



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2021 – 10:29 AM JST

PDB ID : 7D5W
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate of O at 1.84 angstrom resolution
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2020-09-28
Resolution : 1.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

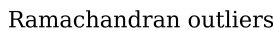
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

i

X-RAY DIFFRACTION

A.

| Metric | Percentile Rank | Value |
|--------|-----------------|-------|
|--------|-----------------|-------|



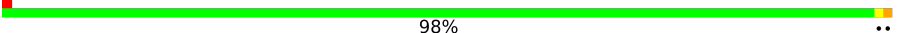














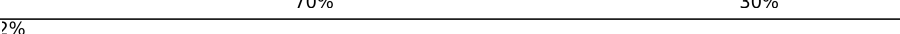


Ramachandran outliers

The numeric value for each fraction is indicated below the corresponding segment, with a dot

[illegible]

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | D | 144 |  |
| 4 | Q | 144 |  |
| 5 | E | 105 |  |
| 5 | R | 105 |  |
| 6 | F | 94 |  |
| 6 | S | 94 |  |
| 7 | G | 84 |  |
| 7 | T | 84 |  |
| 8 | H | 79 |  |
| 8 | U | 79 |  |
| 9 | I | 73 |  |
| 9 | V | 73 |  |
| 10 | J | 58 |  |
| 10 | W | 58 |  |
| 11 | K | 49 |  |
| 11 | X | 49 |  |
| 12 | L | 46 |  |
| 12 | Y | 46 |  |
| 13 | M | 43 |  |
| 13 | Z | 43 |  |

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 |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 14 | HEA | A | 601[A] | X | - | - | - |
| 14 | HEA | A | 601[B] | X | - | - | - |
| 14 | HEA | A | 601[C] | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 14 | HEA | A | 602 | X | - | - | - |
| 14 | HEA | N | 602[A] | X | - | - | - |
| 14 | HEA | N | 602[B] | X | - | - | - |
| 14 | HEA | N | 602[C] | X | - | - | - |
| 14 | HEA | N | 603 | X | - | - | - |
| 23 | DMU | X | 104 | - | - | - | X |
| 25 | CHD | J | 101 | - | - | - | X |
| 9 | SAC | V | 1 | - | - | - | X |

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 514 | Total | C | N | O | S | 0 | 34 | 0 |
| | | | 4193 | 2793 | 646 | 714 | 40 | | | |
| 1 | N | 514 | Total | C | N | O | S | 0 | 38 | 0 |
| | | | 4199 | 2799 | 644 | 714 | 42 | | | |

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 227 | Total | C | N | O | S | 0 | 8 | 0 |
| | | | 1851 | 1202 | 281 | 347 | 21 | | | |
| 2 | O | 227 | Total | C | N | O | S | 0 | 12 | 0 |
| | | | 1872 | 1217 | 288 | 346 | 21 | | | |

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 259 | Total | C | N | O | S | 0 | 11 | 0 |
| | | | 2144 | 1430 | 340 | 359 | 15 | | | |
| 3 | P | 259 | Total | C | N | O | S | 0 | 11 | 0 |
| | | | 2143 | 1431 | 341 | 357 | 14 | | | |

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | D | 144 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 1209 | 788 | 199 | 218 | 4 | | | |
| 4 | Q | 144 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 1197 | 779 | 196 | 218 | 4 | | | |

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 852 | 544 | 144 | 162 | 2 | | | |
| 5 | R | 105 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 858 | 547 | 147 | 162 | 2 | | | |

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 94 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 731 | 451 | 129 | 145 | 6 | | | |
| 6 | S | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 716 | 444 | 127 | 140 | 5 | | | |

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 84 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 690 | 445 | 130 | 114 | 1 | | | |
| 7 | T | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 672 | 431 | 129 | 111 | 1 | | | |

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 79 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 665 | 418 | 122 | 120 | 5 | | | |
| 8 | U | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 417 | 121 | 119 | 5 | | | |

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | I | 73 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 605 | 392 | 107 | 102 | 4 | | | |
| 9 | V | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 601 | 390 | 107 | 100 | 4 | | | |

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | J | 58 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 462 | 297 | 78 | 84 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | W | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 461 | 297 | 78 | 83 | 3 | | | |

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11 | K | 49 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 390 | 254 | 65 | 69 | 2 | | | |
| 11 | X | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 250 | 65 | 67 | 2 | | | |

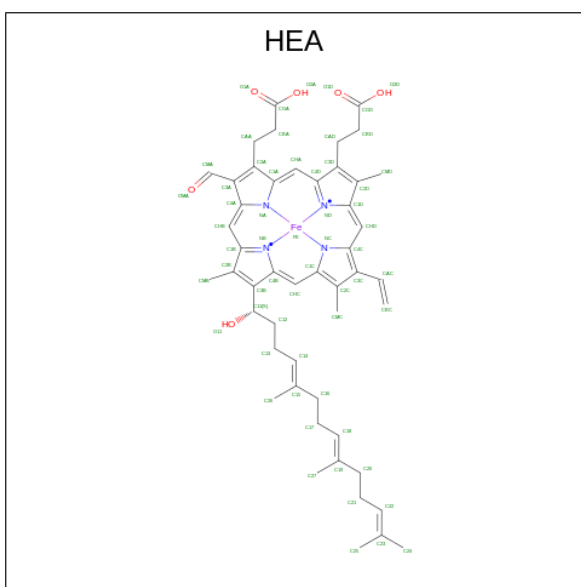
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | L | 46 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 386 | 259 | 64 | 60 | 3 | | | |
| 12 | Y | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 380 | 254 | 64 | 60 | 2 | | | |

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 13 | M | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 336 | 223 | 53 | 60 | | | |
| 13 | Z | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53 | 59 | | | |

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14 | A | 1 | Total 81 | C 69 | Fe 1 | N 4 | O 7 | 0 | 1 |
| 14 | A | 1 | Total 60 | C 49 | Fe 1 | N 4 | O 6 | 0 | 0 |
| 14 | N | 1 | Total 81 | C 69 | Fe 1 | N 4 | O 7 | 0 | 1 |
| 14 | N | 1 | Total 60 | C 49 | Fe 1 | N 4 | O 6 | 0 | 0 |

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 15 | N | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

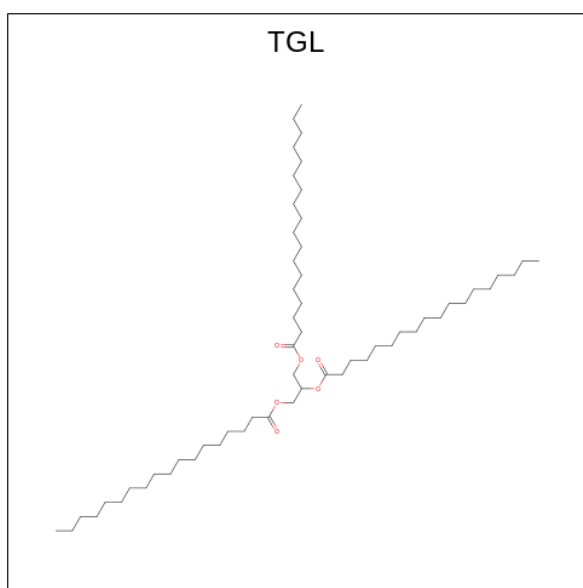
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 16 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

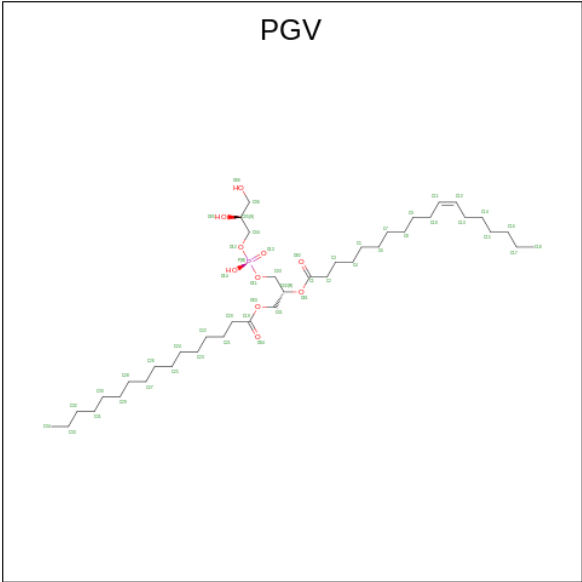
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 17 | C | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 17 | N | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 17 | P | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



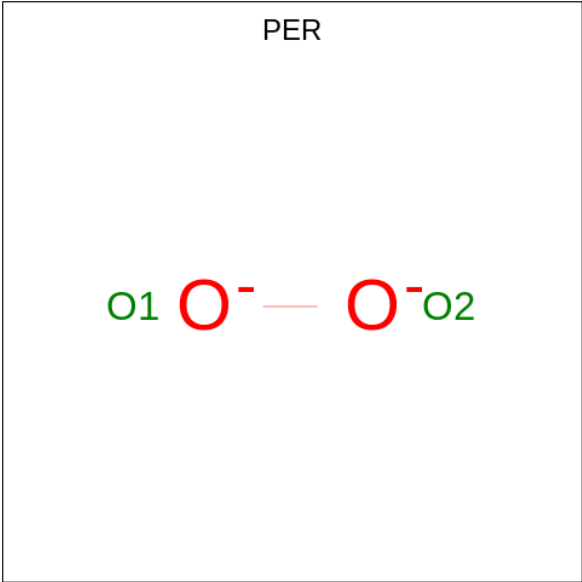
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 18 | A | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | A | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | L | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | N | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 18 | N | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



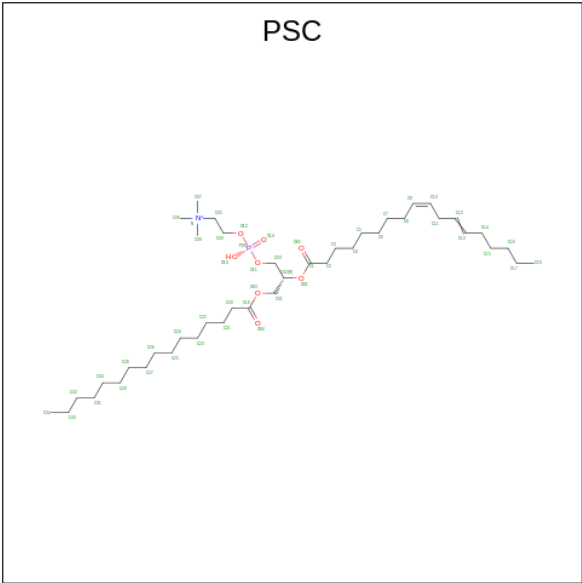
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 19 | A | 1 | Total | C | O | 0 | 0 |
| | | | 34 | 32 | 2 | | |
| 19 | A | 1 | Total | C | O | P | 0 |
| | | | 51 | 40 | 10 | 1 | 0 |
| 19 | C | 1 | Total | C | O | P | 0 |
| | | | 48 | 37 | 10 | 1 | 0 |
| 19 | C | 1 | Total | C | O | | 0 |
| | | | 36 | 32 | 4 | | 0 |
| 19 | N | 1 | Total | C | O | P | 0 |
| | | | 51 | 40 | 10 | 1 | 0 |
| 19 | N | 1 | Total | C | O | P | 0 |
| | | | 51 | 40 | 10 | 1 | 0 |
| 19 | P | 1 | Total | C | O | P | 0 |
| | | | 51 | 40 | 10 | 1 | 0 |
| 19 | P | 1 | Total | C | O | | 0 |
| | | | 31 | 29 | 2 | | 0 |

- Molecule 20 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 20 | A | 1 | Total | O | 0 | 1 |
| | | | 2 | 2 | | |
| 20 | N | 1 | Total | O | 0 | 1 |
| | | | 2 | 2 | | |

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



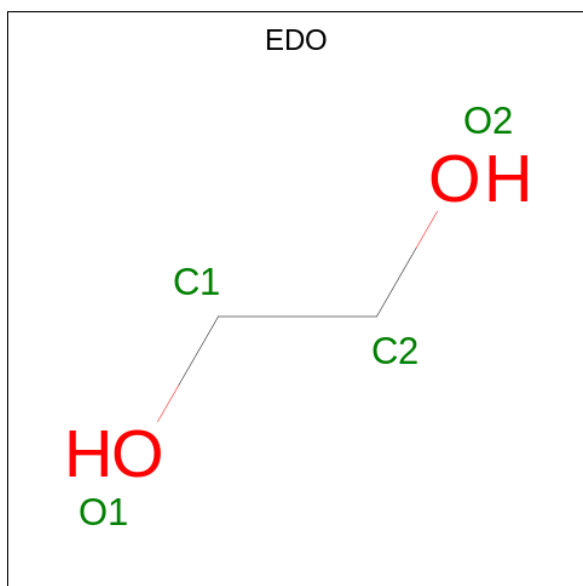
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21 | A | 1 | Total | C | 0 | 0 |
| | | | 25 | 25 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21 | O | 1 | Total | C | O | 0 | 0 |
| | | | 31 | 29 | 2 | | |

- Molecule 22 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 22 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | D | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | D | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | D | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | D | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | D | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | E | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 22 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | E | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | F | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | G | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | J | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | L | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | L | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | M | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | N | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | N | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | N | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | N | 1 | Total 4 | C 2 | O 2 | 0 | 0 |
| 22 | N | 1 | Total 4 | C 2 | O 2 | 0 | 0 |

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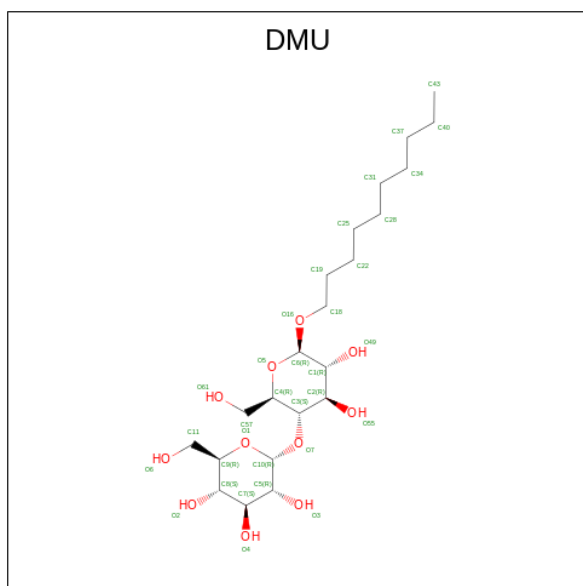
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 22 | N | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | N | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | N | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | N | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | N | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | O | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | O | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | O | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | P | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | Q | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | S | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | S | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | S | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 22 | S | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 22 | S | 1 | Total C O 4 2 2 | 0 | 0 |
| 22 | T | 1 | Total C O 4 2 2 | 0 | 0 |
| 22 | T | 1 | Total C O 4 2 2 | 0 | 0 |
| 22 | T | 1 | Total C O 4 2 2 | 0 | 0 |
| 22 | W | 1 | Total C O 4 2 2 | 0 | 0 |
| 22 | W | 1 | Total C O 4 2 2 | 0 | 0 |
| 22 | Y | 1 | Total C O 4 2 2 | 0 | 0 |

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



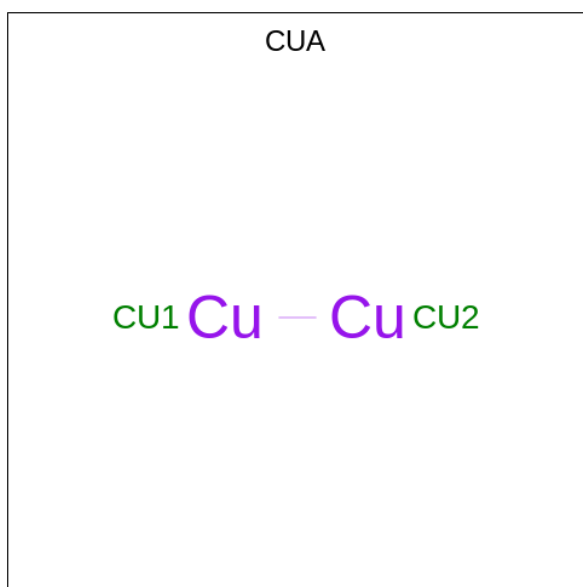
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|---------|
| 23 | A | 1 | Total 11 | C 10 | O 1 | 0 | 0 |
| 23 | C | 1 | Total 33 | C 22 | O 11 | 0 | 0 |
| 23 | C | 1 | Total 12 | C 11 | O 1 | 0 | 0 |
| 23 | D | 1 | Total 33 | C 22 | O 11 | 0 | 0 |

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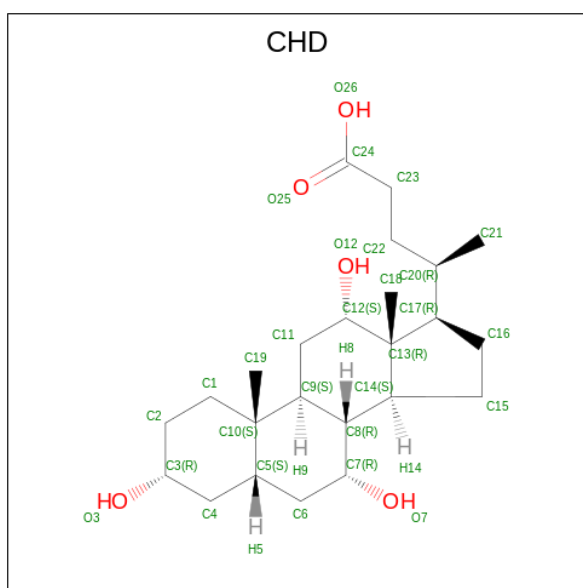
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 23 | D | 1 | Total C O 11 10 1 | 0 | 0 |
| 23 | J | 1 | Total C O 11 10 1 | 0 | 0 |
| 23 | K | 1 | Total C 8 8 | 0 | 0 |
| 23 | K | 1 | Total C O 11 10 1 | 0 | 0 |
| 23 | K | 1 | Total C 10 10 | 0 | 0 |
| 23 | K | 1 | Total C O 11 10 1 | 0 | 0 |
| 23 | K | 1 | Total C 9 9 | 0 | 0 |
| 23 | L | 1 | Total C O 21 16 5 | 0 | 0 |
| 23 | M | 1 | Total C O 33 22 11 | 0 | 0 |
| 23 | O | 1 | Total C O 13 11 2 | 0 | 0 |
| 23 | P | 1 | Total C O 33 22 11 | 0 | 0 |
| 23 | P | 1 | Total C O 21 16 5 | 0 | 0 |
| 23 | P | 1 | Total C O 32 21 11 | 0 | 0 |
| 23 | Q | 1 | Total C O 11 10 1 | 0 | 0 |
| 23 | X | 1 | Total C 10 10 | 0 | 0 |
| 23 | X | 1 | Total C 9 9 | 0 | 0 |
| 23 | X | 1 | Total C 9 9 | 0 | 0 |
| 23 | X | 1 | Total C O 22 16 6 | 0 | 0 |
| 23 | Z | 1 | Total C O 33 22 11 | 0 | 0 |

- Molecule 24 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 24 | B | 1 | Total | Cu | 0 | 0 |
| | | | 2 | 2 | | |
| 24 | O | 1 | Total | Cu | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 25 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



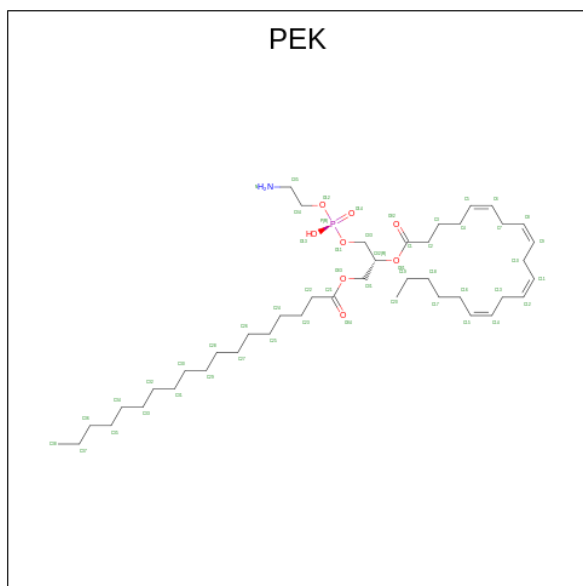
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 25 | B | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 25 | C | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 25 | C | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 25 | G | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 25 | J | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 25 | L | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 25 | P | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 25 | Y | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |

- Molecule 26 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



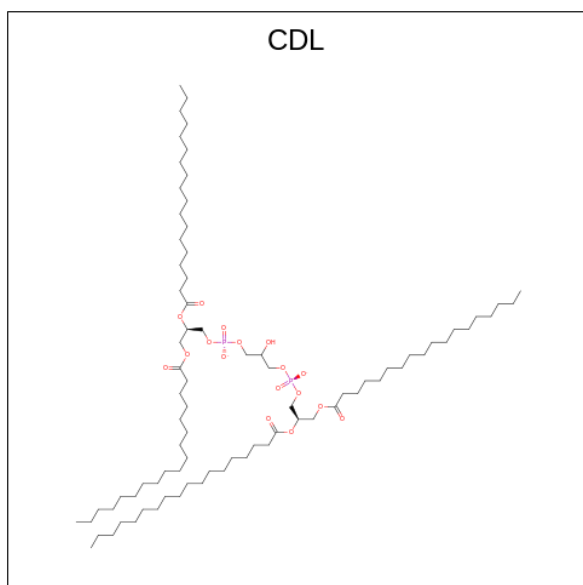
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 26 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | | |
| 26 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |
| 26 | C | 1 | Total | C | | | | 0 | 0 |
| | | | 36 | 36 | | | | | |
| 26 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 26 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |
| 26 | T | 1 | Total | C | O | | | 0 | 0 |
| | | | 37 | 35 | 2 | | | | |

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

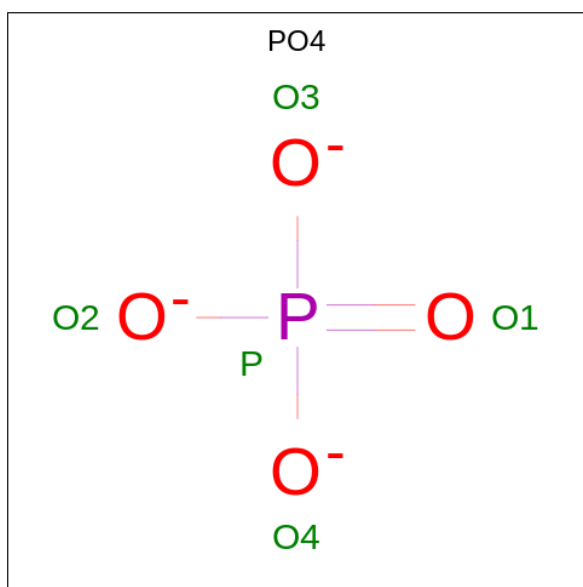


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 27 | C | 1 | Total | C | O | 0 | 0 |
| | | | 65 | 61 | 4 | | |
| 27 | N | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 60 | 2 | | |
| 27 | P | 1 | Total | C | O | 0 | 0 |
| | | | 68 | 64 | 4 | | |
| 27 | T | 1 | Total | C | O | 0 | 0 |
| | | | 61 | 59 | 2 | | |

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 28 | F | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 28 | S | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 29 | H | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 29 | U | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 30 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 30 | A | 274 | Total | O | 0 | 14 |
| | | | 274 | 274 | | |
| 30 | B | 229 | Total | O | 0 | 4 |
| | | | 229 | 229 | | |
| 30 | C | 153 | Total | O | 0 | 0 |
| | | | 153 | 153 | | |
| 30 | D | 206 | Total | O | 0 | 2 |
| | | | 207 | 207 | | |
| 30 | E | 162 | Total | O | 0 | 0 |
| | | | 162 | 162 | | |
| 30 | F | 161 | Total | O | 0 | 0 |
| | | | 161 | 161 | | |
| 30 | G | 87 | Total | O | 0 | 0 |
| | | | 87 | 87 | | |
| 30 | H | 92 | Total | O | 0 | 0 |
| | | | 92 | 92 | | |
| 30 | I | 71 | Total | O | 0 | 0 |
| | | | 71 | 71 | | |
| 30 | J | 61 | Total | O | 0 | 0 |
| | | | 61 | 61 | | |

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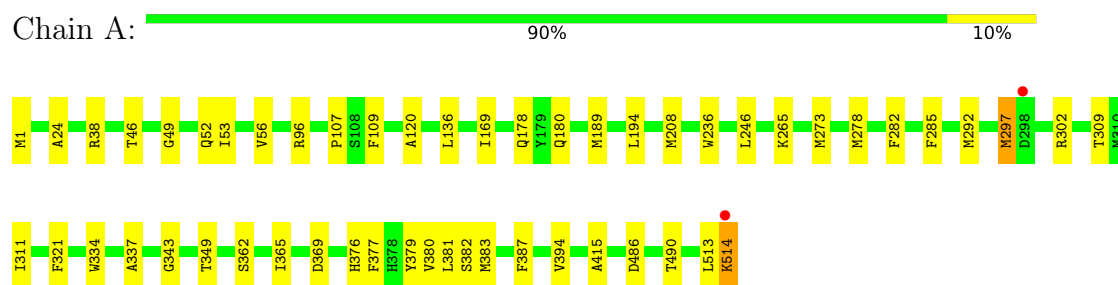
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 30 | K | 45 | Total 45 | O 45 | 0 | 0 |
| 30 | L | 40 | Total 40 | O 40 | 0 | 1 |
| 30 | M | 37 | Total 37 | O 37 | 0 | 0 |
| 30 | N | 282 | Total 282 | O 282 | 0 | 10 |
| 30 | O | 199 | Total 199 | O 199 | 0 | 2 |
| 30 | P | 161 | Total 161 | O 161 | 0 | 3 |
| 30 | Q | 119 | Total 119 | O 119 | 0 | 0 |
| 30 | R | 112 | Total 113 | O 113 | 0 | 1 |
| 30 | S | 141 | Total 141 | O 141 | 0 | 0 |
| 30 | T | 66 | Total 66 | O 66 | 0 | 0 |
| 30 | U | 96 | Total 96 | O 96 | 0 | 0 |
| 30 | V | 65 | Total 66 | O 66 | 0 | 1 |
| 30 | W | 41 | Total 41 | O 41 | 0 | 0 |
| 30 | X | 33 | Total 33 | O 33 | 0 | 0 |
| 30 | Y | 31 | Total 31 | O 31 | 0 | 1 |
| 30 | Z | 28 | Total 28 | O 28 | 0 | 0 |

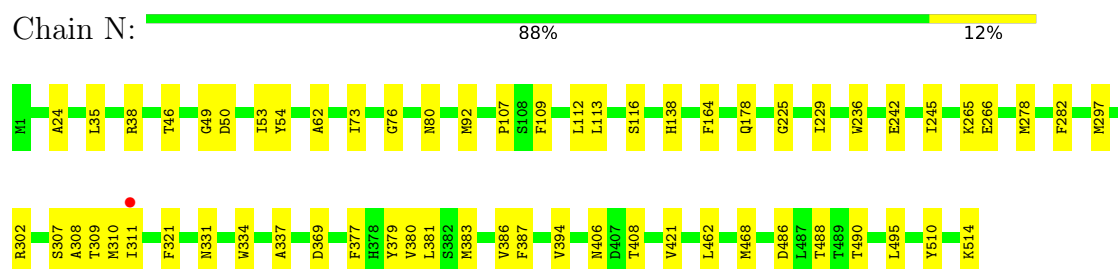
3 Residue-property plots [i](#)

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

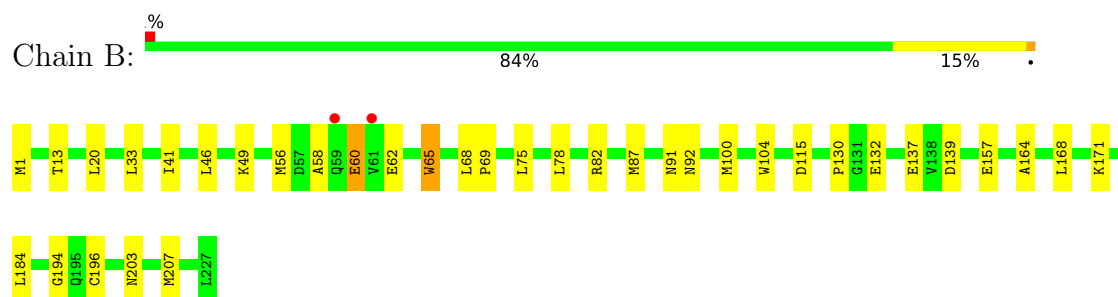
• Molecule 1: Cytochrome c oxidase subunit 1



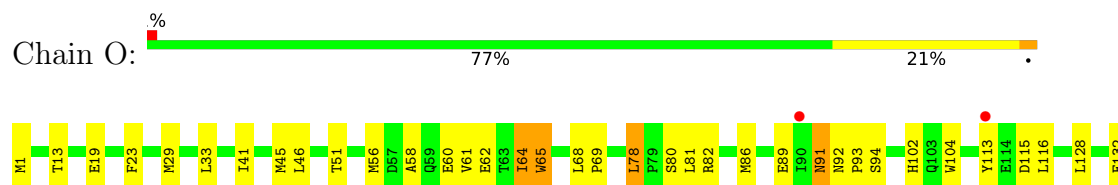
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2

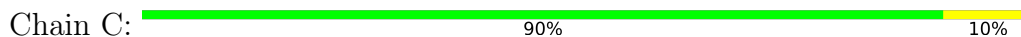


• Molecule 2: Cytochrome c oxidase subunit 2





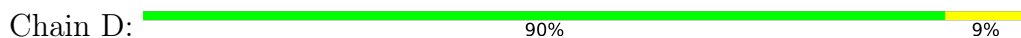
- Molecule 3: Cytochrome c oxidase subunit 3



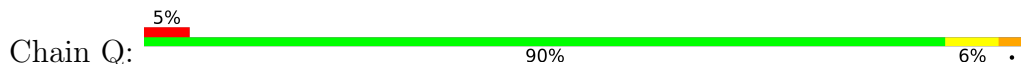
- Molecule 3: Cytochrome c oxidase subunit 3



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



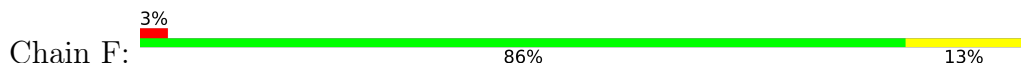
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

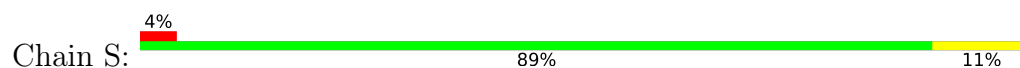


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

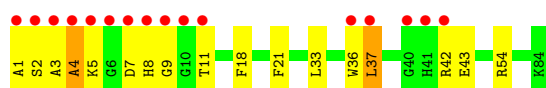
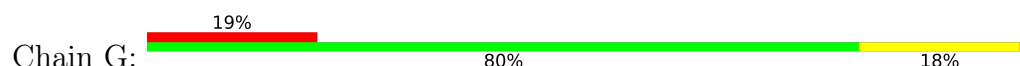




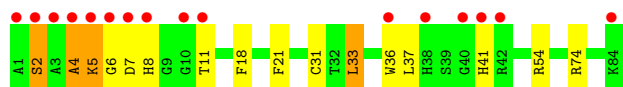
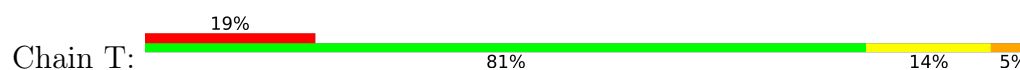
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



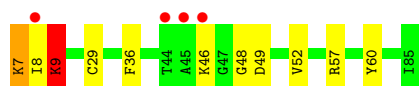
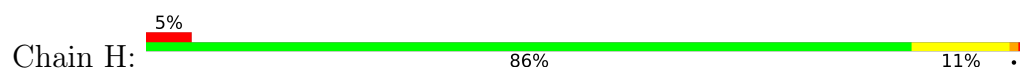
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



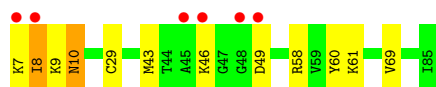
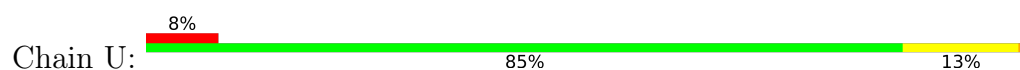
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



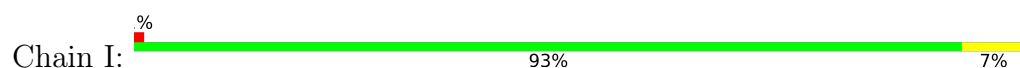
- Molecule 8: Cytochrome c oxidase subunit 6B1



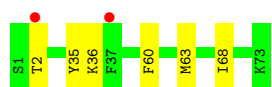
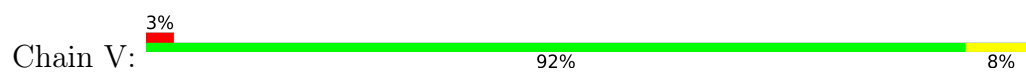
- Molecule 8: Cytochrome c oxidase subunit 6B1



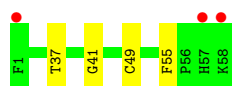
- Molecule 9: Cytochrome c oxidase subunit 6C



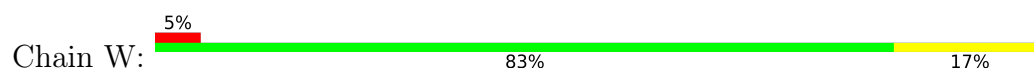
- Molecule 9: Cytochrome c oxidase subunit 6C



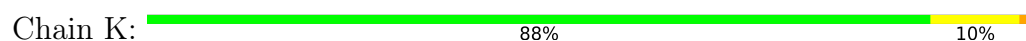
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



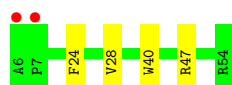
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



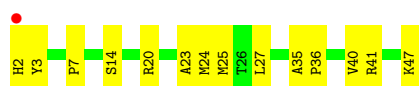
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



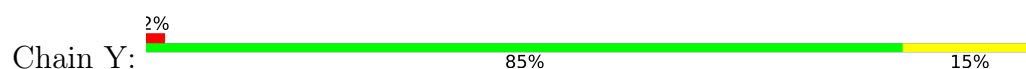
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial




- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

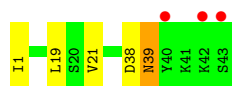


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial




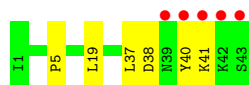
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  7% 88% 9% .



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain Z:  12% 86% 14%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 181.44Å 203.09Å 177.79Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 39.91 – 1.84 133.77 – 1.84 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (39.91-1.84) 99.8 (133.77-1.84) | Depositor EDS |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.08 (at 1.84Å) | Xtriage |
| Refinement program | PHENIX (1.11.1_2575: ???) | Depositor |
| R, R_{free} | 0.154 , 0.184 0.154 , 0.184 | Depositor DCC |
| R_{free} test set | 28294 reflections (5.04%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 25.7 | Xtriage |
| Anisotropy | 0.805 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 82.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | 0.007 for l,-k,h | Xtriage |
| F_o, F_c correlation | 0.97 | EDS |
| Total number of atoms | 34545 | wwPDB-VP |
| Average B, all atoms (Å ²) | 41.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PER, FME, PO4, PEK, NA, EDO, CUA, CU, PGV, TGL, ZN, HEA, PSC, MG, DMU, SAC, CHD

