14 |
| 29 | Z | 101 | LMG | C12-C13-C14-C15 |
| 30 | a | 616 | LHG | C12-C13-C14-C15 |
| 29 | D | 408 | LMG | C35-C36-C37-C38 |
| 29 | a | 613 | LMG | C15-C16-C17-C18 |
| 30 | a | 616 | LHG | C16-C17-C18-C19 |
| 28 | B | 622 | SQD | C28-C29-C30-C31 |
| 30 | e | 101 | LHG | C11-C10-C9-C8 |
| 29 | C | 519 | LMG | C18-C19-C20-C21 |
| 32 | C | 515 | DGD | C4D-C5D-C6D-O5D |
| 29 | A | 613 | LMG | C4-C5-C6-O5 |
| 32 | C | 516 | DGD | C7B-C8B-C9B-CAB |
| 29 | b | 622 | LMG | C15-C16-C17-C18 |
| 28 | b | 601 | SQD | C28-C29-C30-C31 |
| 29 | c | 520 | LMG | C15-C16-C17-C18 |
| 28 | a | 612 | SQD | C27-C28-C29-C30 |
| 30 | d | 406 | LHG | C24-C25-C26-C27 |
| 32 | C | 517 | DGD | C4A-C5A-C6A-C7A |
| 29 | B | 621 | LMG | C36-C37-C38-C39 |
| 32 | E | 101 | DGD | CBA-CCA-CDA-CEA |
| 29 | c | 519 | LMG | C13-C14-C15-C16 |
| 28 | A | 612 | SQD | C27-C28-C29-C30 |
| 24 | a | 609 | CLA | C16-C17-C18-C19 |
| 24 | a | 607 | CLA | C16-C17-C18-C19 |
| 24 | A | 607 | CLA | C16-C17-C18-C19 |
| 29 | Z | 101 | LMG | O1-C7-C8-C9 |
| 29 | b | 622 | LMG | C18-C19-C20-C21 |
| 28 | a | 614 | SQD | O6-C44-C45-C46 |
| 29 | z | 101 | LMG | O1-C7-C8-C9 |
| 28 | X | 101 | SQD | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | A | 614 | SQD | O6-C44-C45-C46 |
| 29 | a | 613 | LMG | C7-C8-C9-O8 |
| 24 | C | 509 | CLA | C10-C11-C12-C13 |
| 24 | c | 509 | CLA | C10-C11-C12-C13 |
| 28 | x | 101 | SQD | C35-C36-C37-C38 |
| 32 | E | 101 | DGD | CAB-CBB-CCB-CDB |
| 32 | c | 517 | DGD | C5D-C6D-O5D-C1E |
| 29 | c | 520 | LMG | C8-C7-O1-C1 |
| 24 | C | 506 | CLA | O1D-CGD-O2D-CED |
| 24 | C | 502 | CLA | O1D-CGD-O2D-CED |
| 32 | h | 102 | DGD | C9A-CAA-CBA-CCA |
| 32 | h | 102 | DGD | CCB-CDB-CEB-CFB |
| 30 | d | 407 | LHG | C34-C35-C36-C37 |
| 28 | b | 601 | SQD | C13-C14-C15-C16 |
| 28 | b | 601 | SQD | C35-C36-C37-C38 |
| 28 | B | 622 | SQD | C13-C14-C15-C16 |
| 28 | B | 622 | SQD | C35-C36-C37-C38 |
| 32 | C | 517 | DGD | C8B-C9B-CAB-CBB |
| 29 | D | 408 | LMG | O6-C1-O1-C7 |
| 24 | C | 511 | CLA | O1D-CGD-O2D-CED |
| 32 | c | 517 | DGD | C5B-C6B-C7B-C8B |
| 28 | A | 614 | SQD | C19-C20-C21-C22 |
| 26 | A | 610 | BCR | C15-C16-C17-C18 |
| 28 | a | 614 | SQD | C19-C20-C21-C22 |
| 32 | h | 102 | DGD | CCA-CDA-CEA-CFA |
| 30 | a | 616 | LHG | O10-C23-O8-C6 |
| 29 | B | 621 | LMG | C28-C29-C30-C31 |
| 29 | C | 518 | LMG | C29-C30-C31-C32 |
| 30 | D | 406 | LHG | C24-C25-C26-C27 |
| 32 | h | 102 | DGD | CBB-CCB-CDB-CEB |
| 28 | a | 612 | SQD | C35-C36-C37-C38 |
| 30 | e | 101 | LHG | C15-C16-C17-C18 |
| 32 | E | 101 | DGD | C3A-C4A-C5A-C6A |
| 28 | A | 612 | SQD | C35-C36-C37-C38 |
| 24 | b | 614 | CLA | C13-C15-C16-C17 |
| 26 | h | 101 | BCR | C35-C13-C14-C15 |
| 25 | A | 608 | PHO | C4-C3-C5-C6 |
| 29 | B | 621 | LMG | C15-C16-C17-C18 |
| 24 | C | 511 | CLA | CBA-CGA-O2A-C1 |
| 24 | A | 609 | CLA | C5-C6-C7-C8 |
| 32 | h | 102 | DGD | CDB-CEB-CFB-CGB |
| 24 | a | 609 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | c | 509 | CLA | C2-C1-O2A-CGA |
| 32 | d | 405 | DGD | CAA-CBA-CCA-CDA |
| 29 | B | 621 | LMG | C30-C31-C32-C33 |
| 30 | D | 407 | LHG | C9-C10-C11-C12 |
| 30 | a | 616 | LHG | C10-C11-C12-C13 |
| 32 | H | 102 | DGD | CAA-CBA-CCA-CDA |
| 24 | B | 608 | CLA | O1A-CGA-O2A-C1 |
| 32 | C | 516 | DGD | C8B-C9B-CAB-CBB |
| 28 | l | 101 | SQD | C19-C20-C21-C22 |
| 30 | e | 101 | LHG | C26-C27-C28-C29 |
| 28 | L | 102 | SQD | C19-C20-C21-C22 |
| 24 | B | 613 | CLA | C13-C15-C16-C17 |
| 30 | A | 615 | LHG | C25-C26-C27-C28 |
| 32 | c | 518 | DGD | CBA-CCA-CDA-CEA |
| 32 | C | 515 | DGD | C2E-C1E-O5D-C6D |
| 26 | A | 610 | BCR | C11-C10-C9-C8 |
| 32 | c | 517 | DGD | C2E-C1E-O5D-C6D |
| 30 | A | 615 | LHG | C33-C34-C35-C36 |
| 29 | c | 519 | LMG | C34-C35-C36-C37 |
| 24 | b | 614 | CLA | O1A-CGA-O2A-C1 |
| 24 | a | 609 | CLA | C16-C17-C18-C20 |
| 32 | C | 516 | DGD | CDA-CEA-CFA-CGA |
| 32 | E | 101 | DGD | C6A-C7A-C8A-C9A |
| 29 | c | 519 | LMG | C39-C40-C41-C42 |
| 29 | z | 101 | LMG | C15-C16-C17-C18 |
| 24 | C | 508 | CLA | C11-C10-C8-C7 |
| 24 | B | 617 | CLA | C11-C12-C13-C15 |
| 24 | a | 609 | CLA | C11-C10-C8-C7 |
| 24 | C | 512 | CLA | C11-C10-C8-C7 |
| 24 | c | 513 | CLA | C6-C7-C8-C10 |
| 24 | C | 501 | CLA | C11-C12-C13-C15 |
| 24 | b | 603 | CLA | C6-C7-C8-C10 |
| 24 | b | 603 | CLA | C11-C10-C8-C7 |
| 24 | c | 501 | CLA | C11-C12-C13-C15 |
| 24 | c | 508 | CLA | C11-C10-C8-C7 |
| 24 | C | 506 | CLA | C11-C12-C13-C15 |
| 24 | C | 513 | CLA | C6-C7-C8-C10 |
| 24 | D | 404 | CLA | C11-C10-C8-C7 |
| 24 | d | 403 | CLA | C11-C10-C8-C7 |
| 27 | d | 404 | PL9 | C13-C14-C16-C17 |
| 24 | B | 616 | CLA | C12-C13-C15-C16 |
| 24 | A | 609 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | c | 512 | CLA | C11-C10-C8-C7 |
| 24 | b | 618 | CLA | C11-C12-C13-C15 |
| 24 | b | 617 | CLA | C12-C13-C15-C16 |
| 24 | c | 506 | CLA | C11-C12-C13-C15 |
| 24 | B | 602 | CLA | C6-C7-C8-C10 |
| 24 | B | 602 | CLA | C11-C10-C8-C7 |
| 24 | c | 504 | CLA | O1A-CGA-O2A-C1 |
| 24 | C | 508 | CLA | C11-C10-C8-C9 |
| 24 | B | 617 | CLA | C11-C12-C13-C14 |
| 24 | c | 513 | CLA | C11-C12-C13-C14 |
| 24 | C | 501 | CLA | C14-C13-C15-C16 |
| 24 | c | 501 | CLA | C14-C13-C15-C16 |
| 24 | c | 508 | CLA | C11-C10-C8-C9 |
| 24 | C | 506 | CLA | C11-C12-C13-C14 |
| 24 | C | 513 | CLA | C11-C12-C13-C14 |
| 24 | b | 618 | CLA | C11-C12-C13-C14 |
| 24 | c | 506 | CLA | C11-C12-C13-C14 |
| 26 | K | 101 | BCR | C15-C16-C17-C18 |
| 26 | K | 102 | BCR | C15-C16-C17-C18 |
| 26 | t | 101 | BCR | C15-C16-C17-C18 |
| 28 | a | 612 | SQD | C14-C15-C16-C17 |
| 29 | Z | 101 | LMG | C13-C14-C15-C16 |
| 30 | E | 102 | LHG | C26-C27-C28-C29 |
| 28 | A | 612 | SQD | C14-C15-C16-C17 |
| 26 | t | 101 | BCR | C36-C18-C19-C20 |
| 24 | B | 617 | CLA | C16-C17-C18-C20 |
| 24 | B | 605 | CLA | C16-C17-C18-C19 |
| 24 | b | 606 | CLA | C16-C17-C18-C19 |
| 24 | A | 609 | CLA | C16-C17-C18-C20 |
| 24 | b | 618 | CLA | C16-C17-C18-C20 |
| 29 | A | 613 | LMG | C22-C23-C24-C25 |
| 28 | A | 614 | SQD | C25-C26-C27-C28 |
| 26 | c | 521 | BCR | C21-C22-C23-C24 |
| 26 | F | 101 | BCR | C17-C18-C19-C20 |
| 28 | a | 614 | SQD | C25-C26-C27-C28 |
| 29 | A | 613 | LMG | C21-C22-C23-C24 |
| 32 | E | 101 | DGD | C4B-C5B-C6B-C7B |
| 32 | E | 101 | DGD | O1A-C1A-O1G-C1G |
| 28 | b | 601 | SQD | C24-C23-O48-C46 |
| 28 | B | 622 | SQD | C24-C23-O48-C46 |
| 28 | a | 612 | SQD | C19-C20-C21-C22 |
| 32 | c | 517 | DGD | CDA-CEA-CFA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | B | 621 | LMG | C31-C32-C33-C34 |
| 30 | E | 102 | LHG | C9-C10-C11-C12 |
| 28 | A | 612 | SQD | C19-C20-C21-C22 |
| 29 | Z | 101 | LMG | C4-C5-C6-O5 |
| 30 | A | 615 | LHG | C17-C18-C19-C20 |
| 29 | D | 408 | LMG | C30-C31-C32-C33 |
| 32 | C | 517 | DGD | C5B-C6B-C7B-C8B |
| 26 | c | 515 | BCR | C22-C23-C24-C25 |
| 26 | B | 618 | BCR | C6-C7-C8-C9 |
| 24 | a | 607 | CLA | CBD-CGD-O2D-CED |
| 28 | a | 614 | SQD | C31-C32-C33-C34 |
| 28 | a | 614 | SQD | O5-C1-O6-C44 |
| 28 | A | 614 | SQD | O5-C1-O6-C44 |
| 30 | L | 101 | LHG | O6-C4-C5-C6 |
| 30 | l | 102 | LHG | O6-C4-C5-C6 |
| 28 | A | 614 | SQD | C31-C32-C33-C34 |
| 30 | d | 407 | LHG | C13-C14-C15-C16 |
| 29 | c | 519 | LMG | C20-C21-C22-C23 |
| 27 | A | 611 | PL9 | C28-C29-C31-C32 |
| 27 | d | 404 | PL9 | C43-C44-C46-C47 |
| 24 | D | 403 | CLA | O1D-CGD-O2D-CED |
| 24 | B | 609 | CLA | C13-C15-C16-C17 |
| 24 | b | 610 | CLA | C13-C15-C16-C17 |
| 24 | b | 605 | CLA | C16-C17-C18-C20 |
| 24 | B | 604 | CLA | C16-C17-C18-C20 |
| 29 | z | 101 | LMG | C13-C14-C15-C16 |
| 32 | E | 101 | DGD | CAA-CBA-CCA-CDA |
| 29 | C | 518 | LMG | C14-C15-C16-C17 |
| 24 | B | 602 | CLA | C3A-C2A-CAA-CBA |
| 24 | B | 605 | CLA | C4C-C3C-CAC-CBC |
| 29 | C | 519 | LMG | C33-C34-C35-C36 |
| 28 | l | 101 | SQD | C35-C36-C37-C38 |
| 24 | C | 508 | CLA | C5-C6-C7-C8 |
| 24 | c | 508 | CLA | C5-C6-C7-C8 |
| 24 | b | 617 | CLA | C13-C15-C16-C17 |
| 29 | C | 518 | LMG | C34-C35-C36-C37 |
| 30 | D | 406 | LHG | C27-C28-C29-C30 |
| 30 | l | 102 | LHG | C14-C15-C16-C17 |
| 28 | L | 102 | SQD | C35-C36-C37-C38 |
| 30 | D | 406 | LHG | C31-C32-C33-C34 |
| 28 | a | 614 | SQD | C32-C33-C34-C35 |
| 28 | A | 614 | SQD | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 28 | l | 101 | SQD | C44-C45-C46-O48 |
| 29 | D | 408 | LMG | C7-C8-C9-O8 |
| 28 | b | 601 | SQD | C44-C45-C46-O48 |
| 28 | B | 622 | SQD | C44-C45-C46-O48 |
| 28 | L | 102 | SQD | C44-C45-C46-O48 |
| 29 | C | 519 | LMG | O9-C10-O7-C8 |
| 32 | C | 516 | DGD | C5A-C6A-C7A-C8A |
| 30 | A | 615 | LHG | C24-C25-C26-C27 |
| 29 | a | 613 | LMG | C39-C40-C41-C42 |
| 24 | B | 616 | CLA | C13-C15-C16-C17 |
| 32 | C | 515 | DGD | CBA-CCA-CDA-CEA |
| 30 | E | 102 | LHG | C19-C20-C21-C22 |
| 30 | A | 615 | LHG | C27-C28-C29-C30 |
| 32 | C | 516 | DGD | C9B-CAB-CBB-CCB |
| 24 | B | 605 | CLA | C2C-C3C-CAC-CBC |
| 30 | A | 615 | LHG | C18-C19-C20-C21 |
| 24 | b | 606 | CLA | C2C-C3C-CAC-CBC |
| 30 | E | 102 | LHG | C3-O3-P-O6 |
| 30 | D | 407 | LHG | O10-C23-O8-C6 |
| 24 | B | 613 | CLA | O1D-CGD-O2D-CED |
| 32 | C | 516 | DGD | CDB-CEB-CFB-CGB |
| 32 | d | 405 | DGD | C6A-C7A-C8A-C9A |
| 28 | a | 614 | SQD | C35-C36-C37-C38 |
| 28 | A | 614 | SQD | C35-C36-C37-C38 |
| 32 | E | 101 | DGD | CBB-CCB-CDB-CEB |
| 24 | B | 616 | CLA | C10-C11-C12-C13 |
| 24 | b | 617 | CLA | C10-C11-C12-C13 |
| 24 | B | 602 | CLA | O1A-CGA-O2A-C1 |
| 30 | D | 406 | LHG | C15-C16-C17-C18 |
| 28 | l | 101 | SQD | O47-C45-C46-O48 |
| 32 | d | 405 | DGD | O1G-C1G-C2G-O2G |
| 28 | b | 601 | SQD | O47-C45-C46-O48 |
| 28 | B | 622 | SQD | O47-C45-C46-O48 |
| 32 | E | 101 | DGD | O1G-C1G-C2G-O2G |
| 28 | L | 102 | SQD | O47-C45-C46-O48 |
| 24 | b | 615 | CLA | O1D-CGD-O2D-CED |
| 28 | L | 102 | SQD | C30-C31-C32-C33 |
| 26 | I | 101 | BCR | C15-C16-C17-C18 |
| 26 | c | 515 | BCR | C15-C16-C17-C18 |
| 29 | c | 520 | LMG | C11-C10-O7-C8 |
| 24 | b | 603 | CLA | C16-C17-C18-C20 |
| 24 | B | 602 | CLA | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 28 | l | 101 | SQD | C30-C31-C32-C33 |
| 27 | D | 405 | PL9 | C39-C41-C42-C43 |
| 24 | b | 603 | CLA | C2-C1-O2A-CGA |
| 27 | D | 405 | PL9 | C13-C14-C16-C17 |
| 30 | d | 407 | LHG | C32-C33-C34-C35 |
| 24 | c | 507 | CLA | C11-C10-C8-C9 |
| 24 | b | 616 | CLA | C11-C12-C13-C14 |
| 24 | b | 616 | CLA | C14-C13-C15-C16 |
| 24 | C | 507 | CLA | C11-C10-C8-C9 |
| 24 | B | 615 | CLA | C11-C12-C13-C14 |
| 24 | B | 615 | CLA | C14-C13-C15-C16 |
| 29 | B | 621 | LMG | C33-C34-C35-C36 |
| 29 | B | 621 | LMG | C34-C35-C36-C37 |
| 29 | c | 520 | LMG | C11-C12-C13-C14 |
| 24 | B | 607[A] | CLA | C8-C10-C11-C12 |
| 24 | b | 603 | CLA | C15-C16-C17-C18 |
| 24 | b | 608[A] | CLA | C8-C10-C11-C12 |
| 24 | B | 602 | CLA | C15-C16-C17-C18 |
| 30 | A | 615 | LHG | C2-C3-O3-P |
| 29 | C | 518 | LMG | C20-C21-C22-C23 |
| 30 | L | 101 | LHG | C32-C33-C34-C35 |
| 32 | H | 102 | DGD | C5A-C6A-C7A-C8A |
| 24 | B | 606 | CLA | CBD-CGD-O2D-CED |
| 26 | K | 101 | BCR | C1-C6-C7-C8 |
| 26 | T | 101 | BCR | C5-C6-C7-C8 |
| 26 | k | 101 | BCR | C23-C24-C25-C30 |
| 26 | b | 619 | BCR | C23-C24-C25-C26 |
| 29 | a | 613 | LMG | C22-C23-C24-C25 |
| 32 | H | 102 | DGD | O2G-C1B-C2B-C3B |
| 26 | K | 102 | BCR | C36-C18-C19-C20 |
| 27 | A | 611 | PL9 | C47-C48-C49-C50 |
| 28 | B | 622 | SQD | C16-C17-C18-C19 |
| 24 | B | 612 | CLA | O1D-CGD-O2D-CED |
| 26 | H | 101 | BCR | C21-C22-C23-C24 |
| 26 | k | 101 | BCR | C21-C22-C23-C24 |
| 24 | c | 502 | CLA | C15-C16-C17-C18 |
| 24 | C | 502 | CLA | C15-C16-C17-C18 |
| 28 | b | 601 | SQD | C16-C17-C18-C19 |
| 30 | l | 102 | LHG | C25-C26-C27-C28 |
| 24 | a | 615 | CLA | C4C-C3C-CAC-CBC |
| 29 | c | 520 | LMG | C40-C41-C42-C43 |
| 30 | D | 406 | LHG | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | B | 607[B] | CLA | C16-C17-C18-C19 |
| 24 | C | 501 | CLA | C16-C17-C18-C19 |
| 24 | c | 501 | CLA | C16-C17-C18-C19 |
| 24 | c | 502 | CLA | C16-C17-C18-C20 |
| 24 | b | 608[B] | CLA | C16-C17-C18-C19 |
| 24 | C | 502 | CLA | C16-C17-C18-C20 |
| 30 | D | 407 | LHG | O6-C4-C5-C6 |
| 24 | B | 617 | CLA | C12-C13-C15-C16 |
| 24 | c | 513 | CLA | C11-C12-C13-C15 |
| 24 | C | 501 | CLA | C12-C13-C15-C16 |
| 24 | c | 507 | CLA | C11-C10-C8-C7 |
| 24 | b | 616 | CLA | C11-C12-C13-C15 |
| 24 | c | 501 | CLA | C12-C13-C15-C16 |
| 24 | C | 513 | CLA | C11-C12-C13-C15 |
| 24 | C | 507 | CLA | C11-C10-C8-C7 |
| 24 | D | 404 | CLA | C6-C7-C8-C10 |
| 24 | d | 403 | CLA | C6-C7-C8-C10 |
| 24 | B | 616 | CLA | C11-C10-C8-C7 |
| 24 | B | 615 | CLA | C11-C12-C13-C15 |
| 24 | b | 613 | CLA | C12-C13-C15-C16 |
| 24 | B | 612 | CLA | C12-C13-C15-C16 |
| 24 | b | 618 | CLA | C12-C13-C15-C16 |
| 24 | b | 617 | CLA | C11-C10-C8-C7 |
| 32 | c | 516 | DGD | O1A-C1A-O1G-C1G |
| 28 | b | 601 | SQD | O10-C23-O48-C46 |
| 29 | A | 613 | LMG | C15-C16-C17-C18 |
| 26 | H | 101 | BCR | C13-C14-C15-C16 |
| 26 | F | 101 | BCR | C19-C20-C21-C22 |
| 26 | t | 101 | BCR | C9-C10-C11-C12 |
| 26 | b | 620 | BCR | C15-C16-C17-C18 |
| 24 | B | 617 | CLA | C16-C17-C18-C19 |
| 28 | B | 622 | SQD | O10-C23-O48-C46 |
| 26 | I | 101 | BCR | C11-C10-C9-C34 |
| 26 | c | 521 | BCR | C16-C17-C18-C36 |
| 30 | L | 101 | LHG | C24-C25-C26-C27 |
| 32 | d | 405 | DGD | O6D-C5D-C6D-O5D |
| 32 | H | 102 | DGD | CDB-CEB-CFB-CGB |
| 24 | b | 618 | CLA | C16-C17-C18-C19 |
| 30 | D | 407 | LHG | C24-C23-O8-C6 |
| 24 | A | 609 | CLA | CBA-CGA-O2A-C1 |
| 32 | E | 101 | DGD | C4D-C5D-C6D-O5D |
| 28 | x | 101 | SQD | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 29 | c | 519 | LMG | C30-C31-C32-C33 |
| 32 | c | 518 | DGD | C3A-C4A-C5A-C6A |
| 32 | d | 405 | DGD | CAB-CBB-CCB-CDB |
| 30 | d | 406 | LHG | C34-C35-C36-C37 |
| 24 | c | 503 | CLA | C8-C10-C11-C12 |
| 24 | C | 503 | CLA | C8-C10-C11-C12 |
| 24 | c | 513 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 501 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 603 | CLA | CAD-CBD-CGD-O2D |
| 24 | A | 606 | CLA | CAD-CBD-CGD-O2D |
| 25 | A | 608 | PHO | CAD-CBD-CGD-O2D |
| 24 | C | 509 | CLA | CAD-CBD-CGD-O2D |
| 24 | A | 609 | CLA | CAD-CBD-CGD-O2D |
| 29 | c | 519 | LMG | O9-C10-O7-C8 |
| 28 | X | 101 | SQD | C11-C10-C9-C8 |
| 32 | C | 517 | DGD | C7A-C8A-C9A-CAA |
| 30 | D | 406 | LHG | C11-C10-C9-C8 |
| 26 | B | 620 | BCR | C6-C7-C8-C9 |
| 29 | A | 613 | LMG | C7-C8-C9-O8 |
| 32 | E | 101 | DGD | O1G-C1G-C2G-C3G |
| 32 | H | 102 | DGD | O1G-C1G-C2G-C3G |
| 24 | B | 606 | CLA | O1A-CGA-O2A-C1 |
| 30 | L | 101 | LHG | O6-C4-C5-O7 |
| 28 | a | 614 | SQD | C24-C25-C26-C27 |
| 28 | A | 614 | SQD | C24-C25-C26-C27 |
| 24 | C | 510 | CLA | CBA-CGA-O2A-C1 |
| 24 | B | 615 | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 605 | CLA | C16-C17-C18-C19 |
| 24 | B | 604 | CLA | C16-C17-C18-C19 |
| 29 | C | 518 | LMG | C22-C23-C24-C25 |
| 24 | C | 508 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 607 | CLA | CHA-CBD-CGD-O2D |
| 24 | c | 504 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 504 | CLA | CHA-CBD-CGD-O2D |
| 24 | B | 607[A] | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 607[B] | CLA | CHA-CBD-CGD-O1D |
| 24 | c | 507 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 505 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 510 | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 610 | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 610 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 507 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | C | 507 | CLA | CHA-CBD-CGD-O2D |
| 24 | b | 608[A] | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 604 | CLA | CHA-CBD-CGD-O2D |
| 24 | b | 608[B] | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 604 | CLA | CHA-CBD-CGD-O2D |
| 24 | c | 510 | CLA | CHA-CBD-CGD-O1D |
| 24 | c | 510 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 503 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 614 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 614 | CLA | CHA-CBD-CGD-O2D |
| 24 | B | 608 | CLA | CHA-CBD-CGD-O2D |
| 24 | B | 602 | CLA | CHA-CBD-CGD-O2D |
| 24 | C | 502 | CLA | CHA-CBD-CGD-O2D |
| 32 | C | 515 | DGD | CBB-CCB-CDB-CEB |
| 28 | a | 614 | SQD | C2-C1-O6-C44 |
| 28 | A | 614 | SQD | C2-C1-O6-C44 |
| 32 | C | 515 | DGD | CDA-CEA-CFA-CGA |
| 32 | C | 517 | DGD | CAB-CBB-CCB-CDB |
| 29 | C | 519 | LMG | C11-C12-C13-C14 |
| 29 | a | 613 | LMG | O7-C8-C9-O8 |
| 30 | d | 407 | LHG | C10-C11-C12-C13 |
| 24 | b | 609 | CLA | O1A-CGA-O2A-C1 |
| 32 | C | 517 | DGD | O1A-C1A-O1G-C1G |
| 28 | a | 614 | SQD | C29-C30-C31-C32 |
| 28 | A | 614 | SQD | C29-C30-C31-C32 |
| 29 | B | 621 | LMG | C18-C19-C20-C21 |
| 24 | C | 501 | CLA | C16-C17-C18-C20 |
| 24 | b | 603 | CLA | C16-C17-C18-C19 |
| 24 | c | 501 | CLA | C16-C17-C18-C20 |
| 24 | B | 602 | CLA | C16-C17-C18-C19 |
| 32 | c | 517 | DGD | CDB-CEB-CFB-CGB |
| 30 | E | 102 | LHG | C12-C13-C14-C15 |
| 27 | a | 611 | PL9 | C15-C14-C16-C17 |
| 32 | C | 516 | DGD | CCA-CDA-CEA-CFA |
| 32 | C | 515 | DGD | O1A-C1A-O1G-C1G |
| 25 | A | 608 | PHO | C2-C3-C5-C6 |
| 27 | a | 611 | PL9 | C28-C29-C31-C32 |
| 28 | a | 614 | SQD | C27-C28-C29-C30 |
| 28 | A | 614 | SQD | C27-C28-C29-C30 |
| 24 | a | 609 | CLA | C11-C12-C13-C14 |
| 24 | D | 404 | CLA | C6-C7-C8-C9 |
| 24 | d | 403 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | A | 609 | CLA | C11-C12-C13-C14 |
| 24 | b | 613 | CLA | C14-C13-C15-C16 |
| 24 | B | 612 | CLA | C14-C13-C15-C16 |
| 24 | C | 512 | CLA | O1D-CGD-O2D-CED |
| 29 | c | 519 | LMG | C14-C15-C16-C17 |
| 29 | a | 613 | LMG | O6-C5-C6-O5 |
| 32 | C | 516 | DGD | C8A-C9A-CAA-CBA |
| 32 | C | 516 | DGD | CBA-CCA-CDA-CEA |
| 26 | T | 101 | BCR | C36-C18-C19-C20 |
| 26 | c | 521 | BCR | C36-C18-C19-C20 |
| 30 | E | 102 | LHG | O1-C1-C2-C3 |
| 26 | I | 101 | BCR | C17-C18-C19-C20 |
| 26 | b | 619 | BCR | C17-C18-C19-C20 |
| 26 | t | 101 | BCR | C17-C18-C19-C20 |
| 26 | b | 621 | BCR | C17-C18-C19-C20 |
| 24 | b | 612 | CLA | C8-C10-C11-C12 |
| 29 | j | 101 | LMG | C17-C18-C19-C20 |
| 24 | a | 606 | CLA | C2-C1-O2A-CGA |
| 24 | b | 618 | CLA | C2-C1-O2A-CGA |
| 24 | B | 602 | CLA | C2-C1-O2A-CGA |
| 29 | C | 518 | LMG | C19-C20-C21-C22 |
| 29 | A | 613 | LMG | C11-C12-C13-C14 |
| 26 | T | 101 | BCR | C9-C10-C11-C12 |
| 30 | E | 102 | LHG | C4-O6-P-O3 |
| 30 | a | 616 | LHG | C11-C10-C9-C8 |
| 24 | b | 606 | CLA | C4C-C3C-CAC-CBC |
| 24 | B | 614 | CLA | C13-C15-C16-C17 |
| 30 | a | 616 | LHG | C2-C3-O3-P |
| 32 | C | 516 | DGD | C7A-C8A-C9A-CAA |
| 29 | C | 518 | LMG | C31-C32-C33-C34 |
| 30 | L | 101 | LHG | C14-C15-C16-C17 |
| 30 | D | 407 | LHG | C3-O3-P-O4 |
| 30 | e | 101 | LHG | C3-O3-P-O4 |
| 30 | L | 101 | LHG | C4-O6-P-O5 |
| 30 | l | 102 | LHG | C4-O6-P-O5 |
| 24 | b | 612 | CLA | C16-C17-C18-C19 |
| 24 | B | 611 | CLA | C16-C17-C18-C19 |
| 32 | c | 516 | DGD | C9A-CAA-CBA-CCA |
| 30 | d | 406 | LHG | C15-C16-C17-C18 |
| 32 | c | 516 | DGD | O6D-C1D-O3G-C3G |
| 24 | b | 615 | CLA | C13-C15-C16-C17 |
| 24 | B | 611 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | A | 613 | LMG | C29-C28-O8-C9 |
| 24 | B | 615 | CLA | CBD-CGD-O2D-CED |
| 29 | c | 519 | LMG | O10-C28-O8-C9 |
| 28 | a | 614 | SQD | C9-C10-C11-C12 |
| 28 | A | 614 | SQD | C9-C10-C11-C12 |
| 32 | C | 515 | DGD | C5A-C6A-C7A-C8A |
| 29 | j | 101 | LMG | C11-C12-C13-C14 |
| 29 | Z | 101 | LMG | C18-C19-C20-C21 |
| 24 | C | 504 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 603 | CLA | CAD-CBD-CGD-O1D |
| 24 | C | 510 | CLA | CAD-CBD-CGD-O1D |
| 24 | c | 502 | CLA | CAD-CBD-CGD-O1D |
| 24 | B | 615 | CLA | CAD-CBD-CGD-O1D |
| 24 | C | 503 | CLA | CAD-CBD-CGD-O1D |
| 24 | B | 602 | CLA | CAD-CBD-CGD-O1D |
| 24 | C | 502 | CLA | CAD-CBD-CGD-O1D |
| 28 | a | 612 | SQD | C23-C24-C25-C26 |
| 28 | A | 612 | SQD | C23-C24-C25-C26 |
| 32 | c | 517 | DGD | C5A-C6A-C7A-C8A |
| 29 | a | 613 | LMG | C29-C30-C31-C32 |
| 32 | H | 102 | DGD | C8A-C9A-CAA-CBA |
| 24 | B | 605 | CLA | C3-C5-C6-C7 |
| 24 | b | 606 | CLA | C3-C5-C6-C7 |
| 28 | b | 601 | SQD | C19-C20-C21-C22 |
| 28 | B | 622 | SQD | C19-C20-C21-C22 |
| 24 | D | 402 | CLA | C2C-C3C-CAC-CBC |
| 28 | X | 101 | SQD | C28-C29-C30-C31 |
| 32 | c | 517 | DGD | C6A-C7A-C8A-C9A |
| 24 | b | 603 | CLA | CBA-CGA-O2A-C1 |
| 24 | B | 602 | CLA | CBA-CGA-O2A-C1 |
| 28 | x | 101 | SQD | C28-C29-C30-C31 |
| 32 | c | 518 | DGD | CAB-CBB-CCB-CDB |
| 24 | b | 617 | CLA | C16-C17-C18-C20 |
| 24 | c | 502 | CLA | CBD-CGD-O2D-CED |
| 24 | c | 504 | CLA | C12-C13-C15-C16 |
| 24 | C | 504 | CLA | C12-C13-C15-C16 |
| 24 | b | 616 | CLA | C12-C13-C15-C16 |
| 24 | C | 506 | CLA | C6-C7-C8-C10 |
| 24 | a | 607 | CLA | C11-C10-C8-C7 |
| 24 | D | 404 | CLA | C11-C12-C13-C15 |
| 24 | D | 404 | CLA | C12-C13-C15-C16 |
| 24 | d | 403 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 30 | l | 102 | LHG | O6-C4-C5-O7 |
| 24 | A | 607 | CLA | C11-C10-C8-C7 |
| 24 | C | 509 | CLA | C6-C7-C8-C10 |
| 24 | B | 615 | CLA | C12-C13-C15-C16 |
| 29 | a | 613 | LMG | C10-C11-C12-C13 |
| 24 | c | 506 | CLA | C6-C7-C8-C10 |
| 24 | c | 509 | CLA | C6-C7-C8-C10 |
| 32 | C | 515 | DGD | C9A-CAA-CBA-CCA |
| 32 | c | 518 | DGD | CDB-CEB-CFB-CGB |
| 32 | c | 516 | DGD | C5A-C6A-C7A-C8A |
| 27 | A | 611 | PL9 | C2-C3-C7-C8 |
| 29 | A | 613 | LMG | C10-C11-C12-C13 |
| 29 | A | 613 | LMG | C17-C18-C19-C20 |
| 29 | j | 101 | LMG | C34-C35-C36-C37 |
| 30 | a | 616 | LHG | C17-C18-C19-C20 |
| 32 | h | 102 | DGD | C5A-C6A-C7A-C8A |
| 24 | B | 616 | CLA | C16-C17-C18-C20 |
| 29 | C | 519 | LMG | C40-C41-C42-C43 |
| 30 | A | 615 | LHG | C30-C31-C32-C33 |
| 32 | c | 518 | DGD | C3B-C4B-C5B-C6B |
| 32 | c | 518 | DGD | CBB-CCB-CDB-CEB |
| 32 | d | 405 | DGD | O1G-C1G-C2G-C3G |
| 33 | v | 201 | HEM | C4D-C3D-CAD-CBD |
| 29 | C | 519 | LMG | C16-C17-C18-C19 |
| 29 | a | 613 | LMG | O1-C7-C8-C9 |
| 29 | A | 613 | LMG | O1-C7-C8-O7 |
| 29 | A | 613 | LMG | O7-C8-C9-O8 |
| 29 | D | 408 | LMG | O7-C8-C9-O8 |
| 32 | h | 102 | DGD | O1G-C1G-C2G-O2G |
| 30 | E | 102 | LHG | O7-C5-C6-O8 |
| 29 | a | 613 | LMG | O1-C7-C8-O7 |
| 30 | e | 101 | LHG | C9-C10-C11-C12 |
| 32 | C | 516 | DGD | C2G-C3G-O3G-C1D |
| 32 | C | 516 | DGD | C5D-C6D-O5D-C1E |
| 32 | c | 517 | DGD | C2G-C3G-O3G-C1D |
| 29 | C | 519 | LMG | C8-C7-O1-C1 |
| 24 | c | 513 | CLA | C3-C5-C6-C7 |
| 27 | A | 611 | PL9 | C15-C14-C16-C17 |
| 29 | a | 613 | LMG | C33-C34-C35-C36 |
| 29 | A | 613 | LMG | C39-C40-C41-C42 |
| 32 | d | 405 | DGD | CBB-CCB-CDB-CEB |
| 24 | c | 504 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | B | 617 | CLA | C14-C13-C15-C16 |
| 24 | C | 504 | CLA | C14-C13-C15-C16 |
| 24 | a | 607 | CLA | C11-C10-C8-C9 |
| 24 | A | 607 | CLA | C11-C10-C8-C9 |
| 24 | A | 609 | CLA | C11-C10-C8-C9 |
| 24 | c | 512 | CLA | C11-C10-C8-C9 |
| 24 | b | 618 | CLA | C14-C13-C15-C16 |
| 26 | t | 101 | BCR | C6-C7-C8-C9 |
| 24 | C | 513 | CLA | C3-C5-C6-C7 |
| 28 | l | 101 | SQD | C13-C14-C15-C16 |
| 30 | E | 102 | LHG | O1-C1-C2-O2 |
| 29 | b | 622 | LMG | C35-C36-C37-C38 |
| 30 | E | 102 | LHG | C17-C18-C19-C20 |
| 30 | d | 407 | LHG | C11-C10-C9-C8 |
| 26 | c | 515 | BCR | C13-C14-C15-C16 |
| 29 | a | 613 | LMG | C17-C18-C19-C20 |
| 28 | L | 102 | SQD | C13-C14-C15-C16 |
| 29 | D | 408 | LMG | C11-C12-C13-C14 |
| 28 | b | 601 | SQD | C14-C15-C16-C17 |
| 28 | B | 622 | SQD | C14-C15-C16-C17 |
| 29 | C | 519 | LMG | C36-C37-C38-C39 |
| 29 | B | 621 | LMG | C39-C40-C41-C42 |
| 29 | Z | 101 | LMG | C15-C16-C17-C18 |
| 32 | c | 518 | DGD | C7A-C8A-C9A-CAA |
| 28 | b | 601 | SQD | C46-C45-O47-C7 |
| 28 | B | 622 | SQD | C46-C45-O47-C7 |
| 29 | c | 520 | LMG | C16-C17-C18-C19 |
| 29 | C | 518 | LMG | O9-C10-O7-C8 |
| 24 | B | 617 | CLA | C2-C1-O2A-CGA |
| 24 | C | 506 | CLA | C2-C1-O2A-CGA |
| 29 | C | 518 | LMG | C30-C31-C32-C33 |
| 29 | c | 519 | LMG | C29-C28-O8-C9 |
| 26 | K | 102 | BCR | C19-C20-C21-C22 |
| 30 | L | 101 | LHG | O10-C23-O8-C6 |
| 30 | D | 407 | LHG | O6-C4-C5-O7 |
| 24 | B | 603 | CLA | O1D-CGD-O2D-CED |
| 27 | a | 611 | PL9 | C35-C34-C36-C37 |
| 32 | c | 517 | DGD | C7A-C8A-C9A-CAA |
| 29 | c | 520 | LMG | C36-C37-C38-C39 |
| 26 | T | 101 | BCR | C23-C24-C25-C30 |
| 26 | F | 101 | BCR | C1-C6-C7-C8 |
| 26 | A | 610 | BCR | C1-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | t | 101 | BCR | C23-C24-C25-C26 |
| 24 | b | 603 | CLA | CAA-CBA-CGA-O2A |
| 29 | B | 621 | LMG | O8-C28-C29-C30 |
| 30 | l | 102 | LHG | C28-C29-C30-C31 |
| 24 | C | 512 | CLA | C16-C17-C18-C19 |
| 24 | c | 512 | CLA | C16-C17-C18-C19 |
| 24 | b | 612 | CLA | C2A-CAA-CBA-CGA |
| 26 | K | 101 | BCR | C20-C21-C22-C23 |
| 29 | A | 613 | LMG | C2-C1-O1-C7 |
| 30 | D | 406 | LHG | C3-O3-P-O6 |
| 30 | e | 101 | LHG | C4-O6-P-O3 |
| 29 | A | 613 | LMG | O1-C7-C8-C9 |
| 29 | b | 622 | LMG | C30-C31-C32-C33 |
| 24 | C | 506 | CLA | C12-C13-C15-C16 |
| 24 | d | 403 | CLA | C11-C12-C13-C15 |
| 24 | c | 506 | CLA | C12-C13-C15-C16 |
| 32 | c | 516 | DGD | CBA-CCA-CDA-CEA |
| 24 | a | 609 | CLA | C11-C10-C8-C9 |
| 24 | C | 512 | CLA | C11-C10-C8-C9 |
| 24 | c | 513 | CLA | C6-C7-C8-C9 |
| 24 | b | 603 | CLA | C6-C7-C8-C9 |
| 24 | C | 506 | CLA | C6-C7-C8-C9 |
| 24 | C | 513 | CLA | C6-C7-C8-C9 |
| 24 | B | 616 | CLA | C11-C10-C8-C9 |
| 24 | b | 617 | CLA | C11-C10-C8-C9 |
| 24 | c | 506 | CLA | C6-C7-C8-C9 |
| 24 | B | 602 | CLA | C6-C7-C8-C9 |
| 26 | B | 619 | BCR | C19-C20-C21-C22 |
| 24 | b | 612 | CLA | C16-C17-C18-C20 |
| 24 | B | 611 | CLA | C16-C17-C18-C20 |
| 29 | A | 613 | LMG | C19-C20-C21-C22 |
| 30 | l | 102 | LHG | C9-C10-C11-C12 |
| 24 | c | 502 | CLA | C16-C17-C18-C19 |
| 24 | C | 502 | CLA | C16-C17-C18-C19 |
| 29 | C | 519 | LMG | C39-C40-C41-C42 |
| 32 | E | 101 | DGD | C5A-C6A-C7A-C8A |
| 27 | D | 405 | PL9 | C36-C37-C38-C39 |
| 30 | D | 406 | LHG | O1-C1-C2-O2 |
| 24 | B | 616 | CLA | C16-C17-C18-C19 |
| 24 | b | 617 | CLA | C16-C17-C18-C19 |
| 24 | c | 504 | CLA | CBA-CGA-O2A-C1 |
| 32 | d | 405 | DGD | C2A-C1A-O1G-C1G |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 30 | d | 406 | LHG | C17-C18-C19-C20 |
| 24 | a | 609 | CLA | O1A-CGA-O2A-C1 |
| 24 | C | 510 | CLA | CBD-CGD-O2D-CED |
| 32 | C | 515 | DGD | CCA-CDA-CEA-CFA |
| 32 | E | 101 | DGD | CDB-CEB-CFB-CGB |
| 24 | C | 501 | CLA | O1A-CGA-O2A-C1 |
| 24 | b | 615 | CLA | O1A-CGA-O2A-C1 |
| 29 | A | 613 | LMG | O6-C1-O1-C7 |
| 26 | b | 620 | BCR | C9-C10-C11-C12 |
| 24 | b | 613 | CLA | O1A-CGA-O2A-C1 |
| 24 | A | 607 | CLA | C2C-C3C-CAC-CBC |
| 24 | A | 607 | CLA | C4C-C3C-CAC-CBC |
| 32 | h | 102 | DGD | C8B-C9B-CAB-CBB |
| 29 | B | 621 | LMG | C13-C14-C15-C16 |
| 26 | k | 101 | BCR | C18-C19-C20-C21 |
| 24 | d | 403 | CLA | O1A-CGA-O2A-C1 |
| 32 | H | 102 | DGD | C7B-C8B-C9B-CAB |
| 27 | d | 404 | PL9 | C15-C14-C16-C17 |
| 24 | b | 612 | CLA | C13-C15-C16-C17 |
| 24 | B | 611 | CLA | C13-C15-C16-C17 |
| 29 | c | 519 | LMG | C21-C22-C23-C24 |
| 30 | L | 101 | LHG | C16-C17-C18-C19 |
| 32 | c | 518 | DGD | O6D-C5D-C6D-O5D |
| 28 | a | 614 | SQD | C10-C11-C12-C13 |
| 28 | A | 614 | SQD | C10-C11-C12-C13 |
| 27 | d | 404 | PL9 | C42-C43-C44-C45 |
| 24 | B | 611 | CLA | C2A-CAA-CBA-CGA |
| 24 | c | 509 | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 610 | CLA | C2A-CAA-CBA-CGA |
| 32 | C | 516 | DGD | C2B-C3B-C4B-C5B |
| 24 | b | 603 | CLA | C3A-C2A-CAA-CBA |
| 24 | B | 616 | CLA | C3A-C2A-CAA-CBA |
| 29 | z | 101 | LMG | C14-C15-C16-C17 |
| 30 | e | 101 | LHG | C19-C20-C21-C22 |
| 29 | c | 519 | LMG | C22-C23-C24-C25 |
| 24 | B | 617 | CLA | C13-C15-C16-C17 |
| 26 | B | 619 | BCR | C35-C13-C14-C15 |
| 30 | A | 615 | LHG | C13-C14-C15-C16 |
| 24 | C | 512 | CLA | C16-C17-C18-C20 |
| 24 | c | 512 | CLA | C16-C17-C18-C20 |
| 24 | C | 506 | CLA | CBA-CGA-O2A-C1 |
| 24 | C | 510 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | c | 510 | CLA | C8-C10-C11-C12 |
| 24 | b | 618 | CLA | C13-C15-C16-C17 |
| 24 | c | 505 | CLA | CBD-CGD-O2D-CED |
| 29 | C | 519 | LMG | C12-C13-C14-C15 |
| 27 | d | 404 | PL9 | C35-C34-C36-C37 |
| 24 | D | 403 | CLA | C1A-C2A-CAA-CBA |
| 24 | C | 513 | CLA | C1A-C2A-CAA-CBA |
| 24 | B | 603 | CLA | C1A-C2A-CAA-CBA |
| 24 | B | 611 | CLA | C1A-C2A-CAA-CBA |
| 29 | b | 622 | LMG | C39-C40-C41-C42 |
| 24 | c | 504 | CLA | C11-C10-C8-C7 |
| 24 | C | 504 | CLA | C11-C10-C8-C7 |
| 24 | a | 609 | CLA | C12-C13-C15-C16 |
| 24 | B | 607[B] | CLA | C11-C10-C8-C7 |
| 24 | c | 502 | CLA | C12-C13-C15-C16 |
| 24 | b | 608[B] | CLA | C11-C10-C8-C7 |
| 24 | A | 609 | CLA | C12-C13-C15-C16 |
| 24 | C | 502 | CLA | C12-C13-C15-C16 |
| 24 | C | 505 | CLA | C2A-CAA-CBA-CGA |
| 30 | D | 407 | LHG | C35-C36-C37-C38 |
| 29 | a | 613 | LMG | C21-C22-C23-C24 |
| 29 | Z | 101 | LMG | O6-C5-C6-O5 |
| 24 | B | 608 | CLA | CBA-CGA-O2A-C1 |
| 27 | a | 611 | PL9 | C45-C44-C46-C47 |
| 27 | d | 404 | PL9 | C12-C11-C9-C10 |
| 32 | C | 515 | DGD | C1B-C2B-C3B-C4B |
| 24 | c | 513 | CLA | C16-C17-C18-C19 |
| 24 | C | 513 | CLA | C16-C17-C18-C19 |
| 30 | d | 406 | LHG | C11-C12-C13-C14 |
| 29 | c | 520 | LMG | C39-C40-C41-C42 |
| 29 | C | 518 | LMG | C33-C34-C35-C36 |
| 28 | a | 612 | SQD | O6-C44-C45-O47 |
| 32 | E | 101 | DGD | O2G-C2G-C3G-O3G |
| 28 | A | 612 | SQD | O6-C44-C45-O47 |
| 32 | H | 102 | DGD | O1G-C1G-C2G-O2G |
| 32 | C | 517 | DGD | CBA-CCA-CDA-CEA |
| 30 | d | 407 | LHG | C26-C27-C28-C29 |
| 24 | c | 502 | CLA | O1A-CGA-O2A-C1 |
| 24 | C | 510 | CLA | C6-C7-C8-C9 |
| 29 | c | 520 | LMG | C32-C33-C34-C35 |
| 24 | c | 501 | CLA | C2A-CAA-CBA-CGA |
| 24 | c | 505 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | c | 515 | BCR | C1-C6-C7-C8 |
| 26 | B | 619 | BCR | C1-C6-C7-C8 |
| 26 | a | 610 | BCR | C23-C24-C25-C30 |
| 26 | K | 101 | BCR | C23-C24-C25-C30 |
| 26 | C | 514 | BCR | C1-C6-C7-C8 |
| 32 | d | 405 | DGD | CDB-CEB-CFB-CGB |
| 24 | b | 610 | CLA | C4C-C3C-CAC-CBC |
| 29 | c | 520 | LMG | C37-C38-C39-C40 |
| 24 | c | 513 | CLA | C4-C3-C5-C6 |
| 27 | A | 611 | PL9 | C45-C44-C46-C47 |
| 25 | a | 608 | PHO | C4-C3-C5-C6 |
| 24 | C | 513 | CLA | C4-C3-C5-C6 |
| 32 | E | 101 | DGD | O6E-C5E-C6E-O5E |
| 26 | K | 101 | BCR | C21-C22-C23-C24 |
| 30 | d | 407 | LHG | C16-C17-C18-C19 |
| 24 | B | 610 | CLA | C2-C3-C5-C6 |
| 25 | a | 608 | PHO | C2-C3-C5-C6 |
| 24 | b | 611 | CLA | C2-C3-C5-C6 |
| 24 | B | 602 | CLA | CAA-CBA-CGA-O2A |
| 29 | A | 613 | LMG | C20-C21-C22-C23 |
| 30 | e | 101 | LHG | O6-C4-C5-O7 |
| 32 | c | 516 | DGD | CCA-CDA-CEA-CFA |
| 32 | h | 102 | DGD | CDA-CEA-CFA-CGA |
| 24 | C | 506 | CLA | CBD-CGD-O2D-CED |
| 24 | B | 613 | CLA | CBA-CGA-O2A-C1 |
| 24 | B | 615 | CLA | CBA-CGA-O2A-C1 |
| 32 | d | 405 | DGD | C4E-C5E-C6E-O5E |
| 25 | D | 401 | PHO | C8-C10-C11-C12 |
| 24 | c | 507 | CLA | C4-C3-C5-C6 |
| 27 | D | 405 | PL9 | C19-C21-C22-C23 |
| 26 | b | 620 | BCR | C19-C20-C21-C22 |
| 32 | H | 102 | DGD | CDA-CEA-CFA-CGA |
| 30 | a | 616 | LHG | O7-C5-C6-O8 |
| 32 | C | 515 | DGD | C8B-C9B-CAB-CBB |
| 24 | a | 615 | CLA | C2A-CAA-CBA-CGA |
| 25 | D | 401 | PHO | C5-C6-C7-C8 |
| 30 | D | 407 | LHG | C25-C26-C27-C28 |
| 30 | l | 102 | LHG | C17-C18-C19-C20 |
| 30 | D | 407 | LHG | C13-C14-C15-C16 |
| 26 | k | 101 | BCR | C35-C13-C14-C15 |
| 32 | C | 517 | DGD | C2B-C3B-C4B-C5B |
| 24 | a | 609 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | C | 507 | CLA | C4-C3-C5-C6 |
| 27 | D | 405 | PL9 | C12-C11-C9-C10 |
| 29 | C | 518 | LMG | C29-C28-O8-C9 |
| 30 | l | 102 | LHG | O7-C7-C8-C9 |
| 32 | c | 518 | DGD | C6B-C7B-C8B-C9B |
| 28 | b | 601 | SQD | C33-C34-C35-C36 |
| 24 | B | 607[A] | CLA | C11-C12-C13-C14 |
| 24 | B | 607[B] | CLA | C11-C10-C8-C9 |
| 24 | D | 404 | CLA | C11-C12-C13-C14 |
| 24 | d | 403 | CLA | C11-C12-C13-C14 |
| 24 | b | 608[A] | CLA | C11-C12-C13-C14 |
| 24 | b | 608[B] | CLA | C11-C10-C8-C9 |
| 24 | c | 510 | CLA | C6-C7-C8-C9 |
| 32 | c | 516 | DGD | C3B-C4B-C5B-C6B |
| 28 | B | 622 | SQD | C33-C34-C35-C36 |
| 24 | b | 605 | CLA | C13-C15-C16-C17 |
| 24 | C | 512 | CLA | C3A-C2A-CAA-CBA |
| 24 | A | 609 | CLA | C3A-C2A-CAA-CBA |
| 24 | b | 617 | CLA | C3A-C2A-CAA-CBA |
| 25 | d | 401 | PHO | C4C-C3C-CAC-CBC |
| 24 | B | 604 | CLA | C13-C15-C16-C17 |
| 24 | C | 510 | CLA | CAA-CBA-CGA-O2A |
| 24 | D | 403 | CLA | CAA-CBA-CGA-O2A |
| 30 | E | 102 | LHG | O7-C7-C8-C9 |
| 32 | d | 405 | DGD | C4B-C5B-C6B-C7B |
| 24 | C | 508 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 512 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 606 | CLA | CAD-CBD-CGD-O2D |
| 24 | c | 501 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 510 | CLA | CAD-CBD-CGD-O2D |
| 24 | c | 502 | CLA | CAD-CBD-CGD-O2D |
| 24 | C | 513 | CLA | CAD-CBD-CGD-O2D |
| 24 | B | 606 | CLA | CAD-CBD-CGD-O2D |
| 24 | b | 615 | CLA | CAD-CBD-CGD-O2D |
| 24 | c | 506 | CLA | CAD-CBD-CGD-O2D |
| 24 | B | 611 | CLA | CAD-CBD-CGD-O2D |
| 24 | c | 509 | CLA | CAD-CBD-CGD-O2D |
| 30 | D | 406 | LHG | C17-C18-C19-C20 |
| 24 | D | 402 | CLA | C4C-C3C-CAC-CBC |
| 28 | B | 622 | SQD | C17-C18-C19-C20 |
| 28 | L | 102 | SQD | O48-C23-C24-C25 |
| 24 | A | 609 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 28 | l | 101 | SQD | O48-C23-C24-C25 |
| 29 | j | 101 | LMG | O7-C10-C11-C12 |
| 30 | L | 101 | LHG | O7-C7-C8-C9 |
| 28 | b | 601 | SQD | C17-C18-C19-C20 |
| 26 | h | 101 | BCR | C7-C8-C9-C10 |
| 26 | A | 610 | BCR | C21-C22-C23-C24 |
| 26 | C | 514 | BCR | C11-C12-C13-C14 |
| 30 | d | 406 | LHG | C27-C28-C29-C30 |
| 29 | c | 520 | LMG | C14-C15-C16-C17 |
| 30 | E | 102 | LHG | C4-C5-C6-O8 |
| 27 | A | 611 | PL9 | C21-C22-C23-C24 |
| 32 | c | 518 | DGD | O1G-C1A-C2A-C3A |
| 24 | c | 510 | CLA | CAA-CBA-CGA-O2A |
| 24 | d | 402 | CLA | O2A-C1-C2-C3 |
| 24 | B | 605 | CLA | O2A-C1-C2-C3 |
| 24 | C | 512 | CLA | O2A-C1-C2-C3 |
| 24 | b | 606 | CLA | O2A-C1-C2-C3 |
| 24 | D | 403 | CLA | O2A-C1-C2-C3 |
| 25 | a | 608 | PHO | O2A-C1-C2-C3 |
| 25 | A | 608 | PHO | O2A-C1-C2-C3 |
| 24 | b | 604 | CLA | O2A-C1-C2-C3 |
| 24 | c | 512 | CLA | O2A-C1-C2-C3 |
| 24 | c | 509 | CLA | O2A-C1-C2-C3 |
| 32 | c | 518 | DGD | C5B-C6B-C7B-C8B |
| 24 | c | 507 | CLA | CHA-CBD-CGD-O1D |
| 24 | b | 605 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 608 | PHO | CHA-CBD-CGD-O2D |
| 24 | a | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | D | 401 | PHO | CHA-CBD-CGD-O2D |
| 24 | D | 402 | CLA | CHA-CBD-CGD-O2D |
| 24 | B | 603 | CLA | CHA-CBD-CGD-O2D |
| 24 | c | 505 | CLA | CHA-CBD-CGD-O2D |
| 24 | A | 607 | CLA | CHA-CBD-CGD-O1D |
| 24 | B | 615 | CLA | CHA-CBD-CGD-O2D |
| 24 | c | 509 | CLA | CHA-CBD-CGD-O1D |
| 29 | a | 613 | LMG | C19-C20-C21-C22 |
| 24 | B | 607[A] | CLA | C16-C17-C18-C20 |
| 24 | b | 608[A] | CLA | C16-C17-C18-C20 |
| 27 | a | 611 | PL9 | C2-C3-C7-C8 |
| 32 | C | 517 | DGD | O1G-C1A-C2A-C3A |
| 30 | D | 406 | LHG | O7-C5-C6-O8 |
| 24 | a | 607 | CLA | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | D | 408 | LMG | O7-C10-C11-C12 |
| 24 | b | 614 | CLA | CAA-CBA-CGA-O2A |
| 30 | d | 406 | LHG | C10-C11-C12-C13 |
| 29 | a | 613 | LMG | C16-C17-C18-C19 |
| 24 | C | 501 | CLA | C2A-CAA-CBA-CGA |
| 24 | b | 605 | CLA | C2A-CAA-CBA-CGA |
| 30 | a | 616 | LHG | O1-C1-C2-O2 |
| 32 | C | 517 | DGD | CDB-CEB-CFB-CGB |
| 32 | h | 102 | DGD | O2G-C1B-C2B-C3B |
| 27 | d | 404 | PL9 | C36-C37-C38-C39 |
| 24 | B | 610 | CLA | C4-C3-C5-C6 |
| 24 | a | 609 | CLA | C11-C12-C13-C15 |
| 24 | A | 609 | CLA | C11-C12-C13-C15 |
| 32 | H | 102 | DGD | C9B-CAB-CBB-CCB |
| 24 | B | 614 | CLA | CAA-CBA-CGA-O2A |
| 30 | e | 101 | LHG | O7-C7-C8-C9 |
| 24 | c | 504 | CLA | C11-C10-C8-C9 |
| 24 | C | 504 | CLA | C11-C10-C8-C9 |
| 24 | B | 605 | CLA | C6-C7-C8-C9 |
| 24 | C | 505 | CLA | C14-C13-C15-C16 |
| 24 | b | 606 | CLA | C6-C7-C8-C9 |
| 24 | C | 506 | CLA | C14-C13-C15-C16 |
| 24 | D | 404 | CLA | C14-C13-C15-C16 |
| 24 | d | 403 | CLA | C14-C13-C15-C16 |
| 24 | c | 505 | CLA | C14-C13-C15-C16 |
| 24 | c | 506 | CLA | C14-C13-C15-C16 |
| 30 | A | 615 | LHG | O10-C23-C24-C25 |
| 26 | t | 101 | BCR | C19-C20-C21-C22 |
| 32 | E | 101 | DGD | C3B-C4B-C5B-C6B |
| 28 | A | 612 | SQD | C18-C19-C20-C21 |
| 28 | a | 612 | SQD | C18-C19-C20-C21 |
| 29 | D | 408 | LMG | C32-C33-C34-C35 |
| 32 | d | 405 | DGD | C3B-C4B-C5B-C6B |
| 32 | c | 517 | DGD | O1B-C1B-C2B-C3B |
| 30 | D | 406 | LHG | C34-C35-C36-C37 |
| 24 | c | 513 | CLA | C16-C17-C18-C20 |
| 24 | C | 513 | CLA | C16-C17-C18-C20 |
| 24 | b | 611 | CLA | C4-C3-C5-C6 |
| 29 | C | 518 | LMG | C21-C22-C23-C24 |
| 24 | a | 607 | CLA | C2C-C3C-CAC-CBC |
| 30 | e | 101 | LHG | O9-C7-C8-C9 |
| 25 | A | 608 | PHO | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | B | 609 | CLA | C1A-C2A-CAA-CBA |
| 24 | b | 612 | CLA | C1A-C2A-CAA-CBA |
| 24 | c | 505 | CLA | C1A-C2A-CAA-CBA |
| 24 | b | 604 | CLA | C1A-C2A-CAA-CBA |
| 24 | b | 610 | CLA | C1A-C2A-CAA-CBA |
| 32 | c | 516 | DGD | C7B-C8B-C9B-CAB |
| 32 | C | 516 | DGD | O1B-C1B-C2B-C3B |
| 24 | c | 509 | CLA | O1D-CGD-O2D-CED |
| 24 | d | 402 | CLA | C2-C1-O2A-CGA |
| 24 | B | 608 | CLA | C2-C1-O2A-CGA |
| 29 | c | 519 | LMG | C17-C18-C19-C20 |
| 28 | A | 614 | SQD | C11-C12-C13-C14 |
| 32 | E | 101 | DGD | C2A-C1A-O1G-C1G |
| 32 | E | 101 | DGD | C1G-C2G-C3G-O3G |
| 28 | a | 614 | SQD | C11-C12-C13-C14 |
| 24 | D | 403 | CLA | CAA-CBA-CGA-O1A |
| 24 | b | 607 | CLA | C13-C15-C16-C17 |
| 24 | B | 606 | CLA | C13-C15-C16-C17 |
| 32 | c | 517 | DGD | C8A-C9A-CAA-CBA |
| 27 | D | 405 | PL9 | C18-C19-C21-C22 |
| 32 | c | 516 | DGD | C2E-C1E-O5D-C6D |
| 30 | A | 615 | LHG | C4-O6-P-O5 |
| 30 | d | 407 | LHG | C4-O6-P-O5 |
| 28 | L | 102 | SQD | O10-C23-C24-C25 |
| 30 | a | 616 | LHG | O8-C23-C24-C25 |
| 24 | B | 610 | CLA | O1A-CGA-O2A-C1 |
| 28 | l | 101 | SQD | O10-C23-C24-C25 |
| 29 | z | 101 | LMG | O7-C10-C11-C12 |
| 24 | c | 512 | CLA | CAA-CBA-CGA-O2A |
| 29 | A | 613 | LMG | O10-C28-C29-C30 |
| 27 | d | 404 | PL9 | C45-C44-C46-C47 |
| 30 | D | 406 | LHG | C28-C29-C30-C31 |
| 27 | d | 404 | PL9 | C38-C39-C41-C42 |
| 24 | B | 613 | CLA | CAD-CBD-CGD-O1D |
| 24 | B | 610 | CLA | CAD-CBD-CGD-O1D |
| 24 | c | 510 | CLA | CAD-CBD-CGD-O1D |
| 24 | b | 614 | CLA | CAD-CBD-CGD-O1D |
| 24 | c | 511 | CLA | C6-C7-C8-C9 |
| 24 | a | 609 | CLA | C14-C13-C15-C16 |
| 24 | B | 607[B] | CLA | C14-C13-C15-C16 |
| 24 | C | 511 | CLA | C6-C7-C8-C9 |
| 24 | D | 402 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|-----------------|
| 24 | b | 608[B] | CLA | C14-C13-C15-C16 |
| 24 | A | 609 | CLA | C14-C13-C15-C16 |
| 24 | a | 615 | CLA | C11-C12-C13-C14 |
| 29 | a | 613 | LMG | C36-C37-C38-C39 |
| 24 | c | 501 | CLA | CAA-CBA-CGA-O2A |
| 29 | D | 408 | LMG | C19-C20-C21-C22 |
| 24 | B | 616 | CLA | C15-C16-C17-C18 |
| 32 | H | 102 | DGD | C5B-C6B-C7B-C8B |
| 28 | b | 601 | SQD | C45-C46-O48-C23 |
| 28 | B | 622 | SQD | C45-C46-O48-C23 |
| 24 | b | 604 | CLA | C2A-CAA-CBA-CGA |
| 32 | C | 516 | DGD | O2G-C1B-C2B-C3B |
| 24 | C | 505 | CLA | CAA-CBA-CGA-O2A |
| 27 | D | 405 | PL9 | C25-C24-C26-C27 |
| 24 | b | 617 | CLA | C15-C16-C17-C18 |
| 24 | c | 511 | CLA | C6-C7-C8-C10 |
| 24 | d | 402 | CLA | C12-C13-C15-C16 |
| 24 | B | 607[B] | CLA | C12-C13-C15-C16 |
| 24 | c | 507 | CLA | C11-C12-C13-C15 |
| 24 | C | 505 | CLA | C12-C13-C15-C16 |
| 24 | b | 616 | CLA | C11-C10-C8-C7 |
| 24 | C | 511 | CLA | C6-C7-C8-C10 |
| 24 | C | 510 | CLA | C6-C7-C8-C10 |
| 24 | D | 403 | CLA | C12-C13-C15-C16 |
| 24 | C | 507 | CLA | C11-C12-C13-C15 |
| 24 | c | 505 | CLA | C12-C13-C15-C16 |
| 24 | b | 608[B] | CLA | C12-C13-C15-C16 |
| 24 | B | 615 | CLA | C11-C10-C8-C7 |
| 24 | c | 510 | CLA | C6-C7-C8-C10 |
| 24 | C | 501 | CLA | CAA-CBA-CGA-O1A |
| 32 | c | 517 | DGD | O2G-C1B-C2B-C3B |
| 32 | C | 517 | DGD | CCA-CDA-CEA-CFA |
| 30 | d | 407 | LHG | C12-C13-C14-C15 |
| 26 | B | 618 | BCR | C17-C18-C19-C20 |
| 26 | b | 621 | BCR | C21-C22-C23-C24 |
| 24 | B | 613 | CLA | CAA-CBA-CGA-O1A |
| 24 | B | 613 | CLA | C8-C10-C11-C12 |
| 24 | b | 614 | CLA | C8-C10-C11-C12 |
| 32 | c | 518 | DGD | O6E-C5E-C6E-O5E |
| 29 | C | 518 | LMG | O8-C28-C29-C30 |
| 24 | C | 506 | CLA | C15-C16-C17-C18 |
| 24 | c | 506 | CLA | C15-C16-C17-C18 |

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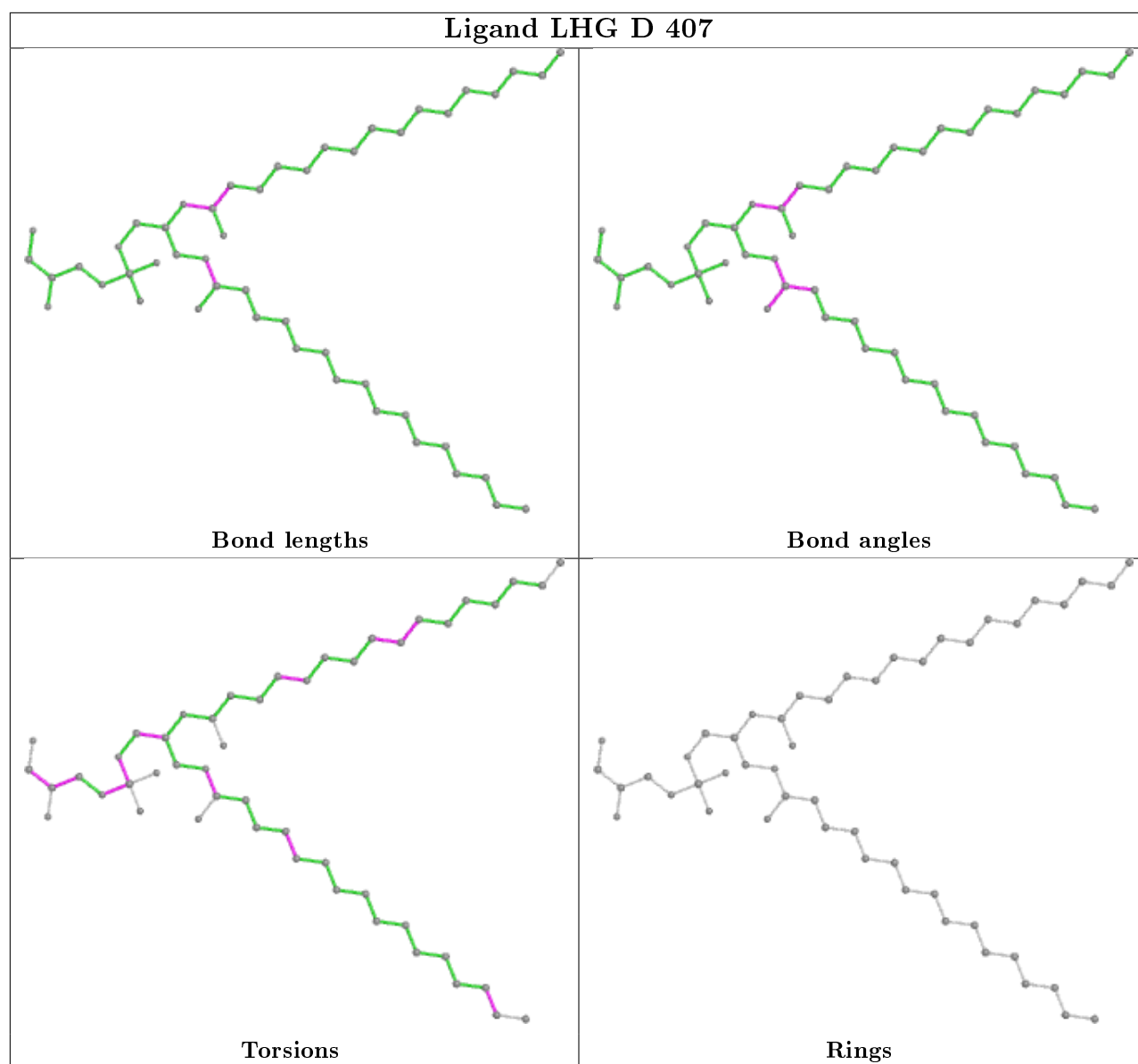
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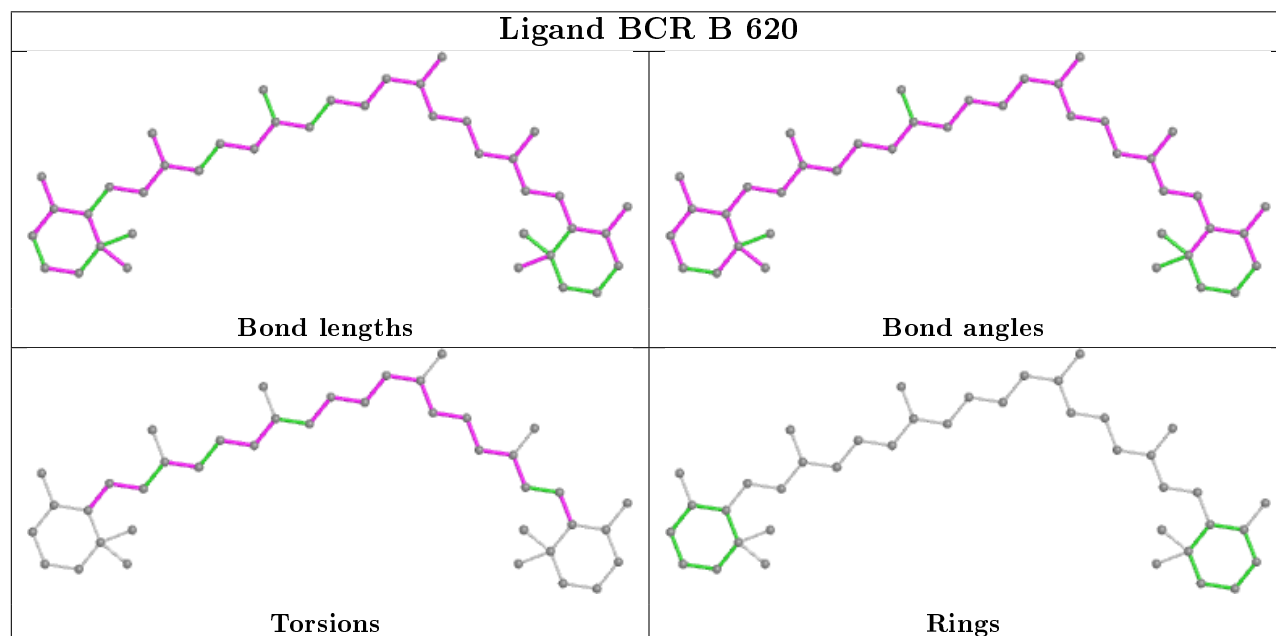
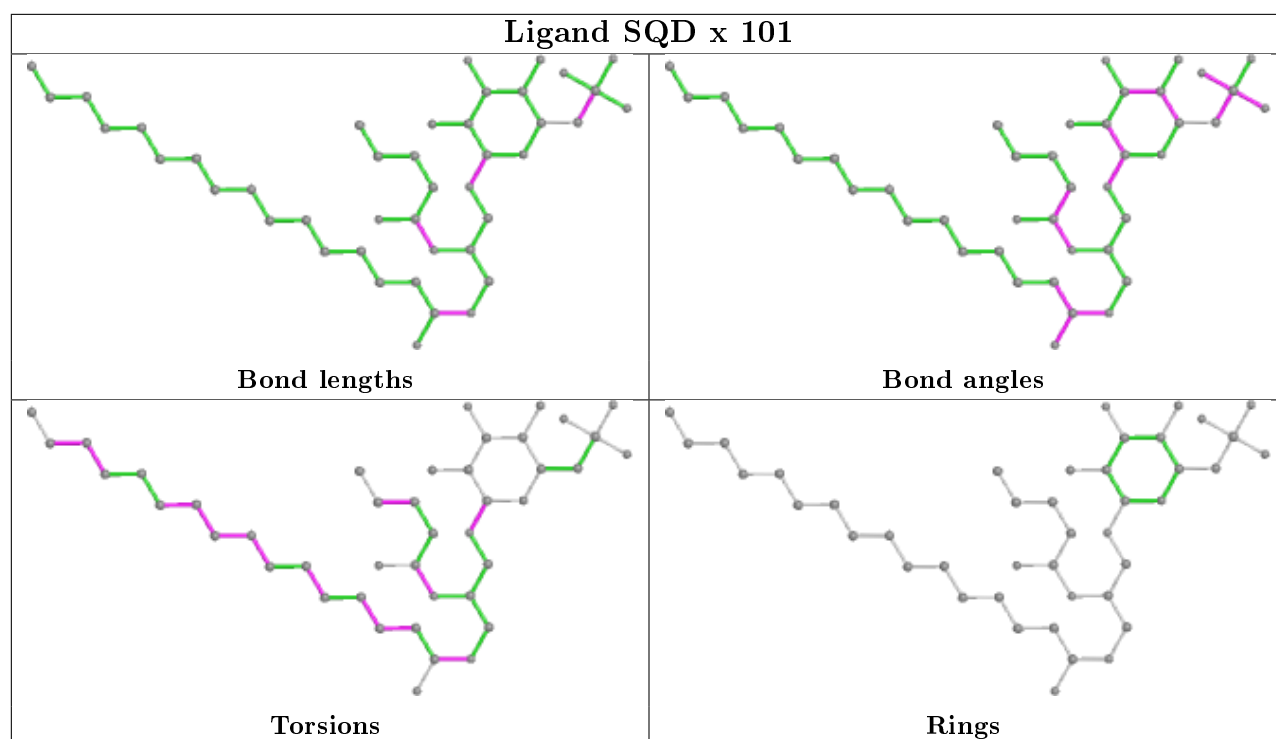
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 30 | a | 616 | LHG | O10-C23-C24-C25 |
| 30 | E | 102 | LHG | O9-C7-C8-C9 |
| 32 | d | 405 | DGD | O1A-C1A-C2A-C3A |
| 30 | l | 102 | LHG | O9-C7-C8-C9 |
| 30 | d | 407 | LHG | O8-C23-C24-C25 |

There are no ring outliers.

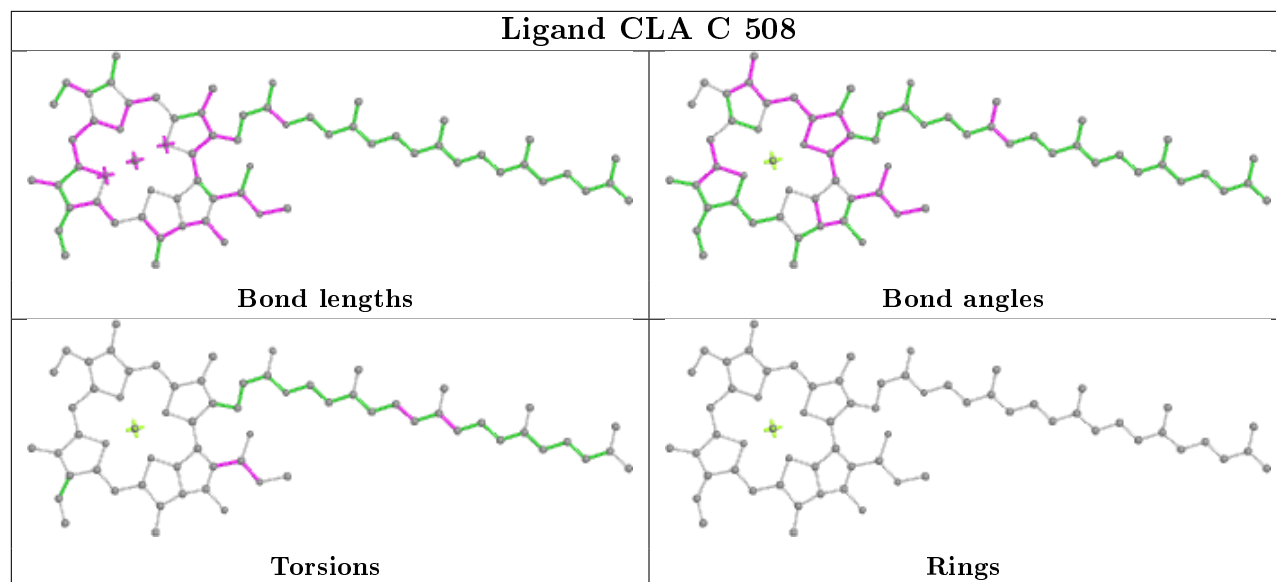
No monomer is involved in short contacts.

