



Full wwPDB EM Validation Report ⓘ

Apr 16, 2025 – 04:38 PM JST

PDB ID : 9J2F / pdb_00009j2f
EMDB ID : EMD-61095
Title : Structure of photosynthetic LH1-RC complex from the purple bacterium *Blautia* *tepidus*
Authors : Kimura, Y.; Kanno, R.; Mori, K.; Matsuda, Y.; Seto, R.; Takenaka, S.; Mino, H.; Ohkubo, T.; Honda, M.; Sasaki, Y.C.; Kishikawa, J.; Mitsuoka, K.; Mio, K.; Hall, M.; Purba, E.R.; Mochizuki, T.; Mizoguchi, A.; Humbel, B.M.; Madigan, M.T.; Wang-Otomo, Z.-Y.; Tani, K.
Deposited on : 2024-08-06
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

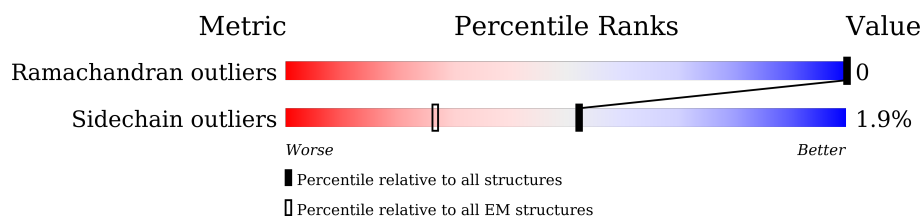
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

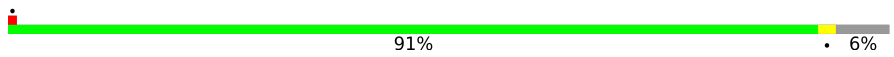
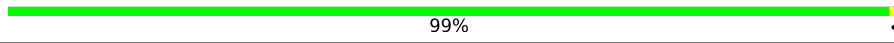
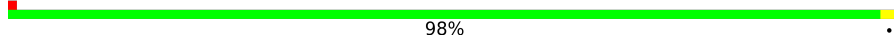
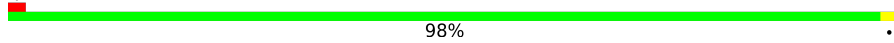





The reported resolution of this entry is 2.20 Å.

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.









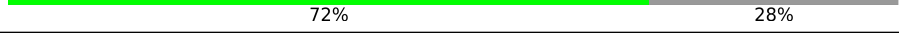
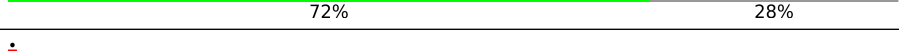
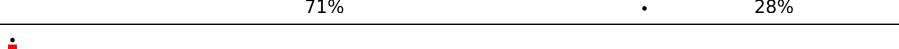
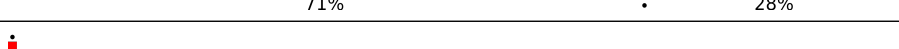
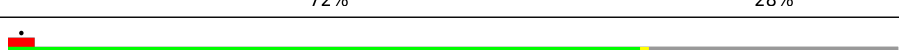

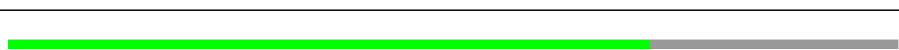

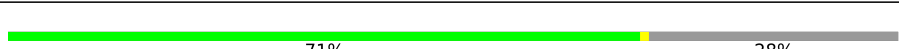





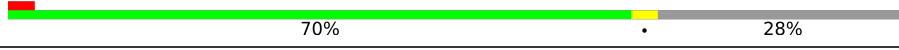
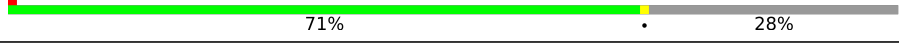



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | C | 354 |  91% 6% |
| 2 | L | 274 |  99% |
| 3 | M | 332 |  98% |
| 4 | H | 260 |  98% |
| 5 | 3 | 69 |  72% 28% |
| 5 | 6 | 69 |  71% 28% |
| 5 | 9 | 69 |  71% 28% |
| 5 | A | 69 |  70% 28% |
| 5 | D | 69 |  71% 28% |



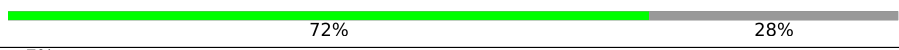



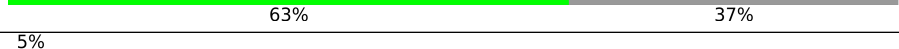
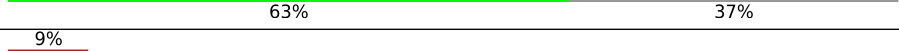
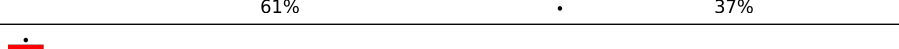
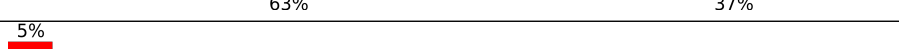
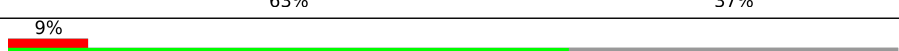



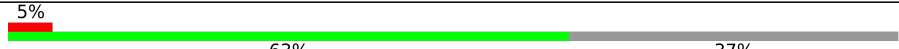





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | I | 69 |  |
| 5 | N | 69 |  |
| 5 | Q | 69 |  |
| 5 | T | 69 |  |
| 5 | W | 69 |  |
| 5 | Z | 69 |  |
| 5 | b | 69 |  |
| 5 | e | 69 |  |
| 5 | h | 69 |  |
| 5 | k | 69 |  |
| 5 | n | 69 |  |
| 5 | q | 69 |  |
| 6 | 0 | 69 |  |
| 6 | 1 | 69 |  |
| 6 | 4 | 69 |  |
| 6 | 7 | 69 |  |
| 6 | B | 69 |  |
| 6 | E | 69 |  |
| 6 | J | 69 |  |
| 6 | O | 69 |  |
| 6 | R | 69 |  |
| 6 | U | 69 |  |
| 6 | X | 69 |  |
| 6 | c | 69 |  |
| 6 | f | 69 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 6 | i | 69 |  |
| 6 | l | 69 |  |
| 6 | o | 69 |  |
| 6 | r | 69 |  |
| 7 | G | 56 |  |
| 8 | 2 | 57 |  |
| 8 | 5 | 57 |  |
| 8 | 8 | 57 |  |
| 8 | F | 57 |  |
| 8 | K | 57 |  |
| 8 | P | 57 |  |
| 8 | S | 57 |  |
| 8 | V | 57 |  |
| 8 | Y | 57 |  |
| 8 | a | 57 |  |
| 8 | d | 57 |  |
| 8 | g | 57 |  |
| 8 | j | 57 |  |
| 8 | m | 57 |  |
| 8 | p | 57 |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13 | BCB | 0 | 102 | X | - | - | - |
| 13 | BCB | 1 | 101 | X | - | - | - |
| 13 | BCB | 3 | 101 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13 | BCB | 4 | 101 | X | - | - | - |
| 13 | BCB | 6 | 101 | X | - | - | - |
| 13 | BCB | 7 | 102 | X | - | - | - |
| 13 | BCB | 9 | 101 | X | - | - | - |
| 13 | BCB | A | 102 | X | - | - | - |
| 13 | BCB | B | 202 | X | - | - | - |
| 13 | BCB | D | 101 | X | - | - | - |
| 13 | BCB | E | 101 | X | - | - | - |
| 13 | BCB | I | 101 | X | - | - | - |
| 13 | BCB | J | 101 | X | - | - | - |
| 13 | BCB | L | 302 | X | - | - | - |
| 13 | BCB | L | 303 | X | - | - | - |
| 13 | BCB | M | 402 | X | - | - | - |
| 13 | BCB | M | 403 | X | - | - | - |
| 13 | BCB | N | 101 | X | - | - | - |
| 13 | BCB | O | 102 | X | - | - | - |
| 13 | BCB | Q | 402 | X | - | - | - |
| 13 | BCB | R | 102 | X | - | - | - |
| 13 | BCB | T | 101 | X | - | - | - |
| 13 | BCB | U | 102 | X | - | - | - |
| 13 | BCB | W | 302 | X | - | - | - |
| 13 | BCB | X | 102 | X | - | - | - |
| 13 | BCB | Z | 101 | X | - | - | - |
| 13 | BCB | b | 101 | X | - | - | - |
| 13 | BCB | c | 101 | X | - | - | - |
| 13 | BCB | e | 101 | X | - | - | - |
| 13 | BCB | f | 101 | X | - | - | - |
| 13 | BCB | h | 102 | X | - | - | - |
| 13 | BCB | i | 101 | X | - | - | - |
| 13 | BCB | k | 102 | X | - | - | - |
| 13 | BCB | l | 102 | X | - | - | - |
| 13 | BCB | n | 101 | X | - | - | - |
| 13 | BCB | o | 102 | X | - | - | - |
| 13 | BCB | q | 101 | X | - | - | - |
| 13 | BCB | r | 101 | X | - | - | - |

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 32918 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Photosynthetic reaction center cytochrome c subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | C | 331 | Total | C | N | O | S | 0 | 0 |
| | | | 2585 | 1637 | 455 | 471 | 22 | | |

- Molecule 2 is a protein called Reaction center protein L chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | L | 273 | Total | C | N | O | S | 0 | 0 |
| | | | 2159 | 1454 | 347 | 352 | 6 | | |

- Molecule 3 is a protein called Reaction center protein M chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | M | 331 | Total | C | N | O | S | 0 | 0 |
| | | | 2621 | 1746 | 433 | 427 | 15 | | |

- Molecule 4 is a protein called Photosynthetic reaction center subunit H.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | H | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2041 | 1313 | 343 | 382 | 3 | | |

- Molecule 5 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5 | A | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | D | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | I | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | N | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5 | Q | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | T | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | W | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | Z | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | 3 | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | 6 | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | 9 | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | b | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | e | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | h | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | k | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | n | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |
| 5 | q | 50 | Total | C | N | O | 0 | 0 |
| | | | 424 | 288 | 72 | 64 | | |

- Molecule 6 is a protein called Antenna complex alpha/beta subunit domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6 | B | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 407 | 274 | 63 | 69 | 1 | | |
| 6 | E | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 407 | 274 | 63 | 69 | 1 | | |
| 6 | J | 48 | Total | C | N | O | S | 0 | 0 |
| | | | 386 | 260 | 60 | 65 | 1 | | |
| 6 | O | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 407 | 274 | 63 | 69 | 1 | | |
| 6 | R | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 400 | 269 | 62 | 68 | 1 | | |
| 6 | U | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 400 | 269 | 62 | 68 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 6 | X | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | 1 | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | 4 | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | 7 | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | 0 | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | c | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | f | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | i | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | l | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | o | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |
| 6 | r | 50 | Total 400 | C 269 | N 62 | O 68 | S 1 | 0 | 0 |

- Molecule 7 is a protein called Light-harvesting protein gamma1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 7 | G | 28 | Total 232 | C 159 | N 36 | O 37 | 0 | 0 |

- Molecule 8 is a protein called Light-harvesting protein B-1015 gamma chain.

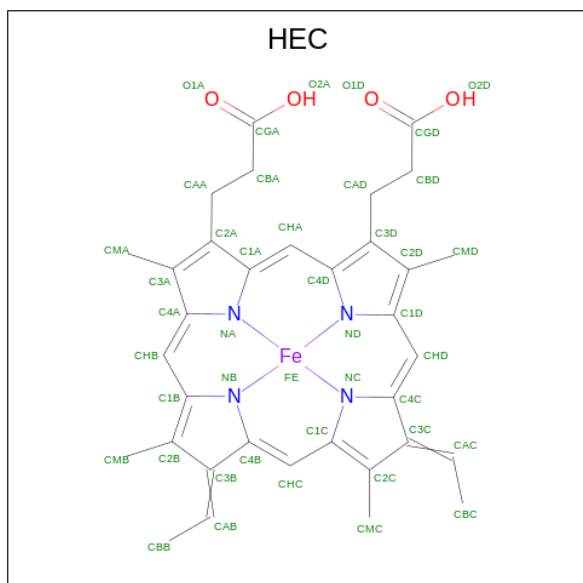
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 8 | F | 36 | Total 279 | C 189 | N 42 | O 48 | 0 | 0 |
| 8 | K | 36 | Total 279 | C 189 | N 42 | O 48 | 0 | 0 |
| 8 | P | 36 | Total 279 | C 189 | N 42 | O 48 | 0 | 0 |
| 8 | S | 36 | Total 279 | C 189 | N 42 | O 48 | 0 | 0 |
| 8 | V | 36 | Total 279 | C 189 | N 42 | O 48 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 8 | Y | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | 2 | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | 5 | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | 8 | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | a | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | d | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | g | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | j | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | m | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |
| 8 | p | 36 | Total | C | N | O | 0 | 0 |
| | | | 279 | 189 | 42 | 48 | | |

- Molecule 9 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 9 | C | 1 | Total | C | Fe | N | O |
| | | | 43 | 34 | 1 | 4 | 4 |
| | | | | | | | 0 |

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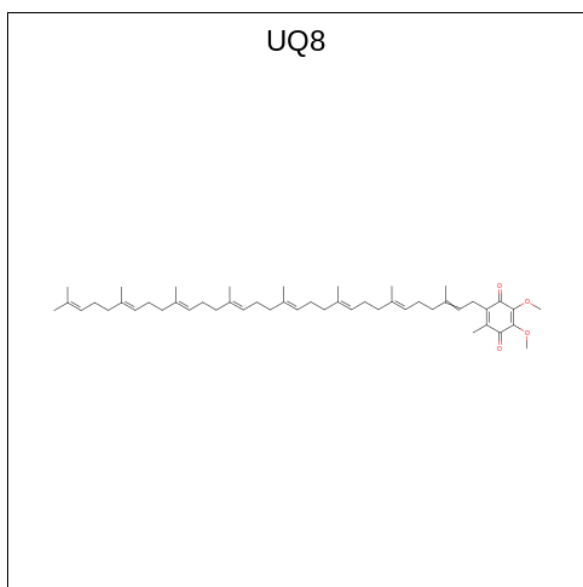
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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 9 | C | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |
| 9 | C | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |
| 9 | C | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

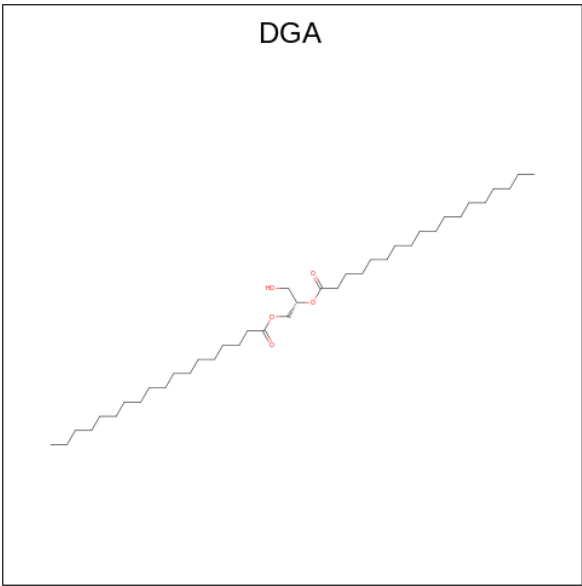
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 10 | C | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 11 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



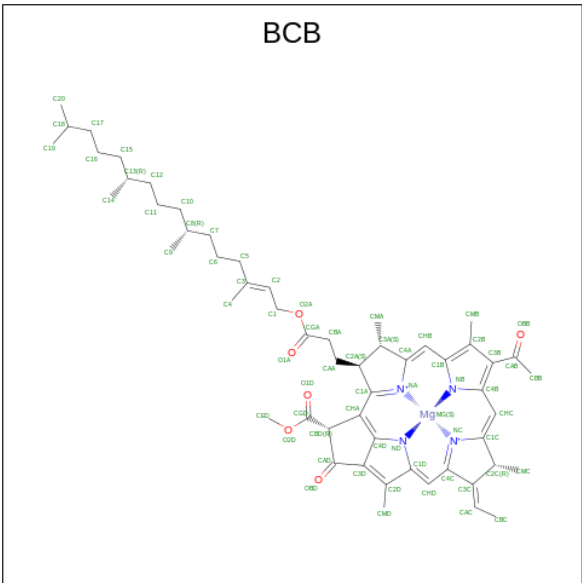
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 11 | C | 1 | Total | C | O | 0 |
| | | | 15 | 11 | 4 | |
| 11 | L | 1 | Total | C | O | 0 |
| | | | 31 | 27 | 4 | |
| 11 | M | 1 | Total | C | O | 0 |
| | | | 25 | 21 | 4 | |
| 11 | M | 1 | Total | C | O | 0 |
| | | | 53 | 49 | 4 | |
| 11 | A | 1 | Total | C | O | 0 |
| | | | 53 | 49 | 4 | |

- Molecule 12 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 12 | L | 1 | Total | C | O | 0 |
| | | | 23 | 19 | 4 | |

- Molecule 13 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |

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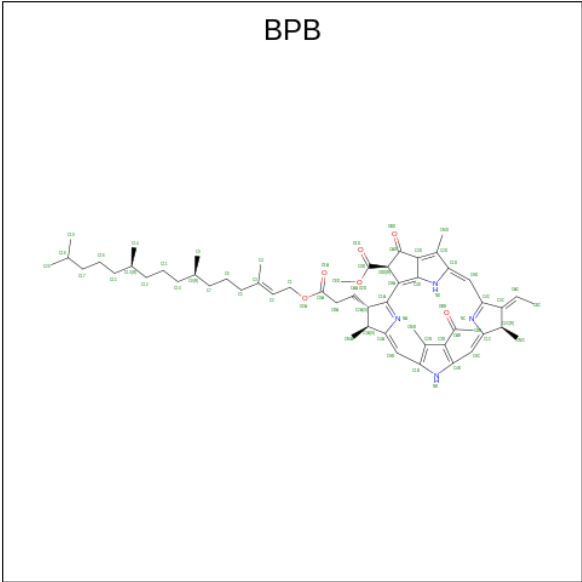
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13 | L | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | M | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | M | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | A | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | B | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | D | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | E | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | I | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | J | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | N | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | O | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | Q | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | R | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | T | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | U | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | W | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | X | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | Z | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | 1 | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | 3 | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 13 | 4 | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |

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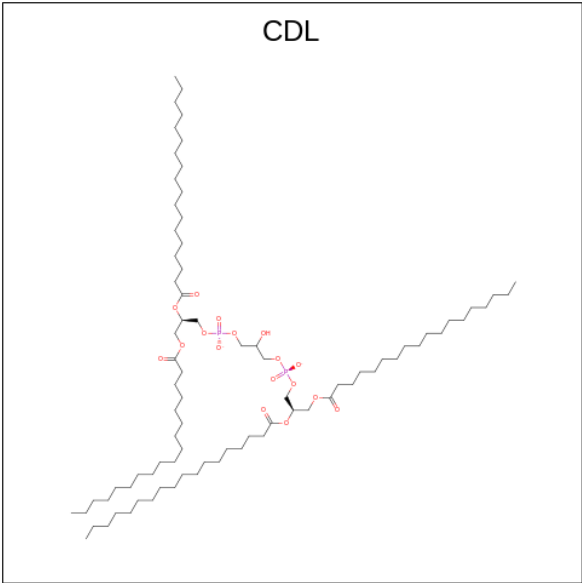
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | 0 | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | h | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | i | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | k | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | l | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | n | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | o | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 13 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |

- Molecule 14 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 14 | L | 1 | Total | C | N | O | 0 |
| | | | 65 | 55 | 4 | 6 | |
| 14 | M | 1 | Total | C | N | O | 0 |
| | | | 65 | 55 | 4 | 6 | |

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 15 | L | 1 | Total | C | O | P | 0 |
| | | | 75 | 56 | 17 | 2 | |
| 15 | M | 1 | Total | C | O | P | 0 |
| | | | 85 | 66 | 17 | 2 | |

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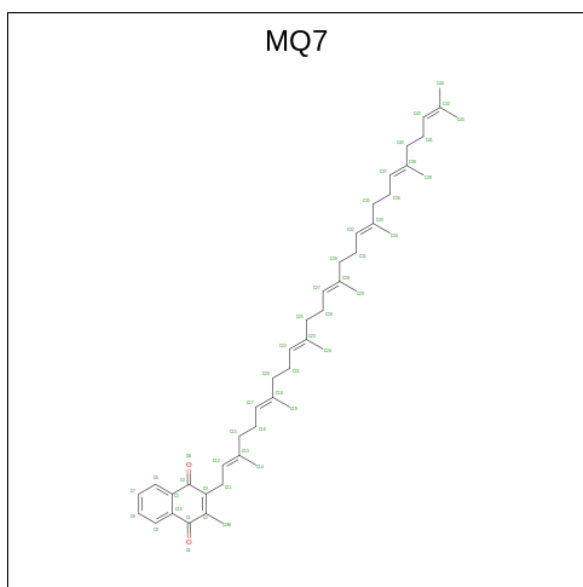
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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 15 | H | 1 | Total | C | O | P | 0 |
| | | | 98 | 79 | 17 | 2 | |
| 15 | H | 1 | Total | C | O | P | 0 |
| | | | 72 | 53 | 17 | 2 | |
| 15 | r | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |

- Molecule 16 is FE (III) ION (CCD ID: FE) (formula: Fe).

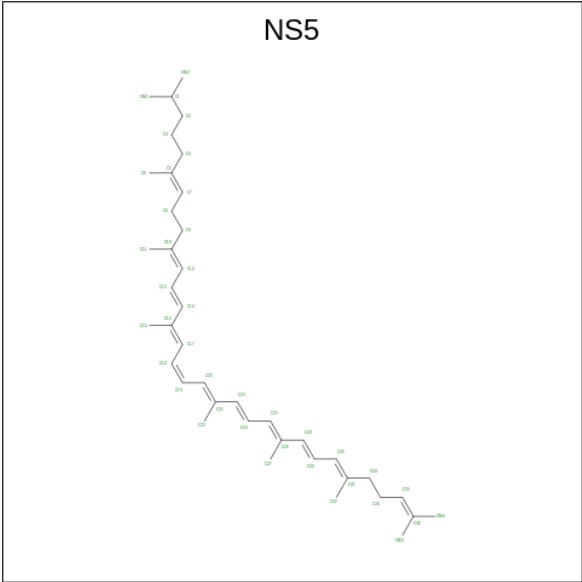
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 16 | M | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |

- Molecule 17 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



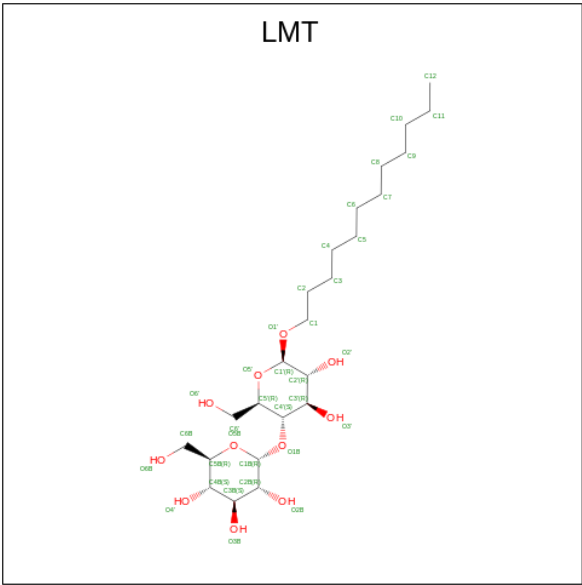
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 17 | M | 1 | Total | C | O | 0 |
| | | | 48 | 46 | 2 | |

- Molecule 18 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|--|---------|
| 18 | M | 1 | Total | C | | 0 |
| | | | 40 | 40 | | |

- Molecule 19 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



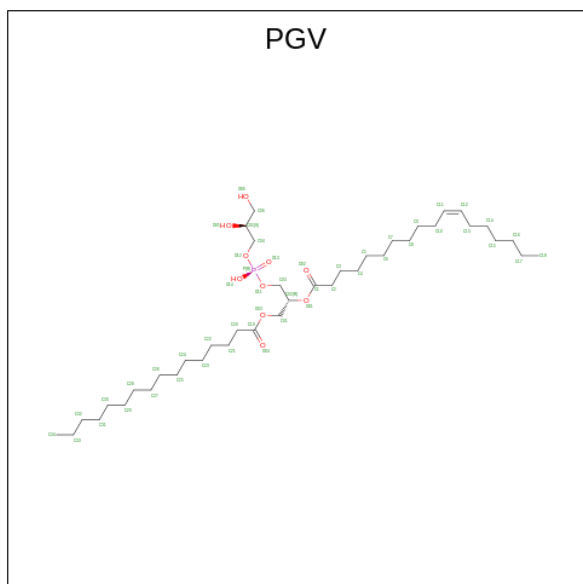
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 19 | M | 1 | Total | C | O | 0 |
| | | | 25 | 19 | 6 | |
| 19 | B | 1 | Total | C | O | 0 |
| | | | 15 | 13 | 2 | |
| 19 | T | 1 | Total | C | O | 0 |
| | | | 26 | 19 | 7 | |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 19 | b | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | b | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | h | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | k | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | n | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |

- Molecule 20 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



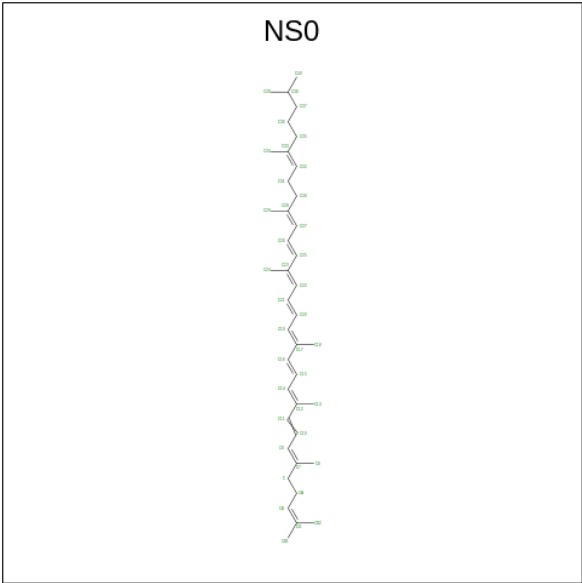
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 20 | M | 1 | Total | C | O | P | 0 |
| | | | 45 | 34 | 10 | 1 | |
| 20 | D | 1 | Total | C | O | P | 0 |
| | | | 47 | 36 | 10 | 1 | |
| 20 | I | 1 | Total | C | O | P | 0 |
| | | | 51 | 40 | 10 | 1 | |
| 20 | N | 1 | Total | C | O | P | 0 |
| | | | 38 | 27 | 10 | 1 | |
| 20 | Q | 1 | Total | C | O | P | 0 |
| | | | 49 | 39 | 9 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 20 | W | 1 | Total | C | O | P | 0 |
| | | | 48 | 37 | 10 | 1 | |

- Molecule 21 is all-trans-1,2-dihydroneurosporene (CCD ID: NS0) (formula: C₄₀H₆₀).



| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 21 | A | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | D | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | O | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | R | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | U | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | W | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | X | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | 2 | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | 7 | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 21 | 9 | 1 | Total | C | 0 |
| | | | 40 | 40 | |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 21 | 0 | 1 | Total C 40 40 | 0 |
| 21 | h | 1 | Total C 40 40 | 0 |
| 21 | k | 1 | Total C 40 40 | 0 |
| 21 | l | 1 | Total C 40 40 | 0 |
| 21 | o | 1 | Total C 40 40 | 0 |
| 21 | q | 1 | Total C 40 40 | 0 |

- Molecule 22 is water.

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 22 | C | 98 | Total O 98 98 | 0 |
| 22 | L | 59 | Total O 59 59 | 0 |
| 22 | M | 75 | Total O 75 75 | 0 |
| 22 | H | 22 | Total O 22 22 | 0 |
| 22 | A | 6 | Total O 6 6 | 0 |
| 22 | B | 2 | Total O 2 2 | 0 |
| 22 | D | 6 | Total O 6 6 | 0 |
| 22 | E | 3 | Total O 3 3 | 0 |
| 22 | I | 7 | Total O 7 7 | 0 |
| 22 | J | 3 | Total O 3 3 | 0 |
| 22 | K | 2 | Total O 2 2 | 0 |
| 22 | N | 6 | Total O 6 6 | 0 |
| 22 | O | 3 | Total O 3 3 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 22 | Q | 6 | Total O 6 6 | 0 |
| 22 | R | 5 | Total O 5 5 | 0 |
| 22 | S | 1 | Total O 1 1 | 0 |
| 22 | T | 6 | Total O 6 6 | 0 |
| 22 | U | 5 | Total O 5 5 | 0 |
| 22 | V | 2 | Total O 2 2 | 0 |
| 22 | W | 3 | Total O 3 3 | 0 |
| 22 | X | 5 | Total O 5 5 | 0 |
| 22 | Y | 2 | Total O 2 2 | 0 |
| 22 | Z | 4 | Total O 4 4 | 0 |
| 22 | 1 | 3 | Total O 3 3 | 0 |
| 22 | 2 | 3 | Total O 3 3 | 0 |
| 22 | 3 | 5 | Total O 5 5 | 0 |
| 22 | 4 | 7 | Total O 7 7 | 0 |
| 22 | 5 | 5 | Total O 5 5 | 0 |
| 22 | 6 | 10 | Total O 10 10 | 0 |
| 22 | 7 | 4 | Total O 4 4 | 0 |
| 22 | 8 | 1 | Total O 1 1 | 0 |
| 22 | 9 | 6 | Total O 6 6 | 0 |
| 22 | 0 | 1 | Total O 1 1 | 0 |
| 22 | b | 10 | Total O 10 10 | 0 |

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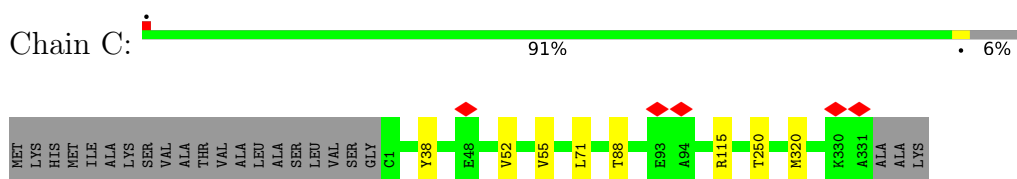
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 22 | c | 4 | Total 4 | O 4 | 0 |
| 22 | e | 9 | Total 9 | O 9 | 0 |
| 22 | f | 2 | Total 2 | O 2 | 0 |
| 22 | g | 1 | Total 1 | O 1 | 0 |
| 22 | h | 4 | Total 4 | O 4 | 0 |
| 22 | i | 1 | Total 1 | O 1 | 0 |
| 22 | j | 2 | Total 2 | O 2 | 0 |
| 22 | k | 5 | Total 5 | O 5 | 0 |
| 22 | l | 1 | Total 1 | O 1 | 0 |
| 22 | n | 4 | Total 4 | O 4 | 0 |
| 22 | o | 1 | Total 1 | O 1 | 0 |
| 22 | p | 1 | Total 1 | O 1 | 0 |
| 22 | q | 2 | Total 2 | O 2 | 0 |

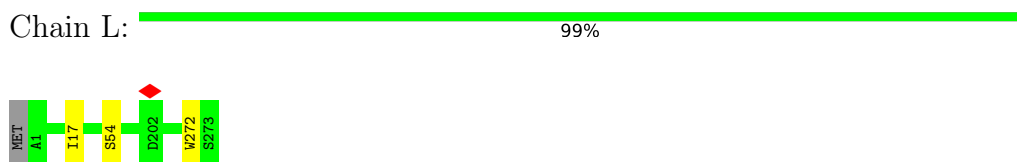
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

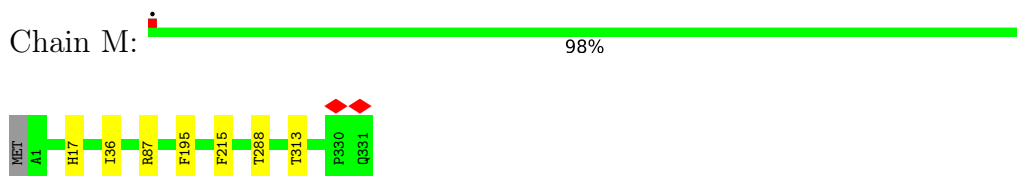
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



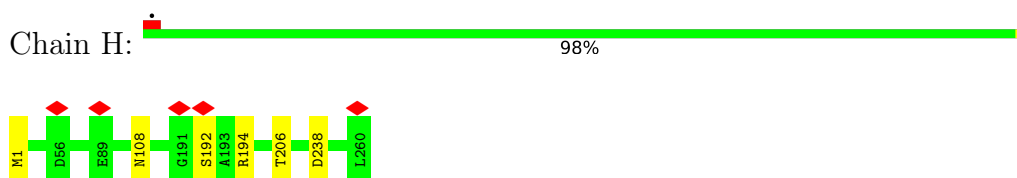
- Molecule 2: Reaction center protein L chain



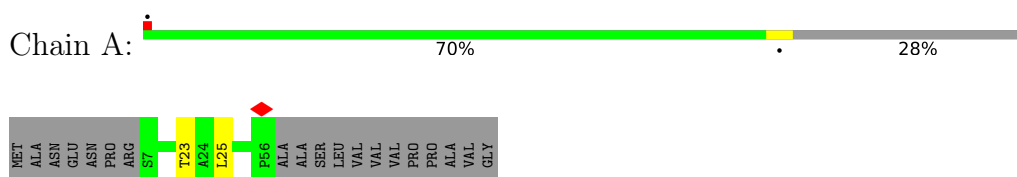
- Molecule 3: Reaction center protein M chain



- Molecule 4: Photosynthetic reaction center subunit H

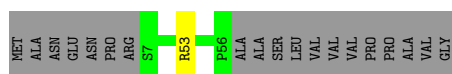


- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



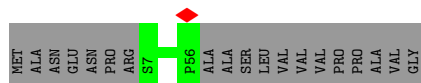
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain D:  71% 28%



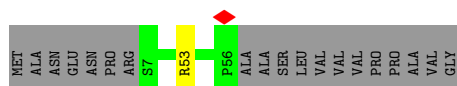
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain I:  72% 28%



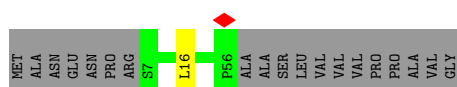
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain N:  71% 28%



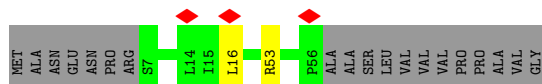
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain Q:  71% 28%



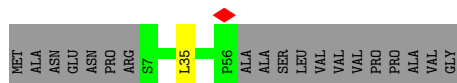
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain T:  70% 28%



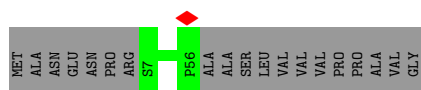
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

Chain W:  71% 28%

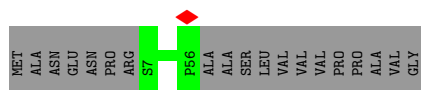


- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein

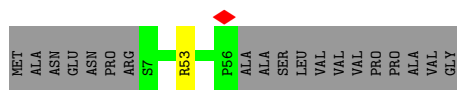
Chain Z:  72% 28%



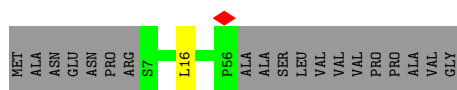
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



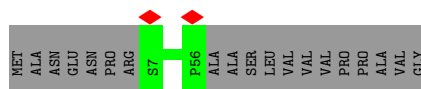
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



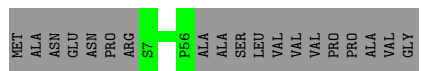
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



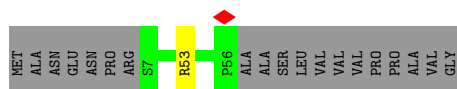
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



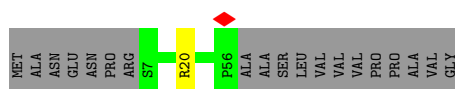
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



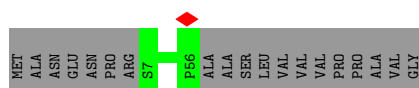
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



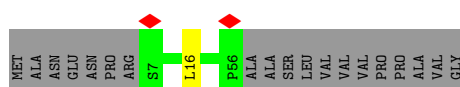
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



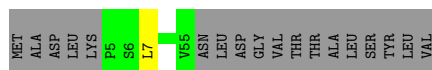
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



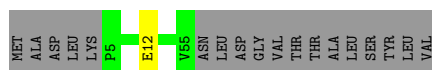
- Molecule 5: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



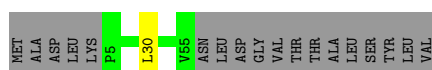
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



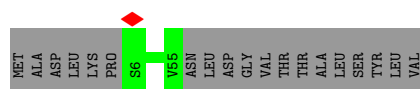
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



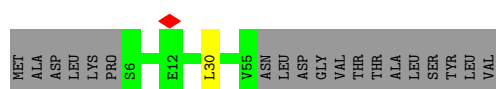
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



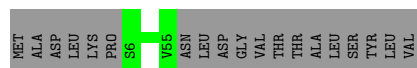
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



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- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



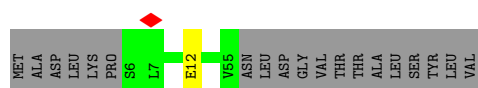
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

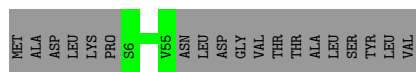


- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein



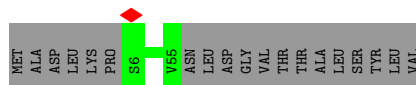
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain c:  72% 28%



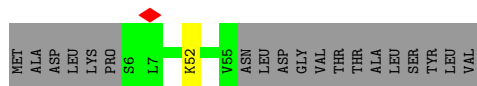
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain f:  72% 28%



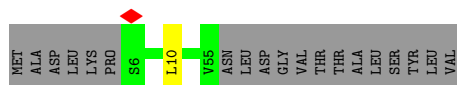
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain i:  71% 28%



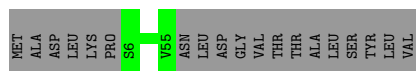
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain l:  71% 28%



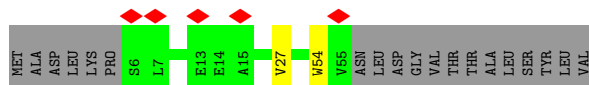
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain o:  72% 28%



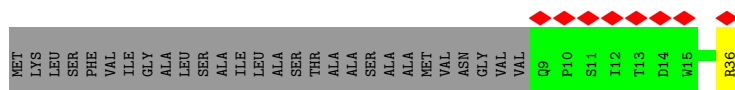
- Molecule 6: Antenna complex alpha/beta subunit domain-containing protein

Chain r:  7% 70% 28%

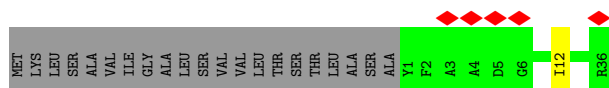


- Molecule 7: Light-harvesting protein gamma1

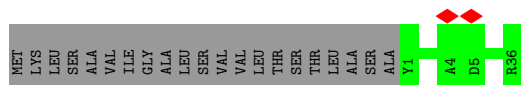
Chain G:  14% 48% 50%



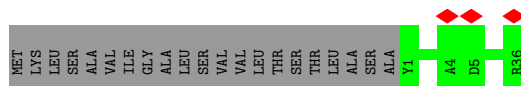
- Molecule 8: Light-harvesting protein B-1015 gamma chain



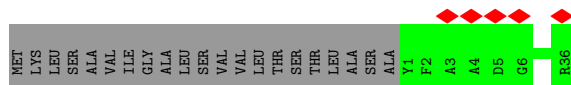
- Molecule 8: Light-harvesting protein B-1015 gamma chain



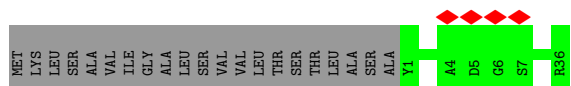
- Molecule 8: Light-harvesting protein B-1015 gamma chain



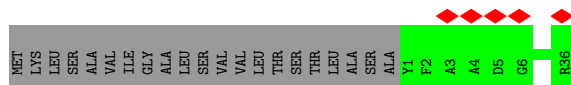
- Molecule 8: Light-harvesting protein B-1015 gamma chain



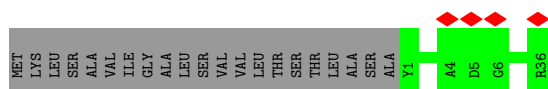
- Molecule 8: Light-harvesting protein B-1015 gamma chain



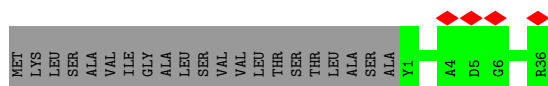
- Molecule 8: Light-harvesting protein B-1015 gamma chain



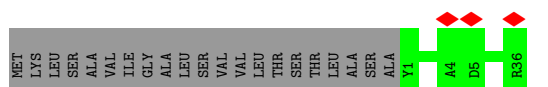
- Molecule 8: Light-harvesting protein B-1015 gamma chain



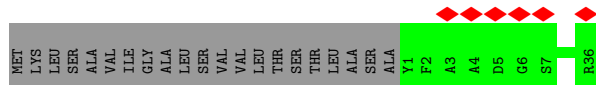
- Molecule 8: Light-harvesting protein B-1015 gamma chain



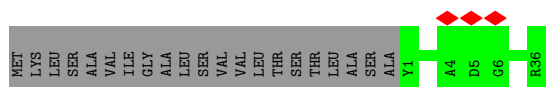
- Molecule 8: Light-harvesting protein B-1015 gamma chain



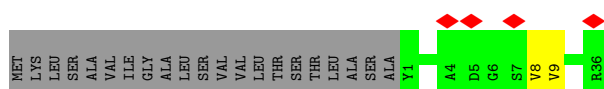
- Molecule 8: Light-harvesting protein B-1015 gamma chain



- Molecule 8: Light-harvesting protein B-1015 gamma chain

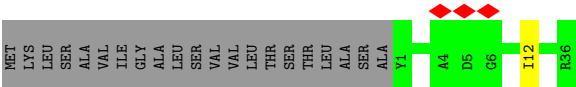


- Molecule 8: Light-harvesting protein B-1015 gamma chain

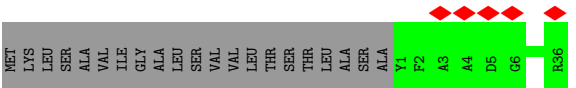


- Molecule 8: Light-harvesting protein B-1015 gamma chain

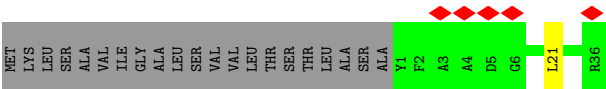




● Molecule 8: Light-harvesting protein B-1015 gamma chain



● Molecule 8: Light-harvesting protein B-1015 gamma chain



4 Experimental information

| Property | Value | Source |
|--------------------------------------|--------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 294012 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 40 | Depositor |
| Minimum defocus (nm) | 900 | Depositor |
| Maximum defocus (nm) | 2700 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.434 | Depositor |
| Minimum map value | -0.179 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.012 | Depositor |
| Recommended contour level | 0.045 | Depositor |
| Map size (\AA) | 328.0, 328.0, 328.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 0.82, 0.82, 0.82 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, BCB, NS0, MQ7, LMT, HEC, MG, UQ8, DGA, CDL, NS5, PGV, BPB, FE

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 | C | 0.31 | 0/2657 | 0.53 | 0/3614 |
| 2 | L | 0.31 | 0/2246 | 0.48 | 0/3062 |
| 3 | M | 0.31 | 0/2725 | 0.50 | 0/3718 |
| 4 | H | 0.30 | 0/2087 | 0.54 | 0/2848 |
| 5 | 3 | 0.28 | 0/438 | 0.51 | 0/599 |
| 5 | 6 | 0.28 | 0/438 | 0.52 | 0/599 |
| 5 | 9 | 0.28 | 0/438 | 0.51 | 0/599 |
| 5 | A | 0.29 | 0/438 | 0.51 | 0/599 |
| 5 | D | 0.28 | 0/438 | 0.49 | 0/599 |
| 5 | I | 0.28 | 0/438 | 0.49 | 0/599 |
| 5 | N | 0.27 | 0/438 | 0.49 | 0/599 |
| 5 | Q | 0.26 | 0/438 | 0.49 | 0/599 |
| 5 | T | 0.26 | 0/438 | 0.51 | 0/599 |
| 5 | W | 0.26 | 0/438 | 0.50 | 0/599 |
| 5 | Z | 0.28 | 0/438 | 0.52 | 0/599 |
| 5 | b | 0.27 | 0/438 | 0.49 | 0/599 |
| 5 | e | 0.26 | 0/438 | 0.49 | 0/599 |
| 5 | h | 0.25 | 0/438 | 0.51 | 0/599 |
| 5 | k | 0.28 | 0/438 | 0.50 | 0/599 |
| 5 | n | 0.26 | 0/438 | 0.51 | 0/599 |
| 5 | q | 0.26 | 0/438 | 0.50 | 0/599 |
| 6 | 0 | 0.29 | 0/414 | 0.45 | 0/569 |
| 6 | 1 | 0.31 | 0/414 | 0.43 | 0/569 |
| 6 | 4 | 0.30 | 0/414 | 0.44 | 0/569 |
| 6 | 7 | 0.30 | 0/414 | 0.44 | 0/569 |
| 6 | B | 0.28 | 0/422 | 0.44 | 0/580 |
| 6 | E | 0.30 | 0/422 | 0.44 | 0/580 |
| 6 | J | 0.30 | 0/400 | 0.43 | 0/550 |
| 6 | O | 0.29 | 0/422 | 0.45 | 0/580 |
| 6 | R | 0.29 | 0/414 | 0.45 | 0/569 |
| 6 | U | 0.29 | 0/414 | 0.50 | 0/569 |
| 6 | X | 0.29 | 0/414 | 0.46 | 0/569 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 6 | c | 0.29 | 0/414 | 0.46 | 0/569 |
| 6 | f | 0.30 | 0/414 | 0.43 | 0/569 |
| 6 | i | 0.28 | 0/414 | 0.46 | 0/569 |
| 6 | l | 0.28 | 0/414 | 0.44 | 0/569 |
| 6 | o | 0.28 | 0/414 | 0.43 | 0/569 |
| 6 | r | 0.29 | 0/414 | 0.45 | 0/569 |
| 7 | G | 0.27 | 0/241 | 0.52 | 0/333 |
| 8 | 2 | 0.28 | 0/288 | 0.53 | 0/397 |
| 8 | 5 | 0.29 | 0/288 | 0.52 | 0/397 |
| 8 | 8 | 0.29 | 0/288 | 0.50 | 0/397 |
| 8 | F | 0.28 | 0/288 | 0.50 | 0/397 |
| 8 | K | 0.27 | 0/288 | 0.51 | 0/397 |
| 8 | P | 0.28 | 0/288 | 0.49 | 0/397 |
| 8 | S | 0.28 | 0/288 | 0.53 | 0/397 |
| 8 | V | 0.29 | 0/288 | 0.51 | 0/397 |
| 8 | Y | 0.27 | 0/288 | 0.51 | 0/397 |
| 8 | a | 0.27 | 0/288 | 0.50 | 0/397 |
| 8 | d | 0.29 | 0/288 | 0.52 | 0/397 |
| 8 | g | 0.29 | 0/288 | 0.50 | 0/397 |
| 8 | j | 0.30 | 0/288 | 0.50 | 0/397 |
| 8 | m | 0.28 | 0/288 | 0.49 | 0/397 |
| 8 | p | 0.28 | 0/288 | 0.50 | 0/397 |
| All | All | 0.29 | 0/28770 | 0.49 | 0/39400 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | C | 329/354 (93%) | 323 (98%) | 6 (2%) | 0 | 100 | 100 |
| 2 | L | 271/274 (99%) | 262 (97%) | 9 (3%) | 0 | 100 | 100 |
| 3 | M | 329/332 (99%) | 320 (97%) | 9 (3%) | 0 | 100 | 100 |
| 4 | H | 258/260 (99%) | 251 (97%) | 7 (3%) | 0 | 100 | 100 |
| 5 | 3 | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | 6 | 48/69 (70%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 5 | 9 | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | A | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | D | 48/69 (70%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 5 | I | 48/69 (70%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 5 | N | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | Q | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | T | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | W | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | Z | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | b | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | e | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | h | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | k | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | n | 48/69 (70%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 5 | q | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 6 | 0 | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 6 | 1 | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | 4 | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 6 | 7 | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 6 | B | 49/69 (71%) | 47 (96%) | 2 (4%) | 0 | 100 | 100 |
| 6 | E | 49/69 (71%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | J | 46/69 (67%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | O | 49/69 (71%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | R | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 6 | U | 48/69 (70%) | 44 (92%) | 4 (8%) | 0 | 100 | 100 |
| 6 | X | 48/69 (70%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 6 | c | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | f | 48/69 (70%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | i | 48/69 (70%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 6 | l | 48/69 (70%) | 43 (90%) | 5 (10%) | 0 | 100 | 100 |
| 6 | o | 48/69 (70%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 6 | r | 48/69 (70%) | 44 (92%) | 4 (8%) | 0 | 100 | 100 |
| 7 | G | 26/56 (46%) | 26 (100%) | 0 | 0 | 100 | 100 |
| 8 | 2 | 34/57 (60%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | 5 | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | 8 | 34/57 (60%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | F | 34/57 (60%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | K | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | P | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | S | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | V | 34/57 (60%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | Y | 34/57 (60%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | a | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | d | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | g | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | j | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 8 | m | 34/57 (60%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | p | 34/57 (60%) | 34 (100%) | 0 | 0 | 100 | 100 |
| All | All | 3356/4477 (75%) | 3250 (97%) | 106 (3%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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 | C | 279/295 (95%) | 271 (97%) | 8 (3%) | 37 | 50 |
| 2 | L | 213/214 (100%) | 210 (99%) | 3 (1%) | 62 | 77 |
| 3 | M | 257/258 (100%) | 250 (97%) | 7 (3%) | 40 | 53 |
| 4 | H | 209/209 (100%) | 204 (98%) | 5 (2%) | 44 | 57 |
| 5 | 3 | 45/59 (76%) | 45 (100%) | 0 | 100 | 100 |
| 5 | 6 | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | 9 | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | A | 45/59 (76%) | 43 (96%) | 2 (4%) | 24 | 31 |
| 5 | D | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | I | 45/59 (76%) | 45 (100%) | 0 | 100 | 100 |
| 5 | N | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | Q | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | T | 45/59 (76%) | 43 (96%) | 2 (4%) | 24 | 31 |
| 5 | W | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | Z | 45/59 (76%) | 45 (100%) | 0 | 100 | 100 |
| 5 | b | 45/59 (76%) | 45 (100%) | 0 | 100 | 100 |
| 5 | e | 45/59 (76%) | 45 (100%) | 0 | 100 | 100 |
| 5 | h | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | k | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 5 | n | 45/59 (76%) | 45 (100%) | 0 | 100 | 100 |
| 5 | q | 45/59 (76%) | 44 (98%) | 1 (2%) | 47 | 61 |
| 6 | 0 | 43/59 (73%) | 42 (98%) | 1 (2%) | 45 | 59 |
| 6 | 1 | 43/59 (73%) | 43 (100%) | 0 | 100 | 100 |
| 6 | 4 | 43/59 (73%) | 42 (98%) | 1 (2%) | 45 | 59 |
| 6 | 7 | 43/59 (73%) | 42 (98%) | 1 (2%) | 45 | 59 |
| 6 | B | 44/59 (75%) | 43 (98%) | 1 (2%) | 45 | 59 |
| 6 | E | 44/59 (75%) | 43 (98%) | 1 (2%) | 45 | 59 |
| 6 | J | 41/59 (70%) | 41 (100%) | 0 | 100 | 100 |
| 6 | O | 44/59 (75%) | 43 (98%) | 1 (2%) | 45 | 59 |
| 6 | R | 43/59 (73%) | 43 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 6 | U | 43/59 (73%) | 41 (95%) | 2 (5%) | 22 | 29 |
| 6 | X | 43/59 (73%) | 42 (98%) | 1 (2%) | 45 | 59 |
| 6 | c | 43/59 (73%) | 43 (100%) | 0 | 100 | 100 |
| 6 | f | 43/59 (73%) | 43 (100%) | 0 | 100 | 100 |
| 6 | i | 43/59 (73%) | 42 (98%) | 1 (2%) | 45 | 59 |
| 6 | l | 43/59 (73%) | 42 (98%) | 1 (2%) | 45 | 59 |
| 6 | o | 43/59 (73%) | 43 (100%) | 0 | 100 | 100 |
| 6 | r | 43/59 (73%) | 41 (95%) | 2 (5%) | 22 | 29 |
| 7 | G | 25/44 (57%) | 24 (96%) | 1 (4%) | 27 | 35 |
| 8 | 2 | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | 5 | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | 8 | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | F | 29/45 (64%) | 28 (97%) | 1 (3%) | 32 | 42 |
| 8 | K | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | P | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | S | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | V | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | Y | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | a | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | d | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | g | 29/45 (64%) | 27 (93%) | 2 (7%) | 13 | 14 |
| 8 | j | 29/45 (64%) | 28 (97%) | 1 (3%) | 32 | 42 |
| 8 | m | 29/45 (64%) | 29 (100%) | 0 | 100 | 100 |
| 8 | p | 29/45 (64%) | 28 (97%) | 1 (3%) | 32 | 42 |
| All | All | 2915/3701 (79%) | 2860 (98%) | 55 (2%) | 52 | 67 |

All (55) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 38 | TYR |
| 1 | C | 52 | VAL |
| 1 | C | 55 | VAL |
| 1 | C | 71 | LEU |
| 1 | C | 88 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 115 | ARG |
| 1 | C | 250 | THR |
| 1 | C | 320 | MET |
| 2 | L | 17 | ILE |
| 2 | L | 54 | SER |
| 2 | L | 272 | TRP |
| 3 | M | 17 | HIS |
| 3 | M | 36 | ILE |
| 3 | M | 87 | ARG |
| 3 | M | 195 | PHE |
| 3 | M | 215 | PHE |
| 3 | M | 288 | THR |
| 3 | M | 313 | THR |
| 4 | H | 108 | ASN |
| 4 | H | 192 | SER |
| 4 | H | 194 | ARG |
| 4 | H | 206 | THR |
| 4 | H | 238 | ASP |
| 5 | A | 23 | THR |
| 5 | A | 25 | LEU |
| 6 | B | 7 | LEU |
| 7 | G | 36 | ARG |
| 5 | D | 53 | ARG |
| 6 | E | 12 | GLU |
| 8 | F | 12 | ILE |
| 5 | N | 53 | ARG |
| 6 | O | 30 | LEU |
| 5 | Q | 16 | LEU |
| 5 | T | 16 | LEU |
| 5 | T | 53 | ARG |
| 6 | U | 10 | LEU |
| 6 | U | 11 | THR |
| 5 | W | 35 | LEU |
| 6 | X | 30 | LEU |
| 6 | 4 | 45 | PRO |
| 5 | 6 | 53 | ARG |
| 6 | 7 | 52 | LYS |
| 5 | 9 | 16 | LEU |
| 6 | 0 | 12 | GLU |
| 8 | g | 8 | VAL |
| 8 | g | 9 | VAL |
| 5 | h | 53 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | i | 52 | LYS |
| 8 | j | 12 | ILE |
| 5 | k | 20 | ARG |
| 6 | l | 10 | LEU |
| 8 | p | 21 | LEU |
| 5 | q | 16 | LEU |
| 6 | r | 27 | VAL |
| 6 | r | 54 | TRP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 267 | GLN |
| 1 | C | 295 | GLN |
| 4 | H | 94 | GLN |
| 4 | H | 108 | ASN |
| 7 | G | 16 | ASN |
| 5 | D | 44 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | FME | H | 1 | 4 | 8,9,10 | 0.46 | 0 | 7,9,11 | 1.24 | 2 (28%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 4 | FME | H | 1 | 4 | - | 3/7/9/11 | - |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | H | 1 | FME | O-C-CA | -2.52 | 118.19 | 124.78 |
| 4 | H | 1 | FME | CA-N-CN | -2.09 | 119.61 | 122.82 |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 4 | H | 1 | FME | O1-CN-N-CA |
| 4 | H | 1 | FME | CB-CA-N-CN |
| 4 | H | 1 | FME | CA-CB-CG-SD |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 2 are monoatomic - leaving 87 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 |
| 15 | CDL | H | 302 | - | 71,71,99 | 1.10 | 4 (5%) | 77,83,111 | 1.09 | 5 (6%) |
| 21 | NS0 | X | 101 | - | 39,39,39 | 1.39 | 6 (15%) | 44,46,46 | 1.30 | 7 (15%) |
| 13 | BCB | 0 | 102 | - | 63,74,74 | 2.98 | 14 (22%) | 74,115,115 | 2.80 | 22 (29%) |
| 20 | PGV | N | 102 | - | 37,37,50 | 1.08 | 2 (5%) | 40,43,56 | 1.04 | 3 (7%) |
| 15 | CDL | M | 409 | - | 84,84,99 | 0.99 | 4 (4%) | 90,96,111 | 1.11 | 8 (8%) |
| 13 | BCB | q | 101 | - | 63,74,74 | 2.97 | 16 (25%) | 74,115,115 | 2.87 | 22 (29%) |
| 9 | HEC | C | 401 | 1 | 32,50,50 | 1.61 | 4 (12%) | 24,82,82 | 1.51 | 3 (12%) |
| 13 | BCB | W | 302 | - | 63,74,74 | 2.98 | 15 (23%) | 74,115,115 | 2.90 | 21 (28%) |
| 13 | BCB | l | 102 | - | 63,74,74 | 3.01 | 15 (23%) | 74,115,115 | 2.89 | 22 (29%) |
| 13 | BCB | I | 101 | - | 63,74,74 | 2.96 | 15 (23%) | 74,115,115 | 2.88 | 20 (27%) |
| 13 | BCB | A | 102 | - | 63,74,74 | 2.98 | 15 (23%) | 74,115,115 | 2.91 | 22 (29%) |
| 13 | BCB | 9 | 101 | - | 63,74,74 | 2.97 | 15 (23%) | 74,115,115 | 2.87 | 23 (31%) |
| 13 | BCB | L | 302 | - | 63,74,74 | 2.92 | 14 (22%) | 74,115,115 | 2.92 | 20 (27%) |
| 13 | BCB | J | 101 | - | 63,74,74 | 2.99 | 15 (23%) | 74,115,115 | 2.81 | 22 (29%) |
| 20 | PGV | M | 411 | - | 44,44,50 | 0.96 | 2 (4%) | 46,50,56 | 0.95 | 3 (6%) |
| 13 | BCB | c | 101 | - | 63,74,74 | 3.00 | 15 (23%) | 74,115,115 | 2.86 | 21 (28%) |
| 13 | BCB | B | 202 | - | 63,74,74 | 3.00 | 15 (23%) | 74,115,115 | 2.88 | 23 (31%) |
| 19 | LMT | B | 201 | - | 14,14,36 | 0.69 | 0 | 14,14,47 | 0.59 | 0 |
| 19 | LMT | T | 102 | - | 26,26,36 | 0.41 | 0 | 31,31,47 | 1.05 | 2 (6%) |
| 11 | UQ8 | A | 101 | - | 53,53,53 | 1.21 | 2 (3%) | 64,67,67 | 1.59 | 15 (23%) |
| 19 | LMT | b | 103 | - | 36,36,36 | 0.40 | 0 | 47,47,47 | 0.94 | 2 (4%) |
| 21 | NS0 | 2 | 101 | - | 39,39,39 | 1.41 | 6 (15%) | 44,46,46 | 1.24 | 8 (18%) |
| 13 | BCB | M | 402 | - | 63,74,74 | 2.98 | 15 (23%) | 74,115,115 | 2.91 | 20 (27%) |
| 11 | UQ8 | M | 407 | - | 25,25,53 | 1.70 | 2 (8%) | 30,33,67 | 1.53 | 7 (23%) |
| 13 | BCB | r | 101 | - | 63,74,74 | 3.02 | 14 (22%) | 74,115,115 | 2.80 | 22 (29%) |
| 20 | PGV | I | 102 | - | 50,50,50 | 0.89 | 2 (4%) | 53,56,56 | 1.03 | 3 (5%) |
| 21 | NS0 | A | 103 | - | 39,39,39 | 1.41 | 6 (15%) | 44,46,46 | 1.26 | 8 (18%) |
| 21 | NS0 | W | 303 | - | 39,39,39 | 1.38 | 8 (20%) | 44,46,46 | 1.28 | 7 (15%) |
| 20 | PGV | Q | 401 | - | 48,48,50 | 0.96 | 2 (4%) | 51,53,56 | 0.99 | 2 (3%) |
| 15 | CDL | H | 301 | - | 97,97,99 | 0.92 | 4 (4%) | 103,109,111 | 1.06 | 5 (4%) |
| 13 | BCB | k | 102 | - | 63,74,74 | 2.97 | 15 (23%) | 74,115,115 | 2.81 | 21 (28%) |
| 9 | HEC | C | 404 | 1 | 32,50,50 | 1.62 | 5 (15%) | 24,82,82 | 1.30 | 1 (4%) |
| 21 | NS0 | D | 103 | - | 39,39,39 | 1.43 | 6 (15%) | 44,46,46 | 1.25 | 7 (15%) |
| 18 | NS5 | M | 406 | - | 39,39,39 | 1.43 | 6 (15%) | 44,46,46 | 1.28 | 7 (15%) |
| 13 | BCB | 1 | 101 | - | 63,74,74 | 2.98 | 14 (22%) | 74,115,115 | 2.89 | 22 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 21 | NS0 | h | 101 | - | 39,39,39 | 1.42 | 6 (15%) | 44,46,46 | 1.25 | 7 (15%) |
| 11 | UQ8 | M | 408 | - | 53,53,53 | 1.25 | 2 (3%) | 64,67,67 | 1.61 | 17 (26%) |
| 13 | BCB | n | 101 | - | 63,74,74 | 3.01 | 14 (22%) | 74,115,115 | 2.85 | 23 (31%) |
| 13 | BCB | o | 102 | - | 63,74,74 | 3.01 | 15 (23%) | 74,115,115 | 2.84 | 21 (28%) |
| 13 | BCB | b | 101 | - | 63,74,74 | 2.93 | 15 (23%) | 74,115,115 | 2.93 | 23 (31%) |
| 11 | UQ8 | L | 305 | - | 31,31,53 | 1.56 | 2 (6%) | 37,40,67 | 1.43 | 6 (16%) |
| 19 | LMT | k | 103 | - | 36,36,36 | 0.43 | 0 | 47,47,47 | 0.86 | 1 (2%) |
| 19 | LMT | b | 102 | - | 36,36,36 | 0.44 | 0 | 47,47,47 | 0.78 | 0 |
| 13 | BCB | 3 | 101 | - | 63,74,74 | 2.92 | 15 (23%) | 74,115,115 | 2.95 | 24 (32%) |
| 21 | NS0 | q | 102 | - | 39,39,39 | 1.40 | 6 (15%) | 44,46,46 | 1.29 | 7 (15%) |
| 13 | BCB | X | 102 | - | 63,74,74 | 3.00 | 14 (22%) | 74,115,115 | 2.82 | 23 (31%) |
| 20 | PGV | W | 301 | - | 47,47,50 | 0.95 | 2 (4%) | 50,53,56 | 1.07 | 4 (8%) |
| 13 | BCB | M | 403 | - | 63,74,74 | 2.98 | 16 (25%) | 74,115,115 | 2.88 | 21 (28%) |
| 13 | BCB | 6 | 101 | - | 63,74,74 | 2.98 | 15 (23%) | 74,115,115 | 2.81 | 22 (29%) |
| 13 | BCB | f | 101 | - | 63,74,74 | 2.98 | 15 (23%) | 74,115,115 | 2.85 | 23 (31%) |
| 13 | BCB | D | 101 | - | 63,74,74 | 2.96 | 16 (25%) | 74,115,115 | 2.87 | 23 (31%) |
| 21 | NS0 | R | 101 | - | 39,39,39 | 1.41 | 6 (15%) | 44,46,46 | 1.32 | 6 (13%) |
| 19 | LMT | n | 102 | - | 36,36,36 | 0.40 | 0 | 47,47,47 | 0.78 | 1 (2%) |
| 15 | CDL | r | 102 | - | 67,67,99 | 1.11 | 4 (5%) | 73,79,111 | 1.14 | 4 (5%) |
| 19 | LMT | M | 410 | - | 25,25,36 | 0.42 | 0 | 30,30,47 | 0.63 | 0 |
| 13 | BCB | h | 102 | - | 63,74,74 | 2.99 | 15 (23%) | 74,115,115 | 2.94 | 23 (31%) |
| 21 | NS0 | 0 | 101 | - | 39,39,39 | 1.41 | 6 (15%) | 44,46,46 | 1.20 | 6 (13%) |
| 13 | BCB | E | 101 | - | 63,74,74 | 2.97 | 15 (23%) | 74,115,115 | 2.82 | 22 (29%) |
| 13 | BCB | i | 101 | - | 63,74,74 | 2.96 | 15 (23%) | 74,115,115 | 2.86 | 25 (33%) |
| 21 | NS0 | k | 101 | - | 39,39,39 | 1.41 | 6 (15%) | 44,46,46 | 1.36 | 8 (18%) |
| 13 | BCB | e | 101 | - | 63,74,74 | 2.99 | 15 (23%) | 74,115,115 | 2.88 | 22 (29%) |
| 13 | BCB | N | 101 | - | 63,74,74 | 2.94 | 15 (23%) | 74,115,115 | 2.87 | 20 (27%) |
| 13 | BCB | 7 | 102 | - | 63,74,74 | 2.99 | 14 (22%) | 74,115,115 | 2.80 | 23 (31%) |
| 11 | UQ8 | C | 406 | - | 15,15,53 | 2.16 | 2 (13%) | 19,21,67 | 1.42 | 2 (10%) |
| 21 | NS0 | 7 | 101 | - | 39,39,39 | 1.41 | 6 (15%) | 44,46,46 | 1.25 | 6 (13%) |
| 21 | NS0 | 9 | 102 | - | 39,39,39 | 1.42 | 6 (15%) | 44,46,46 | 1.27 | 8 (18%) |
| 21 | NS0 | l | 101 | - | 39,39,39 | 1.38 | 6 (15%) | 44,46,46 | 1.30 | 8 (18%) |
| 13 | BCB | T | 101 | - | 63,74,74 | 3.00 | 16 (25%) | 74,115,115 | 2.85 | 20 (27%) |
| 21 | NS0 | O | 101 | - | 39,39,39 | 1.38 | 6 (15%) | 44,46,46 | 1.24 | 6 (13%) |
| 20 | PGV | D | 102 | - | 46,46,50 | 0.95 | 2 (4%) | 48,52,56 | 1.07 | 2 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 13 | BCB | O | 102 | - | 63,74,74 | 2.94 | 15 (23%) | 74,115,115 | 2.87 | 20 (27%) |
| 14 | BPB | M | 404 | - | 49,70,70 | 0.56 | 1 (2%) | 47,101,101 | 0.81 | 2 (4%) |
| 13 | BCB | L | 303 | - | 63,74,74 | 2.96 | 15 (23%) | 74,115,115 | 2.97 | 24 (32%) |
| 15 | CDL | L | 306 | - | 74,74,99 | 1.05 | 4 (5%) | 80,86,111 | 1.17 | 8 (10%) |
| 17 | MQ7 | M | 405 | - | 49,49,49 | 1.36 | 2 (4%) | 60,63,63 | 1.48 | 13 (21%) |
| 19 | LMT | h | 103 | - | 36,36,36 | 0.36 | 0 | 47,47,47 | 0.70 | 1 (2%) |
| 9 | HEC | C | 402 | 1 | 32,50,50 | 1.56 | 4 (12%) | 24,82,82 | 1.43 | 3 (12%) |
| 9 | HEC | C | 403 | 1 | 32,50,50 | 1.64 | 5 (15%) | 24,82,82 | 1.37 | 3 (12%) |
| 13 | BCB | Z | 101 | - | 63,74,74 | 2.94 | 15 (23%) | 74,115,115 | 2.90 | 21 (28%) |
| 13 | BCB | Q | 402 | - | 63,74,74 | 2.96 | 14 (22%) | 74,115,115 | 2.87 | 21 (28%) |
| 21 | NS0 | o | 101 | - | 39,39,39 | 1.40 | 6 (15%) | 44,46,46 | 1.26 | 7 (15%) |
| 13 | BCB | R | 102 | - | 63,74,74 | 3.01 | 15 (23%) | 74,115,115 | 2.90 | 22 (29%) |
| 13 | BCB | 4 | 101 | - | 63,74,74 | 2.97 | 15 (23%) | 74,115,115 | 2.85 | 21 (28%) |
| 13 | BCB | U | 102 | - | 63,74,74 | 3.00 | 15 (23%) | 74,115,115 | 2.83 | 24 (32%) |
| 14 | BPB | L | 304 | - | 49,70,70 | 0.58 | 1 (2%) | 47,101,101 | 0.77 | 1 (2%) |
| 21 | NS0 | U | 101 | - | 39,39,39 | 1.39 | 6 (15%) | 44,46,46 | 1.31 | 8 (18%) |
| 12 | DGA | L | 301 | 1 | 22,22,43 | 1.37 | 3 (13%) | 24,24,45 | 1.83 | 5 (20%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|-------|
| 15 | CDL | H | 302 | - | - | 36/82/82/110 | - |
| 21 | NS0 | X | 101 | - | - | 4/43/43/43 | - |
| 13 | BCB | 0 | 102 | - | 2/2/21/26 | 13/37/137/137 | - |
| 20 | PGV | N | 102 | - | - | 11/42/42/55 | - |
| 15 | CDL | M | 409 | - | - | 38/95/95/110 | - |
| 13 | BCB | q | 101 | - | 2/2/21/26 | 14/37/137/137 | - |
| 9 | HEC | C | 401 | 1 | - | 2/10/54/54 | - |
| 13 | BCB | W | 302 | - | 2/2/21/26 | 10/37/137/137 | - |
| 13 | BCB | l | 102 | - | 2/2/21/26 | 6/37/137/137 | - |
| 13 | BCB | I | 101 | - | 2/2/21/26 | 8/37/137/137 | - |
| 13 | BCB | A | 102 | - | 2/2/21/26 | 17/37/137/137 | - |
| 13 | BCB | 9 | 101 | - | 2/2/21/26 | 12/37/137/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|----------------|---------|
| 13 | BCB | L | 302 | - | 2/2/21/26 | 5/37/137/137 | - |
| 13 | BCB | J | 101 | - | 2/2/21/26 | 13/37/137/137 | - |
| 20 | PGV | M | 411 | - | - | 13/49/49/55 | - |
| 13 | BCB | c | 101 | - | 2/2/21/26 | 14/37/137/137 | - |
| 13 | BCB | B | 202 | - | 2/2/21/26 | 4/37/137/137 | - |
| 19 | LMT | B | 201 | - | - | 6/13/13/61 | - |
| 19 | LMT | T | 102 | - | - | 1/17/38/61 | 0/1/1/2 |
| 11 | UQ8 | A | 101 | - | - | 14/51/75/75 | 0/1/1/1 |
| 19 | LMT | b | 103 | - | - | 6/21/61/61 | 0/2/2/2 |
| 21 | NS0 | 2 | 101 | - | - | 6/43/43/43 | - |
| 13 | BCB | M | 402 | - | 2/2/21/26 | 8/37/137/137 | - |
| 11 | UQ8 | M | 407 | - | - | 0/18/42/75 | 0/1/1/1 |
| 13 | BCB | r | 101 | - | 2/2/21/26 | 14/37/137/137 | - |
| 20 | PGV | I | 102 | - | - | 16/55/55/55 | - |
| 21 | NS0 | A | 103 | - | - | 2/43/43/43 | - |
| 21 | NS0 | W | 303 | - | - | 7/43/43/43 | - |
| 20 | PGV | Q | 401 | - | - | 17/52/52/55 | - |
| 15 | CDL | H | 301 | - | - | 41/108/108/110 | - |
| 13 | BCB | k | 102 | - | 2/2/21/26 | 11/37/137/137 | - |
| 9 | HEC | C | 404 | 1 | - | 3/10/54/54 | - |
| 21 | NS0 | D | 103 | - | - | 3/43/43/43 | - |
| 18 | NS5 | M | 406 | - | - | 2/43/43/43 | - |
| 13 | BCB | l | 101 | - | 2/2/21/26 | 14/37/137/137 | - |
| 21 | NS0 | h | 101 | - | - | 1/43/43/43 | - |
| 11 | UQ8 | M | 408 | - | - | 12/51/75/75 | 0/1/1/1 |
| 13 | BCB | n | 101 | - | 2/2/21/26 | 4/37/137/137 | - |
| 13 | BCB | o | 102 | - | 2/2/21/26 | 18/37/137/137 | - |
| 13 | BCB | b | 101 | - | 2/2/21/26 | 10/37/137/137 | - |
| 11 | UQ8 | L | 305 | - | - | 6/25/49/75 | 0/1/1/1 |
| 19 | LMT | k | 103 | - | - | 3/21/61/61 | 0/2/2/2 |
| 19 | LMT | b | 102 | - | - | 11/21/61/61 | 0/2/2/2 |
| 13 | BCB | 3 | 101 | - | 2/2/21/26 | 12/37/137/137 | - |
| 21 | NS0 | q | 102 | - | - | 7/43/43/43 | - |
| 13 | BCB | X | 102 | - | 2/2/21/26 | 19/37/137/137 | - |
| 20 | PGV | W | 301 | - | - | 16/52/52/55 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 13 | BCB | M | 403 | - | 2/2/21/26 | 8/37/137/137 | - |
| 13 | BCB | 6 | 101 | - | 2/2/21/26 | 6/37/137/137 | - |
| 13 | BCB | f | 101 | - | 2/2/21/26 | 17/37/137/137 | - |
| 13 | BCB | D | 101 | - | 2/2/21/26 | 10/37/137/137 | - |
| 21 | NS0 | R | 101 | - | - | 6/43/43/43 | - |
| 19 | LMT | n | 102 | - | - | 4/21/61/61 | 0/2/2/2 |
| 15 | CDL | r | 102 | - | - | 42/78/78/110 | - |
| 19 | LMT | M | 410 | - | - | 6/17/37/61 | 0/1/1/2 |
| 13 | BCB | h | 102 | - | 2/2/21/26 | 4/37/137/137 | - |
| 21 | NS0 | 0 | 101 | - | - | 4/43/43/43 | - |
| 13 | BCB | E | 101 | - | 2/2/21/26 | 14/37/137/137 | - |
| 13 | BCB | i | 101 | - | 2/2/21/26 | 14/37/137/137 | - |
| 21 | NS0 | k | 101 | - | - | 4/43/43/43 | - |
| 13 | BCB | e | 101 | - | 2/2/21/26 | 10/37/137/137 | - |
| 13 | BCB | N | 101 | - | 2/2/21/26 | 17/37/137/137 | - |
| 13 | BCB | 7 | 102 | - | 2/2/21/26 | 21/37/137/137 | - |
| 11 | UQ8 | C | 406 | - | - | 0/6/30/75 | 0/1/1/1 |
| 21 | NS0 | 7 | 101 | - | - | 6/43/43/43 | - |
| 21 | NS0 | 9 | 102 | - | - | 6/43/43/43 | - |
| 21 | NS0 | l | 101 | - | - | 7/43/43/43 | - |
| 13 | BCB | T | 101 | - | 2/2/21/26 | 10/37/137/137 | - |
| 21 | NS0 | O | 101 | - | - | 8/43/43/43 | - |
| 20 | PGV | D | 102 | - | - | 14/51/51/55 | - |
| 13 | BCB | O | 102 | - | 2/2/21/26 | 17/37/137/137 | - |
| 14 | BPB | M | 404 | - | - | 5/37/105/105 | 0/5/6/6 |
| 13 | BCB | L | 303 | - | 2/2/21/26 | 3/37/137/137 | - |
| 15 | CDL | L | 306 | - | - | 31/85/85/110 | - |
| 17 | MQ7 | M | 405 | - | - | 0/41/61/61 | 0/2/2/2 |
| 19 | LMT | h | 103 | - | - | 4/21/61/61 | 0/2/2/2 |
| 9 | HEC | C | 402 | 1 | - | 3/10/54/54 | - |
| 9 | HEC | C | 403 | 1 | - | 0/10/54/54 | - |
| 13 | BCB | Z | 101 | - | 2/2/21/26 | 6/37/137/137 | - |
| 13 | BCB | Q | 402 | - | 2/2/21/26 | 6/37/137/137 | - |
| 21 | NS0 | o | 101 | - | - | 6/43/43/43 | - |
| 13 | BCB | R | 102 | - | 2/2/21/26 | 10/37/137/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 13 | BCB | 4 | 101 | - | 2/2/21/26 | 12/37/137/137 | - |
| 13 | BCB | U | 102 | - | 2/2/21/26 | 11/37/137/137 | - |
| 14 | BPB | L | 304 | - | - | 3/37/105/105 | 0/5/6/6 |
| 21 | NS0 | U | 101 | - | - | 6/43/43/43 | - |
| 12 | DGA | L | 301 | 1 | - | 13/23/23/45 | - |

