



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 3, 2023 – 02:29 PM JST

PDB ID : 8IJN
Title : Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-Bound Fully Reduced State at 100 K
Authors : Tsukihara, T.; Shimada, A.; Muramoto, K.
Deposited on : 2023-02-27
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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 : 2.32.2
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) : 2.32.2

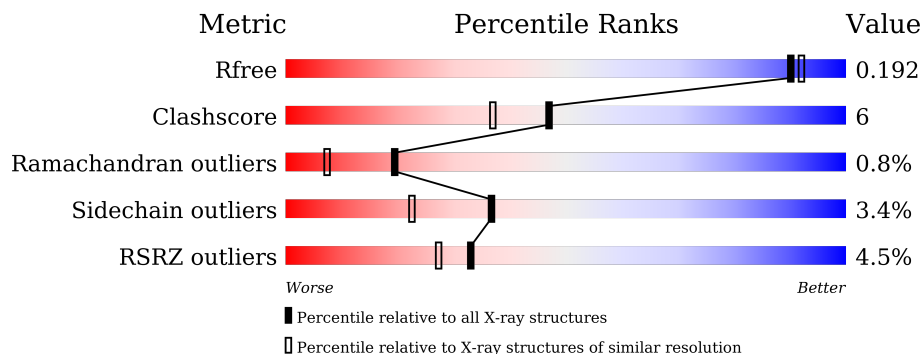
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 5950 (1.80-1.80) |
| Clashscore | 141614 | 6793 (1.80-1.80) |
| Ramachandran outliers | 138981 | 6697 (1.80-1.80) |
| Sidechain outliers | 138945 | 6696 (1.80-1.80) |
| RSRZ outliers | 127900 | 5850 (1.80-1.80) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 514 | 89% 10% . |
| 1 | N | 514 | 91% 8% |
| 2 | B | 227 | % 82% 16% .. |
| 2 | O | 227 | 2% 77% 21% . |
| 3 | C | 261 | 89% 10% . |
| 3 | P | 261 | % 89% 10% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | D | 147 | 10% 88% 8% |
| 4 | Q | 147 | 10% 88% 9% |
| 5 | E | 109 | 2% 89% 6% |
| 5 | R | 109 | 7% 90% 6% |
| 6 | F | 98 | 7% 87% 10% |
| 6 | S | 98 | 8% 89% 7% |
| 7 | G | 85 | 21% 73% 21% |
| 7 | T | 85 | 19% 71% 18% 9% |
| 8 | H | 85 | 14% 80% 11% 7% |
| 8 | U | 85 | 14% 81% 8% 7% |
| 9 | I | 73 | 4% 88% 11% |
| 9 | V | 73 | 10% 84% 15% |
| 10 | J | 59 | 10% 88% 10% |
| 10 | W | 59 | 12% 90% 7% |
| 11 | K | 56 | 5% 80% 7% 12% |
| 11 | X | 56 | 20% 79% 7% 12% |
| 12 | L | 47 | 2% 85% 13% |
| 12 | Y | 47 | 81% 13% |
| 13 | M | 46 | 9% 72% 17% 9% |
| 13 | Z | 46 | 13% 80% 9% 7% |

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 | X | - | - | - |
| 14 | HEA | A | 602 | X | - | - | - |
| 14 | HEA | N | 601 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 14 | HEA | N | 602 | X | - | - | - |
| 23 | CHD | J | 101 | - | - | - | X |
| 23 | CHD | W | 101 | - | - | - | X |
| 25 | CDL | G | 102 | - | - | X | - |
| 26 | DMU | W | 102 | - | - | - | X |
| 9 | SAC | V | 1 | - | - | - | X |

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32780 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 |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 514 | 4072 | 2716 | 631 | 687 | 38 | 0 | 10 | 0 |
| 1 | N | 514 | 4072 | 2717 | 631 | 686 | 38 | 0 | 9 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | B | 227 | 1831 | 1191 | 281 | 341 | 18 | 0 | 2 | 0 |
| 2 | O | 227 | 1824 | 1185 | 281 | 340 | 18 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | C | 259 | 2116 | 1415 | 336 | 351 | 14 | 0 | 3 | 0 |
| 3 | P | 259 | 2110 | 1412 | 336 | 350 | 12 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | D | 144 | 1195 | 777 | 196 | 218 | 4 | 0 | 0 | 0 |
| 4 | Q | 144 | 1195 | 777 | 196 | 218 | 4 | 0 | 0 | 0 |

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

| 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 | 0 | 0 |
| | | | 852 | 544 | 144 | 162 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 748 | 464 | 134 | 145 | 5 | | | |
| 6 | S | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 748 | 464 | 134 | 145 | 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 | P | S | 0 | 0 | 0 |
| | | | 675 | 431 | 129 | 113 | 1 | 1 | | | |
| 7 | T | 84 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 675 | 431 | 129 | 113 | 1 | 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 | 0 | 0 |
| | | | 662 | 417 | 121 | 119 | 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 | 0 | 0 |
| | | | 601 | 390 | 107 | 100 | 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.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | J | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 460 | 297 | 78 | 82 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | W | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 460 | 297 | 78 | 82 | 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 | 0 | 0 |
| | | | 384 | 250 | 65 | 67 | 2 | | | |
| 11 | X | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 250 | 65 | 67 | 2 | | | |

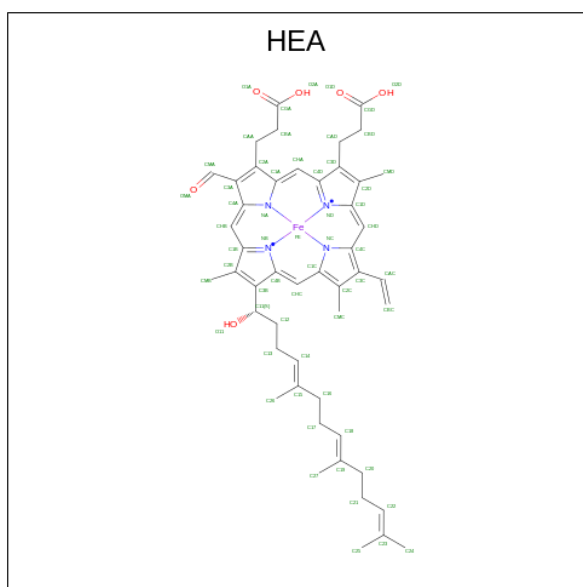
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

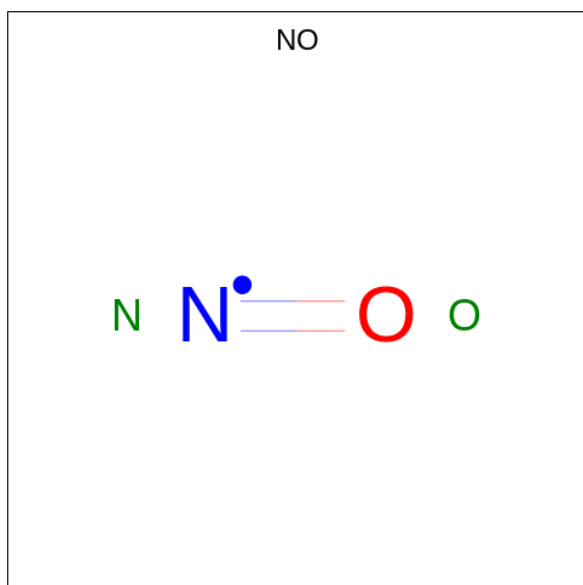
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 13 | M | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53 | 59 | | | |
| 13 | Z | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53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

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



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

- Molecule 15 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 15 | A | 1 | Total | N | O | 0 | 0 |
| | | | 2 | 1 | 1 | | |
| 15 | N | 1 | Total | N | O | 0 | 0 |
| | | | 2 | 1 | 1 | | |