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

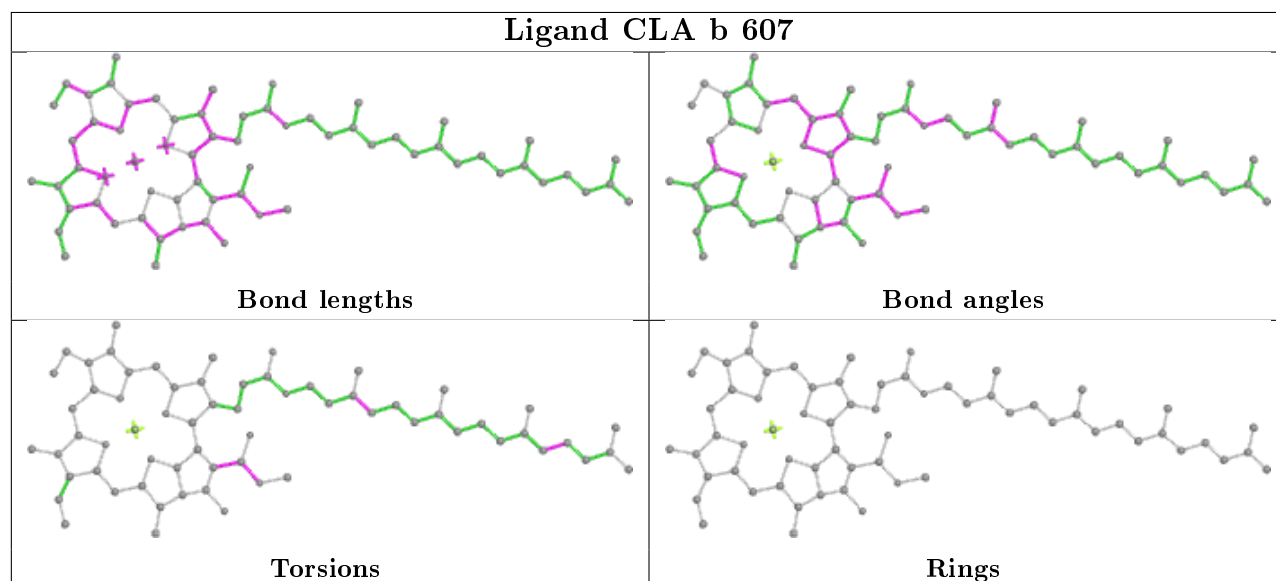




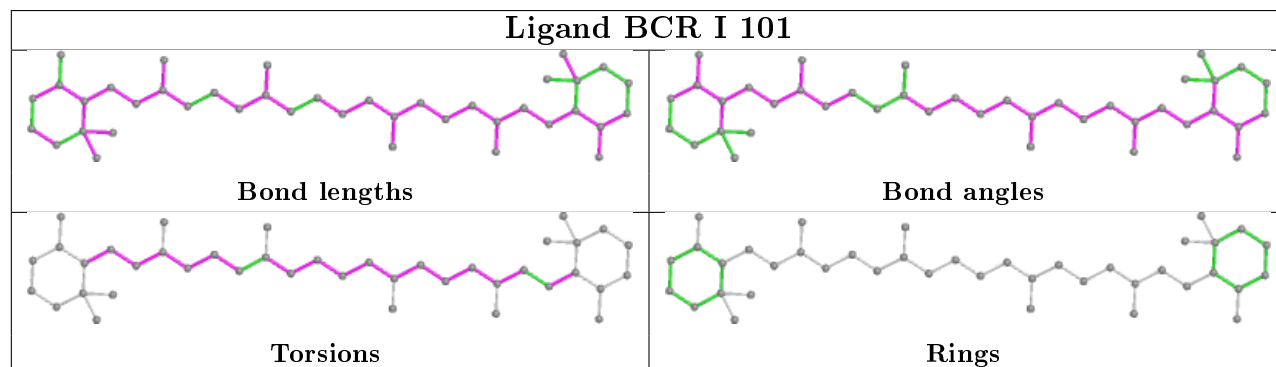
Ligand CLA C 508

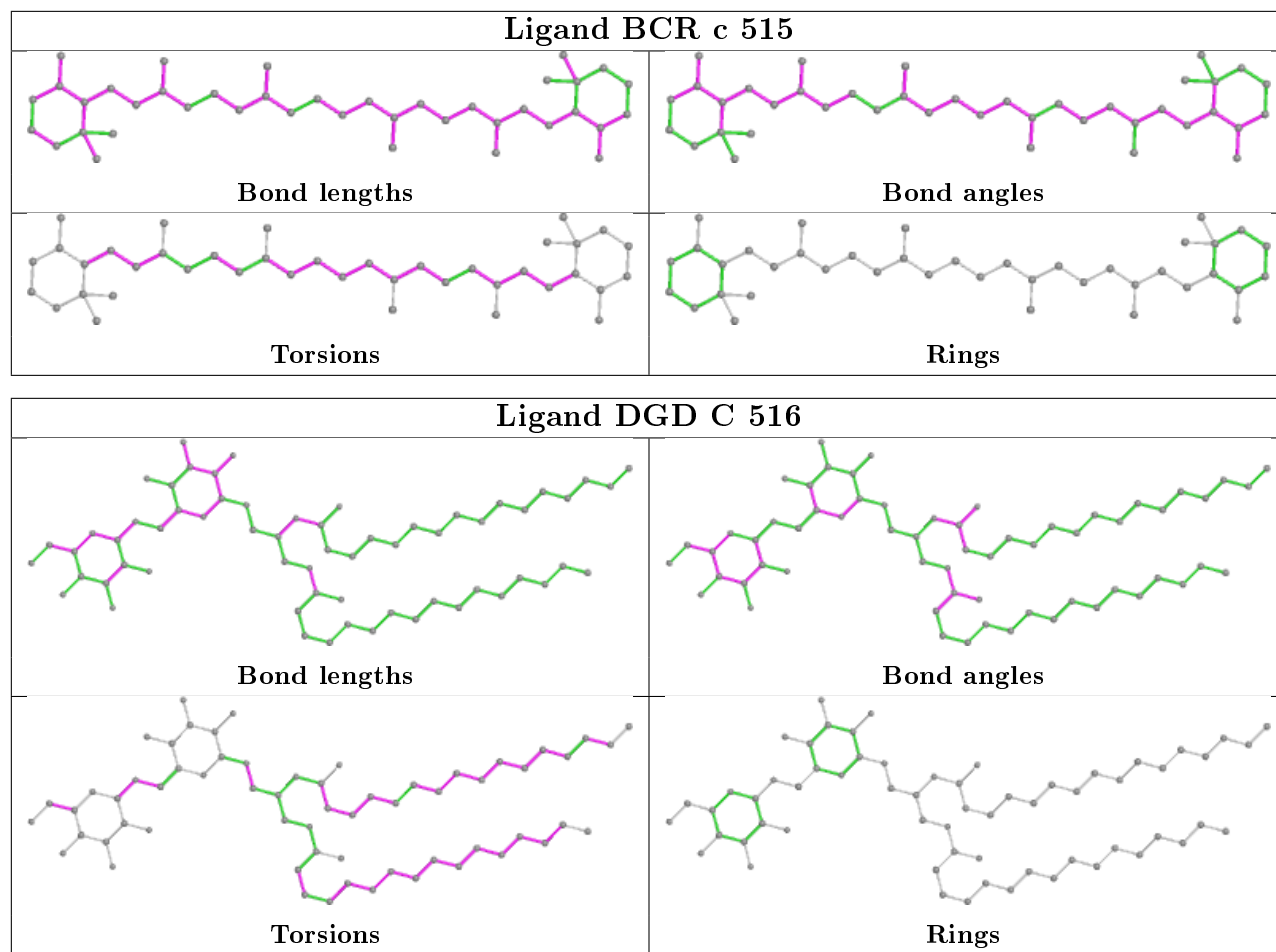


Ligand CLA b 607

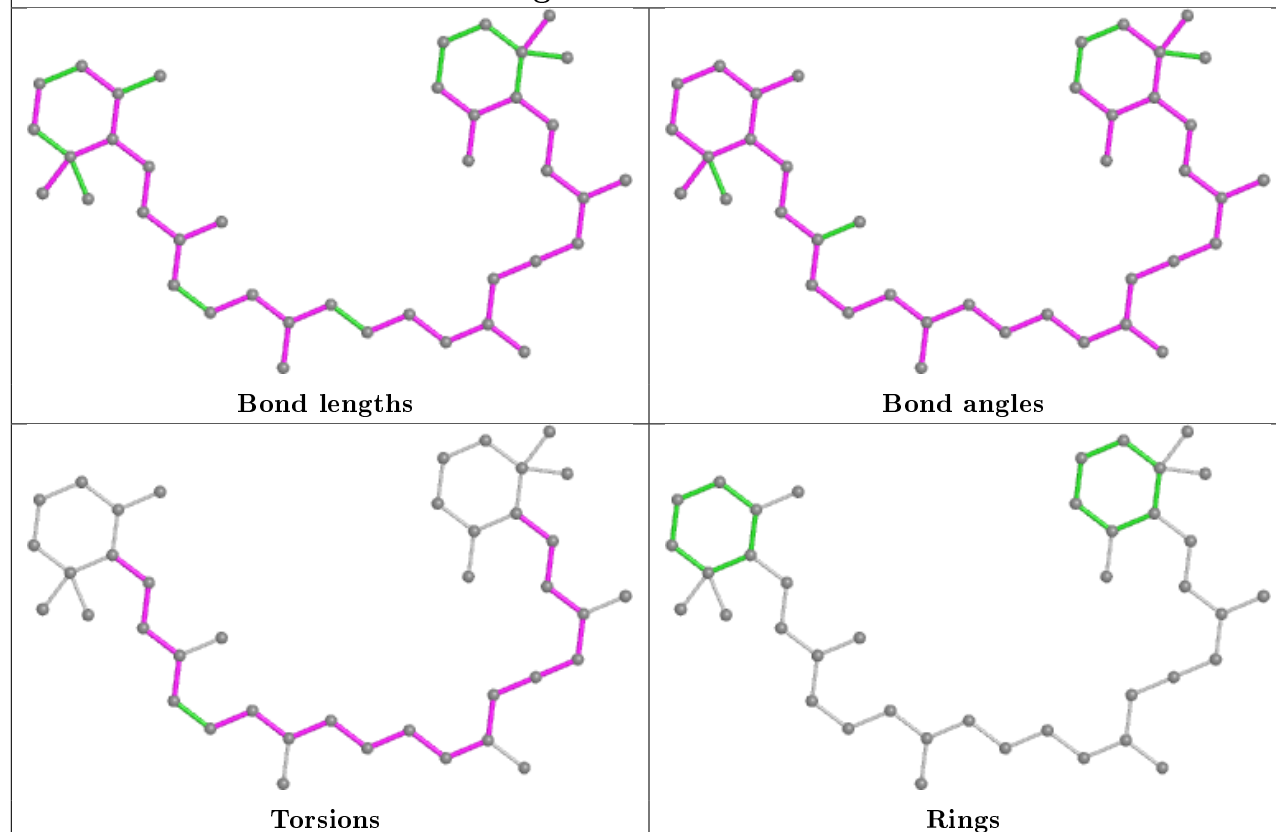


Ligand BCR I 101

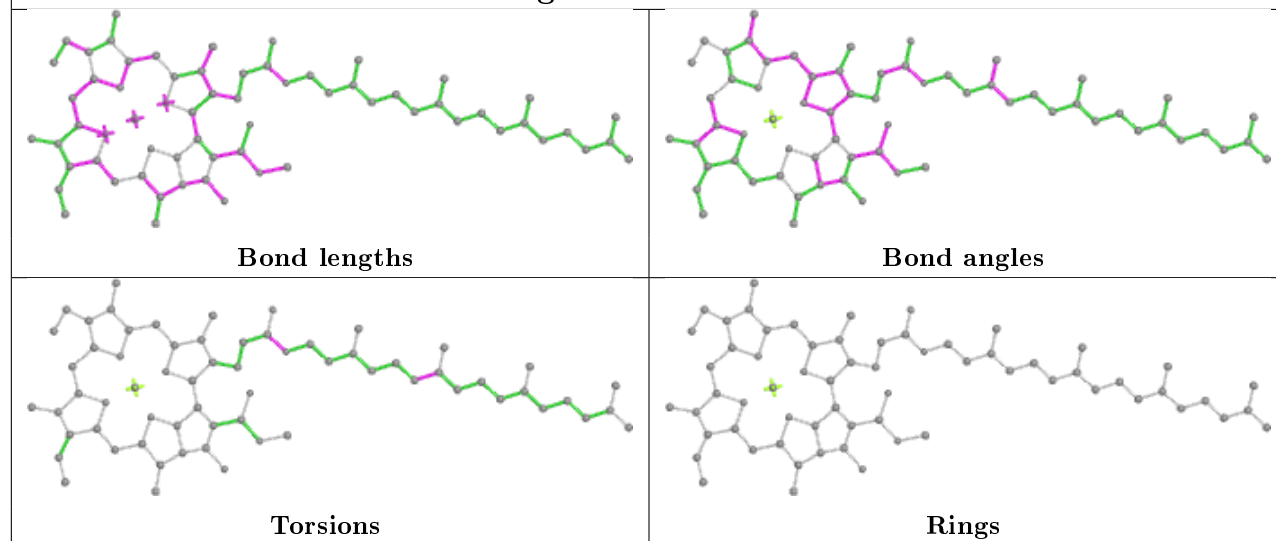




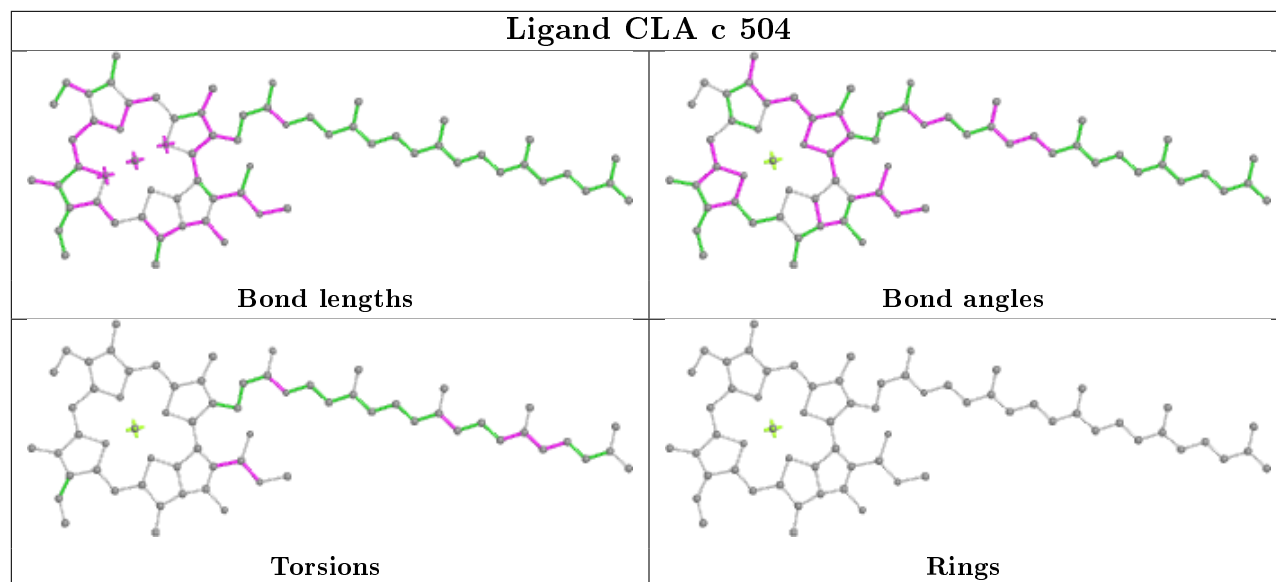
Ligand BCR h 101



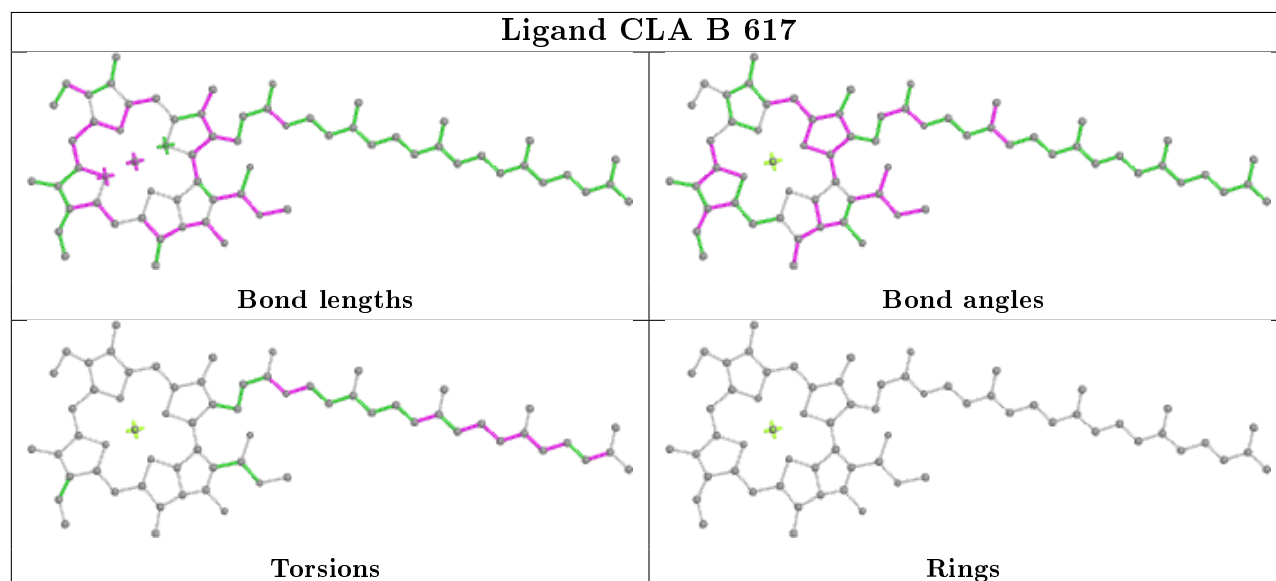
Ligand CLA c 511



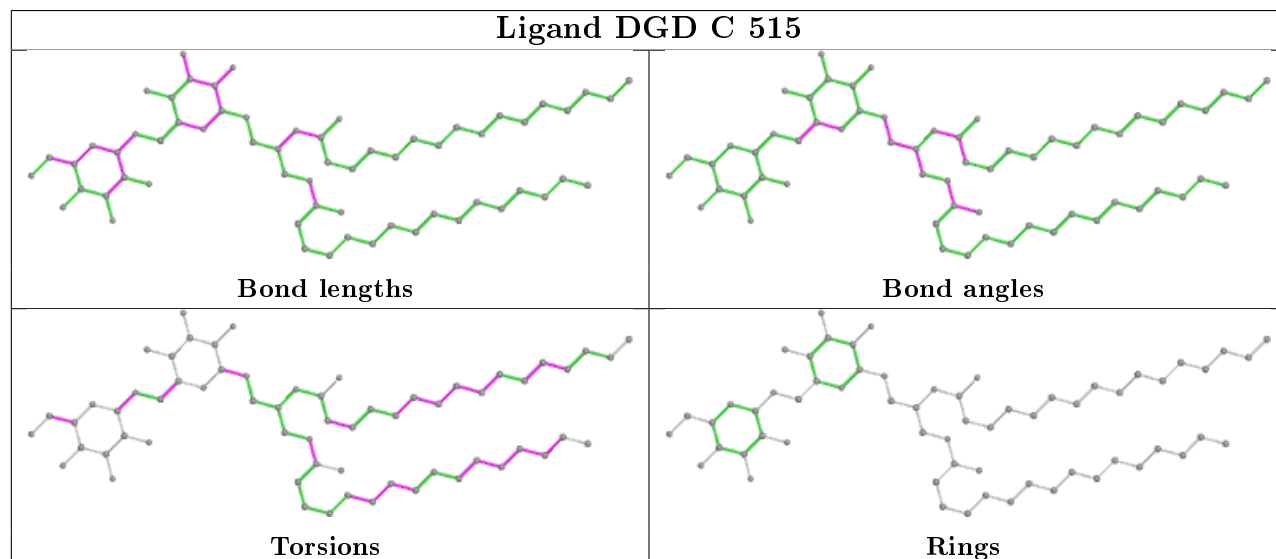
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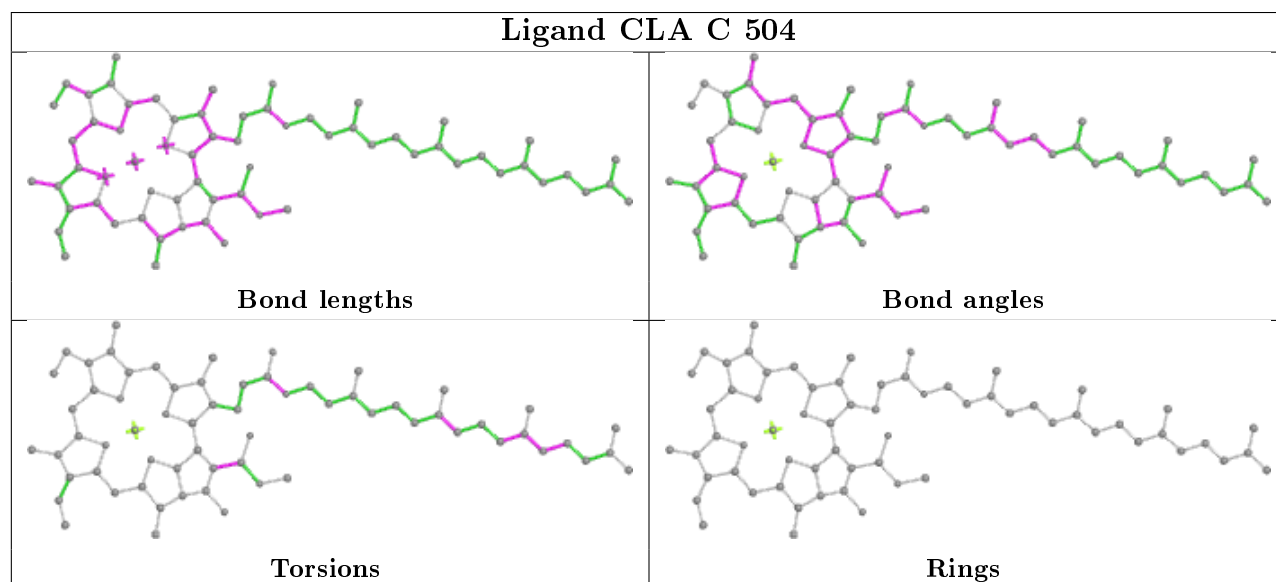
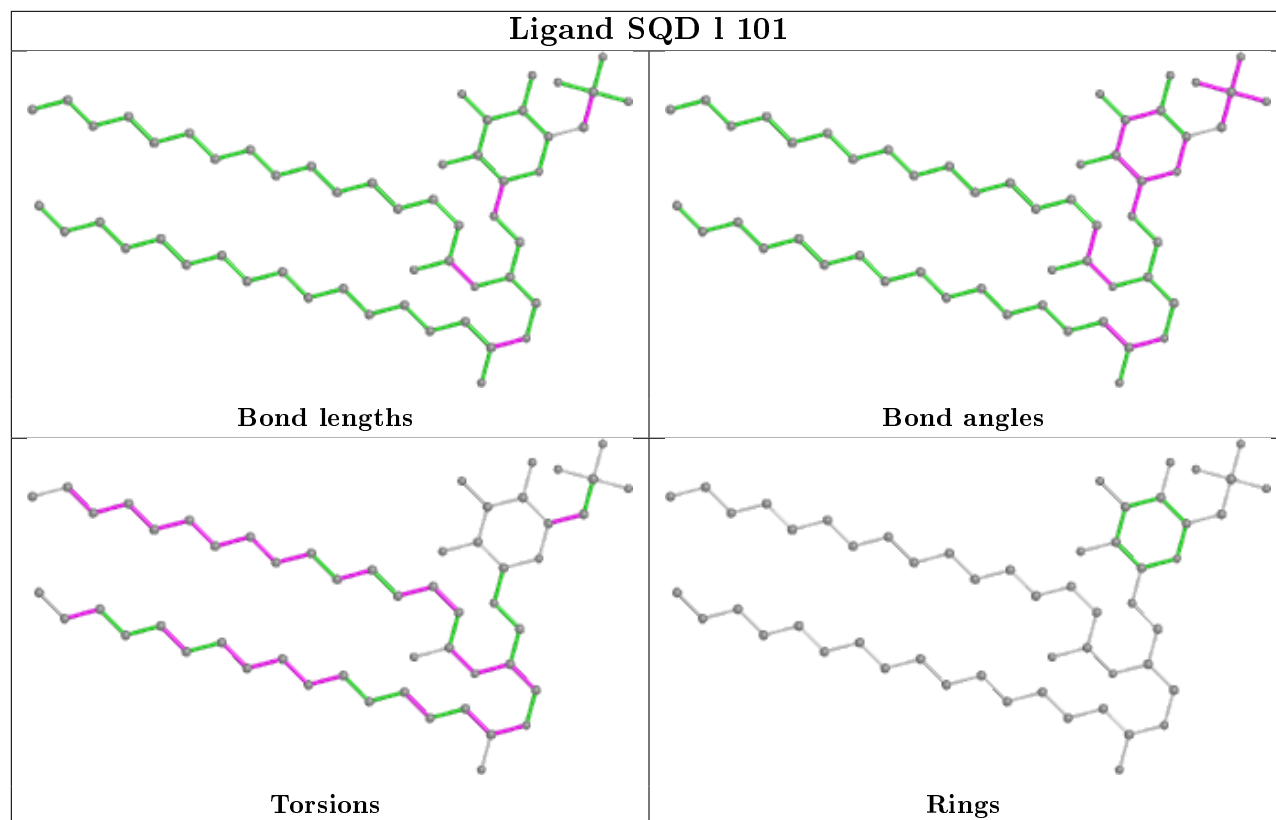


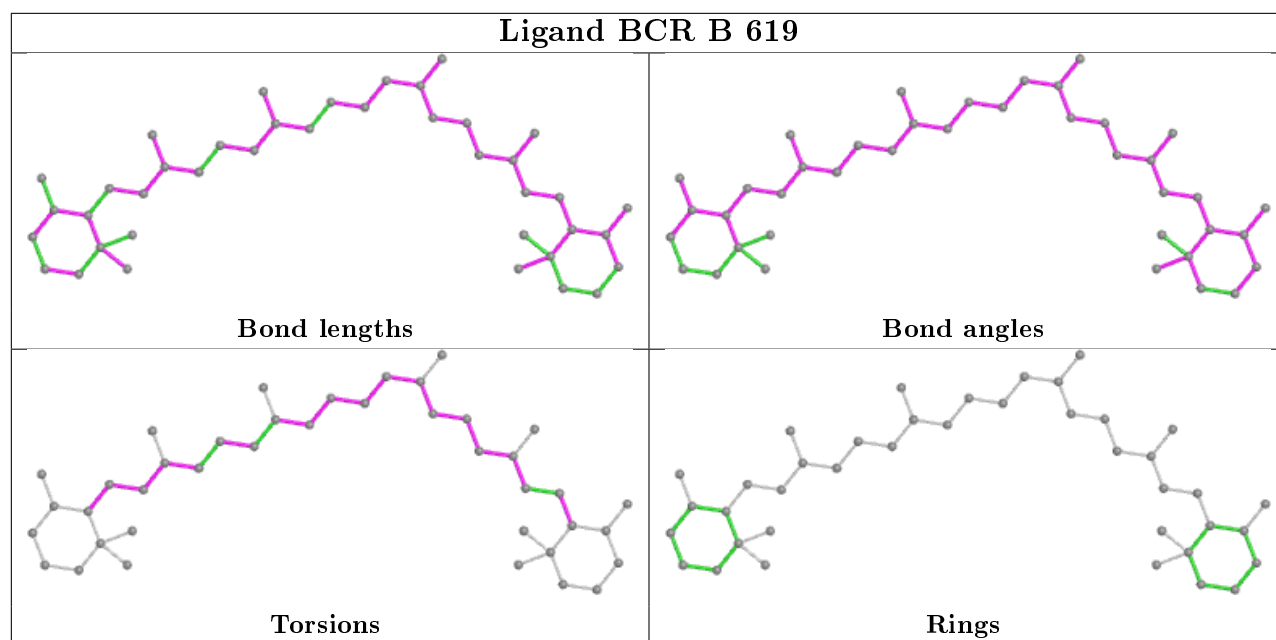
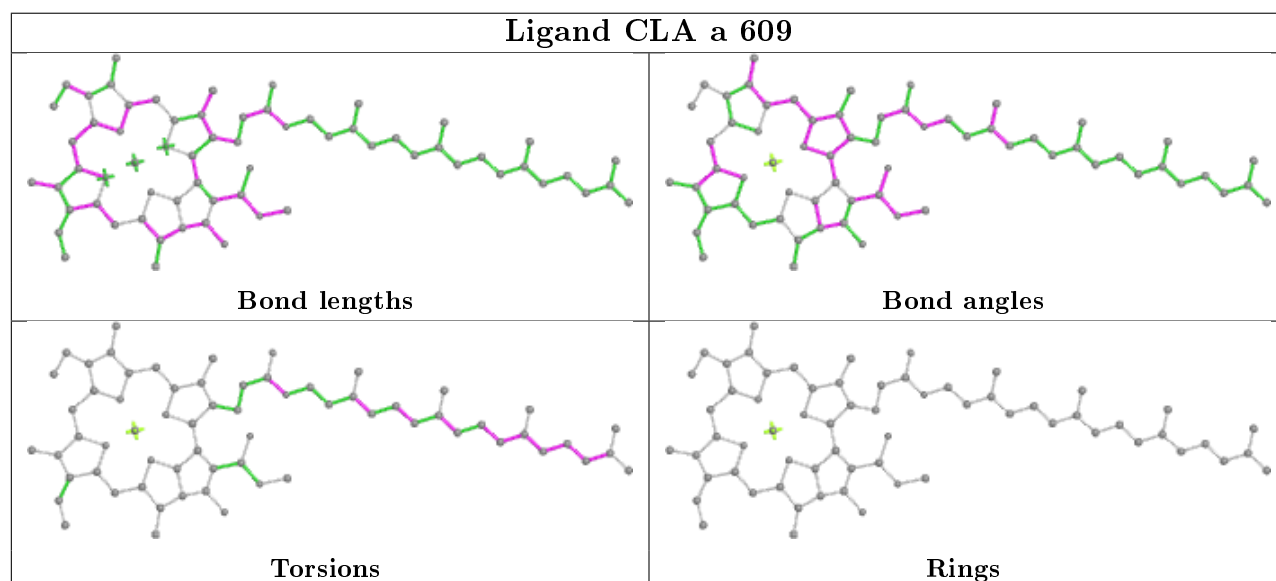
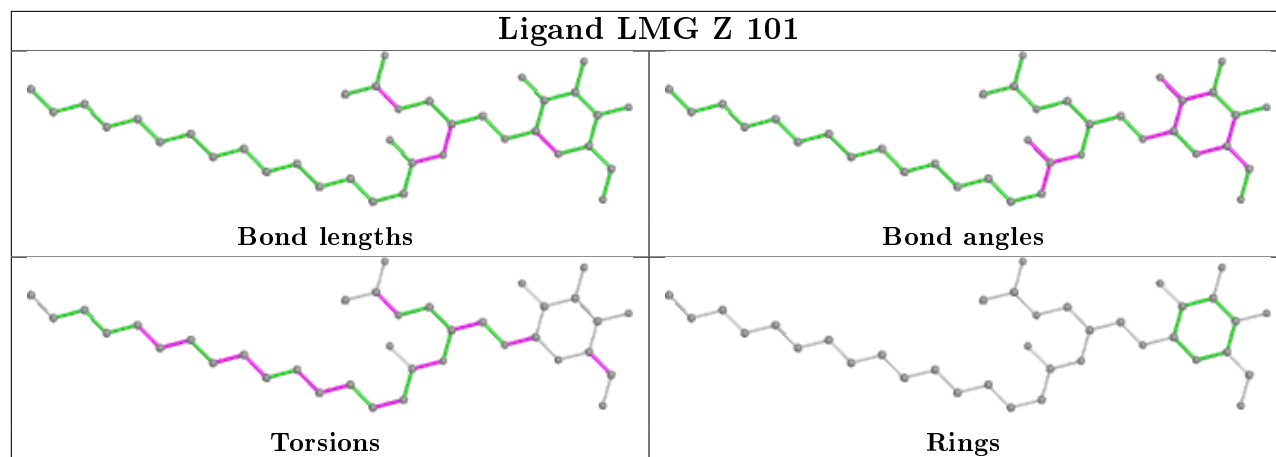
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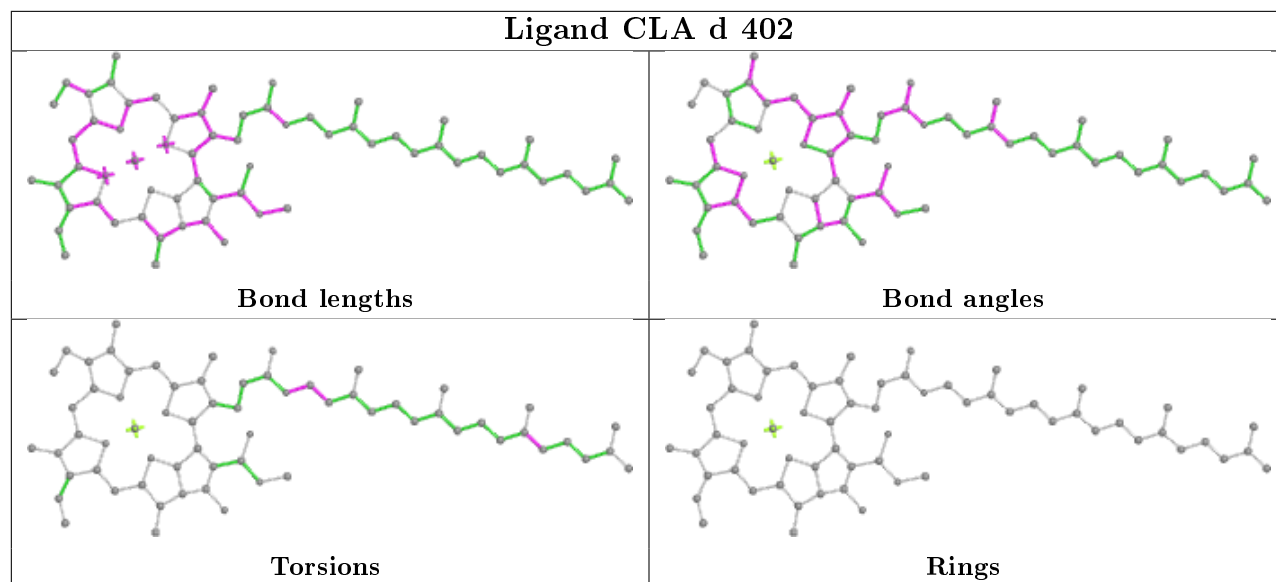
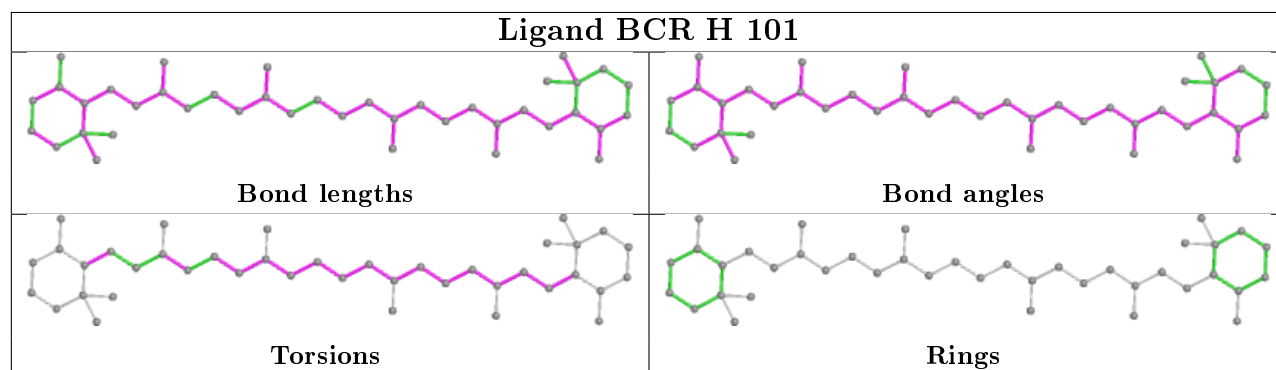
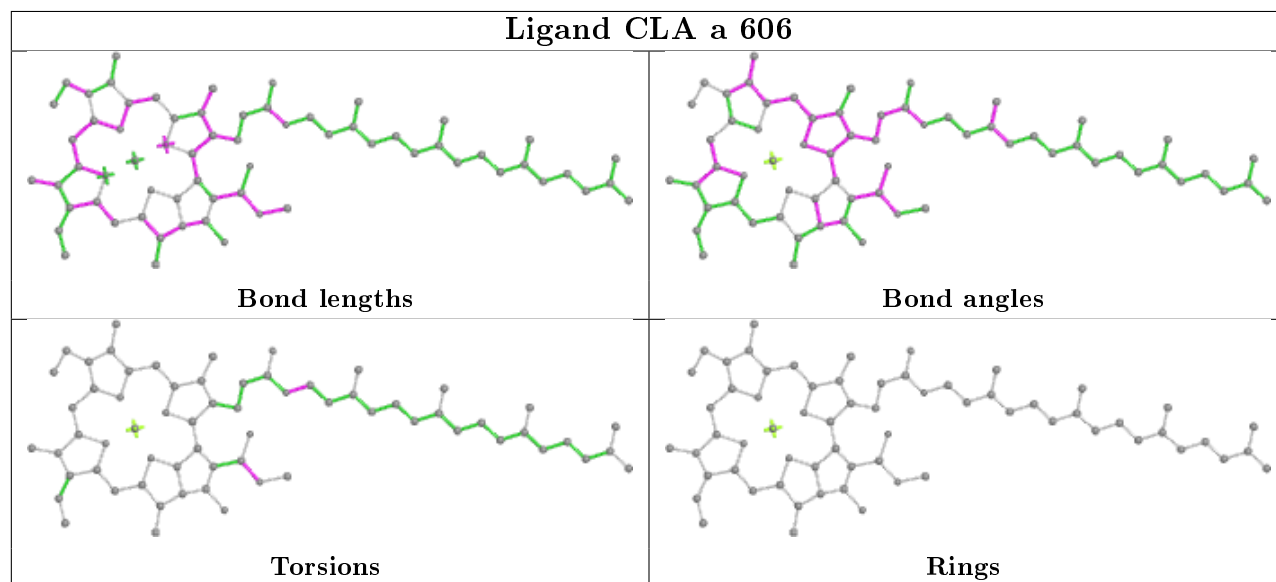


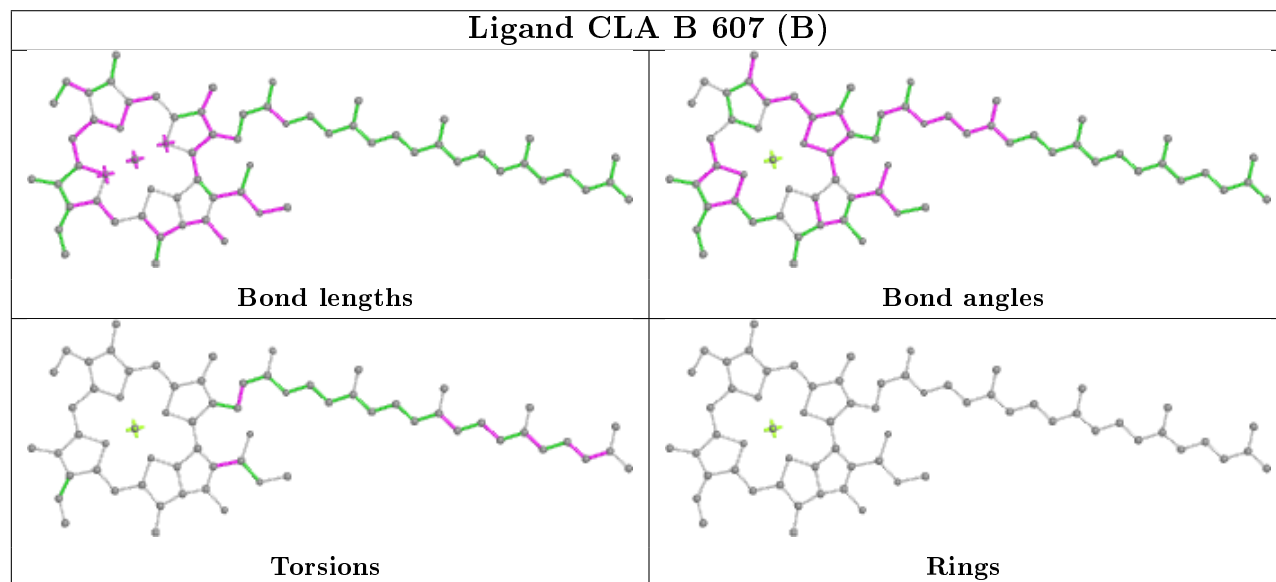
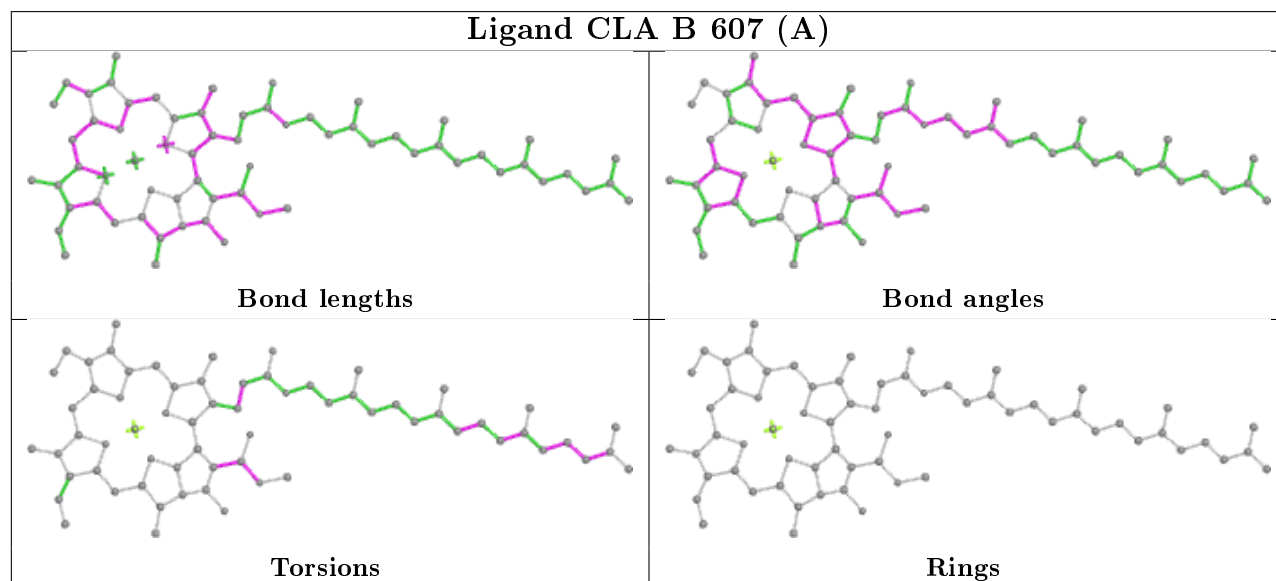
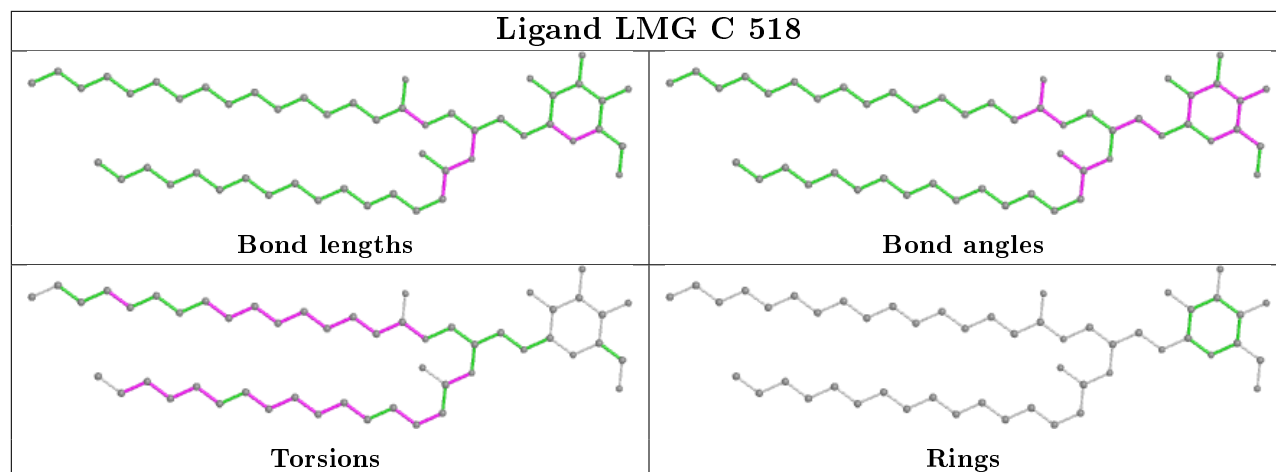
Ligand DGD C 515

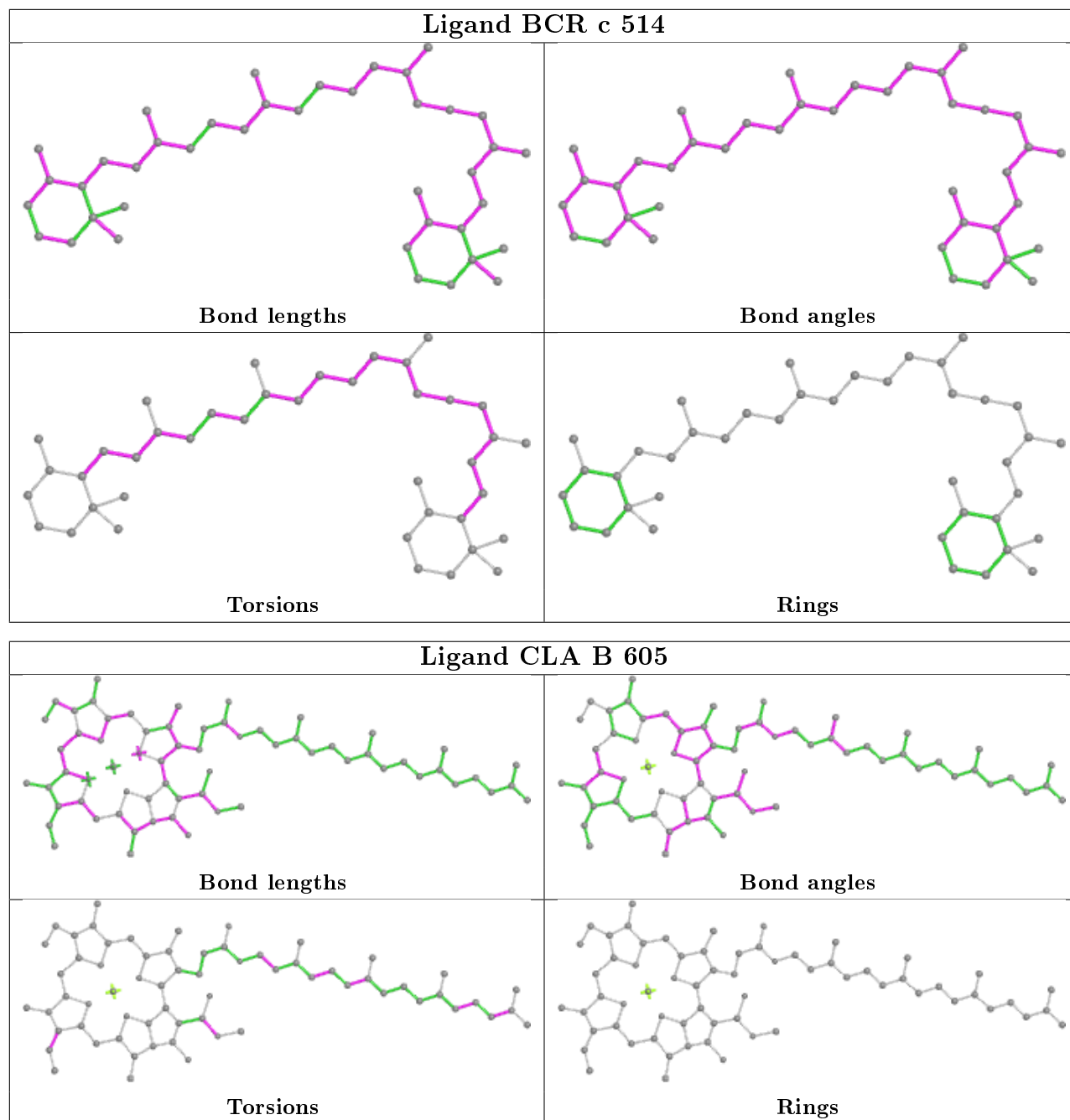


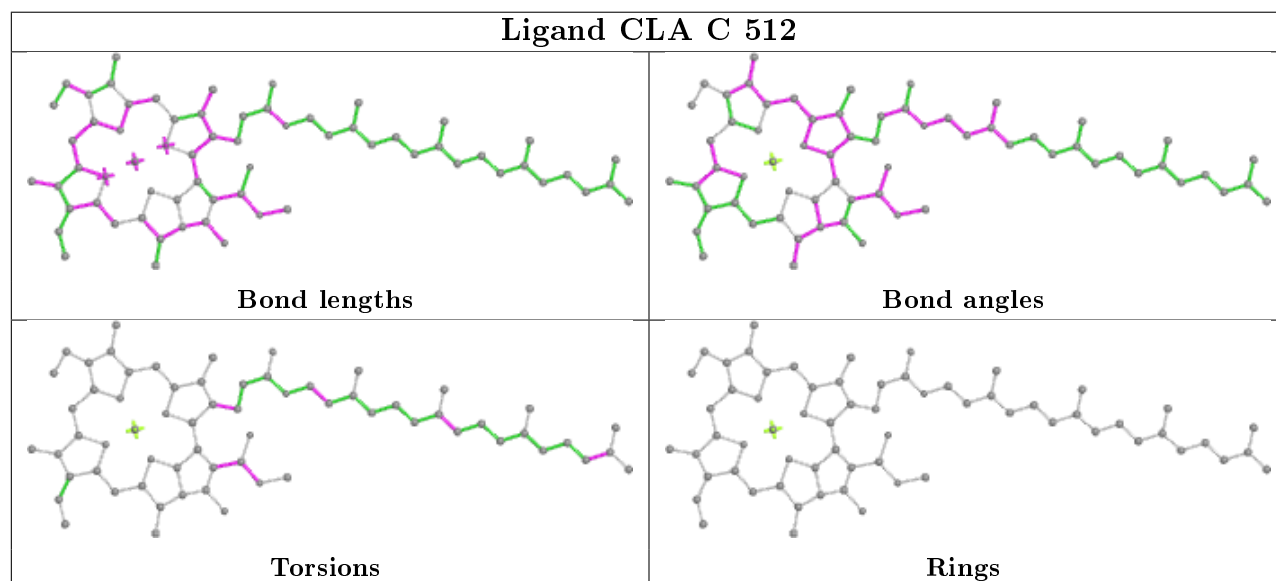
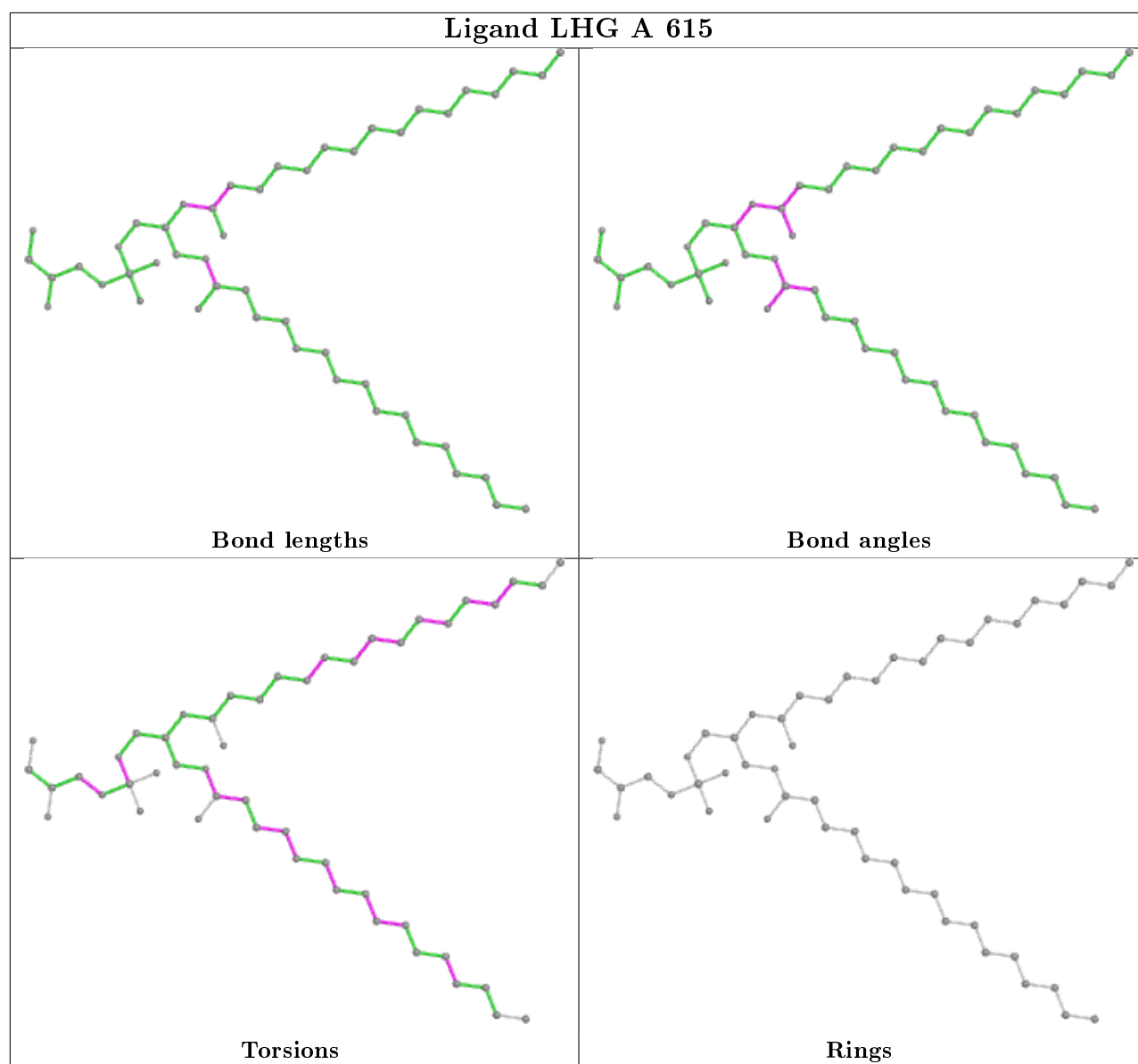




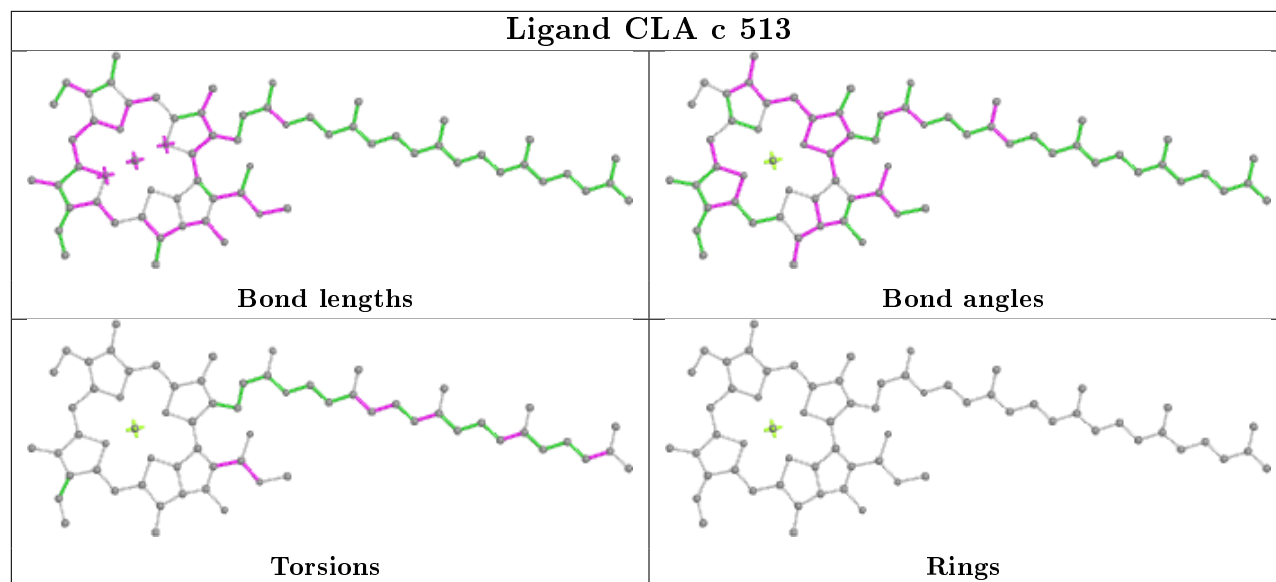
Ligand CLA d 402**Ligand BCR H 101****Ligand CLA a 606**



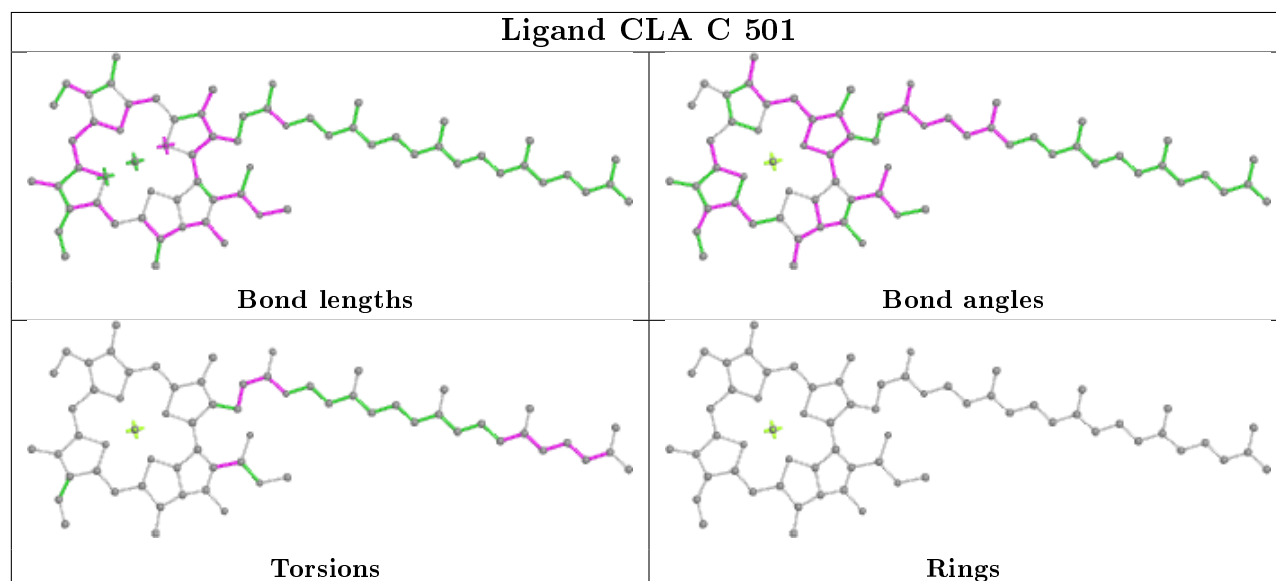




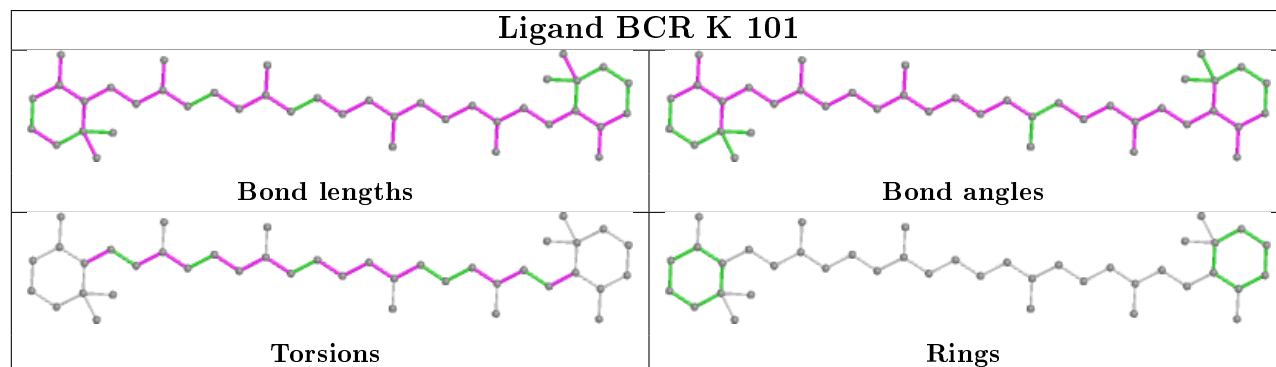
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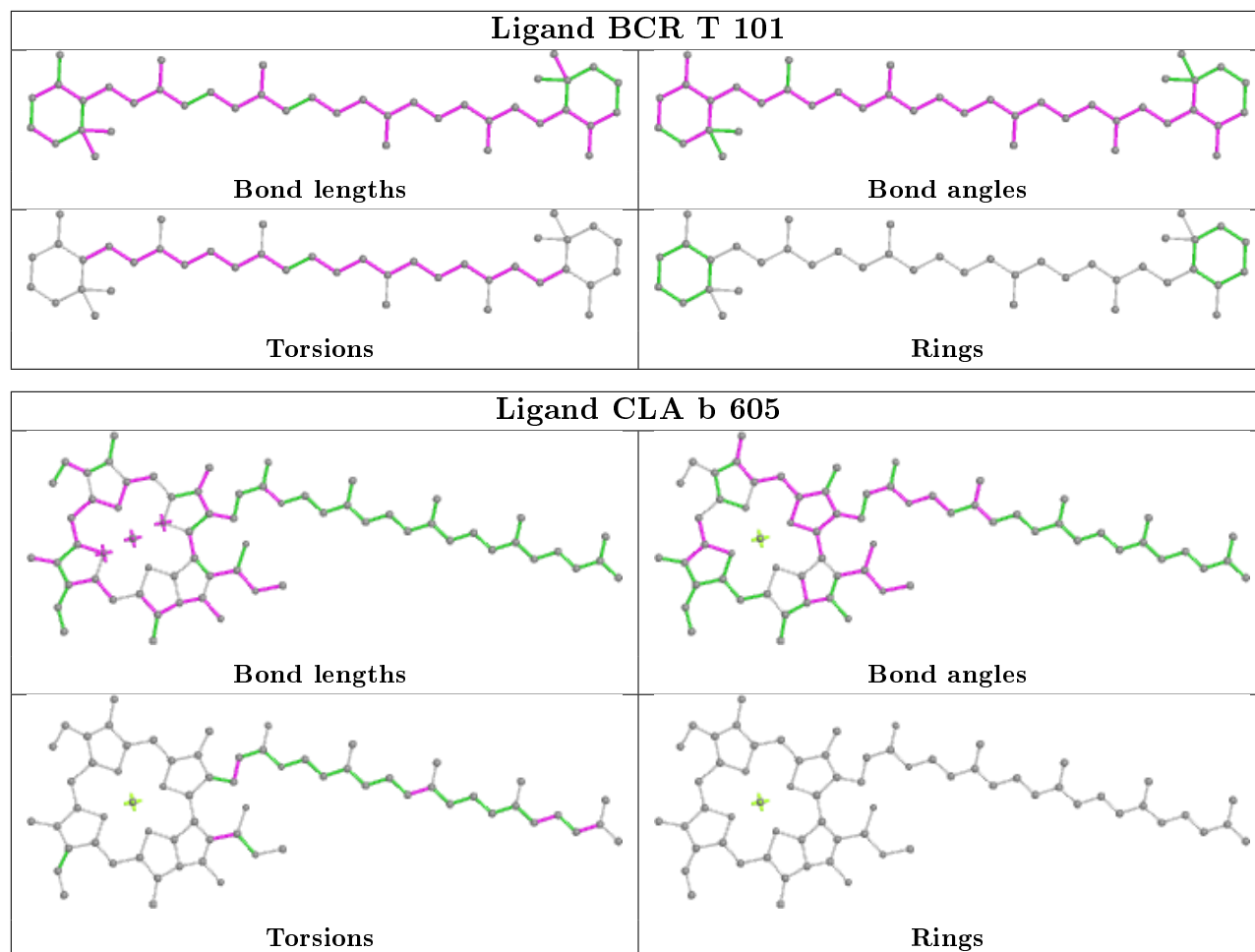


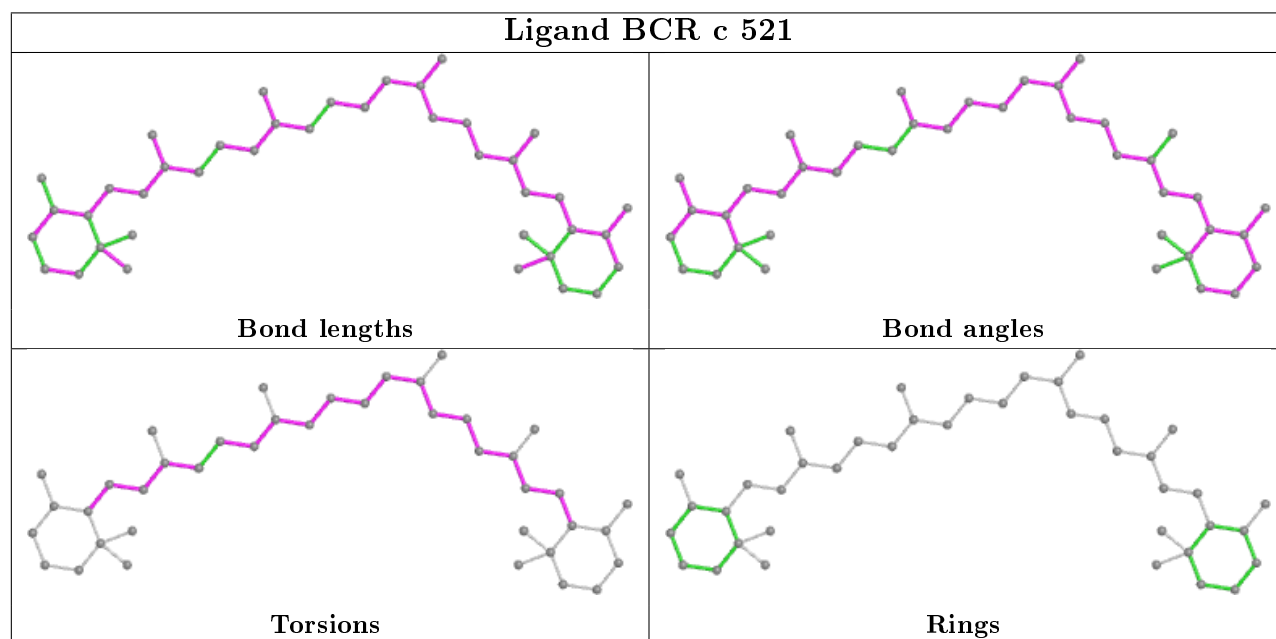
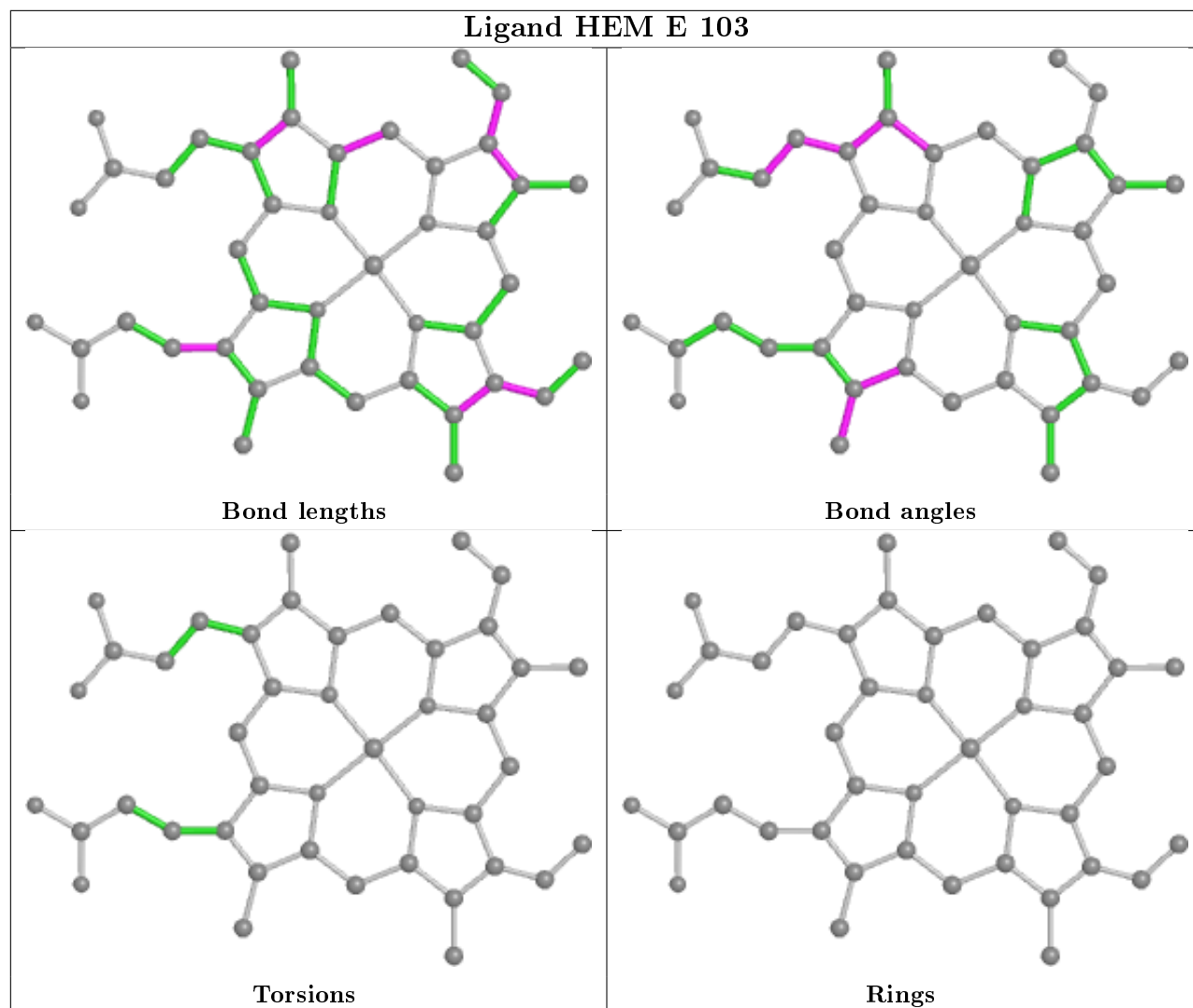
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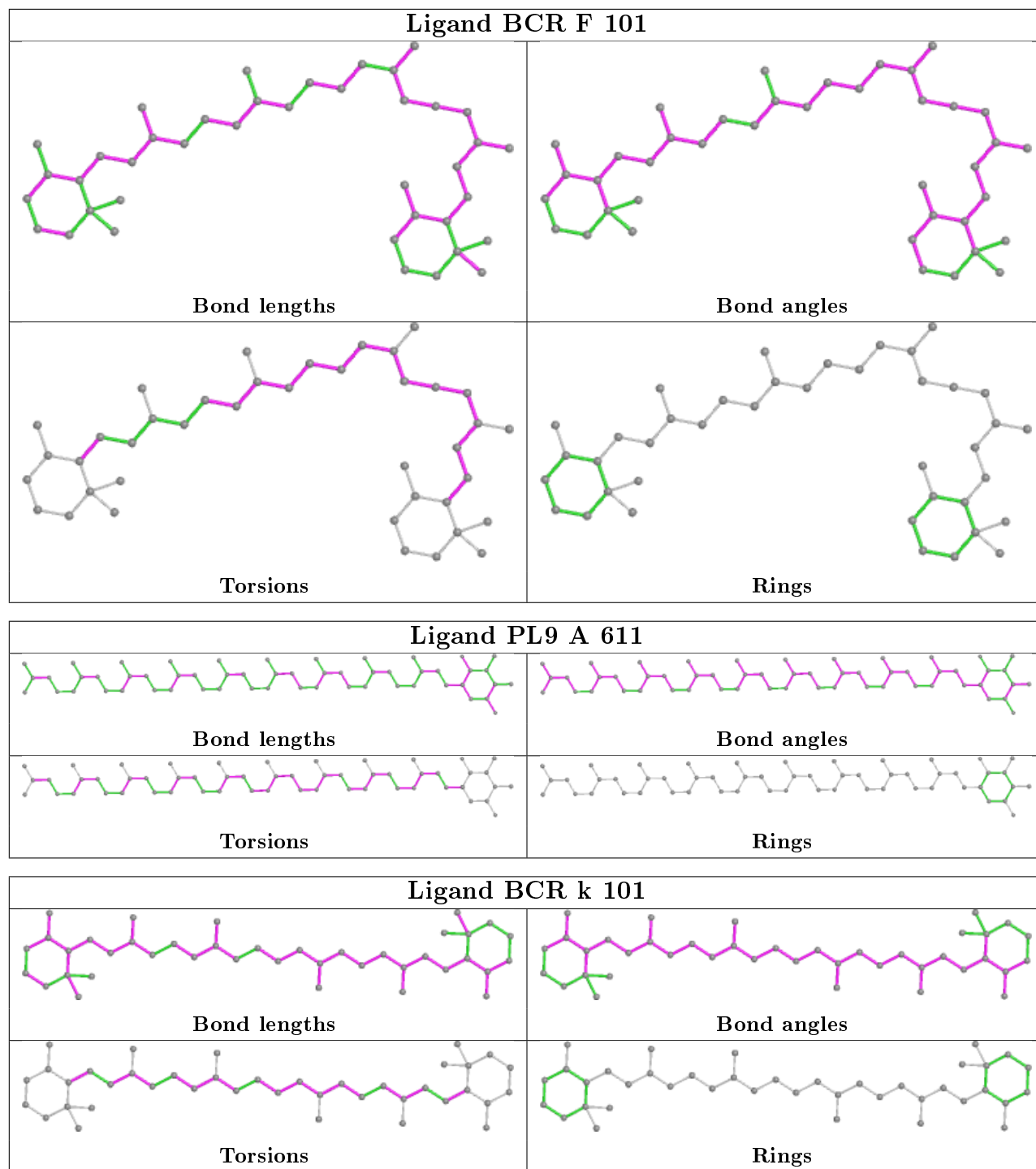


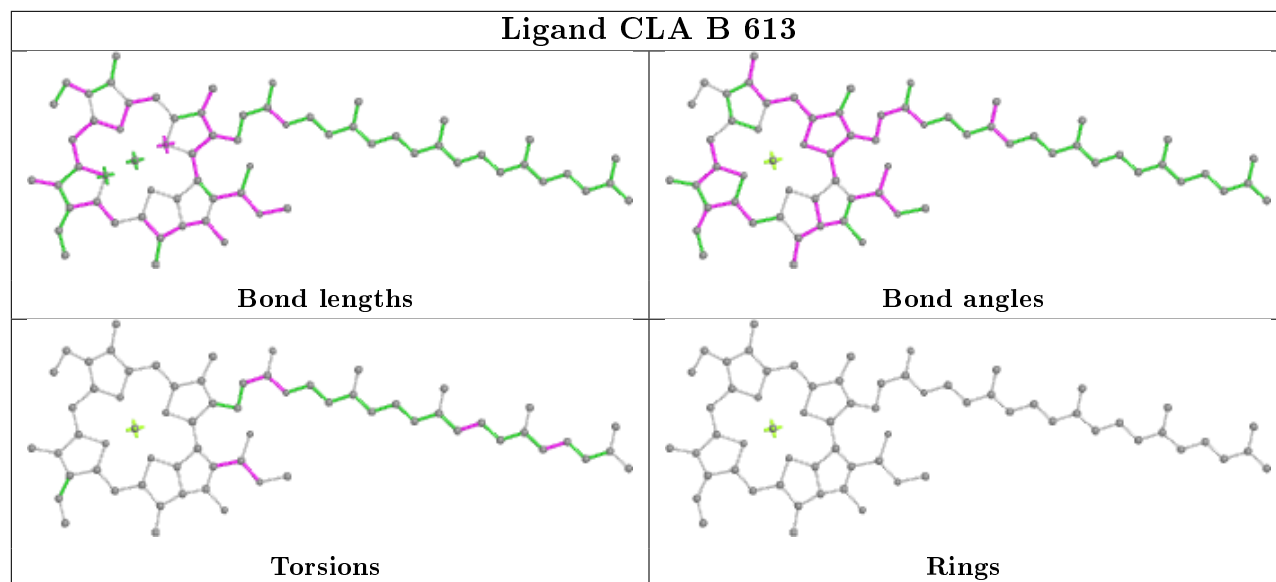
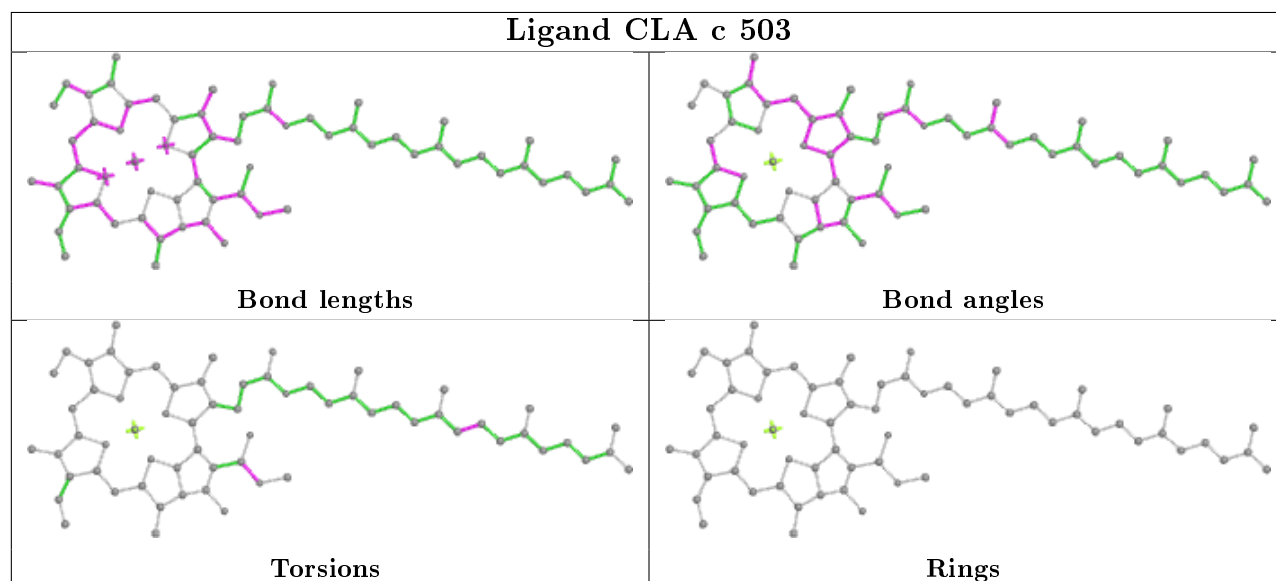
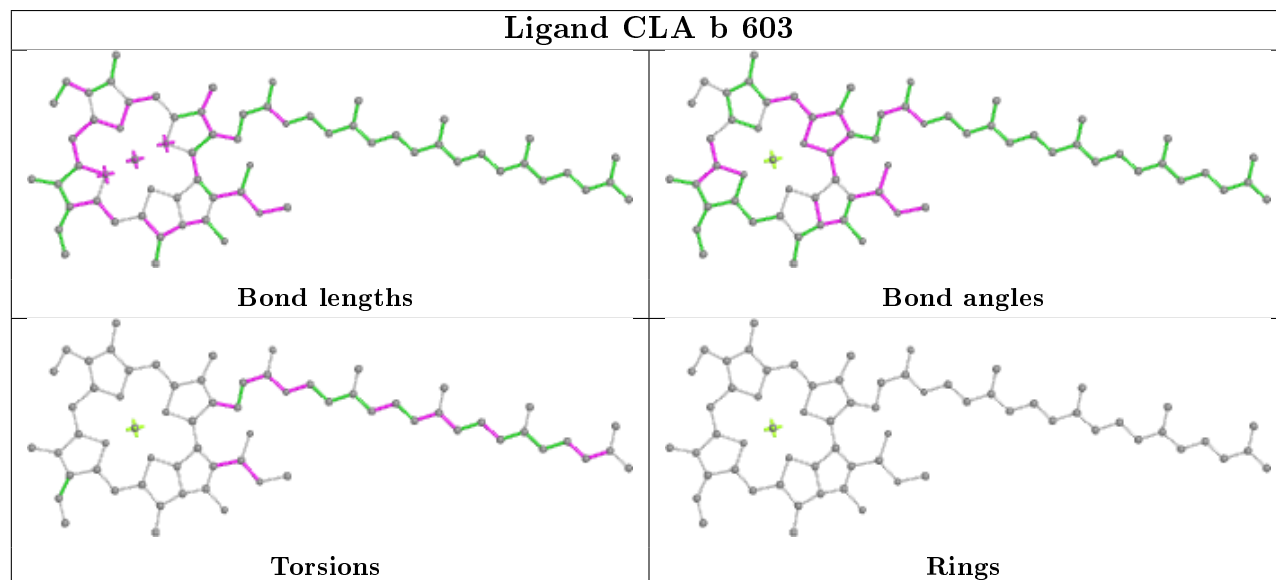
Ligand BCR K 101



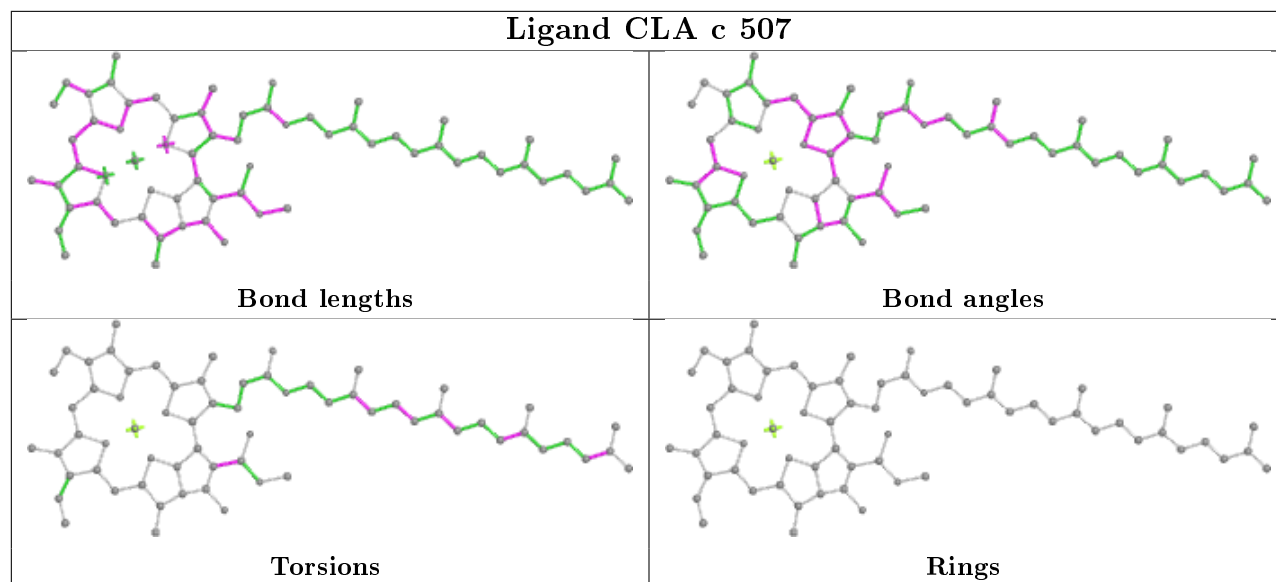




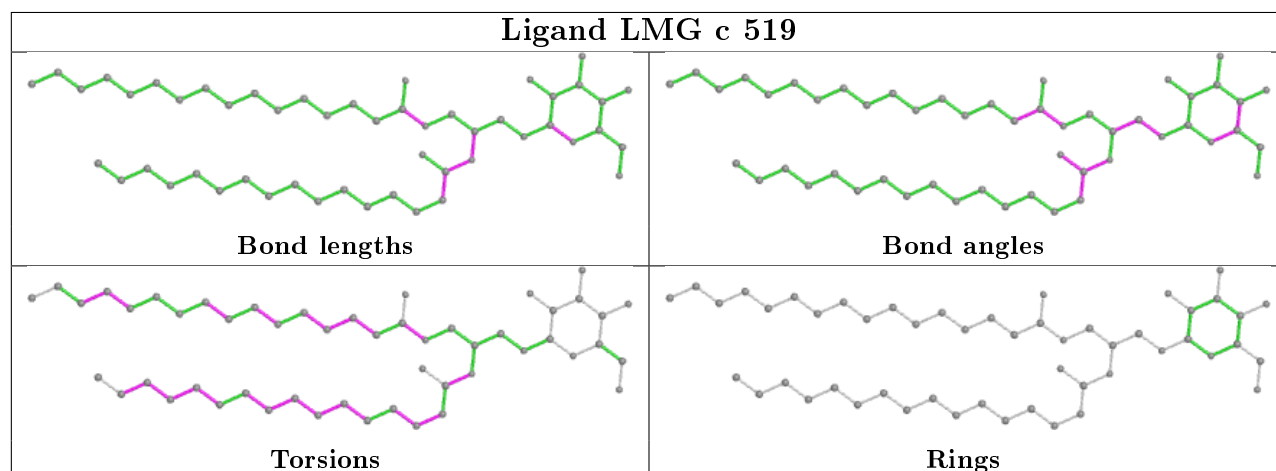


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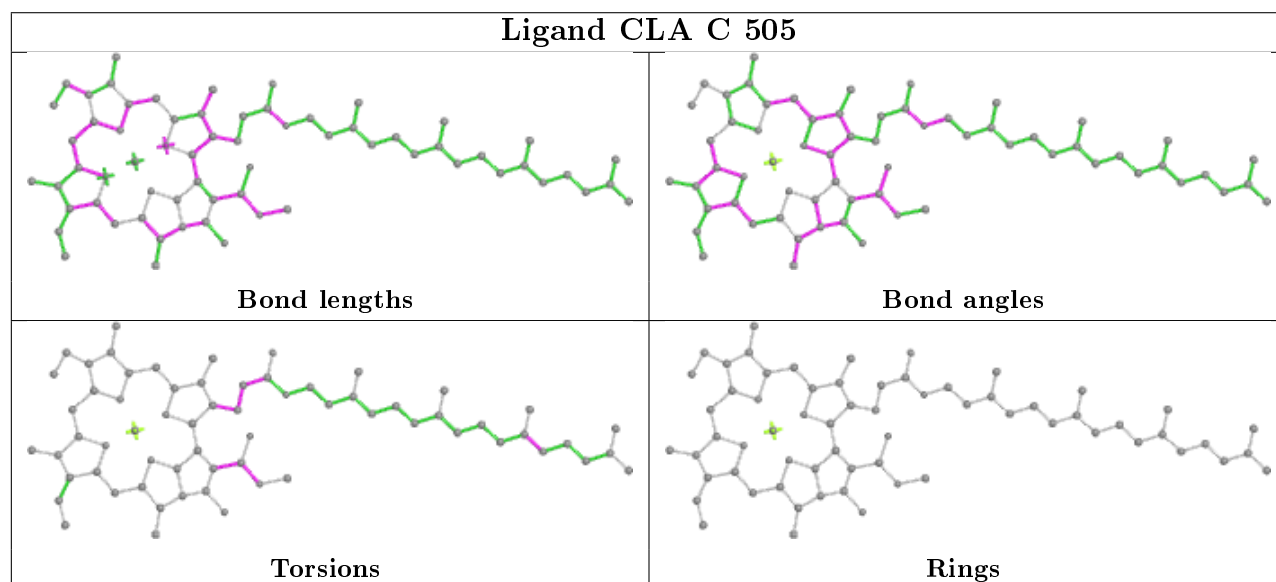
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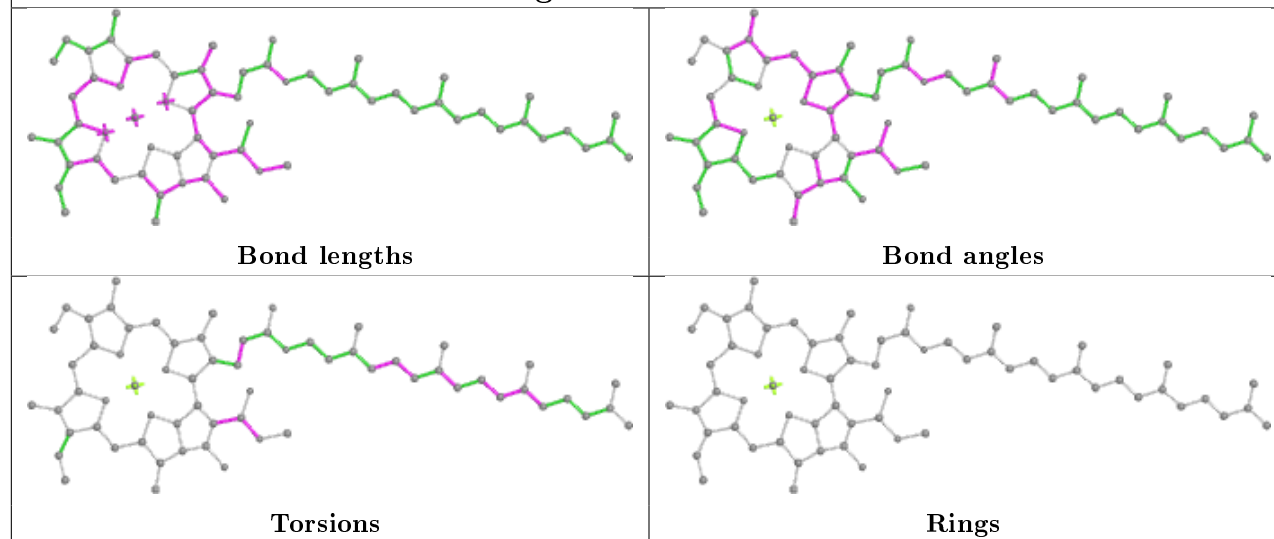
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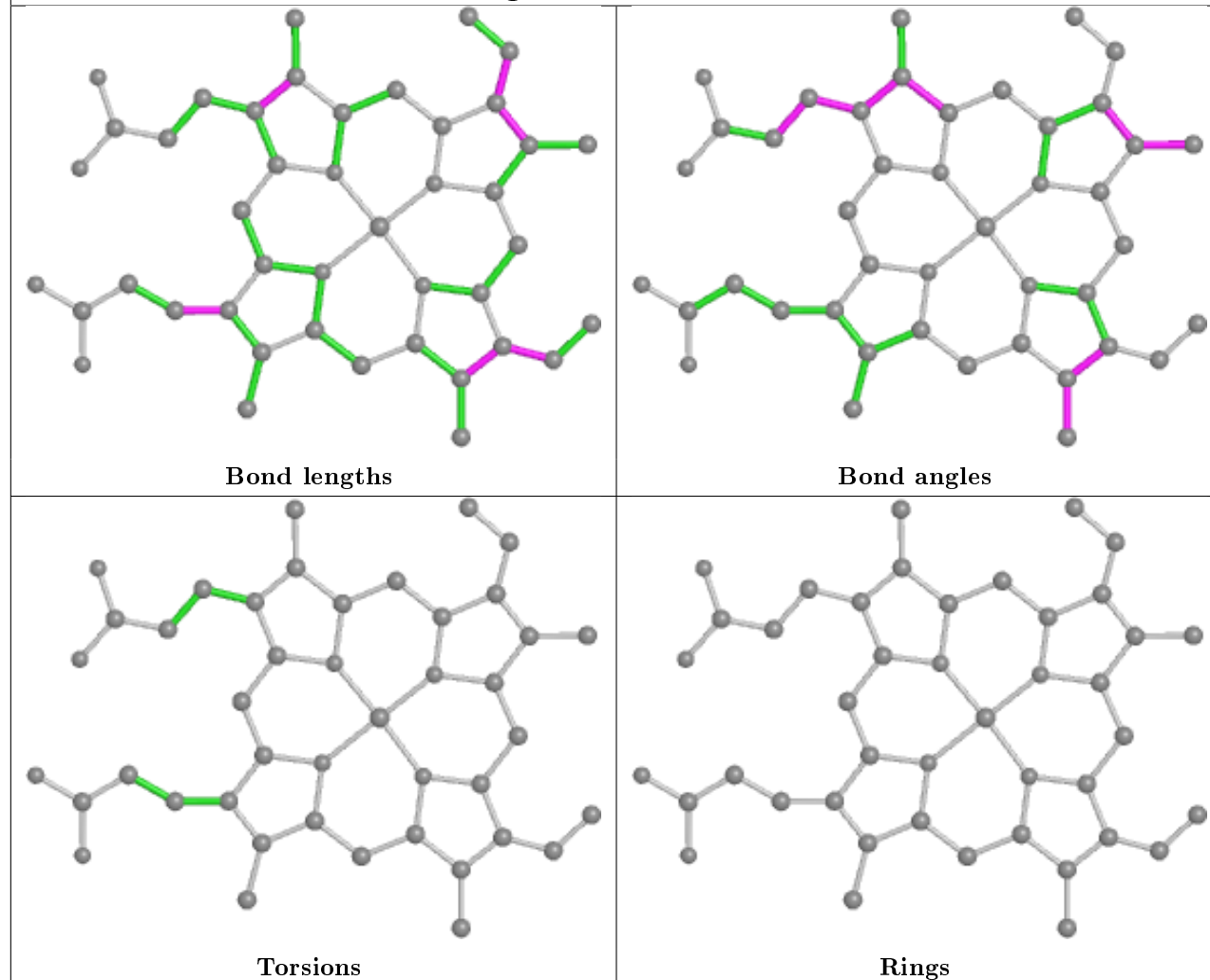
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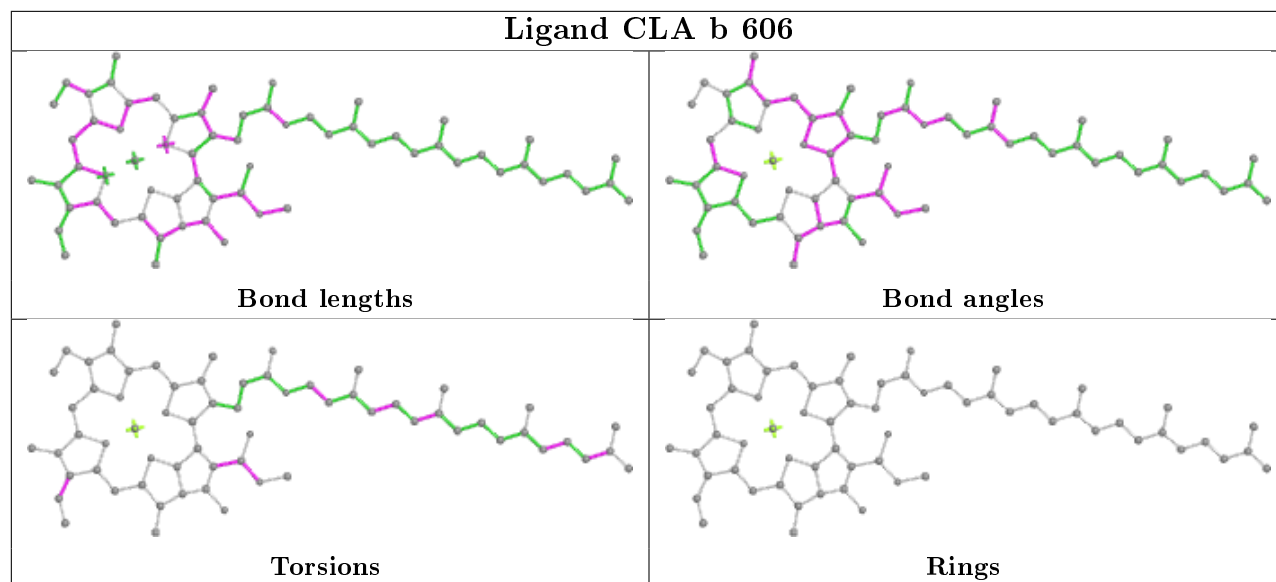
Ligand CLA b 616