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.81 | 0/4432 | 0.78 | 3/6043 (0.0%) |
| 1 | N | 0.76 | 0/4457 | 0.74 | 1/6082 (0.0%) |
| 2 | B | 0.74 | 0/1928 | 0.80 | 2/2623 (0.1%) |
| 2 | O | 0.62 | 0/1973 | 0.76 | 2/2686 (0.1%) |
| 3 | C | 0.73 | 2/2288 (0.1%) | 0.67 | 0/3125 |
| 3 | P | 0.69 | 0/2287 | 0.65 | 0/3124 |
| 4 | D | 0.68 | 0/1259 | 0.68 | 0/1698 |
| 4 | Q | 0.48 | 0/1236 | 0.59 | 0/1668 |
| 5 | E | 0.62 | 0/871 | 0.71 | 0/1182 |
| 5 | R | 0.52 | 0/882 | 0.62 | 0/1196 |
| 6 | F | 0.67 | 0/773 | 0.70 | 0/1048 |
| 6 | S | 0.68 | 0/732 | 0.72 | 0/993 |
| 7 | G | 0.63 | 0/743 | 0.70 | 0/1009 |
| 7 | T | 0.53 | 0/699 | 0.73 | 1/950 (0.1%) |
| 8 | H | 0.64 | 0/690 | 0.66 | 0/932 |
| 8 | U | 0.60 | 1/682 (0.1%) | 0.69 | 0/921 |
| 9 | I | 0.52 | 0/614 | 0.63 | 0/814 |
| 9 | V | 0.48 | 0/605 | 0.62 | 0/802 |
| 10 | J | 0.52 | 0/478 | 0.60 | 0/644 |
| 10 | W | 0.47 | 0/472 | 0.59 | 0/636 |
| 11 | K | 0.57 | 0/419 | 0.65 | 1/574 (0.2%) |
| 11 | X | 0.50 | 0/398 | 0.57 | 0/544 |
| 12 | L | 0.67 | 0/409 | 0.62 | 0/547 |
| 12 | Y | 0.58 | 0/393 | 0.60 | 0/526 |
| 13 | M | 0.69 | 0/346 | 0.66 | 0/470 |
| 13 | Z | 0.54 | 0/345 | 0.60 | 0/470 |
| All | All | 0.68 | 3/30411 (0.0%) | 0.71 | 10/41307 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 3 | C | 246[A] | ASP | CB-CG | 6.16 | 1.64 | 1.51 |
| 3 | C | 246[B] | ASP | CB-CG | 6.16 | 1.64 | 1.51 |
| 8 | U | 69 | VAL | CB-CG1 | 5.04 | 1.63 | 1.52 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 1 | A | 189 | MET | CG-SD-CE | -7.68 | 87.90 | 100.20 |
| 1 | N | 310 | MET | CG-SD-CE | -7.37 | 88.41 | 100.20 |
| 2 | O | 65[A] | TRP | CA-CB-CG | 6.37 | 125.81 | 113.70 |
| 2 | O | 65[B] | TRP | CA-CB-CG | 6.37 | 125.81 | 113.70 |
| 1 | A | 96 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 2 | B | 82 | ARG | NE-CZ-NH2 | -5.95 | 117.32 | 120.30 |
| 1 | A | 208 | MET | CG-SD-CE | 5.55 | 109.09 | 100.20 |
| 11 | K | 47 | ARG | NE-CZ-NH1 | 5.41 | 123.01 | 120.30 |
| 7 | T | 33 | LEU | CA-CB-CG | 5.07 | 126.97 | 115.30 |
| 2 | B | 139 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4193 | 0 | 4162 | 51 | 0 |
| 1 | N | 4199 | 0 | 4190 | 58 | 0 |
| 2 | B | 1851 | 0 | 1858 | 22 | 0 |
| 2 | O | 1872 | 0 | 1876 | 29 | 0 |
| 3 | C | 2144 | 0 | 2062 | 24 | 0 |
| 3 | P | 2143 | 0 | 2069 | 24 | 0 |
| 4 | D | 1209 | 0 | 1202 | 14 | 0 |
| 4 | Q | 1197 | 0 | 1188 | 11 | 0 |
| 5 | E | 852 | 0 | 845 | 1 | 0 |
| 5 | R | 858 | 0 | 854 | 5 | 0 |
| 6 | F | 731 | 0 | 709 | 13 | 0 |
| 6 | S | 716 | 0 | 697 | 8 | 0 |
| 7 | G | 690 | 0 | 669 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7 | T | 672 | 0 | 645 | 13 | 0 |
| 8 | H | 665 | 0 | 625 | 6 | 0 |
| 8 | U | 662 | 0 | 623 | 7 | 0 |
| 9 | I | 605 | 0 | 615 | 2 | 0 |
| 9 | V | 601 | 0 | 613 | 5 | 0 |
| 10 | J | 462 | 0 | 460 | 5 | 0 |
| 10 | W | 461 | 0 | 459 | 5 | 0 |
| 11 | K | 390 | 0 | 377 | 6 | 0 |
| 11 | X | 384 | 0 | 366 | 3 | 0 |
| 12 | L | 386 | 0 | 392 | 19 | 0 |
| 12 | Y | 380 | 0 | 380 | 5 | 0 |
| 13 | M | 336 | 0 | 352 | 7 | 0 |
| 13 | Z | 335 | 0 | 352 | 5 | 0 |
| 14 | A | 141 | 0 | 115 | 9 | 0 |
| 14 | N | 141 | 0 | 115 | 10 | 0 |
| 15 | A | 1 | 0 | 0 | 0 | 0 |
| 15 | N | 1 | 0 | 0 | 0 | 0 |
| 16 | A | 1 | 0 | 0 | 0 | 0 |
| 16 | N | 1 | 0 | 0 | 0 | 0 |
| 17 | A | 1 | 0 | 0 | 0 | 0 |
| 17 | C | 1 | 0 | 0 | 0 | 0 |
| 17 | N | 1 | 0 | 0 | 0 | 0 |
| 17 | P | 1 | 0 | 0 | 0 | 0 |
| 18 | A | 126 | 0 | 220 | 17 | 0 |
| 18 | L | 63 | 0 | 110 | 15 | 0 |
| 18 | N | 173 | 0 | 312 | 11 | 0 |
| 19 | A | 85 | 0 | 136 | 2 | 0 |
| 19 | C | 84 | 0 | 121 | 3 | 0 |
| 19 | N | 102 | 0 | 152 | 4 | 0 |
| 19 | P | 82 | 0 | 130 | 2 | 0 |
| 20 | A | 2 | 0 | 0 | 1 | 0 |
| 20 | N | 2 | 0 | 0 | 1 | 0 |
| 21 | A | 25 | 0 | 44 | 3 | 0 |
| 21 | O | 31 | 0 | 52 | 4 | 0 |
| 22 | A | 44 | 0 | 66 | 5 | 0 |
| 22 | B | 16 | 0 | 24 | 0 | 0 |
| 22 | C | 40 | 0 | 60 | 2 | 0 |
| 22 | D | 20 | 0 | 30 | 5 | 0 |
| 22 | E | 12 | 0 | 18 | 0 | 0 |
| 22 | F | 32 | 0 | 48 | 0 | 0 |
| 22 | G | 4 | 0 | 6 | 0 | 0 |
| 22 | J | 8 | 0 | 12 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22 | L | 8 | 0 | 12 | 0 | 0 |
| 22 | M | 4 | 0 | 6 | 0 | 0 |
| 22 | N | 40 | 0 | 60 | 2 | 0 |
| 22 | O | 12 | 0 | 18 | 0 | 0 |
| 22 | P | 28 | 0 | 42 | 0 | 0 |
| 22 | Q | 4 | 0 | 6 | 0 | 0 |
| 22 | S | 24 | 0 | 36 | 1 | 0 |
| 22 | T | 12 | 0 | 18 | 0 | 0 |
| 22 | W | 8 | 0 | 12 | 0 | 0 |
| 22 | Y | 4 | 0 | 6 | 1 | 0 |
| 23 | A | 11 | 0 | 21 | 0 | 0 |
| 23 | C | 45 | 0 | 63 | 3 | 0 |
| 23 | D | 44 | 0 | 63 | 3 | 0 |
| 23 | J | 11 | 0 | 21 | 1 | 0 |
| 23 | K | 49 | 0 | 93 | 2 | 0 |
| 23 | L | 21 | 0 | 30 | 6 | 0 |
| 23 | M | 33 | 0 | 42 | 2 | 0 |
| 23 | O | 13 | 0 | 21 | 0 | 0 |
| 23 | P | 86 | 0 | 109 | 5 | 0 |
| 23 | Q | 11 | 0 | 21 | 2 | 0 |
| 23 | X | 50 | 0 | 84 | 2 | 0 |
| 23 | Z | 33 | 0 | 42 | 1 | 0 |
| 24 | B | 2 | 0 | 0 | 0 | 0 |
| 24 | O | 2 | 0 | 0 | 0 | 0 |
| 25 | B | 29 | 0 | 39 | 0 | 0 |
| 25 | C | 58 | 0 | 78 | 2 | 0 |
| 25 | G | 29 | 0 | 39 | 1 | 0 |
| 25 | J | 29 | 0 | 39 | 2 | 0 |
| 25 | L | 29 | 0 | 39 | 2 | 0 |
| 25 | P | 29 | 0 | 39 | 0 | 0 |
| 25 | Y | 29 | 0 | 39 | 0 | 0 |
| 26 | C | 133 | 0 | 192 | 7 | 0 |
| 26 | P | 90 | 0 | 116 | 2 | 0 |
| 26 | T | 37 | 0 | 59 | 6 | 0 |
| 27 | C | 65 | 0 | 113 | 7 | 0 |
| 27 | N | 62 | 0 | 109 | 5 | 0 |
| 27 | P | 68 | 0 | 119 | 7 | 0 |
| 27 | T | 61 | 0 | 110 | 9 | 0 |
| 28 | F | 1 | 0 | 0 | 0 | 0 |
| 28 | S | 1 | 0 | 0 | 0 | 0 |
| 29 | H | 5 | 0 | 0 | 0 | 0 |
| 29 | U | 5 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30 | A | 274 | 0 | 0 | 7 | 0 |
| 30 | B | 229 | 0 | 0 | 1 | 0 |
| 30 | C | 153 | 0 | 0 | 5 | 0 |
| 30 | D | 207 | 0 | 0 | 0 | 0 |
| 30 | E | 162 | 0 | 0 | 0 | 0 |
| 30 | F | 161 | 0 | 0 | 2 | 0 |
| 30 | G | 87 | 0 | 0 | 1 | 0 |
| 30 | H | 92 | 0 | 0 | 0 | 0 |
| 30 | I | 71 | 0 | 0 | 1 | 0 |
| 30 | J | 61 | 0 | 0 | 0 | 0 |
| 30 | K | 45 | 0 | 0 | 0 | 0 |
| 30 | L | 40 | 0 | 0 | 2 | 0 |
| 30 | M | 37 | 0 | 0 | 0 | 0 |
| 30 | N | 282 | 0 | 0 | 7 | 0 |
| 30 | O | 199 | 0 | 0 | 1 | 0 |
| 30 | P | 161 | 0 | 0 | 0 | 0 |
| 30 | Q | 119 | 0 | 0 | 2 | 0 |
| 30 | R | 113 | 0 | 0 | 1 | 0 |
| 30 | S | 141 | 0 | 0 | 2 | 0 |
| 30 | T | 66 | 0 | 0 | 1 | 0 |
| 30 | U | 96 | 0 | 0 | 1 | 0 |
| 30 | V | 66 | 0 | 0 | 0 | 0 |
| 30 | W | 41 | 0 | 0 | 0 | 0 |
| 30 | X | 33 | 0 | 0 | 0 | 0 |
| 30 | Y | 31 | 0 | 0 | 0 | 0 |
| 30 | Z | 28 | 0 | 0 | 0 | 0 |
| All | All | 34545 | 0 | 32367 | 372 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:A:609[A]:PER:O2 | 20:A:609[A]:PER:O1 | 1.55 | 1.24 |
| 20:N:611[A]:PER:O2 | 20:N:611[A]:PER:O1 | 1.55 | 1.21 |
| 12:L:20:ARG:HH22 | 18:L:101:TGL:HC52 | 1.31 | 0.95 |
| 1:N:113:LEU:HB2 | 18:N:608:TGL:H301 | 1.58 | 0.85 |
| 6:F:85:CYS:SG | 6:F:87[A]:THR:HG23 | 2.16 | 0.85 |
| 23:P:308:DMU:H9 | 10:W:49:CYS:HB3 | 1.57 | 0.85 |
| 18:A:607:TGL:HB21 | 4:D:78:TRP:HB3 | 1.57 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 1:A:178[B]:GLN:NE2 | 7:T:7:ASP:O | 2.10 | 0.84 |
| 8:H:7:LYS:HD2 | 8:H:8:ILE:HG23 | 1.63 | 0.80 |
| 12:L:20:ARG:HH12 | 18:L:101:TGL:HC32 | 1.46 | 0.79 |
| 1:N:510:TYR:HA | 22:N:621:EDO:H12 | 1.69 | 0.74 |
| 19:A:608:PGV:H311 | 13:M:19:LEU:HD23 | 1.71 | 0.73 |
| 12:L:24[B]:MET:HE1 | 18:L:101:TGL:HC81 | 1.68 | 0.73 |
| 27:C:308:CDL:H322 | 27:C:308:CDL:H471 | 1.70 | 0.72 |
| 13:M:39:ASN:HD22 | 13:M:39:ASN:H | 1.38 | 0.72 |
| 27:T:102:CDL:H531 | 27:T:102:CDL:H251 | 1.73 | 0.71 |
| 26:C:304:PEK:H101 | 26:C:304:PEK:H42 | 1.72 | 0.69 |
| 1:A:194:LEU:HD11 | 7:T:4:ALA:HB1 | 1.75 | 0.69 |
| 12:L:14:SER:H | 18:L:101:TGL:HC31 | 1.58 | 0.68 |
| 3:P:62:ILE:HD12 | 27:P:307:CDL:H522 | 1.77 | 0.67 |
| 5:R:80:GLU:N | 5:R:80:GLU:OE1 | 2.28 | 0.67 |
| 27:P:307:CDL:H521 | 27:P:307:CDL:HB62 | 1.77 | 0.67 |
| 26:P:304:PEK:H101 | 26:P:304:PEK:H42 | 1.76 | 0.66 |
| 12:L:20:ARG:NH2 | 18:L:101:TGL:HC52 | 2.06 | 0.66 |
| 18:L:101:TGL:OC1 | 18:L:101:TGL:HC41 | 1.95 | 0.66 |
| 19:C:307:PGV:H21 | 19:C:307:PGV:H71 | 1.77 | 0.65 |
| 7:T:74:ARG:NH1 | 30:T:201:HOH:O | 2.29 | 0.65 |
| 22:A:616:EDO:H22 | 30:A:912:HOH:O | 1.97 | 0.65 |
| 2:B:100[B]:MET:HG2 | 2:B:157:GLU:HG3 | 1.78 | 0.65 |
| 18:A:607:TGL:HC71 | 2:B:49:LYS:HE3 | 1.80 | 0.64 |
| 12:L:25:MET:HG2 | 18:L:101:TGL:HA62 | 1.79 | 0.64 |
| 3:P:33:MET:HE1 | 3:P:42:LEU:H | 1.62 | 0.63 |
| 1:N:24:ALA:HB2 | 14:N:602[A]:HEA:H253 | 1.80 | 0.63 |
| 4:D:4:SER:HB2 | 22:D:204:EDO:O1 | 1.97 | 0.63 |
| 3:P:80[B]:ARG:NH2 | 3:P:236:GLU:OE1 | 2.31 | 0.63 |
| 3:P:34:TRP:HE1 | 23:P:316:DMU:H29 | 1.63 | 0.61 |
| 12:L:2:HIS:CG | 12:L:3:TYR:H | 2.18 | 0.61 |
| 13:M:39:ASN:H | 13:M:39:ASN:ND2 | 1.99 | 0.61 |
| 1:N:377:PHE:HA | 1:N:380[B]:VAL:HG12 | 1.83 | 0.61 |
| 18:A:606:TGL:H322 | 18:A:606:TGL:H261 | 1.83 | 0.60 |
| 1:N:334:TRP:CD1 | 18:N:609:TGL:HC41 | 2.36 | 0.60 |
| 1:A:169:ILE:HG23 | 7:T:8:HIS:O | 2.02 | 0.59 |
| 7:G:11:THR:HA | 30:N:867:HOH:O | 2.02 | 0.59 |
| 18:A:607:TGL:HA31 | 18:A:607:TGL:HB51 | 1.83 | 0.59 |
| 18:N:608:TGL:HC51 | 12:Y:20:ARG:NH2 | 2.17 | 0.59 |
| 27:T:102:CDL:H781 | 27:T:102:CDL:H561 | 1.83 | 0.59 |
| 7:G:37:LEU:HD23 | 27:N:601:CDL:H381 | 1.84 | 0.59 |
| 4:D:94:LEU:HB3 | 23:D:206:DMU:H18 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:G:1:ALA:HB2 | 19:P:306:PGV:H342 | 1.85 | 0.59 |
| 26:C:304:PEK:H14 | 30:C:535:HOH:O | 2.03 | 0.59 |
| 9:I:8:GLN:HG2 | 30:I:140:HOH:O | 2.02 | 0.59 |
| 1:N:514:LYS:OXT | 6:S:37:LYS:NZ | 2.34 | 0.59 |
| 3:C:203:PHE:CE1 | 26:C:304:PEK:H9 | 2.38 | 0.58 |
| 7:G:5:LYS:HB3 | 1:N:278[B]:MET:HE3 | 1.84 | 0.58 |
| 1:N:49[B]:GLY:HA3 | 13:Z:41:LYS:HE3 | 1.86 | 0.58 |
| 11:X:40:TRP:CD2 | 23:X:102:DMU:H14 | 2.38 | 0.58 |
| 2:O:19:GLU:HG3 | 2:O:86[A]:MET:HE1 | 1.85 | 0.58 |
| 2:O:196:CYS:HB2 | 2:O:207:MET:HG3 | 1.86 | 0.58 |
| 6:F:54[A]:ASN:ND2 | 30:F:203:HOH:O | 2.36 | 0.58 |
| 10:J:55:PHE:CE1 | 23:L:105:DMU:H29 | 2.39 | 0.58 |
| 2:B:196:CYS:HB2 | 2:B:207:MET:HG3 | 1.85 | 0.57 |
| 1:N:35[B]:LEU:HD23 | 23:Z:101:DMU:H24 | 1.86 | 0.57 |
| 1:N:53[B]:ILE:HG12 | 30:N:895:HOH:O | 2.04 | 0.57 |
| 1:N:308:ALA:O | 1:N:311[A]:ILE:HG12 | 2.04 | 0.57 |
| 2:B:130:PRO:HB3 | 22:D:205:EDO:H21 | 1.85 | 0.57 |
| 3:C:127:LEU:HD22 | 27:N:601:CDL:HB61 | 1.87 | 0.57 |
| 1:N:297[C]:MET:HG2 | 1:N:302:ARG:HG3 | 1.85 | 0.57 |
| 1:A:194:LEU:CD1 | 7:T:4:ALA:HB1 | 2.35 | 0.56 |
| 3:P:168:THR:HG21 | 26:T:101:PEK:H12 | 1.87 | 0.56 |
| 30:C:411:HOH:O | 6:F:52:ILE:HD11 | 2.05 | 0.56 |
| 7:G:4:ALA:HB3 | 1:N:282:PHE:HA | 1.88 | 0.56 |
| 4:Q:20:ARG:HG2 | 30:Q:386:HOH:O | 2.05 | 0.56 |
| 1:A:321[A]:PHE:CD2 | 2:B:65:TRP:HB2 | 2.40 | 0.55 |
| 1:A:321[B]:PHE:CD1 | 21:A:610:PSC:H341 | 2.41 | 0.55 |
| 21:A:610:PSC:H242 | 2:B:56:MET:HB3 | 1.88 | 0.55 |
| 19:N:610:PGV:H311 | 13:Z:19:LEU:HD23 | 1.89 | 0.55 |
| 23:D:206:DMU:H29 | 11:K:36:ILE:HB | 1.88 | 0.55 |
| 18:A:607:TGL:HC42 | 18:A:607:TGL:OG3 | 2.07 | 0.55 |
| 3:C:156:ARG:HE | 25:C:309:CHD:C24 | 2.20 | 0.55 |
| 1:A:334:TRP:CD1 | 18:A:607:TGL:HC41 | 2.42 | 0.55 |
| 27:T:102:CDL:H561 | 27:T:102:CDL:H761 | 1.89 | 0.55 |
| 1:N:379:TYR:O | 1:N:383[B]:MET:HB2 | 2.06 | 0.55 |
| 1:A:337:ALA:HB2 | 1:A:394[A]:VAL:HG23 | 1.89 | 0.55 |
| 1:A:377:PHE:O | 1:A:381[B]:LEU:HB3 | 2.07 | 0.55 |
| 14:N:603:HEA:HMC1 | 14:N:603:HEA:HBC1 | 1.89 | 0.55 |
| 2:B:13:THR:HB | 2:B:168:LEU:HD23 | 1.89 | 0.54 |
| 2:B:132:GLU:HB3 | 2:B:137:GLU:HG3 | 1.90 | 0.54 |
| 2:O:116:LEU:HD13 | 2:O:226:MET:HG2 | 1.88 | 0.54 |
| 5:R:43:PRO:HB2 | 5:R:48:ILE:HD11 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 8:U:43:MET:HE3 | 8:U:49:ASP:N | 2.23 | 0.54 |
| 19:N:612:PGV:H183 | 26:P:304:PEK:H342 | 1.90 | 0.54 |
| 1:N:331[B]:ASN:ND2 | 4:Q:21:ASP:HB3 | 2.22 | 0.53 |
| 1:A:278[B]:MET:HB3 | 7:T:5:LYS:HG2 | 1.90 | 0.53 |
| 3:C:210:ILE:HG12 | 19:C:306:PGV:H132 | 1.90 | 0.53 |
| 1:A:265:LYS:HB2 | 1:A:490:THR:HG21 | 1.91 | 0.53 |
| 12:L:24[B]:MET:SD | 18:L:101:TGL:HC22 | 2.48 | 0.53 |
| 1:N:297[C]:MET:CG | 1:N:302:ARG:HG3 | 2.38 | 0.53 |
| 7:T:41:HIS:HB3 | 7:T:74:ARG:NH2 | 2.24 | 0.53 |
| 1:N:514:LYS:HD2 | 30:S:278:HOH:O | 2.07 | 0.53 |
| 26:T:101:PEK:H382 | 27:T:102:CDL:H273 | 1.91 | 0.53 |
| 1:A:107:PRO:HB3 | 3:C:25:LEU:HB2 | 1.90 | 0.53 |
| 1:N:113:LEU:HB2 | 18:N:608:TGL:C32 | 2.39 | 0.53 |
| 4:Q:6:VAL:HG12 | 4:Q:7:LYS:H | 1.74 | 0.53 |
| 1:A:24:ALA:HB2 | 14:A:601[A]:HEA:H253 | 1.91 | 0.52 |
| 4:D:40:LEU:CD2 | 4:D:58:GLU:HG2 | 2.39 | 0.52 |
| 1:A:349:THR:OG1 | 1:A:349:THR:CA | 2.57 | 0.52 |
| 1:N:488:THR:HB | 1:N:495:LEU:HD13 | 1.91 | 0.52 |
| 4:D:120:THR:HG21 | 11:K:48[B]:VAL:CG1 | 2.40 | 0.52 |
| 2:O:132:GLU:HB3 | 2:O:137:GLU:HG3 | 1.91 | 0.52 |
| 10:J:41:GLY:HA3 | 23:J:104:DMU:H23 | 1.90 | 0.52 |
| 4:D:98:TRP:CE2 | 23:M:101:DMU:H11 | 2.44 | 0.52 |
| 14:A:602:HEA:HBC1 | 14:A:602:HEA:HMC1 | 1.91 | 0.52 |
| 3:C:52:LEU:HD21 | 27:C:308:CDL:H432 | 1.92 | 0.51 |
| 2:B:104:TRP:CG | 2:B:203:ASN:HB2 | 2.45 | 0.51 |
| 21:O:302:PSC:H111 | 21:O:302:PSC:H321 | 1.92 | 0.51 |
| 1:A:514[A]:LYS:HD2 | 30:A:731:HOH:O | 2.11 | 0.51 |
| 30:A:787:HOH:O | 12:L:7:PRO:HG3 | 2.09 | 0.51 |
| 1:A:379:TYR:O | 1:A:383[B]:MET:HB2 | 2.11 | 0.51 |
| 27:N:601:CDL:H371 | 2:O:81:LEU:HD12 | 1.93 | 0.51 |
| 1:A:343:GLY:HA2 | 18:A:607:TGL:H212 | 1.93 | 0.50 |
| 1:A:53[A]:ILE:HD11 | 12:L:40:VAL:HG13 | 1.93 | 0.50 |
| 10:J:55:PHE:HE1 | 23:L:105:DMU:H29 | 1.75 | 0.50 |
| 1:A:377:PHE:HA | 1:A:380[B]:VAL:HG12 | 1.94 | 0.50 |
| 22:A:612:EDO:H22 | 13:M:1:ILE:H1 | 1.77 | 0.50 |
| 18:L:101:TGL:CC1 | 18:L:101:TGL:HC61 | 2.41 | 0.50 |
| 18:L:101:TGL:CC1 | 18:L:101:TGL:HG12 | 2.39 | 0.50 |
| 1:N:297[C]:MET:SD | 1:N:302:ARG:HG3 | 2.51 | 0.50 |
| 2:O:93:PRO:HG3 | 2:O:151:ARG:HB2 | 1.91 | 0.50 |
| 1:A:46:THR:HG22 | 1:A:49[B]:GLY:H | 1.77 | 0.50 |
| 26:C:305:PEK:H231 | 7:G:21:PHE:CD1 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:H:49:ASP:O | 8:H:52:VAL:HG22 | 2.12 | 0.50 |
| 1:N:265:LYS:HB2 | 1:N:490:THR:HG21 | 1.93 | 0.50 |
| 8:U:7:LYS:O | 8:U:8:ILE:HB | 2.11 | 0.50 |
| 3:P:52:LEU:HD21 | 27:P:307:CDL:H412 | 1.94 | 0.50 |
| 2:B:87:MET:HE2 | 30:B:417:HOH:O | 2.10 | 0.50 |
| 2:O:78:LEU:O | 2:O:82[B]:ARG:HG3 | 2.12 | 0.50 |
| 3:C:180[B]:GLU:HG3 | 30:C:416:HOH:O | 2.10 | 0.50 |
| 3:C:258:TRP:HZ3 | 27:N:601:CDL:H651 | 1.77 | 0.50 |
| 8:U:46:LYS:O | 30:U:201:HOH:O | 2.19 | 0.50 |
| 21:A:610:PSC:H342 | 2:B:41:ILE:HD13 | 1.93 | 0.49 |
| 3:C:37:PHE:CE2 | 23:C:310:DMU:H13 | 2.47 | 0.49 |
| 7:T:31:CYS:SG | 27:T:102:CDL:H532 | 2.52 | 0.49 |
| 23:L:105:DMU:H5 | 30:L:216:HOH:O | 2.12 | 0.49 |
| 1:A:282:PHE:HA | 7:T:4:ALA:HB3 | 1.93 | 0.49 |
| 4:Q:65:LYS:HE3 | 30:Q:410:HOH:O | 2.12 | 0.49 |
| 27:T:102:CDL:H781 | 27:T:102:CDL:C56 | 2.42 | 0.49 |
| 3:C:180[B]:GLU:HG2 | 30:C:422:HOH:O | 2.11 | 0.49 |
| 11:X:40:TRP:CD1 | 23:X:102:DMU:H10 | 2.47 | 0.49 |
| 1:A:311:ILE:CD1 | 27:T:102:CDL:H441 | 2.42 | 0.49 |
| 8:H:36:PHE:CD1 | 8:H:57:ARG:HB2 | 2.48 | 0.49 |
| 1:N:113:LEU:CB | 18:N:608:TGL:H301 | 2.36 | 0.49 |
| 1:A:513:LEU:O | 1:A:514[A]:LYS:HB2 | 2.13 | 0.49 |
| 2:O:58:ALA:O | 2:O:62:GLU:HG3 | 2.13 | 0.49 |
| 3:P:257:TYR:O | 3:P:261:SER:HB3 | 2.12 | 0.49 |
| 1:N:468:MET:HG3 | 30:N:969:HOH:O | 2.11 | 0.49 |
| 12:Y:3:TYR:CE2 | 22:Y:101:EDO:H21 | 2.48 | 0.49 |
| 3:P:33:MET:CE | 3:P:42:LEU:H | 2.25 | 0.49 |
| 2:O:13:THR:HB | 2:O:168:LEU:HD23 | 1.95 | 0.49 |
| 2:B:168:LEU:HD13 | 2:B:184:LEU:HG | 1.94 | 0.49 |
| 3:C:258:TRP:CE3 | 22:C:315:EDO:H21 | 2.48 | 0.49 |
| 2:O:56:MET:HB3 | 21:O:302:PSC:H232 | 1.94 | 0.49 |
| 4:Q:101:HIS:ND1 | 23:Q:201:DMU:H6 | 2.28 | 0.49 |
| 1:N:383[C]:MET:O | 1:N:387:PHE:N | 2.46 | 0.48 |
| 4:Q:101:HIS:CG | 23:Q:201:DMU:H6 | 2.48 | 0.48 |
| 7:G:7:ASP:O | 1:N:178[B]:GLN:NE2 | 2.46 | 0.48 |
| 25:L:102:CHD:H232 | 13:M:21:VAL:HG21 | 1.95 | 0.48 |
| 3:P:41:THR:HA | 3:P:44[A]:MET:HE2 | 1.95 | 0.48 |
| 1:A:381[B]:LEU:HB2 | 14:A:602:HEA:CAC | 2.43 | 0.48 |
| 1:N:46:THR:HG22 | 1:N:49[B]:GLY:H | 1.78 | 0.48 |
| 2:O:23:PHE:CZ | 2:O:80:SER:HB2 | 2.48 | 0.48 |
| 3:P:40:MET:SD | 23:P:316:DMU:H6 | 2.54 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:P:210:ILE:HD13 | 19:P:305:PGV:H301 | 1.96 | 0.48 |
| 12:L:24[A]:MET:SD | 18:L:101:TGL:H152 | 2.54 | 0.48 |
| 3:P:34:TRP:CD1 | 3:P:40:MET:HG2 | 2.48 | 0.48 |
| 7:G:4:ALA:CB | 1:N:282:PHE:HA | 2.43 | 0.48 |
| 4:D:120:THR:HG21 | 11:K:48[B]:VAL:HG11 | 1.95 | 0.48 |
| 1:A:321[B]:PHE:HB3 | 2:B:65:TRP:CE3 | 2.49 | 0.47 |
| 27:P:307:CDL:H161 | 27:P:307:CDL:H132 | 1.65 | 0.47 |
| 4:D:4:SER:HB2 | 22:D:204:EDO:C1 | 2.45 | 0.47 |
| 8:H:46:LYS:HE3 | 8:U:7:LYS:HB2 | 1.96 | 0.47 |
| 10:W:29:ASN:O | 10:W:33:ARG:HG3 | 2.13 | 0.47 |
| 4:Q:126:MET:HG3 | 4:Q:128:VAL:HG23 | 1.96 | 0.47 |
| 11:X:24:PHE:O | 11:X:28:VAL:HG12 | 2.15 | 0.47 |
| 18:A:606:TGL:HA72 | 18:A:606:TGL:H142 | 1.96 | 0.47 |
| 1:N:406:ASN:HD21 | 19:N:610:PGV:H21 | 1.79 | 0.47 |
| 8:H:9:LYS:HA | 8:H:9:LYS:HD3 | 1.38 | 0.47 |
| 1:N:107:PRO:HB3 | 3:P:25:LEU:HB2 | 1.96 | 0.47 |
| 1:N:486[B]:ASP:OD2 | 4:Q:19:ARG:NE | 2.47 | 0.47 |
| 18:A:606:TGL:H142 | 18:A:606:TGL:H112 | 1.43 | 0.47 |
| 8:U:43:MET:HE3 | 8:U:49:ASP:H | 1.80 | 0.46 |
| 11:K:42:PRO:O | 11:K:47:ARG:NH2 | 2.49 | 0.46 |
| 1:N:381[B]:LEU:HB2 | 14:N:603:HEA:CAC | 2.46 | 0.46 |
| 2:O:61:VAL:O | 2:O:64[A]:ILE:HG23 | 2.16 | 0.46 |
| 1:A:273:MET:HE2 | 30:A:756:HOH:O | 2.15 | 0.46 |
| 18:L:101:TGL:H261 | 18:L:101:TGL:H232 | 1.71 | 0.46 |
| 3:C:51[A]:MET:SD | 27:C:308:CDL:H622 | 2.56 | 0.46 |
| 6:F:50:PRO:HG2 | 30:F:265:HOH:O | 2.16 | 0.46 |
| 2:O:215:PRO:HD3 | 9:V:60:PHE:CD1 | 2.50 | 0.46 |
| 3:C:220:PHE:HB2 | 27:C:308:CDL:H712 | 1.96 | 0.46 |
| 18:A:606:TGL:H101 | 18:A:606:TGL:C28 | 2.46 | 0.46 |
| 1:A:376:HIS:CE1 | 1:A:380[B]:VAL:HG11 | 2.50 | 0.46 |
| 1:A:383[C]:MET:O | 1:A:387:PHE:N | 2.48 | 0.46 |
| 26:C:304:PEK:H221 | 26:C:304:PEK:H251 | 1.54 | 0.46 |
| 27:C:308:CDL:H822 | 27:C:308:CDL:H851 | 1.66 | 0.46 |
| 2:O:89:GLU:O | 2:O:91:ASN:ND2 | 2.49 | 0.46 |
| 18:N:607:TGL:HB91 | 18:N:607:TGL:H122 | 1.72 | 0.46 |
| 30:N:825:HOH:O | 3:P:77:LYS:HE3 | 2.15 | 0.46 |
| 5:R:7:THR:HB | 5:R:9:GLU:OE2 | 2.16 | 0.46 |
| 18:A:607:TGL:HB42 | 4:D:78:TRP:HA | 1.98 | 0.46 |
| 18:N:608:TGL:H222 | 18:N:608:TGL:HA91 | 1.54 | 0.46 |
| 27:P:307:CDL:H821 | 27:P:307:CDL:H851 | 1.58 | 0.46 |
| 1:A:285:PHE:CE2 | 7:T:4:ALA:HB2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:A:309:THR:HG22 | 14:A:602:HEA:HMB2 | 1.99 | 0.45 |
| 4:Q:48:TRP:HA | 4:Q:51:LEU:HD22 | 1.99 | 0.45 |
| 18:N:607:TGL:H222 | 18:N:607:TGL:H271 | 1.99 | 0.45 |
| 14:A:601[B]:HEA:H122 | 30:A:860:HOH:O | 2.17 | 0.45 |
| 8:U:9:LYS:O | 8:U:10:ASN:HB2 | 2.16 | 0.45 |
| 1:A:53[B]:ILE:HG12 | 30:L:235:HOH:O | 2.17 | 0.45 |
| 5:E:90:ARG:NH2 | 5:E:103:GLU:OE2 | 2.49 | 0.45 |
| 1:N:408:THR:HB | 19:N:610:PGV:H51 | 1.97 | 0.45 |
| 1:N:35[A]:LEU:HD11 | 1:N:462:LEU:HB2 | 1.98 | 0.45 |
| 3:P:224[B]:LYS:HE3 | 27:P:307:CDL:H131 | 1.98 | 0.45 |
| 14:A:602:HEA:H243 | 2:B:69:PRO:HB3 | 1.99 | 0.45 |
| 1:N:297[C]:MET:SD | 1:N:302:ARG:CG | 3.05 | 0.45 |
| 1:N:383[A]:MET:HG2 | 1:N:421:VAL:HG21 | 1.99 | 0.45 |
| 6:S:22:LEU:HD12 | 30:S:306:HOH:O | 2.15 | 0.45 |
| 2:O:65[B]:TRP:CD1 | 21:O:302:PSC:H12 | 2.52 | 0.45 |
| 1:A:285:PHE:CD2 | 7:T:4:ALA:HB2 | 2.52 | 0.45 |
| 1:N:337:ALA:HB2 | 1:N:394[A]:VAL:HG23 | 1.98 | 0.45 |
| 27:C:308:CDL:H662 | 27:C:308:CDL:H631 | 1.72 | 0.44 |
| 7:G:9:GLY:HA2 | 30:N:892:HOH:O | 2.17 | 0.44 |
| 7:T:21:PHE:CG | 26:T:101:PEK:H222 | 2.51 | 0.44 |
| 3:C:207:HIS:CE1 | 19:C:306:PGV:H343 | 2.52 | 0.44 |
| 2:O:164:ALA:O | 2:O:194:GLY:HA3 | 2.17 | 0.44 |
| 6:S:76:LYS:HE3 | 6:S:76:LYS:HB3 | 1.69 | 0.44 |
| 3:C:164:PHE:CD1 | 25:C:309:CHD:H192 | 2.52 | 0.44 |
| 3:P:168:THR:HG22 | 26:T:101:PEK:H14 | 2.00 | 0.44 |
| 7:T:41:HIS:HB3 | 7:T:74:ARG:CZ | 2.47 | 0.44 |
| 1:A:236:TRP:CH2 | 14:A:602:HEA:HBD1 | 2.51 | 0.44 |
| 1:A:334:TRP:CZ3 | 18:A:607:TGL:HA51 | 2.52 | 0.44 |
| 22:A:620:EDO:H22 | 6:F:66:ASN:ND2 | 2.31 | 0.44 |
| 1:A:311:ILE:HD11 | 27:T:102:CDL:H421 | 2.00 | 0.44 |
| 22:C:318:EDO:H11 | 6:F:16:LEU:HD13 | 1.99 | 0.44 |
| 12:L:24[B]:MET:CG | 18:L:101:TGL:HA22 | 2.47 | 0.44 |
| 1:N:73:ILE:HD11 | 14:N:602[C]:HEA:H22 | 1.98 | 0.44 |
| 14:N:602[C]:HEA:H212 | 14:N:602[C]:HEA:H271 | 1.87 | 0.44 |
| 1:N:307:SER:O | 1:N:311[A]:ILE:HG23 | 2.17 | 0.44 |
| 2:O:41:ILE:O | 2:O:45:MET:HG2 | 2.18 | 0.44 |
| 1:A:334:TRP:CH2 | 2:B:46:LEU:HD13 | 2.52 | 0.44 |
| 1:A:334:TRP:CE3 | 18:A:607:TGL:HA51 | 2.53 | 0.44 |
| 13:Z:37:LEU:HD23 | 13:Z:37:LEU:HA | 1.86 | 0.44 |
| 1:N:92:MET:HE1 | 1:N:164:PHE:CD1 | 2.52 | 0.44 |
| 1:A:136[B]:LEU:HD11 | 30:A:962:HOH:O | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 1:A:292:MET:O | 1:A:297[B]:MET:HE3 | 2.17 | 0.43 |
| 26:C:304:PEK:H42 | 26:C:304:PEK:H72 | 1.59 | 0.43 |
| 3:P:47:LEU:O | 3:P:51[B]:MET:HG2 | 2.18 | 0.43 |
| 12:L:41:ARG:NH1 | 23:L:105:DMU:H2 | 2.33 | 0.43 |
| 3:P:168:THR:CG2 | 26:T:101:PEK:H12 | 2.46 | 0.43 |
| 2:B:164:ALA:O | 2:B:194:GLY:HA3 | 2.17 | 0.43 |
| 12:L:35:ALA:HB3 | 12:L:36:PRO:HD3 | 2.00 | 0.43 |
| 1:N:377:PHE:O | 1:N:381[B]:LEU:HB3 | 2.18 | 0.43 |
| 4:Q:5:VAL:H | 13:Z:5:PRO:HD3 | 1.83 | 0.43 |
| 3:C:158:HIS:CE1 | 6:F:1:ALA:HB3 | 2.53 | 0.43 |
| 23:K:101:DMU:H21 | 23:K:102:DMU:H17 | 2.00 | 0.43 |
| 12:L:2:HIS:CG | 12:L:3:TYR:N | 2.85 | 0.43 |
| 1:N:76:GLY:O | 1:N:80:ASN:HB2 | 2.18 | 0.43 |
| 1:A:334:TRP:HZ3 | 18:A:607:TGL:HA71 | 1.83 | 0.43 |
| 12:L:41:ARG:HH12 | 23:L:105:DMU:H2 | 1.83 | 0.43 |
| 1:N:334:TRP:CH2 | 2:O:46:LEU:HD13 | 2.54 | 0.43 |
| 3:P:59:ARG:HA | 27:P:307:CDL:H522 | 1.99 | 0.43 |
| 5:R:79:LYS:HD2 | 5:R:79:LYS:HA | 1.89 | 0.43 |
| 6:S:54:ASN:HB2 | 6:S:76:LYS:HE2 | 2.00 | 0.43 |
| 10:W:54:SER:O | 12:Y:46:LYS:HD3 | 2.18 | 0.43 |
| 1:A:52[B]:GLN:O | 1:A:56:VAL:HG23 | 2.19 | 0.43 |
| 3:C:37:PHE:CD2 | 23:C:310:DMU:H13 | 2.53 | 0.43 |
| 1:N:116:SER:HB3 | 30:N:834:HOH:O | 2.18 | 0.43 |
| 1:A:362[B]:SER:HB2 | 2:B:20:LEU:HD21 | 2.01 | 0.43 |
| 22:A:612:EDO:H22 | 13:M:1:ILE:N | 2.34 | 0.43 |
| 12:Y:45:LEU:HD21 | 13:Z:40:TYR:CD1 | 2.54 | 0.43 |
| 18:A:607:TGL:HG32 | 30:A:924:HOH:O | 2.18 | 0.43 |
| 6:F:21[B]:MET:HE2 | 6:F:21[B]:MET:HB2 | 1.64 | 0.42 |
| 1:N:54[A]:TYR:HB2 | 30:N:788[A]:HOH:O | 2.19 | 0.42 |
| 7:G:5:LYS:HB3 | 1:N:278[B]:MET:CE | 2.49 | 0.42 |
| 1:N:321:PHE:CD1 | 21:O:302:PSC:H341 | 2.54 | 0.42 |
| 14:N:603:HEA:H243 | 2:O:69:PRO:HB3 | 2.01 | 0.42 |
| 1:A:321[A]:PHE:HB3 | 2:B:65:TRP:CE3 | 2.54 | 0.42 |
| 4:D:98:TRP:CD2 | 23:M:101:DMU:H11 | 2.54 | 0.42 |
| 23:L:105:DMU:H13 | 23:L:105:DMU:H18 | 1.62 | 0.42 |
| 2:B:196:CYS:CB | 2:B:207:MET:HG3 | 2.50 | 0.42 |
| 1:N:266:GLU:OE1 | 22:S:106:EDO:H11 | 2.19 | 0.42 |
| 2:O:183:THR:HG22 | 30:O:567:HOH:O | 2.19 | 0.42 |
| 10:W:4:ARG:O | 10:W:7:GLU:HG2 | 2.20 | 0.42 |
| 14:A:601[C]:HEA:H212 | 14:A:601[C]:HEA:H271 | 1.69 | 0.42 |
| 3:P:47:LEU:O | 3:P:51[A]:MET:HG3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:B:58:ALA:O | 2:B:62:GLU:HG3 | 2.20 | 0.42 |
| 3:C:58:TRP:HB2 | 27:C:308:CDL:H552 | 2.02 | 0.42 |
| 11:K:47:ARG:HG2 | 11:K:48[A]:VAL:HG23 | 2.02 | 0.42 |
| 1:N:309:THR:HG22 | 14:N:603:HEA:HMB2 | 2.00 | 0.42 |
| 2:O:168:LEU:HD13 | 2:O:184:LEU:HG | 2.01 | 0.42 |
| 5:R:108:LYS:HB3 | 30:R:298:HOH:O | 2.20 | 0.42 |
| 2:B:100[B]:MET:CG | 2:B:157:GLU:HG3 | 2.49 | 0.42 |
| 3:C:244:PHE:HA | 26:C:303:PEK:H101 | 2.01 | 0.42 |
| 4:D:115:TRP:HE3 | 22:D:205:EDO:H11 | 1.85 | 0.42 |
| 19:A:611:PGV:H182 | 3:C:28:THR:HG22 | 2.02 | 0.42 |
| 12:L:24[B]:MET:SD | 18:L:101:TGL:CC2 | 3.07 | 0.42 |
| 18:N:607:TGL:H311 | 18:N:607:TGL:H141 | 1.77 | 0.42 |
| 3:C:158:HIS:HE1 | 6:F:1:ALA:HB3 | 1.85 | 0.41 |
| 3:C:191:GLY:HA3 | 30:G:212:HOH:O | 2.19 | 0.41 |
| 12:L:24[B]:MET:HG2 | 18:L:101:TGL:HA22 | 2.02 | 0.41 |
| 1:N:112:LEU:HD23 | 1:N:112:LEU:C | 2.40 | 0.41 |
| 1:A:311:ILE:CD1 | 27:T:102:CDL:H421 | 2.51 | 0.41 |
| 10:J:37:THR:HG23 | 25:J:101:CHD:H191 | 2.02 | 0.41 |
| 25:J:101:CHD:H21 | 25:J:101:CHD:H9 | 1.79 | 0.41 |
| 2:O:113:TYR:HD1 | 8:U:58:ARG:NH2 | 2.17 | 0.41 |
| 9:V:63:MET:HB3 | 9:V:68:ILE:CD1 | 2.50 | 0.41 |
| 3:C:3:HIS:N | 30:C:410:HOH:O | 2.53 | 0.41 |
| 6:F:75:HIS:H | 6:F:80[B]:GLN:HE22 | 1.68 | 0.41 |
| 2:O:104:TRP:CG | 2:O:203:ASN:HB2 | 2.55 | 0.41 |
| 4:D:19[B]:ARG:NH1 | 4:D:22:TYR:HB2 | 2.36 | 0.41 |
| 1:N:229:ILE:HD11 | 2:O:175:ILE:HD13 | 2.03 | 0.41 |
| 1:N:236:TRP:CH2 | 14:N:603:HEA:HBD1 | 2.56 | 0.41 |
| 27:N:601:CDL:H801 | 27:N:601:CDL:H832 | 1.77 | 0.41 |
| 1:A:415:ALA:HB1 | 18:A:607:TGL:H131 | 2.02 | 0.41 |
| 2:O:102:HIS:O | 2:O:104:TRP:HA | 2.21 | 0.41 |
| 6:S:62:CYS:HB3 | 6:S:85:CYS:HB3 | 2.03 | 0.41 |
| 9:V:63:MET:HB3 | 9:V:68:ILE:HG12 | 2.02 | 0.41 |
| 1:A:246:LEU:HD13 | 1:A:381[B]:LEU:HD11 | 2.02 | 0.41 |
| 1:A:513:LEU:HD23 | 1:A:513:LEU:HA | 1.52 | 0.41 |
| 1:N:225:GLY:HA3 | 3:P:112:LEU:HD21 | 2.02 | 0.41 |
| 3:P:154:GLY:HA2 | 6:S:6:VAL:HB | 2.02 | 0.41 |
| 25:L:102:CHD:H183 | 25:L:102:CHD:H212 | 2.02 | 0.41 |
| 3:P:165:ILE:HG12 | 26:T:101:PEK:H11 | 2.03 | 0.41 |
| 9:V:36:LYS:HE3 | 9:V:36:LYS:HB3 | 1.86 | 0.41 |
| 10:W:18:LEU:HB2 | 10:W:23:LYS:HG3 | 2.02 | 0.41 |
| 3:C:157:LYS:HE2 | 3:C:161[B]:GLN:NE2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 25:G:101:CHD:H212 | 25:G:101:CHD:H12 | 2.02 | 0.41 |
| 2:O:128:LEU:HD11 | 2:O:134:ARG:HA | 2.02 | 0.41 |
| 23:P:308:DMU:H41 | 23:P:308:DMU:H36 | 1.74 | 0.41 |
| 23:P:308:DMU:H29 | 23:P:308:DMU:H32 | 2.03 | 0.41 |
| 1:A:120:ALA:HB2 | 22:A:618:EDO:H12 | 2.03 | 0.41 |
| 9:I:57:MET:O | 9:I:61[B]:GLU:HG2 | 2.20 | 0.41 |
| 18:A:607:TGL:H132 | 18:A:607:TGL:H101 | 1.89 | 0.40 |
| 18:N:608:TGL:HC31 | 12:Y:13:PHE:HA | 2.04 | 0.40 |
| 3:P:207:HIS:HD2 | 3:P:241:TYR:OH | 2.04 | 0.40 |
| 23:C:310:DMU:C22 | 10:J:49:CYS:HB3 | 2.51 | 0.40 |
| 4:D:5:VAL:H | 22:D:204:EDO:C1 | 2.35 | 0.40 |
| 1:A:302[B]:ARG:HH22 | 1:A:365[B]:ILE:HD11 | 1.86 | 0.40 |
| 12:L:23:ALA:O | 12:L:27[A]:LEU:HG | 2.21 | 0.40 |
| 1:N:242:GLU:HA | 1:N:245:ILE:HD12 | 2.02 | 0.40 |
| 1:N:331[B]:ASN:ND2 | 2:O:51:THR:HG21 | 2.36 | 0.40 |
| 18:N:608:TGL:HC22 | 18:N:608:TGL:HC52 | 1.78 | 0.40 |
| 4:D:101:HIS:HB2 | 23:D:206:DMU:H30 | 2.03 | 0.40 |
| 11:K:24:PHE:HB2 | 23:K:103:DMU:H9 | 2.02 | 0.40 |
| 1:N:50[B]:ASP:CG | 1:N:53[B]:ILE:HG13 | 2.42 | 0.40 |
| 1:N:331[B]:ASN:HD21 | 4:Q:21:ASP:HB3 | 1.86 | 0.40 |
| 13:M:39:ASN:ND2 | 13:M:39:ASN:N | 2.68 | 0.40 |
| 1:N:386[B]:VAL:HG21 | 14:N:602[B]:HEA:H162 | 2.04 | 0.40 |
| 22:N:620:EDO:H22 | 6:S:66:ASN:ND2 | 2.37 | 0.40 |
| 6:S:25:ARG:HE | 6:S:25:ARG:HB2 | 1.68 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|----------------|-----------|---------|----------|-----------------------|
| 1 | A | 548/514 (107%) | 529 (96%) | 19 (4%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1 | N | 553/514 (108%) | 534 (97%) | 19 (3%) | 0 | 100 | 100 |
| 2 | B | 233/227 (103%) | 227 (97%) | 5 (2%) | 1 (0%) | 34 | 20 |
| 2 | O | 237/227 (104%) | 230 (97%) | 5 (2%) | 2 (1%) | 19 | 7 |
| 3 | C | 268/259 (104%) | 263 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | P | 268/259 (104%) | 263 (98%) | 5 (2%) | 0 | 100 | 100 |
| 4 | D | 145/144 (101%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 4 | Q | 143/144 (99%) | 138 (96%) | 3 (2%) | 2 (1%) | 11 | 3 |
| 5 | E | 103/105 (98%) | 102 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | R | 104/105 (99%) | 103 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | F | 97/94 (103%) | 95 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | S | 92/94 (98%) | 90 (98%) | 1 (1%) | 1 (1%) | 14 | 4 |
| 7 | G | 87/84 (104%) | 77 (88%) | 8 (9%) | 2 (2%) | 6 | 1 |
| 7 | T | 82/84 (98%) | 72 (88%) | 6 (7%) | 4 (5%) | 2 | 0 |
| 8 | H | 78/79 (99%) | 73 (94%) | 3 (4%) | 2 (3%) | 5 | 0 |
| 8 | U | 77/79 (98%) | 72 (94%) | 3 (4%) | 2 (3%) | 5 | 0 |
| 9 | I | 72/73 (99%) | 71 (99%) | 1 (1%) | 0 | 100 | 100 |
| 9 | V | 71/73 (97%) | 68 (96%) | 3 (4%) | 0 | 100 | 100 |
| 10 | J | 57/58 (98%) | 57 (100%) | 0 | 0 | 100 | 100 |
| 10 | W | 56/58 (97%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 11 | K | 50/49 (102%) | 49 (98%) | 1 (2%) | 0 | 100 | 100 |
| 11 | X | 47/49 (96%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 12 | L | 46/46 (100%) | 44 (96%) | 2 (4%) | 0 | 100 | 100 |
| 12 | Y | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 13 | M | 41/43 (95%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| 13 | Z | 41/43 (95%) | 39 (95%) | 2 (5%) | 0 | 100 | 100 |
| All | All | 3640/3550 (102%) | 3522 (97%) | 102 (3%) | 16 (0%) | 34 | 20 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 4 | ALA |
| 7 | T | 2 | SER |
| 8 | U | 8 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 6 | S | 2 | SER |
| 8 | H | 9 | LYS |
| 8 | H | 48 | GLY |
| 2 | O | 92[A] | ASN |
| 2 | O | 92[B] | ASN |
| 7 | G | 3 | ALA |
| 7 | T | 4 | ALA |
| 8 | U | 10 | ASN |
| 7 | T | 5 | LYS |
| 4 | Q | 5 | VAL |
| 4 | Q | 6 | VAL |
| 7 | T | 6 | GLY |
| 2 | B | 92 | ASN |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1 | A | 458/426 (108%) | 445 (97%) | 13 (3%) | 43 | 26 |
| 1 | N | 463/426 (109%) | 459 (99%) | 4 (1%) | 78 | 71 |
| 2 | B | 218/210 (104%) | 207 (95%) | 11 (5%) | 24 | 8 |
| 2 | O | 221/210 (105%) | 209 (95%) | 12 (5%) | 22 | 7 |
| 3 | C | 235/224 (105%) | 230 (98%) | 5 (2%) | 53 | 38 |
| 3 | P | 235/224 (105%) | 231 (98%) | 4 (2%) | 60 | 47 |
| 4 | D | 131/128 (102%) | 128 (98%) | 3 (2%) | 50 | 34 |
| 4 | Q | 129/128 (101%) | 124 (96%) | 5 (4%) | 32 | 14 |
| 5 | E | 92/92 (100%) | 91 (99%) | 1 (1%) | 73 | 64 |
| 5 | R | 93/92 (101%) | 93 (100%) | 0 | 100 | 100 |
| 6 | F | 83/78 (106%) | 80 (96%) | 3 (4%) | 35 | 17 |
| 6 | S | 78/78 (100%) | 78 (100%) | 0 | 100 | 100 |
| 7 | G | 73/68 (107%) | 63 (86%) | 10 (14%) | 3 | 0 |
| 7 | T | 68/68 (100%) | 61 (90%) | 7 (10%) | 7 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 8 | H | 72/71 (101%) | 68 (94%) | 4 (6%) | 21 | 6 |
| 8 | U | 71/71 (100%) | 68 (96%) | 3 (4%) | 30 | 12 |
| 9 | I | 58/57 (102%) | 57 (98%) | 1 (2%) | 60 | 47 |
| 9 | V | 57/57 (100%) | 56 (98%) | 1 (2%) | 59 | 44 |
| 10 | J | 50/49 (102%) | 50 (100%) | 0 | 100 | 100 |
| 10 | W | 49/49 (100%) | 47 (96%) | 2 (4%) | 30 | 13 |
| 11 | K | 42/39 (108%) | 41 (98%) | 1 (2%) | 49 | 32 |
| 11 | X | 39/39 (100%) | 38 (97%) | 1 (3%) | 46 | 29 |
| 12 | L | 41/39 (105%) | 40 (98%) | 1 (2%) | 49 | 32 |
| 12 | Y | 39/39 (100%) | 37 (95%) | 2 (5%) | 24 | 8 |
| 13 | M | 37/37 (100%) | 35 (95%) | 2 (5%) | 22 | 7 |
| 13 | Z | 37/37 (100%) | 36 (97%) | 1 (3%) | 44 | 28 |
| All | All | 3169/3036 (104%) | 3072 (97%) | 97 (3%) | 42 | 23 |

All (97) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 38 | ARG |
| 1 | A | 109 | PHE |
| 1 | A | 180 | GLN |
| 1 | A | 297[A] | MET |
| 1 | A | 297[B] | MET |
| 1 | A | 369 | ASP |
| 1 | A | 382[A] | SER |
| 1 | A | 382[B] | SER |
| 1 | A | 382[C] | SER |
| 1 | A | 486[A] | ASP |
| 1 | A | 486[B] | ASP |
| 1 | A | 514[A] | LYS |
| 1 | A | 514[B] | LYS |
| 2 | B | 33 | LEU |
| 2 | B | 60[A] | GLU |
| 2 | B | 60[B] | GLU |
| 2 | B | 65 | TRP |
| 2 | B | 68 | LEU |
| 2 | B | 75 | LEU |
| 2 | B | 78 | LEU |
| 2 | B | 91 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 2 | B | 115[A] | ASP |
| 2 | B | 115[B] | ASP |
| 2 | B | 171 | LYS |
| 3 | C | 40 | MET |
| 3 | C | 76 | GLN |
| 3 | C | 159 | MET |
| 3 | C | 214 | PHE |
| 3 | C | 230 | ASN |
| 4 | D | 4 | SER |
| 4 | D | 31 | LYS |
| 4 | D | 147 | LYS |
| 5 | E | 90 | ARG |
| 6 | F | 37 | LYS |
| 6 | F | 54[A] | ASN |
| 6 | F | 54[B] | ASN |
| 7 | G | 2 | SER |
| 7 | G | 8 | HIS |
| 7 | G | 18 | PHE |
| 7 | G | 33[A] | LEU |
| 7 | G | 33[B] | LEU |
| 7 | G | 36 | TRP |
| 7 | G | 37 | LEU |
| 7 | G | 42 | ARG |
| 7 | G | 43 | GLU |
| 7 | G | 54 | ARG |
| 8 | H | 7 | LYS |
| 8 | H | 9 | LYS |
| 8 | H | 29 | CYS |
| 8 | H | 60 | TYR |
| 9 | I | 37 | PHE |
| 11 | K | 54 | ARG |
| 12 | L | 47 | LYS |
| 13 | M | 38 | ASP |
| 13 | M | 39 | ASN |
| 1 | N | 38 | ARG |
| 1 | N | 109 | PHE |
| 1 | N | 138 | HIS |
| 1 | N | 369 | ASP |
| 2 | O | 33 | LEU |
| 2 | O | 64[A] | ILE |
| 2 | O | 64[B] | ILE |
| 2 | O | 68 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | O | 78 | LEU |
| 2 | O | 91 | ASN |
| 2 | O | 94 | SER |
| 2 | O | 115 | ASP |
| 2 | O | 158 | ASP |
| 2 | O | 171 | LYS |
| 2 | O | 225 | SER |
| 2 | O | 226 | MET |
| 3 | P | 3 | HIS |
| 3 | P | 159 | MET |
| 3 | P | 214 | PHE |
| 3 | P | 230 | ASN |
| 4 | Q | 4 | SER |
| 4 | Q | 7 | LYS |
| 4 | Q | 20 | ARG |
| 4 | Q | 51 | LEU |
| 4 | Q | 58 | GLU |
| 7 | T | 2 | SER |
| 7 | T | 11 | THR |
| 7 | T | 18 | PHE |
| 7 | T | 33 | LEU |
| 7 | T | 36 | TRP |
| 7 | T | 37 | LEU |
| 7 | T | 54 | ARG |
| 8 | U | 29 | CYS |
| 8 | U | 60 | TYR |
| 8 | U | 61 | LYS |
| 9 | V | 2 | THR |
| 10 | W | 50 | LEU |
| 10 | W | 58 | LYS |
| 11 | X | 47 | ARG |
| 12 | Y | 2 | HIS |
| 12 | Y | 47 | LYS |
| 13 | Z | 38 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 91 | ASN |
| 2 | B | 181 | GLN |
| 4 | D | 109 | HIS |
| 6 | F | 32 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 94 | HIS |
| 13 | M | 39 | ASN |
| 2 | O | 91 | ASN |
| 2 | O | 195 | GLN |
| 3 | P | 158 | HIS |
| 4 | Q | 101 | HIS |
| 4 | Q | 109 | HIS |
| 7 | T | 8 | HIS |
| 8 | U | 31 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 9 | SAC | I | 1 | 9 | 7,8,9 | 0.63 | 0 | 8,9,11 | 1.02 | 1 (12%) |
| 9 | SAC | V | 1 | 9 | 7,8,9 | 0.60 | 0 | 8,9,11 | 0.80 | 0 |
| 2 | FME | B | 1 | 2 | 8,9,10 | 0.76 | 0 | 7,9,11 | 2.24 | 1 (14%) |
| 1 | FME | A | 1 | 1 | 8,9,10 | 0.43 | 0 | 7,9,11 | 1.47 | 2 (28%) |
| 2 | FME | O | 1 | 2 | 8,9,10 | 0.72 | 0 | 7,9,11 | 1.53 | 2 (28%) |
| 1 | FME | N | 1 | 1 | 8,9,10 | 0.43 | 0 | 7,9,11 | 1.31 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 9 | SAC | I | 1 | 9 | - | 3/7/8/10 | - |
| 9 | SAC | V | 1 | 9 | - | 2/7/8/10 | - |
| 2 | FME | B | 1 | 2 | - | 0/7/9/11 | - |
| 1 | FME | A | 1 | 1 | - | 4/7/9/11 | - |
| 2 | FME | O | 1 | 2 | - | 0/7/9/11 | - |
| 1 | FME | N | 1 | 1 | - | 2/7/9/11 | - |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | B | 1 | FME | CG-CB-CA | -4.65 | 100.04 | 112.95 |
| 2 | O | 1 | FME | CG-CB-CA | -3.17 | 104.15 | 112.95 |
| 1 | A | 1 | FME | C-CA-N | 2.40 | 114.06 | 109.73 |
| 9 | I | 1 | SAC | O-C-CA | -2.16 | 119.11 | 124.78 |
| 1 | A | 1 | FME | O1-CN-N | -2.12 | 119.69 | 125.27 |
| 2 | O | 1 | FME | O-C-CA | -2.03 | 119.45 | 124.78 |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | A | 1 | FME | N-CA-CB-CG |
| 9 | I | 1 | SAC | O-C-CA-CB |
| 1 | N | 1 | FME | N-CA-CB-CG |
| 9 | V | 1 | SAC | C2A-C1A-N-CA |
| 9 | V | 1 | SAC | OAC-C1A-N-CA |
| 9 | I | 1 | SAC | C2A-C1A-N-CA |
| 9 | I | 1 | SAC | OAC-C1A-N-CA |
| 1 | A | 1 | FME | CA-CB-CG-SD |
| 1 | A | 1 | FME | C-CA-CB-CG |
| 1 | N | 1 | FME | C-CA-CB-CG |
| 1 | A | 1 | FME | CB-CG-SD-CE |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 161 ligands modelled in this entry, 10 are monoatomic - leaving 151 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 |
| 23 | DMU | Q | 201 | - | 10,10,34 | 0.36 | 0 | 9,9,45 | 0.36 | 0 |
| 22 | EDO | P | 315 | - | 3,3,3 | 0.53 | 0 | 2,2,2 | 0.13 | 0 |
| 22 | EDO | N | 615 | - | 3,3,3 | 0.54 | 0 | 2,2,2 | 0.34 | 0 |
| 22 | EDO | O | 305 | - | 3,3,3 | 0.55 | 0 | 2,2,2 | 0.11 | 0 |
| 14 | HEA | N | 602[A] | - | 44,67,67 | 0.95 | 2 (4%) | 37,103,103 | 2.02 | 7 (18%) |
| 25 | CHD | B | 302 | - | 29,32,32 | 0.81 | 0 | 48,51,51 | 1.40 | 6 (12%) |
| 26 | PEK | C | 303 | - | 44,44,52 | 1.21 | 2 (4%) | 47,49,57 | 1.41 | 8 (17%) |
| 18 | TGL | L | 101 | - | 62,62,62 | 1.12 | 3 (4%) | 65,65,65 | 1.39 | 7 (10%) |
| 22 | EDO | S | 103 | - | 3,3,3 | 0.59 | 0 | 2,2,2 | 0.12 | 0 |
| 22 | EDO | F | 103 | - | 3,3,3 | 0.47 | 0 | 2,2,2 | 0.52 | 0 |
| 23 | DMU | D | 207 | - | 10,10,34 | 0.33 | 0 | 9,9,45 | 0.57 | 0 |
| 18 | TGL | N | 608 | - | 52,52,62 | 0.73 | 1 (1%) | 50,50,65 | 0.88 | 2 (4%) |
| 22 | EDO | F | 106 | - | 3,3,3 | 0.61 | 0 | 2,2,2 | 0.54 | 0 |
| 22 | EDO | N | 617 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.15 | 0 |
| 22 | EDO | A | 612 | - | 3,3,3 | 0.71 | 0 | 2,2,2 | 0.35 | 0 |
| 22 | EDO | A | 614 | - | 3,3,3 | 0.45 | 0 | 2,2,2 | 0.28 | 0 |
| 14 | HEA | N | 603 | 20,1,30 | 44,67,67 | 1.03 | 2 (4%) | 37,103,103 | 1.61 | 10 (27%) |
| 24 | CUA | B | 301 | 2 | 0,1,1 | 0.00 | - | - | - | - |
| 22 | EDO | S | 106 | - | 3,3,3 | 0.37 | 0 | 2,2,2 | 0.91 | 0 |
| 22 | EDO | W | 101 | - | 3,3,3 | 0.38 | 0 | 2,2,2 | 0.45 | 0 |
| 25 | CHD | L | 102 | - | 29,32,32 | 0.63 | 0 | 48,51,51 | 2.49 | 23 (47%) |
| 22 | EDO | T | 104 | - | 3,3,3 | 0.49 | 0 | 2,2,2 | 0.28 | 0 |
| 23 | DMU | C | 321 | - | 11,11,34 | 0.40 | 0 | 10,10,45 | 0.32 | 0 |
| 25 | CHD | C | 309 | - | 29,32,32 | 0.69 | 0 | 48,51,51 | 1.30 | 7 (14%) |
| 22 | EDO | Y | 101 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.17 | 0 |
| 22 | EDO | B | 306 | - | 3,3,3 | 0.57 | 0 | 2,2,2 | 0.32 | 0 |
| 22 | EDO | A | 620 | - | 3,3,3 | 0.67 | 0 | 2,2,2 | 0.14 | 0 |
| 23 | DMU | L | 105 | - | 21,21,34 | 0.90 | 1 (4%) | 24,25,45 | 2.08 | 5 (20%) |
| 22 | EDO | A | 613 | - | 3,3,3 | 0.79 | 0 | 2,2,2 | 0.68 | 0 |
| 22 | EDO | P | 309 | - | 3,3,3 | 0.53 | 0 | 2,2,2 | 0.21 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | EDO | A | 622 | - | 3,3,3 | 0.56 | 0 | 2,2,2 | 0.61 | 0 |
| 22 | EDO | B | 303 | - | 3,3,3 | 0.72 | 0 | 2,2,2 | 0.30 | 0 |
| 25 | CHD | P | 301 | - | 29,32,32 | 0.64 | 0 | 48,51,51 | 1.42 | 10 (20%) |
| 20 | PER | A | 609[A] | 15,14 | 0,1,1 | 0.00 | - | - | | |
| 14 | HEA | A | 602 | 20,1,30 | 44,67,67 | 1.00 | 2 (4%) | 37,103,103 | 1.89 | 14 (37%) |
| 22 | EDO | N | 621 | - | 3,3,3 | 0.34 | 0 | 2,2,2 | 0.50 | 0 |
| 22 | EDO | J | 102 | - | 3,3,3 | 0.51 | 0 | 2,2,2 | 0.16 | 0 |
| 27 | CDL | N | 601 | - | 58,58,99 | 1.30 | 9 (15%) | 55,55,111 | 0.98 | 4 (7%) |
| 22 | EDO | M | 102 | - | 3,3,3 | 0.45 | 0 | 2,2,2 | 0.34 | 0 |
| 18 | TGL | A | 607 | - | 62,62,62 | 1.08 | 3 (4%) | 65,65,65 | 1.11 | 6 (9%) |
| 19 | PGV | N | 610 | - | 50,50,50 | 0.96 | 2 (4%) | 53,56,56 | 1.06 | 3 (5%) |
| 22 | EDO | A | 617 | - | 3,3,3 | 0.50 | 0 | 2,2,2 | 0.59 | 0 |
| 23 | DMU | Z | 101 | - | 34,34,34 | 0.46 | 0 | 45,45,45 | 0.82 | 2 (4%) |
| 22 | EDO | P | 313 | - | 3,3,3 | 0.43 | 0 | 2,2,2 | 0.97 | 0 |
| 22 | EDO | A | 621 | - | 3,3,3 | 0.61 | 0 | 2,2,2 | 0.51 | 0 |
| 19 | PGV | A | 608 | - | 31,31,50 | 0.41 | 0 | 29,29,56 | 0.58 | 0 |
| 22 | EDO | E | 203 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.40 | 0 |
| 27 | CDL | T | 102 | - | 57,57,99 | 1.26 | 8 (14%) | 54,54,111 | 0.87 | 1 (1%) |
| 23 | DMU | D | 206 | - | 34,34,34 | 0.70 | 1 (2%) | 45,45,45 | 1.40 | 8 (17%) |
| 29 | PO4 | H | 101 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.74 | 0 |
| 21 | PSC | O | 302 | - | 27,27,51 | 0.77 | 1 (3%) | 25,25,59 | 0.72 | 1 (4%) |
| 22 | EDO | N | 614 | - | 3,3,3 | 0.65 | 0 | 2,2,2 | 0.18 | 0 |
| 23 | DMU | X | 102 | - | 8,8,34 | 0.29 | 0 | 7,7,45 | 0.48 | 0 |
| 26 | PEK | C | 305 | - | 34,34,52 | 0.32 | 0 | 32,32,57 | 0.58 | 0 |
| 27 | CDL | C | 308 | - | 62,62,99 | 1.32 | 8 (12%) | 61,61,111 | 1.41 | 11 (18%) |
| 19 | PGV | C | 307 | - | 35,35,50 | 1.31 | 2 (5%) | 37,37,56 | 1.95 | 9 (24%) |
| 22 | EDO | D | 203 | - | 3,3,3 | 0.50 | 0 | 2,2,2 | 0.22 | 0 |
| 22 | EDO | N | 620 | - | 3,3,3 | 0.58 | 0 | 2,2,2 | 0.15 | 0 |
| 22 | EDO | B | 304 | - | 3,3,3 | 0.40 | 0 | 2,2,2 | 0.53 | 0 |
| 22 | EDO | S | 105 | - | 3,3,3 | 0.64 | 0 | 2,2,2 | 0.71 | 0 |
| 22 | EDO | T | 105 | - | 3,3,3 | 0.62 | 0 | 2,2,2 | 0.32 | 0 |
| 22 | EDO | W | 102 | - | 3,3,3 | 0.49 | 0 | 2,2,2 | 0.45 | 0 |
| 22 | EDO | S | 107 | - | 3,3,3 | 0.52 | 0 | 2,2,2 | 0.58 | 0 |
| 22 | EDO | C | 311 | - | 3,3,3 | 0.53 | 0 | 2,2,2 | 0.17 | 0 |
| 29 | PO4 | U | 101 | - | 4,4,4 | 1.06 | 0 | 6,6,6 | 0.56 | 0 |
| 22 | EDO | G | 102 | - | 3,3,3 | 0.83 | 0 | 2,2,2 | 0.50 | 0 |
| 21 | PSC | A | 610 | - | 23,23,51 | 0.84 | 1 (4%) | 20,21,59 | 0.79 | 0 |
| 22 | EDO | C | 312 | - | 3,3,3 | 0.63 | 0 | 2,2,2 | 0.34 | 0 |
| 22 | EDO | P | 311 | - | 3,3,3 | 0.70 | 0 | 2,2,2 | 0.18 | 0 |
| 22 | EDO | J | 103 | - | 3,3,3 | 0.36 | 0 | 2,2,2 | 0.76 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | EDO | C | 317 | - | 3,3,3 | 0.54 | 0 | 2,2,2 | 0.15 | 0 |
| 22 | EDO | F | 102 | - | 3,3,3 | 0.56 | 0 | 2,2,2 | 0.43 | 0 |
| 26 | PEK | C | 304 | - | 51,51,52 | 0.80 | 2 (3%) | 54,56,57 | 1.16 | 4 (7%) |
| 22 | EDO | D | 202 | - | 3,3,3 | 0.50 | 0 | 2,2,2 | 0.31 | 0 |
| 22 | EDO | N | 613 | - | 3,3,3 | 0.63 | 0 | 2,2,2 | 0.64 | 0 |
| 24 | CUA | O | 301 | 2 | 0,1,1 | 0.00 | - | - | | |
| 23 | DMU | M | 101 | - | 34,34,34 | 0.44 | 0 | 45,45,45 | 1.03 | 1 (2%) |
| 22 | EDO | A | 618 | - | 3,3,3 | 0.75 | 0 | 2,2,2 | 0.29 | 0 |
| 22 | EDO | L | 104 | - | 3,3,3 | 0.59 | 0 | 2,2,2 | 0.49 | 0 |
| 25 | CHD | C | 301 | - | 29,32,32 | 0.59 | 0 | 48,51,51 | 1.60 | 9 (18%) |
| 19 | PGV | C | 306 | - | 47,47,50 | 0.84 | 2 (4%) | 50,53,56 | 0.90 | 3 (6%) |
| 22 | EDO | T | 103 | - | 3,3,3 | 0.73 | 0 | 2,2,2 | 0.36 | 0 |
| 22 | EDO | A | 619 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.16 | 0 |
| 22 | EDO | F | 107 | - | 3,3,3 | 0.50 | 0 | 2,2,2 | 0.38 | 0 |
| 25 | CHD | J | 101 | - | 29,32,32 | 0.63 | 0 | 48,51,51 | 2.82 | 18 (37%) |
| 19 | PGV | P | 306 | - | 26,29,50 | 0.40 | 0 | 24,28,56 | 0.58 | 0 |
| 19 | PGV | P | 305 | - | 50,50,50 | 0.76 | 2 (4%) | 53,56,56 | 1.00 | 1 (1%) |
| 22 | EDO | A | 616 | - | 3,3,3 | 0.45 | 0 | 2,2,2 | 0.50 | 0 |
| 22 | EDO | P | 312 | - | 3,3,3 | 0.44 | 0 | 2,2,2 | 0.97 | 0 |
| 22 | EDO | P | 310 | - | 3,3,3 | 0.54 | 0 | 2,2,2 | 0.19 | 0 |
| 23 | DMU | K | 101 | - | 7,7,34 | 0.25 | 0 | 6,6,45 | 0.37 | 0 |
| 22 | EDO | O | 303 | - | 3,3,3 | 0.76 | 0 | 2,2,2 | 0.48 | 0 |
| 22 | EDO | C | 313 | - | 3,3,3 | 0.80 | 0 | 2,2,2 | 0.35 | 0 |
| 22 | EDO | Q | 202 | - | 3,3,3 | 0.54 | 0 | 2,2,2 | 0.39 | 0 |
| 22 | EDO | F | 109 | - | 3,3,3 | 0.61 | 0 | 2,2,2 | 0.75 | 0 |
| 23 | DMU | O | 306 | - | 11,11,34 | 0.22 | 0 | 9,9,45 | 0.65 | 0 |
| 18 | TGL | N | 609 | - | 52,52,62 | 0.69 | 1 (1%) | 50,50,65 | 0.69 | 2 (4%) |
| 22 | EDO | C | 318 | - | 3,3,3 | 0.56 | 0 | 2,2,2 | 0.35 | 0 |
| 23 | DMU | C | 310 | - | 34,34,34 | 0.55 | 1 (2%) | 45,45,45 | 1.20 | 6 (13%) |
| 22 | EDO | N | 618 | - | 3,3,3 | 0.53 | 0 | 2,2,2 | 0.32 | 0 |
| 20 | PER | N | 611[A] | 15,14 | 0,1,1 | 0.00 | - | - | | |
| 23 | DMU | X | 101 | - | 9,9,34 | 0.31 | 0 | 8,8,45 | 0.51 | 0 |
| 25 | CHD | Y | 102 | - | 29,32,32 | 0.62 | 0 | 48,51,51 | 2.25 | 16 (33%) |
| 23 | DMU | K | 104 | - | 10,10,34 | 0.25 | 0 | 9,9,45 | 0.52 | 0 |
| 23 | DMU | J | 104 | - | 10,10,34 | 0.33 | 0 | 9,9,45 | 0.41 | 0 |
| 22 | EDO | L | 103 | - | 3,3,3 | 0.24 | 0 | 2,2,2 | 1.02 | 0 |
| 26 | PEK | P | 304 | - | 51,51,52 | 0.77 | 2 (3%) | 54,56,57 | 1.07 | 4 (7%) |
| 18 | TGL | N | 607 | - | 62,62,62 | 1.04 | 3 (4%) | 65,65,65 | 1.20 | 4 (6%) |
| 22 | EDO | N | 616 | - | 3,3,3 | 0.40 | 0 | 2,2,2 | 0.69 | 0 |
| 22 | EDO | F | 105 | - | 3,3,3 | 0.62 | 0 | 2,2,2 | 0.23 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | EDO | E | 201 | - | 3,3,3 | 0.56 | 0 | 2,2,2 | 0.25 | 0 |
| 23 | DMU | P | 308 | - | 34,34,34 | 0.51 | 0 | 45,45,45 | 1.21 | 7 (15%) |
| 23 | DMU | P | 316 | - | 21,21,34 | 0.61 | 1 (4%) | 24,25,45 | 0.81 | 1 (4%) |
| 22 | EDO | P | 314 | - | 3,3,3 | 0.57 | 0 | 2,2,2 | 0.14 | 0 |
| 23 | DMU | K | 105 | - | 8,8,34 | 0.30 | 0 | 7,7,45 | 0.57 | 0 |
| 23 | DMU | X | 103 | - | 8,8,34 | 0.30 | 0 | 7,7,45 | 0.61 | 0 |
| 19 | PGV | A | 611 | - | 50,50,50 | 0.90 | 3 (6%) | 53,56,56 | 1.20 | 4 (7%) |
| 22 | EDO | B | 305 | - | 3,3,3 | 0.71 | 0 | 2,2,2 | 0.10 | 0 |
| 22 | EDO | C | 315 | - | 3,3,3 | 0.56 | 0 | 2,2,2 | 0.18 | 0 |
| 22 | EDO | D | 201 | - | 3,3,3 | 0.57 | 0 | 2,2,2 | 0.29 | 0 |
| 22 | EDO | S | 104 | - | 3,3,3 | 0.49 | 0 | 2,2,2 | 0.77 | 0 |
| 22 | EDO | D | 204 | - | 3,3,3 | 0.50 | 0 | 2,2,2 | 0.46 | 0 |
| 23 | DMU | X | 104 | - | 22,22,34 | 0.57 | 1 (4%) | 27,27,45 | 0.77 | 0 |
| 27 | CDL | P | 307 | - | 65,65,99 | 1.37 | 9 (13%) | 64,64,111 | 1.24 | 6 (9%) |
| 25 | CHD | G | 101 | - | 29,32,32 | 0.72 | 1 (3%) | 48,51,51 | 1.14 | 3 (6%) |
| 22 | EDO | F | 108 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.37 | 0 |
| 23 | DMU | A | 623 | - | 10,10,34 | 0.31 | 0 | 9,9,45 | 0.48 | 0 |
| 22 | EDO | S | 102 | - | 3,3,3 | 0.77 | 0 | 2,2,2 | 0.72 | 0 |
| 26 | PEK | T | 101 | - | 35,35,52 | 0.86 | 1 (2%) | 34,34,57 | 1.07 | 3 (8%) |
| 19 | PGV | N | 612 | - | 50,50,50 | 0.89 | 3 (6%) | 53,56,56 | 1.12 | 6 (11%) |
| 18 | TGL | A | 606 | - | 62,62,62 | 1.04 | 3 (4%) | 65,65,65 | 1.28 | 5 (7%) |
| 22 | EDO | C | 314 | - | 3,3,3 | 0.34 | 0 | 2,2,2 | 0.67 | 0 |
| 22 | EDO | D | 205 | - | 3,3,3 | 0.37 | 0 | 2,2,2 | 0.39 | 0 |
| 22 | EDO | E | 202 | - | 3,3,3 | 0.45 | 0 | 2,2,2 | 0.12 | 0 |
| 22 | EDO | N | 619 | - | 3,3,3 | 0.56 | 0 | 2,2,2 | 0.13 | 0 |
| 14 | HEA | A | 601[A] | - | 44,67,67 | 1.11 | 2 (4%) | 37,103,103 | 2.08 | 10 (27%) |
| 22 | EDO | A | 615 | - | 3,3,3 | 0.68 | 0 | 2,2,2 | 0.98 | 0 |
| 22 | EDO | O | 304 | - | 3,3,3 | 0.65 | 0 | 2,2,2 | 0.08 | 0 |
| 22 | EDO | C | 316 | - | 3,3,3 | 0.38 | 0 | 2,2,2 | 0.35 | 0 |
| 23 | DMU | K | 102 | - | 10,10,34 | 0.34 | 0 | 9,9,45 | 0.62 | 0 |
| 22 | EDO | C | 319 | - | 3,3,3 | 0.60 | 0 | 2,2,2 | 0.31 | 0 |
| 23 | DMU | P | 317 | - | 33,33,34 | 0.73 | 1 (3%) | 44,44,45 | 1.66 | 8 (18%) |
| 22 | EDO | N | 622 | - | 3,3,3 | 0.75 | 0 | 2,2,2 | 0.28 | 0 |
| 23 | DMU | K | 103 | - | 9,9,34 | 0.34 | 0 | 8,8,45 | 0.34 | 0 |
| 22 | EDO | F | 104 | - | 3,3,3 | 0.58 | 0 | 2,2,2 | 0.33 | 0 |
| 22 | EDO | C | 320 | - | 3,3,3 | 0.71 | 0 | 2,2,2 | 0.45 | 0 |
| 26 | PEK | P | 303 | - | 37,37,52 | 1.14 | 2 (5%) | 40,42,57 | 1.27 | 4 (10%) |