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

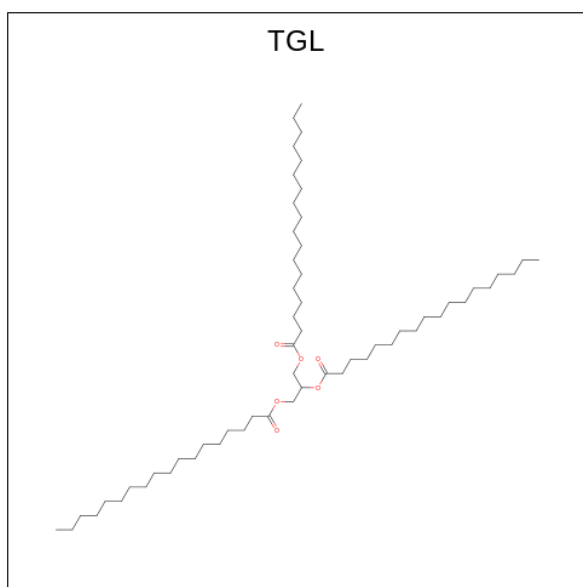
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 17 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

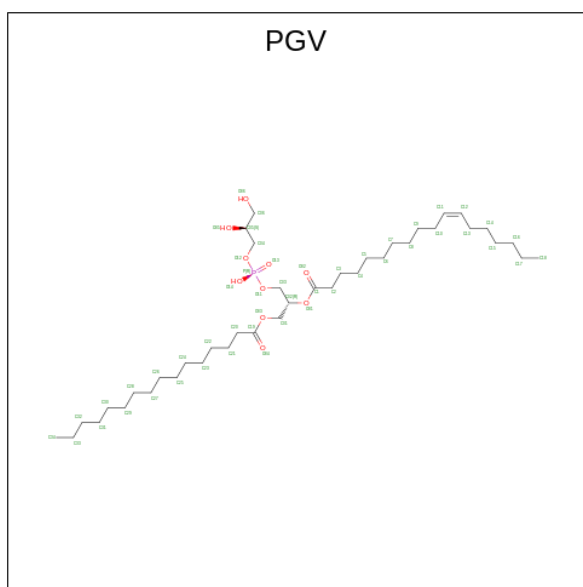
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 18 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 18 | N | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



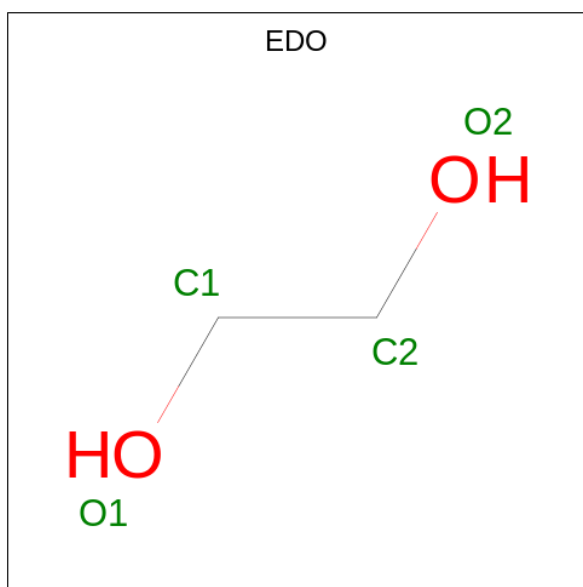
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 19 | A | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 19 | D | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 19 | L | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 19 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 19 | O | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 19 | Q | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

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



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| | | | Total | C | O | P | | |
| 20 | A | 1 | 51 | 40 | 10 | 1 | 0 | 0 |
| 20 | A | 1 | 51 | 40 | 10 | 1 | 0 | 0 |
| 20 | C | 1 | 51 | 40 | 10 | 1 | 0 | 0 |
| 20 | C | 1 | 51 | 40 | 10 | 1 | 0 | 0 |
| 20 | N | 1 | 46 | 37 | 8 | 1 | 0 | 0 |
| 20 | N | 1 | 51 | 40 | 10 | 1 | 0 | 0 |
| 20 | P | 1 | 51 | 40 | 10 | 1 | 0 | 0 |
| 20 | P | 1 | 51 | 40 | 10 | 1 | 0 | 0 |

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



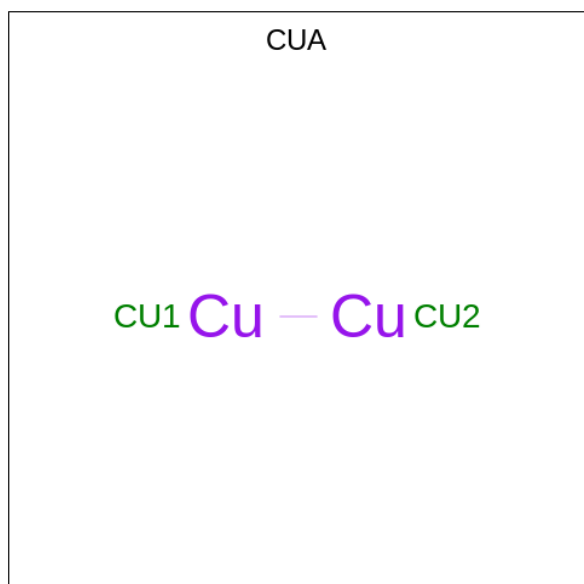
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 21 | A | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | A | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | A | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | A | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | B | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | C | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | F | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | N | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | N | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | N | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | N | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | N | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | N | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | O | 1 | Total C O 4 2 2 | 0 | 0 |

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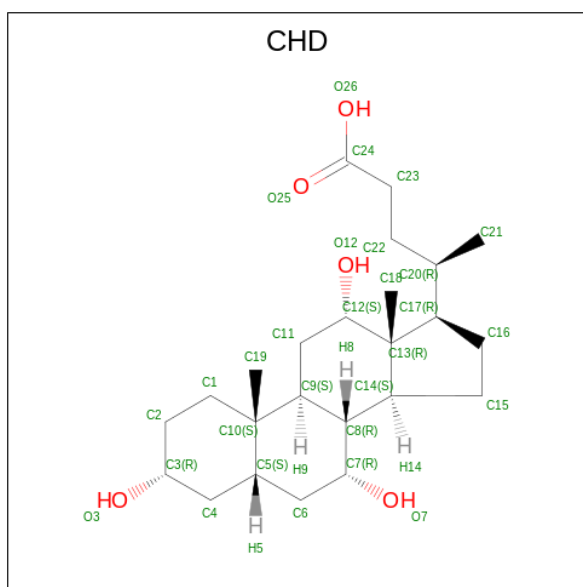
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 21 | O | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | P | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | P | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | Q | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | Q | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | S | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | S | 1 | Total C O 4 2 2 | 0 | 0 |
| 21 | S | 1 | Total C O 4 2 2 | 0 | 0 |

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



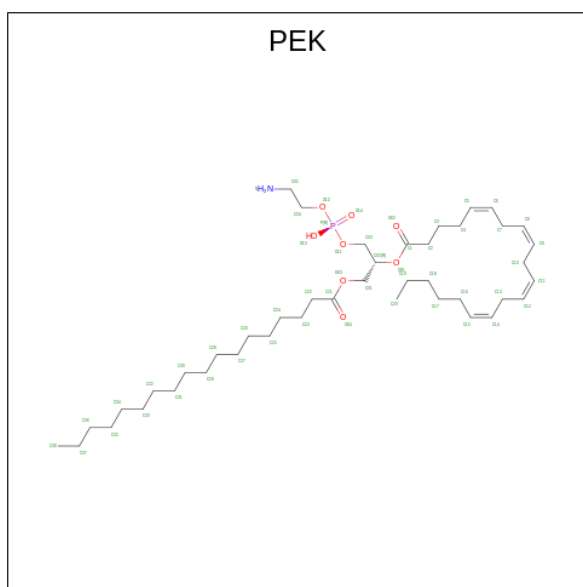
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 22 | B | 1 | Total Cu 2 2 | 0 | 0 |
| 22 | O | 1 | Total Cu 2 2 | 0 | 0 |

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



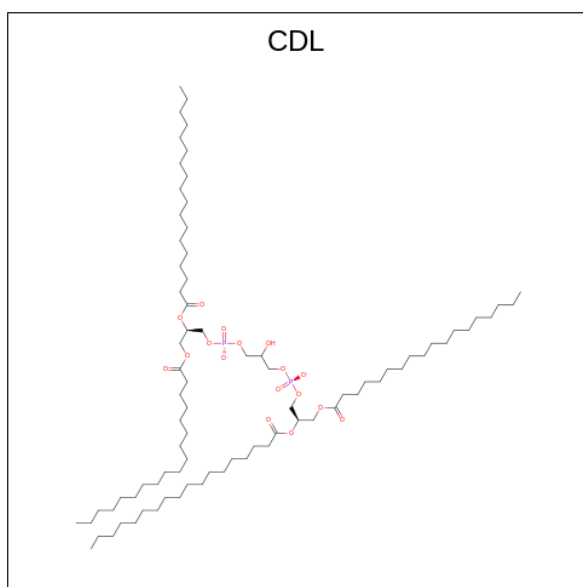
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 23 | B | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | C | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | C | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | J | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | O | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | P | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | P | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | W | 1 | Total C O 29 24 5 | 0 | 0 |

- Molecule 24 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).