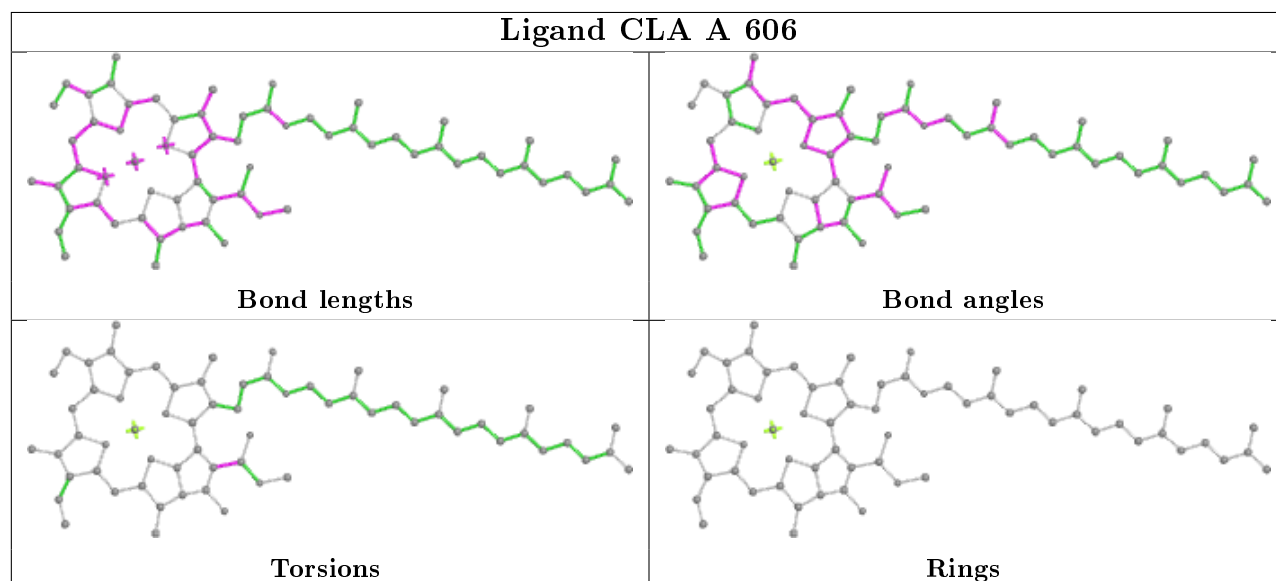
Ligand HEM e 102



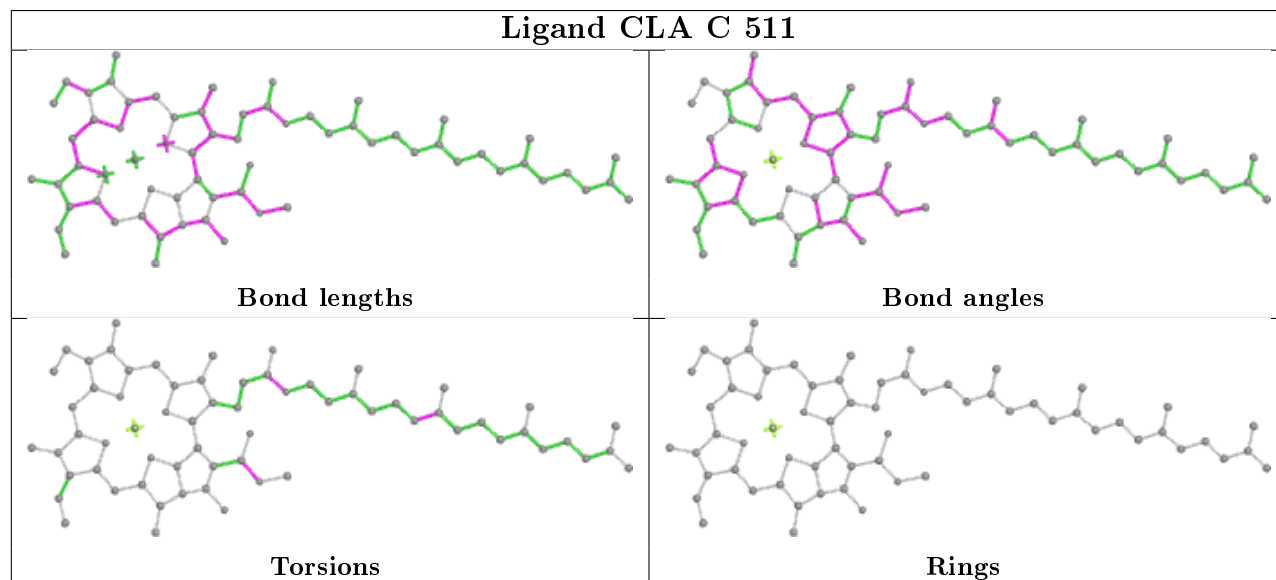
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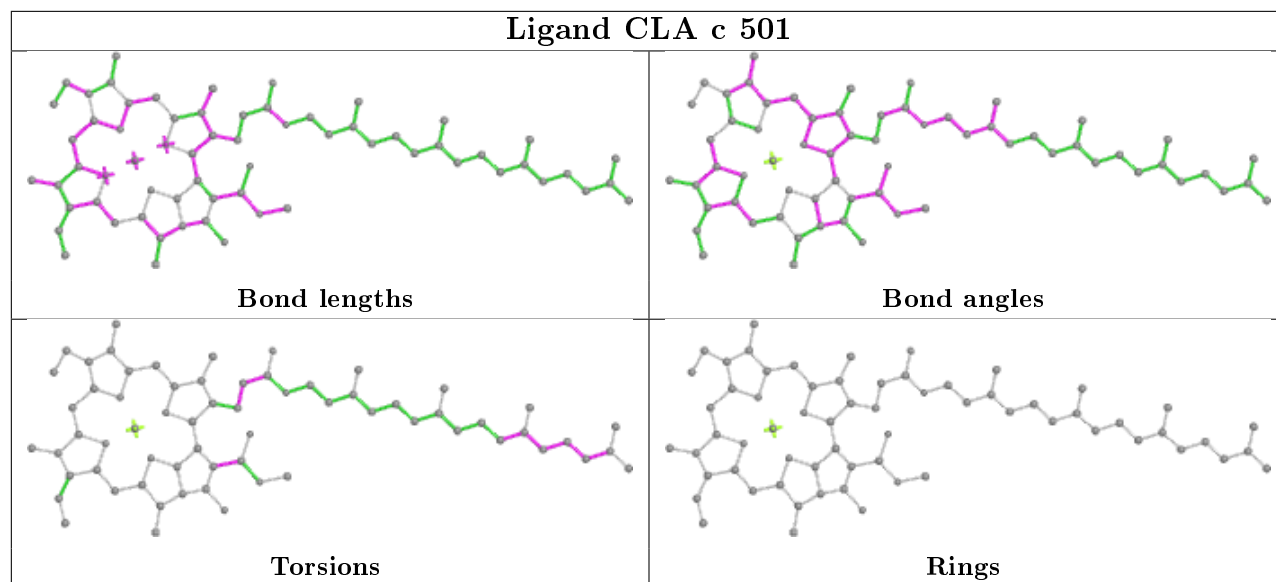
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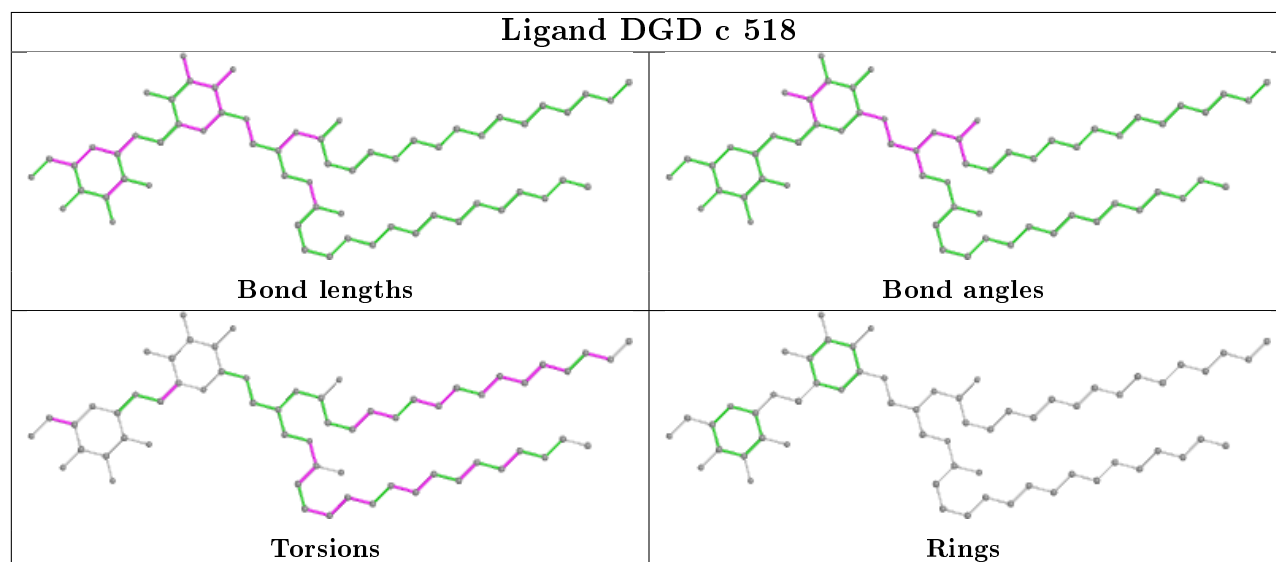
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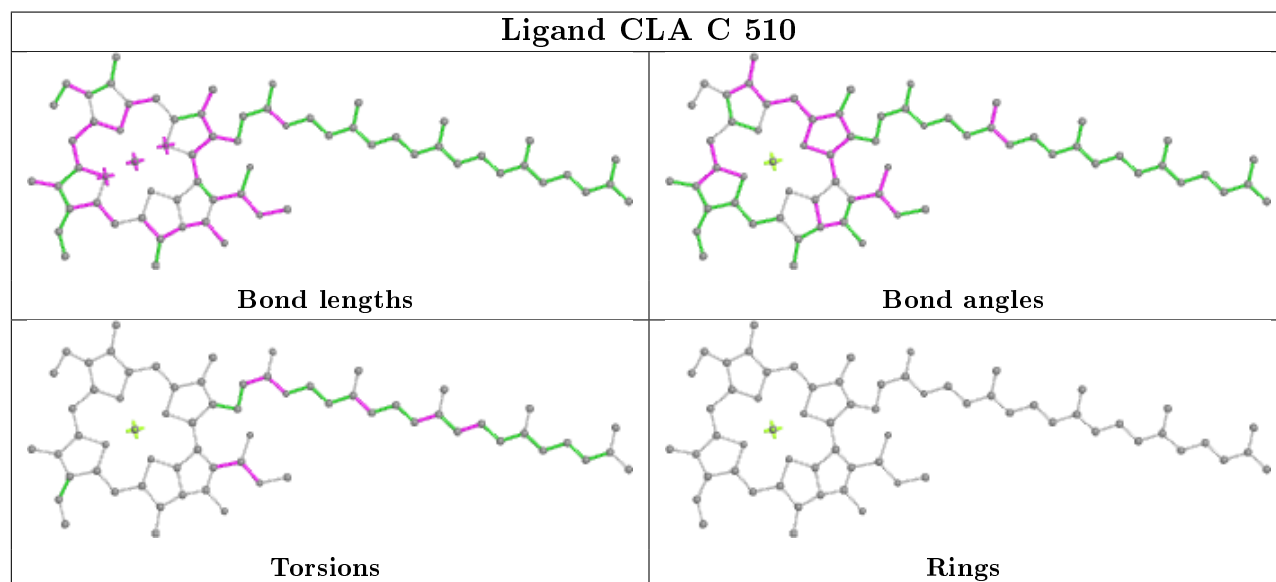
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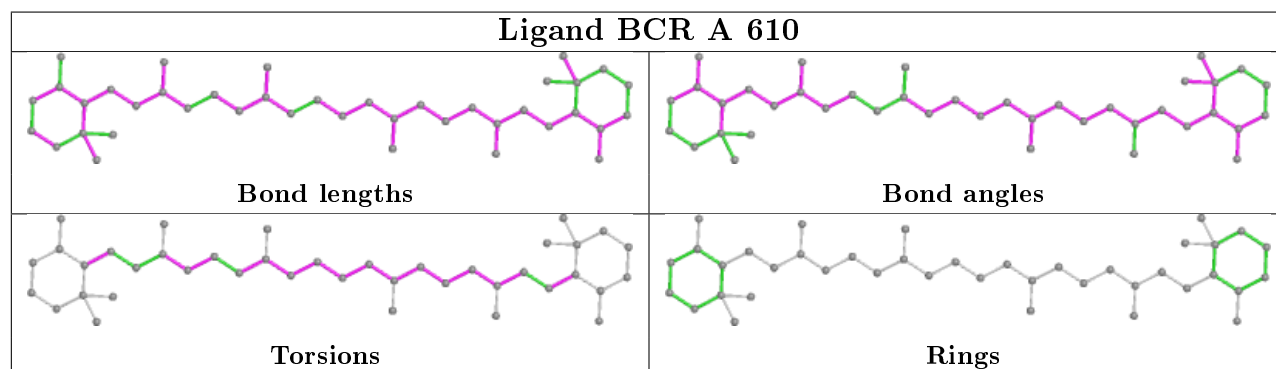
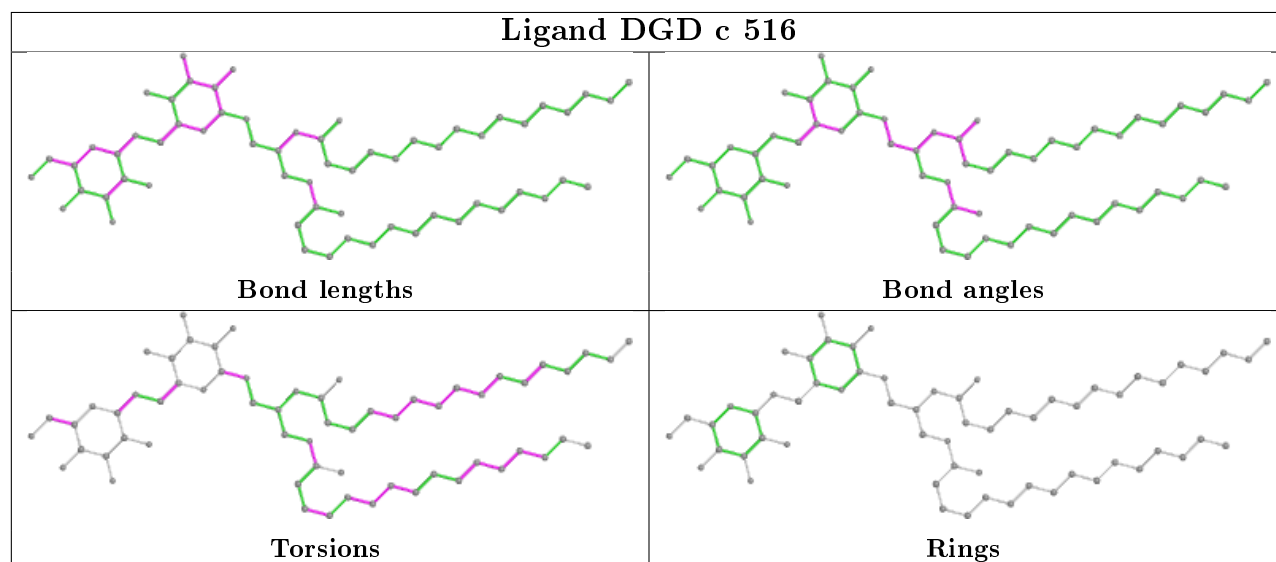
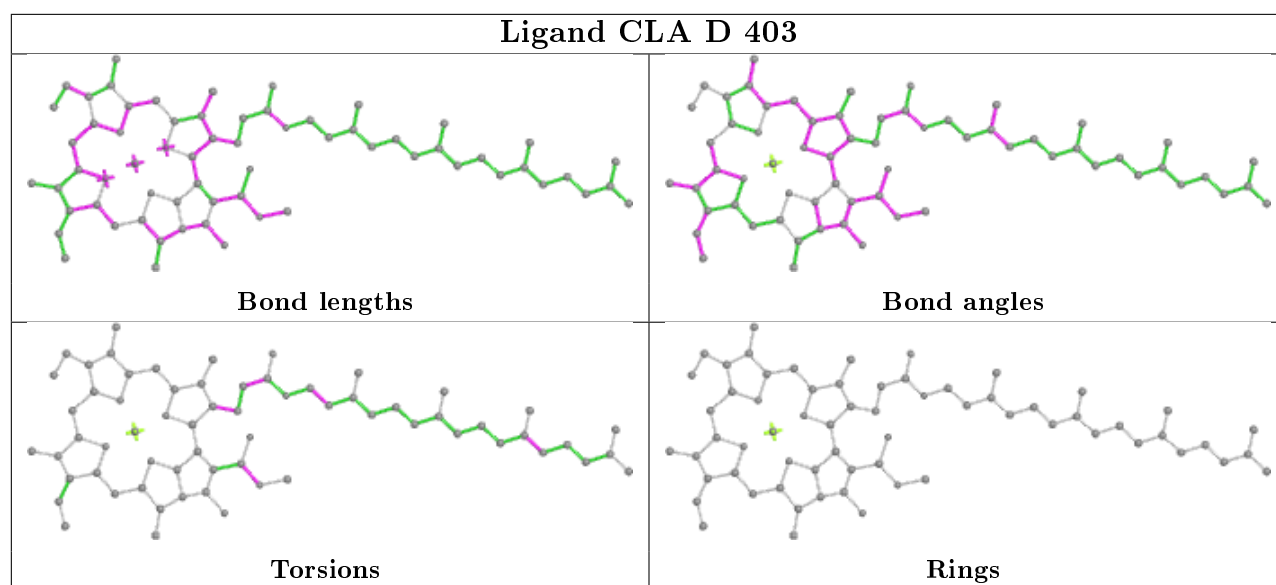


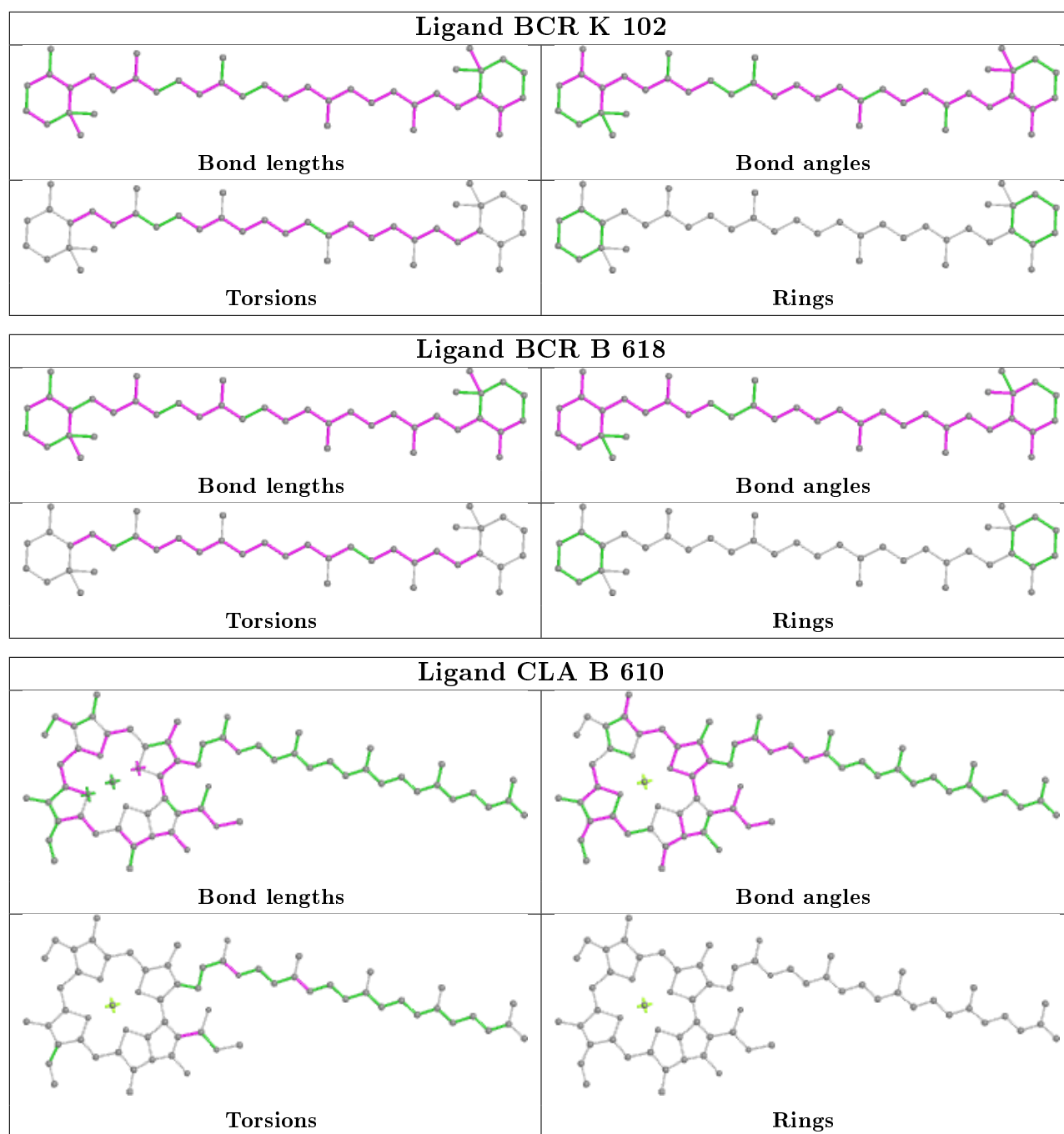
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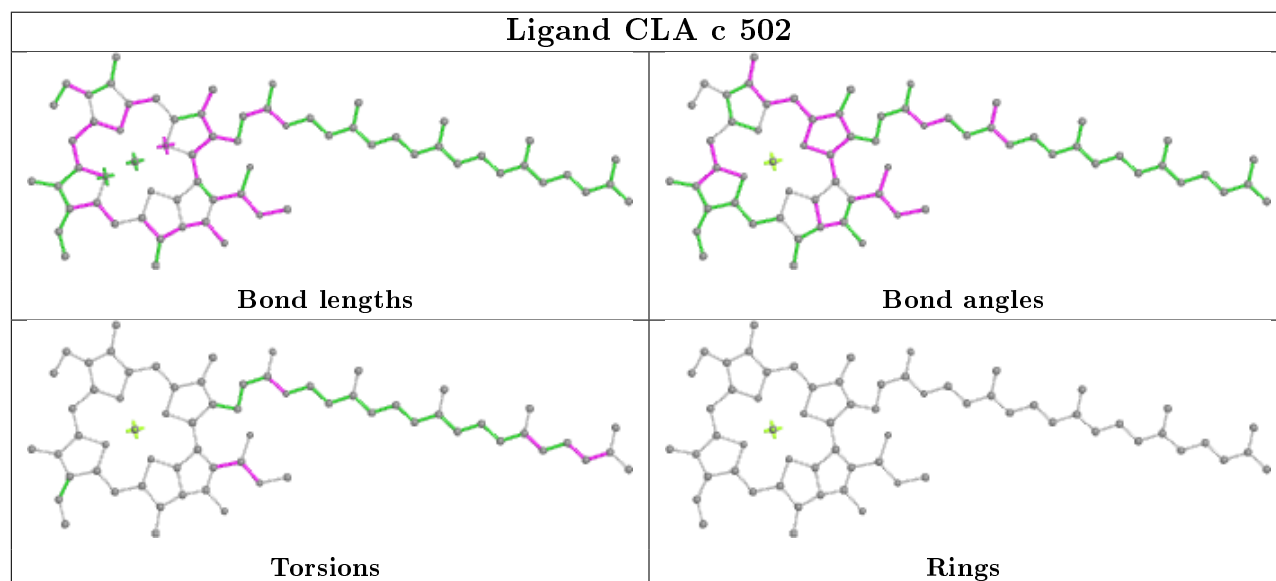
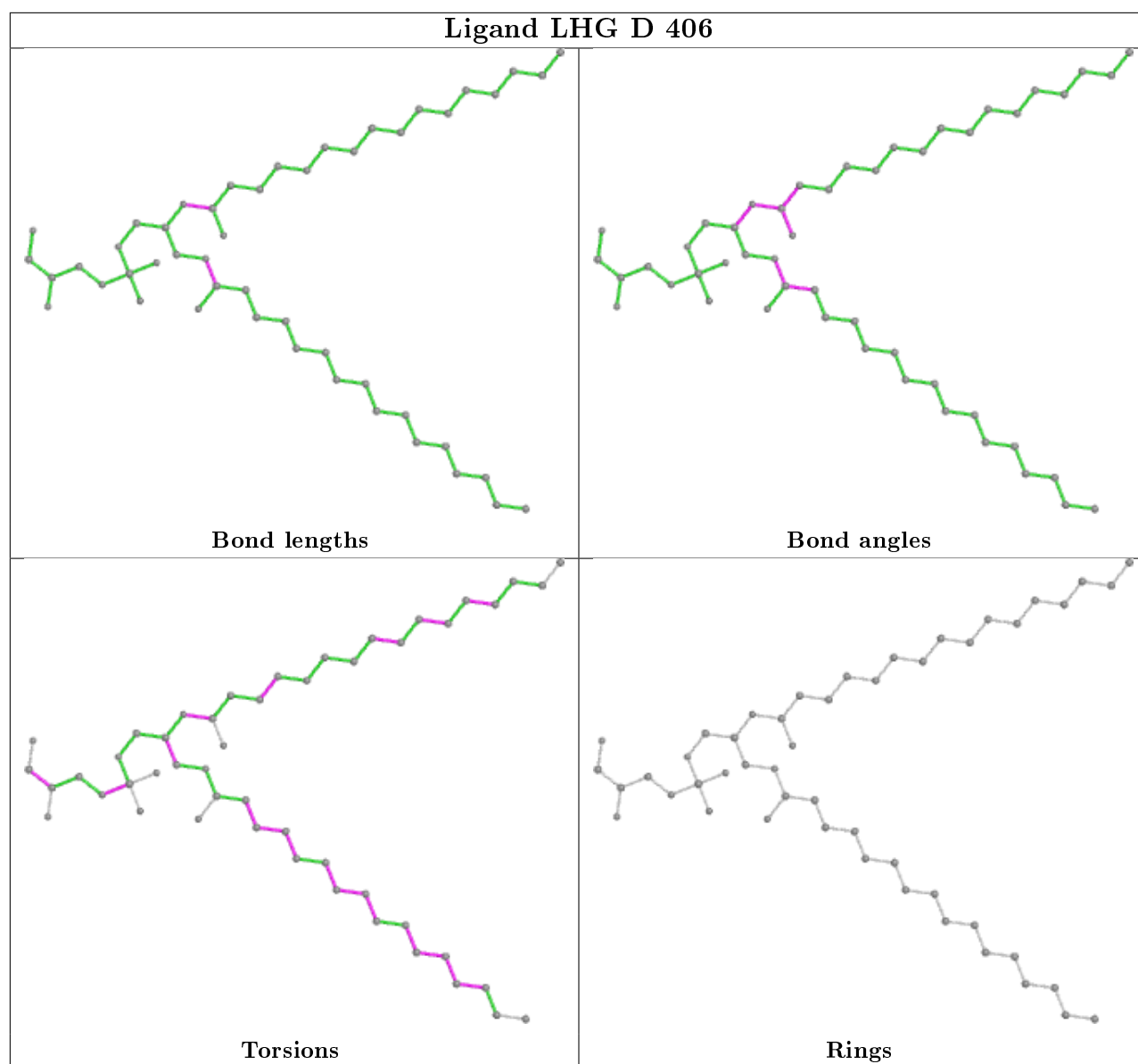


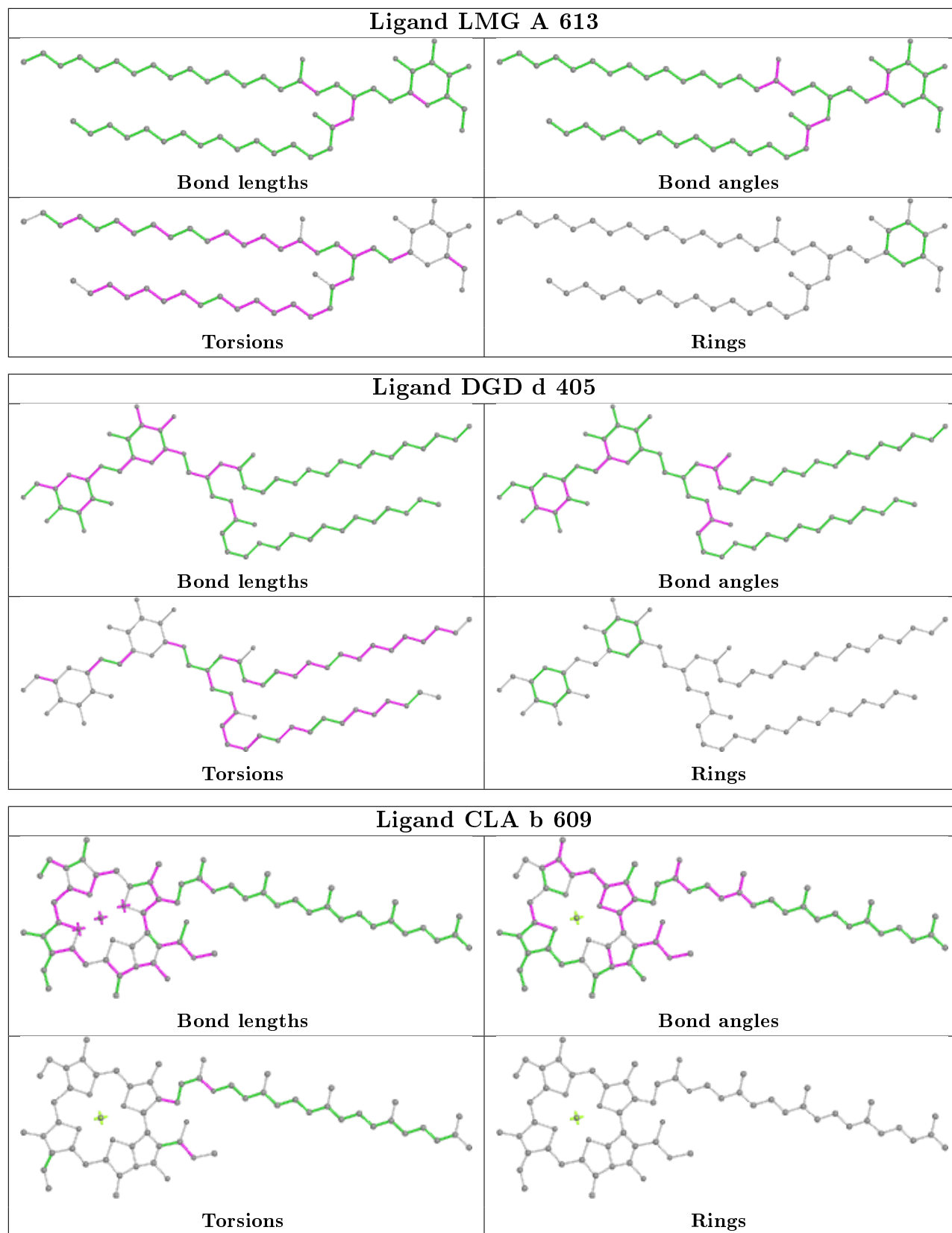
Ligand CLA C 510

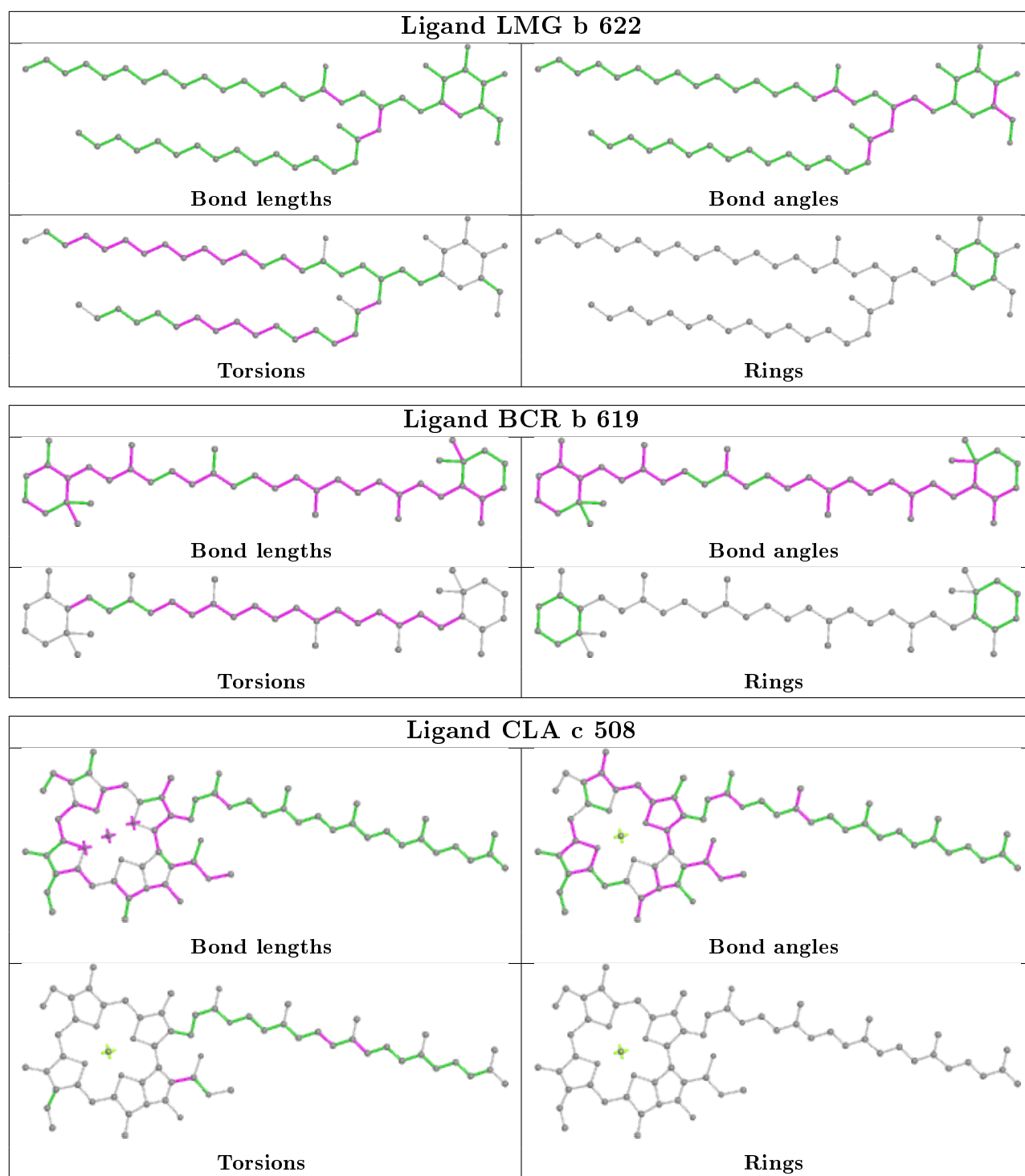


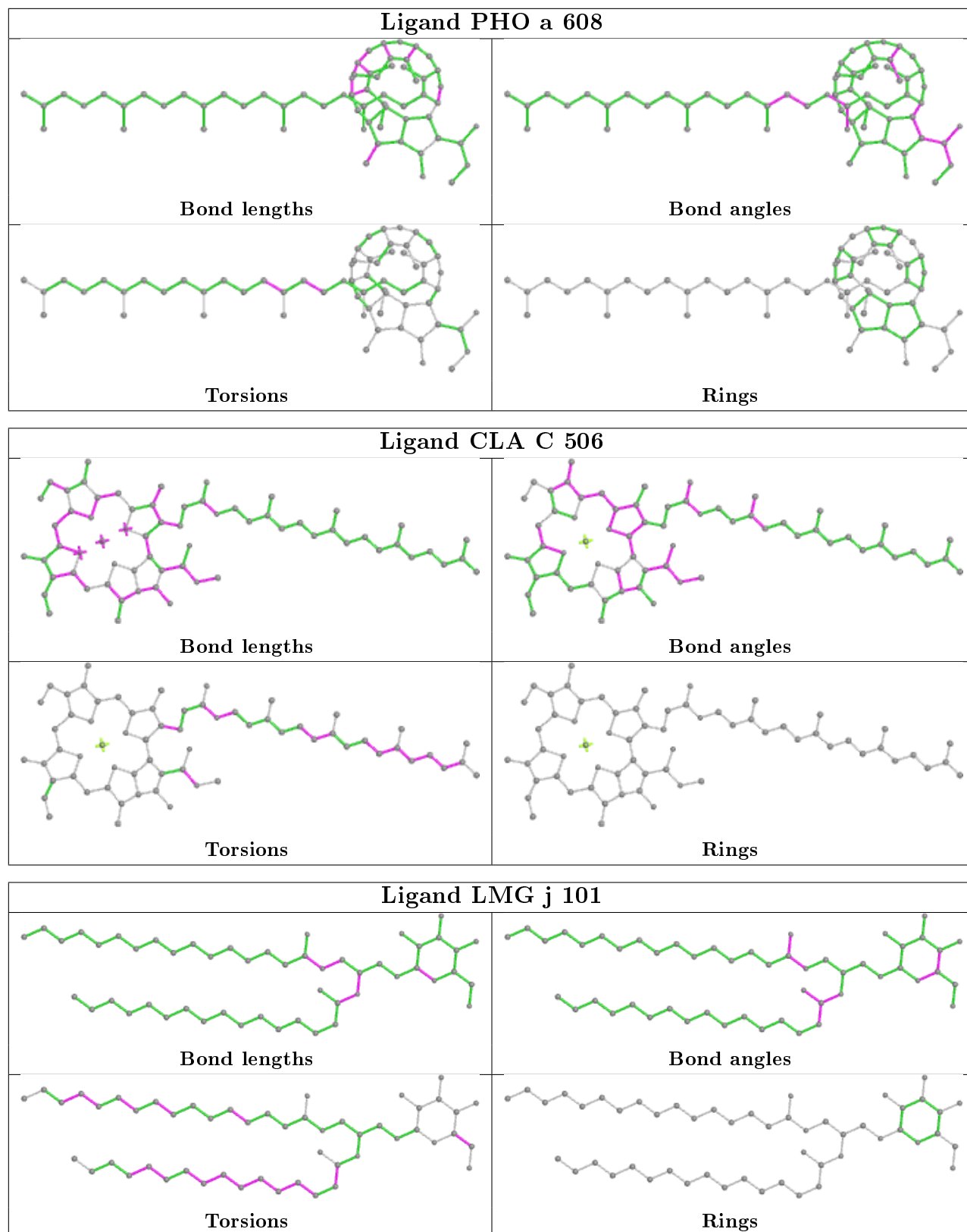




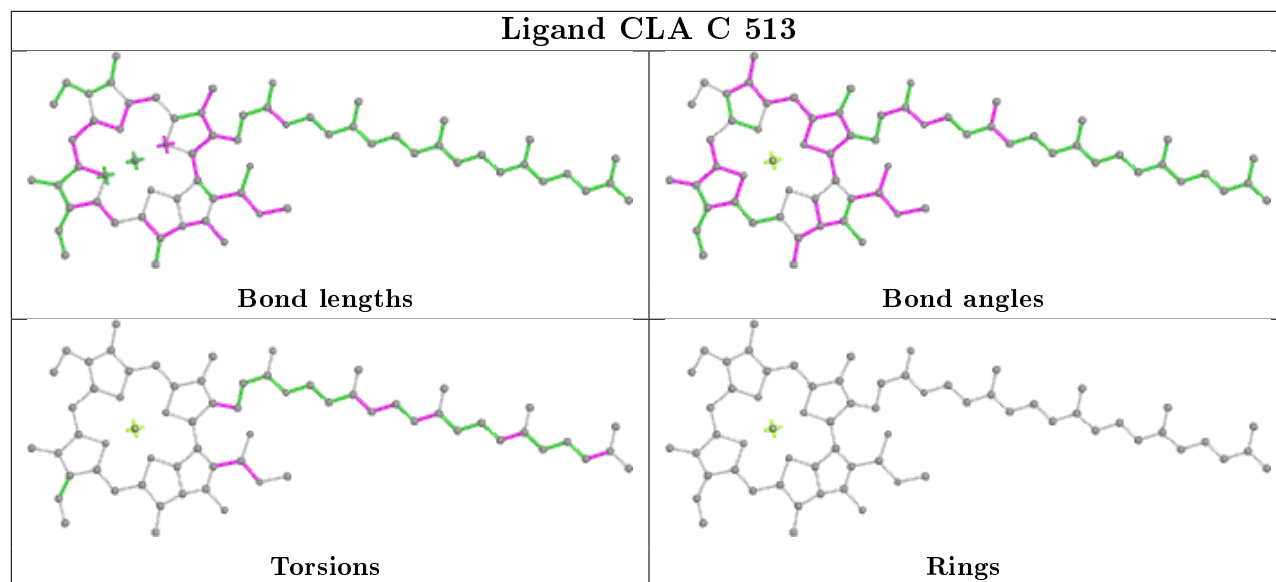




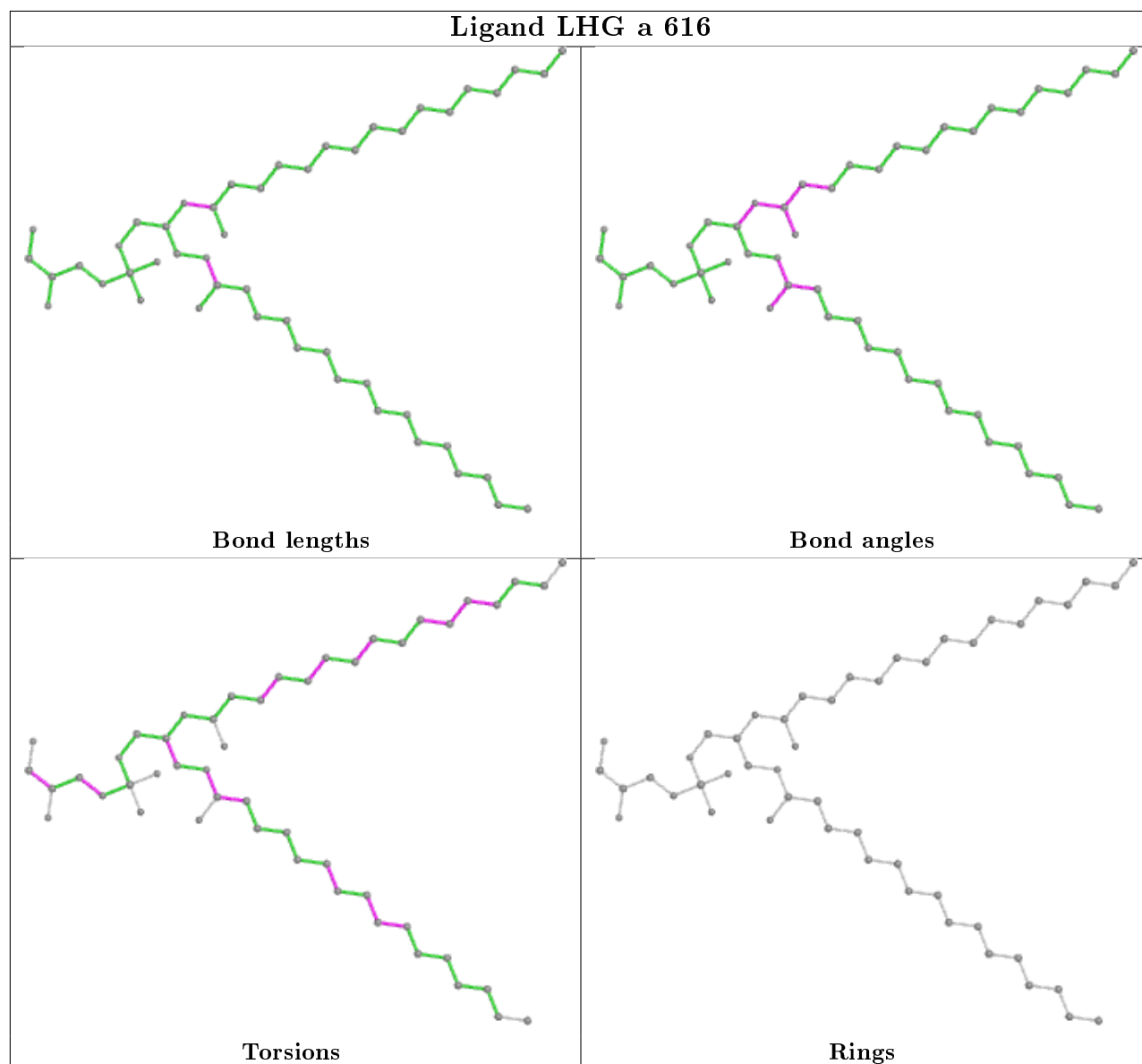




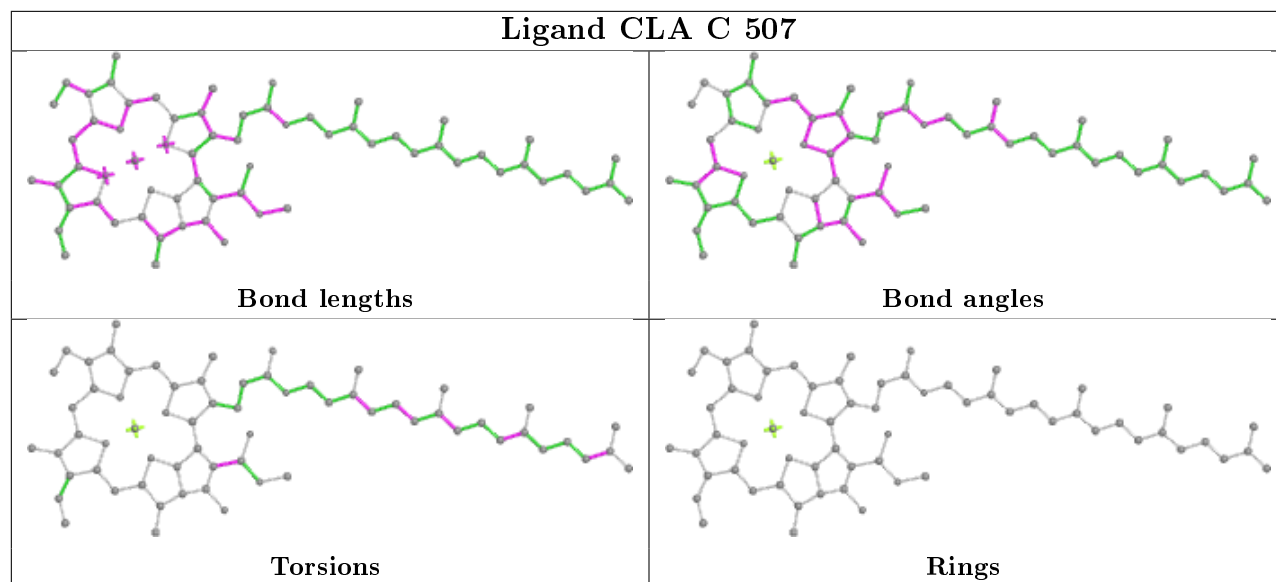
Ligand CLA C 513



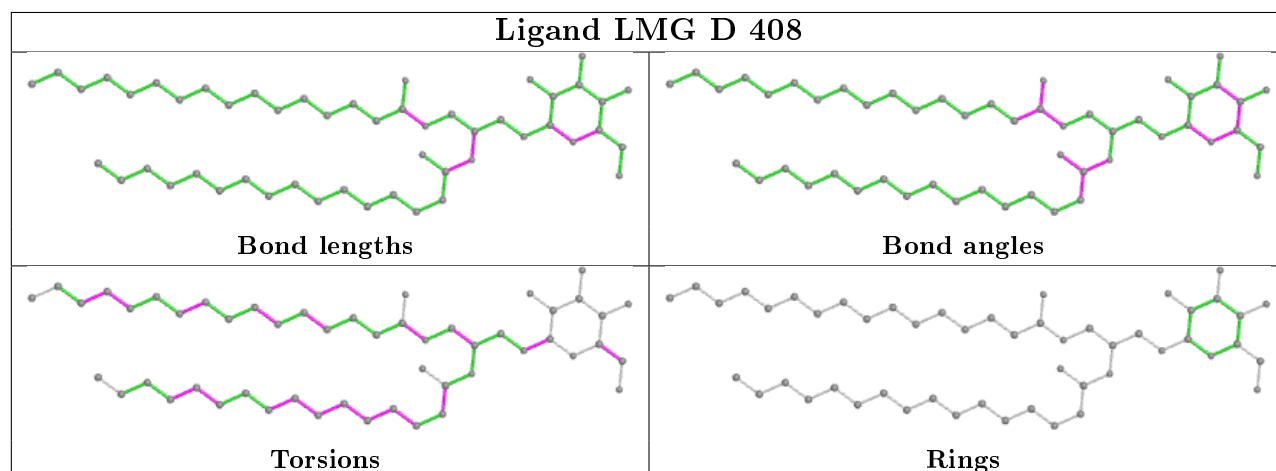
Ligand LHG a 616



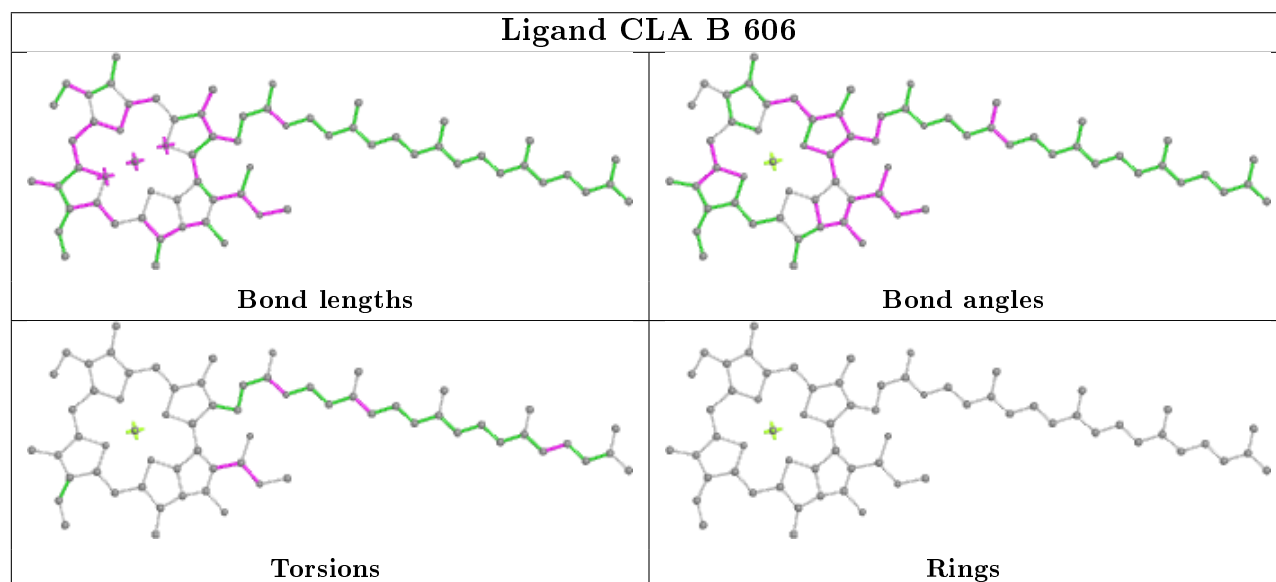
Ligand CLA C 507

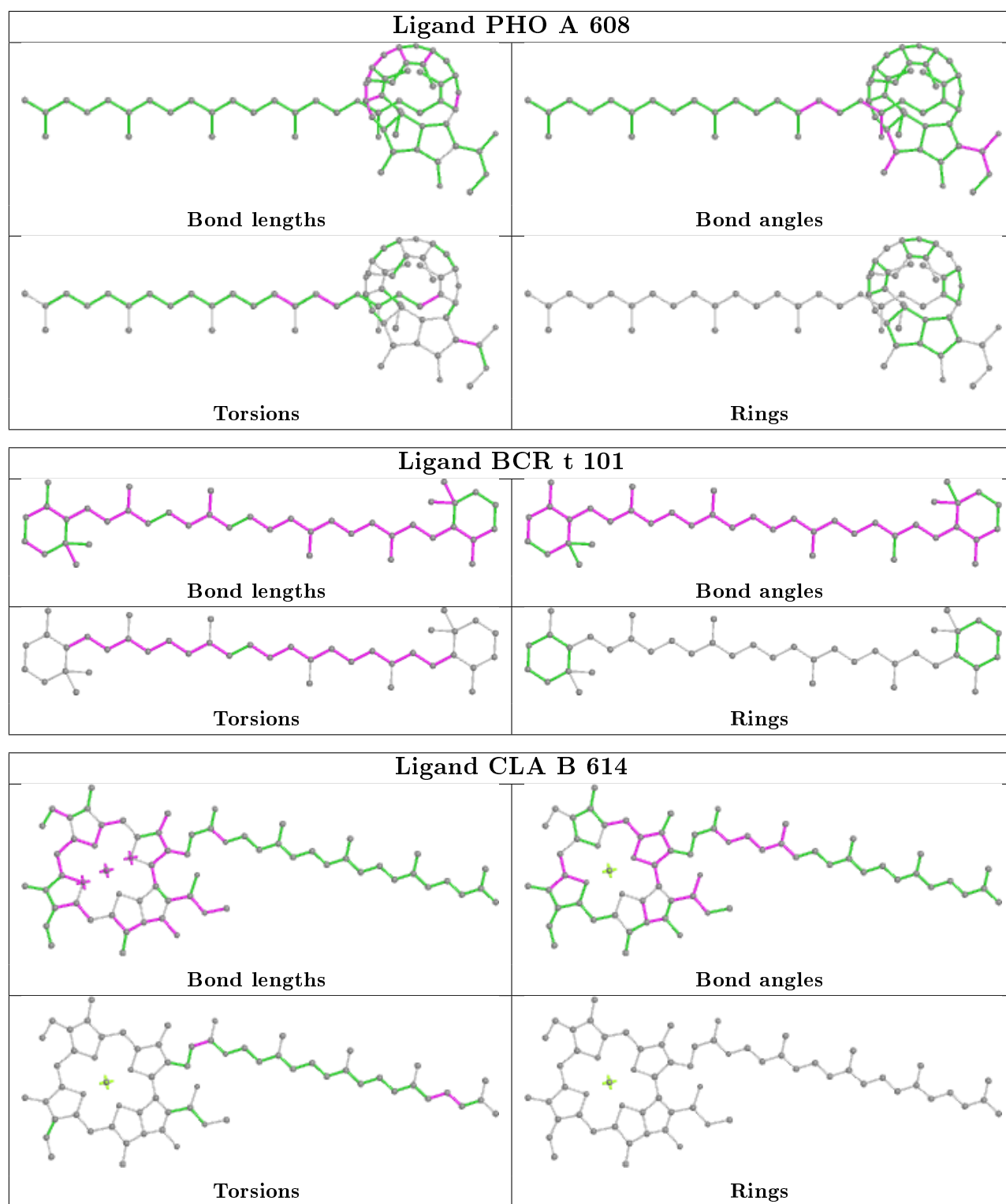


Ligand LMG D 408

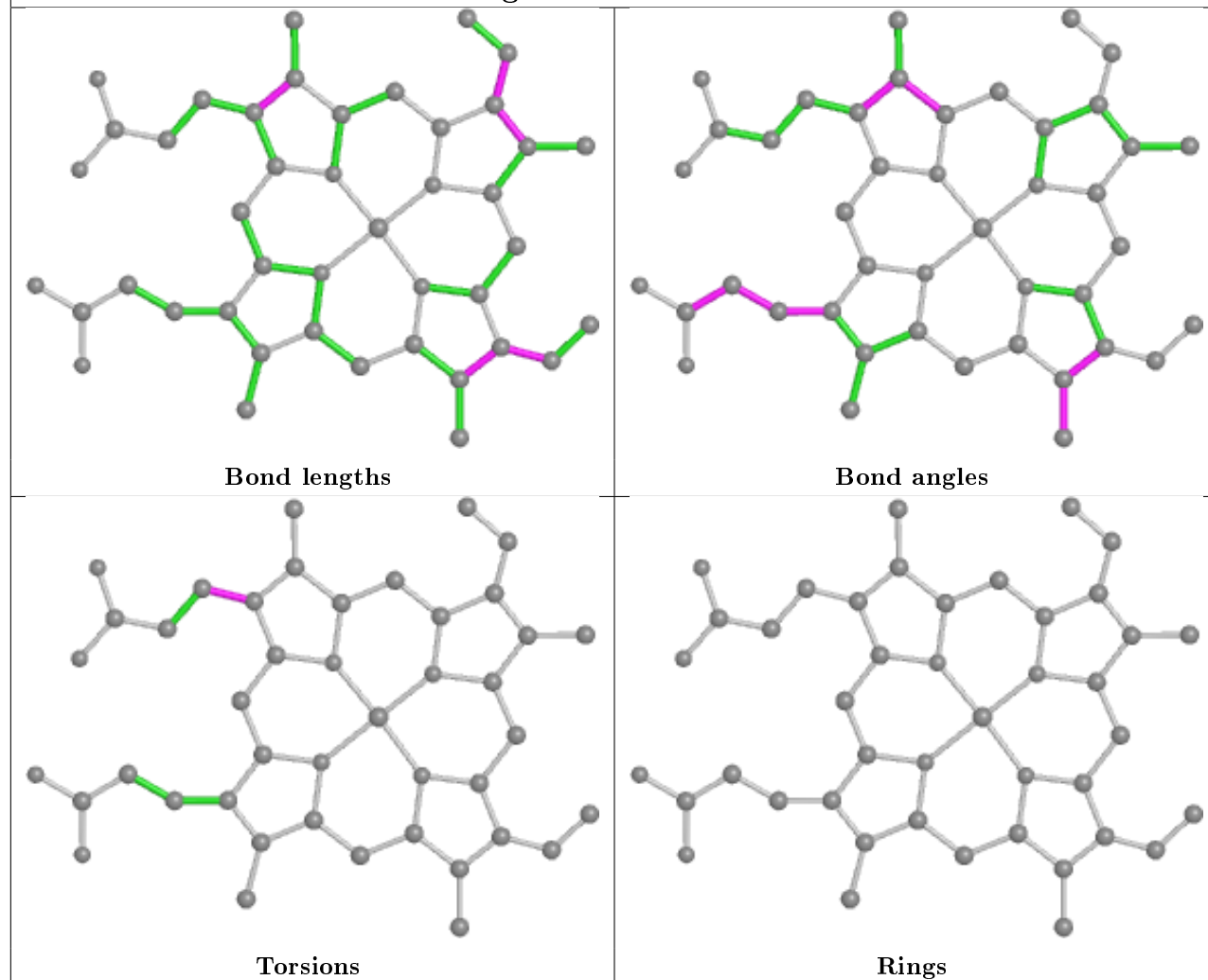


Ligand CLA B 606

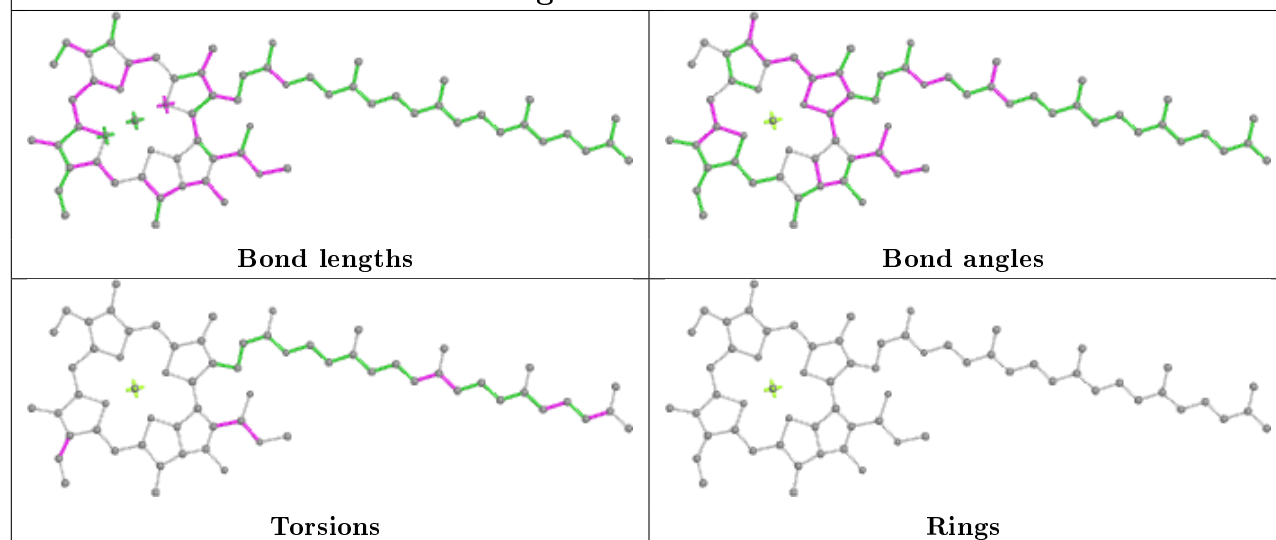


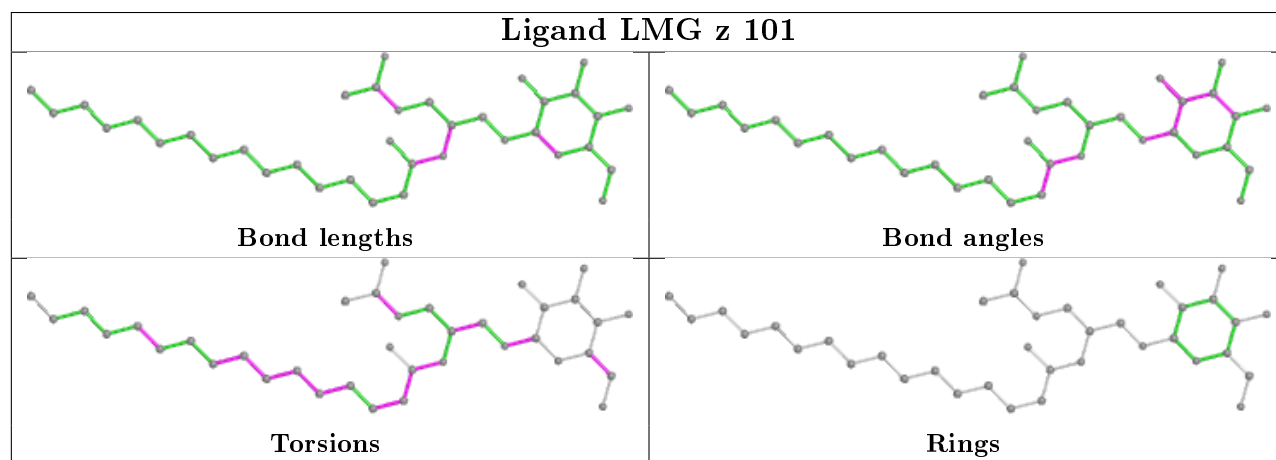
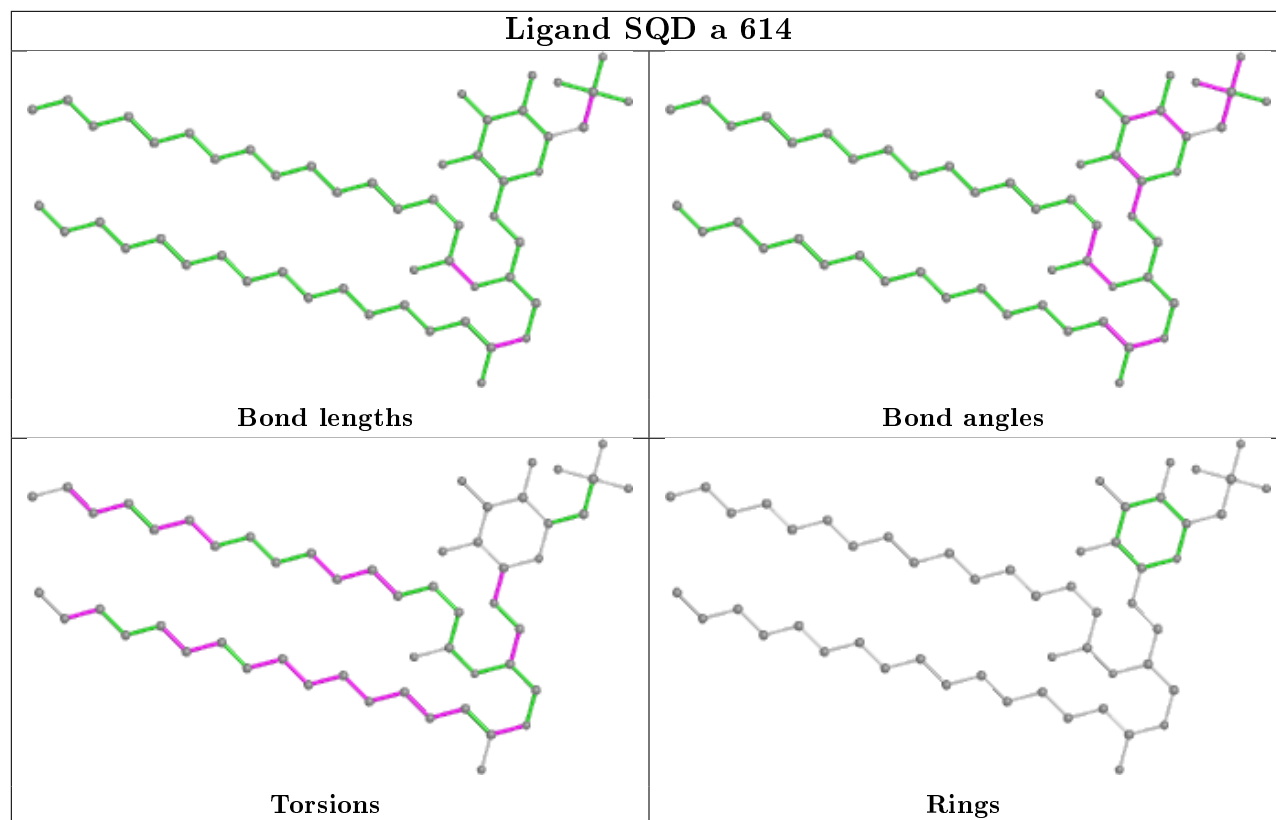


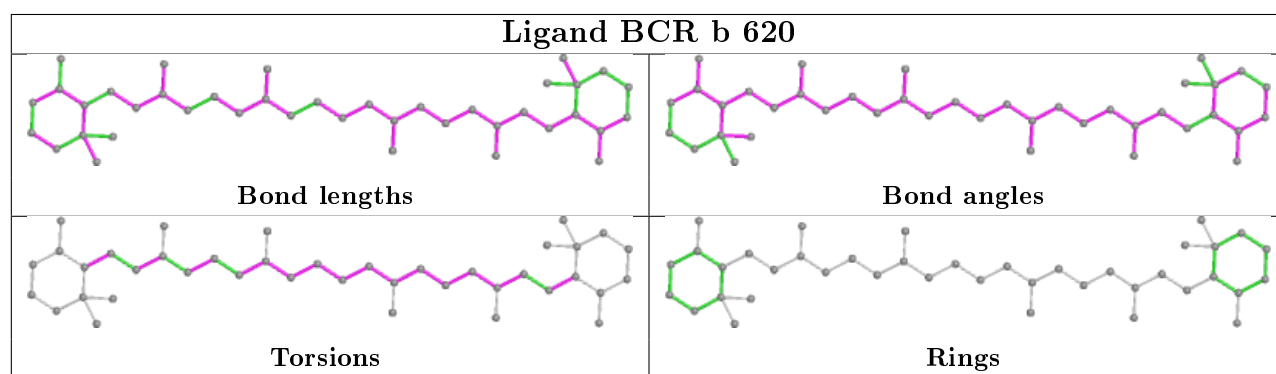
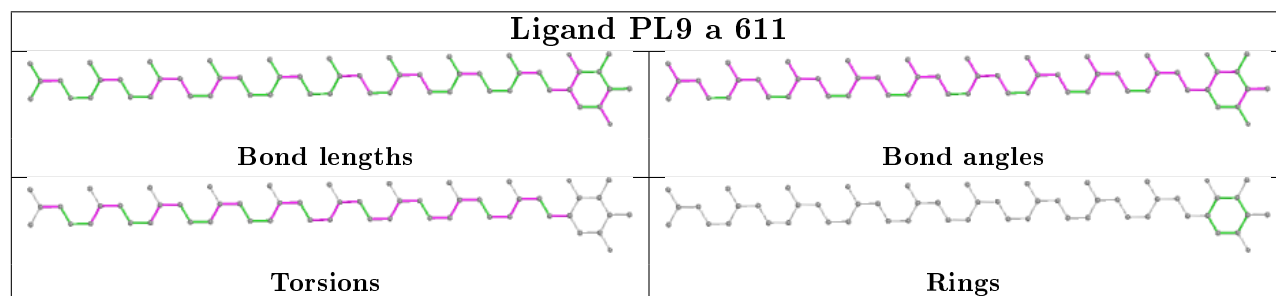
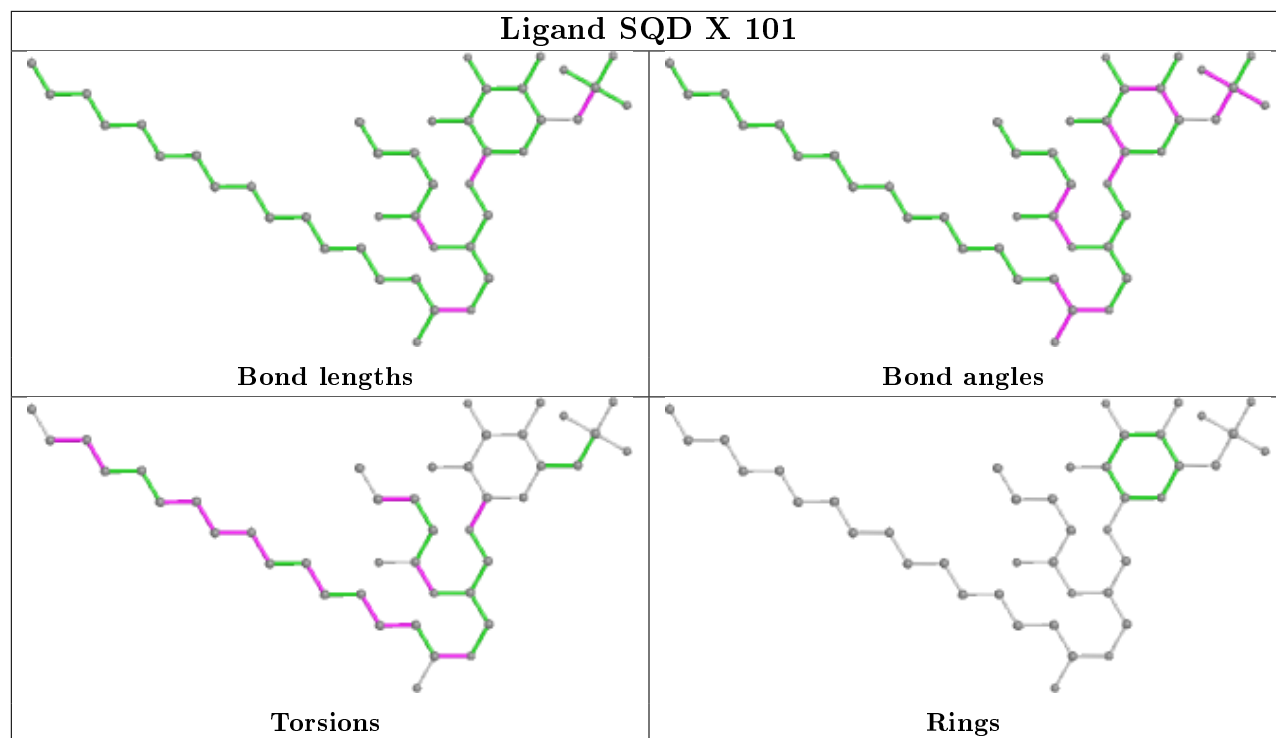
Ligand HEM v 201

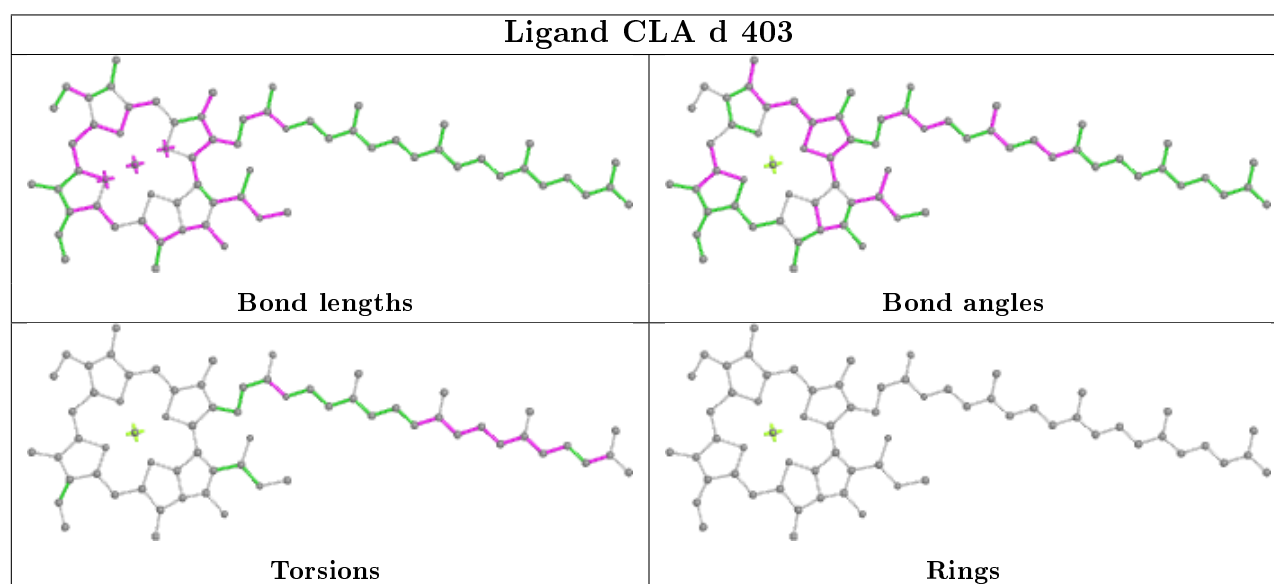
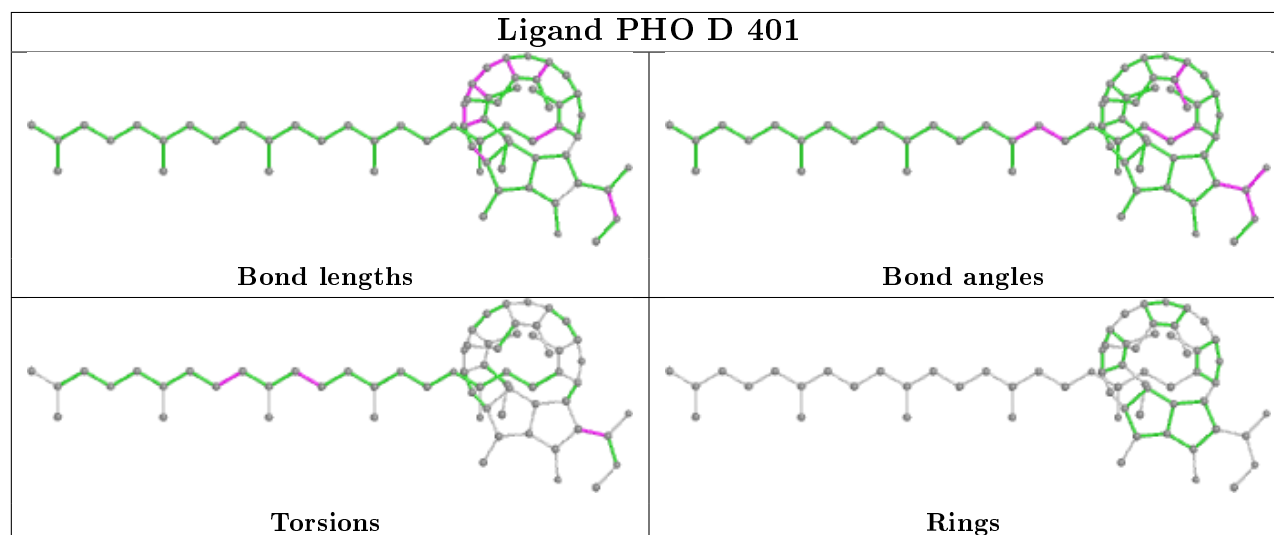
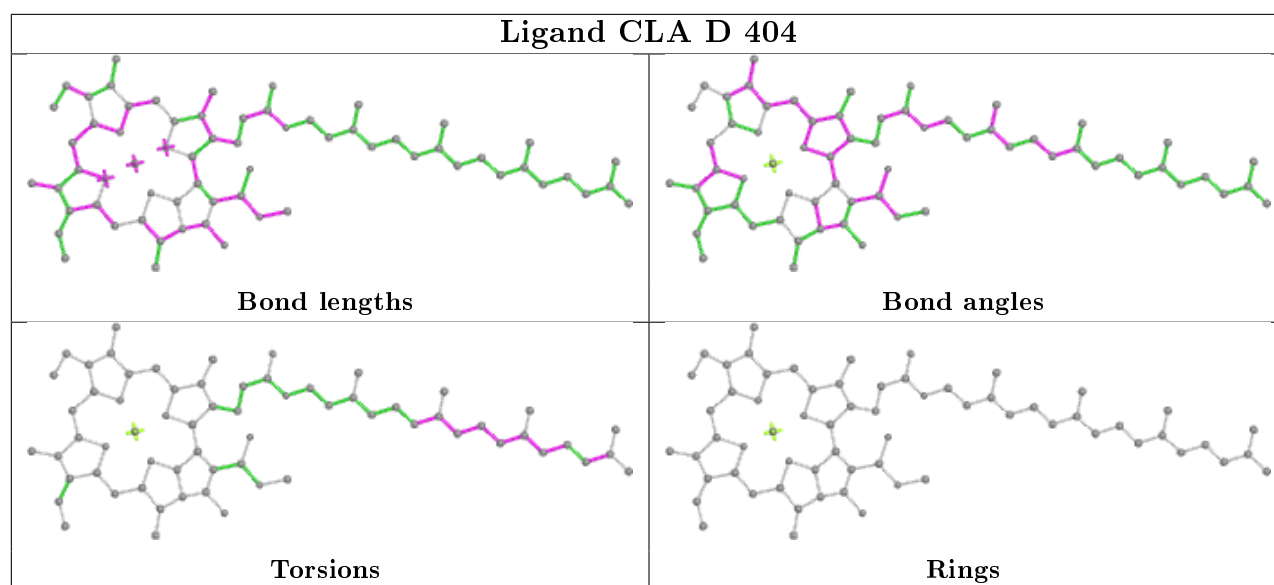