All (737) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13 | R | 102 | BCB | C4B-NB | 12.73 | 1.46 | 1.35 |
| 13 | J | 101 | BCB | C4B-NB | 12.71 | 1.46 | 1.35 |
| 13 | o | 102 | BCB | C4B-NB | 12.65 | 1.46 | 1.35 |
| 13 | B | 202 | BCB | C4B-NB | 12.59 | 1.46 | 1.35 |
| 13 | c | 101 | BCB | C4B-NB | 12.58 | 1.46 | 1.35 |
| 13 | X | 102 | BCB | C4B-NB | 12.51 | 1.46 | 1.35 |
| 13 | 0 | 102 | BCB | C4B-NB | 12.44 | 1.46 | 1.35 |
| 13 | 7 | 102 | BCB | C4B-NB | 12.42 | 1.46 | 1.35 |
| 13 | 4 | 101 | BCB | C4B-NB | 12.42 | 1.46 | 1.35 |
| 13 | U | 102 | BCB | C4B-NB | 12.38 | 1.46 | 1.35 |
| 13 | n | 101 | BCB | C4B-NB | 12.37 | 1.46 | 1.35 |
| 13 | 6 | 101 | BCB | C4B-NB | 12.33 | 1.46 | 1.35 |
| 13 | l | 102 | BCB | C4B-NB | 12.31 | 1.46 | 1.35 |
| 13 | e | 101 | BCB | C4B-NB | 12.30 | 1.46 | 1.35 |
| 13 | W | 302 | BCB | C4B-NB | 12.29 | 1.46 | 1.35 |
| 13 | f | 101 | BCB | C4B-NB | 12.26 | 1.46 | 1.35 |
| 13 | h | 102 | BCB | C4B-NB | 12.23 | 1.46 | 1.35 |
| 13 | i | 101 | BCB | C4B-NB | 12.23 | 1.46 | 1.35 |
| 13 | T | 101 | BCB | C4B-NB | 12.18 | 1.46 | 1.35 |
| 13 | k | 102 | BCB | C4B-NB | 12.15 | 1.46 | 1.35 |
| 13 | Q | 402 | BCB | C4B-NB | 12.14 | 1.46 | 1.35 |
| 13 | E | 101 | BCB | C4B-NB | 12.11 | 1.46 | 1.35 |
| 13 | 9 | 101 | BCB | C4B-NB | 12.10 | 1.46 | 1.35 |
| 13 | r | 101 | BCB | C4B-NB | 12.10 | 1.46 | 1.35 |
| 13 | O | 102 | BCB | C4B-NB | 12.09 | 1.46 | 1.35 |
| 13 | 1 | 101 | BCB | C4B-NB | 12.08 | 1.46 | 1.35 |
| 13 | M | 402 | BCB | C4B-NB | 12.03 | 1.45 | 1.35 |
| 13 | Z | 101 | BCB | C4B-NB | 12.02 | 1.45 | 1.35 |
| 13 | L | 303 | BCB | C4B-NB | 11.88 | 1.45 | 1.35 |
| 13 | b | 101 | BCB | C4B-NB | 11.88 | 1.45 | 1.35 |
| 13 | I | 101 | BCB | C4B-NB | 11.88 | 1.45 | 1.35 |
| 13 | r | 101 | BCB | C1B-NB | 11.84 | 1.45 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13 | N | 101 | BCB | C4B-NB | 11.79 | 1.45 | 1.35 |
| 13 | D | 101 | BCB | C4B-NB | 11.59 | 1.45 | 1.35 |
| 13 | A | 102 | BCB | C4B-NB | 11.58 | 1.45 | 1.35 |
| 13 | 3 | 101 | BCB | C4B-NB | 11.58 | 1.45 | 1.35 |
| 13 | q | 101 | BCB | C4B-NB | 11.54 | 1.45 | 1.35 |
| 13 | M | 403 | BCB | C4B-NB | 11.52 | 1.45 | 1.35 |
| 13 | M | 402 | BCB | C1B-NB | 11.40 | 1.45 | 1.35 |
| 13 | U | 102 | BCB | C1B-NB | 11.32 | 1.45 | 1.35 |
| 13 | L | 302 | BCB | C4B-NB | 11.31 | 1.45 | 1.35 |
| 13 | l | 102 | BCB | C1B-NB | 11.28 | 1.45 | 1.35 |
| 13 | J | 101 | BCB | C1B-NB | 11.14 | 1.45 | 1.35 |
| 13 | T | 101 | BCB | C1B-NB | 11.14 | 1.45 | 1.35 |
| 13 | o | 102 | BCB | C1B-NB | 11.14 | 1.45 | 1.35 |
| 13 | 1 | 101 | BCB | C1B-NB | 11.12 | 1.45 | 1.35 |
| 13 | q | 101 | BCB | C1B-NB | 11.12 | 1.45 | 1.35 |
| 13 | X | 102 | BCB | C1B-NB | 11.06 | 1.45 | 1.35 |
| 13 | A | 102 | BCB | C1B-NB | 10.99 | 1.45 | 1.35 |
| 13 | 0 | 102 | BCB | C1B-NB | 10.97 | 1.45 | 1.35 |
| 13 | L | 303 | BCB | C1B-NB | 10.96 | 1.45 | 1.35 |
| 13 | n | 101 | BCB | C1B-NB | 10.95 | 1.45 | 1.35 |
| 13 | E | 101 | BCB | C1B-NB | 10.95 | 1.45 | 1.35 |
| 13 | B | 202 | BCB | C1B-NB | 10.94 | 1.45 | 1.35 |
| 13 | f | 101 | BCB | C1B-NB | 10.93 | 1.45 | 1.35 |
| 13 | h | 102 | BCB | C1B-NB | 10.91 | 1.44 | 1.35 |
| 13 | L | 302 | BCB | C1B-NB | 10.91 | 1.44 | 1.35 |
| 13 | c | 101 | BCB | C1B-NB | 10.88 | 1.44 | 1.35 |
| 13 | D | 101 | BCB | C1B-NB | 10.88 | 1.44 | 1.35 |
| 13 | 7 | 102 | BCB | C1B-NB | 10.84 | 1.44 | 1.35 |
| 13 | 4 | 101 | BCB | C1B-NB | 10.84 | 1.44 | 1.35 |
| 13 | i | 101 | BCB | C1B-NB | 10.83 | 1.44 | 1.35 |
| 13 | 6 | 101 | BCB | C1B-NB | 10.82 | 1.44 | 1.35 |
| 13 | R | 102 | BCB | C1B-NB | 10.79 | 1.44 | 1.35 |
| 13 | Q | 402 | BCB | C1B-NB | 10.78 | 1.44 | 1.35 |
| 13 | k | 102 | BCB | C1B-NB | 10.76 | 1.44 | 1.35 |
| 13 | Z | 101 | BCB | C1B-NB | 10.74 | 1.44 | 1.35 |
| 13 | O | 102 | BCB | C1B-NB | 10.73 | 1.44 | 1.35 |
| 13 | N | 101 | BCB | C1B-NB | 10.69 | 1.44 | 1.35 |
| 13 | e | 101 | BCB | C1B-NB | 10.68 | 1.44 | 1.35 |
| 13 | 9 | 101 | BCB | C1B-NB | 10.66 | 1.44 | 1.35 |
| 13 | M | 403 | BCB | C1B-NB | 10.65 | 1.44 | 1.35 |
| 13 | W | 302 | BCB | C1B-NB | 10.59 | 1.44 | 1.35 |
| 13 | 3 | 101 | BCB | C1B-NB | 10.54 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13 | I | 101 | BCB | C1B-NB | 10.51 | 1.44 | 1.35 |
| 13 | b | 101 | BCB | C1B-NB | 10.33 | 1.44 | 1.35 |
| 11 | M | 408 | UQ8 | C6-C1 | 7.83 | 1.49 | 1.35 |
| 13 | M | 403 | BCB | C1D-ND | 7.69 | 1.47 | 1.37 |
| 17 | M | 405 | MQ7 | C3-C2 | 7.66 | 1.49 | 1.35 |
| 11 | M | 407 | UQ8 | C6-C1 | 7.64 | 1.49 | 1.35 |
| 13 | A | 102 | BCB | C1D-ND | 7.62 | 1.47 | 1.37 |
| 11 | L | 305 | UQ8 | C6-C1 | 7.58 | 1.49 | 1.35 |
| 13 | 9 | 101 | BCB | C1D-ND | 7.51 | 1.47 | 1.37 |
| 11 | C | 406 | UQ8 | C6-C1 | 7.49 | 1.48 | 1.35 |
| 11 | A | 101 | UQ8 | C6-C1 | 7.43 | 1.48 | 1.35 |
| 13 | D | 101 | BCB | C1D-ND | 7.42 | 1.46 | 1.37 |
| 13 | b | 101 | BCB | C1D-ND | 7.41 | 1.46 | 1.37 |
| 13 | T | 101 | BCB | C1D-ND | 7.40 | 1.46 | 1.37 |
| 13 | n | 101 | BCB | C1D-ND | 7.39 | 1.46 | 1.37 |
| 13 | I | 101 | BCB | C1D-ND | 7.38 | 1.46 | 1.37 |
| 13 | L | 302 | BCB | C1D-ND | 7.38 | 1.46 | 1.37 |
| 13 | q | 101 | BCB | C1D-ND | 7.37 | 1.46 | 1.37 |
| 13 | e | 101 | BCB | C1D-ND | 7.35 | 1.46 | 1.37 |
| 13 | h | 102 | BCB | C1D-ND | 7.31 | 1.46 | 1.37 |
| 13 | W | 302 | BCB | C1D-ND | 7.28 | 1.46 | 1.37 |
| 13 | 6 | 101 | BCB | C1D-ND | 7.27 | 1.46 | 1.37 |
| 13 | M | 402 | BCB | C1D-ND | 7.25 | 1.46 | 1.37 |
| 13 | 3 | 101 | BCB | C1D-ND | 7.25 | 1.46 | 1.37 |
| 13 | L | 303 | BCB | C1D-ND | 7.17 | 1.46 | 1.37 |
| 13 | k | 102 | BCB | C1D-ND | 7.14 | 1.46 | 1.37 |
| 13 | Q | 402 | BCB | C1D-ND | 7.10 | 1.46 | 1.37 |
| 13 | Z | 101 | BCB | C1D-ND | 7.09 | 1.46 | 1.37 |
| 13 | N | 101 | BCB | C1D-ND | 7.07 | 1.46 | 1.37 |
| 13 | o | 102 | BCB | C1D-ND | 7.07 | 1.46 | 1.37 |
| 13 | 7 | 102 | BCB | C1D-ND | 6.99 | 1.46 | 1.37 |
| 13 | X | 102 | BCB | C1D-ND | 6.92 | 1.46 | 1.37 |
| 13 | r | 101 | BCB | C1D-ND | 6.91 | 1.46 | 1.37 |
| 13 | B | 202 | BCB | C1D-ND | 6.90 | 1.46 | 1.37 |
| 13 | O | 102 | BCB | C1D-ND | 6.90 | 1.46 | 1.37 |
| 13 | E | 101 | BCB | C1D-ND | 6.83 | 1.46 | 1.37 |
| 13 | 4 | 101 | BCB | C1D-ND | 6.81 | 1.46 | 1.37 |
| 13 | R | 102 | BCB | C1D-ND | 6.75 | 1.46 | 1.37 |
| 13 | f | 101 | BCB | C1D-ND | 6.71 | 1.46 | 1.37 |
| 13 | c | 101 | BCB | C1D-ND | 6.69 | 1.46 | 1.37 |
| 13 | i | 101 | BCB | C1D-ND | 6.69 | 1.46 | 1.37 |
| 13 | 0 | 102 | BCB | C1D-ND | 6.65 | 1.46 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | U | 102 | BCB | C1D-ND | 6.64 | 1.45 | 1.37 |
| 13 | J | 101 | BCB | C1D-ND | 6.62 | 1.45 | 1.37 |
| 13 | l | 102 | BCB | C1D-ND | 6.60 | 1.45 | 1.37 |
| 13 | 1 | 101 | BCB | C1D-ND | 6.57 | 1.45 | 1.37 |
| 13 | 3 | 101 | BCB | C3B-C2B | 6.36 | 1.50 | 1.39 |
| 13 | I | 101 | BCB | C3B-C2B | 6.33 | 1.50 | 1.39 |
| 13 | M | 403 | BCB | C3B-C2B | 6.29 | 1.50 | 1.39 |
| 13 | R | 102 | BCB | C3B-C2B | 6.29 | 1.50 | 1.39 |
| 13 | b | 101 | BCB | C3B-C2B | 6.28 | 1.50 | 1.39 |
| 13 | D | 101 | BCB | C3B-C2B | 6.27 | 1.50 | 1.39 |
| 13 | T | 101 | BCB | C3B-C2B | 6.26 | 1.50 | 1.39 |
| 13 | W | 302 | BCB | C3B-C2B | 6.26 | 1.50 | 1.39 |
| 13 | N | 101 | BCB | C3B-C2B | 6.24 | 1.50 | 1.39 |
| 13 | k | 102 | BCB | C3B-C2B | 6.21 | 1.50 | 1.39 |
| 13 | n | 101 | BCB | C3B-C2B | 6.20 | 1.50 | 1.39 |
| 13 | L | 303 | BCB | C3B-C2B | 6.19 | 1.50 | 1.39 |
| 13 | 1 | 101 | BCB | C3B-C2B | 6.18 | 1.50 | 1.39 |
| 13 | q | 101 | BCB | C3B-C2B | 6.18 | 1.50 | 1.39 |
| 13 | c | 101 | BCB | C3B-C2B | 6.17 | 1.50 | 1.39 |
| 13 | 6 | 101 | BCB | C3B-C2B | 6.17 | 1.50 | 1.39 |
| 13 | o | 102 | BCB | C3B-C2B | 6.17 | 1.50 | 1.39 |
| 13 | h | 102 | BCB | C3B-C2B | 6.16 | 1.50 | 1.39 |
| 13 | l | 102 | BCB | C3B-C2B | 6.15 | 1.50 | 1.39 |
| 13 | A | 102 | BCB | C3B-C2B | 6.15 | 1.50 | 1.39 |
| 13 | f | 101 | BCB | C3B-C2B | 6.13 | 1.50 | 1.39 |
| 13 | B | 202 | BCB | C3B-C2B | 6.13 | 1.50 | 1.39 |
| 13 | e | 101 | BCB | C3B-C2B | 6.12 | 1.50 | 1.39 |
| 13 | Q | 402 | BCB | C3B-C2B | 6.12 | 1.50 | 1.39 |
| 13 | U | 102 | BCB | C3B-C2B | 6.11 | 1.50 | 1.39 |
| 13 | 7 | 102 | BCB | C3B-C2B | 6.11 | 1.50 | 1.39 |
| 13 | 9 | 101 | BCB | C3B-C2B | 6.10 | 1.50 | 1.39 |
| 13 | M | 403 | BCB | C2C-C3C | -6.09 | 1.43 | 1.51 |
| 13 | L | 302 | BCB | C3B-C2B | 6.09 | 1.50 | 1.39 |
| 13 | 4 | 101 | BCB | C3B-C2B | 6.08 | 1.50 | 1.39 |
| 13 | i | 101 | BCB | C3B-C2B | 6.04 | 1.50 | 1.39 |
| 13 | O | 102 | BCB | C3B-C2B | 6.04 | 1.50 | 1.39 |
| 13 | E | 101 | BCB | C3B-C2B | 6.03 | 1.50 | 1.39 |
| 13 | 0 | 102 | BCB | C3B-C2B | 6.03 | 1.50 | 1.39 |
| 13 | c | 101 | BCB | C2C-C3C | -6.01 | 1.43 | 1.51 |
| 13 | X | 102 | BCB | C3B-C2B | 5.96 | 1.50 | 1.39 |
| 13 | r | 101 | BCB | C3B-C2B | 5.96 | 1.50 | 1.39 |
| 13 | Z | 101 | BCB | C3B-C2B | 5.95 | 1.50 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | J | 101 | BCB | C3B-C2B | 5.91 | 1.50 | 1.39 |
| 13 | e | 101 | BCB | CAC-C3C | 5.90 | 1.49 | 1.33 |
| 13 | I | 101 | BCB | CAC-C3C | 5.89 | 1.49 | 1.33 |
| 13 | Q | 402 | BCB | CAC-C3C | 5.88 | 1.49 | 1.33 |
| 13 | l | 102 | BCB | CAC-C3C | 5.88 | 1.49 | 1.33 |
| 13 | B | 202 | BCB | CAC-C3C | 5.87 | 1.49 | 1.33 |
| 13 | n | 101 | BCB | CAC-C3C | 5.87 | 1.49 | 1.33 |
| 13 | R | 102 | BCB | C2C-C3C | -5.86 | 1.44 | 1.51 |
| 13 | U | 102 | BCB | CAC-C3C | 5.86 | 1.49 | 1.33 |
| 13 | Z | 101 | BCB | CAC-C3C | 5.85 | 1.49 | 1.33 |
| 13 | h | 102 | BCB | CAC-C3C | 5.85 | 1.49 | 1.33 |
| 13 | T | 101 | BCB | CAC-C3C | 5.85 | 1.49 | 1.33 |
| 13 | 6 | 101 | BCB | CAC-C3C | 5.85 | 1.49 | 1.33 |
| 13 | b | 101 | BCB | CAC-C3C | 5.84 | 1.49 | 1.33 |
| 13 | c | 101 | BCB | CAC-C3C | 5.83 | 1.49 | 1.33 |
| 13 | 0 | 102 | BCB | CAC-C3C | 5.83 | 1.49 | 1.33 |
| 13 | E | 101 | BCB | CAC-C3C | 5.83 | 1.49 | 1.33 |
| 13 | k | 102 | BCB | CAC-C3C | 5.82 | 1.49 | 1.33 |
| 13 | L | 302 | BCB | CAC-C3C | 5.82 | 1.49 | 1.33 |
| 13 | 1 | 101 | BCB | C2C-C3C | -5.81 | 1.44 | 1.51 |
| 13 | q | 101 | BCB | CAC-C3C | 5.81 | 1.49 | 1.33 |
| 13 | W | 302 | BCB | CAC-C3C | 5.80 | 1.49 | 1.33 |
| 13 | A | 102 | BCB | C2C-C3C | -5.80 | 1.44 | 1.51 |
| 13 | r | 101 | BCB | CAC-C3C | 5.80 | 1.49 | 1.33 |
| 13 | O | 102 | BCB | C2C-C3C | -5.79 | 1.44 | 1.51 |
| 13 | 3 | 101 | BCB | CAC-C3C | 5.79 | 1.49 | 1.33 |
| 13 | 1 | 101 | BCB | CAC-C3C | 5.78 | 1.49 | 1.33 |
| 13 | N | 101 | BCB | CAC-C3C | 5.78 | 1.49 | 1.33 |
| 13 | 9 | 101 | BCB | CAC-C3C | 5.78 | 1.49 | 1.33 |
| 13 | 4 | 101 | BCB | CAC-C3C | 5.78 | 1.49 | 1.33 |
| 13 | D | 101 | BCB | CAC-C3C | 5.77 | 1.49 | 1.33 |
| 13 | 7 | 102 | BCB | CAC-C3C | 5.77 | 1.49 | 1.33 |
| 13 | o | 102 | BCB | CAC-C3C | 5.76 | 1.49 | 1.33 |
| 13 | A | 102 | BCB | CAC-C3C | 5.75 | 1.49 | 1.33 |
| 13 | M | 403 | BCB | CAC-C3C | 5.75 | 1.49 | 1.33 |
| 13 | L | 303 | BCB | CAC-C3C | 5.74 | 1.49 | 1.33 |
| 13 | i | 101 | BCB | CAC-C3C | 5.74 | 1.49 | 1.33 |
| 13 | X | 102 | BCB | CAC-C3C | 5.72 | 1.49 | 1.33 |
| 13 | J | 101 | BCB | CAC-C3C | 5.72 | 1.49 | 1.33 |
| 13 | O | 102 | BCB | CAC-C3C | 5.71 | 1.49 | 1.33 |
| 13 | l | 102 | BCB | C2C-C3C | -5.71 | 1.44 | 1.51 |
| 13 | R | 102 | BCB | CAC-C3C | 5.71 | 1.49 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | f | 101 | BCB | C2C-C3C | -5.70 | 1.44 | 1.51 |
| 13 | 4 | 101 | BCB | C2C-C3C | -5.70 | 1.44 | 1.51 |
| 13 | M | 402 | BCB | C2C-C3C | -5.70 | 1.44 | 1.51 |
| 13 | f | 101 | BCB | CAC-C3C | 5.69 | 1.49 | 1.33 |
| 13 | 7 | 102 | BCB | C2C-C3C | -5.69 | 1.44 | 1.51 |
| 13 | M | 402 | BCB | CAC-C3C | 5.68 | 1.49 | 1.33 |
| 13 | E | 101 | BCB | C2C-C3C | -5.68 | 1.44 | 1.51 |
| 13 | X | 102 | BCB | C2C-C3C | -5.68 | 1.44 | 1.51 |
| 13 | U | 102 | BCB | C2C-C3C | -5.61 | 1.44 | 1.51 |
| 13 | r | 101 | BCB | C2C-C3C | -5.56 | 1.44 | 1.51 |
| 13 | 0 | 102 | BCB | C2C-C3C | -5.56 | 1.44 | 1.51 |
| 13 | i | 101 | BCB | C2C-C3C | -5.55 | 1.44 | 1.51 |
| 13 | o | 102 | BCB | C2C-C3C | -5.54 | 1.44 | 1.51 |
| 13 | 6 | 101 | BCB | C2C-C3C | -5.53 | 1.44 | 1.51 |
| 13 | D | 101 | BCB | C2C-C3C | -5.50 | 1.44 | 1.51 |
| 13 | W | 302 | BCB | C2C-C3C | -5.50 | 1.44 | 1.51 |
| 13 | I | 101 | BCB | C2C-C3C | -5.48 | 1.44 | 1.51 |
| 13 | b | 101 | BCB | C2C-C3C | -5.47 | 1.44 | 1.51 |
| 13 | N | 101 | BCB | C2C-C3C | -5.45 | 1.44 | 1.51 |
| 13 | L | 302 | BCB | C2C-C3C | -5.41 | 1.44 | 1.51 |
| 13 | h | 102 | BCB | C2C-C3C | -5.41 | 1.44 | 1.51 |
| 13 | 3 | 101 | BCB | C2C-C3C | -5.38 | 1.44 | 1.51 |
| 13 | B | 202 | BCB | C2C-C3C | -5.36 | 1.44 | 1.51 |
| 13 | e | 101 | BCB | C2C-C3C | -5.31 | 1.44 | 1.51 |
| 13 | J | 101 | BCB | C2C-C3C | -5.31 | 1.44 | 1.51 |
| 13 | n | 101 | BCB | C2C-C3C | -5.31 | 1.44 | 1.51 |
| 13 | Q | 402 | BCB | C2C-C3C | -5.24 | 1.44 | 1.51 |
| 13 | L | 303 | BCB | C2C-C3C | -5.21 | 1.45 | 1.51 |
| 13 | Z | 101 | BCB | C2C-C3C | -5.19 | 1.45 | 1.51 |
| 13 | 9 | 101 | BCB | C2C-C3C | -5.16 | 1.45 | 1.51 |
| 13 | q | 101 | BCB | C2C-C3C | -5.15 | 1.45 | 1.51 |
| 13 | n | 101 | BCB | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 13 | L | 302 | BCB | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 13 | M | 402 | BCB | C3B-C2B | 5.11 | 1.48 | 1.39 |
| 13 | e | 101 | BCB | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 13 | 1 | 101 | BCB | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 13 | k | 102 | BCB | C2C-C3C | -5.06 | 1.45 | 1.51 |
| 13 | R | 102 | BCB | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 13 | f | 101 | BCB | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 13 | h | 102 | BCB | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 13 | T | 101 | BCB | C2C-C3C | -5.02 | 1.45 | 1.51 |
| 13 | 9 | 101 | BCB | O2D-CGD | 5.02 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | X | 102 | BCB | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 13 | i | 101 | BCB | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 13 | W | 302 | BCB | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 13 | U | 102 | BCB | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 13 | 0 | 102 | BCB | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 13 | 6 | 101 | BCB | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 13 | k | 102 | BCB | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 13 | l | 102 | BCB | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 13 | 3 | 101 | BCB | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 13 | 7 | 102 | BCB | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 13 | B | 202 | BCB | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 13 | b | 101 | BCB | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 13 | c | 101 | BCB | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 13 | E | 101 | BCB | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 13 | M | 403 | BCB | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 13 | o | 102 | BCB | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 13 | Z | 101 | BCB | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 17 | M | 405 | MQ7 | C10-C5 | 4.90 | 1.48 | 1.40 |
| 13 | r | 101 | BCB | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 13 | D | 101 | BCB | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 13 | q | 101 | BCB | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 13 | M | 403 | BCB | C3D-C4D | -4.89 | 1.33 | 1.44 |
| 13 | 4 | 101 | BCB | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 13 | A | 102 | BCB | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 13 | T | 101 | BCB | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 13 | J | 101 | BCB | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 13 | Q | 402 | BCB | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 13 | L | 303 | BCB | C3D-C4D | -4.84 | 1.33 | 1.44 |
| 13 | I | 101 | BCB | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 13 | R | 102 | BCB | C3D-C4D | -4.79 | 1.33 | 1.44 |
| 13 | N | 101 | BCB | O2D-CGD | 4.79 | 1.44 | 1.33 |
| 13 | 1 | 101 | BCB | C3D-C4D | -4.78 | 1.33 | 1.44 |
| 13 | c | 101 | BCB | C3D-C4D | -4.78 | 1.33 | 1.44 |
| 13 | O | 102 | BCB | O2D-CGD | 4.77 | 1.44 | 1.33 |
| 13 | 0 | 102 | BCB | C3D-C4D | -4.76 | 1.33 | 1.44 |
| 13 | B | 202 | BCB | C3D-C4D | -4.74 | 1.33 | 1.44 |
| 13 | L | 303 | BCB | O2D-CGD | 4.74 | 1.44 | 1.33 |
| 9 | C | 403 | HEC | C2B-C3B | -4.73 | 1.35 | 1.40 |
| 13 | E | 101 | BCB | C3D-C4D | -4.73 | 1.33 | 1.44 |
| 13 | M | 402 | BCB | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 13 | 7 | 102 | BCB | C3D-C4D | -4.71 | 1.33 | 1.44 |
| 13 | M | 402 | BCB | C3D-C4D | -4.70 | 1.33 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | o | 102 | BCB | C3D-C4D | -4.69 | 1.33 | 1.44 |
| 13 | i | 101 | BCB | C3D-C4D | -4.69 | 1.33 | 1.44 |
| 13 | f | 101 | BCB | C3D-C4D | -4.68 | 1.33 | 1.44 |
| 13 | U | 102 | BCB | C3D-C4D | -4.68 | 1.33 | 1.44 |
| 13 | l | 102 | BCB | C3D-C4D | -4.64 | 1.33 | 1.44 |
| 13 | A | 102 | BCB | C3D-C4D | -4.64 | 1.33 | 1.44 |
| 13 | r | 101 | BCB | C3D-C4D | -4.64 | 1.33 | 1.44 |
| 9 | C | 401 | HEC | C2B-C3B | -4.62 | 1.35 | 1.40 |
| 13 | I | 101 | BCB | C3D-C4D | -4.61 | 1.33 | 1.44 |
| 13 | 4 | 101 | BCB | C3D-C4D | -4.59 | 1.33 | 1.44 |
| 13 | b | 101 | BCB | C3D-C4D | -4.59 | 1.33 | 1.44 |
| 13 | X | 102 | BCB | C3D-C4D | -4.59 | 1.33 | 1.44 |
| 13 | L | 302 | BCB | C3D-C4D | -4.57 | 1.33 | 1.44 |
| 13 | D | 101 | BCB | C3D-C4D | -4.57 | 1.33 | 1.44 |
| 13 | 9 | 101 | BCB | C3D-C4D | -4.56 | 1.33 | 1.44 |
| 13 | q | 101 | BCB | C3D-C4D | -4.56 | 1.33 | 1.44 |
| 13 | J | 101 | BCB | C3D-C4D | -4.53 | 1.33 | 1.44 |
| 13 | Z | 101 | BCB | C3D-C4D | -4.52 | 1.34 | 1.44 |
| 13 | O | 102 | BCB | C3D-C4D | -4.51 | 1.34 | 1.44 |
| 13 | Q | 402 | BCB | C3D-C4D | -4.51 | 1.34 | 1.44 |
| 13 | h | 102 | BCB | C3D-C4D | -4.50 | 1.34 | 1.44 |
| 13 | W | 302 | BCB | C3D-C4D | -4.49 | 1.34 | 1.44 |
| 13 | e | 101 | BCB | C3D-C4D | -4.47 | 1.34 | 1.44 |
| 13 | k | 102 | BCB | C3D-C4D | -4.45 | 1.34 | 1.44 |
| 13 | n | 101 | BCB | C3D-C4D | -4.43 | 1.34 | 1.44 |
| 15 | H | 302 | CDL | OA8-CA7 | 4.43 | 1.46 | 1.33 |
| 9 | C | 404 | HEC | C2B-C3B | -4.43 | 1.36 | 1.40 |
| 9 | C | 403 | HEC | CBB-CAB | -4.42 | 1.32 | 1.49 |
| 9 | C | 402 | HEC | CBC-CAC | -4.42 | 1.32 | 1.49 |
| 13 | N | 101 | BCB | C3D-C4D | -4.41 | 1.34 | 1.44 |
| 13 | 3 | 101 | BCB | C3D-C4D | -4.40 | 1.34 | 1.44 |
| 13 | 6 | 101 | BCB | C3D-C4D | -4.38 | 1.34 | 1.44 |
| 9 | C | 404 | HEC | CBC-CAC | -4.37 | 1.33 | 1.49 |
| 13 | c | 101 | BCB | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 13 | f | 101 | BCB | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 13 | J | 101 | BCB | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 15 | H | 301 | CDL | OA8-CA7 | 4.34 | 1.46 | 1.33 |
| 13 | L | 303 | BCB | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 13 | T | 101 | BCB | C3D-C4D | -4.34 | 1.34 | 1.44 |
| 20 | D | 102 | PGV | O01-C1 | 4.33 | 1.46 | 1.34 |
| 20 | Q | 401 | PGV | O03-C19 | 4.33 | 1.46 | 1.33 |
| 9 | C | 401 | HEC | CBB-CAB | -4.33 | 1.33 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15 | H | 302 | CDL | OA6-CA5 | 4.33 | 1.46 | 1.34 |
| 13 | l | 101 | BCB | O2A-CGA | 4.32 | 1.46 | 1.33 |
| 13 | X | 102 | BCB | O2A-CGA | 4.32 | 1.46 | 1.33 |
| 13 | D | 101 | BCB | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 20 | W | 301 | PGV | O03-C19 | 4.31 | 1.45 | 1.33 |
| 13 | r | 101 | BCB | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 20 | N | 102 | PGV | O03-C19 | 4.31 | 1.45 | 1.33 |
| 20 | N | 102 | PGV | O01-C1 | 4.29 | 1.46 | 1.34 |
| 13 | 4 | 101 | BCB | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 13 | B | 202 | BCB | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 13 | i | 101 | BCB | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 13 | T | 101 | BCB | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 9 | C | 404 | HEC | CBB-CAB | -4.27 | 1.33 | 1.49 |
| 15 | r | 102 | CDL | OA6-CA5 | 4.27 | 1.46 | 1.34 |
| 15 | r | 102 | CDL | OB6-CB5 | 4.27 | 1.46 | 1.34 |
| 9 | C | 403 | HEC | CBC-CAC | -4.27 | 1.33 | 1.49 |
| 13 | 3 | 101 | BCB | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 15 | L | 306 | CDL | OA8-CA7 | 4.26 | 1.45 | 1.33 |
| 13 | M | 403 | BCB | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 13 | E | 101 | BCB | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 13 | l | 102 | BCB | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 13 | Z | 101 | BCB | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 13 | W | 302 | BCB | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 9 | C | 401 | HEC | CBC-CAC | -4.25 | 1.33 | 1.49 |
| 13 | O | 102 | BCB | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 15 | H | 302 | CDL | OB8-CB7 | 4.24 | 1.45 | 1.33 |
| 13 | 0 | 102 | BCB | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 15 | H | 301 | CDL | OA6-CA5 | 4.22 | 1.46 | 1.34 |
| 9 | C | 402 | HEC | CBB-CAB | -4.21 | 1.33 | 1.49 |
| 13 | N | 101 | BCB | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 13 | o | 102 | BCB | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 13 | R | 102 | BCB | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 15 | M | 409 | CDL | OA8-CA7 | 4.19 | 1.45 | 1.33 |
| 13 | e | 101 | BCB | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 20 | Q | 401 | PGV | O01-C1 | 4.18 | 1.46 | 1.34 |
| 13 | b | 101 | BCB | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 13 | U | 102 | BCB | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 13 | 7 | 102 | BCB | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 20 | I | 102 | PGV | O03-C19 | 4.16 | 1.45 | 1.33 |
| 15 | r | 102 | CDL | OA8-CA7 | 4.15 | 1.45 | 1.33 |
| 13 | n | 101 | BCB | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 13 | A | 102 | BCB | O2A-CGA | 4.14 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | L | 301 | DGA | OG1-CA1 | 4.11 | 1.45 | 1.33 |
| 15 | r | 102 | CDL | OB8-CB7 | 4.11 | 1.45 | 1.33 |
| 20 | D | 102 | PGV | O03-C19 | 4.11 | 1.45 | 1.33 |
| 13 | q | 101 | BCB | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 13 | 9 | 101 | BCB | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 13 | M | 402 | BCB | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 20 | M | 411 | PGV | O03-C19 | 4.09 | 1.45 | 1.33 |
| 13 | I | 101 | BCB | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 15 | L | 306 | CDL | OB6-CB5 | 4.08 | 1.45 | 1.34 |
| 15 | L | 306 | CDL | OB8-CB7 | 4.06 | 1.45 | 1.33 |
| 13 | 6 | 101 | BCB | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 15 | M | 409 | CDL | OA6-CA5 | 4.05 | 1.45 | 1.34 |
| 13 | h | 102 | BCB | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 13 | k | 102 | BCB | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 15 | M | 409 | CDL | OB6-CB5 | 4.04 | 1.45 | 1.34 |
| 20 | M | 411 | PGV | O01-C1 | 4.04 | 1.45 | 1.34 |
| 13 | Q | 402 | BCB | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 15 | L | 306 | CDL | OA6-CA5 | 4.02 | 1.45 | 1.34 |
| 20 | I | 102 | PGV | O01-C1 | 3.98 | 1.45 | 1.34 |
| 15 | M | 409 | CDL | OB8-CB7 | 3.98 | 1.45 | 1.33 |
| 15 | H | 301 | CDL | OB6-CB5 | 3.97 | 1.45 | 1.34 |
| 18 | M | 406 | NS5 | C25-C26 | 3.93 | 1.41 | 1.35 |
| 15 | H | 302 | CDL | OB6-CB5 | 3.89 | 1.45 | 1.34 |
| 20 | W | 301 | PGV | O01-C1 | 3.89 | 1.45 | 1.34 |
| 12 | L | 301 | DGA | OG2-CB1 | 3.88 | 1.45 | 1.34 |
| 9 | C | 402 | HEC | C2B-C3B | -3.86 | 1.36 | 1.40 |
| 13 | M | 402 | BCB | CHD-C1D | 3.79 | 1.45 | 1.38 |
| 13 | e | 101 | BCB | CHD-C1D | 3.78 | 1.45 | 1.38 |
| 13 | L | 302 | BCB | O2A-CGA | 3.78 | 1.44 | 1.33 |
| 15 | H | 301 | CDL | OB8-CB7 | 3.75 | 1.44 | 1.33 |
| 13 | A | 102 | BCB | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 13 | L | 303 | BCB | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 13 | 9 | 101 | BCB | CHD-C1D | 3.69 | 1.45 | 1.38 |
| 21 | k | 101 | NS0 | C19-C17 | 3.68 | 1.40 | 1.35 |
| 21 | 9 | 102 | NS0 | C19-C17 | 3.67 | 1.40 | 1.35 |
| 13 | I | 101 | BCB | CHD-C1D | 3.67 | 1.45 | 1.38 |
| 13 | k | 102 | BCB | CHD-C1D | 3.65 | 1.45 | 1.38 |
| 13 | M | 403 | BCB | CHD-C1D | 3.64 | 1.45 | 1.38 |
| 13 | q | 101 | BCB | CHD-C1D | 3.64 | 1.45 | 1.38 |
| 13 | X | 102 | BCB | CHD-C1D | 3.64 | 1.45 | 1.38 |
| 13 | n | 101 | BCB | CHD-C1D | 3.62 | 1.45 | 1.38 |
| 18 | M | 406 | NS5 | C20-C21 | 3.62 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 13 | 7 | 102 | BCB | CHD-C1D | 3.61 | 1.45 | 1.38 |
| 13 | l | 102 | BCB | CHD-C1D | 3.60 | 1.45 | 1.38 |
| 13 | L | 302 | BCB | CHD-C1D | 3.59 | 1.45 | 1.38 |
| 13 | i | 101 | BCB | CHD-C1D | 3.58 | 1.45 | 1.38 |
| 13 | E | 101 | BCB | CHD-C1D | 3.58 | 1.45 | 1.38 |
| 13 | Q | 402 | BCB | CHD-C1D | 3.57 | 1.45 | 1.38 |
| 13 | f | 101 | BCB | CHD-C1D | 3.56 | 1.45 | 1.38 |
| 13 | l | 102 | BCB | C3D-C2D | 3.55 | 1.48 | 1.39 |
| 21 | h | 101 | NS0 | C22-C23 | 3.55 | 1.40 | 1.35 |
| 13 | N | 101 | BCB | CHD-C1D | 3.55 | 1.45 | 1.38 |
| 13 | T | 101 | BCB | CHD-C1D | 3.52 | 1.45 | 1.38 |
| 21 | A | 103 | NS0 | C19-C17 | 3.52 | 1.40 | 1.35 |
| 13 | n | 101 | BCB | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 13 | r | 101 | BCB | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 13 | B | 202 | BCB | CHD-C1D | 3.50 | 1.45 | 1.38 |
| 21 | D | 103 | NS0 | C22-C23 | 3.50 | 1.40 | 1.35 |
| 21 | R | 101 | NS0 | C22-C23 | 3.49 | 1.40 | 1.35 |
| 21 | R | 101 | NS0 | C19-C17 | 3.49 | 1.40 | 1.35 |
| 13 | h | 102 | BCB | CHD-C1D | 3.49 | 1.45 | 1.38 |
| 13 | Q | 402 | BCB | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 13 | q | 101 | BCB | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 13 | J | 101 | BCB | CHD-C1D | 3.48 | 1.45 | 1.38 |
| 13 | n | 101 | BCB | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 13 | W | 302 | BCB | CHD-C1D | 3.47 | 1.45 | 1.38 |
| 13 | M | 403 | BCB | CHD-C4C | 3.47 | 1.47 | 1.39 |
| 21 | h | 101 | NS0 | C19-C17 | 3.46 | 1.40 | 1.35 |
| 13 | 4 | 101 | BCB | CHD-C1D | 3.46 | 1.45 | 1.38 |
| 21 | q | 102 | NS0 | C19-C17 | 3.46 | 1.40 | 1.35 |
| 13 | 3 | 101 | BCB | CHD-C1D | 3.46 | 1.45 | 1.38 |
| 13 | R | 102 | BCB | CHD-C1D | 3.45 | 1.45 | 1.38 |
| 13 | 0 | 102 | BCB | CHD-C1D | 3.45 | 1.45 | 1.38 |
| 13 | 1 | 101 | BCB | CHD-C1D | 3.45 | 1.45 | 1.38 |
| 13 | f | 101 | BCB | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 13 | h | 102 | BCB | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 13 | r | 101 | BCB | CHD-C1D | 3.44 | 1.45 | 1.38 |
| 13 | D | 101 | BCB | CHD-C1D | 3.43 | 1.45 | 1.38 |
| 13 | o | 102 | BCB | C3D-C2D | 3.43 | 1.48 | 1.39 |
| 13 | O | 102 | BCB | C3D-C2D | 3.43 | 1.48 | 1.39 |
| 13 | U | 102 | BCB | CHD-C1D | 3.43 | 1.45 | 1.38 |
| 13 | T | 101 | BCB | C3D-C2D | 3.42 | 1.48 | 1.39 |
| 13 | e | 101 | BCB | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 13 | k | 102 | BCB | C3D-C2D | 3.42 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 13 | D | 101 | BCB | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 21 | o | 101 | NS0 | C19-C17 | 3.41 | 1.40 | 1.35 |
| 13 | e | 101 | BCB | C3D-C2D | 3.41 | 1.48 | 1.39 |
| 21 | 9 | 102 | NS0 | C22-C23 | 3.41 | 1.40 | 1.35 |
| 13 | N | 101 | BCB | C3D-C2D | 3.41 | 1.48 | 1.39 |
| 13 | r | 101 | BCB | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 13 | 0 | 102 | BCB | C3D-C2D | 3.40 | 1.48 | 1.39 |
| 13 | A | 102 | BCB | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 13 | T | 101 | BCB | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 13 | O | 102 | BCB | CHD-C1D | 3.40 | 1.45 | 1.38 |
| 13 | 9 | 101 | BCB | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 13 | J | 101 | BCB | C3D-C2D | 3.39 | 1.48 | 1.39 |
| 13 | k | 102 | BCB | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 13 | q | 101 | BCB | C3D-C2D | 3.39 | 1.48 | 1.39 |
| 21 | U | 101 | NS0 | C19-C17 | 3.39 | 1.40 | 1.35 |
| 21 | 0 | 101 | NS0 | C19-C17 | 3.39 | 1.40 | 1.35 |
| 13 | k | 102 | BCB | CHD-C4C | 3.38 | 1.47 | 1.39 |
| 13 | Z | 101 | BCB | C3D-C2D | 3.38 | 1.48 | 1.39 |
| 21 | o | 101 | NS0 | C22-C23 | 3.38 | 1.40 | 1.35 |
| 21 | X | 101 | NS0 | C14-C12 | 3.38 | 1.40 | 1.35 |
| 13 | o | 102 | BCB | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 21 | q | 102 | NS0 | C22-C23 | 3.37 | 1.40 | 1.35 |
| 13 | 4 | 101 | BCB | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 13 | W | 302 | BCB | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 13 | U | 102 | BCB | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 13 | 7 | 102 | BCB | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 13 | Z | 101 | BCB | CHD-C1D | 3.36 | 1.44 | 1.38 |
| 13 | X | 102 | BCB | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 13 | O | 102 | BCB | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 13 | o | 102 | BCB | CHD-C1D | 3.36 | 1.44 | 1.38 |
| 21 | D | 103 | NS0 | C19-C17 | 3.36 | 1.40 | 1.35 |
| 21 | 7 | 101 | NS0 | C19-C17 | 3.35 | 1.40 | 1.35 |
| 13 | L | 303 | BCB | OBD-CAD | 3.35 | 1.28 | 1.22 |
| 21 | U | 101 | NS0 | C22-C23 | 3.35 | 1.40 | 1.35 |
| 21 | 7 | 101 | NS0 | C22-C23 | 3.35 | 1.40 | 1.35 |
| 13 | B | 202 | BCB | C3D-C2D | 3.34 | 1.48 | 1.39 |
| 13 | A | 102 | BCB | C3D-C2D | 3.33 | 1.48 | 1.39 |
| 21 | k | 101 | NS0 | C22-C23 | 3.33 | 1.40 | 1.35 |
| 13 | c | 101 | BCB | C3D-C2D | 3.33 | 1.48 | 1.39 |
| 21 | 2 | 101 | NS0 | C19-C17 | 3.32 | 1.40 | 1.35 |
| 13 | 9 | 101 | BCB | CHD-C4C | 3.32 | 1.46 | 1.39 |
| 21 | A | 103 | NS0 | C22-C23 | 3.32 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 13 | M | 402 | BCB | C3D-C2D | 3.32 | 1.48 | 1.39 |
| 13 | L | 302 | BCB | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 13 | 6 | 101 | BCB | CHD-C1D | 3.31 | 1.44 | 1.38 |
| 13 | A | 102 | BCB | CHD-C4C | 3.31 | 1.46 | 1.39 |
| 11 | A | 101 | UQ8 | C4-C3 | 3.31 | 1.49 | 1.36 |
| 13 | 6 | 101 | BCB | C3D-C2D | 3.31 | 1.48 | 1.39 |
| 21 | l | 101 | NS0 | C22-C23 | 3.30 | 1.40 | 1.35 |
| 13 | M | 402 | BCB | CHD-C4C | 3.30 | 1.46 | 1.39 |
| 13 | B | 202 | BCB | OBD-CAD | 3.30 | 1.28 | 1.22 |
| 13 | 1 | 101 | BCB | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 13 | Z | 101 | BCB | OBD-CAD | 3.30 | 1.28 | 1.22 |
| 13 | h | 102 | BCB | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 13 | W | 302 | BCB | OBD-CAD | 3.30 | 1.28 | 1.22 |
| 13 | 3 | 101 | BCB | OBD-CAD | 3.30 | 1.28 | 1.22 |
| 13 | I | 101 | BCB | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 13 | E | 101 | BCB | C3D-C2D | 3.29 | 1.48 | 1.39 |
| 13 | I | 101 | BCB | OBD-CAD | 3.29 | 1.28 | 1.22 |
| 13 | 6 | 101 | BCB | OBD-CAD | 3.29 | 1.28 | 1.22 |
| 21 | O | 101 | NS0 | C19-C17 | 3.28 | 1.40 | 1.35 |
| 13 | 9 | 101 | BCB | C3D-C2D | 3.28 | 1.48 | 1.39 |
| 13 | i | 101 | BCB | C3D-C2D | 3.28 | 1.48 | 1.39 |
| 13 | M | 402 | BCB | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 21 | h | 101 | NS0 | C14-C12 | 3.28 | 1.40 | 1.35 |
| 21 | 0 | 101 | NS0 | C22-C23 | 3.28 | 1.40 | 1.35 |
| 13 | b | 101 | BCB | CHD-C1D | 3.28 | 1.44 | 1.38 |
| 13 | l | 102 | BCB | OBD-CAD | 3.26 | 1.28 | 1.22 |
| 13 | Q | 402 | BCB | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 21 | X | 101 | NS0 | C19-C17 | 3.25 | 1.40 | 1.35 |
| 13 | X | 102 | BCB | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 13 | 3 | 101 | BCB | C3D-C2D | 3.25 | 1.48 | 1.39 |
| 13 | c | 101 | BCB | CHD-C1D | 3.24 | 1.44 | 1.38 |
| 13 | E | 101 | BCB | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 13 | 1 | 101 | BCB | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 13 | D | 101 | BCB | C3D-C2D | 3.24 | 1.48 | 1.39 |
| 13 | N | 101 | BCB | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 13 | R | 102 | BCB | C3D-C2D | 3.23 | 1.47 | 1.39 |
| 13 | b | 101 | BCB | C3D-C2D | 3.23 | 1.47 | 1.39 |
| 21 | A | 103 | NS0 | C14-C12 | 3.22 | 1.40 | 1.35 |
| 13 | M | 403 | BCB | C3D-C2D | 3.22 | 1.47 | 1.39 |
| 13 | L | 303 | BCB | CHD-C4C | 3.22 | 1.46 | 1.39 |
| 21 | l | 101 | NS0 | C19-C17 | 3.21 | 1.40 | 1.35 |
| 13 | J | 101 | BCB | OBD-CAD | 3.21 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | E | 101 | BCB | CHD-C4C | 3.20 | 1.46 | 1.39 |
| 13 | c | 101 | BCB | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 21 | k | 101 | NS0 | C14-C12 | 3.19 | 1.40 | 1.35 |
| 13 | R | 102 | BCB | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 21 | o | 101 | NS0 | C14-C12 | 3.18 | 1.40 | 1.35 |
| 13 | I | 101 | BCB | CHD-C4C | 3.18 | 1.46 | 1.39 |
| 13 | f | 101 | BCB | OBD-CAD | 3.17 | 1.27 | 1.22 |
| 13 | U | 102 | BCB | OBD-CAD | 3.17 | 1.27 | 1.22 |
| 13 | Q | 402 | BCB | CHD-C4C | 3.16 | 1.46 | 1.39 |
| 13 | b | 101 | BCB | OBD-CAD | 3.16 | 1.27 | 1.22 |
| 18 | M | 406 | NS5 | C17-C15 | 3.16 | 1.40 | 1.35 |
| 13 | 0 | 102 | BCB | OBD-CAD | 3.15 | 1.27 | 1.22 |
| 13 | T | 101 | BCB | CHD-C4C | 3.15 | 1.46 | 1.39 |
| 13 | L | 303 | BCB | C3D-C2D | 3.14 | 1.47 | 1.39 |
| 13 | 7 | 102 | BCB | OBD-CAD | 3.14 | 1.27 | 1.22 |
| 11 | L | 305 | UQ8 | C4-C3 | 3.13 | 1.49 | 1.36 |
| 13 | n | 101 | BCB | CHD-C4C | 3.13 | 1.46 | 1.39 |
| 21 | 2 | 101 | NS0 | C22-C23 | 3.12 | 1.39 | 1.35 |
| 13 | 4 | 101 | BCB | OBD-CAD | 3.12 | 1.27 | 1.22 |
| 13 | 3 | 101 | BCB | CHD-C4C | 3.12 | 1.46 | 1.39 |
| 13 | D | 101 | BCB | CHD-C4C | 3.11 | 1.46 | 1.39 |
| 13 | L | 302 | BCB | CHD-C4C | 3.10 | 1.46 | 1.39 |
| 13 | Z | 101 | BCB | CHD-C4C | 3.10 | 1.46 | 1.39 |
| 21 | O | 101 | NS0 | C22-C23 | 3.10 | 1.39 | 1.35 |
| 21 | X | 101 | NS0 | C22-C23 | 3.10 | 1.39 | 1.35 |
| 21 | O | 101 | NS0 | C14-C12 | 3.10 | 1.39 | 1.35 |
| 13 | i | 101 | BCB | OBD-CAD | 3.09 | 1.27 | 1.22 |
| 13 | L | 302 | BCB | C3D-C2D | 3.09 | 1.47 | 1.39 |
| 13 | J | 101 | BCB | CHD-C4C | 3.09 | 1.46 | 1.39 |
| 21 | 2 | 101 | NS0 | C16-C17 | -3.09 | 1.39 | 1.45 |
| 13 | e | 101 | BCB | CHD-C4C | 3.08 | 1.46 | 1.39 |
| 13 | q | 101 | BCB | CHD-C4C | 3.08 | 1.46 | 1.39 |
| 13 | 7 | 102 | BCB | CHD-C4C | 3.08 | 1.46 | 1.39 |
| 13 | r | 101 | BCB | CHD-C4C | 3.08 | 1.46 | 1.39 |
| 13 | h | 102 | BCB | CHD-C4C | 3.07 | 1.46 | 1.39 |
| 13 | i | 101 | BCB | CHD-C4C | 3.07 | 1.46 | 1.39 |
| 21 | D | 103 | NS0 | C14-C12 | 3.07 | 1.39 | 1.35 |
| 21 | 0 | 101 | NS0 | C14-C12 | 3.07 | 1.39 | 1.35 |
| 13 | U | 102 | BCB | CHD-C4C | 3.06 | 1.46 | 1.39 |
| 21 | W | 303 | NS0 | C19-C17 | 3.06 | 1.39 | 1.35 |
| 21 | l | 101 | NS0 | C14-C12 | 3.06 | 1.39 | 1.35 |
| 13 | N | 101 | BCB | CHD-C4C | 3.05 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21 | q | 102 | NS0 | C14-C12 | 3.05 | 1.39 | 1.35 |
| 13 | B | 202 | BCB | CHD-C4C | 3.05 | 1.46 | 1.39 |
| 21 | U | 101 | NS0 | C14-C12 | 3.05 | 1.39 | 1.35 |
| 13 | 6 | 101 | BCB | CHD-C4C | 3.04 | 1.46 | 1.39 |
| 13 | l | 102 | BCB | CHD-C4C | 3.04 | 1.46 | 1.39 |
| 13 | W | 302 | BCB | CHD-C4C | 3.03 | 1.46 | 1.39 |
| 13 | X | 102 | BCB | CHD-C4C | 3.02 | 1.46 | 1.39 |
| 21 | 2 | 101 | NS0 | C14-C12 | 3.01 | 1.39 | 1.35 |
| 13 | 1 | 101 | BCB | CHD-C4C | 3.00 | 1.46 | 1.39 |
| 13 | b | 101 | BCB | CHD-C4C | 2.99 | 1.46 | 1.39 |
| 13 | 0 | 102 | BCB | CHD-C4C | 2.98 | 1.46 | 1.39 |
| 21 | R | 101 | NS0 | C14-C12 | 2.98 | 1.39 | 1.35 |
| 13 | R | 102 | BCB | CHD-C4C | 2.98 | 1.46 | 1.39 |
| 21 | W | 303 | NS0 | C16-C17 | -2.97 | 1.39 | 1.45 |
| 11 | C | 406 | UQ8 | C4-C3 | 2.97 | 1.48 | 1.36 |
| 13 | f | 101 | BCB | CHD-C4C | 2.97 | 1.46 | 1.39 |
| 11 | M | 407 | UQ8 | C4-C3 | 2.94 | 1.48 | 1.36 |
| 21 | 7 | 101 | NS0 | C14-C12 | 2.94 | 1.39 | 1.35 |
| 21 | 9 | 102 | NS0 | C16-C17 | -2.93 | 1.39 | 1.45 |
| 13 | o | 102 | BCB | CHD-C4C | 2.90 | 1.45 | 1.39 |
| 13 | 4 | 101 | BCB | CHD-C4C | 2.89 | 1.45 | 1.39 |
| 13 | O | 102 | BCB | CHD-C4C | 2.89 | 1.45 | 1.39 |
| 9 | C | 402 | HEC | C4B-C3B | 2.87 | 1.48 | 1.43 |
| 21 | 7 | 101 | NS0 | C16-C17 | -2.86 | 1.39 | 1.45 |
| 21 | D | 103 | NS0 | C11-C12 | -2.86 | 1.39 | 1.45 |
| 21 | W | 303 | NS0 | C14-C12 | 2.85 | 1.39 | 1.35 |
| 13 | M | 403 | BCB | OBD-CAD | 2.85 | 1.27 | 1.22 |
| 11 | M | 408 | UQ8 | C4-C3 | 2.82 | 1.47 | 1.36 |
| 21 | 9 | 102 | NS0 | C14-C12 | 2.82 | 1.39 | 1.35 |
| 21 | 0 | 101 | NS0 | C16-C17 | -2.81 | 1.39 | 1.45 |
| 13 | c | 101 | BCB | CHD-C4C | 2.81 | 1.45 | 1.39 |
| 21 | W | 303 | NS0 | C22-C23 | 2.81 | 1.39 | 1.35 |
| 21 | D | 103 | NS0 | C16-C17 | -2.79 | 1.40 | 1.45 |
| 21 | O | 101 | NS0 | C16-C17 | -2.78 | 1.40 | 1.45 |
| 21 | R | 101 | NS0 | C16-C17 | -2.77 | 1.40 | 1.45 |
| 21 | q | 102 | NS0 | C16-C17 | -2.76 | 1.40 | 1.45 |
| 21 | W | 303 | NS0 | C25-C23 | -2.76 | 1.40 | 1.45 |
| 21 | h | 101 | NS0 | C16-C17 | -2.75 | 1.40 | 1.45 |
| 21 | A | 103 | NS0 | C16-C17 | -2.73 | 1.40 | 1.45 |
| 21 | U | 101 | NS0 | C16-C17 | -2.70 | 1.40 | 1.45 |
| 21 | o | 101 | NS0 | C16-C17 | -2.69 | 1.40 | 1.45 |
| 9 | C | 401 | HEC | C4B-C3B | 2.69 | 1.47 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21 | 2 | 101 | NS0 | C11-C12 | -2.68 | 1.40 | 1.45 |
| 21 | 7 | 101 | NS0 | C11-C12 | -2.67 | 1.40 | 1.45 |
| 21 | R | 101 | NS0 | C11-C12 | -2.67 | 1.40 | 1.45 |
| 21 | 0 | 101 | NS0 | C25-C23 | -2.67 | 1.40 | 1.45 |
| 21 | k | 101 | NS0 | C16-C17 | -2.66 | 1.40 | 1.45 |
| 21 | 9 | 102 | NS0 | C11-C12 | -2.63 | 1.40 | 1.45 |
| 21 | X | 101 | NS0 | C16-C17 | -2.63 | 1.40 | 1.45 |
| 21 | 2 | 101 | NS0 | C25-C23 | -2.62 | 1.40 | 1.45 |
| 13 | D | 101 | BCB | C4B-CHC | 2.62 | 1.48 | 1.41 |
| 21 | X | 101 | NS0 | C11-C12 | -2.62 | 1.40 | 1.45 |
| 21 | D | 103 | NS0 | C25-C23 | -2.61 | 1.40 | 1.45 |
| 21 | o | 101 | NS0 | C11-C12 | -2.61 | 1.40 | 1.45 |
| 9 | C | 404 | HEC | C4B-C3B | 2.61 | 1.47 | 1.43 |
| 21 | l | 101 | NS0 | C16-C17 | -2.60 | 1.40 | 1.45 |
| 13 | Q | 402 | BCB | C4B-CHC | 2.60 | 1.48 | 1.41 |
| 21 | l | 101 | NS0 | C11-C12 | -2.60 | 1.40 | 1.45 |
| 13 | 6 | 101 | BCB | C4B-CHC | 2.59 | 1.48 | 1.41 |
| 21 | A | 103 | NS0 | C25-C23 | -2.59 | 1.40 | 1.45 |
| 21 | W | 303 | NS0 | C11-C12 | -2.59 | 1.40 | 1.45 |
| 21 | q | 102 | NS0 | C11-C12 | -2.59 | 1.40 | 1.45 |
| 13 | A | 102 | BCB | C4B-CHC | 2.58 | 1.48 | 1.41 |
| 21 | 0 | 101 | NS0 | C11-C12 | -2.58 | 1.40 | 1.45 |
| 18 | M | 406 | NS5 | C14-C15 | -2.58 | 1.40 | 1.45 |
| 13 | M | 403 | BCB | C4B-CHC | 2.56 | 1.48 | 1.41 |
| 13 | T | 101 | BCB | C4B-CHC | 2.56 | 1.48 | 1.41 |
| 12 | L | 301 | DGA | OG2-CG2 | -2.56 | 1.42 | 1.47 |
| 21 | q | 102 | NS0 | C25-C23 | -2.55 | 1.40 | 1.45 |
| 13 | N | 101 | BCB | C4B-CHC | 2.54 | 1.48 | 1.41 |
| 13 | q | 101 | BCB | C4B-CHC | 2.54 | 1.48 | 1.41 |
| 21 | 7 | 101 | NS0 | C25-C23 | -2.53 | 1.40 | 1.45 |
| 13 | h | 102 | BCB | C4B-CHC | 2.52 | 1.48 | 1.41 |
| 13 | L | 303 | BCB | C4B-CHC | 2.52 | 1.48 | 1.41 |
| 21 | O | 101 | NS0 | C11-C12 | -2.51 | 1.40 | 1.45 |
| 21 | h | 101 | NS0 | C11-C12 | -2.51 | 1.40 | 1.45 |
| 13 | n | 101 | BCB | C4B-CHC | 2.51 | 1.48 | 1.41 |
| 21 | A | 103 | NS0 | C11-C12 | -2.51 | 1.40 | 1.45 |
| 21 | U | 101 | NS0 | C11-C12 | -2.51 | 1.40 | 1.45 |
| 21 | U | 101 | NS0 | C25-C23 | -2.51 | 1.40 | 1.45 |
| 21 | X | 101 | NS0 | C25-C23 | -2.51 | 1.40 | 1.45 |
| 9 | C | 403 | HEC | C4B-C3B | 2.51 | 1.47 | 1.43 |
| 21 | k | 101 | NS0 | C25-C23 | -2.51 | 1.40 | 1.45 |
| 13 | I | 101 | BCB | C4B-CHC | 2.51 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | 3 | 101 | BCB | C4B-CHC | 2.50 | 1.47 | 1.41 |
| 21 | 9 | 102 | NS0 | C25-C23 | -2.49 | 1.40 | 1.45 |
| 21 | k | 101 | NS0 | C11-C12 | -2.49 | 1.40 | 1.45 |
| 21 | O | 101 | NS0 | C25-C23 | -2.49 | 1.40 | 1.45 |
| 13 | Z | 101 | BCB | C4B-CHC | 2.48 | 1.47 | 1.41 |
| 21 | l | 101 | NS0 | C25-C23 | -2.48 | 1.40 | 1.45 |
| 21 | h | 101 | NS0 | C25-C23 | -2.45 | 1.40 | 1.45 |
| 13 | e | 101 | BCB | C4B-CHC | 2.44 | 1.47 | 1.41 |
| 13 | c | 101 | BCB | C4B-CHC | 2.43 | 1.47 | 1.41 |
| 18 | M | 406 | NS5 | C28-C26 | -2.43 | 1.40 | 1.45 |
| 13 | b | 101 | BCB | C4B-CHC | 2.43 | 1.47 | 1.41 |
| 13 | M | 402 | BCB | C1D-C2D | 2.41 | 1.50 | 1.45 |
| 21 | R | 101 | NS0 | C25-C23 | -2.41 | 1.40 | 1.45 |
| 13 | W | 302 | BCB | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 21 | o | 101 | NS0 | C25-C23 | -2.40 | 1.40 | 1.45 |
| 13 | U | 102 | BCB | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 13 | R | 102 | BCB | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 13 | 9 | 101 | BCB | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 13 | M | 402 | BCB | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 13 | r | 101 | BCB | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 18 | M | 406 | NS5 | C23-C21 | -2.38 | 1.40 | 1.45 |
| 13 | k | 102 | BCB | C4B-CHC | 2.38 | 1.47 | 1.41 |
| 13 | l | 102 | BCB | C4B-CHC | 2.37 | 1.47 | 1.41 |
| 13 | B | 202 | BCB | C4B-CHC | 2.35 | 1.47 | 1.41 |
| 13 | 4 | 101 | BCB | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 13 | E | 101 | BCB | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 13 | X | 102 | BCB | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 13 | f | 101 | BCB | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 13 | 0 | 102 | BCB | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 13 | L | 302 | BCB | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 13 | 1 | 101 | BCB | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 13 | J | 101 | BCB | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 13 | 9 | 101 | BCB | C1D-C2D | 2.29 | 1.49 | 1.45 |
| 13 | 7 | 102 | BCB | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 14 | M | 404 | BPB | C3A-C2A | -2.28 | 1.52 | 1.54 |
| 13 | o | 102 | BCB | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 9 | C | 403 | HEC | C3C-C2C | -2.26 | 1.38 | 1.40 |
| 13 | L | 303 | BCB | C1D-C2D | 2.24 | 1.49 | 1.45 |
| 13 | i | 101 | BCB | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 13 | O | 102 | BCB | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 13 | c | 101 | BCB | C1B-CHB | 2.18 | 1.47 | 1.41 |
| 9 | C | 404 | HEC | C3C-C2C | -2.17 | 1.38 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13 | b | 101 | BCB | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 14 | L | 304 | BPB | C3A-C2A | -2.14 | 1.52 | 1.54 |
| 13 | i | 101 | BCB | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 13 | o | 102 | BCB | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 13 | J | 101 | BCB | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 13 | R | 102 | BCB | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 13 | I | 101 | BCB | C1D-C2D | 2.12 | 1.49 | 1.45 |
| 13 | U | 102 | BCB | C1B-CHB | 2.11 | 1.46 | 1.41 |
| 13 | A | 102 | BCB | C1D-C2D | 2.09 | 1.49 | 1.45 |
| 13 | O | 102 | BCB | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 13 | M | 403 | BCB | C1B-CHB | 2.08 | 1.46 | 1.41 |
| 13 | l | 102 | BCB | C1B-CHB | 2.08 | 1.46 | 1.41 |
| 13 | B | 202 | BCB | C1B-CHB | 2.08 | 1.46 | 1.41 |
| 13 | D | 101 | BCB | C1D-C2D | 2.07 | 1.49 | 1.45 |
| 13 | E | 101 | BCB | C1B-CHB | 2.07 | 1.46 | 1.41 |
| 13 | k | 102 | BCB | C1D-C2D | 2.07 | 1.49 | 1.45 |
| 13 | 3 | 101 | BCB | C1B-CHB | 2.07 | 1.46 | 1.41 |
| 13 | 4 | 101 | BCB | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 13 | f | 101 | BCB | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 13 | e | 101 | BCB | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 13 | Z | 101 | BCB | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 13 | T | 101 | BCB | C1D-C2D | 2.04 | 1.49 | 1.45 |
| 13 | 6 | 101 | BCB | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 13 | W | 302 | BCB | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 13 | h | 102 | BCB | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 21 | W | 303 | NS0 | C21-C22 | -2.03 | 1.37 | 1.43 |
| 13 | M | 403 | BCB | C1D-C2D | 2.03 | 1.49 | 1.45 |
| 13 | T | 101 | BCB | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 13 | D | 101 | BCB | C1B-CHB | 2.01 | 1.46 | 1.41 |
| 21 | W | 303 | NS0 | C20-C19 | -2.01 | 1.37 | 1.43 |
| 13 | N | 101 | BCB | C1B-CHB | 2.01 | 1.46 | 1.41 |
| 13 | q | 101 | BCB | C1B-CHB | 2.01 | 1.46 | 1.41 |
| 13 | q | 101 | BCB | C1D-C2D | 2.00 | 1.49 | 1.45 |