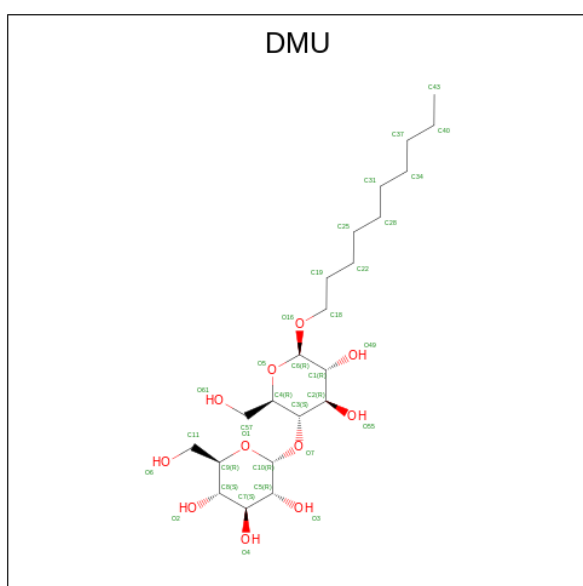
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 24 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 24 | G | 1 | Total | C | O | P | | 0 | 0 |
| | | | 50 | 41 | 8 | 1 | | | |
| 24 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 24 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 24 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 24 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



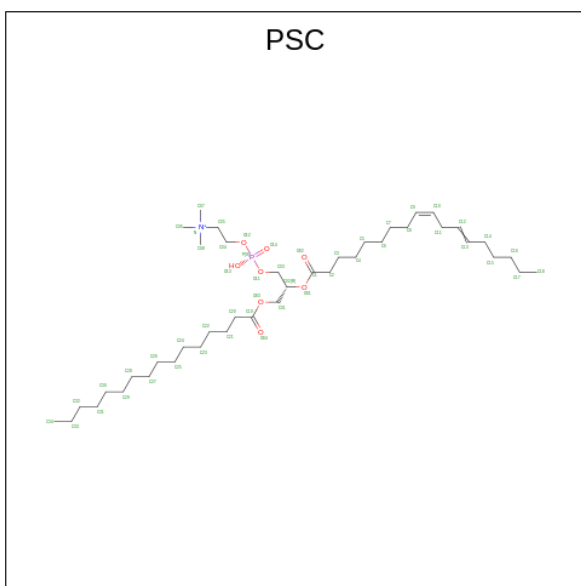
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | |
|-----|-------|----------|--------------|---------|---------|---------|---------|---|
| | | | Total | C | O | | | P |
| 25 | C | 1 | Total 100 | C 81 | O 17 | P 2 | 0 | 0 |
| 25 | G | 1 | Total 100 | C 81 | O 17 | P 2 | 0 | 0 |
| 25 | P | 1 | Total 100 | C 81 | O 17 | P 2 | 0 | 0 |
| 25 | T | 1 | Total 100 | C 81 | O 17 | P 2 | 0 | 0 |

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 26 | C | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 26 | M | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 26 | O | 1 | Total | C | O | 0 | 0 |
| | | | 22 | 16 | 6 | | |
| 26 | P | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 26 | W | 1 | Total | C | O | 0 | 0 |
| | | | 32 | 21 | 11 | | |
| 26 | Z | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |

- Molecule 27 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)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 |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 27 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |
| 27 | R | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |

- 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 | | |

Continued on next page...

Continued from previous page...

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

- Molecule 29 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 29 | A | 229 | Total 229 | O 229 | 0 | 0 |
| 29 | B | 148 | Total 149 | O 149 | 0 | 1 |
| 29 | C | 120 | Total 120 | O 120 | 0 | 0 |
| 29 | D | 79 | Total 79 | O 79 | 0 | 0 |
| 29 | E | 48 | Total 48 | O 48 | 0 | 0 |
| 29 | F | 68 | Total 68 | O 68 | 0 | 0 |
| 29 | G | 48 | Total 48 | O 48 | 0 | 0 |
| 29 | H | 51 | Total 51 | O 51 | 0 | 0 |
| 29 | I | 39 | Total 39 | O 39 | 0 | 0 |
| 29 | J | 26 | Total 26 | O 26 | 0 | 0 |
| 29 | K | 30 | Total 30 | O 30 | 0 | 0 |
| 29 | L | 23 | Total 23 | O 23 | 0 | 0 |
| 29 | M | 24 | Total 24 | O 24 | 0 | 0 |
| 29 | N | 231 | Total 231 | O 231 | 0 | 0 |
| 29 | O | 146 | Total 146 | O 146 | 0 | 2 |
| 29 | P | 106 | Total 106 | O 106 | 0 | 0 |
| 29 | Q | 59 | Total 59 | O 59 | 0 | 0 |
| 29 | R | 55 | Total 55 | O 55 | 0 | 0 |

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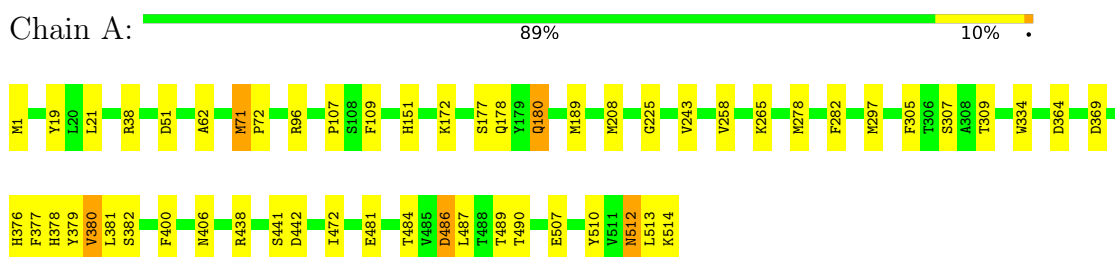
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|---------|----------------|----------------|
| 29 | S | 72 | Total 72 | O 72 | 0 | 0 |
| 29 | T | 51 | Total 51 | O 51 | 0 | 0 |
| 29 | U | 48 | Total 48 | O 48 | 0 | 0 |
| 29 | V | 29 | Total 29 | O 29 | 0 | 0 |
| 29 | W | 22 | Total 22 | O 22 | 0 | 0 |
| 29 | X | 22 | Total 22 | O 22 | 0 | 0 |
| 29 | Y | 17 | Total 17 | O 17 | 0 | 0 |
| 29 | Z | 17 | Total 17 | O 17 | 0 | 0 |

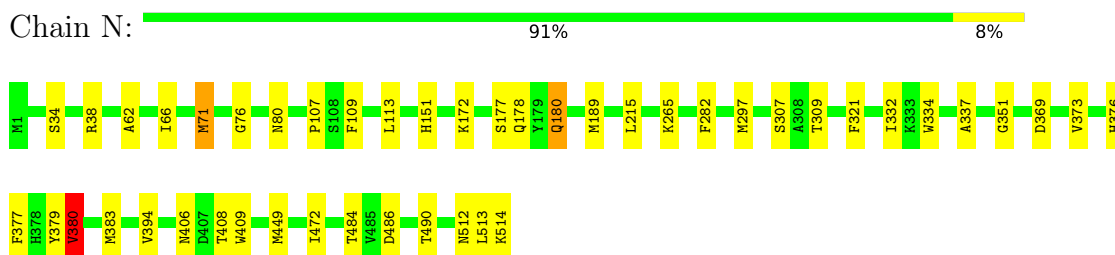
3 Residue-property plots [i](#)

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.