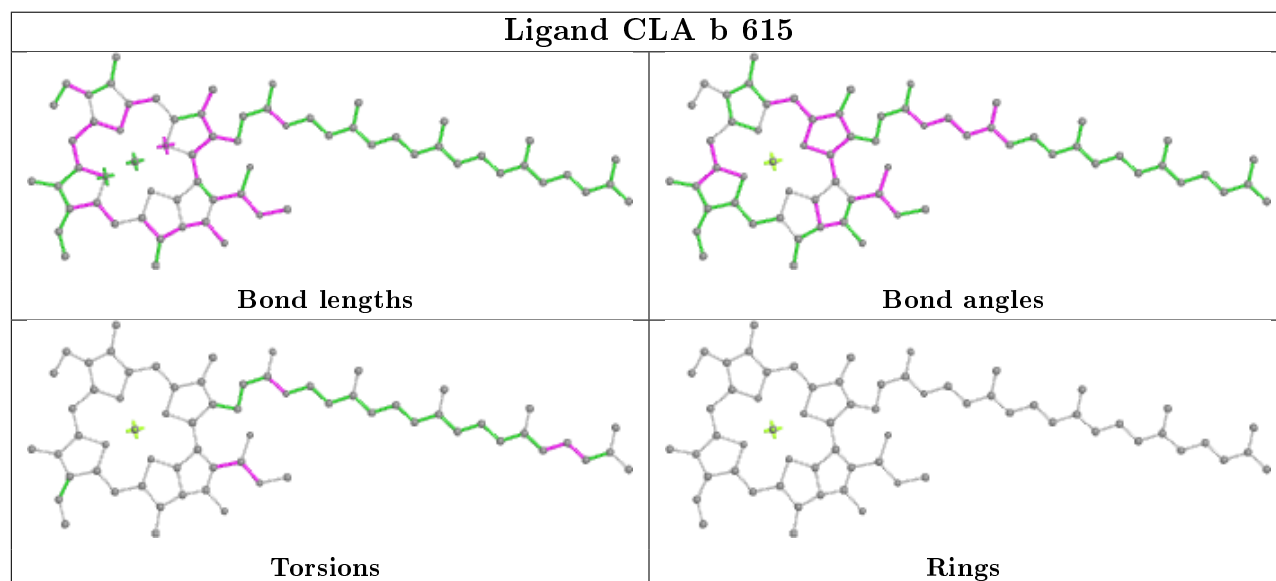
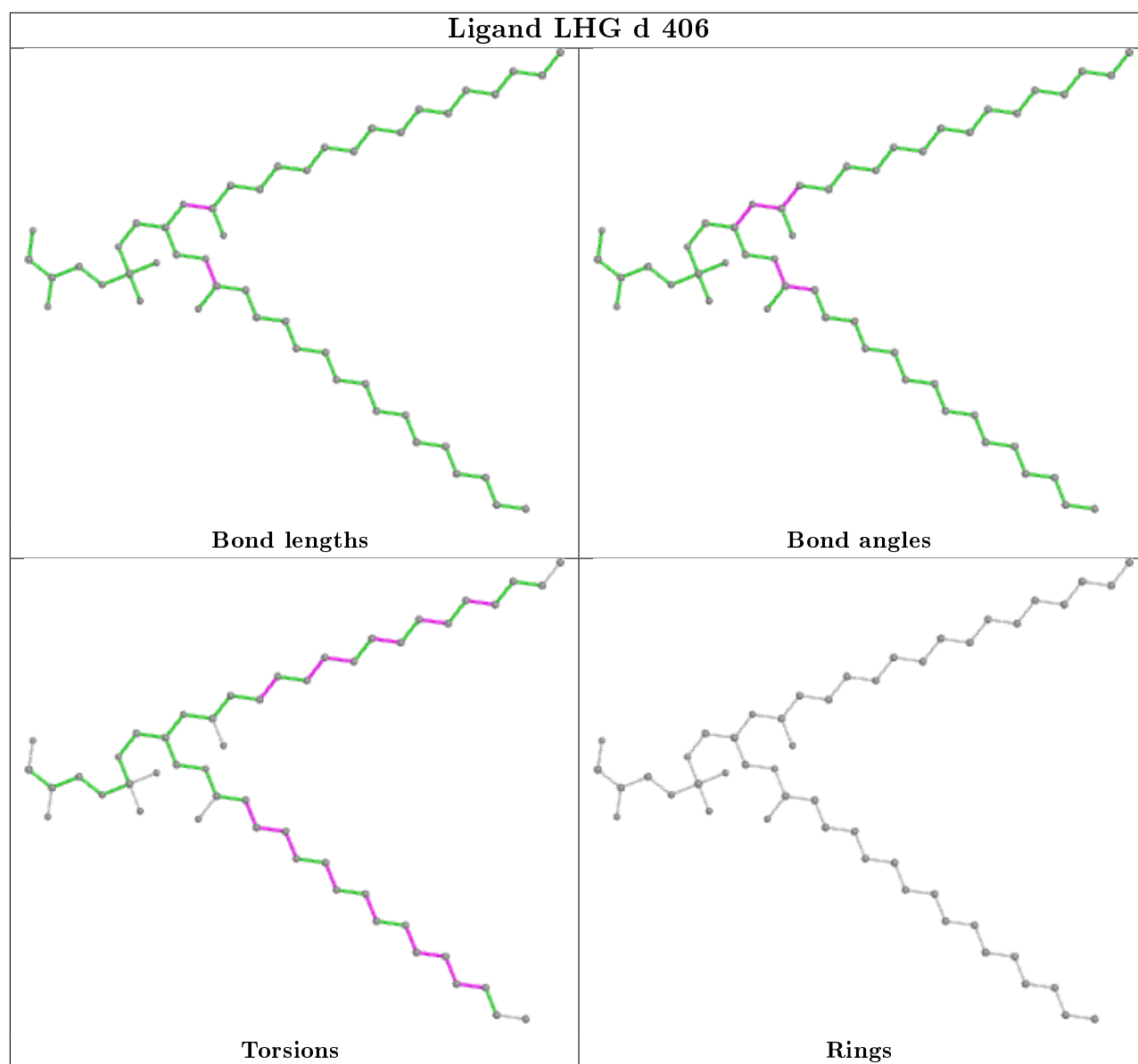
Ligand CLA a 607

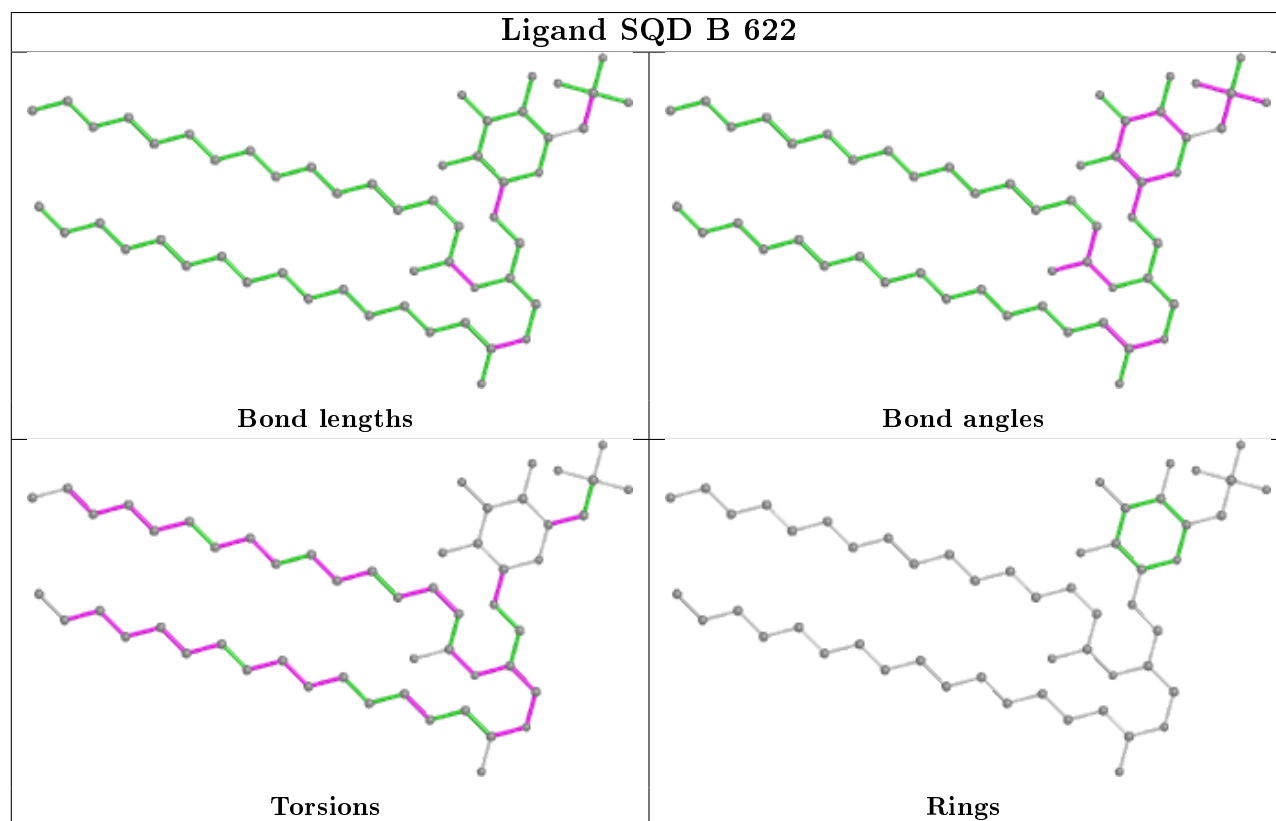
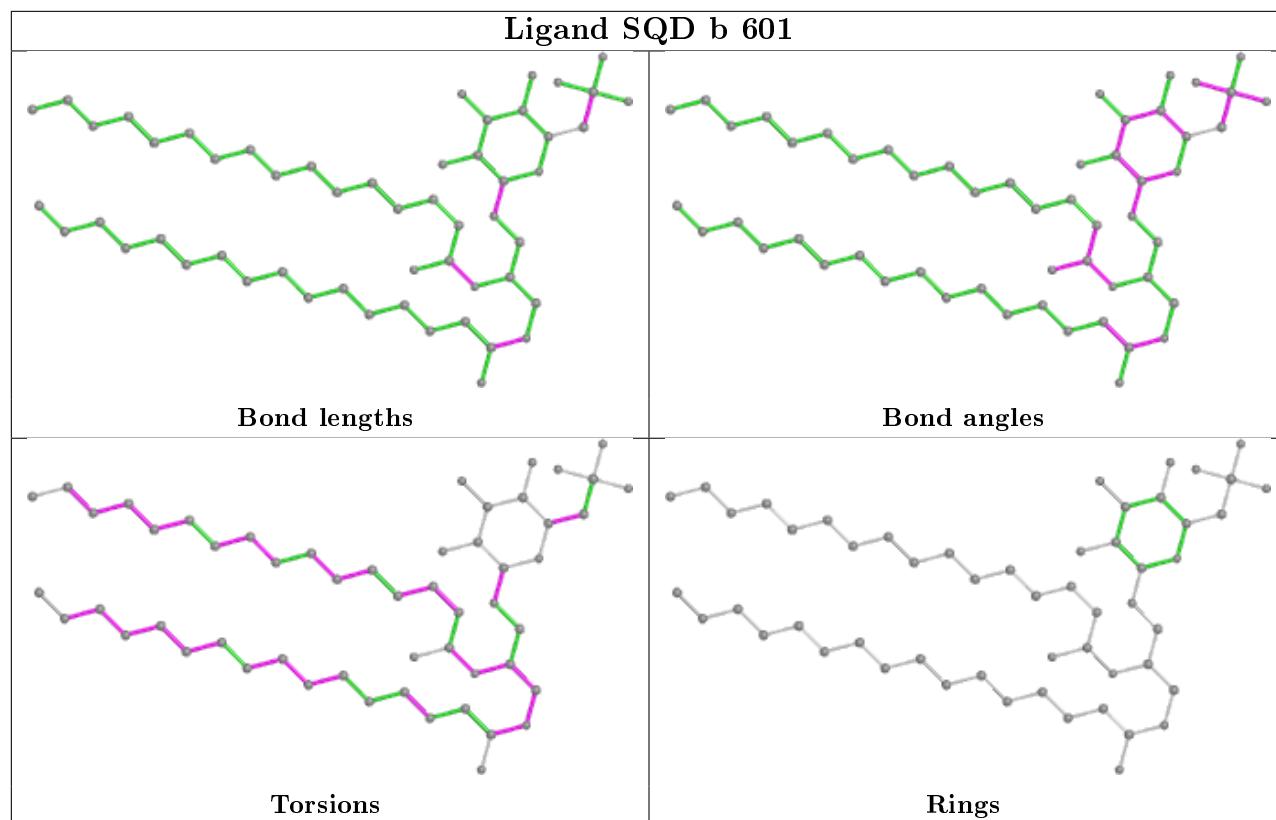


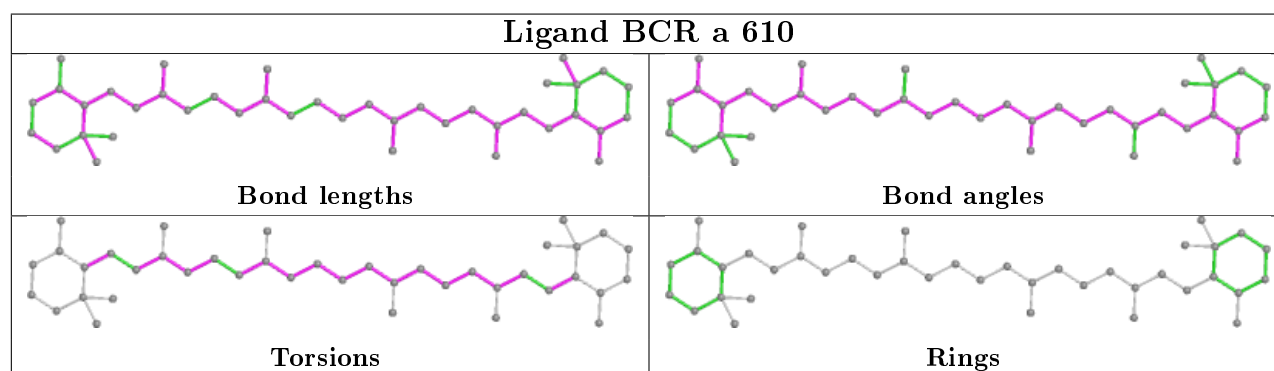
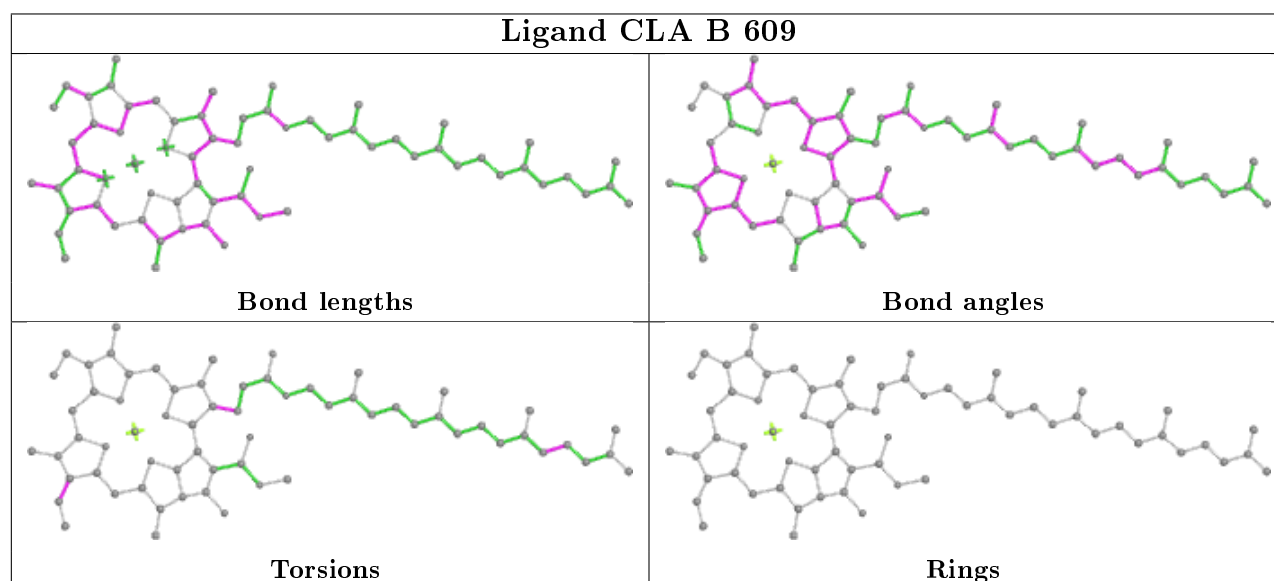
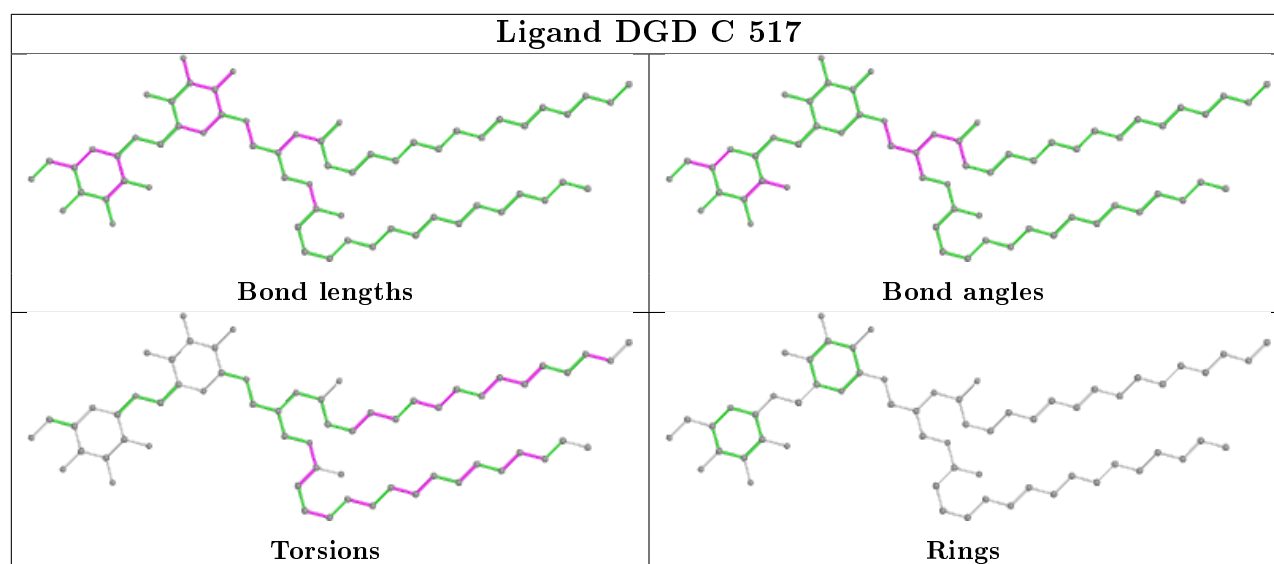


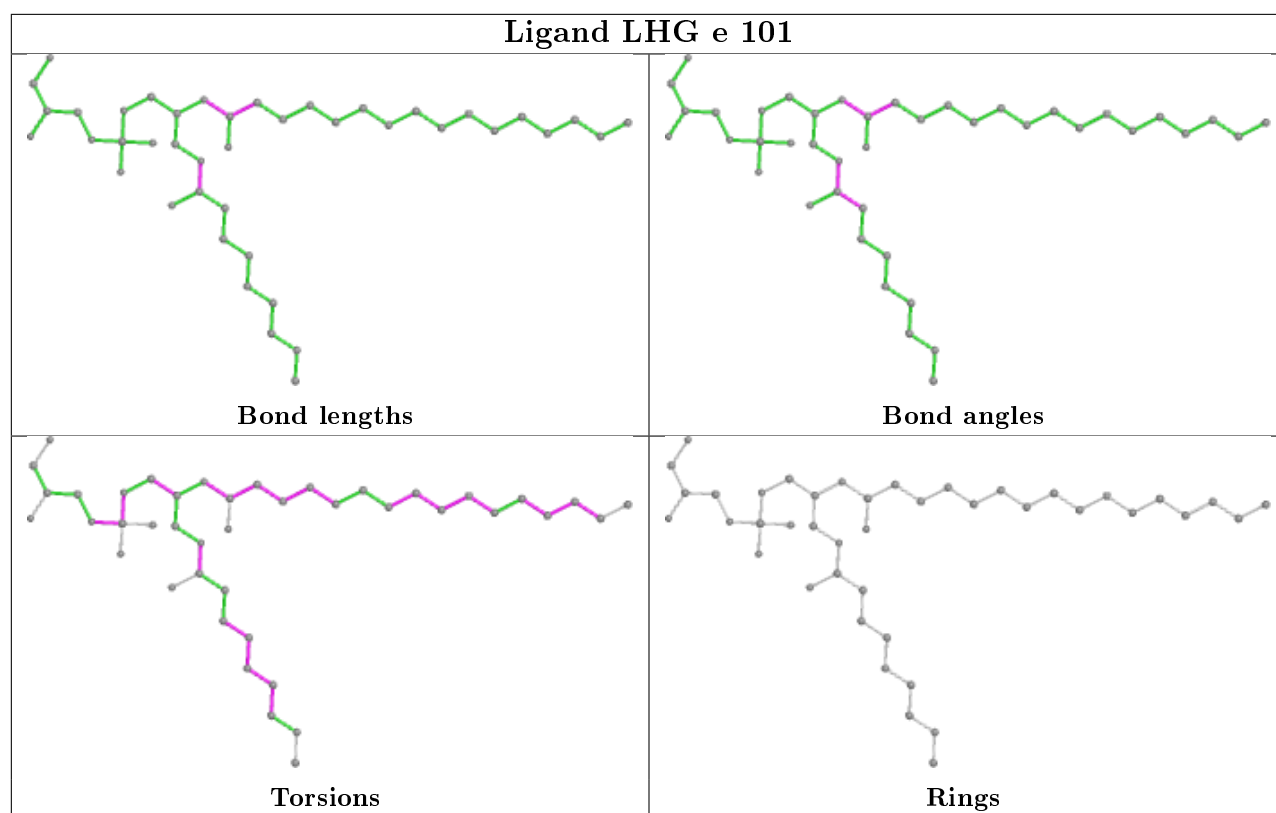


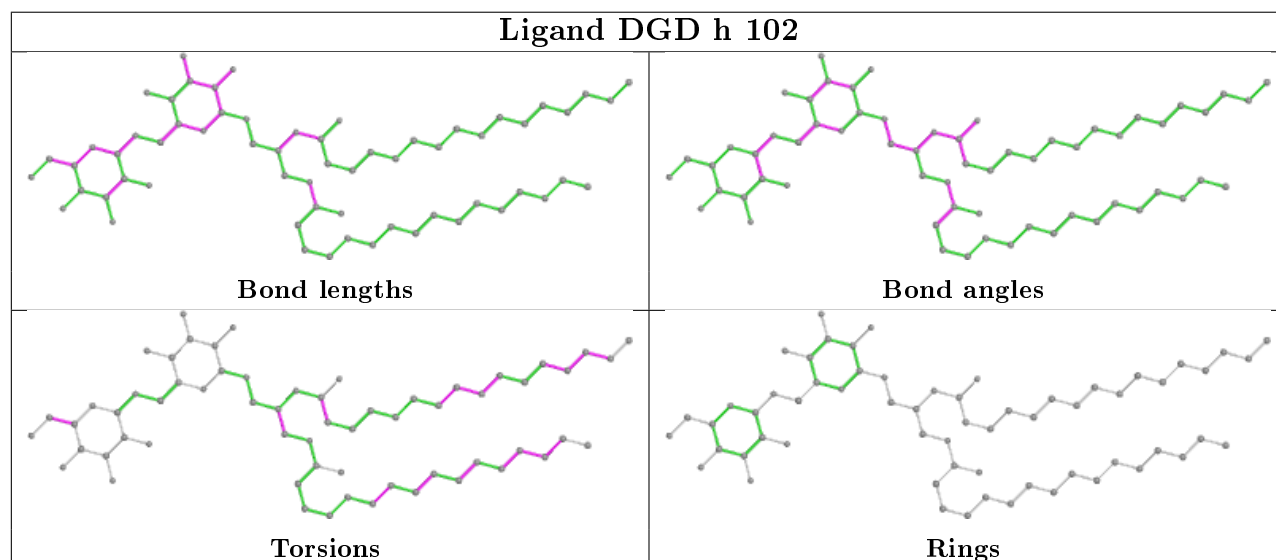
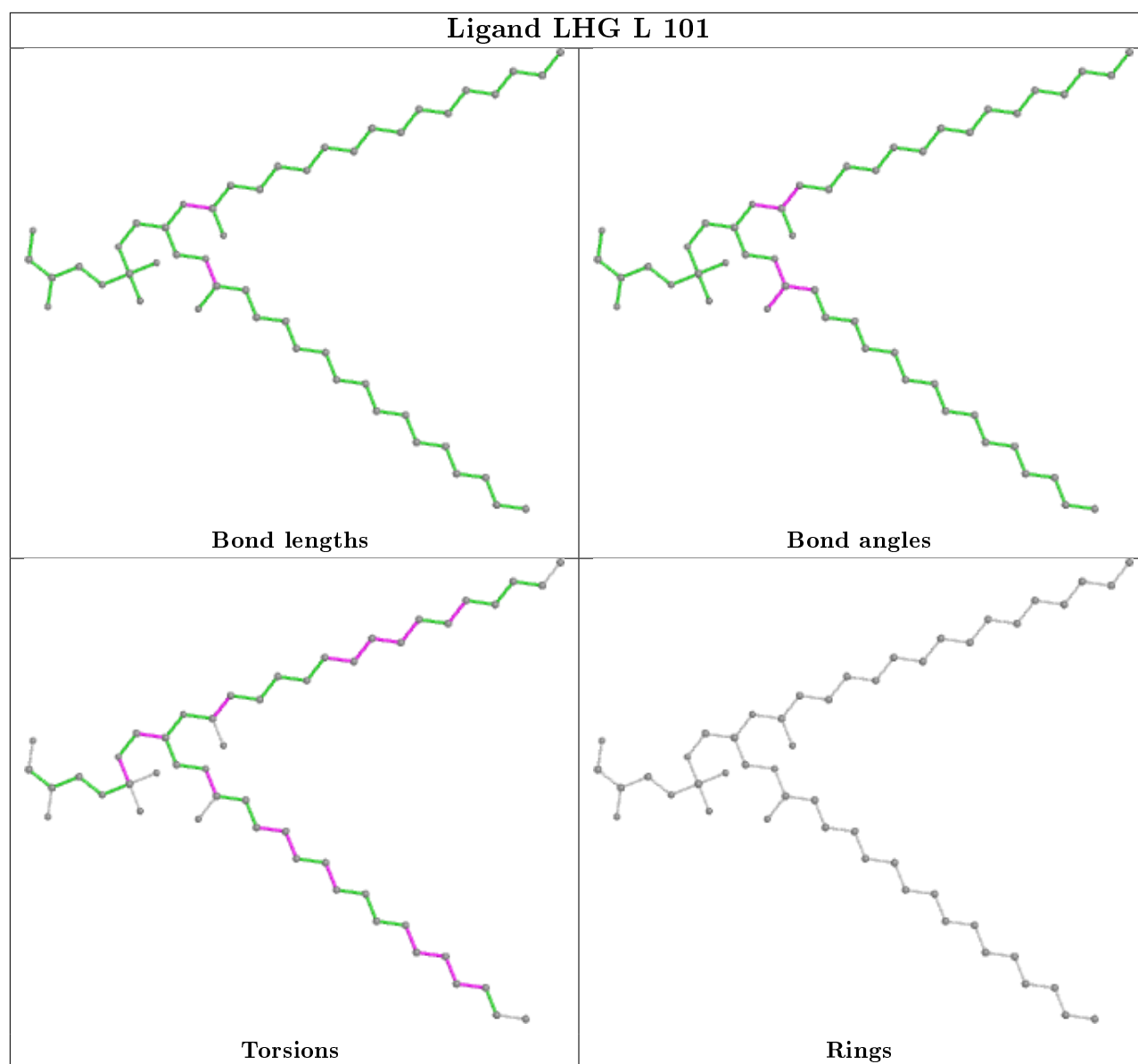




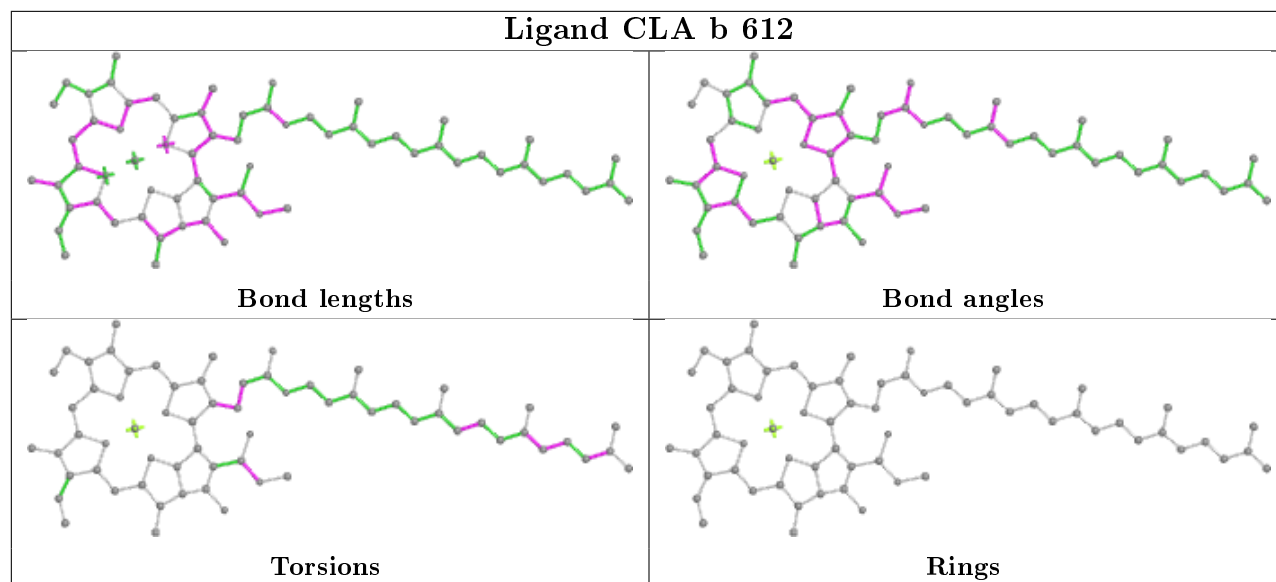




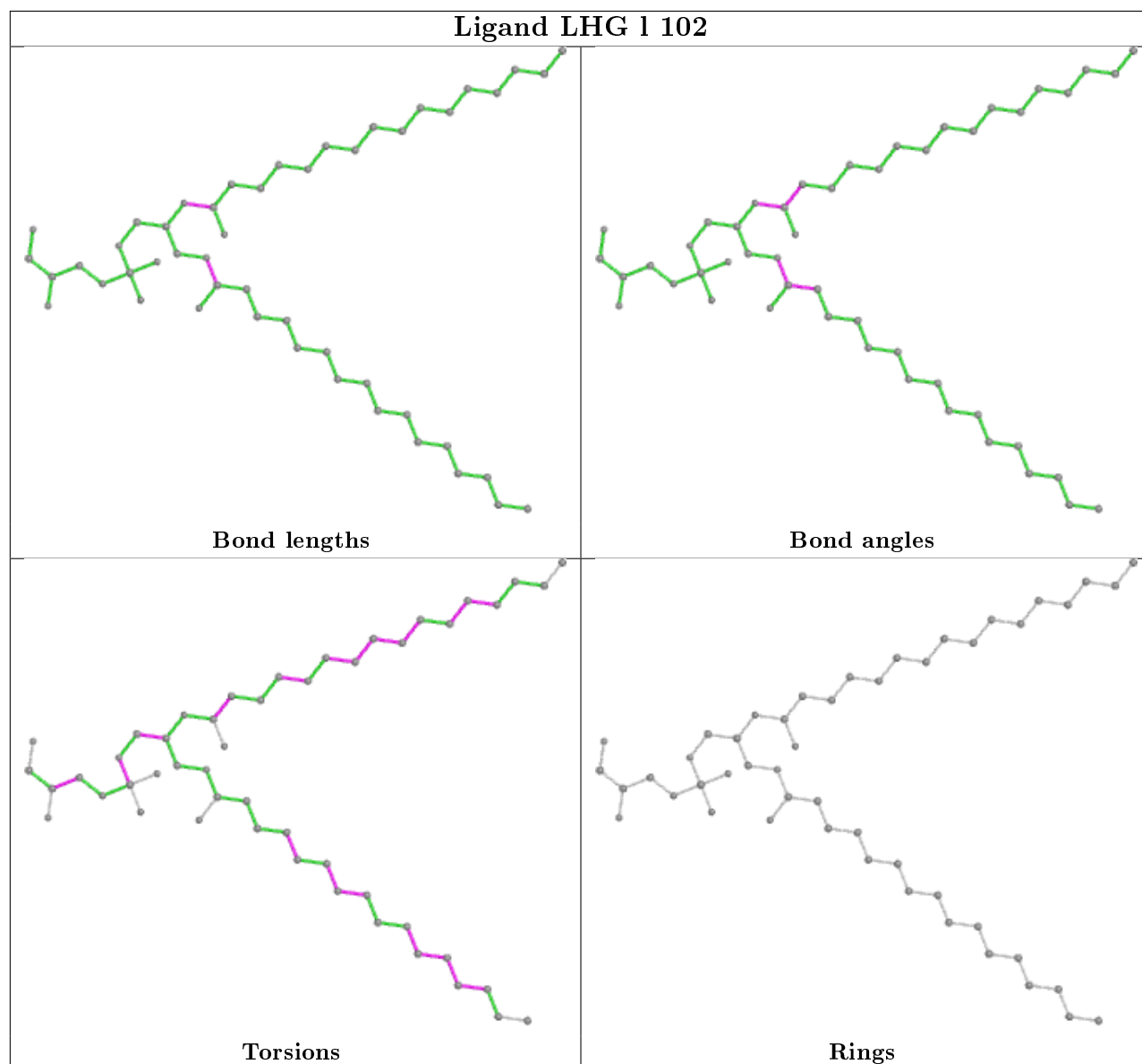


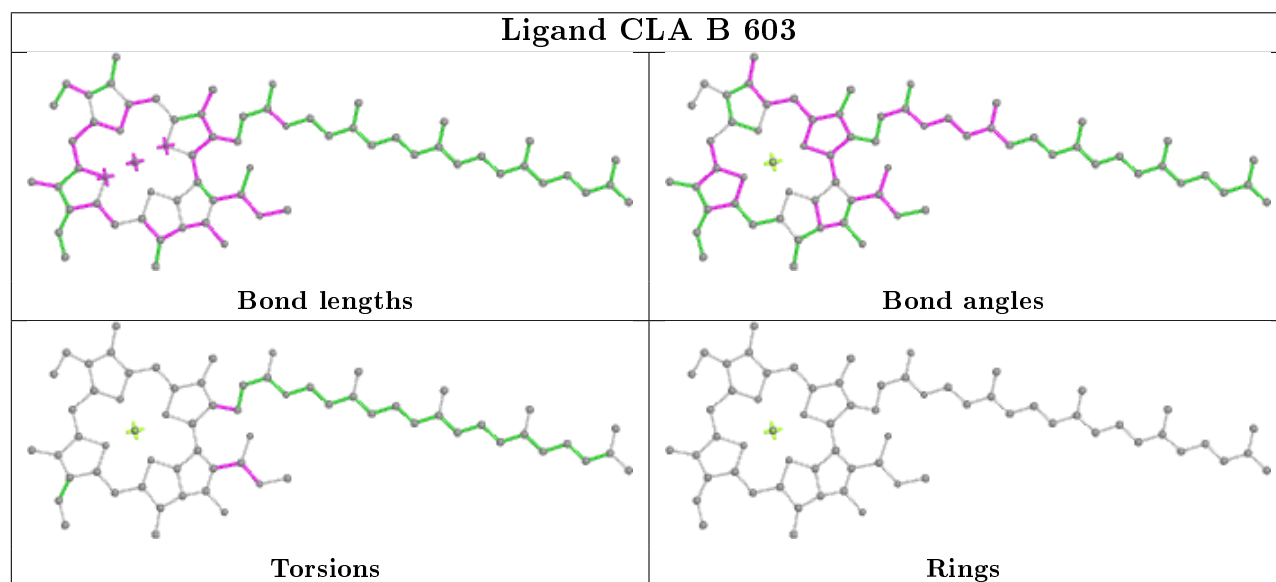
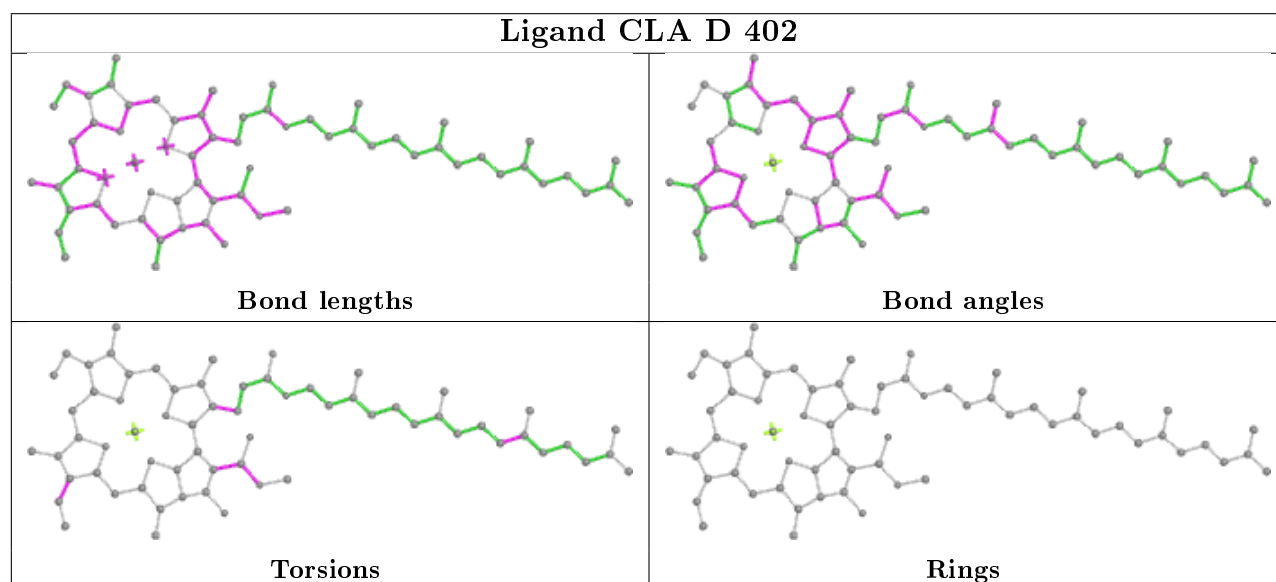
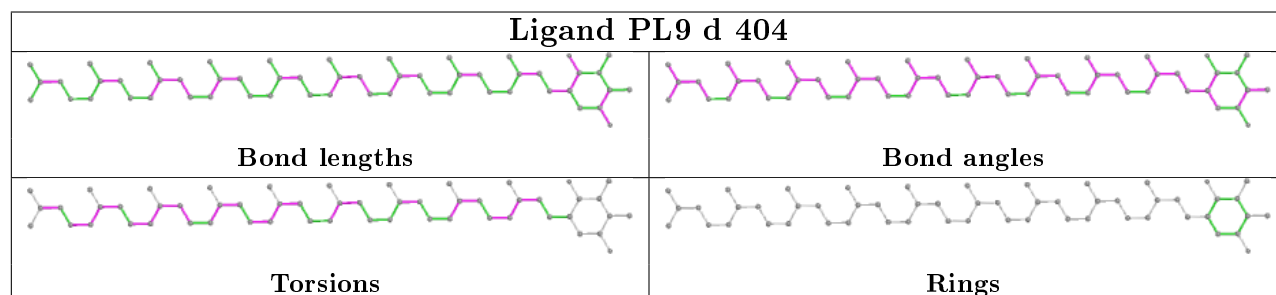
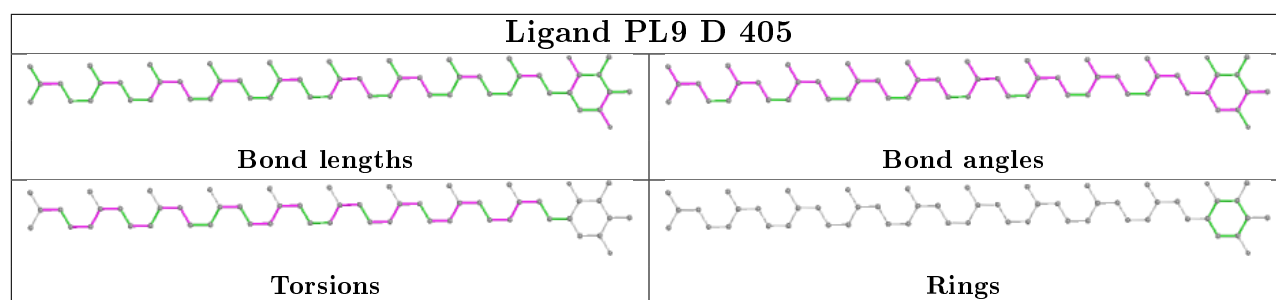


Ligand CLA b 612

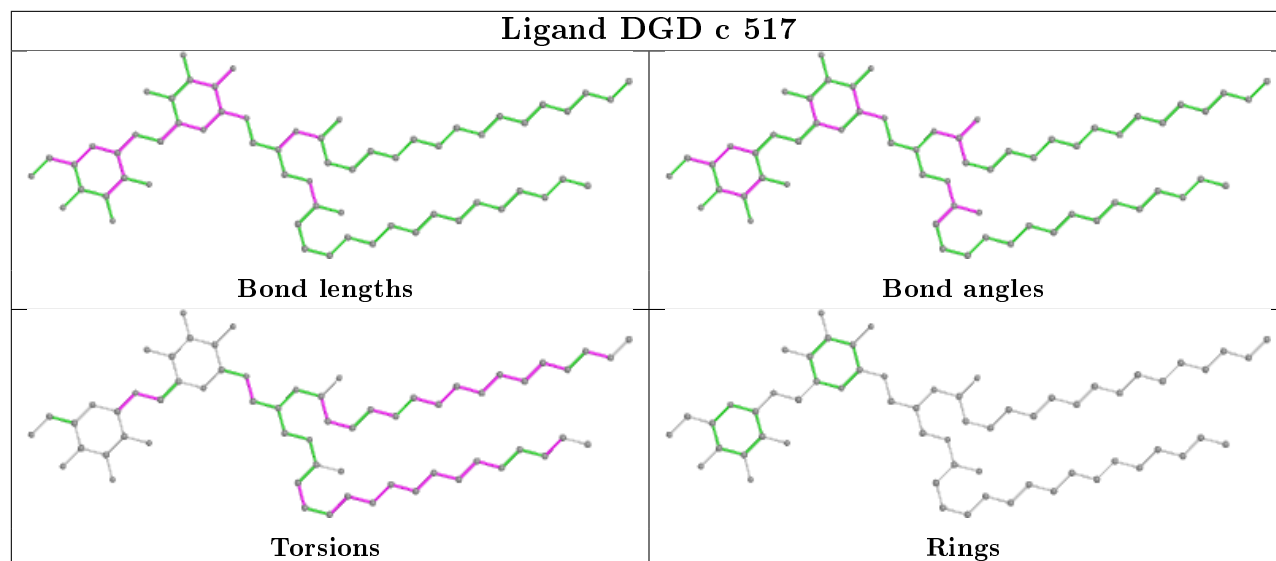


Ligand LHG 1 102

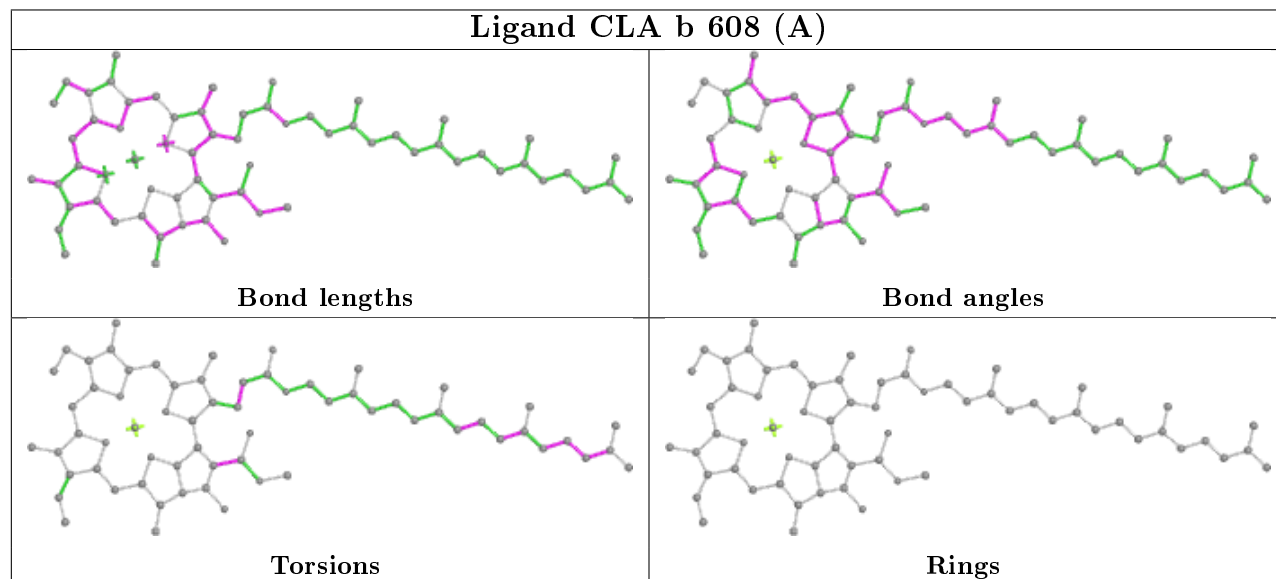


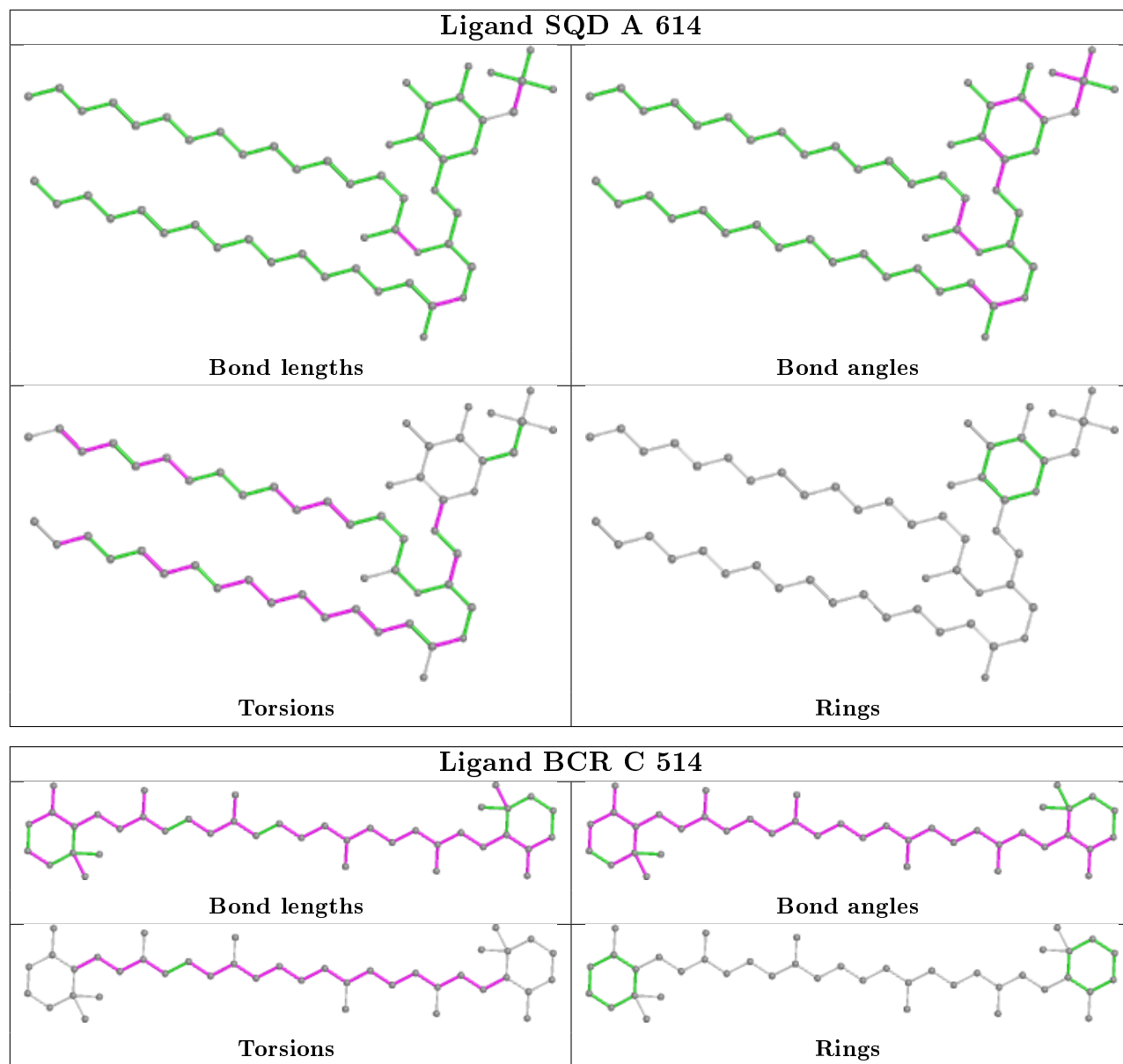


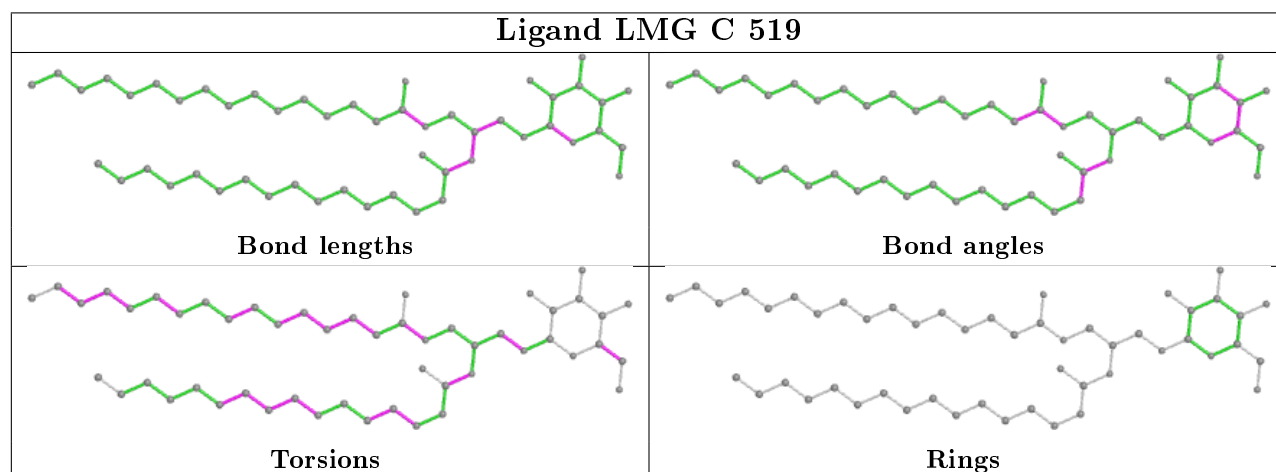
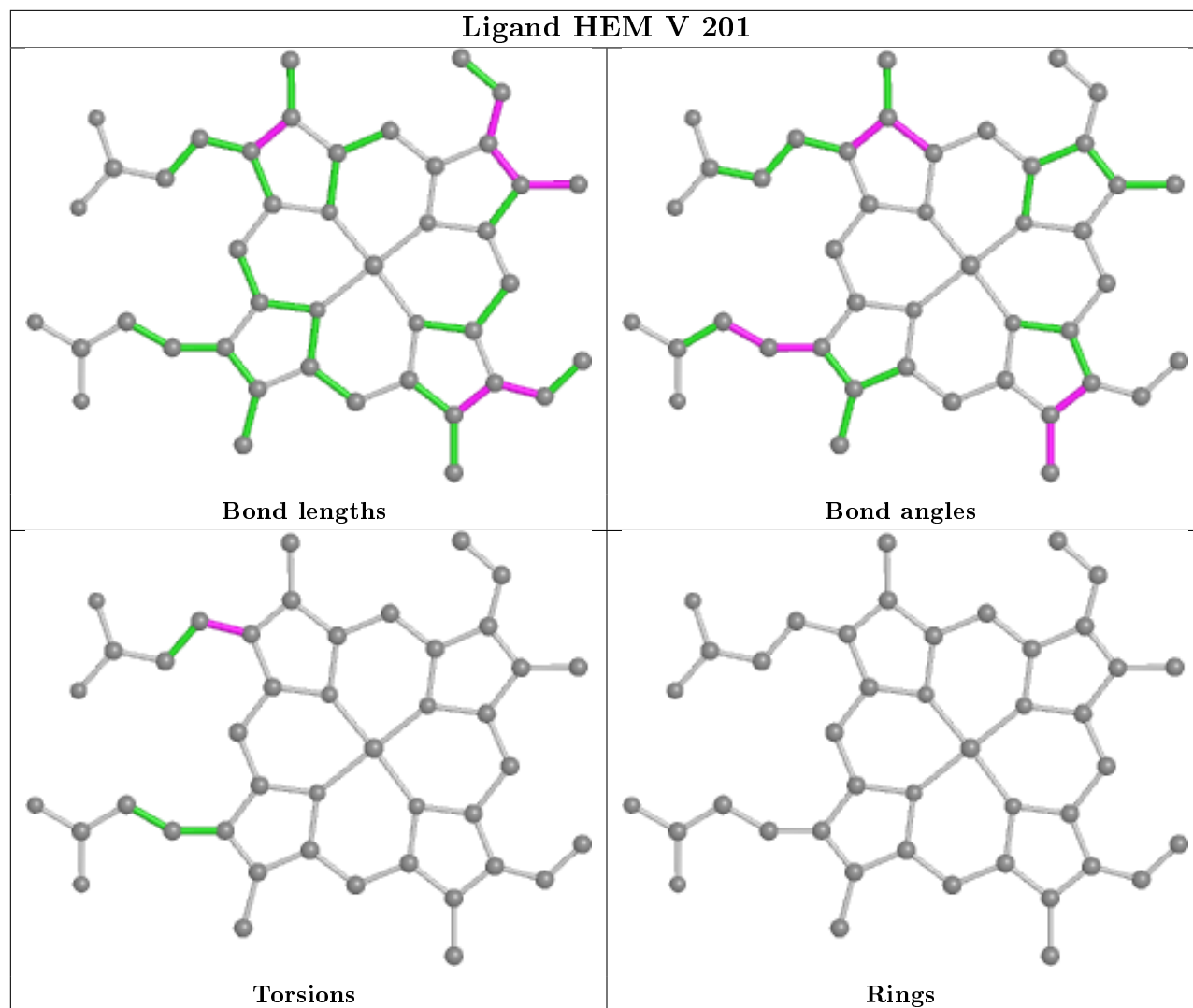
Ligand DGD c 517



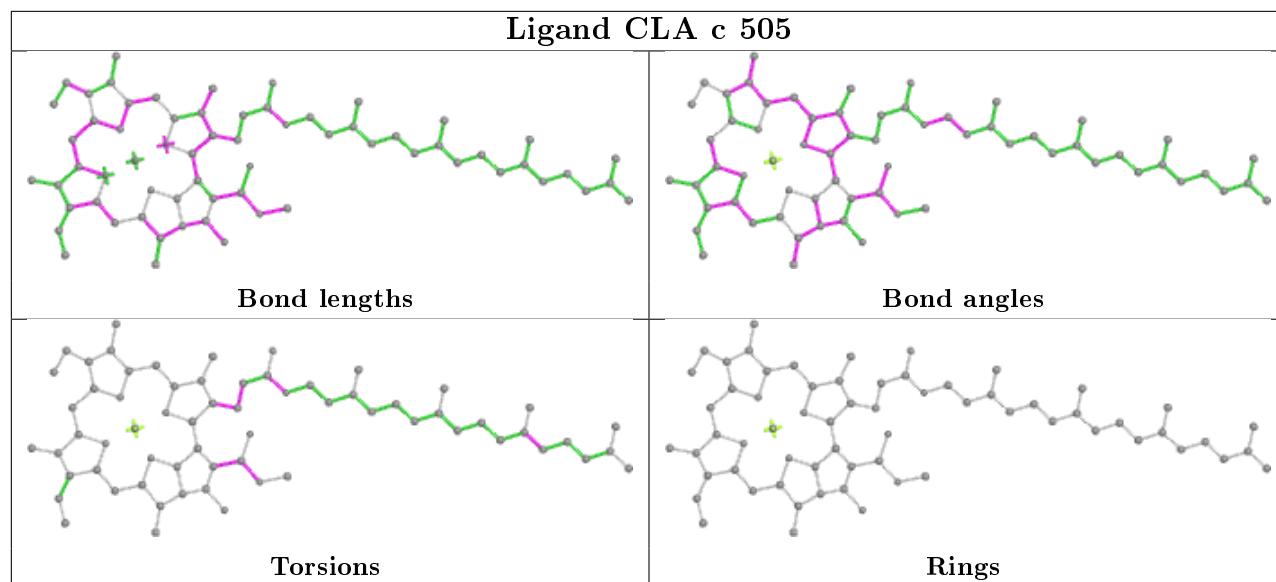
Ligand CLA b 608 (A)



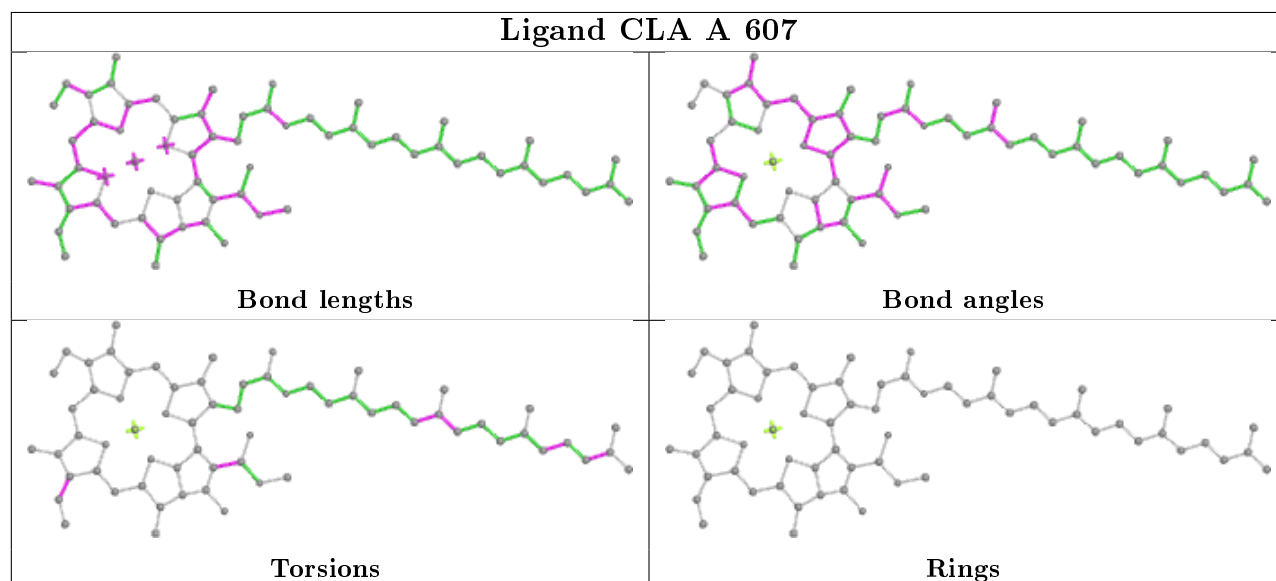




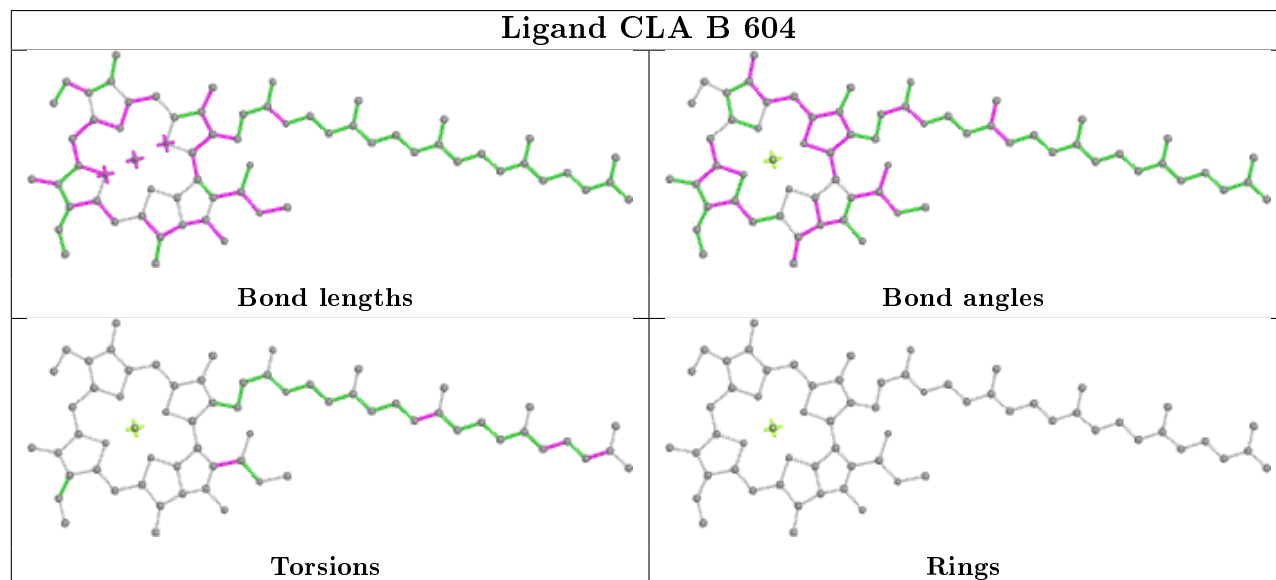
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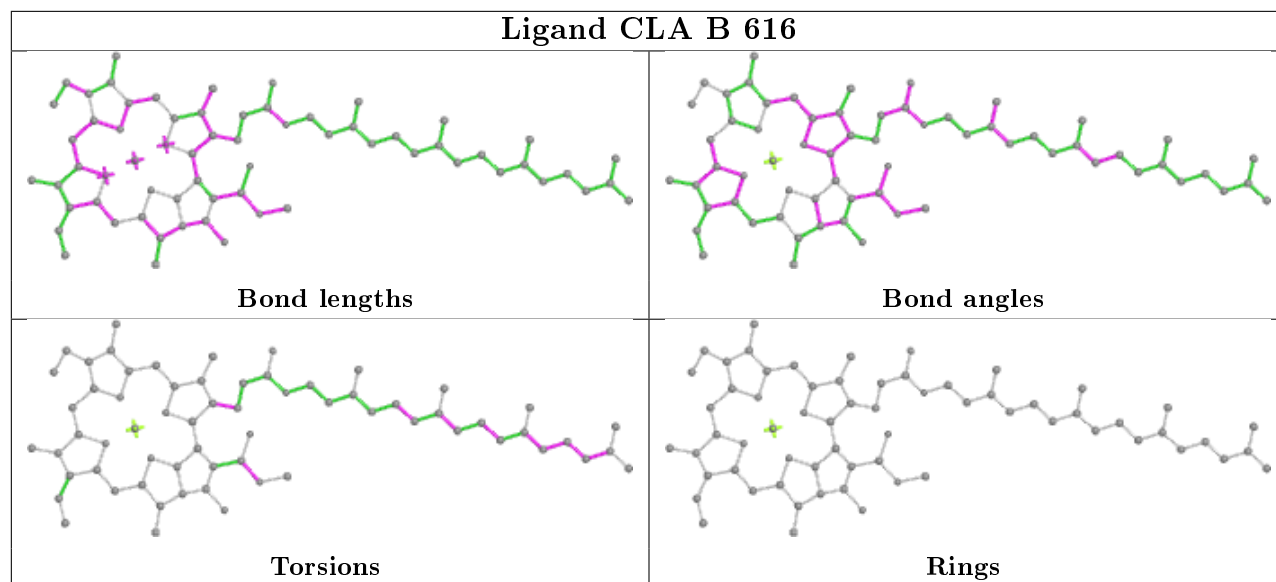
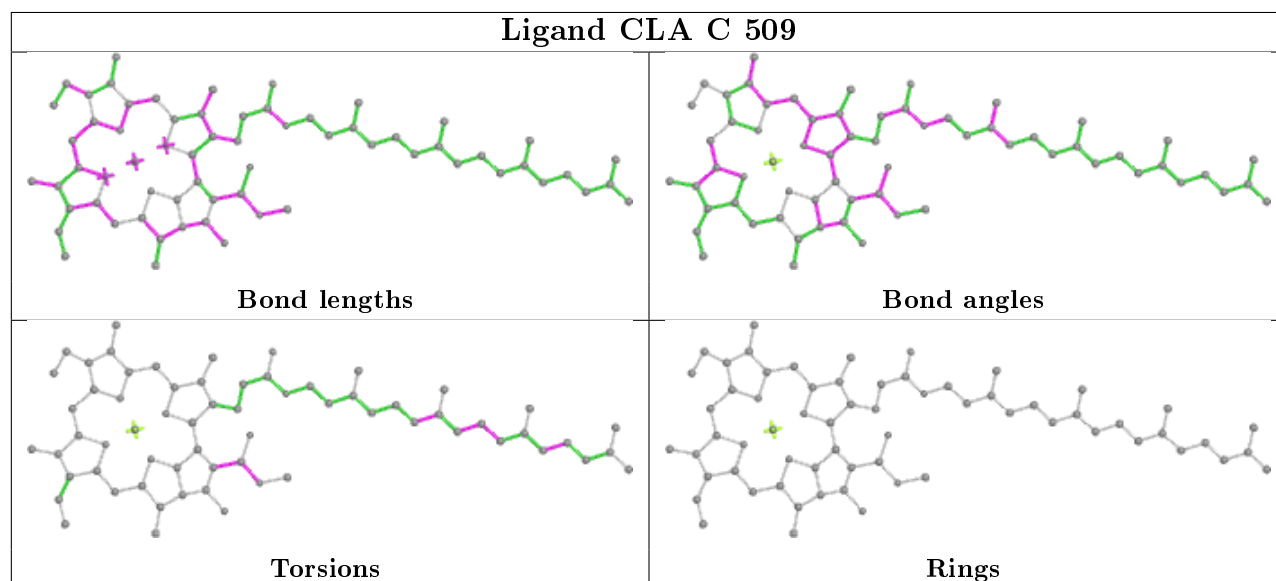
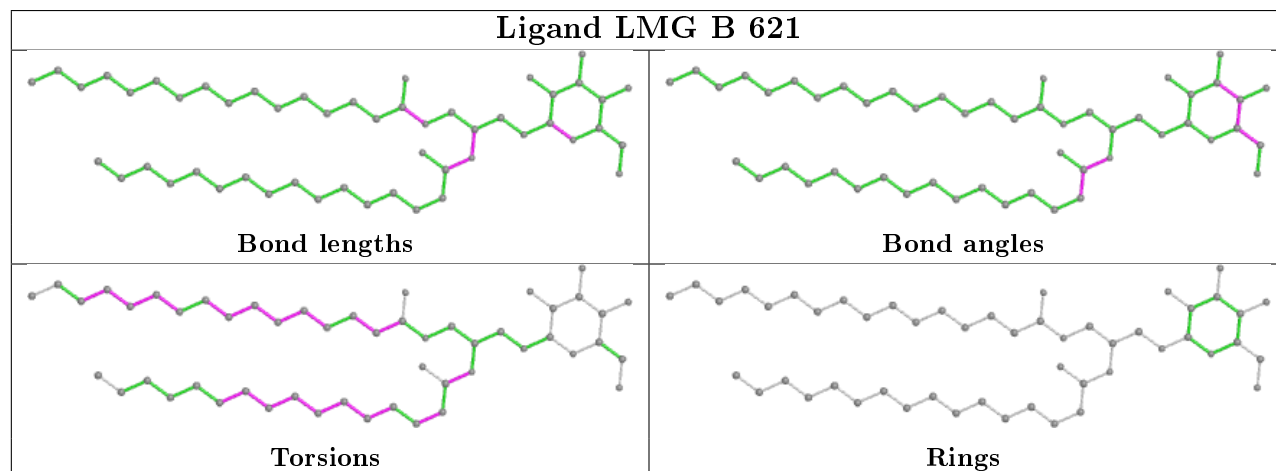


Ligand CLA A 607

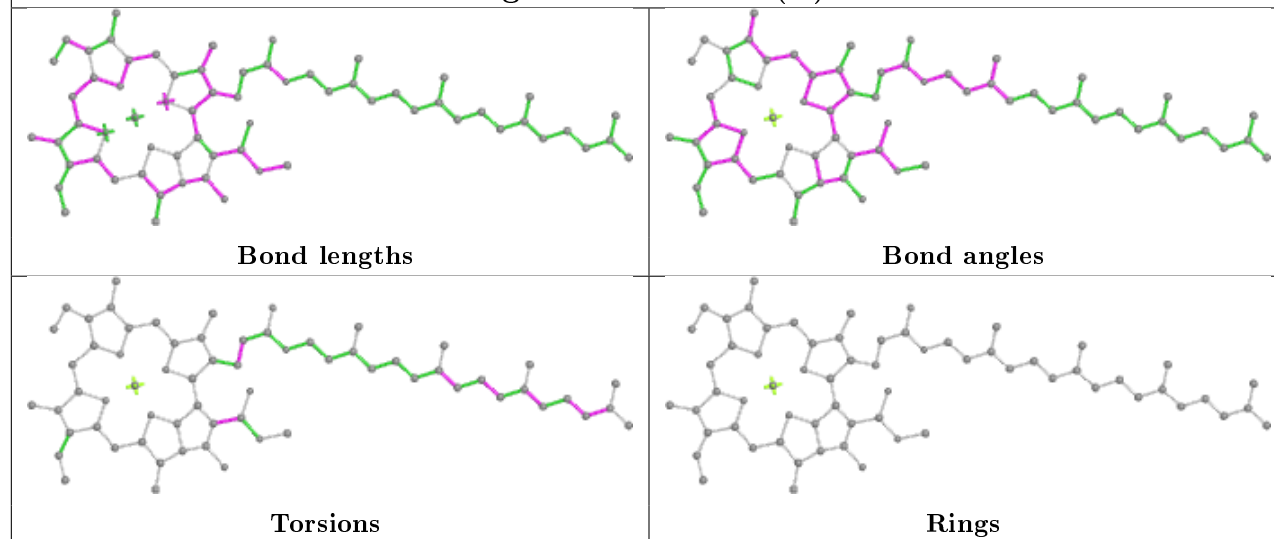


Ligand CLA B 604

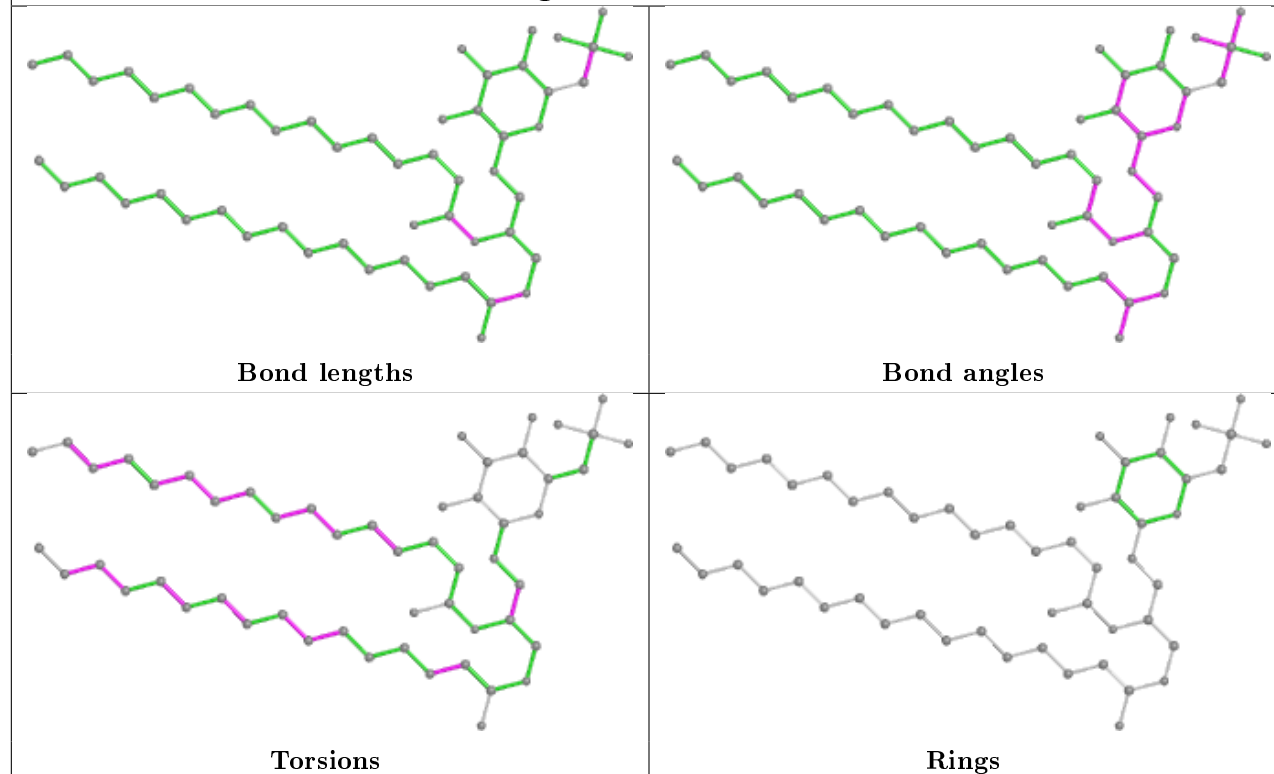


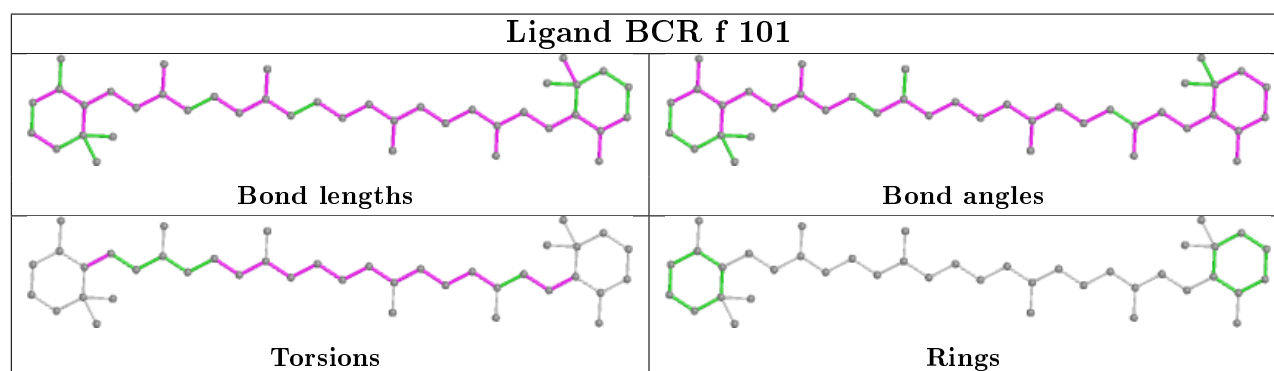
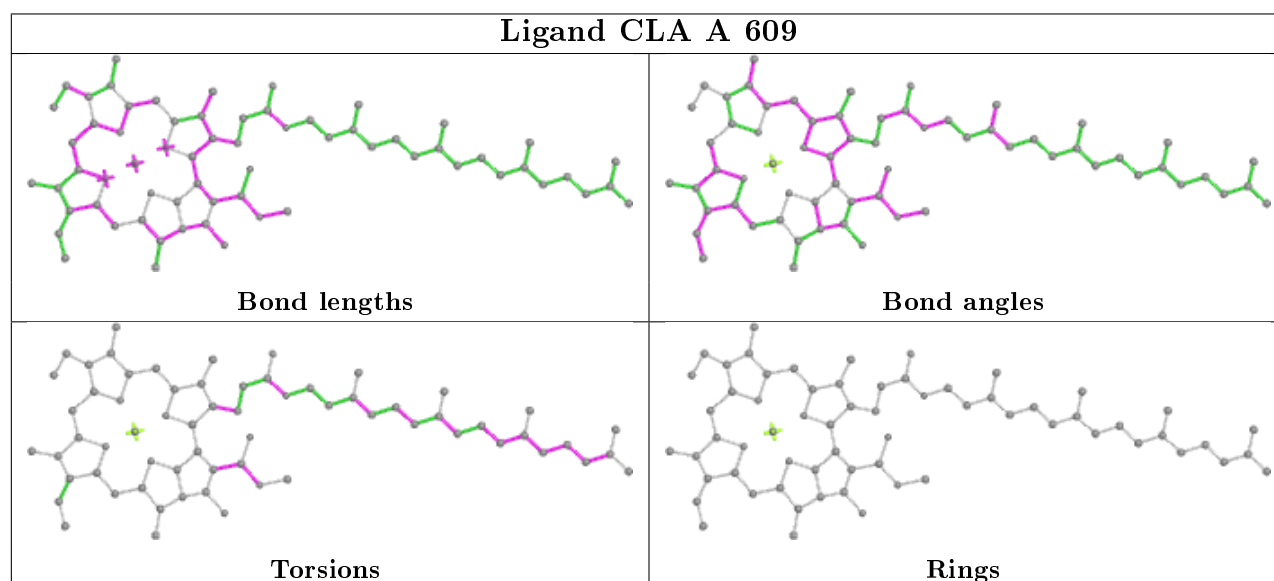
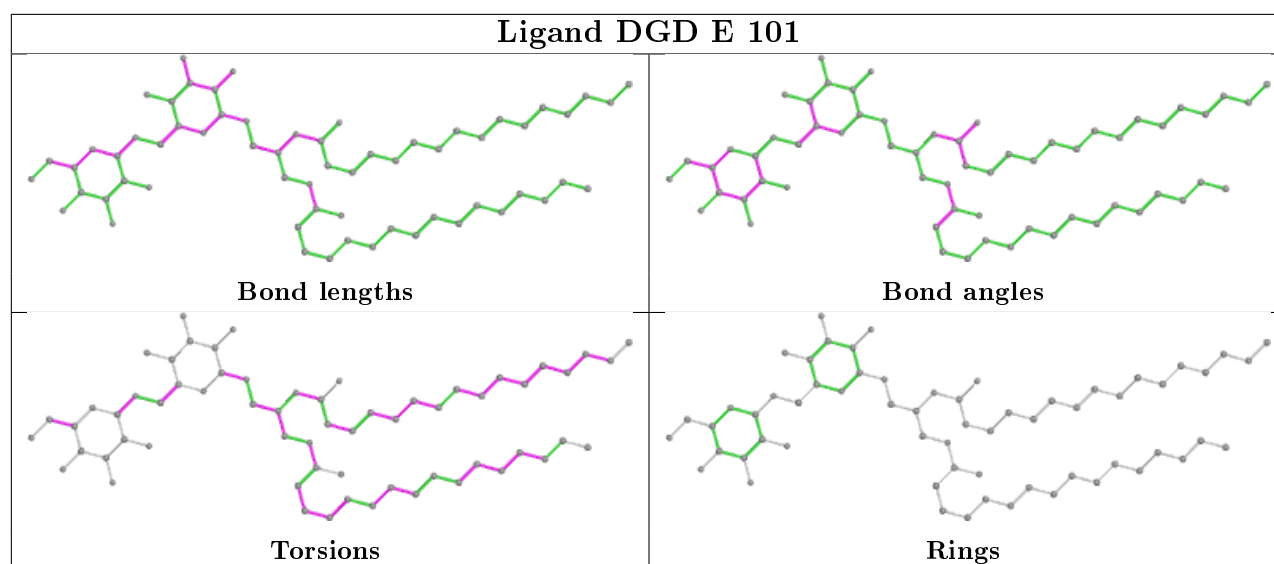
Ligand CLA B 616**Ligand CLA C 509****Ligand LMG B 621**

Ligand CLA b 608 (B)