All (1087) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 13 | h | 102 | BCB | C1C-NC-C4C | -18.83 | 98.24 | 106.71 |
| 13 | 3 | 101 | BCB | C1C-NC-C4C | -18.76 | 98.27 | 106.71 |
| 13 | O | 102 | BCB | C1C-NC-C4C | -18.72 | 98.29 | 106.71 |
| 13 | l | 102 | BCB | C1C-NC-C4C | -18.68 | 98.31 | 106.71 |
| 13 | 1 | 101 | BCB | C1C-NC-C4C | -18.61 | 98.34 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 13 | 4 | 101 | BCB | C1C-NC-C4C | -18.59 | 98.35 | 106.71 |
| 13 | R | 102 | BCB | C1C-NC-C4C | -18.52 | 98.38 | 106.71 |
| 13 | b | 101 | BCB | C1C-NC-C4C | -18.44 | 98.42 | 106.71 |
| 13 | f | 101 | BCB | C1C-NC-C4C | -18.40 | 98.43 | 106.71 |
| 13 | B | 202 | BCB | C1C-NC-C4C | -18.39 | 98.44 | 106.71 |
| 13 | c | 101 | BCB | C1C-NC-C4C | -18.38 | 98.44 | 106.71 |
| 13 | Z | 101 | BCB | C1C-NC-C4C | -18.36 | 98.45 | 106.71 |
| 13 | Q | 402 | BCB | C1C-NC-C4C | -18.20 | 98.52 | 106.71 |
| 13 | i | 101 | BCB | C1C-NC-C4C | -18.19 | 98.53 | 106.71 |
| 13 | W | 302 | BCB | C1C-NC-C4C | -18.18 | 98.53 | 106.71 |
| 13 | L | 302 | BCB | C1C-NC-C4C | -18.16 | 98.54 | 106.71 |
| 13 | o | 102 | BCB | C1C-NC-C4C | -18.14 | 98.55 | 106.71 |
| 13 | U | 102 | BCB | C1C-NC-C4C | -18.03 | 98.60 | 106.71 |
| 13 | 7 | 102 | BCB | C1C-NC-C4C | -18.02 | 98.61 | 106.71 |
| 13 | N | 101 | BCB | C1C-NC-C4C | -18.01 | 98.61 | 106.71 |
| 13 | e | 101 | BCB | C1C-NC-C4C | -17.98 | 98.62 | 106.71 |
| 13 | I | 101 | BCB | C1C-NC-C4C | -17.95 | 98.63 | 106.71 |
| 13 | T | 101 | BCB | C1C-NC-C4C | -17.95 | 98.64 | 106.71 |
| 13 | n | 101 | BCB | C1C-NC-C4C | -17.94 | 98.64 | 106.71 |
| 13 | r | 101 | BCB | C1C-NC-C4C | -17.89 | 98.66 | 106.71 |
| 13 | E | 101 | BCB | C1C-NC-C4C | -17.88 | 98.67 | 106.71 |
| 13 | X | 102 | BCB | C1C-NC-C4C | -17.87 | 98.67 | 106.71 |
| 13 | J | 101 | BCB | C1C-NC-C4C | -17.85 | 98.68 | 106.71 |
| 13 | q | 101 | BCB | C1C-NC-C4C | -17.85 | 98.68 | 106.71 |
| 13 | A | 102 | BCB | C1C-NC-C4C | -17.82 | 98.69 | 106.71 |
| 13 | k | 102 | BCB | C1C-NC-C4C | -17.70 | 98.75 | 106.71 |
| 13 | L | 303 | BCB | C1C-NC-C4C | -17.66 | 98.77 | 106.71 |
| 13 | D | 101 | BCB | C1C-NC-C4C | -17.45 | 98.86 | 106.71 |
| 13 | 0 | 102 | BCB | C1C-NC-C4C | -17.40 | 98.88 | 106.71 |
| 13 | M | 402 | BCB | C1C-NC-C4C | -17.35 | 98.91 | 106.71 |
| 13 | 6 | 101 | BCB | C1C-NC-C4C | -17.32 | 98.92 | 106.71 |
| 13 | 9 | 101 | BCB | C1C-NC-C4C | -17.04 | 99.05 | 106.71 |
| 13 | M | 403 | BCB | C1C-NC-C4C | -16.24 | 99.41 | 106.71 |
| 13 | M | 403 | BCB | CMD-C2D-C1D | 7.06 | 137.15 | 124.71 |
| 13 | L | 303 | BCB | CMD-C2D-C1D | 6.91 | 136.88 | 124.71 |
| 13 | M | 402 | BCB | CMD-C2D-C1D | 6.78 | 136.66 | 124.71 |
| 13 | 9 | 101 | BCB | CMD-C2D-C1D | 6.75 | 136.61 | 124.71 |
| 13 | A | 102 | BCB | CMD-C2D-C1D | 6.66 | 136.45 | 124.71 |
| 13 | D | 101 | BCB | CMD-C2D-C1D | 6.58 | 136.30 | 124.71 |
| 13 | I | 101 | BCB | CMD-C2D-C1D | 6.56 | 136.27 | 124.71 |
| 13 | L | 302 | BCB | CMD-C2D-C1D | 6.55 | 136.25 | 124.71 |
| 13 | q | 101 | BCB | CMD-C2D-C1D | 6.42 | 136.03 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | b | 101 | BCB | CMD-C2D-C1D | 6.38 | 135.96 | 124.71 |
| 13 | 3 | 101 | BCB | CMD-C2D-C1D | 6.30 | 135.82 | 124.71 |
| 13 | J | 101 | BCB | C1D-ND-C4D | -6.30 | 101.86 | 106.33 |
| 13 | 6 | 101 | BCB | CMD-C2D-C1D | 6.29 | 135.79 | 124.71 |
| 13 | M | 402 | BCB | C1D-ND-C4D | -6.21 | 101.93 | 106.33 |
| 13 | e | 101 | BCB | CMD-C2D-C1D | 6.19 | 135.62 | 124.71 |
| 13 | k | 102 | BCB | CMD-C2D-C1D | 6.17 | 135.58 | 124.71 |
| 13 | T | 101 | BCB | CMD-C2D-C1D | 6.16 | 135.58 | 124.71 |
| 13 | N | 101 | BCB | CMD-C2D-C1D | 6.06 | 135.39 | 124.71 |
| 13 | h | 102 | BCB | CMD-C2D-C1D | 6.06 | 135.39 | 124.71 |
| 13 | W | 302 | BCB | CMD-C2D-C1D | 6.03 | 135.34 | 124.71 |
| 13 | Q | 402 | BCB | CMD-C2D-C1D | 6.02 | 135.31 | 124.71 |
| 13 | c | 101 | BCB | C1D-ND-C4D | -5.92 | 102.13 | 106.33 |
| 13 | n | 101 | BCB | CMD-C2D-C1D | 5.92 | 135.14 | 124.71 |
| 13 | L | 303 | BCB | C1D-ND-C4D | -5.91 | 102.14 | 106.33 |
| 13 | f | 101 | BCB | C1D-ND-C4D | -5.90 | 102.14 | 106.33 |
| 13 | L | 303 | BCB | O2D-CGD-CBD | 5.84 | 121.65 | 111.27 |
| 13 | Z | 101 | BCB | CMD-C2D-C1D | 5.82 | 134.96 | 124.71 |
| 13 | 1 | 101 | BCB | C1D-ND-C4D | -5.80 | 102.22 | 106.33 |
| 13 | i | 101 | BCB | C1D-ND-C4D | -5.79 | 102.22 | 106.33 |
| 13 | 0 | 102 | BCB | C1D-ND-C4D | -5.77 | 102.24 | 106.33 |
| 13 | U | 102 | BCB | C1D-ND-C4D | -5.74 | 102.25 | 106.33 |
| 13 | 4 | 101 | BCB | C1D-ND-C4D | -5.72 | 102.27 | 106.33 |
| 13 | o | 102 | BCB | C1D-ND-C4D | -5.69 | 102.30 | 106.33 |
| 12 | L | 301 | DGA | CG2-OG2-CB1 | -5.64 | 110.62 | 117.88 |
| 13 | O | 102 | BCB | C1D-ND-C4D | -5.59 | 102.36 | 106.33 |
| 13 | B | 202 | BCB | C1D-ND-C4D | -5.57 | 102.38 | 106.33 |
| 13 | E | 101 | BCB | C1D-ND-C4D | -5.56 | 102.39 | 106.33 |
| 13 | 9 | 101 | BCB | C1D-ND-C4D | -5.55 | 102.39 | 106.33 |
| 13 | D | 101 | BCB | C1D-ND-C4D | -5.52 | 102.41 | 106.33 |
| 13 | X | 102 | BCB | C1D-ND-C4D | -5.45 | 102.46 | 106.33 |
| 13 | M | 403 | BCB | C1D-ND-C4D | -5.45 | 102.47 | 106.33 |
| 13 | R | 102 | BCB | C1D-ND-C4D | -5.39 | 102.50 | 106.33 |
| 13 | M | 402 | BCB | CHD-C1D-ND | -5.35 | 119.53 | 124.45 |
| 13 | l | 102 | BCB | C1D-ND-C4D | -5.25 | 102.61 | 106.33 |
| 13 | M | 402 | BCB | O2D-CGD-CBD | 5.24 | 120.58 | 111.27 |
| 13 | E | 101 | BCB | CMD-C2D-C1D | 5.20 | 133.88 | 124.71 |
| 13 | L | 302 | BCB | C1D-ND-C4D | -5.20 | 102.64 | 106.33 |
| 13 | B | 202 | BCB | CMD-C2D-C1D | 5.17 | 133.83 | 124.71 |
| 13 | r | 101 | BCB | C1D-ND-C4D | -5.13 | 102.69 | 106.33 |
| 13 | X | 102 | BCB | CMD-C2D-C1D | 5.11 | 133.72 | 124.71 |
| 13 | M | 402 | BCB | C2C-C1C-CHC | -5.11 | 111.61 | 123.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | R | 102 | BCB | CMD-C2D-C1D | 5.09 | 133.68 | 124.71 |
| 13 | 7 | 102 | BCB | C1D-ND-C4D | -5.08 | 102.73 | 106.33 |
| 13 | q | 101 | BCB | C1D-ND-C4D | -5.08 | 102.73 | 106.33 |
| 13 | M | 403 | BCB | O2D-CGD-CBD | 5.06 | 120.26 | 111.27 |
| 13 | 6 | 101 | BCB | C1D-ND-C4D | -5.01 | 102.77 | 106.33 |
| 13 | A | 102 | BCB | C1D-ND-C4D | -5.01 | 102.78 | 106.33 |
| 13 | L | 302 | BCB | C2C-C1C-CHC | -4.98 | 111.91 | 123.64 |
| 13 | h | 102 | BCB | C1D-ND-C4D | -4.96 | 102.81 | 106.33 |
| 13 | b | 101 | BCB | C1D-ND-C4D | -4.96 | 102.81 | 106.33 |
| 13 | M | 403 | BCB | C2C-C1C-CHC | -4.93 | 112.03 | 123.64 |
| 13 | k | 102 | BCB | C2C-C1C-CHC | -4.92 | 112.05 | 123.64 |
| 13 | M | 403 | BCB | CHD-C1D-ND | -4.89 | 119.96 | 124.45 |
| 13 | 4 | 101 | BCB | C2C-C1C-CHC | -4.88 | 112.16 | 123.64 |
| 13 | f | 101 | BCB | C2C-C1C-CHC | -4.87 | 112.18 | 123.64 |
| 13 | O | 102 | BCB | C2C-C1C-CHC | -4.86 | 112.20 | 123.64 |
| 13 | L | 303 | BCB | C2C-C1C-CHC | -4.83 | 112.26 | 123.64 |
| 13 | 7 | 102 | BCB | C2C-C1C-CHC | -4.82 | 112.30 | 123.64 |
| 13 | h | 102 | BCB | C2C-C1C-CHC | -4.81 | 112.31 | 123.64 |
| 13 | e | 101 | BCB | C2C-C1C-CHC | -4.81 | 112.31 | 123.64 |
| 13 | 0 | 102 | BCB | CMD-C2D-C1D | 4.80 | 133.18 | 124.71 |
| 13 | 1 | 101 | BCB | C2C-C1C-CHC | -4.80 | 112.33 | 123.64 |
| 13 | A | 102 | BCB | O2D-CGD-CBD | 4.80 | 119.79 | 111.27 |
| 13 | n | 101 | BCB | C2C-C1C-CHC | -4.77 | 112.41 | 123.64 |
| 13 | 3 | 101 | BCB | C1D-ND-C4D | -4.76 | 102.95 | 106.33 |
| 13 | 9 | 101 | BCB | C2C-C1C-CHC | -4.76 | 112.42 | 123.64 |
| 13 | J | 101 | BCB | C2C-C1C-CHC | -4.76 | 112.43 | 123.64 |
| 13 | o | 102 | BCB | C2C-C1C-CHC | -4.75 | 112.45 | 123.64 |
| 13 | E | 101 | BCB | C2C-C1C-CHC | -4.75 | 112.47 | 123.64 |
| 13 | W | 302 | BCB | C1D-ND-C4D | -4.73 | 102.97 | 106.33 |
| 13 | r | 101 | BCB | CMD-C2D-C1D | 4.73 | 133.05 | 124.71 |
| 13 | I | 101 | BCB | C2C-C1C-CHC | -4.73 | 112.50 | 123.64 |
| 13 | b | 101 | BCB | C2C-C1C-CHC | -4.72 | 112.52 | 123.64 |
| 13 | A | 102 | BCB | C2C-C1C-CHC | -4.69 | 112.61 | 123.64 |
| 13 | 0 | 102 | BCB | C2C-C1C-CHC | -4.68 | 112.61 | 123.64 |
| 13 | 1 | 101 | BCB | CMD-C2D-C1D | 4.68 | 132.96 | 124.71 |
| 13 | R | 102 | BCB | C2C-C1C-CHC | -4.67 | 112.64 | 123.64 |
| 13 | B | 202 | BCB | C2C-C1C-CHC | -4.67 | 112.65 | 123.64 |
| 12 | L | 301 | DGA | OG2-CB1-CB2 | 4.66 | 121.54 | 111.50 |
| 13 | X | 102 | BCB | C2C-C1C-CHC | -4.66 | 112.67 | 123.64 |
| 13 | c | 101 | BCB | C2C-C1C-CHC | -4.62 | 112.77 | 123.64 |
| 13 | e | 101 | BCB | C1D-ND-C4D | -4.61 | 103.06 | 106.33 |
| 13 | i | 101 | BCB | C2C-C1C-CHC | -4.60 | 112.80 | 123.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | r | 101 | BCB | C2C-C1C-CHC | -4.60 | 112.80 | 123.64 |
| 13 | T | 101 | BCB | C2C-C1C-CHC | -4.60 | 112.81 | 123.64 |
| 13 | 3 | 101 | BCB | C2C-C1C-CHC | -4.59 | 112.82 | 123.64 |
| 13 | D | 101 | BCB | C2C-C1C-CHC | -4.58 | 112.85 | 123.64 |
| 13 | M | 403 | BCB | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 13 | 7 | 102 | BCB | CMD-C2D-C1D | 4.57 | 132.77 | 124.71 |
| 13 | U | 102 | BCB | C2C-C1C-CHC | -4.57 | 112.89 | 123.64 |
| 15 | r | 102 | CDL | OB6-CB5-C51 | 4.56 | 121.33 | 111.50 |
| 13 | l | 102 | BCB | C2C-C1C-CHC | -4.56 | 112.91 | 123.64 |
| 13 | O | 102 | BCB | O2D-CGD-CBD | 4.54 | 119.33 | 111.27 |
| 13 | Z | 101 | BCB | C1D-ND-C4D | -4.54 | 103.11 | 106.33 |
| 13 | o | 102 | BCB | CMD-C2D-C1D | 4.53 | 132.69 | 124.71 |
| 13 | Q | 402 | BCB | C2C-C1C-CHC | -4.52 | 112.99 | 123.64 |
| 13 | i | 101 | BCB | O2D-CGD-CBD | 4.52 | 119.29 | 111.27 |
| 13 | J | 101 | BCB | CMD-C2D-C1D | 4.51 | 132.66 | 124.71 |
| 13 | W | 302 | BCB | C2C-C1C-CHC | -4.50 | 113.04 | 123.64 |
| 13 | q | 101 | BCB | C2C-C1C-CHC | -4.49 | 113.06 | 123.64 |
| 13 | 6 | 101 | BCB | C2C-C1C-CHC | -4.49 | 113.06 | 123.64 |
| 13 | R | 102 | BCB | O2D-CGD-CBD | 4.48 | 119.23 | 111.27 |
| 13 | Z | 101 | BCB | C2C-C1C-CHC | -4.47 | 113.11 | 123.64 |
| 13 | O | 102 | BCB | CMD-C2D-C1D | 4.46 | 132.57 | 124.71 |
| 13 | N | 101 | BCB | C2C-C1C-CHC | -4.43 | 113.21 | 123.64 |
| 13 | i | 101 | BCB | CMD-C2D-C1D | 4.38 | 132.44 | 124.71 |
| 13 | Q | 402 | BCB | C1D-ND-C4D | -4.36 | 103.24 | 106.33 |
| 13 | N | 101 | BCB | CMB-C2B-C3B | 4.35 | 132.81 | 124.68 |
| 13 | c | 101 | BCB | O2D-CGD-CBD | 4.35 | 118.99 | 111.27 |
| 15 | H | 301 | CDL | OA6-CA5-C11 | 4.34 | 120.86 | 111.50 |
| 13 | n | 101 | BCB | C1D-ND-C4D | -4.32 | 103.27 | 106.33 |
| 13 | D | 101 | BCB | C3D-C2D-C1D | -4.31 | 99.94 | 105.83 |
| 13 | f | 101 | BCB | CMD-C2D-C1D | 4.29 | 132.27 | 124.71 |
| 13 | o | 102 | BCB | O2D-CGD-CBD | 4.29 | 118.89 | 111.27 |
| 11 | A | 101 | UQ8 | C7-C8-C9 | -4.28 | 119.66 | 126.79 |
| 13 | I | 101 | BCB | C1D-ND-C4D | -4.27 | 103.31 | 106.33 |
| 15 | H | 302 | CDL | OA6-CA5-C11 | 4.26 | 120.68 | 111.50 |
| 13 | B | 202 | BCB | O2D-CGD-CBD | 4.25 | 118.82 | 111.27 |
| 13 | T | 101 | BCB | C1D-ND-C4D | -4.24 | 103.32 | 106.33 |
| 13 | U | 102 | BCB | CMD-C2D-C1D | 4.24 | 132.18 | 124.71 |
| 13 | 3 | 101 | BCB | C1-C2-C3 | -4.23 | 118.72 | 126.04 |
| 13 | c | 101 | BCB | CMD-C2D-C1D | 4.22 | 132.15 | 124.71 |
| 13 | l | 101 | BCB | CMB-C2B-C3B | 4.22 | 132.57 | 124.68 |
| 13 | f | 101 | BCB | O2D-CGD-CBD | 4.21 | 118.75 | 111.27 |
| 21 | R | 101 | NS0 | C21-C20-C19 | 4.21 | 132.10 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | L | 303 | BCB | CHD-C1D-ND | -4.21 | 120.58 | 124.45 |
| 13 | U | 102 | BCB | O2D-CGD-CBD | 4.20 | 118.74 | 111.27 |
| 13 | 6 | 101 | BCB | C3D-C2D-C1D | -4.20 | 100.11 | 105.83 |
| 13 | l | 102 | BCB | O2D-CGD-CBD | 4.19 | 118.72 | 111.27 |
| 13 | L | 303 | BCB | CMB-C2B-C3B | 4.19 | 132.52 | 124.68 |
| 13 | N | 101 | BCB | C1D-ND-C4D | -4.19 | 103.36 | 106.33 |
| 15 | M | 409 | CDL | OA6-CA5-C11 | 4.19 | 120.52 | 111.50 |
| 20 | I | 102 | PGV | O01-C1-C2 | 4.18 | 120.51 | 111.50 |
| 13 | 9 | 101 | BCB | O2D-CGD-CBD | 4.18 | 118.69 | 111.27 |
| 13 | b | 101 | BCB | C3D-C2D-C1D | -4.18 | 100.13 | 105.83 |
| 15 | M | 409 | CDL | OB6-CB5-C51 | 4.16 | 120.46 | 111.50 |
| 13 | 0 | 102 | BCB | O2D-CGD-CBD | 4.14 | 118.62 | 111.27 |
| 13 | l | 102 | BCB | CMB-C2B-C3B | 4.12 | 132.39 | 124.68 |
| 13 | q | 101 | BCB | CMB-C2B-C3B | 4.10 | 132.36 | 124.68 |
| 13 | I | 101 | BCB | O2D-CGD-CBD | 4.10 | 118.55 | 111.27 |
| 13 | e | 101 | BCB | C1-C2-C3 | -4.09 | 118.96 | 126.04 |
| 13 | Q | 402 | BCB | C1-C2-C3 | -4.09 | 118.97 | 126.04 |
| 13 | k | 102 | BCB | C1D-ND-C4D | -4.09 | 103.43 | 106.33 |
| 13 | k | 102 | BCB | CMB-C2B-C3B | 4.08 | 132.32 | 124.68 |
| 13 | M | 402 | BCB | C3D-C2D-C1D | -4.08 | 100.27 | 105.83 |
| 15 | L | 306 | CDL | OB6-CB5-C51 | 4.07 | 120.28 | 111.50 |
| 13 | r | 101 | BCB | O2D-CGD-CBD | 4.07 | 118.50 | 111.27 |
| 13 | L | 302 | BCB | C3D-C2D-C1D | -4.07 | 100.28 | 105.83 |
| 13 | W | 302 | BCB | C3D-C2D-C1D | -4.07 | 100.28 | 105.83 |
| 13 | 3 | 101 | BCB | C3D-C2D-C1D | -4.06 | 100.29 | 105.83 |
| 13 | q | 101 | BCB | C3D-C2D-C1D | -4.06 | 100.29 | 105.83 |
| 13 | e | 101 | BCB | O2D-CGD-CBD | 4.06 | 118.48 | 111.27 |
| 13 | D | 101 | BCB | CMB-C2B-C3B | 4.06 | 132.27 | 124.68 |
| 13 | I | 101 | BCB | CMB-C2B-C3B | 4.06 | 132.27 | 124.68 |
| 13 | Z | 101 | BCB | C3D-C2D-C1D | -4.05 | 100.30 | 105.83 |
| 15 | r | 102 | CDL | OA6-CA5-C11 | 4.05 | 120.23 | 111.50 |
| 15 | H | 301 | CDL | OB6-CB5-C51 | 4.04 | 120.21 | 111.50 |
| 13 | N | 101 | BCB | C3D-C2D-C1D | -4.04 | 100.32 | 105.83 |
| 13 | 0 | 102 | BCB | CMB-C2B-C3B | 4.04 | 132.23 | 124.68 |
| 13 | 4 | 101 | BCB | O2D-CGD-CBD | 4.03 | 118.42 | 111.27 |
| 13 | 7 | 102 | BCB | O2D-CGD-CBD | 4.03 | 118.42 | 111.27 |
| 13 | Z | 101 | BCB | C1-C2-C3 | -4.02 | 119.09 | 126.04 |
| 13 | e | 101 | BCB | C3D-C2D-C1D | -4.01 | 100.36 | 105.83 |
| 13 | A | 102 | BCB | C3D-C2D-C1D | -4.00 | 100.37 | 105.83 |
| 20 | W | 301 | PGV | O01-C1-C2 | 3.99 | 120.11 | 111.50 |
| 13 | 7 | 102 | BCB | CMB-C2B-C3B | 3.99 | 132.15 | 124.68 |
| 13 | R | 102 | BCB | CMB-C2B-C3B | 3.99 | 132.14 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | W | 302 | BCB | CMB-C2B-C3B | 3.98 | 132.13 | 124.68 |
| 13 | 9 | 101 | BCB | CHD-C1D-ND | -3.97 | 120.81 | 124.45 |
| 13 | E | 101 | BCB | O2D-CGD-CBD | 3.97 | 118.32 | 111.27 |
| 13 | T | 101 | BCB | C3D-C2D-C1D | -3.96 | 100.43 | 105.83 |
| 21 | X | 101 | NS0 | C21-C20-C19 | 3.96 | 131.58 | 123.47 |
| 13 | 9 | 101 | BCB | C3D-C2D-C1D | -3.95 | 100.44 | 105.83 |
| 13 | h | 102 | BCB | C3D-C2D-C1D | -3.95 | 100.44 | 105.83 |
| 13 | Z | 101 | BCB | O2D-CGD-CBD | 3.95 | 118.28 | 111.27 |
| 9 | C | 401 | HEC | CBD-CAD-C3D | -3.95 | 105.89 | 112.62 |
| 13 | Q | 402 | BCB | CMB-C2B-C3B | 3.95 | 132.06 | 124.68 |
| 13 | Q | 402 | BCB | O2D-CGD-CBD | 3.94 | 118.26 | 111.27 |
| 13 | l | 102 | BCB | CMD-C2D-C1D | 3.93 | 131.64 | 124.71 |
| 13 | U | 102 | BCB | CMB-C2B-C3B | 3.93 | 132.03 | 124.68 |
| 13 | o | 102 | BCB | CMB-C2B-C3B | 3.92 | 132.02 | 124.68 |
| 13 | 4 | 101 | BCB | CMB-C2B-C3B | 3.92 | 132.01 | 124.68 |
| 13 | h | 102 | BCB | CMB-C2B-C3B | 3.91 | 132.00 | 124.68 |
| 13 | X | 102 | BCB | O2D-CGD-CBD | 3.90 | 118.20 | 111.27 |
| 13 | N | 101 | BCB | O2D-CGD-CBD | 3.90 | 118.20 | 111.27 |
| 13 | L | 302 | BCB | O2D-CGD-CBD | 3.90 | 118.19 | 111.27 |
| 13 | I | 101 | BCB | C1-C2-C3 | -3.89 | 119.31 | 126.04 |
| 13 | M | 403 | BCB | C1-C2-C3 | -3.89 | 119.31 | 126.04 |
| 13 | 4 | 101 | BCB | CMD-C2D-C1D | 3.89 | 131.57 | 124.71 |
| 13 | D | 101 | BCB | O2D-CGD-CBD | 3.89 | 118.17 | 111.27 |
| 13 | B | 202 | BCB | CMB-C2B-C3B | 3.88 | 131.94 | 124.68 |
| 13 | I | 101 | BCB | C3D-C2D-C1D | -3.88 | 100.53 | 105.83 |
| 13 | X | 102 | BCB | CMB-C2B-C3B | 3.88 | 131.94 | 124.68 |
| 13 | Q | 402 | BCB | C3D-C2D-C1D | -3.88 | 100.54 | 105.83 |
| 13 | b | 101 | BCB | CMB-C2B-C3B | 3.87 | 131.91 | 124.68 |
| 13 | T | 101 | BCB | CMB-C2B-C3B | 3.86 | 131.89 | 124.68 |
| 13 | l | 101 | BCB | O2D-CGD-CBD | 3.85 | 118.11 | 111.27 |
| 13 | n | 101 | BCB | C1-C2-C3 | -3.85 | 119.39 | 126.04 |
| 13 | k | 102 | BCB | C3D-C2D-C1D | -3.83 | 100.60 | 105.83 |
| 13 | n | 101 | BCB | C3D-C2D-C1D | -3.82 | 100.61 | 105.83 |
| 13 | W | 302 | BCB | O2D-CGD-CBD | 3.82 | 118.05 | 111.27 |
| 13 | A | 102 | BCB | CMB-C2B-C3B | 3.81 | 131.81 | 124.68 |
| 13 | n | 101 | BCB | O2D-CGD-CBD | 3.81 | 118.04 | 111.27 |
| 13 | 3 | 101 | BCB | O2D-CGD-CBD | 3.80 | 118.01 | 111.27 |
| 13 | A | 102 | BCB | CHD-C1D-ND | -3.79 | 120.97 | 124.45 |
| 13 | h | 102 | BCB | O2D-CGD-CBD | 3.79 | 118.00 | 111.27 |
| 13 | L | 302 | BCB | C1-C2-C3 | -3.78 | 119.50 | 126.04 |
| 21 | W | 303 | NS0 | C21-C20-C19 | 3.78 | 131.21 | 123.47 |
| 13 | O | 102 | BCB | CMB-C2B-C3B | 3.77 | 131.74 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | M | 403 | BCB | CMB-C2B-C3B | 3.77 | 131.73 | 124.68 |
| 13 | n | 101 | BCB | CMB-C2B-C3B | 3.76 | 131.72 | 124.68 |
| 13 | f | 101 | BCB | CMB-C2B-C3B | 3.76 | 131.71 | 124.68 |
| 13 | W | 302 | BCB | C1-C2-C3 | -3.76 | 119.54 | 126.04 |
| 13 | A | 102 | BCB | C1-C2-C3 | -3.76 | 119.55 | 126.04 |
| 13 | b | 101 | BCB | O2D-CGD-CBD | 3.75 | 117.93 | 111.27 |
| 13 | 9 | 101 | BCB | CMB-C2B-C3B | 3.75 | 131.69 | 124.68 |
| 13 | J | 101 | BCB | O2D-CGD-CBD | 3.73 | 117.89 | 111.27 |
| 21 | 9 | 102 | NS0 | C21-C20-C19 | 3.72 | 131.09 | 123.47 |
| 13 | L | 303 | BCB | C3D-C2D-C1D | -3.72 | 100.76 | 105.83 |
| 13 | N | 101 | BCB | C1-C2-C3 | -3.70 | 119.64 | 126.04 |
| 13 | r | 101 | BCB | CHB-C4A-NA | 3.67 | 129.59 | 124.51 |
| 13 | 3 | 101 | BCB | CMB-C2B-C3B | 3.67 | 131.54 | 124.68 |
| 13 | 6 | 101 | BCB | O2D-CGD-CBD | 3.67 | 117.78 | 111.27 |
| 13 | Z | 101 | BCB | CMB-C2B-C3B | 3.64 | 131.48 | 124.68 |
| 13 | e | 101 | BCB | CMB-C2B-C3B | 3.63 | 131.47 | 124.68 |
| 13 | q | 101 | BCB | O2D-CGD-CBD | 3.63 | 117.72 | 111.27 |
| 13 | L | 302 | BCB | C4-C3-C5 | 3.62 | 121.36 | 115.27 |
| 15 | H | 302 | CDL | OB6-CB5-C51 | 3.61 | 119.27 | 111.50 |
| 20 | Q | 401 | PGV | O01-C1-C2 | 3.60 | 119.27 | 111.50 |
| 15 | L | 306 | CDL | OA6-CA5-C11 | 3.60 | 119.27 | 111.50 |
| 13 | E | 101 | BCB | CMB-C2B-C3B | 3.59 | 131.40 | 124.68 |
| 13 | M | 402 | BCB | C1-C2-C3 | -3.58 | 119.84 | 126.04 |
| 11 | M | 408 | UQ8 | C17-C18-C19 | -3.56 | 119.09 | 127.66 |
| 13 | i | 101 | BCB | C4D-CHA-C1A | -3.56 | 116.92 | 121.25 |
| 13 | r | 101 | BCB | CMB-C2B-C3B | 3.55 | 131.32 | 124.68 |
| 13 | c | 101 | BCB | CMB-C2B-C3B | 3.55 | 131.32 | 124.68 |
| 13 | D | 101 | BCB | CHD-C1D-ND | -3.55 | 121.20 | 124.45 |
| 13 | J | 101 | BCB | C3D-C4D-ND | 3.54 | 115.97 | 110.24 |
| 13 | 6 | 101 | BCB | CMB-C2B-C3B | 3.54 | 131.31 | 124.68 |
| 13 | T | 101 | BCB | O2D-CGD-CBD | 3.54 | 117.55 | 111.27 |
| 20 | D | 102 | PGV | O01-C1-C2 | 3.53 | 119.12 | 111.50 |
| 13 | 9 | 101 | BCB | C1-C2-C3 | -3.53 | 119.94 | 126.04 |
| 13 | O | 102 | BCB | C3D-C2D-C1D | -3.52 | 101.02 | 105.83 |
| 13 | J | 101 | BCB | CHD-C1D-ND | -3.52 | 121.22 | 124.45 |
| 13 | E | 101 | BCB | C3D-C2D-C1D | -3.51 | 101.03 | 105.83 |
| 13 | N | 101 | BCB | CMB-C2B-C1B | -3.51 | 123.07 | 128.46 |
| 21 | o | 101 | NS0 | C21-C20-C19 | 3.51 | 130.67 | 123.47 |
| 13 | J | 101 | BCB | CMB-C2B-C3B | 3.51 | 131.25 | 124.68 |
| 13 | T | 101 | BCB | CHD-C4C-C3C | -3.51 | 121.50 | 125.89 |
| 21 | q | 102 | NS0 | C21-C20-C19 | 3.51 | 130.66 | 123.47 |
| 13 | L | 303 | BCB | C3D-C4D-ND | 3.51 | 115.91 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | J | 101 | BCB | C3D-C2D-C1D | -3.50 | 101.05 | 105.83 |
| 13 | L | 302 | BCB | CMB-C2B-C3B | 3.50 | 131.23 | 124.68 |
| 13 | c | 101 | BCB | CHD-C4C-C3C | -3.50 | 121.51 | 125.89 |
| 13 | o | 102 | BCB | C3D-C2D-C1D | -3.49 | 101.06 | 105.83 |
| 21 | l | 101 | NS0 | C21-C20-C19 | 3.48 | 130.61 | 123.47 |
| 20 | M | 411 | PGV | O01-C1-C2 | 3.47 | 118.99 | 111.50 |
| 13 | b | 101 | BCB | C1-C2-C3 | -3.47 | 120.04 | 126.04 |
| 11 | M | 408 | UQ8 | C25-C24-C26 | 3.47 | 121.10 | 115.27 |
| 21 | k | 101 | NS0 | C21-C20-C19 | 3.46 | 130.57 | 123.47 |
| 11 | L | 305 | UQ8 | C7-C8-C9 | -3.46 | 121.03 | 126.79 |
| 13 | M | 402 | BCB | C3D-C4D-ND | 3.45 | 115.82 | 110.24 |
| 21 | U | 101 | NS0 | C21-C20-C19 | 3.44 | 130.51 | 123.47 |
| 13 | Q | 402 | BCB | CHD-C1D-ND | -3.43 | 121.30 | 124.45 |
| 13 | Z | 101 | BCB | CHD-C4C-C3C | -3.43 | 121.60 | 125.89 |
| 13 | B | 202 | BCB | C3D-C2D-C1D | -3.42 | 101.16 | 105.83 |
| 13 | L | 302 | BCB | CHD-C1D-ND | -3.42 | 121.31 | 124.45 |
| 18 | M | 406 | NS5 | C22-C21-C20 | -3.42 | 118.13 | 122.92 |
| 13 | c | 101 | BCB | C3D-C2D-C1D | -3.41 | 101.17 | 105.83 |
| 13 | f | 101 | BCB | C3D-C4D-ND | 3.41 | 115.75 | 110.24 |
| 13 | M | 402 | BCB | C4-C3-C5 | 3.40 | 120.99 | 115.27 |
| 13 | k | 102 | BCB | O2D-CGD-CBD | 3.40 | 117.31 | 111.27 |
| 13 | l | 101 | BCB | C3D-C2D-C1D | -3.40 | 101.20 | 105.83 |
| 13 | 0 | 102 | BCB | C3D-C4D-ND | 3.39 | 115.73 | 110.24 |
| 13 | R | 102 | BCB | CMB-C2B-C1B | -3.39 | 123.25 | 128.46 |
| 13 | E | 101 | BCB | CHD-C1D-ND | -3.39 | 121.34 | 124.45 |
| 21 | h | 101 | NS0 | C21-C20-C19 | 3.39 | 130.41 | 123.47 |
| 13 | i | 101 | BCB | CMB-C2B-C3B | 3.38 | 131.01 | 124.68 |
| 13 | M | 403 | BCB | C1D-CHD-C4C | -3.38 | 118.77 | 126.06 |
| 13 | r | 101 | BCB | C3D-C2D-C1D | -3.38 | 101.22 | 105.83 |
| 13 | W | 302 | BCB | CHD-C4C-C3C | -3.38 | 121.67 | 125.89 |
| 13 | f | 101 | BCB | C3D-C2D-C1D | -3.37 | 101.23 | 105.83 |
| 13 | h | 102 | BCB | C1-C2-C3 | -3.37 | 120.22 | 126.04 |
| 13 | k | 102 | BCB | C1-C2-C3 | -3.37 | 120.22 | 126.04 |
| 13 | W | 302 | BCB | CHD-C1D-ND | -3.36 | 121.36 | 124.45 |
| 21 | 7 | 101 | NS0 | C21-C20-C19 | 3.36 | 130.35 | 123.47 |
| 13 | X | 102 | BCB | CHD-C1D-ND | -3.36 | 121.37 | 124.45 |
| 13 | e | 101 | BCB | C4D-CHA-C1A | -3.36 | 117.17 | 121.25 |
| 13 | W | 302 | BCB | CMB-C2B-C1B | -3.35 | 123.31 | 128.46 |
| 11 | M | 407 | UQ8 | C17-C16-C14 | -3.35 | 109.14 | 114.62 |
| 13 | q | 101 | BCB | CHD-C1D-ND | -3.35 | 121.38 | 124.45 |
| 13 | T | 101 | BCB | C1-C2-C3 | -3.35 | 120.26 | 126.04 |
| 13 | N | 101 | BCB | CHD-C4C-C3C | -3.35 | 121.70 | 125.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15 | L | 306 | CDL | CA4-OA6-CA5 | -3.34 | 109.56 | 117.79 |
| 13 | U | 102 | BCB | C3D-C2D-C1D | -3.34 | 101.28 | 105.83 |
| 13 | i | 101 | BCB | C3D-C4D-ND | 3.33 | 115.63 | 110.24 |
| 13 | R | 102 | BCB | C3D-C2D-C1D | -3.33 | 101.29 | 105.83 |
| 13 | l | 102 | BCB | CMB-C2B-C1B | -3.32 | 123.36 | 128.46 |
| 13 | 7 | 102 | BCB | CMB-C2B-C1B | -3.32 | 123.36 | 128.46 |
| 13 | l | 102 | BCB | C3D-C2D-C1D | -3.32 | 101.31 | 105.83 |
| 21 | 2 | 101 | NS0 | C21-C20-C19 | 3.30 | 130.23 | 123.47 |
| 13 | 6 | 101 | BCB | CHD-C1D-ND | -3.29 | 121.43 | 124.45 |
| 13 | 0 | 102 | BCB | C4D-CHA-C1A | -3.28 | 117.25 | 121.25 |
| 13 | 1 | 101 | BCB | C3D-C4D-ND | 3.28 | 115.55 | 110.24 |
| 17 | M | 405 | MQ7 | C39-C38-C40 | 3.28 | 120.79 | 115.27 |
| 13 | k | 102 | BCB | CMB-C2B-C1B | -3.28 | 123.43 | 128.46 |
| 13 | Q | 402 | BCB | CHD-C4C-C3C | -3.27 | 121.80 | 125.89 |
| 13 | 3 | 101 | BCB | CHD-C4C-C3C | -3.26 | 121.82 | 125.89 |
| 21 | D | 103 | NS0 | C21-C20-C19 | 3.25 | 130.13 | 123.47 |
| 13 | 4 | 101 | BCB | C4D-CHA-C1A | -3.25 | 117.30 | 121.25 |
| 13 | X | 102 | BCB | C3D-C4D-ND | 3.25 | 115.49 | 110.24 |
| 20 | D | 102 | PGV | O03-C19-C20 | 3.24 | 122.07 | 111.91 |
| 13 | R | 102 | BCB | C4D-CHA-C1A | -3.24 | 117.31 | 121.25 |
| 13 | U | 102 | BCB | C3D-C4D-ND | 3.23 | 115.46 | 110.24 |
| 13 | 7 | 102 | BCB | C4D-CHA-C1A | -3.23 | 117.32 | 121.25 |
| 13 | n | 101 | BCB | CHD-C1D-ND | -3.22 | 121.49 | 124.45 |
| 13 | 6 | 101 | BCB | CHD-C4C-C3C | -3.22 | 121.86 | 125.89 |
| 21 | O | 101 | NS0 | C13-C12-C14 | -3.21 | 118.42 | 122.92 |
| 13 | c | 101 | BCB | C3D-C4D-ND | 3.21 | 115.43 | 110.24 |
| 13 | 4 | 101 | BCB | C3D-C4D-ND | 3.20 | 115.41 | 110.24 |
| 13 | B | 202 | BCB | C3D-C4D-ND | 3.19 | 115.40 | 110.24 |
| 13 | U | 102 | BCB | C4D-CHA-C1A | -3.19 | 117.37 | 121.25 |
| 13 | X | 102 | BCB | C3D-C2D-C1D | -3.19 | 101.48 | 105.83 |
| 21 | X | 101 | NS0 | C18-C17-C19 | -3.19 | 118.46 | 122.92 |
| 13 | B | 202 | BCB | CMB-C2B-C1B | -3.19 | 123.56 | 128.46 |
| 13 | 0 | 102 | BCB | CHB-C4A-NA | 3.18 | 128.91 | 124.51 |
| 13 | q | 101 | BCB | CHD-C4C-C3C | -3.18 | 121.91 | 125.89 |
| 13 | e | 101 | BCB | CHD-C1D-ND | -3.18 | 121.53 | 124.45 |
| 13 | 1 | 101 | BCB | CMB-C2B-C1B | -3.18 | 123.58 | 128.46 |
| 21 | A | 103 | NS0 | C21-C20-C19 | 3.17 | 129.97 | 123.47 |
| 13 | 4 | 101 | BCB | C3D-C2D-C1D | -3.17 | 101.50 | 105.83 |
| 13 | 4 | 101 | BCB | CMB-C2B-C1B | -3.17 | 123.59 | 128.46 |
| 13 | R | 102 | BCB | C4-C3-C5 | 3.17 | 120.60 | 115.27 |
| 13 | 7 | 102 | BCB | C3D-C4D-ND | 3.17 | 115.36 | 110.24 |
| 21 | U | 101 | NS0 | C24-C23-C22 | -3.16 | 118.49 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | B | 202 | BCB | CHD-C1D-ND | -3.16 | 121.55 | 124.45 |
| 21 | q | 102 | NS0 | C13-C12-C14 | -3.16 | 118.50 | 122.92 |
| 13 | B | 202 | BCB | C4D-CHA-C1A | -3.16 | 117.40 | 121.25 |
| 13 | A | 102 | BCB | CHB-C4A-NA | 3.15 | 128.87 | 124.51 |
| 13 | 0 | 102 | BCB | CHD-C1D-ND | -3.15 | 121.56 | 124.45 |
| 13 | L | 303 | BCB | CMB-C2B-C1B | -3.15 | 123.62 | 128.46 |
| 13 | 7 | 102 | BCB | C3D-C2D-C1D | -3.15 | 101.54 | 105.83 |
| 13 | o | 102 | BCB | CMB-C2B-C1B | -3.14 | 123.63 | 128.46 |
| 13 | L | 302 | BCB | CHB-C4A-NA | 3.14 | 128.85 | 124.51 |
| 13 | c | 101 | BCB | C4D-CHA-C1A | -3.14 | 117.43 | 121.25 |
| 13 | W | 302 | BCB | O2A-CGA-CBA | 3.14 | 121.75 | 111.91 |
| 21 | k | 101 | NS0 | C24-C23-C22 | -3.13 | 118.53 | 122.92 |
| 11 | A | 101 | UQ8 | C40-C39-C41 | 3.13 | 120.54 | 115.27 |
| 13 | 0 | 102 | BCB | C3D-C2D-C1D | -3.13 | 101.55 | 105.83 |
| 19 | k | 103 | LMT | C1B-O1B-C4' | -3.13 | 110.21 | 117.96 |
| 19 | T | 102 | LMT | C1-O1'-C1' | -3.12 | 108.66 | 113.84 |
| 13 | b | 101 | BCB | CMB-C2B-C1B | -3.12 | 123.67 | 128.46 |
| 11 | M | 408 | UQ8 | C35-C34-C36 | 3.12 | 120.52 | 115.27 |
| 13 | l | 102 | BCB | C3D-C4D-ND | 3.12 | 115.28 | 110.24 |
| 21 | 2 | 101 | NS0 | C24-C23-C22 | -3.12 | 118.56 | 122.92 |
| 21 | k | 101 | NS0 | C13-C12-C14 | -3.12 | 118.56 | 122.92 |
| 13 | 0 | 102 | BCB | CMB-C2B-C1B | -3.11 | 123.68 | 128.46 |
| 13 | O | 102 | BCB | CHD-C4C-C3C | -3.11 | 122.00 | 125.89 |
| 13 | 6 | 101 | BCB | C1-C2-C3 | -3.11 | 120.66 | 126.04 |
| 21 | U | 101 | NS0 | C13-C12-C14 | -3.11 | 118.57 | 122.92 |
| 13 | b | 101 | BCB | CHD-C4C-C3C | -3.10 | 122.01 | 125.89 |
| 13 | L | 303 | BCB | C1-C2-C3 | -3.10 | 120.69 | 126.04 |
| 18 | M | 406 | NS5 | C27-C26-C25 | -3.10 | 118.58 | 122.92 |
| 13 | 9 | 101 | BCB | C4-C3-C5 | 3.10 | 120.48 | 115.27 |
| 13 | X | 102 | BCB | CMB-C2B-C1B | -3.09 | 123.71 | 128.46 |
| 11 | A | 101 | UQ8 | C25-C24-C26 | 3.09 | 120.47 | 115.27 |
| 21 | O | 101 | NS0 | C21-C20-C19 | 3.09 | 129.80 | 123.47 |
| 13 | D | 101 | BCB | CHD-C4C-C3C | -3.09 | 122.03 | 125.89 |
| 13 | 6 | 101 | BCB | C4D-CHA-C1A | -3.08 | 117.50 | 121.25 |
| 13 | B | 202 | BCB | CHD-C4C-C3C | -3.08 | 122.03 | 125.89 |
| 13 | O | 102 | BCB | C3D-C4D-ND | 3.08 | 115.22 | 110.24 |
| 21 | k | 101 | NS0 | C18-C17-C19 | -3.08 | 118.61 | 122.92 |
| 13 | E | 101 | BCB | C3D-C4D-ND | 3.08 | 115.22 | 110.24 |
| 21 | W | 303 | NS0 | C13-C12-C14 | -3.08 | 118.61 | 122.92 |
| 13 | f | 101 | BCB | C4D-CHA-C1A | -3.08 | 117.51 | 121.25 |
| 13 | E | 101 | BCB | C4D-CHA-C1A | -3.07 | 117.52 | 121.25 |
| 21 | R | 101 | NS0 | C18-C17-C19 | -3.07 | 118.63 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21 | l | 101 | NS0 | C24-C23-C22 | -3.07 | 118.63 | 122.92 |
| 13 | h | 102 | BCB | CMB-C2B-C1B | -3.06 | 123.76 | 128.46 |
| 21 | 2 | 101 | NS0 | C13-C12-C14 | -3.06 | 118.63 | 122.92 |
| 13 | T | 101 | BCB | CMB-C2B-C1B | -3.06 | 123.76 | 128.46 |
| 17 | M | 405 | MQ7 | C34-C33-C35 | 3.05 | 120.41 | 115.27 |
| 13 | c | 101 | BCB | O2A-CGA-CBA | 3.05 | 121.49 | 111.91 |
| 21 | l | 101 | NS0 | C13-C12-C14 | -3.05 | 118.65 | 122.92 |
| 13 | I | 101 | BCB | CMB-C2B-C1B | -3.05 | 123.77 | 128.46 |
| 13 | R | 102 | BCB | CHD-C4C-C3C | -3.05 | 122.08 | 125.89 |
| 13 | R | 102 | BCB | C3D-C4D-ND | 3.05 | 115.17 | 110.24 |
| 21 | l | 101 | NS0 | C18-C17-C19 | -3.05 | 118.66 | 122.92 |
| 13 | U | 102 | BCB | CMB-C2B-C1B | -3.05 | 123.78 | 128.46 |
| 13 | i | 101 | BCB | C3D-C2D-C1D | -3.05 | 101.67 | 105.83 |
| 21 | D | 103 | NS0 | C18-C17-C19 | -3.04 | 118.66 | 122.92 |
| 13 | r | 101 | BCB | C4D-CHA-C1A | -3.04 | 117.55 | 121.25 |
| 13 | Z | 101 | BCB | C4D-CHA-C1A | -3.04 | 117.55 | 121.25 |
| 21 | q | 102 | NS0 | C18-C17-C19 | -3.04 | 118.67 | 122.92 |
| 11 | M | 408 | UQ8 | C27-C28-C29 | -3.04 | 120.35 | 127.66 |
| 13 | I | 101 | BCB | CHD-C4C-C3C | -3.03 | 122.09 | 125.89 |
| 13 | h | 102 | BCB | CHD-C4C-C3C | -3.03 | 122.09 | 125.89 |
| 11 | A | 101 | UQ8 | C10-C9-C11 | 3.03 | 120.38 | 115.27 |
| 13 | o | 102 | BCB | C3D-C4D-ND | 3.03 | 115.14 | 110.24 |
| 13 | R | 102 | BCB | CHB-C4A-NA | 3.03 | 128.70 | 124.51 |
| 13 | l | 102 | BCB | C1B-CHB-C4A | -3.03 | 124.12 | 130.12 |
| 21 | k | 101 | NS0 | C20-C21-C22 | 3.02 | 129.67 | 123.47 |
| 11 | M | 408 | UQ8 | C30-C29-C31 | 3.02 | 120.36 | 115.27 |
| 13 | L | 303 | BCB | CHB-C4A-NA | 3.02 | 128.69 | 124.51 |
| 13 | D | 101 | BCB | CHB-C4A-NA | 3.02 | 128.69 | 124.51 |
| 13 | c | 101 | BCB | CHB-C4A-NA | 3.01 | 128.67 | 124.51 |
| 13 | N | 101 | BCB | C1B-CHB-C4A | -3.01 | 124.16 | 130.12 |
| 13 | B | 202 | BCB | CHB-C4A-NA | 3.00 | 128.67 | 124.51 |
| 13 | q | 101 | BCB | CMB-C2B-C1B | -3.00 | 123.86 | 128.46 |
| 13 | 9 | 101 | BCB | C2A-C1A-CHA | -2.99 | 118.62 | 123.86 |
| 13 | T | 101 | BCB | C6-C5-C3 | -2.99 | 105.61 | 113.45 |
| 13 | h | 102 | BCB | C4-C3-C5 | 2.98 | 120.29 | 115.27 |
| 13 | 1 | 101 | BCB | CHD-C1D-ND | -2.98 | 121.72 | 124.45 |
| 13 | o | 102 | BCB | CHD-C4C-C3C | -2.98 | 122.16 | 125.89 |
| 13 | f | 101 | BCB | CHD-C1D-ND | -2.98 | 121.72 | 124.45 |
| 13 | q | 101 | BCB | C1B-CHB-C4A | -2.98 | 124.22 | 130.12 |
| 13 | h | 102 | BCB | CHD-C1D-ND | -2.97 | 121.72 | 124.45 |
| 13 | r | 101 | BCB | CHD-C1D-ND | -2.97 | 121.72 | 124.45 |
| 21 | 7 | 101 | NS0 | C24-C23-C22 | -2.97 | 118.76 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | f | 101 | BCB | CMB-C2B-C1B | -2.97 | 123.90 | 128.46 |
| 13 | 9 | 101 | BCB | C4D-CHA-C1A | -2.97 | 117.64 | 121.25 |
| 13 | l | 102 | BCB | CHD-C1D-ND | -2.97 | 121.72 | 124.45 |
| 21 | R | 101 | NS0 | C13-C12-C14 | -2.97 | 118.77 | 122.92 |
| 11 | A | 101 | UQ8 | C22-C23-C24 | -2.97 | 120.51 | 127.66 |
| 21 | 0 | 101 | NS0 | C21-C20-C19 | 2.97 | 129.55 | 123.47 |
| 13 | l | 102 | BCB | C4D-CHA-C1A | -2.96 | 117.64 | 121.25 |
| 19 | b | 103 | LMT | C1-O1'-C1' | -2.96 | 108.93 | 113.84 |
| 13 | 4 | 101 | BCB | CHB-C4A-NA | 2.96 | 128.60 | 124.51 |
| 21 | W | 303 | NS0 | C18-C17-C19 | -2.96 | 118.78 | 122.92 |
| 11 | M | 408 | UQ8 | C7-C8-C9 | 2.96 | 131.72 | 126.79 |
| 13 | E | 101 | BCB | O2A-CGA-CBA | 2.96 | 121.19 | 111.91 |
| 13 | I | 101 | BCB | CHD-C1D-ND | -2.96 | 121.74 | 124.45 |
| 21 | X | 101 | NS0 | C24-C23-C22 | -2.96 | 118.78 | 122.92 |
| 13 | k | 102 | BCB | CHD-C1D-ND | -2.96 | 121.74 | 124.45 |
| 11 | M | 408 | UQ8 | C20-C19-C21 | 2.95 | 120.24 | 115.27 |
| 13 | b | 101 | BCB | C4-C3-C5 | 2.95 | 120.23 | 115.27 |
| 13 | r | 101 | BCB | C3D-C4D-ND | 2.95 | 115.01 | 110.24 |
| 13 | J | 101 | BCB | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 21 | 9 | 102 | NS0 | C13-C12-C14 | -2.95 | 118.79 | 122.92 |
| 13 | 9 | 101 | BCB | CMB-C2B-C1B | -2.95 | 123.94 | 128.46 |
| 13 | X | 102 | BCB | C4D-CHA-C1A | -2.95 | 117.66 | 121.25 |
| 13 | e | 101 | BCB | CMB-C2B-C1B | -2.94 | 123.94 | 128.46 |
| 21 | W | 303 | NS0 | C24-C23-C22 | -2.94 | 118.80 | 122.92 |
| 11 | M | 407 | UQ8 | C10-C9-C11 | 2.94 | 120.21 | 115.27 |
| 11 | A | 101 | UQ8 | C17-C18-C19 | -2.93 | 120.59 | 127.66 |
| 13 | A | 102 | BCB | C1B-CHB-C4A | -2.93 | 124.31 | 130.12 |
| 21 | 0 | 101 | NS0 | C13-C12-C14 | -2.93 | 118.81 | 122.92 |
| 13 | 0 | 102 | BCB | O2A-CGA-CBA | 2.93 | 121.11 | 111.91 |
| 13 | T | 101 | BCB | O2A-CGA-CBA | 2.93 | 121.11 | 111.91 |
| 13 | N | 101 | BCB | CHD-C1D-ND | -2.93 | 121.76 | 124.45 |
| 21 | U | 101 | NS0 | C18-C17-C19 | -2.93 | 118.82 | 122.92 |
| 13 | n | 101 | BCB | CMB-C2B-C1B | -2.93 | 123.97 | 128.46 |
| 21 | R | 101 | NS0 | C24-C23-C22 | -2.92 | 118.83 | 122.92 |
| 15 | L | 306 | CDL | OA8-CA7-C31 | 2.92 | 121.07 | 111.91 |
| 13 | 6 | 101 | BCB | C4-C3-C5 | 2.92 | 120.18 | 115.27 |
| 13 | 3 | 101 | BCB | CHD-C1D-ND | -2.92 | 121.77 | 124.45 |
| 13 | N | 101 | BCB | O2A-CGA-CBA | 2.92 | 121.06 | 111.91 |
| 13 | X | 102 | BCB | CHB-C4A-NA | 2.91 | 128.54 | 124.51 |
| 11 | M | 408 | UQ8 | C15-C14-C16 | 2.91 | 120.17 | 115.27 |
| 13 | D | 101 | BCB | CMB-C2B-C1B | -2.91 | 123.99 | 128.46 |
| 15 | H | 302 | CDL | OA8-CA7-C31 | 2.91 | 121.04 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | L | 303 | BCB | CHD-C4C-C3C | -2.91 | 122.25 | 125.89 |
| 13 | Q | 402 | BCB | C4-C3-C5 | 2.91 | 120.16 | 115.27 |
| 21 | D | 103 | NS0 | C24-C23-C22 | -2.91 | 118.85 | 122.92 |
| 13 | i | 101 | BCB | CHB-C4A-NA | 2.91 | 128.53 | 124.51 |
| 13 | c | 101 | BCB | C1D-CHD-C4C | -2.91 | 119.79 | 126.06 |
| 21 | A | 103 | NS0 | C18-C17-C19 | -2.90 | 118.86 | 122.92 |
| 13 | 9 | 101 | BCB | CHB-C4A-NA | 2.90 | 128.53 | 124.51 |
| 13 | O | 102 | BCB | C1D-CHD-C4C | -2.90 | 119.80 | 126.06 |
| 13 | b | 101 | BCB | CHD-C1D-ND | -2.90 | 121.79 | 124.45 |
| 13 | U | 102 | BCB | CHD-C4C-C3C | -2.90 | 122.26 | 125.89 |
| 13 | r | 101 | BCB | O2A-CGA-CBA | 2.90 | 120.99 | 111.91 |
| 21 | h | 101 | NS0 | C24-C23-C22 | -2.89 | 118.87 | 122.92 |
| 11 | M | 408 | UQ8 | C16-C14-C13 | -2.89 | 115.27 | 121.12 |
| 13 | 0 | 102 | BCB | C2A-C1A-CHA | -2.89 | 118.81 | 123.86 |
| 13 | 9 | 101 | BCB | CHD-C4C-C3C | -2.88 | 122.28 | 125.89 |
| 18 | M | 406 | NS5 | C18-C19-C20 | 2.88 | 129.37 | 123.47 |
| 13 | o | 102 | BCB | O2A-CGA-CBA | 2.88 | 120.94 | 111.91 |
| 13 | 1 | 101 | BCB | C4D-CHA-C1A | -2.87 | 117.75 | 121.25 |
| 21 | A | 103 | NS0 | C24-C23-C22 | -2.87 | 118.90 | 122.92 |
| 13 | A | 102 | BCB | CHD-C4C-C3C | -2.87 | 122.30 | 125.89 |
| 13 | T | 101 | BCB | C1B-CHB-C4A | -2.87 | 124.44 | 130.12 |
| 13 | k | 102 | BCB | C1B-CHB-C4A | -2.87 | 124.44 | 130.12 |
| 13 | f | 101 | BCB | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 13 | U | 102 | BCB | O2A-CGA-CBA | 2.86 | 120.90 | 111.91 |
| 13 | L | 302 | BCB | CED-O2D-CGD | 2.86 | 122.41 | 115.94 |
| 11 | M | 407 | UQ8 | C12-C13-C14 | -2.86 | 120.77 | 127.66 |
| 21 | 0 | 101 | NS0 | C18-C17-C19 | -2.86 | 118.92 | 122.92 |
| 13 | O | 102 | BCB | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 20 | W | 301 | PGV | C02-O01-C1 | -2.86 | 110.76 | 117.79 |
| 21 | 7 | 101 | NS0 | C13-C12-C14 | -2.86 | 118.92 | 122.92 |
| 13 | i | 101 | BCB | C4-C3-C5 | 2.85 | 120.07 | 115.27 |
| 13 | J | 101 | BCB | O2A-CGA-CBA | 2.85 | 120.86 | 111.91 |
| 13 | o | 102 | BCB | C4-C3-C5 | 2.85 | 120.07 | 115.27 |
| 13 | i | 101 | BCB | CHD-C4C-C3C | -2.85 | 122.32 | 125.89 |
| 19 | n | 102 | LMT | C1B-O1B-C4' | -2.85 | 110.92 | 117.96 |
| 21 | 9 | 102 | NS0 | C24-C23-C22 | -2.85 | 118.94 | 122.92 |
| 21 | o | 101 | NS0 | C18-C17-C19 | -2.84 | 118.94 | 122.92 |
| 12 | L | 301 | DGA | OG1-CA1-CA2 | 2.84 | 120.83 | 111.91 |
| 13 | 9 | 101 | BCB | C3D-C4D-ND | 2.84 | 114.83 | 110.24 |
| 13 | Q | 402 | BCB | C4D-CHA-C1A | -2.84 | 117.80 | 121.25 |
| 21 | h | 101 | NS0 | C18-C17-C19 | -2.84 | 118.95 | 122.92 |
| 13 | o | 102 | BCB | C4D-CHA-C1A | -2.84 | 117.80 | 121.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21 | q | 102 | NS0 | C24-C23-C22 | -2.84 | 118.95 | 122.92 |
| 13 | O | 102 | BCB | C4-C3-C5 | 2.84 | 120.04 | 115.27 |
| 13 | T | 101 | BCB | CHD-C1D-ND | -2.83 | 121.85 | 124.45 |
| 13 | l | 102 | BCB | C1-C2-C3 | -2.83 | 121.14 | 126.04 |
| 13 | Z | 101 | BCB | CMB-C2B-C1B | -2.83 | 124.12 | 128.46 |
| 13 | M | 403 | BCB | O2A-CGA-CBA | 2.83 | 120.78 | 111.91 |
| 21 | 9 | 102 | NS0 | C18-C17-C19 | -2.83 | 118.96 | 122.92 |
| 21 | 2 | 101 | NS0 | C18-C17-C19 | -2.82 | 118.97 | 122.92 |
| 21 | o | 101 | NS0 | C13-C12-C14 | -2.82 | 118.97 | 122.92 |
| 13 | r | 101 | BCB | C1-C2-C3 | -2.82 | 121.17 | 126.04 |
| 13 | k | 102 | BCB | C4D-CHA-C1A | -2.82 | 117.82 | 121.25 |
| 11 | C | 406 | UQ8 | C7-C6-C1 | -2.82 | 119.55 | 124.27 |
| 13 | e | 101 | BCB | O2A-CGA-CBA | 2.82 | 120.74 | 111.91 |
| 13 | X | 102 | BCB | O2A-CGA-CBA | 2.81 | 120.74 | 111.91 |
| 13 | 4 | 101 | BCB | O2A-CGA-CBA | 2.81 | 120.74 | 111.91 |
| 13 | o | 102 | BCB | C1D-CHD-C4C | -2.81 | 119.99 | 126.06 |
| 13 | B | 202 | BCB | C4-C3-C5 | 2.81 | 120.00 | 115.27 |
| 13 | D | 101 | BCB | C2A-C1A-CHA | -2.81 | 118.95 | 123.86 |
| 13 | M | 403 | BCB | O2D-CGD-O1D | -2.81 | 118.35 | 123.84 |
| 13 | O | 102 | BCB | CMB-C2B-C1B | -2.81 | 124.15 | 128.46 |
| 13 | W | 302 | BCB | CHB-C4A-NA | 2.81 | 128.39 | 124.51 |
| 13 | l | 102 | BCB | CHB-C4A-NA | 2.81 | 128.39 | 124.51 |
| 14 | M | 404 | BPB | CMC-C2C-C1C | -2.81 | 109.65 | 114.36 |
| 13 | A | 102 | BCB | C4D-CHA-C1A | -2.81 | 117.83 | 121.25 |
| 13 | e | 101 | BCB | CHD-C4C-C3C | -2.81 | 122.38 | 125.89 |
| 13 | c | 101 | BCB | CMB-C2B-C1B | -2.80 | 124.17 | 128.46 |
| 13 | q | 101 | BCB | C1-C2-C3 | -2.79 | 121.21 | 126.04 |
| 13 | 7 | 102 | BCB | C1B-CHB-C4A | -2.79 | 124.58 | 130.12 |
| 18 | M | 406 | NS5 | C23-C21-C20 | 2.79 | 123.23 | 118.94 |
| 13 | 4 | 101 | BCB | C4-C3-C5 | 2.79 | 119.97 | 115.27 |
| 21 | O | 101 | NS0 | C24-C23-C22 | -2.79 | 119.02 | 122.92 |
| 21 | h | 101 | NS0 | C13-C12-C14 | -2.79 | 119.02 | 122.92 |
| 13 | k | 102 | BCB | C4-C3-C5 | 2.78 | 119.95 | 115.27 |
| 13 | M | 403 | BCB | C4B-CHC-C1C | -2.78 | 124.61 | 130.12 |
| 13 | X | 102 | BCB | CHD-C4C-C3C | -2.78 | 122.41 | 125.89 |
| 13 | i | 101 | BCB | O2A-CGA-CBA | 2.78 | 120.63 | 111.91 |
| 21 | X | 101 | NS0 | C13-C12-C14 | -2.78 | 119.03 | 122.92 |
| 13 | M | 403 | BCB | C3D-C4D-ND | 2.77 | 114.72 | 110.24 |
| 17 | M | 405 | MQ7 | C26-C27-C28 | -2.76 | 121.01 | 127.66 |
| 17 | M | 405 | MQ7 | C29-C28-C30 | 2.76 | 119.92 | 115.27 |
| 13 | M | 402 | BCB | C2A-C1A-CHA | -2.76 | 119.04 | 123.86 |
| 13 | 1 | 101 | BCB | O2A-CGA-CBA | 2.76 | 120.56 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21 | O | 101 | NS0 | C18-C17-C19 | -2.76 | 119.06 | 122.92 |
| 13 | l | 102 | BCB | O2A-CGA-CBA | 2.76 | 120.56 | 111.91 |
| 13 | L | 302 | BCB | C1D-CHD-C4C | -2.76 | 120.11 | 126.06 |
| 13 | 7 | 102 | BCB | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 13 | 7 | 102 | BCB | C1-C2-C3 | -2.75 | 121.29 | 126.04 |
| 13 | O | 102 | BCB | O2A-CGA-CBA | 2.75 | 120.53 | 111.91 |
| 13 | h | 102 | BCB | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 18 | M | 406 | NS5 | C28-C26-C25 | 2.74 | 123.15 | 118.94 |
| 13 | X | 102 | BCB | C1-C2-C3 | -2.74 | 121.30 | 126.04 |
| 13 | J | 101 | BCB | C4D-CHA-C1A | -2.74 | 117.91 | 121.25 |
| 20 | W | 301 | PGV | O03-C19-C20 | 2.74 | 120.52 | 111.91 |
| 13 | D | 101 | BCB | C3D-C4D-ND | 2.74 | 114.67 | 110.24 |
| 13 | L | 303 | BCB | C4-C3-C5 | 2.74 | 119.88 | 115.27 |
| 13 | 7 | 102 | BCB | CHD-C1D-ND | -2.74 | 121.94 | 124.45 |
| 13 | U | 102 | BCB | C4-C3-C5 | 2.74 | 119.88 | 115.27 |
| 13 | E | 101 | BCB | CMB-C2B-C1B | -2.74 | 124.26 | 128.46 |
| 13 | b | 101 | BCB | C4D-CHA-C1A | -2.73 | 117.92 | 121.25 |
| 13 | r | 101 | BCB | CHD-C4C-C3C | -2.73 | 122.47 | 125.89 |
| 13 | E | 101 | BCB | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 13 | D | 101 | BCB | O2A-CGA-CBA | 2.73 | 120.47 | 111.91 |
| 13 | i | 101 | BCB | C1D-CHD-C4C | -2.73 | 120.17 | 126.06 |
| 13 | Q | 402 | BCB | CMB-C2B-C1B | -2.73 | 124.27 | 128.46 |
| 13 | n | 101 | BCB | C4D-CHA-C1A | -2.73 | 117.93 | 121.25 |
| 21 | o | 101 | NS0 | C24-C23-C22 | -2.73 | 119.10 | 122.92 |
| 21 | 7 | 101 | NS0 | C18-C17-C19 | -2.72 | 119.11 | 122.92 |
| 13 | o | 102 | BCB | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 13 | l | 102 | BCB | CHD-C4C-C3C | -2.72 | 122.49 | 125.89 |
| 13 | 0 | 102 | BCB | C4-C3-C5 | 2.72 | 119.84 | 115.27 |
| 13 | J | 101 | BCB | C4-C3-C5 | 2.72 | 119.84 | 115.27 |
| 13 | Z | 101 | BCB | O2A-CGA-CBA | 2.72 | 120.43 | 111.91 |
| 13 | J | 101 | BCB | CMB-C2B-C1B | -2.72 | 124.29 | 128.46 |
| 13 | U | 102 | BCB | C1D-CHD-C4C | -2.71 | 120.20 | 126.06 |
| 13 | 0 | 102 | BCB | CHD-C4C-C3C | -2.71 | 122.50 | 125.89 |
| 13 | q | 101 | BCB | C4-C3-C5 | 2.71 | 119.83 | 115.27 |
| 13 | U | 102 | BCB | C2A-C1A-CHA | -2.71 | 119.12 | 123.86 |
| 13 | R | 102 | BCB | C2A-C1A-CHA | -2.71 | 119.13 | 123.86 |
| 13 | f | 101 | BCB | O2A-CGA-CBA | 2.70 | 120.38 | 111.91 |
| 13 | L | 302 | BCB | C3D-C4D-ND | 2.70 | 114.60 | 110.24 |
| 11 | L | 305 | UQ8 | C1M-C1-C6 | -2.70 | 120.00 | 124.40 |
| 13 | f | 101 | BCB | C1B-CHB-C4A | -2.70 | 124.78 | 130.12 |
| 20 | N | 102 | PGV | O01-C1-C2 | 2.70 | 117.31 | 111.50 |
| 13 | 7 | 102 | BCB | O2A-CGA-CBA | 2.69 | 120.36 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | 3 | 101 | BCB | CMB-C2B-C1B | -2.69 | 124.33 | 128.46 |
| 13 | 4 | 101 | BCB | C1D-CHD-C4C | -2.69 | 120.26 | 126.06 |
| 21 | D | 103 | NS0 | C20-C21-C22 | 2.69 | 128.98 | 123.47 |
| 13 | e | 101 | BCB | CHB-C4A-NA | 2.69 | 128.22 | 124.51 |
| 13 | M | 403 | BCB | CMB-C2B-C1B | -2.68 | 124.34 | 128.46 |
| 13 | 1 | 101 | BCB | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 13 | n | 101 | BCB | C1B-CHB-C4A | -2.68 | 124.81 | 130.12 |
| 13 | I | 101 | BCB | C1B-CHB-C4A | -2.68 | 124.82 | 130.12 |
| 13 | M | 402 | BCB | CHD-C4C-C3C | -2.68 | 122.54 | 125.89 |
| 13 | l | 102 | BCB | C4-C3-C5 | 2.68 | 119.77 | 115.27 |
| 13 | n | 101 | BCB | CHD-C4C-C3C | -2.67 | 122.54 | 125.89 |
| 13 | I | 101 | BCB | C6-C5-C3 | -2.67 | 106.46 | 113.45 |
| 13 | 3 | 101 | BCB | O2A-CGA-CBA | 2.66 | 120.26 | 111.91 |
| 21 | 0 | 101 | NS0 | C24-C23-C22 | -2.66 | 119.20 | 122.92 |
| 11 | L | 305 | UQ8 | C17-C18-C19 | -2.66 | 121.25 | 127.66 |
| 13 | n | 101 | BCB | CAA-CBA-CGA | -2.66 | 105.48 | 113.25 |
| 13 | D | 101 | BCB | C1B-CHB-C4A | -2.66 | 124.85 | 130.12 |
| 11 | L | 305 | UQ8 | C10-C9-C11 | 2.66 | 119.74 | 115.27 |
| 13 | q | 101 | BCB | C2A-C1A-CHA | -2.66 | 119.21 | 123.86 |
| 13 | k | 102 | BCB | CHD-C4C-C3C | -2.65 | 122.57 | 125.89 |
| 20 | N | 102 | PGV | O03-C19-C20 | 2.65 | 120.22 | 111.91 |
| 13 | Z | 101 | BCB | CHD-C1D-ND | -2.65 | 122.02 | 124.45 |
| 13 | h | 102 | BCB | C4D-CHA-C1A | -2.65 | 118.03 | 121.25 |
| 13 | 6 | 101 | BCB | CMB-C2B-C1B | -2.64 | 124.40 | 128.46 |
| 13 | b | 101 | BCB | O2A-CGA-CBA | 2.64 | 120.20 | 111.91 |
| 13 | 3 | 101 | BCB | C6-C5-C3 | -2.64 | 106.53 | 113.45 |
| 13 | Z | 101 | BCB | C1B-CHB-C4A | -2.64 | 124.88 | 130.12 |
| 13 | E | 101 | BCB | C1-C2-C3 | -2.64 | 121.47 | 126.04 |
| 17 | M | 405 | MQ7 | C36-C37-C38 | -2.64 | 121.31 | 127.66 |
| 13 | q | 101 | BCB | C4D-CHA-C1A | -2.64 | 118.04 | 121.25 |
| 13 | U | 102 | BCB | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 13 | h | 102 | BCB | CAA-CBA-CGA | -2.63 | 105.56 | 113.25 |
| 13 | 6 | 101 | BCB | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 15 | L | 306 | CDL | OB8-CB7-C71 | 2.63 | 120.16 | 111.91 |
| 15 | L | 306 | CDL | CB4-OB6-CB5 | -2.63 | 111.32 | 117.79 |
| 13 | B | 202 | BCB | C2A-C1A-CHA | -2.63 | 119.27 | 123.86 |
| 15 | M | 409 | CDL | OA8-CA7-C31 | 2.63 | 120.15 | 111.91 |
| 13 | L | 302 | BCB | O2A-CGA-CBA | 2.63 | 120.15 | 111.91 |
| 13 | I | 101 | BCB | O2A-CGA-CBA | 2.62 | 120.14 | 111.91 |
| 9 | C | 403 | HEC | CBD-CAD-C3D | -2.62 | 108.15 | 112.62 |
| 13 | 7 | 102 | BCB | C1D-CHD-C4C | -2.62 | 120.41 | 126.06 |
| 11 | M | 408 | UQ8 | C41-C42-C43 | -2.62 | 103.28 | 111.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | R | 102 | BCB | CHD-C1D-ND | -2.62 | 122.05 | 124.45 |
| 13 | i | 101 | BCB | C1B-CHB-C4A | -2.62 | 124.93 | 130.12 |
| 13 | Z | 101 | BCB | CHB-C4A-NA | 2.62 | 128.13 | 124.51 |
| 13 | A | 102 | BCB | C2A-C1A-CHA | -2.61 | 119.29 | 123.86 |
| 13 | q | 101 | BCB | CHB-C4A-NA | 2.61 | 128.13 | 124.51 |
| 13 | 0 | 102 | BCB | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 13 | R | 102 | BCB | C1D-CHD-C4C | -2.61 | 120.43 | 126.06 |
| 13 | r | 101 | BCB | C4-C3-C5 | 2.61 | 119.66 | 115.27 |
| 13 | A | 102 | BCB | C3D-C4D-ND | 2.61 | 114.45 | 110.24 |
| 13 | n | 101 | BCB | O2A-CGA-CBA | 2.61 | 120.08 | 111.91 |
| 21 | R | 101 | NS0 | C16-C17-C19 | 2.60 | 122.94 | 118.94 |
| 13 | M | 402 | BCB | CHB-C4A-NA | 2.60 | 128.11 | 124.51 |
| 13 | c | 101 | BCB | C4-C3-C5 | 2.60 | 119.65 | 115.27 |
| 13 | I | 101 | BCB | CHB-C4A-NA | 2.60 | 128.11 | 124.51 |
| 12 | L | 301 | DGA | OG2-CB1-OB1 | -2.60 | 117.42 | 123.70 |
| 11 | A | 101 | UQ8 | C37-C38-C39 | -2.60 | 121.40 | 127.66 |
| 13 | q | 101 | BCB | C3D-C4D-ND | 2.59 | 114.43 | 110.24 |
| 21 | A | 103 | NS0 | C20-C21-C22 | 2.59 | 128.78 | 123.47 |
| 13 | R | 102 | BCB | O2A-CGA-CBA | 2.59 | 120.04 | 111.91 |
| 13 | J | 101 | BCB | CHD-C4C-C3C | -2.59 | 122.65 | 125.89 |
| 13 | f | 101 | BCB | C1D-CHD-C4C | -2.58 | 120.49 | 126.06 |
| 13 | O | 102 | BCB | O2D-CGD-O1D | -2.58 | 118.79 | 123.84 |
| 13 | 1 | 101 | BCB | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 21 | U | 101 | NS0 | C20-C21-C22 | 2.58 | 128.75 | 123.47 |
| 13 | N | 101 | BCB | C4D-CHA-C1A | -2.57 | 118.12 | 121.25 |
| 13 | 6 | 101 | BCB | O2A-CGA-CBA | 2.57 | 119.99 | 111.91 |
| 13 | L | 303 | BCB | C2A-C1A-CHA | -2.57 | 119.36 | 123.86 |
| 13 | Z | 101 | BCB | CAA-CBA-CGA | -2.57 | 105.73 | 113.25 |
| 13 | 6 | 101 | BCB | CAA-CBA-CGA | -2.57 | 105.74 | 113.25 |
| 21 | h | 101 | NS0 | C20-C21-C22 | 2.57 | 128.74 | 123.47 |
| 13 | Q | 402 | BCB | O2A-CGA-CBA | 2.56 | 119.96 | 111.91 |
| 20 | M | 411 | PGV | O03-C19-C20 | 2.56 | 119.96 | 111.91 |
| 13 | n | 101 | BCB | CHB-C4A-NA | 2.56 | 128.06 | 124.51 |
| 13 | B | 202 | BCB | O2A-CGA-CBA | 2.56 | 119.94 | 111.91 |
| 19 | b | 103 | LMT | O1'-C1'-C2' | 2.56 | 112.30 | 108.30 |
| 11 | M | 407 | UQ8 | C1M-C1-C6 | -2.56 | 120.23 | 124.40 |
| 13 | o | 102 | BCB | CHD-C1D-ND | -2.56 | 122.11 | 124.45 |
| 13 | D | 101 | BCB | C1D-CHD-C4C | -2.55 | 120.55 | 126.06 |
| 19 | T | 102 | LMT | O1'-C1'-C2' | 2.55 | 112.29 | 108.30 |
| 13 | A | 102 | BCB | CMB-C2B-C1B | -2.55 | 124.54 | 128.46 |
| 11 | C | 406 | UQ8 | C1M-C1-C6 | -2.55 | 120.24 | 124.40 |
| 13 | i | 101 | BCB | C2A-C1A-CHA | -2.55 | 119.40 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | I | 101 | BCB | C1D-CHD-C4C | -2.54 | 120.57 | 126.06 |
| 13 | 1 | 101 | BCB | C1D-CHD-C4C | -2.54 | 120.57 | 126.06 |
| 15 | H | 301 | CDL | OA8-CA7-C31 | 2.54 | 119.89 | 111.91 |
| 21 | q | 102 | NS0 | C16-C17-C19 | 2.54 | 122.84 | 118.94 |
| 13 | o | 102 | BCB | C1-C2-C3 | -2.54 | 121.66 | 126.04 |
| 13 | L | 302 | BCB | CHD-C4C-C3C | -2.53 | 122.72 | 125.89 |
| 13 | 0 | 102 | BCB | C1-C2-C3 | -2.53 | 121.66 | 126.04 |
| 13 | 6 | 101 | BCB | C1B-CHB-C4A | -2.53 | 125.10 | 130.12 |
| 13 | O | 102 | BCB | CHD-C1D-ND | -2.53 | 122.13 | 124.45 |
| 13 | D | 101 | BCB | C1-C2-C3 | -2.53 | 121.67 | 126.04 |
| 20 | Q | 401 | PGV | O03-C19-C20 | 2.53 | 119.85 | 111.91 |
| 13 | q | 101 | BCB | O2A-CGA-CBA | 2.53 | 119.84 | 111.91 |
| 13 | X | 102 | BCB | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 13 | b | 101 | BCB | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 13 | N | 101 | BCB | CHC-C1C-NC | -2.52 | 121.02 | 124.51 |
| 13 | q | 101 | BCB | CAA-CBA-CGA | -2.52 | 105.88 | 113.25 |
| 13 | A | 102 | BCB | C1D-CHD-C4C | -2.52 | 120.61 | 126.06 |
| 13 | f | 101 | BCB | C4-C3-C5 | 2.52 | 119.51 | 115.27 |
| 13 | L | 303 | BCB | O2D-CGD-O1D | -2.52 | 118.92 | 123.84 |
| 13 | D | 101 | BCB | C6-C5-C3 | -2.52 | 106.86 | 113.45 |
| 15 | M | 409 | CDL | OB8-CB7-C71 | 2.52 | 119.80 | 111.91 |
| 21 | A | 103 | NS0 | C13-C12-C14 | -2.51 | 119.40 | 122.92 |
| 20 | N | 102 | PGV | C03-C02-C01 | -2.51 | 105.85 | 111.79 |
| 21 | 7 | 101 | NS0 | C20-C21-C22 | 2.51 | 128.62 | 123.47 |
| 13 | 1 | 101 | BCB | CHD-C4C-C3C | -2.51 | 122.75 | 125.89 |
| 21 | D | 103 | NS0 | C13-C12-C14 | -2.51 | 119.41 | 122.92 |
| 13 | r | 101 | BCB | C1B-CHB-C4A | -2.51 | 125.15 | 130.12 |
| 13 | W | 302 | BCB | C6-C5-C3 | -2.51 | 106.89 | 113.45 |
| 21 | k | 101 | NS0 | C11-C12-C14 | 2.50 | 122.78 | 118.94 |
| 9 | C | 404 | HEC | CAD-CBD-CGD | -2.50 | 106.75 | 113.76 |
| 11 | A | 101 | UQ8 | C15-C14-C16 | 2.50 | 119.47 | 115.27 |
| 13 | n | 101 | BCB | CED-O2D-CGD | 2.50 | 121.58 | 115.94 |
| 13 | L | 303 | BCB | O1D-CGD-CBD | -2.49 | 119.39 | 124.48 |
| 13 | B | 202 | BCB | O2D-CGD-O1D | -2.49 | 118.97 | 123.84 |
| 13 | I | 101 | BCB | C4D-CHA-C1A | -2.49 | 118.22 | 121.25 |
| 21 | k | 101 | NS0 | C16-C17-C19 | 2.49 | 122.76 | 118.94 |
| 13 | U | 102 | BCB | C1B-CHB-C4A | -2.49 | 125.19 | 130.12 |
| 13 | b | 101 | BCB | CHB-C4A-NA | 2.49 | 127.95 | 124.51 |
| 13 | 7 | 102 | BCB | CHD-C4C-C3C | -2.48 | 122.79 | 125.89 |
| 13 | L | 303 | BCB | C1B-CHB-C4A | -2.48 | 125.21 | 130.12 |
| 17 | M | 405 | MQ7 | C21-C22-C23 | -2.47 | 121.70 | 127.66 |
| 13 | W | 302 | BCB | C4D-CHA-C1A | -2.47 | 118.24 | 121.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | h | 102 | BCB | C3D-C4D-ND | 2.46 | 114.22 | 110.24 |
| 13 | l | 101 | BCB | C4-C3-C5 | 2.46 | 119.41 | 115.27 |
| 13 | r | 101 | BCB | C1D-CHD-C4C | -2.46 | 120.75 | 126.06 |
| 21 | k | 101 | NS0 | C25-C23-C22 | 2.46 | 122.72 | 118.94 |
| 11 | A | 101 | UQ8 | C30-C29-C31 | 2.46 | 119.41 | 115.27 |
| 15 | H | 302 | CDL | CB4-OB6-CB5 | -2.46 | 111.74 | 117.79 |
| 13 | N | 101 | BCB | CAA-CBA-CGA | -2.46 | 106.07 | 113.25 |
| 20 | I | 102 | PGV | C02-O01-C1 | -2.46 | 111.74 | 117.79 |
| 9 | C | 401 | HEC | CBA-CAA-C2A | -2.46 | 108.47 | 112.60 |
| 13 | i | 101 | BCB | CMB-C2B-C1B | -2.45 | 124.70 | 128.46 |
| 11 | A | 101 | UQ8 | C36-C37-C38 | -2.45 | 103.83 | 111.88 |
| 13 | 3 | 101 | BCB | C4D-CHA-C1A | -2.45 | 118.27 | 121.25 |
| 13 | Q | 402 | BCB | CHB-C4A-NA | 2.45 | 127.90 | 124.51 |
| 21 | q | 102 | NS0 | C20-C21-C22 | 2.45 | 128.49 | 123.47 |
| 13 | 4 | 101 | BCB | CHD-C4C-C3C | -2.45 | 122.83 | 125.89 |
| 13 | l | 102 | BCB | C1D-CHD-C4C | -2.45 | 120.78 | 126.06 |
| 13 | 1 | 101 | BCB | CED-O2D-CGD | 2.44 | 121.47 | 115.94 |
| 13 | r | 101 | BCB | C4B-CHC-C1C | -2.44 | 125.28 | 130.12 |
| 13 | B | 202 | BCB | C1-C2-C3 | -2.44 | 121.82 | 126.04 |
| 13 | l | 102 | BCB | CHC-C1C-NC | -2.44 | 121.13 | 124.51 |
| 13 | b | 101 | BCB | C1D-CHD-C4C | -2.44 | 120.79 | 126.06 |
| 13 | E | 101 | BCB | C4-C3-C5 | 2.44 | 119.37 | 115.27 |
| 11 | M | 407 | UQ8 | C15-C14-C16 | 2.44 | 119.37 | 115.27 |
| 11 | L | 305 | UQ8 | C12-C13-C14 | -2.44 | 121.80 | 127.66 |
| 13 | W | 302 | BCB | CAA-CBA-CGA | -2.43 | 106.14 | 113.25 |
| 21 | l | 101 | NS0 | C20-C21-C22 | 2.43 | 128.45 | 123.47 |
| 21 | X | 101 | NS0 | C16-C17-C19 | 2.43 | 122.67 | 118.94 |
| 17 | M | 405 | MQ7 | C45-C43-C44 | 2.43 | 119.97 | 114.60 |
| 21 | D | 103 | NS0 | C16-C17-C19 | 2.43 | 122.67 | 118.94 |
| 13 | O | 102 | BCB | C4D-CHA-C1A | -2.42 | 118.30 | 121.25 |
| 11 | M | 407 | UQ8 | C8-C7-C6 | -2.42 | 105.51 | 112.05 |
| 13 | E | 101 | BCB | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 13 | T | 101 | BCB | C1D-CHD-C4C | -2.42 | 120.83 | 126.06 |
| 13 | 3 | 101 | BCB | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 13 | k | 102 | BCB | O2A-CGA-CBA | 2.42 | 119.50 | 111.91 |
| 13 | q | 101 | BCB | CHC-C1C-NC | -2.42 | 121.17 | 124.51 |
| 14 | L | 304 | BPB | CMA-C3A-C4A | -2.42 | 109.09 | 114.38 |
| 13 | B | 202 | BCB | C1D-CHD-C4C | -2.41 | 120.85 | 126.06 |
| 13 | U | 102 | BCB | CHD-C1D-ND | -2.41 | 122.24 | 124.45 |
| 13 | o | 102 | BCB | C1B-CHB-C4A | -2.41 | 125.34 | 130.12 |
| 13 | 0 | 102 | BCB | C1D-CHD-C4C | -2.41 | 120.86 | 126.06 |
| 13 | e | 101 | BCB | C1B-CHB-C4A | -2.41 | 125.35 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21 | 2 | 101 | NS0 | C25-C23-C22 | 2.41 | 122.63 | 118.94 |
| 13 | r | 101 | BCB | O2D-CGD-O1D | -2.41 | 119.14 | 123.84 |
| 13 | B | 202 | BCB | C4B-CHC-C1C | -2.40 | 125.36 | 130.12 |
| 13 | 4 | 101 | BCB | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 13 | L | 303 | BCB | C1D-CHD-C4C | -2.39 | 120.89 | 126.06 |
| 13 | h | 102 | BCB | O2A-CGA-CBA | 2.39 | 119.42 | 111.91 |
| 13 | E | 101 | BCB | CHD-C4C-C3C | -2.39 | 122.90 | 125.89 |
| 13 | 4 | 101 | BCB | O2D-CGD-O1D | -2.39 | 119.16 | 123.84 |
| 13 | A | 102 | BCB | O2A-CGA-CBA | 2.39 | 119.39 | 111.91 |
| 13 | 3 | 101 | BCB | CHC-C1C-NC | -2.38 | 121.22 | 124.51 |
| 13 | h | 102 | BCB | C1B-CHB-C4A | -2.38 | 125.41 | 130.12 |
| 13 | N | 101 | BCB | C1D-CHD-C4C | -2.38 | 120.93 | 126.06 |
| 13 | i | 101 | BCB | CHD-C1D-ND | -2.38 | 122.27 | 124.45 |
| 14 | M | 404 | BPB | CMA-C3A-C4A | -2.38 | 109.17 | 114.38 |
| 13 | M | 402 | BCB | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 13 | M | 403 | BCB | C2A-C1A-CHA | -2.37 | 119.72 | 123.86 |
| 21 | q | 102 | NS0 | C11-C12-C14 | 2.37 | 122.58 | 118.94 |
| 13 | X | 102 | BCB | C4B-CHC-C1C | -2.37 | 125.43 | 130.12 |
| 13 | E | 101 | BCB | O2D-CGD-O1D | -2.37 | 119.21 | 123.84 |
| 13 | L | 303 | BCB | O2A-CGA-CBA | 2.37 | 119.33 | 111.91 |
| 13 | Z | 101 | BCB | CHC-C1C-NC | -2.36 | 121.24 | 124.51 |
| 13 | i | 101 | BCB | C1-O2A-CGA | 2.36 | 122.64 | 116.44 |
| 13 | 3 | 101 | BCB | C1D-CHD-C4C | -2.36 | 120.97 | 126.06 |
| 13 | E | 101 | BCB | C4B-CHC-C1C | -2.36 | 125.44 | 130.12 |
| 13 | 9 | 101 | BCB | O2A-CGA-CBA | 2.36 | 119.31 | 111.91 |
| 13 | 4 | 101 | BCB | CHD-C1D-ND | -2.36 | 122.29 | 124.45 |
| 13 | W | 302 | BCB | C1B-CHB-C4A | -2.36 | 125.45 | 130.12 |
| 13 | X | 102 | BCB | C2A-C1A-CHA | -2.35 | 119.74 | 123.86 |
| 17 | M | 405 | MQ7 | C19-C18-C20 | 2.35 | 119.23 | 115.27 |
| 13 | D | 101 | BCB | C4D-CHA-C1A | -2.35 | 118.39 | 121.25 |
| 13 | i | 101 | BCB | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 13 | R | 102 | BCB | C1-C2-C3 | -2.35 | 121.98 | 126.04 |
| 13 | R | 102 | BCB | O2D-CGD-O1D | -2.34 | 119.25 | 123.84 |
| 21 | A | 103 | NS0 | C16-C17-C19 | 2.34 | 122.54 | 118.94 |
| 13 | r | 101 | BCB | C2A-C1A-CHA | -2.34 | 119.76 | 123.86 |
| 13 | J | 101 | BCB | C1D-CHD-C4C | -2.34 | 121.00 | 126.06 |
| 13 | c | 101 | BCB | CHD-C1D-ND | -2.34 | 122.31 | 124.45 |
| 21 | l | 101 | NS0 | C11-C12-C14 | 2.34 | 122.53 | 118.94 |
| 20 | I | 102 | PGV | O03-C19-C20 | 2.34 | 119.24 | 111.91 |
| 21 | U | 101 | NS0 | C25-C23-C22 | 2.33 | 122.52 | 118.94 |
| 13 | D | 101 | BCB | O2D-CGD-O1D | -2.33 | 119.27 | 123.84 |
| 21 | O | 101 | NS0 | C11-C12-C14 | 2.33 | 122.52 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | f | 101 | BCB | CHD-C4C-C3C | -2.33 | 122.97 | 125.89 |
| 13 | X | 102 | BCB | C1D-CHD-C4C | -2.33 | 121.03 | 126.06 |
| 13 | 0 | 102 | BCB | C4B-CHC-C1C | -2.33 | 125.50 | 130.12 |
| 13 | q | 101 | BCB | C1D-CHD-C4C | -2.33 | 121.03 | 126.06 |
| 13 | 7 | 102 | BCB | O2D-CGD-O1D | -2.33 | 119.29 | 123.84 |
| 18 | M | 406 | NS5 | C16-C15-C17 | -2.33 | 119.67 | 122.92 |
| 17 | M | 405 | MQ7 | C2M-C2-C3 | -2.33 | 120.61 | 124.40 |
| 13 | 3 | 101 | BCB | CHB-C4A-NA | 2.32 | 127.73 | 124.51 |
| 13 | 1 | 101 | BCB | C2A-C1A-CHA | -2.32 | 119.80 | 123.86 |
| 13 | 3 | 101 | BCB | C3D-C4D-ND | 2.32 | 113.99 | 110.24 |
| 15 | M | 409 | CDL | CA4-OA6-CA5 | -2.32 | 112.08 | 117.79 |
| 13 | L | 303 | BCB | CMD-C2D-C3D | -2.32 | 122.27 | 127.61 |
| 15 | H | 301 | CDL | OB8-CB7-C71 | 2.32 | 119.19 | 111.91 |
| 13 | Q | 402 | BCB | C1B-CHB-C4A | -2.32 | 125.53 | 130.12 |
| 13 | W | 302 | BCB | C3D-C4D-ND | 2.32 | 113.98 | 110.24 |
| 13 | o | 102 | BCB | C2A-C1A-CHA | -2.32 | 119.81 | 123.86 |
| 21 | U | 101 | NS0 | C11-C12-C14 | 2.31 | 122.49 | 118.94 |
| 13 | Q | 402 | BCB | CAA-CBA-CGA | -2.31 | 106.50 | 113.25 |
| 13 | J | 101 | BCB | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 13 | f | 101 | BCB | C2A-C1A-CHA | -2.31 | 119.82 | 123.86 |
| 13 | L | 302 | BCB | C4B-CHC-C1C | -2.31 | 125.55 | 130.12 |
| 13 | B | 202 | BCB | C1B-CHB-C4A | -2.31 | 125.55 | 130.12 |
| 21 | l | 101 | NS0 | C16-C17-C19 | 2.31 | 122.48 | 118.94 |
| 13 | M | 403 | BCB | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 13 | Z | 101 | BCB | C1D-CHD-C4C | -2.30 | 121.11 | 126.06 |
| 13 | k | 102 | BCB | CED-O2D-CGD | 2.30 | 121.13 | 115.94 |
| 13 | R | 102 | BCB | C1B-CHB-C4A | -2.29 | 125.57 | 130.12 |
| 13 | E | 101 | BCB | C1D-CHD-C4C | -2.29 | 121.11 | 126.06 |
| 13 | M | 403 | BCB | CED-O2D-CGD | 2.29 | 121.12 | 115.94 |
| 11 | A | 101 | UQ8 | C1M-C1-C6 | -2.29 | 120.66 | 124.40 |
| 17 | M | 405 | MQ7 | C24-C23-C25 | 2.29 | 119.13 | 115.27 |
| 13 | Q | 402 | BCB | CHC-C1C-NC | -2.29 | 121.35 | 124.51 |
| 13 | n | 101 | BCB | C3D-C4D-ND | 2.29 | 113.94 | 110.24 |
| 13 | 9 | 101 | BCB | C1B-CHB-C4A | -2.28 | 125.59 | 130.12 |
| 13 | 6 | 101 | BCB | C3D-C4D-ND | 2.28 | 113.93 | 110.24 |
| 13 | 6 | 101 | BCB | C1D-CHD-C4C | -2.28 | 121.14 | 126.06 |
| 13 | X | 102 | BCB | C4-C3-C5 | 2.28 | 119.10 | 115.27 |
| 13 | i | 101 | BCB | C1-C2-C3 | -2.27 | 122.11 | 126.04 |
| 13 | k | 102 | BCB | CAA-CBA-CGA | -2.27 | 106.61 | 113.25 |
| 9 | C | 403 | HEC | O2D-CGD-CBD | 2.27 | 121.33 | 114.03 |
| 11 | M | 408 | UQ8 | C46-C44-C45 | 2.27 | 119.61 | 114.60 |
| 13 | 3 | 101 | BCB | C2A-C1A-CHA | -2.27 | 119.89 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | J | 101 | BCB | C2A-C1A-CHA | -2.27 | 119.89 | 123.86 |
| 13 | U | 102 | BCB | CED-O2D-CGD | 2.27 | 121.06 | 115.94 |
| 21 | R | 101 | NS0 | C11-C12-C14 | 2.27 | 122.42 | 118.94 |
| 21 | l | 101 | NS0 | C25-C23-C22 | 2.26 | 122.41 | 118.94 |
| 13 | 7 | 102 | BCB | C2A-C1A-CHA | -2.26 | 119.91 | 123.86 |
| 13 | 7 | 102 | BCB | C4B-CHC-C1C | -2.26 | 125.64 | 130.12 |
| 13 | I | 101 | BCB | C3D-C4D-ND | 2.26 | 113.89 | 110.24 |
| 13 | 0 | 102 | BCB | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 13 | O | 102 | BCB | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 13 | Z | 101 | BCB | C4-C3-C5 | 2.25 | 119.06 | 115.27 |
| 13 | n | 101 | BCB | C4-C3-C5 | 2.25 | 119.06 | 115.27 |
| 9 | C | 402 | HEC | CMC-C2C-C1C | -2.25 | 125.00 | 128.46 |
| 9 | C | 403 | HEC | CMC-C2C-C1C | -2.25 | 125.01 | 128.46 |
| 11 | L | 305 | UQ8 | C20-C19-C21 | 2.25 | 119.05 | 115.27 |
| 13 | T | 101 | BCB | C4D-CHA-C1A | -2.25 | 118.52 | 121.25 |
| 21 | A | 103 | NS0 | C15-C14-C12 | 2.25 | 130.51 | 127.31 |
| 13 | k | 102 | BCB | CHB-C4A-NA | 2.25 | 127.62 | 124.51 |
| 13 | M | 402 | BCB | O2D-CGD-O1D | -2.24 | 119.45 | 123.84 |
| 13 | 4 | 101 | BCB | C4B-CHC-C1C | -2.24 | 125.67 | 130.12 |
| 13 | h | 102 | BCB | C1D-CHD-C4C | -2.24 | 121.22 | 126.06 |
| 13 | Q | 402 | BCB | C3D-C4D-ND | 2.24 | 113.86 | 110.24 |
| 13 | f | 101 | BCB | C4B-CHC-C1C | -2.24 | 125.68 | 130.12 |
| 13 | T | 101 | BCB | CHB-C4A-NA | 2.24 | 127.61 | 124.51 |
| 13 | U | 102 | BCB | C1-C2-C3 | -2.24 | 122.17 | 126.04 |
| 13 | e | 101 | BCB | C3D-C4D-ND | 2.24 | 113.86 | 110.24 |
| 13 | b | 101 | BCB | C4A-NA-C1A | 2.24 | 107.71 | 106.71 |
| 13 | e | 101 | BCB | C4B-CHC-C1C | -2.24 | 125.69 | 130.12 |
| 17 | M | 405 | MQ7 | C31-C32-C33 | -2.24 | 122.27 | 127.66 |
| 13 | L | 302 | BCB | O2A-CGA-O1A | -2.24 | 117.95 | 123.59 |
| 13 | e | 101 | BCB | CAA-CBA-CGA | -2.23 | 106.72 | 113.25 |
| 21 | 2 | 101 | NS0 | C11-C12-C14 | 2.23 | 122.37 | 118.94 |
| 13 | o | 102 | BCB | O2D-CGD-O1D | -2.23 | 119.47 | 123.84 |
| 11 | A | 101 | UQ8 | C7-C6-C5 | 2.23 | 121.16 | 118.48 |
| 13 | r | 101 | BCB | CHC-C1C-NC | -2.23 | 121.43 | 124.51 |
| 21 | W | 303 | NS0 | C16-C17-C19 | 2.23 | 122.36 | 118.94 |
| 13 | M | 403 | BCB | C4-C3-C5 | 2.23 | 119.02 | 115.27 |
| 11 | M | 408 | UQ8 | C1M-C1-C6 | -2.23 | 120.77 | 124.40 |
| 13 | l | 102 | BCB | C2A-C1A-CHA | -2.23 | 119.97 | 123.86 |
| 13 | M | 402 | BCB | O1D-CGD-CBD | -2.23 | 119.93 | 124.48 |
| 13 | i | 101 | BCB | CHC-C1C-NC | -2.22 | 121.44 | 124.51 |
| 21 | 9 | 102 | NS0 | C16-C17-C19 | 2.22 | 122.35 | 118.94 |
| 15 | M | 409 | CDL | OB6-CB5-OB7 | -2.22 | 118.33 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | c | 101 | BCB | C4B-CHC-C1C | -2.22 | 125.72 | 130.12 |
| 13 | c | 101 | BCB | C2A-C1A-CHA | -2.22 | 119.97 | 123.86 |
| 21 | U | 101 | NS0 | C16-C17-C19 | 2.22 | 122.35 | 118.94 |
| 13 | M | 402 | BCB | C4B-CHC-C1C | -2.22 | 125.72 | 130.12 |
| 13 | W | 302 | BCB | C1D-CHD-C4C | -2.22 | 121.27 | 126.06 |
| 9 | C | 401 | HEC | O2D-CGD-CBD | 2.22 | 121.15 | 114.03 |
| 17 | M | 405 | MQ7 | C14-C13-C15 | 2.21 | 119.00 | 115.27 |
| 13 | e | 101 | BCB | CED-O2D-CGD | 2.21 | 120.95 | 115.94 |
| 13 | M | 402 | BCB | C4D-CHA-C1A | -2.21 | 118.55 | 121.25 |
| 13 | b | 101 | BCB | CAA-CBA-CGA | -2.21 | 106.78 | 113.25 |
| 13 | M | 402 | BCB | C1D-CHD-C4C | -2.21 | 121.29 | 126.06 |
| 13 | Z | 101 | BCB | C3D-C4D-ND | 2.21 | 113.81 | 110.24 |
| 11 | M | 407 | UQ8 | C7-C8-C9 | -2.21 | 123.12 | 126.79 |
| 13 | T | 101 | BCB | CAA-CBA-CGA | -2.20 | 106.82 | 113.25 |
| 13 | M | 403 | BCB | C1-O2A-CGA | 2.20 | 122.21 | 116.44 |
| 13 | h | 102 | BCB | C2A-C1A-CHA | -2.20 | 120.02 | 123.86 |
| 13 | E | 101 | BCB | O2A-CGA-O1A | -2.19 | 118.06 | 123.59 |
| 21 | 9 | 102 | NS0 | C20-C21-C22 | 2.19 | 127.97 | 123.47 |
| 13 | k | 102 | BCB | C1D-CHD-C4C | -2.19 | 121.33 | 126.06 |
| 13 | o | 102 | BCB | C4B-CHC-C1C | -2.19 | 125.77 | 130.12 |
| 13 | T | 101 | BCB | C3D-C4D-ND | 2.19 | 113.78 | 110.24 |
| 11 | M | 408 | UQ8 | C31-C32-C33 | -2.19 | 104.68 | 111.88 |
| 13 | b | 101 | BCB | C2A-C1A-CHA | -2.19 | 120.03 | 123.86 |
| 13 | 0 | 102 | BCB | O2A-CGA-O1A | -2.19 | 118.07 | 123.59 |
| 13 | b | 101 | BCB | C3D-C4D-ND | 2.19 | 113.78 | 110.24 |
| 13 | L | 303 | BCB | C4D-CHA-C1A | -2.19 | 118.59 | 121.25 |
| 12 | L | 301 | DGA | OG1-CA1-OA1 | -2.19 | 118.08 | 123.59 |
| 15 | H | 301 | CDL | CB4-OB6-CB5 | -2.19 | 112.41 | 117.79 |
| 13 | 7 | 102 | BCB | C4-C3-C5 | 2.18 | 118.93 | 115.27 |
| 9 | C | 402 | HEC | CAD-CBD-CGD | -2.17 | 107.66 | 113.76 |
| 13 | A | 102 | BCB | O2D-CGD-O1D | -2.17 | 119.59 | 123.84 |
| 13 | k | 102 | BCB | C3D-C4D-ND | 2.17 | 113.75 | 110.24 |
| 11 | M | 408 | UQ8 | C32-C33-C34 | -2.17 | 122.43 | 127.66 |
| 21 | h | 101 | NS0 | C16-C17-C19 | 2.17 | 122.28 | 118.94 |
| 13 | b | 101 | BCB | C16-C15-C13 | -2.17 | 108.90 | 115.92 |
| 13 | L | 302 | BCB | C4D-CHA-C1A | -2.17 | 118.61 | 121.25 |
| 19 | h | 103 | LMT | C1B-O1B-C4' | -2.17 | 112.60 | 117.96 |
| 13 | M | 403 | BCB | CHB-C4A-NA | 2.17 | 127.51 | 124.51 |
| 13 | 6 | 101 | BCB | C2A-C1A-CHA | -2.16 | 120.08 | 123.86 |
| 21 | X | 101 | NS0 | C25-C23-C22 | 2.16 | 122.25 | 118.94 |
| 13 | 4 | 101 | BCB | C1-C2-C3 | -2.16 | 122.31 | 126.04 |
| 13 | R | 102 | BCB | C4B-CHC-C1C | -2.16 | 125.84 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | n | 101 | BCB | C6-C5-C3 | -2.16 | 107.80 | 113.45 |
| 11 | A | 101 | UQ8 | C12-C13-C14 | -2.16 | 122.47 | 127.66 |
| 21 | 0 | 101 | NS0 | C20-C21-C22 | 2.16 | 127.89 | 123.47 |
| 13 | c | 101 | BCB | C1B-CHB-C4A | -2.15 | 125.85 | 130.12 |
| 13 | e | 101 | BCB | C4-C3-C5 | 2.15 | 118.89 | 115.27 |
| 21 | 9 | 102 | NS0 | C11-C12-C14 | 2.15 | 122.24 | 118.94 |
| 13 | i | 101 | BCB | C4B-C3B-CAB | -2.15 | 122.98 | 127.13 |
| 13 | U | 102 | BCB | O2D-CGD-O1D | -2.15 | 119.64 | 123.84 |
| 13 | h | 102 | BCB | C4B-CHC-C1C | -2.15 | 125.87 | 130.12 |
| 15 | H | 302 | CDL | OB8-CB7-C71 | 2.15 | 118.64 | 111.91 |
| 13 | O | 102 | BCB | C2A-C1A-CHA | -2.15 | 120.11 | 123.86 |
| 13 | f | 101 | BCB | O2D-CGD-O1D | -2.15 | 119.64 | 123.84 |
| 21 | 2 | 101 | NS0 | C16-C17-C19 | 2.14 | 122.23 | 118.94 |
| 13 | 1 | 101 | BCB | C4B-CHC-C1C | -2.14 | 125.87 | 130.12 |
| 18 | M | 406 | NS5 | C18-C17-C15 | 2.14 | 130.37 | 127.31 |
| 13 | I | 101 | BCB | CAA-CBA-CGA | -2.14 | 107.00 | 113.25 |
| 13 | n | 101 | BCB | C4B-CHC-C1C | -2.14 | 125.88 | 130.12 |
| 13 | X | 102 | BCB | O2D-CGD-O1D | -2.14 | 119.65 | 123.84 |
| 13 | c | 101 | BCB | C1-C2-C3 | -2.14 | 122.34 | 126.04 |
| 13 | c | 101 | BCB | O2D-CGD-O1D | -2.14 | 119.66 | 123.84 |
| 21 | W | 303 | NS0 | C25-C23-C22 | 2.14 | 122.22 | 118.94 |
| 13 | 9 | 101 | BCB | C11-C10-C8 | -2.14 | 109.01 | 115.92 |
| 13 | U | 102 | BCB | C4B-CHC-C1C | -2.14 | 125.88 | 130.12 |
| 21 | 0 | 101 | NS0 | C16-C17-C19 | 2.14 | 122.22 | 118.94 |
| 13 | Q | 402 | BCB | C4B-CHC-C1C | -2.14 | 125.88 | 130.12 |
| 21 | A | 103 | NS0 | C25-C23-C22 | 2.14 | 122.22 | 118.94 |
| 13 | B | 202 | BCB | CHC-C1C-NC | -2.13 | 121.56 | 124.51 |
| 13 | W | 302 | BCB | CHC-C1C-NC | -2.13 | 121.56 | 124.51 |
| 13 | D | 101 | BCB | C4B-C3B-CAB | -2.13 | 123.01 | 127.13 |
| 20 | W | 301 | PGV | O01-C1-O02 | -2.13 | 118.55 | 123.70 |
| 13 | e | 101 | BCB | C6-C5-C3 | -2.13 | 107.86 | 113.45 |
| 13 | b | 101 | BCB | CHC-C1C-NC | -2.13 | 121.57 | 124.51 |
| 13 | B | 202 | BCB | O2A-CGA-O1A | -2.13 | 118.22 | 123.59 |
| 13 | N | 101 | BCB | CHB-C4A-NA | 2.13 | 127.46 | 124.51 |
| 13 | N | 101 | BCB | C6-C5-C3 | -2.13 | 107.88 | 113.45 |
| 13 | X | 102 | BCB | CED-O2D-CGD | 2.12 | 120.73 | 115.94 |
| 11 | A | 101 | UQ8 | C46-C44-C45 | 2.12 | 119.28 | 114.60 |
| 13 | J | 101 | BCB | C4B-CHC-C1C | -2.12 | 125.92 | 130.12 |
| 13 | 4 | 101 | BCB | C2A-C1A-CHA | -2.12 | 120.16 | 123.86 |
| 13 | A | 102 | BCB | CHC-C1C-NC | -2.11 | 121.59 | 124.51 |
| 13 | 1 | 101 | BCB | CHC-C1C-NC | -2.11 | 121.59 | 124.51 |
| 13 | R | 102 | BCB | CED-O2D-CGD | 2.11 | 120.71 | 115.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21 | X | 101 | NS0 | C20-C21-C22 | 2.11 | 127.80 | 123.47 |
| 13 | f | 101 | BCB | C1-C2-C3 | -2.10 | 122.41 | 126.04 |
| 15 | L | 306 | CDL | OA8-CA7-OA9 | -2.10 | 118.29 | 123.59 |
| 13 | k | 102 | BCB | C4B-CHC-C1C | -2.10 | 125.96 | 130.12 |
| 21 | O | 101 | NS0 | C20-C21-C22 | 2.10 | 127.77 | 123.47 |
| 13 | D | 101 | BCB | C4-C3-C5 | 2.09 | 118.79 | 115.27 |
| 13 | T | 101 | BCB | CHC-C1C-NC | -2.09 | 121.62 | 124.51 |
| 21 | 9 | 102 | NS0 | C25-C23-C22 | 2.09 | 122.14 | 118.94 |
| 13 | E | 101 | BCB | C2A-C1A-CHA | -2.09 | 120.21 | 123.86 |
| 13 | 9 | 101 | BCB | CED-O2D-CGD | 2.09 | 120.65 | 115.94 |
| 13 | L | 303 | BCB | C1-O2A-CGA | 2.08 | 121.91 | 116.44 |
| 13 | 3 | 101 | BCB | C11-C10-C8 | -2.08 | 109.19 | 115.92 |
| 13 | A | 102 | BCB | C4-C3-C5 | 2.08 | 118.77 | 115.27 |
| 21 | 7 | 101 | NS0 | C25-C23-C22 | 2.08 | 122.14 | 118.94 |
| 13 | l | 102 | BCB | O2D-CGD-O1D | -2.08 | 119.77 | 123.84 |
| 11 | M | 408 | UQ8 | C22-C23-C24 | -2.08 | 122.65 | 127.66 |
| 11 | A | 101 | UQ8 | C26-C27-C28 | -2.08 | 105.04 | 111.88 |
| 13 | J | 101 | BCB | CED-O2D-CGD | 2.08 | 120.64 | 115.94 |
| 13 | h | 102 | BCB | CED-O2D-CGD | 2.08 | 120.63 | 115.94 |
| 15 | r | 102 | CDL | OB6-CB5-OB7 | -2.08 | 118.69 | 123.70 |
| 13 | L | 302 | BCB | C4B-C3B-CAB | -2.07 | 123.12 | 127.13 |
| 13 | h | 102 | BCB | CHC-C1C-NC | -2.07 | 121.65 | 124.51 |
| 15 | M | 409 | CDL | OA6-CA5-OA7 | -2.07 | 118.70 | 123.70 |
| 13 | 7 | 102 | BCB | O2A-CGA-O1A | -2.07 | 118.37 | 123.59 |
| 13 | I | 101 | BCB | O2D-CGD-O1D | -2.07 | 119.80 | 123.84 |
| 13 | 9 | 101 | BCB | C1D-CHD-C4C | -2.07 | 121.60 | 126.06 |
| 21 | o | 101 | NS0 | C15-C14-C12 | 2.07 | 130.26 | 127.31 |
| 13 | 6 | 101 | BCB | CED-O2D-CGD | 2.06 | 120.61 | 115.94 |
| 20 | M | 411 | PGV | O03-C19-O04 | -2.06 | 118.39 | 123.59 |
| 13 | A | 102 | BCB | CBA-CAA-C2A | -2.06 | 107.78 | 113.86 |
| 21 | o | 101 | NS0 | C16-C17-C19 | 2.06 | 122.10 | 118.94 |
| 13 | l | 102 | BCB | C4B-CHC-C1C | -2.06 | 126.04 | 130.12 |
| 17 | M | 405 | MQ7 | C16-C17-C18 | -2.06 | 122.70 | 127.66 |
| 13 | n | 101 | BCB | C1D-CHD-C4C | -2.06 | 121.62 | 126.06 |
| 13 | 3 | 101 | BCB | C4B-C3B-CAB | -2.06 | 123.16 | 127.13 |
| 13 | 3 | 101 | BCB | CED-O2D-CGD | 2.06 | 120.59 | 115.94 |
| 11 | M | 408 | UQ8 | C37-C38-C39 | -2.06 | 122.71 | 127.66 |
| 13 | e | 101 | BCB | C1D-CHD-C4C | -2.06 | 121.62 | 126.06 |
| 13 | 6 | 101 | BCB | C4A-NA-C1A | 2.05 | 107.63 | 106.71 |
| 13 | Q | 402 | BCB | C4B-C3B-CAB | -2.05 | 123.17 | 127.13 |
| 21 | 2 | 101 | NS0 | C20-C21-C22 | 2.05 | 127.67 | 123.47 |
| 13 | O | 102 | BCB | C4B-CHC-C1C | -2.05 | 126.06 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | W | 302 | BCB | C2A-C1A-CHA | -2.04 | 120.28 | 123.86 |
| 13 | 1 | 101 | BCB | C4B-C3B-CAB | -2.04 | 123.18 | 127.13 |
| 13 | 7 | 102 | BCB | CED-O2D-CGD | 2.04 | 120.56 | 115.94 |
| 13 | D | 101 | BCB | CHC-C1C-NC | -2.04 | 121.69 | 124.51 |
| 21 | W | 303 | NS0 | C11-C12-C14 | 2.04 | 122.07 | 118.94 |
| 13 | 9 | 101 | BCB | CMD-C2D-C3D | -2.04 | 122.92 | 127.61 |
| 13 | i | 101 | BCB | C4B-CHC-C1C | -2.04 | 126.08 | 130.12 |
| 9 | C | 402 | HEC | CMB-C2B-C1B | -2.04 | 125.33 | 128.46 |
| 13 | f | 101 | BCB | CED-O2D-CGD | 2.03 | 120.54 | 115.94 |
| 13 | J | 101 | BCB | CHC-C1C-NC | -2.03 | 121.70 | 124.51 |
| 13 | Z | 101 | BCB | CED-O2D-CGD | 2.03 | 120.54 | 115.94 |
| 15 | r | 102 | CDL | OB8-CB7-C71 | 2.03 | 118.28 | 111.91 |
| 21 | o | 101 | NS0 | C11-C12-C14 | 2.03 | 122.06 | 118.94 |
| 13 | q | 101 | BCB | CED-O2D-CGD | 2.03 | 120.53 | 115.94 |
| 13 | 3 | 101 | BCB | C4-C3-C5 | 2.03 | 118.68 | 115.27 |
| 13 | X | 102 | BCB | C6-C5-C3 | -2.03 | 108.14 | 113.45 |
| 13 | n | 101 | BCB | C2A-C1A-CHA | -2.02 | 120.32 | 123.86 |
| 21 | h | 101 | NS0 | C25-C23-C22 | 2.02 | 122.04 | 118.94 |
| 21 | D | 103 | NS0 | C25-C23-C22 | 2.02 | 122.04 | 118.94 |
| 13 | U | 102 | BCB | CAA-CBA-CGA | -2.02 | 107.35 | 113.25 |
| 13 | i | 101 | BCB | C16-C15-C13 | -2.02 | 109.39 | 115.92 |
| 11 | M | 408 | UQ8 | C40-C39-C41 | 2.02 | 118.67 | 115.27 |
| 13 | N | 101 | BCB | C3D-C4D-ND | 2.02 | 113.50 | 110.24 |
| 13 | J | 101 | BCB | O2D-CGD-O1D | -2.02 | 119.89 | 123.84 |
| 13 | 9 | 101 | BCB | C4B-CHC-C1C | -2.01 | 126.13 | 130.12 |
| 15 | M | 409 | CDL | CB6-CB4-CB3 | -2.01 | 107.04 | 111.79 |
| 13 | U | 102 | BCB | CHC-C1C-NC | -2.01 | 121.73 | 124.51 |
| 13 | r | 101 | BCB | C4B-C3B-CAB | -2.01 | 123.25 | 127.13 |
| 15 | L | 306 | CDL | OB6-CB5-OB7 | -2.00 | 118.86 | 123.70 |
| 13 | f | 101 | BCB | CHC-C1C-NC | -2.00 | 121.74 | 124.51 |
| 13 | M | 402 | BCB | CMD-C2D-C3D | -2.00 | 123.01 | 127.61 |
| 13 | L | 303 | BCB | CHC-C1C-NC | -2.00 | 121.75 | 124.51 |