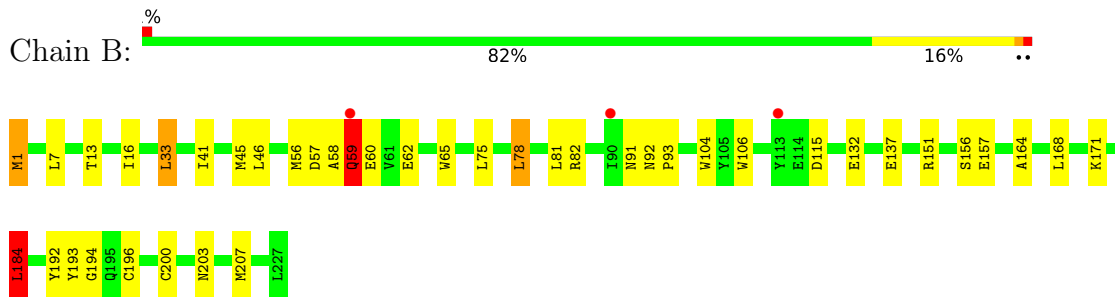
- Molecule 1: Cytochrome c oxidase subunit 1



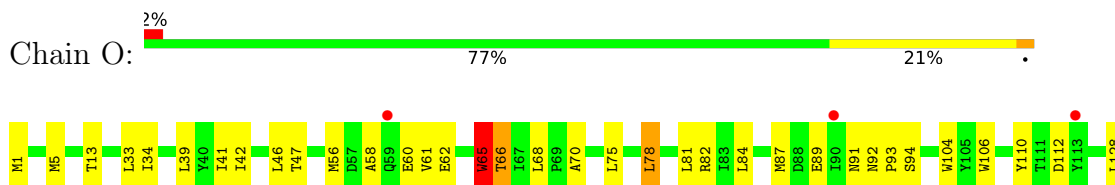
- Molecule 1: Cytochrome c oxidase subunit 1

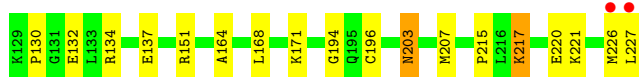


- Molecule 2: Cytochrome c oxidase subunit 2

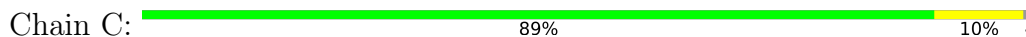


- Molecule 2: Cytochrome c oxidase subunit 2

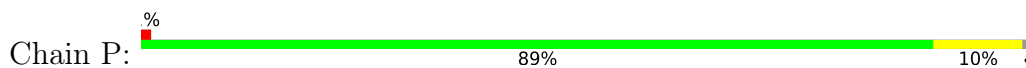




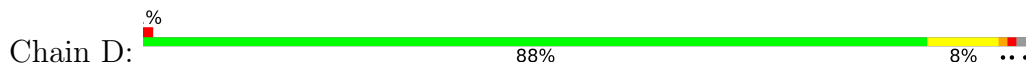
- Molecule 3: Cytochrome c oxidase subunit 3



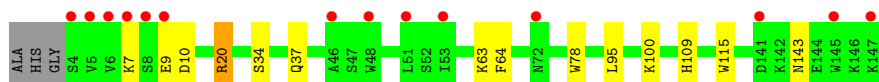
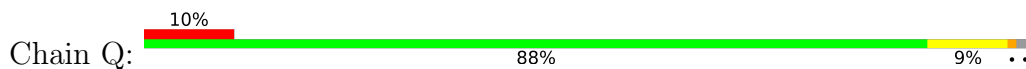
- Molecule 3: Cytochrome c oxidase subunit 3



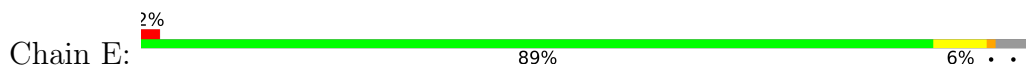
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



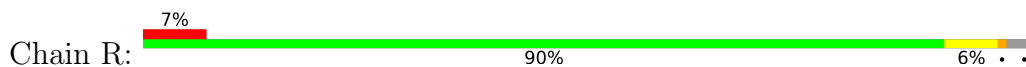
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



- Molecule 5: Cytochrome c oxidase subunit 5A

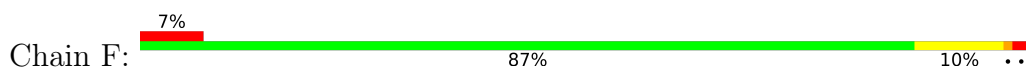


- Molecule 5: Cytochrome c oxidase subunit 5A

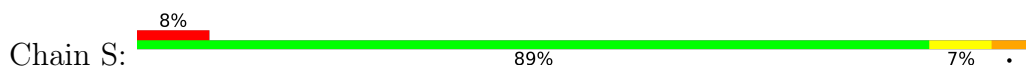




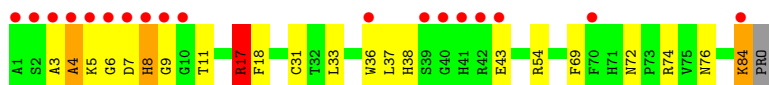
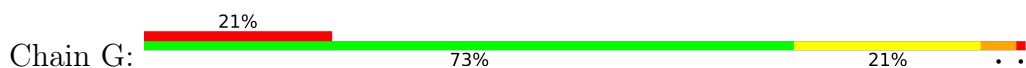
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



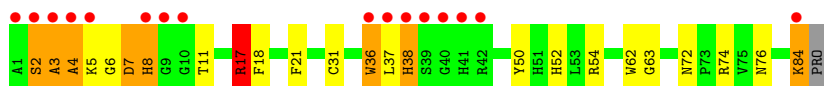
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



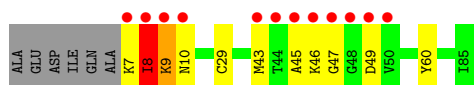
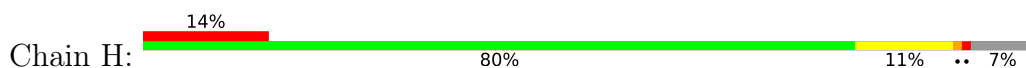
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



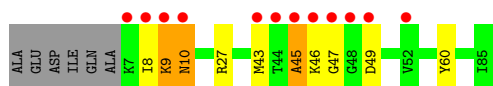
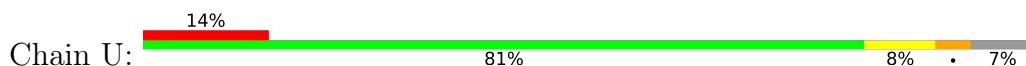
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



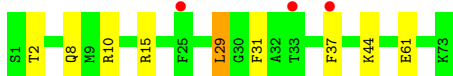
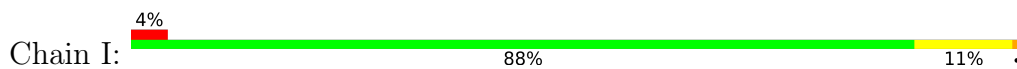
- Molecule 8: Cytochrome c oxidase subunit 6B1



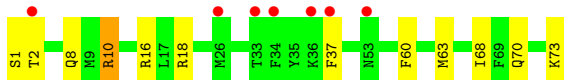
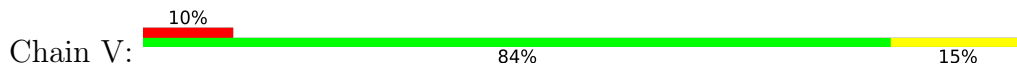
- Molecule 8: Cytochrome c oxidase subunit 6B1



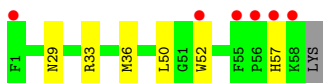
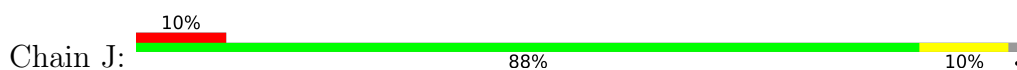
- Molecule 9: Cytochrome c oxidase subunit 6C



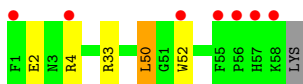
- Molecule 9: Cytochrome c oxidase subunit 6C



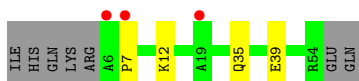
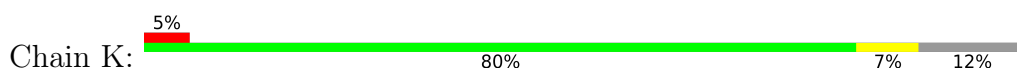
- Molecule 10: Cytochrome c oxidase subunit 7A1



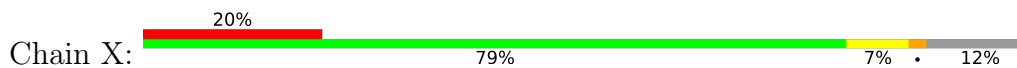
- Molecule 10: Cytochrome c oxidase subunit 7A1



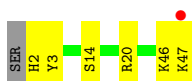
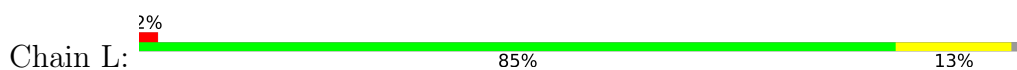
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial




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



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




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

Chain Y:  81% 13% . .