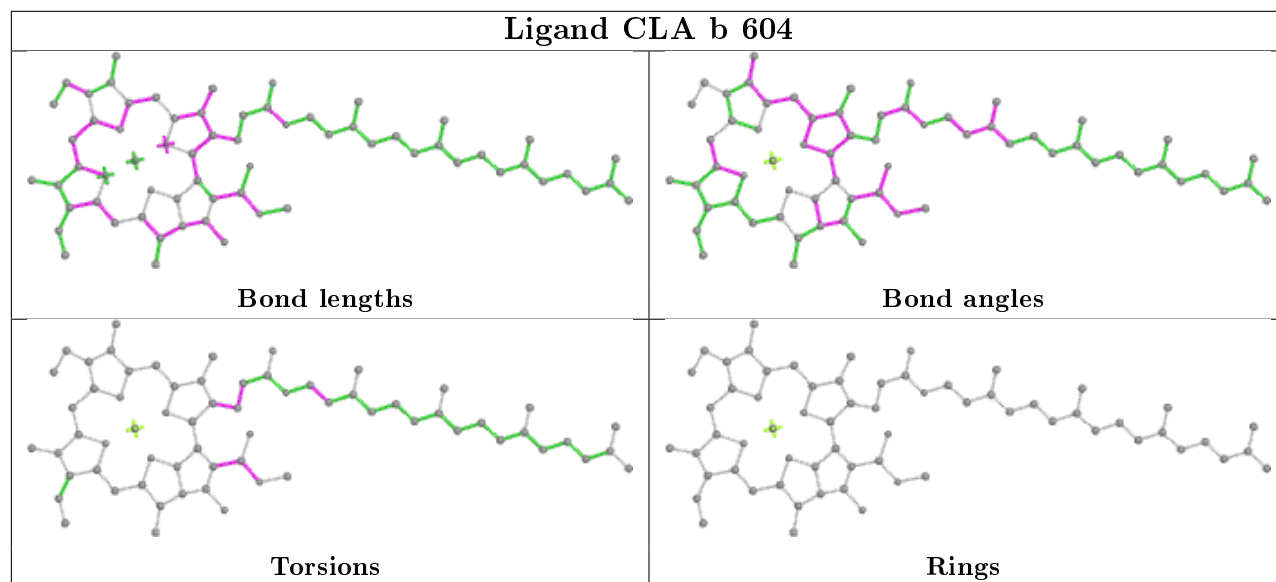


Ligand SQD a 612

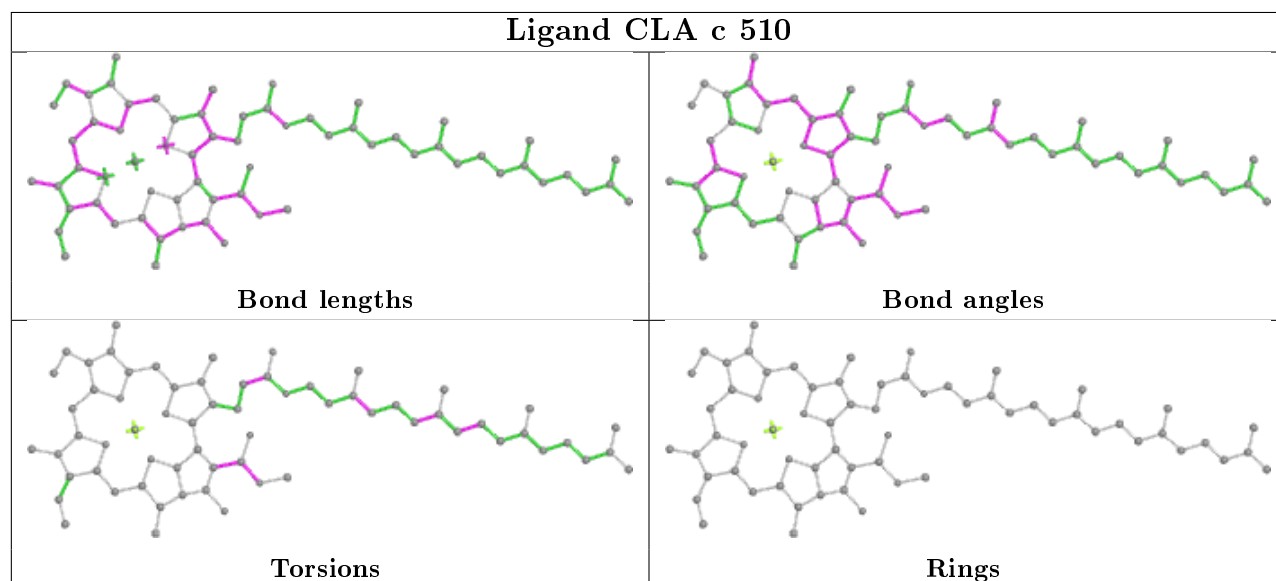




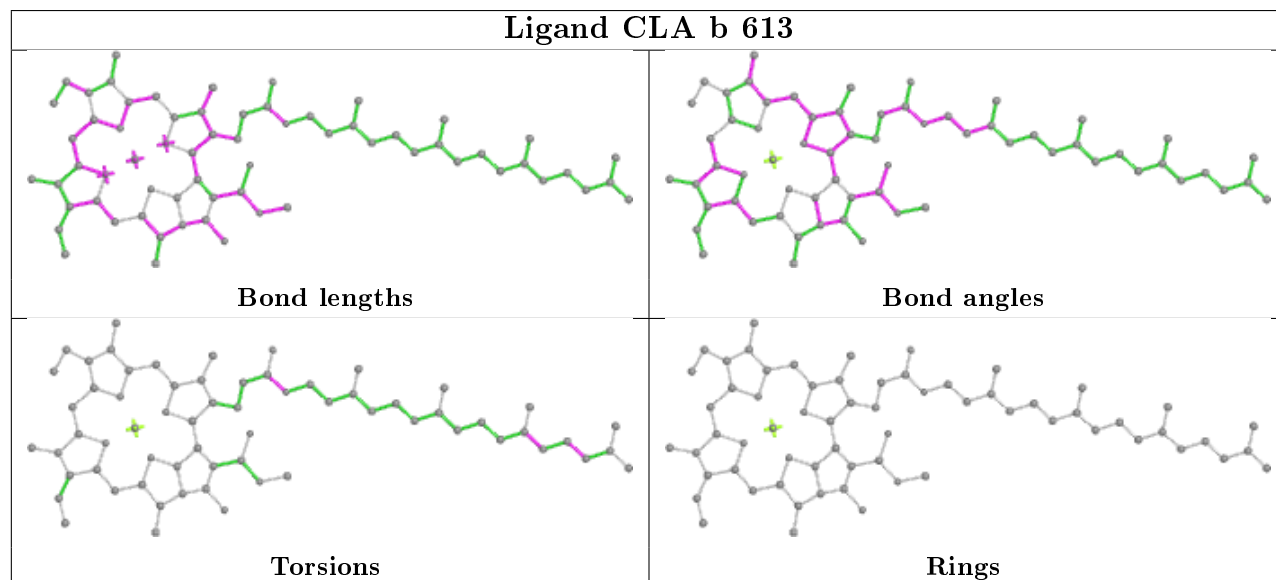
Ligand CLA b 604

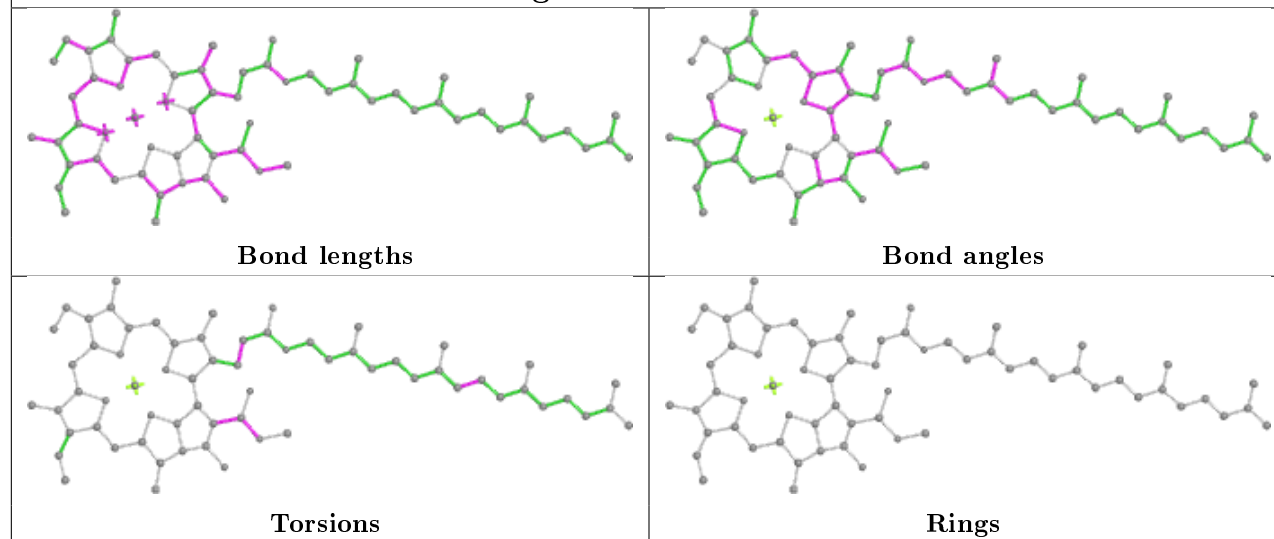
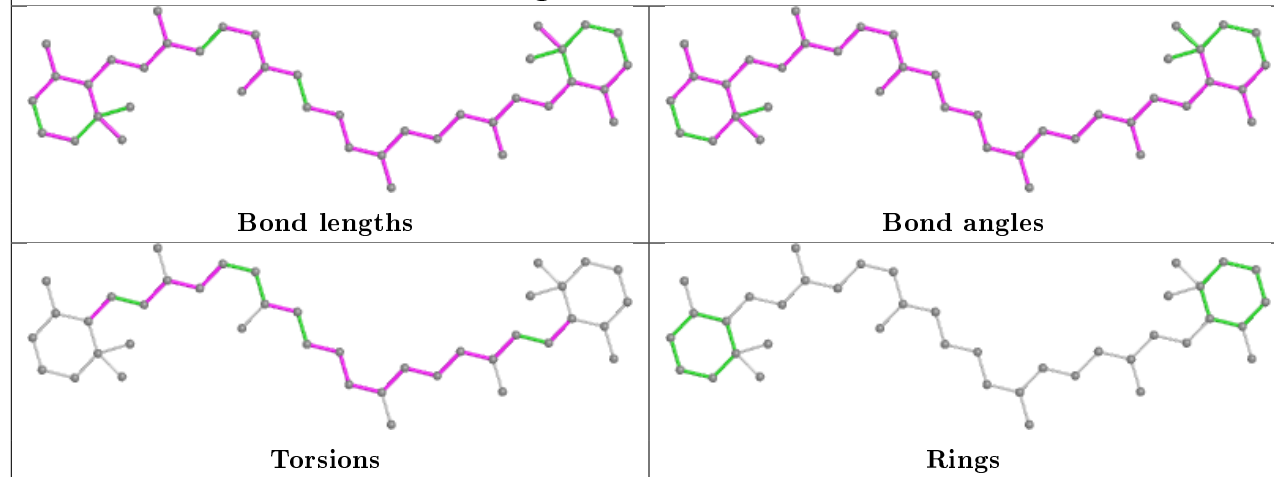


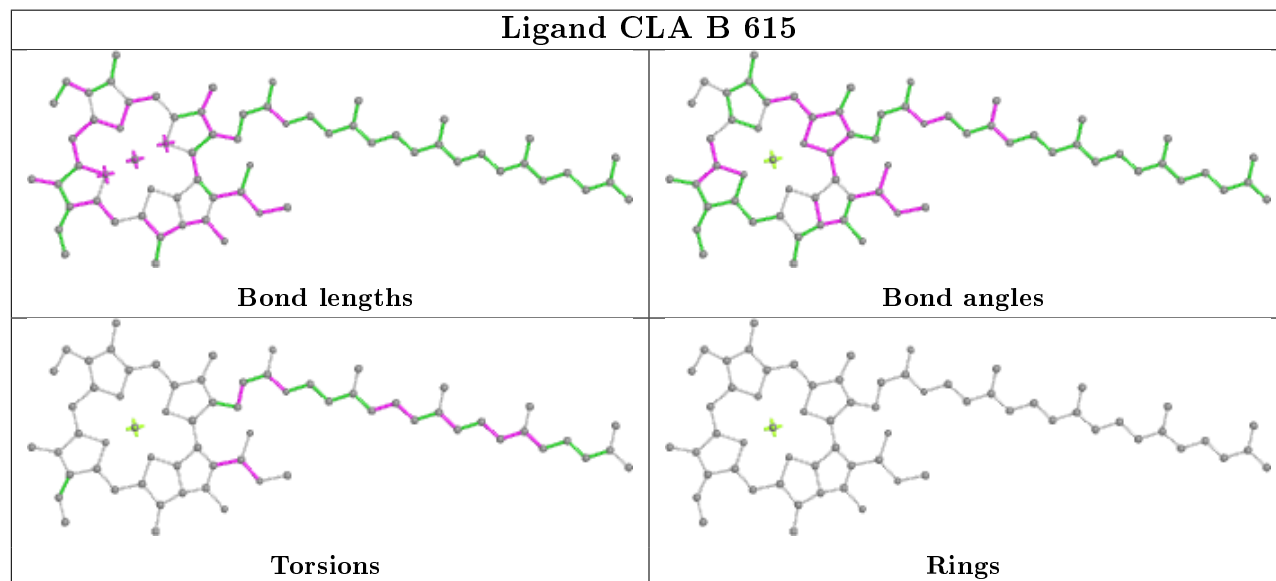
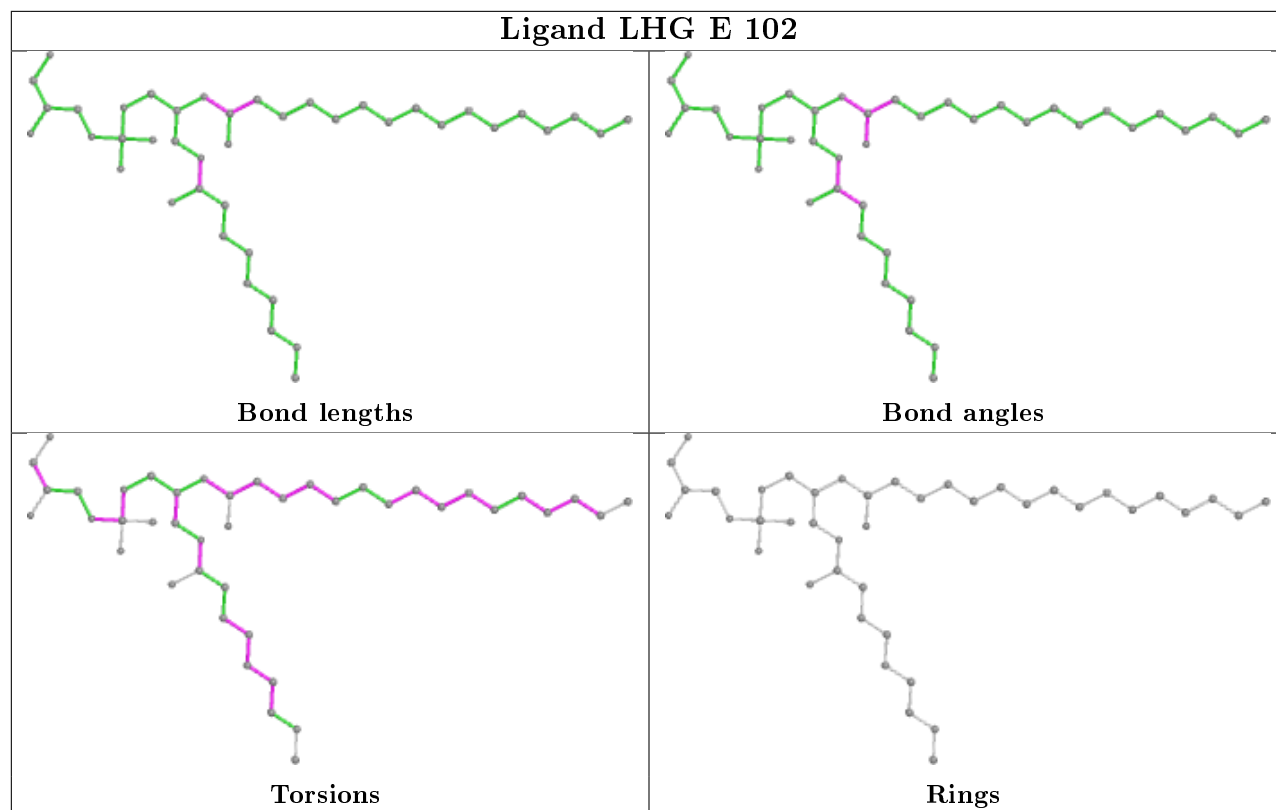
Ligand CLA c 510



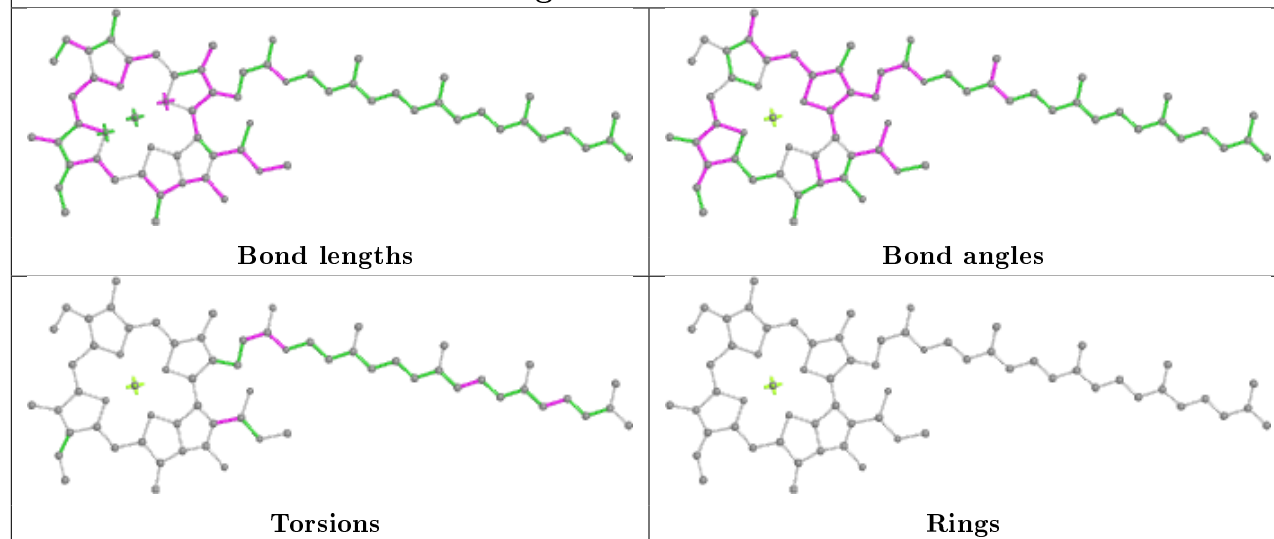
Ligand CLA b 613



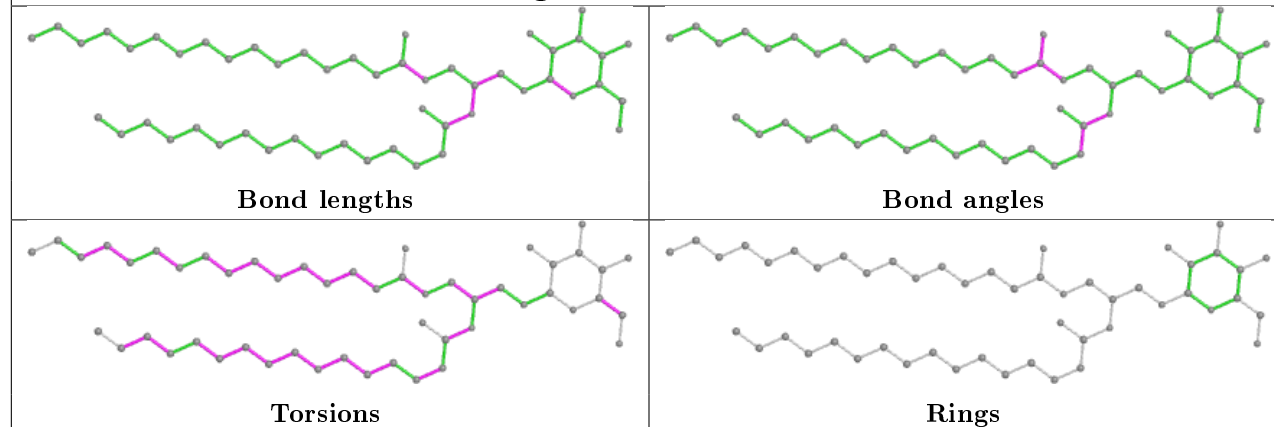
Ligand CLA C 503**Ligand BCR b 621**



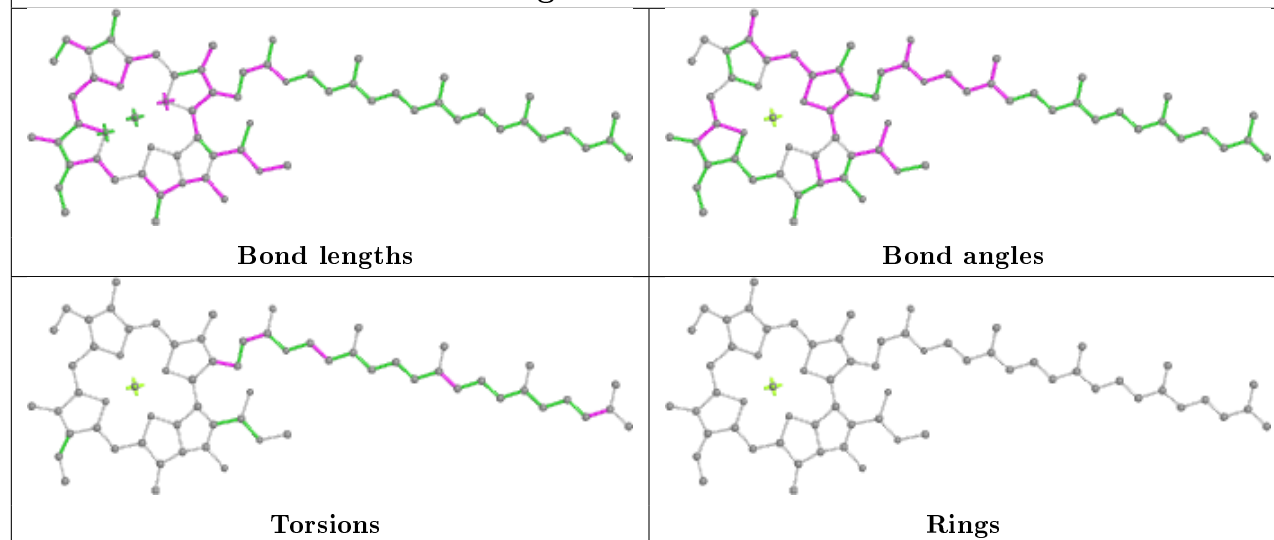
Ligand CLA b 614

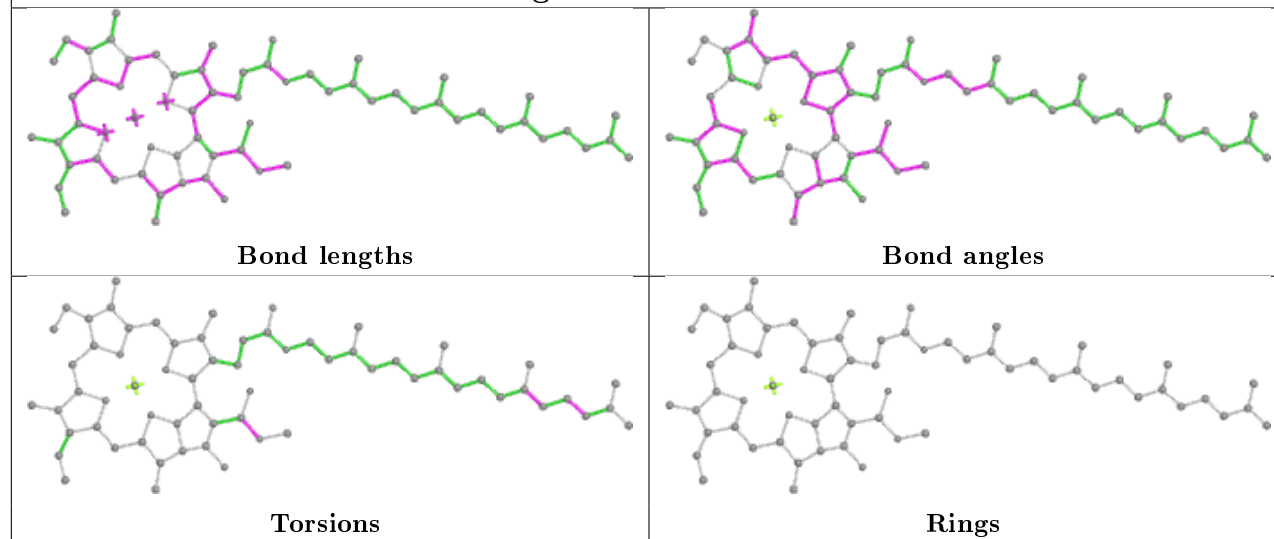
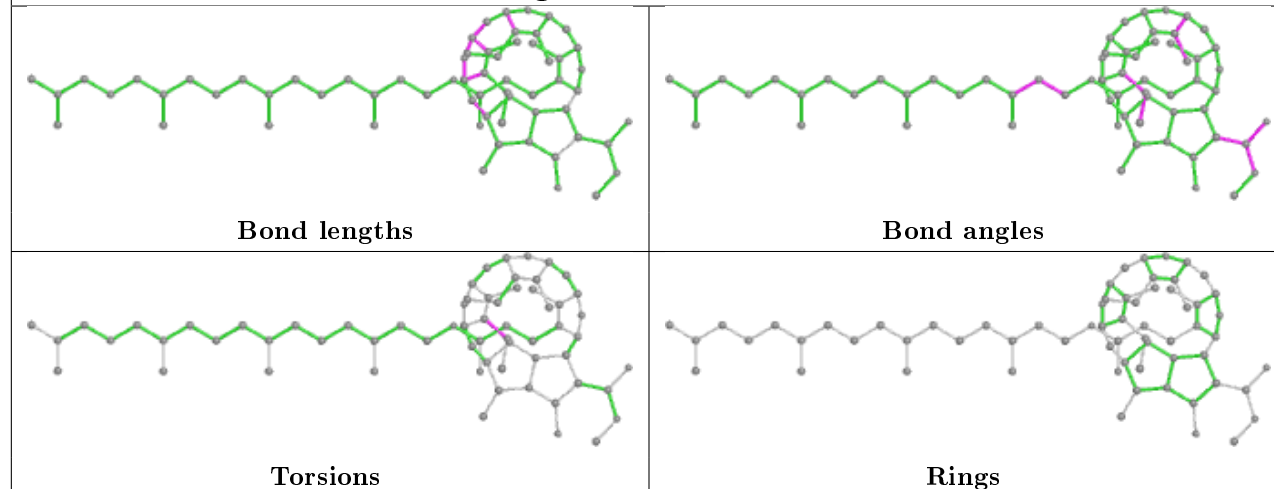
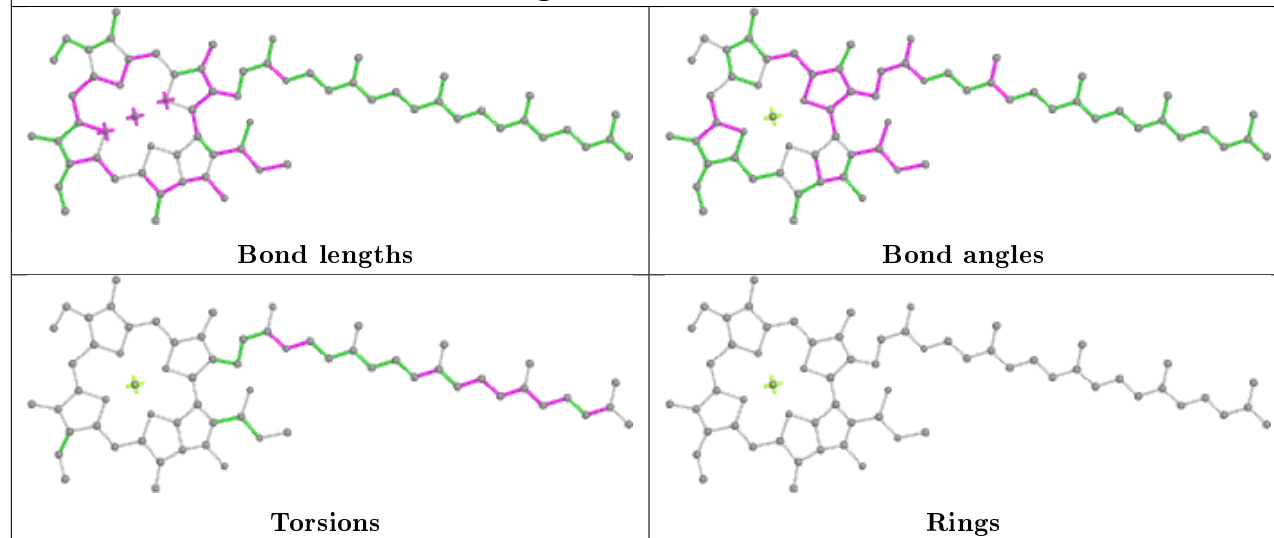


Ligand LMG a 613

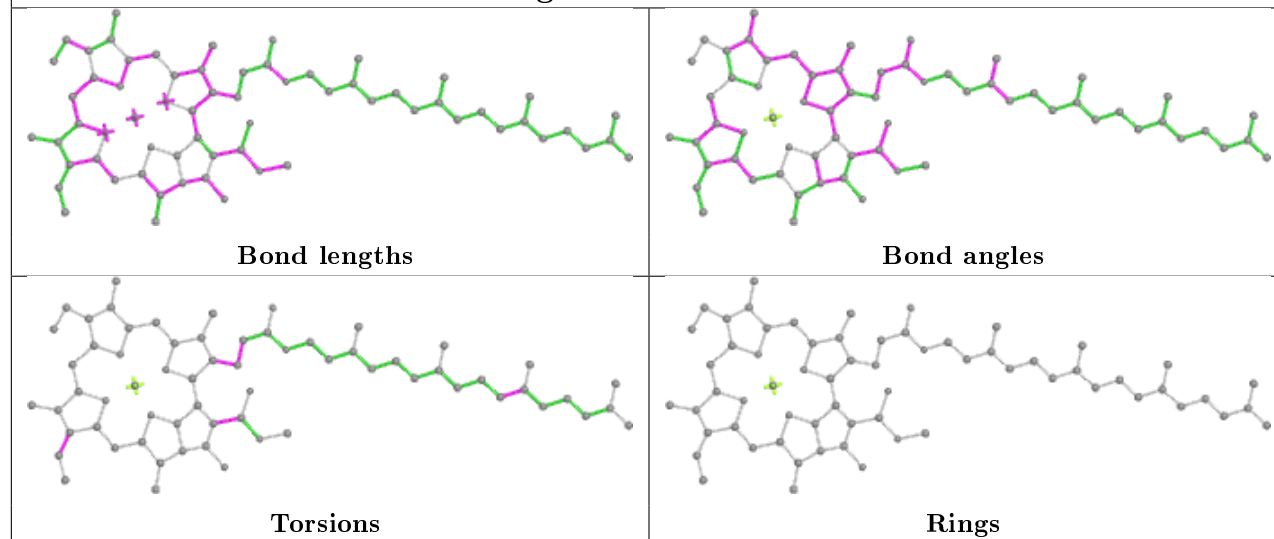


Ligand CLA c 512

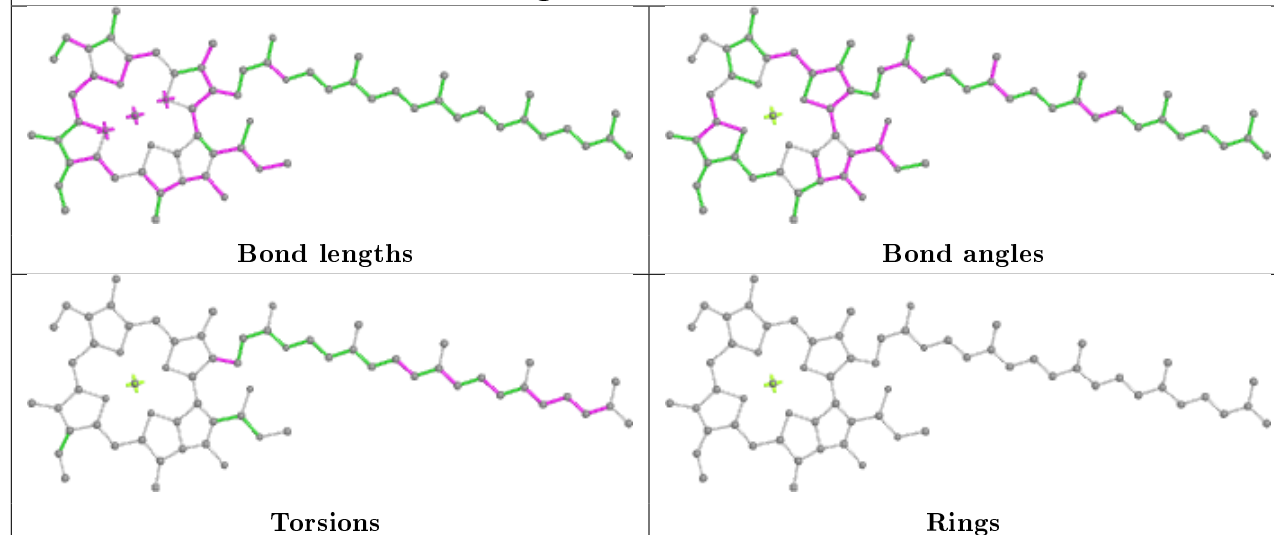


Ligand CLA B 612**Ligand PHO d 401****Ligand CLA b 618**

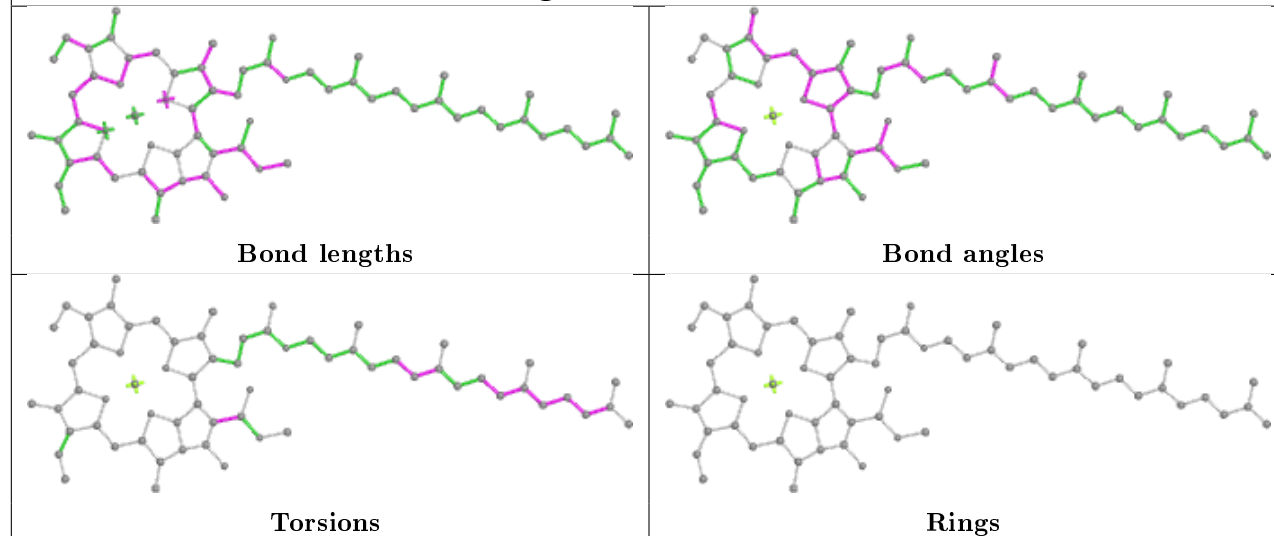
Ligand CLA a 615



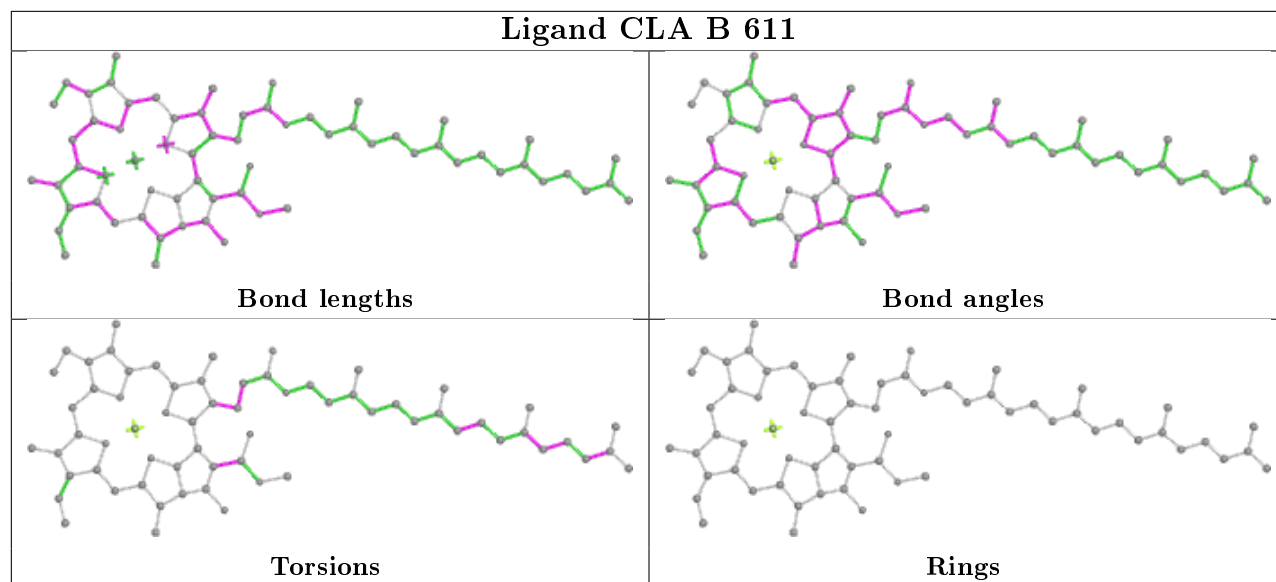
Ligand CLA b 617



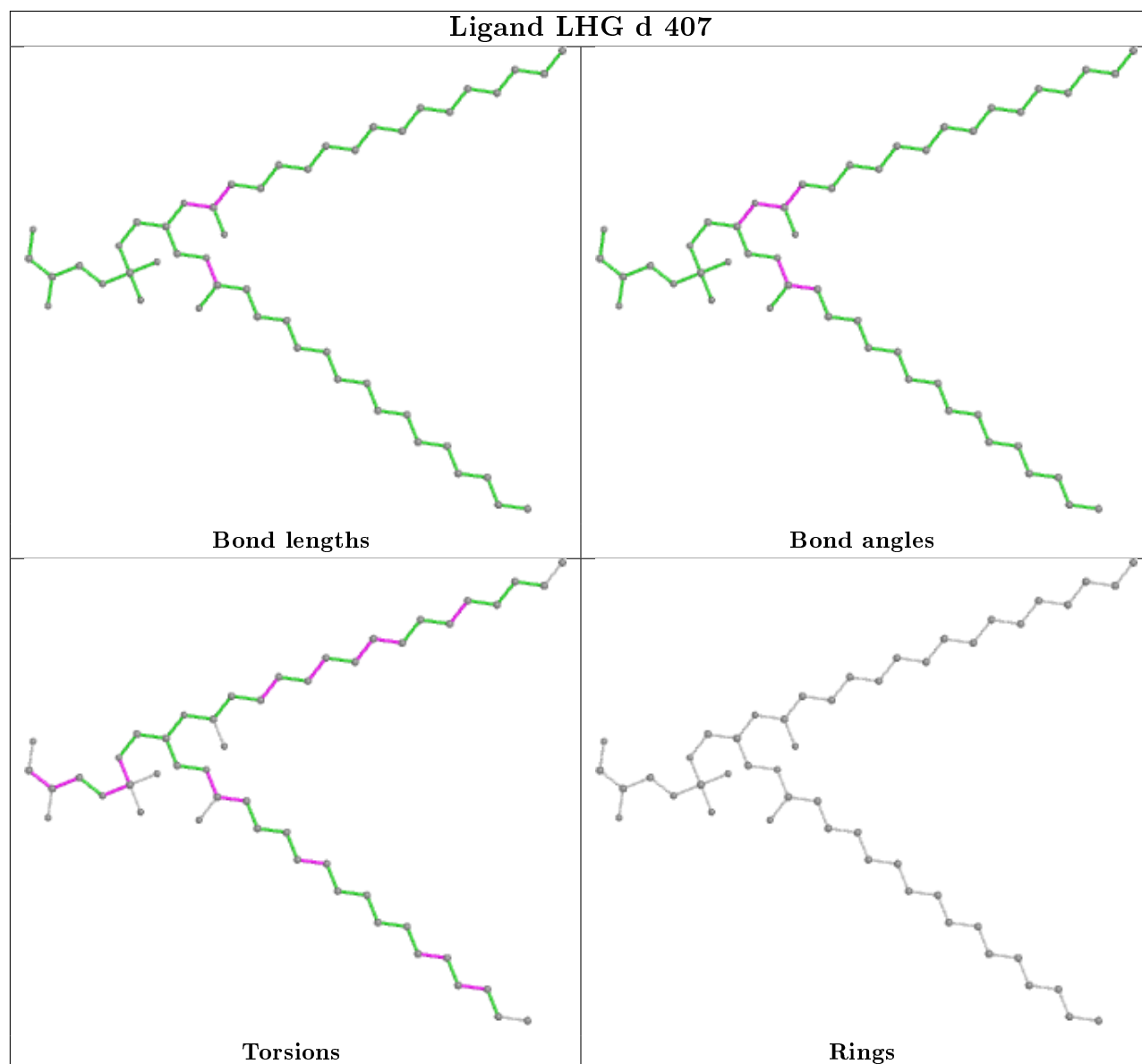
Ligand CLA c 506

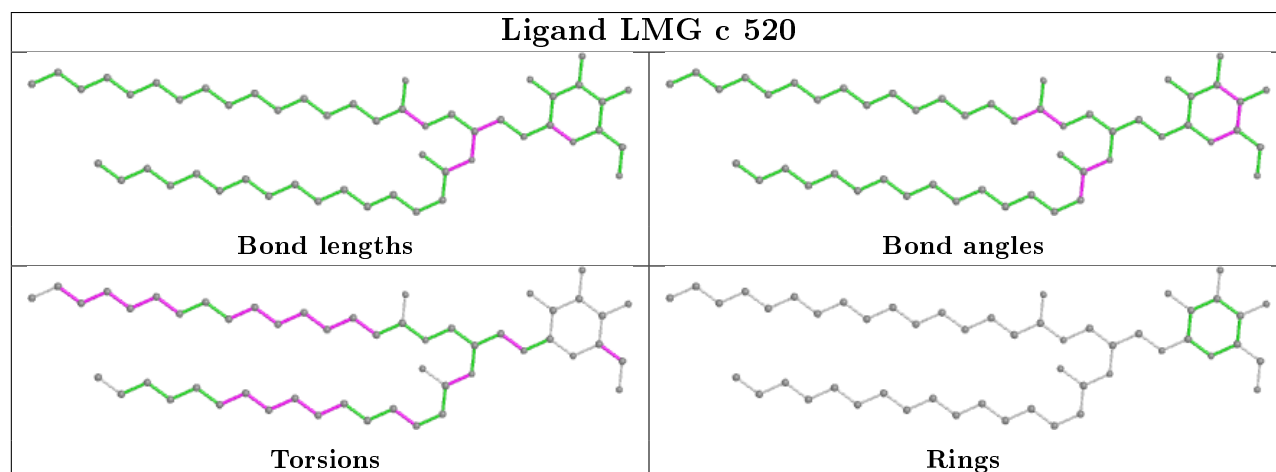
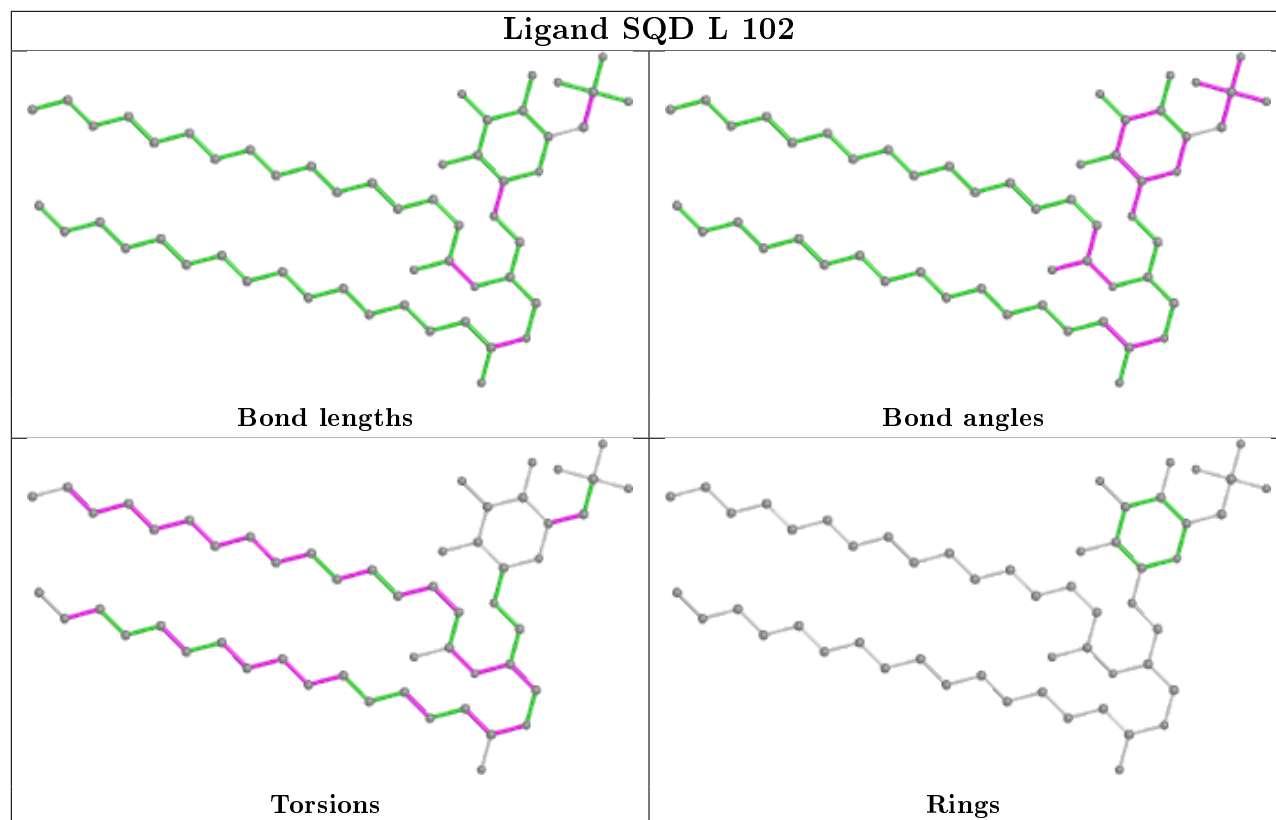


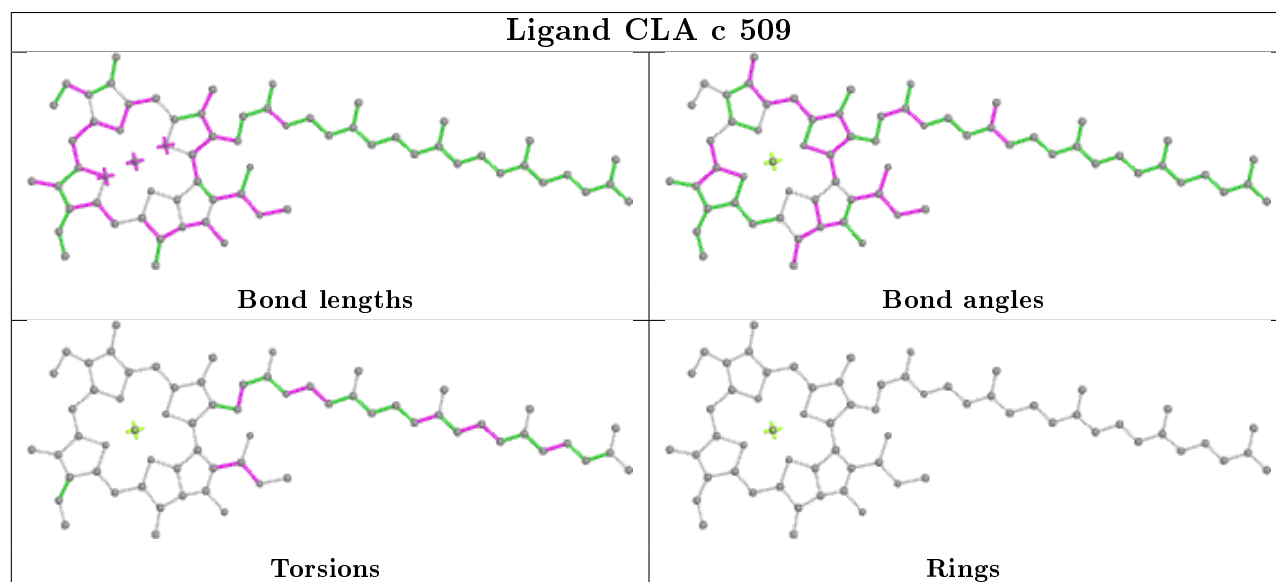
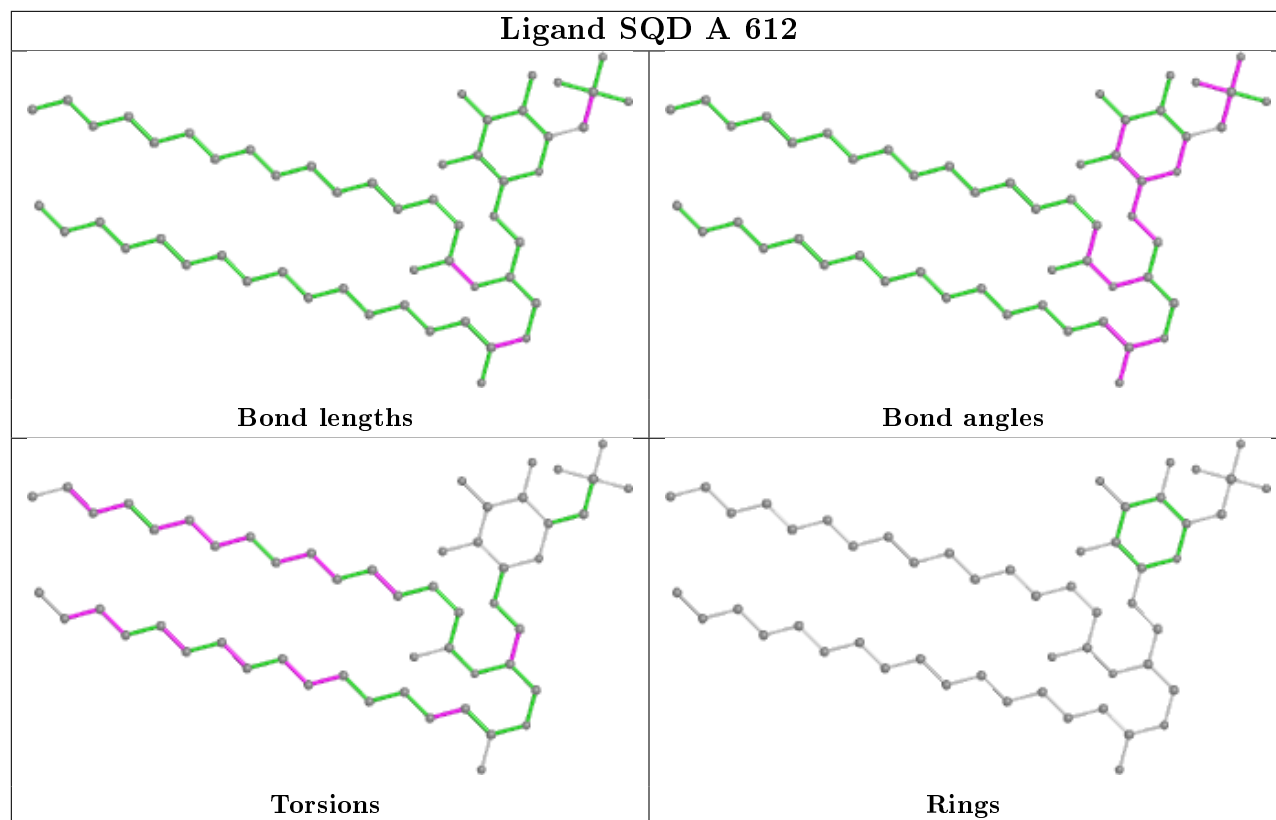
Ligand CLA B 611



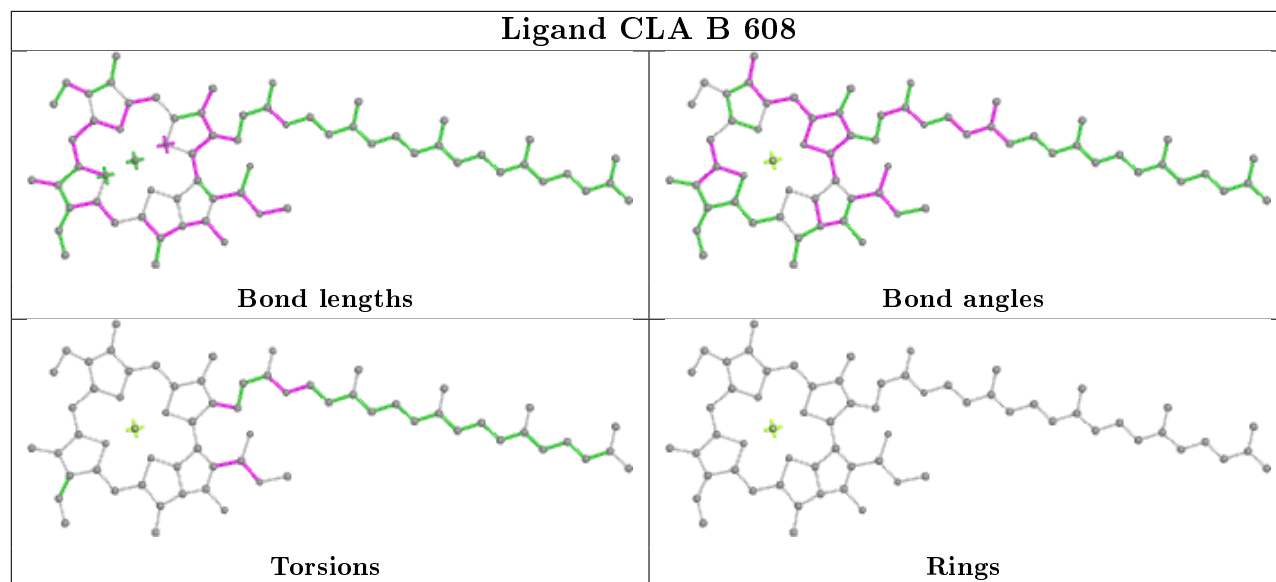
Ligand LHG d 407



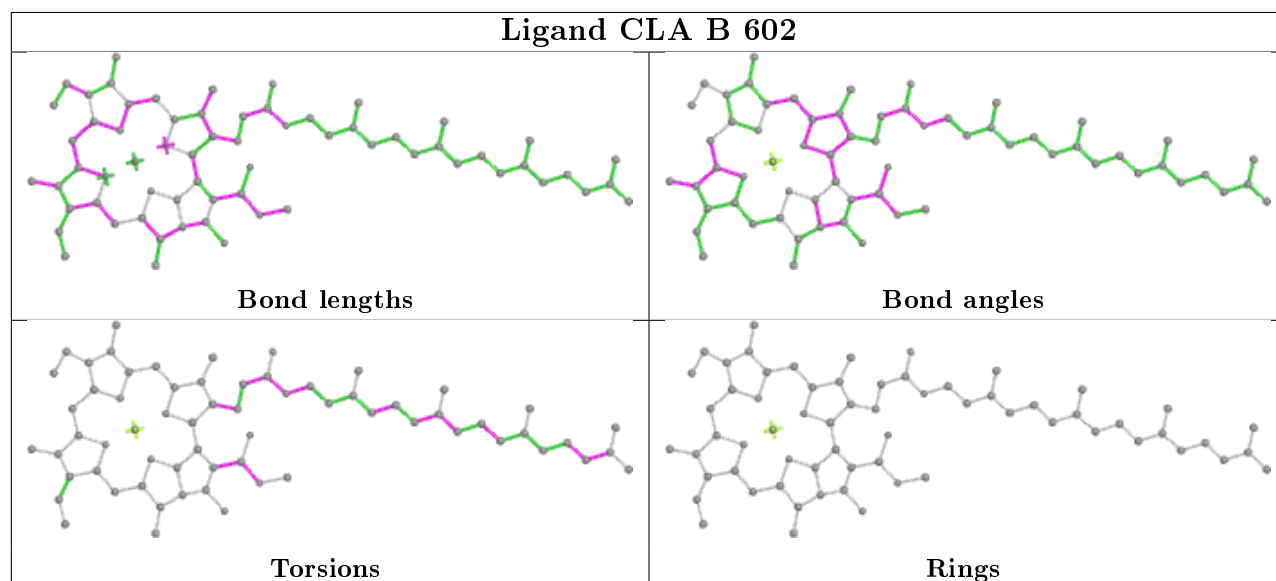




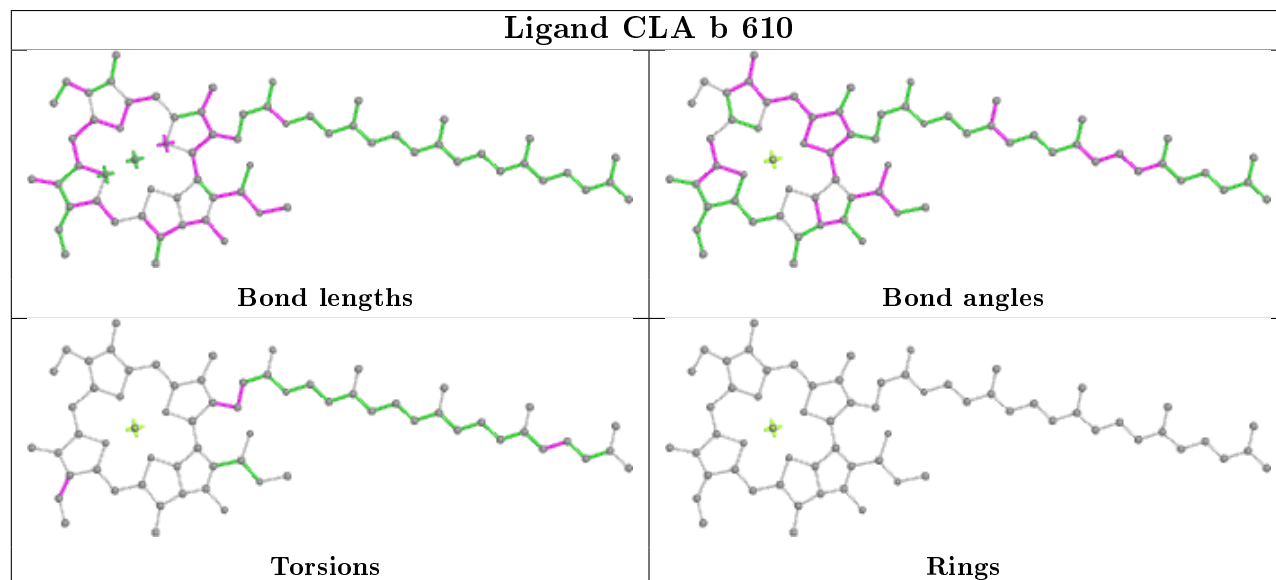
Ligand CLA B 608

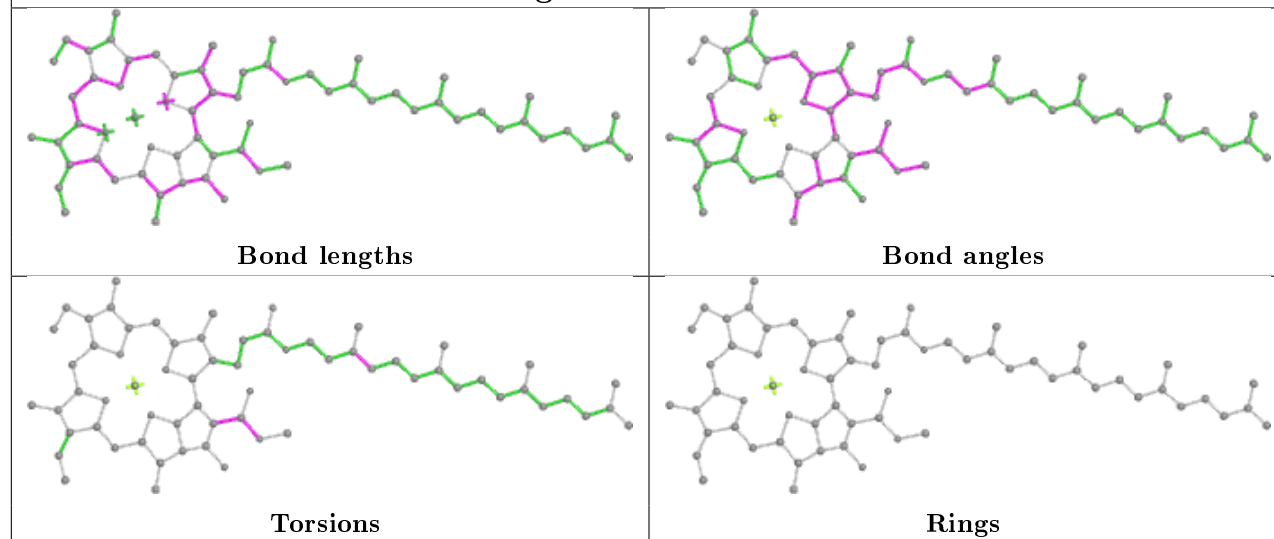
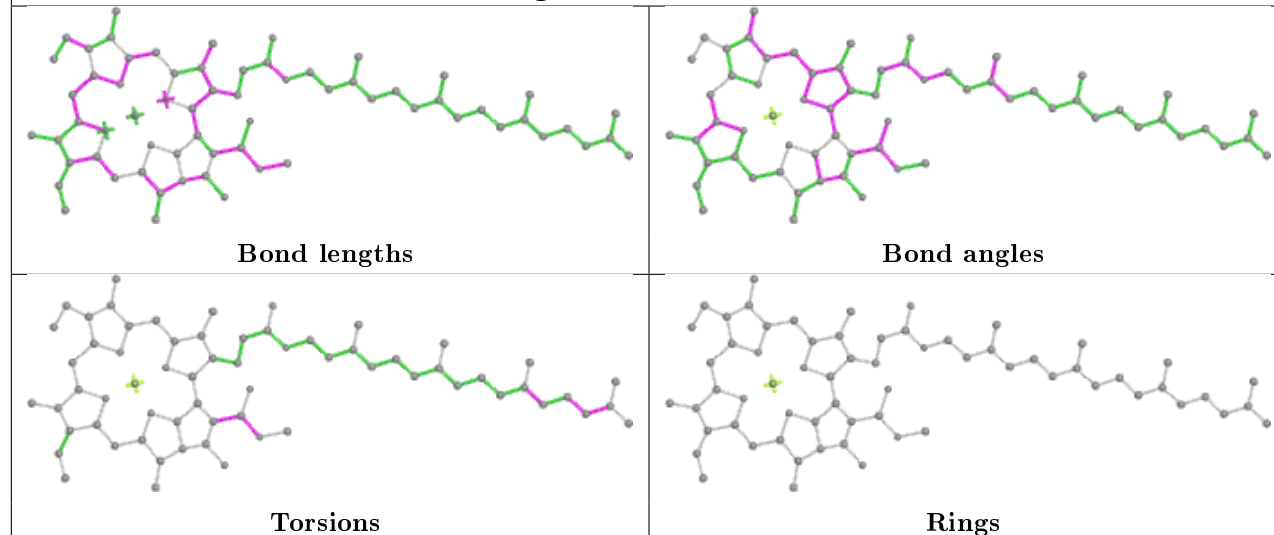
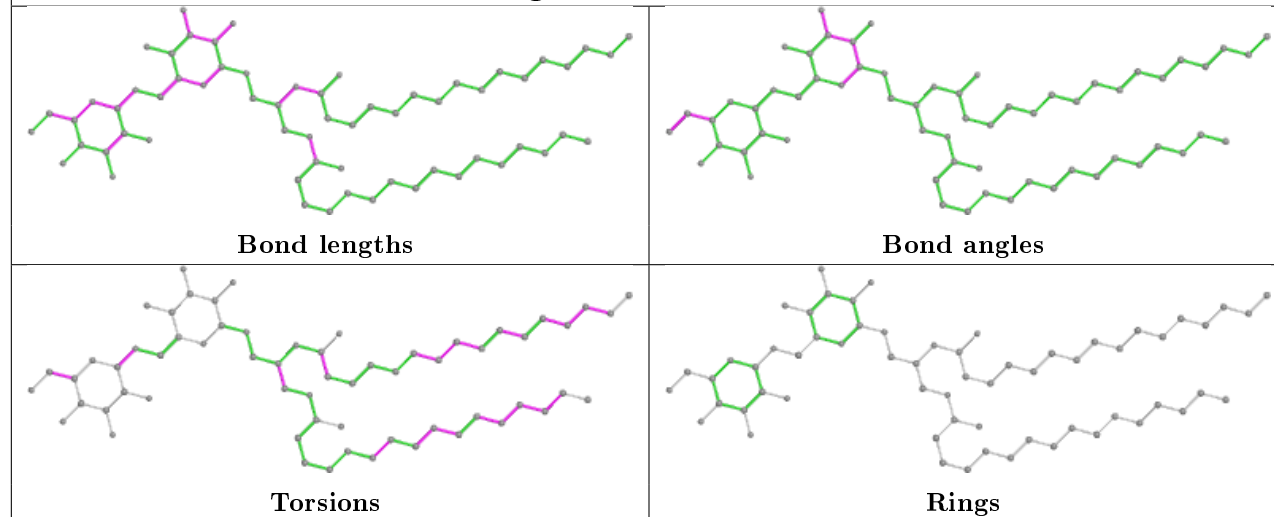


Ligand CLA B 602



Ligand CLA b 610



Ligand CLA b 611**Ligand CLA C 502****Ligand DGD H 102**

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

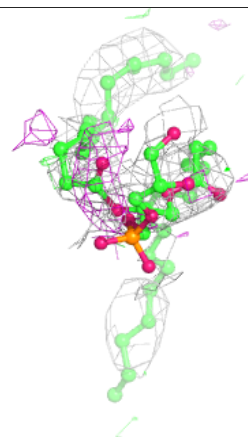
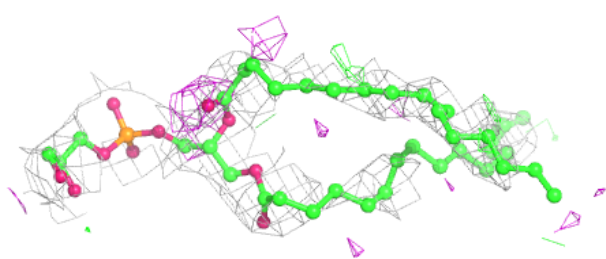
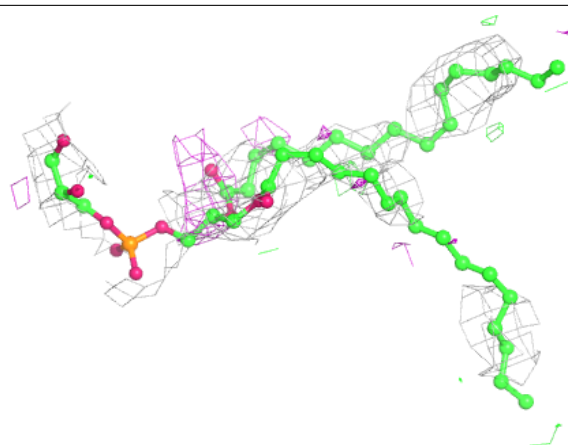
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

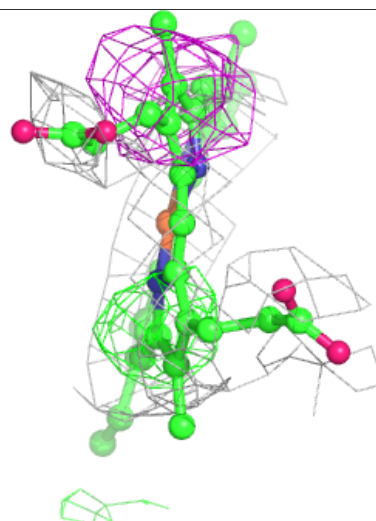
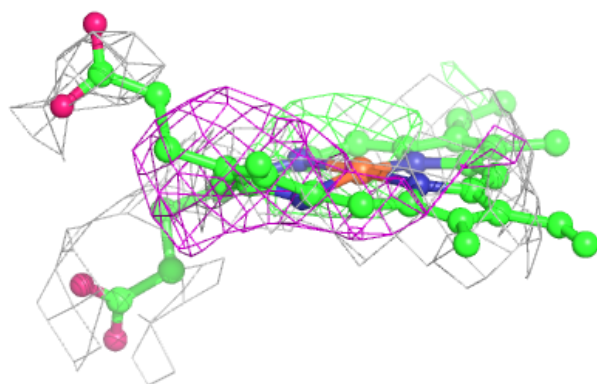
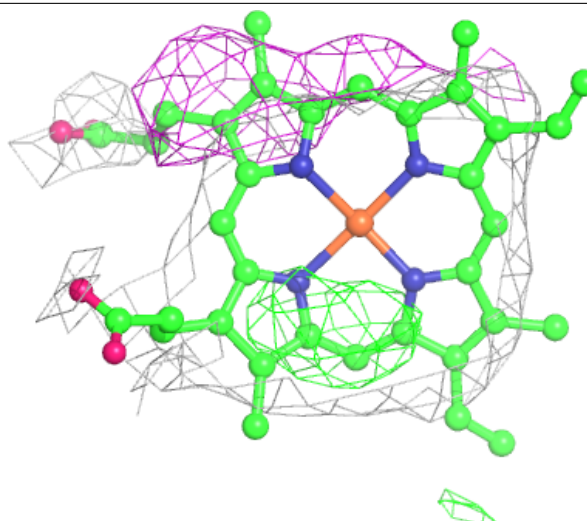
Electron density around LHG D 407:

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



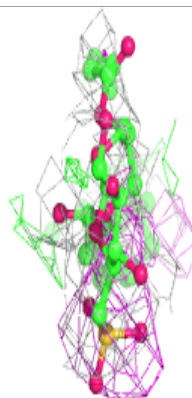
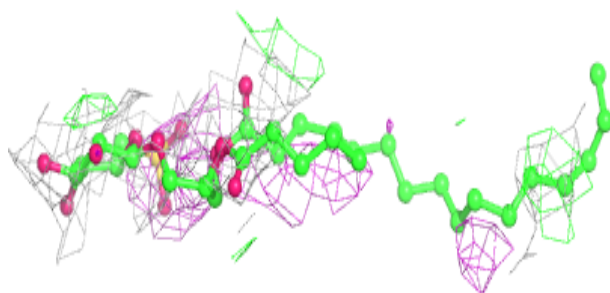
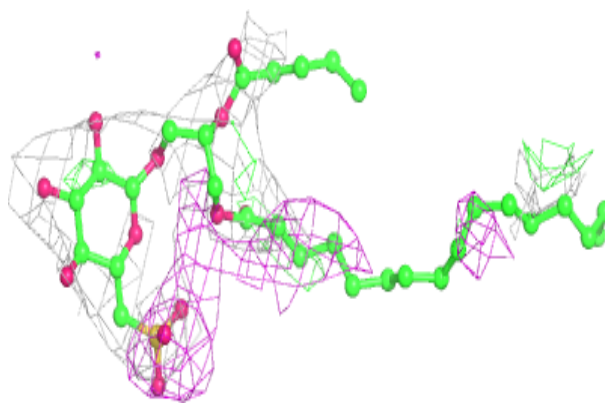
Electron density around HEM e 102:

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

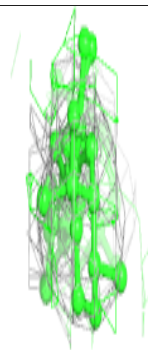
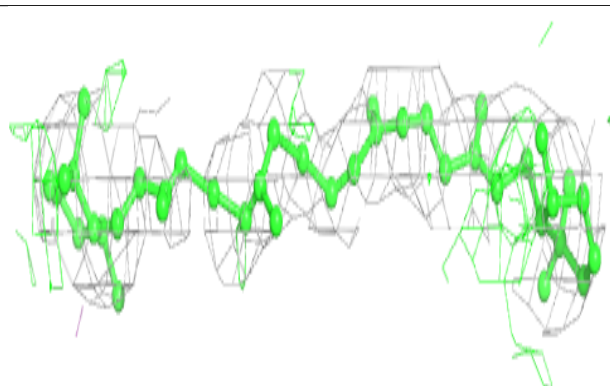
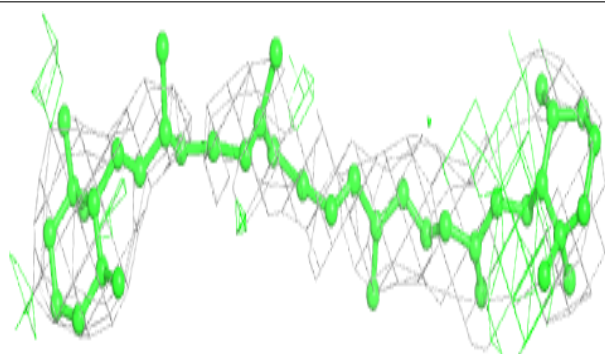


Electron density around SQD x 101:

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

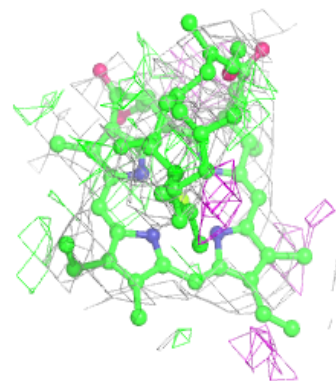
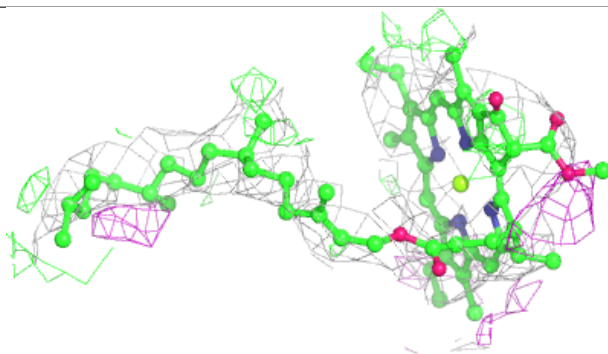
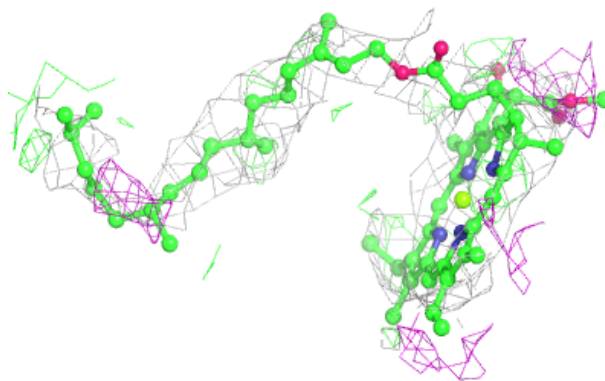
**Electron density around BCR B 620:**

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

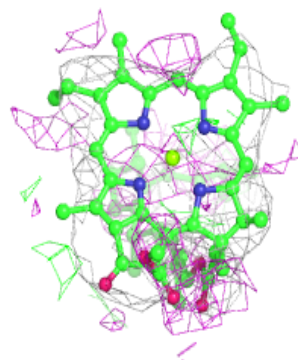
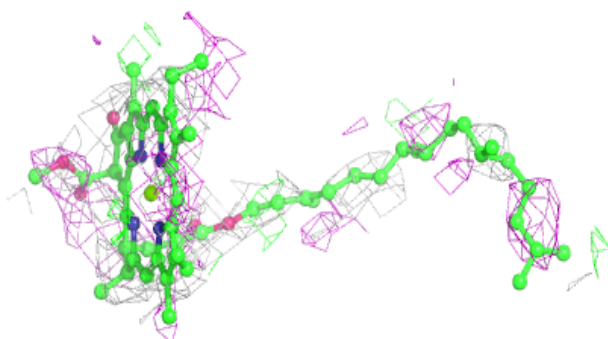
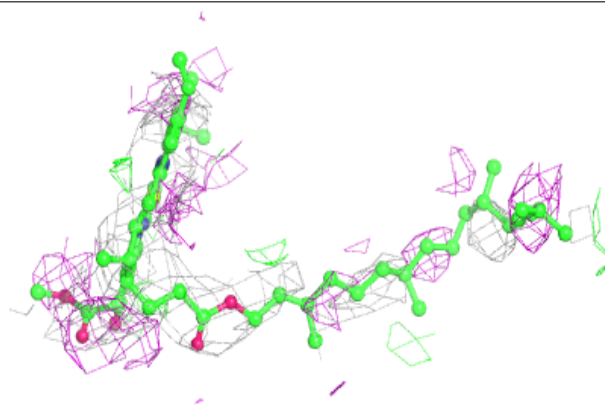


Electron density around CLA C 508:

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

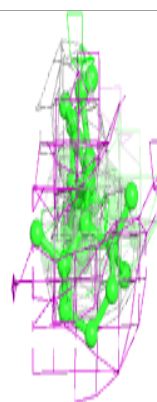
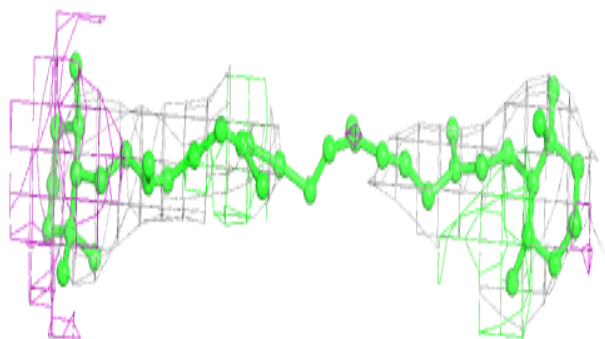
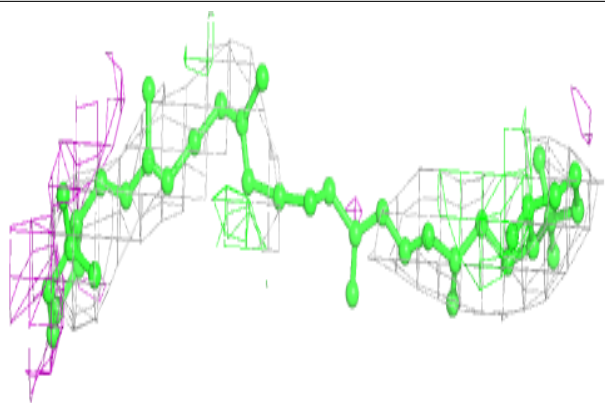
**Electron density around CLA b 607:**

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

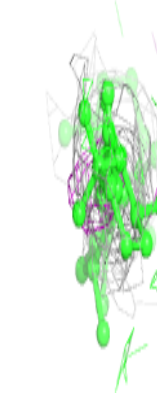
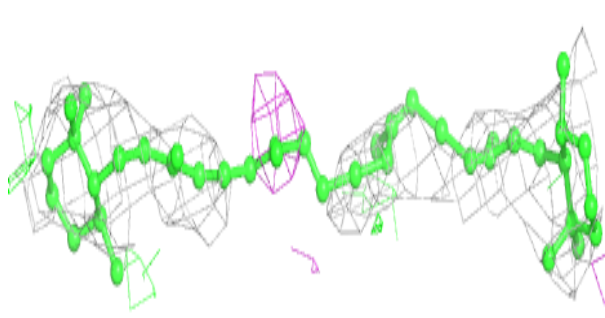
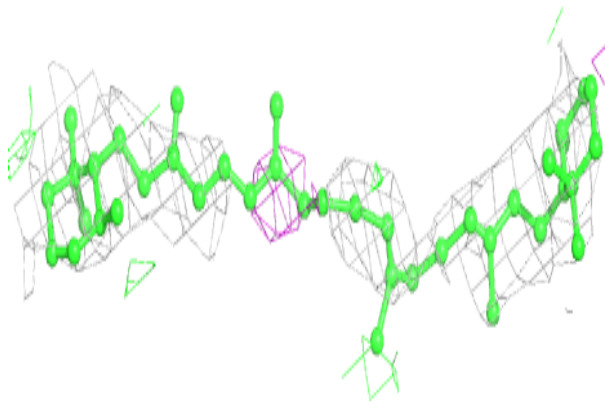


Electron density around BCR I 101:

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

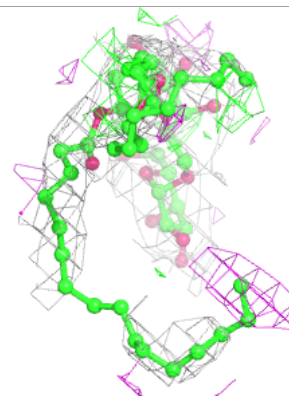
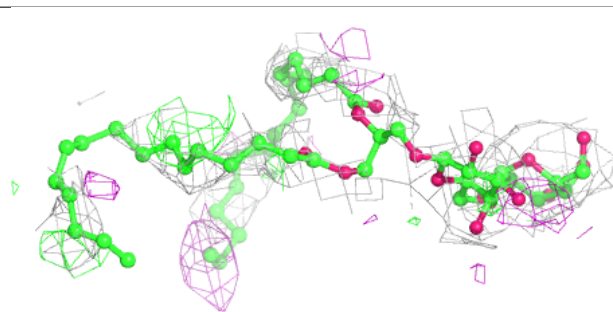
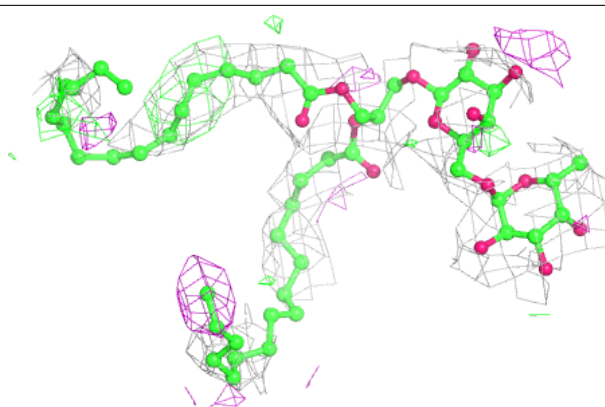
**Electron density around BCR c 515:**

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

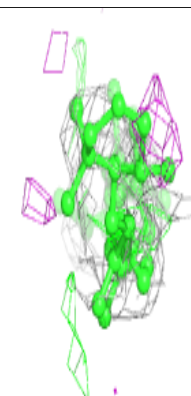
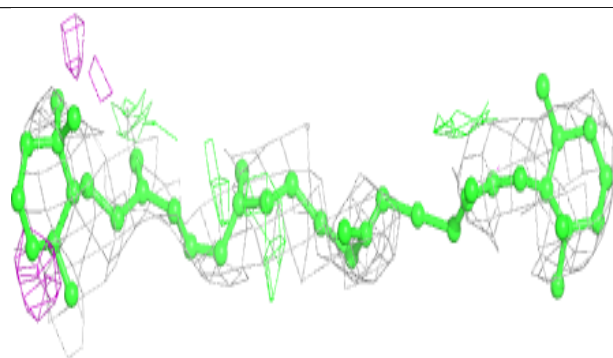
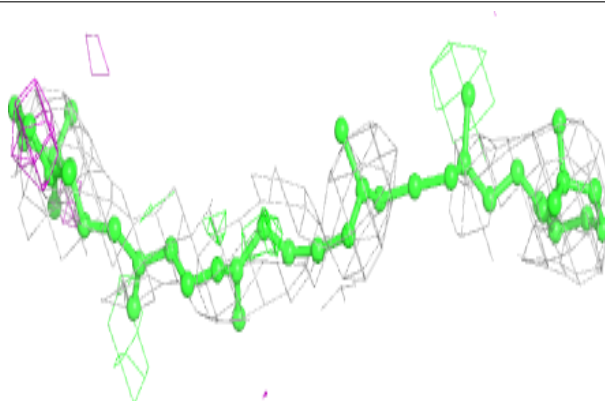


Electron density around DGD C 516:

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

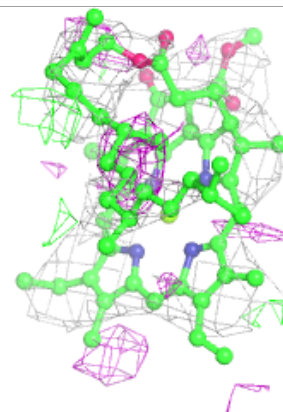
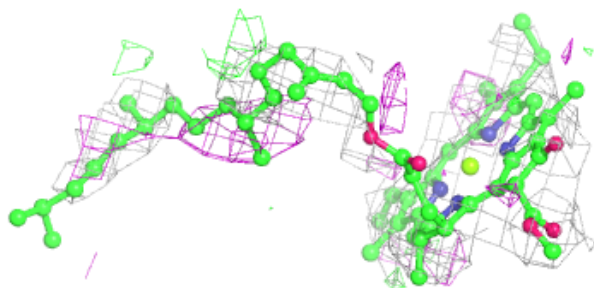
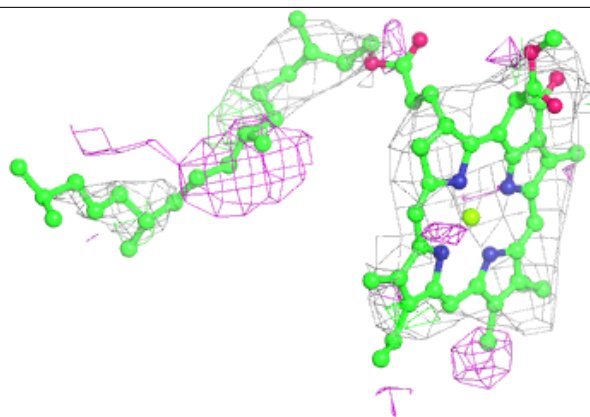
**Electron density around BCR h 101:**

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

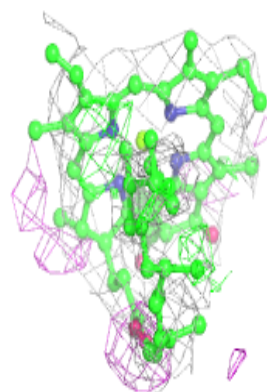
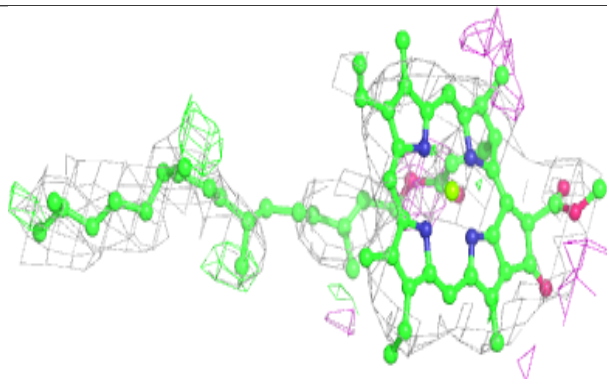
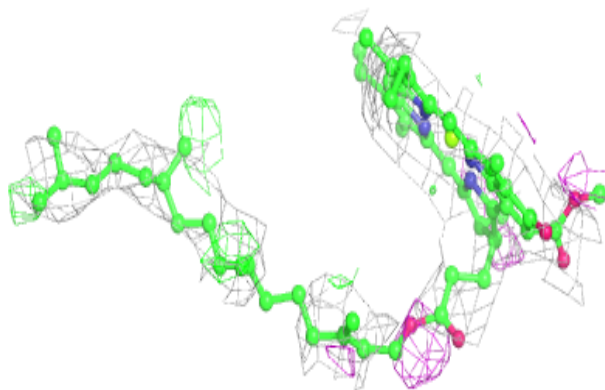