All (76) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 13 | L | 302 | BCB | NA |
| 13 | L | 302 | BCB | NC |
| 13 | L | 303 | BCB | NA |
| 13 | L | 303 | BCB | NC |
| 13 | M | 402 | BCB | NA |
| 13 | M | 402 | BCB | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 13 | M | 403 | BCB | NA |
| 13 | M | 403 | BCB | NC |
| 13 | A | 102 | BCB | NA |
| 13 | A | 102 | BCB | NC |
| 13 | B | 202 | BCB | NA |
| 13 | B | 202 | BCB | NC |
| 13 | D | 101 | BCB | NA |
| 13 | D | 101 | BCB | NC |
| 13 | E | 101 | BCB | NA |
| 13 | E | 101 | BCB | NC |
| 13 | I | 101 | BCB | NA |
| 13 | I | 101 | BCB | NC |
| 13 | J | 101 | BCB | NA |
| 13 | J | 101 | BCB | NC |
| 13 | N | 101 | BCB | NA |
| 13 | N | 101 | BCB | NC |
| 13 | O | 102 | BCB | NA |
| 13 | O | 102 | BCB | NC |
| 13 | Q | 402 | BCB | NA |
| 13 | Q | 402 | BCB | NC |
| 13 | R | 102 | BCB | NA |
| 13 | R | 102 | BCB | NC |
| 13 | T | 101 | BCB | NA |
| 13 | T | 101 | BCB | NC |
| 13 | U | 102 | BCB | NA |
| 13 | U | 102 | BCB | NC |
| 13 | W | 302 | BCB | NA |
| 13 | W | 302 | BCB | NC |
| 13 | X | 102 | BCB | NA |
| 13 | X | 102 | BCB | NC |
| 13 | Z | 101 | BCB | NA |
| 13 | Z | 101 | BCB | NC |
| 13 | 1 | 101 | BCB | NA |
| 13 | 1 | 101 | BCB | NC |
| 13 | 3 | 101 | BCB | NA |
| 13 | 3 | 101 | BCB | NC |
| 13 | 4 | 101 | BCB | NA |
| 13 | 4 | 101 | BCB | NC |
| 13 | 6 | 101 | BCB | NA |
| 13 | 6 | 101 | BCB | NC |
| 13 | 7 | 102 | BCB | NA |
| 13 | 7 | 102 | BCB | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 13 | 9 | 101 | BCB | NA |
| 13 | 9 | 101 | BCB | NC |
| 13 | 0 | 102 | BCB | NA |
| 13 | 0 | 102 | BCB | NC |
| 13 | b | 101 | BCB | NA |
| 13 | b | 101 | BCB | NC |
| 13 | c | 101 | BCB | NA |
| 13 | c | 101 | BCB | NC |
| 13 | e | 101 | BCB | NA |
| 13 | e | 101 | BCB | NC |
| 13 | f | 101 | BCB | NA |
| 13 | f | 101 | BCB | NC |
| 13 | h | 102 | BCB | NA |
| 13 | h | 102 | BCB | NC |
| 13 | i | 101 | BCB | NA |
| 13 | i | 101 | BCB | NC |
| 13 | k | 102 | BCB | NA |
| 13 | k | 102 | BCB | NC |
| 13 | l | 102 | BCB | NA |
| 13 | l | 102 | BCB | NC |
| 13 | n | 101 | BCB | NA |
| 13 | n | 101 | BCB | NC |
| 13 | o | 102 | BCB | NA |
| 13 | o | 102 | BCB | NC |
| 13 | q | 101 | BCB | NA |
| 13 | q | 101 | BCB | NC |
| 13 | r | 101 | BCB | NA |
| 13 | r | 101 | BCB | NC |