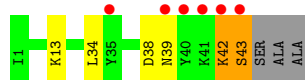
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  9% 72% 17% . 7%



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

Chain Z:  13% 80% 9% . 7%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 35.37 – 1.80 83.50 – 1.80 | Depositor EDS |
| % Data completeness (in resolution range) | 99.6 (35.37-1.80) 99.6 (83.50-1.80) | Depositor EDS |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.29 (at 1.80Å) | Xtrriage |
| Refinement program | PHENIX (1.13_2998: ???) | Depositor |
| R, R_{free} | 0.169 , 0.192 0.169 , 0.192 | Depositor DCC |
| R_{free} test set | 30652 reflections (4.96%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 28.1 | Xtrriage |
| Anisotropy | 0.505 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.37 , 67.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtrriage |
| Estimated twinning fraction | 0.007 for l,-k,h | Xtrriage |
| F_o, F_c correlation | 0.97 | EDS |
| Total number of atoms | 32780 | wwPDB-VP |
| Average B, all atoms (Å ²) | 41.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: ZN, MG, PGV, CDL, HEA, DMU, TGL, EDO, TPO, CUA, NO, CU, NA, CHD, PSC, FME, PEK, SAC

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 | 1.10 | 8/4230 (0.2%) | 0.90 | 6/5775 (0.1%) |
| 1 | N | 0.95 | 4/4224 (0.1%) | 0.81 | 2/5767 (0.0%) |
| 2 | B | 1.03 | 6/1878 (0.3%) | 0.93 | 3/2558 (0.1%) |
| 2 | O | 0.77 | 1/1860 (0.1%) | 0.83 | 3/2534 (0.1%) |
| 3 | C | 0.91 | 1/2219 (0.0%) | 0.77 | 2/3033 (0.1%) |
| 3 | P | 0.85 | 0/2197 | 0.72 | 0/3005 |
| 4 | D | 0.83 | 2/1229 (0.2%) | 0.84 | 3/1658 (0.2%) |
| 4 | Q | 0.64 | 0/1229 | 0.69 | 2/1658 (0.1%) |
| 5 | E | 0.80 | 0/871 | 0.79 | 2/1182 (0.2%) |
| 5 | R | 0.65 | 0/871 | 0.68 | 0/1182 |
| 6 | F | 0.84 | 1/765 (0.1%) | 0.78 | 0/1038 |
| 6 | S | 0.72 | 0/765 | 0.78 | 0/1038 |
| 7 | G | 0.85 | 1/690 (0.1%) | 1.02 | 3/937 (0.3%) |
| 7 | T | 0.76 | 1/690 (0.1%) | 1.01 | 2/937 (0.2%) |
| 8 | H | 0.78 | 0/682 | 0.70 | 0/921 |
| 8 | U | 0.66 | 0/682 | 0.68 | 0/921 |
| 9 | I | 0.68 | 0/605 | 0.68 | 0/802 |
| 9 | V | 0.60 | 0/605 | 0.70 | 1/802 (0.1%) |
| 10 | J | 0.69 | 0/471 | 0.67 | 0/636 |
| 10 | W | 0.57 | 0/471 | 0.63 | 0/636 |
| 11 | K | 0.84 | 1/398 (0.3%) | 0.72 | 0/546 |
| 11 | X | 0.54 | 0/398 | 0.55 | 0/546 |
| 12 | L | 0.92 | 0/393 | 0.76 | 0/526 |
| 12 | Y | 0.71 | 0/393 | 0.59 | 0/526 |
| 13 | M | 0.85 | 0/345 | 0.75 | 1/470 (0.2%) |
| 13 | Z | 0.60 | 0/345 | 0.59 | 0/470 |
| All | All | 0.87 | 26/29506 (0.1%) | 0.80 | 30/40104 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6 | F | 0 | 1 |
| 6 | S | 0 | 1 |
| All | All | 0 | 2 |