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 |
|-----|------|-------|--------|---------|----------|--------------|---------|
| 23 | DMU | Q | 201 | - | - | 4/8/8/59 | - |
| 22 | EDO | P | 315 | - | - | 0/1/1/1 | - |
| 22 | EDO | N | 615 | - | - | 0/1/1/1 | - |
| 22 | EDO | O | 305 | - | - | 0/1/1/1 | - |
| 14 | HEA | N | 602[A] | - | 3/3/7/16 | 0/24/76/76 | - |
| 25 | CHD | B | 302 | - | - | 0/7/74/74 | 0/4/4/4 |
| 26 | PEK | C | 303 | - | - | 19/48/48/56 | - |
| 18 | TGL | L | 101 | - | - | 39/65/65/65 | - |
| 22 | EDO | S | 103 | - | - | 0/1/1/1 | - |
| 22 | EDO | F | 103 | - | - | 0/1/1/1 | - |
| 23 | DMU | D | 207 | - | - | 4/8/8/59 | - |
| 18 | TGL | N | 608 | - | - | 22/47/47/65 | - |
| 22 | EDO | F | 106 | - | - | 0/1/1/1 | - |
| 22 | EDO | N | 617 | - | - | 0/1/1/1 | - |
| 22 | EDO | A | 612 | - | - | 1/1/1/1 | - |
| 22 | EDO | A | 614 | - | - | 1/1/1/1 | - |
| 14 | HEA | N | 603 | 20,1,30 | 3/3/7/16 | 1/24/76/76 | - |
| 22 | EDO | S | 106 | - | - | 1/1/1/1 | - |
| 22 | EDO | W | 101 | - | - | 1/1/1/1 | - |
| 25 | CHD | L | 102 | - | - | 5/7/74/74 | 0/4/4/4 |
| 22 | EDO | T | 104 | - | - | 1/1/1/1 | - |
| 23 | DMU | C | 321 | - | - | 0/9/9/59 | - |
| 25 | CHD | C | 309 | - | - | 3/7/74/74 | 0/4/4/4 |
| 22 | EDO | Y | 101 | - | - | 0/1/1/1 | - |
| 22 | EDO | B | 306 | - | - | 0/1/1/1 | - |
| 22 | EDO | A | 620 | - | - | 1/1/1/1 | - |
| 23 | DMU | L | 105 | - | - | 8/13/29/59 | 0/1/1/2 |
| 22 | EDO | A | 613 | - | - | 0/1/1/1 | - |
| 22 | EDO | P | 309 | - | - | 0/1/1/1 | - |
| 22 | EDO | A | 622 | - | - | 0/1/1/1 | - |
| 22 | EDO | B | 303 | - | - | 0/1/1/1 | - |
| 25 | CHD | P | 301 | - | - | 0/7/74/74 | 0/4/4/4 |
| 14 | HEA | A | 602 | 20,1,30 | 3/3/7/16 | 0/24/76/76 | - |
| 22 | EDO | N | 621 | - | - | 0/1/1/1 | - |
| 22 | EDO | J | 102 | - | - | 1/1/1/1 | - |
| 27 | CDL | N | 601 | - | - | 16/51/51/110 | - |
| 22 | EDO | M | 102 | - | - | 1/1/1/1 | - |
| 18 | TGL | A | 607 | - | - | 26/65/65/65 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|---------|
| 19 | PGV | N | 610 | - | - | 14/55/55/55 | - |
| 22 | EDO | A | 617 | - | - | 1/1/1/1 | - |
| 23 | DMU | Z | 101 | - | - | 7/19/59/59 | 0/2/2/2 |
| 22 | EDO | P | 313 | - | - | 1/1/1/1 | - |
| 22 | EDO | A | 621 | - | - | 0/1/1/1 | - |
| 19 | PGV | A | 608 | - | - | 9/26/27/55 | - |
| 22 | EDO | E | 203 | - | - | 0/1/1/1 | - |
| 27 | CDL | T | 102 | - | - | 18/50/50/110 | - |
| 23 | DMU | D | 206 | - | - | 6/19/59/59 | 0/2/2/2 |
| 21 | PSC | O | 302 | - | - | 5/23/23/55 | - |
| 22 | EDO | N | 614 | - | - | 0/1/1/1 | - |
| 23 | DMU | X | 102 | - | - | 2/6/6/59 | - |
| 26 | PEK | C | 305 | - | - | 13/30/30/56 | - |
| 27 | CDL | C | 308 | - | - | 17/55/58/110 | - |
| 19 | PGV | C | 307 | - | - | 16/36/36/55 | - |
| 22 | EDO | D | 203 | - | - | 0/1/1/1 | - |
| 22 | EDO | N | 620 | - | - | 0/1/1/1 | - |
| 22 | EDO | B | 304 | - | - | 0/1/1/1 | - |
| 22 | EDO | S | 105 | - | - | 0/1/1/1 | - |
| 22 | EDO | T | 105 | - | - | 1/1/1/1 | - |
| 22 | EDO | W | 102 | - | - | 1/1/1/1 | - |
| 22 | EDO | S | 107 | - | - | 0/1/1/1 | - |
| 22 | EDO | C | 311 | - | - | 0/1/1/1 | - |
| 22 | EDO | G | 102 | - | - | 0/1/1/1 | - |
| 21 | PSC | A | 610 | - | - | 11/19/19/55 | - |
| 22 | EDO | C | 312 | - | - | 0/1/1/1 | - |
| 22 | EDO | P | 311 | - | - | 0/1/1/1 | - |
| 22 | EDO | J | 103 | - | - | 1/1/1/1 | - |
| 22 | EDO | C | 317 | - | - | 0/1/1/1 | - |
| 22 | EDO | F | 102 | - | - | 0/1/1/1 | - |
| 26 | PEK | C | 304 | - | - | 17/55/55/56 | - |
| 22 | EDO | D | 202 | - | - | 1/1/1/1 | - |
| 22 | EDO | N | 613 | - | - | 0/1/1/1 | - |
| 23 | DMU | M | 101 | - | - | 4/19/59/59 | 0/2/2/2 |
| 22 | EDO | A | 618 | - | - | 1/1/1/1 | - |
| 22 | EDO | L | 104 | - | - | 1/1/1/1 | - |
| 25 | CHD | C | 301 | - | - | 0/7/74/74 | 0/4/4/4 |
| 19 | PGV | C | 306 | - | - | 13/52/52/55 | - |
| 22 | EDO | T | 103 | - | - | 0/1/1/1 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|----------|-------------|---------|
| 22 | EDO | A | 619 | - | - | 1/1/1/1 | - |
| 22 | EDO | F | 107 | - | - | 0/1/1/1 | - |
| 25 | CHD | J | 101 | - | - | 6/7/74/74 | 0/4/4/4 |
| 19 | PGV | P | 306 | - | - | 5/23/25/55 | - |
| 19 | PGV | P | 305 | - | - | 6/55/55/55 | - |
| 22 | EDO | A | 616 | - | - | 0/1/1/1 | - |
| 22 | EDO | P | 312 | - | - | 1/1/1/1 | - |
| 22 | EDO | P | 310 | - | - | 0/1/1/1 | - |
| 23 | DMU | K | 101 | - | - | 1/5/5/59 | - |
| 22 | EDO | O | 303 | - | - | 0/1/1/1 | - |
| 22 | EDO | C | 313 | - | - | 0/1/1/1 | - |
| 14 | HEA | A | 601[C] | - | 3/3/5/16 | - | - |
| 22 | EDO | Q | 202 | - | - | 0/1/1/1 | - |
| 22 | EDO | F | 109 | - | - | 0/1/1/1 | - |
| 23 | DMU | O | 306 | - | - | 1/8/8/59 | - |
| 18 | TGL | N | 609 | - | - | 20/47/47/65 | - |
| 22 | EDO | C | 318 | - | - | 0/1/1/1 | - |
| 23 | DMU | C | 310 | - | - | 3/19/59/59 | 0/2/2/2 |
| 22 | EDO | N | 618 | - | - | 1/1/1/1 | - |
| 23 | DMU | X | 101 | - | - | 2/7/7/59 | - |
| 25 | CHD | Y | 102 | - | - | 3/7/74/74 | 0/4/4/4 |
| 23 | DMU | K | 104 | - | - | 3/8/8/59 | - |
| 14 | HEA | A | 601[B] | - | 3/3/5/16 | - | - |
| 23 | DMU | J | 104 | - | - | 2/8/8/59 | - |
| 22 | EDO | L | 103 | - | - | 1/1/1/1 | - |
| 26 | PEK | P | 304 | - | - | 10/55/55/56 | - |
| 18 | TGL | N | 607 | - | - | 31/65/65/65 | - |
| 22 | EDO | N | 616 | - | - | 0/1/1/1 | - |
| 14 | HEA | N | 602[C] | - | 3/3/5/16 | - | - |
| 22 | EDO | F | 105 | - | - | 0/1/1/1 | - |
| 22 | EDO | E | 201 | - | - | 0/1/1/1 | - |
| 23 | DMU | P | 308 | - | - | 8/19/59/59 | 0/2/2/2 |
| 23 | DMU | P | 316 | - | - | 5/13/29/59 | 0/1/1/2 |
| 22 | EDO | P | 314 | - | - | 0/1/1/1 | - |
| 23 | DMU | K | 105 | - | - | 0/6/6/59 | - |
| 23 | DMU | X | 103 | - | - | 0/6/6/59 | - |
| 19 | PGV | A | 611 | - | - | 4/55/55/55 | - |
| 22 | EDO | B | 305 | - | - | 0/1/1/1 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|------|----------|--------------|---------|
| 22 | EDO | C | 315 | - | - | 0/1/1/1 | - |
| 22 | EDO | D | 201 | - | - | 0/1/1/1 | - |
| 22 | EDO | S | 104 | - | - | 0/1/1/1 | - |
| 22 | EDO | D | 204 | - | - | 1/1/1/1 | - |
| 23 | DMU | X | 104 | - | - | 2/13/33/59 | 0/1/1/2 |
| 14 | HEA | N | 602[B] | - | 3/3/5/16 | - | - |
| 27 | CDL | P | 307 | - | - | 27/61/61/110 | - |
| 25 | CHD | G | 101 | - | - | 0/7/74/74 | 0/4/4/4 |
| 22 | EDO | F | 108 | - | - | 1/1/1/1 | - |
| 23 | DMU | A | 623 | - | - | 0/8/8/59 | - |
| 22 | EDO | S | 102 | - | - | 0/1/1/1 | - |
| 26 | PEK | T | 101 | - | - | 14/32/32/56 | - |
| 19 | PGV | N | 612 | - | - | 6/55/55/55 | - |
| 18 | TGL | A | 606 | - | - | 37/65/65/65 | - |
| 22 | EDO | C | 314 | - | - | 0/1/1/1 | - |
| 22 | EDO | D | 205 | - | - | 1/1/1/1 | - |
| 22 | EDO | E | 202 | - | - | 1/1/1/1 | - |
| 22 | EDO | N | 619 | - | - | 1/1/1/1 | - |
| 14 | HEA | A | 601[A] | - | 3/3/7/16 | 0/24/76/76 | - |
| 22 | EDO | A | 615 | - | - | 0/1/1/1 | - |
| 22 | EDO | O | 304 | - | - | 0/1/1/1 | - |
| 22 | EDO | C | 316 | - | - | 0/1/1/1 | - |
| 23 | DMU | K | 102 | - | - | 4/8/8/59 | - |
| 22 | EDO | C | 319 | - | - | 0/1/1/1 | - |
| 23 | DMU | P | 317 | - | - | 3/18/58/59 | 0/2/2/2 |
| 22 | EDO | N | 622 | - | - | 0/1/1/1 | - |
| 23 | DMU | K | 103 | - | - | 2/7/7/59 | - |
| 22 | EDO | F | 104 | - | - | 0/1/1/1 | - |
| 22 | EDO | C | 320 | - | - | 1/1/1/1 | - |
| 26 | PEK | P | 303 | - | - | 13/41/41/56 | - |

All (88) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 19 | C | 307 | PGV | O03-C19 | 5.47 | 1.49 | 1.33 |
| 26 | C | 303 | PEK | O03-C21 | 5.28 | 1.48 | 1.33 |
| 18 | L | 101 | TGL | OG2-CB1 | 5.01 | 1.48 | 1.34 |
| 27 | N | 601 | CDL | OB8-CB7 | 4.91 | 1.47 | 1.33 |
| 27 | P | 307 | CDL | OB6-CB5 | 4.82 | 1.47 | 1.33 |
| 18 | A | 607 | TGL | OG1-CA1 | 4.76 | 1.47 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 27 | P | 307 | CDL | OB8-CB7 | 4.71 | 1.47 | 1.33 |
| 18 | L | 101 | TGL | OG1-CA1 | 4.70 | 1.47 | 1.33 |
| 18 | L | 101 | TGL | OG3-CC1 | 4.69 | 1.47 | 1.33 |
| 26 | P | 303 | PEK | O03-C21 | 4.65 | 1.46 | 1.33 |
| 18 | A | 606 | TGL | OG1-CA1 | 4.64 | 1.46 | 1.33 |
| 26 | C | 303 | PEK | O01-C1 | 4.64 | 1.47 | 1.34 |
| 27 | T | 102 | CDL | OB8-CB7 | 4.62 | 1.46 | 1.33 |
| 18 | N | 607 | TGL | OG2-CB1 | 4.60 | 1.47 | 1.34 |
| 18 | N | 608 | TGL | OG3-CC1 | 4.46 | 1.47 | 1.33 |
| 18 | N | 607 | TGL | OG1-CA1 | 4.43 | 1.46 | 1.33 |
| 19 | C | 307 | PGV | O01-C1 | 4.42 | 1.46 | 1.34 |
| 18 | A | 606 | TGL | OG2-CB1 | 4.39 | 1.46 | 1.34 |
| 19 | N | 610 | PGV | O03-C19 | 4.38 | 1.46 | 1.33 |
| 18 | N | 609 | TGL | OG3-CC1 | 4.38 | 1.47 | 1.33 |
| 27 | C | 308 | CDL | OB8-CB7 | 4.36 | 1.46 | 1.33 |
| 26 | T | 101 | PEK | O03-C21 | 4.36 | 1.46 | 1.33 |
| 27 | C | 308 | CDL | OB6-CB5 | 4.36 | 1.46 | 1.33 |
| 26 | P | 303 | PEK | O01-C1 | 4.34 | 1.46 | 1.34 |
| 18 | A | 607 | TGL | OG3-CC1 | 4.32 | 1.46 | 1.33 |
| 18 | A | 606 | TGL | OG3-CC1 | 4.32 | 1.46 | 1.33 |
| 18 | N | 607 | TGL | OG3-CC1 | 4.24 | 1.45 | 1.33 |
| 14 | A | 601[A] | HEA | CAD-C3D | 4.18 | 1.58 | 1.52 |
| 18 | A | 607 | TGL | OG2-CB1 | 4.17 | 1.46 | 1.34 |
| 19 | N | 610 | PGV | O01-C1 | 4.17 | 1.46 | 1.34 |
| 21 | A | 610 | PSC | C13-C12 | 3.74 | 1.53 | 1.31 |
| 21 | O | 302 | PSC | C13-C12 | 3.72 | 1.53 | 1.31 |
| 19 | A | 611 | PGV | O01-C1 | 3.60 | 1.44 | 1.34 |
| 26 | C | 304 | PEK | O03-C21 | 3.60 | 1.43 | 1.33 |
| 27 | C | 308 | CDL | C59-C58 | -3.56 | 1.31 | 1.51 |
| 19 | N | 612 | PGV | O01-C1 | 3.51 | 1.44 | 1.34 |
| 27 | C | 308 | CDL | C82-C81 | -3.49 | 1.32 | 1.51 |
| 27 | C | 308 | CDL | C79-C78 | -3.36 | 1.32 | 1.51 |
| 27 | P | 307 | CDL | C82-C81 | -3.34 | 1.32 | 1.51 |
| 27 | C | 308 | CDL | C62-C61 | -3.32 | 1.32 | 1.51 |
| 27 | P | 307 | CDL | C79-C78 | -3.26 | 1.33 | 1.51 |
| 27 | T | 102 | CDL | C62-C61 | -3.25 | 1.33 | 1.51 |
| 27 | T | 102 | CDL | C82-C81 | -3.24 | 1.33 | 1.51 |
| 23 | L | 105 | DMU | O16-C6 | 3.22 | 1.45 | 1.40 |
| 26 | P | 304 | PEK | O03-C21 | 3.22 | 1.42 | 1.33 |
| 27 | T | 102 | CDL | C59-C58 | -3.21 | 1.33 | 1.51 |
| 27 | P | 307 | CDL | C59-C58 | -3.21 | 1.33 | 1.51 |
| 27 | N | 601 | CDL | C42-C41 | -3.19 | 1.33 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 27 | N | 601 | CDL | C62-C61 | -3.18 | 1.33 | 1.51 |
| 14 | N | 602[A] | HEA | C3B-C11 | -3.17 | 1.50 | 1.52 |
| 27 | P | 307 | CDL | C39-C38 | -3.17 | 1.33 | 1.51 |
| 27 | P | 307 | CDL | C42-C41 | -3.16 | 1.33 | 1.51 |
| 27 | C | 308 | CDL | C39-C38 | -3.12 | 1.34 | 1.51 |
| 27 | P | 307 | CDL | C22-C21 | -3.11 | 1.34 | 1.51 |
| 27 | C | 308 | CDL | C42-C41 | -3.10 | 1.34 | 1.51 |
| 27 | T | 102 | CDL | C79-C78 | -3.08 | 1.34 | 1.51 |
| 27 | N | 601 | CDL | C19-C18 | -3.03 | 1.34 | 1.51 |
| 27 | P | 307 | CDL | C19-C18 | -3.02 | 1.34 | 1.51 |
| 27 | T | 102 | CDL | C19-C18 | -3.00 | 1.34 | 1.51 |
| 27 | N | 601 | CDL | C82-C81 | -3.00 | 1.34 | 1.51 |
| 27 | N | 601 | CDL | C39-C38 | -2.96 | 1.35 | 1.51 |
| 27 | T | 102 | CDL | C22-C21 | -2.95 | 1.35 | 1.51 |
| 27 | N | 601 | CDL | C79-C78 | -2.95 | 1.35 | 1.51 |
| 19 | C | 306 | PGV | O01-C1 | 2.93 | 1.42 | 1.34 |
| 26 | C | 304 | PEK | O01-C1 | 2.89 | 1.42 | 1.34 |
| 19 | A | 611 | PGV | O03-C19 | 2.80 | 1.41 | 1.33 |
| 19 | N | 612 | PGV | O03-C19 | 2.79 | 1.41 | 1.33 |
| 23 | D | 206 | DMU | O16-C6 | 2.57 | 1.44 | 1.40 |
| 27 | N | 601 | CDL | C58-C59 | -2.56 | 1.33 | 1.51 |
| 23 | P | 317 | DMU | O16-C6 | 2.52 | 1.44 | 1.40 |
| 19 | P | 305 | PGV | O03-C19 | 2.51 | 1.40 | 1.33 |
| 19 | P | 305 | PGV | O01-C1 | 2.51 | 1.41 | 1.34 |
| 14 | A | 602 | HEA | O11-C11 | 2.49 | 1.48 | 1.42 |
| 27 | T | 102 | CDL | C41-C42 | -2.48 | 1.34 | 1.51 |
| 14 | N | 603 | HEA | CAD-C3D | 2.47 | 1.55 | 1.52 |
| 14 | N | 603 | HEA | O11-C11 | 2.42 | 1.48 | 1.42 |
| 19 | C | 306 | PGV | O03-C19 | 2.42 | 1.40 | 1.33 |
| 26 | P | 304 | PEK | O01-C1 | 2.39 | 1.41 | 1.34 |
| 27 | N | 601 | CDL | C22-C21 | -2.37 | 1.34 | 1.51 |
| 23 | C | 310 | DMU | O16-C6 | 2.28 | 1.44 | 1.40 |
| 19 | A | 611 | PGV | O01-C02 | -2.27 | 1.40 | 1.46 |
| 19 | N | 612 | PGV | O01-C02 | -2.26 | 1.40 | 1.46 |
| 23 | X | 104 | DMU | O16-C6 | 2.15 | 1.43 | 1.40 |
| 25 | G | 101 | CHD | O7-C7 | 2.09 | 1.47 | 1.43 |
| 23 | P | 316 | DMU | O16-C6 | 2.06 | 1.43 | 1.40 |
| 14 | N | 602[A] | HEA | O11-C11 | 2.06 | 1.47 | 1.42 |
| 14 | A | 602 | HEA | CMC-C2C | 2.05 | 1.55 | 1.51 |
| 14 | A | 601[A] | HEA | CMC-C2C | 2.00 | 1.55 | 1.51 |

All (269) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 25 | J | 101 | CHD | C10-C9-C8 | 7.54 | 119.92 | 111.82 |
| 25 | J | 101 | CHD | C14-C8-C9 | -7.45 | 99.48 | 109.71 |
| 25 | J | 101 | CHD | C14-C8-C7 | 7.39 | 121.60 | 111.81 |
| 14 | N | 602[A] | HEA | C13-C12-C11 | -7.03 | 103.78 | 114.35 |
| 18 | A | 606 | TGL | OG2-CB1-CB2 | 6.40 | 125.30 | 111.50 |
| 19 | C | 307 | PGV | O03-C19-C20 | 6.11 | 131.09 | 111.91 |
| 18 | N | 607 | TGL | OG2-CB1-CB2 | 5.95 | 124.33 | 111.50 |
| 19 | C | 307 | PGV | O01-C1-C2 | 5.68 | 123.75 | 111.50 |
| 14 | A | 601[A] | HEA | C1B-C2B-C3B | -5.65 | 103.06 | 107.00 |
| 25 | L | 102 | CHD | C4-C5-C10 | 5.65 | 118.66 | 112.66 |
| 25 | Y | 102 | CHD | C1-C10-C5 | 5.65 | 116.12 | 107.77 |
| 14 | A | 601[A] | HEA | C13-C12-C11 | -5.54 | 106.02 | 114.35 |
| 25 | L | 102 | CHD | C21-C20-C17 | 5.39 | 121.17 | 112.92 |
| 23 | L | 105 | DMU | C18-O16-C6 | 5.33 | 122.67 | 113.84 |
| 25 | J | 101 | CHD | C14-C13-C12 | 5.27 | 112.31 | 107.40 |
| 25 | Y | 102 | CHD | C9-C11-C12 | -5.19 | 107.44 | 114.30 |
| 25 | C | 301 | CHD | C18-C13-C12 | 5.16 | 114.32 | 109.07 |
| 25 | J | 101 | CHD | C9-C11-C12 | -4.92 | 107.81 | 114.30 |
| 14 | A | 602 | HEA | CAD-CBD-CGD | -4.77 | 104.67 | 112.67 |
| 23 | L | 105 | DMU | O5-C6-O16 | 4.73 | 121.18 | 109.97 |
| 26 | P | 303 | PEK | O03-C21-C22 | 4.73 | 123.79 | 111.38 |
| 14 | N | 602[A] | HEA | C1B-C2B-C3B | -4.70 | 103.73 | 107.00 |
| 25 | Y | 102 | CHD | C6-C5-C4 | -4.66 | 105.82 | 111.19 |
| 23 | P | 317 | DMU | C10-O1-C9 | 4.63 | 122.77 | 113.69 |
| 25 | Y | 102 | CHD | C14-C8-C7 | 4.57 | 117.87 | 111.81 |
| 27 | P | 307 | CDL | OB8-CB7-C71 | 4.55 | 126.19 | 111.91 |
| 25 | J | 101 | CHD | C22-C20-C17 | 4.53 | 119.65 | 110.28 |
| 14 | A | 601[A] | HEA | CAA-CBA-CGA | -4.53 | 105.07 | 112.67 |
| 25 | Y | 102 | CHD | C21-C20-C17 | 4.48 | 119.78 | 112.92 |
| 25 | L | 102 | CHD | C5-C4-C3 | 4.46 | 119.30 | 112.76 |
| 26 | C | 303 | PEK | O03-C21-C22 | 4.43 | 125.82 | 111.91 |
| 25 | L | 102 | CHD | C10-C9-C8 | 4.40 | 116.55 | 111.82 |
| 25 | L | 102 | CHD | C13-C17-C20 | 4.38 | 124.72 | 119.50 |
| 26 | C | 303 | PEK | O01-C1-C2 | 4.37 | 120.92 | 111.50 |
| 18 | L | 101 | TGL | OG2-CB1-CB2 | 4.36 | 120.89 | 111.50 |
| 19 | C | 307 | PGV | C01-O03-C19 | 4.33 | 133.16 | 117.12 |
| 25 | J | 101 | CHD | C13-C17-C20 | 4.21 | 124.53 | 119.50 |
| 25 | L | 102 | CHD | C17-C13-C12 | -4.16 | 113.86 | 117.67 |
| 25 | J | 101 | CHD | C9-C10-C5 | 4.12 | 114.37 | 108.58 |
| 19 | N | 610 | PGV | C02-O01-C1 | -4.12 | 107.65 | 117.79 |
| 25 | L | 102 | CHD | C11-C9-C10 | -4.03 | 109.57 | 113.73 |
| 14 | N | 602[A] | HEA | C26-C15-C16 | 3.97 | 121.96 | 115.27 |
| 25 | B | 302 | CHD | C6-C5-C4 | -3.95 | 106.65 | 111.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23 | L | 105 | DMU | C3-C4-C57 | -3.92 | 105.72 | 112.60 |
| 25 | Y | 102 | CHD | C19-C10-C1 | -3.90 | 101.98 | 108.26 |
| 27 | C | 308 | CDL | C52-C51-CB5 | -3.79 | 99.83 | 113.62 |
| 25 | P | 301 | CHD | C22-C23-C24 | -3.76 | 105.50 | 113.59 |
| 18 | L | 101 | TGL | OG1-CA1-CA2 | 3.70 | 123.53 | 111.91 |
| 23 | L | 105 | DMU | O5-C4-C57 | 3.68 | 112.73 | 106.83 |
| 14 | N | 602[A] | HEA | CAA-CBA-CGA | -3.67 | 106.52 | 112.67 |
| 27 | C | 308 | CDL | OB8-CB7-C71 | 3.67 | 123.41 | 111.91 |
| 23 | M | 101 | DMU | C18-O16-C6 | -3.66 | 107.77 | 113.84 |
| 25 | L | 102 | CHD | C6-C5-C4 | -3.66 | 106.98 | 111.19 |
| 23 | P | 317 | DMU | C10-C5-C7 | 3.60 | 117.49 | 110.00 |
| 18 | L | 101 | TGL | CC3-CC2-CC1 | 3.59 | 126.66 | 113.62 |
| 18 | A | 607 | TGL | OG3-CC1-CC2 | 3.56 | 123.09 | 111.91 |
| 19 | A | 611 | PGV | O03-C19-O04 | -3.55 | 114.63 | 123.59 |
| 19 | C | 307 | PGV | O03-C19-O04 | -3.54 | 114.65 | 123.59 |
| 25 | J | 101 | CHD | C18-C13-C14 | -3.53 | 105.69 | 111.21 |
| 25 | J | 101 | CHD | C1-C10-C9 | -3.52 | 105.81 | 111.35 |
| 18 | A | 607 | TGL | OG1-CA1-CA2 | 3.49 | 122.87 | 111.91 |
| 26 | T | 101 | PEK | O03-C21-C22 | 3.49 | 126.02 | 112.23 |
| 25 | Y | 102 | CHD | C14-C13-C12 | 3.48 | 110.64 | 107.40 |
| 25 | C | 301 | CHD | C1-C2-C3 | -3.47 | 106.02 | 110.47 |
| 25 | L | 102 | CHD | C14-C13-C12 | 3.46 | 110.62 | 107.40 |
| 23 | P | 317 | DMU | C6-C1-C2 | 3.46 | 117.20 | 110.00 |
| 18 | A | 606 | TGL | CB3-CB2-CB1 | -3.44 | 101.09 | 113.62 |
| 25 | C | 301 | CHD | C22-C20-C17 | -3.38 | 103.31 | 110.28 |
| 27 | C | 308 | CDL | OB6-CB5-C51 | 3.37 | 122.50 | 111.91 |
| 25 | Y | 102 | CHD | C4-C3-C2 | -3.37 | 106.53 | 110.55 |
| 23 | P | 317 | DMU | O1-C9-C8 | 3.36 | 115.79 | 109.69 |
| 23 | D | 206 | DMU | C6-O5-C4 | 3.36 | 120.28 | 113.69 |
| 23 | P | 308 | DMU | C18-O16-C6 | -3.33 | 108.32 | 113.84 |
| 26 | P | 303 | PEK | O01-C1-C2 | 3.33 | 118.67 | 111.50 |
| 23 | P | 317 | DMU | O16-C6-C1 | 3.29 | 113.44 | 108.30 |
| 19 | A | 611 | PGV | O03-C19-C20 | 3.28 | 122.20 | 111.91 |
| 27 | P | 307 | CDL | OB8-CB7-OB9 | -3.28 | 115.32 | 123.59 |
| 25 | G | 101 | CHD | C6-C5-C4 | -3.26 | 107.43 | 111.19 |
| 25 | J | 101 | CHD | C15-C14-C8 | 3.26 | 122.89 | 118.33 |
| 14 | A | 602 | HEA | C20-C19-C18 | -3.22 | 114.59 | 121.12 |
| 23 | P | 317 | DMU | O1-C10-C5 | 3.22 | 117.16 | 110.35 |
| 25 | B | 302 | CHD | C13-C17-C20 | -3.21 | 115.66 | 119.50 |
| 25 | J | 101 | CHD | C5-C6-C7 | -3.21 | 110.92 | 114.46 |
| 18 | A | 607 | TGL | OG3-CC1-OC1 | -3.20 | 115.51 | 123.59 |
| 19 | P | 305 | PGV | O01-C1-O02 | -3.19 | 115.98 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 18 | L | 101 | TGL | CG3-CG2-CG1 | -3.14 | 104.36 | 111.79 |
| 25 | Y | 102 | CHD | C10-C9-C8 | 3.12 | 115.17 | 111.82 |
| 19 | N | 612 | PGV | O03-C19-O04 | -3.12 | 115.73 | 123.59 |
| 25 | L | 102 | CHD | C22-C23-C24 | -3.12 | 106.89 | 113.59 |
| 27 | C | 308 | CDL | C61-C60-C59 | -3.11 | 98.64 | 114.42 |
| 14 | A | 602 | HEA | C13-C12-C11 | -3.11 | 109.68 | 114.35 |
| 14 | A | 602 | HEA | CBD-CAD-C3D | 3.04 | 118.09 | 112.49 |
| 14 | N | 603 | HEA | C1B-C2B-C3B | -3.03 | 104.89 | 107.00 |
| 25 | L | 102 | CHD | C1-C10-C5 | 3.03 | 112.24 | 107.77 |
| 26 | C | 304 | PEK | O03-C21-C22 | 3.01 | 121.37 | 111.91 |
| 14 | N | 603 | HEA | CMD-C2D-C3D | 3.00 | 130.60 | 124.94 |
| 14 | N | 603 | HEA | CBD-CAD-C3D | 3.00 | 118.02 | 112.49 |
| 14 | N | 602[A] | HEA | C16-C15-C14 | -2.99 | 115.06 | 121.12 |
| 25 | J | 101 | CHD | C23-C22-C20 | -2.99 | 110.70 | 114.72 |
| 14 | N | 602[A] | HEA | CMB-C2B-C3B | 2.98 | 130.53 | 124.69 |
| 25 | L | 102 | CHD | C14-C8-C7 | 2.98 | 115.76 | 111.81 |
| 18 | L | 101 | TGL | OG3-CC1-OC1 | -2.95 | 116.14 | 123.59 |
| 25 | L | 102 | CHD | C1-C10-C9 | -2.93 | 106.74 | 111.35 |
| 23 | D | 206 | DMU | C10-O1-C9 | 2.93 | 119.44 | 113.69 |
| 19 | N | 610 | PGV | O01-C1-C2 | 2.89 | 117.74 | 111.50 |
| 14 | A | 602 | HEA | C1B-C2B-C3B | -2.89 | 104.99 | 107.00 |
| 14 | A | 601[A] | HEA | CMB-C2B-C3B | 2.88 | 130.33 | 124.69 |
| 25 | L | 102 | CHD | C9-C10-C5 | 2.87 | 112.61 | 108.58 |
| 23 | C | 310 | DMU | C8-C7-C5 | 2.86 | 115.81 | 110.82 |
| 26 | T | 101 | PEK | C01-O03-C21 | 2.84 | 125.45 | 116.11 |
| 27 | N | 601 | CDL | CB6-OB8-CB7 | 2.84 | 126.08 | 116.92 |
| 23 | D | 206 | DMU | C11-C9-C8 | -2.80 | 106.44 | 113.00 |
| 25 | B | 302 | CHD | C16-C17-C13 | 2.79 | 106.29 | 103.55 |
| 14 | N | 603 | HEA | C13-C12-C11 | -2.79 | 110.16 | 114.35 |
| 27 | T | 102 | CDL | OB8-CB7-C71 | 2.79 | 120.65 | 111.91 |
| 27 | P | 307 | CDL | OB6-CB5-C51 | 2.78 | 120.64 | 111.91 |
| 25 | C | 309 | CHD | C11-C9-C10 | -2.77 | 110.87 | 113.73 |
| 23 | P | 317 | DMU | O7-C10-C5 | 2.76 | 115.25 | 108.10 |
| 19 | N | 610 | PGV | O03-C19-C20 | 2.75 | 120.55 | 111.91 |
| 14 | A | 601[A] | HEA | CMD-C2D-C3D | 2.75 | 130.12 | 124.94 |
| 25 | C | 301 | CHD | C18-C13-C17 | -2.75 | 106.91 | 111.21 |
| 25 | L | 102 | CHD | C18-C13-C14 | -2.74 | 106.93 | 111.21 |
| 14 | A | 602 | HEA | C27-C19-C20 | 2.73 | 119.87 | 115.27 |
| 18 | A | 606 | TGL | OG3-CC1-CC2 | 2.71 | 120.42 | 111.91 |
| 23 | D | 206 | DMU | O1-C9-C8 | 2.71 | 114.61 | 109.69 |
| 25 | B | 302 | CHD | C19-C10-C5 | -2.70 | 105.78 | 110.36 |
| 19 | C | 307 | PGV | O01-C1-O02 | -2.69 | 117.19 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 27 | C | 308 | CDL | OB8-CB7-OB9 | -2.69 | 116.79 | 123.59 |
| 25 | J | 101 | CHD | C13-C14-C8 | -2.69 | 111.31 | 114.74 |
| 14 | A | 602 | HEA | CBA-CAA-C2A | -2.68 | 107.54 | 112.48 |
| 25 | C | 309 | CHD | C19-C10-C9 | -2.67 | 107.50 | 111.18 |
| 23 | P | 308 | DMU | O7-C3-C2 | 2.67 | 114.38 | 107.28 |
| 25 | P | 301 | CHD | C22-C20-C17 | -2.67 | 104.78 | 110.28 |
| 26 | C | 303 | PEK | C01-O03-C21 | 2.66 | 126.97 | 117.12 |
| 18 | L | 101 | TGL | OG1-CG1-CG2 | 2.66 | 116.17 | 108.43 |
| 25 | Y | 102 | CHD | C13-C17-C20 | 2.65 | 122.65 | 119.50 |
| 25 | P | 301 | CHD | C11-C9-C10 | -2.63 | 111.02 | 113.73 |
| 18 | A | 606 | TGL | OG1-CA1-CA2 | 2.63 | 120.15 | 111.91 |
| 25 | L | 102 | CHD | C11-C12-C13 | 2.62 | 113.94 | 111.24 |
| 25 | L | 102 | CHD | C23-C22-C20 | -2.62 | 111.20 | 114.72 |
| 23 | L | 105 | DMU | O5-C6-C1 | -2.61 | 104.81 | 110.35 |
| 19 | N | 612 | PGV | O03-C19-C20 | 2.60 | 120.08 | 111.91 |
| 14 | N | 602[A] | HEA | C3C-C4C-NC | 2.60 | 112.57 | 109.21 |
| 14 | A | 602 | HEA | CAA-CBA-CGA | -2.59 | 108.32 | 112.67 |
| 26 | C | 303 | PEK | O03-C21-O04 | -2.59 | 117.06 | 123.59 |
| 18 | N | 608 | TGL | OG3-CC1-OC1 | -2.57 | 115.08 | 123.14 |
| 18 | N | 607 | TGL | OG1-CA1-CA2 | 2.57 | 119.96 | 111.91 |
| 14 | N | 603 | HEA | CAA-CBA-CGA | -2.56 | 108.37 | 112.67 |
| 25 | J | 101 | CHD | C6-C5-C4 | -2.55 | 108.26 | 111.19 |
| 25 | P | 301 | CHD | C6-C5-C10 | -2.54 | 109.96 | 112.66 |
| 26 | P | 304 | PEK | C8-C7-C6 | -2.52 | 99.63 | 112.02 |
| 23 | D | 206 | DMU | C10-C5-C7 | 2.51 | 115.22 | 110.00 |
| 19 | C | 307 | PGV | C21-C20-C19 | -2.50 | 104.52 | 113.62 |
| 25 | Y | 102 | CHD | C15-C14-C8 | 2.50 | 121.83 | 118.33 |
| 14 | N | 603 | HEA | CAD-CBD-CGD | -2.48 | 108.51 | 112.67 |
| 23 | C | 310 | DMU | C10-C5-C7 | 2.48 | 115.15 | 110.00 |
| 26 | T | 101 | PEK | O03-C21-O04 | -2.47 | 115.40 | 123.14 |
| 26 | P | 303 | PEK | C01-O03-C21 | 2.46 | 126.24 | 117.12 |
| 25 | B | 302 | CHD | C11-C9-C10 | -2.46 | 111.19 | 113.73 |
| 26 | P | 304 | PEK | O03-C21-C22 | 2.45 | 119.60 | 111.91 |
| 19 | C | 307 | PGV | O04-C19-C20 | -2.45 | 114.17 | 123.73 |
| 18 | A | 607 | TGL | OG2-CB1-CB2 | 2.44 | 116.77 | 111.50 |
| 25 | Y | 102 | CHD | C2-C1-C10 | 2.44 | 116.96 | 112.78 |
| 26 | P | 303 | PEK | O03-C21-O04 | -2.44 | 117.44 | 123.59 |
| 14 | A | 602 | HEA | C13-C14-C15 | -2.43 | 121.82 | 127.66 |
| 26 | C | 303 | PEK | O01-C1-O02 | -2.42 | 117.84 | 123.70 |
| 26 | C | 303 | PEK | O03-C01-C02 | 2.42 | 115.48 | 108.43 |
| 19 | A | 611 | PGV | C32-C31-C30 | -2.42 | 102.15 | 114.42 |
| 23 | D | 206 | DMU | C7-C8-C9 | 2.42 | 114.55 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 18 | N | 607 | TGL | OG3-CC1-CC2 | 2.41 | 119.46 | 111.91 |
| 19 | C | 306 | PGV | O03-C19-O04 | -2.40 | 117.53 | 123.59 |
| 27 | C | 308 | CDL | C77-C76-C75 | -2.40 | 102.25 | 114.42 |
| 18 | N | 609 | TGL | OG3-CC1-CC2 | 2.40 | 121.71 | 112.23 |
| 25 | J | 101 | CHD | O7-C7-C8 | 2.40 | 114.78 | 109.43 |
| 23 | C | 310 | DMU | C7-C8-C9 | 2.39 | 114.51 | 110.24 |
| 25 | P | 301 | CHD | O12-C12-C13 | -2.39 | 106.98 | 111.03 |
| 18 | N | 608 | TGL | OG3-CC1-CC2 | 2.39 | 121.67 | 112.23 |
| 19 | N | 612 | PGV | O01-C02-C01 | -2.38 | 99.77 | 108.40 |
| 27 | C | 308 | CDL | C80-C79-C78 | 2.38 | 126.51 | 114.42 |
| 27 | P | 307 | CDL | C83-C82-C81 | 2.37 | 126.45 | 114.42 |
| 25 | C | 301 | CHD | C4-C5-C10 | -2.37 | 110.14 | 112.66 |
| 14 | N | 603 | HEA | C3C-C4C-NC | 2.37 | 112.27 | 109.21 |
| 25 | Y | 102 | CHD | C16-C17-C13 | -2.37 | 101.23 | 103.55 |
| 14 | N | 603 | HEA | C27-C19-C20 | 2.36 | 119.25 | 115.27 |
| 25 | J | 101 | CHD | C11-C9-C8 | -2.36 | 107.42 | 110.88 |
| 23 | C | 310 | DMU | C10-O1-C9 | -2.35 | 109.07 | 113.69 |
| 23 | P | 308 | DMU | C1-C2-C3 | -2.35 | 104.31 | 109.68 |
| 25 | L | 102 | CHD | C15-C14-C8 | 2.35 | 121.61 | 118.33 |
| 25 | L | 102 | CHD | C14-C8-C9 | -2.35 | 106.49 | 109.71 |
| 14 | A | 602 | HEA | C26-C15-C16 | 2.35 | 119.22 | 115.27 |
| 26 | C | 303 | PEK | C2-C3-C4 | 2.34 | 117.40 | 113.23 |
| 14 | A | 601[A] | HEA | C26-C15-C16 | 2.34 | 119.20 | 115.27 |
| 27 | C | 308 | CDL | C81-C80-C79 | -2.33 | 102.60 | 114.42 |
| 19 | N | 612 | PGV | C01-O03-C19 | -2.33 | 108.50 | 117.12 |
| 25 | C | 301 | CHD | C5-C4-C3 | -2.32 | 109.34 | 112.76 |
| 23 | C | 310 | DMU | O7-C10-C5 | 2.31 | 114.09 | 108.10 |
| 14 | A | 601[A] | HEA | C13-C14-C15 | -2.31 | 122.10 | 127.66 |
| 14 | A | 601[A] | HEA | C3C-C4C-NC | 2.31 | 112.19 | 109.21 |
| 25 | G | 101 | CHD | C18-C13-C12 | -2.30 | 106.72 | 109.07 |
| 23 | Z | 101 | DMU | O1-C9-C8 | 2.29 | 113.86 | 109.69 |
| 23 | P | 317 | DMU | C1-C2-C3 | 2.28 | 114.90 | 109.68 |
| 23 | P | 308 | DMU | C10-C5-C7 | 2.27 | 114.72 | 110.00 |
| 26 | P | 304 | PEK | C3-C2-C1 | -2.26 | 105.39 | 113.62 |
| 25 | C | 309 | CHD | C14-C8-C9 | -2.26 | 106.61 | 109.71 |
| 25 | P | 301 | CHD | C18-C13-C12 | 2.26 | 111.37 | 109.07 |
| 18 | A | 607 | TGL | CG3-CG2-CG1 | -2.26 | 106.45 | 111.79 |
| 25 | P | 301 | CHD | C18-C13-C17 | -2.25 | 107.69 | 111.21 |
| 25 | C | 301 | CHD | C11-C9-C10 | -2.24 | 111.41 | 113.73 |
| 27 | N | 601 | CDL | C40-C39-C38 | 2.24 | 125.80 | 114.42 |
| 26 | C | 304 | PEK | O03-C21-O04 | -2.24 | 117.94 | 123.59 |
| 26 | C | 304 | PEK | C3-C2-C1 | -2.23 | 105.50 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 14 | N | 603 | HEA | C13-C14-C15 | -2.23 | 122.29 | 127.66 |
| 27 | C | 308 | CDL | C62-C61-C60 | 2.23 | 125.74 | 114.42 |
| 19 | A | 611 | PGV | O01-C1-C2 | 2.22 | 116.29 | 111.50 |
| 19 | C | 307 | PGV | C02-O01-C1 | -2.22 | 115.02 | 117.88 |
| 25 | C | 301 | CHD | C19-C10-C1 | -2.22 | 104.68 | 108.26 |
| 27 | C | 308 | CDL | CB4-OB6-CB5 | -2.22 | 109.75 | 116.92 |
| 23 | D | 206 | DMU | O16-C6-C1 | 2.21 | 111.76 | 108.30 |
| 25 | L | 102 | CHD | C18-C13-C12 | 2.21 | 111.31 | 109.07 |
| 27 | P | 307 | CDL | OB8-CB6-CB4 | 2.20 | 115.12 | 108.61 |
| 19 | N | 612 | PGV | O01-C1-C2 | 2.20 | 116.25 | 111.50 |
| 25 | G | 101 | CHD | C13-C14-C8 | -2.19 | 111.95 | 114.74 |
| 14 | A | 602 | HEA | C16-C15-C14 | -2.18 | 116.71 | 121.12 |
| 26 | C | 303 | PEK | C02-O01-C1 | -2.17 | 112.44 | 117.79 |
| 18 | L | 101 | TGL | OG3-CC1-CC2 | 2.17 | 118.71 | 111.91 |
| 25 | Y | 102 | CHD | C22-C23-C24 | -2.16 | 108.94 | 113.59 |
| 25 | L | 102 | CHD | C22-C20-C17 | -2.16 | 105.82 | 110.28 |
| 18 | N | 607 | TGL | OG2-CB1-OB1 | -2.15 | 118.49 | 123.70 |
| 14 | A | 601[A] | HEA | CBD-CAD-C3D | -2.14 | 108.53 | 112.49 |
| 25 | P | 301 | CHD | C5-C4-C3 | -2.14 | 109.61 | 112.76 |
| 19 | N | 612 | PGV | C9-C10-C11 | -2.14 | 100.17 | 112.43 |
| 25 | J | 101 | CHD | C16-C17-C20 | 2.12 | 115.43 | 112.15 |
| 25 | Y | 102 | CHD | O7-C7-C8 | 2.12 | 114.17 | 109.43 |
| 14 | A | 602 | HEA | CMD-C2D-C3D | 2.11 | 128.92 | 124.94 |
| 26 | P | 304 | PEK | O03-C21-O04 | -2.11 | 118.27 | 123.59 |
| 25 | Y | 102 | CHD | C21-C20-C22 | -2.10 | 107.07 | 110.36 |
| 23 | P | 308 | DMU | C7-C8-C9 | 2.09 | 113.97 | 110.24 |
| 25 | C | 309 | CHD | C22-C23-C24 | -2.09 | 109.09 | 113.59 |
| 23 | P | 316 | DMU | C3-C2-C1 | 2.09 | 113.72 | 110.69 |
| 25 | L | 102 | CHD | C13-C14-C8 | -2.08 | 112.08 | 114.74 |
| 14 | A | 602 | HEA | C4B-C3B-C2B | -2.07 | 105.42 | 106.87 |
| 19 | C | 307 | PGV | C03-C02-C01 | -2.07 | 106.67 | 112.63 |
| 25 | P | 301 | CHD | C21-C20-C22 | -2.07 | 107.12 | 110.36 |
| 25 | L | 102 | CHD | O7-C7-C8 | 2.06 | 114.03 | 109.43 |
| 14 | N | 603 | HEA | C21-C22-C23 | -2.06 | 120.70 | 127.75 |
| 25 | B | 302 | CHD | C13-C14-C8 | -2.06 | 112.11 | 114.74 |
| 23 | C | 310 | DMU | C18-O16-C6 | 2.06 | 117.25 | 113.84 |
| 18 | N | 609 | TGL | CG3-OG3-CC1 | 2.05 | 122.88 | 116.11 |
| 18 | A | 606 | TGL | OB1-CB1-CB2 | -2.05 | 115.72 | 123.73 |
| 27 | N | 601 | CDL | C44-C43-C42 | -2.05 | 104.03 | 114.42 |
| 27 | N | 601 | CDL | C19-C18-C17 | 2.04 | 124.80 | 114.42 |
| 25 | C | 309 | CHD | C1-C10-C5 | 2.04 | 110.79 | 107.77 |
| 23 | D | 206 | DMU | O61-C57-C4 | 2.04 | 118.29 | 111.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 19 | C | 306 | PGV | O03-C19-C20 | 2.04 | 118.31 | 111.91 |
| 26 | C | 304 | PEK | O01-C1-C2 | 2.04 | 115.89 | 111.50 |
| 23 | P | 308 | DMU | C6-O5-C4 | 2.04 | 117.69 | 113.69 |
| 25 | C | 309 | CHD | C17-C13-C14 | 2.03 | 102.14 | 100.09 |
| 23 | P | 308 | DMU | O1-C10-C5 | 2.03 | 114.65 | 110.35 |
| 27 | P | 307 | CDL | OB6-CB4-CB6 | -2.03 | 102.61 | 108.61 |
| 19 | C | 306 | PGV | O03-C01-C02 | -2.03 | 102.53 | 108.43 |
| 23 | Z | 101 | DMU | C10-O7-C3 | -2.02 | 112.96 | 117.96 |
| 25 | P | 301 | CHD | C16-C17-C20 | -2.02 | 109.02 | 112.15 |
| 25 | C | 301 | CHD | O12-C12-C13 | -2.02 | 107.62 | 111.03 |
| 27 | C | 308 | CDL | C84-C83-C82 | -2.02 | 104.17 | 114.42 |
| 21 | O | 302 | PSC | C14-C13-C12 | -2.02 | 109.25 | 124.73 |
| 14 | A | 601[A] | HEA | CMC-C2C-C3C | 2.01 | 128.45 | 124.68 |
| 25 | C | 309 | CHD | C5-C6-C7 | 2.01 | 116.68 | 114.46 |
| 14 | A | 602 | HEA | C21-C20-C19 | 2.01 | 119.58 | 112.98 |
| 18 | A | 607 | TGL | OG1-CA1-OA1 | -2.00 | 118.54 | 123.59 |

All (24) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|--------|------|------|
| 14 | A | 601[A] | HEA | NA |
| 14 | A | 601[A] | HEA | ND |
| 14 | A | 601[A] | HEA | NB |
| 14 | A | 601[B] | HEA | NA |
| 14 | A | 601[B] | HEA | ND |
| 14 | A | 601[B] | HEA | NB |
| 14 | A | 601[C] | HEA | NA |
| 14 | A | 601[C] | HEA | ND |
| 14 | A | 601[C] | HEA | NB |
| 14 | A | 602 | HEA | NA |
| 14 | A | 602 | HEA | ND |
| 14 | A | 602 | HEA | NB |
| 14 | N | 602[A] | HEA | NA |
| 14 | N | 602[A] | HEA | ND |
| 14 | N | 602[A] | HEA | NB |
| 14 | N | 602[B] | HEA | NA |
| 14 | N | 602[B] | HEA | ND |
| 14 | N | 602[B] | HEA | NB |
| 14 | N | 602[C] | HEA | NA |
| 14 | N | 602[C] | HEA | ND |
| 14 | N | 602[C] | HEA | NB |
| 14 | N | 603 | HEA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14 | N | 603 | HEA | ND |
| 14 | N | 603 | HEA | NB |