All (884) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 9 | C | 402 | HEC | C3D-CAD-CBD-CGD |
| 11 | M | 408 | UQ8 | C29-C31-C32-C33 |
| 11 | M | 408 | UQ8 | C6-C7-C8-C9 |
| 11 | A | 101 | UQ8 | C34-C36-C37-C38 |
| 11 | A | 101 | UQ8 | C25-C24-C26-C27 |
| 11 | A | 101 | UQ8 | C23-C24-C26-C27 |
| 12 | L | 301 | DGA | CB2-CB1-OG2-CG2 |
| 13 | M | 403 | BCB | CAD-CBD-CGD-O1D |
| 13 | M | 403 | BCB | CAD-CBD-CGD-O2D |
| 13 | E | 101 | BCB | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | J | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | J | 101 | BCB | CHA-CBD-CGD-O2D |
| 13 | O | 102 | BCB | CHA-CBD-CGD-O1D |
| 13 | O | 102 | BCB | CHA-CBD-CGD-O2D |
| 13 | Q | 402 | BCB | CBD-CGD-O2D-CED |
| 13 | Q | 402 | BCB | C14-C13-C15-C16 |
| 13 | R | 102 | BCB | CHA-CBD-CGD-O1D |
| 13 | R | 102 | BCB | CHA-CBD-CGD-O2D |
| 13 | W | 302 | BCB | CBD-CGD-O2D-CED |
| 13 | X | 102 | BCB | CHA-CBD-CGD-O1D |
| 13 | X | 102 | BCB | CHA-CBD-CGD-O2D |
| 13 | Z | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | 1 | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | 1 | 101 | BCB | CHA-CBD-CGD-O2D |
| 13 | 3 | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | 4 | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | 4 | 101 | BCB | CHA-CBD-CGD-O2D |
| 13 | 7 | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | 7 | 102 | BCB | CHA-CBD-CGD-O1D |
| 13 | 7 | 102 | BCB | CHA-CBD-CGD-O2D |
| 13 | b | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | b | 101 | BCB | C2-C3-C5-C6 |
| 13 | b | 101 | BCB | C4-C3-C5-C6 |
| 13 | c | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | c | 101 | BCB | CHA-CBD-CGD-O2D |
| 13 | f | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | f | 101 | BCB | CHA-CBD-CGD-O2D |
| 13 | h | 102 | BCB | CBD-CGD-O2D-CED |
| 13 | i | 101 | BCB | CBA-CGA-O2A-C1 |
| 13 | i | 101 | BCB | O1A-CGA-O2A-C1 |
| 13 | i | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | i | 101 | BCB | C11-C12-C13-C14 |
| 13 | k | 102 | BCB | CBD-CGD-O2D-CED |
| 13 | o | 102 | BCB | CHA-CBD-CGD-O1D |
| 13 | o | 102 | BCB | CHA-CBD-CGD-O2D |
| 13 | q | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | q | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | r | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | r | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | r | 101 | BCB | CHA-CBD-CGD-O2D |
| 14 | L | 304 | BPB | O2A-C1-C2-C3 |
| 15 | L | 306 | CDL | O1-C1-CB2-OB2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 15 | H | 301 | CDL | CA2-OA2-PA1-OA3 |
| 15 | H | 301 | CDL | CB2-OB2-PB2-OB3 |
| 15 | H | 301 | CDL | CB2-OB2-PB2-OB4 |
| 15 | H | 301 | CDL | CB2-OB2-PB2-OB5 |
| 15 | H | 301 | CDL | CB3-OB5-PB2-OB2 |
| 15 | H | 301 | CDL | CB3-OB5-PB2-OB3 |
| 15 | H | 301 | CDL | CB3-OB5-PB2-OB4 |
| 15 | H | 302 | CDL | CA2-OA2-PA1-OA4 |
| 15 | H | 302 | CDL | CB2-OB2-PB2-OB3 |
| 15 | H | 302 | CDL | CB2-OB2-PB2-OB4 |
| 15 | H | 302 | CDL | CB3-OB5-PB2-OB4 |
| 15 | r | 102 | CDL | CA3-OA5-PA1-OA4 |
| 15 | r | 102 | CDL | CB2-OB2-PB2-OB4 |
| 15 | r | 102 | CDL | CB3-OB5-PB2-OB2 |
| 15 | r | 102 | CDL | OB5-CB3-CB4-OB6 |
| 15 | r | 102 | CDL | OB7-CB5-OB6-CB4 |
| 15 | r | 102 | CDL | C51-CB5-OB6-CB4 |
| 19 | b | 102 | LMT | O5'-C1'-O1'-C1 |
| 19 | b | 102 | LMT | C2-C1-O1'-C1' |
| 19 | k | 103 | LMT | O5'-C1'-O1'-C1 |
| 20 | M | 411 | PGV | C03-O11-P-O14 |
| 20 | M | 411 | PGV | C04-O12-P-O11 |
| 20 | M | 411 | PGV | C04-O12-P-O13 |
| 20 | M | 411 | PGV | C04-O12-P-O14 |
| 20 | I | 102 | PGV | C04-O12-P-O11 |
| 20 | I | 102 | PGV | C04-O12-P-O13 |
| 20 | I | 102 | PGV | C04-O12-P-O14 |
| 20 | Q | 401 | PGV | C04-O12-P-O13 |
| 20 | W | 301 | PGV | C03-O11-P-O12 |
| 20 | W | 301 | PGV | C04-O12-P-O14 |
| 21 | R | 101 | NS0 | C29-C28-C30-C31 |
| 21 | R | 101 | NS0 | C27-C28-C30-C31 |
| 13 | A | 102 | BCB | CBD-CGD-O2D-CED |
| 13 | T | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | 6 | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | 9 | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | e | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | n | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | q | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | Z | 101 | BCB | O1D-CGD-O2D-CED |
| 13 | Q | 402 | BCB | O1D-CGD-O2D-CED |
| 13 | 3 | 101 | BCB | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | h | 102 | BCB | O1D-CGD-O2D-CED |
| 13 | D | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | I | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | N | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | W | 302 | BCB | O1D-CGD-O2D-CED |
| 13 | k | 102 | BCB | O1D-CGD-O2D-CED |
| 12 | L | 301 | DGA | OB1-CB1-OG2-CG2 |
| 15 | H | 302 | CDL | OA7-CA5-OA6-CA4 |
| 13 | A | 102 | BCB | C3-C5-C6-C7 |
| 13 | q | 101 | BCB | C3-C5-C6-C7 |
| 15 | H | 302 | CDL | C11-CA5-OA6-CA4 |
| 13 | b | 101 | BCB | O1D-CGD-O2D-CED |
| 13 | J | 101 | BCB | CBD-CGD-O2D-CED |
| 13 | o | 102 | BCB | CBD-CGD-O2D-CED |
| 19 | n | 102 | LMT | O5B-C5B-C6B-O6B |
| 13 | M | 403 | BCB | C2A-CAA-CBA-CGA |
| 13 | T | 101 | BCB | O1D-CGD-O2D-CED |
| 13 | 6 | 101 | BCB | O1D-CGD-O2D-CED |
| 13 | 9 | 101 | BCB | O1D-CGD-O2D-CED |
| 12 | L | 301 | DGA | OA1-CA1-OG1-CG1 |
| 19 | b | 103 | LMT | O5'-C5'-C6'-O6' |
| 13 | e | 101 | BCB | O1D-CGD-O2D-CED |
| 15 | M | 409 | CDL | O1-C1-CA2-OA2 |
| 15 | M | 409 | CDL | O1-C1-CB2-OB2 |
| 15 | H | 302 | CDL | O1-C1-CB2-OB2 |
| 15 | r | 102 | CDL | O1-C1-CB2-OB2 |
| 13 | i | 101 | BCB | C3-C5-C6-C7 |
| 13 | r | 101 | BCB | C3-C5-C6-C7 |
| 20 | Q | 401 | PGV | C2-C1-O01-C02 |
| 13 | X | 102 | BCB | CBD-CGD-O2D-CED |
| 13 | r | 101 | BCB | CBD-CGD-O2D-CED |
| 19 | M | 410 | LMT | O5'-C5'-C6'-O6' |
| 13 | q | 101 | BCB | O1D-CGD-O2D-CED |
| 13 | q | 101 | BCB | C8-C10-C11-C12 |
| 12 | L | 301 | DGA | CA2-CA1-OG1-CG1 |
| 20 | Q | 401 | PGV | O02-C1-O01-C02 |
| 13 | L | 303 | BCB | C13-C15-C16-C17 |
| 13 | L | 302 | BCB | C4-C3-C5-C6 |
| 18 | M | 406 | NS5 | C11-C10-C9-C8 |
| 21 | q | 102 | NS0 | C29-C28-C30-C31 |
| 13 | L | 302 | BCB | C2-C3-C5-C6 |
| 18 | M | 406 | NS5 | C12-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | q | 102 | NS0 | C27-C28-C30-C31 |
| 19 | n | 102 | LMT | C4B-C5B-C6B-O6B |
| 11 | L | 305 | UQ8 | C14-C16-C17-C18 |
| 11 | M | 408 | UQ8 | C39-C41-C42-C43 |
| 11 | A | 101 | UQ8 | C19-C21-C22-C23 |
| 15 | r | 102 | CDL | C31-CA7-OA8-CA6 |
| 13 | A | 102 | BCB | O1D-CGD-O2D-CED |
| 13 | n | 101 | BCB | O1D-CGD-O2D-CED |
| 15 | r | 102 | CDL | OA9-CA7-OA8-CA6 |
| 15 | L | 306 | CDL | CA2-C1-CB2-OB2 |
| 15 | M | 409 | CDL | CA2-C1-CB2-OB2 |
| 15 | H | 302 | CDL | CA2-C1-CB2-OB2 |
| 20 | I | 102 | PGV | O12-C04-C05-C06 |
| 20 | D | 102 | PGV | C20-C19-O03-C01 |
| 13 | 6 | 101 | BCB | C15-C16-C17-C18 |
| 13 | I | 101 | BCB | O1D-CGD-O2D-CED |
| 13 | D | 101 | BCB | C15-C16-C17-C18 |
| 13 | E | 101 | BCB | C10-C11-C12-C13 |
| 15 | L | 306 | CDL | O1-C1-CA2-OA2 |
| 20 | I | 102 | PGV | O12-C04-C05-O05 |
| 20 | D | 102 | PGV | O04-C19-O03-C01 |
| 13 | A | 102 | BCB | C11-C12-C13-C14 |
| 13 | J | 101 | BCB | C6-C7-C8-C9 |
| 13 | O | 102 | BCB | C11-C12-C13-C14 |
| 13 | U | 102 | BCB | C14-C13-C15-C16 |
| 13 | X | 102 | BCB | C11-C12-C13-C14 |
| 13 | X | 102 | BCB | C14-C13-C15-C16 |
| 13 | 4 | 101 | BCB | C11-C10-C8-C9 |
| 13 | 7 | 102 | BCB | C11-C12-C13-C14 |
| 13 | 0 | 102 | BCB | C11-C12-C13-C14 |
| 13 | c | 101 | BCB | C11-C10-C8-C9 |
| 13 | e | 101 | BCB | C14-C13-C15-C16 |
| 13 | o | 102 | BCB | C6-C7-C8-C9 |
| 13 | o | 102 | BCB | C11-C12-C13-C14 |
| 13 | r | 101 | BCB | C11-C10-C8-C9 |
| 13 | N | 101 | BCB | O1D-CGD-O2D-CED |
| 13 | X | 102 | BCB | C13-C15-C16-C17 |
| 13 | n | 101 | BCB | C13-C15-C16-C17 |
| 21 | O | 101 | NS0 | C10-C11-C12-C13 |
| 15 | M | 409 | CDL | C11-CA5-OA6-CA4 |
| 20 | Q | 401 | PGV | C19-C20-C21-C22 |
| 13 | J | 101 | BCB | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 19 | b | 103 | LMT | C4'-C5'-C6'-O6' |
| 13 | A | 102 | BCB | C5-C6-C7-C8 |
| 13 | D | 101 | BCB | C13-C15-C16-C17 |
| 13 | I | 101 | BCB | C13-C15-C16-C17 |
| 13 | Q | 402 | BCB | C13-C15-C16-C17 |
| 13 | Q | 402 | BCB | C15-C16-C17-C18 |
| 13 | W | 302 | BCB | C10-C11-C12-C13 |
| 13 | Z | 101 | BCB | C8-C10-C11-C12 |
| 13 | 1 | 101 | BCB | C10-C11-C12-C13 |
| 13 | 3 | 101 | BCB | C10-C11-C12-C13 |
| 13 | r | 101 | BCB | C13-C15-C16-C17 |
| 19 | b | 102 | LMT | O5B-C5B-C6B-O6B |
| 15 | L | 306 | CDL | CA5-C11-C12-C13 |
| 13 | E | 101 | BCB | C8-C10-C11-C12 |
| 13 | T | 101 | BCB | C10-C11-C12-C13 |
| 13 | e | 101 | BCB | C5-C6-C7-C8 |
| 13 | r | 101 | BCB | C8-C10-C11-C12 |
| 15 | r | 102 | CDL | CA7-C31-C32-C33 |
| 13 | A | 102 | BCB | C15-C16-C17-C18 |
| 21 | 0 | 101 | NS0 | C33-C35-C36-C37 |
| 15 | r | 102 | CDL | C71-CB7-OB8-CB6 |
| 20 | W | 301 | PGV | C27-C28-C29-C30 |
| 13 | 9 | 101 | BCB | C2-C1-O2A-CGA |
| 13 | D | 101 | BCB | O1D-CGD-O2D-CED |
| 15 | r | 102 | CDL | C11-CA5-OA6-CA4 |
| 13 | k | 102 | BCB | C13-C15-C16-C17 |
| 13 | A | 102 | BCB | C12-C13-C15-C16 |
| 13 | 0 | 102 | BCB | C11-C12-C13-C15 |
| 13 | M | 402 | BCB | C15-C16-C17-C18 |
| 13 | R | 102 | BCB | C10-C11-C12-C13 |
| 13 | E | 101 | BCB | C13-C15-C16-C17 |
| 11 | M | 408 | UQ8 | C19-C21-C22-C23 |
| 11 | A | 101 | UQ8 | C14-C16-C17-C18 |
| 15 | H | 301 | CDL | CB5-C51-C52-C53 |
| 15 | H | 301 | CDL | O1-C1-CA2-OA2 |
| 15 | H | 302 | CDL | O1-C1-CA2-OA2 |
| 13 | W | 302 | BCB | C5-C6-C7-C8 |
| 13 | 1 | 101 | BCB | C8-C10-C11-C12 |
| 13 | r | 101 | BCB | C10-C11-C12-C13 |
| 19 | B | 201 | LMT | O1'-C1-C2-C3 |
| 13 | D | 101 | BCB | C8-C10-C11-C12 |
| 13 | R | 102 | BCB | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | X | 102 | BCB | C15-C16-C17-C18 |
| 13 | 4 | 101 | BCB | C10-C11-C12-C13 |
| 13 | 7 | 102 | BCB | C5-C6-C7-C8 |
| 13 | Z | 101 | BCB | C5-C6-C7-C8 |
| 13 | 1 | 101 | BCB | C15-C16-C17-C18 |
| 13 | 3 | 101 | BCB | C5-C6-C7-C8 |
| 13 | 9 | 101 | BCB | C10-C11-C12-C13 |
| 15 | M | 409 | CDL | CA2-OA2-PA1-OA5 |
| 15 | H | 301 | CDL | CA3-OA5-PA1-OA2 |
| 15 | H | 302 | CDL | CA2-OA2-PA1-OA5 |
| 15 | H | 302 | CDL | CA3-OA5-PA1-OA2 |
| 15 | H | 302 | CDL | CB2-OB2-PB2-OB5 |
| 15 | r | 102 | CDL | CB2-OB2-PB2-OB5 |
| 20 | M | 411 | PGV | C03-O11-P-O12 |
| 20 | D | 102 | PGV | C04-O12-P-O11 |
| 20 | I | 102 | PGV | C03-O11-P-O12 |
| 20 | N | 102 | PGV | C04-O12-P-O11 |
| 20 | W | 301 | PGV | C04-O12-P-O11 |
| 20 | M | 411 | PGV | C1-C2-C3-C4 |
| 13 | J | 101 | BCB | O1D-CGD-O2D-CED |
| 15 | M | 409 | CDL | CB2-C1-CA2-OA2 |
| 15 | H | 301 | CDL | CB2-C1-CA2-OA2 |
| 15 | H | 302 | CDL | CB2-C1-CA2-OA2 |
| 15 | M | 409 | CDL | OA7-CA5-OA6-CA4 |
| 15 | r | 102 | CDL | OA7-CA5-OA6-CA4 |
| 19 | M | 410 | LMT | C4'-C5'-C6'-O6' |
| 13 | A | 102 | BCB | CBA-CGA-O2A-C1 |
| 20 | W | 301 | PGV | C2-C1-O01-C02 |
| 15 | L | 306 | CDL | C79-C80-C81-C82 |
| 15 | M | 409 | CDL | C13-C14-C15-C16 |
| 15 | r | 102 | CDL | C53-C54-C55-C56 |
| 13 | o | 102 | BCB | O1D-CGD-O2D-CED |
| 13 | M | 402 | BCB | C16-C17-C18-C20 |
| 13 | c | 101 | BCB | C8-C10-C11-C12 |
| 15 | H | 301 | CDL | C13-C14-C15-C16 |
| 15 | H | 301 | CDL | C53-C54-C55-C56 |
| 15 | r | 102 | CDL | O1-C1-CA2-OA2 |
| 15 | H | 301 | CDL | C32-C33-C34-C35 |
| 13 | N | 101 | BCB | C16-C17-C18-C19 |
| 13 | 7 | 102 | BCB | C4-C3-C5-C6 |
| 21 | O | 101 | NS0 | C31-C32-C33-C34 |
| 13 | 7 | 102 | BCB | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | L | 303 | BCB | C14-C13-C15-C16 |
| 13 | M | 402 | BCB | C11-C10-C8-C9 |
| 13 | M | 402 | BCB | C14-C13-C15-C16 |
| 15 | H | 302 | CDL | CB5-C51-C52-C53 |
| 13 | X | 102 | BCB | C10-C11-C12-C13 |
| 15 | r | 102 | CDL | OB9-CB7-OB8-CB6 |
| 12 | L | 301 | DGA | CB2-CB3-CB4-CB5 |
| 15 | L | 306 | CDL | C11-C12-C13-C14 |
| 20 | N | 102 | PGV | C04-C05-C06-O06 |
| 20 | W | 301 | PGV | C04-C05-C06-O06 |
| 21 | O | 101 | NS0 | C10-C11-C12-C14 |
| 20 | W | 301 | PGV | O02-C1-O01-C02 |
| 13 | 7 | 102 | BCB | CBD-CGD-O2D-CED |
| 15 | H | 301 | CDL | C33-C34-C35-C36 |
| 19 | M | 410 | LMT | C3-C4-C5-C6 |
| 19 | b | 102 | LMT | C7-C8-C9-C10 |
| 20 | M | 411 | PGV | C3-C4-C5-C6 |
| 20 | M | 411 | PGV | C7-C8-C9-C10 |
| 13 | N | 101 | BCB | C16-C17-C18-C20 |
| 13 | O | 102 | BCB | C16-C17-C18-C19 |
| 13 | O | 102 | BCB | C16-C17-C18-C20 |
| 13 | 9 | 101 | BCB | C16-C17-C18-C20 |
| 13 | f | 101 | BCB | C16-C17-C18-C20 |
| 12 | L | 301 | DGA | CA2-CA3-CA4-CA5 |
| 20 | N | 102 | PGV | C6-C7-C8-C9 |
| 20 | Q | 401 | PGV | C6-C7-C8-C9 |
| 13 | i | 101 | BCB | C13-C15-C16-C17 |
| 13 | A | 102 | BCB | O1A-CGA-O2A-C1 |
| 20 | Q | 401 | PGV | C5-C6-C7-C8 |
| 13 | O | 102 | BCB | C3A-C2A-CAA-CBA |
| 13 | R | 102 | BCB | C3A-C2A-CAA-CBA |
| 13 | X | 102 | BCB | C3A-C2A-CAA-CBA |
| 13 | 7 | 102 | BCB | C3A-C2A-CAA-CBA |
| 13 | 9 | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | 0 | 102 | BCB | C3A-C2A-CAA-CBA |
| 13 | f | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | l | 102 | BCB | C3A-C2A-CAA-CBA |
| 13 | o | 102 | BCB | C3A-C2A-CAA-CBA |
| 13 | r | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | M | 402 | BCB | C16-C17-C18-C19 |
| 19 | B | 201 | LMT | C4-C5-C6-C7 |
| 15 | L | 306 | CDL | C51-CB5-OB6-CB4 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 15 | H | 301 | CDL | C51-CB5-OB6-CB4 |
| 19 | B | 201 | LMT | C1-C2-C3-C4 |
| 13 | W | 302 | BCB | C13-C15-C16-C17 |
| 13 | f | 101 | BCB | C16-C17-C18-C19 |
| 15 | M | 409 | CDL | OB7-CB5-OB6-CB4 |
| 13 | M | 403 | BCB | C2-C1-O2A-CGA |
| 15 | H | 302 | CDL | C59-C60-C61-C62 |
| 20 | W | 301 | PGV | C26-C27-C28-C29 |
| 15 | H | 301 | CDL | CA5-C11-C12-C13 |
| 13 | 9 | 101 | BCB | CBA-CGA-O2A-C1 |
| 13 | N | 101 | BCB | C13-C15-C16-C17 |
| 13 | k | 102 | BCB | C10-C11-C12-C13 |
| 19 | b | 102 | LMT | C1-C2-C3-C4 |
| 15 | M | 409 | CDL | C51-CB5-OB6-CB4 |
| 15 | M | 409 | CDL | C12-C13-C14-C15 |
| 19 | M | 410 | LMT | C4-C5-C6-C7 |
| 13 | o | 102 | BCB | C13-C15-C16-C17 |
| 13 | L | 303 | BCB | C12-C13-C15-C16 |
| 13 | M | 402 | BCB | C11-C10-C8-C7 |
| 13 | M | 402 | BCB | C12-C13-C15-C16 |
| 13 | J | 101 | BCB | C6-C7-C8-C10 |
| 13 | N | 101 | BCB | C11-C12-C13-C15 |
| 13 | X | 102 | BCB | C12-C13-C15-C16 |
| 13 | 4 | 101 | BCB | C11-C10-C8-C7 |
| 13 | 7 | 102 | BCB | C6-C7-C8-C10 |
| 13 | c | 101 | BCB | C6-C7-C8-C10 |
| 13 | i | 101 | BCB | C11-C12-C13-C15 |
| 13 | T | 101 | BCB | C3-C5-C6-C7 |
| 13 | 1 | 101 | BCB | C16-C17-C18-C19 |
| 15 | L | 306 | CDL | OA7-CA5-OA6-CA4 |
| 15 | L | 306 | CDL | OB7-CB5-OB6-CB4 |
| 15 | H | 301 | CDL | OA7-CA5-OA6-CA4 |
| 15 | H | 301 | CDL | OB7-CB5-OB6-CB4 |
| 20 | I | 102 | PGV | O02-C1-O01-C02 |
| 20 | D | 102 | PGV | C1-C2-C3-C4 |
| 20 | D | 102 | PGV | C28-C29-C30-C31 |
| 13 | X | 102 | BCB | O1D-CGD-O2D-CED |
| 13 | N | 101 | BCB | C5-C6-C7-C8 |
| 13 | 1 | 101 | BCB | C13-C15-C16-C17 |
| 13 | 3 | 101 | BCB | C15-C16-C17-C18 |
| 19 | n | 102 | LMT | C6-C7-C8-C9 |
| 13 | E | 101 | BCB | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | N | 101 | BCB | C3-C5-C6-C7 |
| 13 | U | 102 | BCB | C10-C11-C12-C13 |
| 15 | r | 102 | CDL | C33-C34-C35-C36 |
| 15 | L | 306 | CDL | C11-CA5-OA6-CA4 |
| 15 | H | 301 | CDL | C11-CA5-OA6-CA4 |
| 20 | I | 102 | PGV | C2-C1-O01-C02 |
| 19 | B | 201 | LMT | C2-C3-C4-C5 |
| 13 | J | 101 | BCB | C15-C16-C17-C18 |
| 15 | H | 301 | CDL | C51-C52-C53-C54 |
| 15 | H | 302 | CDL | C51-C52-C53-C54 |
| 20 | N | 102 | PGV | C5-C6-C7-C8 |
| 15 | M | 409 | CDL | OB6-CB4-CB6-OB8 |
| 15 | L | 306 | CDL | C32-C33-C34-C35 |
| 19 | b | 102 | LMT | C11-C10-C9-C8 |
| 19 | T | 102 | LMT | O5'-C5'-C6'-O6' |
| 13 | A | 102 | BCB | C14-C13-C15-C16 |
| 13 | I | 101 | BCB | C14-C13-C15-C16 |
| 13 | N | 101 | BCB | C11-C10-C8-C9 |
| 21 | W | 303 | NS0 | CA-CB-CG-CD1 |
| 15 | H | 302 | CDL | C35-C36-C37-C38 |
| 13 | 9 | 101 | BCB | O1A-CGA-O2A-C1 |
| 13 | O | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | 0 | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | o | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | 9 | 101 | BCB | C16-C17-C18-C19 |
| 13 | E | 101 | BCB | C15-C16-C17-C18 |
| 15 | H | 302 | CDL | CB3-OB5-PB2-OB2 |
| 19 | b | 103 | LMT | C1-C2-C3-C4 |
| 15 | L | 306 | CDL | OA5-CA3-CA4-CA6 |
| 15 | r | 102 | CDL | OB5-CB3-CB4-CB6 |
| 19 | M | 410 | LMT | C2-C3-C4-C5 |
| 13 | f | 101 | BCB | C15-C16-C17-C18 |
| 15 | r | 102 | CDL | CA2-C1-CB2-OB2 |
| 20 | W | 301 | PGV | C2-C3-C4-C5 |
| 20 | D | 102 | PGV | C20-C21-C22-C23 |
| 15 | M | 409 | CDL | CB3-CB4-CB6-OB8 |
| 15 | H | 302 | CDL | CA3-CA4-CA6-OA8 |
| 15 | H | 302 | CDL | CB3-CB4-CB6-OB8 |
| 15 | H | 302 | CDL | C58-C59-C60-C61 |
| 15 | r | 102 | CDL | C12-C13-C14-C15 |
| 13 | l | 102 | BCB | C8-C10-C11-C12 |
| 15 | H | 301 | CDL | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 15 | H | 302 | CDL | C53-C54-C55-C56 |
| 13 | c | 101 | BCB | C5-C6-C7-C8 |
| 15 | L | 306 | CDL | C41-C42-C43-C44 |
| 12 | L | 301 | DGA | CB3-CB4-CB5-CB6 |
| 20 | W | 301 | PGV | O05-C05-C06-O06 |
| 20 | W | 301 | PGV | C20-C21-C22-C23 |
| 19 | k | 103 | LMT | C5-C6-C7-C8 |
| 15 | H | 301 | CDL | C71-CB7-OB8-CB6 |
| 15 | M | 409 | CDL | C40-C41-C42-C43 |
| 13 | R | 102 | BCB | C13-C15-C16-C17 |
| 13 | U | 102 | BCB | C13-C15-C16-C17 |
| 13 | 3 | 101 | BCB | C13-C15-C16-C17 |
| 13 | r | 101 | BCB | O1D-CGD-O2D-CED |
| 12 | L | 301 | DGA | CA5-CA6-CA7-CA8 |
| 20 | M | 411 | PGV | C26-C27-C28-C29 |
| 13 | 7 | 102 | BCB | CBA-CGA-O2A-C1 |
| 15 | M | 409 | CDL | C31-CA7-OA8-CA6 |
| 21 | q | 102 | NS0 | C36-C37-C38-C39 |
| 13 | e | 101 | BCB | C13-C15-C16-C17 |
| 13 | f | 101 | BCB | C13-C15-C16-C17 |
| 13 | l | 102 | BCB | C13-C15-C16-C17 |
| 20 | Q | 401 | PGV | C15-C16-C17-C18 |
| 13 | n | 101 | BCB | C15-C16-C17-C18 |
| 13 | 1 | 101 | BCB | C16-C17-C18-C20 |
| 11 | M | 408 | UQ8 | C15-C14-C16-C17 |
| 21 | U | 101 | NS0 | C31-C32-C33-C34 |
| 11 | M | 408 | UQ8 | C13-C14-C16-C17 |
| 13 | E | 101 | BCB | C6-C7-C8-C10 |
| 13 | E | 101 | BCB | C12-C13-C15-C16 |
| 13 | I | 101 | BCB | C12-C13-C15-C16 |
| 13 | N | 101 | BCB | C11-C10-C8-C7 |
| 13 | N | 101 | BCB | C12-C13-C15-C16 |
| 13 | O | 102 | BCB | C11-C12-C13-C15 |
| 13 | O | 102 | BCB | C12-C13-C15-C16 |
| 13 | 3 | 101 | BCB | C11-C10-C8-C7 |
| 13 | 7 | 102 | BCB | C11-C12-C13-C15 |
| 13 | c | 101 | BCB | C11-C10-C8-C7 |
| 13 | i | 101 | BCB | C12-C13-C15-C16 |
| 13 | o | 102 | BCB | C6-C7-C8-C10 |
| 13 | r | 101 | BCB | C11-C10-C8-C7 |
| 14 | M | 404 | BPB | C11-C10-C8-C7 |
| 13 | N | 101 | BCB | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | O | 102 | BCB | C14-C13-C15-C16 |
| 13 | W | 302 | BCB | C14-C13-C15-C16 |
| 13 | 3 | 101 | BCB | C11-C10-C8-C9 |
| 13 | e | 101 | BCB | C11-C10-C8-C9 |
| 13 | i | 101 | BCB | C14-C13-C15-C16 |
| 14 | M | 404 | BPB | C11-C10-C8-C9 |
| 15 | L | 306 | CDL | C53-C54-C55-C56 |
| 15 | r | 102 | CDL | CB2-C1-CA2-OA2 |
| 15 | M | 409 | CDL | C71-CB7-OB8-CB6 |
| 13 | 6 | 101 | BCB | C8-C10-C11-C12 |
| 13 | O | 102 | BCB | C13-C15-C16-C17 |
| 13 | 3 | 101 | BCB | C4-C3-C5-C6 |
| 21 | X | 101 | NS0 | C34-C33-C35-C36 |
| 15 | L | 306 | CDL | C72-C73-C74-C75 |
| 13 | 7 | 102 | BCB | C8-C10-C11-C12 |
| 11 | A | 101 | UQ8 | C31-C32-C33-C34 |
| 19 | h | 103 | LMT | O1'-C1-C2-C3 |
| 21 | W | 303 | NS0 | CA-CB-CG-CD2 |
| 15 | L | 306 | CDL | C52-C53-C54-C55 |
| 13 | O | 102 | BCB | C15-C16-C17-C18 |
| 13 | N | 101 | BCB | C8-C10-C11-C12 |
| 20 | I | 102 | PGV | O03-C01-C02-C03 |
| 15 | r | 102 | CDL | C34-C35-C36-C37 |
| 15 | H | 301 | CDL | C54-C55-C56-C57 |
| 15 | M | 409 | CDL | OA9-CA7-OA8-CA6 |
| 21 | U | 101 | NS0 | CA-C-C7-C8 |
| 13 | A | 102 | BCB | C10-C11-C12-C13 |
| 13 | 4 | 101 | BCB | C15-C16-C17-C18 |
| 15 | H | 302 | CDL | CA7-C31-C32-C33 |
| 20 | N | 102 | PGV | O05-C05-C06-O06 |
| 15 | L | 306 | CDL | OA5-CA3-CA4-OA6 |
| 13 | c | 101 | BCB | CBA-CGA-O2A-C1 |
| 13 | 7 | 102 | BCB | O1A-CGA-O2A-C1 |
| 15 | M | 409 | CDL | C77-C78-C79-C80 |
| 15 | H | 301 | CDL | OA6-CA4-CA6-OA8 |
| 15 | H | 302 | CDL | OB6-CB4-CB6-OB8 |
| 20 | D | 102 | PGV | O03-C01-C02-O01 |
| 20 | I | 102 | PGV | O03-C01-C02-O01 |
| 13 | b | 101 | BCB | C16-C17-C18-C20 |
| 20 | D | 102 | PGV | O12-C04-C05-C06 |
| 19 | B | 201 | LMT | C5-C6-C7-C8 |
| 21 | R | 101 | NS0 | CA-C-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | R | 101 | NS0 | CA-C-C7-C9 |
| 21 | U | 101 | NS0 | CA-C-C7-C9 |
| 21 | X | 101 | NS0 | C32-C33-C35-C36 |
| 13 | M | 403 | BCB | C14-C13-C15-C16 |
| 13 | 7 | 102 | BCB | C11-C10-C8-C9 |
| 13 | k | 102 | BCB | C11-C10-C8-C9 |
| 15 | L | 306 | CDL | C1-CB2-OB2-PB2 |
| 15 | r | 102 | CDL | C1-CB2-OB2-PB2 |
| 19 | k | 103 | LMT | C1-C2-C3-C4 |
| 15 | H | 302 | CDL | C11-C12-C13-C14 |
| 15 | r | 102 | CDL | C32-C33-C34-C35 |
| 20 | M | 411 | PGV | C23-C24-C25-C26 |
| 20 | Q | 401 | PGV | C27-C28-C29-C30 |
| 15 | H | 301 | CDL | OB9-CB7-OB8-CB6 |
| 15 | H | 301 | CDL | C40-C41-C42-C43 |
| 14 | M | 404 | BPB | C13-C15-C16-C17 |
| 20 | Q | 401 | PGV | C26-C27-C28-C29 |
| 20 | N | 102 | PGV | C01-C02-C03-O11 |
| 15 | H | 301 | CDL | C34-C35-C36-C37 |
| 13 | L | 302 | BCB | C12-C13-C15-C16 |
| 13 | M | 403 | BCB | C12-C13-C15-C16 |
| 13 | B | 202 | BCB | C12-C13-C15-C16 |
| 13 | Q | 402 | BCB | C12-C13-C15-C16 |
| 13 | 7 | 102 | BCB | C11-C10-C8-C7 |
| 13 | e | 101 | BCB | C11-C10-C8-C7 |
| 13 | k | 102 | BCB | C11-C10-C8-C7 |
| 13 | o | 102 | BCB | C11-C12-C13-C15 |
| 13 | o | 102 | BCB | C12-C13-C15-C16 |
| 13 | q | 101 | BCB | C11-C10-C8-C7 |
| 13 | Z | 101 | BCB | C10-C11-C12-C13 |
| 13 | X | 102 | BCB | C16-C17-C18-C20 |
| 13 | U | 102 | BCB | C15-C16-C17-C18 |
| 13 | 6 | 101 | BCB | C16-C17-C18-C19 |
| 21 | q | 102 | NS0 | C36-C37-C38-C40 |
| 15 | r | 102 | CDL | C36-C37-C38-C39 |
| 13 | 7 | 102 | BCB | O1D-CGD-O2D-CED |
| 13 | T | 101 | BCB | C13-C15-C16-C17 |
| 15 | H | 302 | CDL | CA6-CA4-OA6-CA5 |
| 15 | r | 102 | CDL | CA6-CA4-OA6-CA5 |
| 21 | A | 103 | NS0 | C26-C27-C28-C29 |
| 21 | U | 101 | NS0 | C8-C7-C9-C10 |
| 21 | W | 303 | NS0 | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | 2 | 101 | NS0 | C26-C27-C28-C29 |
| 21 | 7 | 101 | NS0 | C26-C27-C28-C29 |
| 21 | 9 | 102 | NS0 | C26-C27-C28-C29 |
| 21 | l | 101 | NS0 | C26-C27-C28-C29 |
| 21 | o | 101 | NS0 | C26-C27-C28-C29 |
| 13 | J | 101 | BCB | C13-C15-C16-C17 |
| 11 | M | 408 | UQ8 | C30-C29-C31-C32 |
| 21 | 0 | 101 | NS0 | CA-C-C7-C8 |
| 21 | 9 | 102 | NS0 | CA-C-C7-C9 |
| 15 | r | 102 | CDL | C1-CA2-OA2-PA1 |
| 15 | H | 302 | CDL | OB5-CB3-CB4-OB6 |
| 20 | N | 102 | PGV | O01-C02-C03-O11 |
| 13 | 6 | 101 | BCB | C16-C17-C18-C20 |
| 13 | U | 102 | BCB | CHA-CBD-CGD-O1D |
| 13 | i | 101 | BCB | CHA-CBD-CGD-O2D |
| 13 | l | 102 | BCB | CHA-CBD-CGD-O1D |
| 15 | M | 409 | CDL | OB9-CB7-OB8-CB6 |
| 15 | M | 409 | CDL | C16-C17-C18-C19 |
| 15 | H | 302 | CDL | OA6-CA4-CA6-OA8 |
| 21 | R | 101 | NS0 | C34-C33-C35-C36 |
| 21 | 9 | 102 | NS0 | CA-C-C7-C8 |
| 21 | o | 101 | NS0 | C34-C33-C35-C36 |
| 13 | q | 101 | BCB | O1A-CGA-O2A-C1 |
| 21 | 0 | 101 | NS0 | CA-C-C7-C9 |
| 19 | h | 103 | LMT | C7-C8-C9-C10 |
| 13 | B | 202 | BCB | C14-C13-C15-C16 |
| 13 | q | 101 | BCB | C11-C10-C8-C9 |
| 13 | c | 101 | BCB | O1A-CGA-O2A-C1 |
| 15 | M | 409 | CDL | C60-C61-C62-C63 |
| 13 | R | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | X | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | 9 | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | f | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | e | 101 | BCB | C16-C17-C18-C20 |
| 15 | L | 306 | CDL | CB3-OB5-PB2-OB2 |
| 15 | H | 301 | CDL | CA2-OA2-PA1-OA5 |
| 15 | r | 102 | CDL | CA3-OA5-PA1-OA2 |
| 20 | Q | 401 | PGV | C04-O12-P-O11 |
| 15 | M | 409 | CDL | C73-C74-C75-C76 |
| 15 | H | 302 | CDL | C12-C13-C14-C15 |
| 11 | M | 408 | UQ8 | C40-C39-C41-C42 |
| 21 | U | 101 | NS0 | C34-C33-C35-C36 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | 2 | 101 | NS0 | CA-C-C7-C8 |
| 21 | 7 | 101 | NS0 | C34-C33-C35-C36 |
| 19 | b | 103 | LMT | O1'-C1-C2-C3 |
| 15 | M | 409 | CDL | CA2-OA2-PA1-OA3 |
| 15 | H | 301 | CDL | CA3-OA5-PA1-OA3 |
| 15 | H | 302 | CDL | CA3-OA5-PA1-OA3 |
| 15 | H | 302 | CDL | CB3-OB5-PB2-OB3 |
| 15 | r | 102 | CDL | CB2-OB2-PB2-OB3 |
| 15 | r | 102 | CDL | CB3-OB5-PB2-OB4 |
| 20 | D | 102 | PGV | C04-O12-P-O13 |
| 20 | I | 102 | PGV | C03-O11-P-O13 |
| 20 | N | 102 | PGV | C04-O12-P-O14 |
| 20 | Q | 401 | PGV | C04-O12-P-O14 |
| 20 | W | 301 | PGV | C03-O11-P-O14 |
| 19 | b | 103 | LMT | C2-C3-C4-C5 |
| 13 | q | 101 | BCB | CBA-CGA-O2A-C1 |
| 15 | r | 102 | CDL | C13-C14-C15-C16 |
| 15 | M | 409 | CDL | C35-C36-C37-C38 |
| 20 | W | 301 | PGV | C25-C26-C27-C28 |
| 19 | h | 103 | LMT | C2-C3-C4-C5 |
| 19 | n | 102 | LMT | C5-C6-C7-C8 |
| 20 | N | 102 | PGV | C19-C20-C21-C22 |
| 15 | r | 102 | CDL | C54-C55-C56-C57 |
| 15 | H | 301 | CDL | C44-C45-C46-C47 |
| 13 | o | 102 | BCB | CBA-CGA-O2A-C1 |
| 20 | Q | 401 | PGV | C28-C29-C30-C31 |
| 9 | C | 404 | HEC | C3D-CAD-CBD-CGD |
| 11 | M | 408 | UQ8 | C38-C39-C41-C42 |
| 13 | A | 102 | BCB | C11-C12-C13-C15 |
| 13 | U | 102 | BCB | C12-C13-C15-C16 |
| 13 | X | 102 | BCB | C11-C12-C13-C15 |
| 13 | 1 | 101 | BCB | C12-C13-C15-C16 |
| 13 | 7 | 102 | BCB | C12-C13-C15-C16 |
| 13 | b | 101 | BCB | C11-C12-C13-C15 |
| 13 | e | 101 | BCB | C12-C13-C15-C16 |
| 13 | f | 101 | BCB | C12-C13-C15-C16 |
| 15 | M | 409 | CDL | OA5-CA3-CA4-OA6 |
| 21 | R | 101 | NS0 | C32-C33-C35-C36 |
| 21 | 2 | 101 | NS0 | C26-C27-C28-C30 |
| 21 | 7 | 101 | NS0 | C26-C27-C28-C30 |
| 15 | H | 301 | CDL | C18-C19-C20-C21 |
| 15 | r | 102 | CDL | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | 0 | 102 | BCB | C10-C11-C12-C13 |
| 19 | M | 410 | LMT | C9-C10-C11-C12 |
| 15 | H | 302 | CDL | C57-C58-C59-C60 |
| 19 | b | 102 | LMT | C4B-C5B-C6B-O6B |
| 13 | 4 | 101 | BCB | C13-C15-C16-C17 |
| 15 | L | 306 | CDL | OB6-CB4-CB6-OB8 |
| 15 | H | 301 | CDL | C21-C22-C23-C24 |
| 13 | o | 102 | BCB | O1A-CGA-O2A-C1 |
| 21 | X | 101 | NS0 | CA-C-C7-C8 |
| 21 | 7 | 101 | NS0 | CA-C-C7-C8 |
| 21 | l | 101 | NS0 | C34-C33-C35-C36 |
| 13 | L | 302 | BCB | C14-C13-C15-C16 |
| 13 | T | 101 | BCB | C14-C13-C15-C16 |
| 13 | f | 101 | BCB | C11-C10-C8-C9 |
| 13 | f | 101 | BCB | C11-C12-C13-C14 |
| 13 | b | 101 | BCB | C16-C17-C18-C19 |
| 13 | N | 101 | BCB | C15-C16-C17-C18 |
| 13 | I | 101 | BCB | C3-C5-C6-C7 |
| 11 | L | 305 | UQ8 | C5-C4-O4-C4M |
| 11 | A | 101 | UQ8 | C30-C29-C31-C32 |
| 21 | O | 101 | NS0 | C34-C33-C35-C36 |
| 21 | o | 101 | NS0 | CA-C-C7-C8 |
| 21 | q | 102 | NS0 | CA-C-C7-C8 |
| 20 | I | 102 | PGV | C2-C3-C4-C5 |
| 21 | 7 | 101 | NS0 | C32-C33-C35-C36 |
| 21 | o | 101 | NS0 | C32-C33-C35-C36 |
| 15 | L | 306 | CDL | C81-C82-C83-C84 |
| 20 | D | 102 | PGV | C03-C02-O01-C1 |
| 15 | M | 409 | CDL | OA5-CA3-CA4-CA6 |
| 20 | W | 301 | PGV | O12-C04-C05-C06 |
| 13 | D | 101 | BCB | C2-C1-O2A-CGA |
| 13 | N | 101 | BCB | C2-C1-O2A-CGA |
| 13 | 7 | 102 | BCB | C2-C1-O2A-CGA |
| 13 | e | 101 | BCB | C2-C1-O2A-CGA |
| 13 | O | 102 | BCB | C10-C11-C12-C13 |
| 21 | O | 101 | NS0 | CA-C-C7-C8 |
| 21 | l | 101 | NS0 | CA-C-C7-C8 |
| 11 | M | 408 | UQ8 | C28-C29-C31-C32 |
| 19 | B | 201 | LMT | C3-C4-C5-C6 |
| 13 | X | 102 | BCB | C8-C10-C11-C12 |
| 15 | L | 306 | CDL | CA2-OA2-PA1-OA5 |
| 15 | L | 306 | CDL | CA3-OA5-PA1-OA2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 15 | L | 306 | CDL | CB2-OB2-PB2-OB5 |
| 15 | M | 409 | CDL | CB2-OB2-PB2-OB5 |
| 15 | H | 301 | CDL | CB3-CB4-CB6-OB8 |
| 15 | r | 102 | CDL | CB3-CB4-CB6-OB8 |
| 21 | k | 101 | NS0 | CA-C-C7-C8 |
| 13 | f | 101 | BCB | C11-C10-C8-C7 |
| 21 | 2 | 101 | NS0 | CA-C-C7-C9 |
| 13 | b | 101 | BCB | C11-C12-C13-C14 |
| 13 | f | 101 | BCB | C14-C13-C15-C16 |
| 13 | o | 102 | BCB | C14-C13-C15-C16 |
| 15 | H | 302 | CDL | C32-C33-C34-C35 |
| 21 | O | 101 | NS0 | C31-C32-C33-C35 |
| 13 | 3 | 101 | BCB | C2-C3-C5-C6 |
| 13 | X | 102 | BCB | C16-C17-C18-C19 |
| 20 | W | 301 | PGV | C11-C10-C9-C8 |
| 19 | b | 102 | LMT | C6-C7-C8-C9 |
| 19 | h | 103 | LMT | C9-C10-C11-C12 |
| 13 | M | 403 | BCB | C15-C16-C17-C18 |
| 20 | N | 102 | PGV | C1-C2-C3-C4 |
| 13 | A | 102 | BCB | C4-C3-C5-C6 |
| 21 | D | 103 | NS0 | C34-C33-C35-C36 |
| 20 | M | 411 | PGV | C25-C26-C27-C28 |
| 15 | M | 409 | CDL | C62-C63-C64-C65 |
| 13 | T | 101 | BCB | C2-C1-O2A-CGA |
| 13 | W | 302 | BCB | C2-C1-O2A-CGA |
| 20 | I | 102 | PGV | C1-C2-C3-C4 |
| 13 | E | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | J | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | 1 | 101 | BCB | C3A-C2A-CAA-CBA |
| 11 | A | 101 | UQ8 | C5-C4-O4-C4M |
| 20 | Q | 401 | PGV | C14-C15-C16-C17 |
| 13 | X | 102 | BCB | CBA-CGA-O2A-C1 |
| 21 | 9 | 102 | NS0 | C34-C33-C35-C36 |
| 21 | U | 101 | NS0 | C32-C33-C35-C36 |
| 21 | 7 | 101 | NS0 | CA-C-C7-C9 |
| 21 | q | 102 | NS0 | CA-C-C7-C9 |
| 13 | J | 101 | BCB | C11-C10-C8-C9 |
| 13 | N | 101 | BCB | C11-C12-C13-C14 |
| 13 | W | 302 | BCB | C6-C7-C8-C9 |
| 13 | 4 | 101 | BCB | C6-C7-C8-C9 |
| 13 | k | 102 | BCB | C14-C13-C15-C16 |
| 20 | D | 102 | PGV | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 20 | Q | 401 | PGV | C29-C30-C31-C32 |
| 20 | W | 301 | PGV | C22-C23-C24-C25 |
| 12 | L | 301 | DGA | OG1-CG1-CG2-CG3 |
| 15 | H | 301 | CDL | C61-C62-C63-C64 |
| 13 | f | 101 | BCB | CBA-CGA-O2A-C1 |
| 13 | f | 101 | BCB | C8-C10-C11-C12 |
| 13 | q | 101 | BCB | C5-C6-C7-C8 |
| 21 | 2 | 101 | NS0 | C34-C33-C35-C36 |
| 21 | k | 101 | NS0 | C34-C33-C35-C36 |
| 13 | E | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | J | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | 1 | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | 4 | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | c | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | l | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | W | 302 | BCB | C12-C13-C15-C16 |
| 21 | X | 101 | NS0 | CA-C-C7-C9 |
| 21 | h | 101 | NS0 | C35-C36-C37-C38 |
| 9 | C | 401 | HEC | CAA-CBA-CGA-O1A |
| 9 | C | 402 | HEC | CAA-CBA-CGA-O1A |
| 11 | L | 305 | UQ8 | C3-C4-O4-C4M |
| 15 | M | 409 | CDL | C63-C64-C65-C66 |
| 20 | D | 102 | PGV | C3-C4-C5-C6 |
| 13 | B | 202 | BCB | C13-C15-C16-C17 |
| 13 | O | 102 | BCB | C3-C5-C6-C7 |
| 13 | 0 | 102 | BCB | C5-C6-C7-C8 |
| 20 | M | 411 | PGV | C6-C7-C8-C9 |
| 15 | H | 302 | CDL | OB5-CB3-CB4-CB6 |
| 20 | I | 102 | PGV | C01-C02-C03-O11 |
| 20 | I | 102 | PGV | C20-C21-C22-C23 |
| 13 | J | 101 | BCB | C10-C11-C12-C13 |
| 9 | C | 401 | HEC | CAA-CBA-CGA-O2A |
| 11 | L | 305 | UQ8 | C20-C19-C21-C22 |
| 13 | E | 101 | BCB | C4-C3-C5-C6 |
| 21 | l | 101 | NS0 | C32-C33-C35-C36 |
| 15 | L | 306 | CDL | C80-C81-C82-C83 |
| 19 | b | 102 | LMT | C5'-C4'-O1B-C1B |
| 9 | C | 402 | HEC | CAA-CBA-CGA-O2A |
| 15 | r | 102 | CDL | C14-C15-C16-C17 |
| 21 | D | 103 | NS0 | C-CA-CB-CG |
| 19 | b | 103 | LMT | C3-C4-C5-C6 |
| 11 | A | 101 | UQ8 | C39-C41-C42-C43 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 15 | L | 306 | CDL | CB2-C1-CA2-OA2 |
| 11 | L | 305 | UQ8 | C12-C11-C9-C10 |
| 21 | W | 303 | NS0 | CA-C-C7-C8 |
| 13 | 3 | 101 | BCB | C2-C1-O2A-CGA |
| 13 | q | 101 | BCB | C2-C1-O2A-CGA |
| 21 | D | 103 | NS0 | C32-C33-C35-C36 |
| 21 | O | 101 | NS0 | CA-C-C7-C9 |
| 21 | 9 | 102 | NS0 | C32-C33-C35-C36 |
| 13 | f | 101 | BCB | O1A-CGA-O2A-C1 |
| 13 | D | 101 | BCB | C11-C10-C8-C9 |
| 13 | 0 | 102 | BCB | CBA-CGA-O2A-C1 |
| 13 | X | 102 | BCB | O1A-CGA-O2A-C1 |
| 13 | 0 | 102 | BCB | O1A-CGA-O2A-C1 |
| 19 | b | 102 | LMT | C3'-C4'-O1B-C1B |
| 12 | L | 301 | DGA | CA3-CA4-CA5-CA6 |
| 13 | o | 102 | BCB | C5-C6-C7-C8 |
| 13 | o | 102 | BCB | C10-C11-C12-C13 |
| 11 | A | 101 | UQ8 | C28-C29-C31-C32 |
| 21 | O | 101 | NS0 | C32-C33-C35-C36 |
| 21 | 2 | 101 | NS0 | C32-C33-C35-C36 |
| 21 | k | 101 | NS0 | CA-C-C7-C9 |
| 21 | l | 101 | NS0 | CA-C-C7-C9 |
| 21 | o | 101 | NS0 | CA-C-C7-C9 |
| 20 | M | 411 | PGV | C11-C12-C13-C14 |
| 11 | A | 101 | UQ8 | C2-C3-O3-C3M |
| 13 | c | 101 | BCB | C4-C3-C5-C6 |
| 21 | 0 | 101 | NS0 | C34-C33-C35-C36 |
| 13 | D | 101 | BCB | C11-C10-C8-C7 |
| 13 | O | 102 | BCB | C11-C10-C8-C7 |
| 13 | X | 102 | BCB | C11-C10-C8-C7 |
| 13 | D | 101 | BCB | C5-C6-C7-C8 |
| 20 | Q | 401 | PGV | C13-C14-C15-C16 |
| 13 | 9 | 101 | BCB | CAA-CBA-CGA-O2A |
| 15 | L | 306 | CDL | C32-C31-CA7-OA8 |
| 20 | Q | 401 | PGV | O03-C19-C20-C21 |
| 13 | A | 102 | BCB | C13-C15-C16-C17 |
| 13 | O | 102 | BCB | CBA-CGA-O2A-C1 |
| 11 | M | 408 | UQ8 | C12-C11-C9-C10 |
| 11 | A | 101 | UQ8 | C40-C39-C41-C42 |
| 13 | D | 101 | BCB | C4-C3-C5-C6 |
| 13 | E | 101 | BCB | C2-C3-C5-C6 |
| 15 | M | 409 | CDL | C39-C40-C41-C42 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | R | 102 | BCB | C11-C10-C8-C9 |
| 13 | 1 | 101 | BCB | C14-C13-C15-C16 |
| 13 | c | 101 | BCB | C6-C7-C8-C9 |
| 13 | 4 | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | c | 101 | BCB | C3A-C2A-CAA-CBA |
| 13 | M | 402 | BCB | CAD-CBD-CGD-O2D |
| 14 | L | 304 | BPB | CAD-CBD-CGD-O2D |
| 14 | M | 404 | BPB | CAD-CBD-CGD-O2D |
| 20 | N | 102 | PGV | C03-C02-O01-C1 |
| 13 | 3 | 101 | BCB | C16-C17-C18-C19 |
| 13 | 0 | 102 | BCB | C8-C10-C11-C12 |
| 15 | M | 409 | CDL | C80-C81-C82-C83 |
| 13 | i | 101 | BCB | C4-C3-C5-C6 |
| 13 | i | 101 | BCB | C2-C3-C5-C6 |
| 21 | W | 303 | NS0 | CA-C-C7-C9 |
| 21 | k | 101 | NS0 | C32-C33-C35-C36 |
| 11 | A | 101 | UQ8 | C24-C26-C27-C28 |
| 15 | H | 301 | CDL | CA3-CA4-CA6-OA8 |
| 15 | H | 302 | CDL | C31-C32-C33-C34 |
| 13 | O | 102 | BCB | O1A-CGA-O2A-C1 |
| 12 | L | 301 | DGA | OG2-CB1-CB2-CB3 |
| 15 | M | 409 | CDL | C12-C11-CA5-OA6 |
| 15 | M | 409 | CDL | C61-C62-C63-C64 |
| 15 | H | 301 | CDL | C55-C56-C57-C58 |
| 20 | D | 102 | PGV | O12-C04-C05-O05 |
| 13 | M | 403 | BCB | CHA-CBD-CGD-O2D |
| 13 | E | 101 | BCB | CHA-CBD-CGD-O1D |
| 13 | E | 101 | BCB | CHA-CBD-CGD-O2D |
| 13 | U | 102 | BCB | CHA-CBD-CGD-O2D |
| 13 | 0 | 102 | BCB | CHA-CBD-CGD-O1D |
| 13 | 0 | 102 | BCB | CHA-CBD-CGD-O2D |
| 13 | l | 102 | BCB | CHA-CBD-CGD-O2D |
| 9 | C | 404 | HEC | CAD-CBD-CGD-O1D |
| 13 | B | 202 | BCB | C4-C3-C5-C6 |
| 13 | 1 | 101 | BCB | CBA-CGA-O2A-C1 |
| 15 | M | 409 | CDL | C59-C60-C61-C62 |
| 13 | T | 101 | BCB | CAA-CBA-CGA-O2A |
| 13 | U | 102 | BCB | CAA-CBA-CGA-O2A |
| 15 | L | 306 | CDL | C40-C41-C42-C43 |
| 20 | I | 102 | PGV | C31-C32-C33-C34 |
| 13 | r | 101 | BCB | O1A-CGA-O2A-C1 |
| 13 | b | 101 | BCB | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 15 | H | 301 | CDL | C20-C21-C22-C23 |
| 15 | H | 301 | CDL | C71-C72-C73-C74 |
| 13 | U | 102 | BCB | CBA-CGA-O2A-C1 |
| 13 | 4 | 101 | BCB | C16-C17-C18-C20 |
| 13 | I | 101 | BCB | C11-C10-C8-C9 |
| 13 | 7 | 102 | BCB | C6-C7-C8-C9 |
| 13 | 7 | 102 | BCB | C14-C13-C15-C16 |
| 13 | k | 102 | BCB | C11-C12-C13-C14 |
| 20 | Q | 401 | PGV | O04-C19-C20-C21 |
| 21 | W | 303 | NS0 | C11-C10-C9-C7 |
| 12 | L | 301 | DGA | OB1-CB1-CB2-CB3 |
| 15 | L | 306 | CDL | C82-C83-C84-C85 |
| 13 | q | 101 | BCB | CAA-CBA-CGA-O2A |
| 19 | b | 102 | LMT | C9-C10-C11-C12 |
| 11 | M | 408 | UQ8 | C33-C34-C36-C37 |
| 13 | c | 101 | BCB | C2-C3-C5-C6 |
| 15 | M | 409 | CDL | C36-C37-C38-C39 |
| 13 | R | 102 | BCB | CBA-CGA-O2A-C1 |
| 13 | N | 101 | BCB | C1A-C2A-CAA-CBA |
| 13 | U | 102 | BCB | C1A-C2A-CAA-CBA |
| 13 | i | 101 | BCB | C1A-C2A-CAA-CBA |
| 15 | L | 306 | CDL | C12-C11-CA5-OA6 |
| 13 | r | 101 | BCB | CBA-CGA-O2A-C1 |
| 9 | C | 404 | HEC | CAD-CBD-CGD-O2D |
| 13 | 9 | 101 | BCB | CAA-CBA-CGA-O1A |
| 15 | L | 306 | CDL | C32-C31-CA7-OA9 |
| 15 | r | 102 | CDL | C52-C51-CB5-OB6 |
| 15 | H | 302 | CDL | OB7-CB5-OB6-CB4 |
| 15 | M | 409 | CDL | CA3-OA5-PA1-OA3 |
| 15 | r | 102 | CDL | CA3-OA5-PA1-OA3 |
| 13 | 1 | 101 | BCB | O1A-CGA-O2A-C1 |
| 15 | M | 409 | CDL | C52-C53-C54-C55 |
| 13 | h | 102 | BCB | C13-C15-C16-C17 |
| 13 | b | 101 | BCB | CAA-CBA-CGA-O1A |
| 14 | L | 304 | BPB | C8-C10-C11-C12 |
| 14 | M | 404 | BPB | C15-C16-C17-C18 |
| 13 | q | 101 | BCB | CAA-CBA-CGA-O1A |
| 11 | L | 305 | UQ8 | C12-C11-C9-C8 |
| 11 | A | 101 | UQ8 | C38-C39-C41-C42 |
| 13 | L | 302 | BCB | CAD-CBD-CGD-O1D |
| 13 | A | 102 | BCB | CAD-CBD-CGD-O1D |
| 13 | 0 | 102 | BCB | CAD-CBD-CGD-O1D |

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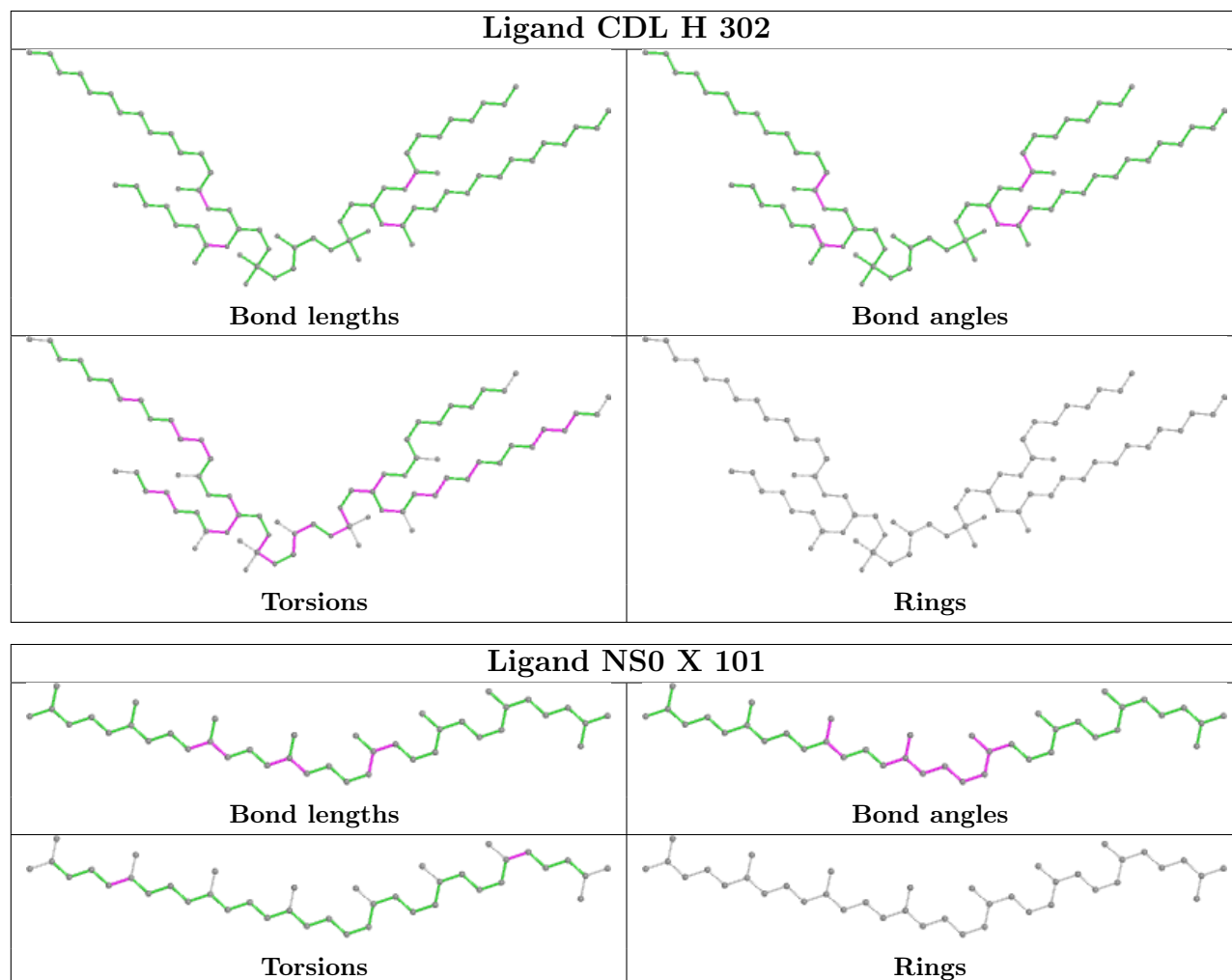
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | T | 101 | BCB | CAA-CBA-CGA-O1A |
| 15 | M | 409 | CDL | C12-C11-CA5-OA7 |
| 13 | k | 102 | BCB | CAA-CBA-CGA-O2A |
| 15 | H | 301 | CDL | C16-C17-C18-C19 |
| 15 | r | 102 | CDL | C12-C11-CA5-OA6 |
| 21 | W | 303 | NS0 | C35-C36-C37-C38 |
| 13 | h | 102 | BCB | CAA-CBA-CGA-O2A |
| 15 | H | 301 | CDL | C12-C11-CA5-OA6 |
| 12 | L | 301 | DGA | CA1-CA2-CA3-CA4 |
| 15 | r | 102 | CDL | C52-C51-CB5-OB7 |
| 13 | A | 102 | BCB | C2-C3-C5-C6 |
| 13 | A | 102 | BCB | C11-C10-C8-C7 |
| 13 | I | 101 | BCB | C11-C10-C8-C7 |
| 13 | R | 102 | BCB | C11-C10-C8-C7 |
| 13 | T | 101 | BCB | C12-C13-C15-C16 |
| 13 | 4 | 101 | BCB | C6-C7-C8-C10 |
| 13 | 0 | 102 | BCB | C12-C13-C15-C16 |
| 21 | 9 | 102 | NS0 | C26-C27-C28-C30 |
| 21 | l | 101 | NS0 | C26-C27-C28-C30 |
| 21 | o | 101 | NS0 | C26-C27-C28-C30 |
| 13 | U | 102 | BCB | CAA-CBA-CGA-O1A |
| 21 | l | 101 | NS0 | C10-C11-C12-C14 |
| 21 | q | 102 | NS0 | C10-C11-C12-C14 |
| 13 | Z | 101 | BCB | CAA-CBA-CGA-O2A |
| 13 | k | 102 | BCB | C8-C10-C11-C12 |
| 21 | A | 103 | NS0 | C35-C36-C37-C38 |
| 13 | W | 302 | BCB | CAA-CBA-CGA-O2A |
| 15 | r | 102 | CDL | C32-C31-CA7-OA8 |
| 13 | f | 101 | BCB | C10-C11-C12-C13 |
| 13 | o | 102 | BCB | C15-C16-C17-C18 |
| 15 | r | 102 | CDL | C55-C56-C57-C58 |
| 20 | D | 102 | PGV | C19-C20-C21-C22 |
| 13 | k | 102 | BCB | CAA-CBA-CGA-O1A |
| 13 | i | 101 | BCB | CAA-CBA-CGA-O2A |

There are no ring outliers.

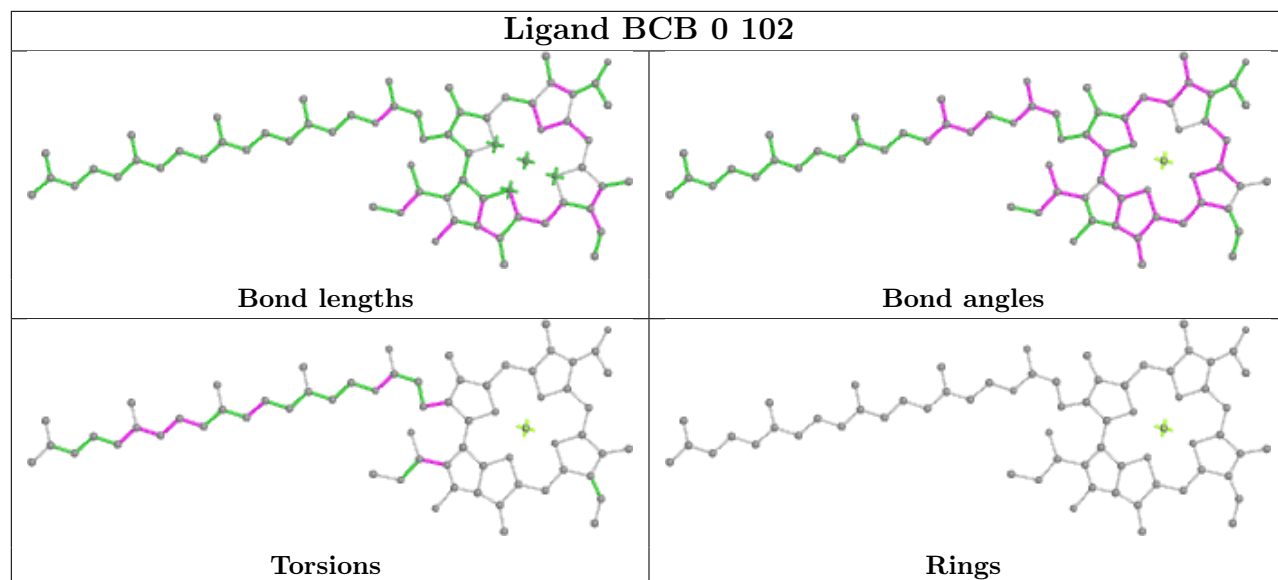
No monomer is involved in short contacts.

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

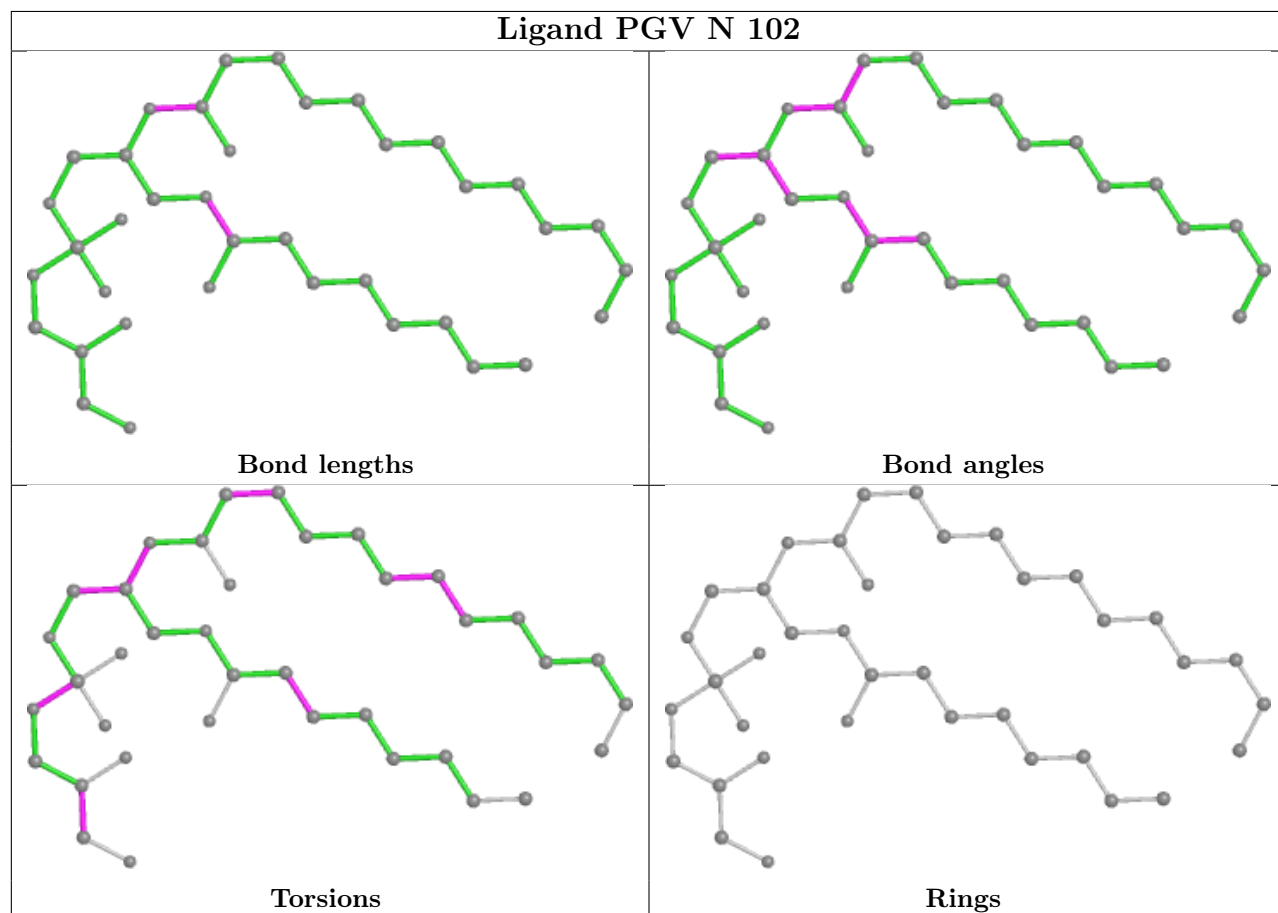
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

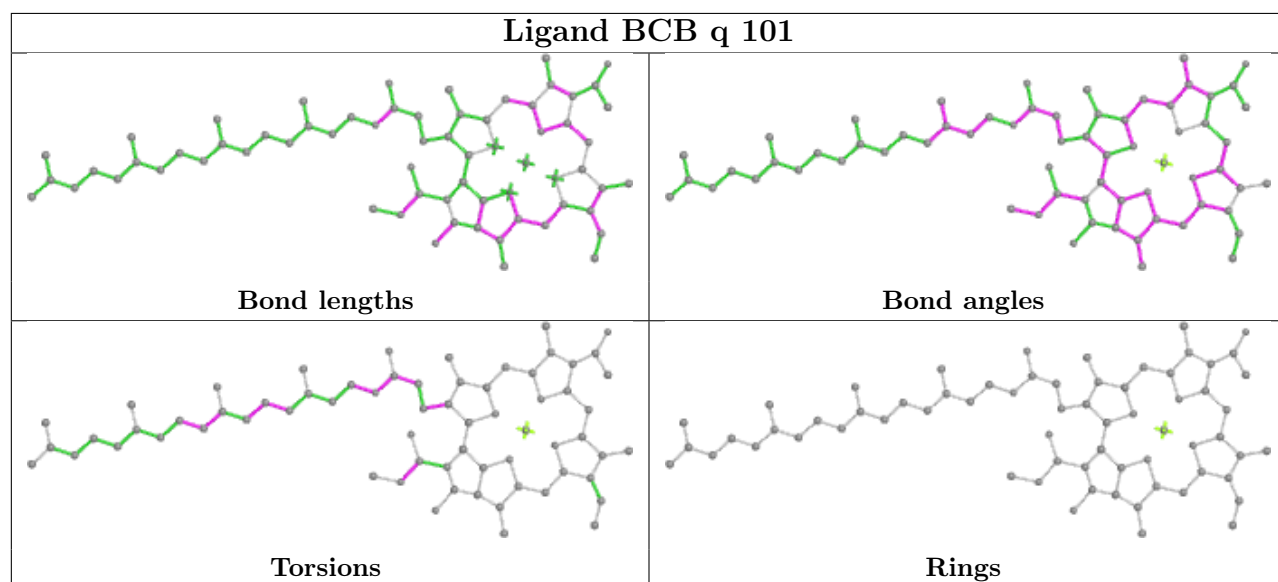
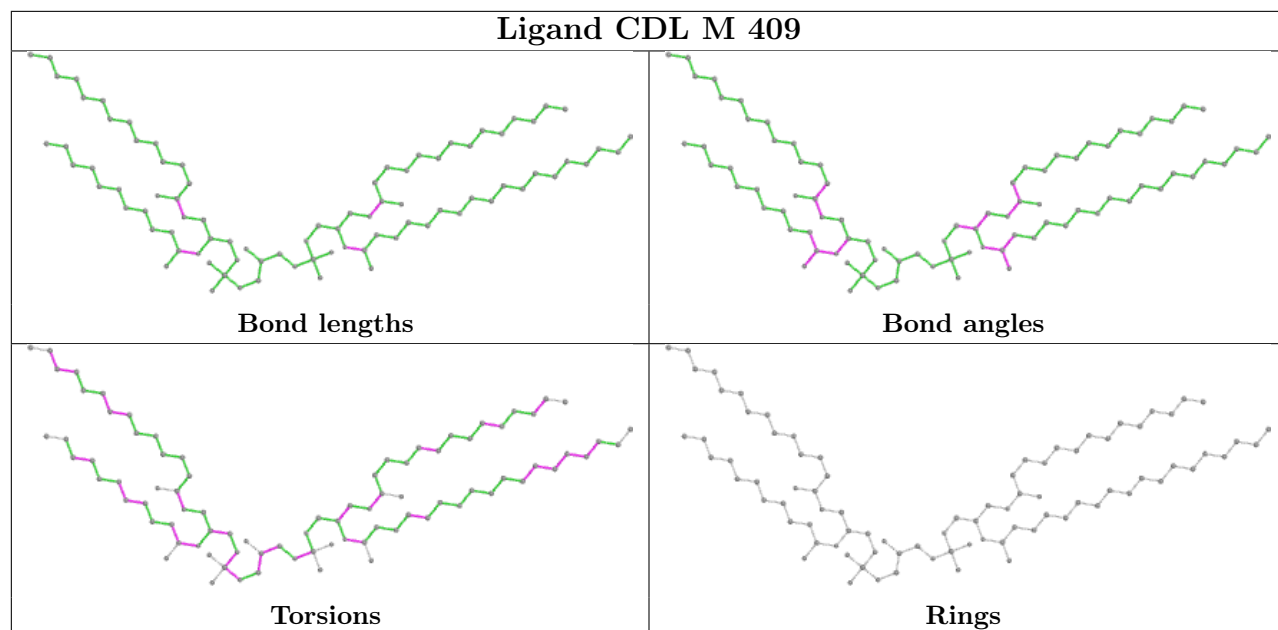


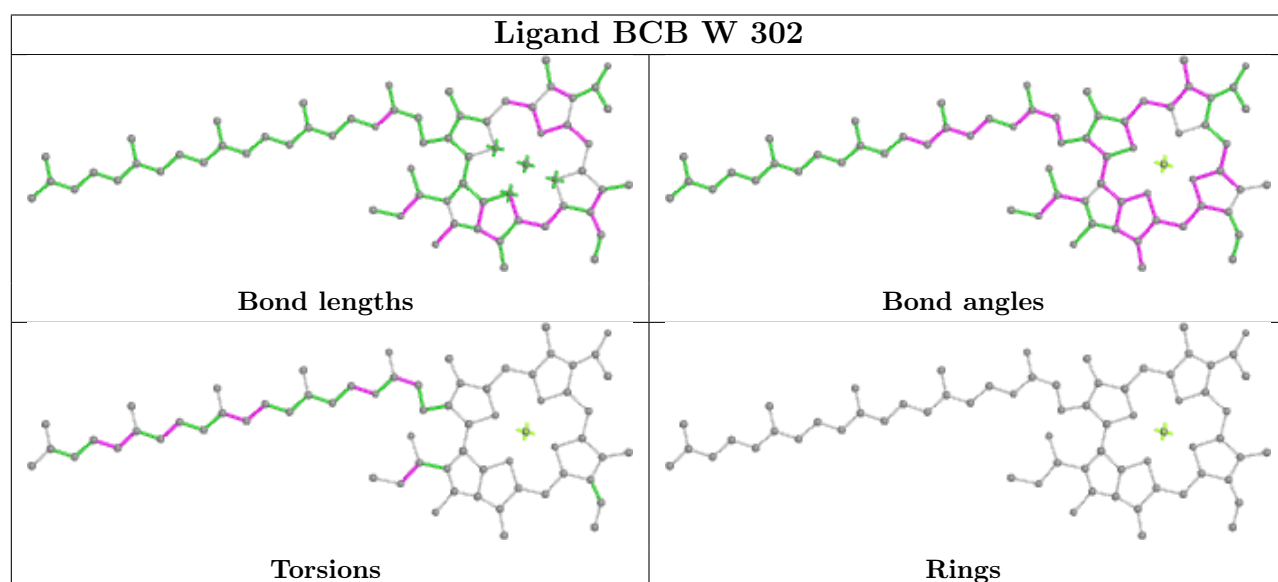
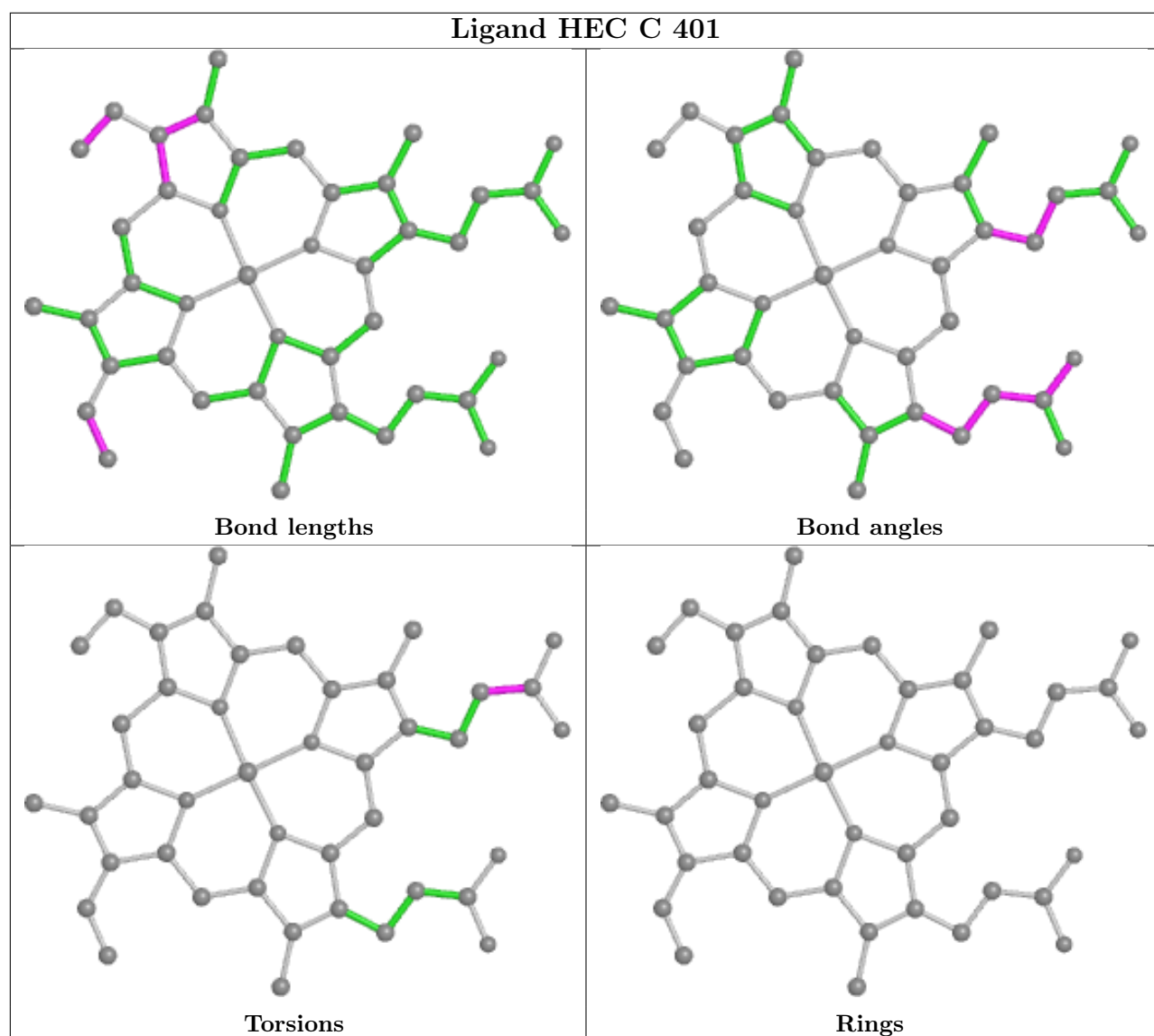
Ligand BCB 0 102