The worst 5 of 26 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | A | 507 | GLU | CG-CD | 6.63 | 1.61 | 1.51 |
| 2 | O | 106 | TRP | CE3-CZ3 | 6.02 | 1.48 | 1.38 |
| 2 | B | 157 | GLU | CB-CG | 5.92 | 1.63 | 1.52 |
| 11 | K | 39 | GLU | CB-CG | 5.69 | 1.62 | 1.52 |
| 1 | A | 19 | TYR | CE2-CZ | 5.68 | 1.46 | 1.38 |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 7 | T | 17 | ARG | NE-CZ-NH1 | 15.52 | 128.06 | 120.30 |
| 1 | A | 71 | MET | CG-SD-CE | -15.23 | 75.84 | 100.20 |
| 7 | G | 17 | ARG | NE-CZ-NH2 | -12.93 | 113.84 | 120.30 |
| 7 | G | 17 | ARG | NE-CZ-NH1 | 12.76 | 126.68 | 120.30 |
| 7 | T | 17 | ARG | NE-CZ-NH2 | -12.59 | 114.01 | 120.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 6 | F | 93 | PRO | Peptide |
| 6 | S | 93 | PRO | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4072 | 0 | 4041 | 36 | 0 |
| 1 | N | 4072 | 0 | 4044 | 41 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | B | 1831 | 0 | 1839 | 24 | 0 |
| 2 | O | 1824 | 0 | 1833 | 31 | 0 |
| 3 | C | 2116 | 0 | 2034 | 24 | 0 |
| 3 | P | 2110 | 0 | 2027 | 32 | 0 |
| 4 | D | 1195 | 0 | 1183 | 10 | 0 |
| 4 | Q | 1195 | 0 | 1183 | 10 | 0 |
| 5 | E | 852 | 0 | 845 | 3 | 0 |
| 5 | R | 852 | 0 | 845 | 5 | 1 |
| 6 | F | 748 | 0 | 728 | 7 | 0 |
| 6 | S | 748 | 0 | 728 | 12 | 0 |
| 7 | G | 675 | 0 | 643 | 17 | 0 |
| 7 | T | 675 | 0 | 643 | 27 | 0 |
| 8 | H | 662 | 0 | 623 | 6 | 0 |
| 8 | U | 662 | 0 | 623 | 5 | 0 |
| 9 | I | 601 | 0 | 613 | 5 | 1 |
| 9 | V | 601 | 0 | 613 | 7 | 0 |
| 10 | J | 460 | 0 | 459 | 4 | 0 |
| 10 | W | 460 | 0 | 459 | 4 | 0 |
| 11 | K | 384 | 0 | 366 | 2 | 0 |
| 11 | X | 384 | 0 | 366 | 4 | 0 |
| 12 | L | 380 | 0 | 380 | 7 | 0 |
| 12 | Y | 380 | 0 | 380 | 6 | 0 |
| 13 | M | 335 | 0 | 352 | 6 | 0 |
| 13 | Z | 335 | 0 | 352 | 2 | 0 |
| 14 | A | 120 | 0 | 108 | 8 | 0 |
| 14 | N | 120 | 0 | 108 | 8 | 0 |
| 15 | A | 2 | 0 | 0 | 0 | 0 |
| 15 | N | 2 | 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 | N | 1 | 0 | 0 | 0 | 0 |
| 18 | A | 1 | 0 | 0 | 0 | 0 |
| 18 | N | 1 | 0 | 0 | 0 | 0 |
| 19 | A | 63 | 0 | 110 | 3 | 0 |
| 19 | D | 63 | 0 | 110 | 8 | 0 |
| 19 | L | 63 | 0 | 110 | 8 | 0 |
| 19 | N | 63 | 0 | 110 | 8 | 0 |
| 19 | O | 63 | 0 | 110 | 0 | 0 |
| 19 | Q | 63 | 0 | 110 | 9 | 0 |
| 20 | A | 102 | 0 | 152 | 4 | 0 |
| 20 | C | 102 | 0 | 152 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20 | N | 97 | 0 | 145 | 5 | 0 |
| 20 | P | 102 | 0 | 152 | 6 | 0 |
| 21 | A | 16 | 0 | 24 | 1 | 0 |
| 21 | B | 4 | 0 | 6 | 0 | 0 |
| 21 | C | 4 | 0 | 6 | 0 | 0 |
| 21 | F | 4 | 0 | 6 | 0 | 0 |
| 21 | N | 24 | 0 | 36 | 2 | 0 |
| 21 | O | 8 | 0 | 12 | 0 | 0 |
| 21 | P | 8 | 0 | 12 | 1 | 0 |
| 21 | Q | 8 | 0 | 12 | 0 | 0 |
| 21 | S | 12 | 0 | 18 | 0 | 0 |
| 22 | B | 2 | 0 | 0 | 0 | 0 |
| 22 | O | 2 | 0 | 0 | 0 | 0 |
| 23 | B | 29 | 0 | 39 | 1 | 0 |
| 23 | C | 58 | 0 | 78 | 3 | 0 |
| 23 | J | 29 | 0 | 38 | 2 | 0 |
| 23 | O | 29 | 0 | 39 | 2 | 0 |
| 23 | P | 58 | 0 | 78 | 1 | 0 |
| 23 | W | 29 | 0 | 38 | 1 | 0 |
| 24 | C | 53 | 0 | 77 | 6 | 0 |
| 24 | G | 103 | 0 | 148 | 5 | 0 |
| 24 | P | 53 | 0 | 77 | 6 | 0 |
| 24 | T | 106 | 0 | 154 | 10 | 0 |
| 25 | C | 100 | 0 | 153 | 14 | 0 |
| 25 | G | 100 | 0 | 156 | 23 | 0 |
| 25 | P | 100 | 0 | 156 | 19 | 0 |
| 25 | T | 100 | 0 | 156 | 14 | 0 |
| 26 | C | 33 | 0 | 42 | 2 | 0 |
| 26 | M | 33 | 0 | 42 | 1 | 0 |
| 26 | O | 22 | 0 | 31 | 1 | 0 |
| 26 | P | 33 | 0 | 42 | 8 | 0 |
| 26 | W | 32 | 0 | 36 | 4 | 0 |
| 26 | Z | 33 | 0 | 42 | 1 | 0 |
| 27 | E | 52 | 0 | 80 | 12 | 0 |
| 27 | R | 52 | 0 | 80 | 10 | 0 |
| 28 | F | 1 | 0 | 0 | 0 | 0 |
| 28 | S | 1 | 0 | 0 | 0 | 0 |
| 29 | A | 229 | 0 | 0 | 1 | 0 |
| 29 | B | 149 | 0 | 0 | 3 | 0 |
| 29 | C | 120 | 0 | 0 | 1 | 0 |
| 29 | D | 79 | 0 | 0 | 1 | 0 |
| 29 | E | 48 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29 | F | 68 | 0 | 0 | 1 | 0 |
| 29 | G | 48 | 0 | 0 | 0 | 0 |
| 29 | H | 51 | 0 | 0 | 0 | 0 |
| 29 | I | 39 | 0 | 0 | 2 | 0 |
| 29 | J | 26 | 0 | 0 | 0 | 0 |
| 29 | K | 30 | 0 | 0 | 1 | 0 |
| 29 | L | 23 | 0 | 0 | 0 | 0 |
| 29 | M | 24 | 0 | 0 | 0 | 0 |
| 29 | N | 231 | 0 | 0 | 4 | 0 |
| 29 | O | 146 | 0 | 0 | 1 | 0 |
| 29 | P | 106 | 0 | 0 | 2 | 0 |
| 29 | Q | 59 | 0 | 0 | 2 | 0 |
| 29 | R | 55 | 0 | 0 | 1 | 0 |
| 29 | S | 72 | 0 | 0 | 1 | 0 |
| 29 | T | 51 | 0 | 0 | 0 | 0 |
| 29 | U | 48 | 0 | 0 | 1 | 0 |
| 29 | V | 29 | 0 | 0 | 0 | 0 |
| 29 | W | 22 | 0 | 0 | 1 | 0 |
| 29 | X | 22 | 0 | 0 | 2 | 0 |
| 29 | Y | 17 | 0 | 0 | 1 | 0 |
| 29 | Z | 17 | 0 | 0 | 0 | 0 |
| All | All | 32780 | 0 | 31593 | 388 | 1 |

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.

The worst 5 of 388 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) |
|-----------------|-------------------|--------------------------|-------------------|
| 6:S:94:HIS:CD2 | 6:S:95:GLN:H | 1.72 | 1.05 |
| 21:N:614:EDO:O2 | 29:N:701:HOH:O | 1.80 | 0.99 |
| 7:T:17:ARG:HH22 | 24:T:101:PEK:H041 | 1.27 | 0.96 |
| 6:S:94:HIS:HD2 | 6:S:95:GLN:H | 1.09 | 0.89 |
| 2:B:81:LEU:HD12 | 25:T:103:CDL:H351 | 1.53 | 0.88 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------------|--------------------------|-------------------|
| 9:I:2:THR:OG1 | 5:R:80:GLU:OE1[3_647] | 2.17 | 0.03 |

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 | 522/514 (102%) | 509 (98%) | 13 (2%) | 0 | 100 | 100 |
| 1 | N | 521/514 (101%) | 509 (98%) | 12 (2%) | 0 | 100 | 100 |
| 2 | B | 227/227 (100%) | 222 (98%) | 4 (2%) | 1 (0%) | 34 | 21 |
| 2 | O | 225/227 (99%) | 217 (96%) | 6 (3%) | 2 (1%) | 17 | 6 |
| 3 | C | 260/261 (100%) | 255 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | P | 257/261 (98%) | 252 (98%) | 5 (2%) | 0 | 100 | 100 |
| 4 | D | 142/147 (97%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 4 | Q | 142/147 (97%) | 136 (96%) | 6 (4%) | 0 | 100 | 100 |
| 5 | E | 103/109 (94%) | 103 (100%) | 0 | 0 | 100 | 100 |
| 5 | R | 103/109 (94%) | 103 (100%) | 0 | 0 | 100 | 100 |
| 6 | F | 96/98 (98%) | 90 (94%) | 2 (2%) | 4 (4%) | 3 | 0 |
| 6 | S | 96/98 (98%) | 90 (94%) | 3 (3%) | 3 (3%) | 4 | 0 |
| 7 | G | 81/85 (95%) | 69 (85%) | 7 (9%) | 5 (6%) | 1 | 0 |
| 7 | T | 81/85 (95%) | 69 (85%) | 7 (9%) | 5 (6%) | 1 | 0 |
| 8 | H | 77/85 (91%) | 70 (91%) | 4 (5%) | 3 (4%) | 3 | 0 |
| 8 | U | 77/85 (91%) | 70 (91%) | 3 (4%) | 4 (5%) | 2 | 0 |
| 9 | I | 71/73 (97%) | 69 (97%) | 2 (3%) | 0 | 100 | 100 |
| 9 | V | 71/73 (97%) | 69 (97%) | 2 (3%) | 0 | 100 | 100 |
| 10 | J | 56/59 (95%) | 56 (100%) | 0 | 0 | 100 | 100 |
| 10 | W | 56/59 (95%) | 56 (100%) | 0 | 0 | 100 | 100 |
| 11 | K | 47/56 (84%) | 47 (100%) | 0 | 0 | 100 | 100 |
| 11 | X | 47/56 (84%) | 45 (96%) | 2 (4%) | 0 | 100 | 100 |
| 12 | L | 44/47 (94%) | 42 (96%) | 2 (4%) | 0 | 100 | 100 |
| 12 | Y | 44/47 (94%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 13 | M | 41/46 (89%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 13 | Z | 41/46 (89%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| All | All | 3528/3614 (98%) | 3410 (97%) | 91 (3%) | 27 (1%) | 19 | 7 |