Electron density around CLA c 511:

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

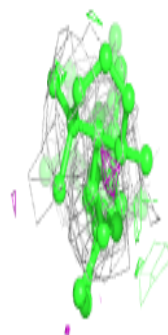
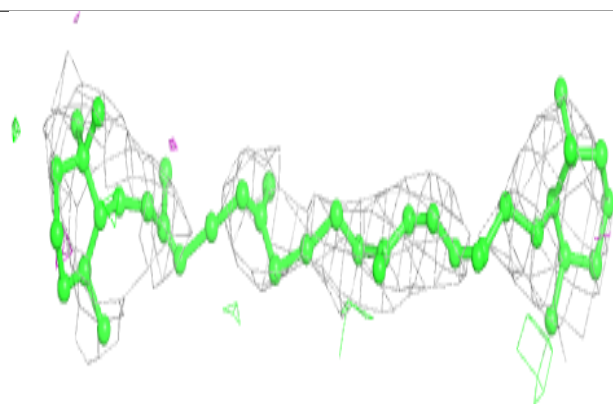
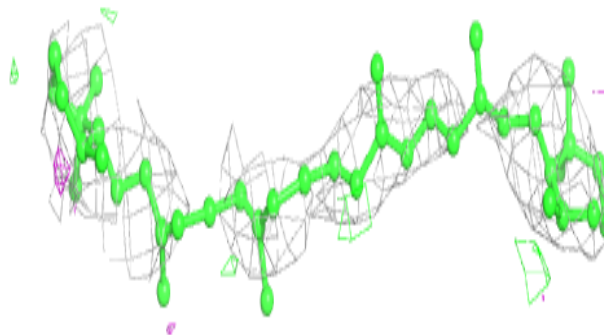
**Electron density around CLA c 504:**

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



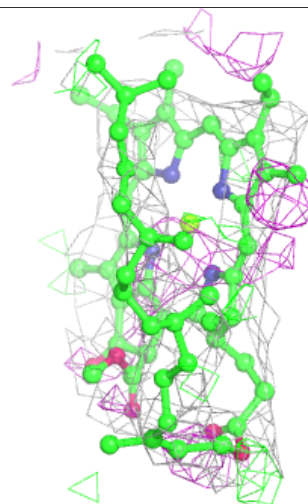
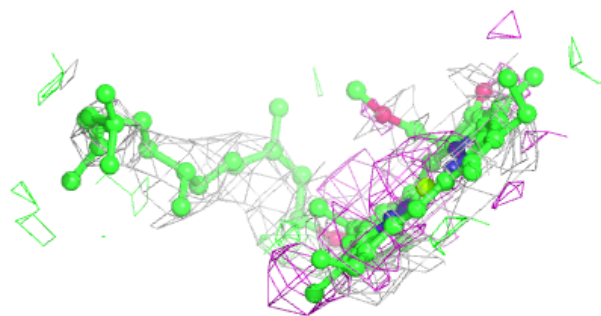
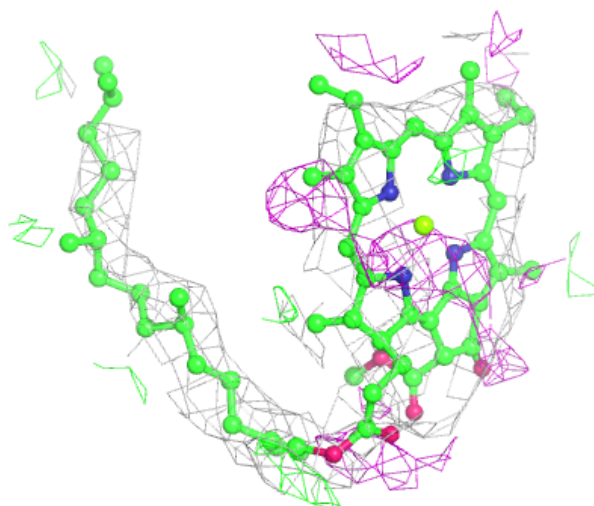
Electron density around BCR c 514:

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



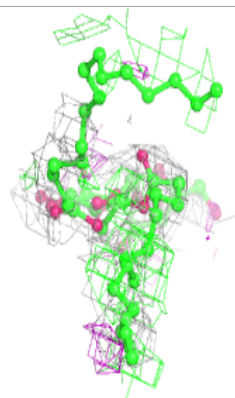
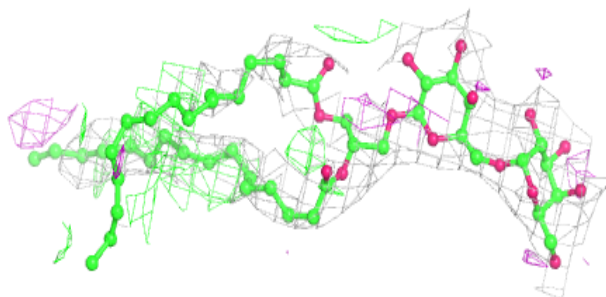
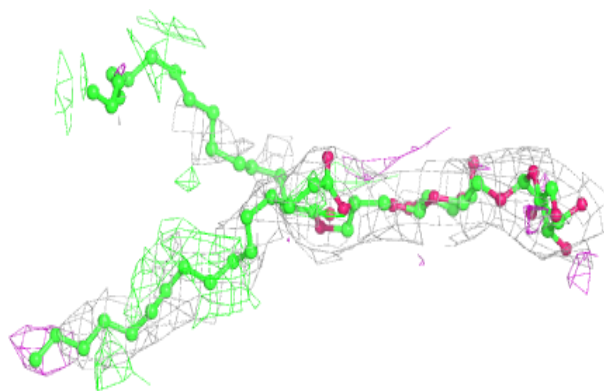
Electron density around CLA B 617:

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

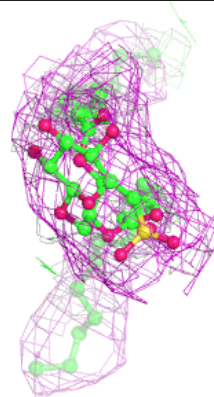
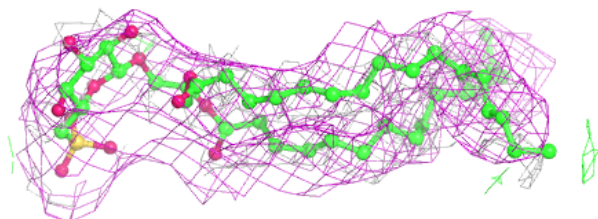
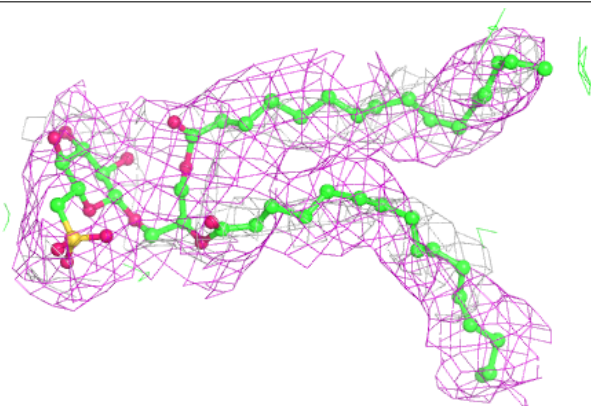


Electron density around DGD C 515:

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

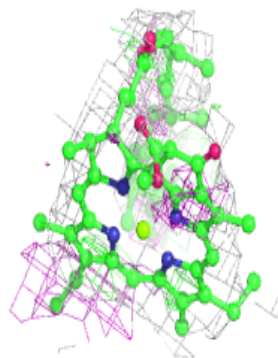
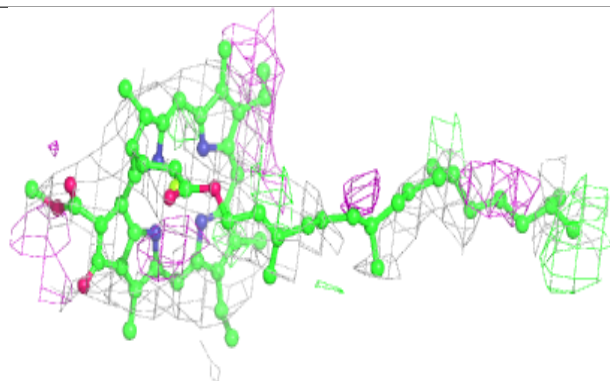
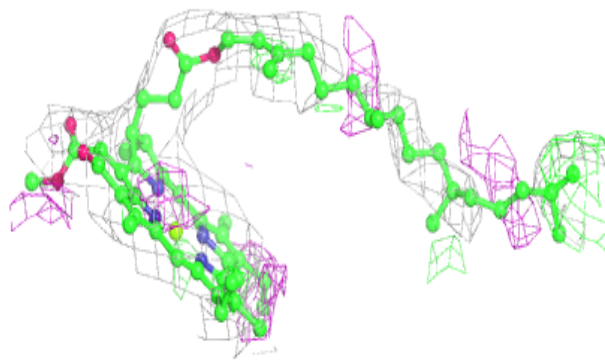
**Electron density around SQD I 101:**

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



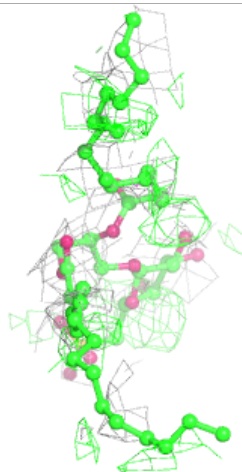
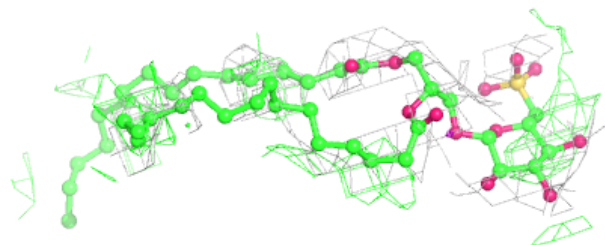
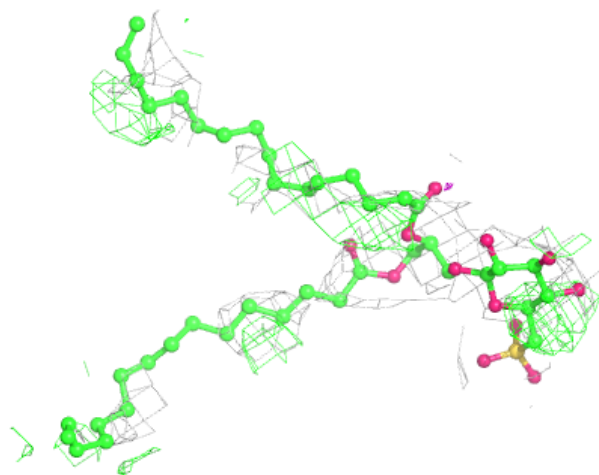
Electron density around CLA C 504:

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



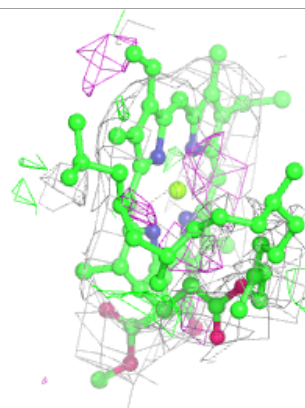
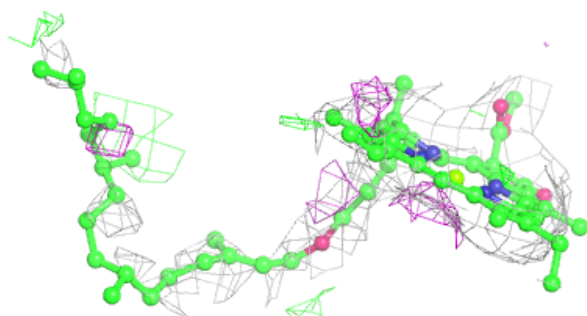
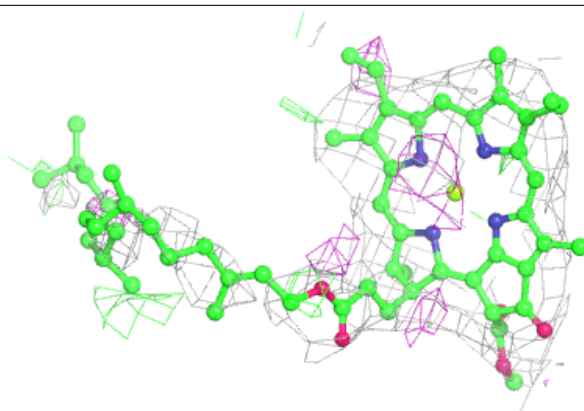
Electron density around SQD a 612:

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

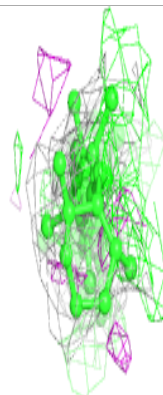
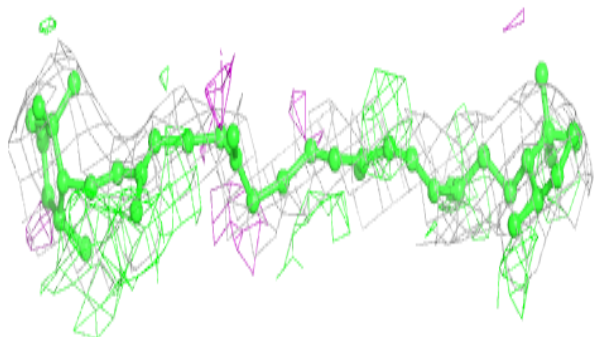
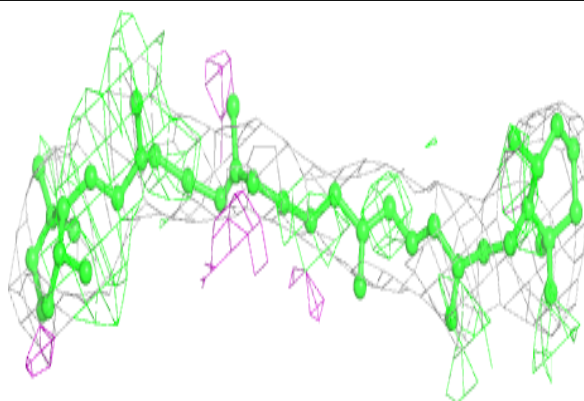


Electron density around CLA a 609:

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

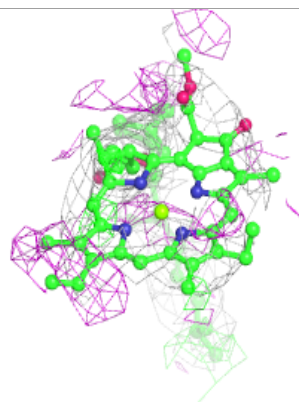
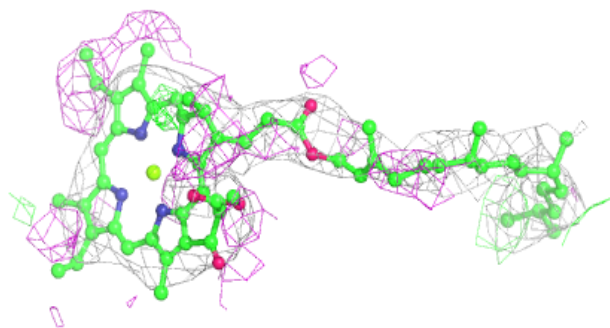
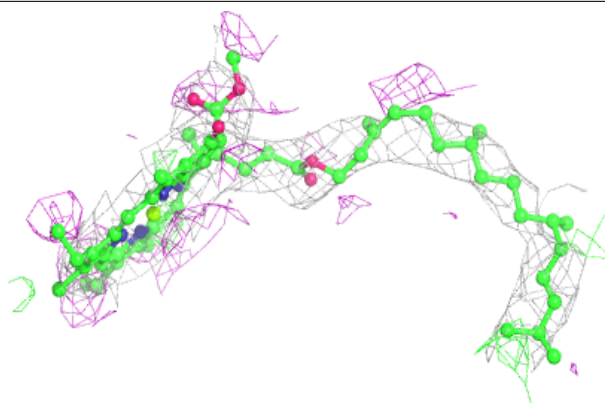
**Electron density around BCR B 619:**

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

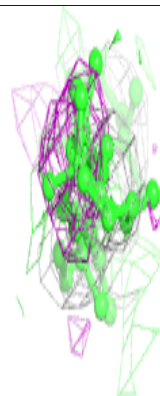
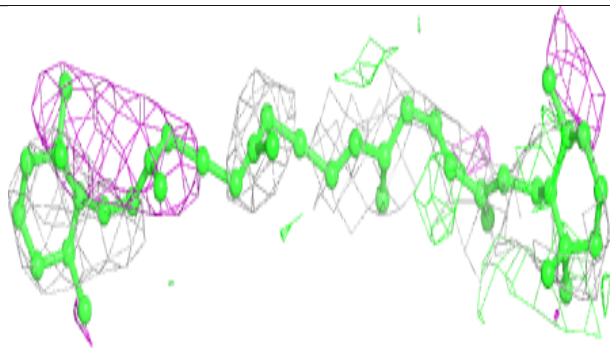
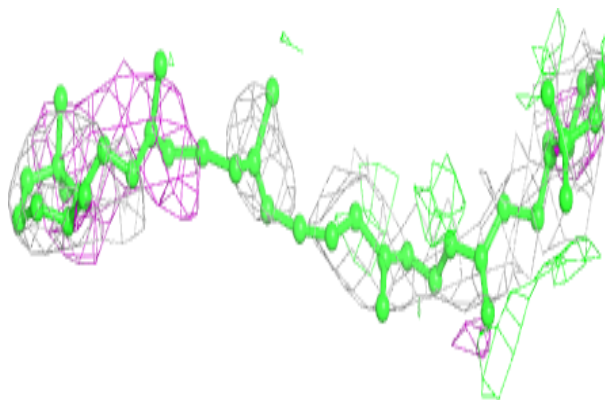


Electron density around CLA d 402:

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

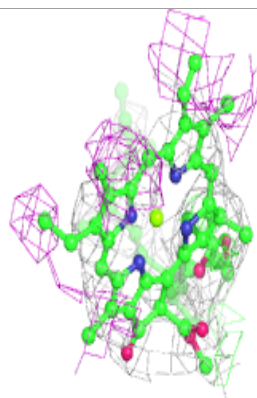
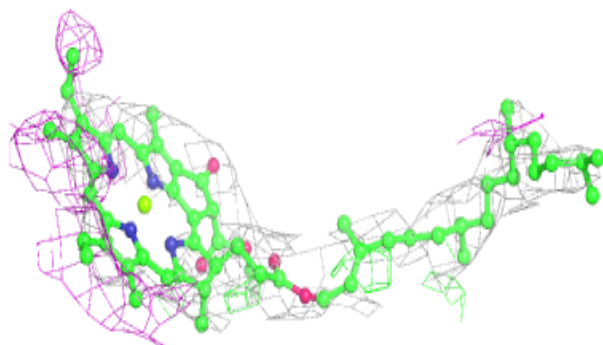
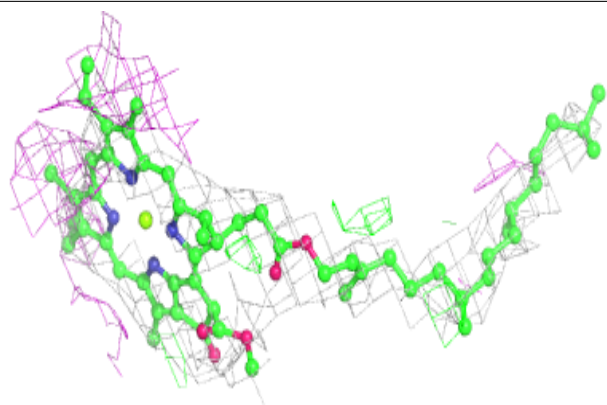
**Electron density around BCR H 101:**

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



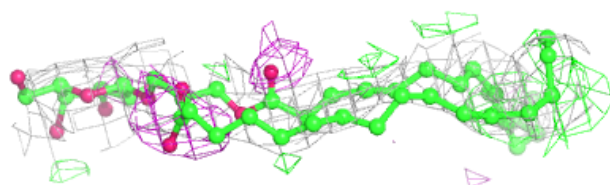
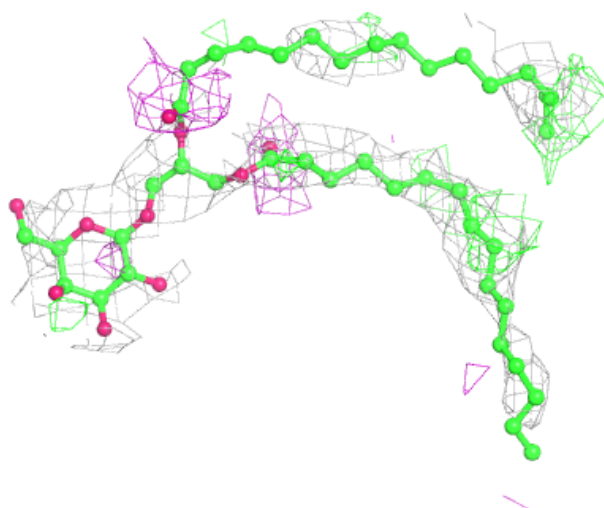
Electron density around CLA a 606:

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



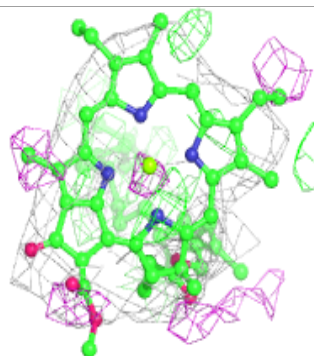
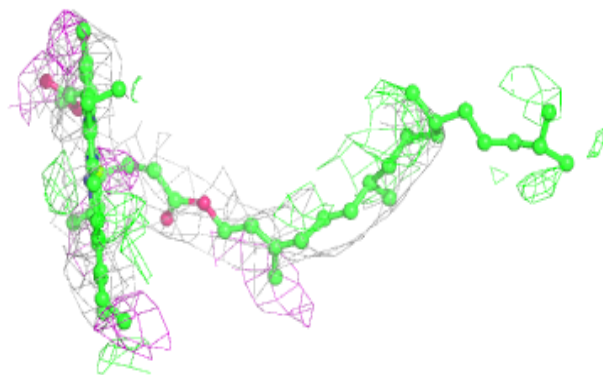
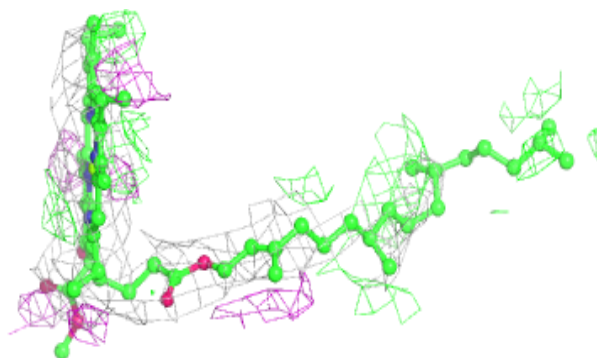
Electron density around LMG C 518:

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



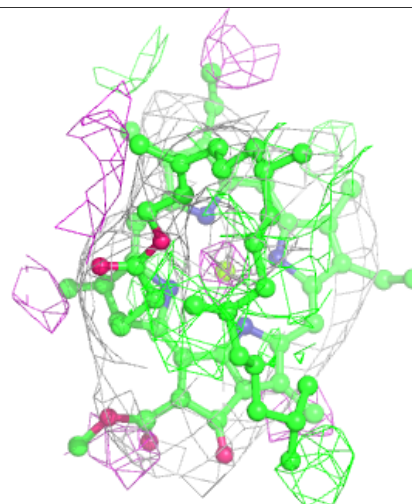
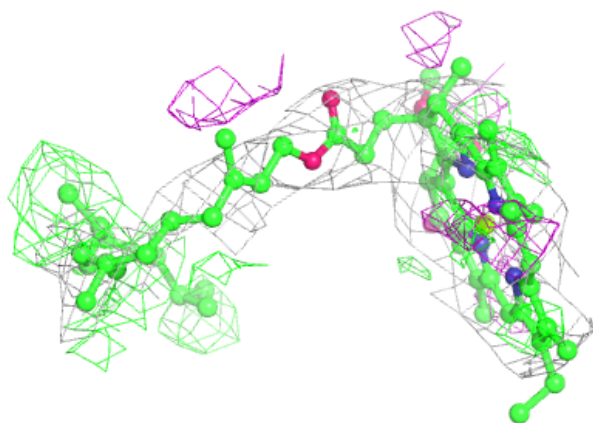
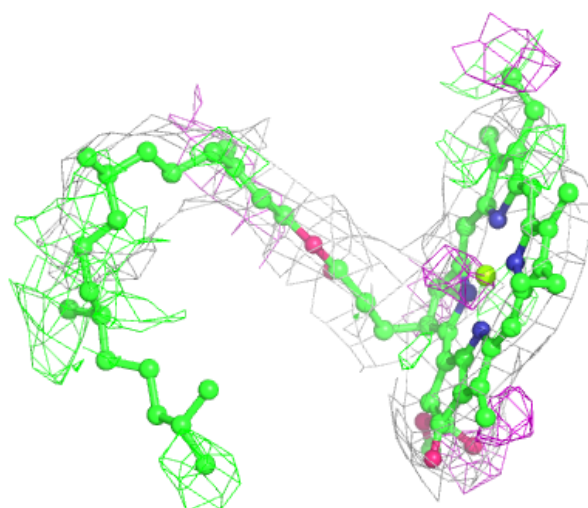
Electron density around CLA B 607 (A):

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



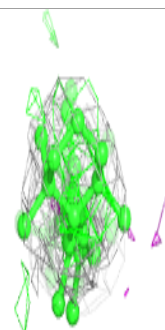
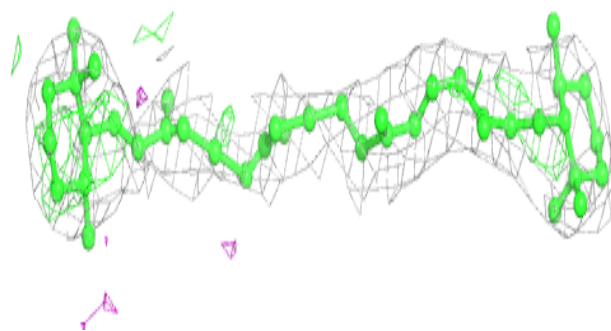
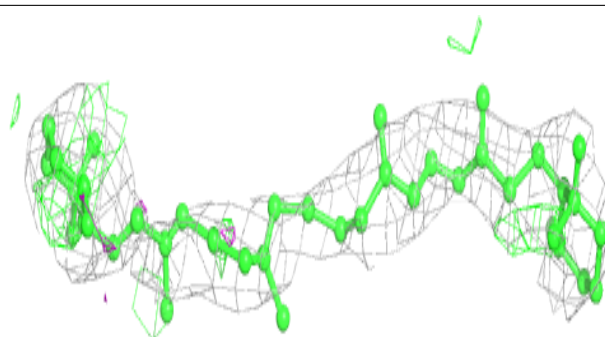
Electron density around CLA B 607 (B):

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

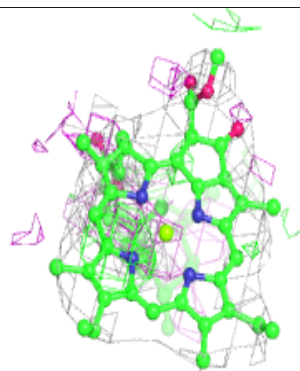
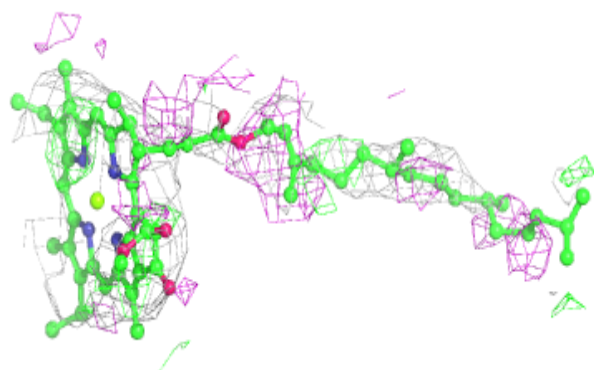
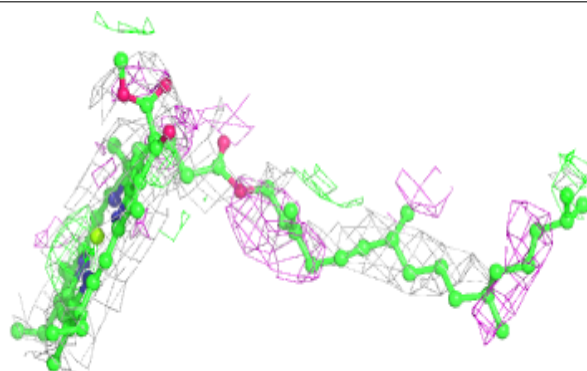


Electron density around BCR a 610:

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

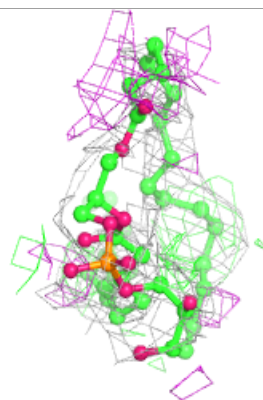
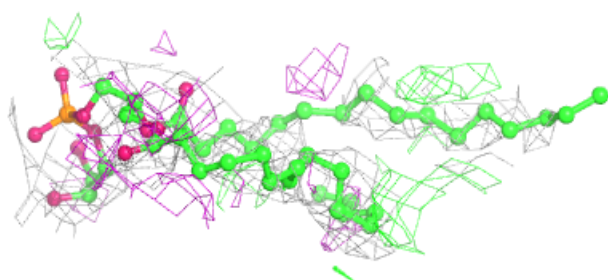
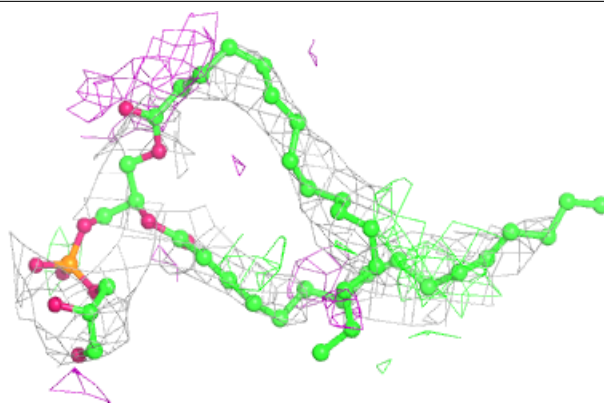
**Electron density around CLA B 605:**

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



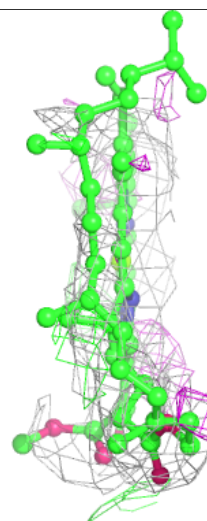
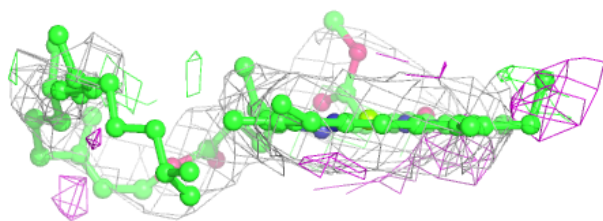
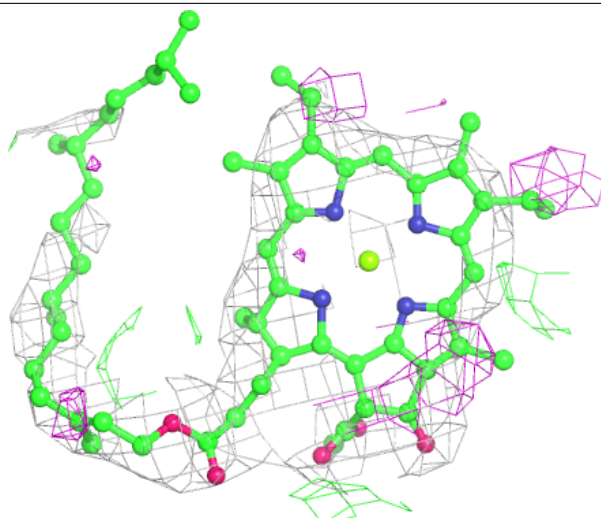
Electron density around LHG A 615:

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



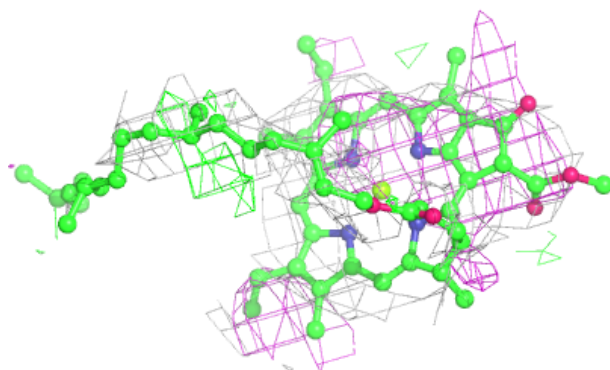
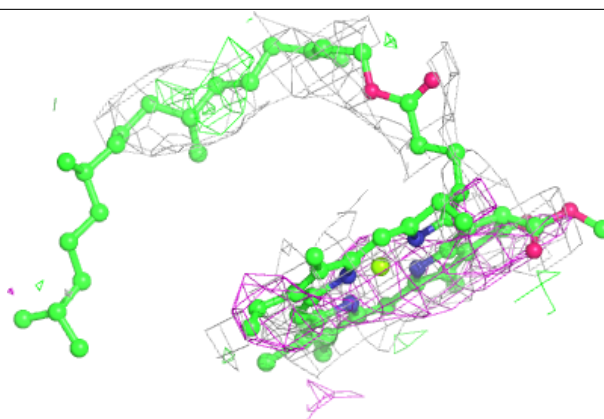
Electron density around CLA C 512:

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

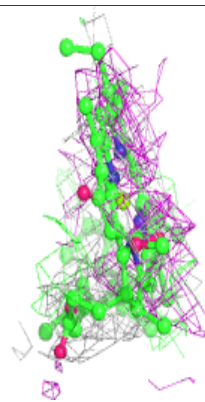
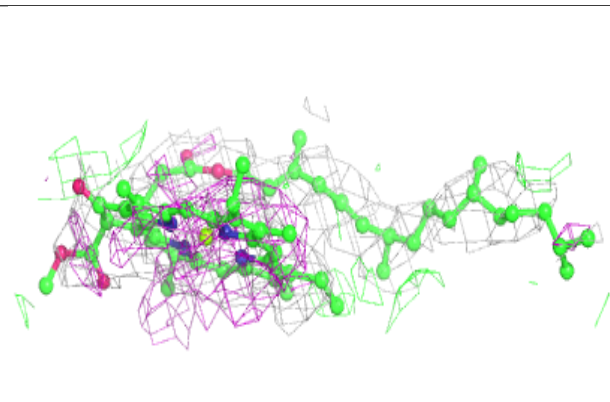
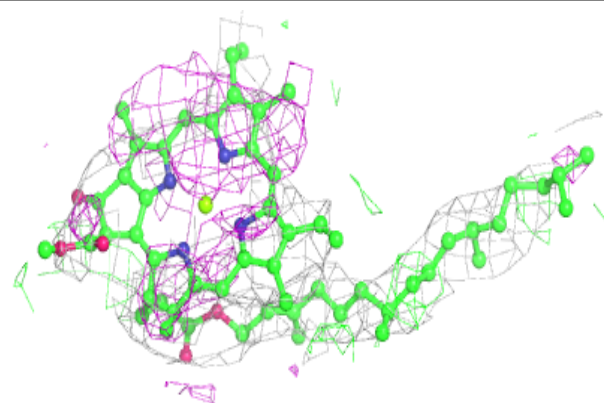


Electron density around CLA c 513:

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

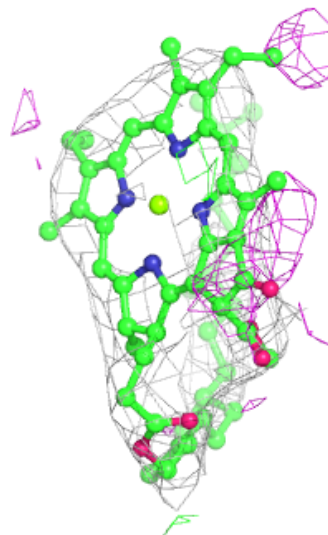
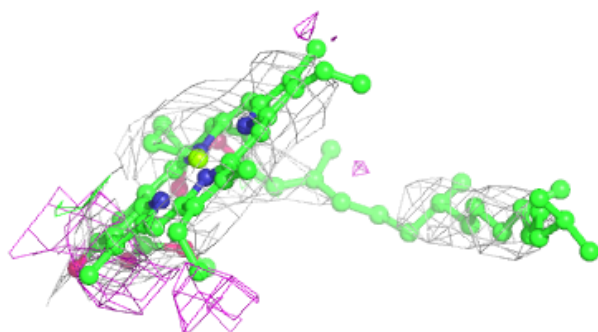
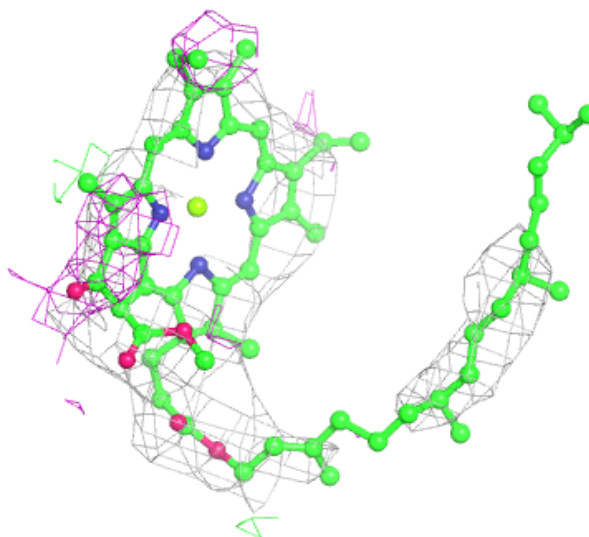
**Electron density around CLA C 501:**

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



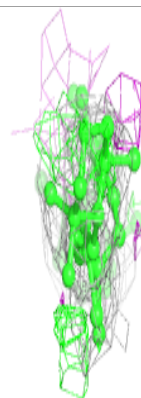
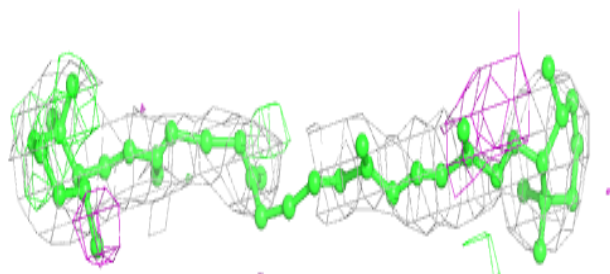
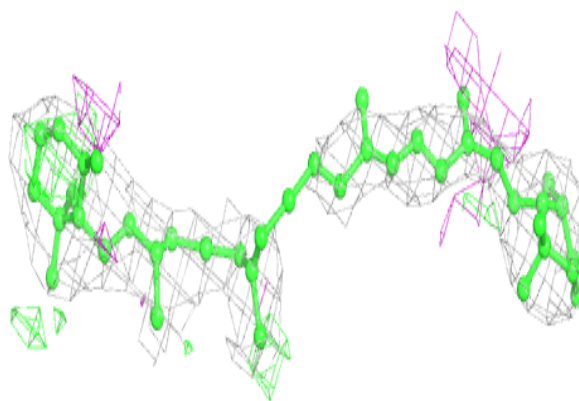
Electron density around CLA c 507:

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

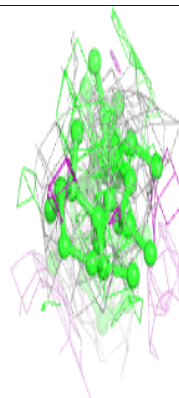
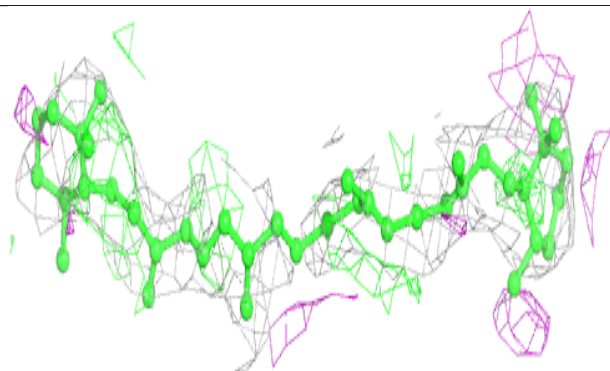
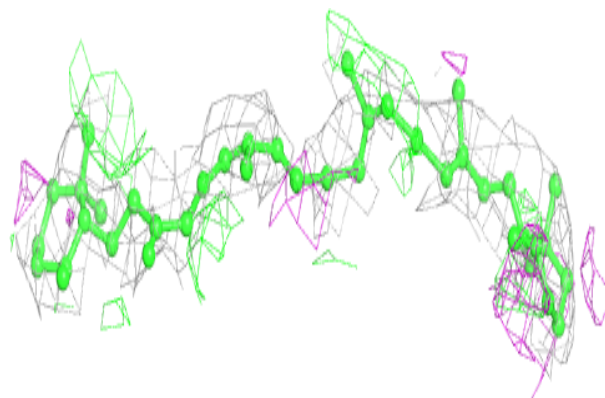


Electron density around BCR K 101:

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

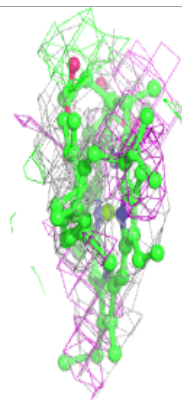
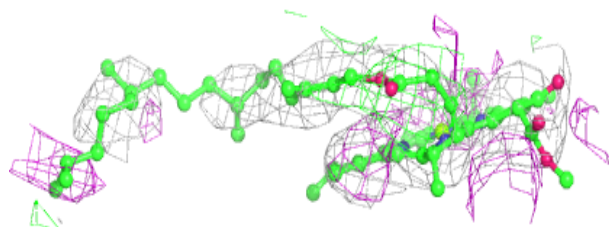
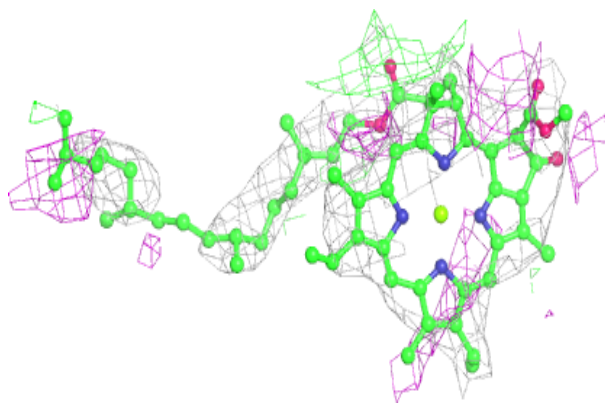
**Electron density around BCR T 101:**

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



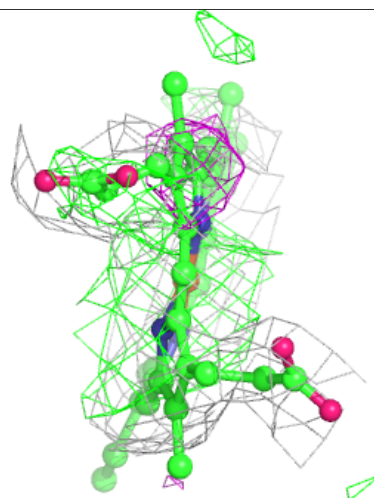
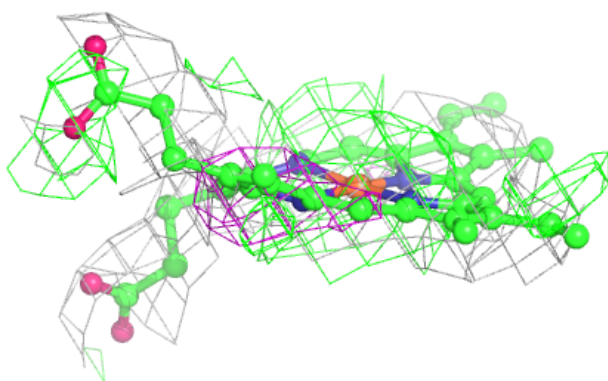
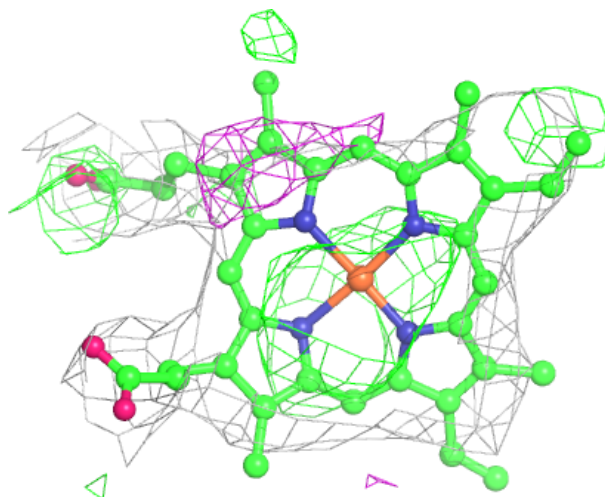
Electron density around CLA b 605:

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



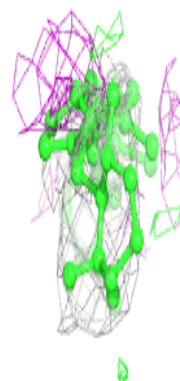
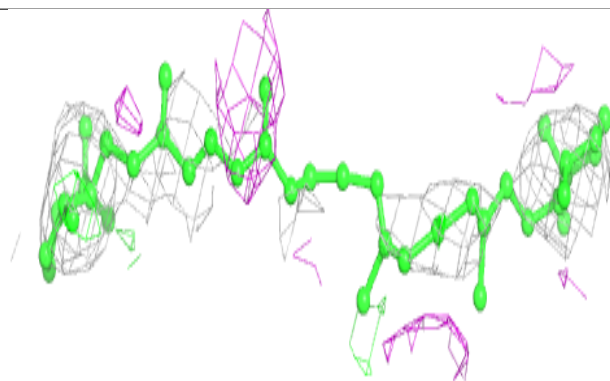
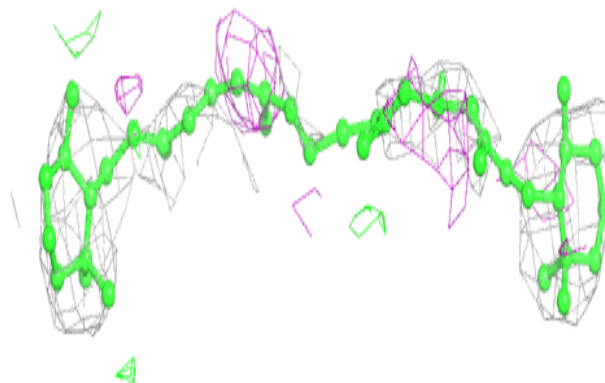
Electron density around HEM E 103:

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

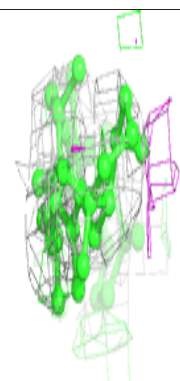
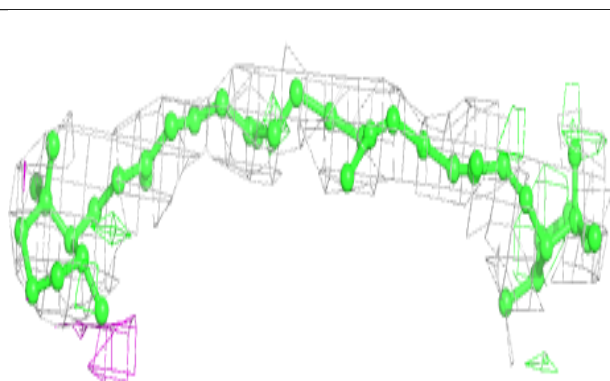
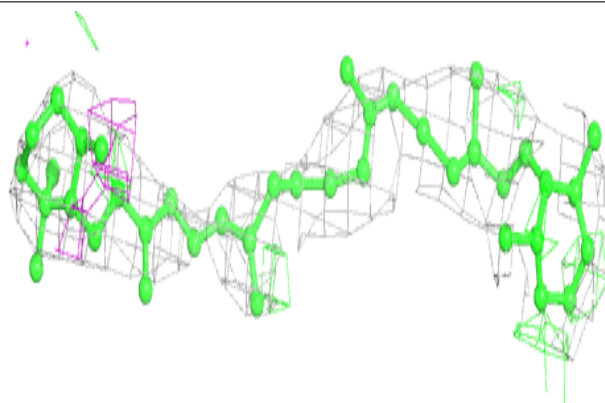


Electron density around BCR c 521:

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

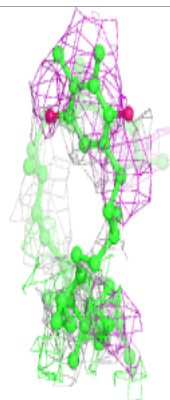
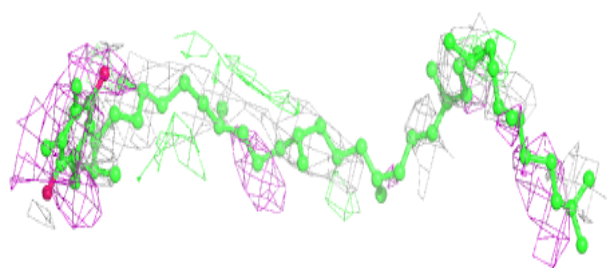
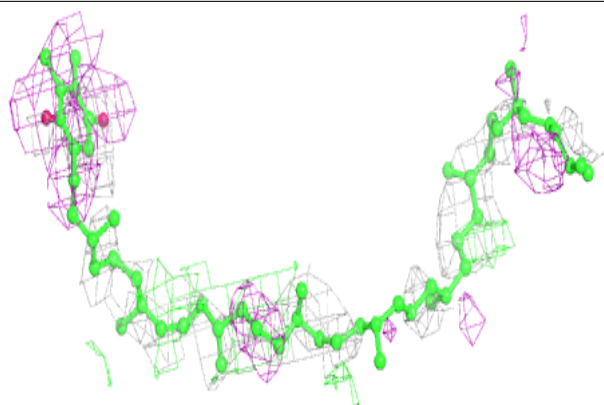
**Electron density around BCR F 101:**

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

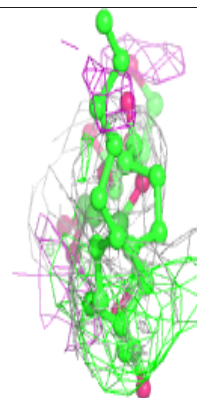
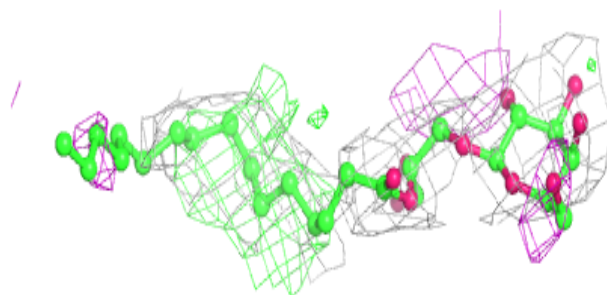
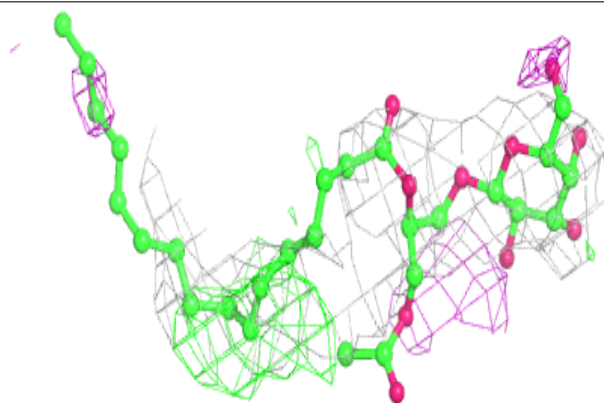


Electron density around PL9 A 611:

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

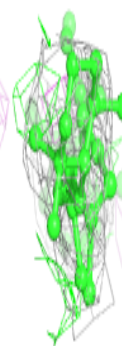
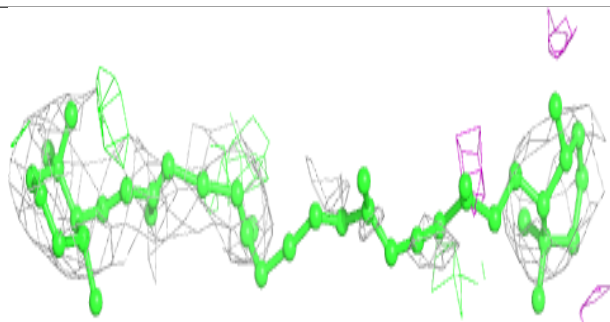
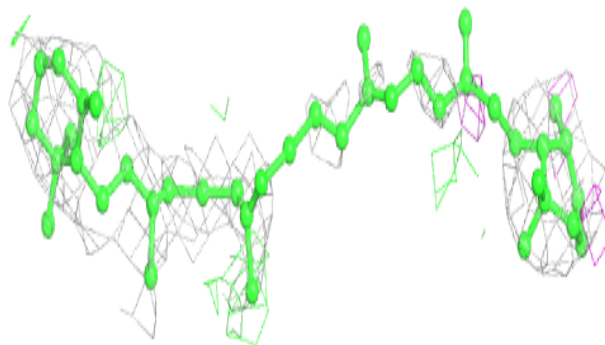
**Electron density around LMG Z 101:**

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

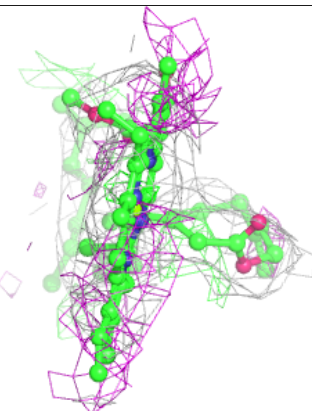
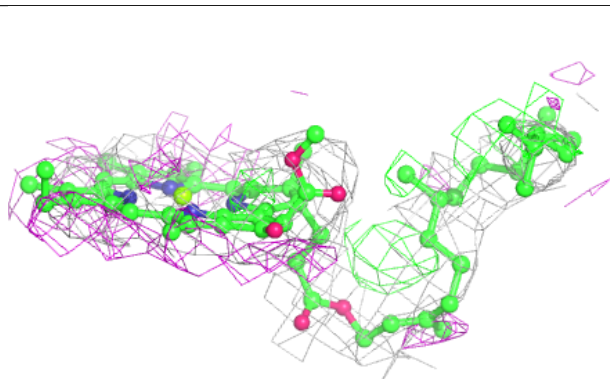
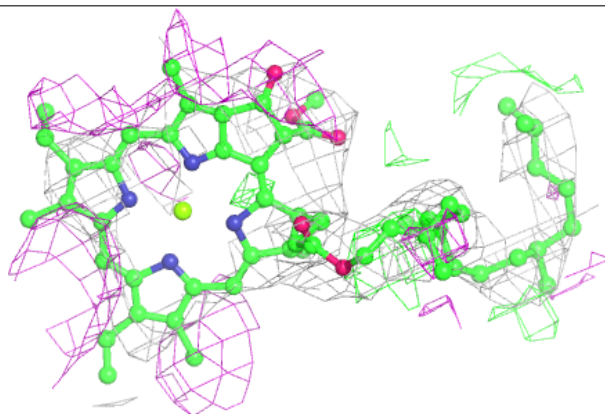


Electron density around BCR k 101:

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

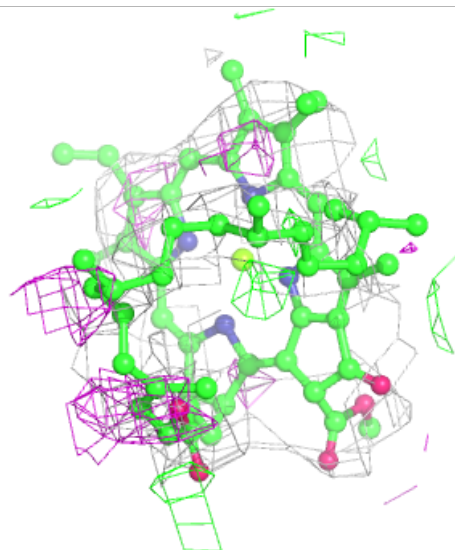
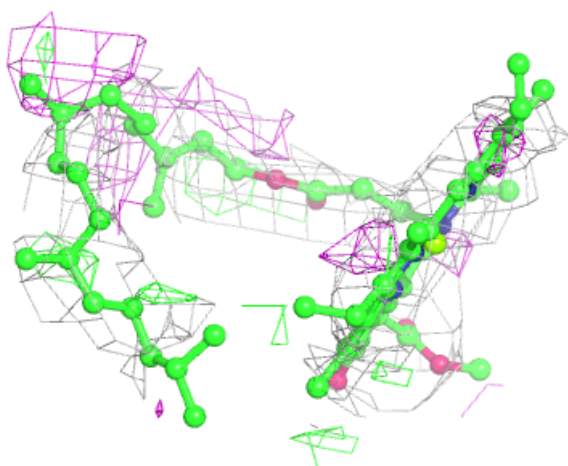
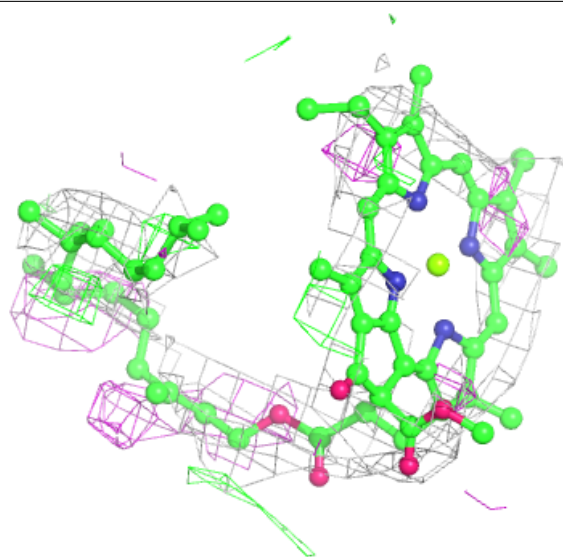
**Electron density around CLA B 613:**

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



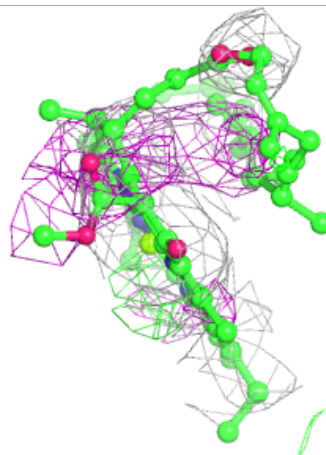
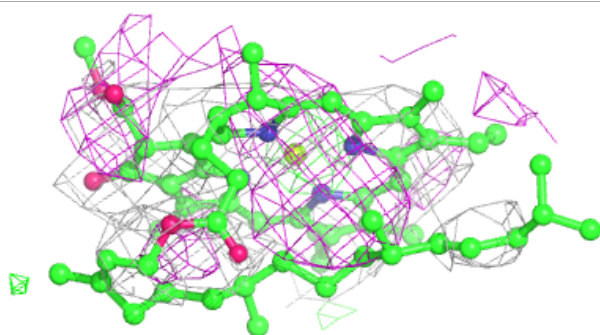
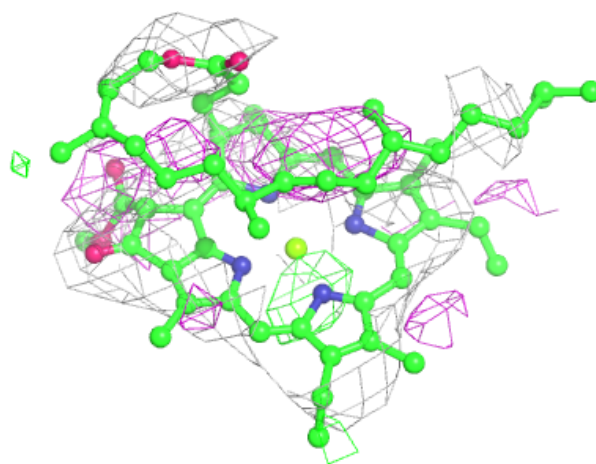
Electron density around CLA c 503:

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



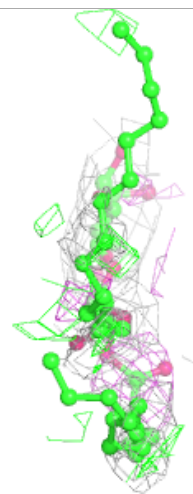
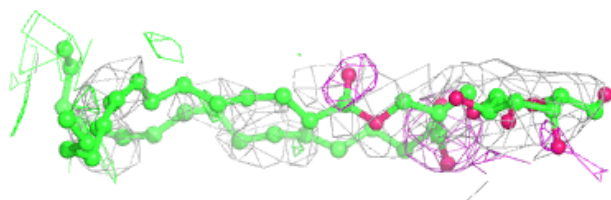
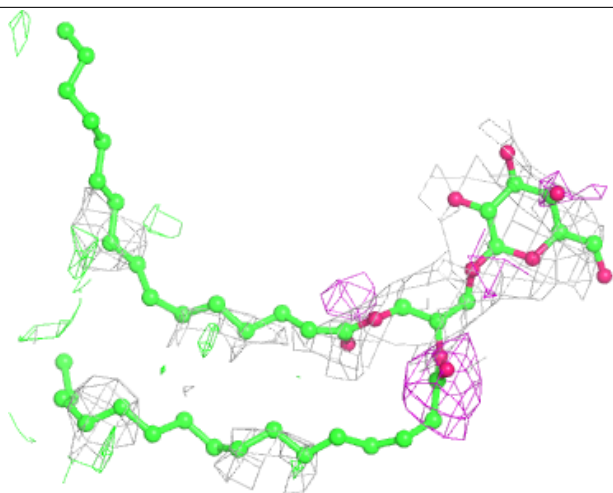
Electron density around CLA b 603:

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



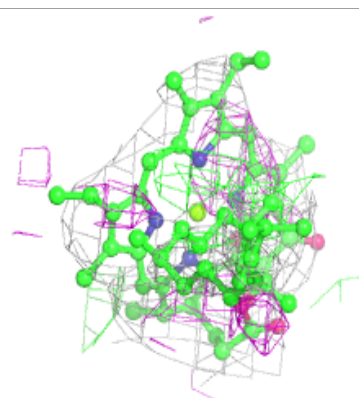
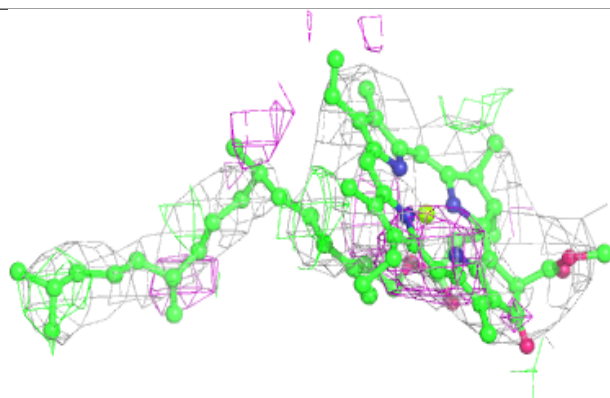
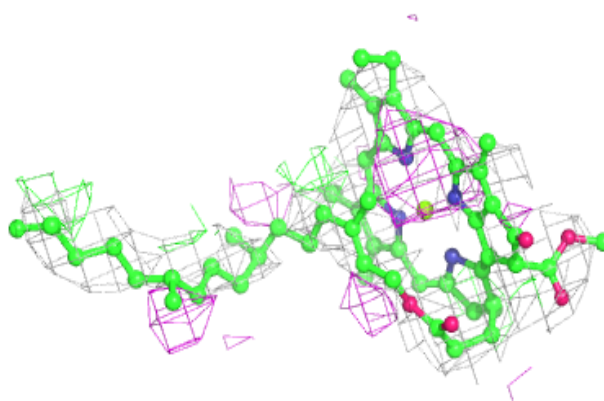
Electron density around LMG c 519:

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

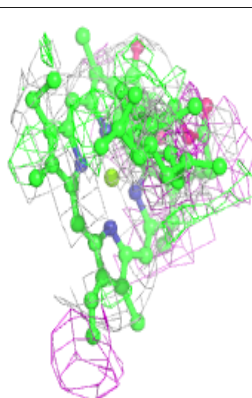
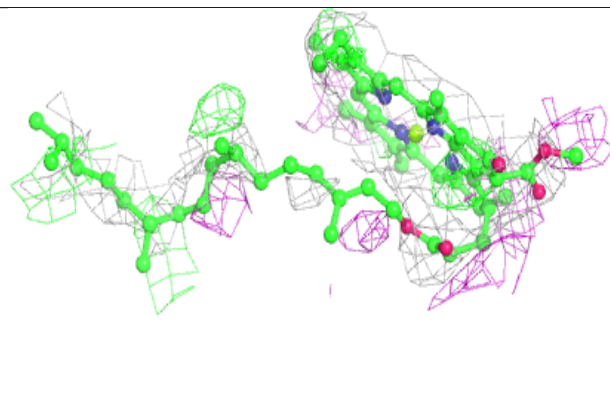
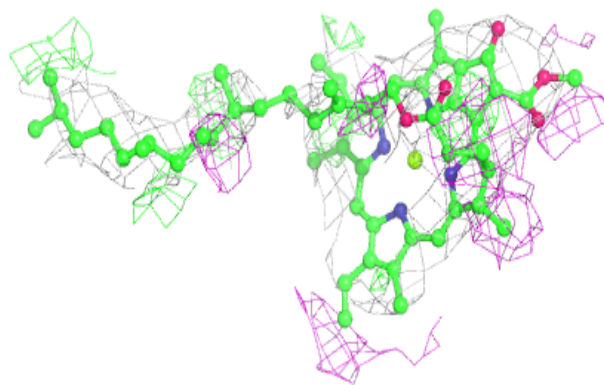


Electron density around CLA C 505:

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

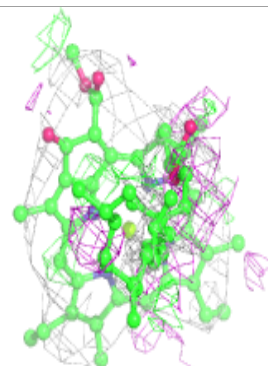
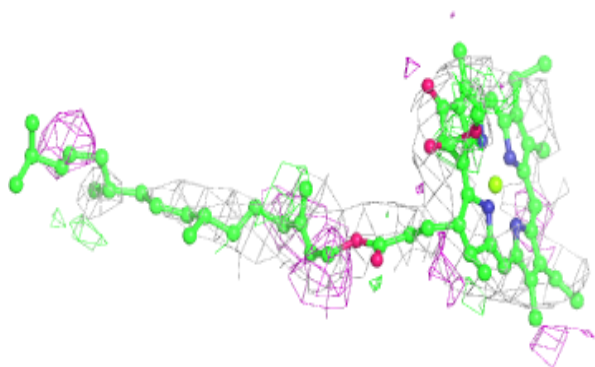
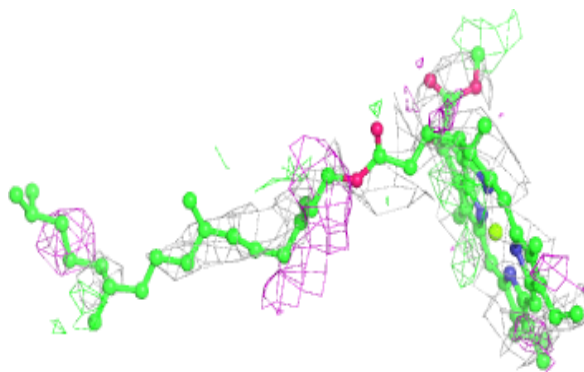
**Electron density around CLA b 616:**

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

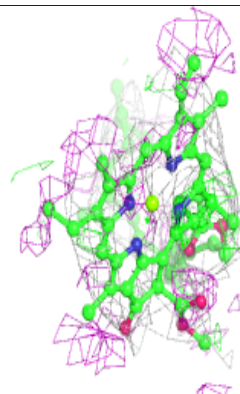
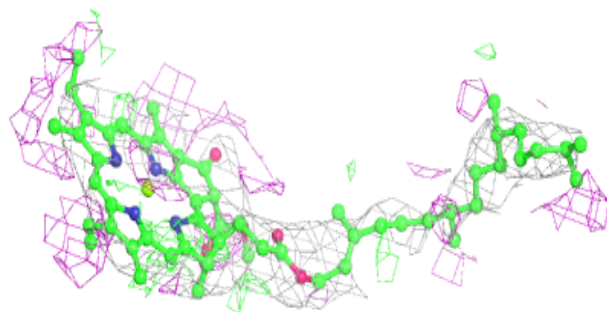
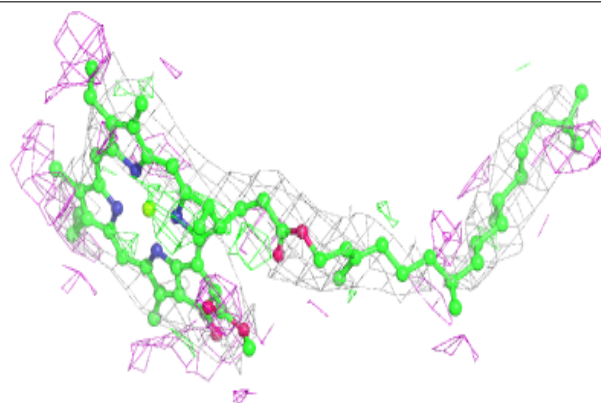


Electron density around CLA b 606:

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

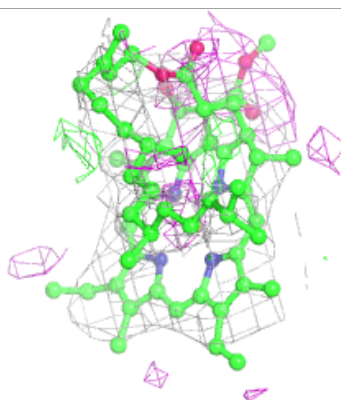
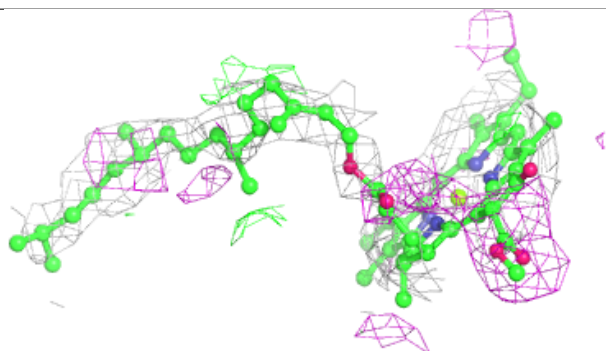
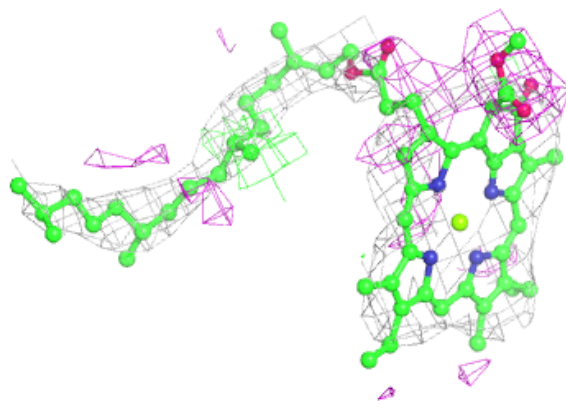
**Electron density around CLA A 606:**

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

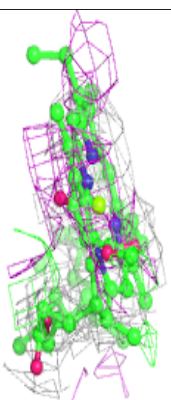
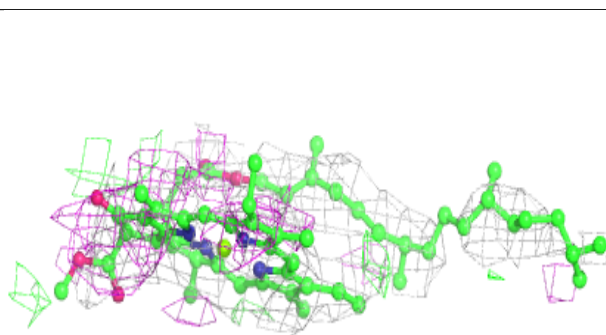
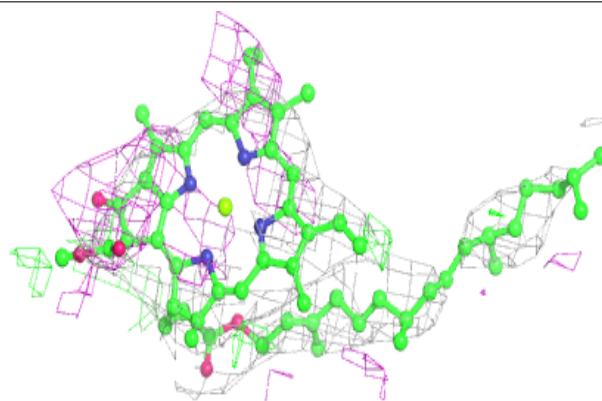


Electron density around CLA C 511:

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

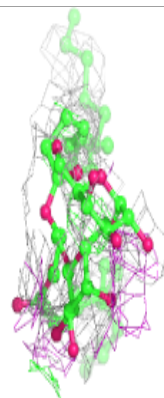
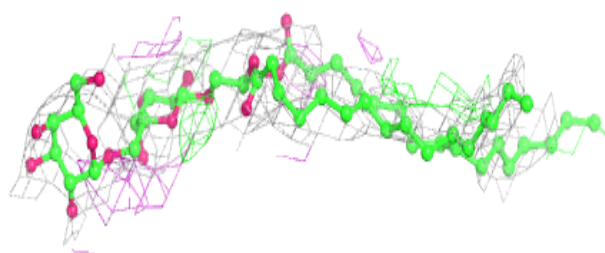
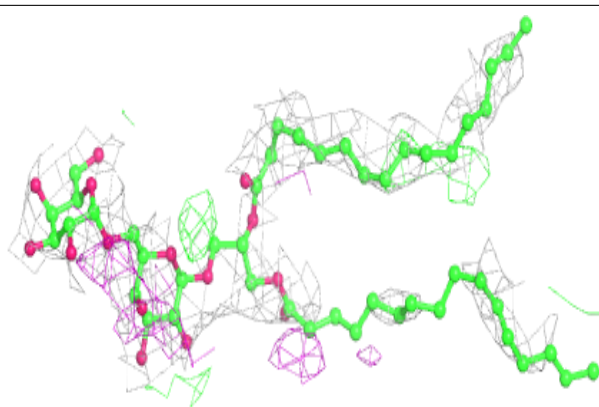
**Electron density around CLA c 501:**

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



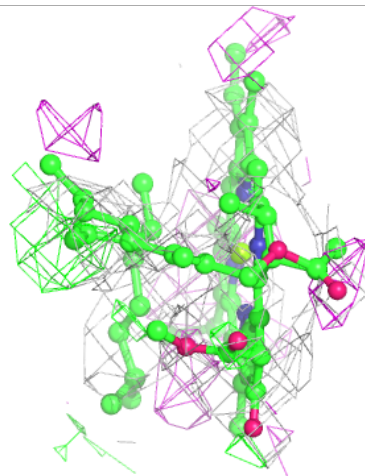
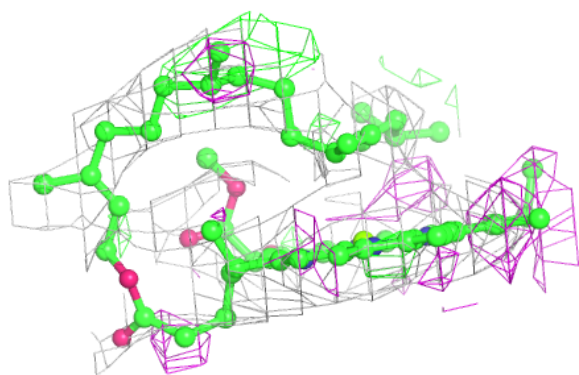
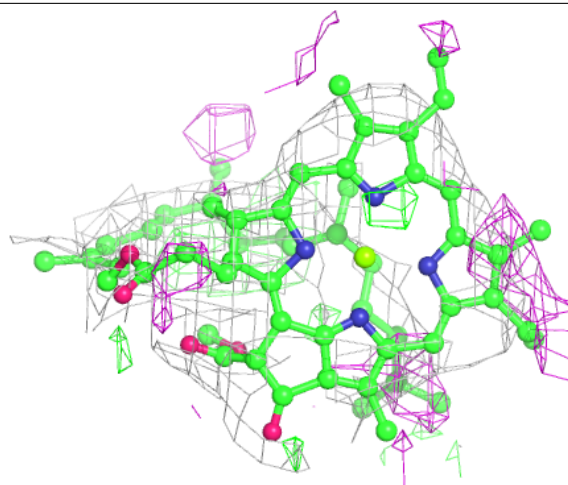
Electron density around DGD c 518:

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



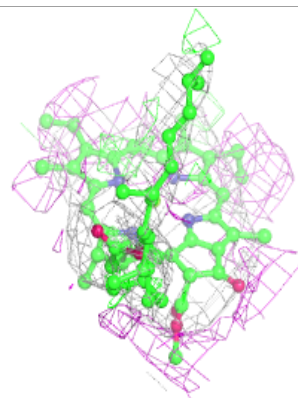
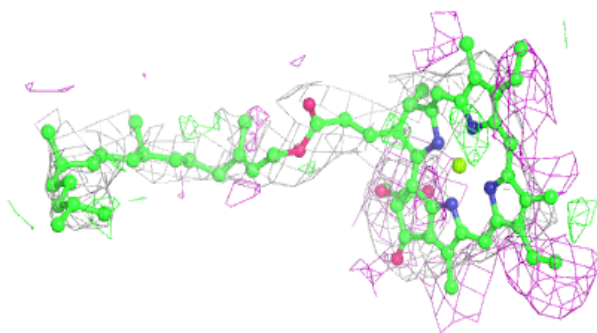
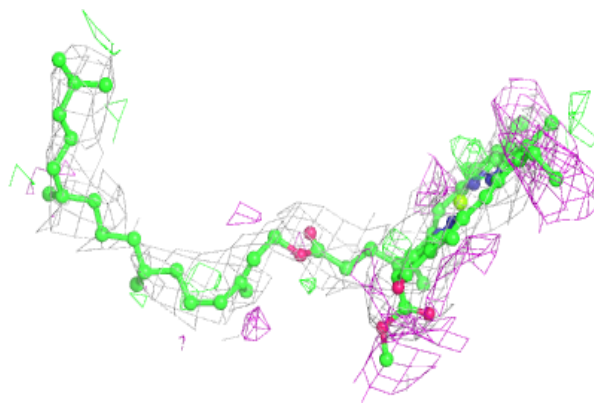
Electron density around CLA C 510:

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

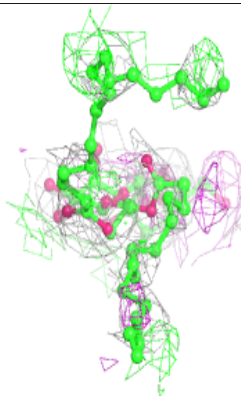
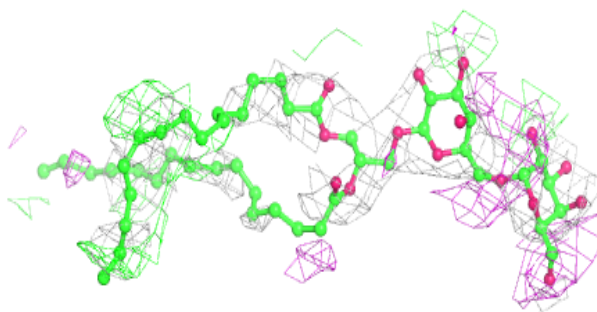
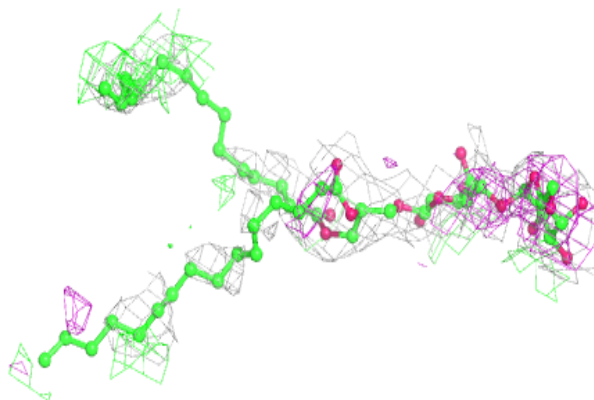


Electron density around CLA D 403:

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

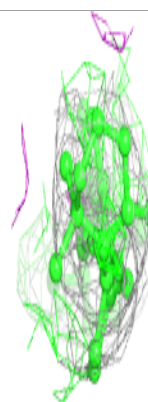
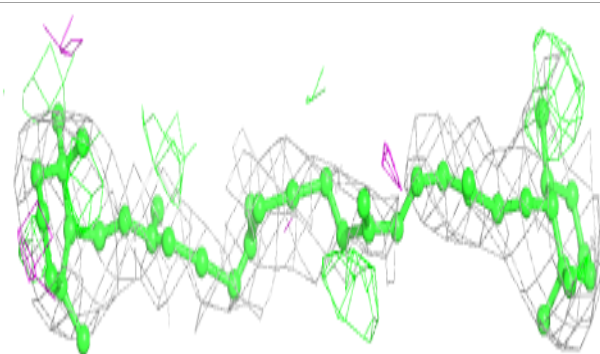
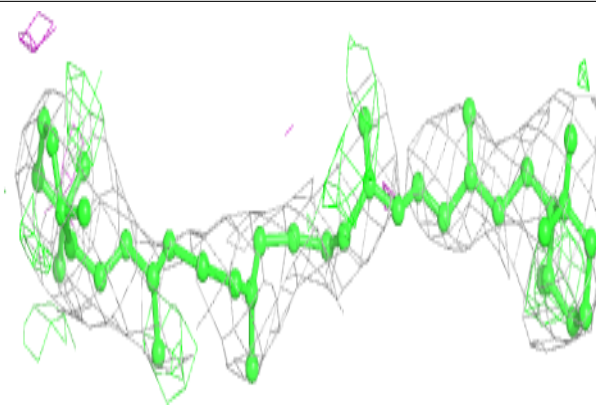
**Electron density around DGD c 516:**

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

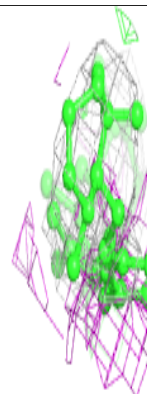
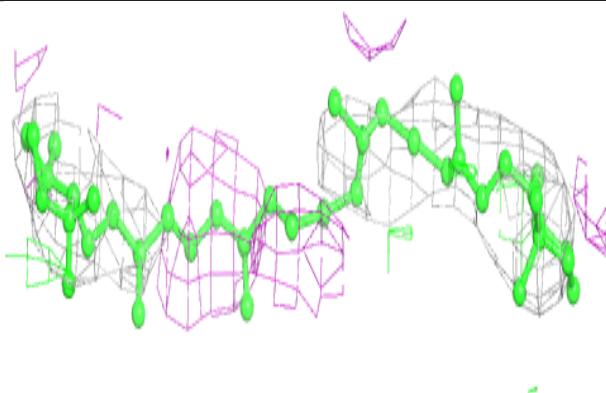
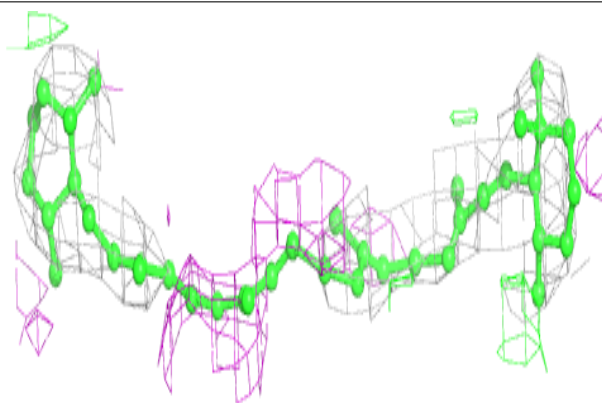