All (543) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | A | 607 | TGL | OB1-CB1-OG2-CG2 |
| 18 | L | 101 | TGL | CB2-CB1-OG2-CG2 |
| 18 | L | 101 | TGL | OB1-CB1-OG2-CG2 |
| 18 | N | 609 | TGL | CC2-CC1-OG3-CG3 |
| 19 | A | 608 | PGV | C1-C2-C3-C4 |
| 19 | C | 307 | PGV | O04-C19-O03-C01 |
| 19 | C | 307 | PGV | C20-C19-O03-C01 |
| 19 | N | 610 | PGV | C04-O12-P-O13 |
| 19 | N | 610 | PGV | O04-C19-O03-C01 |
| 19 | N | 610 | PGV | C20-C19-O03-C01 |
| 21 | A | 610 | PSC | C7-C8-C9-C10 |
| 21 | A | 610 | PSC | C11-C10-C9-C8 |
| 22 | W | 101 | EDO | O1-C1-C2-O2 |
| 23 | L | 105 | DMU | C3-C4-C57-O61 |
| 23 | L | 105 | DMU | O5-C4-C57-O61 |
| 23 | L | 105 | DMU | O5-C6-O16-C18 |
| 25 | J | 101 | CHD | C13-C17-C20-C22 |
| 25 | J | 101 | CHD | C16-C17-C20-C21 |
| 25 | J | 101 | CHD | C16-C17-C20-C22 |
| 26 | C | 305 | PEK | C4-C5-C6-C7 |
| 26 | C | 305 | PEK | C13-C14-C15-C16 |
| 26 | P | 303 | PEK | O04-C21-O03-C01 |
| 26 | P | 303 | PEK | C22-C21-O03-C01 |
| 26 | P | 303 | PEK | C5-C6-C7-C8 |
| 26 | P | 304 | PEK | C7-C8-C9-C10 |
| 26 | T | 101 | PEK | C6-C7-C8-C9 |
| 26 | T | 101 | PEK | C11-C12-C13-C14 |
| 26 | C | 303 | PEK | O04-C21-O03-C01 |
| 26 | T | 101 | PEK | O04-C21-O03-C01 |
| 26 | T | 101 | PEK | C22-C21-O03-C01 |
| 26 | C | 303 | PEK | C22-C21-O03-C01 |
| 23 | D | 206 | DMU | C3-C4-C57-O61 |
| 18 | N | 609 | TGL | OC1-CC1-OG3-CG3 |
| 25 | L | 102 | CHD | C13-C17-C20-C21 |
| 25 | L | 102 | CHD | C16-C17-C20-C22 |
| 18 | A | 607 | TGL | CB2-CB1-OG2-CG2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | L | 102 | CHD | C16-C17-C20-C21 |
| 25 | L | 102 | CHD | C13-C17-C20-C22 |
| 19 | A | 608 | PGV | C10-C11-C12-C13 |
| 26 | C | 303 | PEK | C4-C5-C6-C7 |
| 26 | C | 303 | PEK | C7-C8-C9-C10 |
| 25 | L | 102 | CHD | C20-C22-C23-C24 |
| 19 | N | 610 | PGV | C2-C1-O01-C02 |
| 26 | P | 303 | PEK | C2-C1-O01-C02 |
| 18 | A | 606 | TGL | C22-C23-C24-C25 |
| 25 | J | 101 | CHD | C21-C20-C22-C23 |
| 18 | N | 608 | TGL | C16-C15-CC9-CC8 |
| 27 | C | 308 | CDL | C37-C38-C39-C40 |
| 23 | D | 206 | DMU | O5-C4-C57-O61 |
| 25 | J | 101 | CHD | C13-C17-C20-C21 |
| 23 | P | 308 | DMU | O6-C11-C9-O1 |
| 19 | N | 610 | PGV | O02-C1-O01-C02 |
| 26 | P | 303 | PEK | O02-C1-O01-C02 |
| 27 | C | 308 | CDL | OB6-CB4-CB6-OB8 |
| 18 | A | 606 | TGL | C11-C12-C13-C14 |
| 27 | P | 307 | CDL | C20-C21-C22-C23 |
| 18 | L | 101 | TGL | CC1-CC2-CC3-CC4 |
| 25 | J | 101 | CHD | C17-C20-C22-C23 |
| 26 | C | 303 | PEK | O02-C1-O01-C02 |
| 25 | C | 309 | CHD | C17-C20-C22-C23 |
| 27 | P | 307 | CDL | OB6-CB4-CB6-OB8 |
| 25 | C | 309 | CHD | C21-C20-C22-C23 |
| 26 | C | 303 | PEK | C2-C1-O01-C02 |
| 19 | P | 305 | PGV | C10-C11-C12-C13 |
| 26 | C | 305 | PEK | C10-C11-C12-C13 |
| 26 | P | 304 | PEK | C4-C5-C6-C7 |
| 26 | P | 304 | PEK | C10-C11-C12-C13 |
| 27 | N | 601 | CDL | C80-C81-C82-C83 |
| 27 | P | 307 | CDL | C82-C83-C84-C85 |
| 18 | L | 101 | TGL | C23-C24-C25-C26 |
| 26 | C | 304 | PEK | C22-C23-C24-C25 |
| 18 | L | 101 | TGL | CA9-C20-C21-C22 |
| 23 | C | 310 | DMU | O16-C18-C19-C22 |
| 25 | C | 309 | CHD | C20-C22-C23-C24 |
| 23 | L | 105 | DMU | O16-C18-C19-C22 |
| 19 | N | 610 | PGV | O12-C04-C05-O05 |
| 19 | P | 306 | PGV | C10-C11-C12-C13 |
| 26 | C | 304 | PEK | C7-C8-C9-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | P | 303 | PEK | C4-C5-C6-C7 |
| 26 | T | 101 | PEK | C13-C14-C15-C16 |
| 23 | P | 308 | DMU | C19-C22-C25-C28 |
| 19 | N | 610 | PGV | C04-O12-P-O11 |
| 23 | D | 206 | DMU | C22-C25-C28-C31 |
| 19 | C | 307 | PGV | O02-C1-O01-C02 |
| 23 | P | 308 | DMU | O6-C11-C9-C8 |
| 27 | C | 308 | CDL | C51-CB5-OB6-CB4 |
| 23 | Z | 101 | DMU | O16-C18-C19-C22 |
| 18 | L | 101 | TGL | C19-C33-C34-C35 |
| 18 | N | 607 | TGL | CB9-C10-C11-C12 |
| 23 | K | 102 | DMU | C31-C34-C37-C40 |
| 26 | C | 303 | PEK | C22-C23-C24-C25 |
| 19 | C | 307 | PGV | C2-C1-O01-C02 |
| 18 | A | 606 | TGL | C12-C13-C14-C29 |
| 18 | L | 101 | TGL | C21-C22-C23-C24 |
| 19 | C | 307 | PGV | C24-C25-C26-C27 |
| 23 | K | 103 | DMU | C22-C25-C28-C31 |
| 23 | M | 101 | DMU | C19-C22-C25-C28 |
| 26 | C | 304 | PEK | C23-C24-C25-C26 |
| 23 | K | 103 | DMU | C25-C28-C31-C34 |
| 23 | X | 104 | DMU | O16-C18-C19-C22 |
| 27 | P | 307 | CDL | C37-C38-C39-C40 |
| 27 | T | 102 | CDL | C79-C80-C81-C82 |
| 18 | A | 607 | TGL | C19-C33-C34-C35 |
| 19 | C | 306 | PGV | C7-C8-C9-C10 |
| 27 | N | 601 | CDL | C37-C38-C39-C40 |
| 19 | C | 306 | PGV | C10-C11-C12-C13 |
| 18 | A | 606 | TGL | CA5-CA6-CA7-CA8 |
| 18 | A | 607 | TGL | CC5-CC6-CC7-CC8 |
| 18 | L | 101 | TGL | CA5-CA6-CA7-CA8 |
| 18 | N | 607 | TGL | C24-C25-C26-C27 |
| 19 | C | 307 | PGV | C4-C5-C6-C7 |
| 27 | C | 308 | CDL | C77-C78-C79-C80 |
| 18 | N | 608 | TGL | C19-C33-C34-C35 |
| 27 | T | 102 | CDL | C60-C61-C62-C63 |
| 18 | A | 607 | TGL | CC7-CC8-CC9-C15 |
| 18 | N | 607 | TGL | CB3-CB4-CB5-CB6 |
| 18 | N | 609 | TGL | CC9-C15-C16-C17 |
| 18 | A | 606 | TGL | CC7-CC8-CC9-C15 |
| 18 | A | 606 | TGL | C17-C18-C19-C33 |
| 18 | A | 607 | TGL | CA9-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | L | 101 | TGL | CB6-CB7-CB8-CB9 |
| 18 | L | 101 | TGL | C11-C10-CB9-CB8 |
| 19 | P | 305 | PGV | C7-C8-C9-C10 |
| 27 | P | 307 | CDL | C77-C78-C79-C80 |
| 27 | T | 102 | CDL | C82-C83-C84-C85 |
| 18 | A | 607 | TGL | CB9-C10-C11-C12 |
| 19 | C | 306 | PGV | C20-C21-C22-C23 |
| 23 | P | 308 | DMU | C4-C3-O7-C10 |
| 18 | N | 607 | TGL | OB1-CB1-OG2-CG2 |
| 23 | K | 104 | DMU | C25-C28-C31-C34 |
| 27 | P | 307 | CDL | CB5-C51-C52-C53 |
| 18 | A | 607 | TGL | CB4-CB5-CB6-CB7 |
| 18 | N | 608 | TGL | CC3-CC4-CC5-CC6 |
| 18 | N | 609 | TGL | C22-C23-C24-C25 |
| 21 | A | 610 | PSC | C28-C29-C30-C31 |
| 27 | P | 307 | CDL | C41-C42-C43-C44 |
| 18 | N | 609 | TGL | CA6-CA7-CA8-CA9 |
| 23 | L | 105 | DMU | C25-C28-C31-C34 |
| 23 | P | 316 | DMU | O16-C18-C19-C22 |
| 23 | P | 316 | DMU | C31-C34-C37-C40 |
| 27 | N | 601 | CDL | C40-C41-C42-C43 |
| 18 | A | 606 | TGL | C21-C20-CA9-CA8 |
| 18 | N | 607 | TGL | C19-C33-C34-C35 |
| 18 | N | 608 | TGL | C22-C23-C24-C25 |
| 19 | P | 305 | PGV | C30-C31-C32-C33 |
| 27 | N | 601 | CDL | C32-C33-C34-C35 |
| 18 | L | 101 | TGL | C13-C14-C29-C30 |
| 23 | Z | 101 | DMU | C28-C31-C34-C37 |
| 23 | L | 105 | DMU | C19-C18-O16-C6 |
| 23 | C | 310 | DMU | C18-C19-C22-C25 |
| 21 | O | 302 | PSC | C11-C10-C9-C8 |
| 18 | A | 607 | TGL | CC9-C15-C16-C17 |
| 18 | N | 608 | TGL | C21-C22-C23-C24 |
| 27 | T | 102 | CDL | C20-C21-C22-C23 |
| 27 | C | 308 | CDL | OB7-CB5-OB6-CB4 |
| 23 | P | 308 | DMU | C2-C3-O7-C10 |
| 23 | Z | 101 | DMU | O6-C11-C9-C8 |
| 18 | L | 101 | TGL | C18-C19-C33-C34 |
| 19 | C | 306 | PGV | C19-C20-C21-C22 |
| 27 | P | 307 | CDL | C57-C58-C59-C60 |
| 19 | N | 610 | PGV | O12-C04-C05-C06 |
| 18 | N | 607 | TGL | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | N | 608 | TGL | C21-C20-CA9-CA8 |
| 18 | N | 609 | TGL | CA9-C20-C21-C22 |
| 18 | N | 607 | TGL | CC5-CC6-CC7-CC8 |
| 27 | T | 102 | CDL | C40-C41-C42-C43 |
| 22 | A | 612 | EDO | O1-C1-C2-O2 |
| 22 | D | 204 | EDO | O1-C1-C2-O2 |
| 22 | J | 103 | EDO | O1-C1-C2-O2 |
| 22 | L | 103 | EDO | O1-C1-C2-O2 |
| 22 | L | 104 | EDO | O1-C1-C2-O2 |
| 22 | N | 619 | EDO | O1-C1-C2-O2 |
| 18 | N | 608 | TGL | CB9-C10-C11-C12 |
| 19 | C | 306 | PGV | C27-C28-C29-C30 |
| 23 | Z | 101 | DMU | C25-C28-C31-C34 |
| 27 | N | 601 | CDL | C17-C18-C19-C20 |
| 18 | A | 606 | TGL | CB2-CB1-OG2-CG2 |
| 18 | N | 607 | TGL | CB2-CB1-OG2-CG2 |
| 18 | A | 607 | TGL | C16-C17-C18-C19 |
| 27 | N | 601 | CDL | C33-C34-C35-C36 |
| 23 | D | 206 | DMU | C18-C19-C22-C25 |
| 27 | P | 307 | CDL | CB6-CB4-OB6-CB5 |
| 23 | L | 105 | DMU | C34-C37-C40-C43 |
| 27 | C | 308 | CDL | C55-C56-C57-C58 |
| 27 | N | 601 | CDL | C77-C78-C79-C80 |
| 18 | N | 607 | TGL | C17-C18-C19-C33 |
| 18 | A | 606 | TGL | CB1-CB2-CB3-CB4 |
| 27 | P | 307 | CDL | C51-CB5-OB6-CB4 |
| 18 | N | 607 | TGL | C20-C21-C22-C23 |
| 18 | N | 609 | TGL | CC4-CC5-CC6-CC7 |
| 18 | N | 609 | TGL | C23-C24-C25-C26 |
| 18 | N | 607 | TGL | CB1-CB2-CB3-CB4 |
| 18 | N | 607 | TGL | C14-C29-C30-C31 |
| 18 | N | 608 | TGL | CB4-CB5-CB6-CB7 |
| 27 | C | 308 | CDL | C59-C60-C61-C62 |
| 27 | P | 307 | CDL | C36-C37-C38-C39 |
| 18 | A | 607 | TGL | C20-C21-C22-C23 |
| 23 | Z | 101 | DMU | C22-C25-C28-C31 |
| 18 | N | 609 | TGL | CC5-CC6-CC7-CC8 |
| 18 | N | 607 | TGL | CA4-CA5-CA6-CA7 |
| 27 | N | 601 | CDL | C42-C43-C44-C45 |
| 21 | O | 302 | PSC | C29-C30-C31-C32 |
| 18 | L | 101 | TGL | C15-C16-C17-C18 |
| 18 | N | 607 | TGL | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | N | 609 | TGL | CA4-CA5-CA6-CA7 |
| 19 | P | 306 | PGV | C28-C29-C30-C31 |
| 19 | A | 608 | PGV | C11-C10-C9-C8 |
| 18 | A | 606 | TGL | CB9-C10-C11-C12 |
| 18 | N | 607 | TGL | CB7-CB8-CB9-C10 |
| 19 | N | 610 | PGV | C10-C11-C12-C13 |
| 26 | T | 101 | PEK | C10-C11-C12-C13 |
| 18 | A | 606 | TGL | CC5-CC6-CC7-CC8 |
| 19 | C | 306 | PGV | C28-C29-C30-C31 |
| 23 | Q | 201 | DMU | C18-C19-C22-C25 |
| 27 | P | 307 | CDL | OB7-CB5-OB6-CB4 |
| 18 | A | 606 | TGL | OB1-CB1-OG2-CG2 |
| 18 | A | 606 | TGL | C21-C22-C23-C24 |
| 27 | N | 601 | CDL | C43-C44-C45-C46 |
| 18 | L | 101 | TGL | CC3-CC4-CC5-CC6 |
| 18 | A | 606 | TGL | CC1-CC2-CC3-CC4 |
| 23 | Q | 201 | DMU | C19-C22-C25-C28 |
| 23 | D | 207 | DMU | O16-C18-C19-C22 |
| 21 | A | 610 | PSC | C29-C30-C31-C32 |
| 18 | A | 606 | TGL | C16-C17-C18-C19 |
| 19 | A | 608 | PGV | C4-C5-C6-C7 |
| 23 | O | 306 | DMU | C25-C28-C31-C34 |
| 18 | A | 606 | TGL | C18-C19-C33-C34 |
| 18 | L | 101 | TGL | OG1-CG1-CG2-CG3 |
| 19 | C | 307 | PGV | C10-C11-C12-C13 |
| 18 | N | 609 | TGL | CC6-CC7-CC8-CC9 |
| 23 | M | 101 | DMU | C22-C25-C28-C31 |
| 19 | N | 612 | PGV | C25-C26-C27-C28 |
| 27 | P | 307 | CDL | C81-C82-C83-C84 |
| 18 | N | 609 | TGL | C11-C10-CB9-CB8 |
| 19 | C | 307 | PGV | C23-C24-C25-C26 |
| 23 | P | 316 | DMU | C28-C31-C34-C37 |
| 18 | L | 101 | TGL | OG1-CA1-CA2-CA3 |
| 23 | P | 308 | DMU | O5-C6-O16-C18 |
| 18 | N | 608 | TGL | C29-C30-C31-C32 |
| 18 | N | 608 | TGL | CA3-CA4-CA5-CA6 |
| 18 | A | 606 | TGL | CA2-CA1-OG1-CG1 |
| 23 | Z | 101 | DMU | C34-C37-C40-C43 |
| 27 | P | 307 | CDL | C40-C41-C42-C43 |
| 18 | L | 101 | TGL | CC5-CC6-CC7-CC8 |
| 23 | K | 104 | DMU | C28-C31-C34-C37 |
| 27 | N | 601 | CDL | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 19 | A | 608 | PGV | C21-C22-C23-C24 |
| 19 | P | 305 | PGV | C31-C32-C33-C34 |
| 18 | A | 606 | TGL | CB4-CB5-CB6-CB7 |
| 22 | J | 102 | EDO | O1-C1-C2-O2 |
| 22 | P | 313 | EDO | O1-C1-C2-O2 |
| 18 | N | 608 | TGL | C12-C13-C14-C29 |
| 18 | A | 607 | TGL | CC3-CC4-CC5-CC6 |
| 23 | M | 101 | DMU | C28-C31-C34-C37 |
| 27 | P | 307 | CDL | C73-C74-C75-C76 |
| 18 | N | 607 | TGL | CB4-CB5-CB6-CB7 |
| 23 | D | 207 | DMU | C25-C28-C31-C34 |
| 26 | C | 305 | PEK | C25-C26-C27-C28 |
| 27 | P | 307 | CDL | C53-C54-C55-C56 |
| 23 | L | 105 | DMU | C22-C25-C28-C31 |
| 18 | A | 606 | TGL | CC2-CC1-OG3-CG3 |
| 18 | A | 607 | TGL | CC2-CC1-OG3-CG3 |
| 27 | C | 308 | CDL | C58-C59-C60-C61 |
| 27 | N | 601 | CDL | C81-C82-C83-C84 |
| 19 | C | 307 | PGV | C3-C4-C5-C6 |
| 18 | A | 606 | TGL | CA2-CA3-CA4-CA5 |
| 18 | L | 101 | TGL | CA2-CA1-OG1-CG1 |
| 25 | Y | 102 | CHD | C13-C17-C20-C21 |
| 26 | T | 101 | PEK | C29-C30-C31-C32 |
| 27 | T | 102 | CDL | C80-C81-C82-C83 |
| 18 | A | 606 | TGL | CA1-CA2-CA3-CA4 |
| 18 | L | 101 | TGL | CB4-CB5-CB6-CB7 |
| 18 | N | 607 | TGL | C16-C15-CC9-CC8 |
| 19 | C | 307 | PGV | C13-C14-C15-C16 |
| 18 | L | 101 | TGL | C21-C20-CA9-CA8 |
| 23 | P | 308 | DMU | O16-C18-C19-C22 |
| 18 | N | 608 | TGL | CA2-CA3-CA4-CA5 |
| 19 | A | 611 | PGV | C10-C11-C12-C13 |
| 26 | C | 304 | PEK | C10-C11-C12-C13 |
| 26 | P | 304 | PEK | C13-C14-C15-C16 |
| 27 | T | 102 | CDL | C78-C79-C80-C81 |
| 26 | C | 304 | PEK | O03-C21-C22-C23 |
| 18 | N | 607 | TGL | CA7-CA8-CA9-C20 |
| 18 | N | 607 | TGL | CC6-CC7-CC8-CC9 |
| 27 | C | 308 | CDL | C36-C37-C38-C39 |
| 18 | N | 609 | TGL | CA5-CA6-CA7-CA8 |
| 18 | A | 607 | TGL | C16-C15-CC9-CC8 |
| 21 | A | 610 | PSC | C9-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | A | 610 | PSC | C10-C11-C12-C13 |
| 21 | O | 302 | PSC | C9-C10-C11-C12 |
| 21 | O | 302 | PSC | C10-C11-C12-C13 |
| 26 | C | 303 | PEK | C5-C6-C7-C8 |
| 26 | C | 303 | PEK | C6-C7-C8-C9 |
| 26 | C | 303 | PEK | C11-C10-C9-C8 |
| 26 | C | 303 | PEK | C9-C10-C11-C12 |
| 26 | C | 303 | PEK | C11-C12-C13-C14 |
| 26 | C | 303 | PEK | C12-C13-C14-C15 |
| 26 | C | 304 | PEK | C6-C7-C8-C9 |
| 26 | C | 304 | PEK | C9-C10-C11-C12 |
| 26 | C | 304 | PEK | C12-C13-C14-C15 |
| 26 | C | 305 | PEK | C5-C6-C7-C8 |
| 26 | C | 305 | PEK | C6-C7-C8-C9 |
| 26 | C | 305 | PEK | C11-C10-C9-C8 |
| 26 | C | 305 | PEK | C9-C10-C11-C12 |
| 26 | C | 305 | PEK | C11-C12-C13-C14 |
| 26 | C | 305 | PEK | C12-C13-C14-C15 |
| 26 | P | 303 | PEK | C6-C7-C8-C9 |
| 26 | P | 303 | PEK | C11-C10-C9-C8 |
| 26 | P | 303 | PEK | C11-C12-C13-C14 |
| 26 | P | 303 | PEK | C12-C13-C14-C15 |
| 26 | P | 304 | PEK | C9-C10-C11-C12 |
| 26 | P | 304 | PEK | C12-C13-C14-C15 |
| 26 | T | 101 | PEK | C11-C10-C9-C8 |
| 26 | T | 101 | PEK | C9-C10-C11-C12 |
| 26 | T | 101 | PEK | C12-C13-C14-C15 |
| 18 | A | 606 | TGL | OA1-CA1-OG1-CG1 |
| 27 | T | 102 | CDL | C71-CB7-OB8-CB6 |
| 18 | A | 606 | TGL | C13-C14-C29-C30 |
| 23 | Q | 201 | DMU | C28-C31-C34-C37 |
| 27 | C | 308 | CDL | C64-C65-C66-C67 |
| 18 | L | 101 | TGL | CC4-CC5-CC6-CC7 |
| 19 | P | 305 | PGV | C24-C25-C26-C27 |
| 27 | T | 102 | CDL | C43-C44-C45-C46 |
| 22 | A | 614 | EDO | O1-C1-C2-O2 |
| 22 | A | 619 | EDO | O1-C1-C2-O2 |
| 22 | A | 620 | EDO | O1-C1-C2-O2 |
| 19 | C | 307 | PGV | C6-C7-C8-C9 |
| 18 | N | 608 | TGL | C33-C34-C35-C36 |
| 18 | L | 101 | TGL | C10-C11-C12-C13 |
| 18 | A | 607 | TGL | CA6-CA7-CA8-CA9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | L | 101 | TGL | CB3-CB4-CB5-CB6 |
| 18 | N | 607 | TGL | C21-C20-CA9-CA8 |
| 23 | D | 206 | DMU | C34-C37-C40-C43 |
| 18 | A | 607 | TGL | C18-C19-C33-C34 |
| 26 | P | 304 | PEK | C22-C23-C24-C25 |
| 18 | N | 608 | TGL | C11-C12-C13-C14 |
| 19 | A | 608 | PGV | C2-C3-C4-C5 |
| 21 | A | 610 | PSC | C26-C27-C28-C29 |
| 27 | N | 601 | CDL | C62-C63-C64-C65 |
| 18 | N | 607 | TGL | CA2-CA3-CA4-CA5 |
| 18 | N | 608 | TGL | CA9-C20-C21-C22 |
| 18 | L | 101 | TGL | OA1-CA1-OG1-CG1 |
| 19 | P | 305 | PGV | C02-C03-O11-P |
| 27 | T | 102 | CDL | OB9-CB7-OB8-CB6 |
| 18 | A | 606 | TGL | C20-C21-C22-C23 |
| 18 | N | 608 | TGL | C10-C11-C12-C13 |
| 18 | N | 609 | TGL | CA7-CA8-CA9-C20 |
| 18 | L | 101 | TGL | C24-C25-C26-C27 |
| 18 | A | 607 | TGL | OG1-CG1-CG2-OG2 |
| 18 | L | 101 | TGL | OG2-CG2-CG3-OG3 |
| 18 | A | 607 | TGL | OC1-CC1-OG3-CG3 |
| 18 | A | 606 | TGL | OC1-CC1-OG3-CG3 |
| 21 | A | 610 | PSC | C27-C28-C29-C30 |
| 18 | A | 607 | TGL | CB1-CB2-CB3-CB4 |
| 26 | C | 303 | PEK | C03-O11-P-O12 |
| 23 | M | 101 | DMU | C25-C28-C31-C34 |
| 19 | C | 306 | PGV | C02-C03-O11-P |
| 19 | N | 610 | PGV | C04-O12-P-O14 |
| 26 | T | 101 | PEK | C5-C6-C7-C8 |
| 19 | P | 306 | PGV | C7-C8-C9-C10 |
| 26 | P | 304 | PEK | O12-C04-C05-N |
| 22 | F | 108 | EDO | O1-C1-C2-O2 |
| 23 | P | 317 | DMU | C18-C19-C22-C25 |
| 26 | T | 101 | PEK | C28-C29-C30-C31 |
| 26 | C | 304 | PEK | C16-C17-C18-C19 |
| 19 | N | 612 | PGV | C27-C28-C29-C30 |
| 27 | C | 308 | CDL | C76-C77-C78-C79 |
| 18 | L | 101 | TGL | CA6-CA7-CA8-CA9 |
| 23 | X | 102 | DMU | C34-C37-C40-C43 |
| 18 | A | 607 | TGL | CB3-CB4-CB5-CB6 |
| 18 | L | 101 | TGL | CG1-CG2-CG3-OG3 |
| 18 | N | 607 | TGL | C13-C14-C29-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 18 | N | 607 | TGL | CG1-CG2-CG3-OG3 |
| 18 | L | 101 | TGL | OG1-CG1-CG2-OG2 |
| 18 | N | 607 | TGL | OG2-CG2-CG3-OG3 |
| 27 | P | 307 | CDL | C42-C43-C44-C45 |
| 27 | P | 307 | CDL | C13-C14-C15-C16 |
| 18 | L | 101 | TGL | CC2-CC3-CC4-CC5 |
| 26 | C | 304 | PEK | C26-C27-C28-C29 |
| 27 | N | 601 | CDL | C36-C37-C38-C39 |
| 19 | C | 306 | PGV | C22-C23-C24-C25 |
| 18 | L | 101 | TGL | C11-C12-C13-C14 |
| 23 | K | 102 | DMU | C28-C31-C34-C37 |
| 23 | K | 101 | DMU | C34-C37-C40-C43 |
| 23 | D | 207 | DMU | C28-C31-C34-C37 |
| 18 | L | 101 | TGL | C17-C18-C19-C33 |
| 19 | N | 610 | PGV | C01-C02-O01-C1 |
| 27 | P | 307 | CDL | C72-C73-C74-C75 |
| 18 | N | 607 | TGL | C16-C17-C18-C19 |
| 23 | X | 101 | DMU | C28-C31-C34-C37 |
| 18 | L | 101 | TGL | CA1-CA2-CA3-CA4 |
| 22 | A | 617 | EDO | O1-C1-C2-O2 |
| 22 | A | 618 | EDO | O1-C1-C2-O2 |
| 22 | C | 320 | EDO | O1-C1-C2-O2 |
| 22 | E | 202 | EDO | O1-C1-C2-O2 |
| 23 | J | 104 | DMU | C28-C31-C34-C37 |
| 19 | A | 611 | PGV | C11-C12-C13-C14 |
| 23 | P | 317 | DMU | C1-C6-O16-C18 |
| 19 | C | 306 | PGV | C26-C27-C28-C29 |
| 18 | A | 606 | TGL | C19-C33-C34-C35 |
| 23 | K | 102 | DMU | C22-C25-C28-C31 |
| 25 | Y | 102 | CHD | C16-C17-C20-C22 |
| 27 | T | 102 | CDL | CB3-CB4-CB6-OB8 |
| 27 | P | 307 | CDL | C17-C18-C19-C20 |
| 23 | P | 308 | DMU | C25-C28-C31-C34 |
| 27 | P | 307 | CDL | C12-C13-C14-C15 |
| 18 | L | 101 | TGL | C22-C23-C24-C25 |
| 27 | C | 308 | CDL | C38-C39-C40-C41 |
| 18 | N | 609 | TGL | C20-C21-C22-C23 |
| 19 | C | 307 | PGV | C11-C12-C13-C14 |
| 26 | C | 305 | PEK | C3-C4-C5-C6 |
| 19 | N | 612 | PGV | C26-C27-C28-C29 |
| 23 | D | 207 | DMU | C18-C19-C22-C25 |
| 27 | C | 308 | CDL | C41-C42-C43-C44 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 19 | C | 307 | PGV | C22-C23-C24-C25 |
| 23 | Q | 201 | DMU | C31-C34-C37-C40 |
| 18 | N | 608 | TGL | CB6-CB7-CB8-CB9 |
| 23 | X | 102 | DMU | C22-C25-C28-C31 |
| 25 | Y | 102 | CHD | C16-C17-C20-C21 |
| 26 | T | 101 | PEK | C32-C33-C34-C35 |
| 18 | N | 607 | TGL | CA6-CA7-CA8-CA9 |
| 18 | L | 101 | TGL | OA1-CA1-CA2-CA3 |
| 27 | P | 307 | CDL | C78-C79-C80-C81 |
| 19 | A | 608 | PGV | C11-C12-C13-C14 |
| 19 | C | 306 | PGV | C11-C12-C13-C14 |
| 21 | A | 610 | PSC | C12-C13-C14-C15 |
| 23 | D | 206 | DMU | C28-C31-C34-C37 |
| 18 | N | 607 | TGL | CA3-CA4-CA5-CA6 |
| 18 | A | 606 | TGL | CA7-CA8-CA9-C20 |
| 23 | Z | 101 | DMU | O6-C11-C9-O1 |
| 18 | A | 607 | TGL | OG1-CG1-CG2-CG3 |
| 19 | N | 612 | PGV | C11-C12-C13-C14 |
| 26 | C | 304 | PEK | C4-C5-C6-C7 |
| 23 | P | 317 | DMU | O5-C6-O16-C18 |
| 18 | N | 607 | TGL | C15-C16-C17-C18 |
| 21 | A | 610 | PSC | C30-C31-C32-C33 |
| 27 | N | 601 | CDL | C72-C73-C74-C75 |
| 26 | C | 304 | PEK | C11-C12-C13-C14 |
| 26 | P | 303 | PEK | C9-C10-C11-C12 |
| 26 | P | 304 | PEK | C11-C12-C13-C14 |
| 18 | L | 101 | TGL | CC6-CC7-CC8-CC9 |
| 27 | T | 102 | CDL | C59-C60-C61-C62 |
| 23 | X | 104 | DMU | O5-C4-C57-O61 |
| 18 | N | 608 | TGL | C18-C19-C33-C34 |
| 19 | C | 306 | PGV | C24-C25-C26-C27 |
| 27 | N | 601 | CDL | C31-C32-C33-C34 |
| 18 | N | 609 | TGL | CC3-CC4-CC5-CC6 |
| 23 | P | 316 | DMU | C34-C37-C40-C43 |
| 18 | A | 607 | TGL | C24-C25-C26-C27 |
| 19 | C | 306 | PGV | C1-C2-C3-C4 |
| 27 | C | 308 | CDL | CB6-CB4-OB6-CB5 |
| 22 | M | 102 | EDO | O1-C1-C2-O2 |
| 22 | T | 105 | EDO | O1-C1-C2-O2 |
| 23 | C | 310 | DMU | C28-C31-C34-C37 |
| 27 | P | 307 | CDL | C43-C44-C45-C46 |
| 23 | K | 104 | DMU | C18-C19-C22-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 19 | A | 608 | PGV | C22-C23-C24-C25 |
| 14 | N | 603 | HEA | C26-C15-C16-C17 |
| 19 | A | 611 | PGV | O03-C19-C20-C21 |
| 18 | N | 608 | TGL | CC2-CC3-CC4-CC5 |
| 19 | C | 306 | PGV | C9-C10-C11-C12 |
| 19 | C | 307 | PGV | C9-C10-C11-C12 |
| 26 | C | 305 | PEK | C14-C15-C16-C17 |
| 27 | P | 307 | CDL | C52-C53-C54-C55 |
| 18 | N | 607 | TGL | CC2-CC1-OG3-CG3 |
| 26 | C | 304 | PEK | O12-C04-C05-N |
| 26 | P | 304 | PEK | C14-C15-C16-C17 |
| 18 | A | 606 | TGL | OG2-CG2-CG3-OG3 |
| 26 | P | 303 | PEK | C14-C15-C16-C17 |
| 18 | A | 606 | TGL | OG3-CC1-CC2-CC3 |
| 27 | N | 601 | CDL | OB9-CB7-OB8-CB6 |
| 18 | A | 607 | TGL | CB5-CB6-CB7-CB8 |
| 19 | C | 307 | PGV | O01-C1-C2-C3 |
| 19 | N | 610 | PGV | C9-C10-C11-C12 |
| 19 | N | 610 | PGV | C11-C12-C13-C14 |
| 21 | O | 302 | PSC | C12-C13-C14-C15 |
| 26 | C | 304 | PEK | C14-C15-C16-C17 |
| 19 | A | 611 | PGV | C26-C27-C28-C29 |
| 27 | T | 102 | CDL | C55-C56-C57-C58 |
| 23 | P | 316 | DMU | C19-C18-O16-C6 |
| 18 | N | 608 | TGL | CB3-CB4-CB5-CB6 |
| 26 | C | 304 | PEK | C34-C35-C36-C37 |
| 27 | C | 308 | CDL | C40-C41-C42-C43 |
| 26 | C | 303 | PEK | O03-C21-C22-C23 |
| 18 | A | 606 | TGL | OG1-CA1-CA2-CA3 |
| 27 | P | 307 | CDL | C58-C59-C60-C61 |
| 26 | P | 303 | PEK | C3-C4-C5-C6 |
| 19 | N | 612 | PGV | O03-C19-C20-C21 |
| 21 | A | 610 | PSC | C23-C24-C25-C26 |
| 27 | T | 102 | CDL | C17-C18-C19-C20 |
| 22 | D | 205 | EDO | O1-C1-C2-O2 |
| 22 | N | 618 | EDO | O1-C1-C2-O2 |
| 22 | P | 312 | EDO | O1-C1-C2-O2 |
| 22 | S | 106 | EDO | O1-C1-C2-O2 |
| 22 | T | 104 | EDO | O1-C1-C2-O2 |
| 18 | L | 101 | TGL | CB7-CB8-CB9-C10 |
| 27 | T | 102 | CDL | C24-C25-C26-C27 |
| 19 | P | 306 | PGV | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 27 | C | 308 | CDL | C56-C57-C58-C59 |
| 18 | N | 607 | TGL | C22-C23-C24-C25 |
| 19 | A | 608 | PGV | C9-C10-C11-C12 |
| 26 | T | 101 | PEK | C14-C15-C16-C17 |
| 18 | A | 607 | TGL | C15-C16-C17-C18 |
| 27 | P | 307 | CDL | C52-C51-CB5-OB6 |
| 26 | C | 305 | PEK | C33-C34-C35-C36 |
| 18 | N | 609 | TGL | C11-C12-C13-C14 |
| 18 | N | 608 | TGL | C24-C25-C26-C27 |
| 27 | T | 102 | CDL | C72-C71-CB7-OB8 |
| 26 | C | 303 | PEK | C23-C24-C25-C26 |
| 18 | N | 608 | TGL | CC5-CC6-CC7-CC8 |
| 18 | A | 606 | TGL | OC1-CC1-CC2-CC3 |
| 27 | P | 307 | CDL | C52-C51-CB5-OB7 |
| 18 | A | 606 | TGL | CG1-CG2-CG3-OG3 |
| 26 | C | 303 | PEK | O04-C21-C22-C23 |
| 18 | N | 609 | TGL | C16-C15-CC9-CC8 |
| 23 | J | 104 | DMU | C18-C19-C22-C25 |
| 18 | A | 606 | TGL | C24-C25-C26-C27 |
| 26 | C | 303 | PEK | C03-O11-P-O13 |
| 26 | C | 303 | PEK | C03-O11-P-O14 |
| 18 | A | 606 | TGL | OG1-CG1-CG2-OG2 |
| 18 | L | 101 | TGL | CA4-CA5-CA6-CA7 |
| 27 | C | 308 | CDL | C34-C35-C36-C37 |
| 18 | A | 606 | TGL | OA1-CA1-CA2-CA3 |
| 26 | C | 304 | PEK | O04-C21-C22-C23 |
| 19 | C | 307 | PGV | O02-C1-C2-C3 |
| 22 | D | 202 | EDO | O1-C1-C2-O2 |
| 22 | W | 102 | EDO | O1-C1-C2-O2 |
| 18 | N | 609 | TGL | C10-C11-C12-C13 |
| 18 | A | 607 | TGL | CA7-CA8-CA9-C20 |
| 19 | N | 610 | PGV | O03-C19-C20-C21 |
| 27 | T | 102 | CDL | C57-C58-C59-C60 |
| 26 | C | 304 | PEK | C30-C31-C32-C33 |
| 18 | A | 606 | TGL | C29-C30-C31-C32 |
| 19 | N | 612 | PGV | O04-C19-C20-C21 |
| 27 | T | 102 | CDL | C72-C71-CB7-OB9 |
| 18 | L | 101 | TGL | C14-C29-C30-C31 |
| 18 | N | 607 | TGL | OG3-CC1-CC2-CC3 |
| 19 | P | 306 | PGV | C9-C10-C11-C12 |
| 18 | N | 609 | TGL | C13-C14-C29-C30 |
| 23 | X | 101 | DMU | C19-C22-C25-C28 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | K | 102 | DMU | O16-C18-C19-C22 |
| 18 | A | 606 | TGL | C25-C26-C27-C28 |
| 18 | A | 607 | TGL | OG3-CC1-CC2-CC3 |

There are no ring outliers.

64 monomers are involved in 173 short contacts:

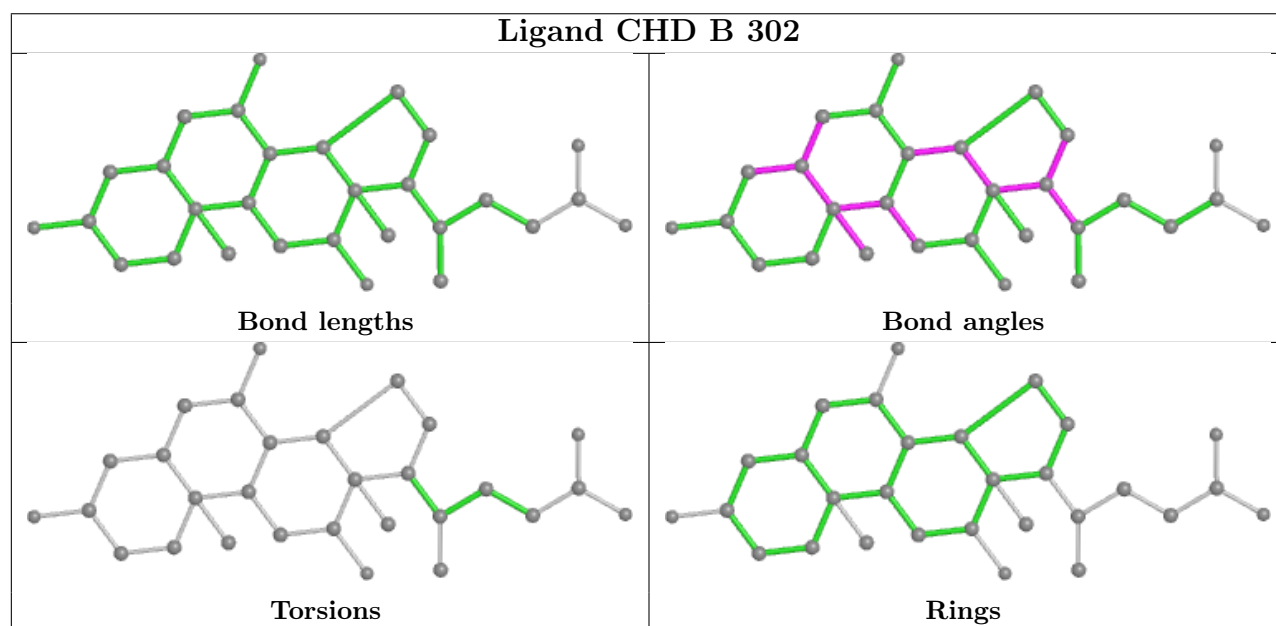
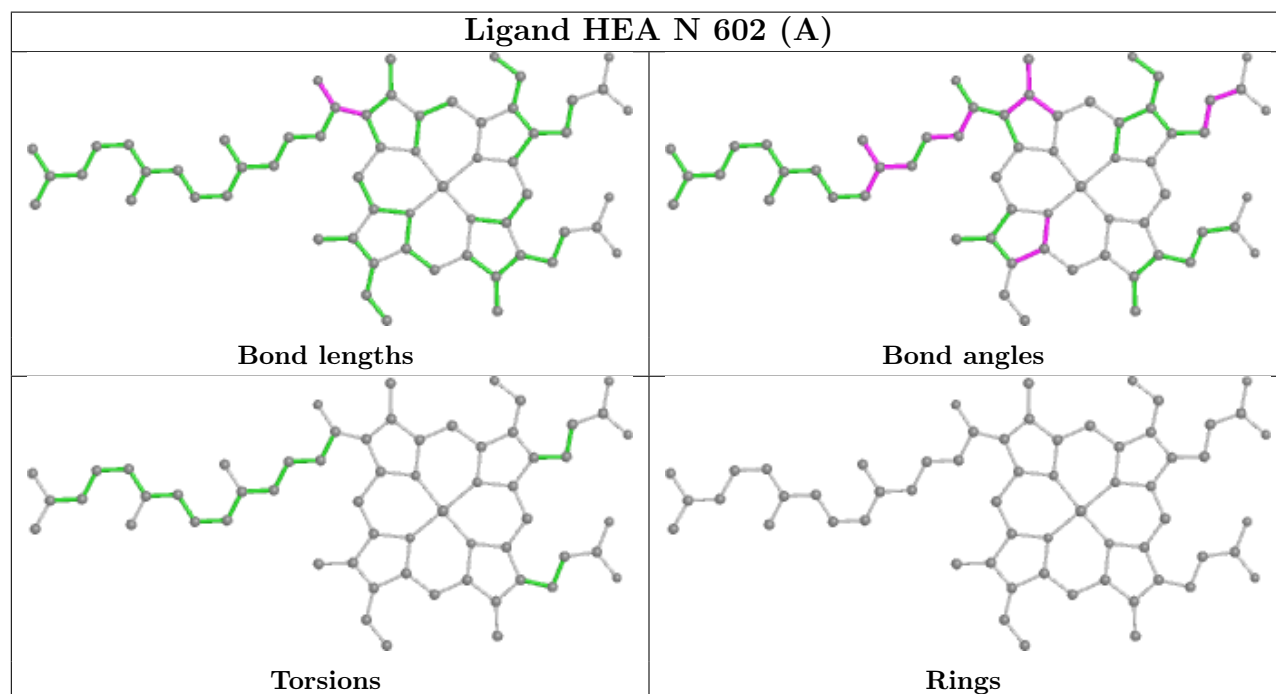
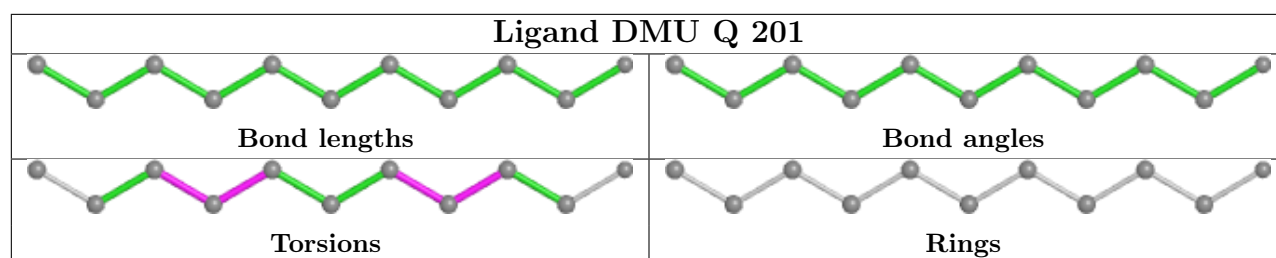
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 23 | Q | 201 | DMU | 2 | 0 |
| 14 | N | 602[A] | HEA | 2 | 0 |
| 26 | C | 303 | PEK | 1 | 0 |
| 18 | L | 101 | TGL | 15 | 0 |
| 18 | N | 608 | TGL | 7 | 0 |
| 22 | A | 612 | EDO | 2 | 0 |
| 14 | N | 603 | HEA | 5 | 0 |
| 22 | S | 106 | EDO | 1 | 0 |
| 25 | L | 102 | CHD | 2 | 0 |
| 25 | C | 309 | CHD | 2 | 0 |
| 22 | Y | 101 | EDO | 1 | 0 |
| 22 | A | 620 | EDO | 1 | 0 |
| 23 | L | 105 | DMU | 6 | 0 |
| 20 | A | 609[A] | PER | 1 | 0 |
| 14 | A | 602 | HEA | 5 | 0 |
| 22 | N | 621 | EDO | 1 | 0 |
| 27 | N | 601 | CDL | 5 | 0 |
| 18 | A | 607 | TGL | 13 | 0 |
| 19 | N | 610 | PGV | 3 | 0 |
| 23 | Z | 101 | DMU | 1 | 0 |
| 19 | A | 608 | PGV | 1 | 0 |
| 27 | T | 102 | CDL | 9 | 0 |
| 23 | D | 206 | DMU | 3 | 0 |
| 21 | O | 302 | PSC | 4 | 0 |
| 23 | X | 102 | DMU | 2 | 0 |
| 26 | C | 305 | PEK | 1 | 0 |
| 27 | C | 308 | CDL | 7 | 0 |
| 19 | C | 307 | PGV | 1 | 0 |
| 22 | N | 620 | EDO | 1 | 0 |
| 21 | A | 610 | PSC | 3 | 0 |
| 26 | C | 304 | PEK | 5 | 0 |
| 23 | M | 101 | DMU | 2 | 0 |
| 22 | A | 618 | EDO | 1 | 0 |
| 19 | C | 306 | PGV | 2 | 0 |

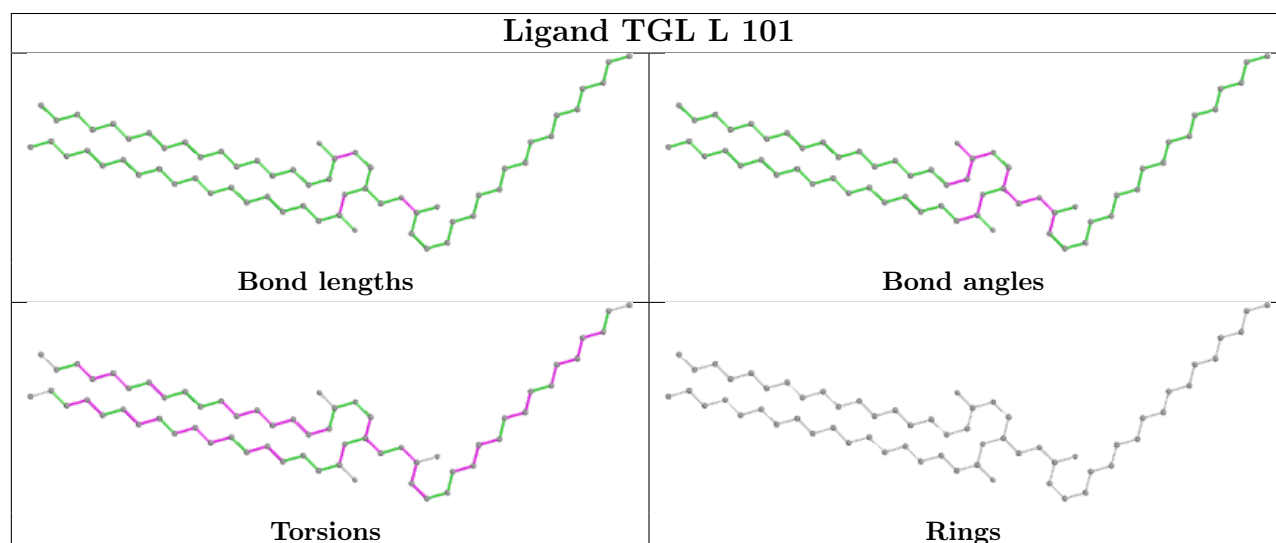
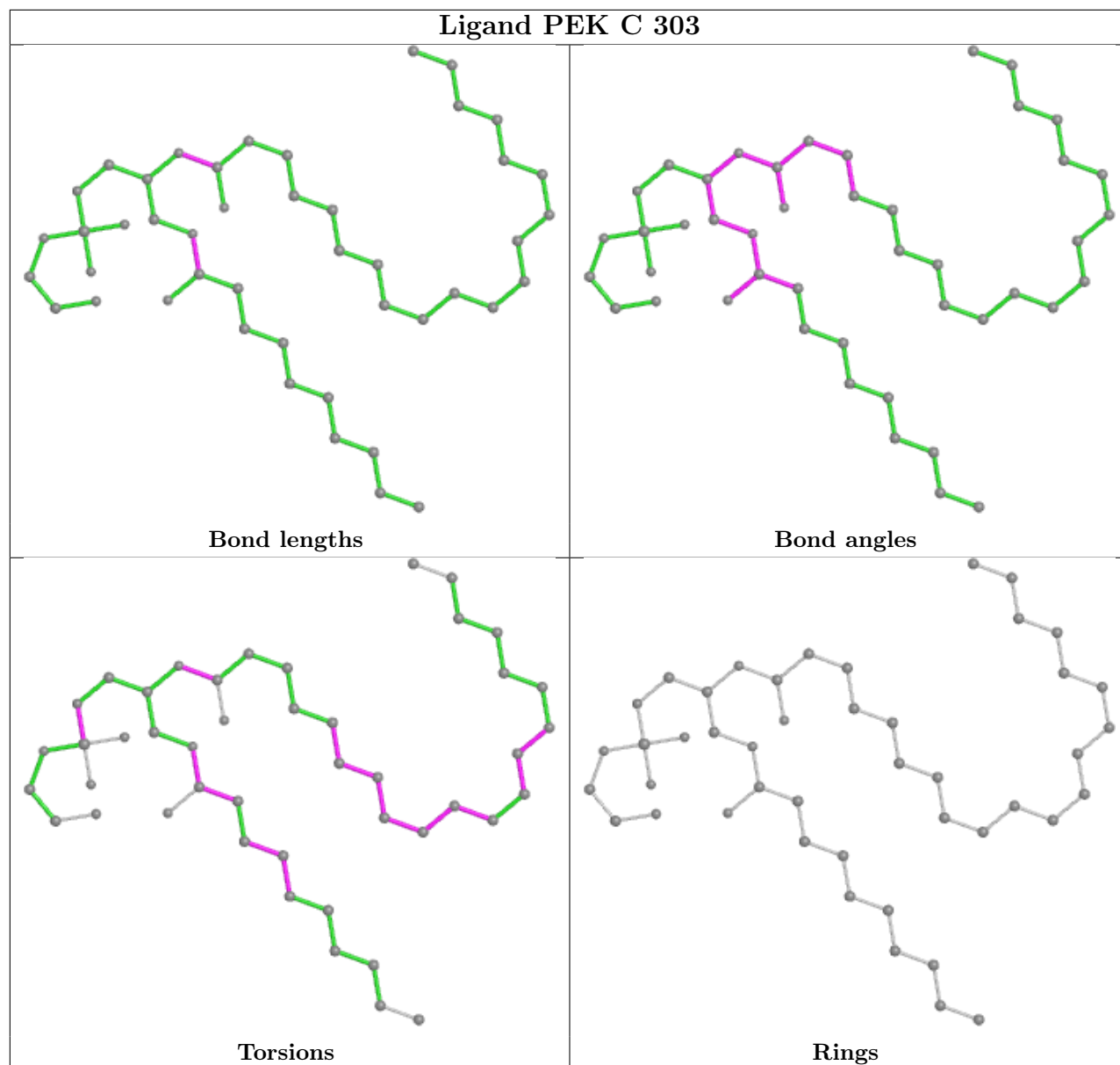
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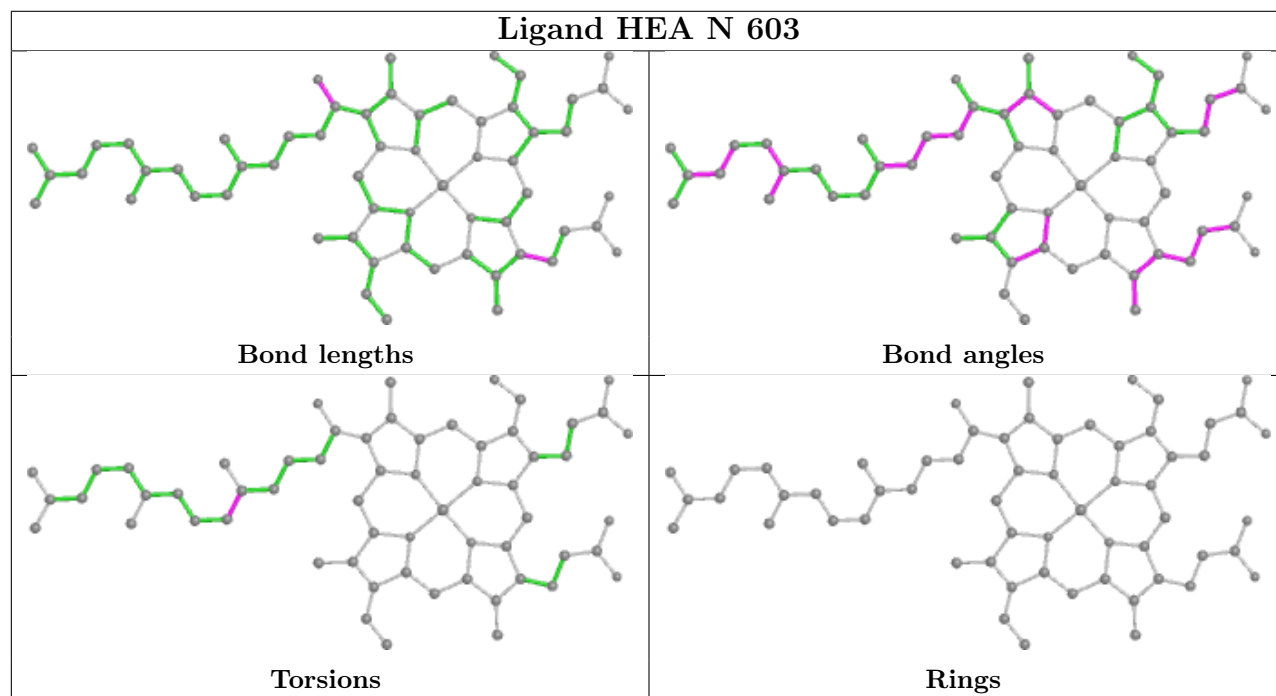
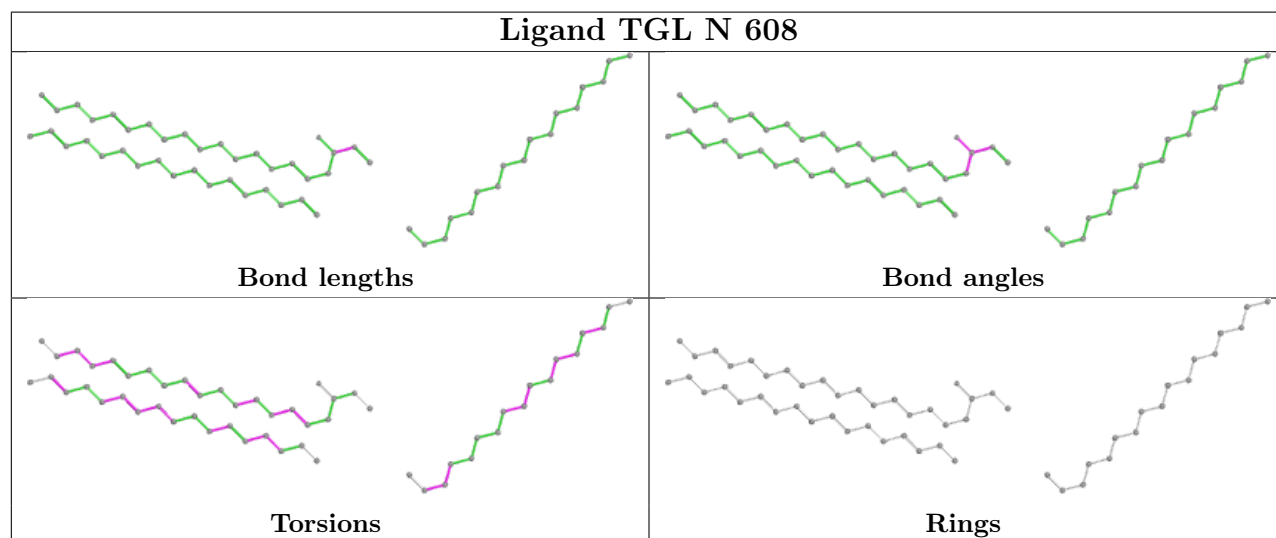
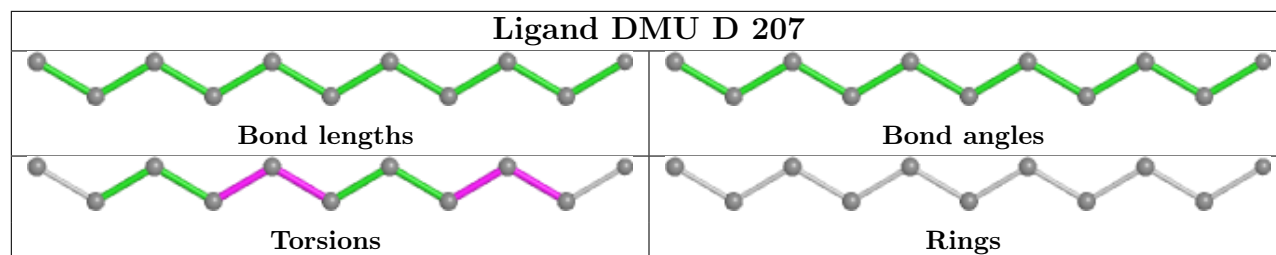
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 25 | J | 101 | CHD | 2 | 0 |
| 19 | P | 306 | PGV | 1 | 0 |
| 19 | P | 305 | PGV | 1 | 0 |
| 22 | A | 616 | EDO | 1 | 0 |
| 23 | K | 101 | DMU | 1 | 0 |
| 14 | A | 601[C] | HEA | 1 | 0 |
| 18 | N | 609 | TGL | 1 | 0 |
| 22 | C | 318 | EDO | 1 | 0 |
| 23 | C | 310 | DMU | 3 | 0 |
| 20 | N | 611[A] | PER | 1 | 0 |
| 14 | A | 601[B] | HEA | 1 | 0 |
| 23 | J | 104 | DMU | 1 | 0 |
| 26 | P | 304 | PEK | 2 | 0 |
| 18 | N | 607 | TGL | 3 | 0 |
| 14 | N | 602[C] | HEA | 2 | 0 |
| 23 | P | 308 | DMU | 3 | 0 |
| 23 | P | 316 | DMU | 2 | 0 |
| 19 | A | 611 | PGV | 1 | 0 |
| 22 | C | 315 | EDO | 1 | 0 |
| 22 | D | 204 | EDO | 3 | 0 |
| 14 | N | 602[B] | HEA | 1 | 0 |
| 27 | P | 307 | CDL | 7 | 0 |
| 25 | G | 101 | CHD | 1 | 0 |
| 26 | T | 101 | PEK | 6 | 0 |
| 19 | N | 612 | PGV | 1 | 0 |
| 18 | A | 606 | TGL | 4 | 0 |
| 22 | D | 205 | EDO | 2 | 0 |
| 14 | A | 601[A] | HEA | 2 | 0 |
| 23 | K | 102 | DMU | 1 | 0 |
| 23 | K | 103 | DMU | 1 | 0 |

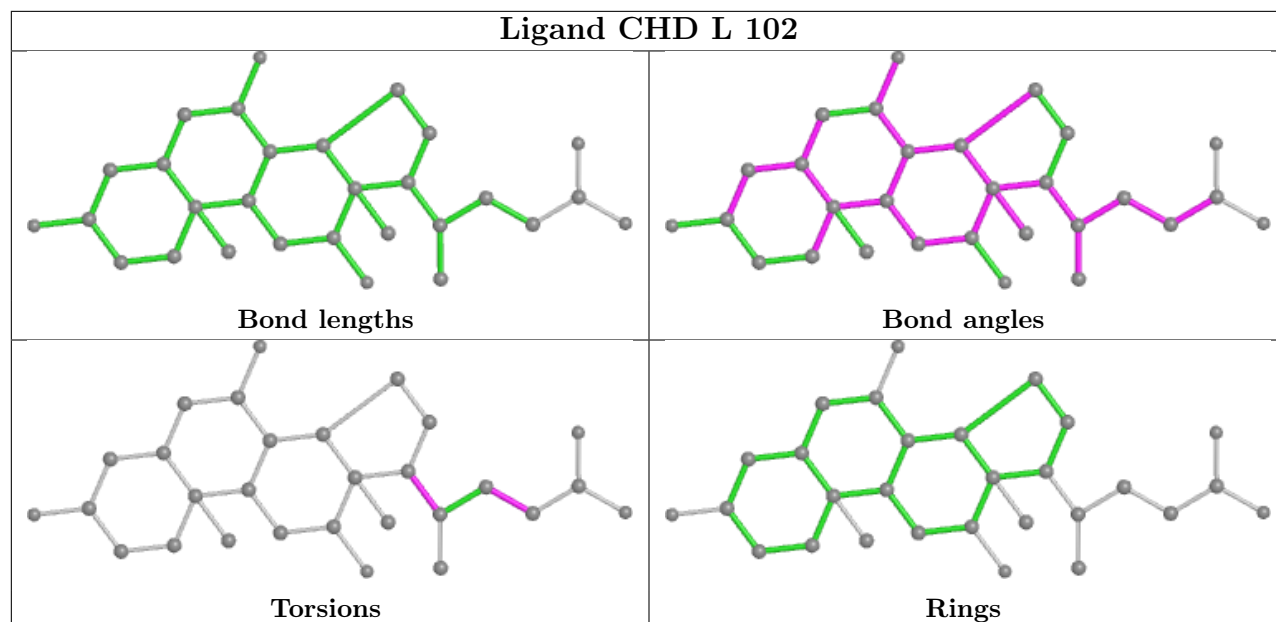
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



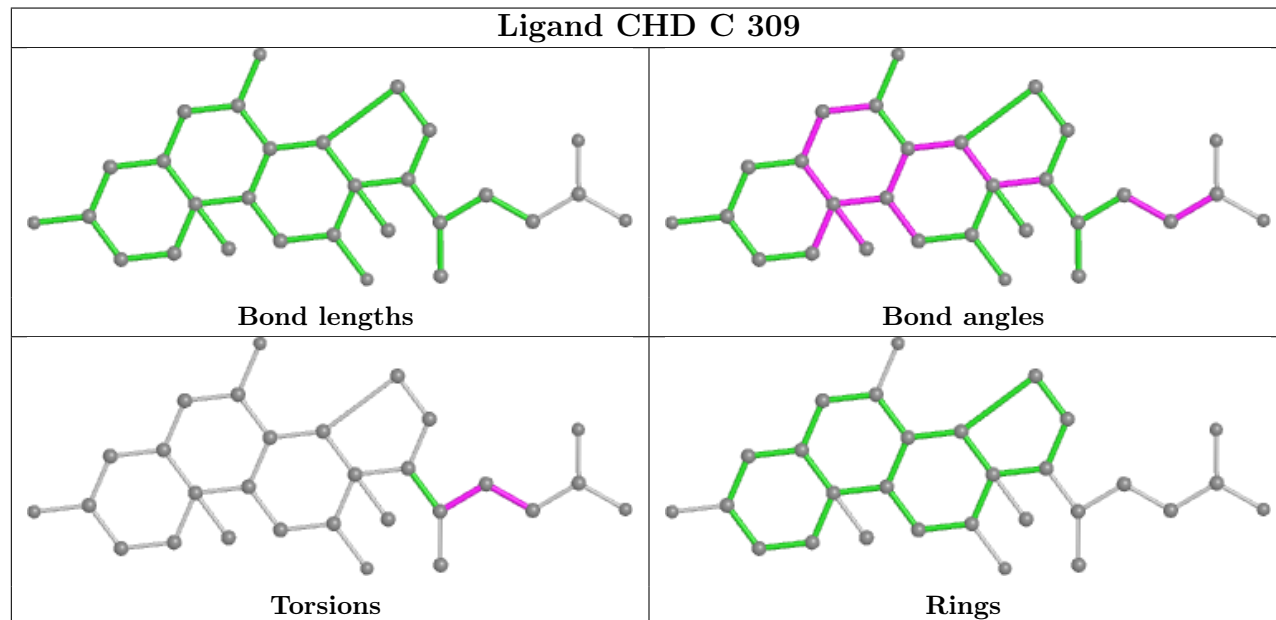


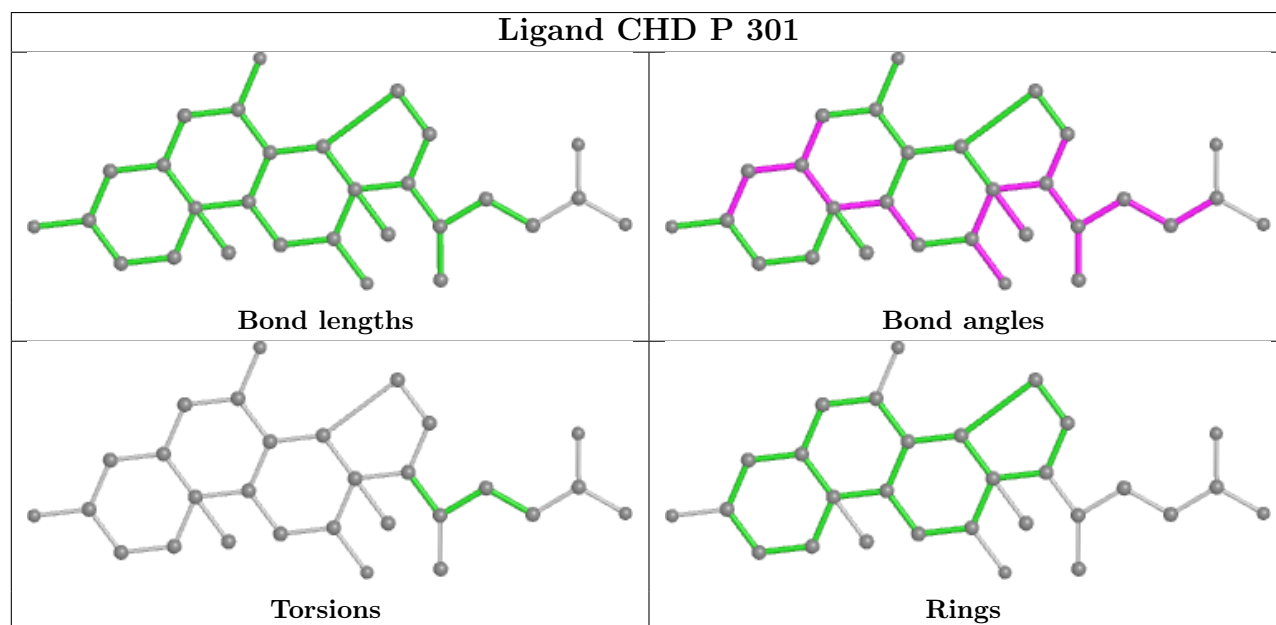
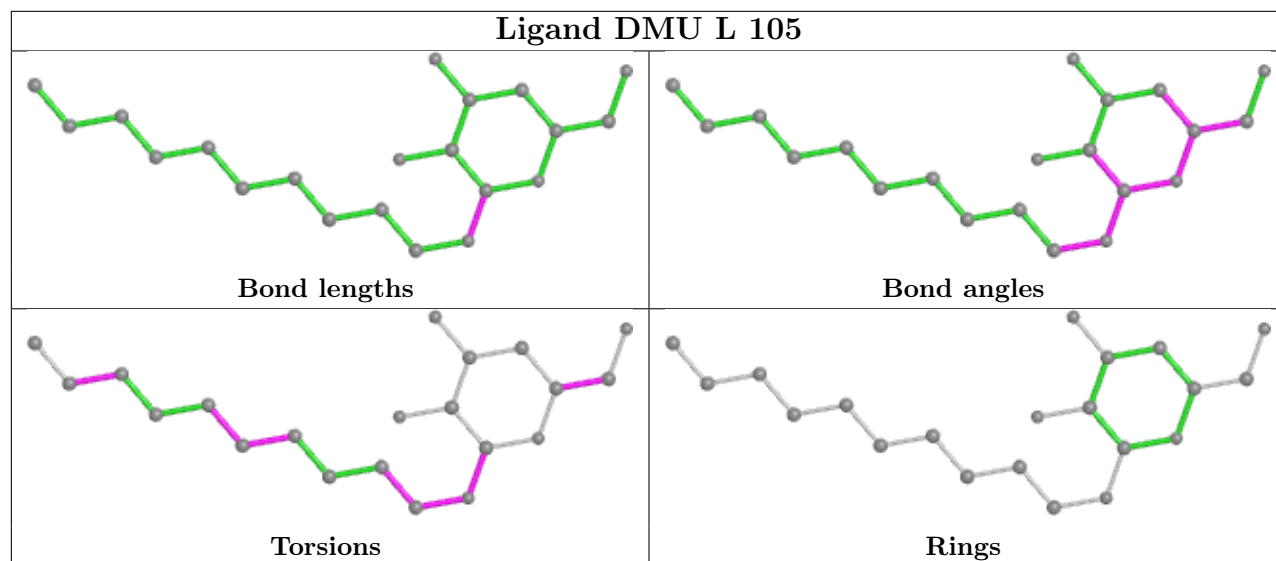