5 of 27 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 2 | SER |
| 6 | F | 94 | HIS |
| 6 | F | 95 | GLN |
| 7 | G | 4 | ALA |
| 7 | G | 7 | ASP |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 435/426 (102%) | 428 (98%) | 7 (2%) | 62 | 54 |
| 1 | N | 434/426 (102%) | 426 (98%) | 8 (2%) | 59 | 48 |
| 2 | B | 212/210 (101%) | 202 (95%) | 10 (5%) | 26 | 12 |
| 2 | O | 210/210 (100%) | 197 (94%) | 13 (6%) | 18 | 6 |
| 3 | C | 227/226 (100%) | 224 (99%) | 3 (1%) | 69 | 62 |
| 3 | P | 224/226 (99%) | 221 (99%) | 3 (1%) | 69 | 62 |
| 4 | D | 128/129 (99%) | 123 (96%) | 5 (4%) | 32 | 17 |
| 4 | Q | 128/129 (99%) | 124 (97%) | 4 (3%) | 40 | 25 |
| 5 | E | 92/95 (97%) | 90 (98%) | 2 (2%) | 52 | 39 |
| 5 | R | 92/95 (97%) | 91 (99%) | 1 (1%) | 73 | 68 |
| 6 | F | 81/81 (100%) | 78 (96%) | 3 (4%) | 34 | 19 |
| 6 | S | 81/81 (100%) | 78 (96%) | 3 (4%) | 34 | 19 |
| 7 | G | 67/68 (98%) | 61 (91%) | 6 (9%) | 9 | 2 |
| 7 | T | 67/68 (98%) | 59 (88%) | 8 (12%) | 5 | 1 |
| 8 | H | 71/75 (95%) | 68 (96%) | 3 (4%) | 30 | 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8 | U | 71/75 (95%) | 69 (97%) | 2 (3%) | 43 | 30 |
| 9 | I | 57/57 (100%) | 52 (91%) | 5 (9%) | 10 | 3 |
| 9 | V | 57/57 (100%) | 52 (91%) | 5 (9%) | 10 | 3 |
| 10 | J | 49/50 (98%) | 48 (98%) | 1 (2%) | 55 | 44 |
| 10 | W | 49/50 (98%) | 48 (98%) | 1 (2%) | 55 | 44 |
| 11 | K | 39/46 (85%) | 39 (100%) | 0 | 100 | 100 |
| 11 | X | 39/46 (85%) | 38 (97%) | 1 (3%) | 46 | 32 |
| 12 | L | 39/40 (98%) | 39 (100%) | 0 | 100 | 100 |
| 12 | Y | 39/40 (98%) | 36 (92%) | 3 (8%) | 13 | 4 |
| 13 | M | 37/38 (97%) | 33 (89%) | 4 (11%) | 6 | 1 |
| 13 | Z | 37/38 (97%) | 32 (86%) | 5 (14%) | 4 | 1 |
| All | All | 3062/3082 (99%) | 2956 (96%) | 106 (4%) | 37 | 21 |

5 of 106 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | O | 33 | LEU |
| 3 | P | 214 | PHE |
| 12 | Y | 20 | ARG |
| 2 | O | 65 | TRP |
| 2 | O | 110 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | O | 91 | ASN |
| 4 | Q | 37 | GLN |
| 2 | O | 181 | GLN |
| 3 | P | 50 | ASN |
| 5 | R | 94 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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 |
| 1 | FME | N | 1 | 1 | 8,9,10 | 0.48 | 0 | 7,9,11 | 1.29 | 0 |
| 2 | FME | O | 1 | 2 | 8,9,10 | 1.25 | 2 (25%) | 7,9,11 | 4.10 | 2 (28%) |
| 9 | SAC | V | 1 | 9 | 7,8,9 | 0.61 | 0 | 8,9,11 | 1.81 | 2 (25%) |
| 7 | TPO | G | 11 | 7 | 8,10,11 | 1.55 | 2 (25%) | 10,14,16 | 1.37 | 1 (10%) |
| 9 | SAC | I | 1 | 9 | 7,8,9 | 0.57 | 0 | 8,9,11 | 0.76 | 0 |
| 1 | FME | A | 1 | 1 | 8,9,10 | 0.55 | 0 | 7,9,11 | 1.84 | 1 (14%) |
| 2 | FME | B | 1 | 2 | 8,9,10 | 2.14 | 3 (37%) | 7,9,11 | 3.73 | 4 (57%) |
| 7 | TPO | T | 11 | 7 | 8,10,11 | 1.61 | 2 (25%) | 10,14,16 | 1.34 | 1 (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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 1 | FME | N | 1 | 1 | - | 5/7/9/11 | - |
| 2 | FME | O | 1 | 2 | - | 2/7/9/11 | - |
| 9 | SAC | V | 1 | 9 | - | 6/7/8/10 | - |
| 7 | TPO | G | 11 | 7 | - | 3/9/11/13 | - |
| 9 | SAC | I | 1 | 9 | - | 4/7/8/10 | - |
| 1 | FME | A | 1 | 1 | - | 4/7/9/11 | - |
| 2 | FME | B | 1 | 2 | - | 1/7/9/11 | - |
| 7 | TPO | T | 11 | 7 | - | 3/9/11/13 | - |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | B | 1 | FME | CA-N | 4.01 | 1.52 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | B | 1 | FME | CN-N | 3.66 | 1.45 | 1.33 |
| 7 | T | 11 | TPO | P-O1P | 2.94 | 1.60 | 1.50 |
| 7 | G | 11 | TPO | P-O1P | 2.94 | 1.60 | 1.50 |
| 2 | O | 1 | FME | O1-CN | -2.54 | 1.15 | 1.22 |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2 | O | 1 | FME | CA-N-CN | -10.11 | 107.27 | 122.82 |
| 2 | B | 1 | FME | C-CA-N | 7.67 | 123.58 | 109.73 |
| 2 | B | 1 | FME | CA-N-CN | -3.91 | 116.80 | 122.82 |
| 7 | G | 11 | TPO | CG2-CB-CA | 3.73 | 120.52 | 113.16 |
| 2 | B | 1 | FME | CG-CB-CA | -3.59 | 102.96 | 112.95 |