Electron density around BCR A 610:

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

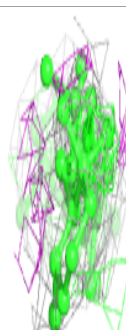
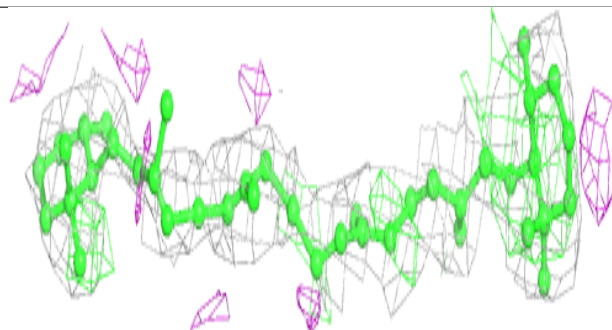
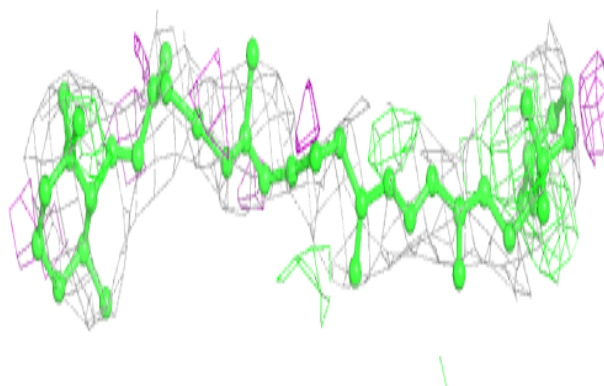
**Electron density around BCR K 102:**

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

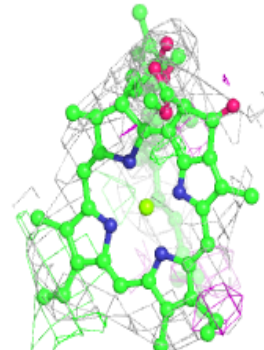
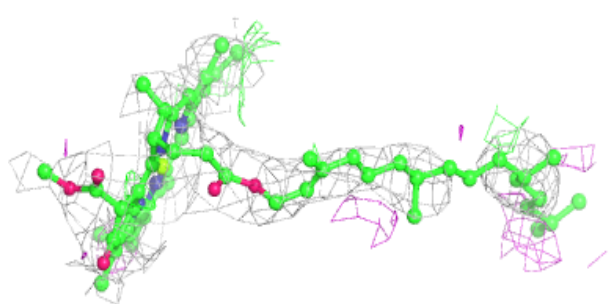
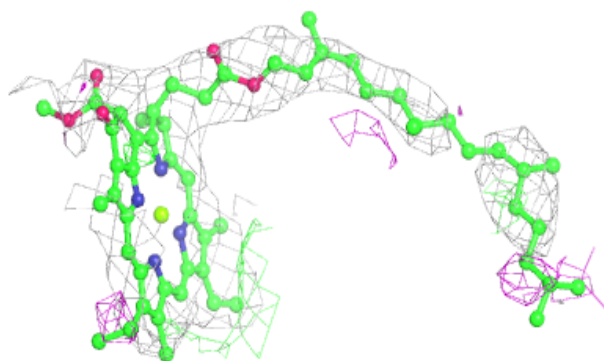


Electron density around BCR B 618:

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

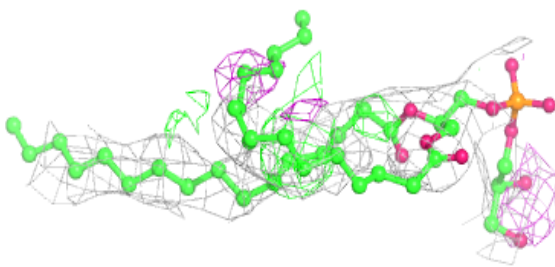
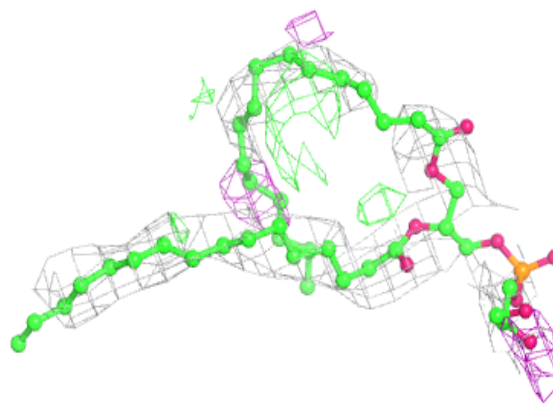
**Electron density around CLA B 610:**

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

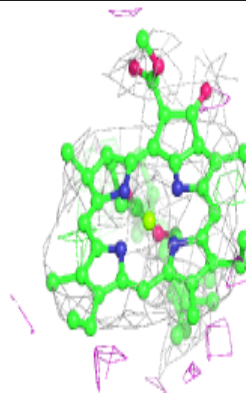
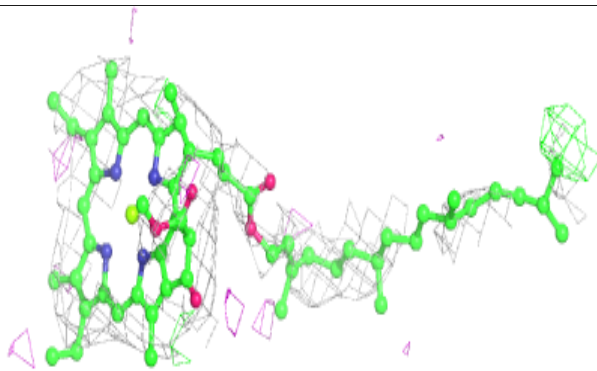
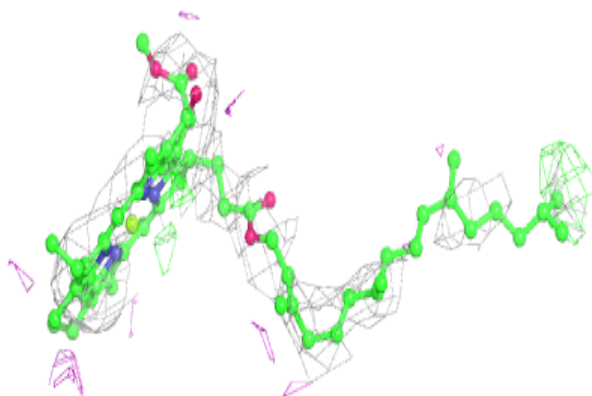


Electron density around LHG D 406:

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

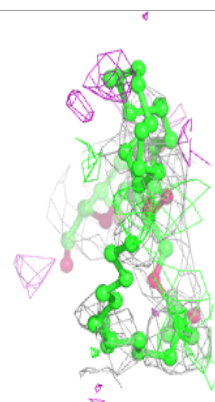
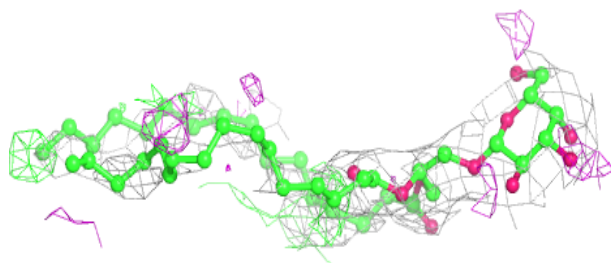
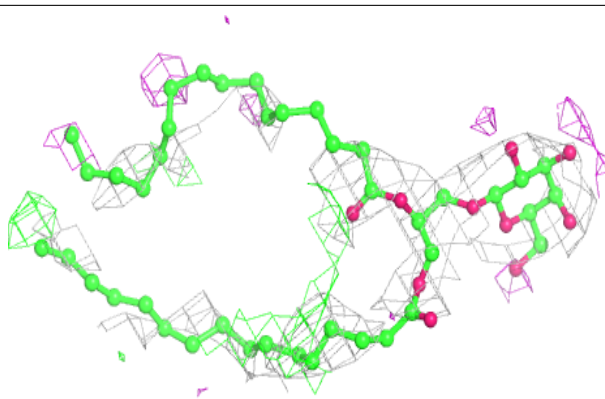
**Electron density around CLA c 502:**

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

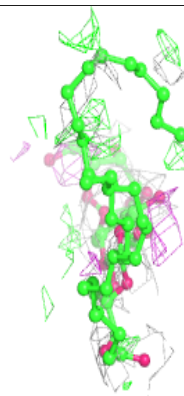
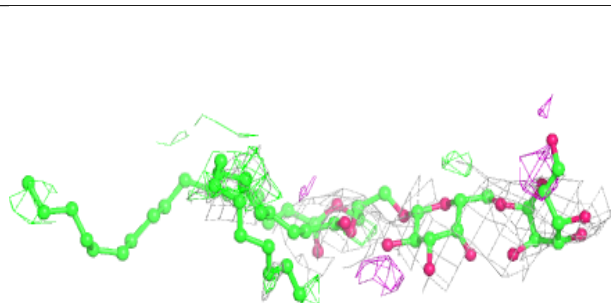
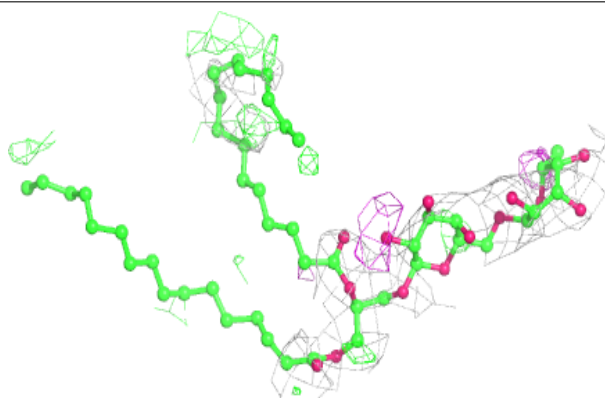


Electron density around LMG A 613:

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

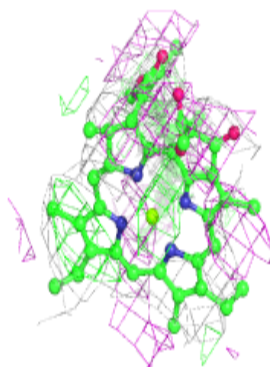
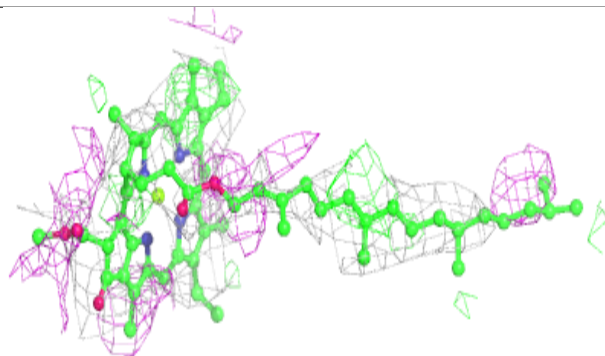
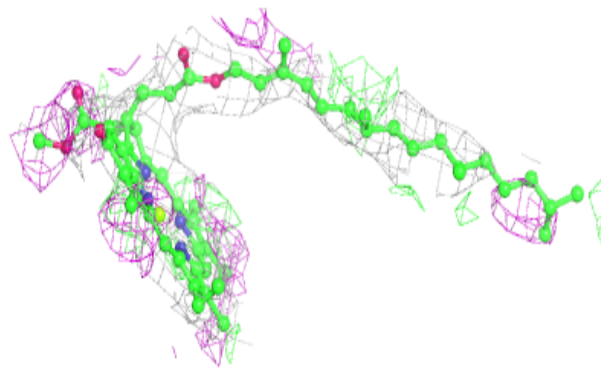
**Electron density around DGD d 405:**

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

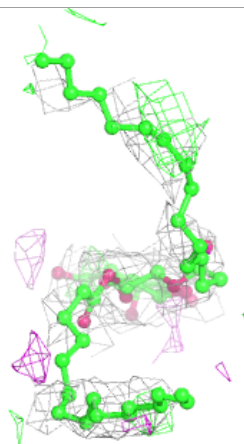
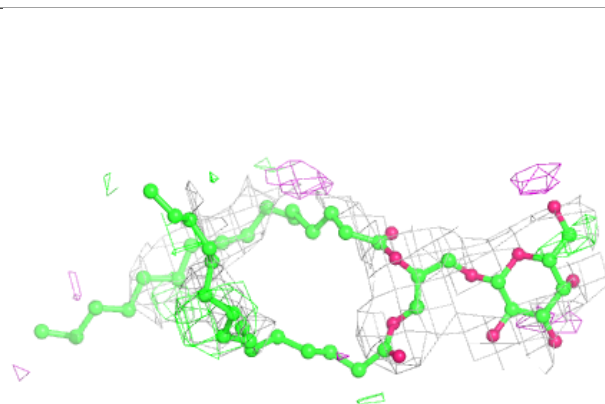
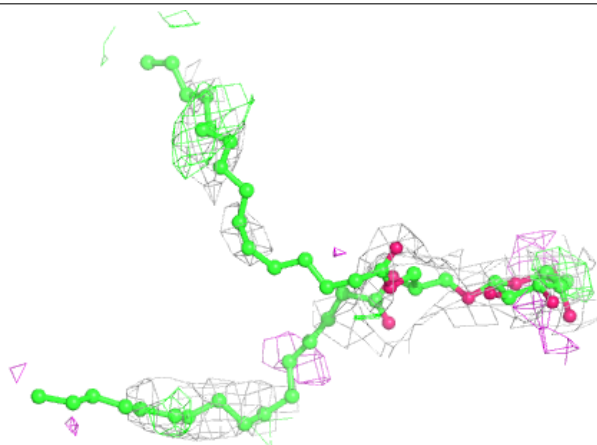


Electron density around CLA b 609:

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

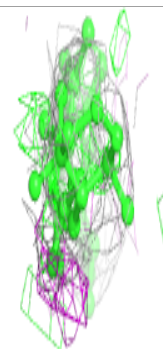
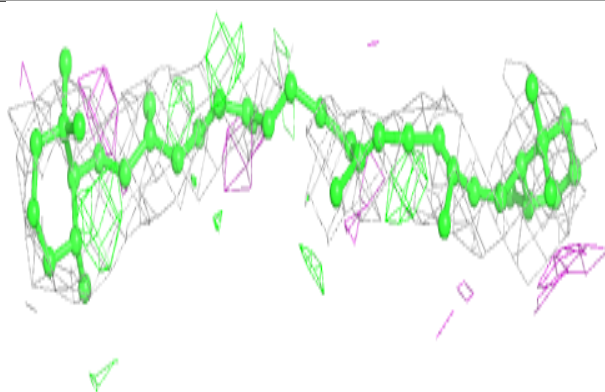
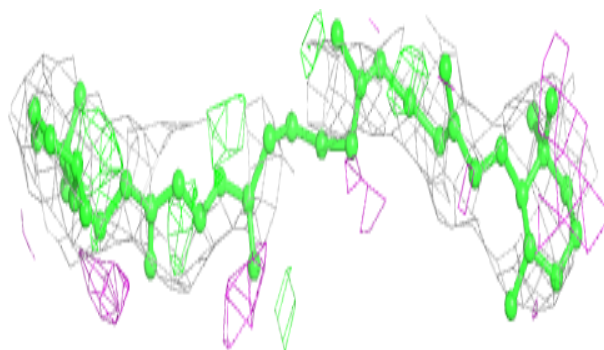
**Electron density around LMG b 622:**

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

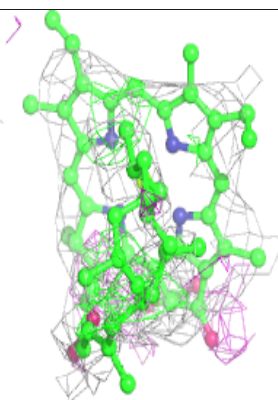
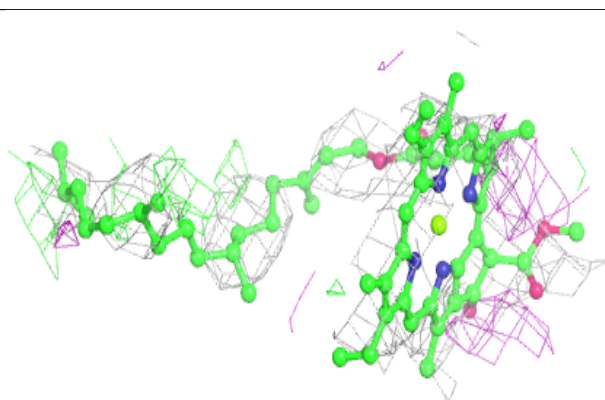
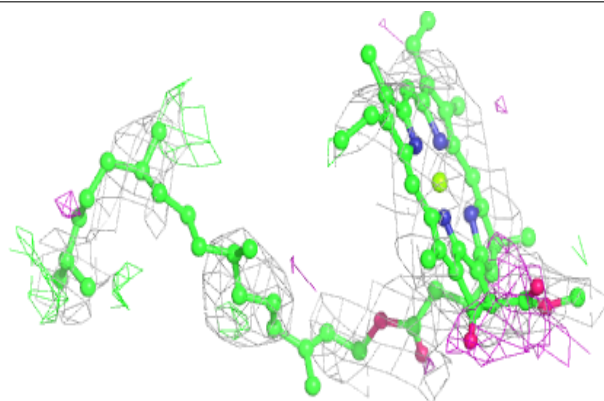


Electron density around BCR b 619:

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

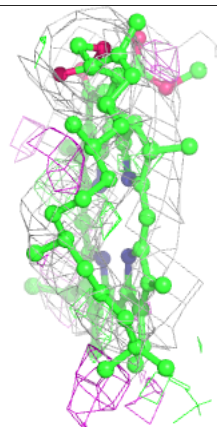
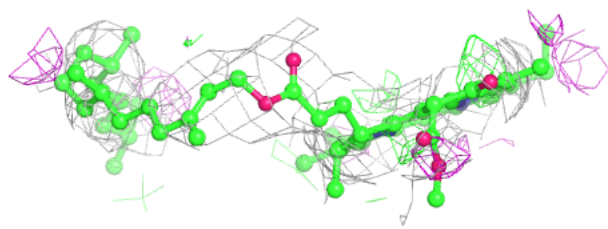
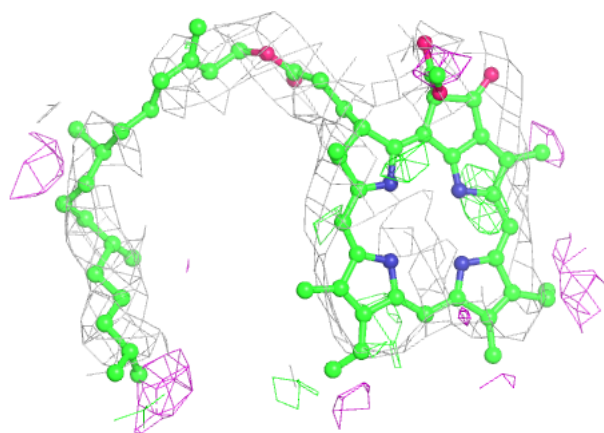
**Electron density around CLA c 508:**

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

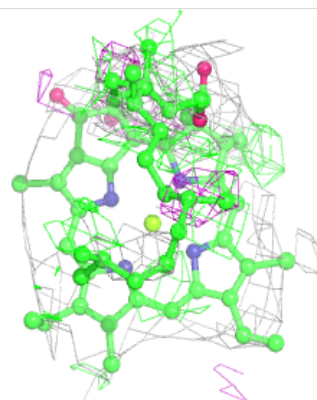
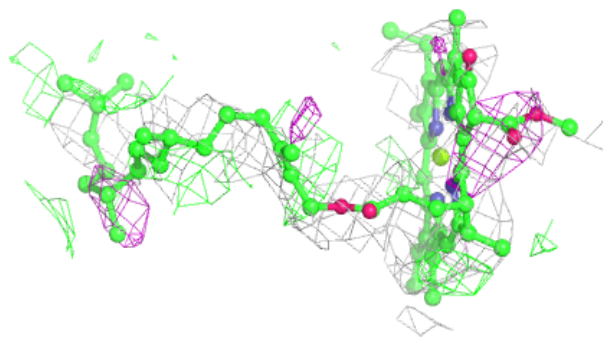
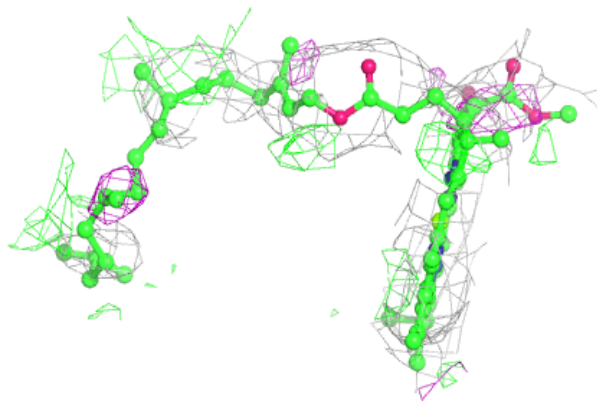


Electron density around PHO a 608:

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

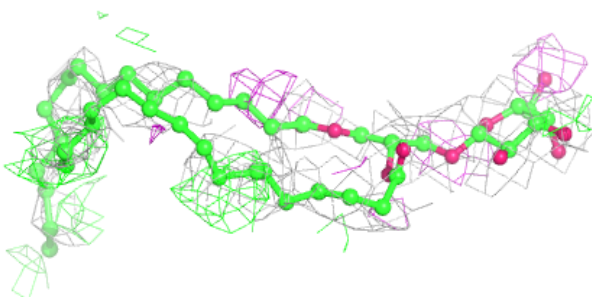
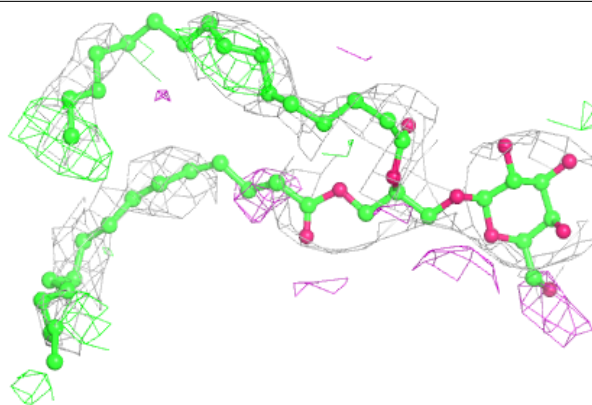
**Electron density around CLA C 506:**

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

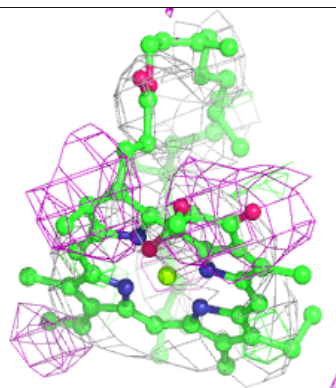
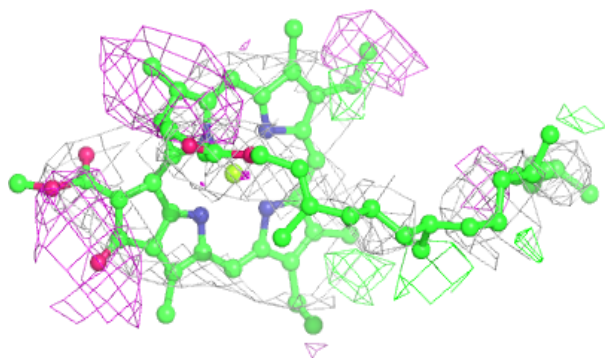
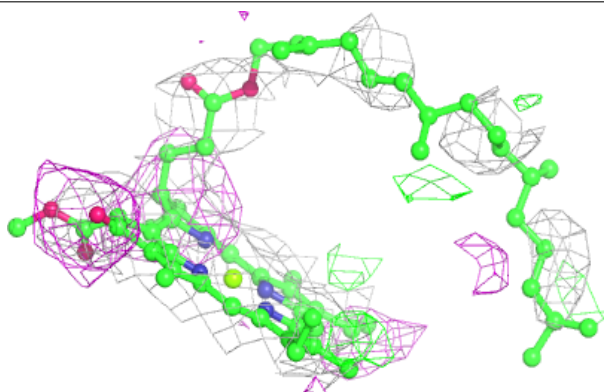


Electron density around LMG j 101:

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

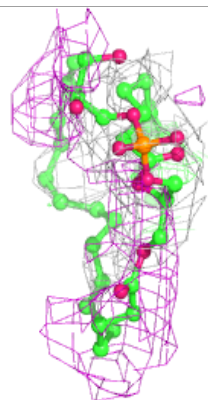
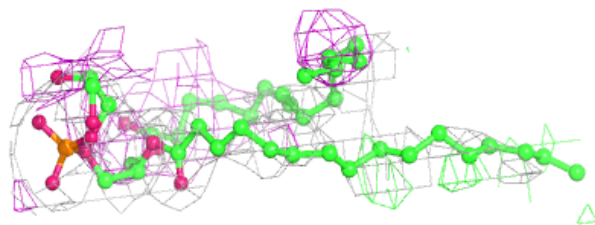
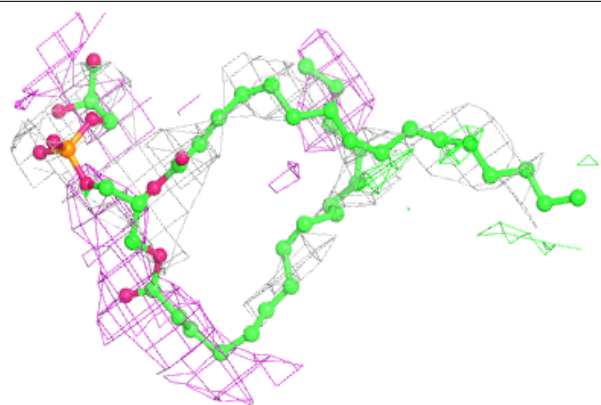
**Electron density around CLA C 513:**

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



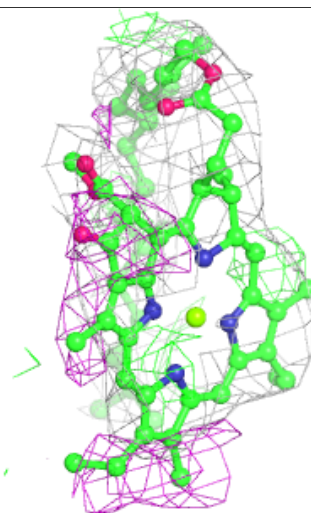
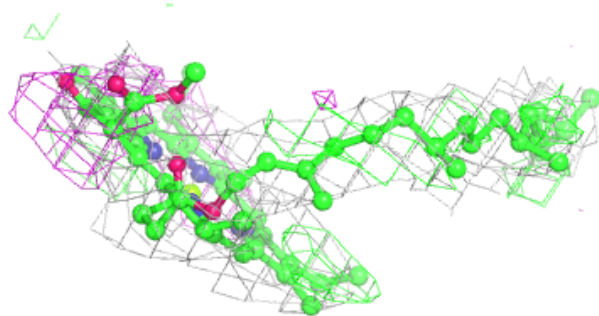
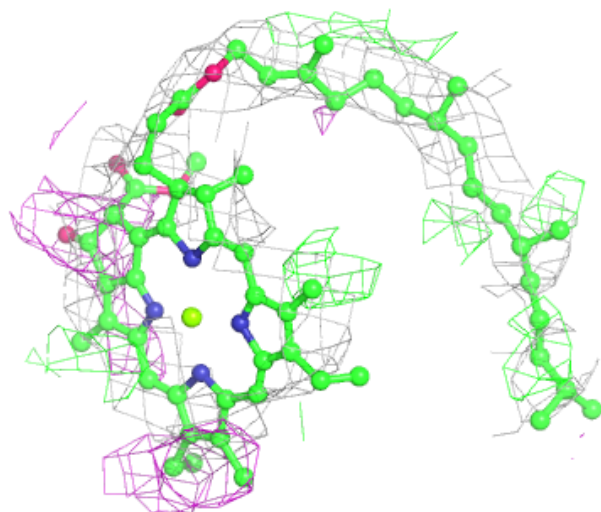
Electron density around LHG a 616:

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



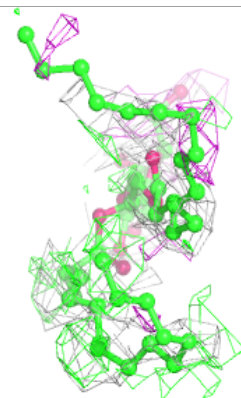
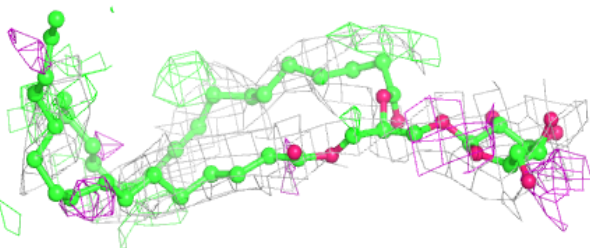
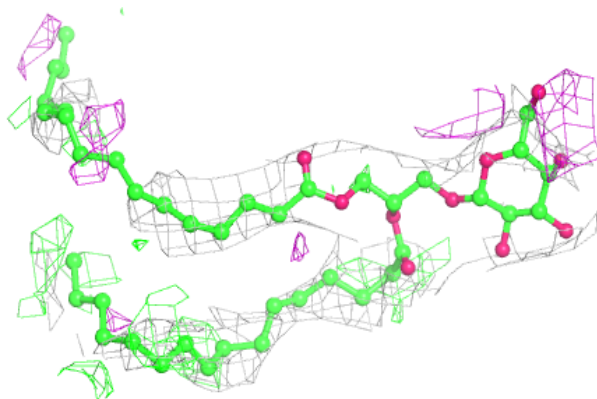
Electron density around CLA C 507:

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

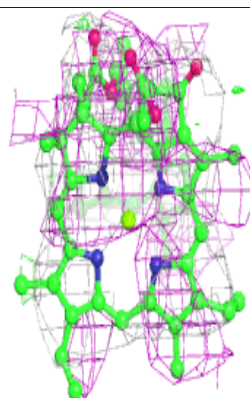
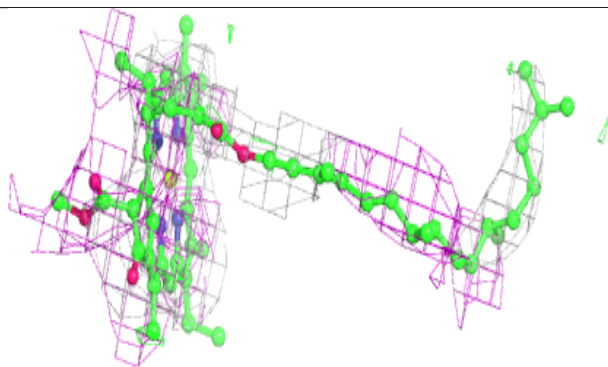
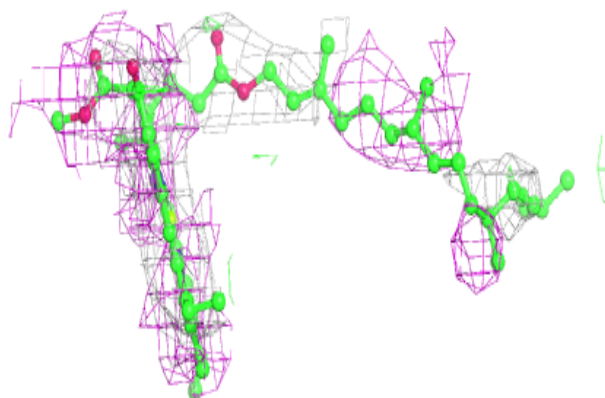


Electron density around LMG D 408:

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

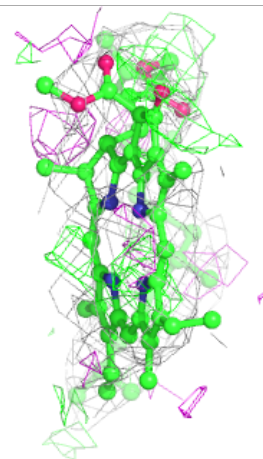
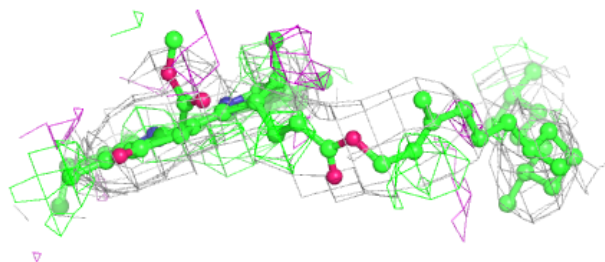
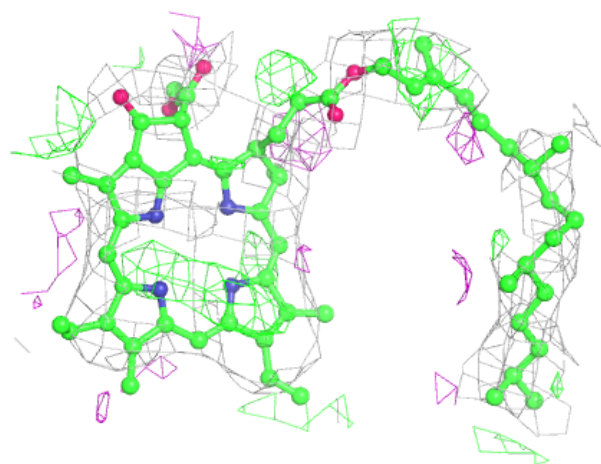
**Electron density around CLA B 606:**

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



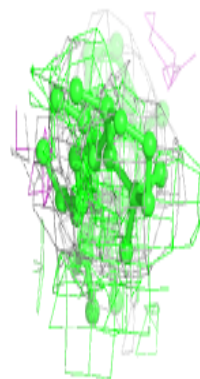
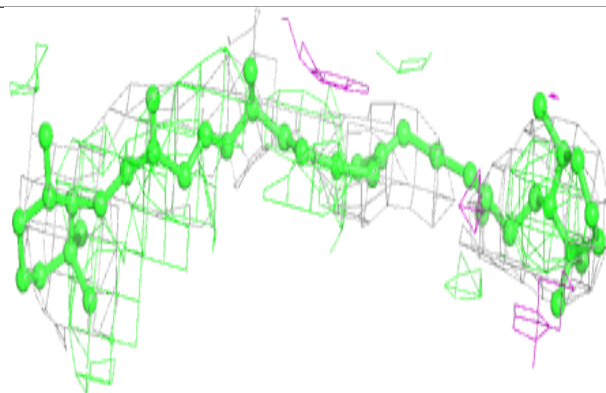
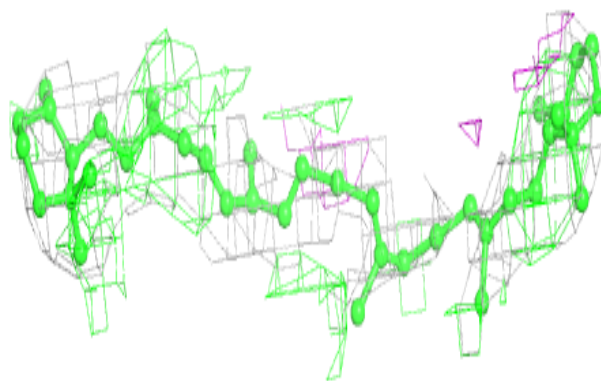
Electron density around PHO A 608:

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



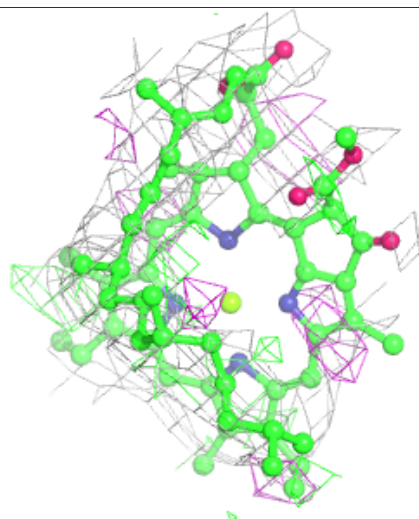
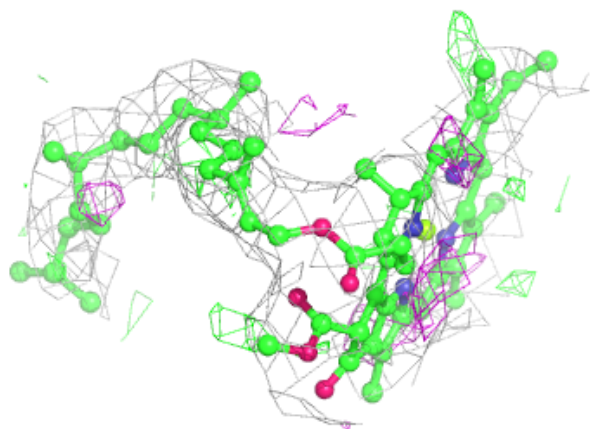
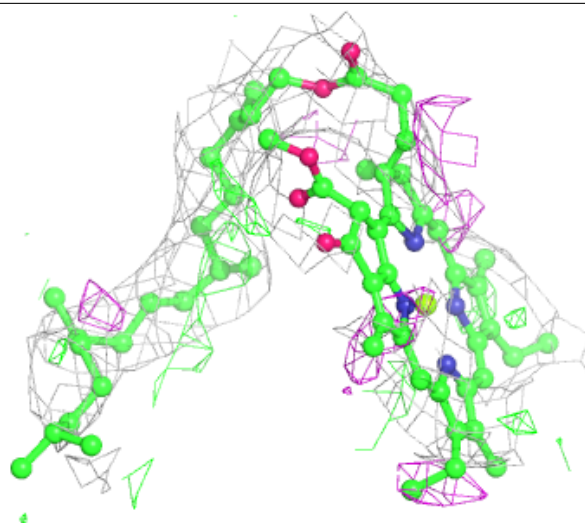
Electron density around BCR t 101:

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



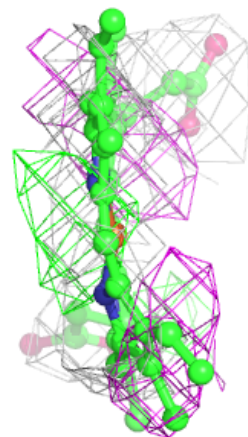
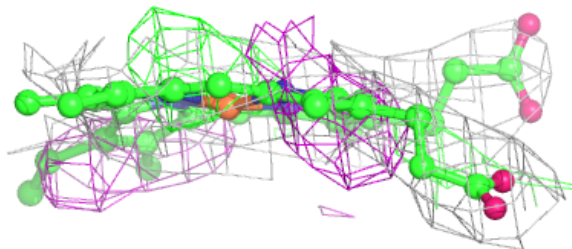
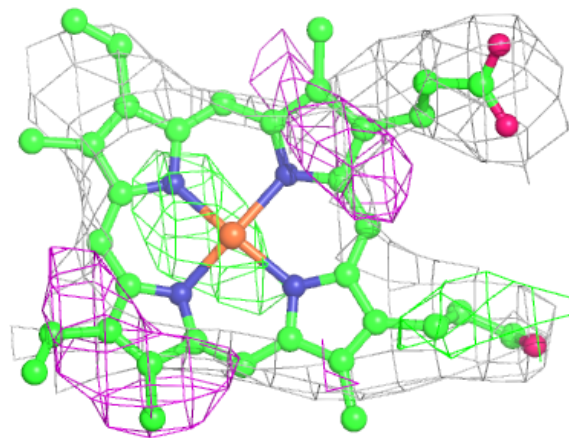
Electron density around CLA B 614:

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



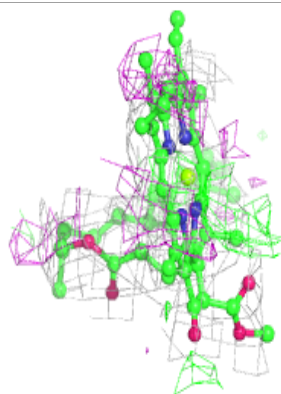
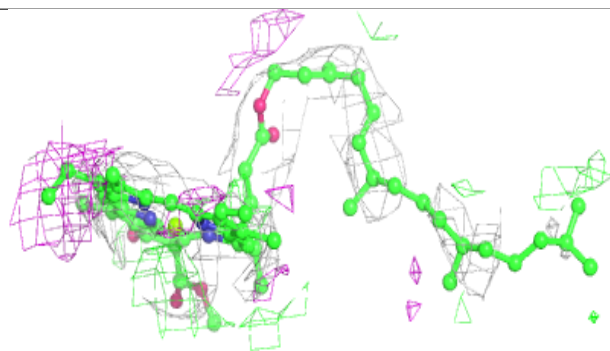
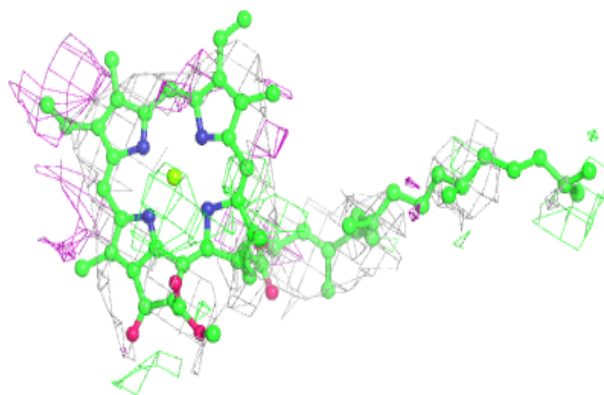
Electron density around HEM v 201:

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

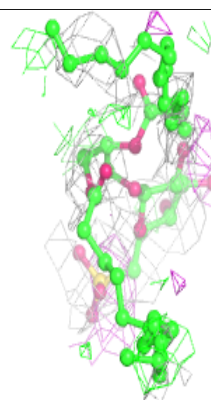
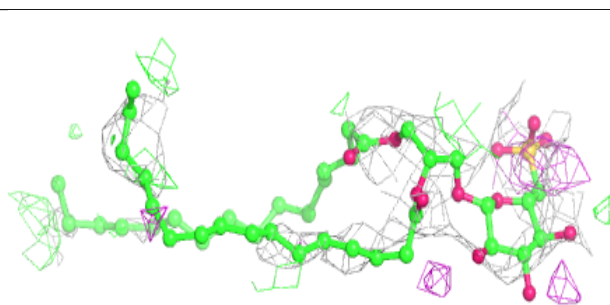
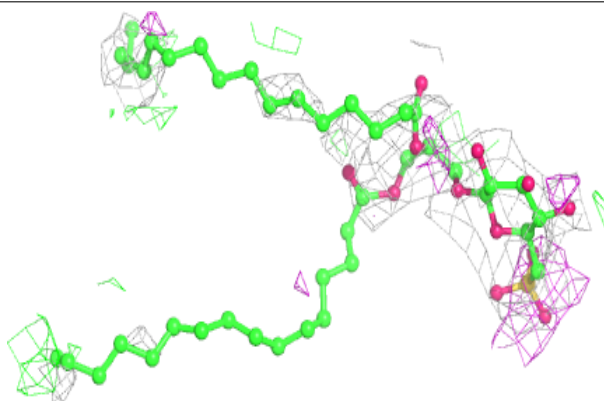


Electron density around CLA a 607:

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

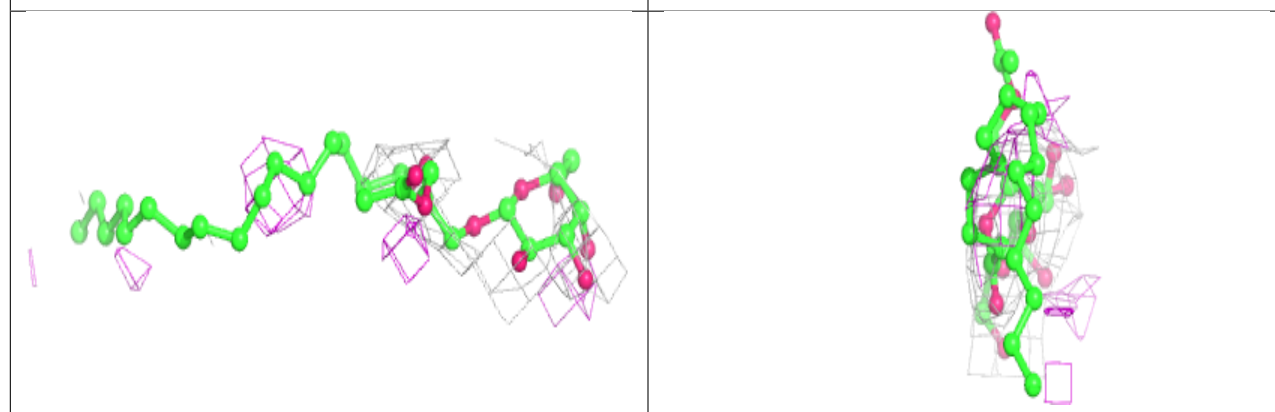
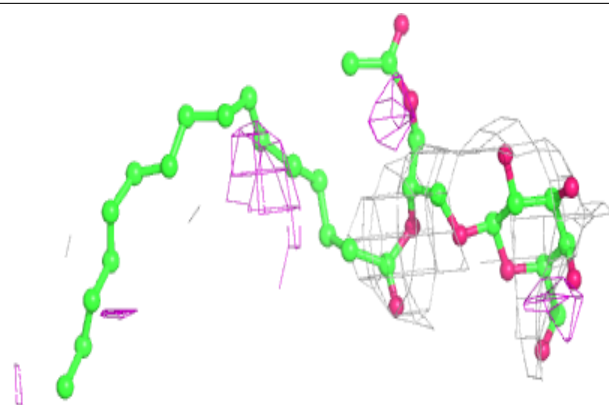
**Electron density around SQD a 614:**

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

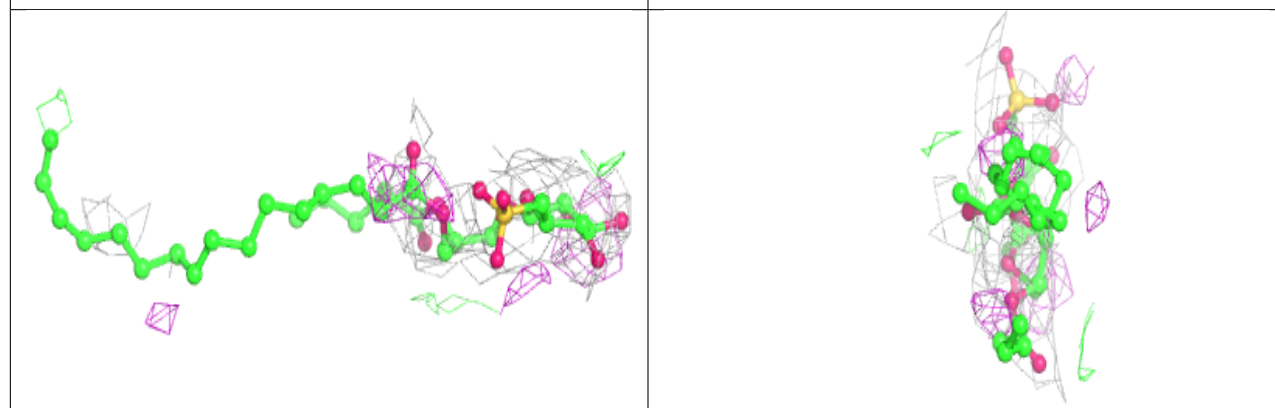
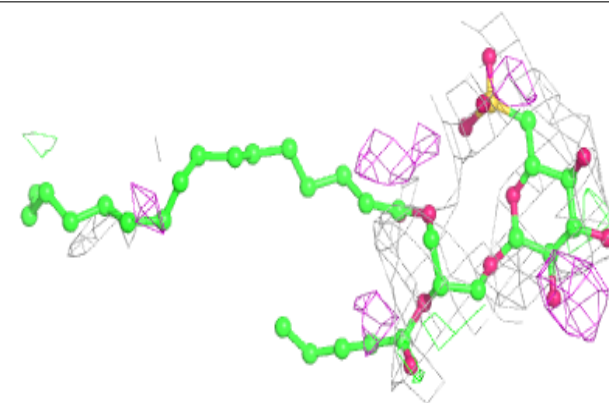


Electron density around LMG z 101:

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

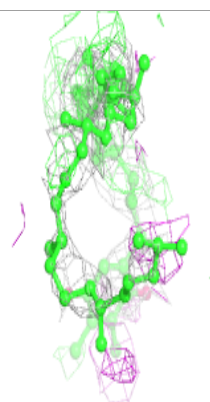
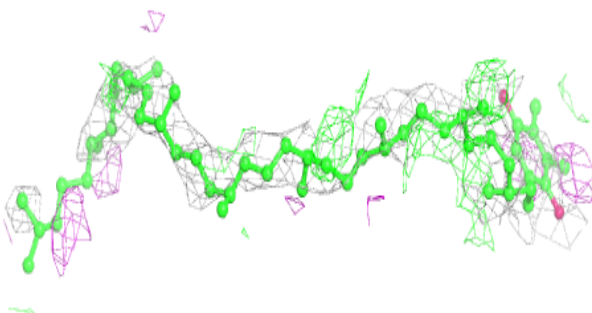
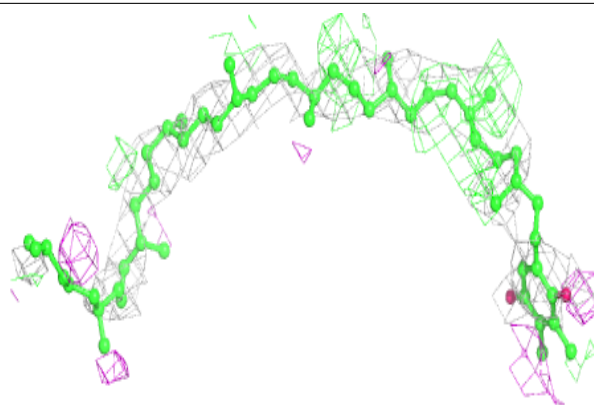
**Electron density around SQD X 101:**

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

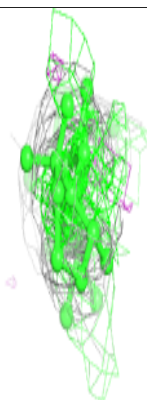
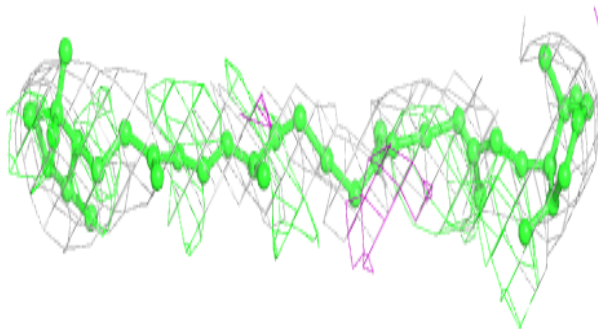
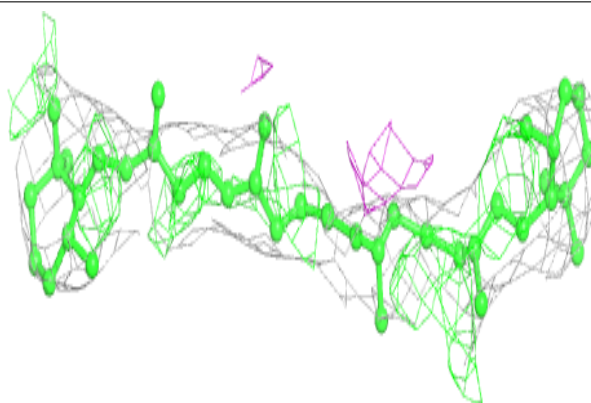


Electron density around PL9 a 611:

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

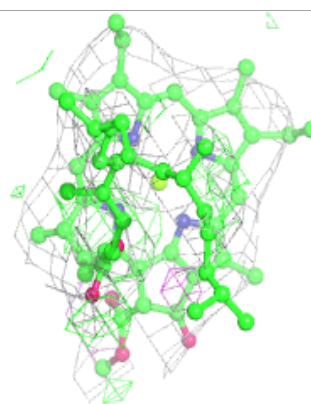
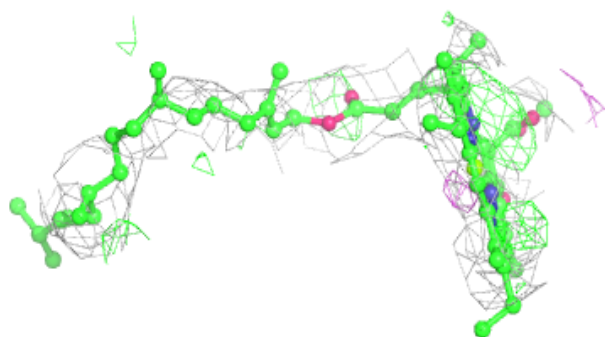
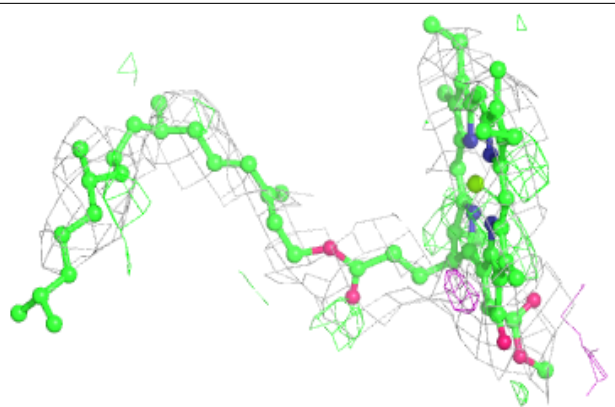
**Electron density around BCR b 620:**

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



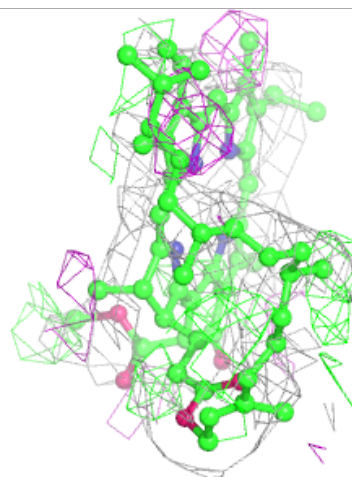
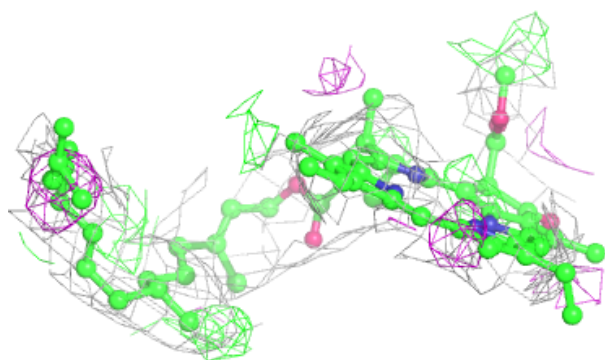
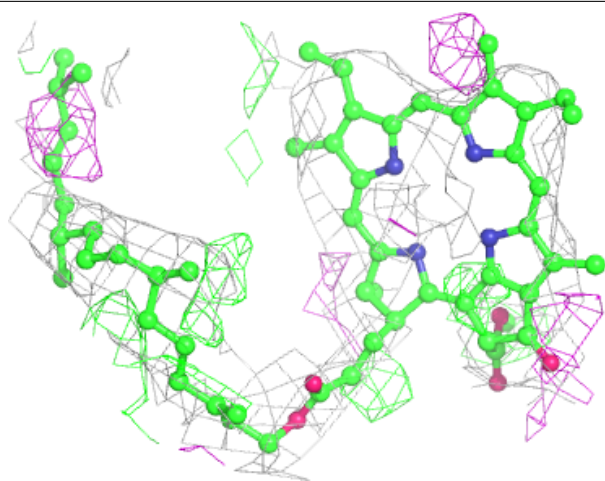
Electron density around CLA D 404:

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



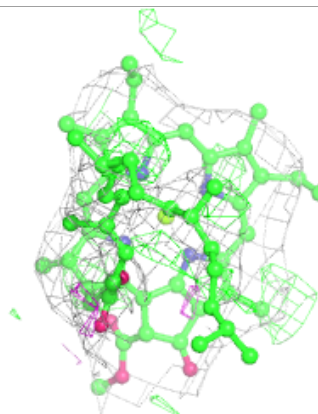
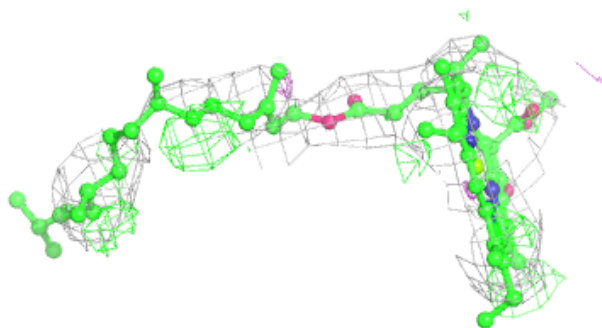
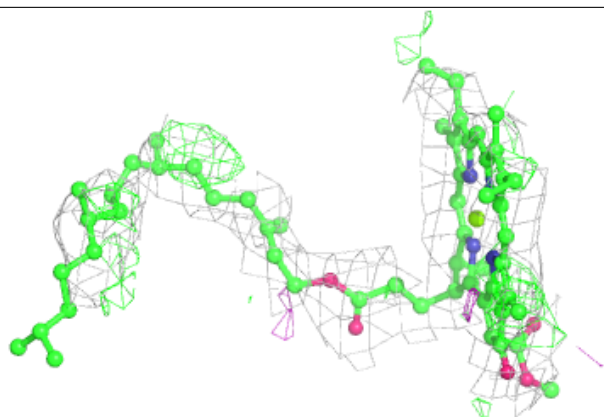
Electron density around PHO D 401:

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

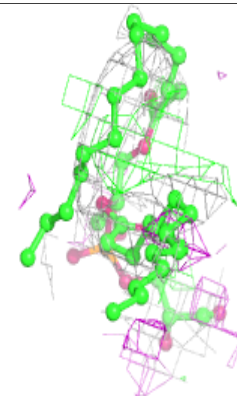
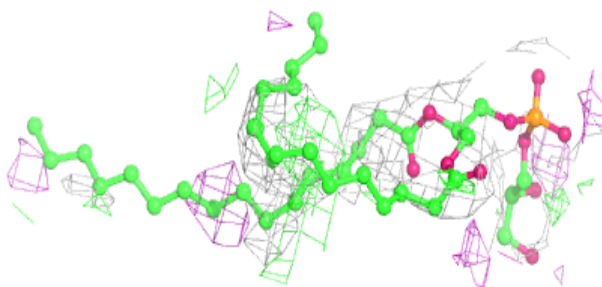
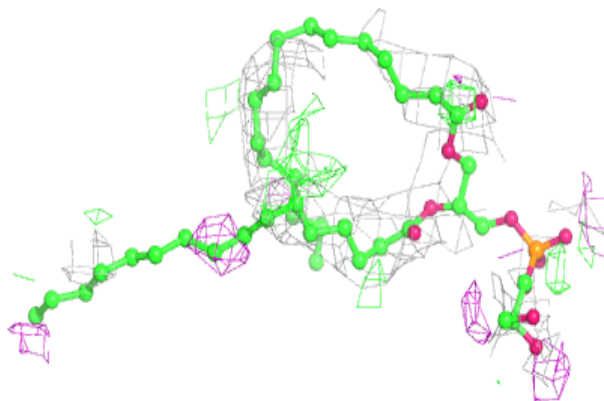


Electron density around CLA d 403:

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

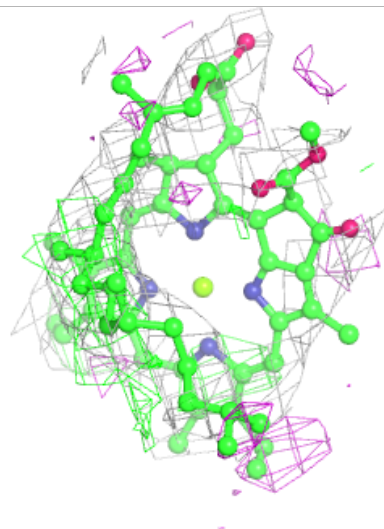
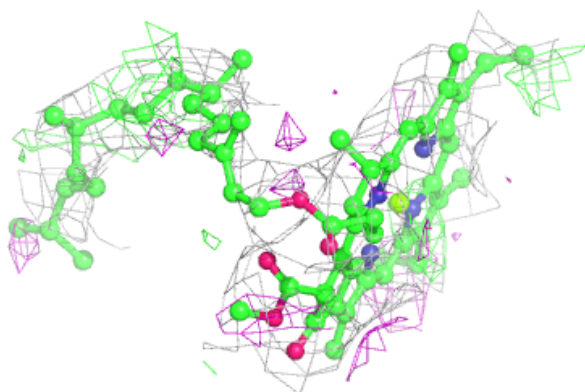
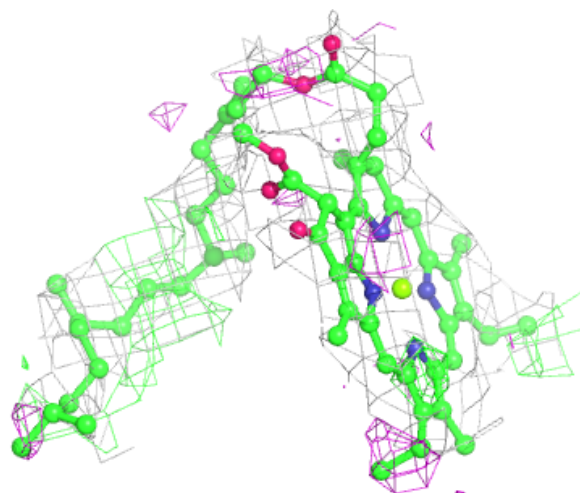
**Electron density around LHG d 406:**

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



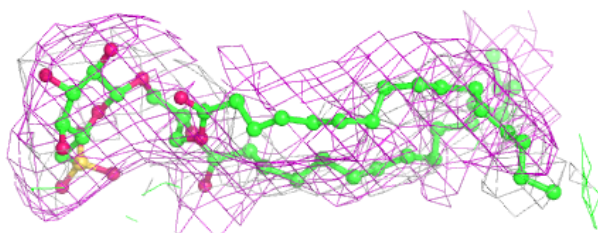
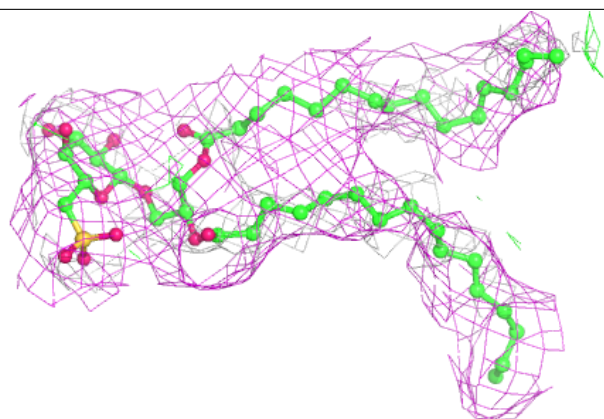
Electron density around CLA b 615:

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

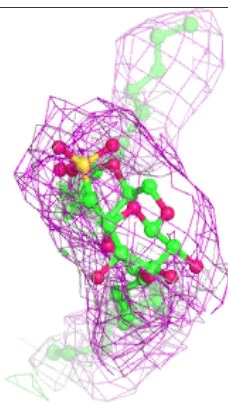
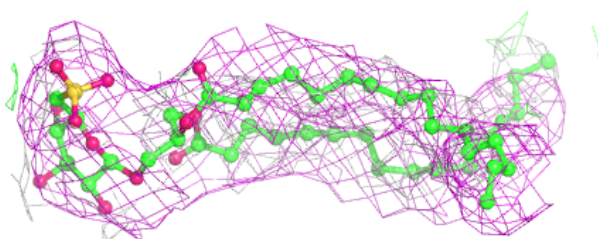
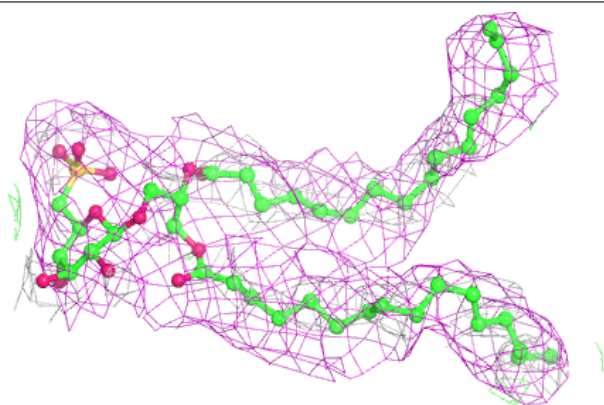


Electron density around SQD b 601:

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

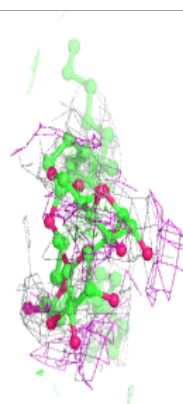
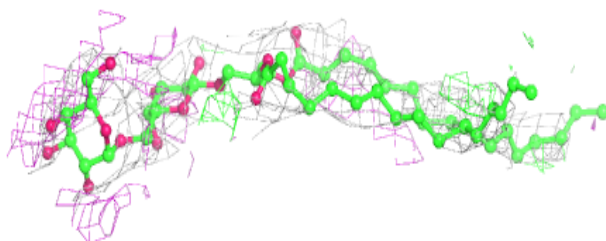
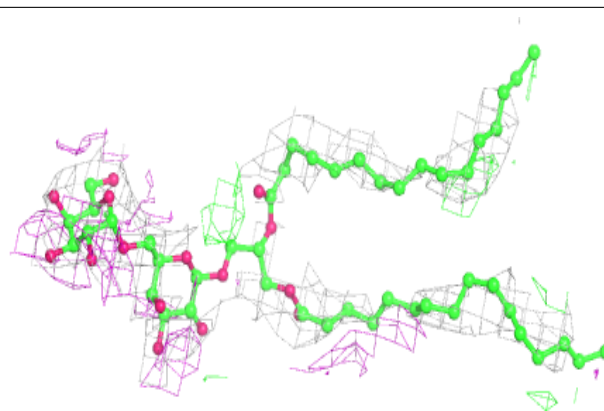
**Electron density around SQD B 622:**

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

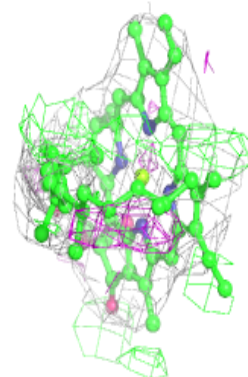
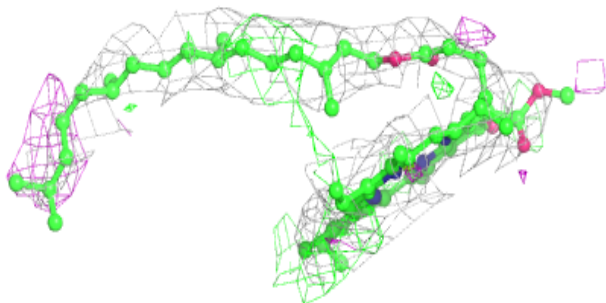
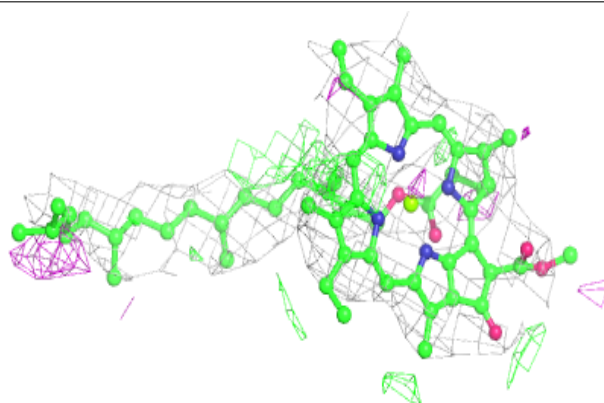


Electron density around DGD C 517:

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

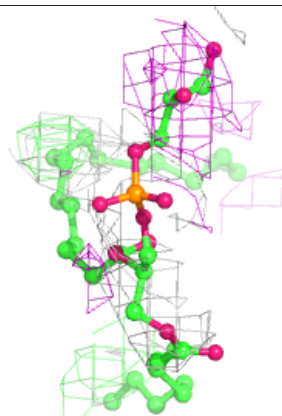
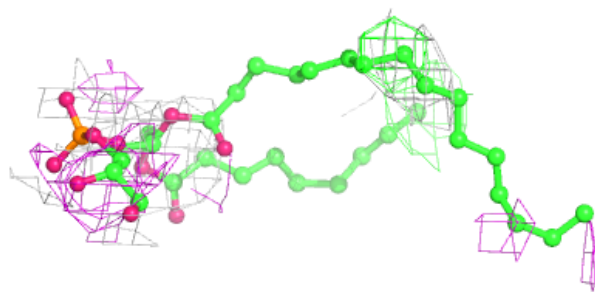
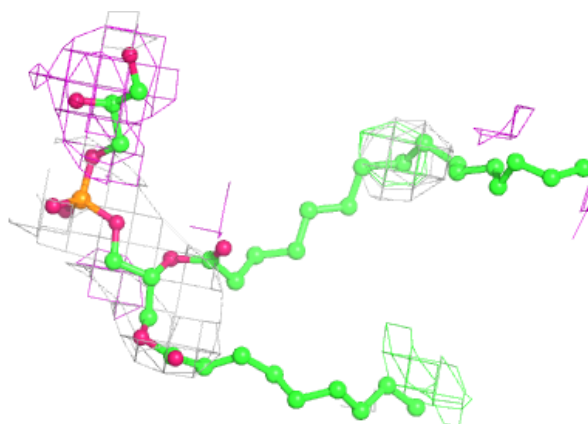
**Electron density around CLA B 609:**

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



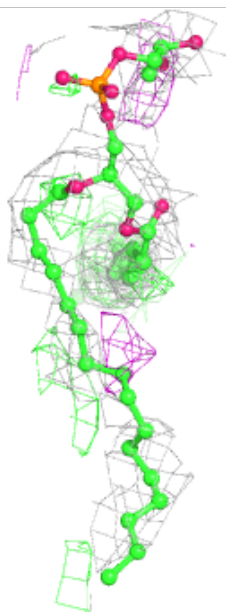
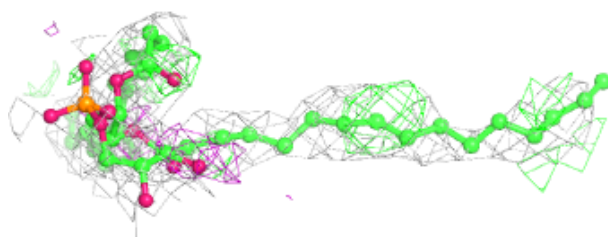
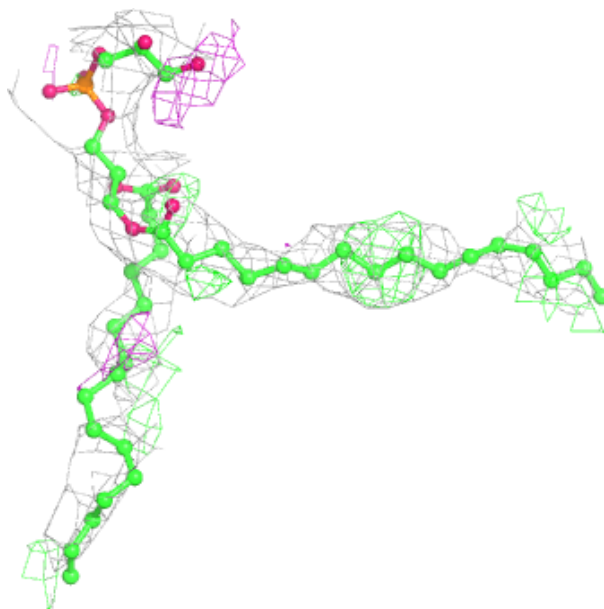
Electron density around LHG e 101:

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



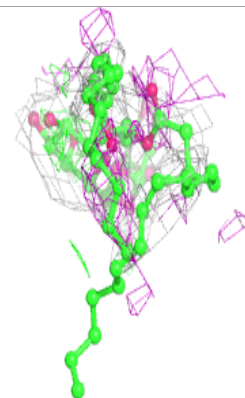
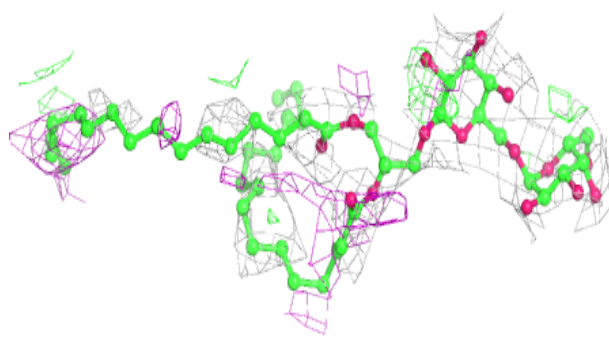
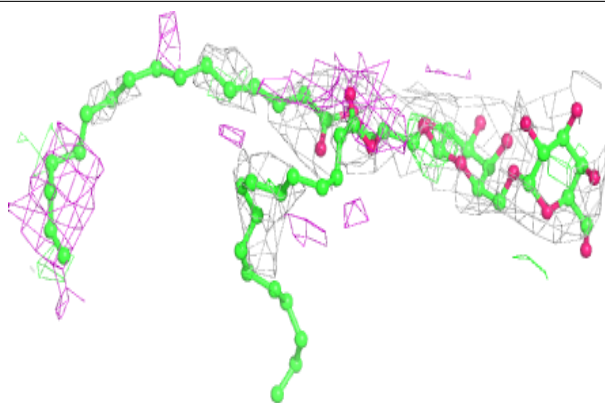
Electron density around LHG L 101:

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

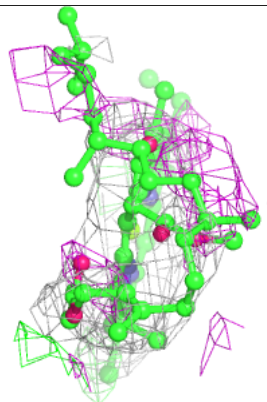
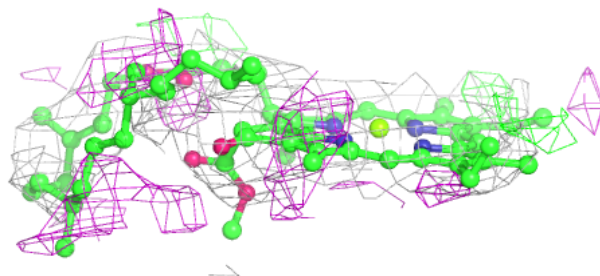
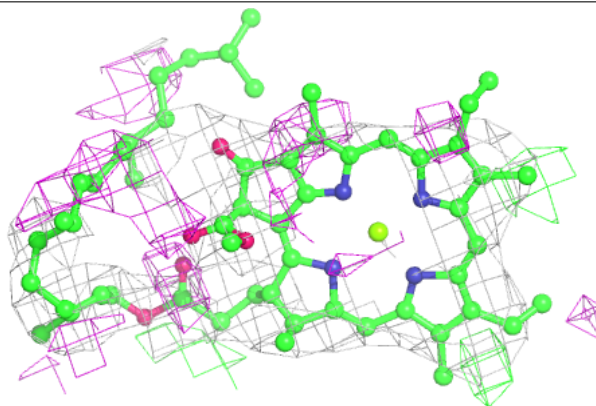


Electron density around DGD h 102:

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

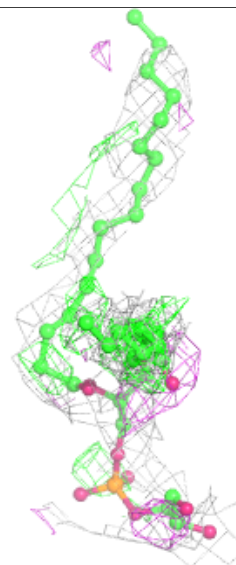
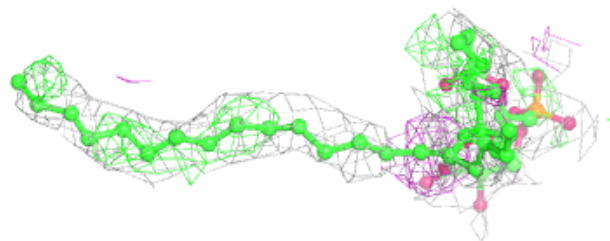
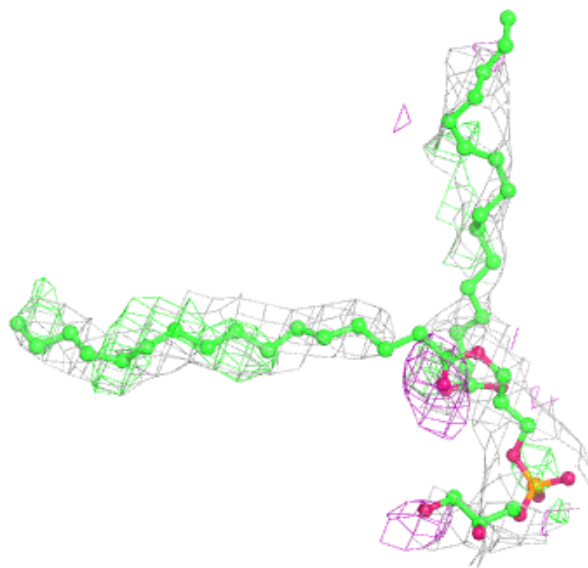
**Electron density around CLA b 612:**

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



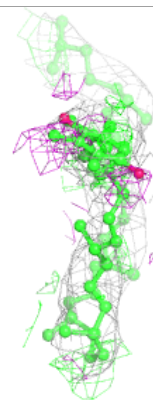
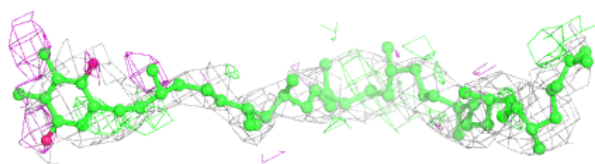
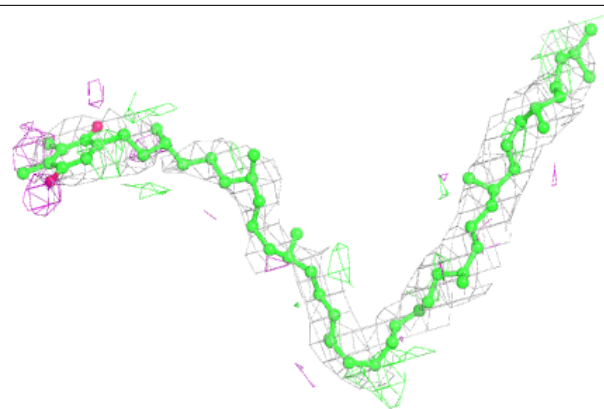
Electron density around LHG 1 102:

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

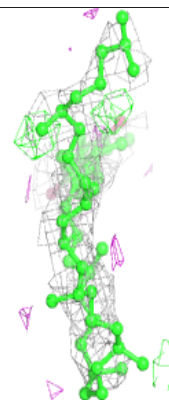
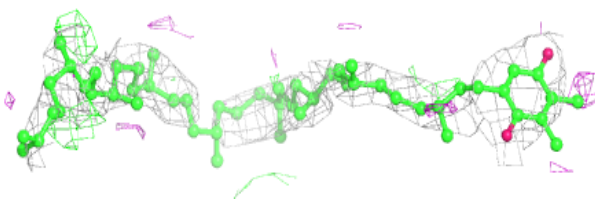
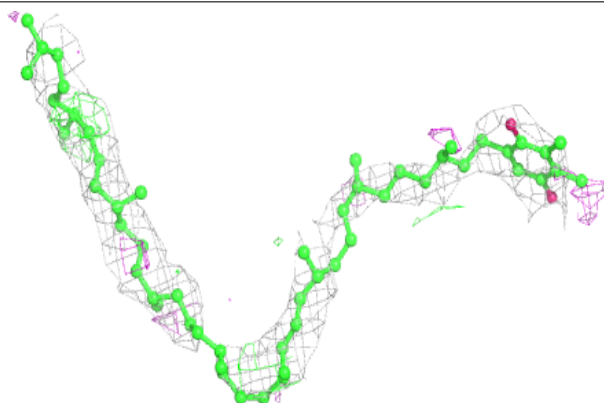


Electron density around PL9 D 405:

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

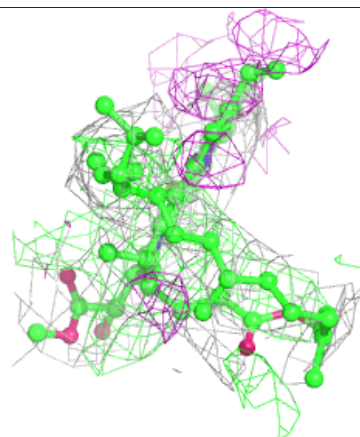
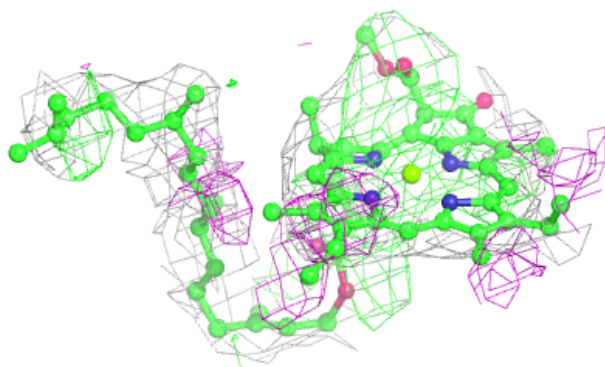
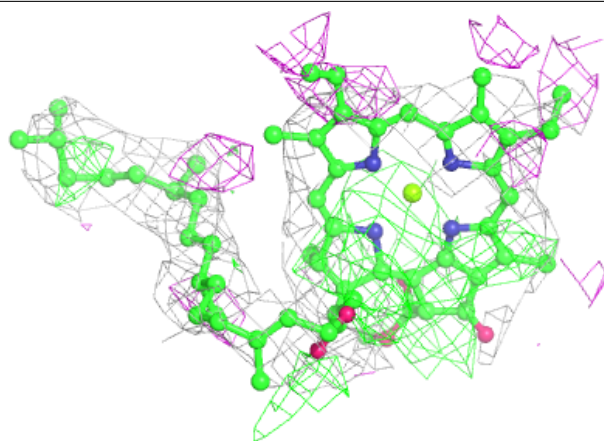
**Electron density around PL9 d 404:**

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

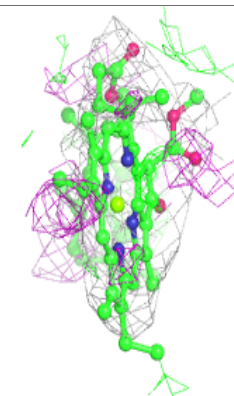
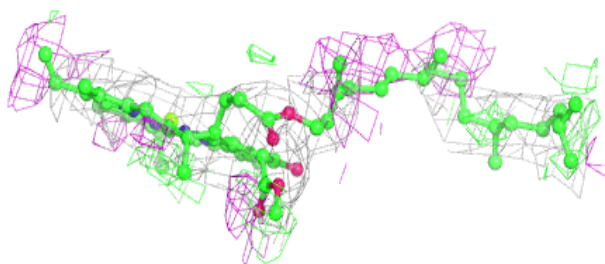
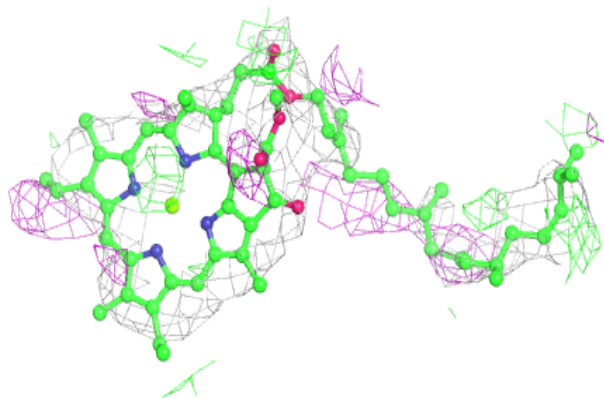