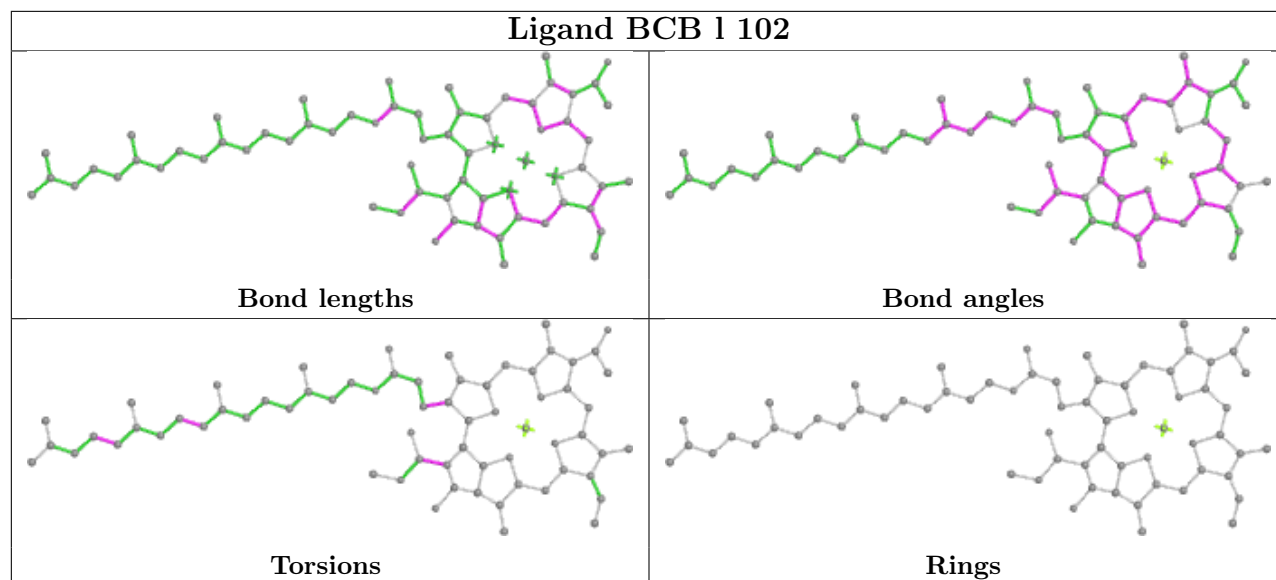
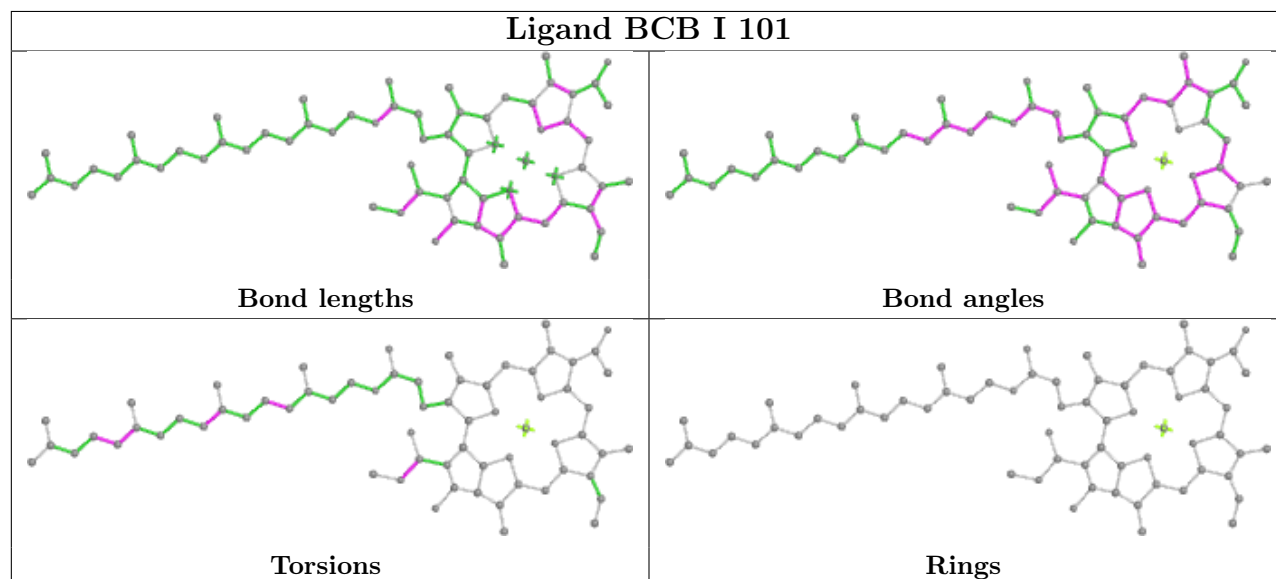
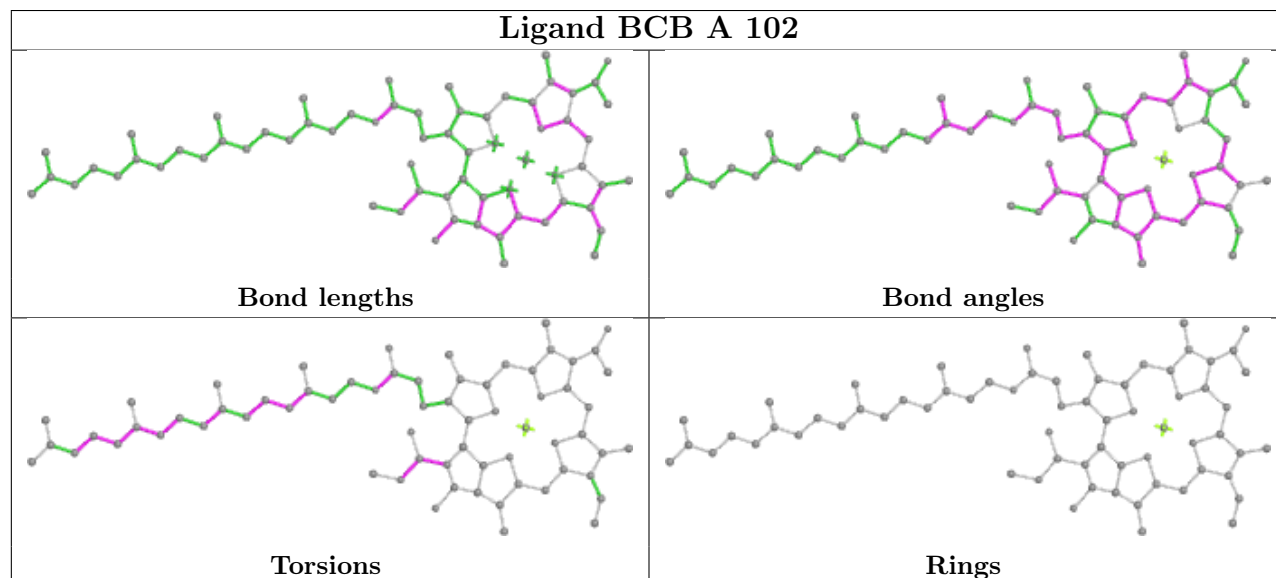


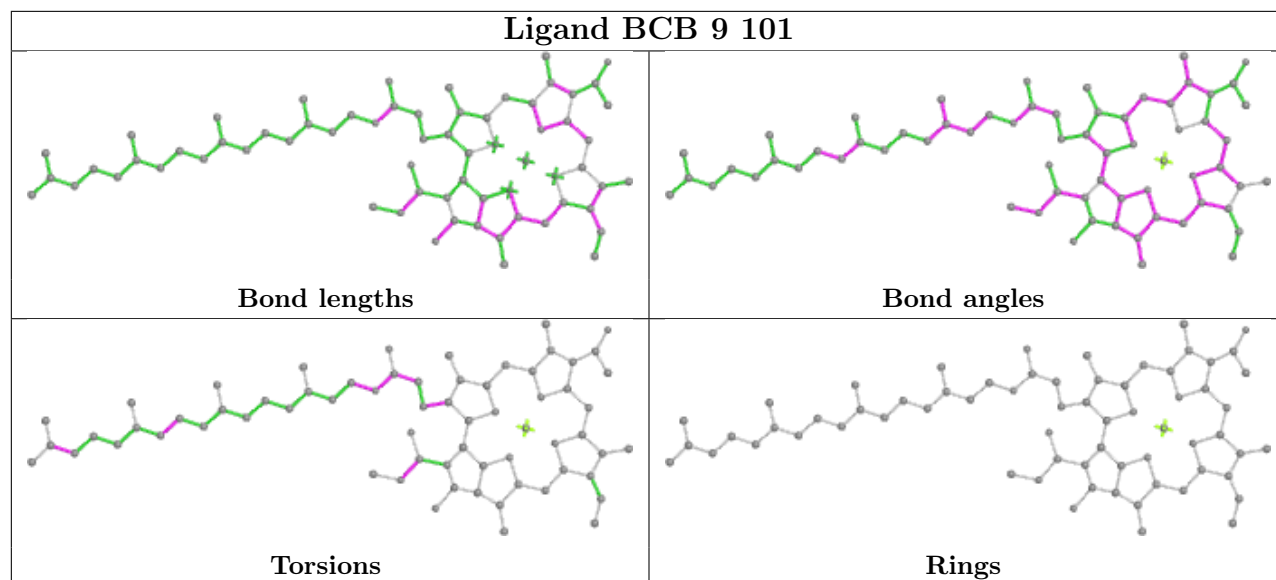
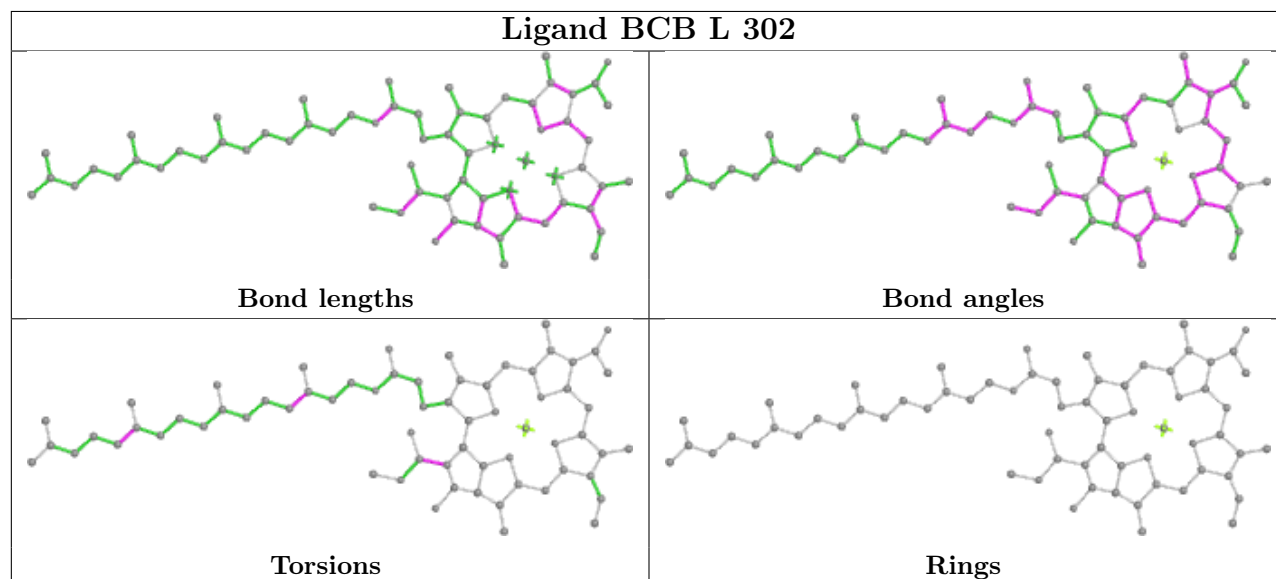
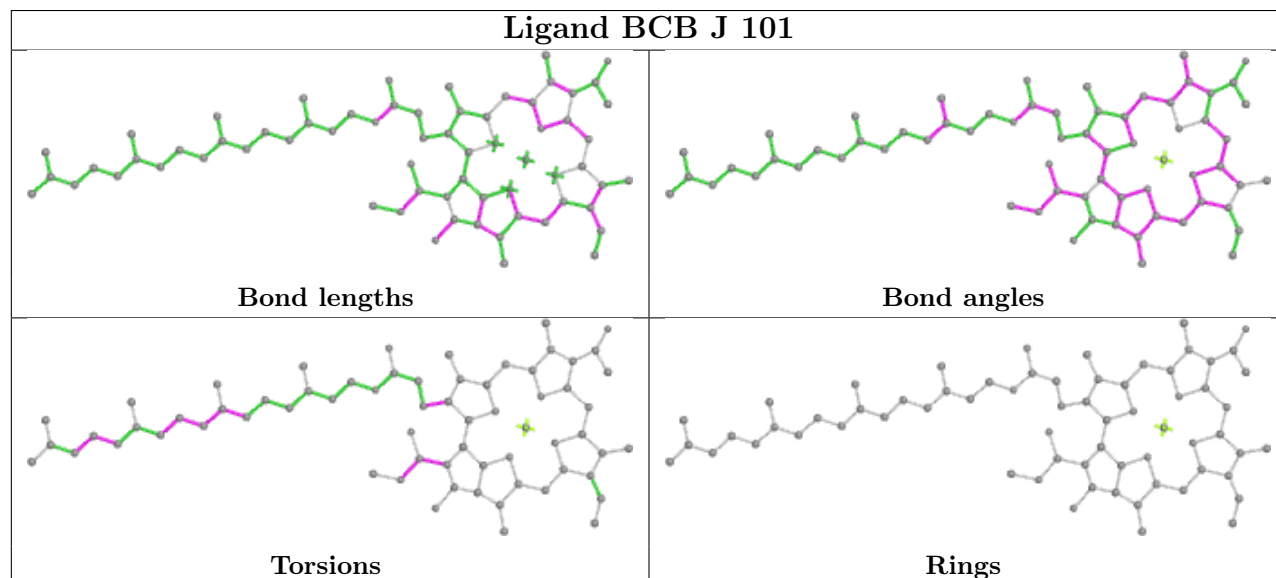
Ligand PGV N 102

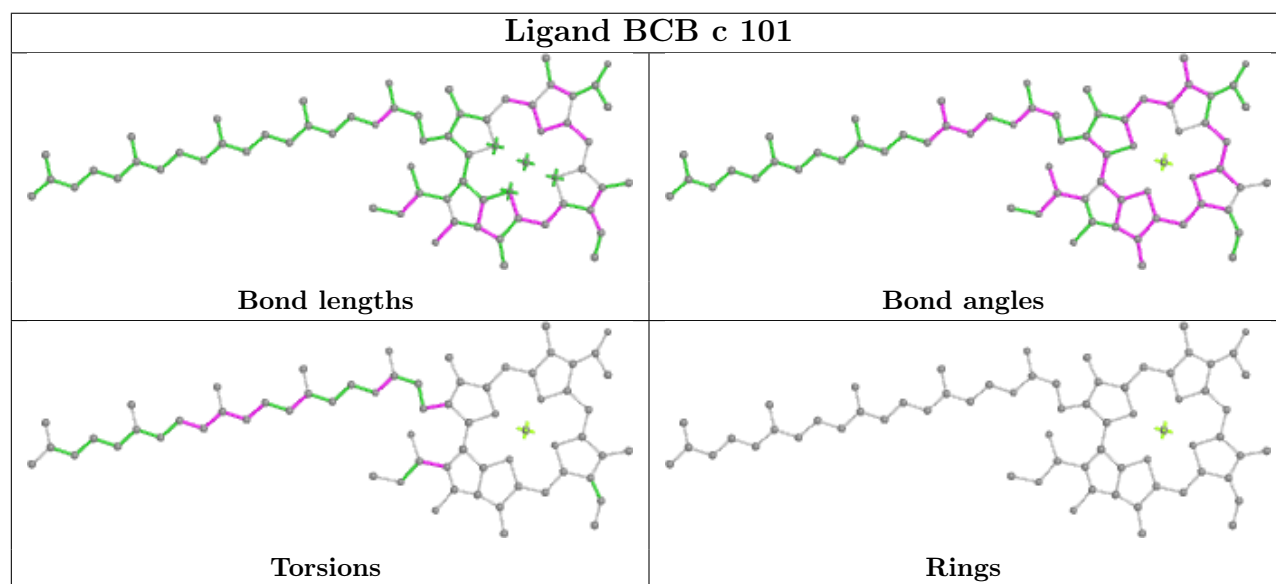
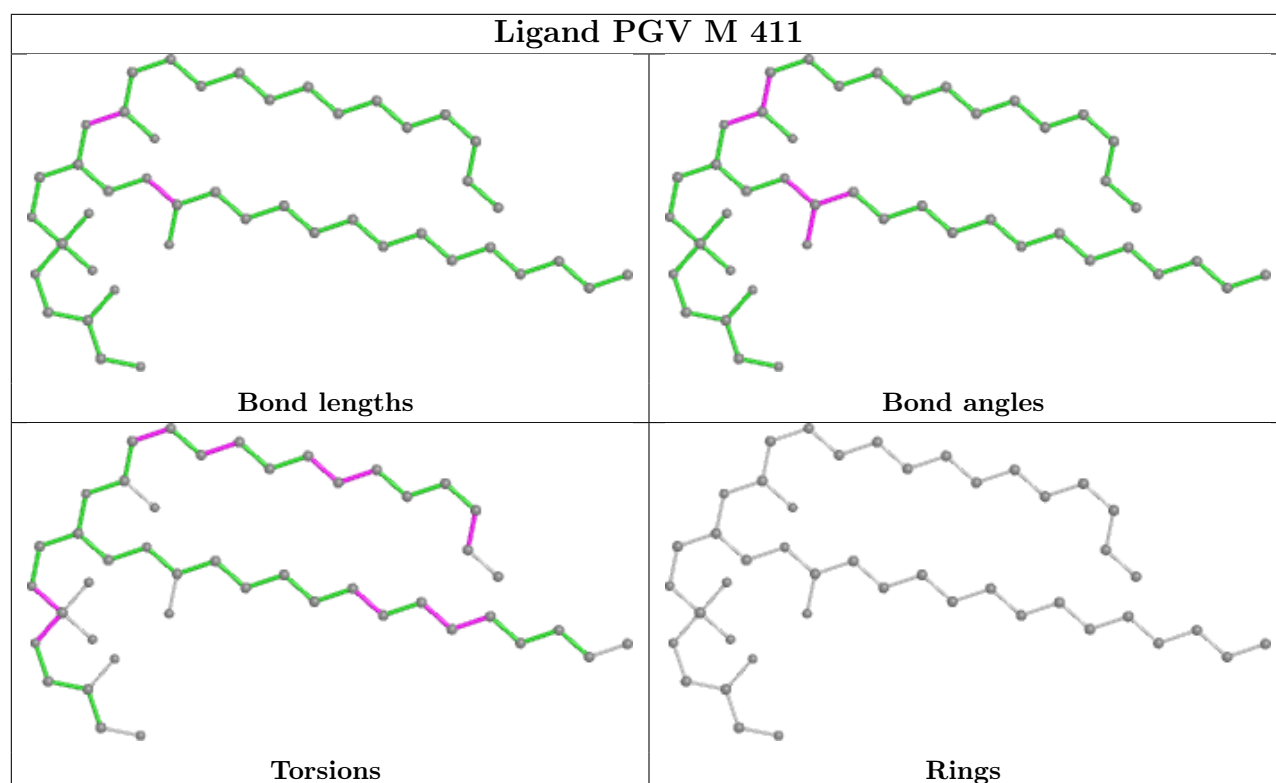


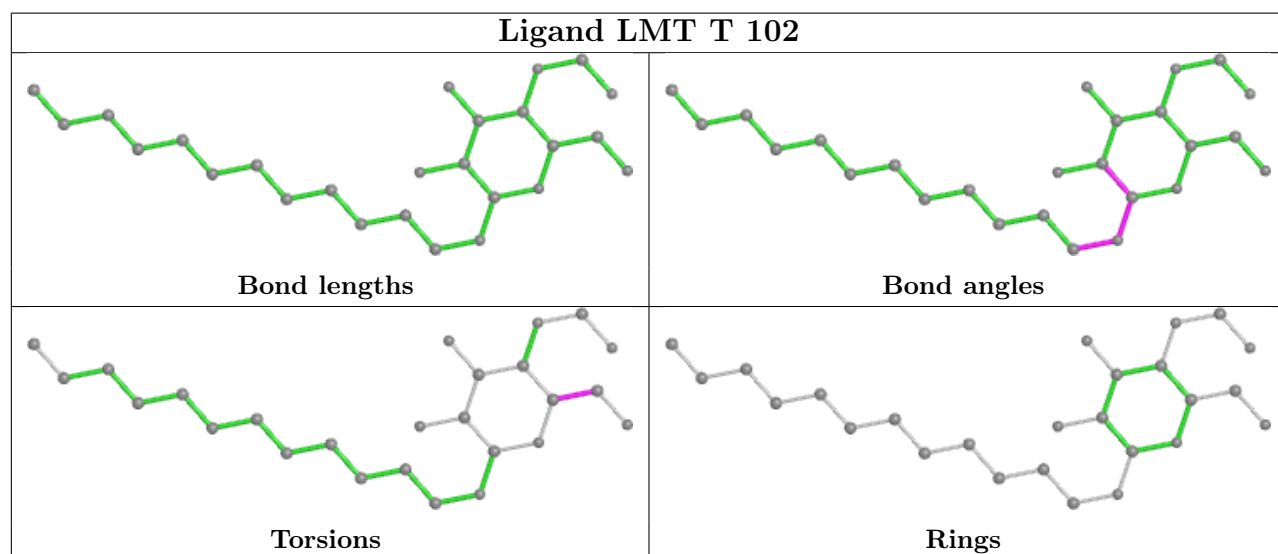
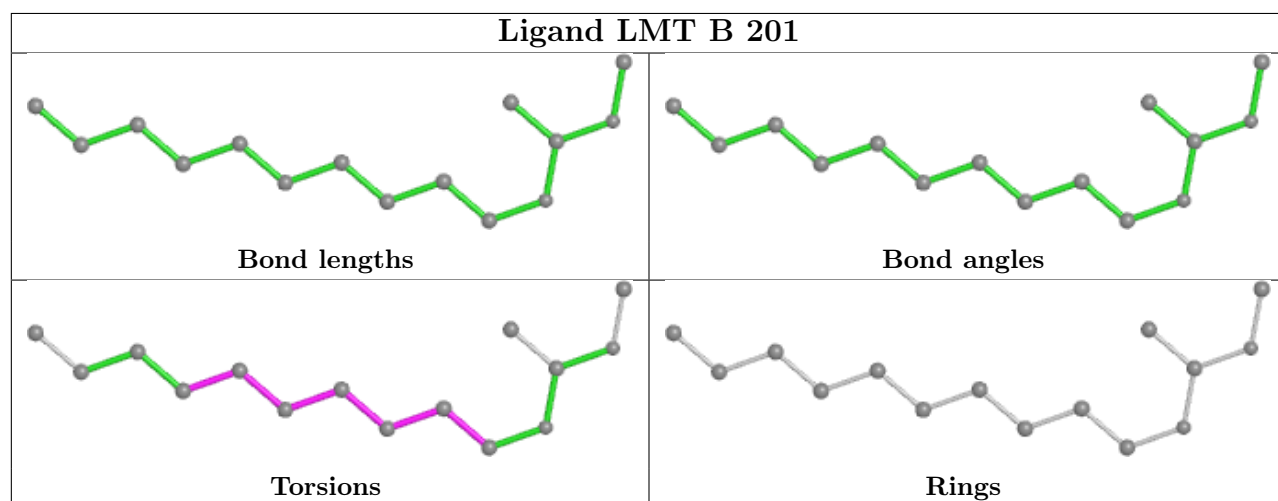
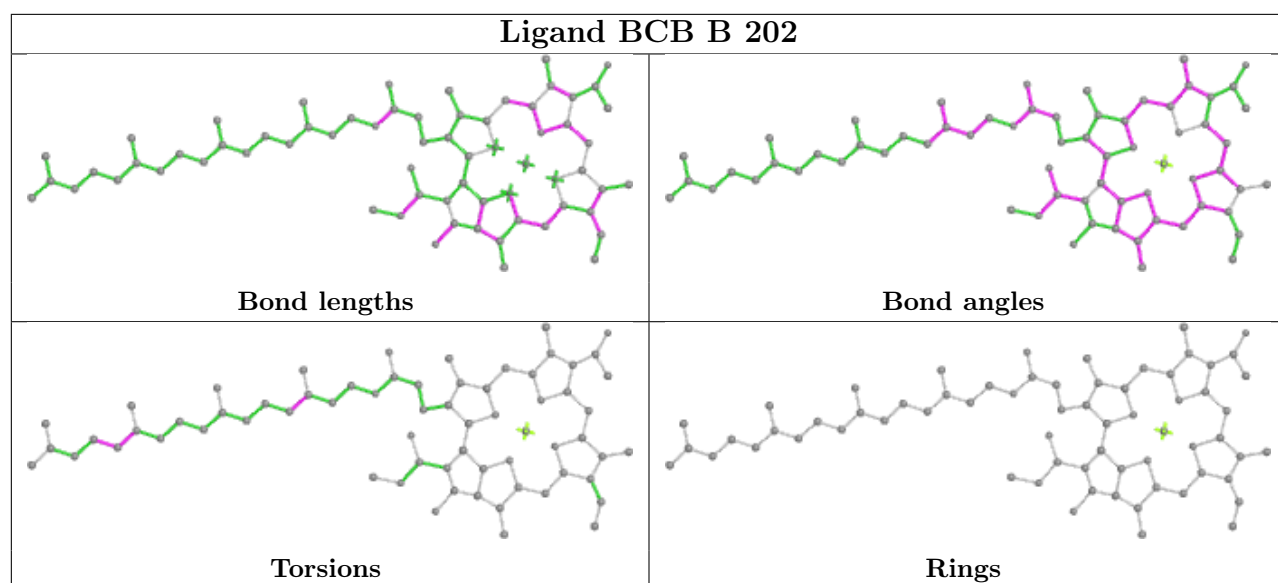


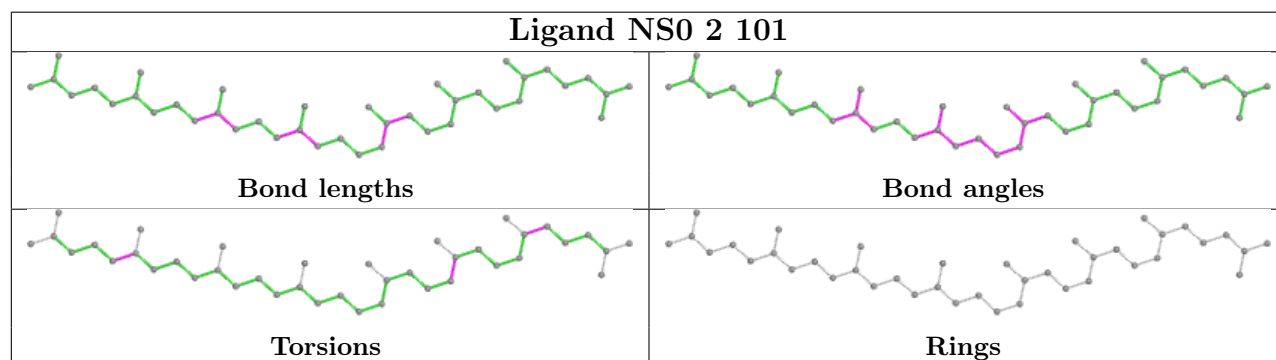
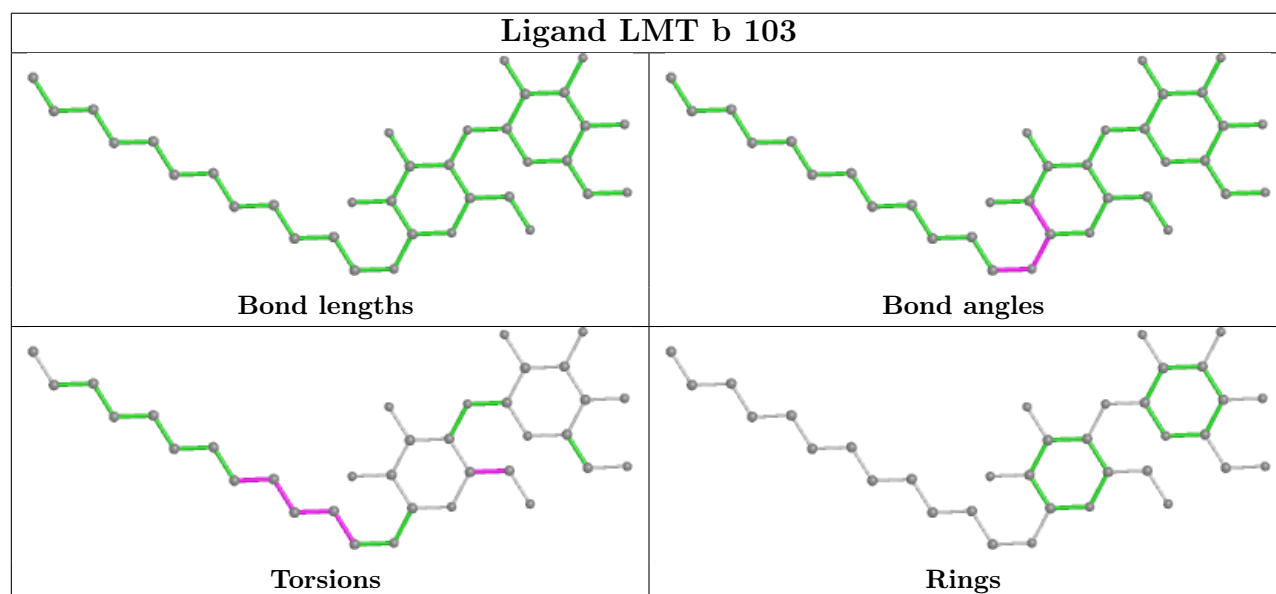
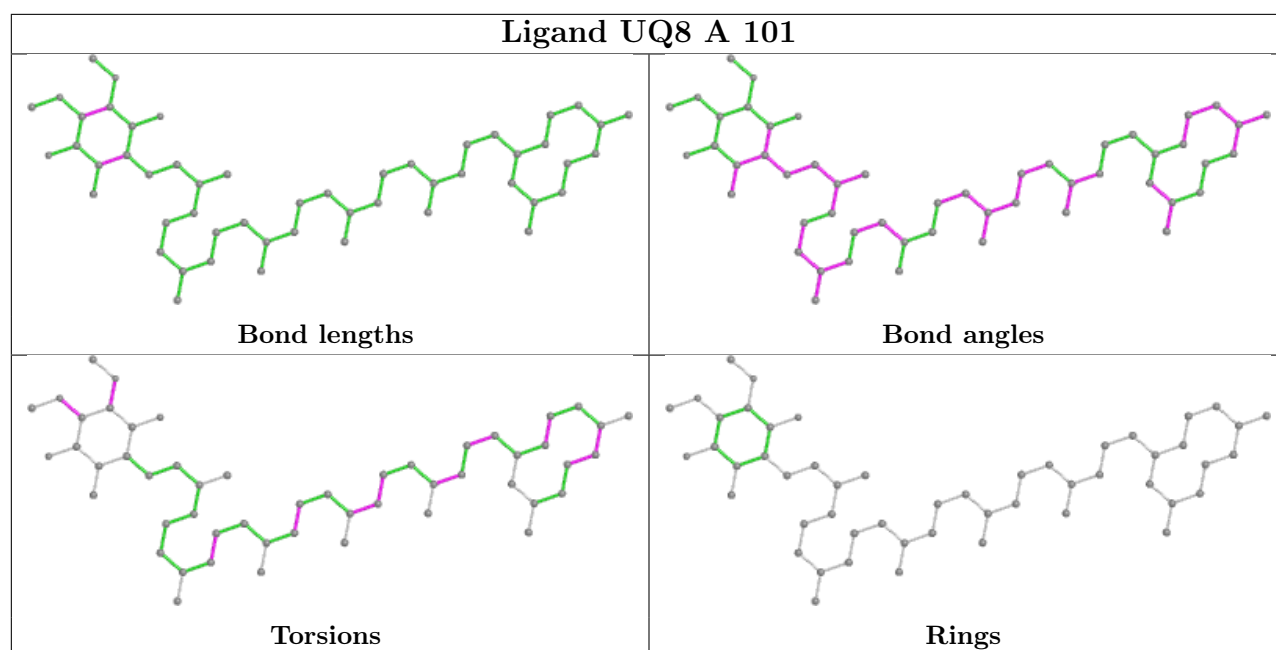


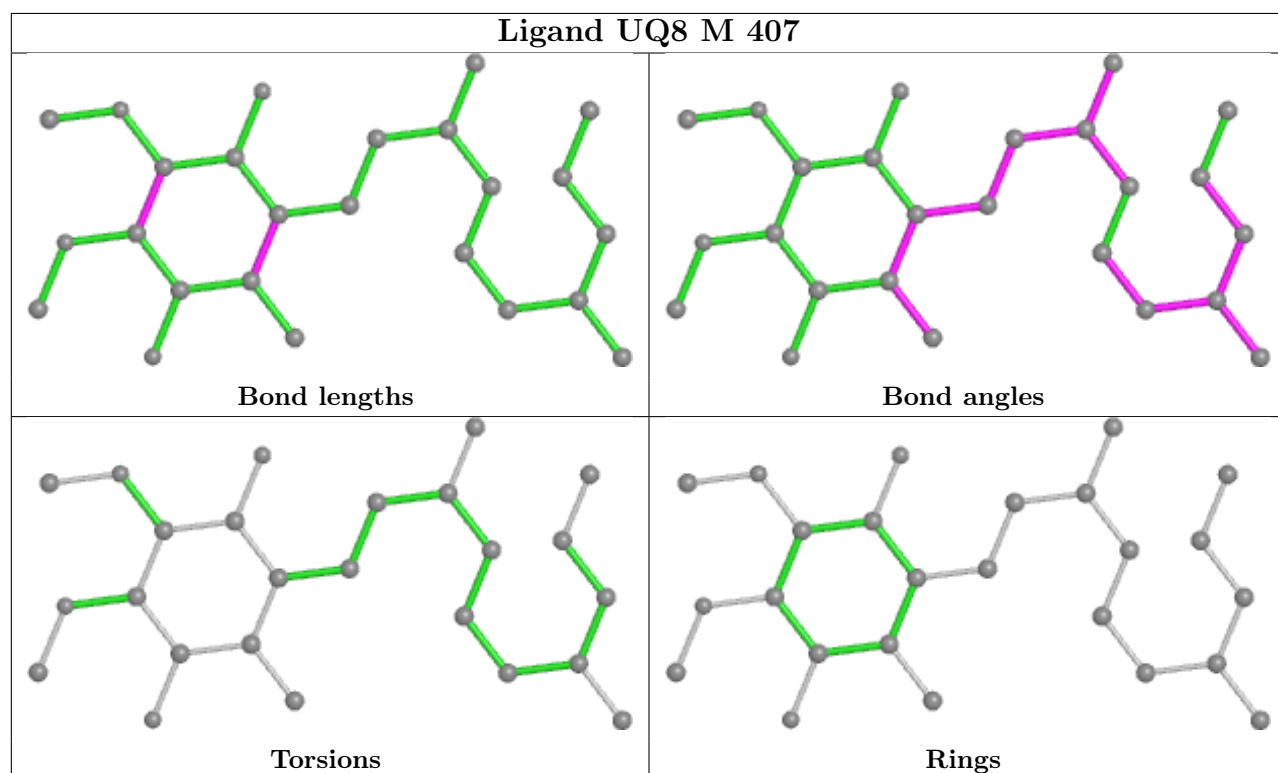
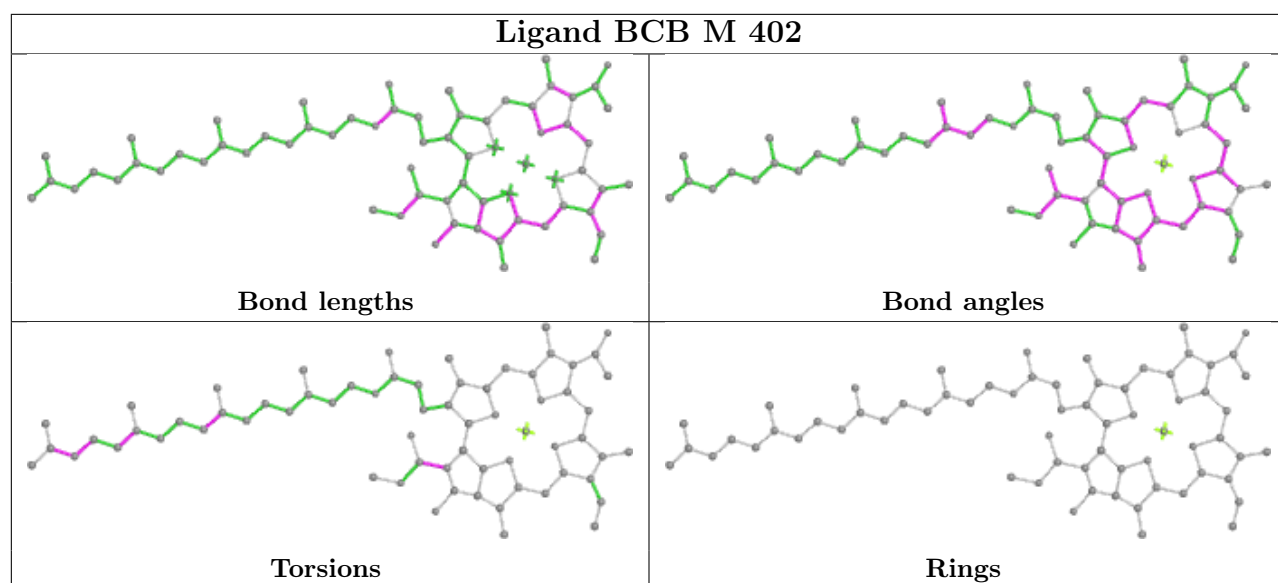
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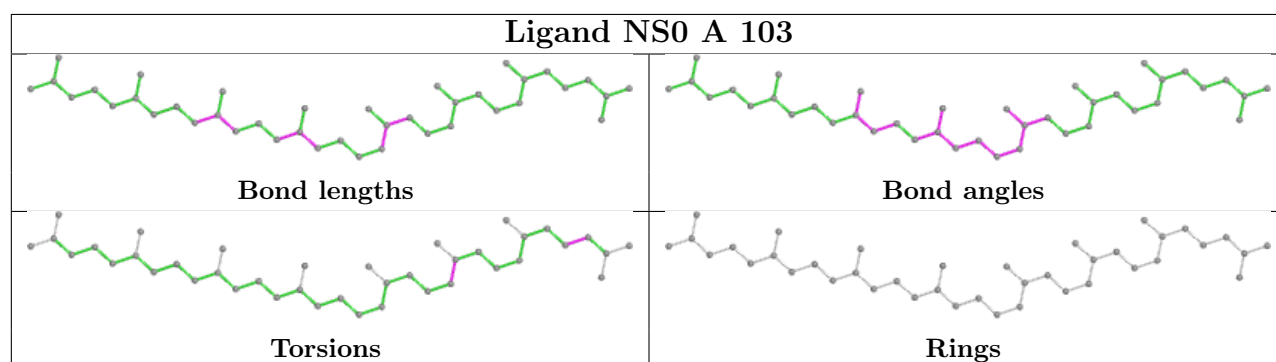
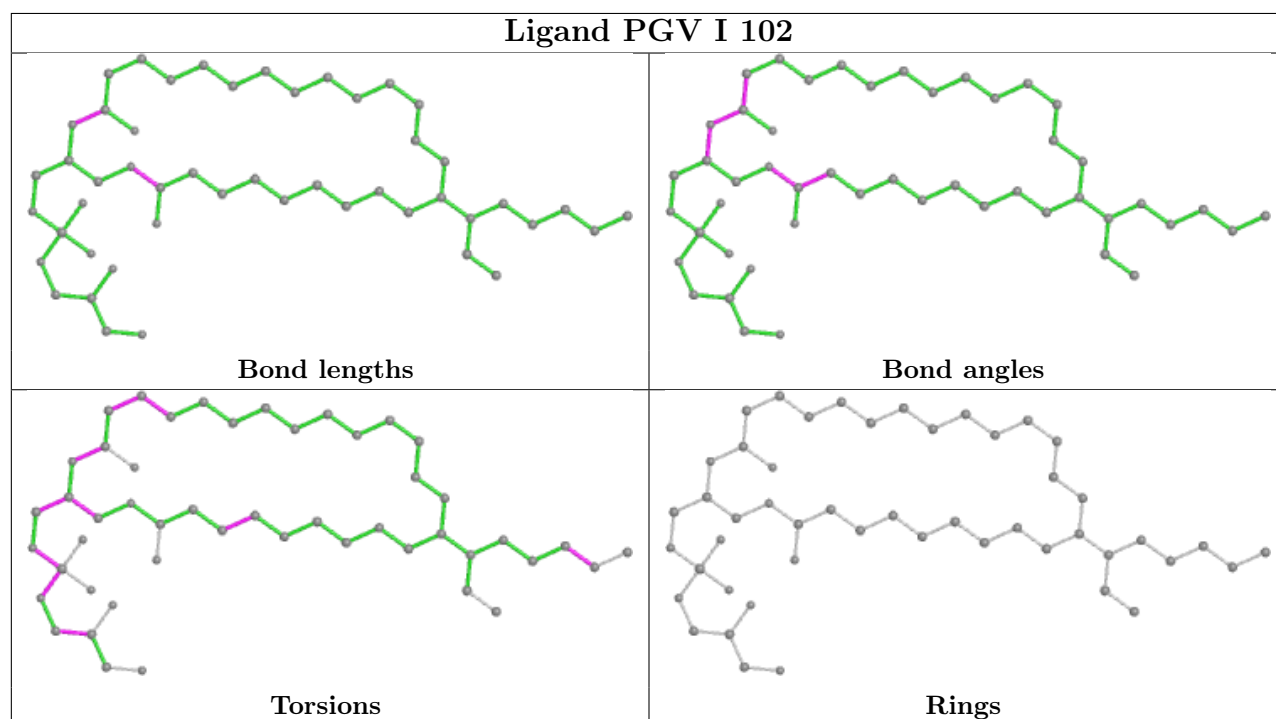
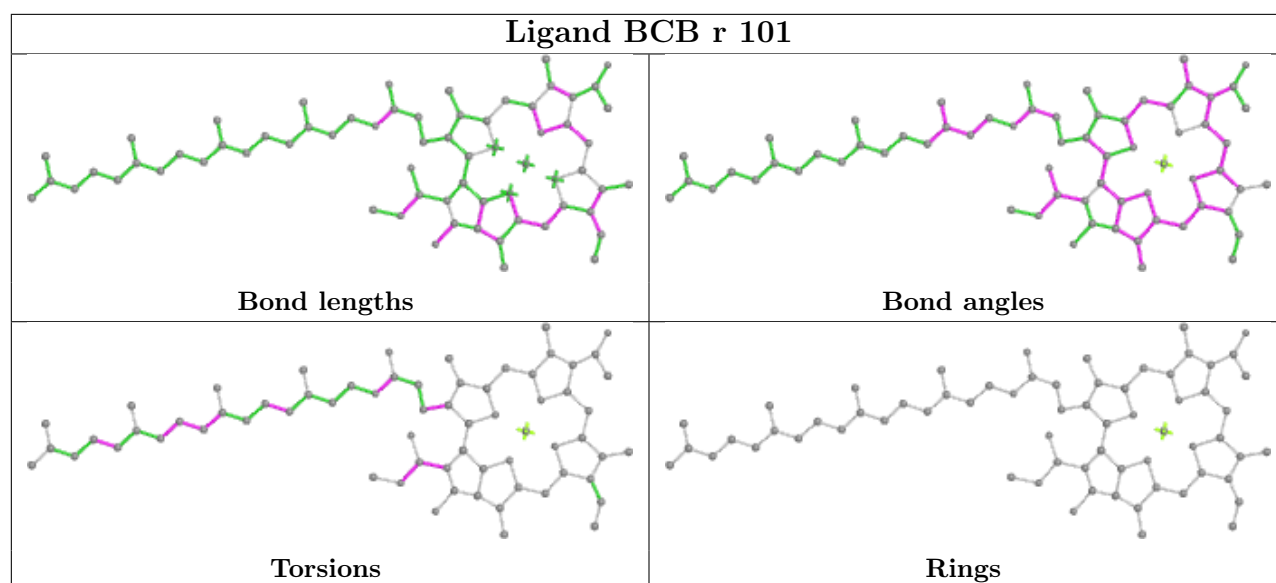
Ligand BCB 9 101**Ligand BCB L 302****Ligand BCB J 101**

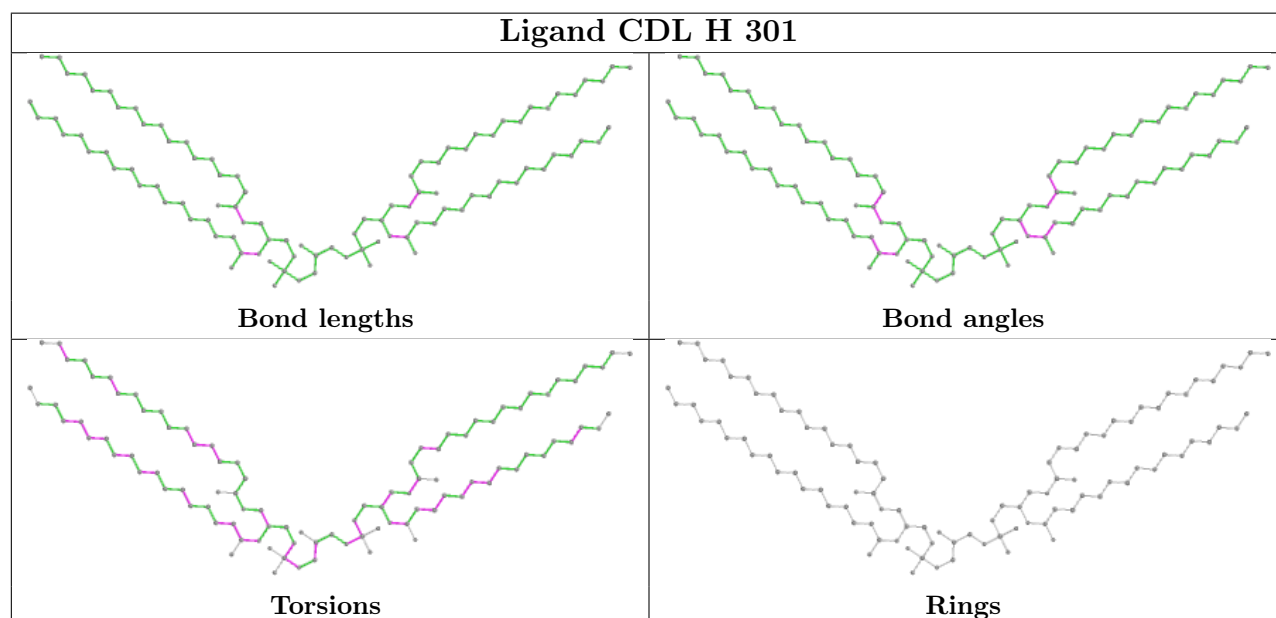
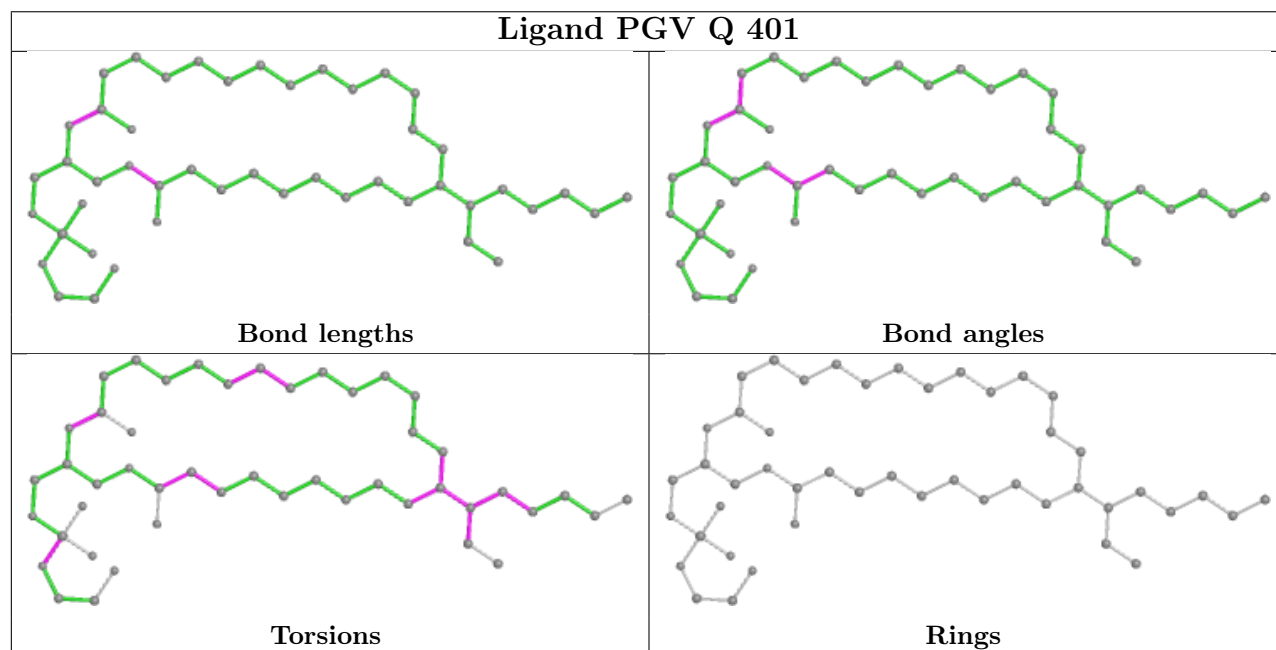
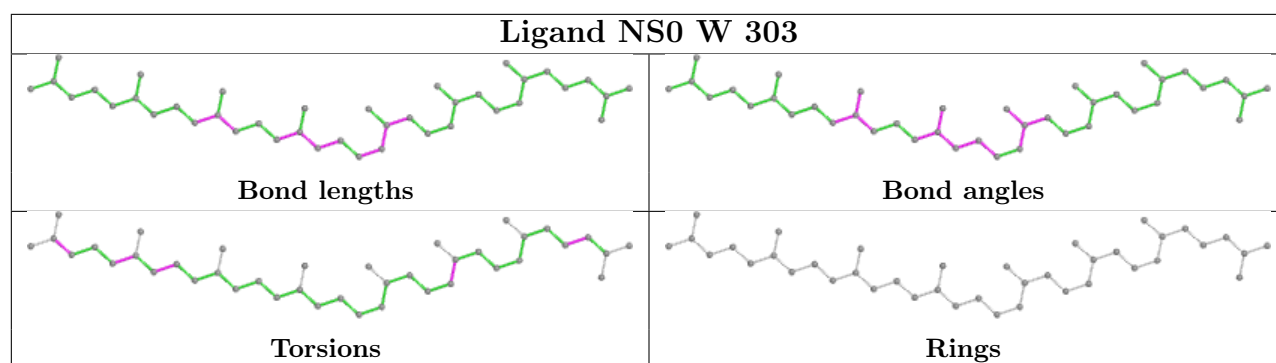




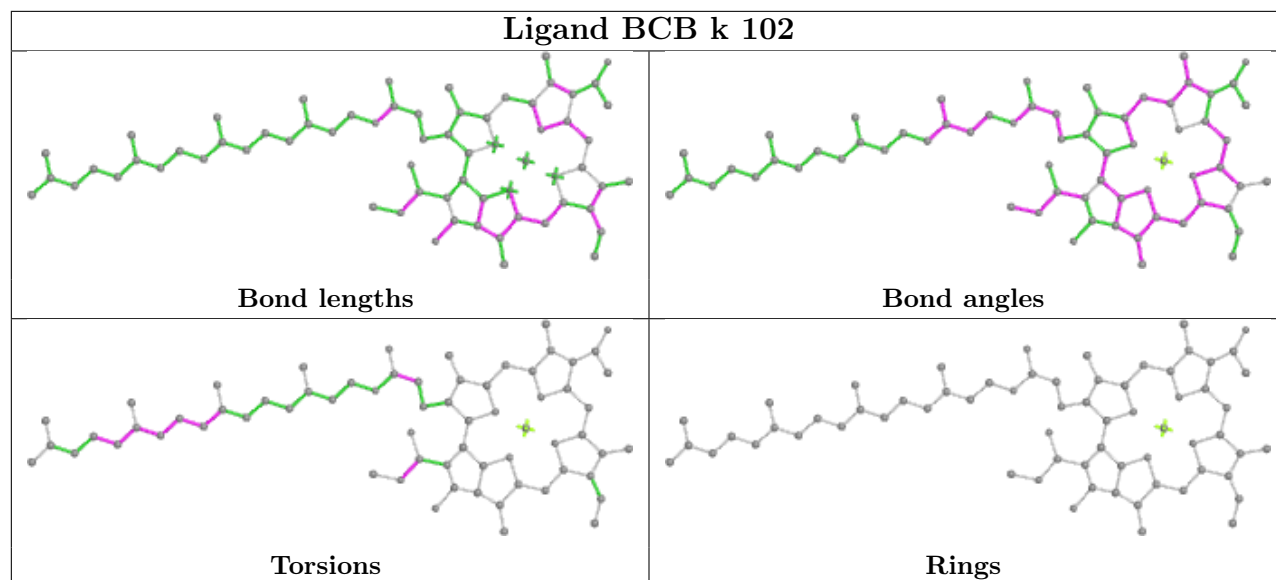




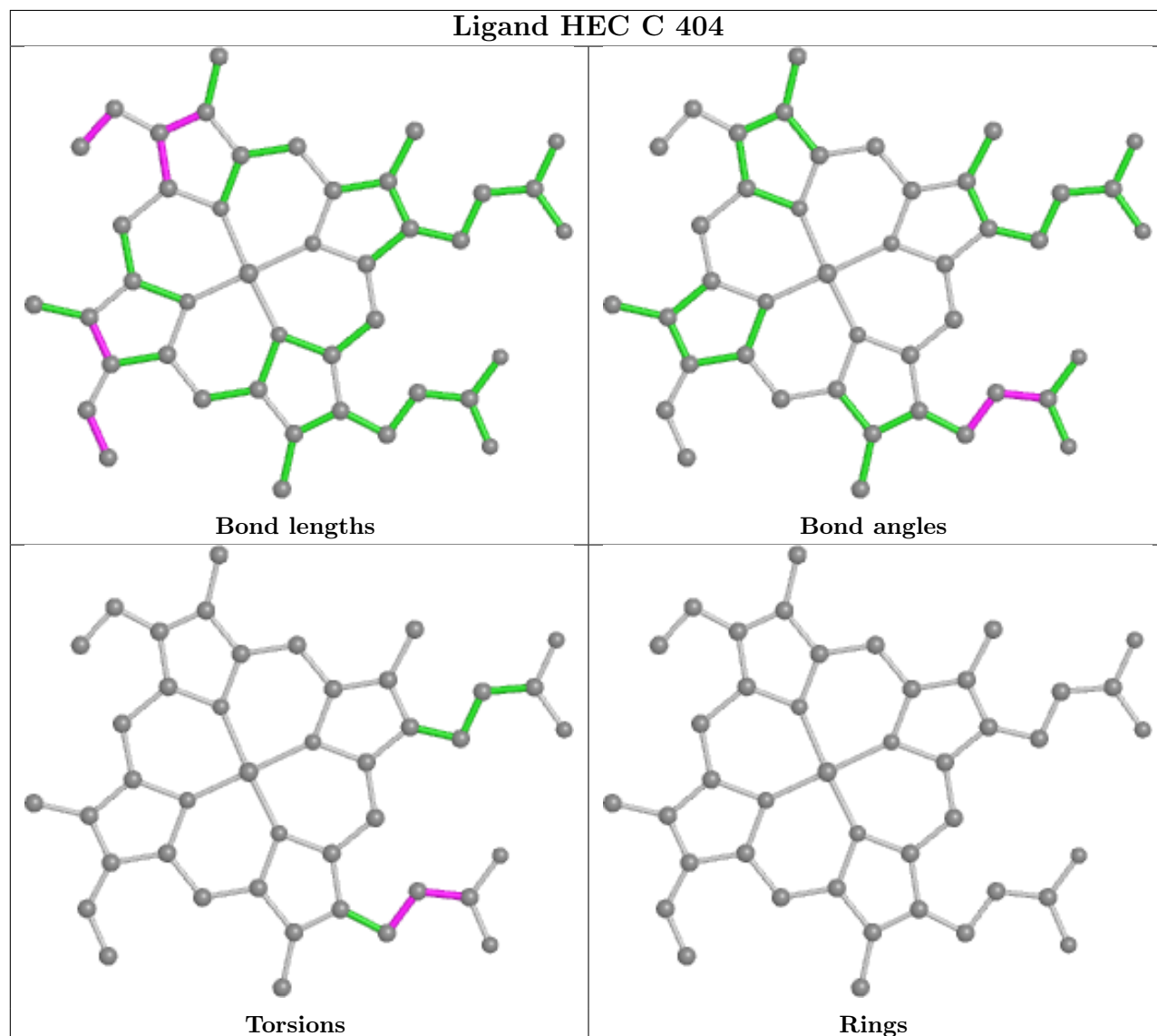


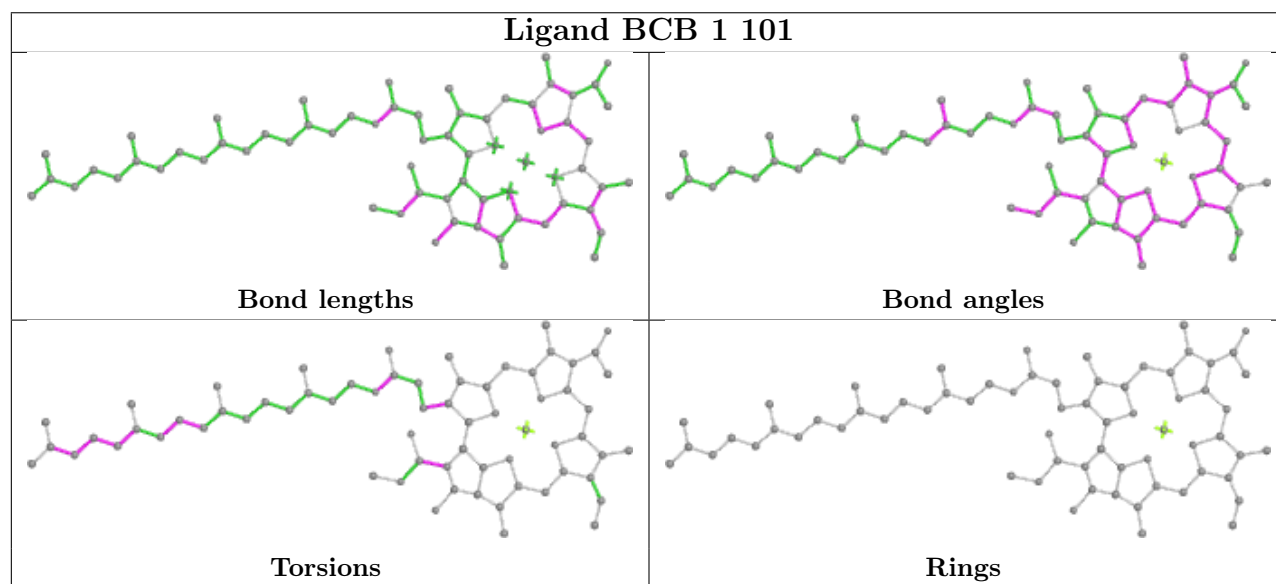
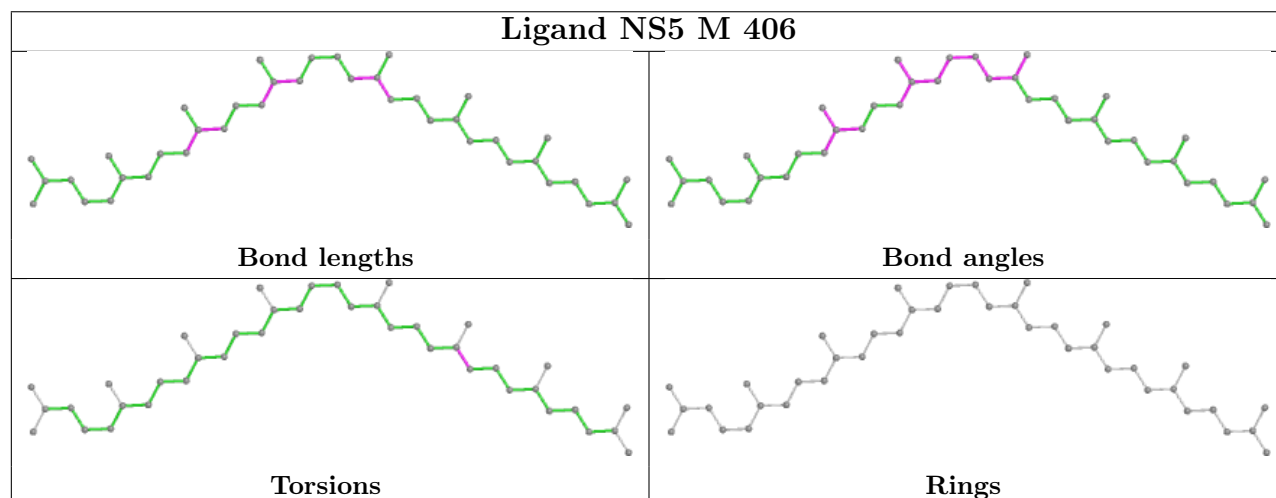
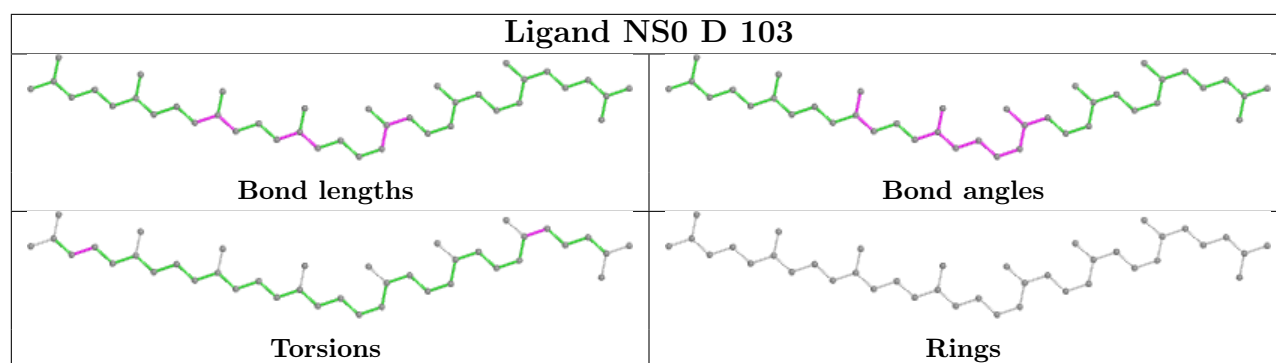


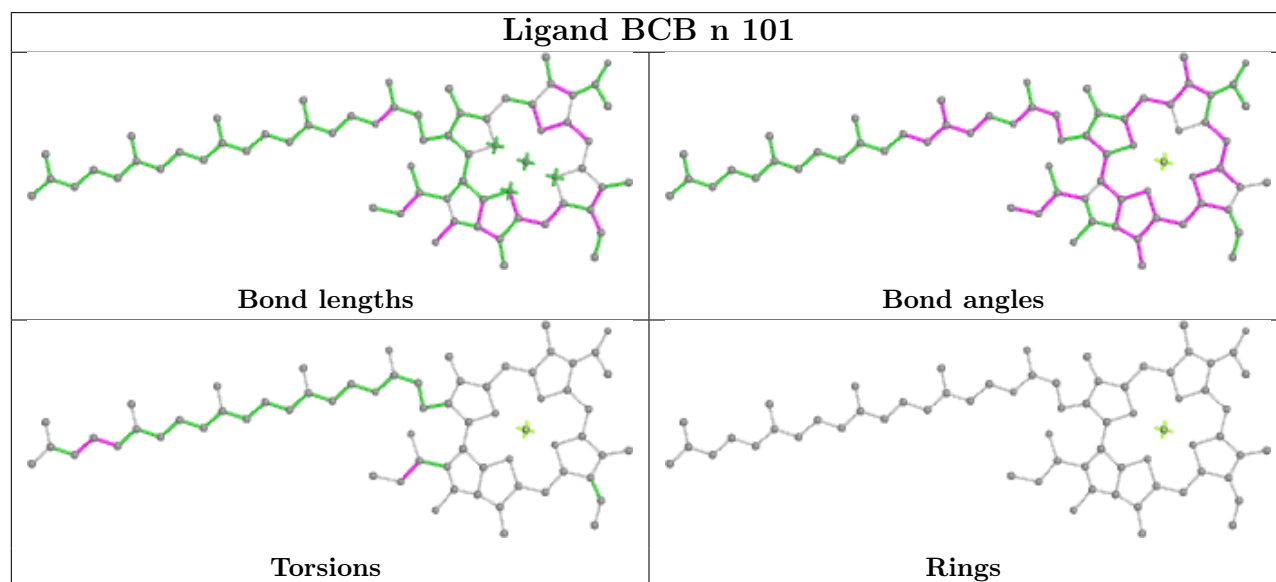
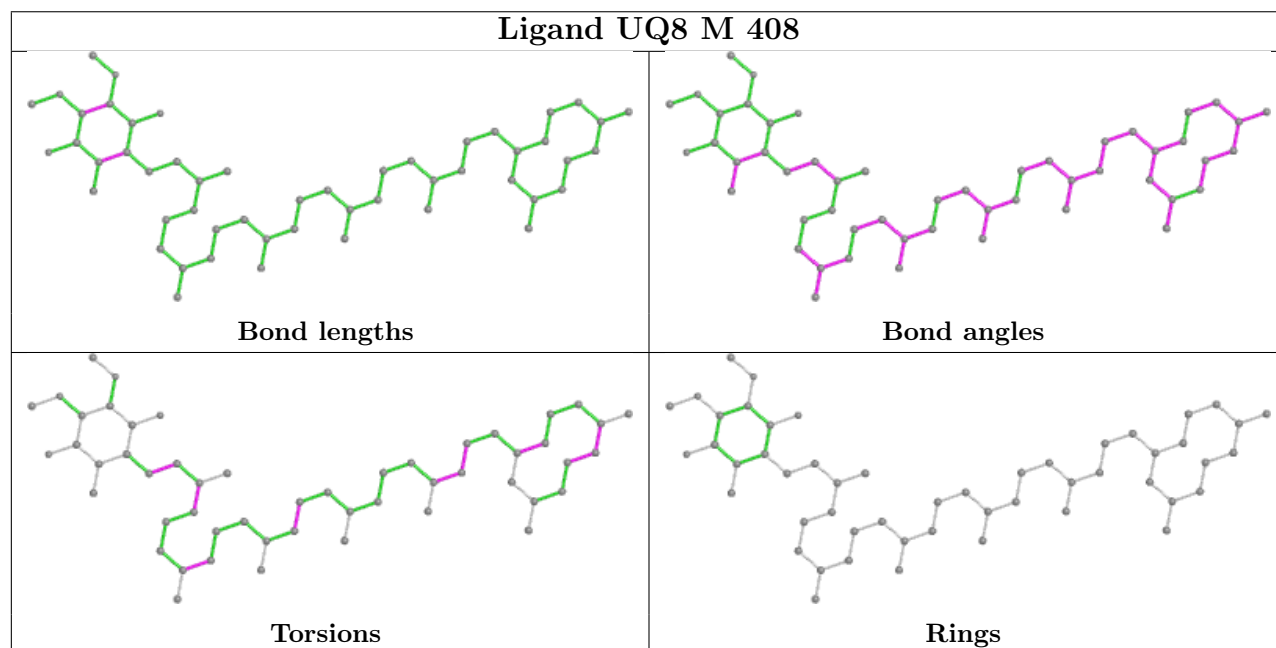
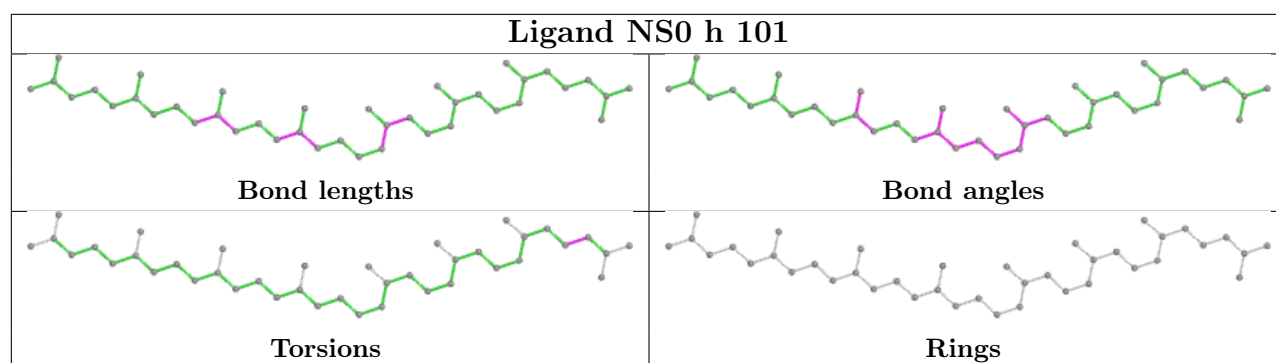
Ligand BCB k 102