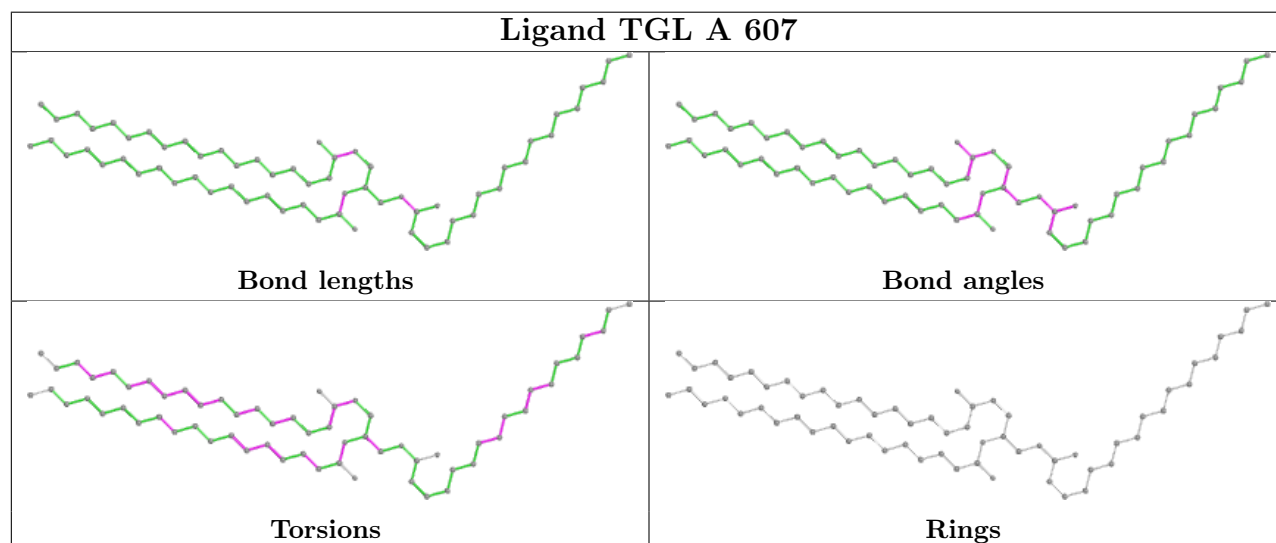
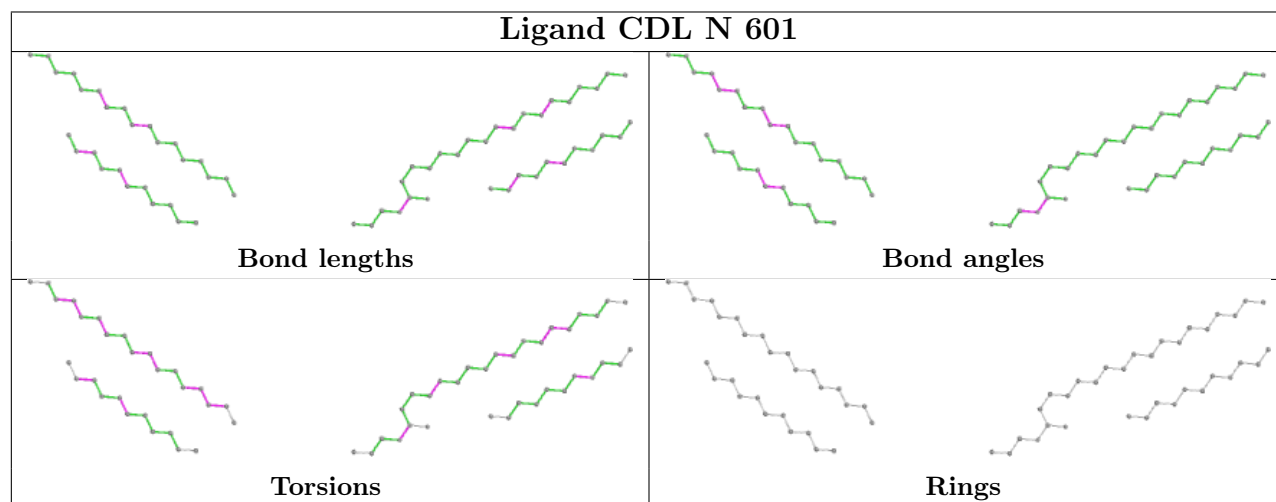
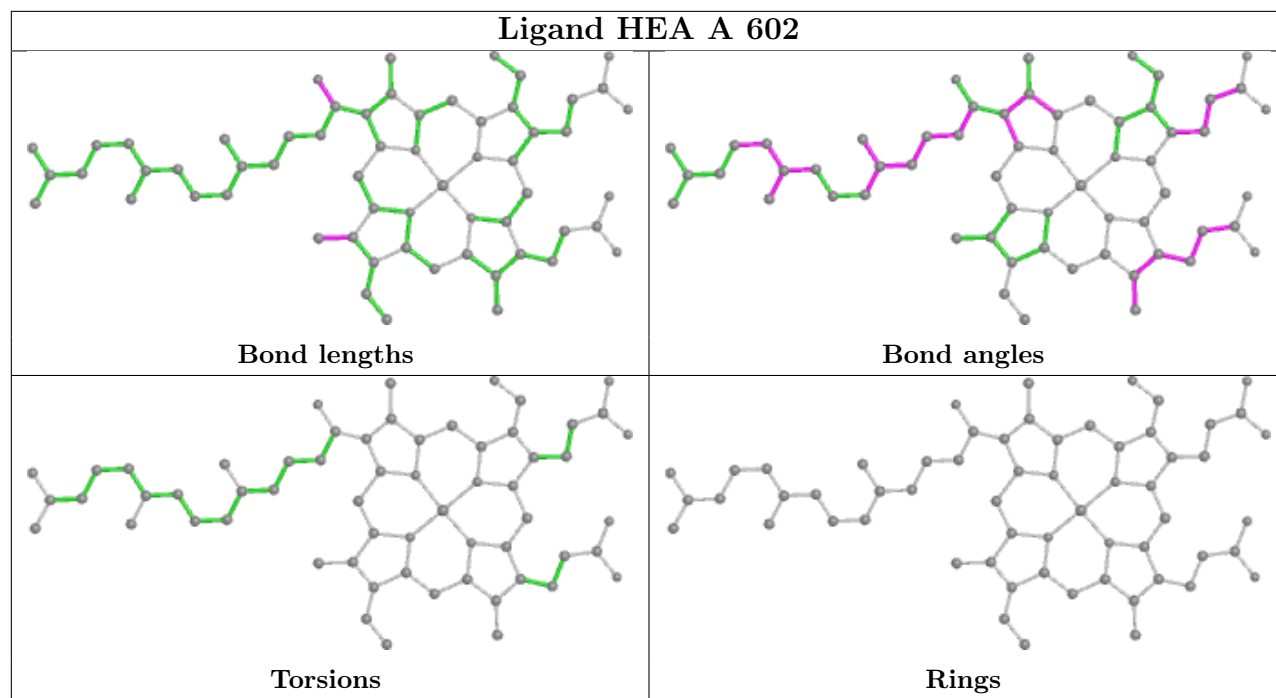
Ligand CHD L 102

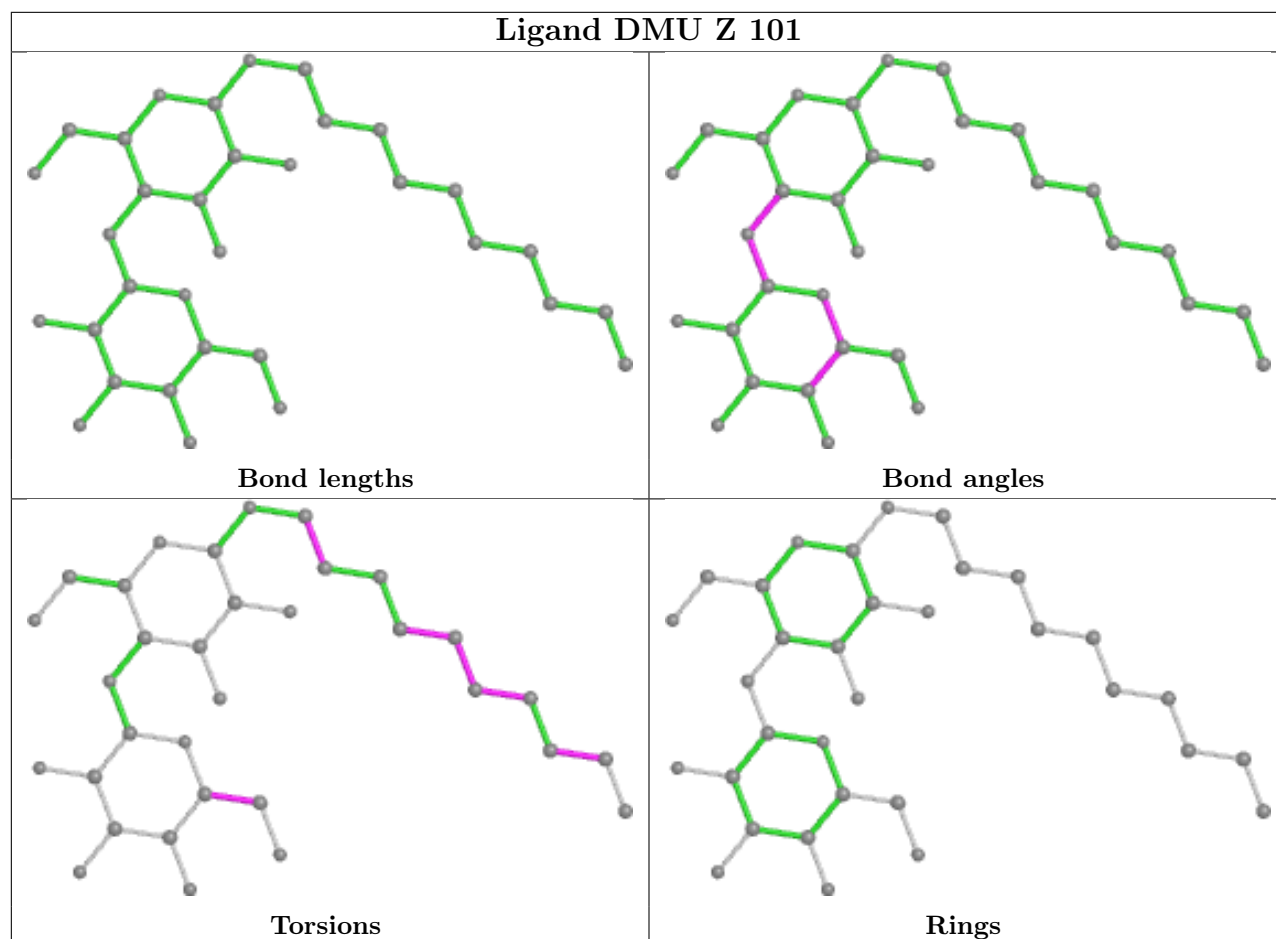
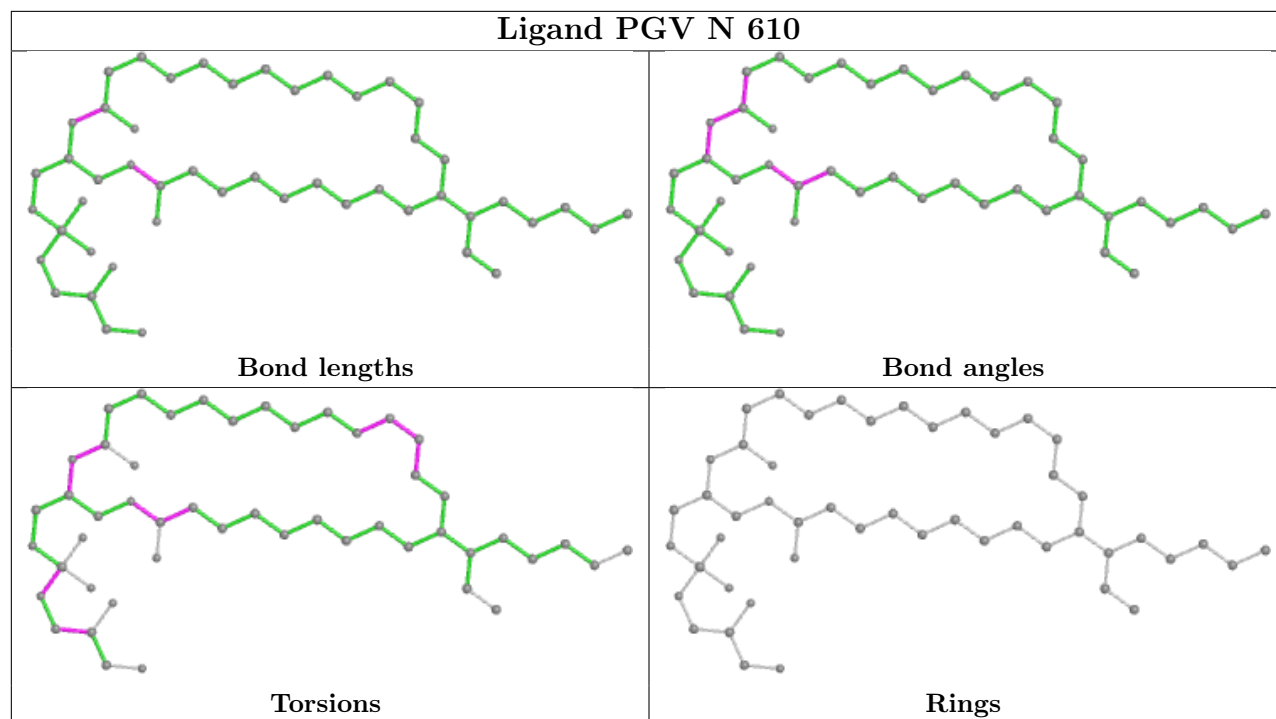


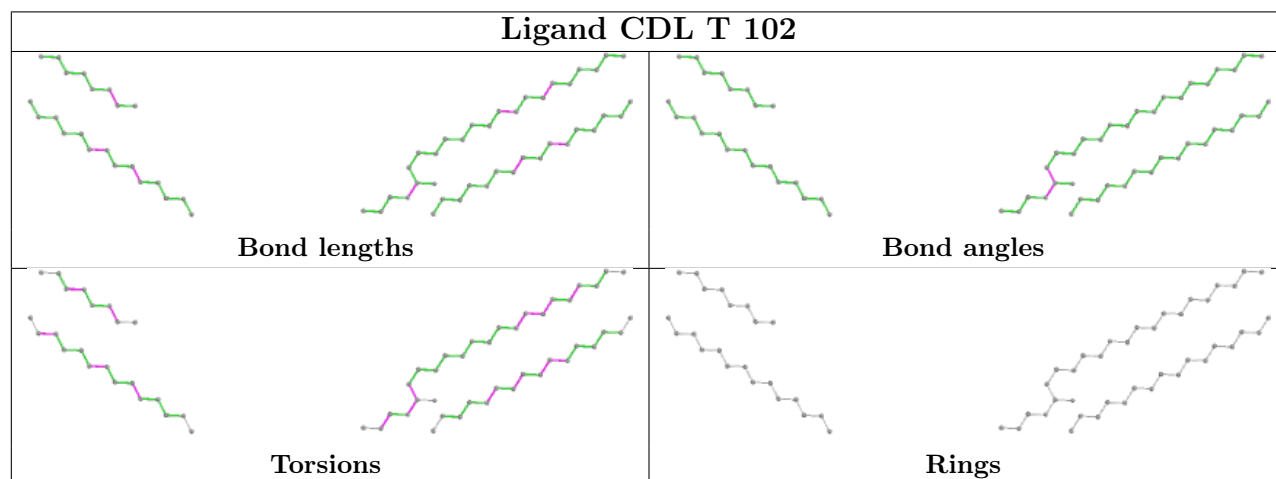
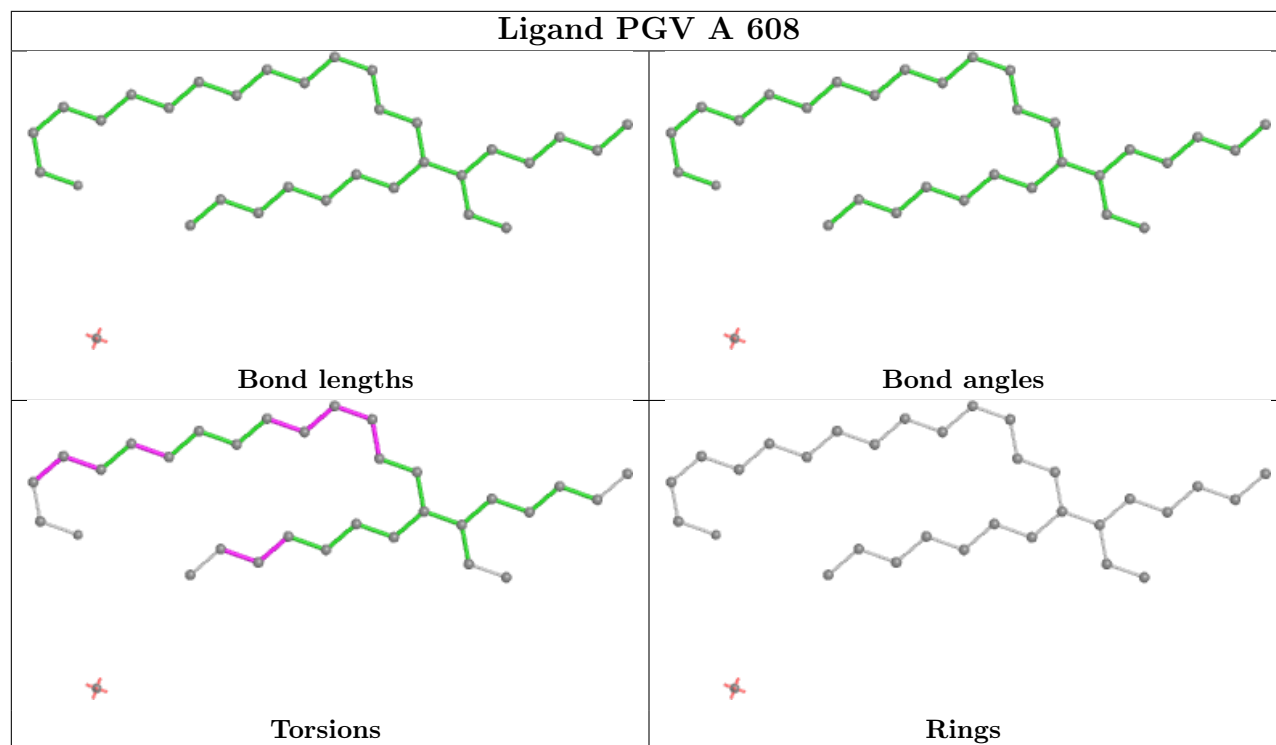
Ligand CHD C 309



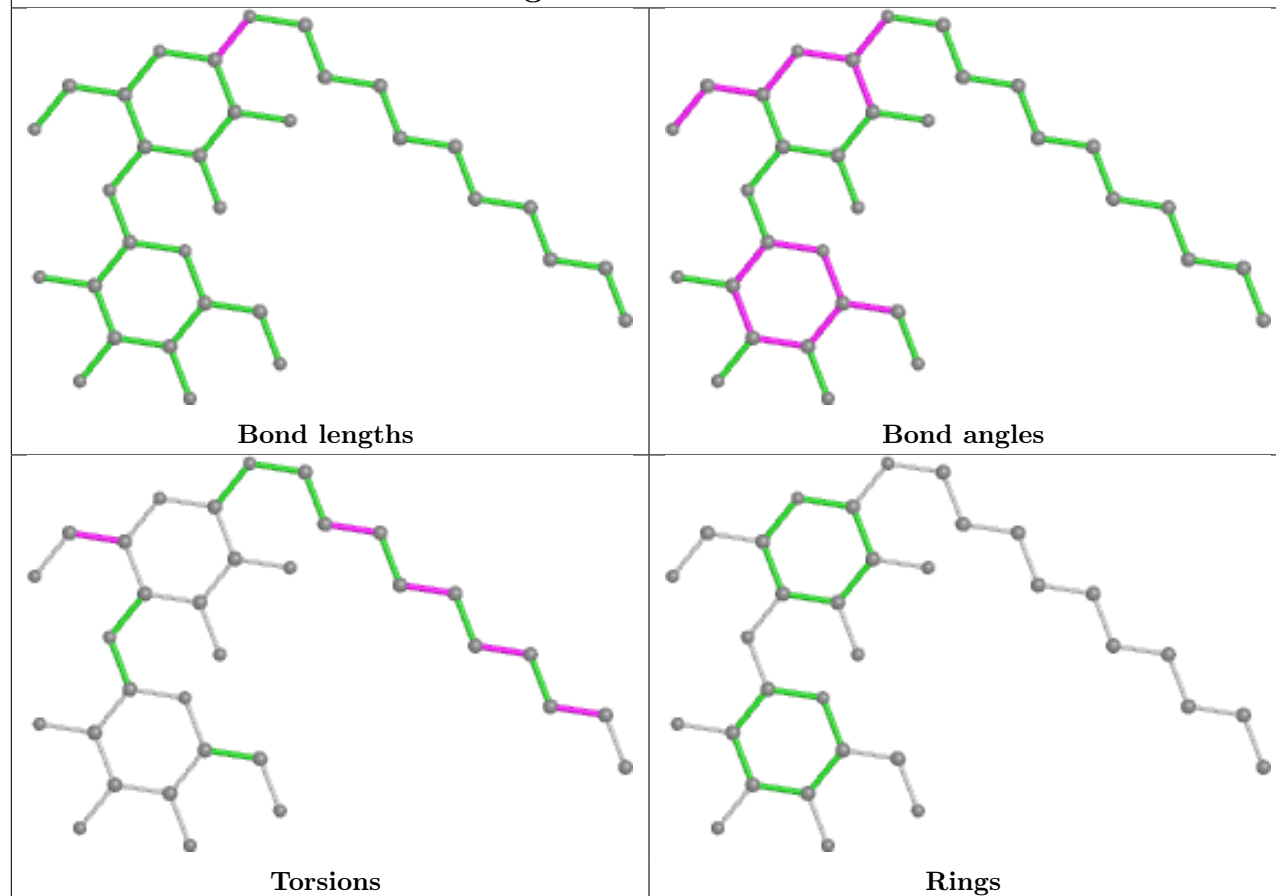




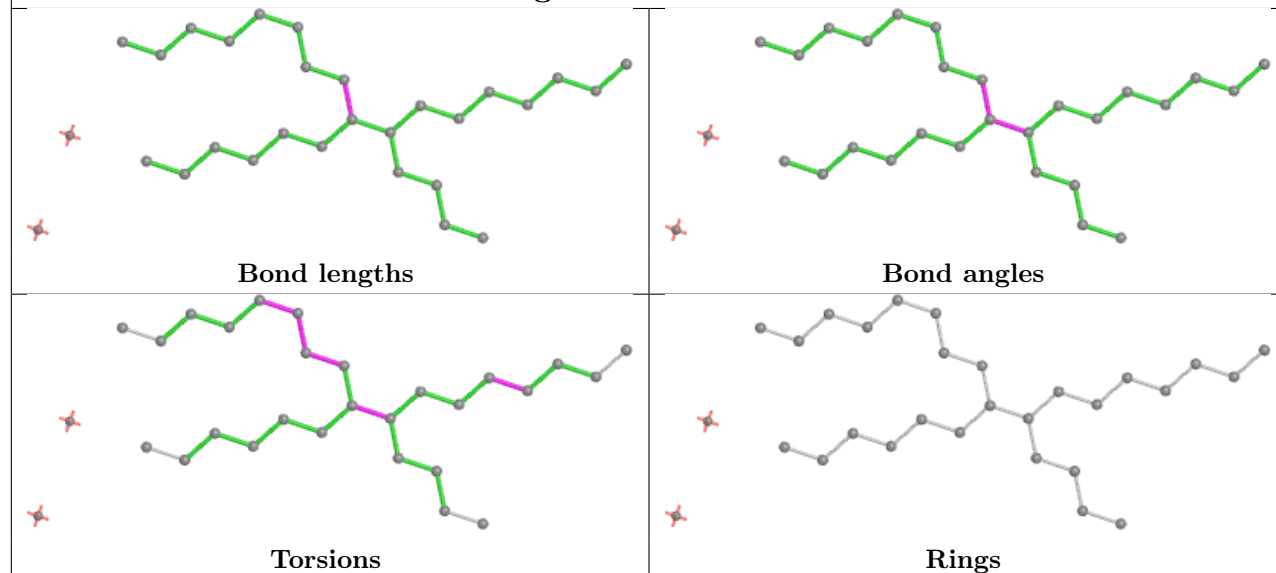


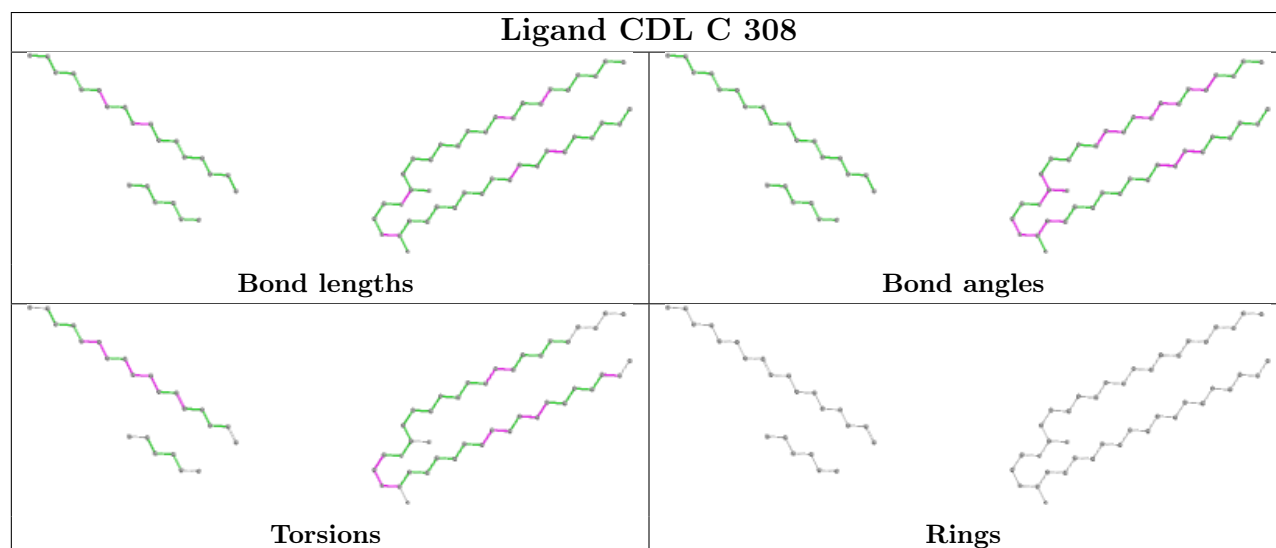
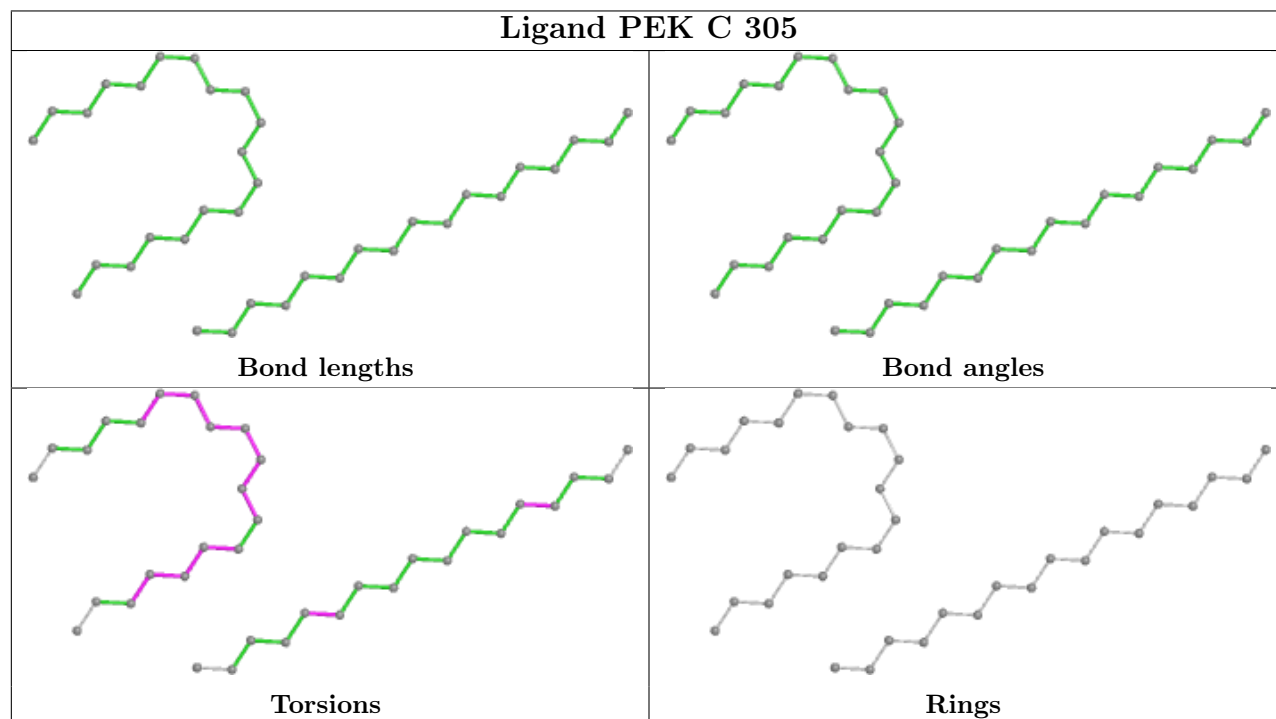
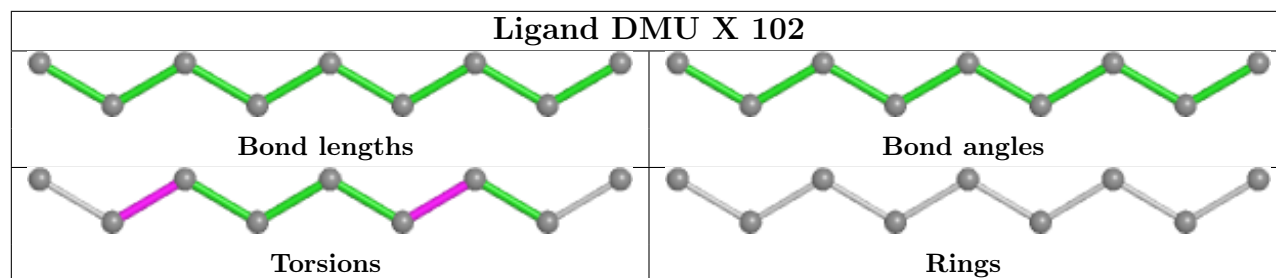


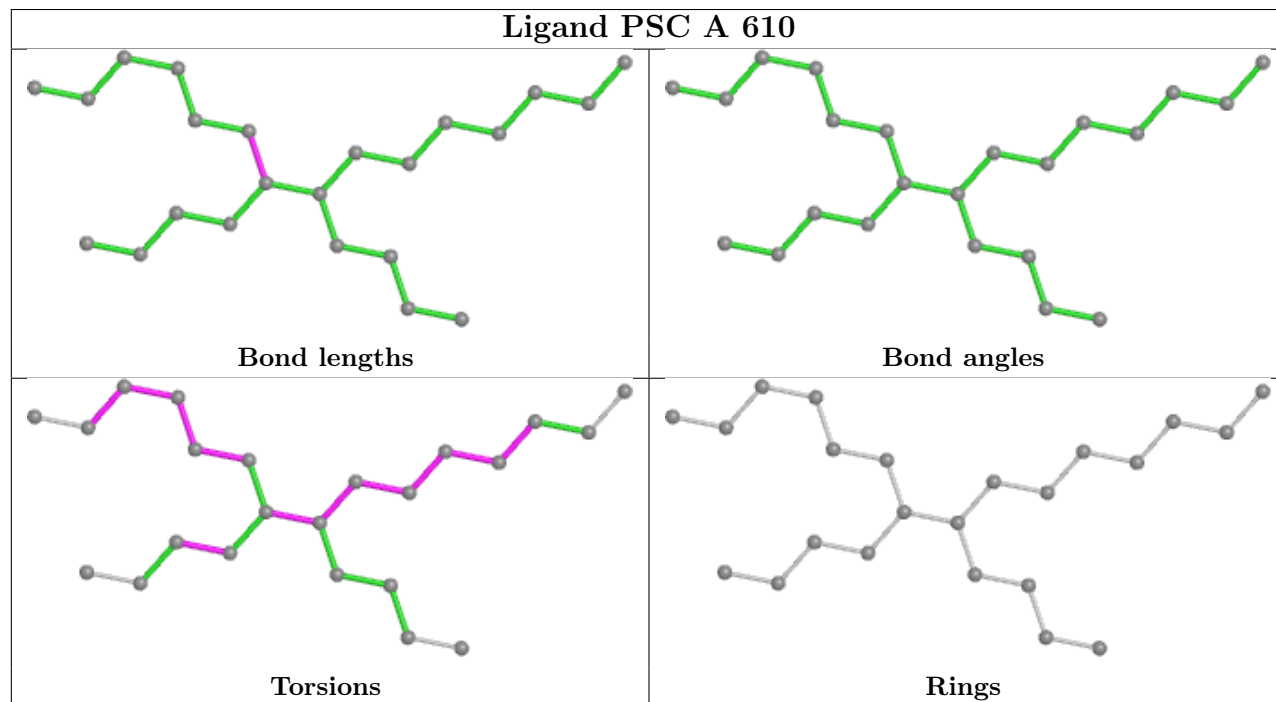
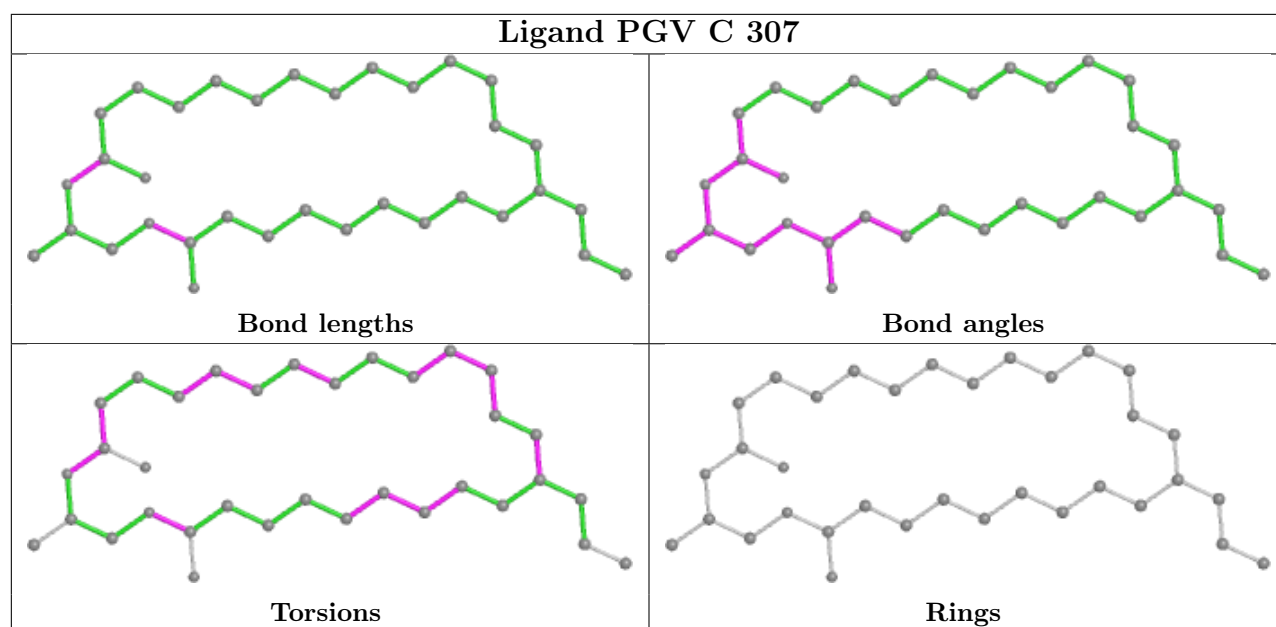
Ligand DMU D 206

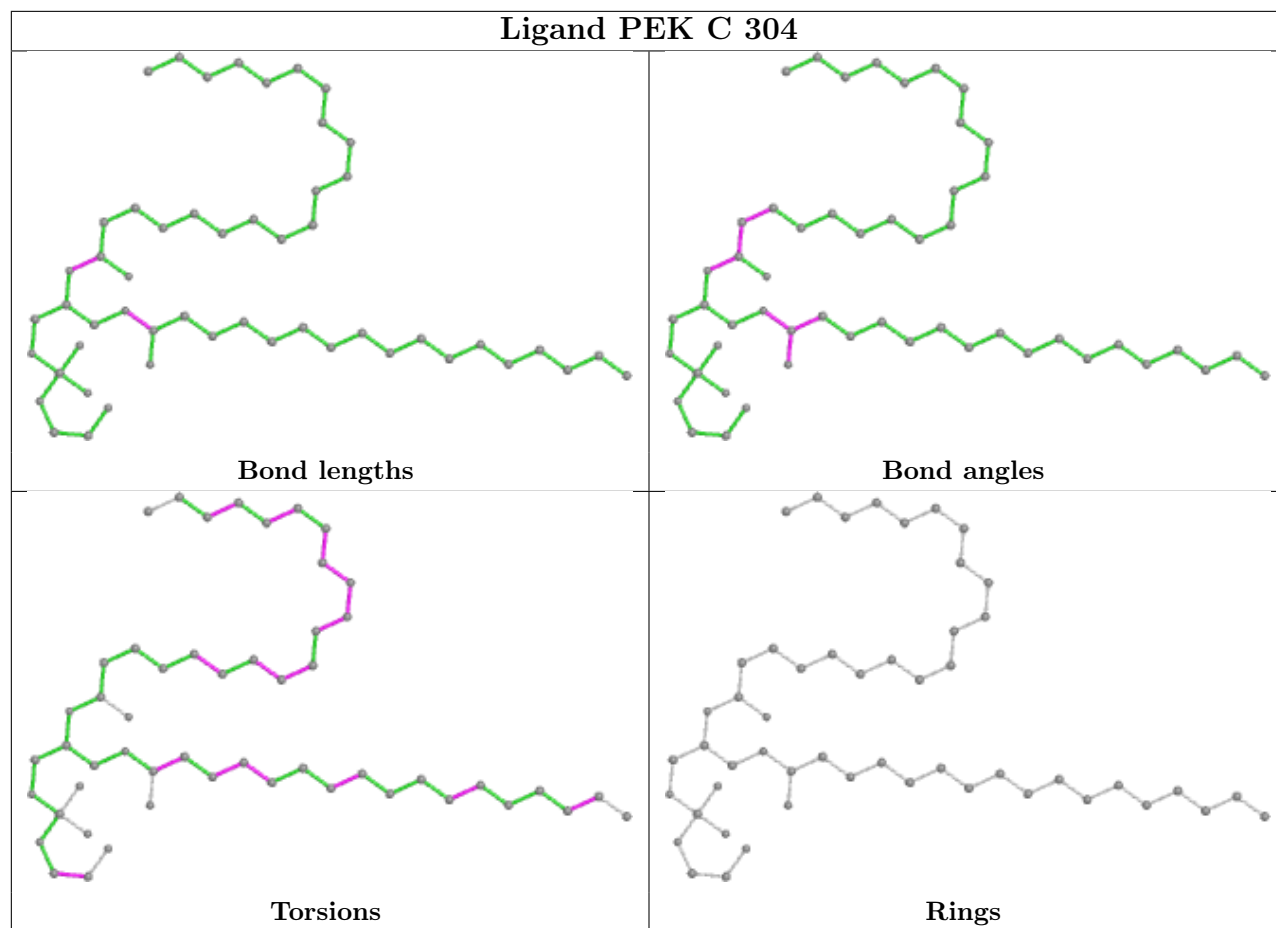


Ligand PSC O 302

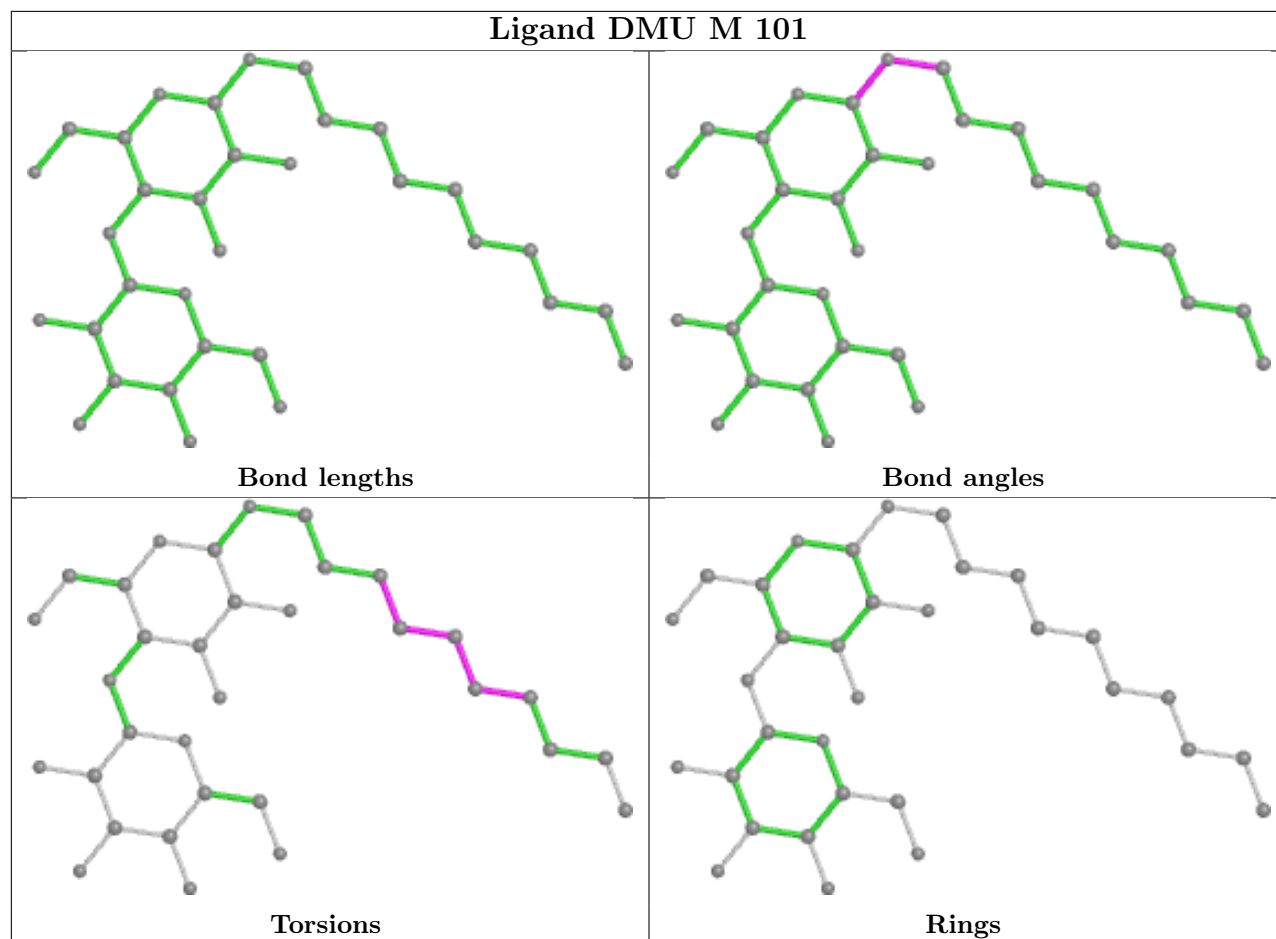




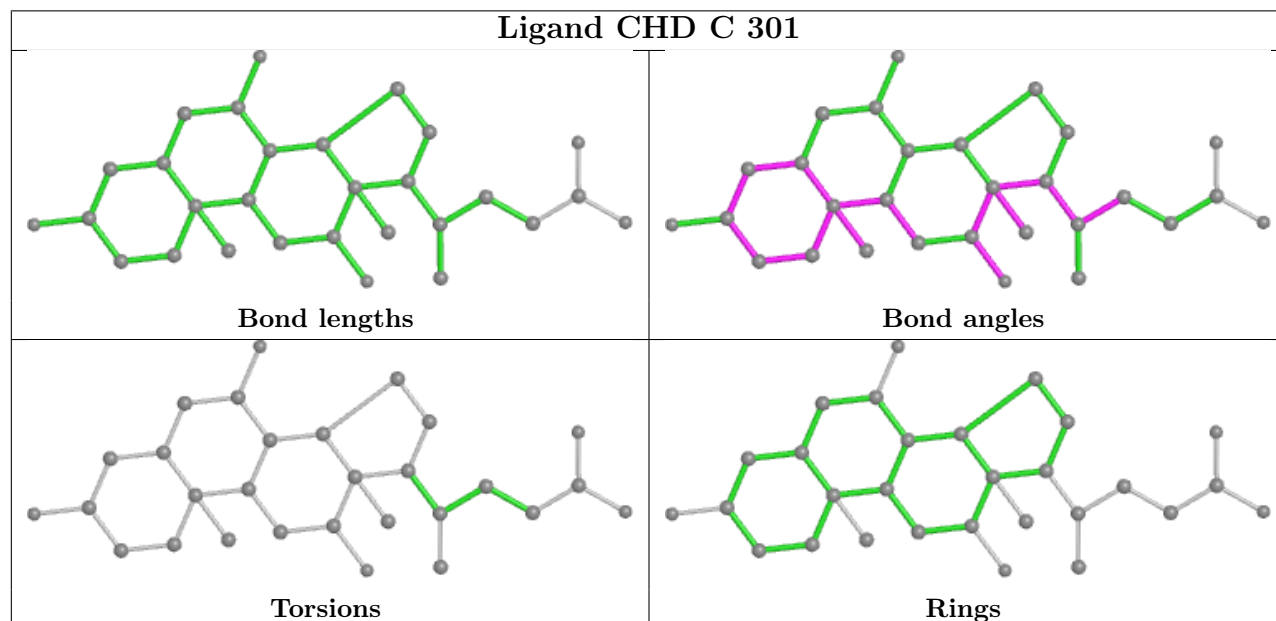




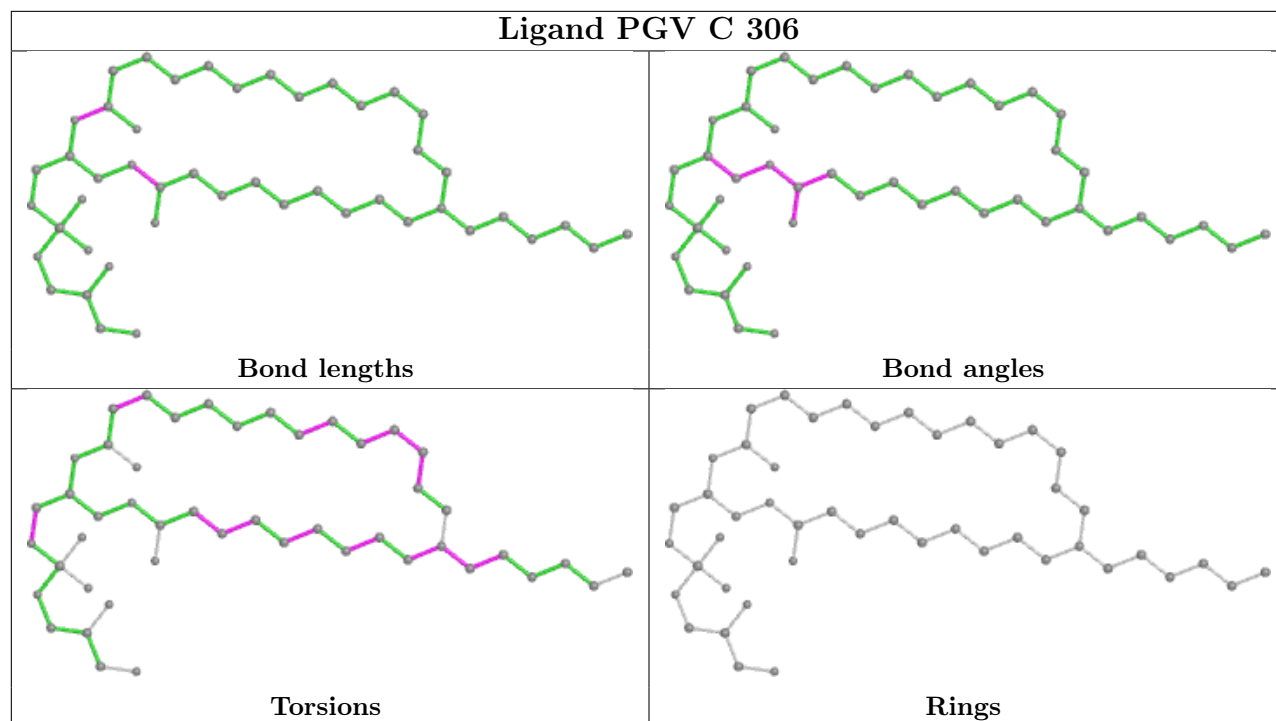
Ligand DMU M 101



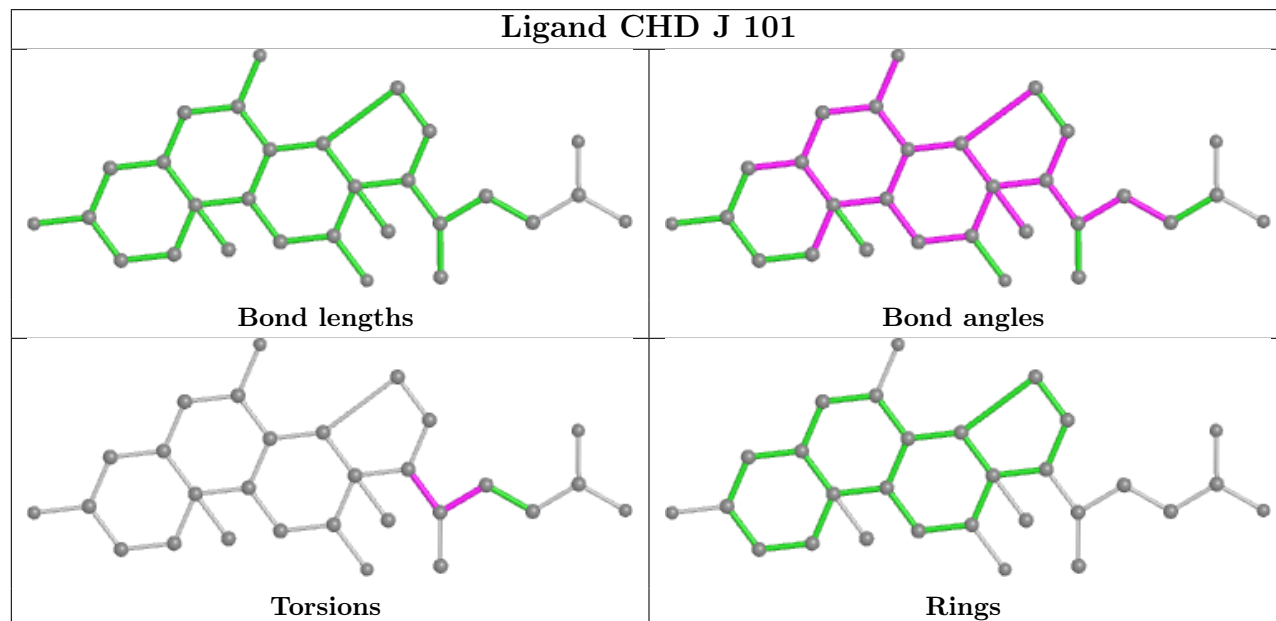
Ligand CHD C 301

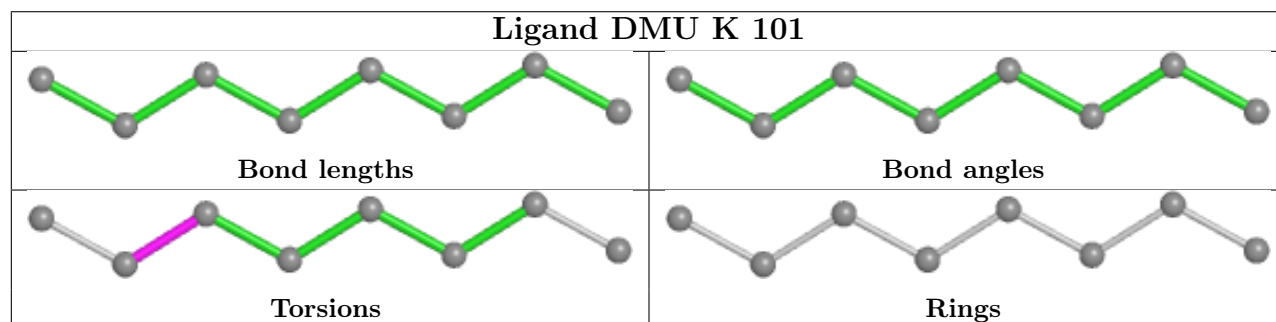
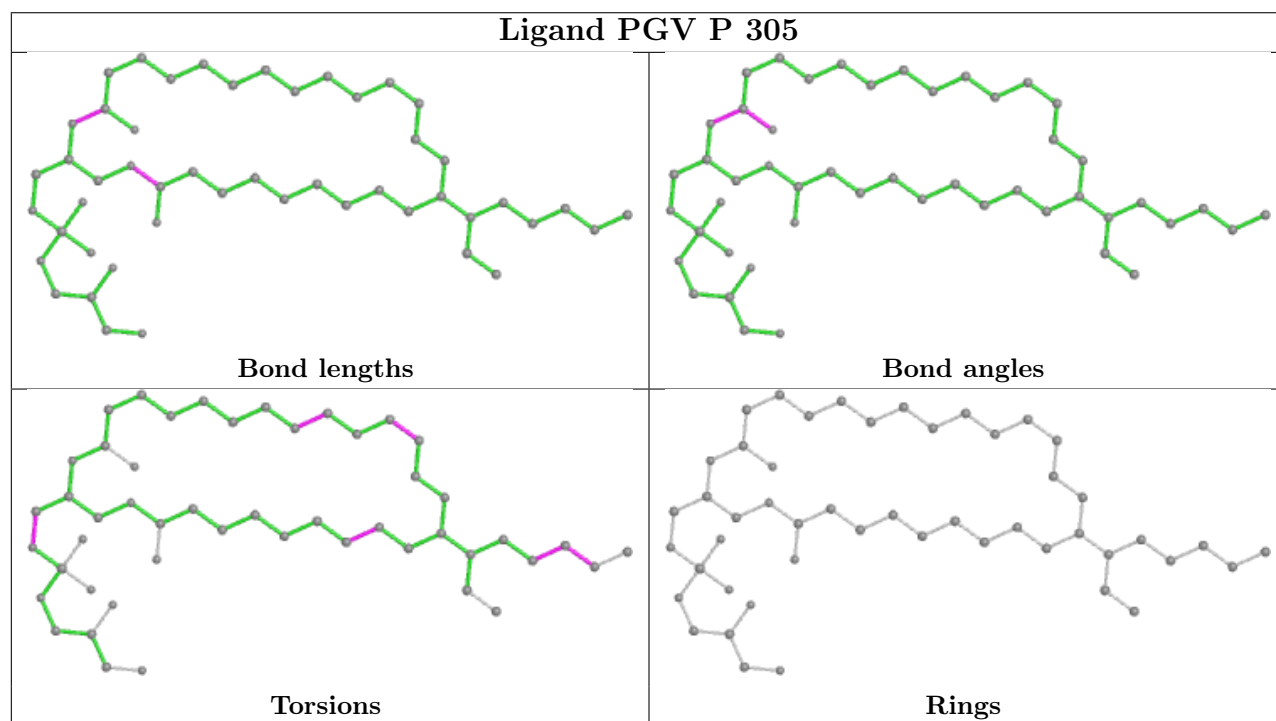
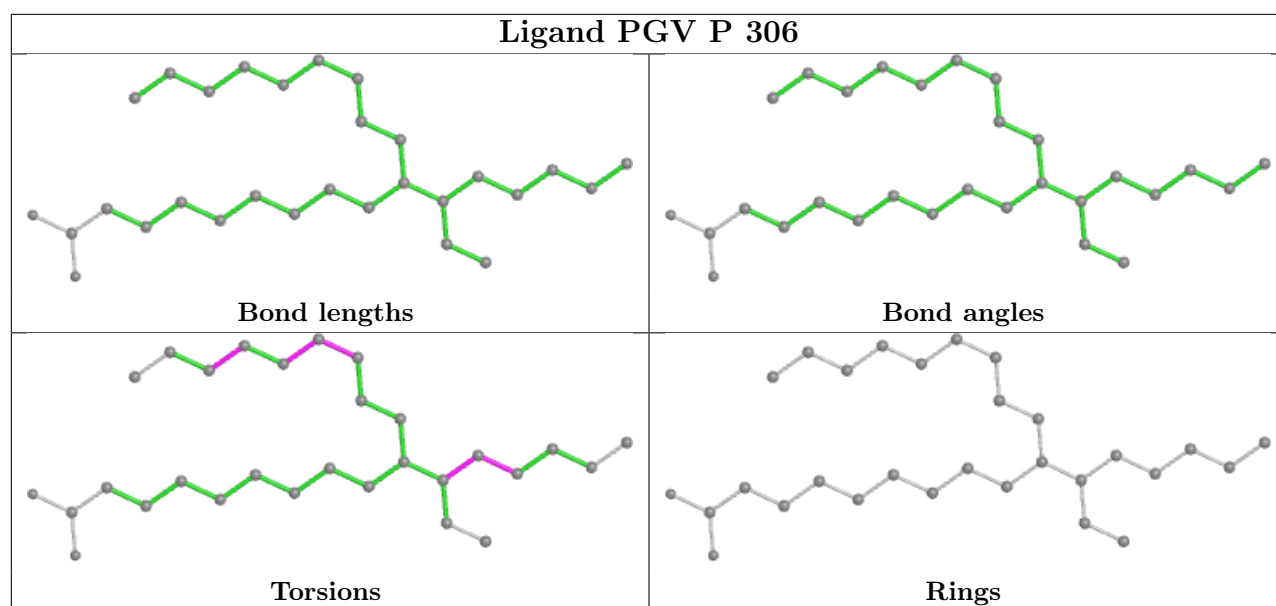