Electron density around CLA D 402:

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

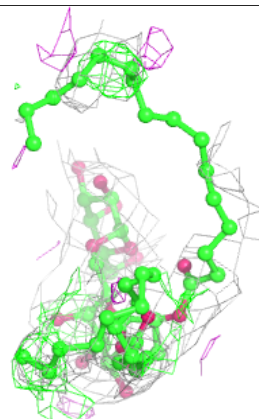
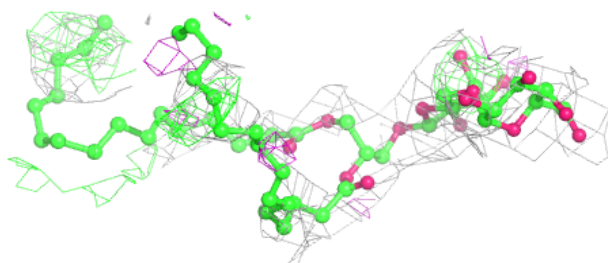
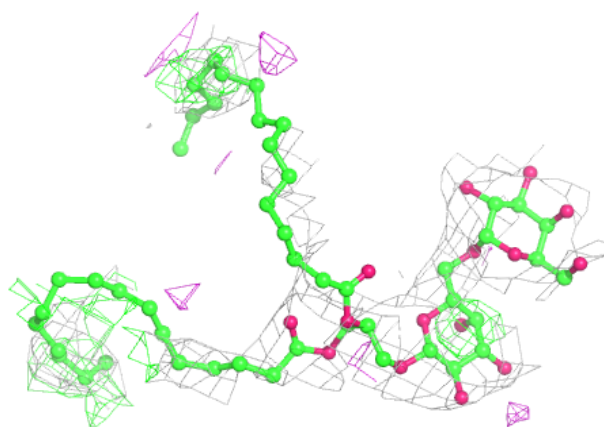
**Electron density around CLA B 603:**

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

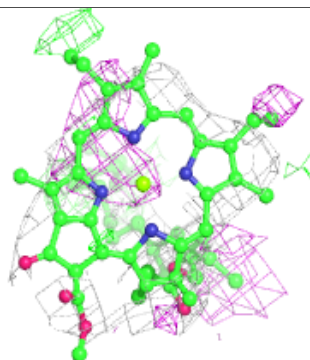
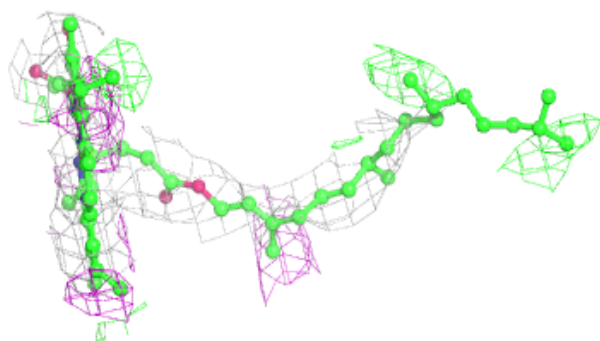
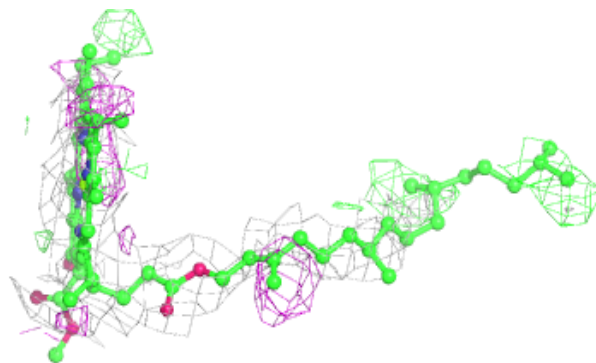


Electron density around DGD c 517:

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

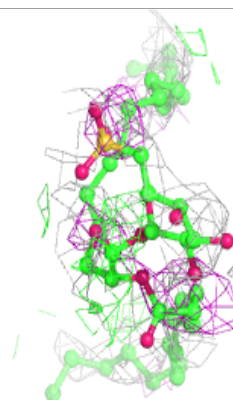
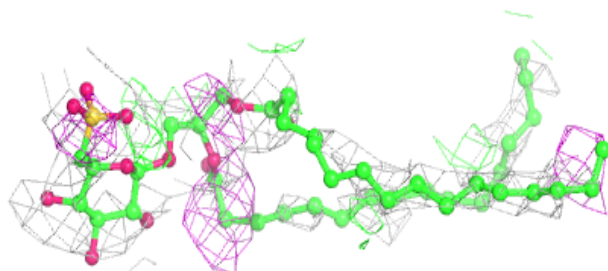
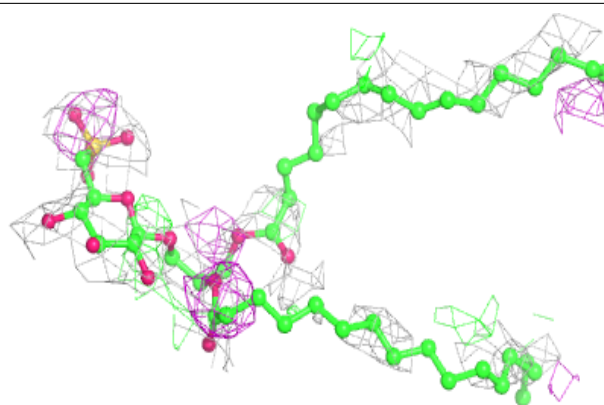
**Electron density around CLA b 608 (A):**

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

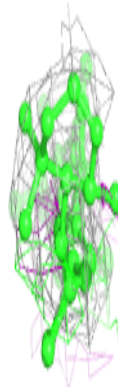
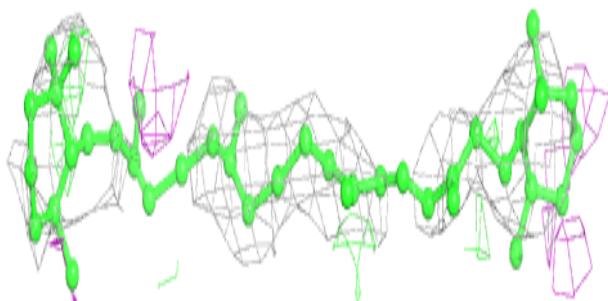
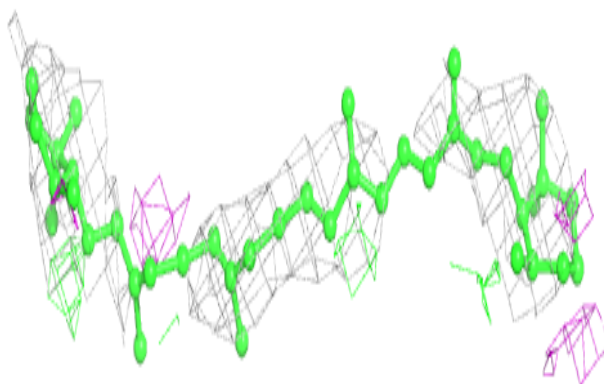


Electron density around SQD A 614:

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

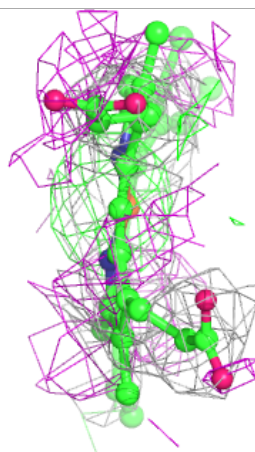
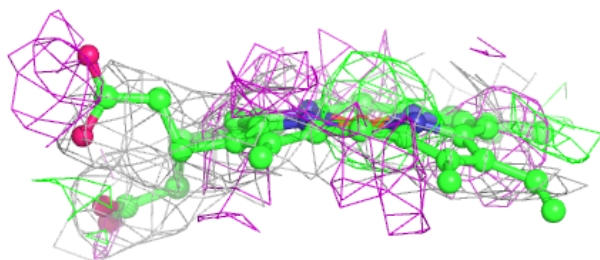
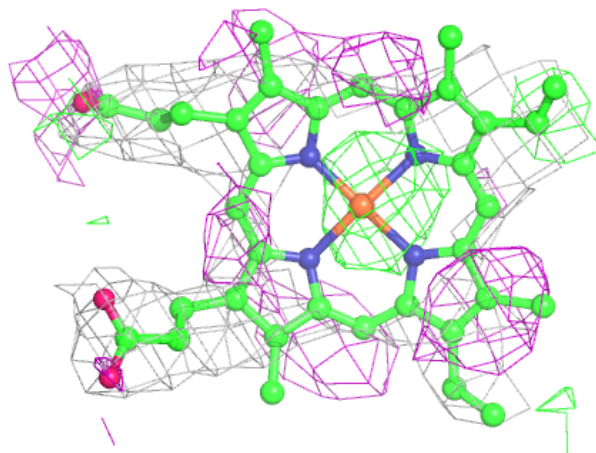
**Electron density around BCR C 514:**

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



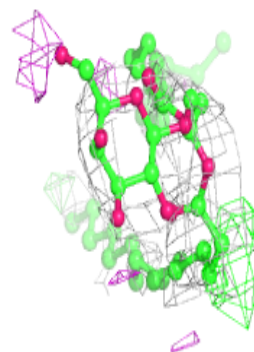
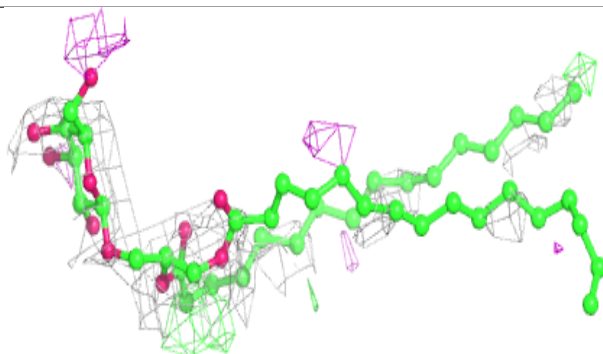
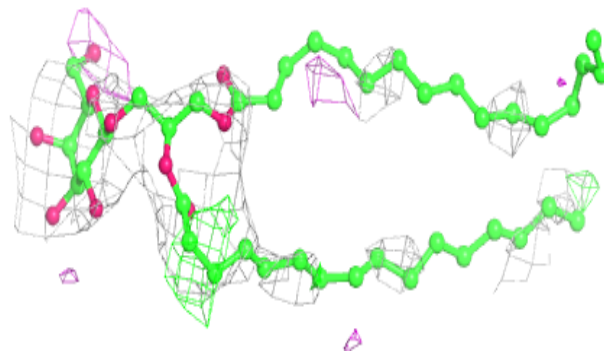
Electron density around HEM V 201:

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

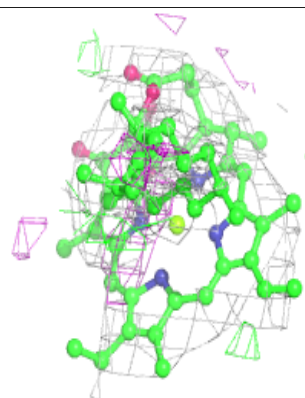
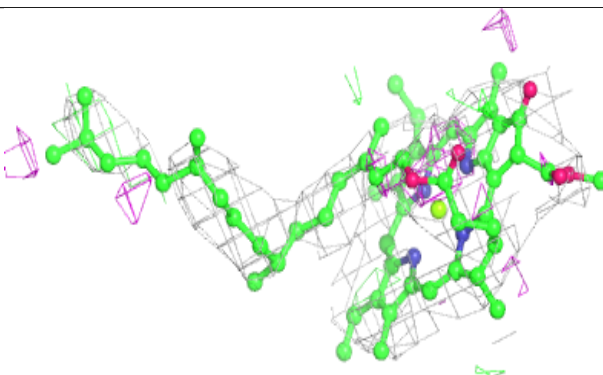
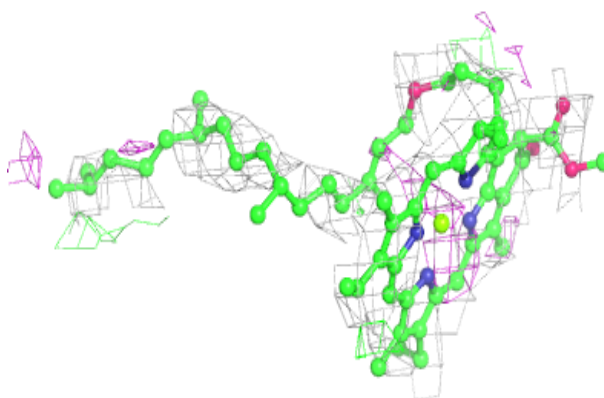


Electron density around LMG C 519:

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

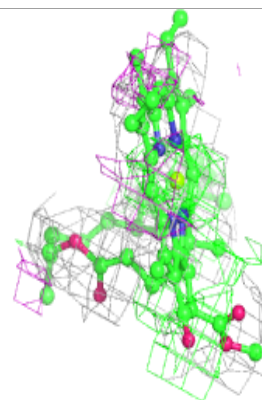
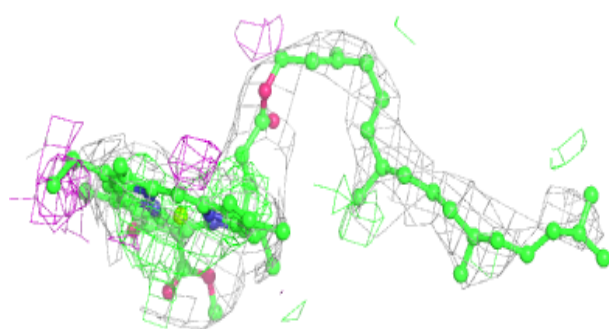
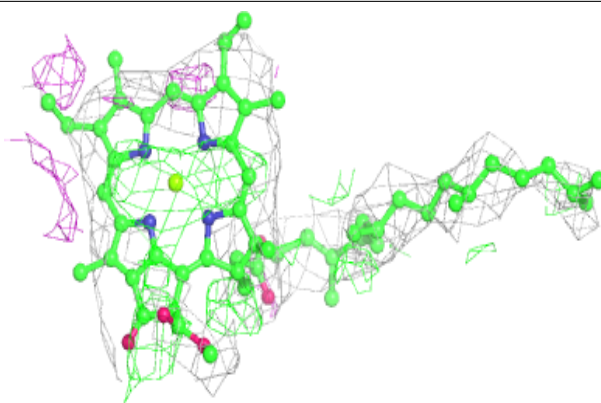
**Electron density around CLA c 505:**

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

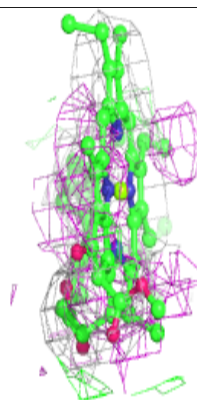
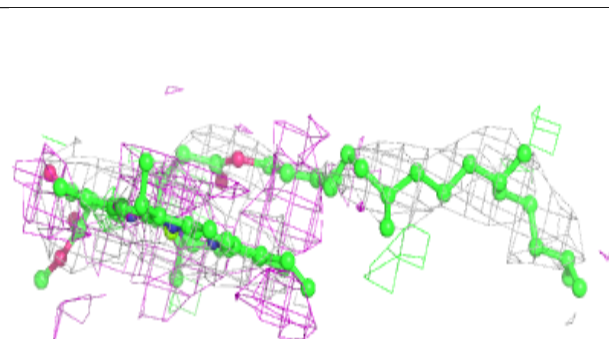
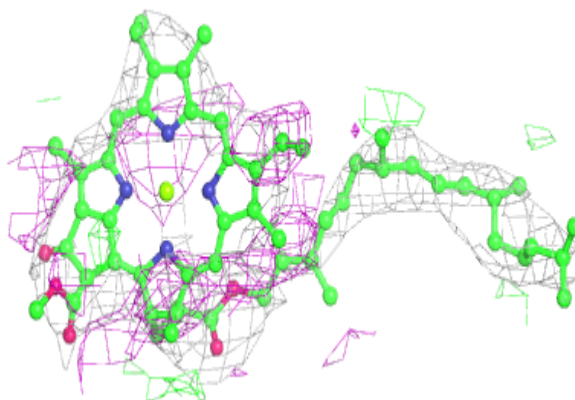


Electron density around CLA A 607:

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

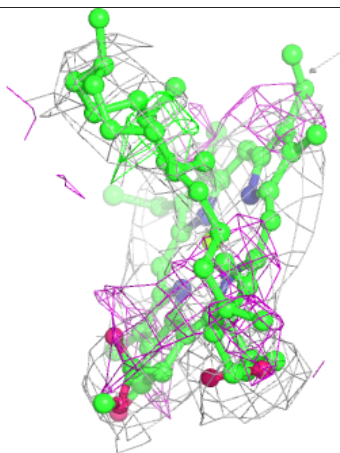
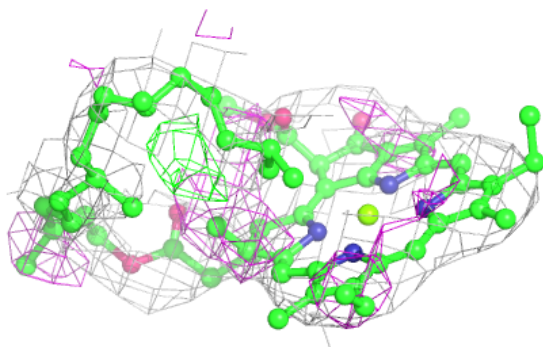
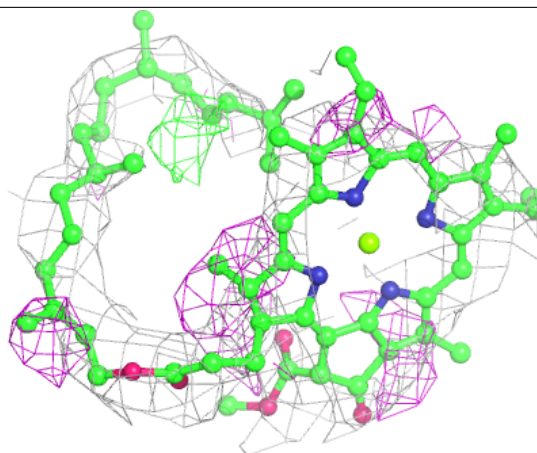
**Electron density around CLA B 604:**

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



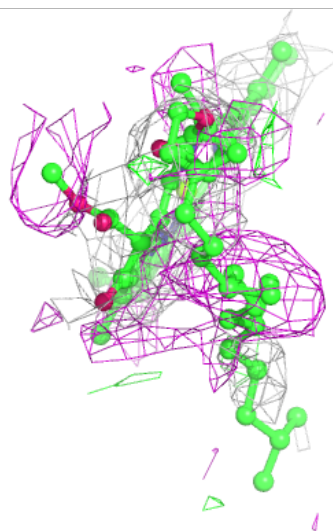
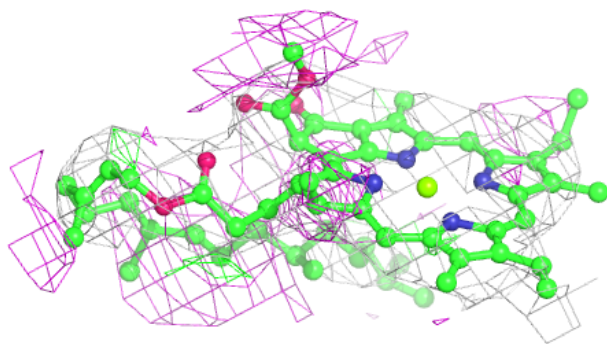
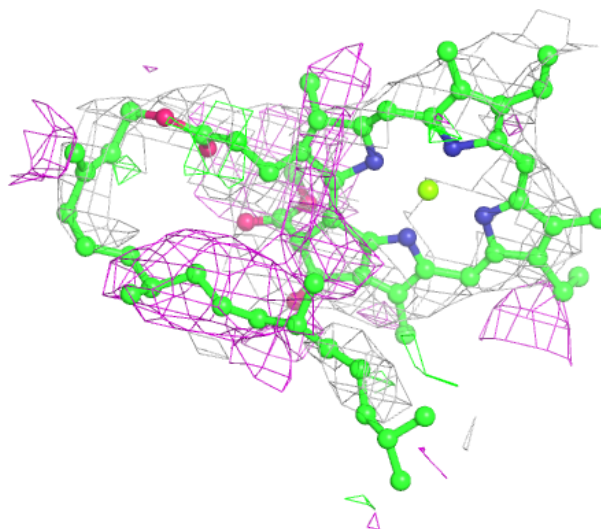
Electron density around CLA B 616:

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



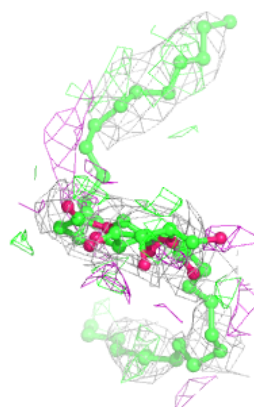
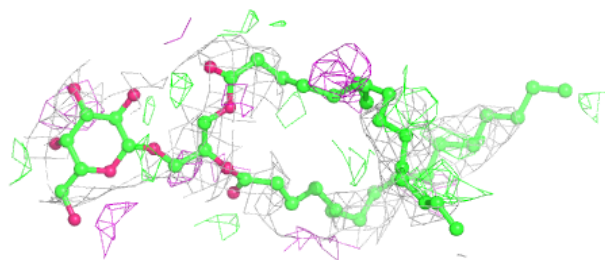
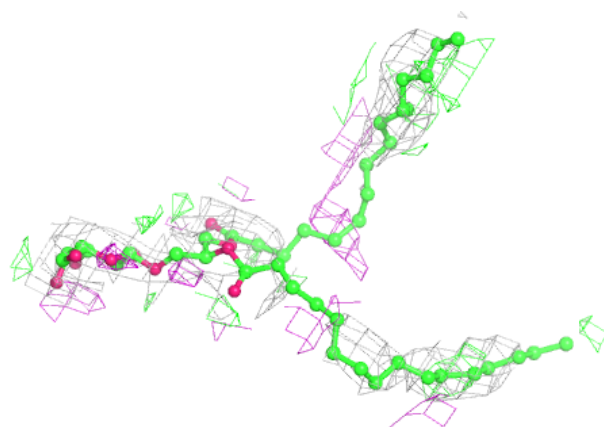
Electron density around CLA C 509:

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



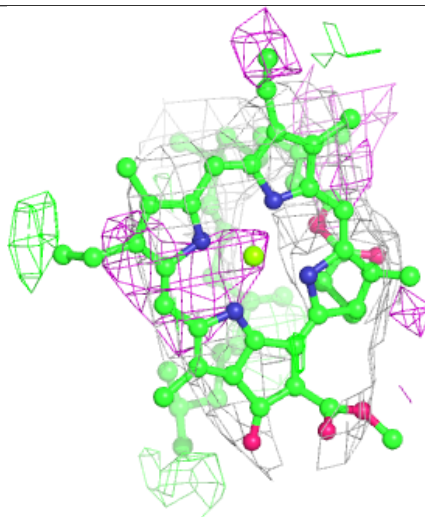
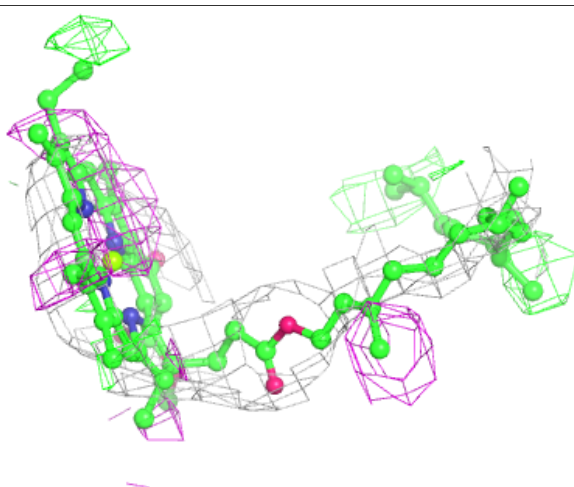
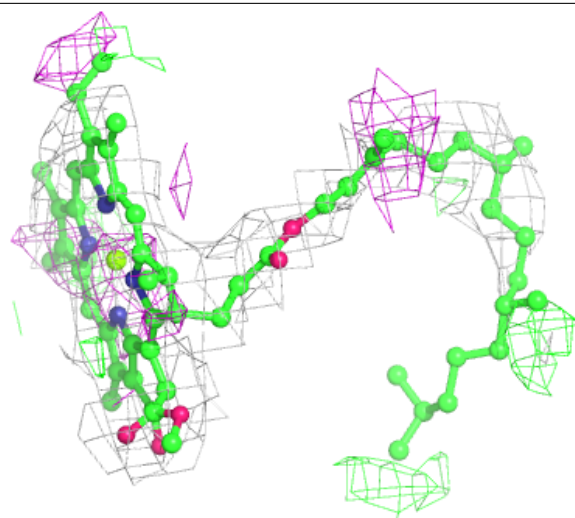
Electron density around LMG B 621:

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



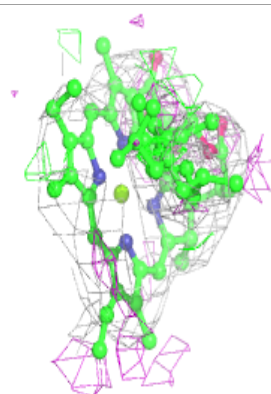
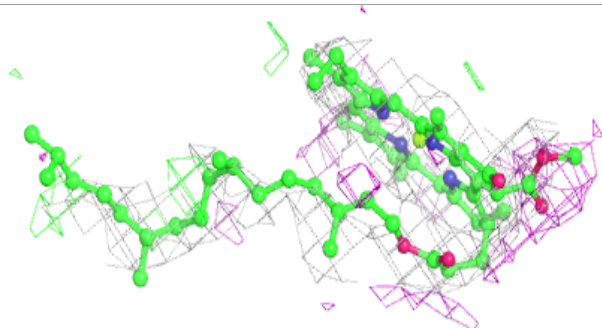
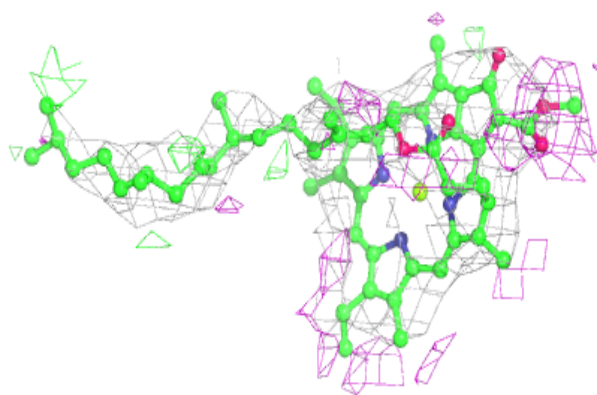
Electron density around CLA b 608 (B):

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

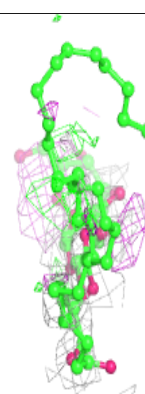
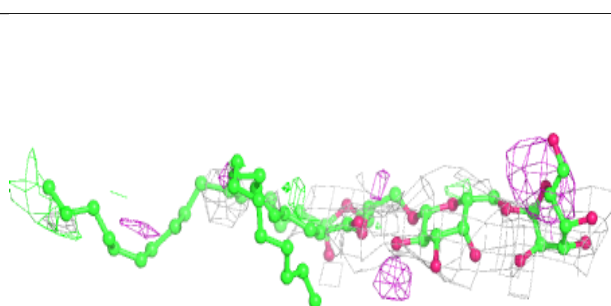
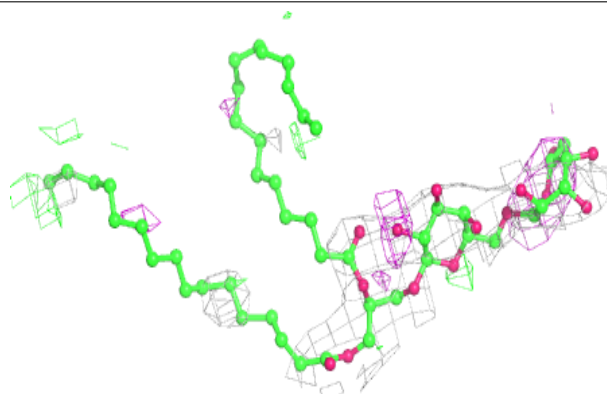


Electron density around CLA B 615:

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

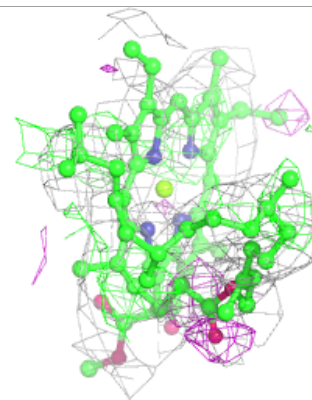
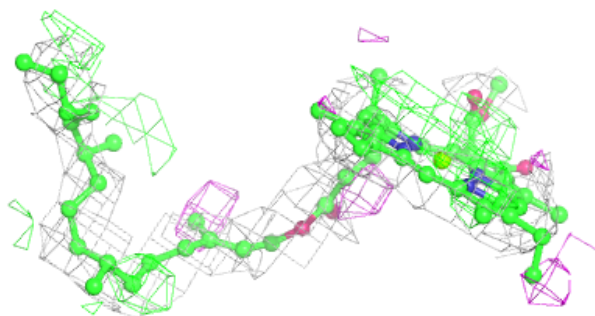
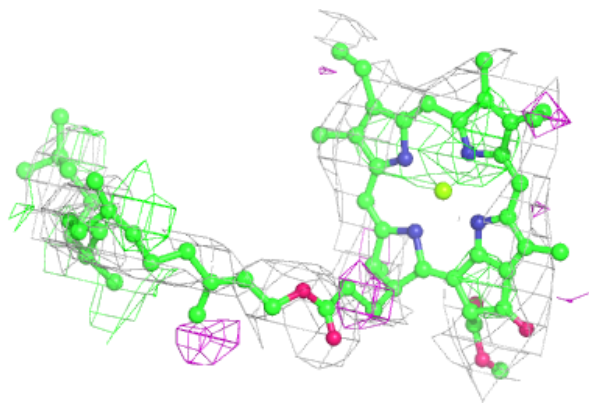
**Electron density around DGD E 101:**

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

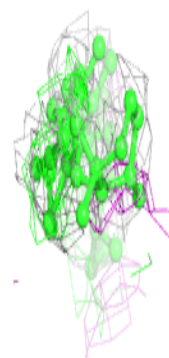
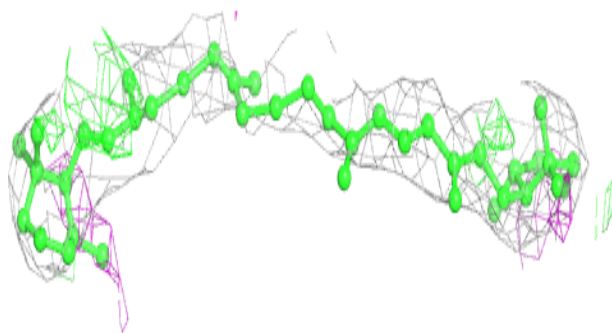
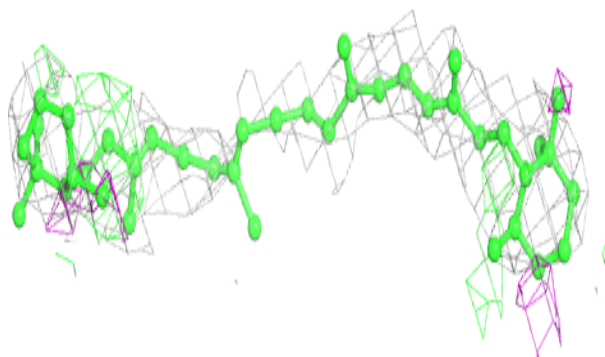


Electron density around CLA A 609:

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

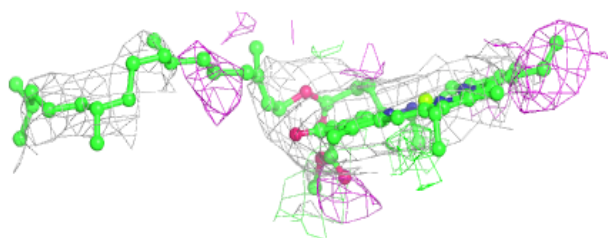
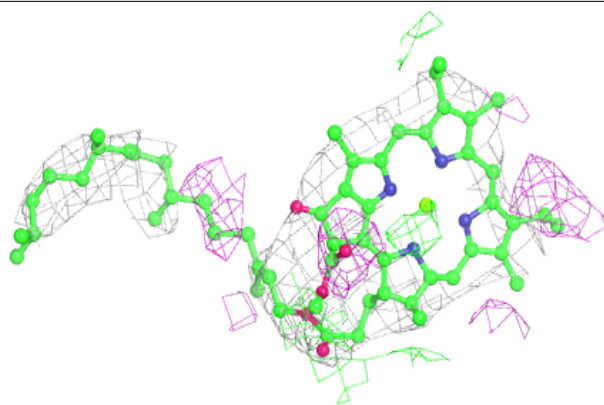
**Electron density around BCR f 101:**

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

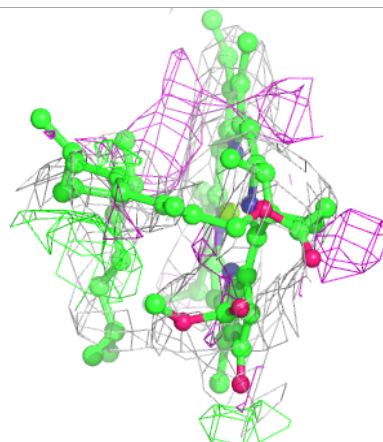
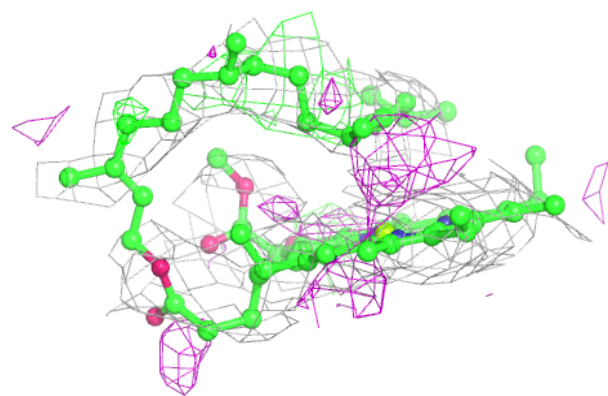
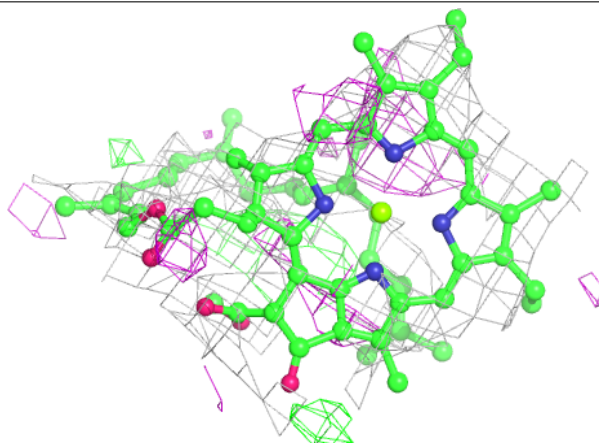


Electron density around CLA b 604:

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

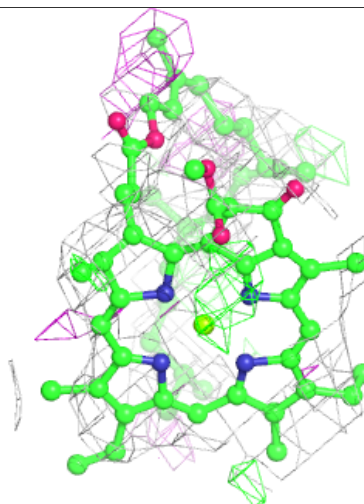
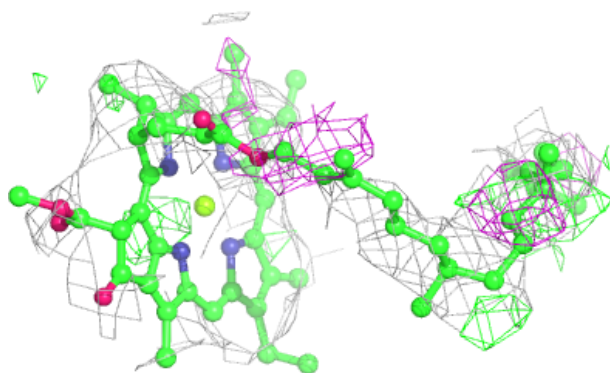
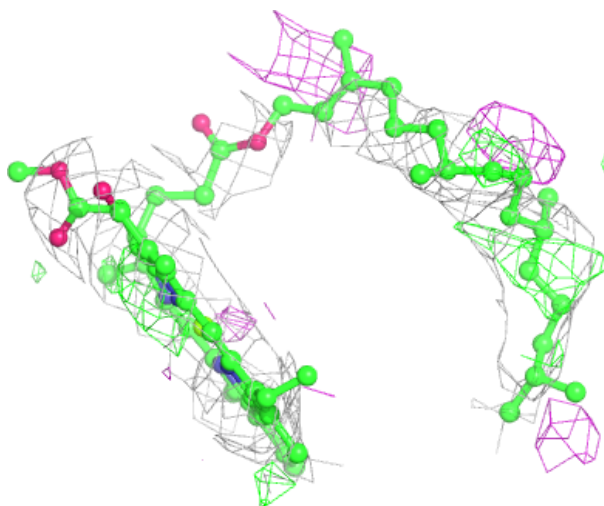
**Electron density around CLA c 510:**

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



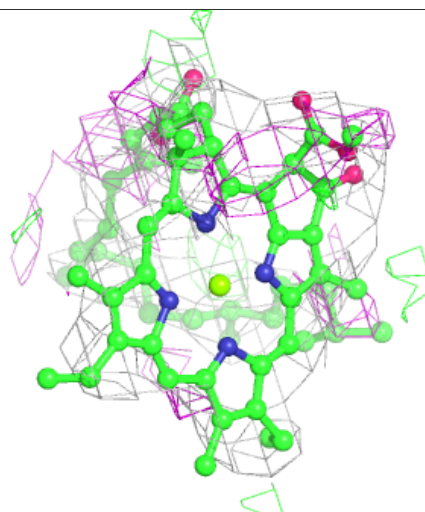
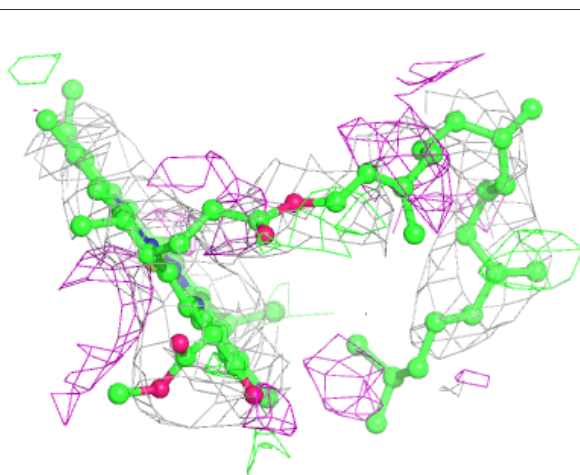
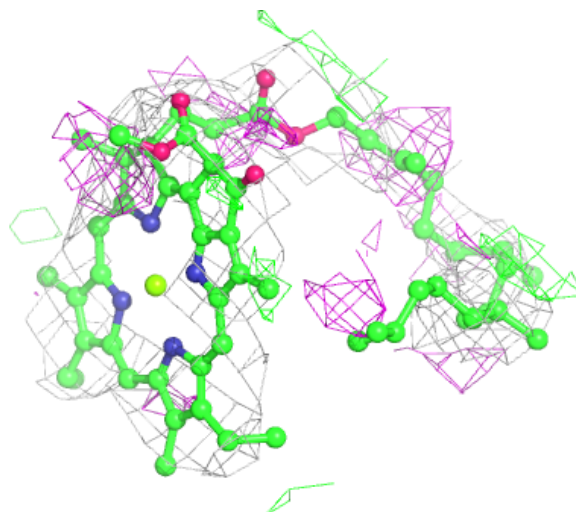
Electron density around CLA b 613:

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



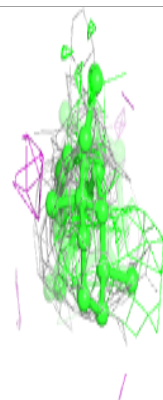
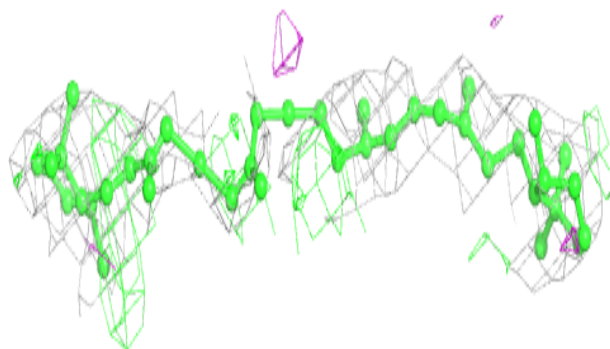
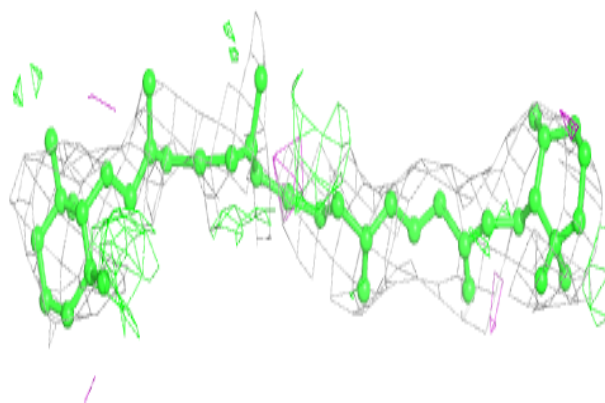
Electron density around CLA C 503:

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



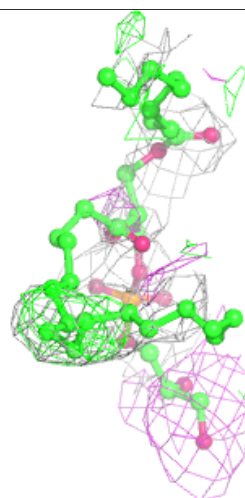
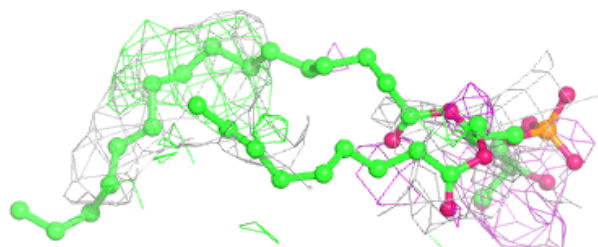
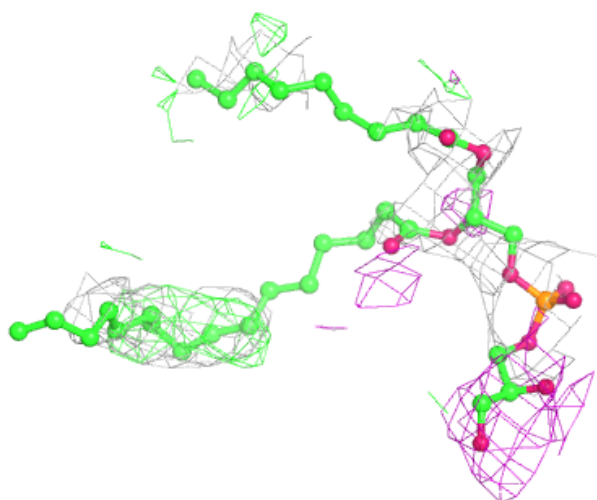
Electron density around BCR b 621:

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



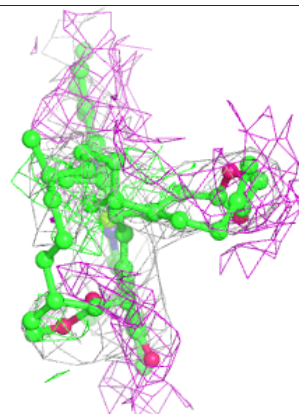
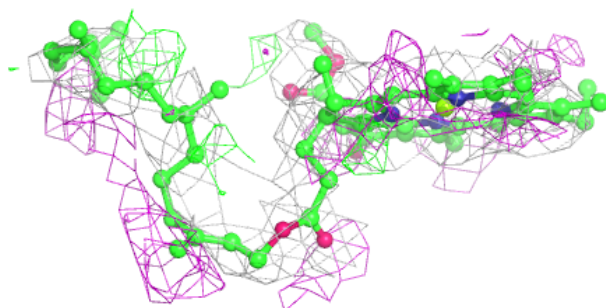
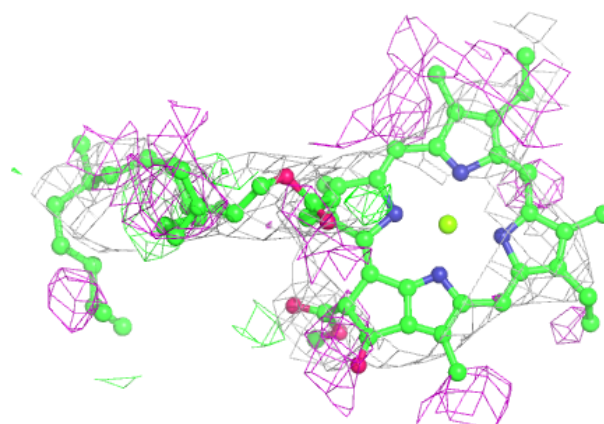
Electron density around LHG E 102:

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

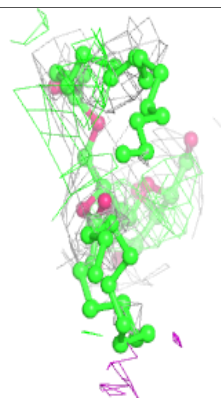
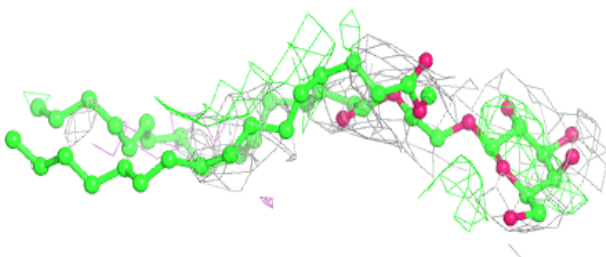
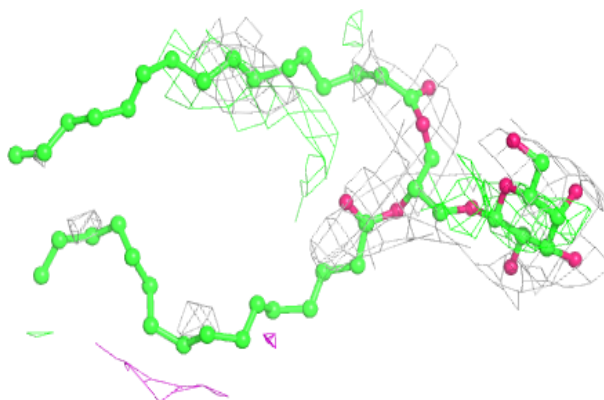


Electron density around CLA b 614:

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

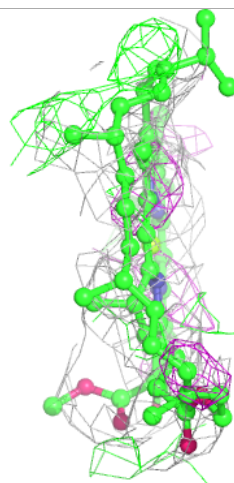
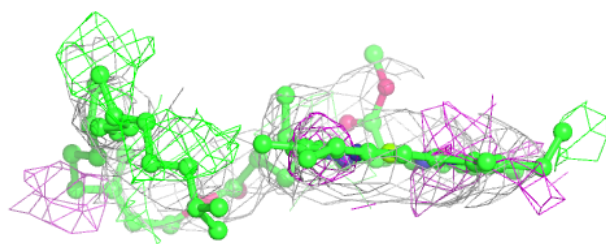
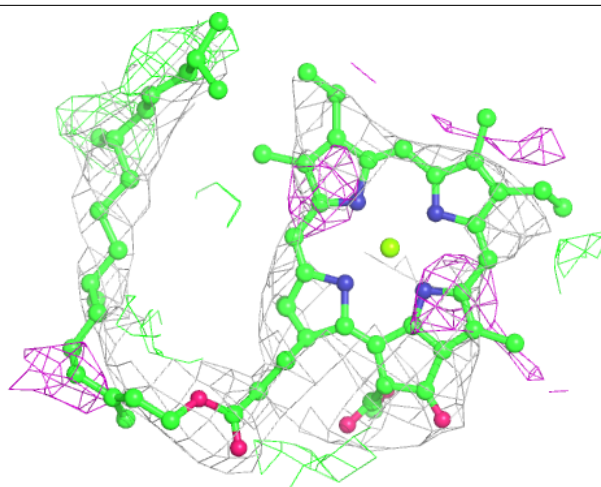
**Electron density around LMG a 613:**

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



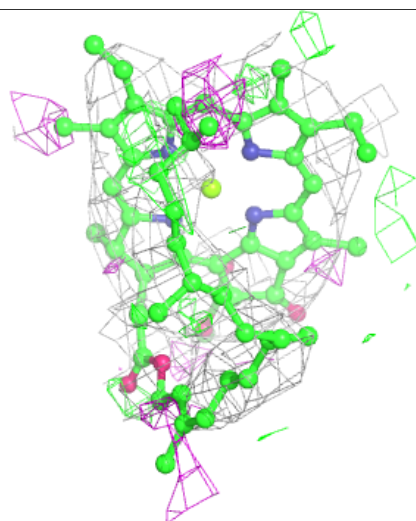
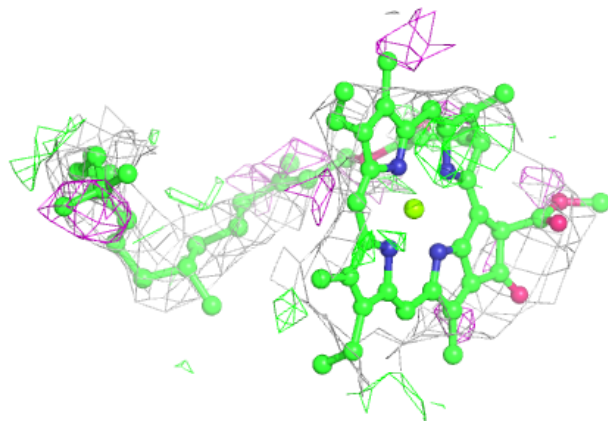
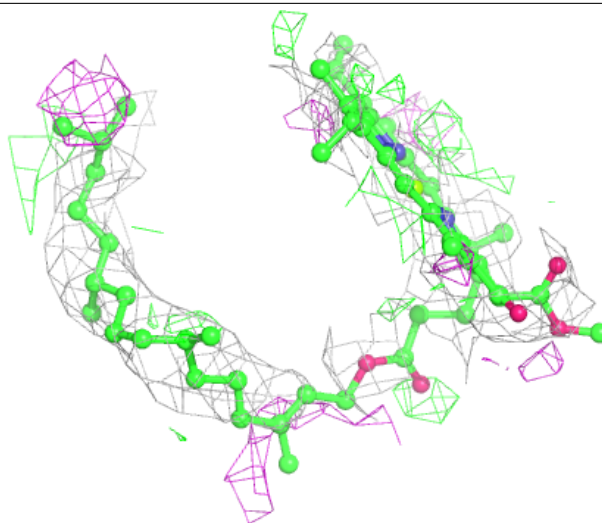
Electron density around CLA c 512:

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



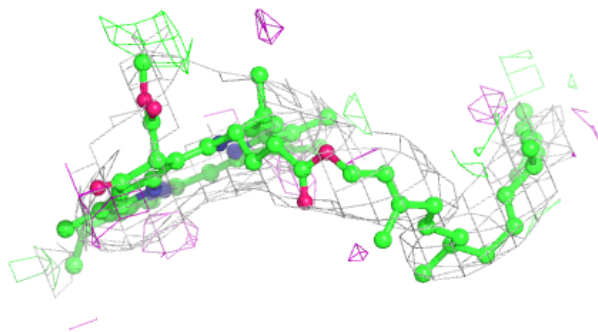
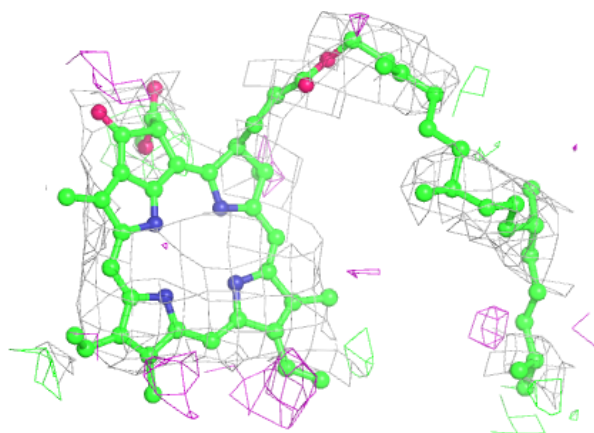
Electron density around CLA B 612:

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



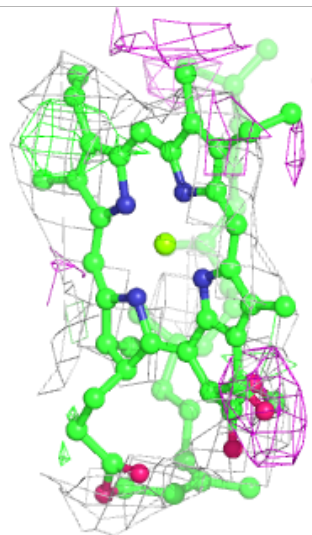
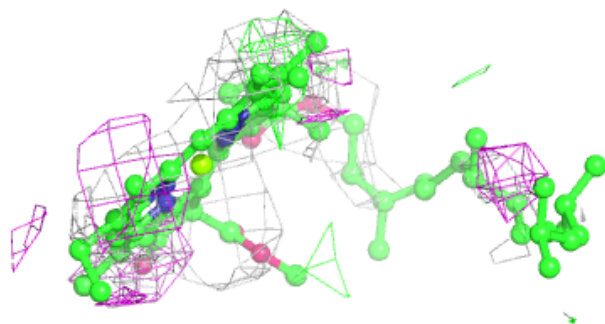
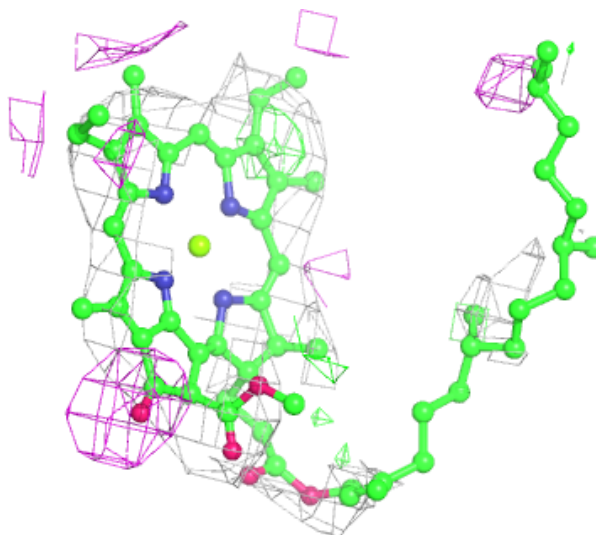
Electron density around PHO d 401:

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



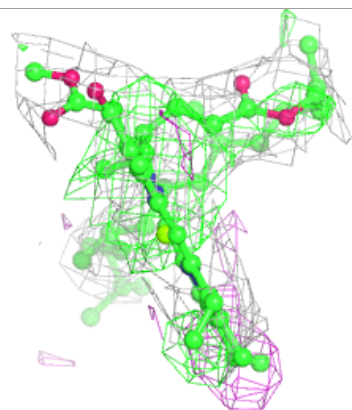
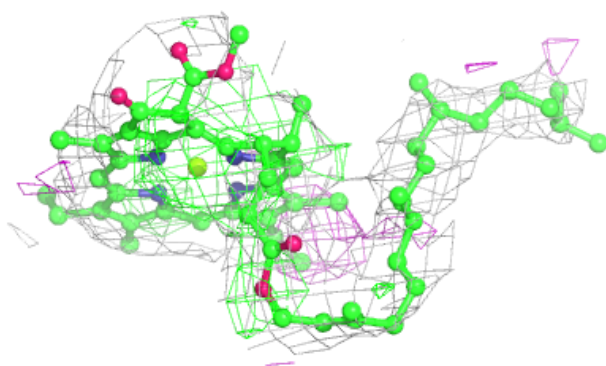
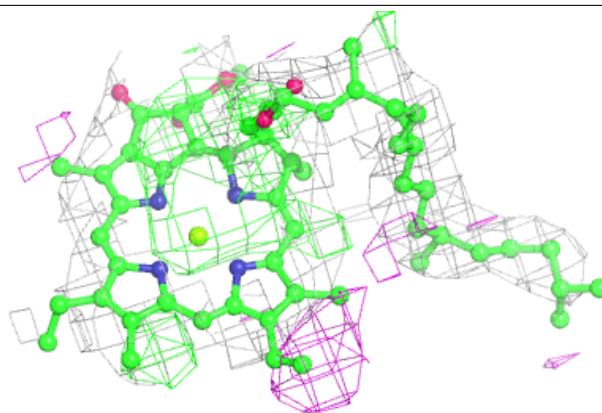
Electron density around CLA b 618:

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



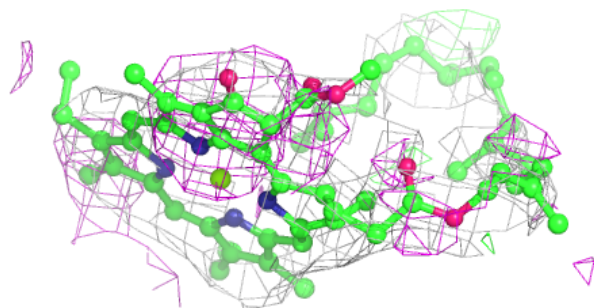
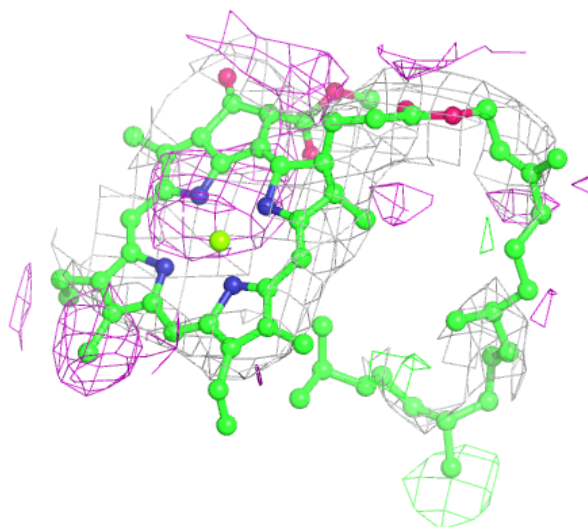
Electron density around CLA a 615:

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



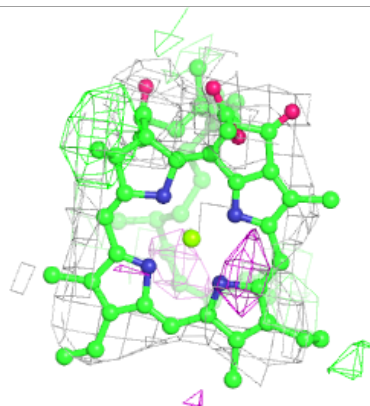
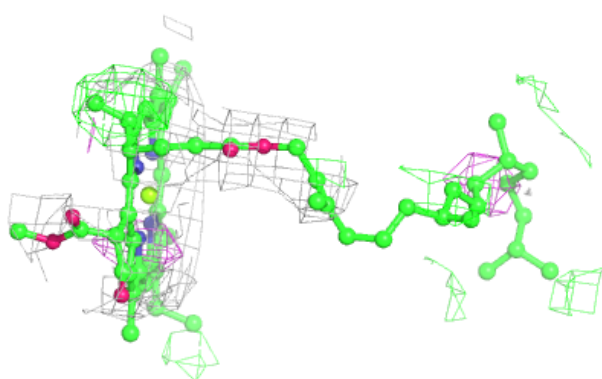
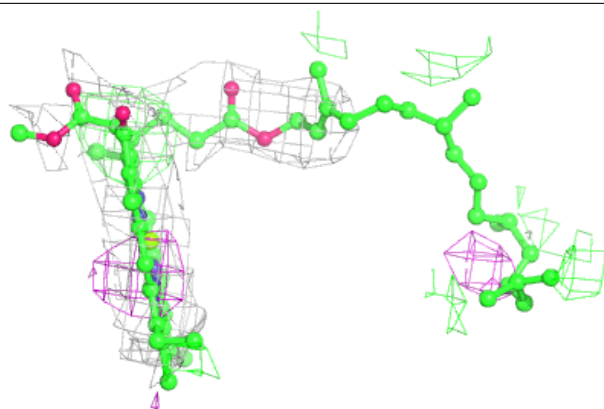
Electron density around CLA b 617:

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

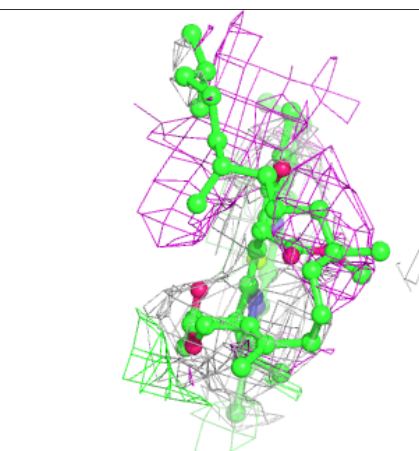
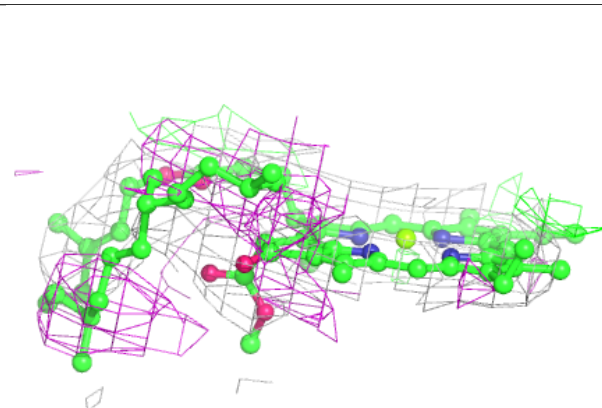
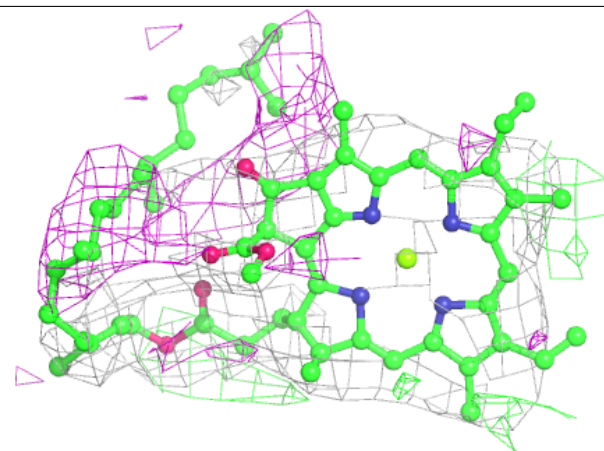


Electron density around CLA c 506:

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

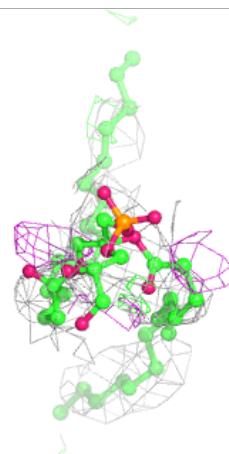
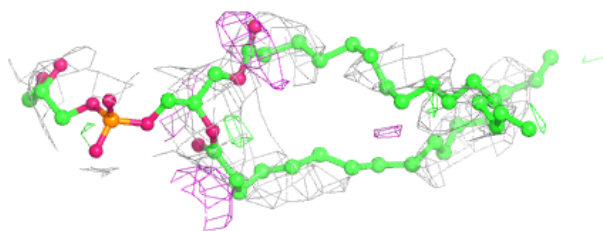
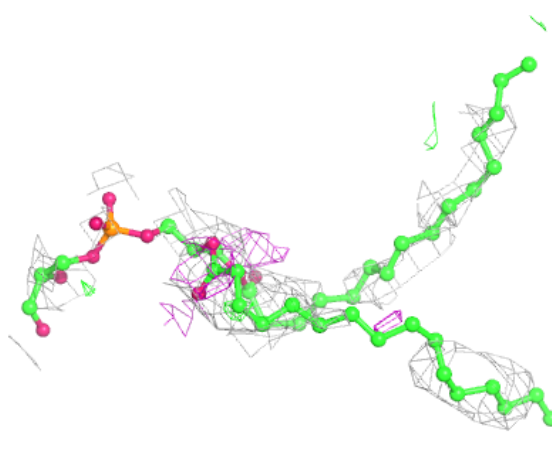
**Electron density around CLA B 611:**

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



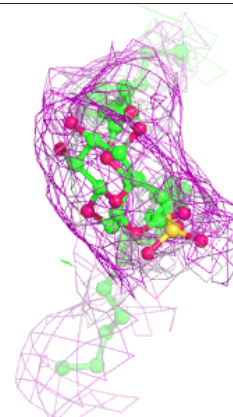
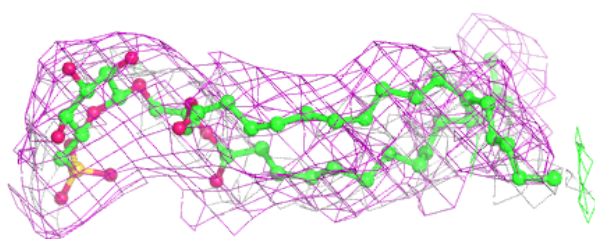
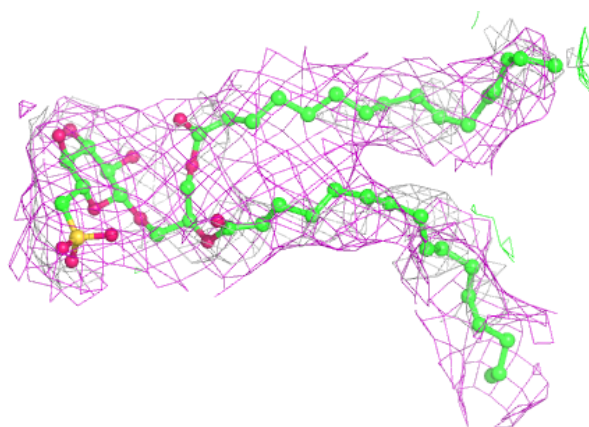
Electron density around LHG d 407:

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

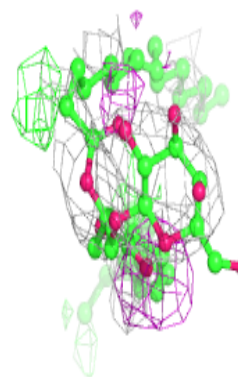
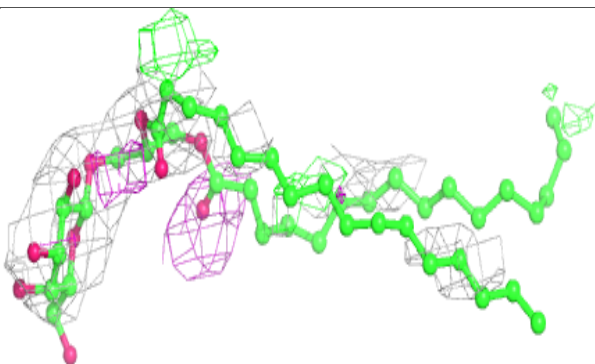
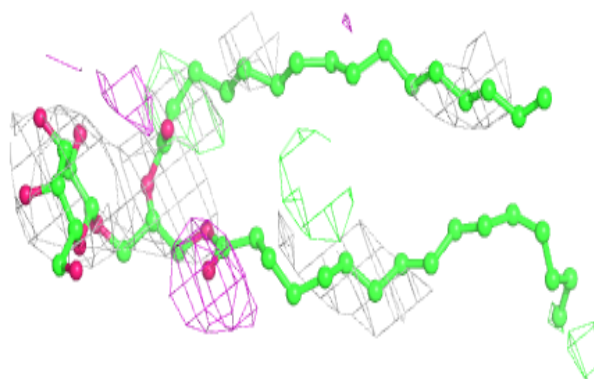


Electron density around SQD L 102:

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

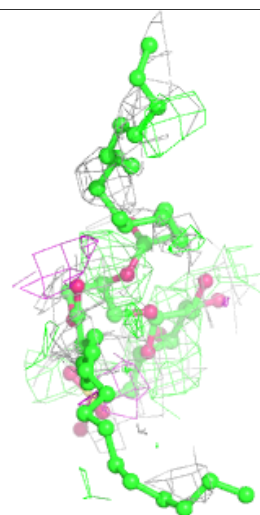
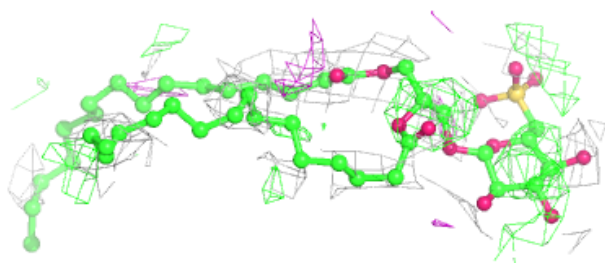
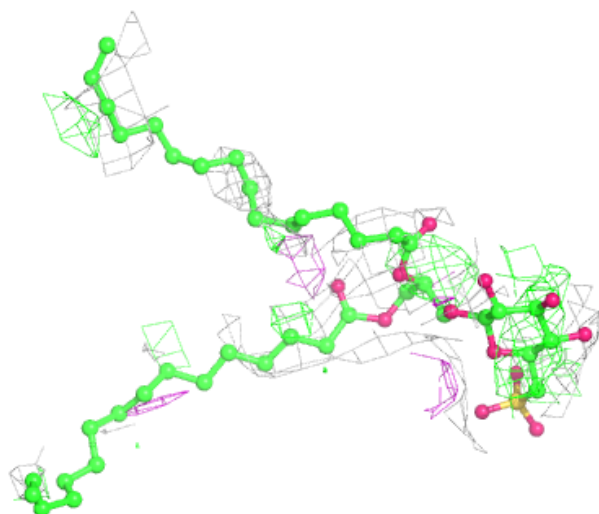
**Electron density around LMG c 520:**

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



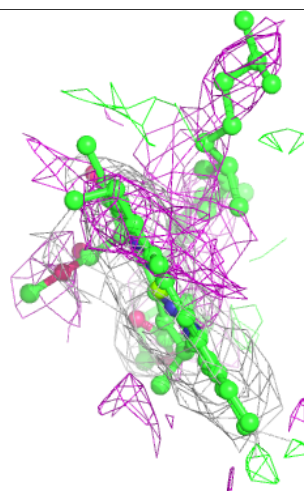
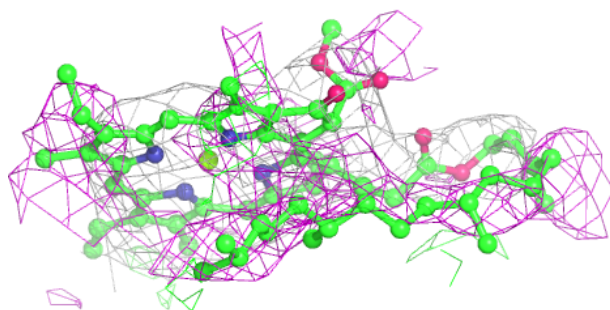
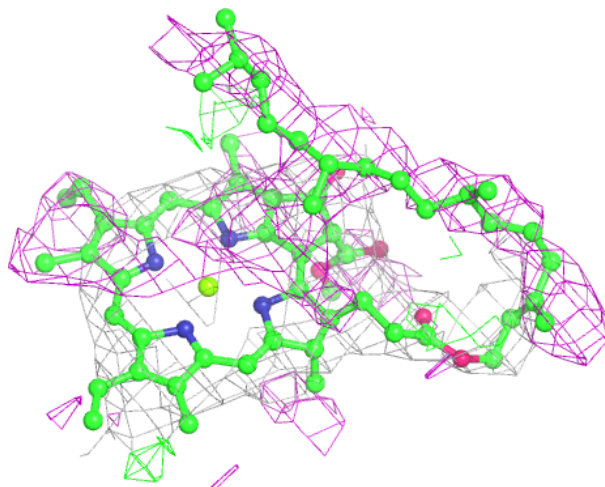
Electron density around SQD A 612:

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



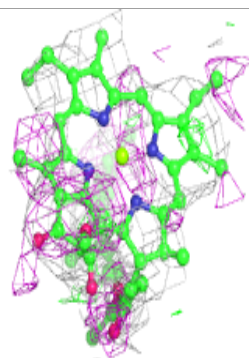
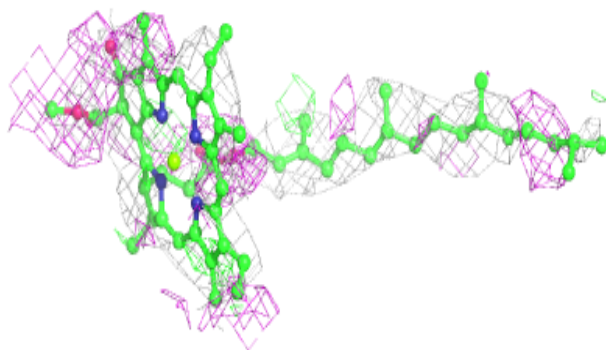
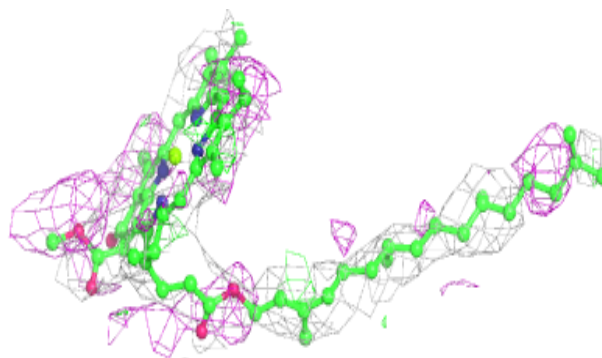
Electron density around CLA c 509:

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

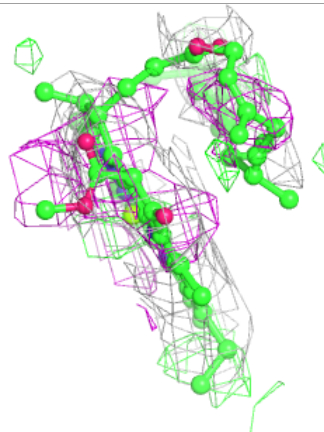
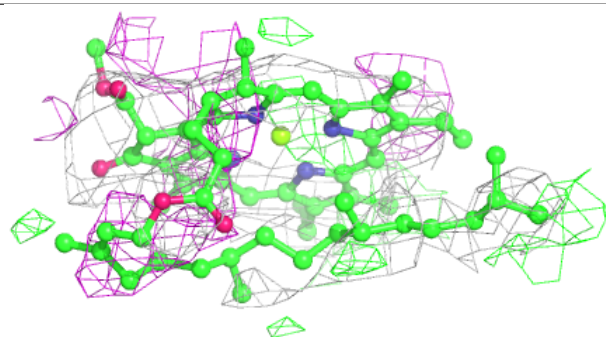
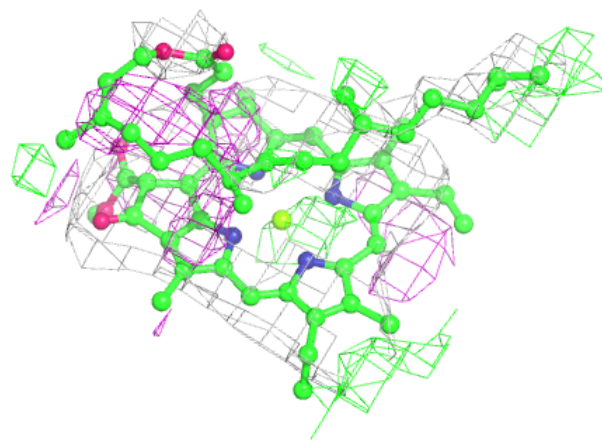


Electron density around CLA B 608:

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

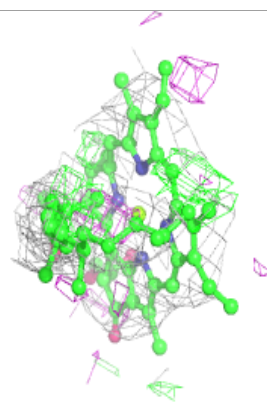
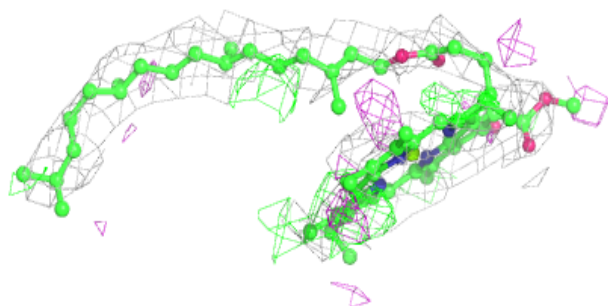
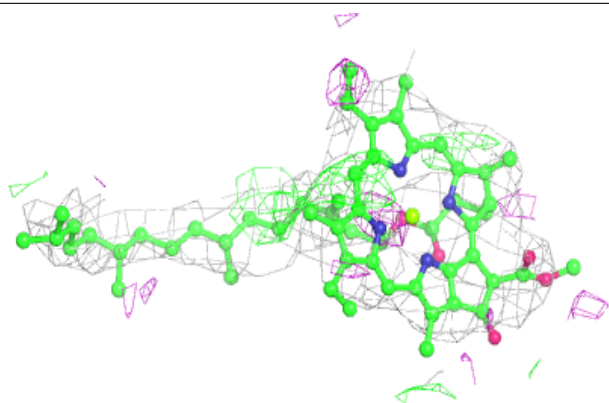
**Electron density around CLA B 602:**

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

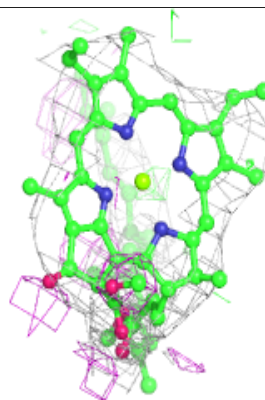
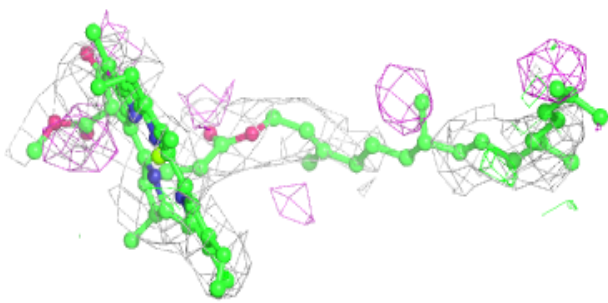
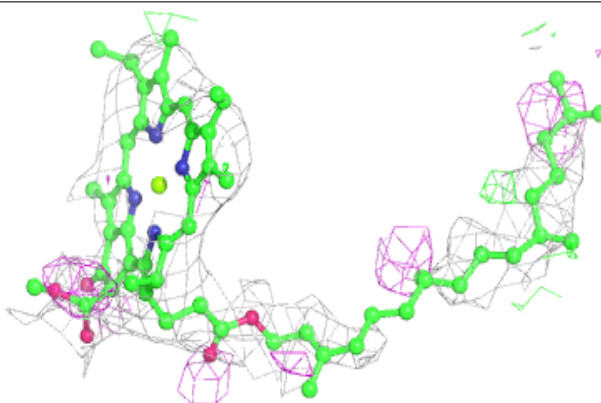


Electron density around CLA b 610:

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

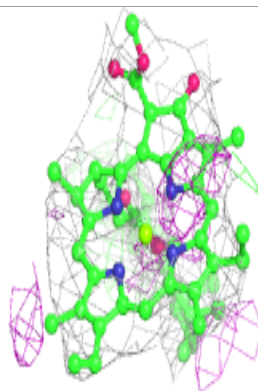
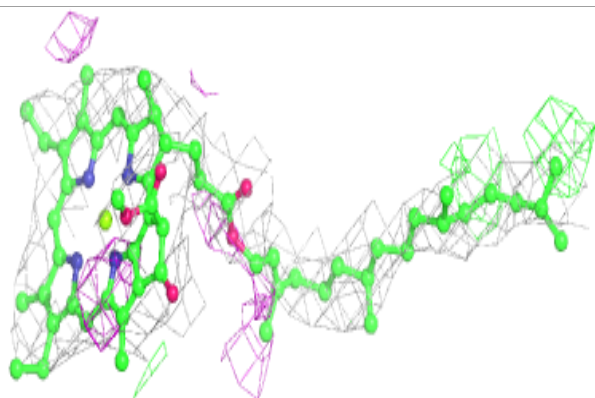
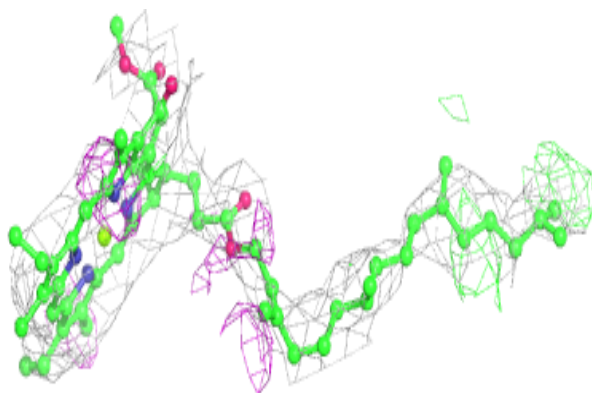
**Electron density around CLA b 611:**

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

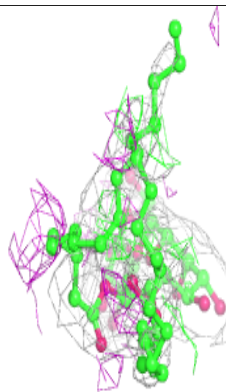
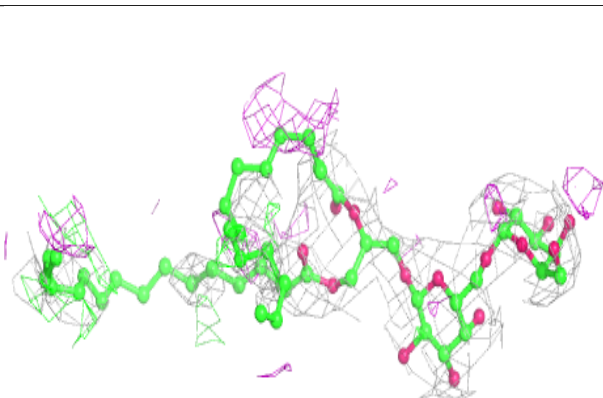
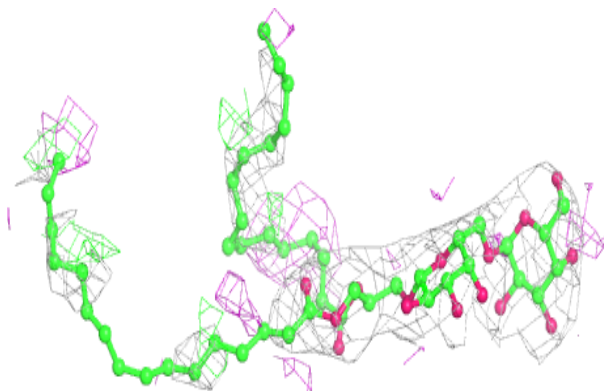


Electron density around CLA C 502:

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

**Electron density around 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)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.