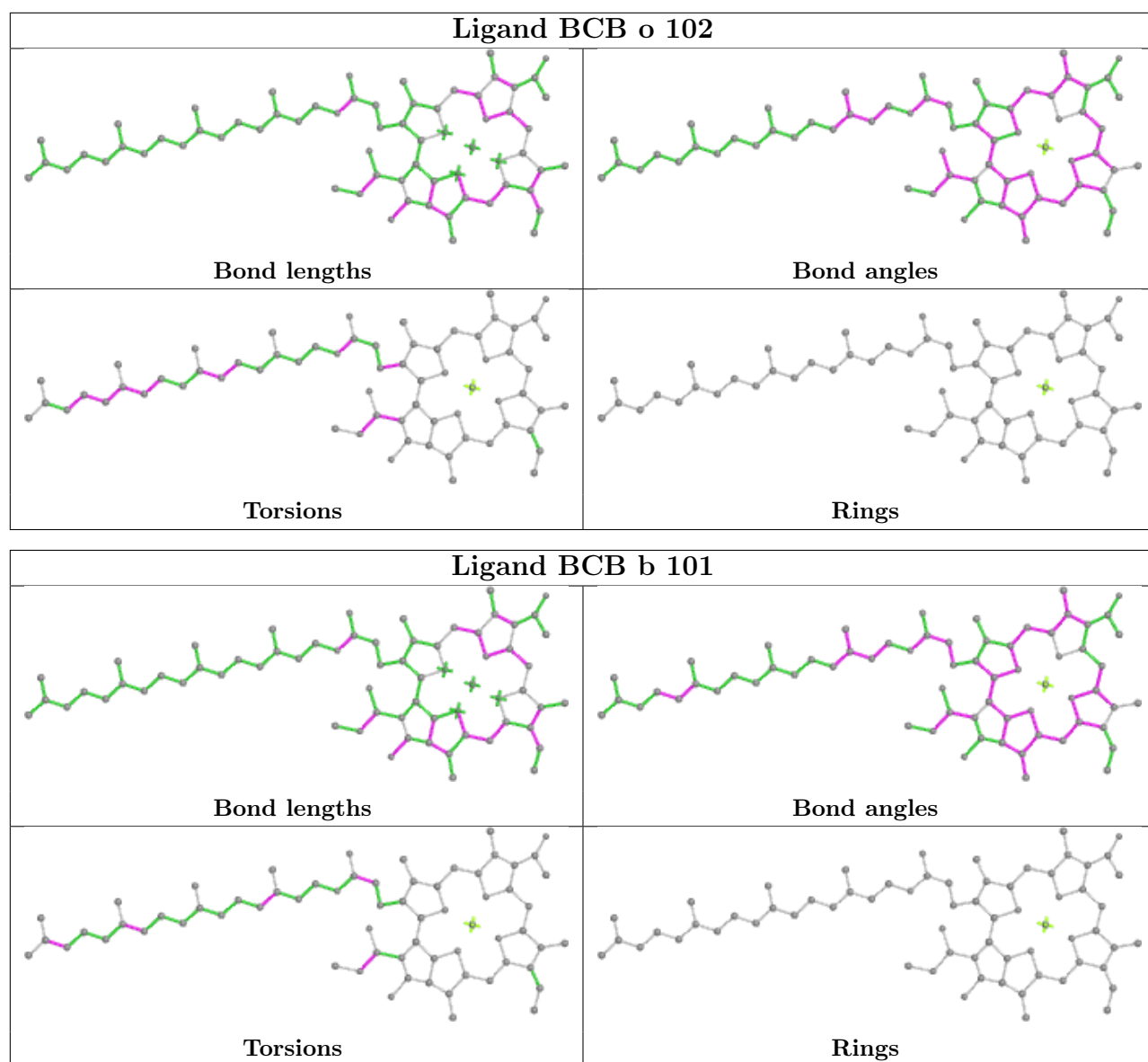


Ligand HEC C 404

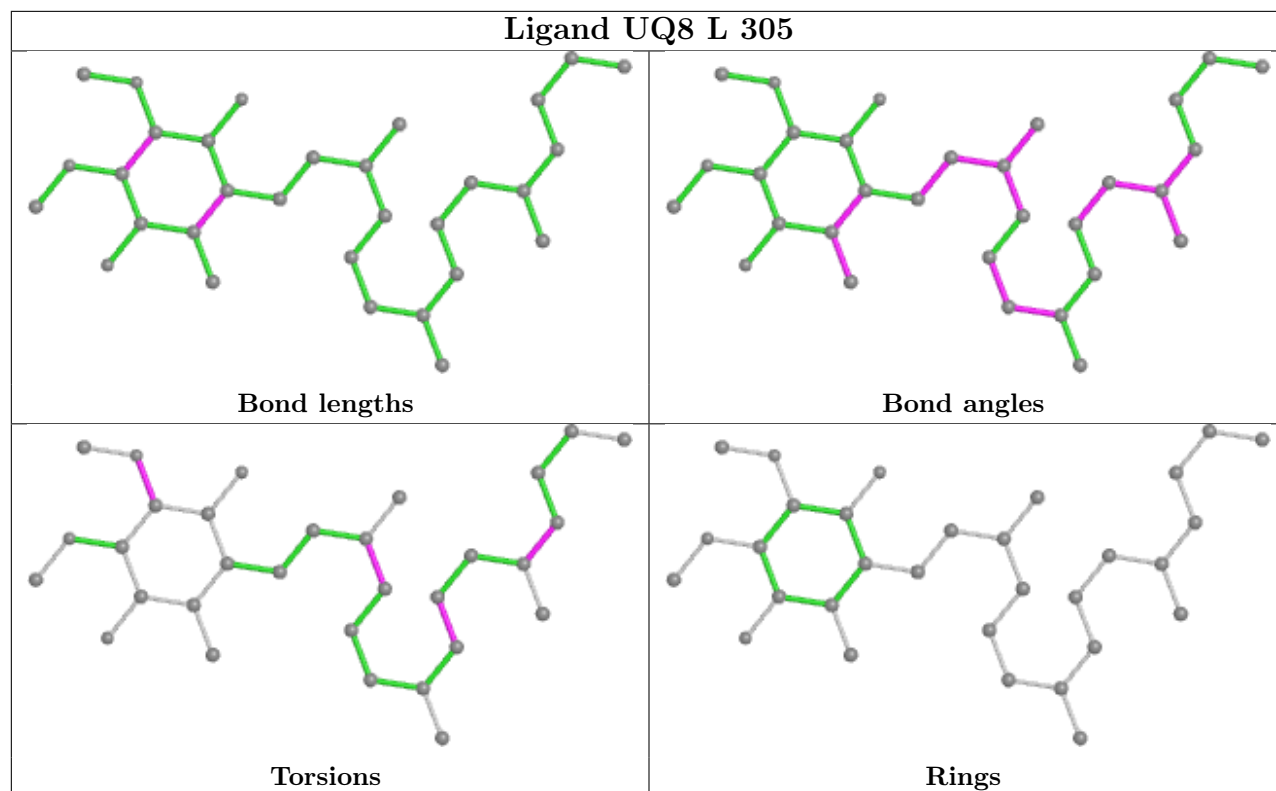




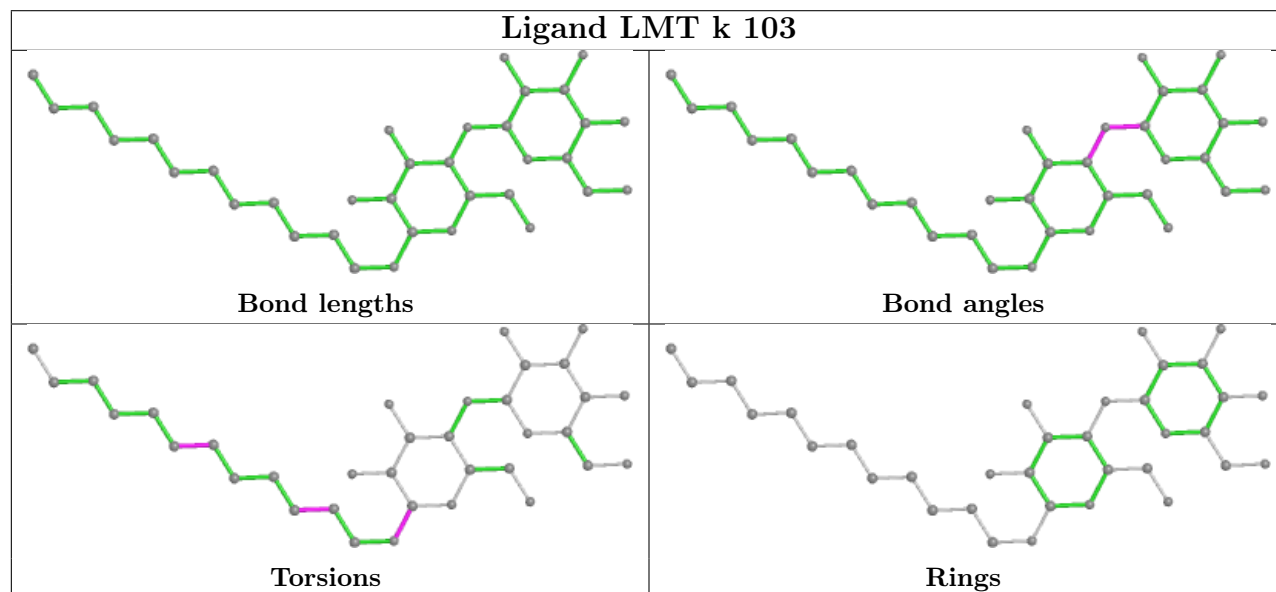


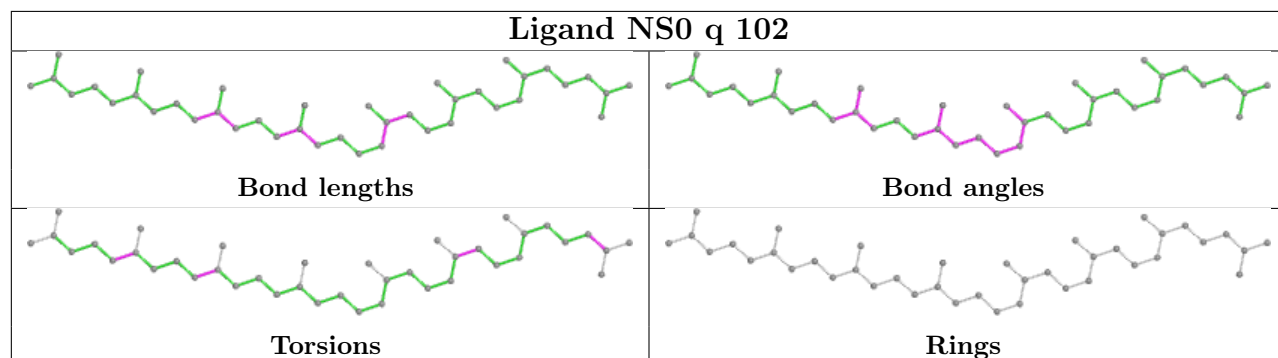
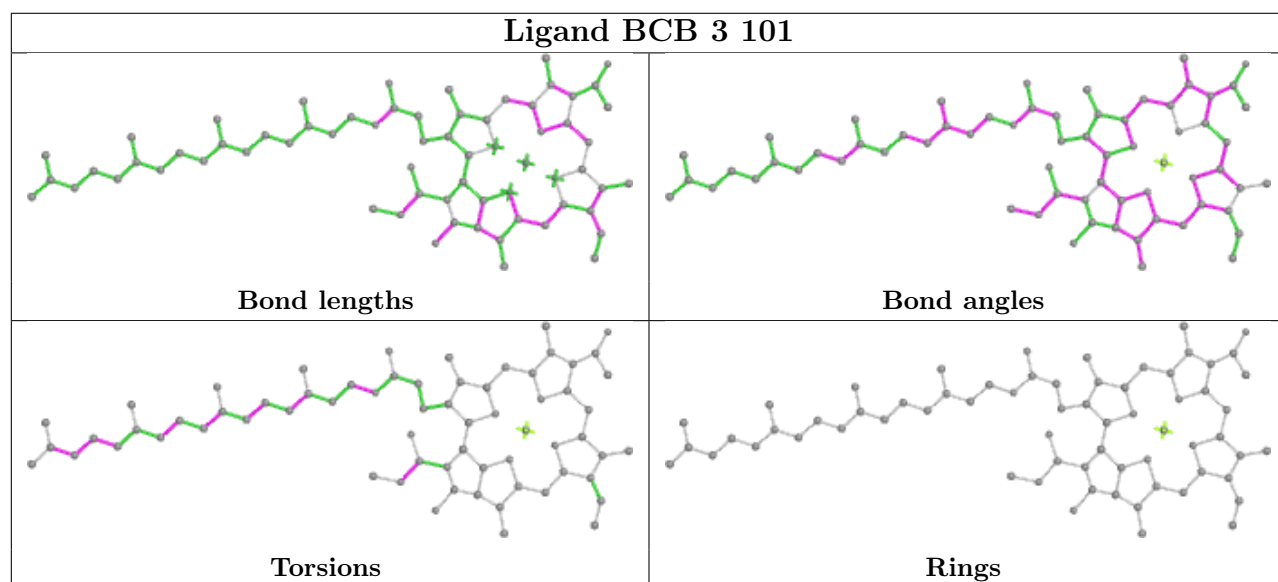
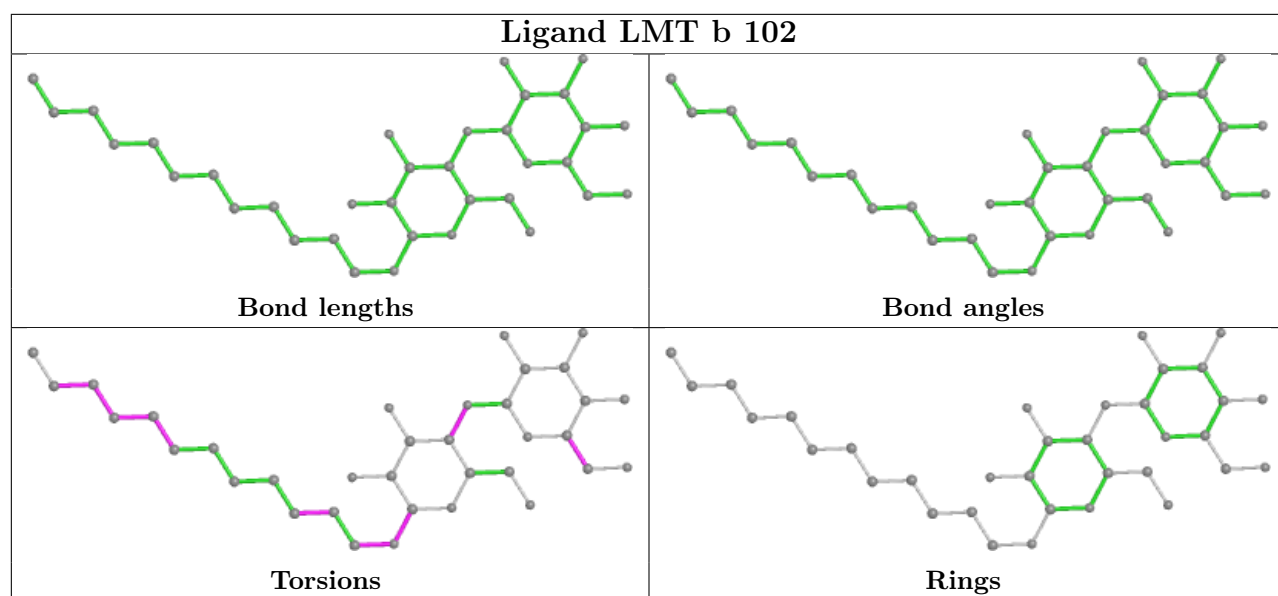


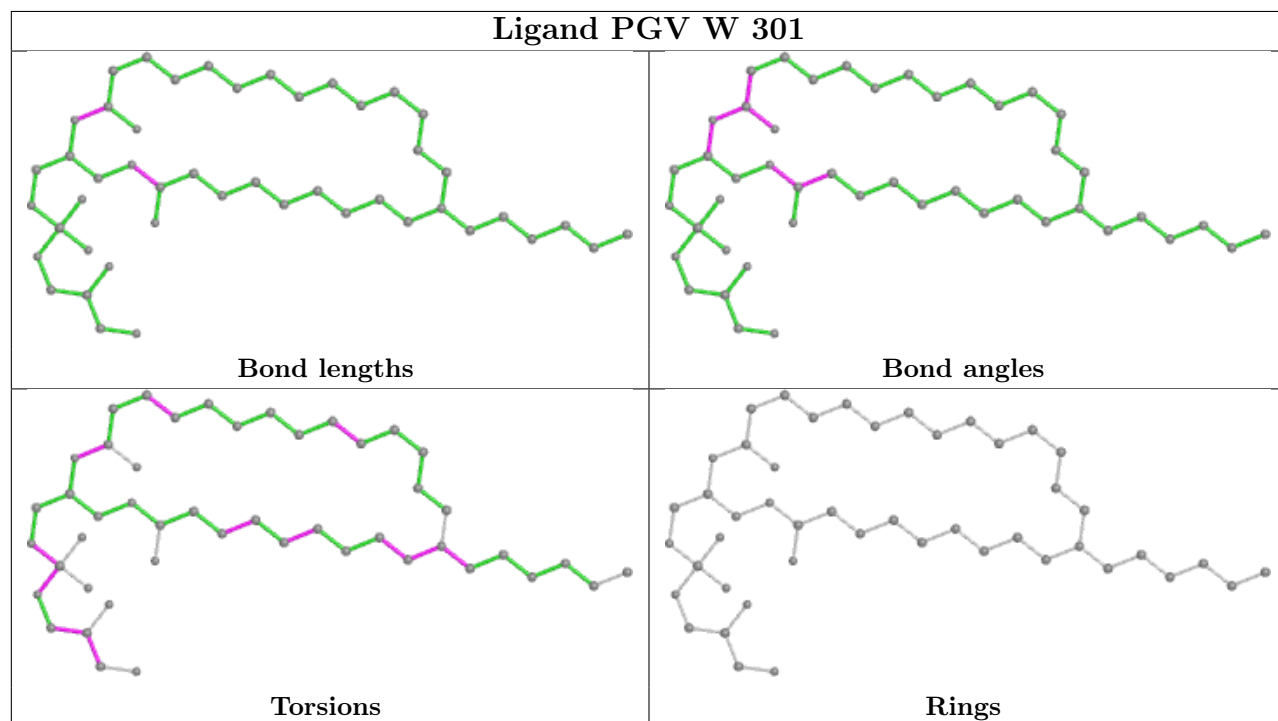
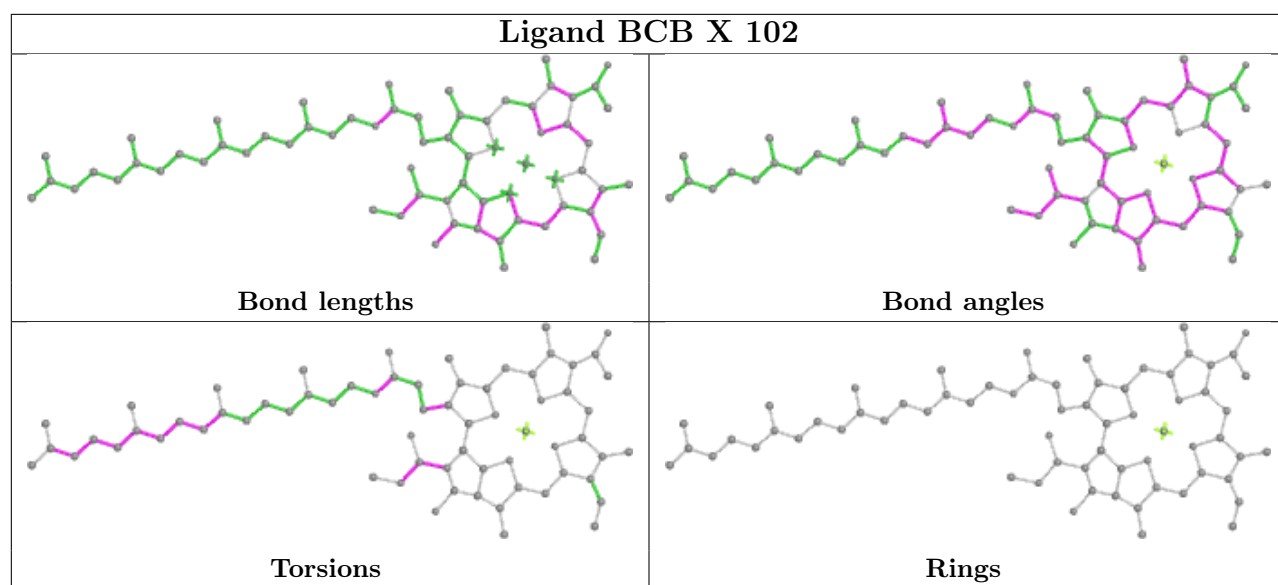
Ligand UQ8 L 305

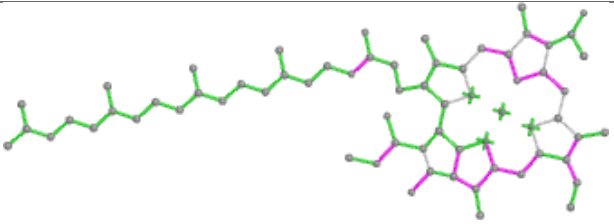
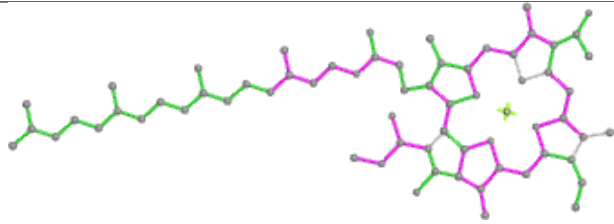
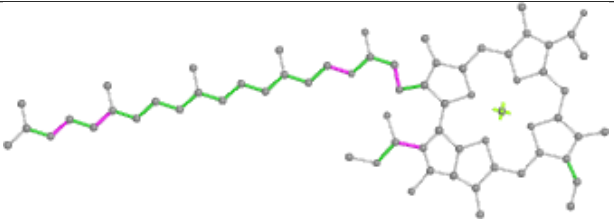
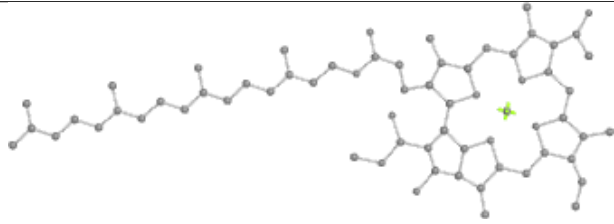
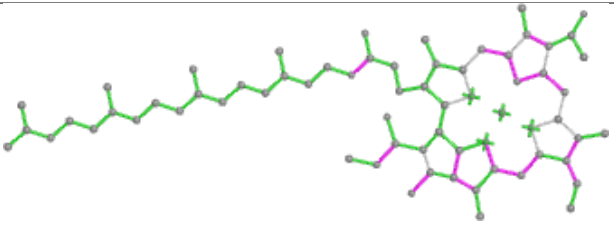
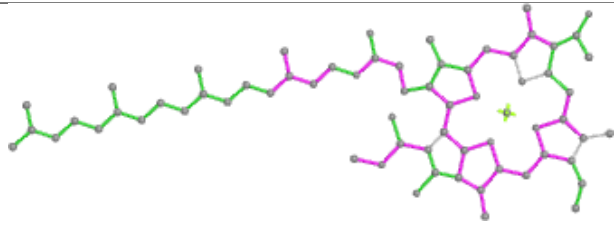
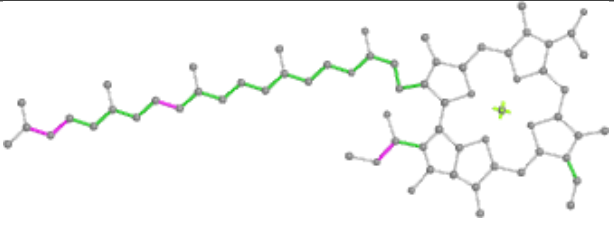
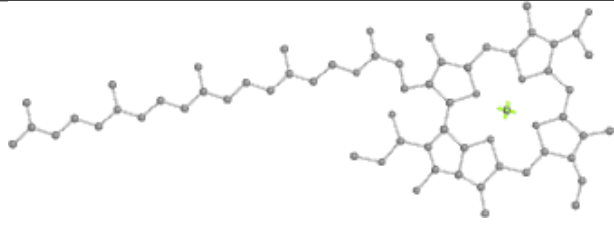
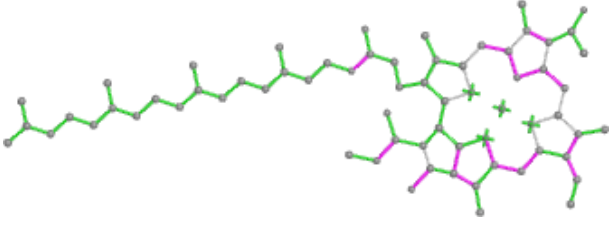
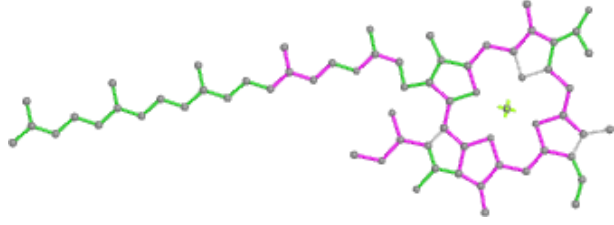
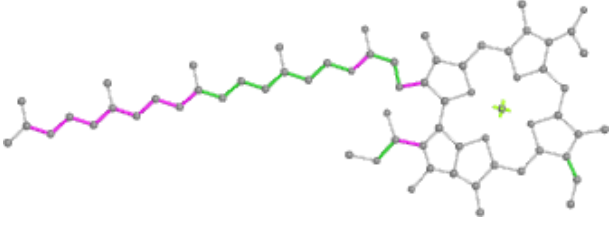
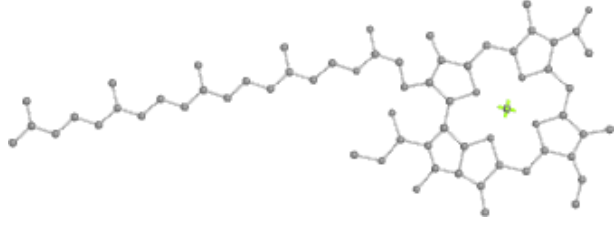


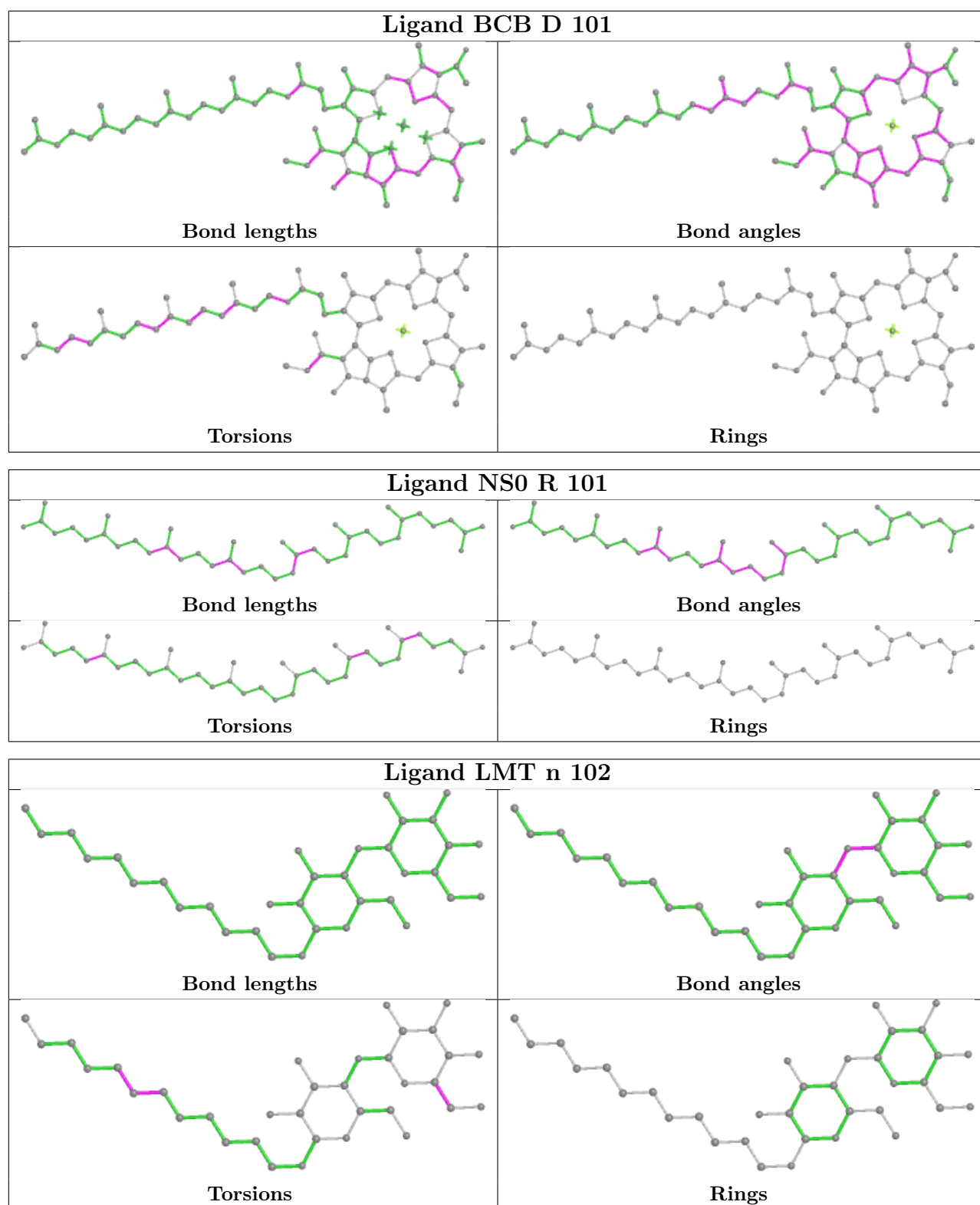
Ligand LMT k 103

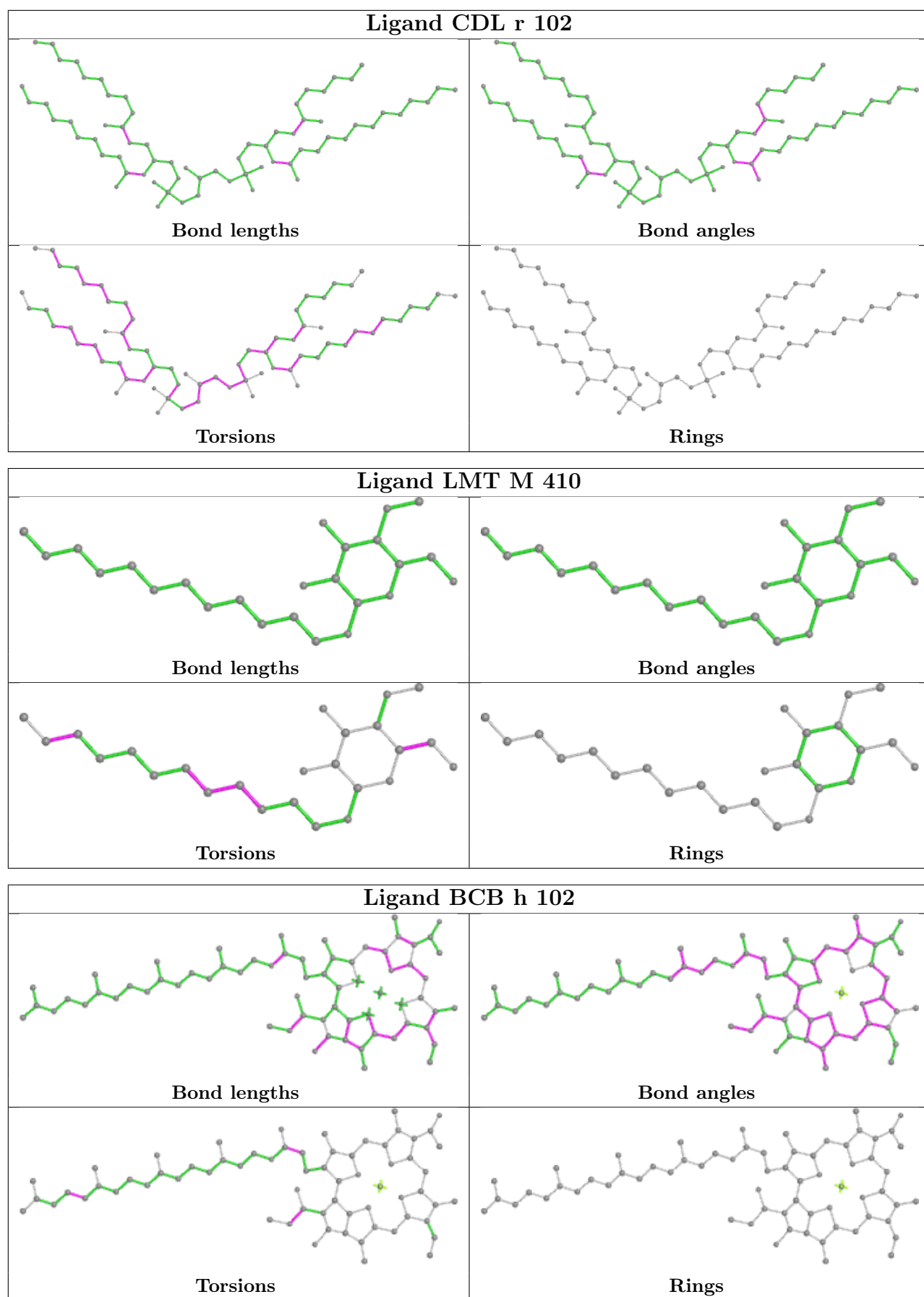


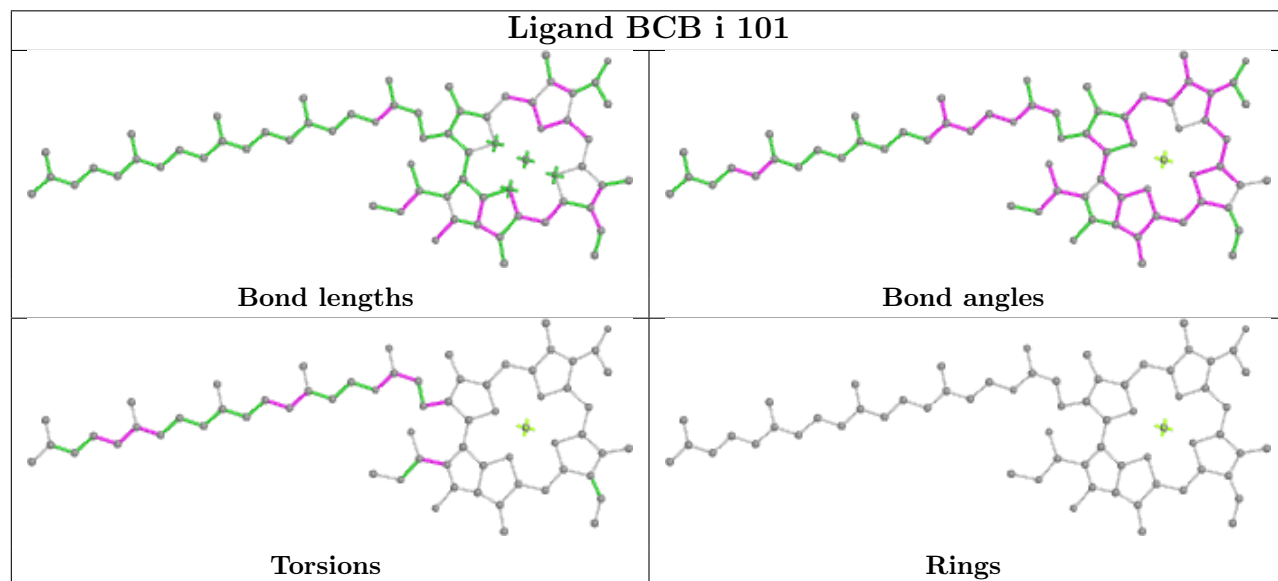
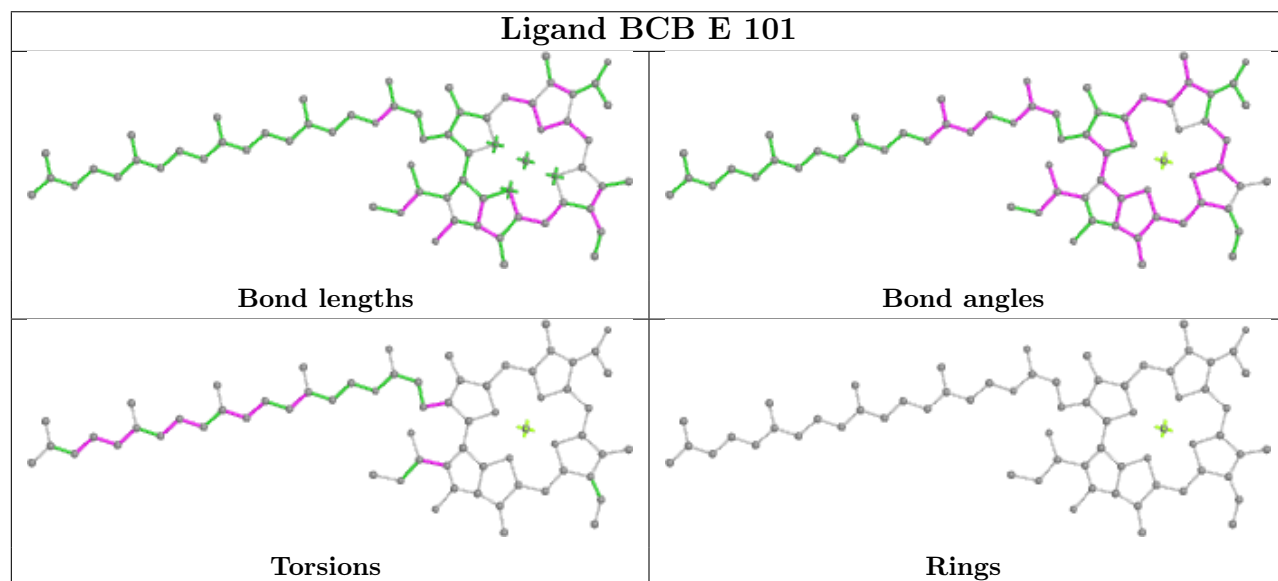
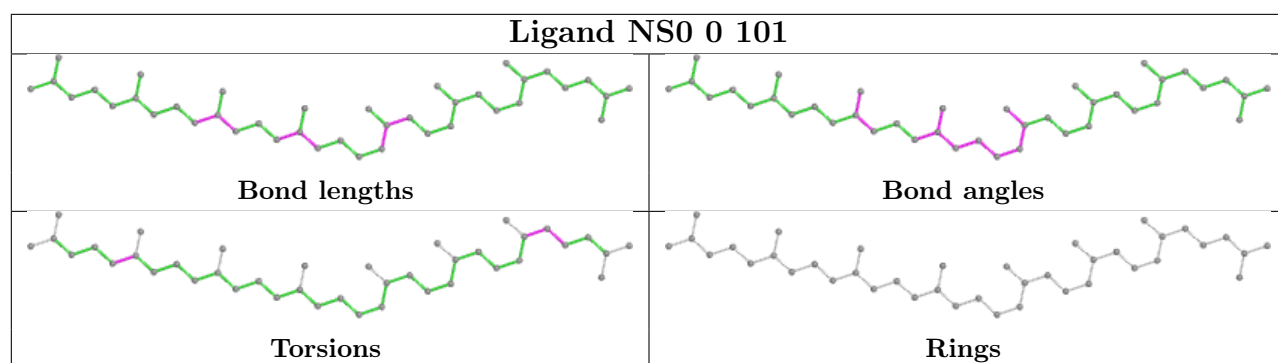


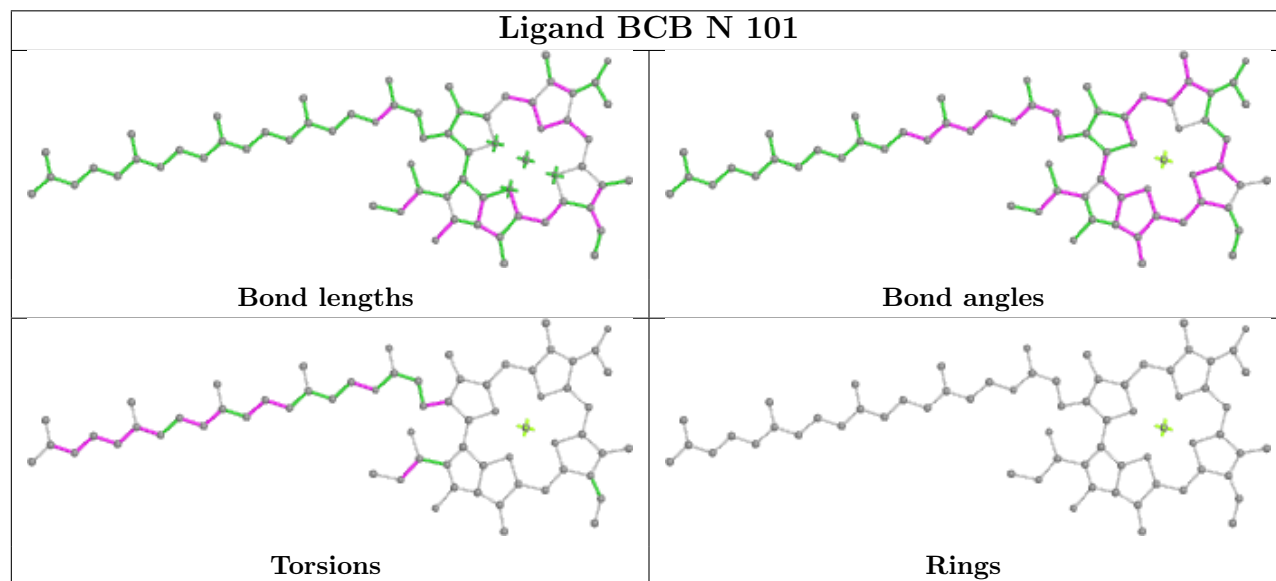
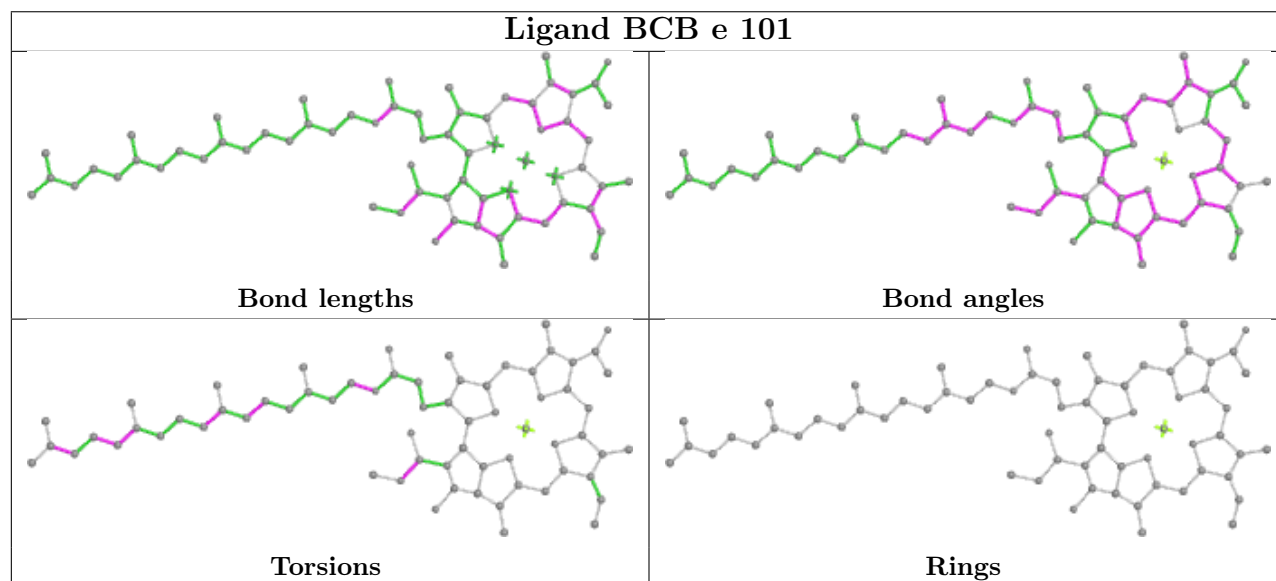
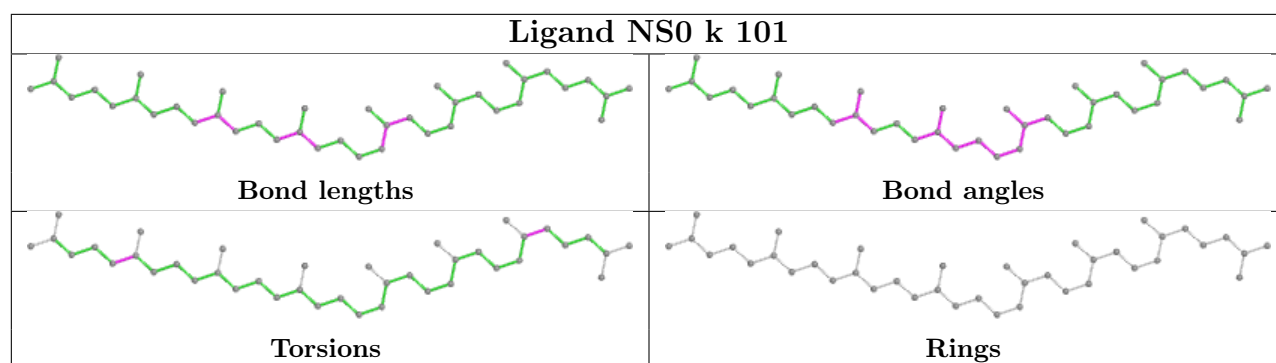


| Ligand BCB M 403 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand BCB 6 101 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand BCB f 101 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |

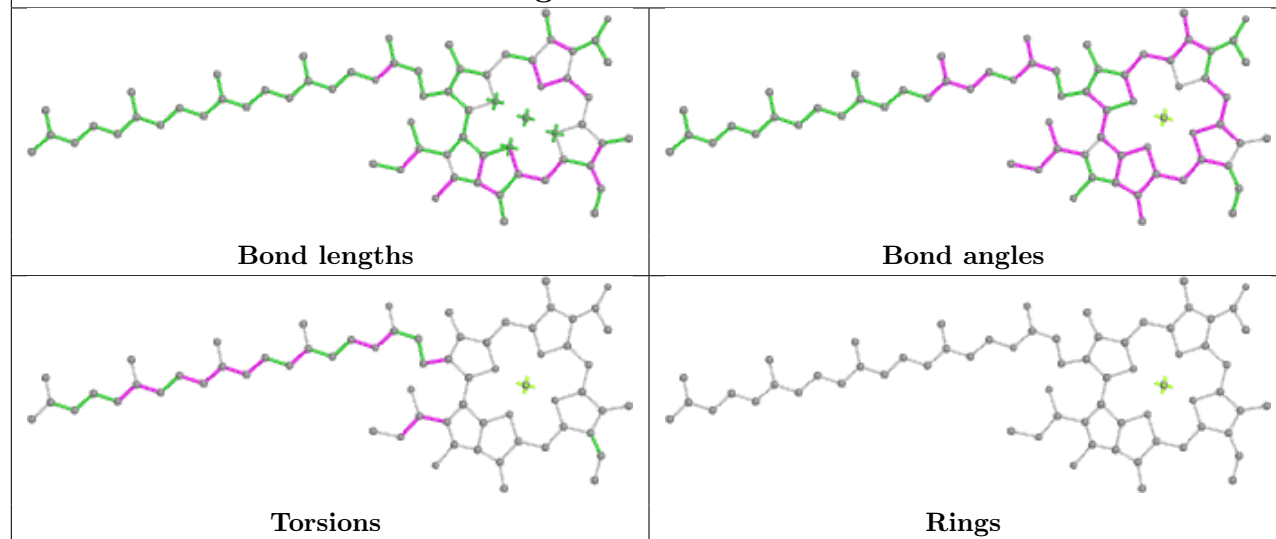




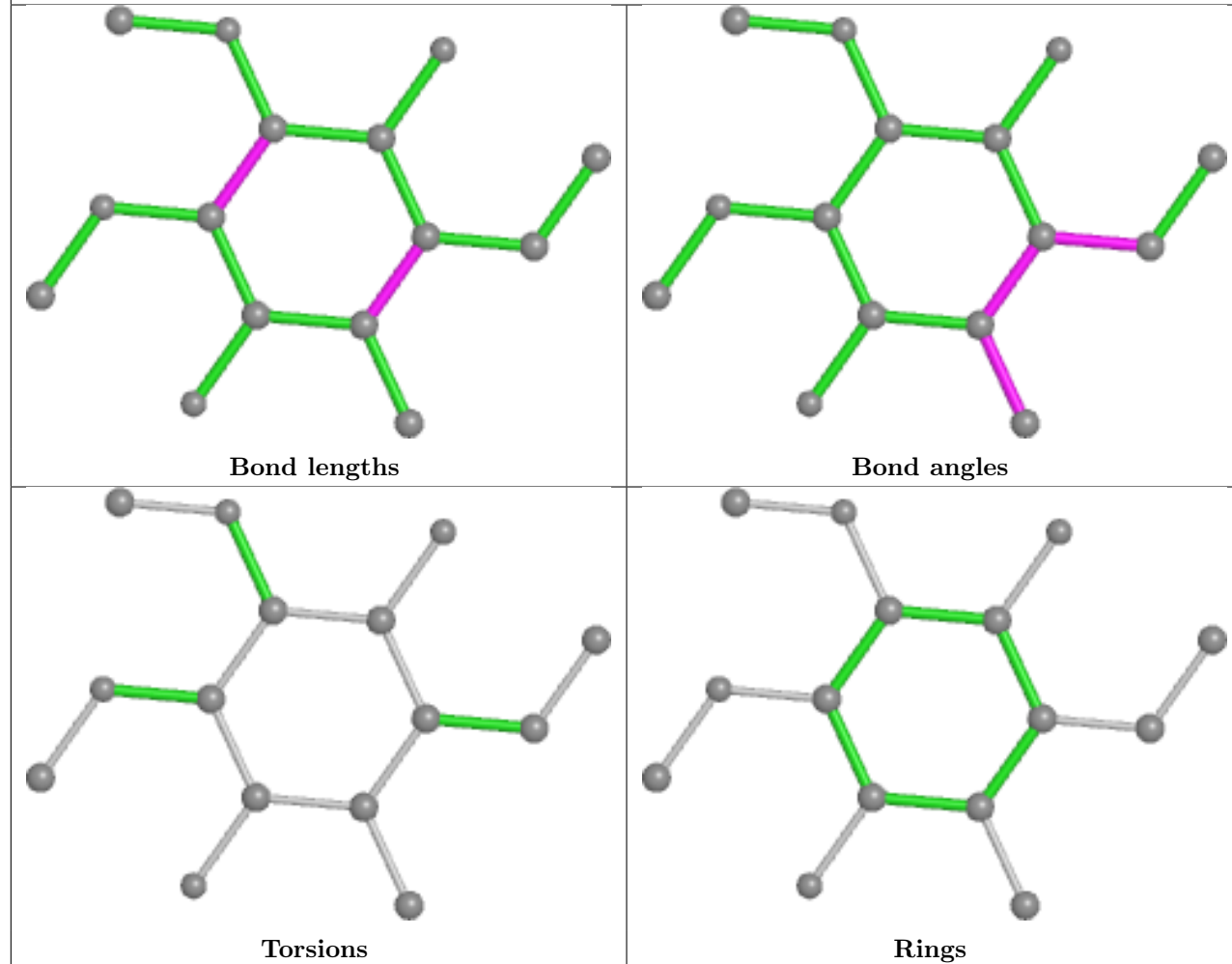


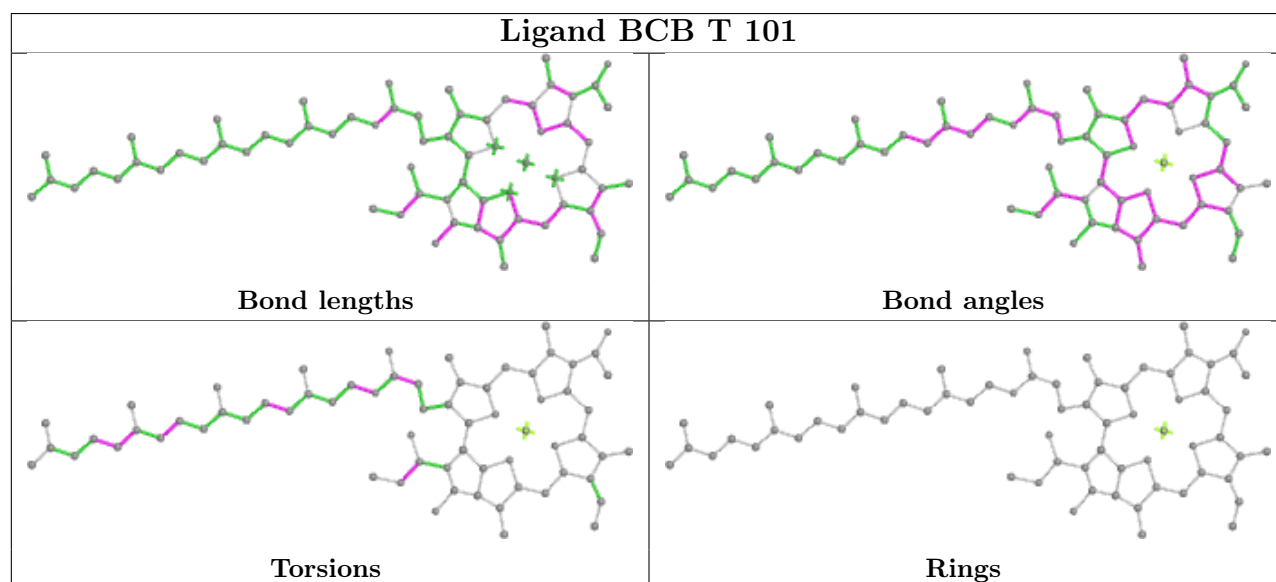
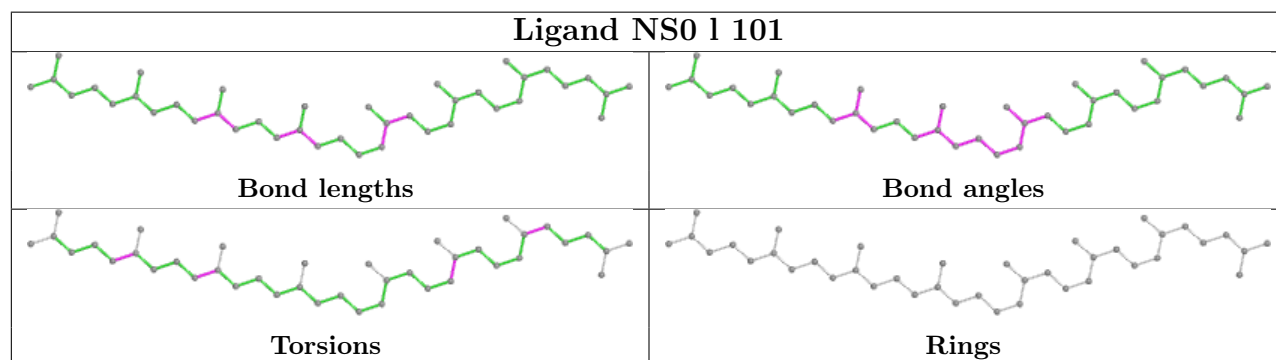
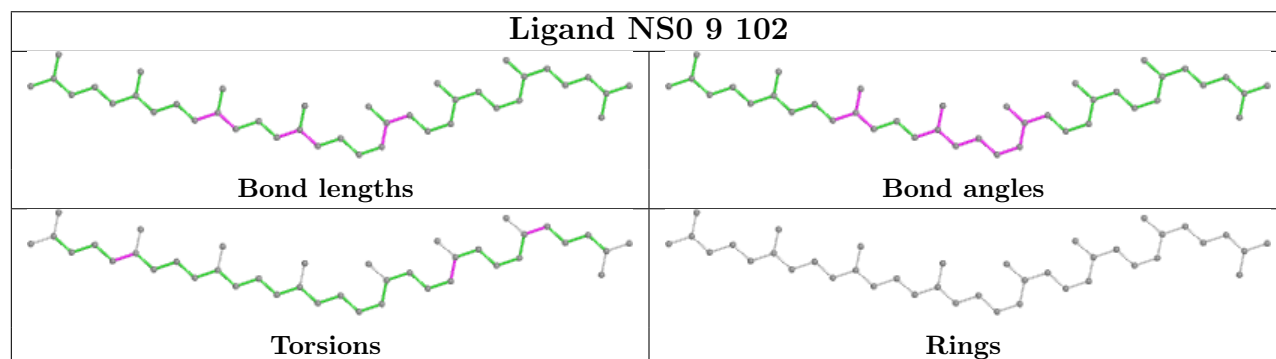
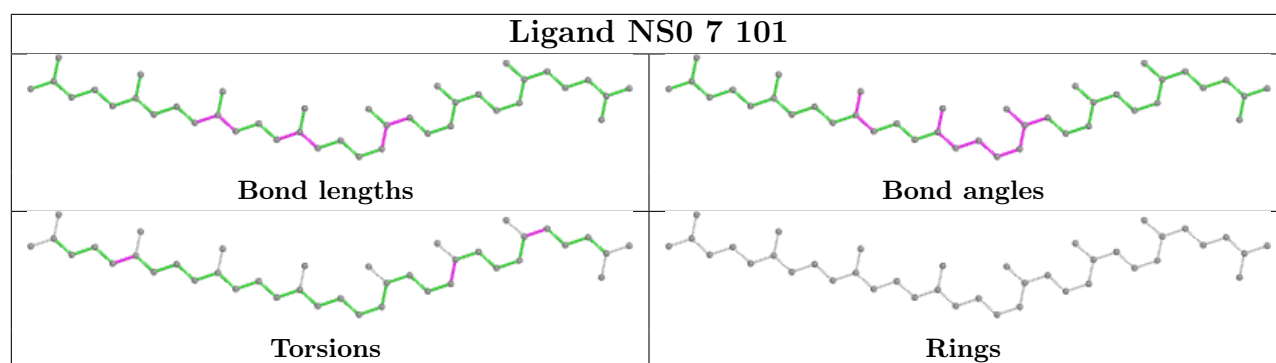


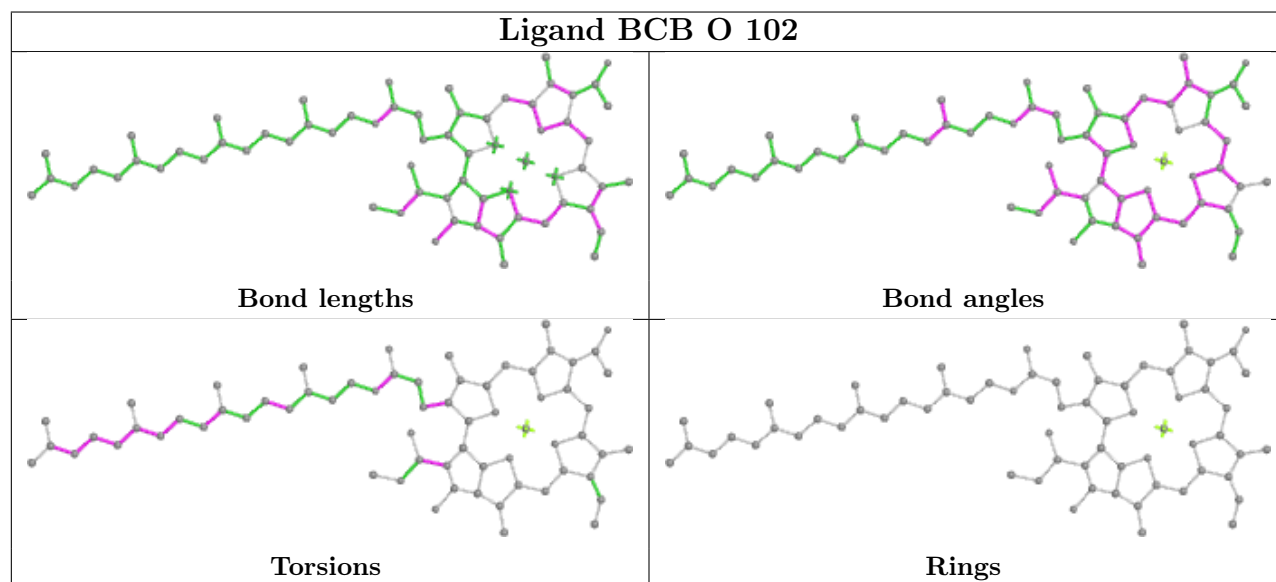
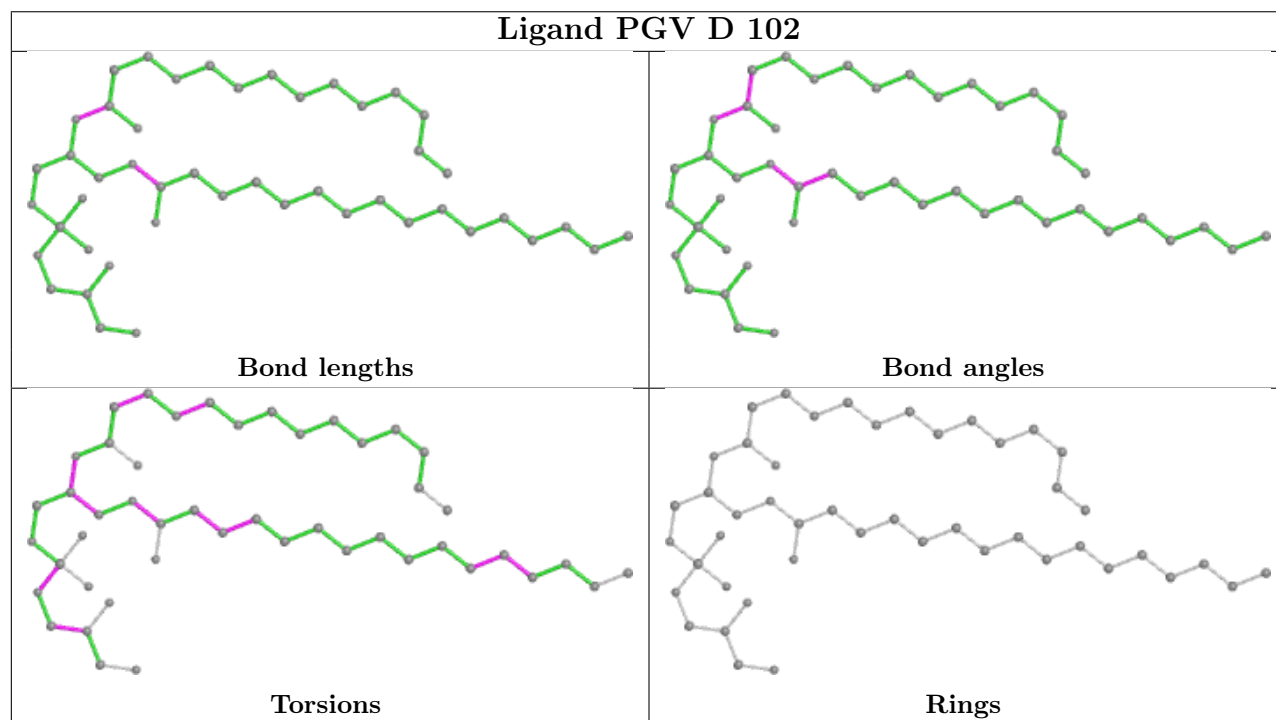
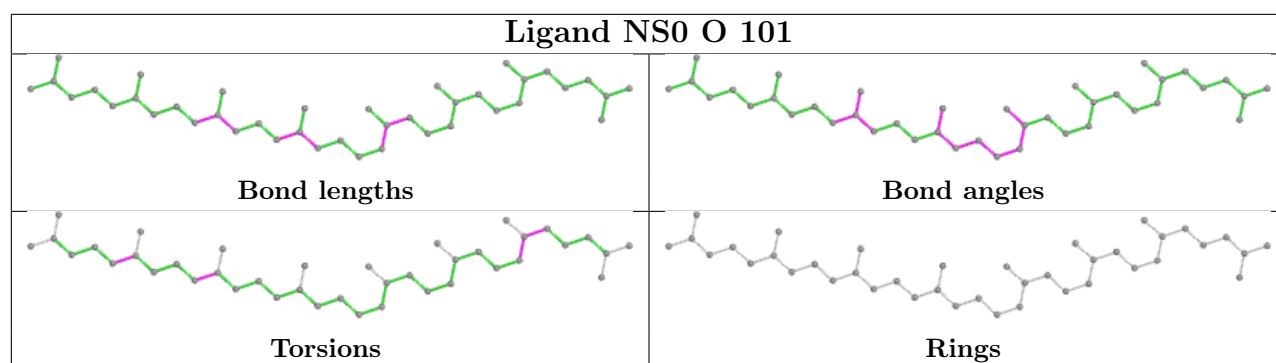
Ligand BCB 7 102

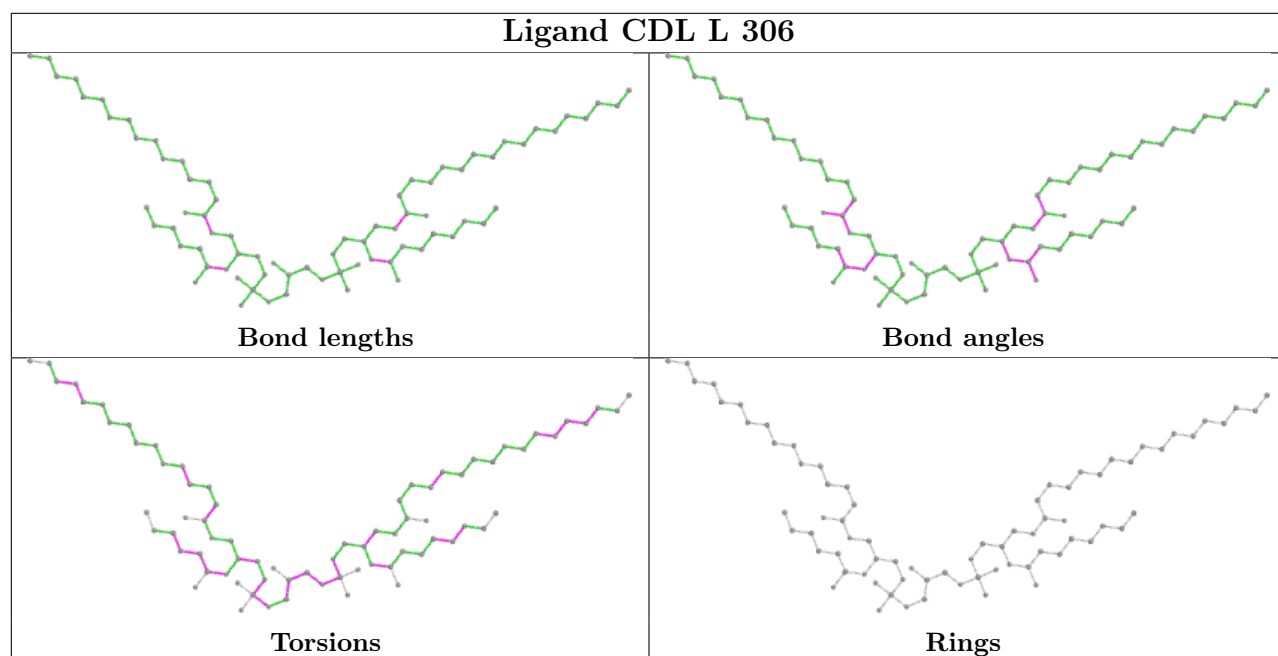
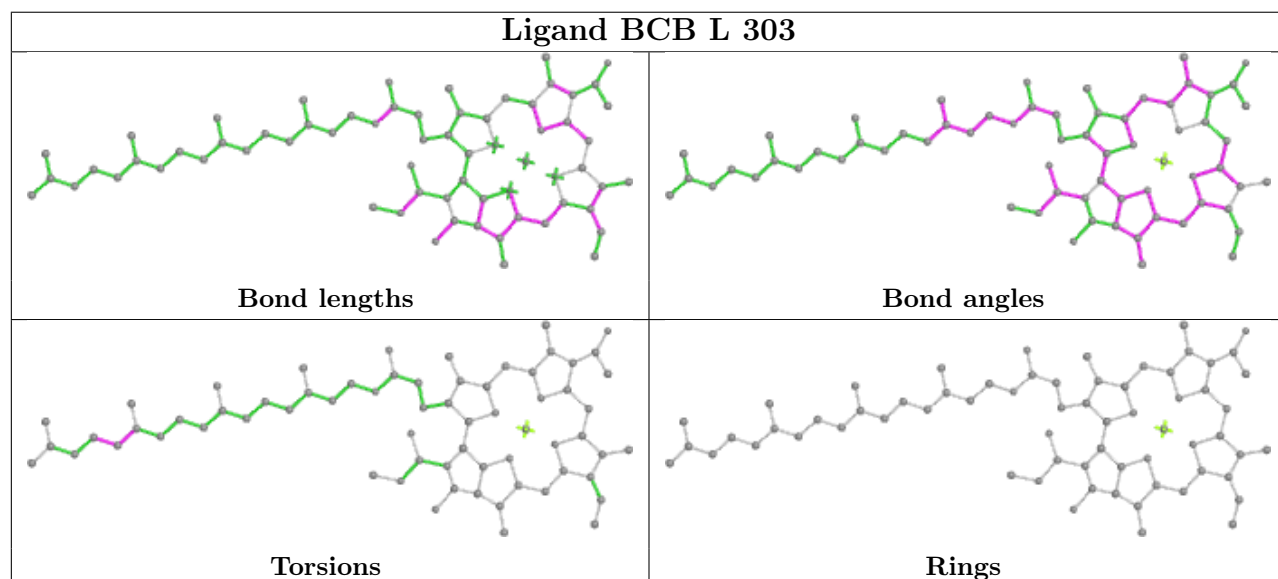
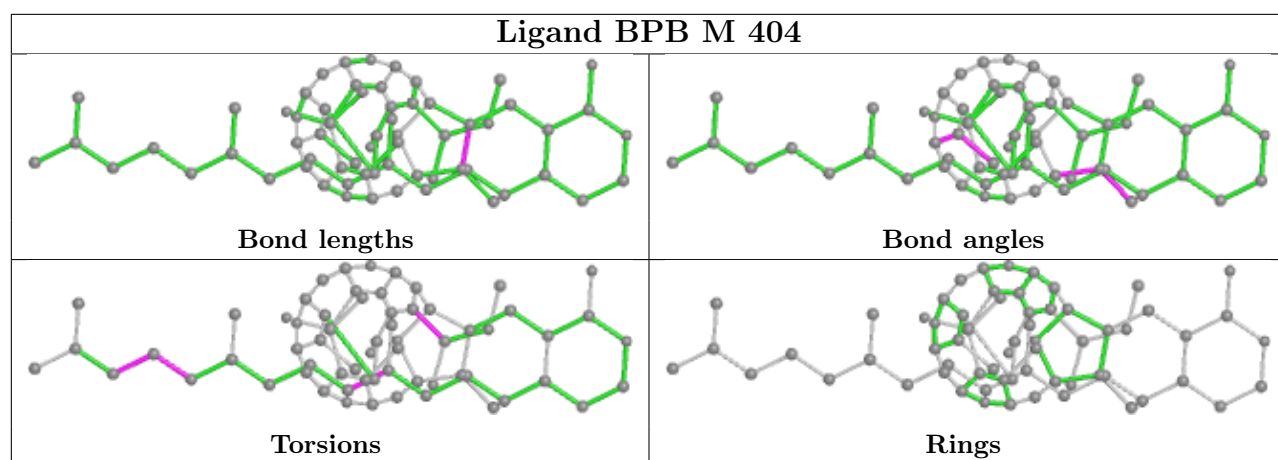