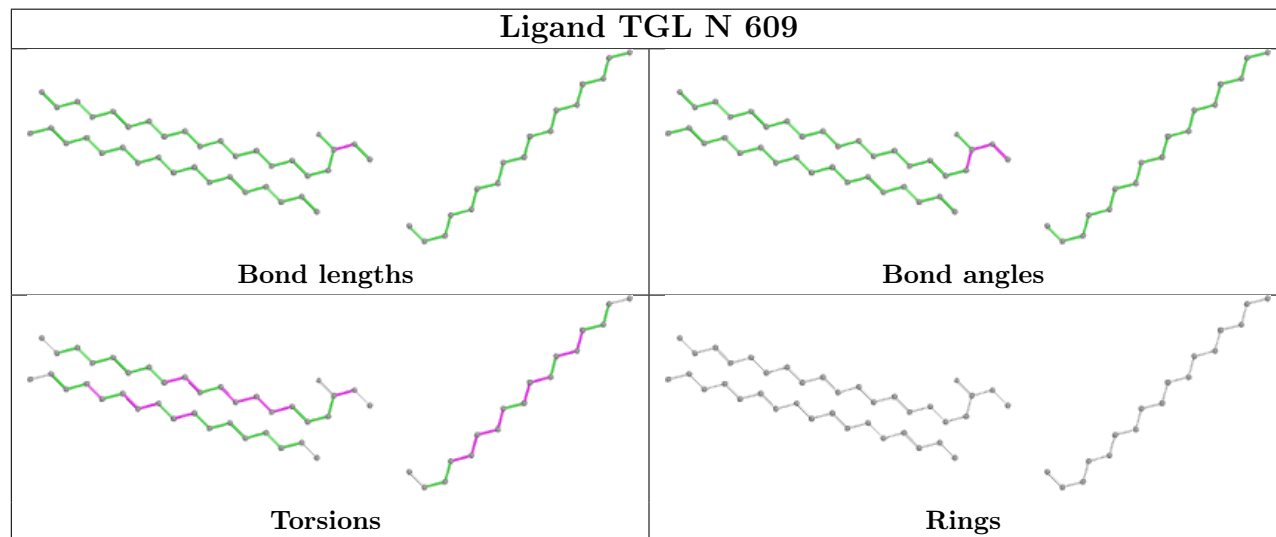
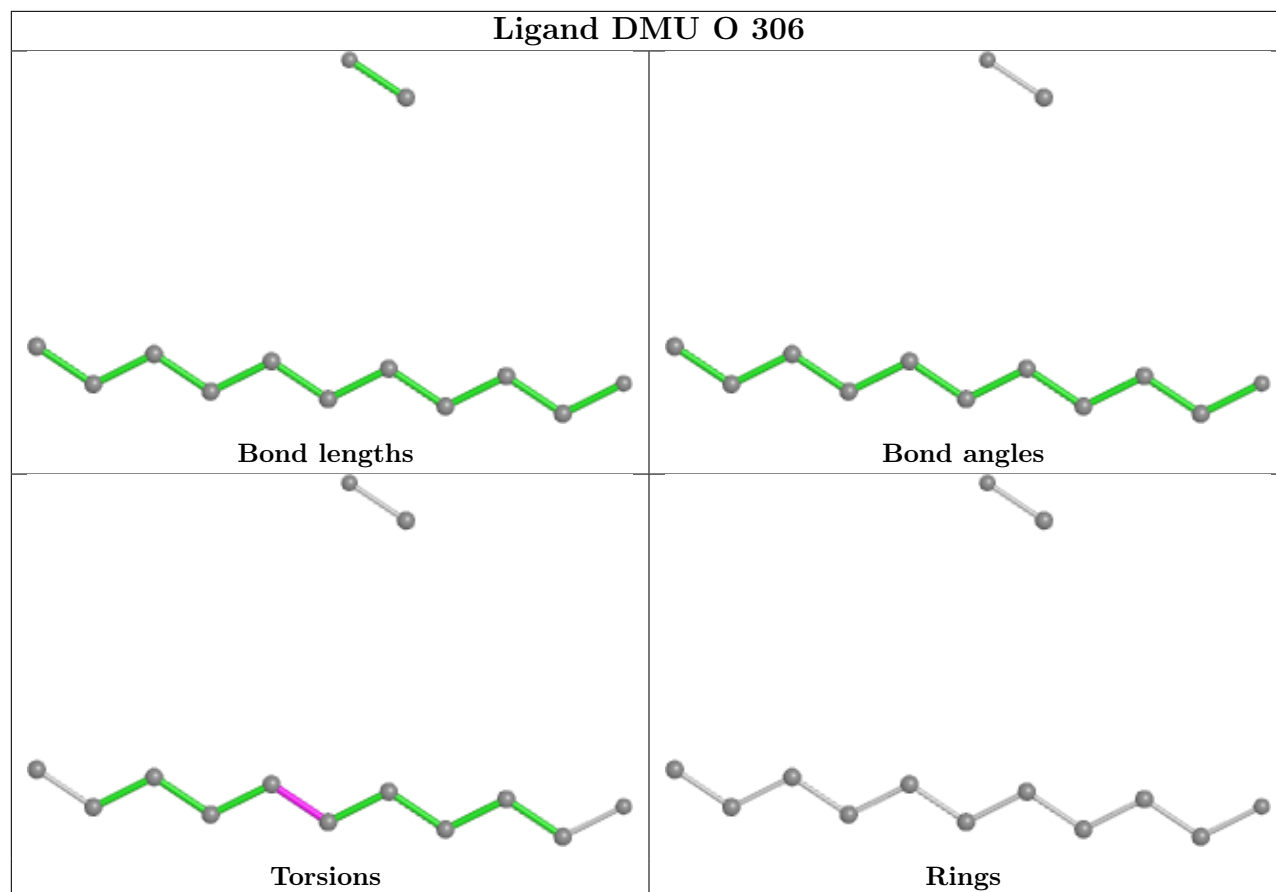
Ligand PGV C 306

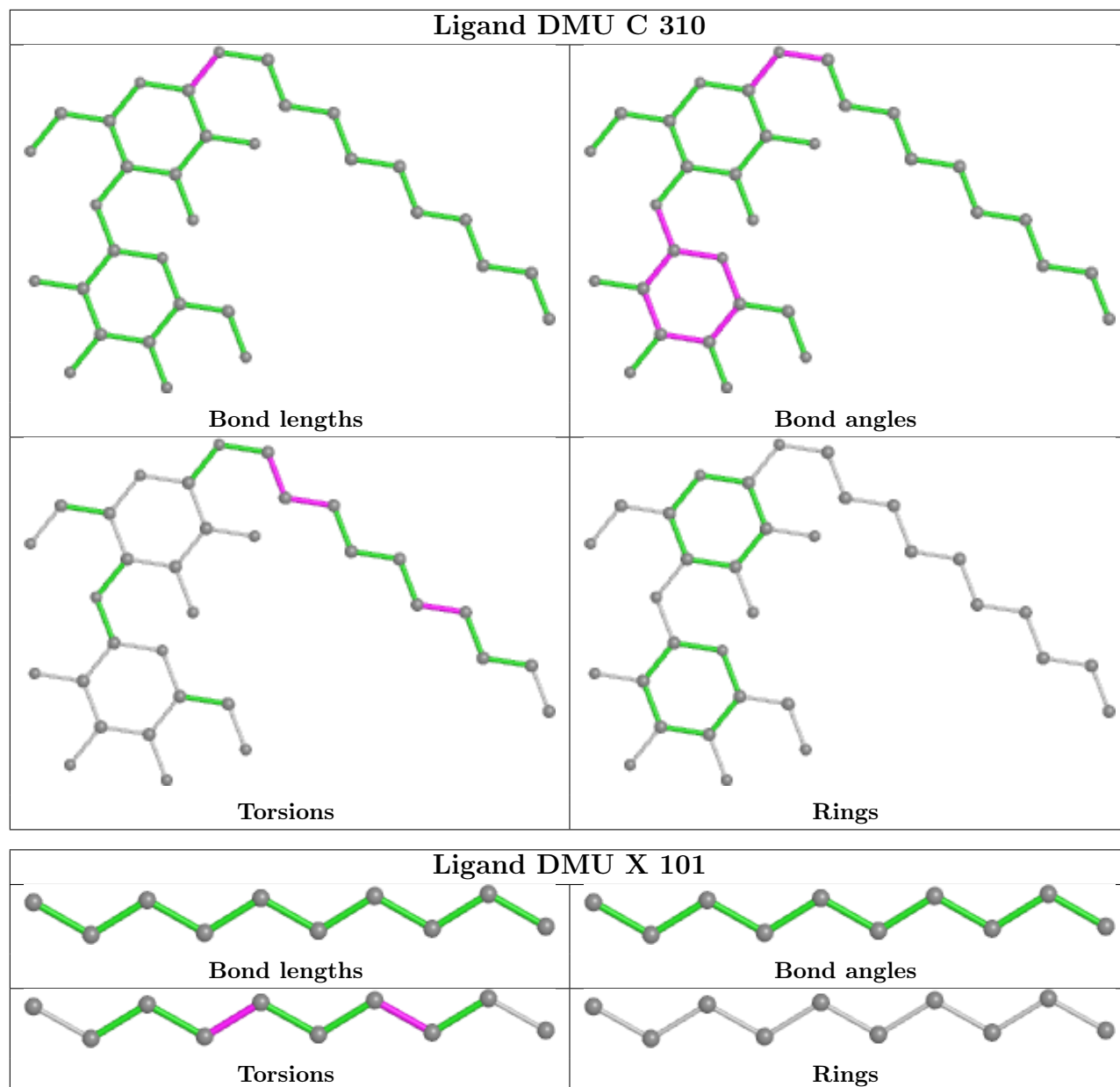


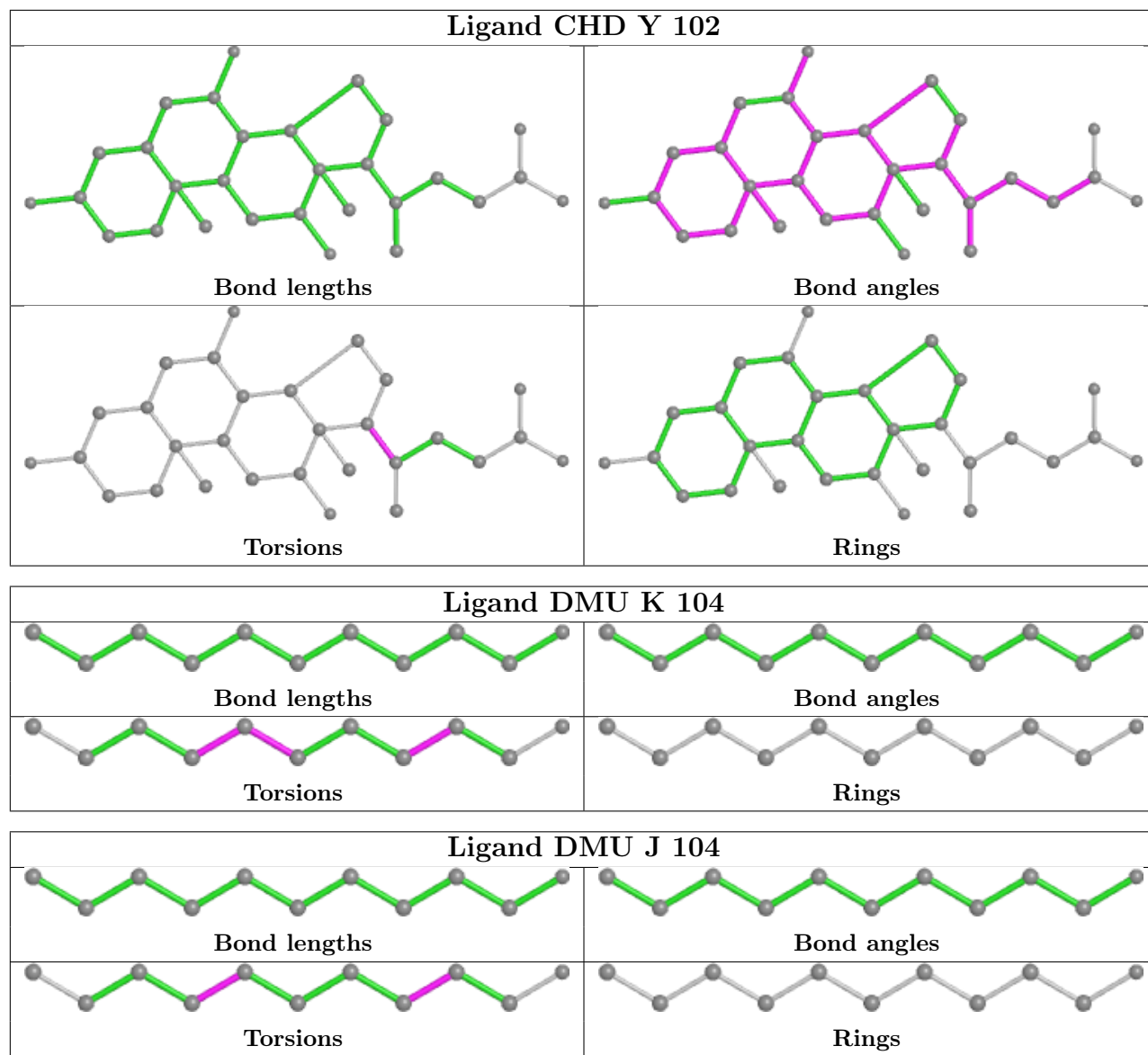
Ligand CHD J 101



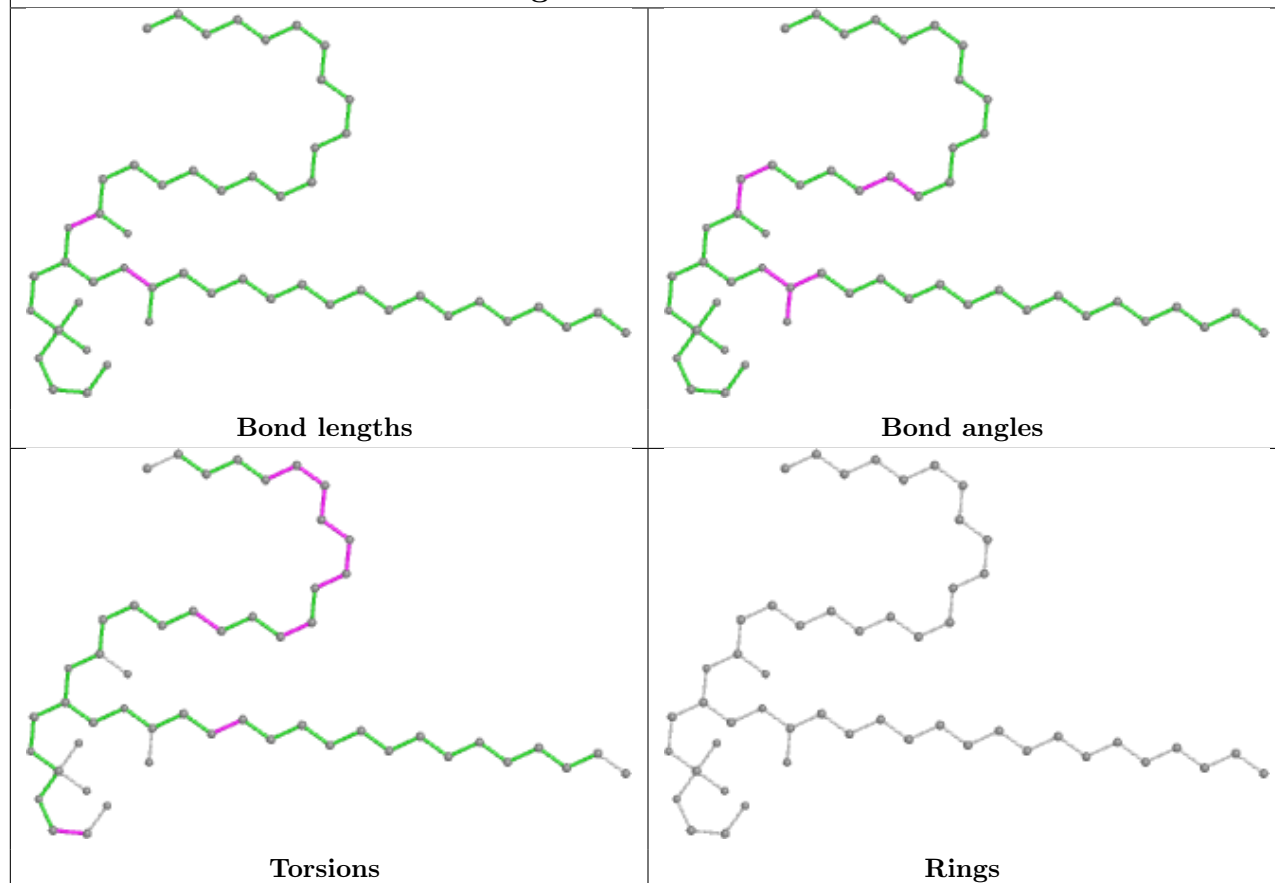




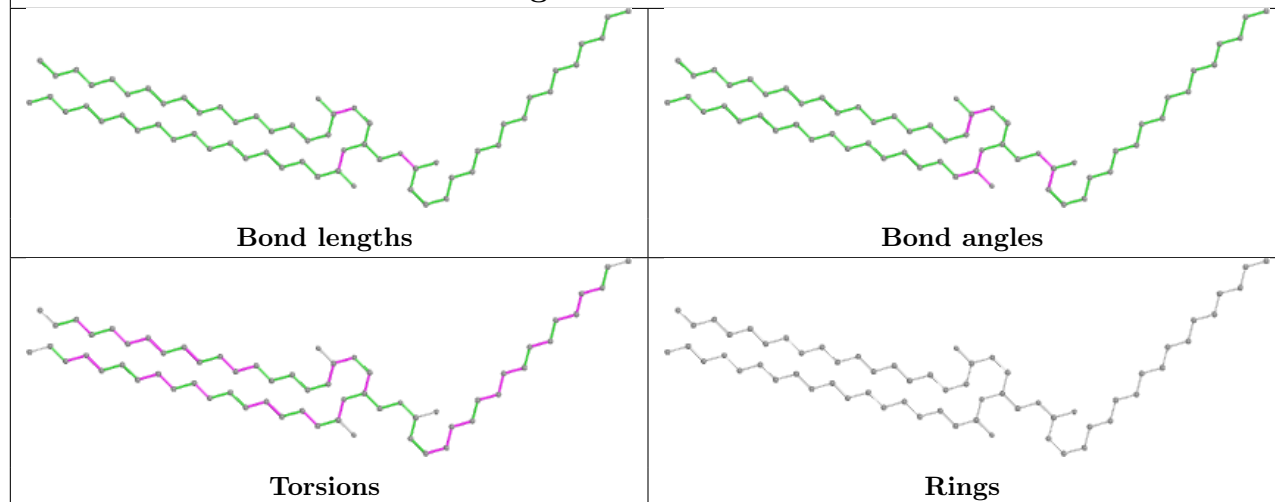


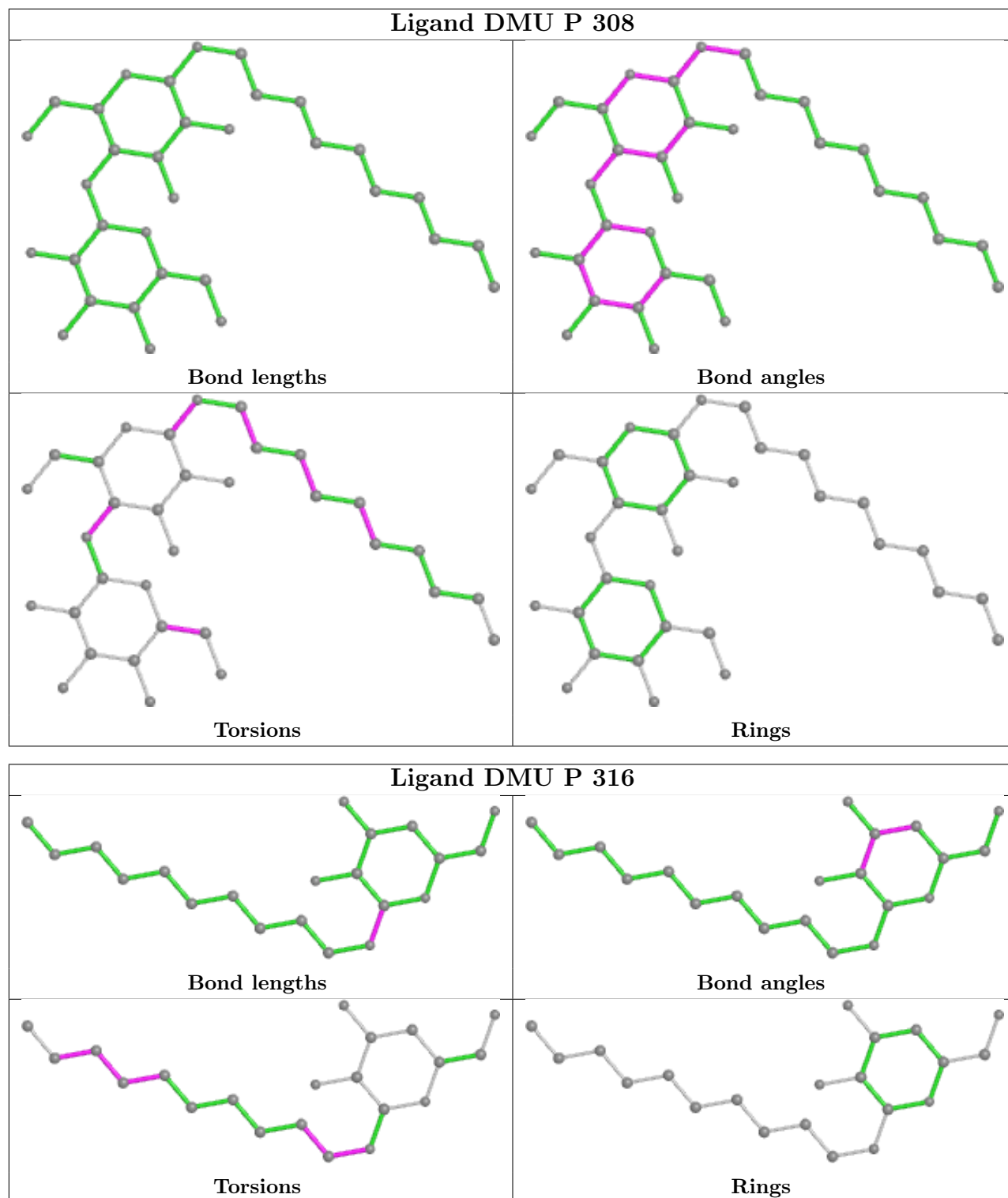


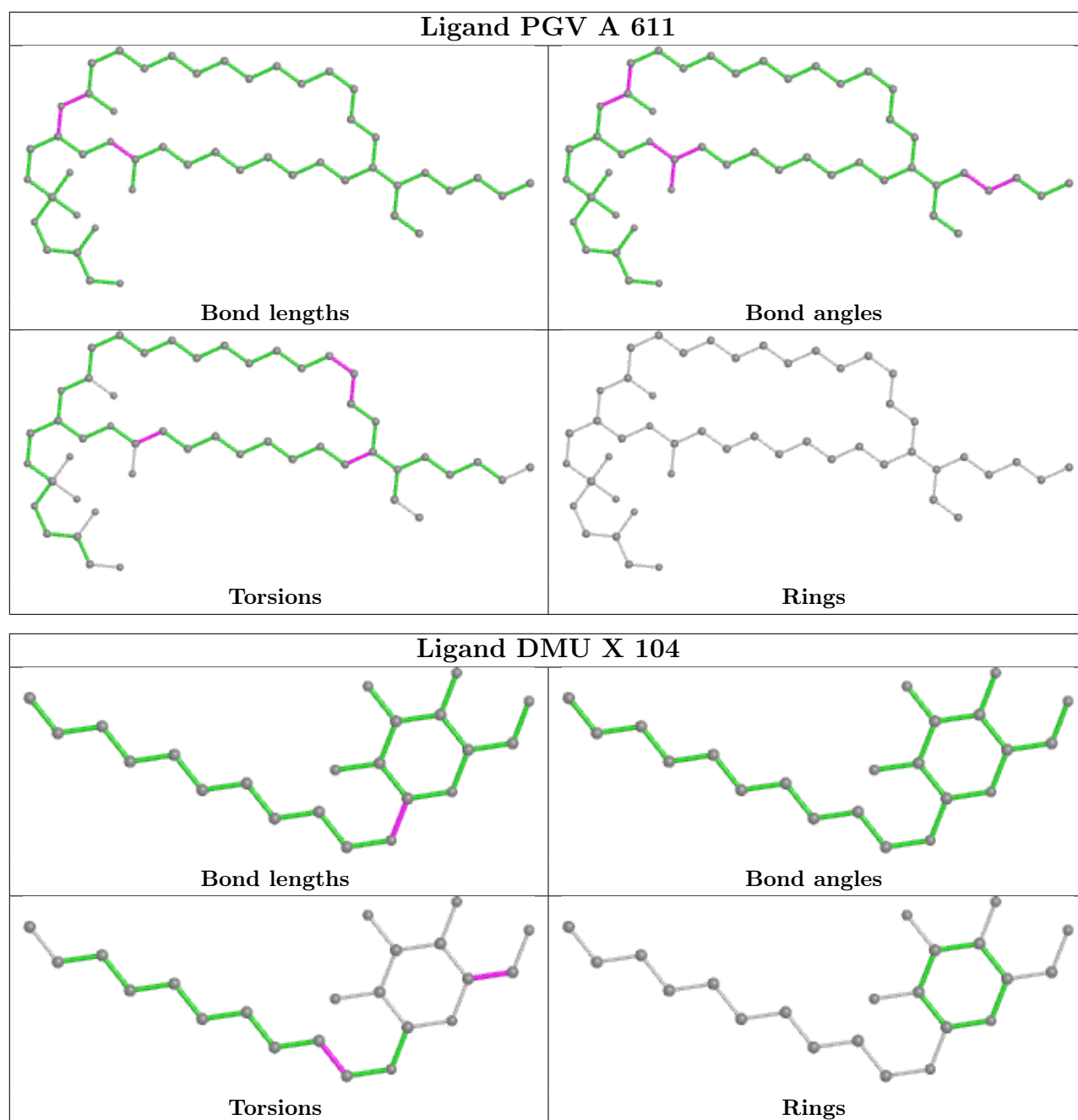
Ligand PEK P 304

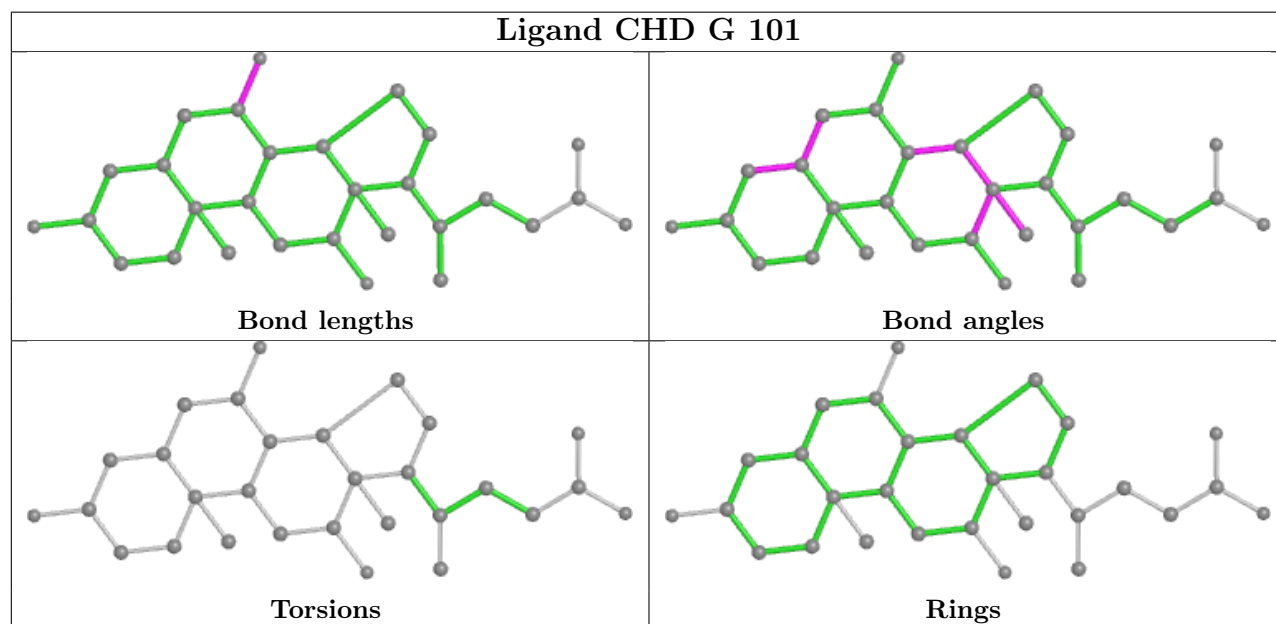
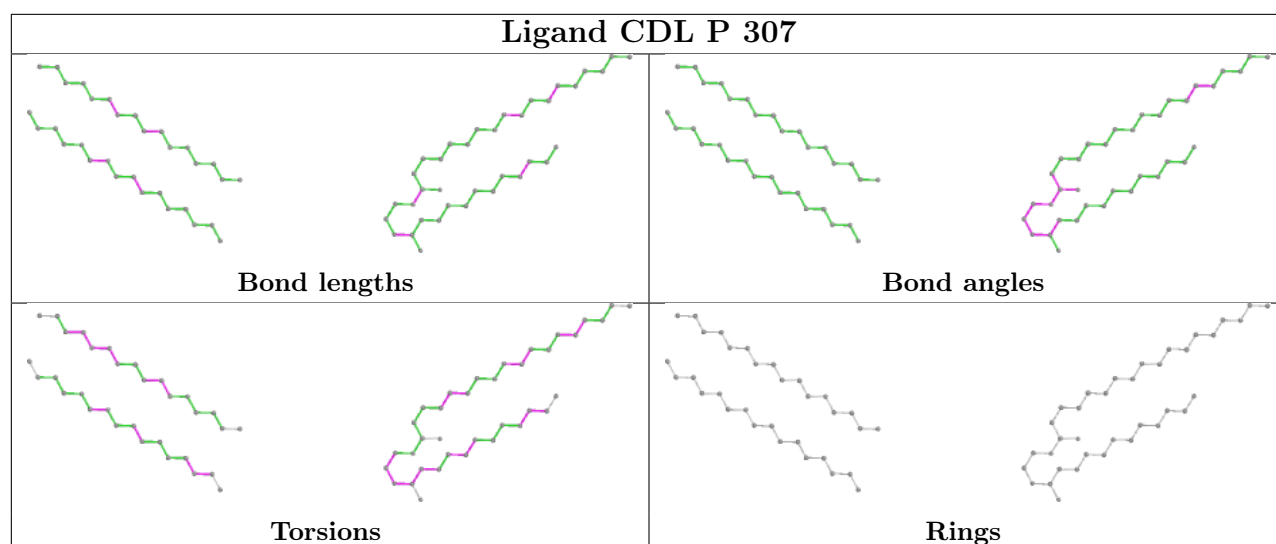


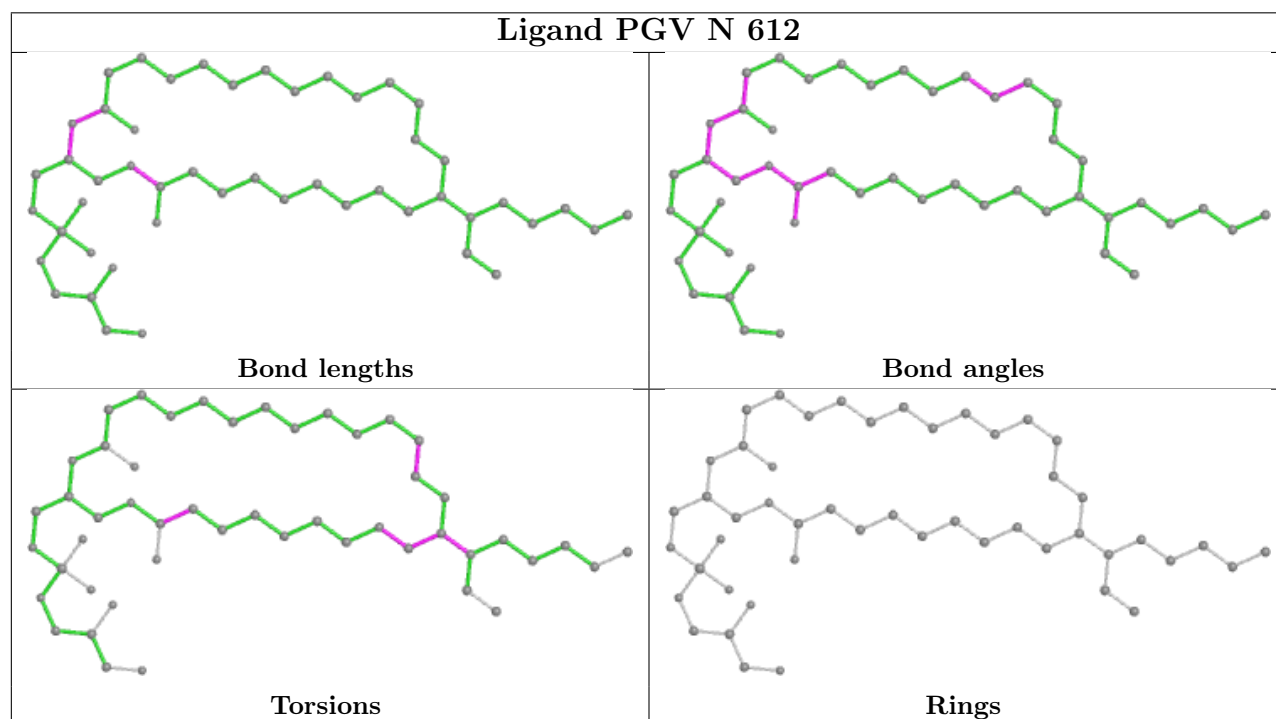
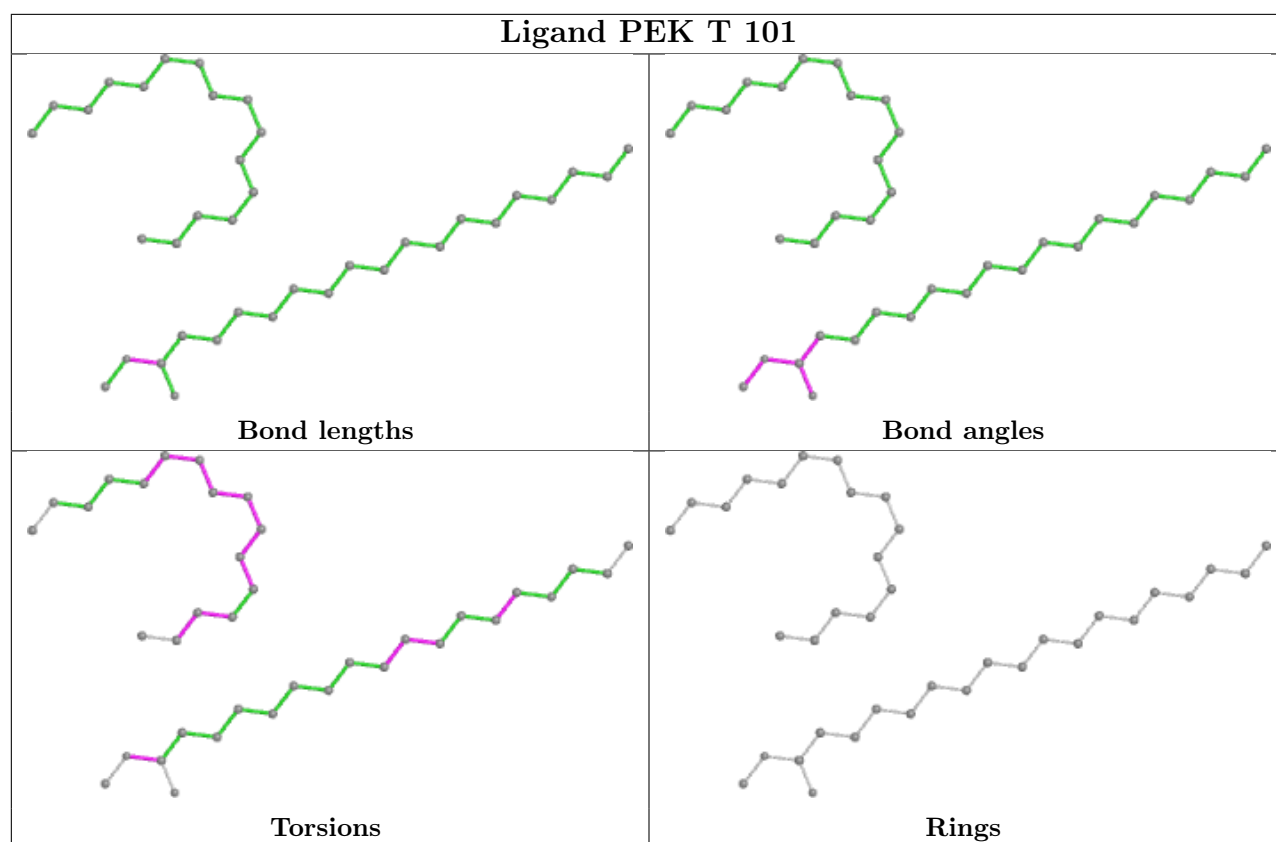
Ligand TGL N 607

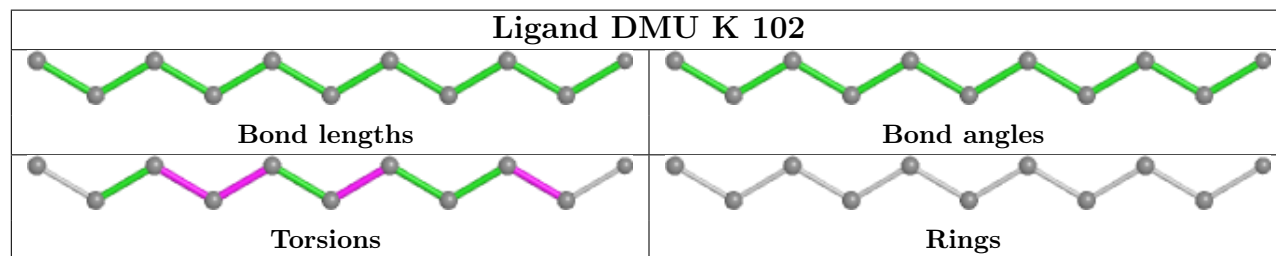
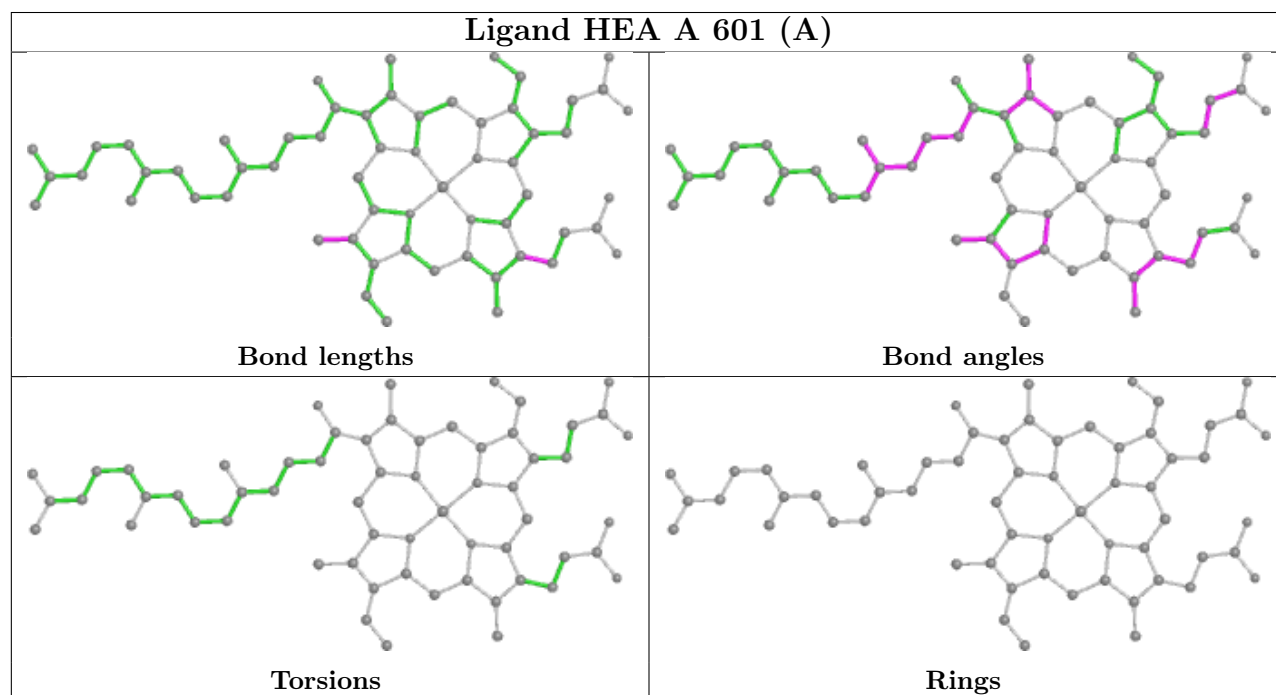
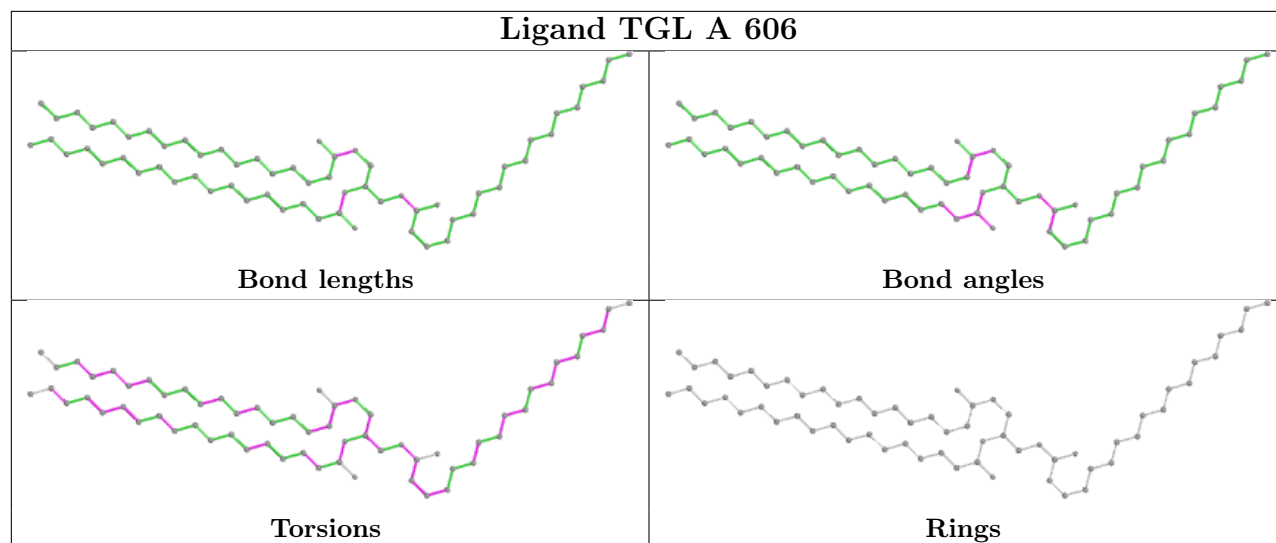


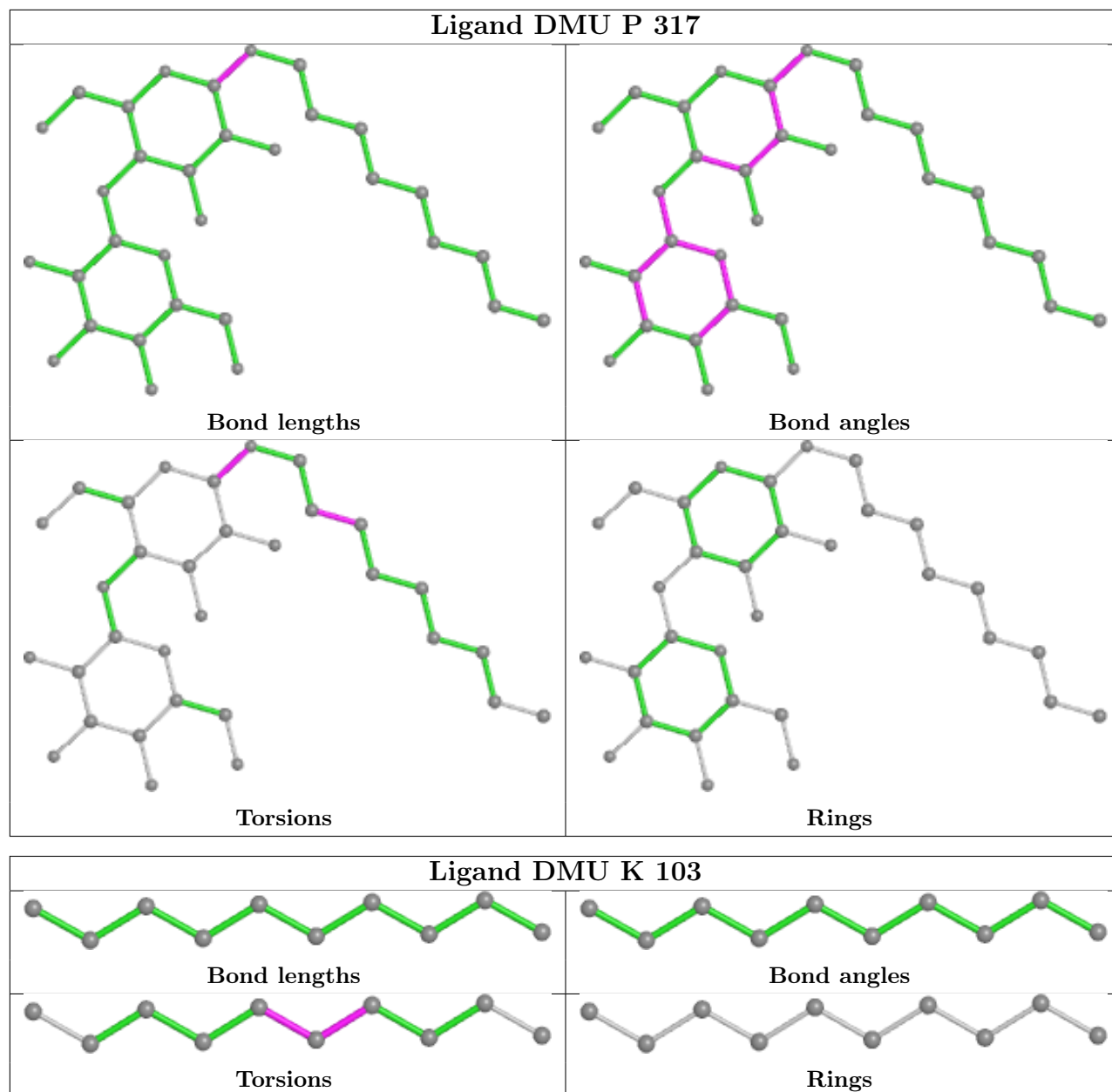


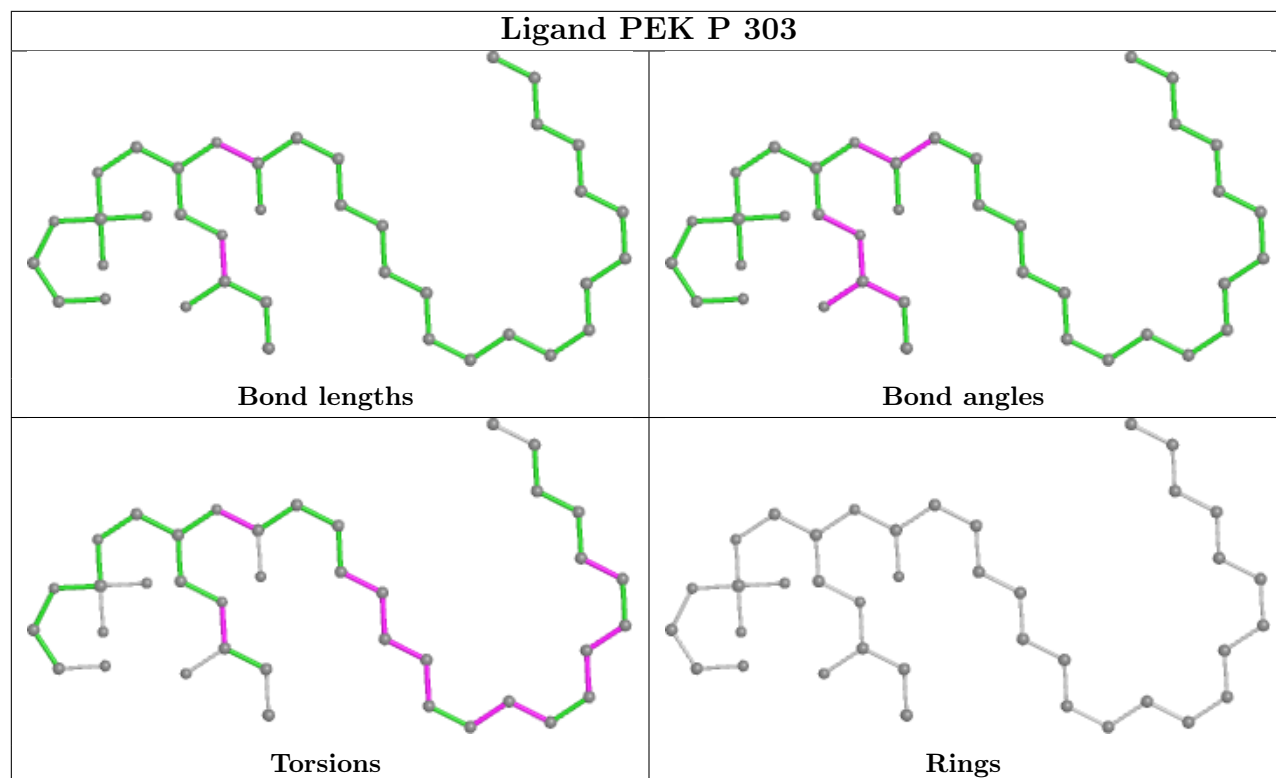












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ > 2 | OWAB(Å ²) | Q < 0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|---------|
| 1 | A | 513/514 (99%) | -0.12 | 2 (0%) 92 92 | 19, 24, 33, 82 | 0 |
| 1 | N | 513/514 (99%) | -0.13 | 1 (0%) 95 94 | 19, 26, 35, 80 | 0 |
| 2 | B | 226/227 (99%) | -0.10 | 2 (0%) 84 84 | 22, 32, 61, 110 | 0 |
| 2 | O | 226/227 (99%) | -0.13 | 2 (0%) 84 84 | 25, 36, 73, 115 | 0 |
| 3 | C | 259/259 (100%) | -0.15 | 0 100 100 | 21, 27, 40, 93 | 0 |
| 3 | P | 259/259 (100%) | -0.13 | 0 100 100 | 21, 28, 43, 90 | 0 |
| 4 | D | 144/144 (100%) | -0.28 | 0 100 100 | 25, 34, 56, 93 | 0 |
| 4 | Q | 144/144 (100%) | 0.34 | 7 (4%) 29 27 | 31, 48, 96, 243 | 0 |
| 5 | E | 105/105 (100%) | -0.26 | 1 (0%) 82 82 | 27, 33, 69, 156 | 0 |
| 5 | R | 105/105 (100%) | -0.17 | 2 (1%) 66 65 | 29, 42, 77, 169 | 0 |
| 6 | F | 94/94 (100%) | -0.05 | 3 (3%) 47 44 | 23, 34, 65, 130 | 0 |
| 6 | S | 94/94 (100%) | -0.02 | 4 (4%) 35 32 | 22, 31, 66, 125 | 0 |
| 7 | G | 84/84 (100%) | 0.88 | 16 (19%) 1 1 | 25, 35, 140, 183 | 0 |
| 7 | T | 84/84 (100%) | 0.73 | 16 (19%) 1 1 | 25, 39, 127, 194 | 0 |
| 8 | H | 79/79 (100%) | 0.15 | 4 (5%) 28 25 | 26, 38, 112, 179 | 0 |
| 8 | U | 79/79 (100%) | 0.16 | 6 (7%) 13 12 | 31, 42, 117, 215 | 0 |
| 9 | I | 72/73 (98%) | 0.14 | 1 (1%) 75 75 | 30, 48, 86, 102 | 0 |
| 9 | V | 72/73 (98%) | 0.17 | 2 (2%) 53 51 | 29, 55, 95, 161 | 0 |
| 10 | J | 58/58 (100%) | 0.17 | 3 (5%) 27 24 | 27, 38, 88, 175 | 0 |
| 10 | W | 58/58 (100%) | 0.04 | 3 (5%) 27 24 | 28, 39, 86, 171 | 0 |
| 11 | K | 49/49 (100%) | -0.11 | 0 100 100 | 30, 38, 59, 72 | 0 |
| 11 | X | 49/49 (100%) | 0.10 | 2 (4%) 37 34 | 36, 47, 86, 100 | 0 |
| 12 | L | 46/46 (100%) | -0.18 | 1 (2%) 62 60 | 25, 30, 56, 105 | 0 |
| 12 | Y | 46/46 (100%) | -0.19 | 1 (2%) 62 60 | 28, 36, 74, 133 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | M | 43/43 (100%) | -0.03 | 3 (6%) 16 14 | 25, 30, 86, 141 | 0 |
| 13 | Z | 43/43 (100%) | 0.09 | 5 (11%) 4 4 | 33, 38, 122, 190 | 0 |
| All | All | 3544/3550 (99%) | -0.03 | 87 (2%) 57 55 | 19, 31, 77, 243 | 0 |