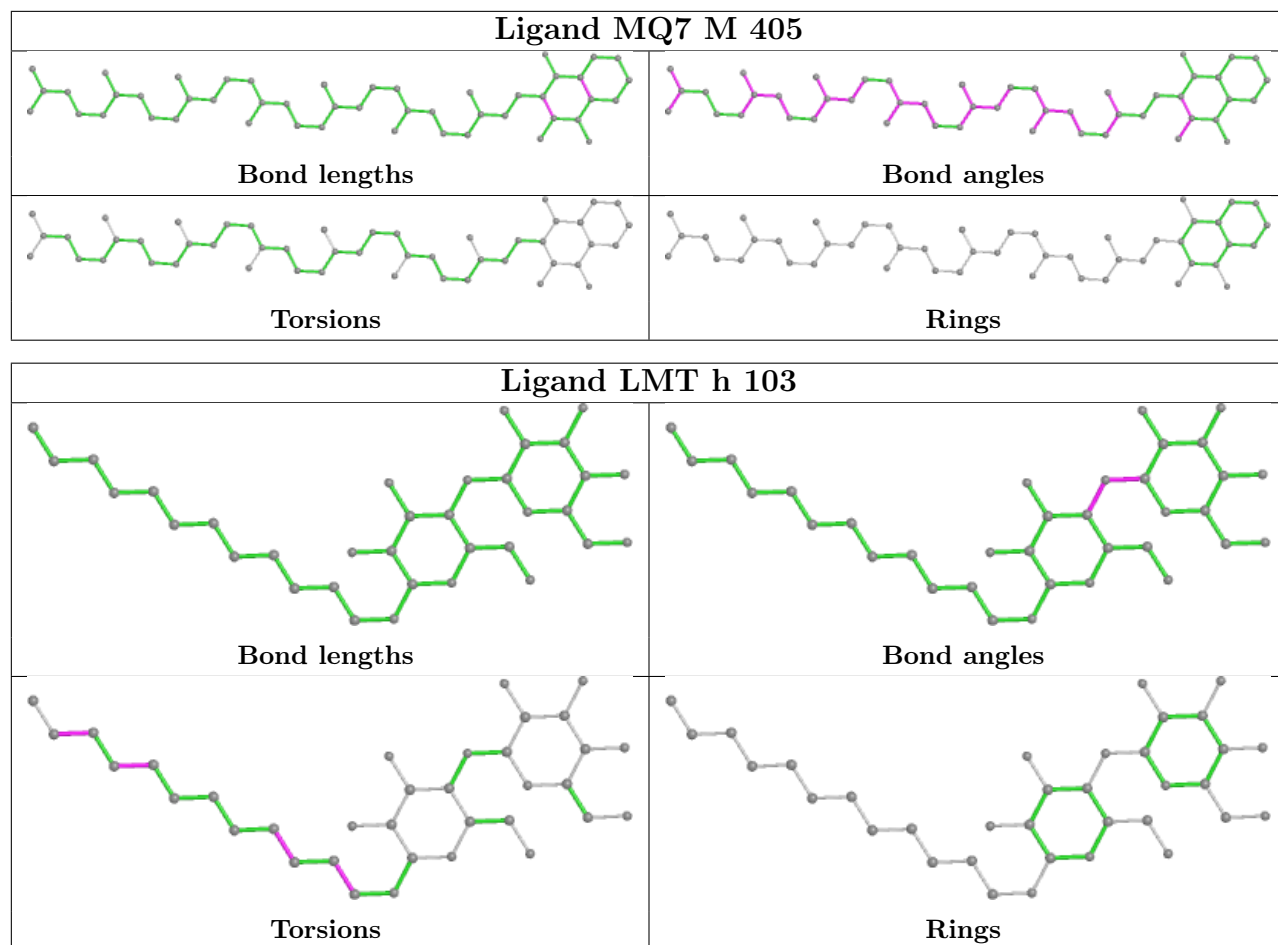
Ligand UQ8 C 406

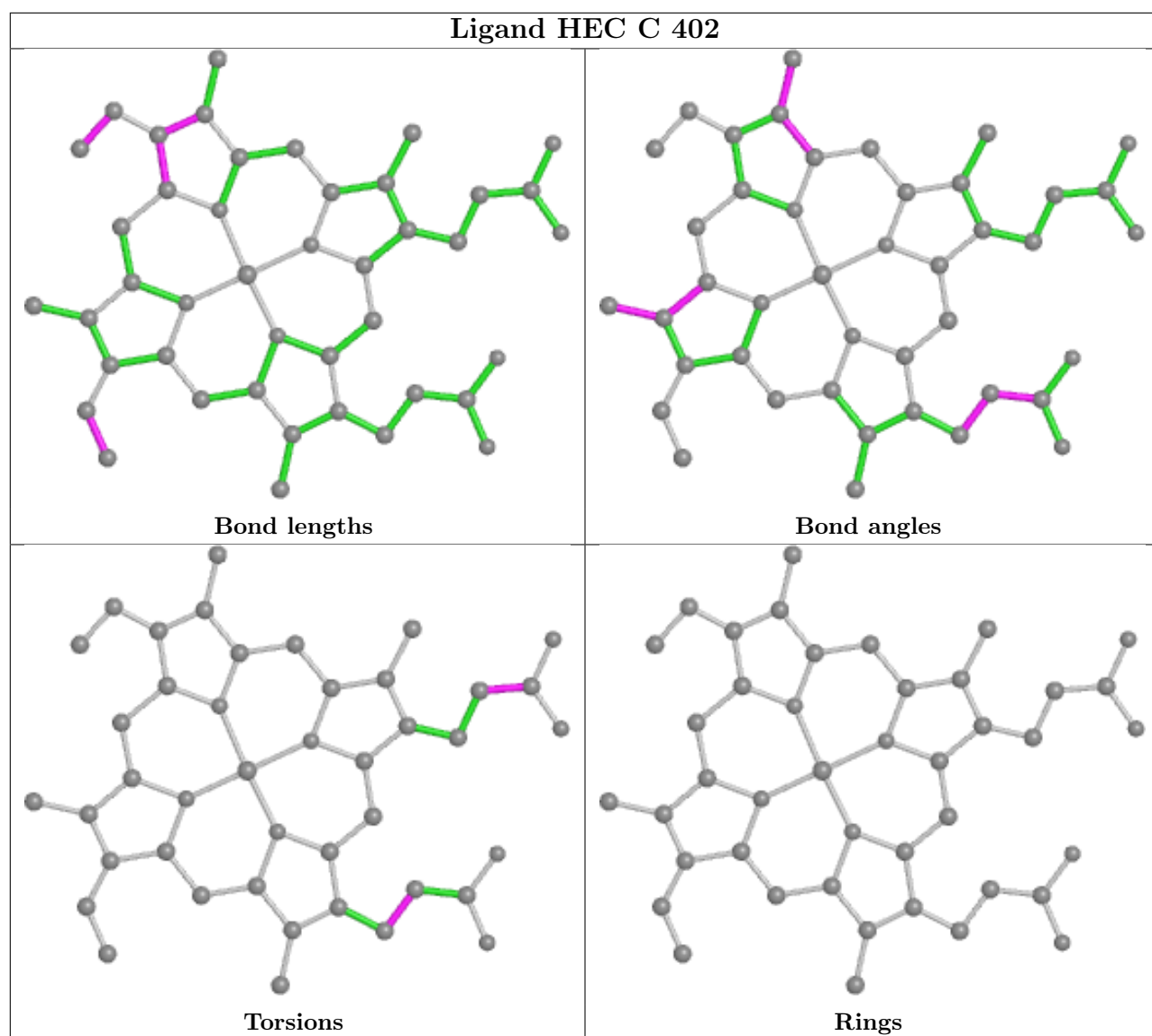




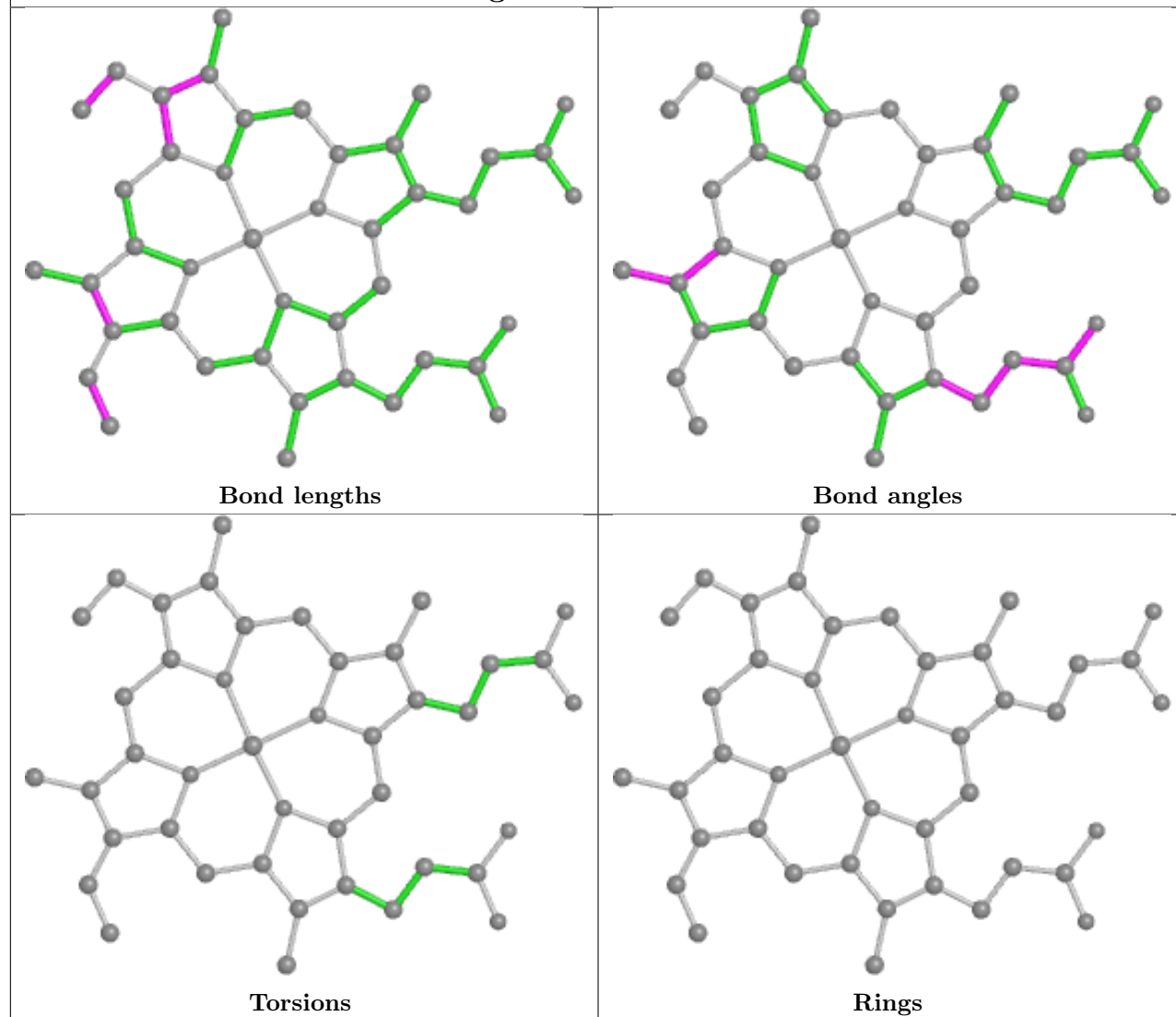




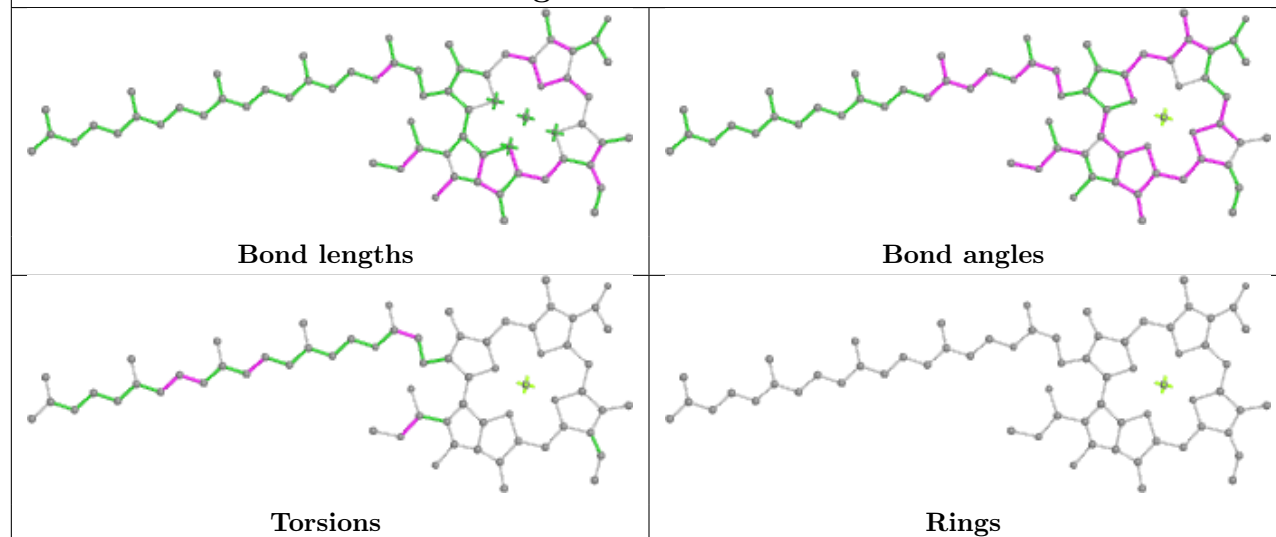


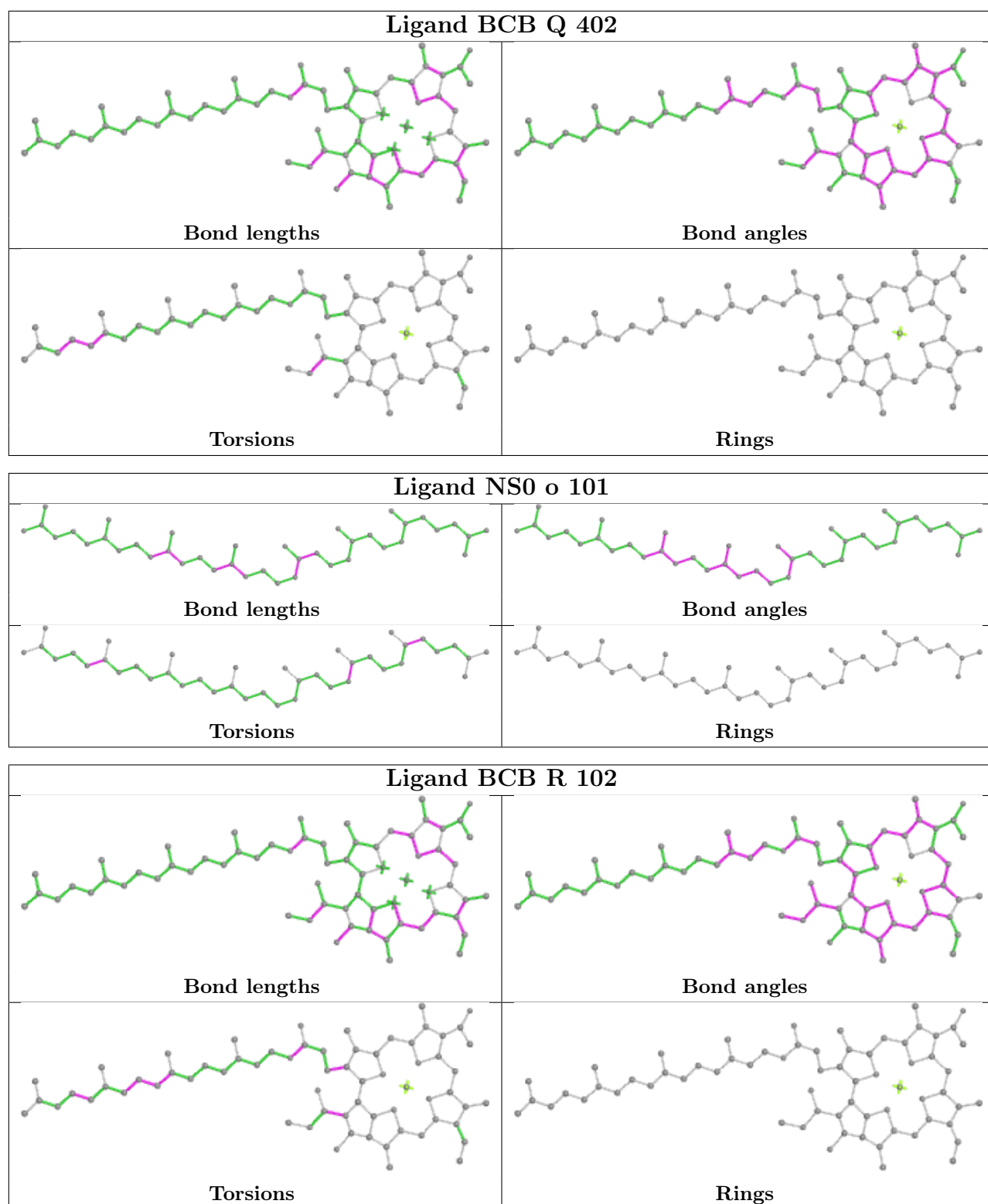


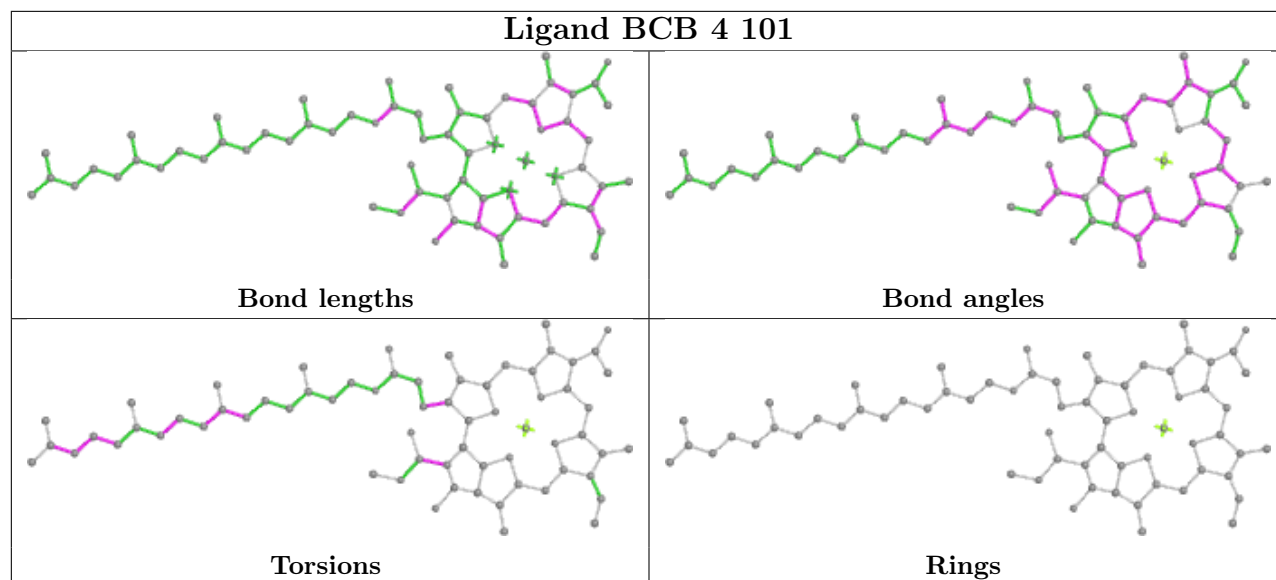
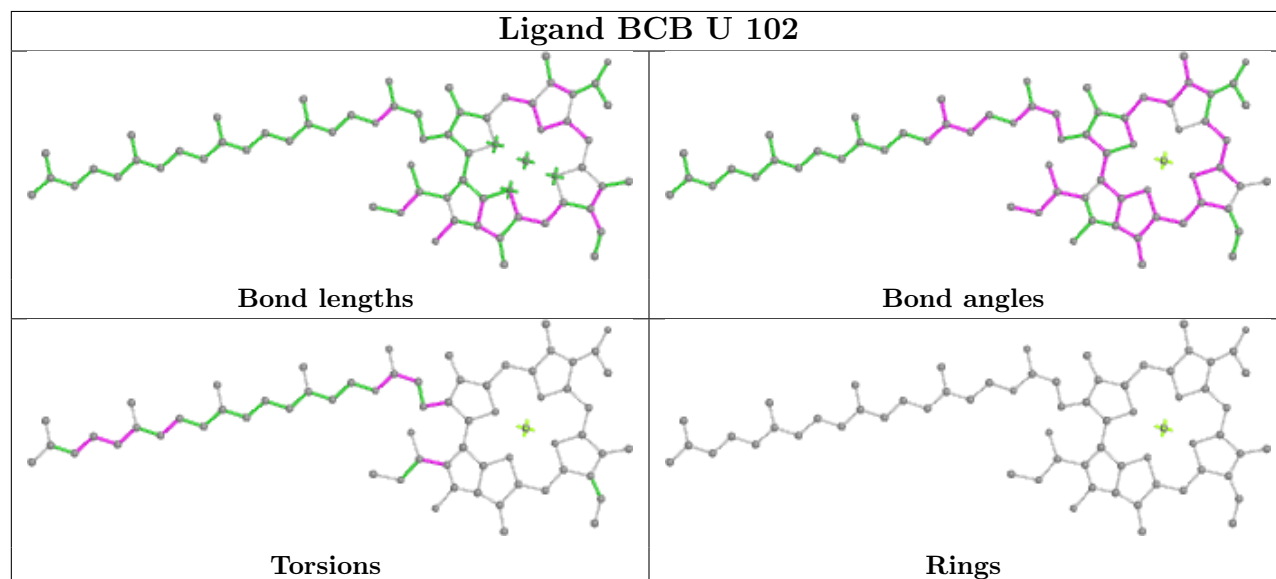
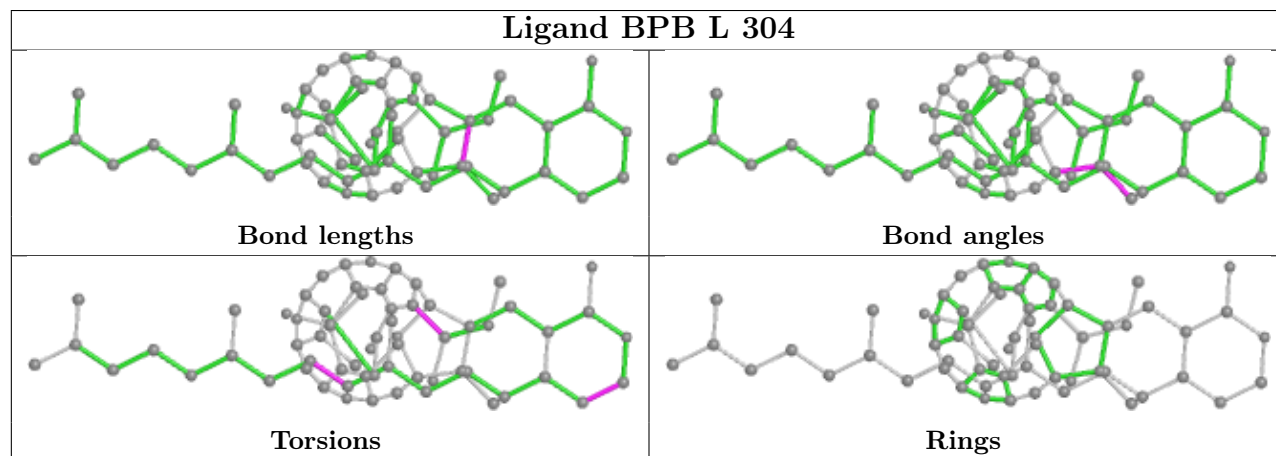
Ligand HEC C 403

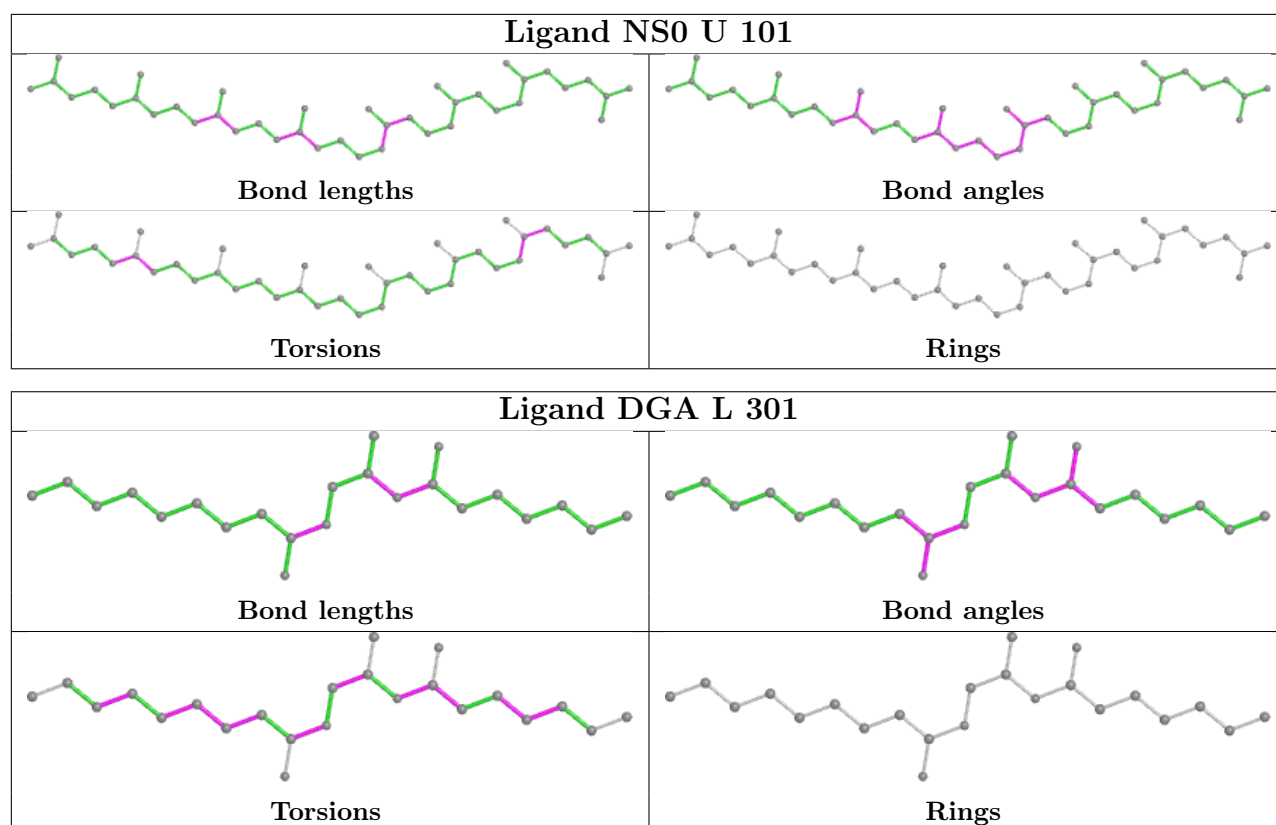


Ligand BCB Z 101





Ligand BCB 4 101**Ligand BCB U 102****Ligand BPB L 304**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

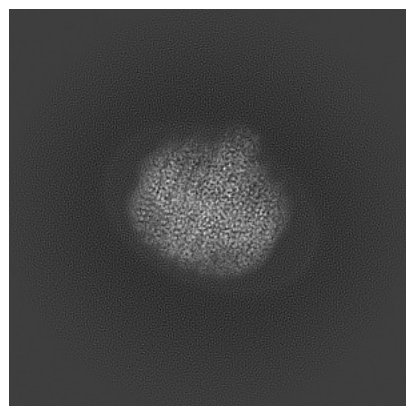
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61095. These allow visual inspection of the internal detail of the map and identification of artifacts.

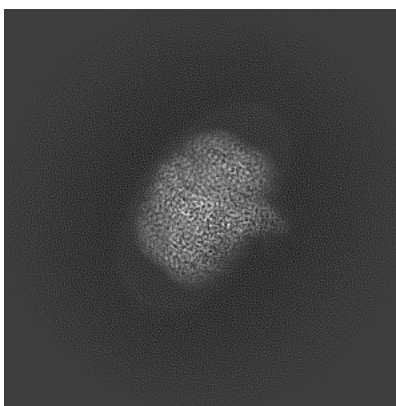
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

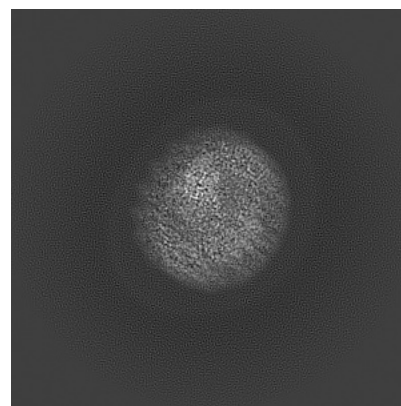
6.1.1 Primary map



X

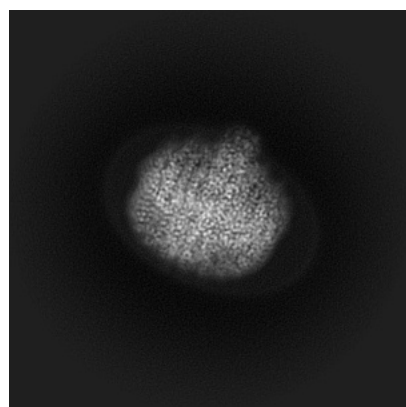


Y

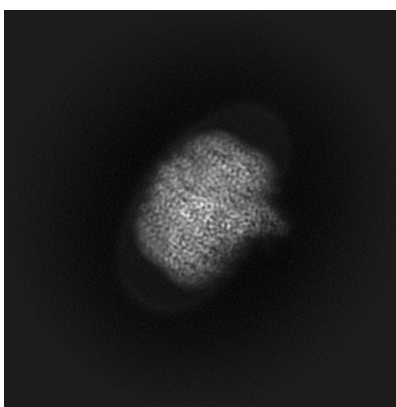


Z

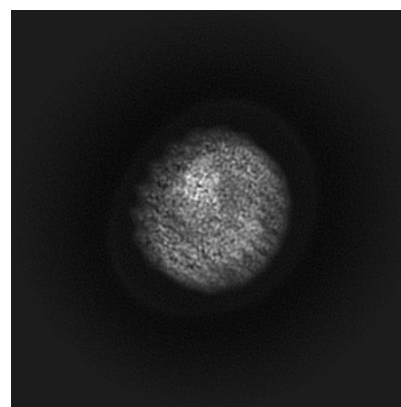
6.1.2 Raw map



X



Y

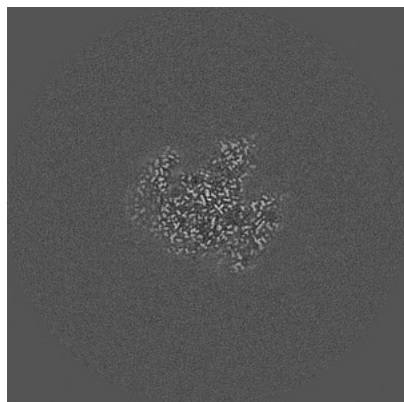


Z

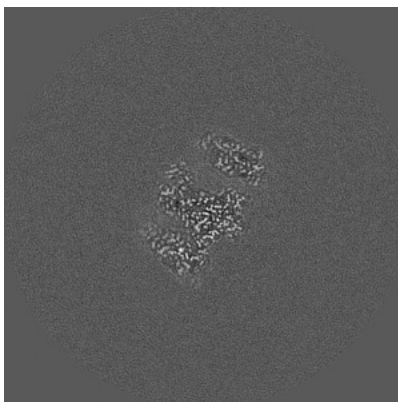
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

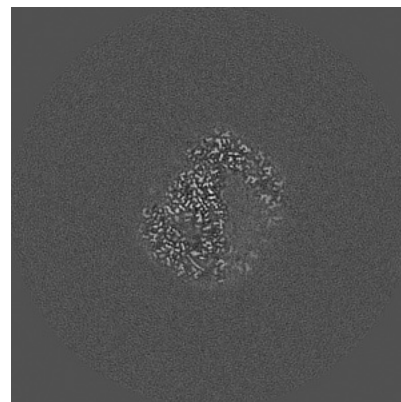
6.2.1 Primary map



X Index: 200

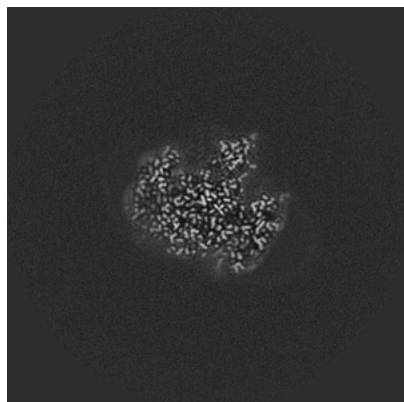


Y Index: 200

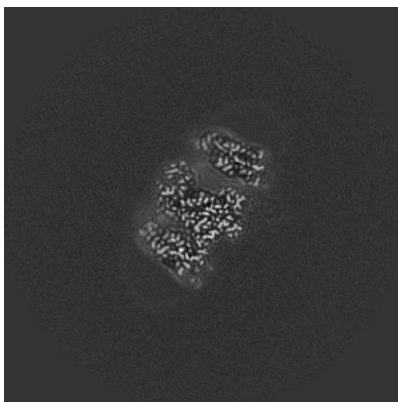


Z Index: 200

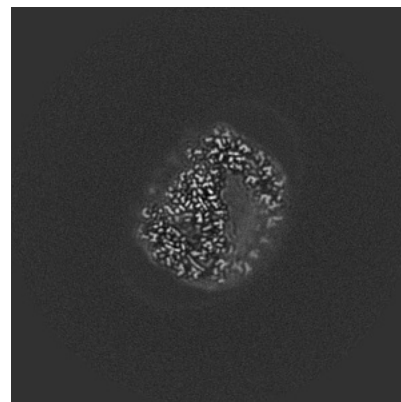
6.2.2 Raw map



X Index: 200



Y Index: 200

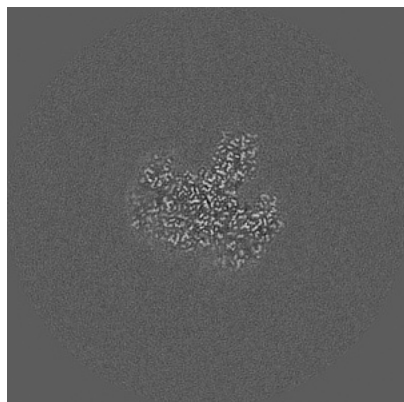


Z Index: 200

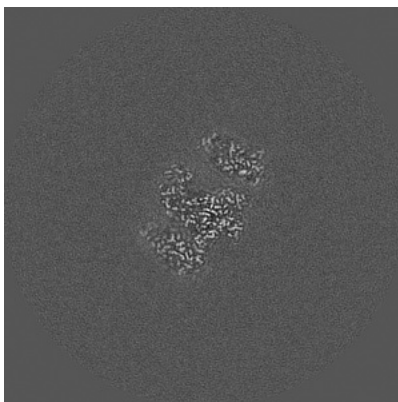
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

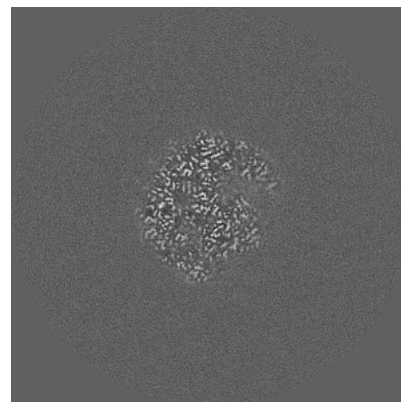
6.3.1 Primary map



X Index: 194

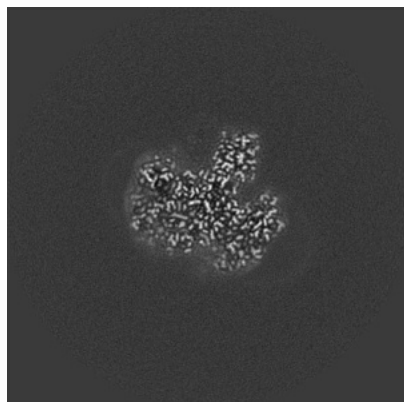


Y Index: 201

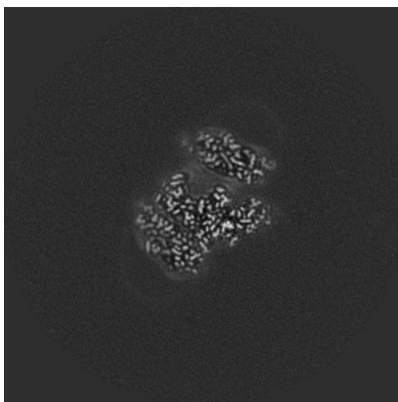


Z Index: 183

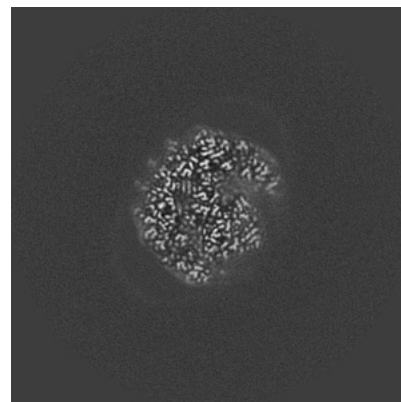
6.3.2 Raw map



X Index: 193



Y Index: 212

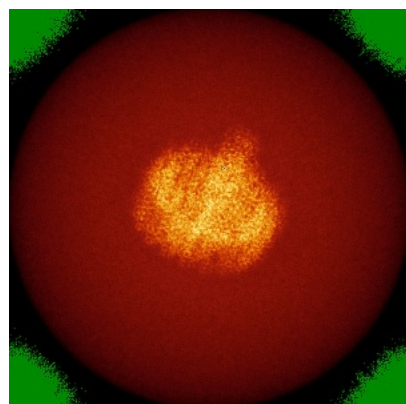


Z Index: 183

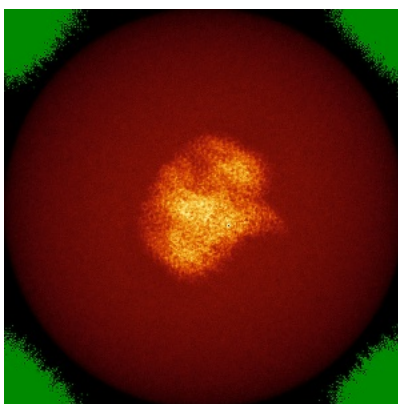
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

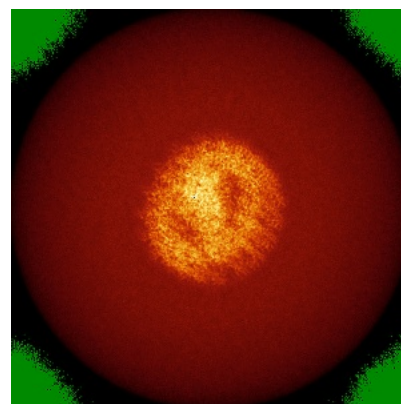
6.4.1 Primary map



X

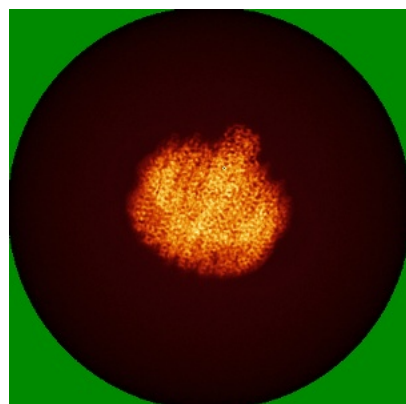


Y

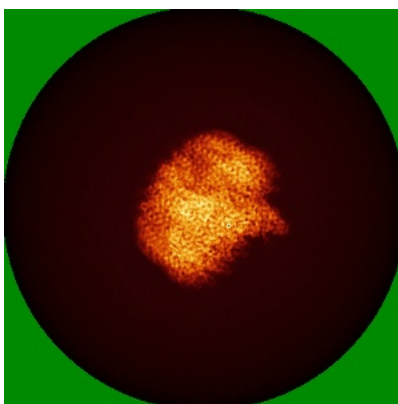


Z

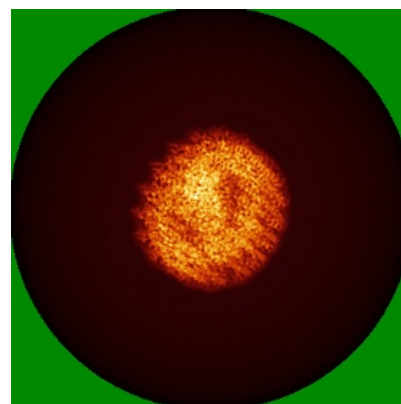
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

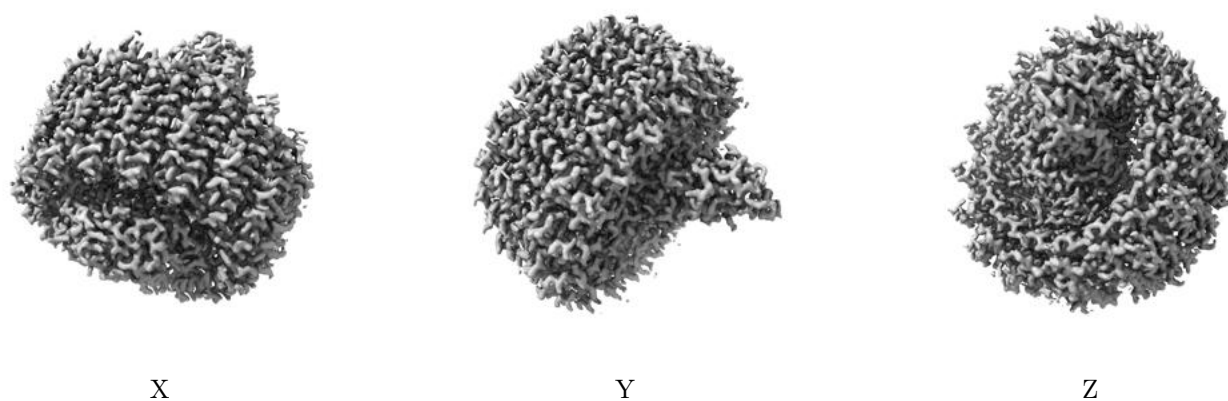
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

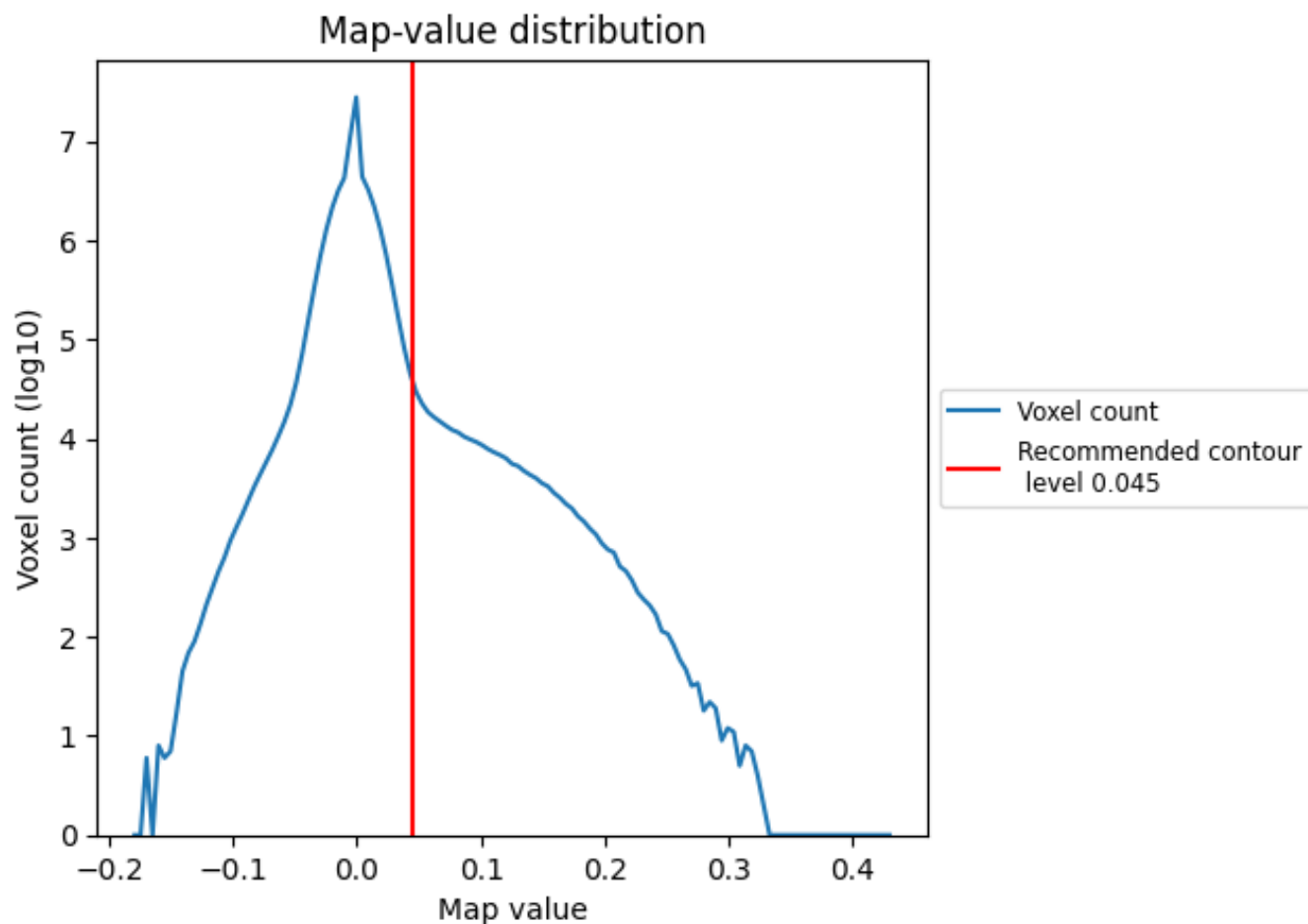
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

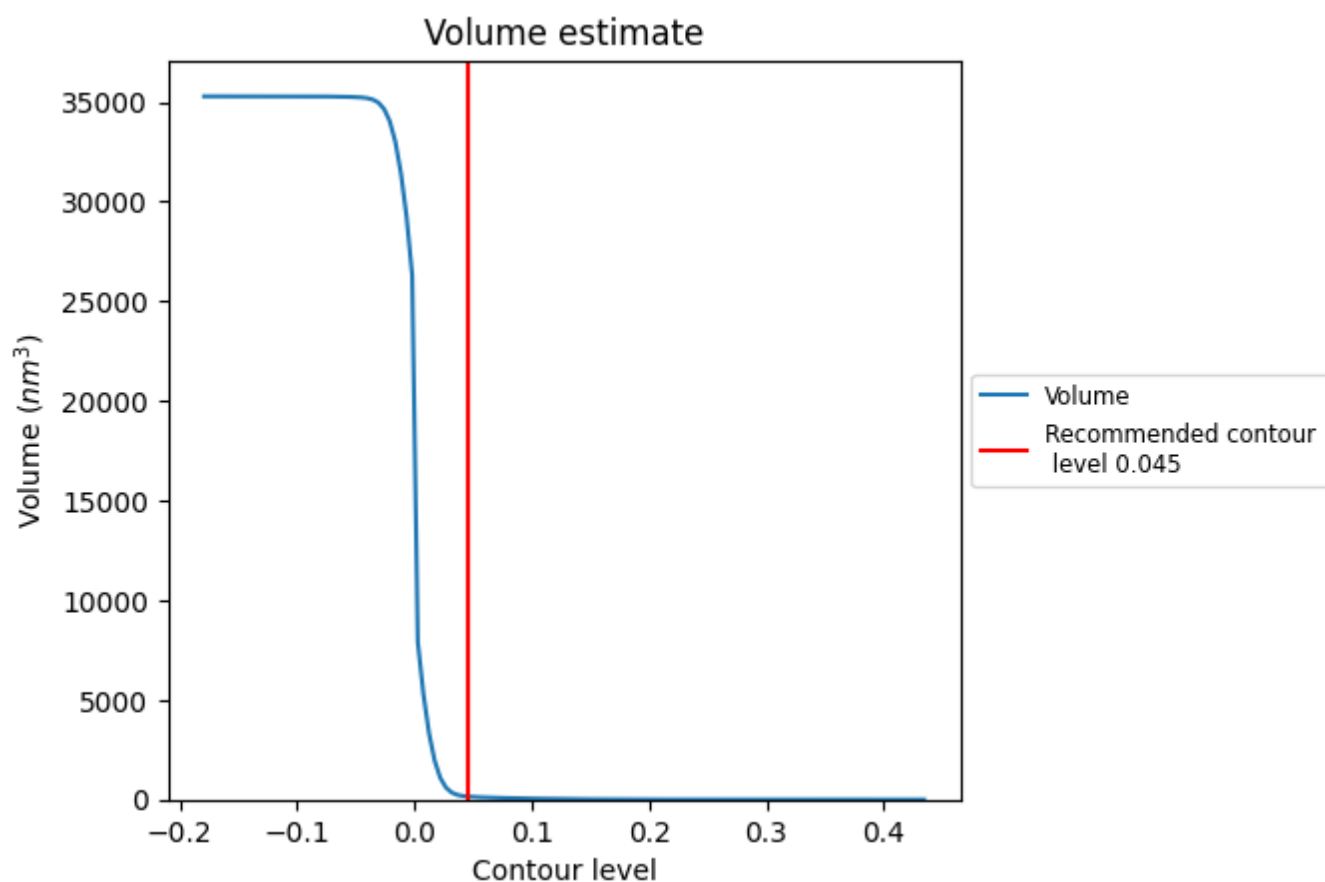
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

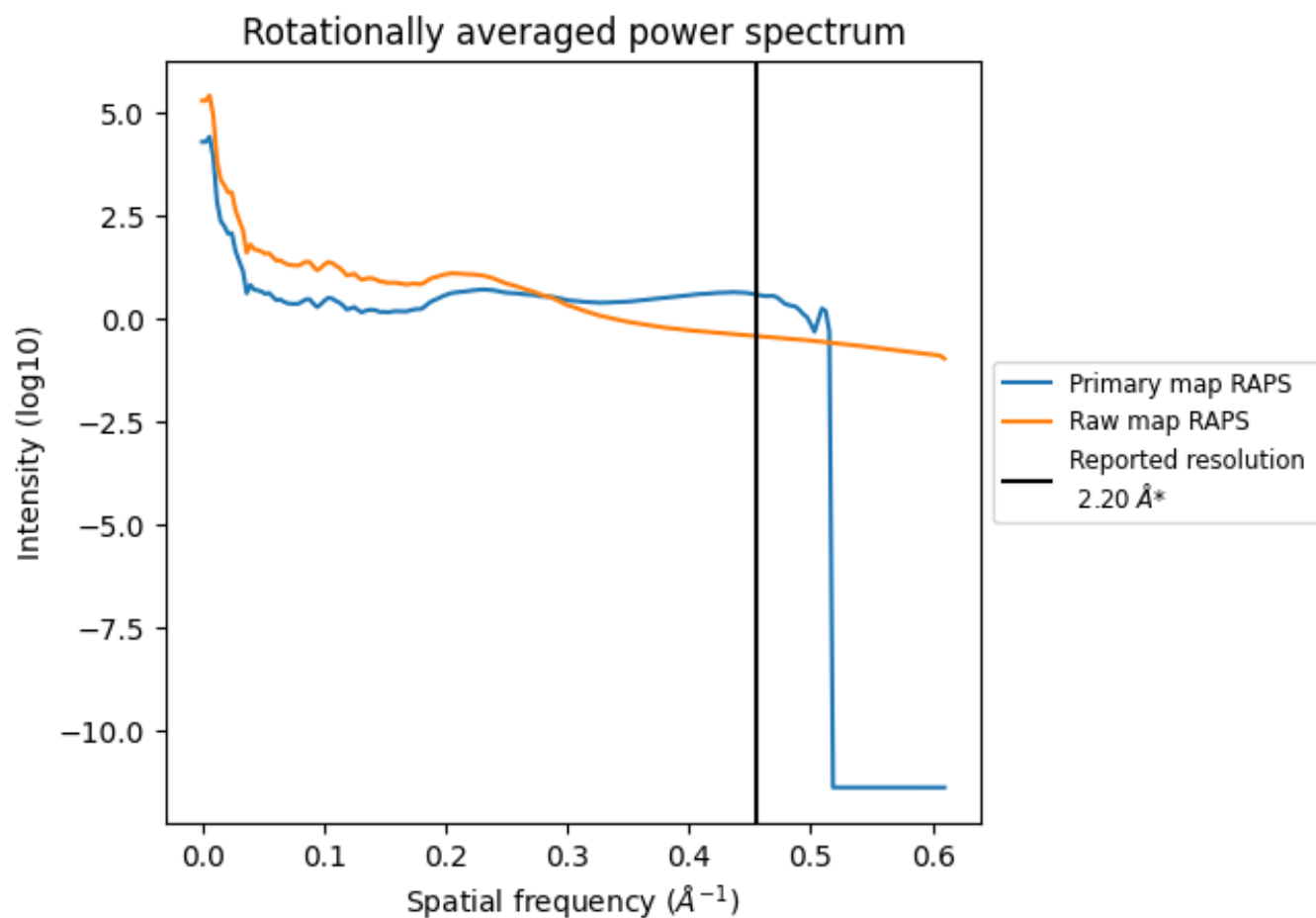
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm³; this corresponds to an approximate mass of 140 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

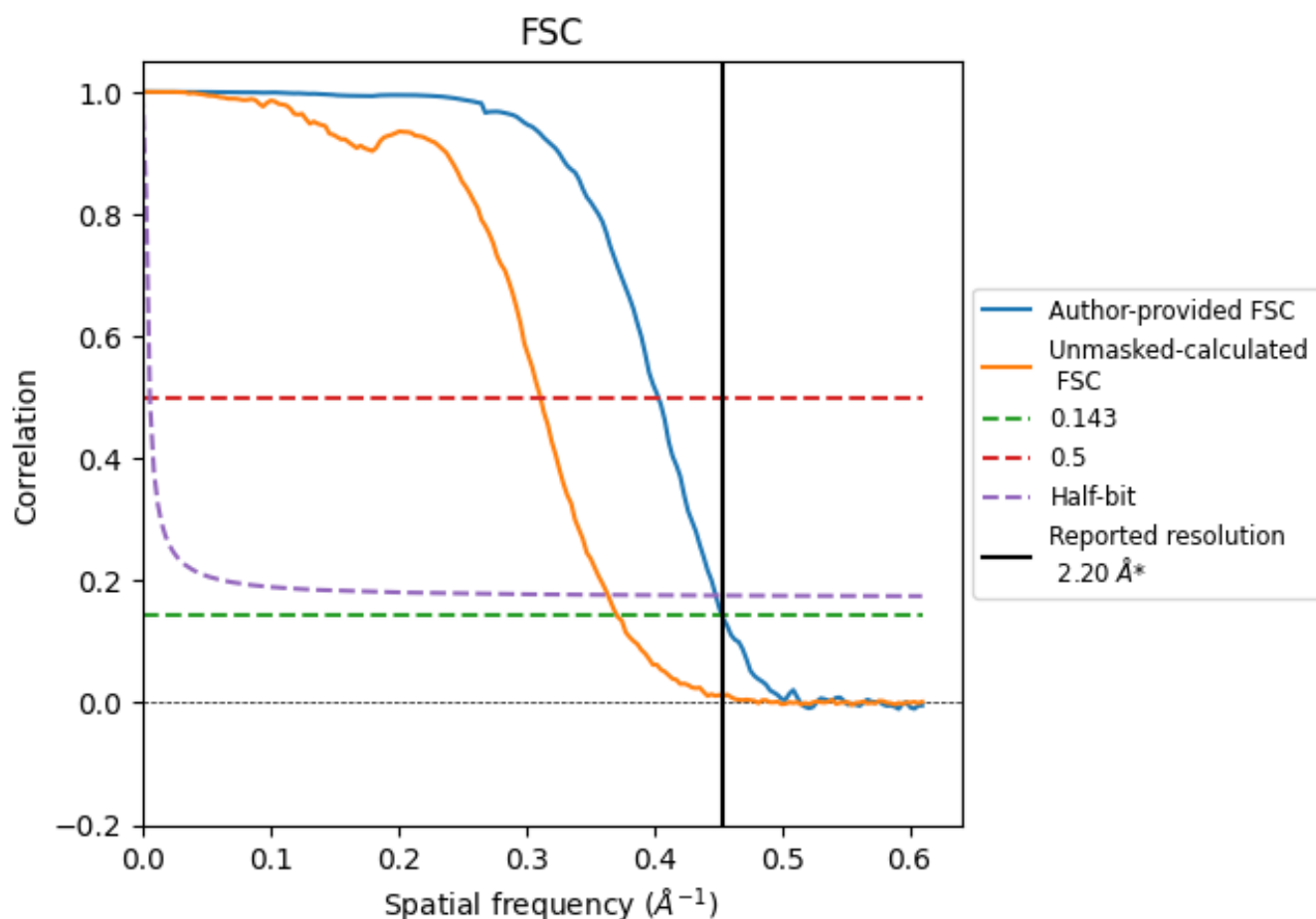


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

8.2 Resolution estimates [i](#)

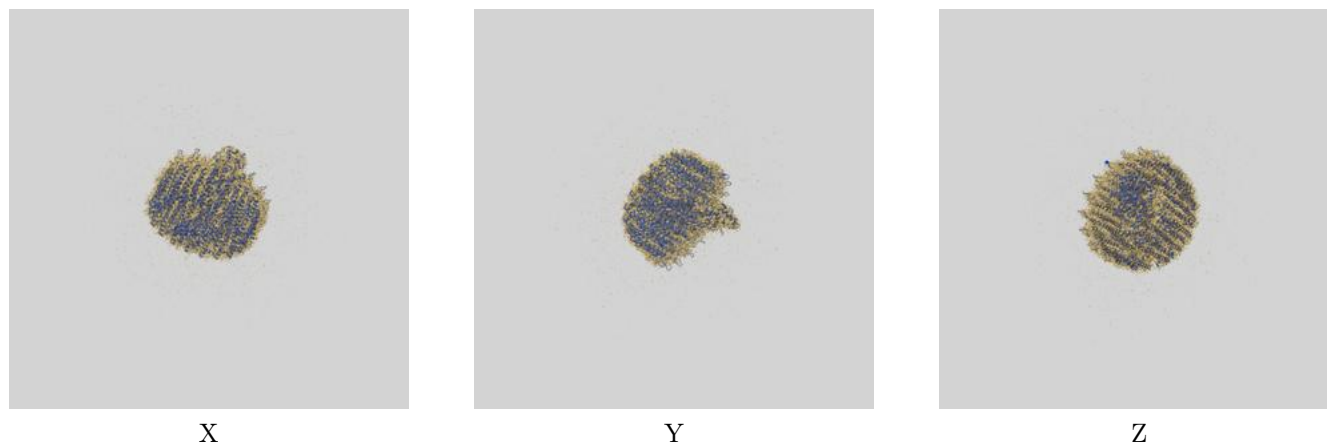
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.20 | - | - |
| Author-provided FSC curve | 2.21 | 2.48 | 2.23 |
| Unmasked-calculated* | 2.69 | 3.21 | 2.75 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.69 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

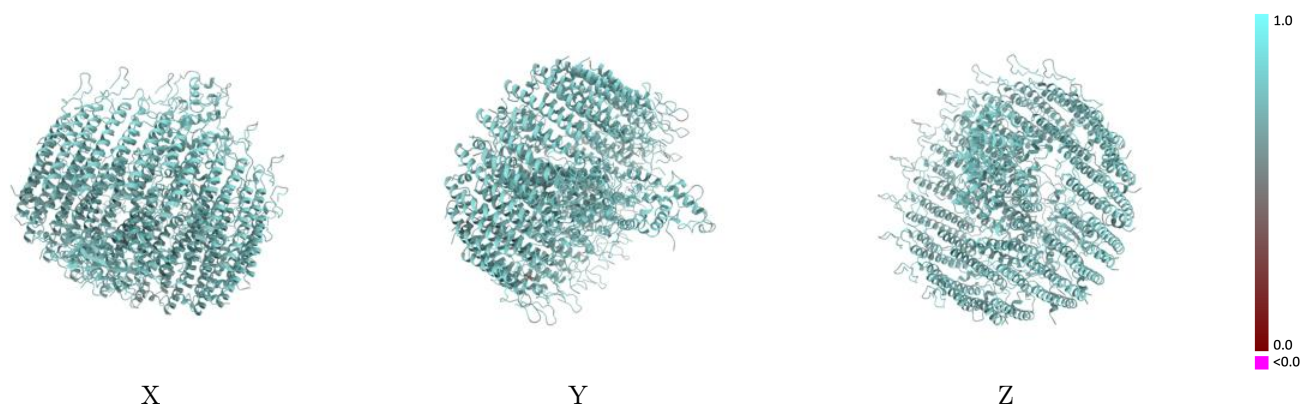
This section contains information regarding the fit between EMDB map EMD-61095 and PDB model 9J2F. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



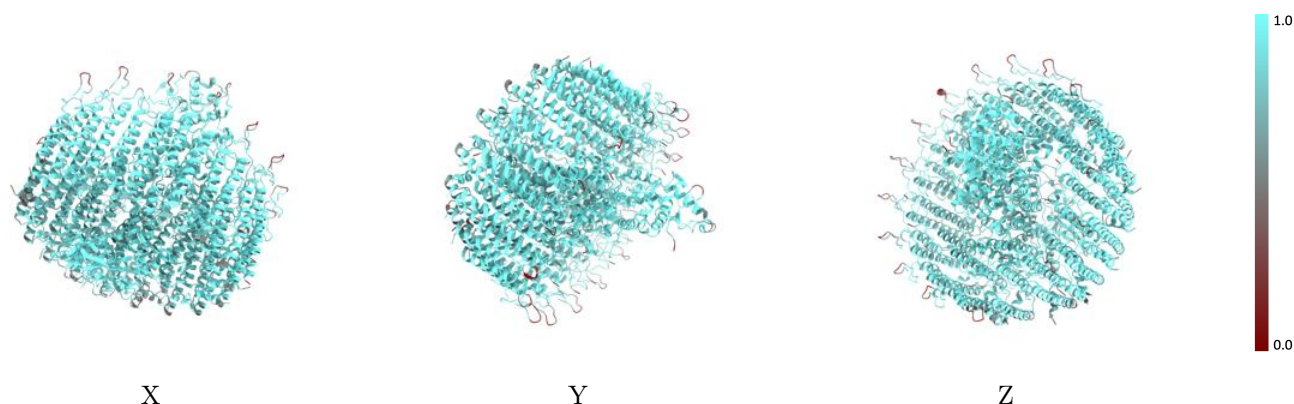
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



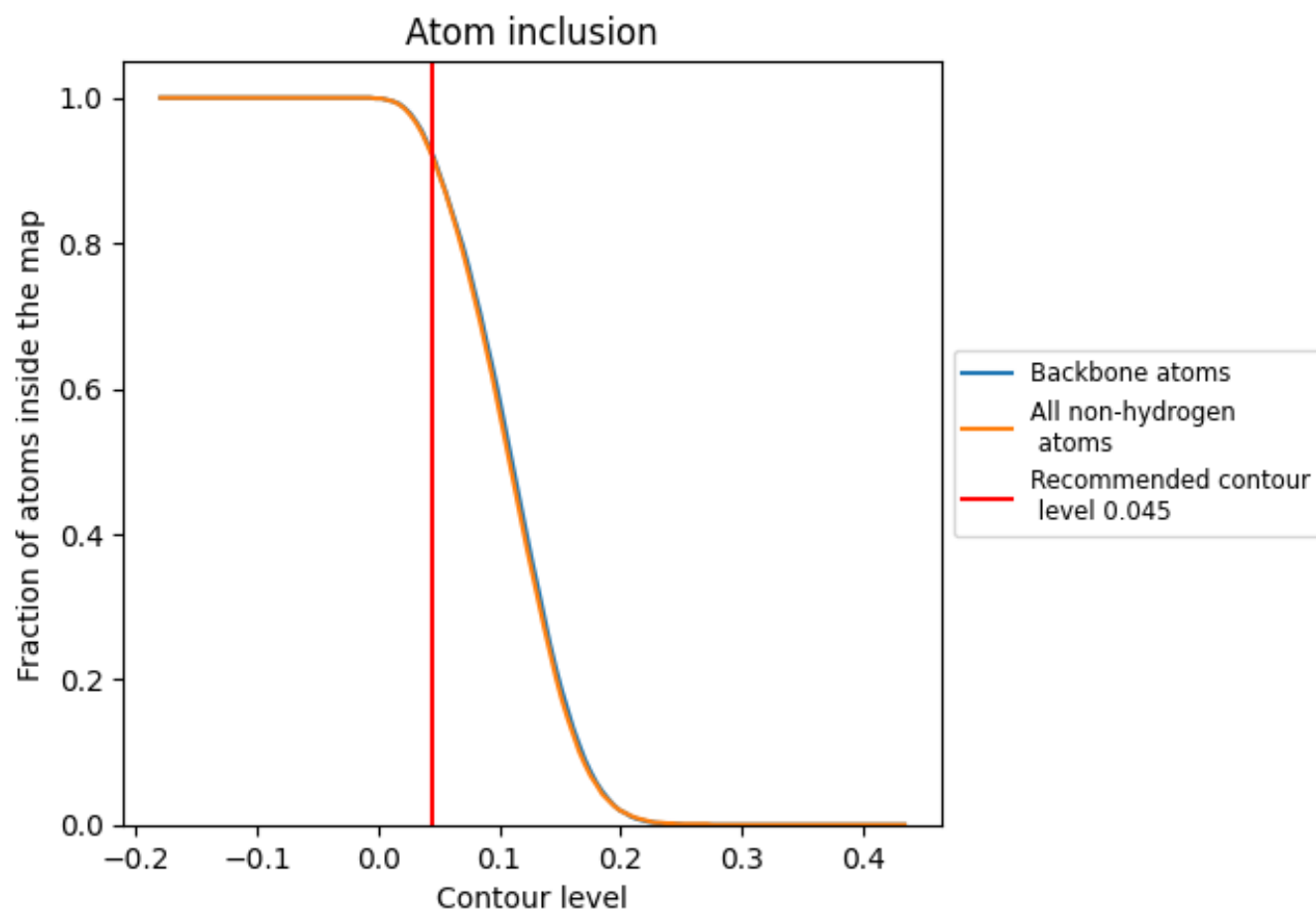
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ









































The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9190 |  0.7250 |
| 0 |  0.9210 |  0.7210 |
| 1 |  0.9600 |  0.7460 |
| 2 |  0.9010 |  0.7020 |
| 3 |  0.9640 |  0.7430 |
| 4 |  0.9320 |  0.7340 |
| 5 |  0.8750 |  0.7030 |
| 6 |  0.9470 |  0.7320 |
| 7 |  0.9310 |  0.7340 |
| 8 |  0.8860 |  0.7010 |
| 9 |  0.9490 |  0.7350 |
| A |  0.9050 |  0.7200 |
| B |  0.8600 |  0.6930 |
| C |  0.9540 |  0.7460 |
| D |  0.9410 |  0.7300 |
| E |  0.9460 |  0.7350 |
| F |  0.8320 |  0.7000 |
| G |  0.6060 |  0.6270 |
| H |  0.9160 |  0.7160 |
| I |  0.9370 |  0.7240 |
| J |  0.9520 |  0.7380 |
| K |  0.9010 |  0.7070 |
| L |  0.9720 |  0.7600 |
| M |  0.9580 |  0.7480 |
| N |  0.9310 |  0.7270 |
| O |  0.9460 |  0.7270 |
| P |  0.8540 |  0.6930 |
| Q |  0.9270 |  0.7230 |
| R |  0.9210 |  0.7220 |
| S |  0.8460 |  0.6950 |
| T |  0.8700 |  0.6950 |
| U |  0.8870 |  0.7000 |
| V |  0.8170 |  0.6830 |
| W |  0.9300 |  0.7230 |
| X |  0.9050 |  0.7210 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Y |  0.8650 |  0.6920 |
| Z |  0.9490 |  0.7400 |
| a |  0.7870 |  0.6870 |
| b |  0.8930 |  0.7150 |
| c |  0.9190 |  0.7290 |
| d |  0.8320 |  0.6880 |
| e |  0.9600 |  0.7360 |
| f |  0.9390 |  0.7290 |
| g |  0.8860 |  0.7030 |
| h |  0.9200 |  0.7200 |
| i |  0.9080 |  0.7130 |
| j |  0.9010 |  0.6970 |
| k |  0.9270 |  0.7180 |
| l |  0.9230 |  0.7200 |
| m |  0.8830 |  0.6970 |
| n |  0.8900 |  0.7140 |
| o |  0.9210 |  0.7170 |
| p |  0.8390 |  0.6920 |
| q |  0.8830 |  0.7010 |
| r |  0.7900 |  0.6730 |