All (87) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | Q | 4 | SER | 17.4 |
| 10 | J | 58 | LYS | 13.6 |
| 6 | F | 1 | ALA | 13.1 |
| 4 | Q | 6 | VAL | 12.9 |
| 4 | Q | 5 | VAL | 12.0 |
| 7 | G | 3 | ALA | 9.0 |
| 7 | T | 3 | ALA | 8.3 |
| 7 | T | 10 | GLY | 8.2 |
| 7 | G | 11 | THR | 7.9 |
| 7 | G | 8 | HIS | 7.8 |
| 7 | T | 8 | HIS | 7.8 |
| 4 | Q | 7 | LYS | 7.6 |
| 6 | S | 1 | ALA | 7.0 |
| 5 | R | 5 | HIS | 6.5 |
| 10 | W | 58 | LYS | 6.4 |
| 7 | G | 9 | GLY | 5.9 |
| 4 | Q | 8 | SER | 5.8 |
| 7 | G | 6 | GLY | 5.8 |
| 8 | H | 8 | ILE | 5.8 |
| 8 | U | 45 | ALA | 5.4 |
| 8 | U | 8 | ILE | 5.4 |
| 7 | T | 11 | THR | 5.3 |
| 7 | G | 7 | ASP | 5.3 |
| 7 | T | 2 | SER | 4.9 |
| 9 | V | 37 | PHE | 4.7 |
| 9 | I | 37 | PHE | 4.5 |
| 7 | G | 42 | ARG | 4.4 |
| 7 | G | 2 | SER | 4.2 |
| 7 | T | 5 | LYS | 4.1 |
| 8 | H | 45 | ALA | 4.1 |
| 7 | T | 1 | ALA | 4.0 |
| 7 | T | 7 | ASP | 3.9 |
| 7 | G | 36 | TRP | 3.9 |
| 6 | S | 2 | SER | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 8 | U | 7 | LYS | 3.9 |
| 7 | T | 36 | TRP | 3.7 |
| 7 | G | 10 | GLY | 3.7 |
| 13 | Z | 43 | SER | 3.6 |
| 10 | J | 1 | PHE | 3.5 |
| 13 | Z | 42 | LYS | 3.5 |
| 7 | T | 4 | ALA | 3.2 |
| 11 | X | 6 | ALA | 3.2 |
| 7 | G | 5 | LYS | 3.2 |
| 10 | J | 57 | HIS | 3.1 |
| 7 | G | 37 | LEU | 3.0 |
| 13 | M | 42 | LYS | 2.9 |
| 7 | T | 40 | GLY | 2.9 |
| 13 | M | 40 | TYR | 2.9 |
| 7 | T | 84 | LYS | 2.9 |
| 6 | F | 2 | SER | 2.8 |
| 2 | O | 113 | TYR | 2.8 |
| 10 | W | 57 | HIS | 2.8 |
| 7 | G | 4 | ALA | 2.6 |
| 2 | O | 90 | ILE | 2.6 |
| 7 | G | 40 | GLY | 2.6 |
| 8 | H | 46 | LYS | 2.6 |
| 13 | Z | 41 | LYS | 2.6 |
| 2 | B | 59 | GLN | 2.6 |
| 7 | T | 6 | GLY | 2.5 |
| 9 | V | 2 | THR | 2.5 |
| 8 | U | 48 | GLY | 2.5 |
| 13 | M | 43 | SER | 2.4 |
| 13 | Z | 40 | TYR | 2.4 |
| 12 | Y | 47 | LYS | 2.4 |
| 6 | S | 94 | HIS | 2.4 |
| 8 | U | 46 | LYS | 2.4 |
| 7 | T | 42 | ARG | 2.3 |
| 7 | T | 38 | HIS | 2.3 |
| 7 | G | 41 | HIS | 2.3 |
| 6 | S | 93 | PRO | 2.3 |
| 1 | A | 514[A] | LYS | 2.2 |
| 5 | R | 109 | VAL | 2.2 |
| 8 | U | 49 | ASP | 2.2 |
| 1 | N | 311[A] | ILE | 2.2 |
| 4 | Q | 72 | ASN | 2.2 |
| 7 | G | 1 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 13 | Z | 39 | ASN | 2.2 |
| 10 | W | 1 | PHE | 2.2 |
| 2 | B | 61 | VAL | 2.2 |
| 11 | X | 7 | PRO | 2.1 |
| 5 | E | 5 | HIS | 2.1 |
| 7 | T | 41 | HIS | 2.1 |
| 12 | L | 2 | HIS | 2.1 |
| 1 | A | 298[A] | ASP | 2.1 |
| 6 | F | 3 | GLY | 2.0 |
| 4 | Q | 51 | LEU | 2.0 |
| 8 | H | 44 | THR | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 9 | SAC | V | 1 | 9/10 | 0.19 | 0.53 | 201,217,238,247 | 0 |
| 9 | SAC | I | 1 | 9/10 | 0.73 | 0.32 | 129,147,176,183 | 0 |
| 1 | FME | N | 1 | 10/11 | 0.95 | 0.10 | 36,45,97,109 | 0 |
| 2 | FME | B | 1 | 10/11 | 0.96 | 0.11 | 28,31,40,126 | 0 |
| 1 | FME | A | 1 | 10/11 | 0.96 | 0.10 | 37,51,85,99 | 0 |
| 2 | FME | O | 1 | 10/11 | 0.97 | 0.12 | 31,36,44,111 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 23 | DMU | X | 102 | 9/33 | 0.52 | 0.31 | 65,70,82,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|--------|------|------|-----------------------------|-------|
| 27 | CDL | N | 601 | 62/100 | 0.52 | 0.35 | 44,76,103,117 | 0 |
| 22 | EDO | P | 310 | 4/4 | 0.54 | 0.17 | 71,72,75,80 | 0 |
| 23 | DMU | X | 104 | 22/33 | 0.56 | 0.43 | 58,94,150,157 | 0 |
| 22 | EDO | A | 618 | 4/4 | 0.58 | 0.26 | 52,59,65,85 | 0 |
| 23 | DMU | A | 623 | 11/33 | 0.64 | 0.37 | 62,76,106,114 | 0 |
| 22 | EDO | F | 105 | 4/4 | 0.66 | 0.18 | 56,58,67,70 | 0 |
| 22 | EDO | C | 315 | 4/4 | 0.66 | 0.23 | 65,78,87,99 | 0 |
| 25 | CHD | J | 101 | 29/29 | 0.68 | 0.41 | 50,120,146,151 | 0 |
| 23 | DMU | L | 105 | 21/33 | 0.68 | 0.20 | 54,80,107,120 | 0 |
| 23 | DMU | D | 207 | 11/33 | 0.69 | 0.33 | 58,81,115,120 | 0 |
| 23 | DMU | P | 317 | 32/33 | 0.69 | 0.22 | 52,107,133,136 | 0 |
| 23 | DMU | Q | 201 | 11/33 | 0.70 | 0.22 | 49,70,93,95 | 0 |
| 22 | EDO | C | 317 | 4/4 | 0.71 | 0.18 | 60,67,70,80 | 0 |
| 23 | DMU | K | 103 | 10/33 | 0.73 | 0.26 | 62,75,106,112 | 0 |
| 26 | PEK | C | 303 | 45/53 | 0.73 | 0.33 | 44,95,175,209 | 0 |
| 23 | DMU | D | 206 | 33/33 | 0.73 | 0.23 | 46,95,141,151 | 0 |
| 27 | CDL | T | 102 | 61/100 | 0.74 | 0.27 | 42,77,110,117 | 0 |
| 26 | PEK | P | 303 | 38/53 | 0.75 | 0.25 | 49,79,163,172 | 0 |
| 23 | DMU | P | 308 | 33/33 | 0.76 | 0.29 | 37,102,137,160 | 0 |
| 26 | PEK | C | 305 | 36/53 | 0.77 | 0.23 | 42,76,101,118 | 0 |
| 22 | EDO | O | 305 | 4/4 | 0.77 | 0.19 | 49,61,62,105 | 0 |
| 25 | CHD | Y | 102 | 29/29 | 0.78 | 0.24 | 56,91,135,152 | 0 |
| 23 | DMU | K | 102 | 11/33 | 0.78 | 0.24 | 55,70,95,105 | 0 |
| 23 | DMU | X | 103 | 9/33 | 0.78 | 0.23 | 56,62,103,104 | 0 |
| 22 | EDO | T | 104 | 4/4 | 0.78 | 0.26 | 56,73,98,107 | 0 |
| 22 | EDO | P | 315 | 4/4 | 0.78 | 0.17 | 66,95,100,113 | 0 |
| 25 | CHD | L | 102 | 29/29 | 0.78 | 0.30 | 51,95,117,134 | 0 |
| 22 | EDO | C | 311 | 4/4 | 0.79 | 0.16 | 44,65,68,73 | 0 |
| 22 | EDO | C | 320 | 4/4 | 0.79 | 0.35 | 33,68,70,73 | 0 |
| 18 | TGL | N | 609 | 55/63 | 0.79 | 0.21 | 46,72,112,119 | 0 |
| 22 | EDO | N | 620 | 4/4 | 0.80 | 0.20 | 52,52,53,80 | 0 |
| 19 | PGV | P | 306 | 31/51 | 0.80 | 0.25 | 32,72,96,109 | 0 |
| 21 | PSC | O | 302 | 31/52 | 0.80 | 0.23 | 36,62,106,153 | 0 |
| 26 | PEK | T | 101 | 37/53 | 0.80 | 0.26 | 43,75,105,131 | 0 |
| 22 | EDO | A | 612 | 4/4 | 0.80 | 0.24 | 51,51,71,101 | 0 |
| 22 | EDO | L | 103 | 4/4 | 0.80 | 0.22 | 42,49,64,119 | 0 |
| 23 | DMU | P | 316 | 21/33 | 0.81 | 0.17 | 51,81,126,136 | 0 |
| 22 | EDO | A | 617 | 4/4 | 0.81 | 0.27 | 57,70,72,73 | 0 |
| 22 | EDO | L | 104 | 4/4 | 0.81 | 0.24 | 50,51,79,128 | 0 |
| 25 | CHD | C | 309 | 29/29 | 0.83 | 0.27 | 47,86,113,140 | 0 |
| 22 | EDO | P | 314 | 4/4 | 0.83 | 0.14 | 37,53,55,74 | 0 |
| 21 | PSC | A | 610 | 25/52 | 0.83 | 0.22 | 44,70,88,111 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|--------|------|------|-----------------------------|-------|
| 19 | PGV | N | 610 | 51/51 | 0.83 | 0.28 | 40,83,151,204 | 0 |
| 18 | TGL | A | 607 | 63/63 | 0.83 | 0.21 | 32,68,117,128 | 0 |
| 19 | PGV | A | 608 | 34/51 | 0.84 | 0.23 | 32,57,110,126 | 0 |
| 18 | TGL | N | 608 | 55/63 | 0.84 | 0.20 | 38,64,110,123 | 0 |
| 22 | EDO | A | 620 | 4/4 | 0.84 | 0.19 | 44,52,61,82 | 0 |
| 18 | TGL | L | 101 | 63/63 | 0.85 | 0.21 | 25,60,114,165 | 0 |
| 18 | TGL | N | 607 | 63/63 | 0.85 | 0.24 | 40,79,108,125 | 0 |
| 23 | DMU | O | 306 | 13/33 | 0.85 | 0.19 | 45,66,128,139 | 0 |
| 27 | CDL | C | 308 | 65/100 | 0.85 | 0.24 | 37,69,123,156 | 0 |
| 19 | PGV | C | 307 | 36/51 | 0.85 | 0.25 | 41,74,140,164 | 0 |
| 18 | TGL | A | 606 | 63/63 | 0.85 | 0.17 | 39,72,108,119 | 0 |
| 22 | EDO | N | 619 | 4/4 | 0.86 | 0.15 | 40,78,80,94 | 0 |
| 22 | EDO | F | 102 | 4/4 | 0.86 | 0.11 | 33,36,53,121 | 0 |
| 27 | CDL | P | 307 | 68/100 | 0.86 | 0.24 | 39,76,127,157 | 0 |
| 23 | DMU | C | 310 | 33/33 | 0.86 | 0.24 | 35,81,151,167 | 0 |
| 22 | EDO | B | 305 | 4/4 | 0.87 | 0.14 | 28,36,44,63 | 0 |
| 22 | EDO | P | 309 | 4/4 | 0.87 | 0.18 | 60,63,63,69 | 0 |
| 23 | DMU | K | 104 | 11/33 | 0.87 | 0.20 | 50,68,100,112 | 0 |
| 23 | DMU | J | 104 | 11/33 | 0.87 | 0.17 | 49,60,84,99 | 0 |
| 22 | EDO | J | 103 | 4/4 | 0.88 | 0.26 | 59,62,62,75 | 0 |
| 22 | EDO | C | 319 | 4/4 | 0.88 | 0.25 | 43,47,61,111 | 0 |
| 22 | EDO | F | 103 | 4/4 | 0.88 | 0.14 | 44,51,53,59 | 0 |
| 22 | EDO | C | 313 | 4/4 | 0.88 | 0.14 | 30,39,40,49 | 0 |
| 23 | DMU | C | 321 | 12/33 | 0.89 | 0.13 | 51,66,84,89 | 0 |
| 23 | DMU | X | 101 | 10/33 | 0.89 | 0.15 | 41,60,84,103 | 0 |
| 22 | EDO | W | 101 | 4/4 | 0.89 | 0.18 | 54,56,71,77 | 0 |
| 22 | EDO | S | 104 | 4/4 | 0.89 | 0.13 | 44,46,48,54 | 0 |
| 22 | EDO | A | 614 | 4/4 | 0.89 | 0.19 | 51,61,65,80 | 0 |
| 23 | DMU | Z | 101 | 33/33 | 0.89 | 0.11 | 37,47,68,72 | 0 |
| 22 | EDO | C | 312 | 4/4 | 0.90 | 0.12 | 32,33,33,82 | 0 |
| 22 | EDO | M | 102 | 4/4 | 0.90 | 0.33 | 68,86,88,93 | 0 |
| 22 | EDO | C | 316 | 4/4 | 0.90 | 0.13 | 49,55,70,77 | 0 |
| 23 | DMU | K | 101 | 8/33 | 0.90 | 0.18 | 48,63,77,85 | 0 |
| 22 | EDO | D | 205 | 4/4 | 0.90 | 0.33 | 53,58,59,61 | 0 |
| 22 | EDO | A | 616 | 4/4 | 0.90 | 0.32 | 31,40,42,78 | 0 |
| 22 | EDO | P | 313 | 4/4 | 0.91 | 0.18 | 49,54,61,76 | 0 |
| 23 | DMU | M | 101 | 33/33 | 0.91 | 0.11 | 35,41,54,65 | 0 |
| 22 | EDO | B | 306 | 4/4 | 0.92 | 0.15 | 38,47,48,48 | 0 |
| 22 | EDO | Q | 202 | 4/4 | 0.92 | 0.17 | 41,46,48,52 | 0 |
| 22 | EDO | J | 102 | 4/4 | 0.92 | 0.17 | 48,48,91,98 | 0 |
| 22 | EDO | D | 201 | 4/4 | 0.92 | 0.21 | 39,49,70,82 | 0 |
| 22 | EDO | P | 311 | 4/4 | 0.92 | 0.13 | 33,37,37,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 22 | EDO | W | 102 | 4/4 | 0.92 | 0.24 | 46,63,67,113 | 0 |
| 22 | EDO | D | 204 | 4/4 | 0.92 | 0.32 | 41,43,50,59 | 0 |
| 22 | EDO | O | 304 | 4/4 | 0.92 | 0.13 | 46,46,48,52 | 0 |
| 29 | PO4 | U | 101 | 5/5 | 0.92 | 0.20 | 51,53,120,124 | 0 |
| 22 | EDO | N | 622 | 4/4 | 0.93 | 0.18 | 30,34,50,92 | 0 |
| 22 | EDO | N | 614 | 4/4 | 0.93 | 0.11 | 38,39,40,40 | 0 |
| 22 | EDO | F | 109 | 4/4 | 0.93 | 0.19 | 35,36,71,71 | 0 |
| 22 | EDO | A | 621 | 4/4 | 0.93 | 0.17 | 37,40,40,52 | 0 |
| 23 | DMU | K | 105 | 9/33 | 0.93 | 0.16 | 38,52,70,105 | 0 |
| 22 | EDO | F | 108 | 4/4 | 0.94 | 0.16 | 37,42,79,101 | 0 |
| 22 | EDO | S | 106 | 4/4 | 0.94 | 0.14 | 37,52,72,76 | 0 |
| 22 | EDO | C | 318 | 4/4 | 0.94 | 0.20 | 40,60,68,94 | 0 |
| 17 | NA | C | 302 | 1/1 | 0.94 | 0.09 | 36,36,36,36 | 0 |
| 22 | EDO | E | 203 | 4/4 | 0.94 | 0.12 | 49,49,49,75 | 0 |
| 22 | EDO | Y | 101 | 4/4 | 0.94 | 0.15 | 48,51,53,64 | 0 |
| 22 | EDO | A | 622 | 4/4 | 0.95 | 0.22 | 32,37,42,42 | 0 |
| 22 | EDO | N | 615 | 4/4 | 0.95 | 0.09 | 38,41,42,58 | 0 |
| 22 | EDO | T | 103 | 4/4 | 0.95 | 0.11 | 30,30,38,40 | 0 |
| 25 | CHD | C | 301 | 29/29 | 0.95 | 0.09 | 26,29,39,44 | 0 |
| 22 | EDO | N | 616 | 4/4 | 0.95 | 0.16 | 33,40,44,86 | 0 |
| 22 | EDO | T | 105 | 4/4 | 0.95 | 0.15 | 37,48,58,62 | 0 |
| 22 | EDO | F | 107 | 4/4 | 0.95 | 0.15 | 45,50,81,119 | 0 |
| 25 | CHD | P | 301 | 29/29 | 0.95 | 0.09 | 26,30,35,44 | 0 |
| 22 | EDO | C | 314 | 4/4 | 0.95 | 0.18 | 31,35,53,60 | 0 |
| 20 | PER | A | 609[A] | 2/2 | 0.96 | 0.12 | 20,20,20,24 | 2 |
| 22 | EDO | A | 615 | 4/4 | 0.96 | 0.11 | 26,26,28,33 | 0 |
| 25 | CHD | G | 101 | 29/29 | 0.96 | 0.10 | 20,26,34,40 | 0 |
| 19 | PGV | N | 612 | 51/51 | 0.96 | 0.13 | 24,31,73,93 | 0 |
| 22 | EDO | D | 203 | 4/4 | 0.96 | 0.14 | 37,40,57,68 | 0 |
| 26 | PEK | P | 304 | 52/53 | 0.96 | 0.13 | 28,43,96,117 | 0 |
| 22 | EDO | N | 613 | 4/4 | 0.97 | 0.10 | 24,27,28,32 | 0 |
| 17 | NA | P | 302 | 1/1 | 0.97 | 0.10 | 38,38,38,38 | 0 |
| 22 | EDO | P | 312 | 4/4 | 0.97 | 0.11 | 28,39,39,57 | 0 |
| 16 | MG | A | 604 | 1/1 | 0.97 | 0.06 | 18,18,18,18 | 0 |
| 20 | PER | N | 611[A] | 2/2 | 0.97 | 0.15 | 20,20,20,31 | 2 |
| 22 | EDO | G | 102 | 4/4 | 0.97 | 0.07 | 25,32,32,34 | 0 |
| 26 | PEK | C | 304 | 52/53 | 0.97 | 0.13 | 25,42,97,111 | 0 |
| 19 | PGV | A | 611 | 51/51 | 0.97 | 0.13 | 19,30,73,90 | 0 |
| 22 | EDO | S | 103 | 4/4 | 0.97 | 0.08 | 32,33,43,43 | 0 |
| 22 | EDO | N | 621 | 4/4 | 0.97 | 0.29 | 39,41,43,116 | 0 |
| 22 | EDO | S | 105 | 4/4 | 0.97 | 0.14 | 29,31,32,32 | 0 |
| 22 | EDO | B | 304 | 4/4 | 0.97 | 0.14 | 33,43,55,80 | 0 |

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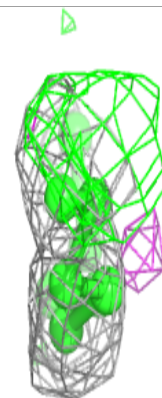
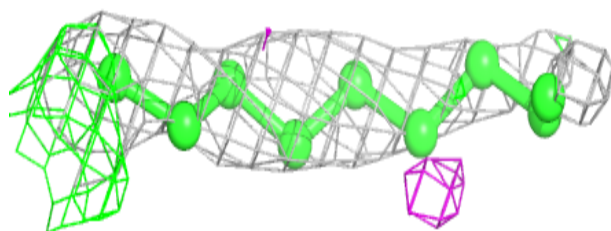
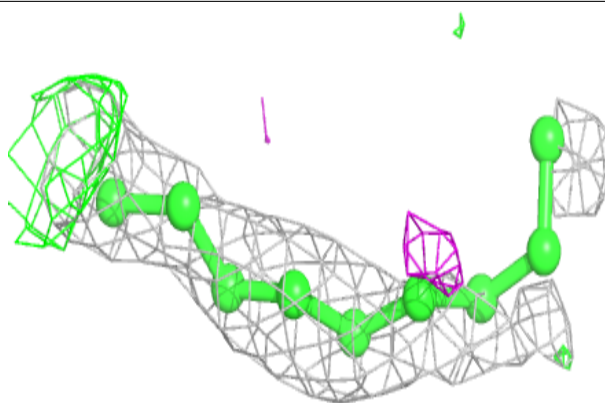
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 19 | PGV | P | 305 | 51/51 | 0.97 | 0.14 | 22,31,87,120 | 0 |
| 25 | CHD | B | 302 | 29/29 | 0.97 | 0.09 | 21,27,36,50 | 0 |
| 22 | EDO | D | 202 | 4/4 | 0.97 | 0.15 | 43,43,57,86 | 0 |
| 29 | PO4 | H | 101 | 5/5 | 0.97 | 0.22 | 62,62,77,101 | 0 |
| 22 | EDO | F | 106 | 4/4 | 0.97 | 0.11 | 30,31,32,32 | 0 |
| 14 | HEA | A | 602 | 60/60 | 0.98 | 0.10 | 16,21,30,37 | 0 |
| 22 | EDO | E | 201 | 4/4 | 0.98 | 0.13 | 38,39,40,40 | 0 |
| 22 | EDO | E | 202 | 4/4 | 0.98 | 0.11 | 37,37,41,43 | 0 |
| 14 | HEA | N | 602[A] | 60/60 | 0.98 | 0.12 | 18,24,38,44 | 18 |
| 14 | HEA | N | 602[B] | 54/60 | 0.98 | 0.12 | 15,24,33,40 | 12 |
| 22 | EDO | S | 102 | 4/4 | 0.98 | 0.12 | 20,22,22,24 | 0 |
| 14 | HEA | N | 602[C] | 51/60 | 0.98 | 0.12 | 16,24,28,33 | 9 |
| 22 | EDO | N | 617 | 4/4 | 0.98 | 0.12 | 20,26,28,31 | 0 |
| 22 | EDO | N | 618 | 4/4 | 0.98 | 0.16 | 29,42,46,46 | 0 |
| 22 | EDO | A | 619 | 4/4 | 0.98 | 0.12 | 28,42,71,95 | 0 |
| 22 | EDO | S | 107 | 4/4 | 0.98 | 0.18 | 28,45,48,62 | 0 |
| 14 | HEA | N | 603 | 60/60 | 0.98 | 0.10 | 18,23,28,37 | 0 |
| 14 | HEA | A | 601[A] | 60/60 | 0.98 | 0.13 | 17,21,40,61 | 18 |
| 14 | HEA | A | 601[B] | 54/60 | 0.98 | 0.13 | 9,20,29,45 | 12 |
| 22 | EDO | O | 303 | 4/4 | 0.98 | 0.11 | 25,29,30,31 | 0 |
| 22 | EDO | B | 303 | 4/4 | 0.98 | 0.09 | 21,25,26,32 | 0 |
| 17 | NA | N | 606 | 1/1 | 0.98 | 0.07 | 30,30,30,30 | 0 |
| 19 | PGV | C | 306 | 48/51 | 0.98 | 0.13 | 21,28,66,92 | 0 |
| 22 | EDO | A | 613 | 4/4 | 0.98 | 0.14 | 21,24,30,30 | 0 |
| 14 | HEA | A | 601[C] | 51/60 | 0.98 | 0.13 | 9,20,24,40 | 9 |
| 16 | MG | N | 605 | 1/1 | 0.99 | 0.05 | 21,21,21,21 | 0 |
| 28 | ZN | S | 101 | 1/1 | 0.99 | 0.11 | 25,25,25,25 | 0 |
| 17 | NA | A | 605 | 1/1 | 0.99 | 0.08 | 24,24,24,24 | 0 |
| 22 | EDO | F | 104 | 4/4 | 0.99 | 0.13 | 22,24,25,27 | 0 |
| 15 | CU | A | 603 | 1/1 | 1.00 | 0.15 | 23,23,23,23 | 0 |
| 28 | ZN | F | 101 | 1/1 | 1.00 | 0.11 | 26,26,26,26 | 0 |
| 24 | CUA | B | 301 | 2/2 | 1.00 | 0.13 | 22,22,22,23 | 0 |
| 24 | CUA | O | 301 | 2/2 | 1.00 | 0.12 | 26,26,26,26 | 0 |
| 15 | CU | N | 604 | 1/1 | 1.00 | 0.14 | 24,24,24,24 | 0 |

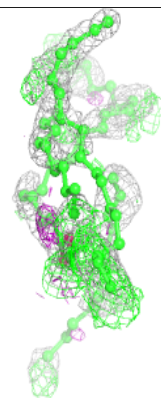
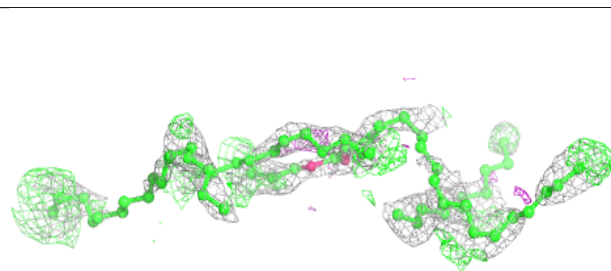
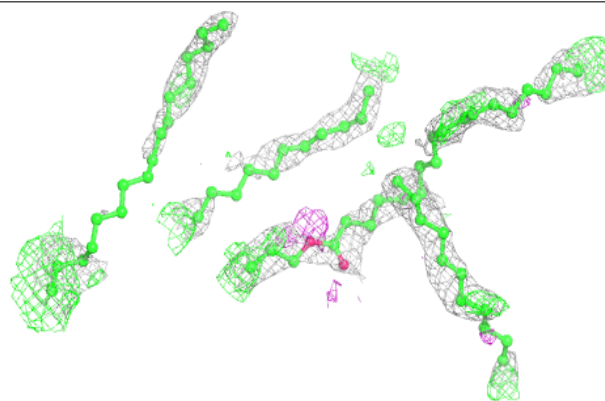
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU X 102:

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

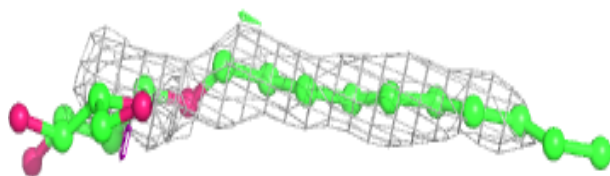
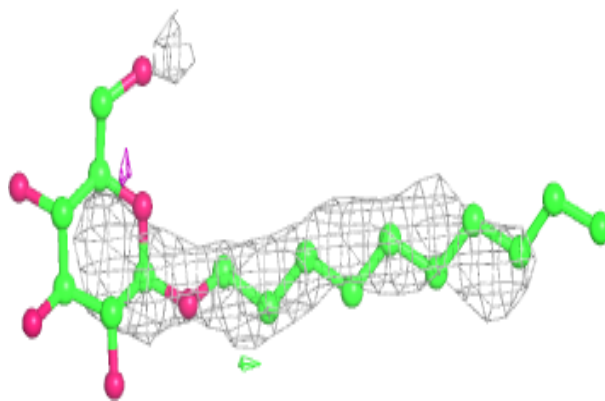
**Electron density around CDL N 601:**

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



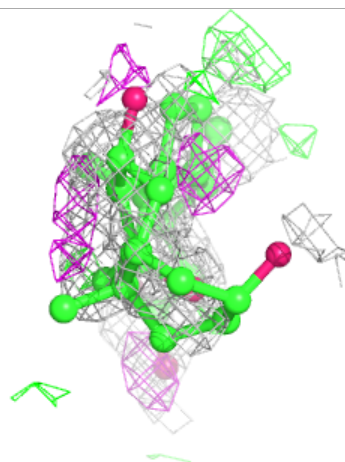
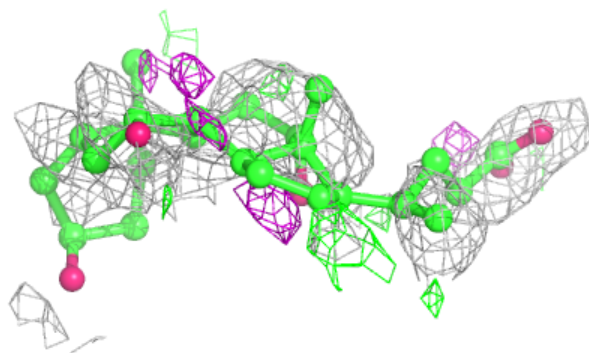
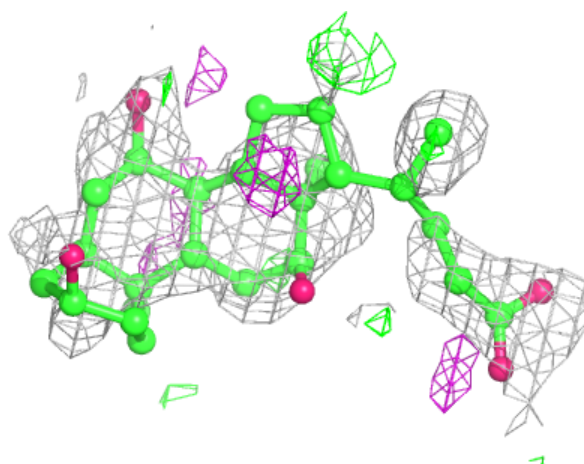
Electron density around DMU X 104:

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



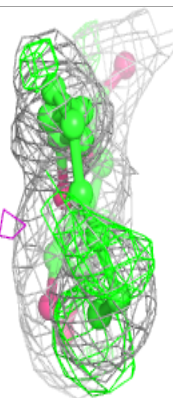
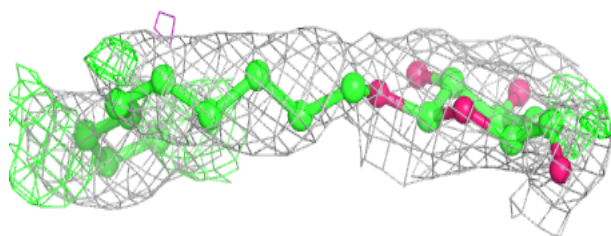
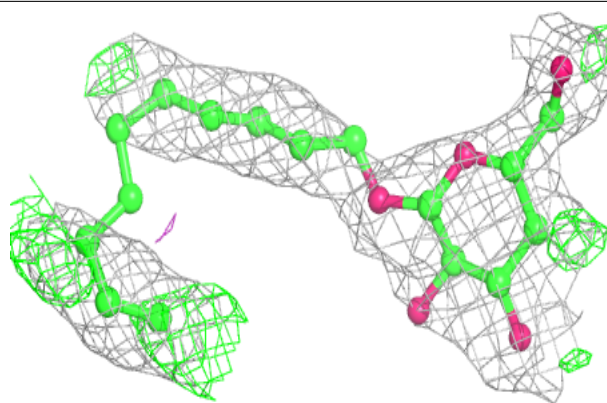
Electron density around CHD J 101:

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

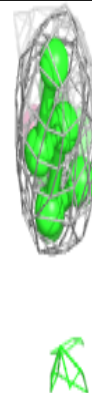
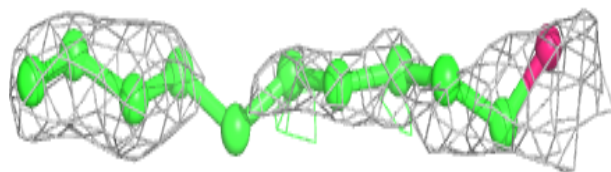
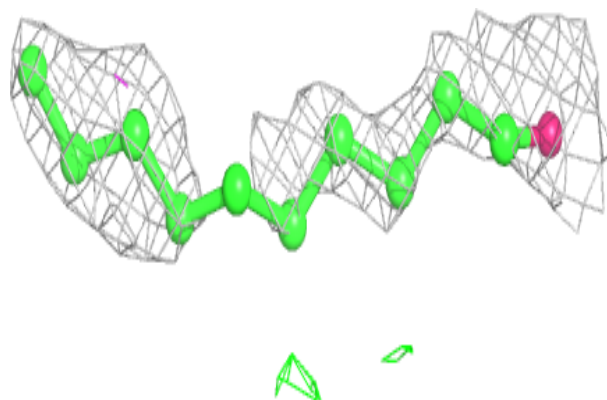


Electron density around DMU L 105:

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

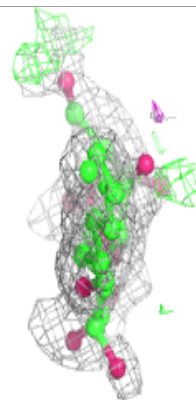
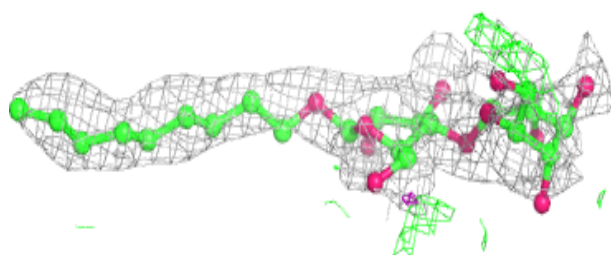
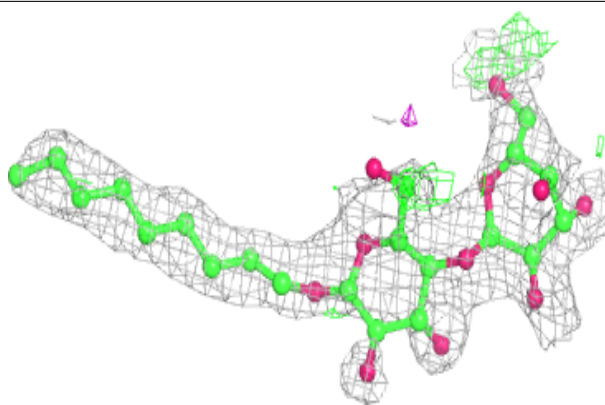
**Electron density around DMU D 207:**

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

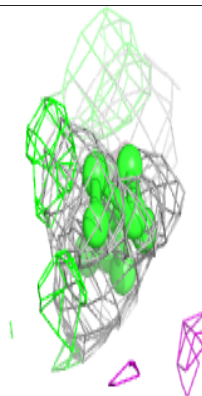
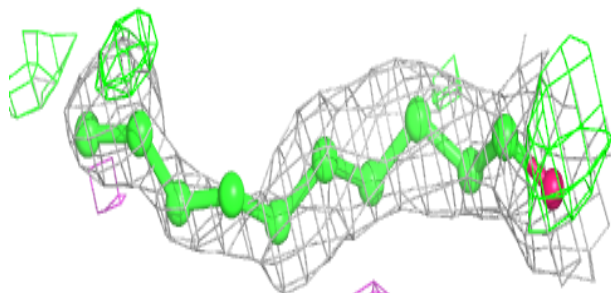
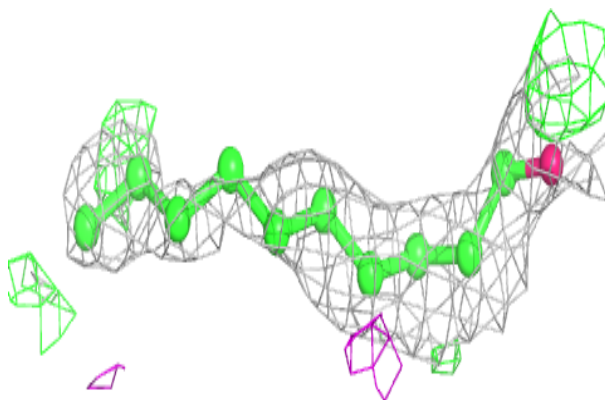


Electron density around DMU P 317:

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

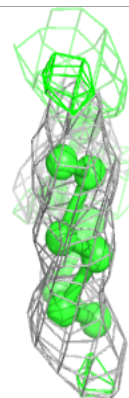
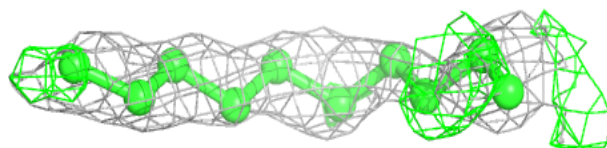
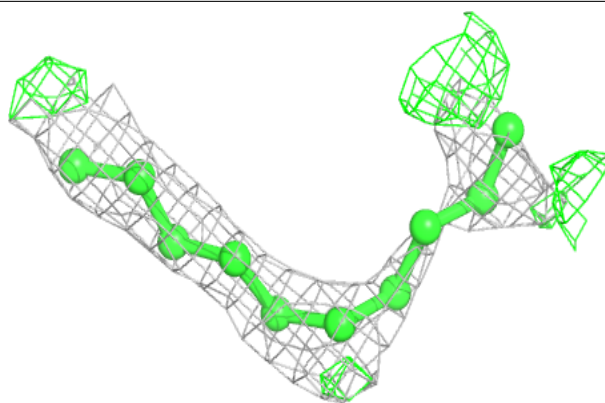
**Electron density around DMU Q 201:**

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



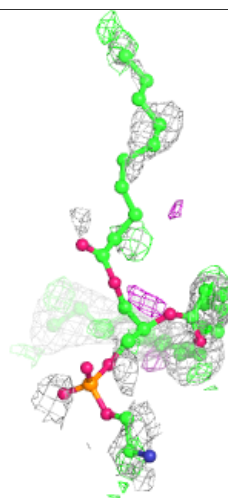
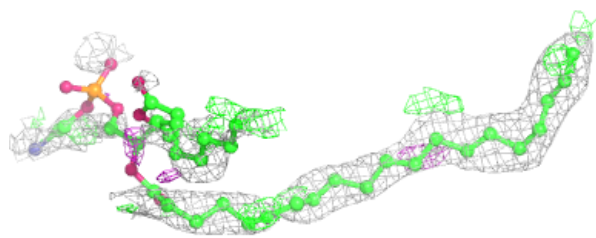
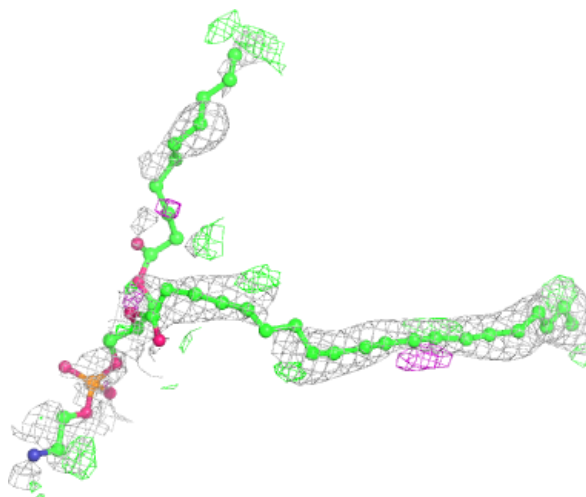
Electron density around DMU K 103:

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



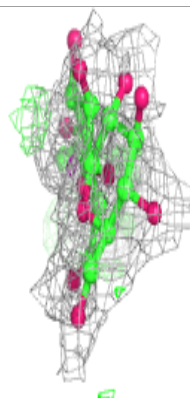
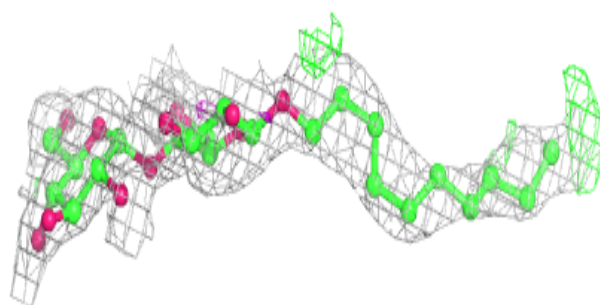
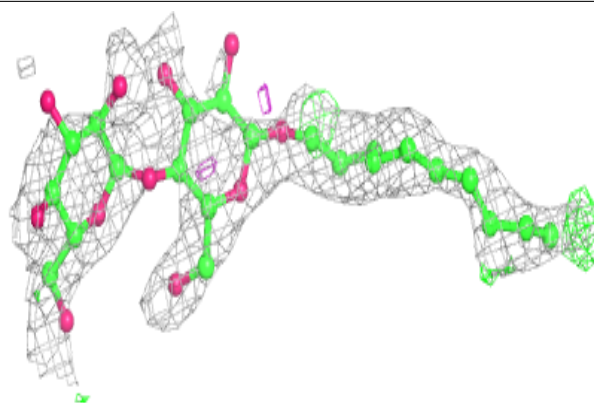
Electron density around PEK C 303:

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

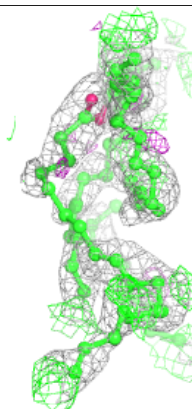
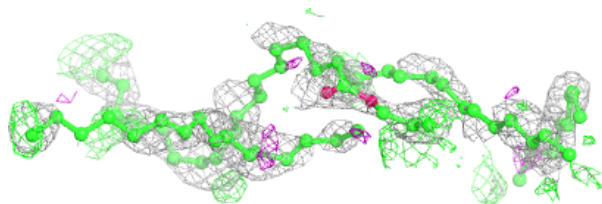
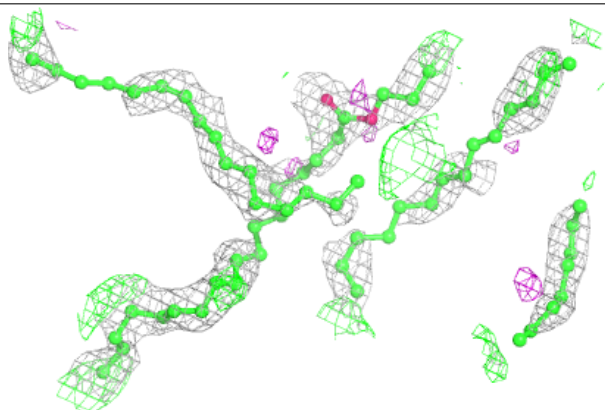


Electron density around DMU D 206:

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

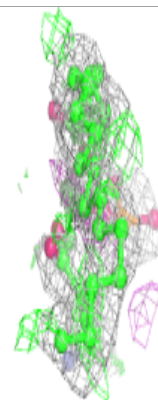
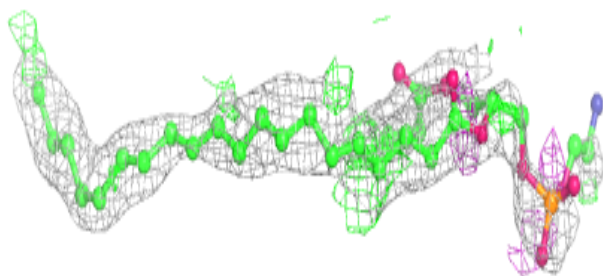
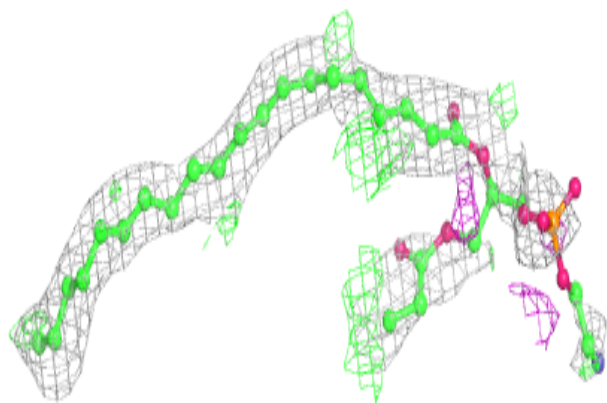
**Electron density around CDL T 102:**

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

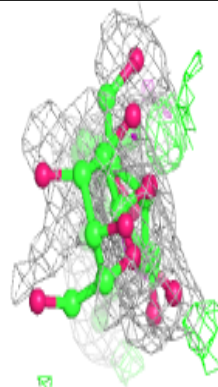
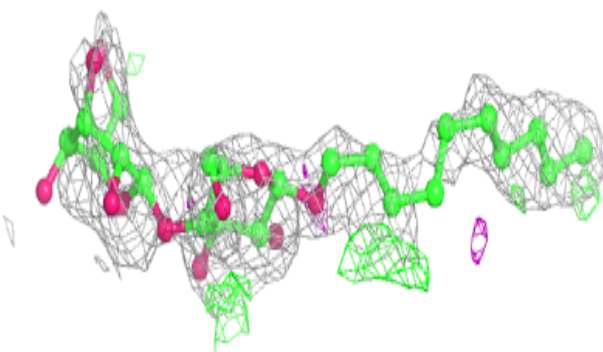
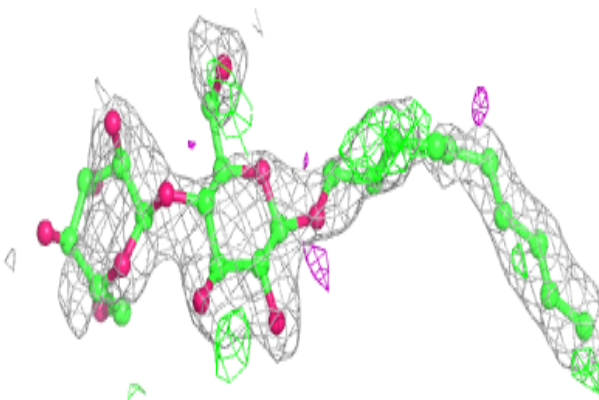


Electron density around PEK P 303:

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

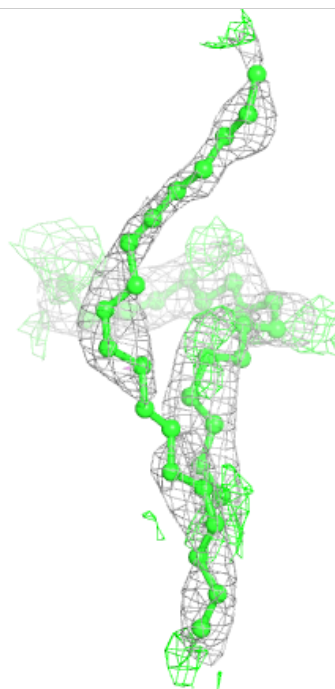
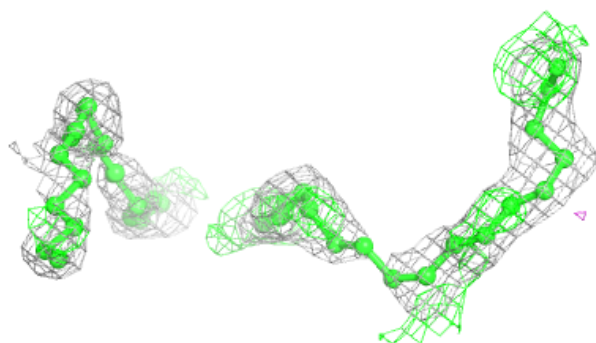
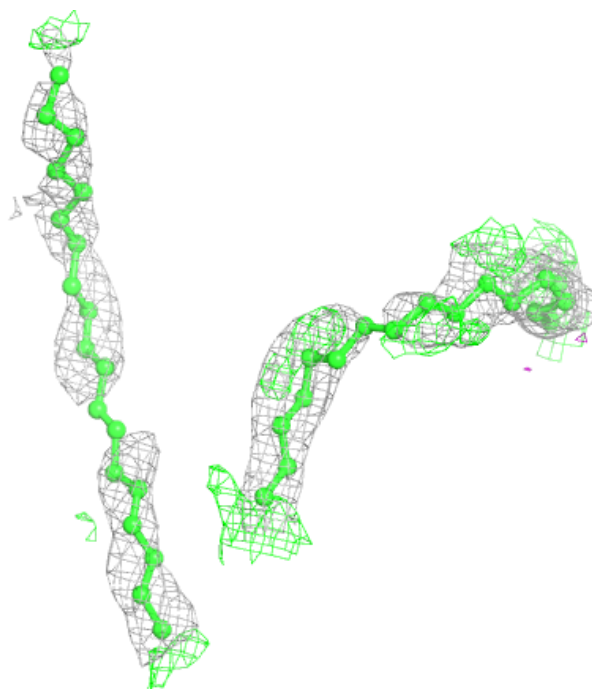
**Electron density around DMU P 308:**

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



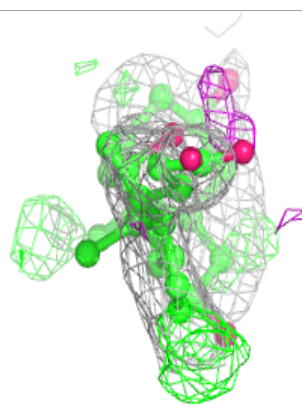
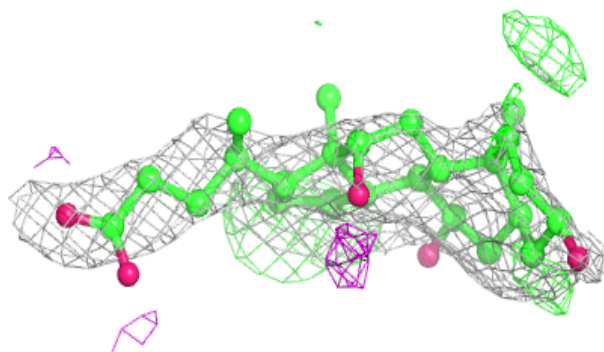
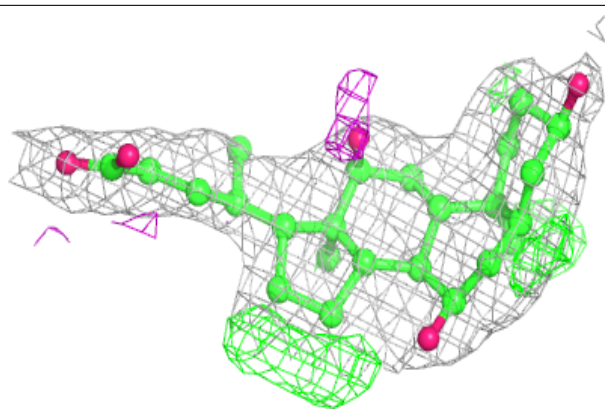
Electron density around PEK C 305:

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

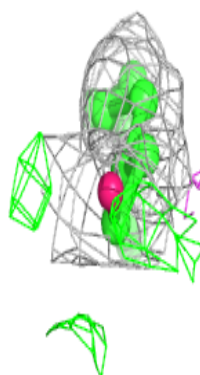
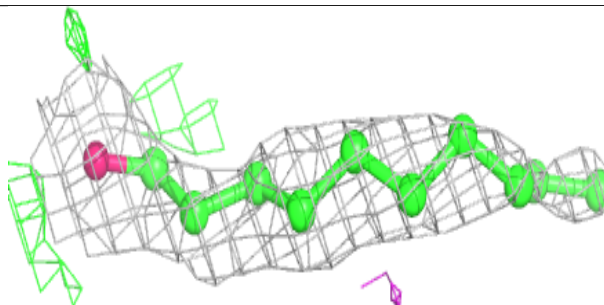
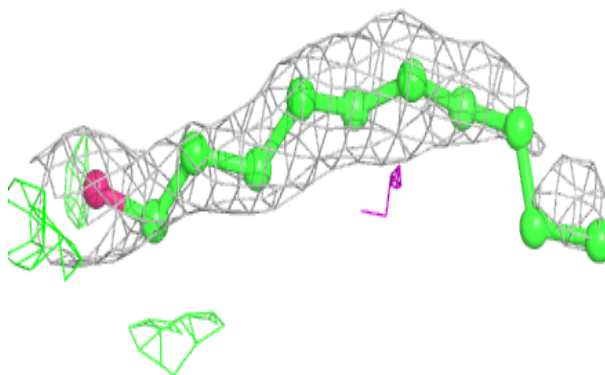


Electron density around CHD Y 102:

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

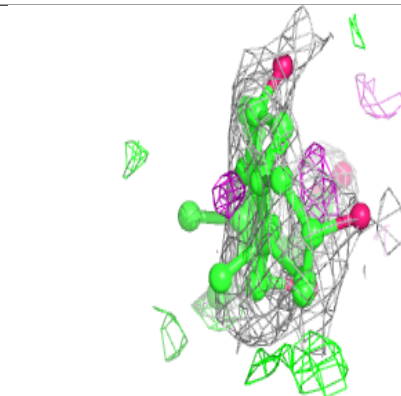
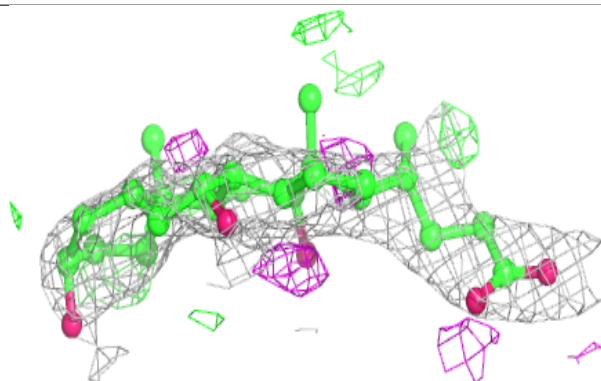
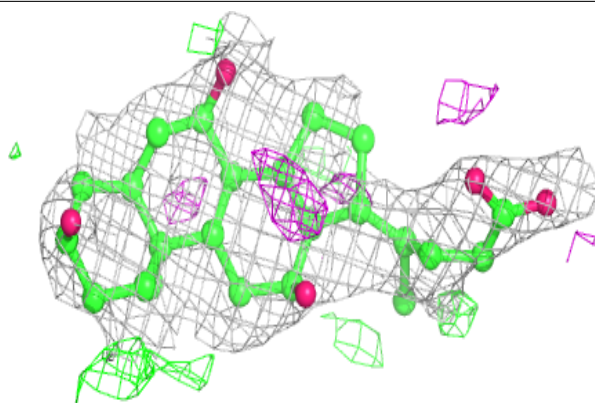
**Electron density around DMU K 102:**

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

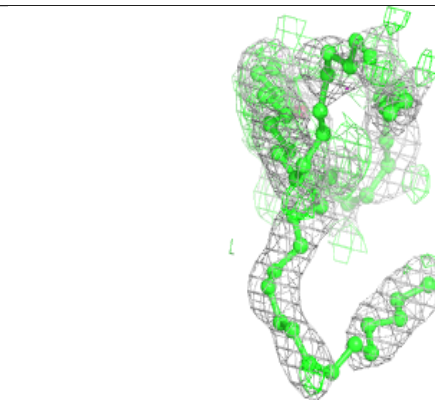
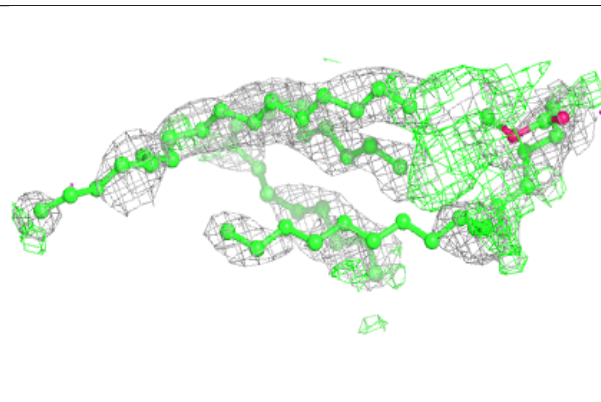
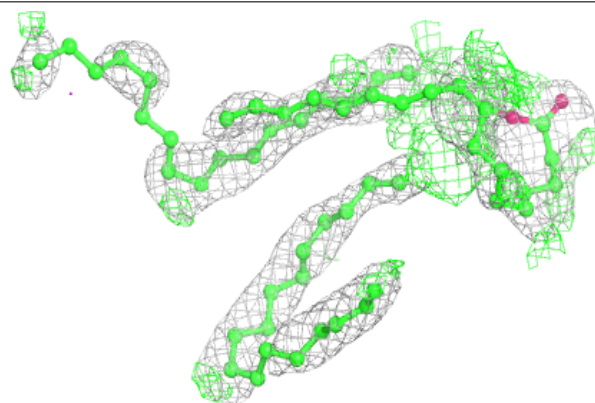


Electron density around CHD L 102:

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

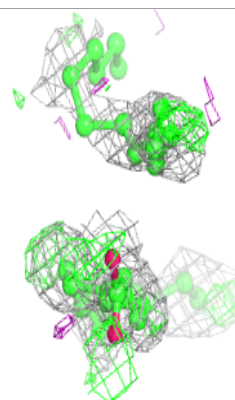
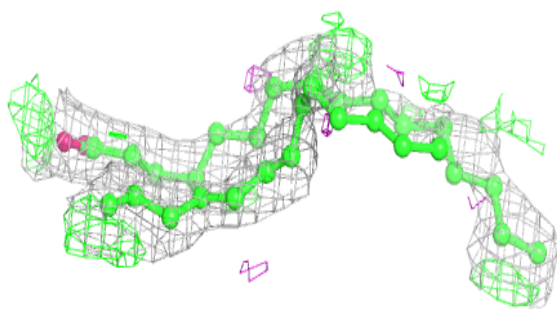
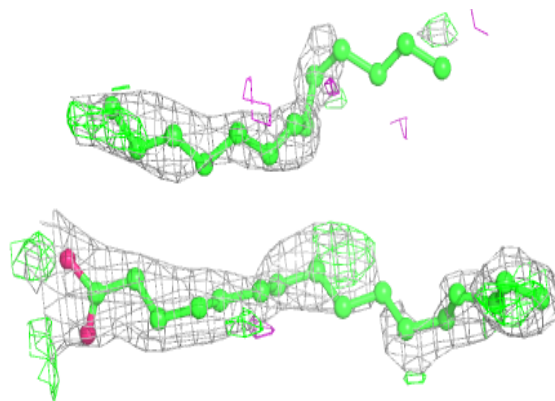
**Electron density around TGL N 609:**

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

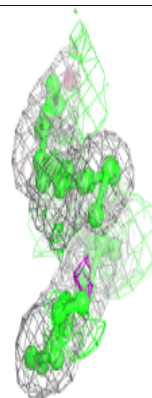
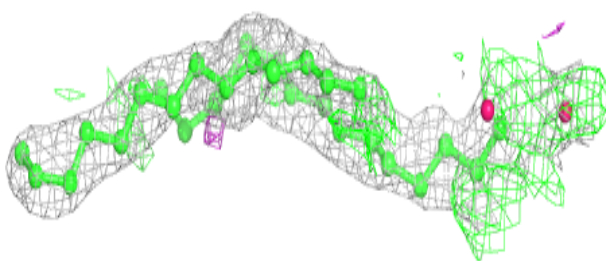
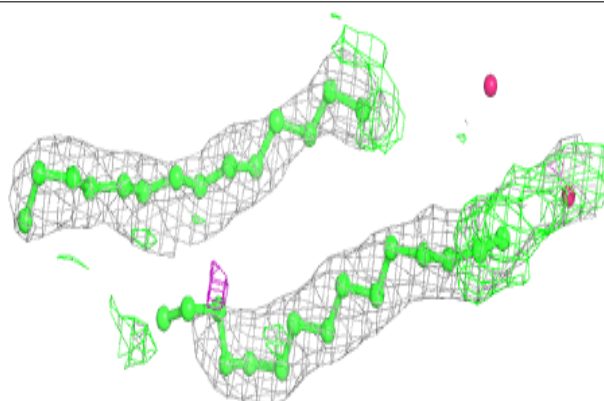


Electron density around PGV P 306:

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

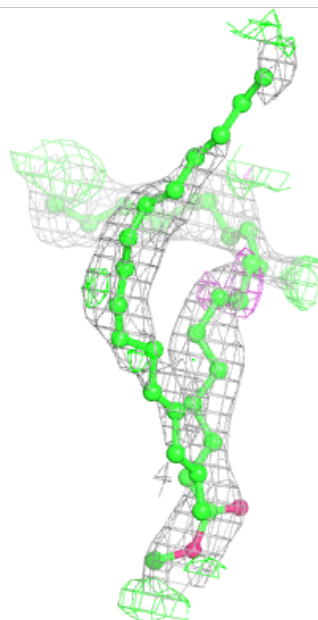
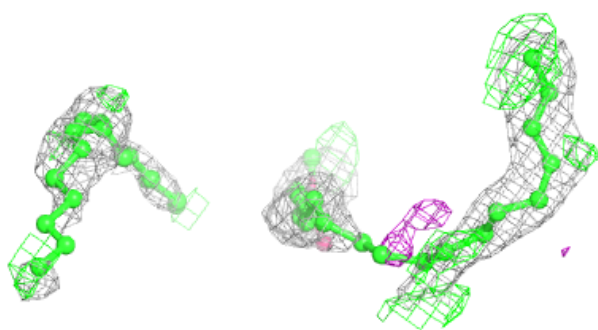
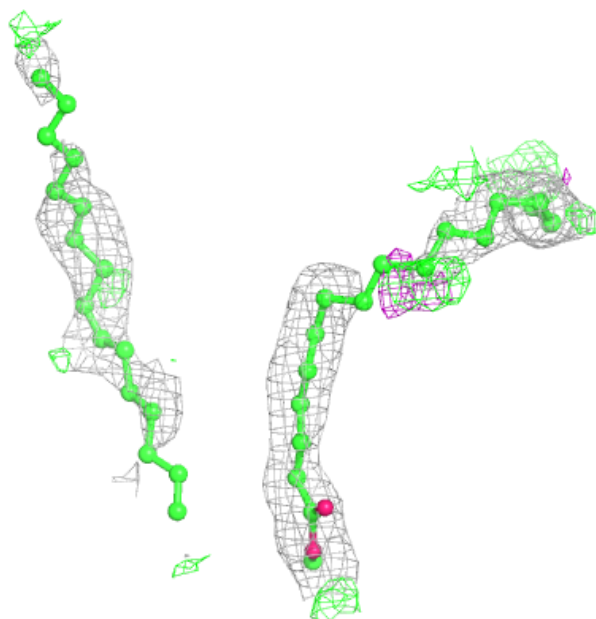
**Electron density around PSC O 302:**

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



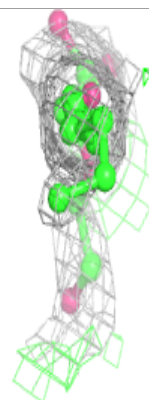
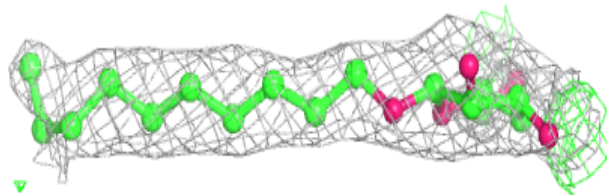
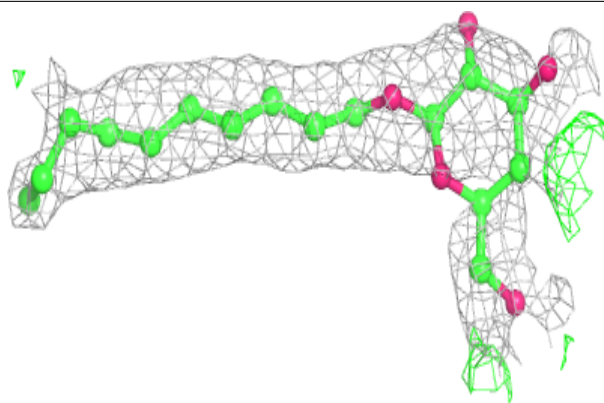
Electron density around PEK T 101:

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

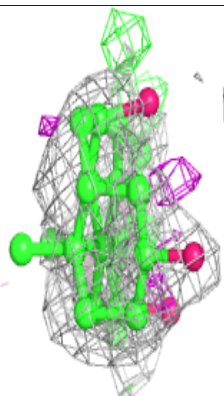
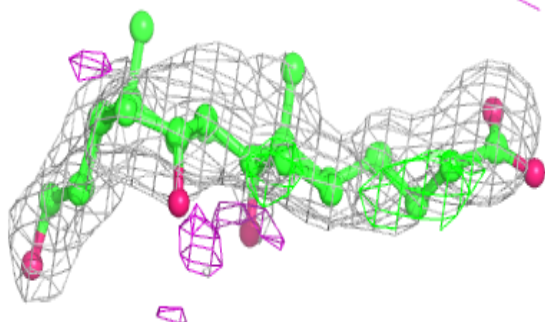
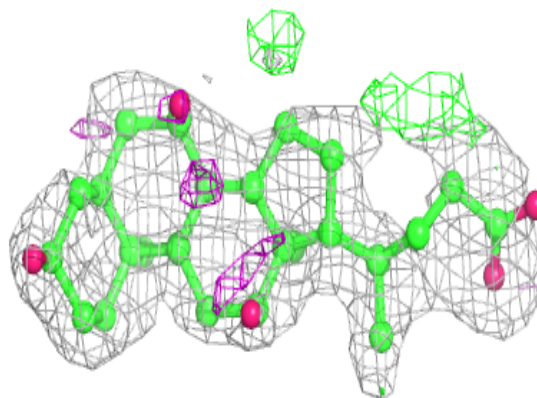


Electron density around DMU P 316:

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

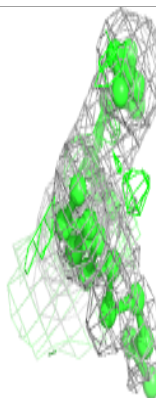
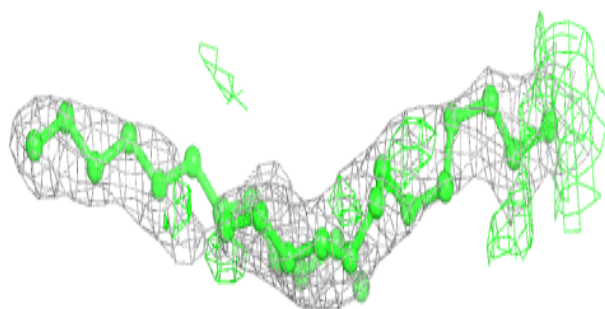
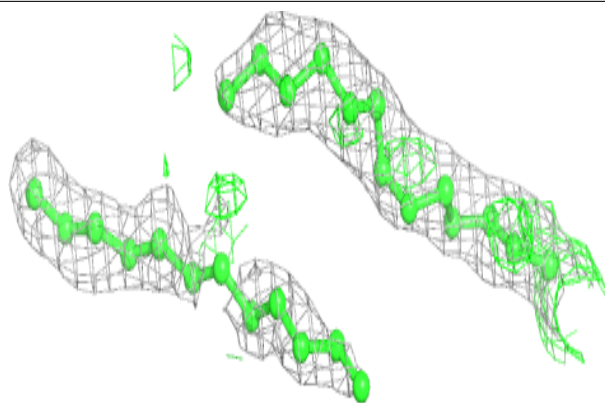
**Electron density around CHD C 309:**

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

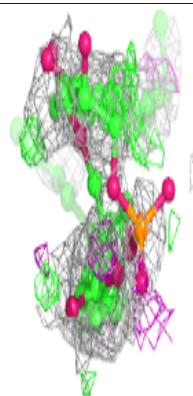
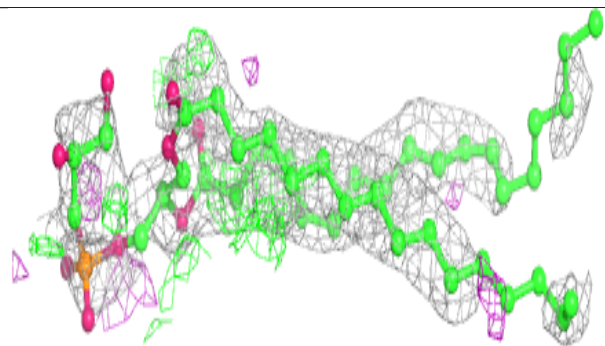
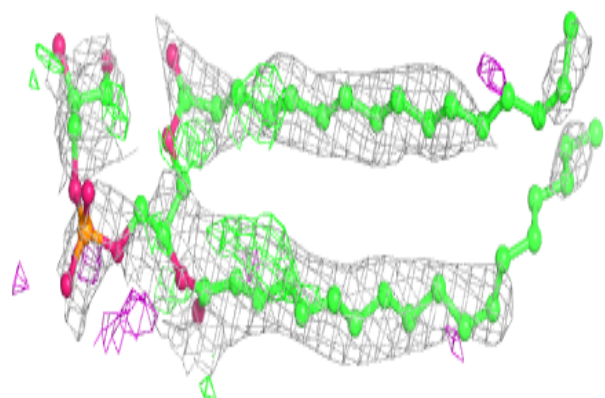


Electron density around PSC A 610:

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

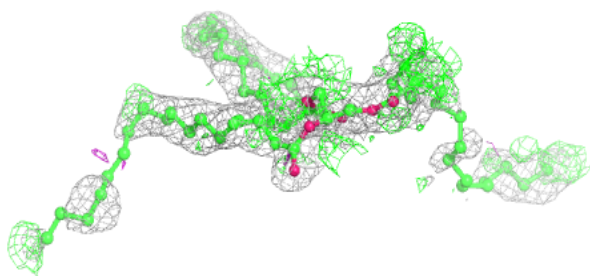
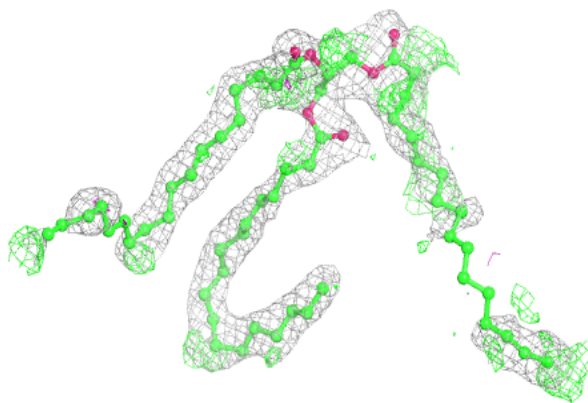
**Electron density around PGV N 610:**

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

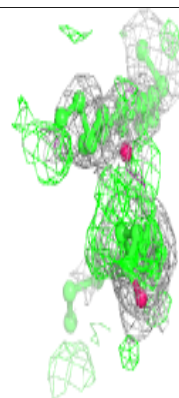
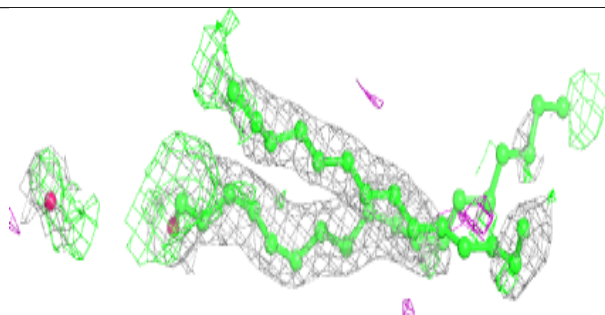
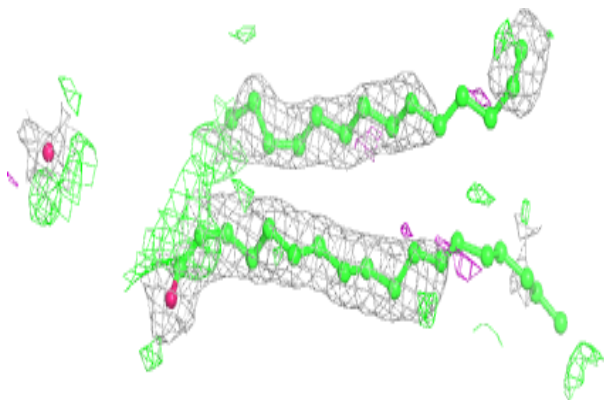


Electron density around TGL A 607:

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

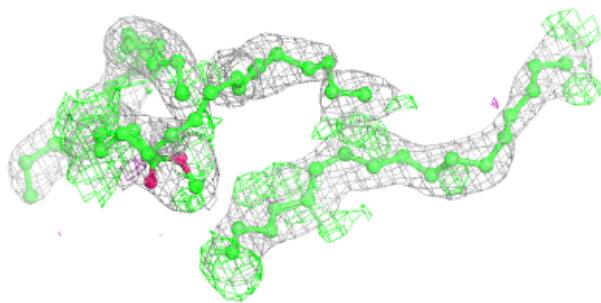
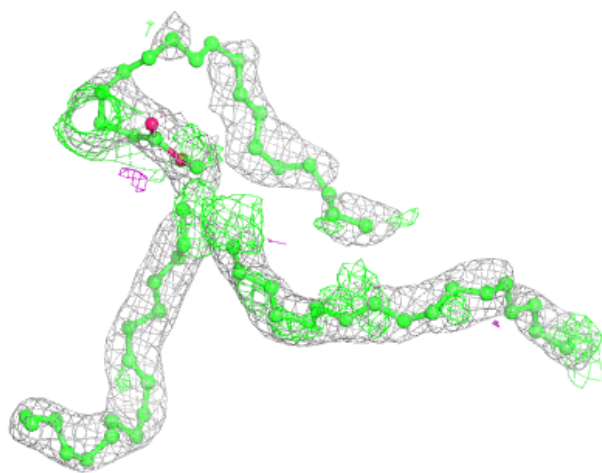
**Electron density around PGV A 608:**

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



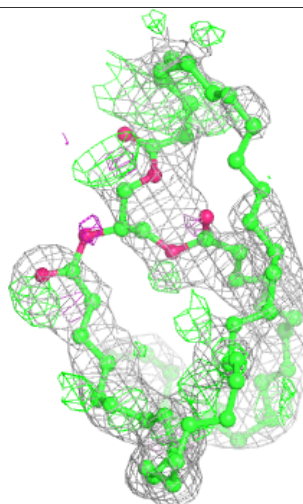
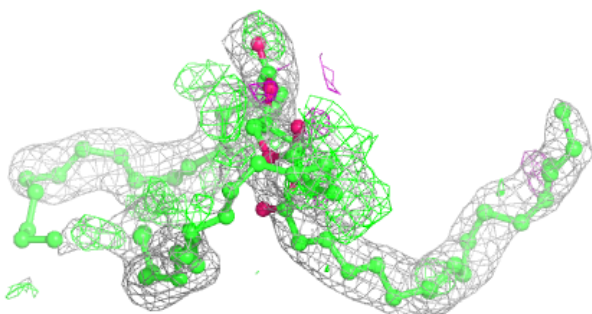
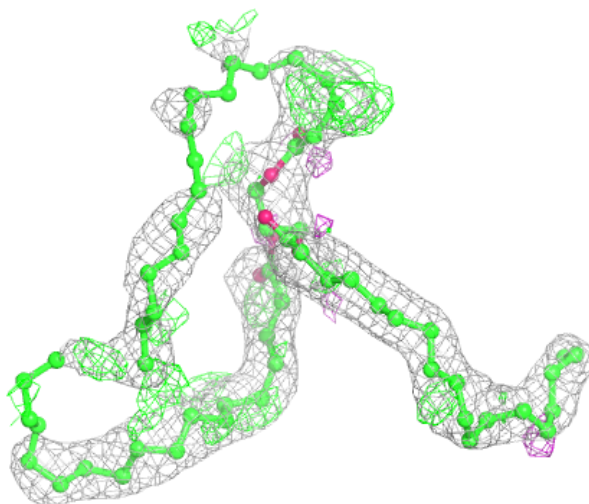
Electron density around TGL N 608:

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



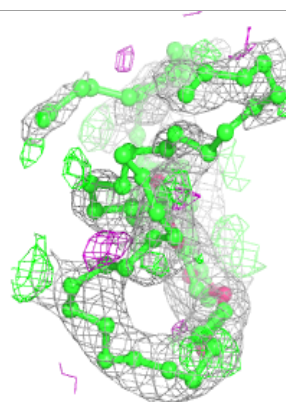
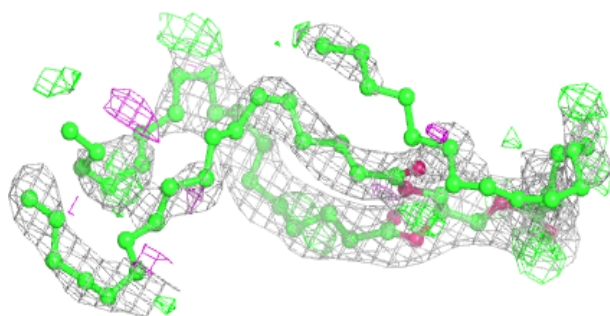
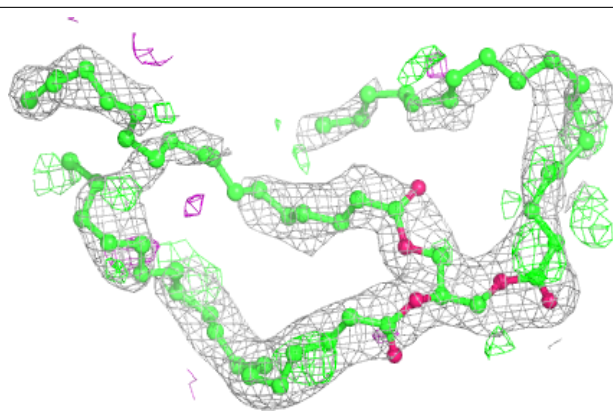
Electron density around TGL L 101:

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

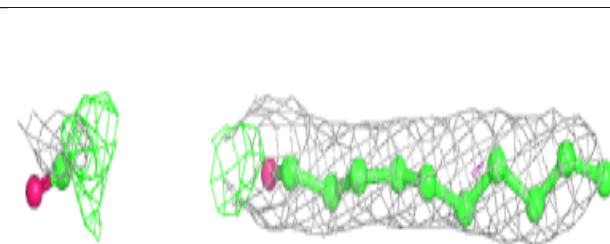
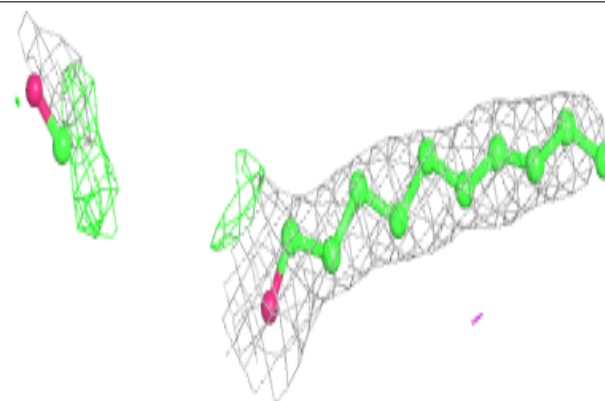


Electron density around TGL N 607:

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

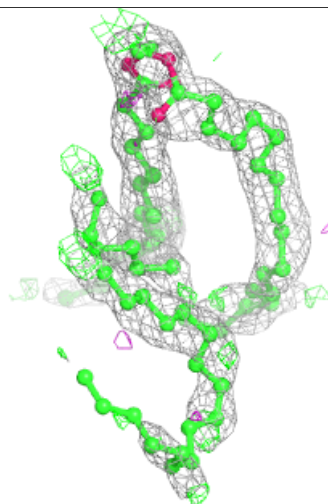
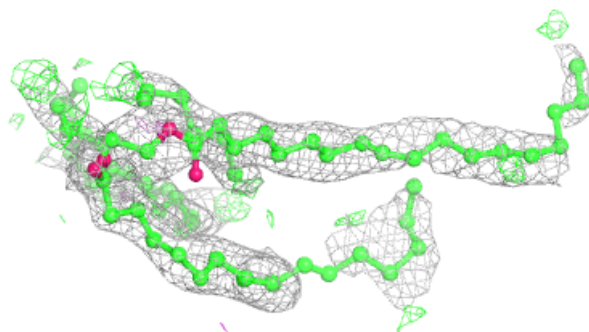
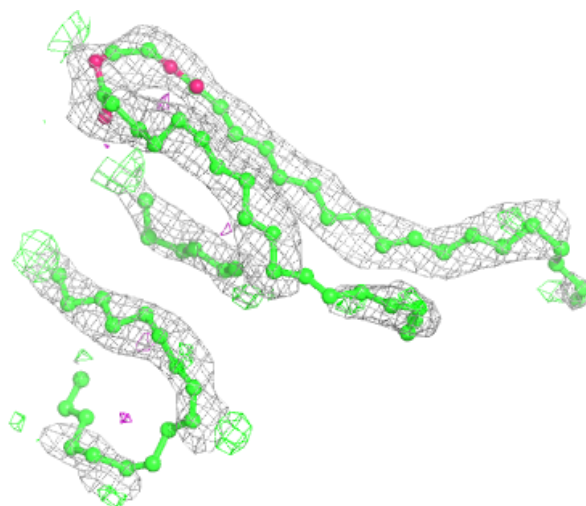
**Electron density around DMU O 306:**

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



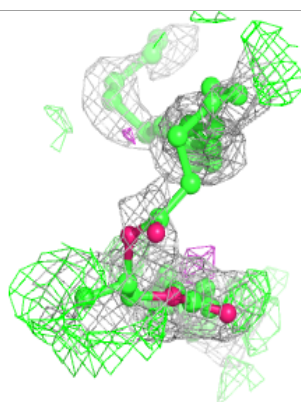
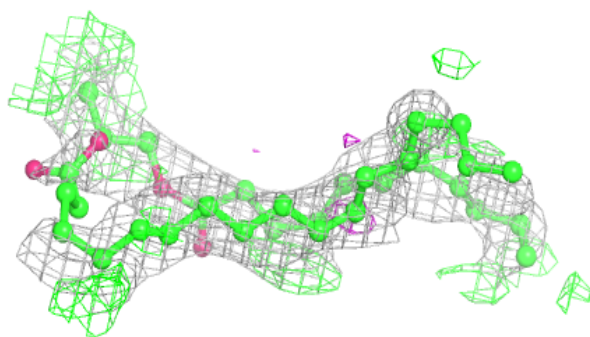
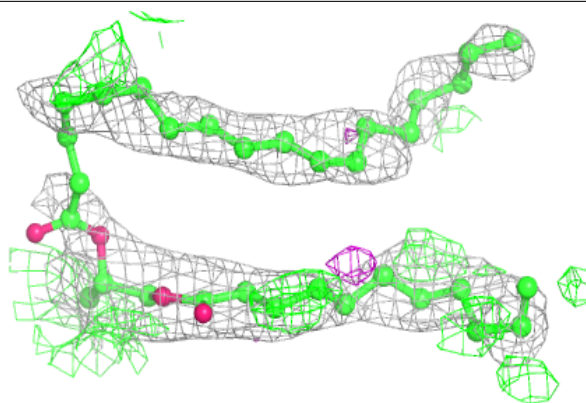
Electron density around CDL C 308:

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

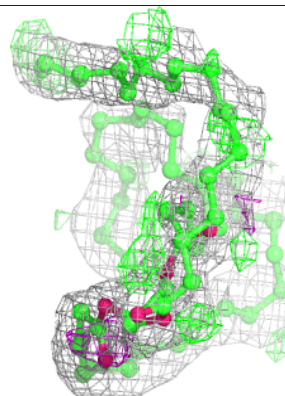
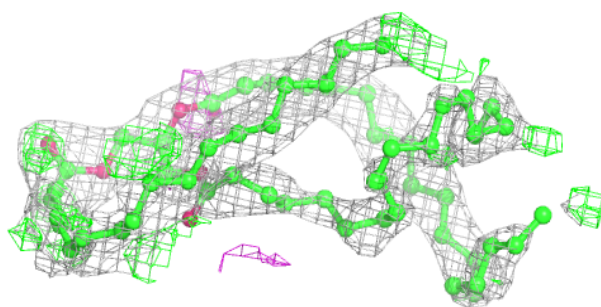
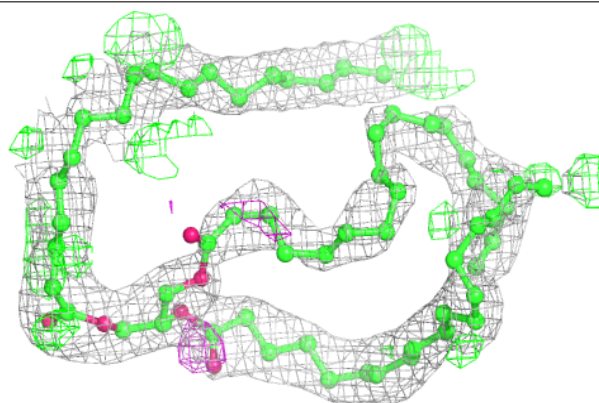


Electron density around PGV C 307:

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

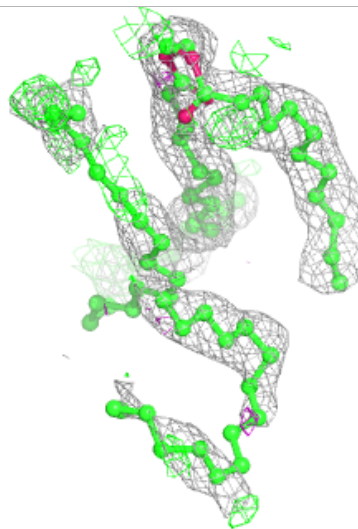
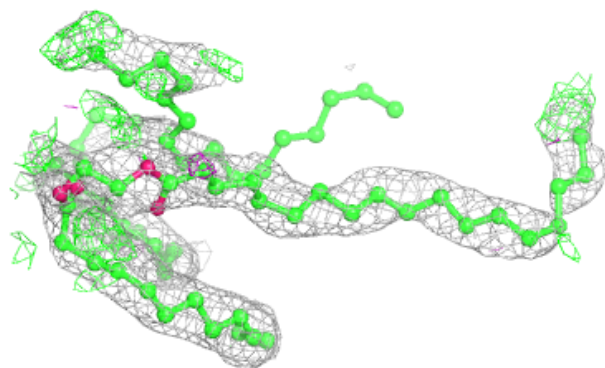
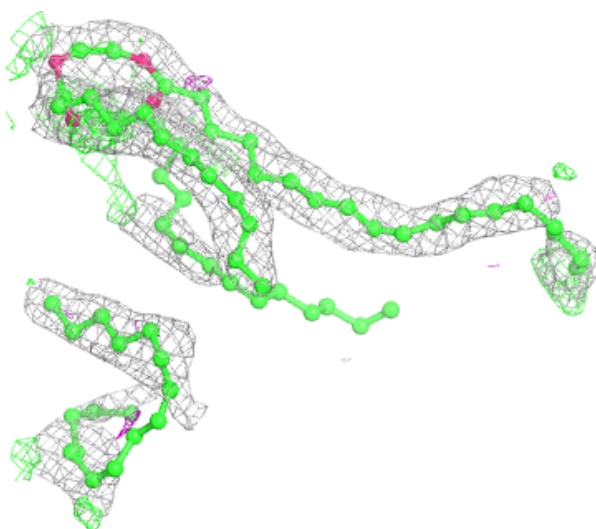
**Electron density around TGL A 606:**

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



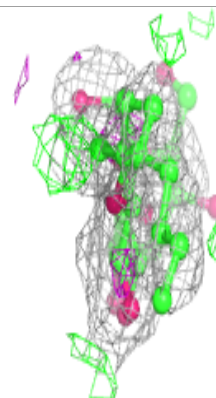
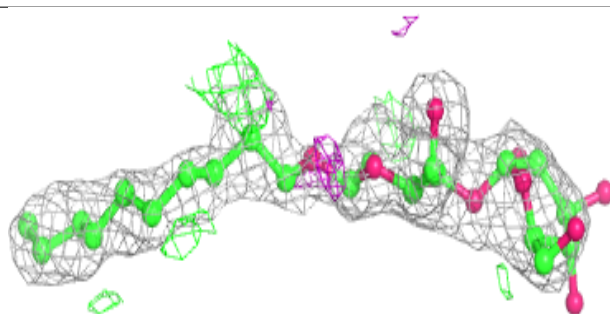
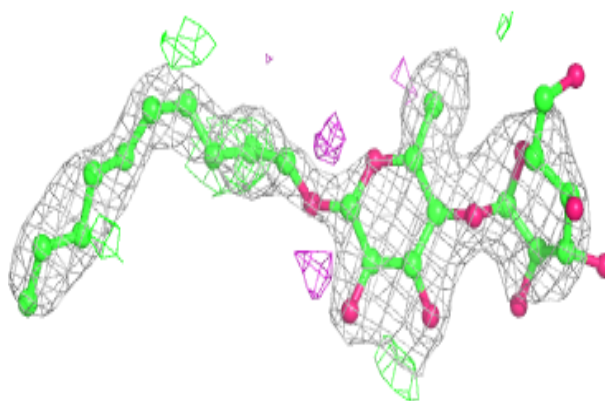
Electron density around CDL P 307:

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

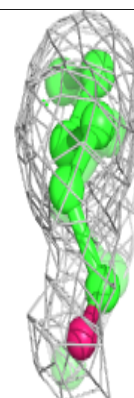
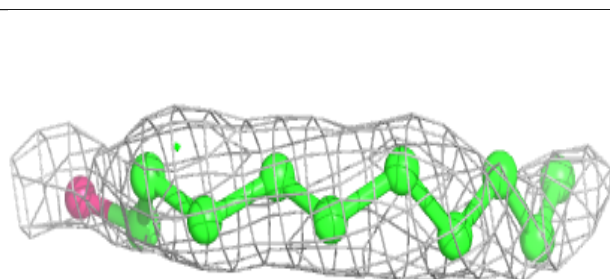
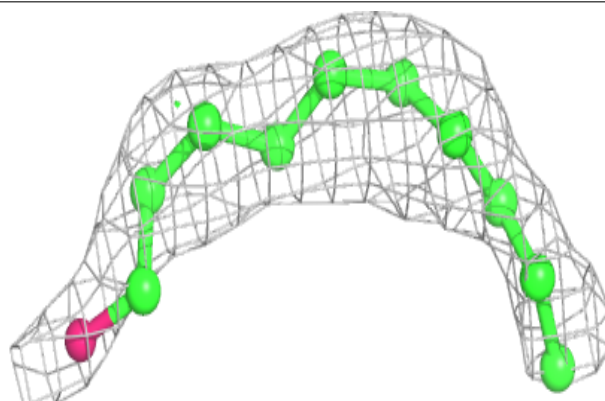


Electron density around DMU C 310:

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

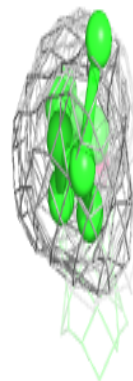
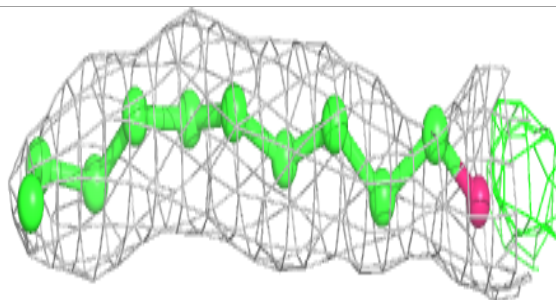
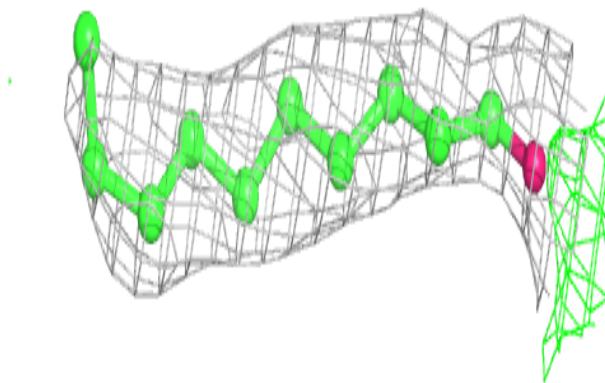
**Electron density around DMU K 104:**

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

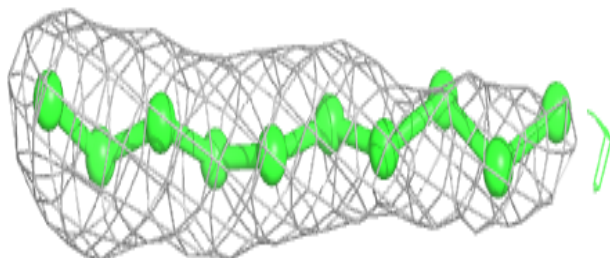
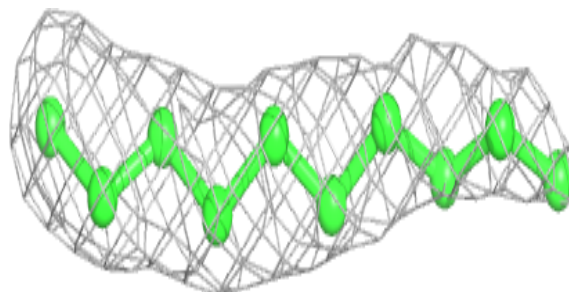


Electron density around DMU J 104:

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

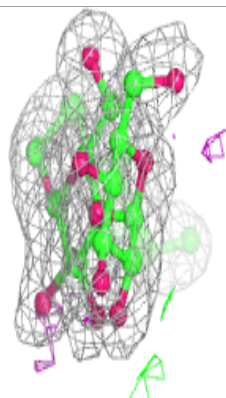
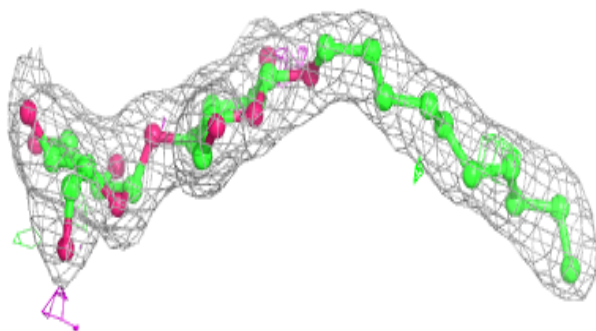
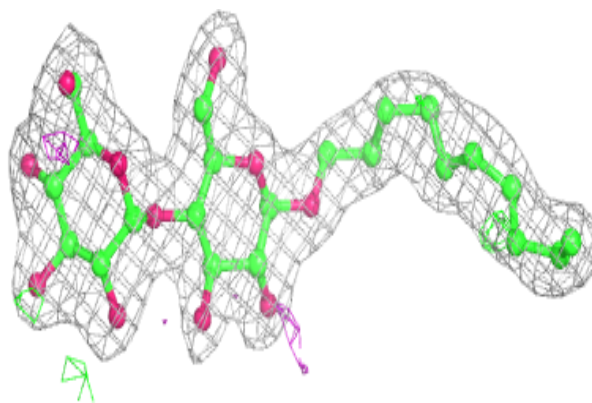
**Electron density around DMU X 101:**

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

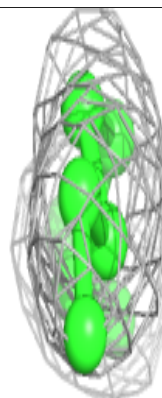
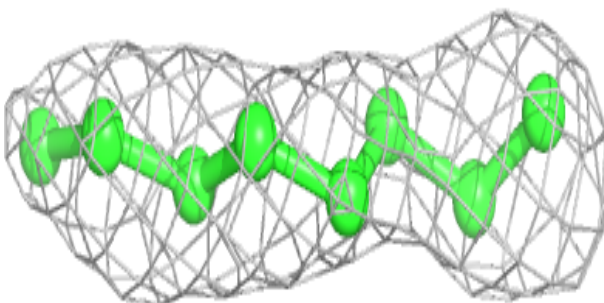
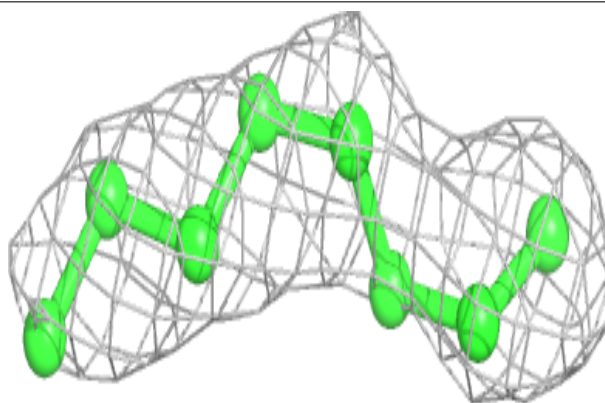


Electron density around DMU Z 101:

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

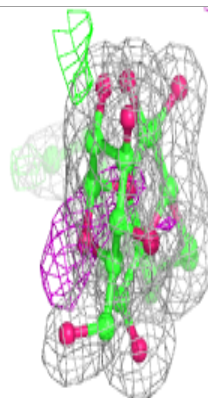
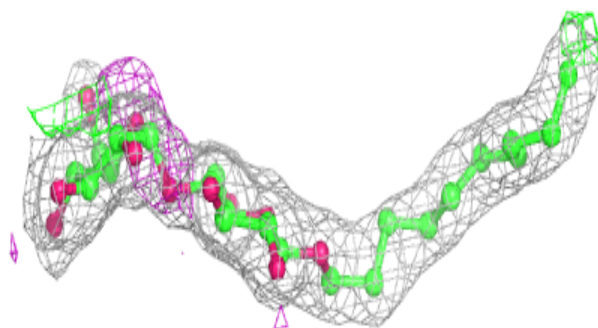
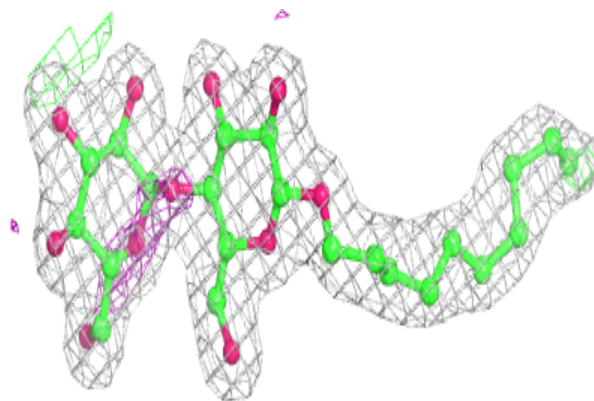
**Electron density around DMU K 101:**

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

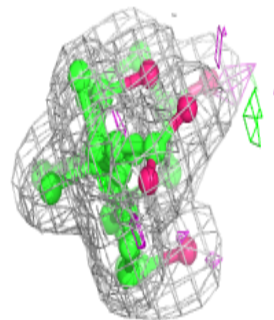
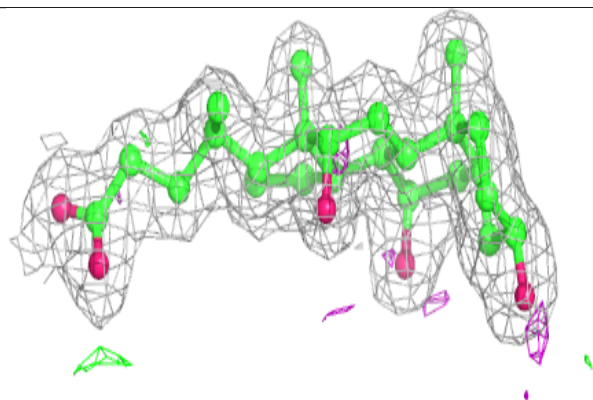
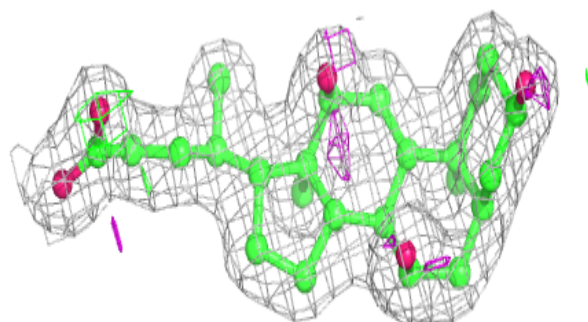


Electron density around DMU M 101:

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

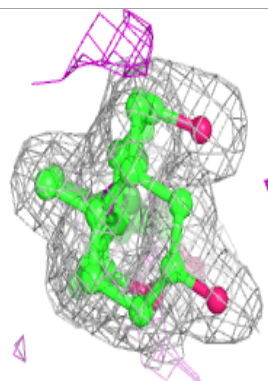
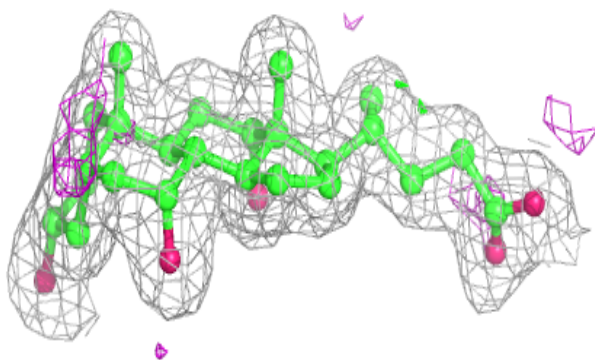
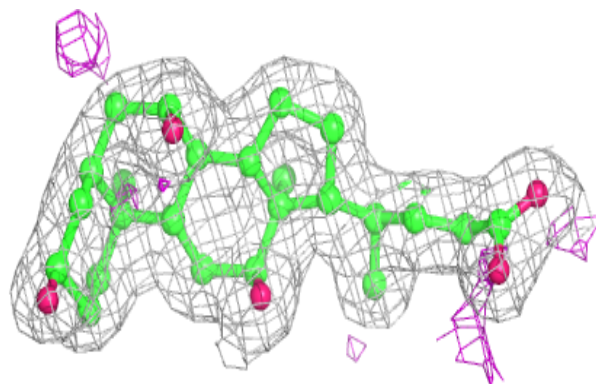
**Electron density around CHD C 301:**

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

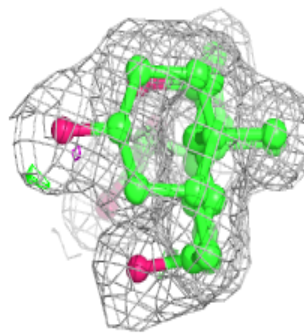
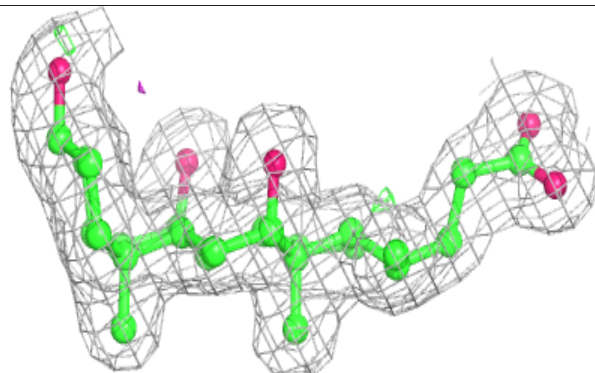
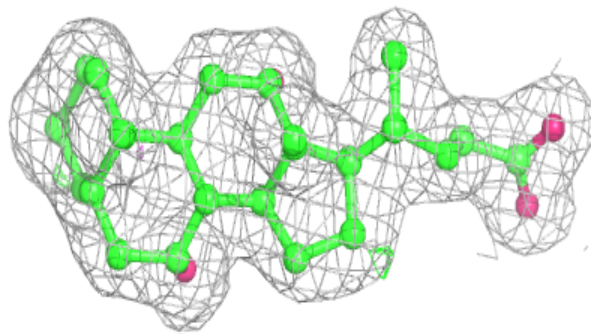


Electron density around CHD P 301:

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

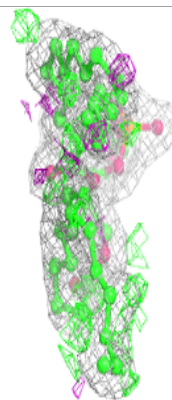
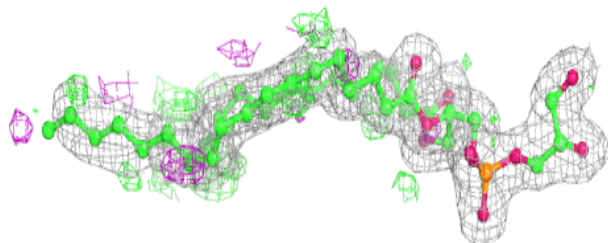
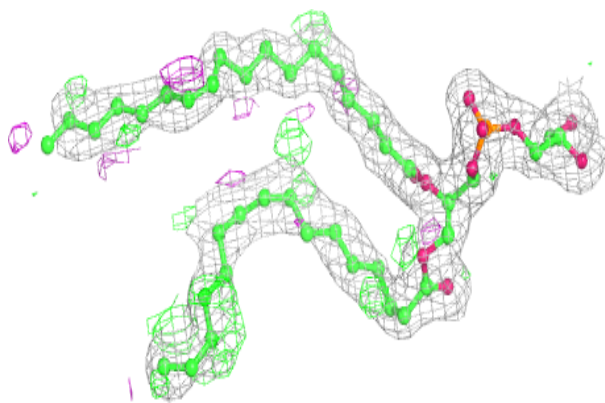
**Electron density around CHD G 101:**

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

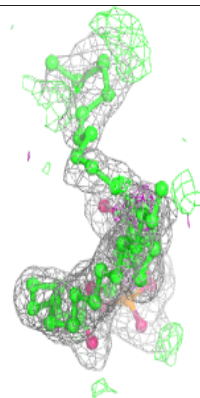
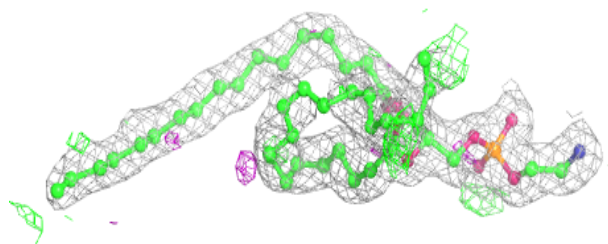
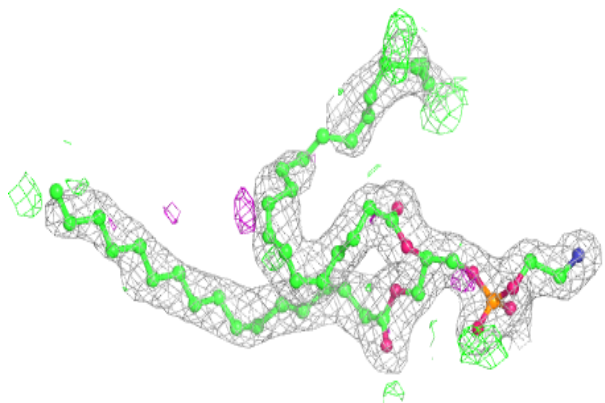


Electron density around PGV N 612:

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

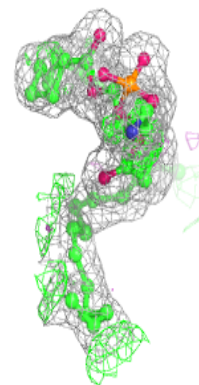
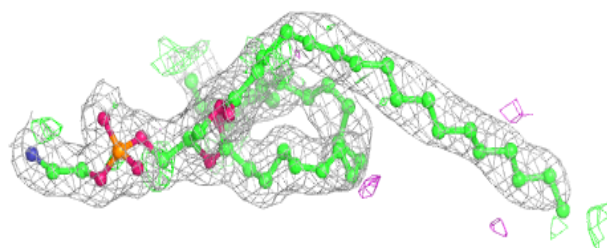
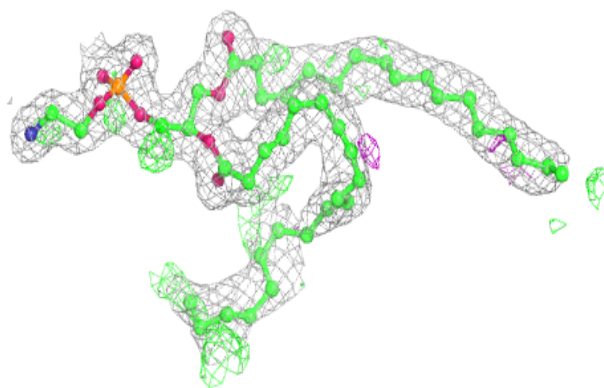
**Electron density around PEK P 304:**

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

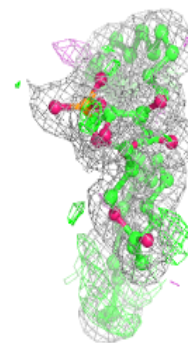
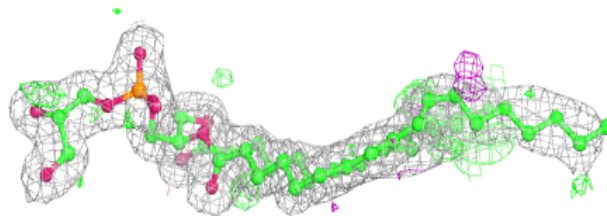
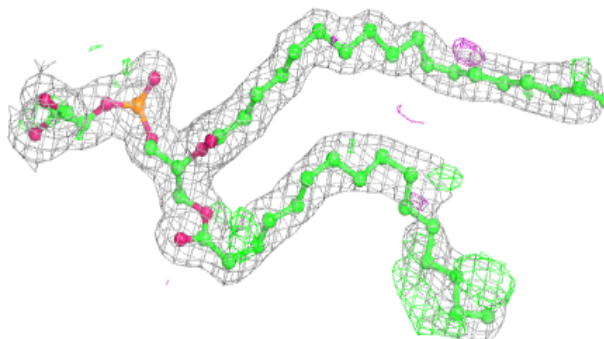


Electron density around PEK C 304:

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

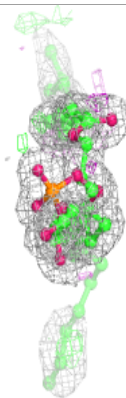
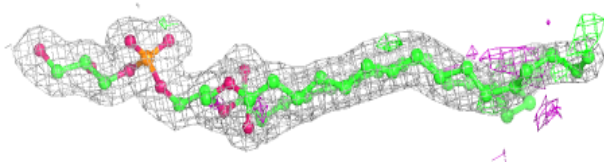
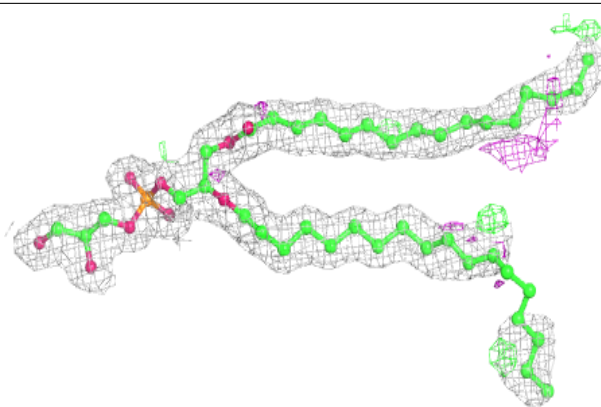
**Electron density around PGV A 611:**

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

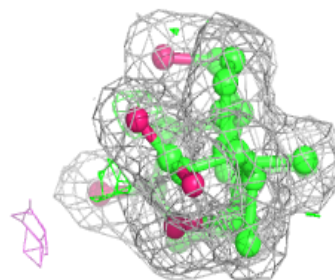
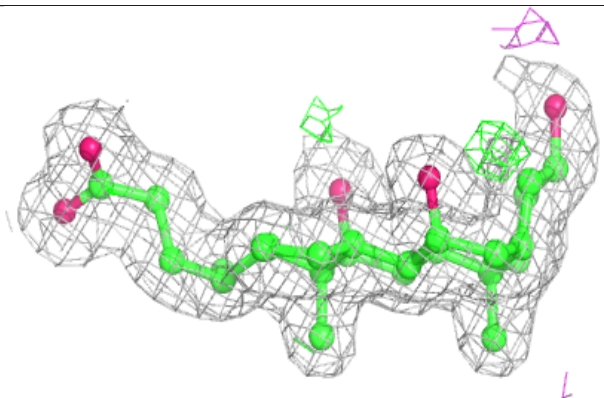
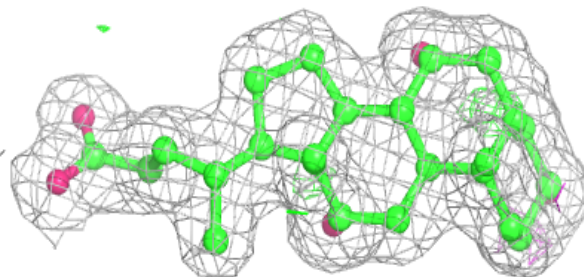


Electron density around PGV P 305:

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

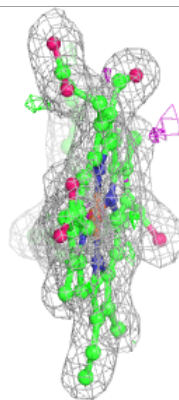
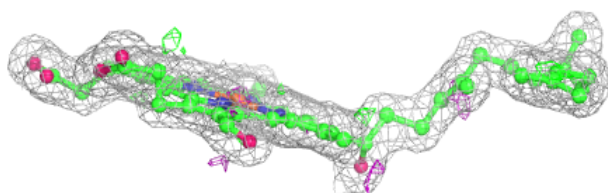
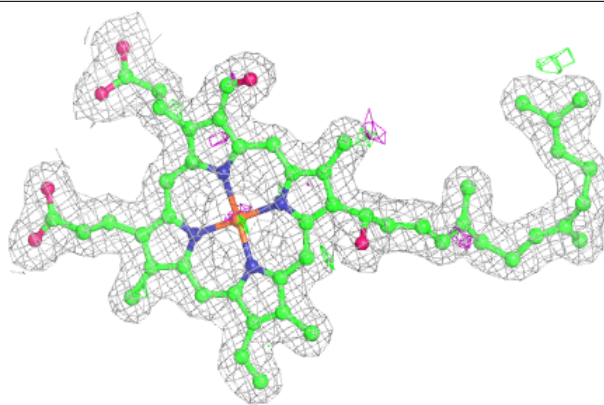
**Electron density around CHD B 302:**

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

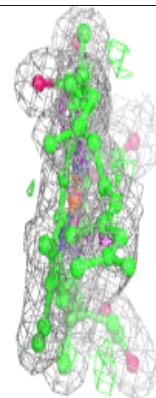
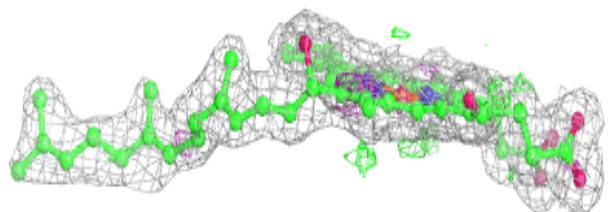
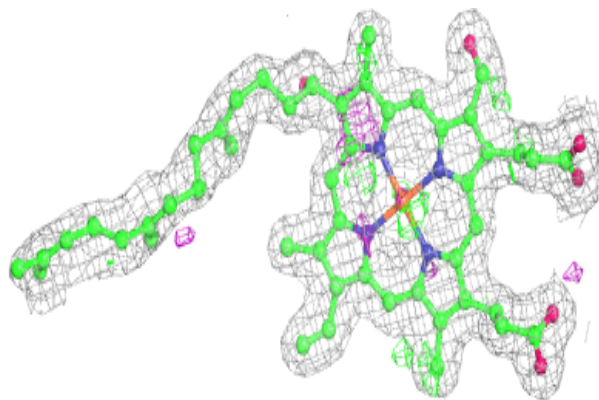


Electron density around HEA A 602:

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

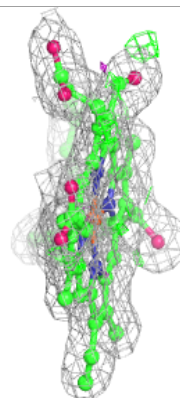
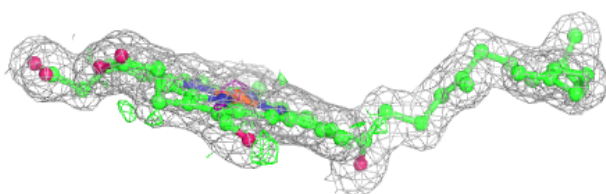
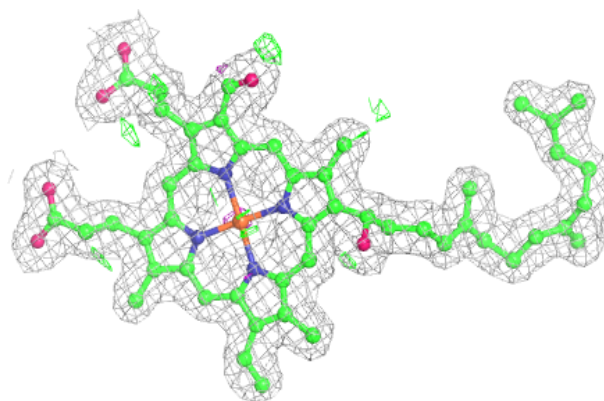
**Electron density around HEA N 602 (A):**

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

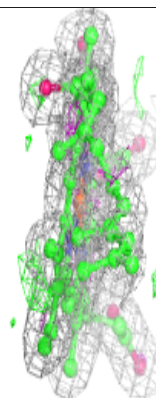
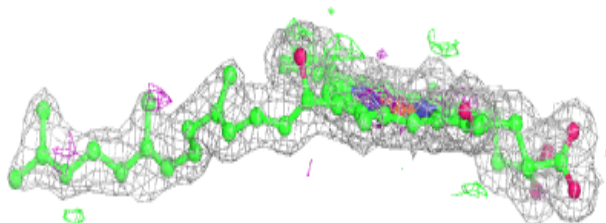
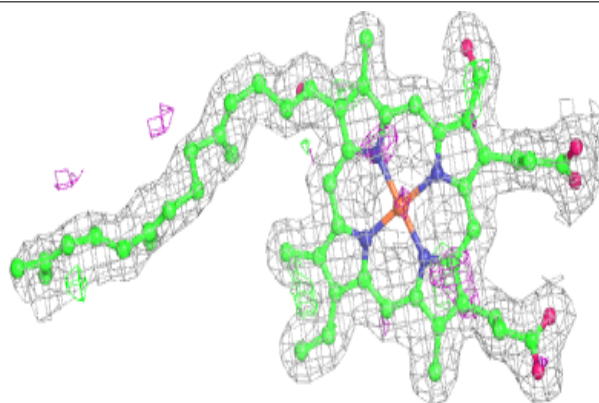


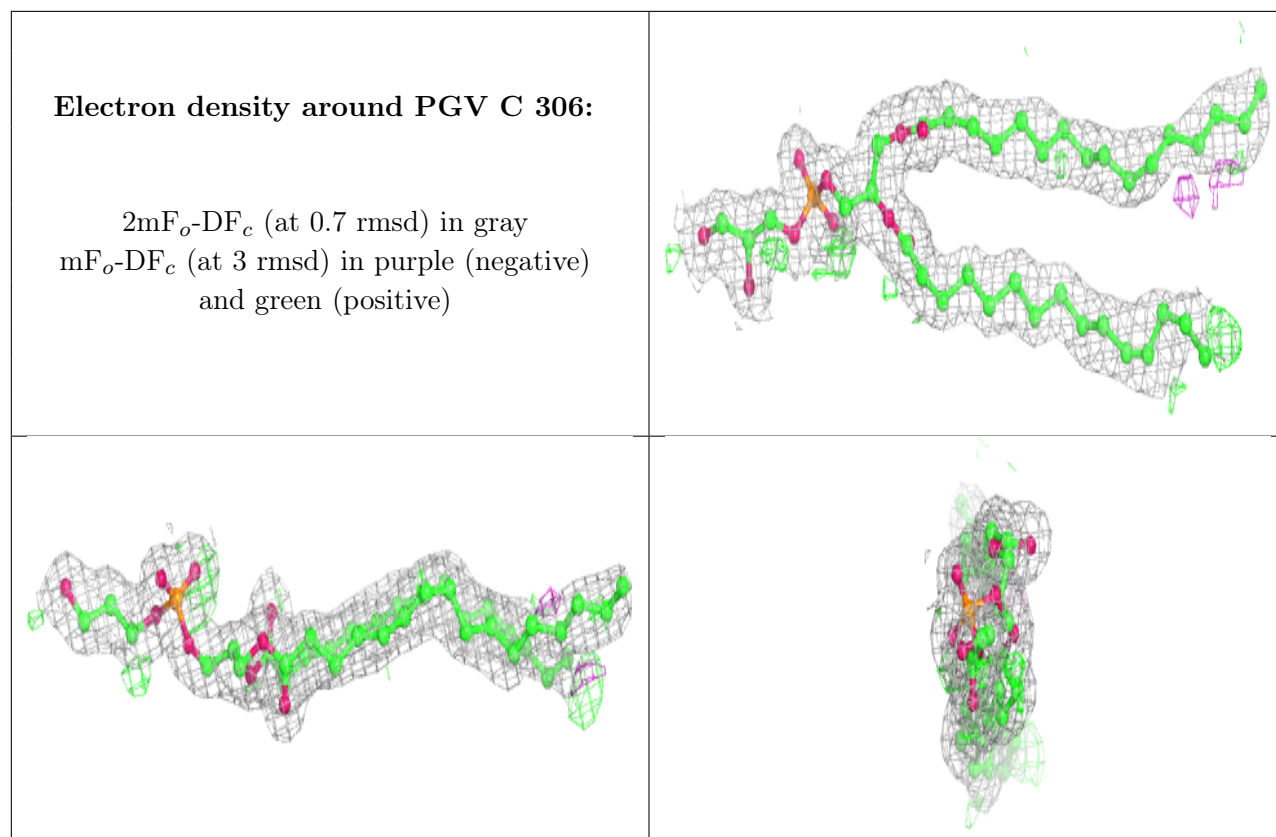
Electron density around HEA N 603:

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

**Electron density around HEA A 601 (A):**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.