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 1 | A | 1 | FME | O1-CN-N-CA |
| 1 | A | 1 | FME | N-CA-CB-CG |
| 2 | B | 1 | FME | O1-CN-N-CA |
| 7 | G | 11 | TPO | N-CA-CB-CG2 |
| 7 | G | 11 | TPO | N-CA-CB-OG1 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | B | 1 | FME | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 8 are monoatomic - leaving 70 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 |
| 14 | HEA | A | 601 | 1 | 57,67,67 | 1.60 | 10 (17%) | 61,103,103 | 2.11 | 21 (34%) |
| 21 | EDO | B | 303 | - | 3,3,3 | 0.73 | 0 | 2,2,2 | 0.55 | 0 |
| 21 | EDO | N | 614 | - | 3,3,3 | 0.71 | 0 | 2,2,2 | 0.47 | 0 |
| 22 | CUA | O | 301 | 2 | 0,1,1 | - | - | - | - | - |
| 21 | EDO | N | 613 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.59 | 0 |
| 21 | EDO | A | 612 | - | 3,3,3 | 0.64 | 0 | 2,2,2 | 0.27 | 0 |
| 20 | PGV | N | 609 | - | 50,50,50 | 1.05 | 3 (6%) | 53,56,56 | 1.12 | 4 (7%) |
| 19 | TGL | L | 101 | - | 62,62,62 | 1.16 | 3 (4%) | 65,65,65 | 1.67 | 10 (15%) |
| 21 | EDO | S | 104 | - | 3,3,3 | 0.66 | 0 | 2,2,2 | 0.36 | 0 |
| 25 | CDL | P | 305 | - | 99,99,99 | 1.36 | 13 (13%) | 105,111,111 | 1.61 | 14 (13%) |
| 27 | PSC | R | 201 | - | 51,51,51 | 1.13 | 3 (5%) | 57,59,59 | 1.20 | 5 (8%) |
| 20 | PGV | A | 608 | - | 50,50,50 | 1.02 | 6 (12%) | 53,56,56 | 1.23 | 5 (9%) |
| 21 | EDO | O | 306 | - | 3,3,3 | 0.53 | 0 | 2,2,2 | 0.13 | 0 |
| 21 | EDO | Q | 203 | - | 3,3,3 | 0.17 | 0 | 2,2,2 | 0.81 | 0 |
| 22 | CUA | B | 301 | 2 | 0,1,1 | - | - | - | - | - |
| 23 | CHD | C | 301 | - | 32,32,32 | 0.96 | 2 (6%) | 51,51,51 | 1.61 | 11 (21%) |
| 21 | EDO | A | 610 | - | 3,3,3 | 1.09 | 0 | 2,2,2 | 0.88 | 0 |
| 24 | PEK | T | 102 | - | 52,52,52 | 1.02 | 2 (3%) | 55,57,57 | 1.67 | 6 (10%) |
| 26 | DMU | P | 307 | - | 34,34,34 | 0.87 | 1 (2%) | 45,45,45 | 2.03 | 11 (24%) |
| 21 | EDO | A | 613 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.30 | 0 |
| 21 | EDO | O | 305 | - | 3,3,3 | 0.90 | 0 | 2,2,2 | 0.25 | 0 |
| 19 | TGL | A | 607 | - | 62,62,62 | 1.06 | 3 (4%) | 65,65,65 | 1.14 | 6 (9%) |
| 21 | EDO | N | 611 | - | 3,3,3 | 0.73 | 0 | 2,2,2 | 0.83 | 0 |
| 14 | HEA | N | 601 | 1 | 57,67,67 | 1.48 | 9 (15%) | 61,103,103 | 1.97 | 22 (36%) |
| 23 | CHD | P | 301 | - | 32,32,32 | 1.00 | 2 (6%) | 51,51,51 | 1.38 | 7 (13%) |
| 21 | EDO | N | 615 | - | 3,3,3 | 0.64 | 0 | 2,2,2 | 0.27 | 0 |
| 20 | PGV | P | 303 | - | 50,50,50 | 0.71 | 1 (2%) | 53,56,56 | 1.13 | 7 (13%) |
| 21 | EDO | S | 102 | - | 3,3,3 | 1.09 | 0 | 2,2,2 | 0.62 | 0 |
| 25 | CDL | G | 102 | - | 99,99,99 | 1.35 | 12 (12%) | 105,111,111 | 1.49 | 12 (11%) |
| 19 | TGL | D | 201 | - | 62,62,62 | 1.11 | 4 (6%) | 65,65,65 | 1.02 | 4 (6%) |
| 24 | PEK | G | 101 | - | 49,49,52 | 1.09 | 3 (6%) | 53,54,57 | 1.32 | 4 (7%) |
| 19 | TGL | O | 303 | - | 62,62,62 | 1.06 | 3 (4%) | 65,65,65 | 1.16 | 4 (6%) |
| 15 | NO | N | 603 | 14,16 | 0,1,1 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 21 | EDO | A | 611 | - | 3,3,3 | 0.92 | 0 | 2,2,2 | 0.70 | 0 |
| 24 | PEK | T | 101 | - | 52,52,52 | 1.06 | 2 (3%) | 55,57,57 | 1.30 | 5 (9%) |
| 14 | HEA | N | 602 | 15,1 | 57,67,67 | 1.56 | 10 (17%) | 61,103,103 | 1.54 | 14 (22%) |
| 20 | PGV | P | 304 | - | 50,50,50 | 1.03 | 2 (4%) | 53,56,56 | 1.44 | 6 (11%) |
| 25 | CDL | T | 103 | - | 99,99,99 | 1.31 | 12 (12%) | 105,111,111 | 1.48 | 10 (9%) |
| 21 | EDO | F | 102 | - | 3,3,3 | 0.99 | 0 | 2,2,2 | 0.65 | 0 |
| 24 | PEK | P | 302 | - | 52,52,52 | 0.74 | 1 (1%) | 55,57,57 | 1.67 | 5 (9%) |
| 23 | CHD | O | 302 | - | 32,32,32 | 1.00 | 1 (3%) | 51,51,51 | 1.48 | 6 (11%) |
| 24 | PEK | G | 103 | - | 52,52,52 | 1.03 | 2 (3%) | 55,57,57 | 1.49 | 5 (9%) |
| 19 | TGL | Q | 201 | - | 62,62,62 | 1.03 | 3 (4%) | 65,65,65 | 0.98 | 3 (4%) |
| 26 | DMU | W | 102 | - | 33,33,34 | 0.86 | 1 (3%) | 44,44,45 | 2.36 | 17 (38%) |
| 26 | DMU | C | 307 | - | 34,34,34 | 0.77 | 1 (2%) | 45,45,45 | 1.64 | 10 (22%) |
| 15 | NO | A | 603 | 14,16 | 0,1,1 | - | - | - | - | - |
| 21 | EDO | S | 103 | - | 3,3,3 | 0.55 | 0 | 2,2,2 | 0.55 | 0 |
| 21 | EDO | P | 308 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.69 | 0 |
| 23 | CHD | P | 306 | - | 32,32,32 | 0.64 | 0 | 51,51,51 | 1.25 | 3 (5%) |
| 19 | TGL | N | 607 | - | 62,62,62 | 1.14 | 3 (4%) | 65,65,65 | 1.33 | 11 (16%) |
| 21 | EDO | C | 308 | - | 3,3,3 | 0.34 | 0 | 2,2,2 | 0.92 | 0 |
| 20 | PGV | C | 304 | - | 50,50,50 | 1.00 | 2 (4%) | 53,56,56 | 1.46 | 6 (11%) |
| 23 | CHD | W | 101 | - | 32,32,32 | 0.69 | 0 | 51,51,51 | 1.98 | 14 (27%) |
| 20 | PGV | N | 608 | - | 45,45,50 | 1.06 | 2 (4%) | 49,50,56 | 1.53 | 9 (18%) |
| 20 | PGV | C | 303 | - | 50,50,50 | 0.89 | 2 (4%) | 53,56,56 | 1.11 | 5 (9%) |
| 21 | EDO | N | 610 | - | 3,3,3 | 0.79 | 0 | 2,2,2 | 0.50 | 0 |
| 21 | EDO | N | 612 | - | 3,3,3 | 0.47 | 0 | 2,2,2 | 0.27 | 0 |
| 26 | DMU | M | 101 | - | 34,34,34 | 0.60 | 1 (2%) | 45,45,45 | 0.96 | 2 (4%) |
| 26 | DMU | O | 304 | - | 22,22,34 | 0.74 | 0 | 27,27,45 | 1.73 | 6 (22%) |
| 21 | EDO | P | 309 | - | 3,3,3 | 0.79 | 0 | 2,2,2 | 0.39 | 0 |
| 23 | CHD | J | 101 | - | 32,32,32 | 0.70 | 0 | 51,51,51 | 1.83 | 13 (25%) |
| 21 | EDO | Q | 202 | - | 3,3,3 | 0.36 | 0 | 2,2,2 | 0.42 | 0 |
| 24 | PEK | C | 302 | - | 52,52,52 | 0.83 | 3 (5%) | 55,57,57 | 1.47 | 10 (18%) |
| 26 | DMU | Z | 101 | - | 34,34,34 | 0.43 | 0 | 45,45,45 | 0.84 | 1 (2%) |
| 27 | PSC | E | 201 | - | 51,51,51 | 1.08 | 3 (5%) | 57,59,59 | 1.20 | 4 (7%) |
| 23 | CHD | B | 302 | - | 32,32,32 | 0.92 | 1 (3%) | 51,51,51 | 1.51 | 11 (21%) |
| 25 | CDL | C | 305 | - | 99,99,99 | 1.35 | 13 (13%) | 105,111,111 | 1.56 | 13 (12%) |
| 20 | PGV | A | 609 | - | 50,50,50 | 1.00 | 2 (4%) | 53,56,56 | 1.23 | 6 (11%) |
| 14 | HEA | A | 602 | 15,1 | 57,67,67 | 1.72 | 14 (24%) | 61,103,103 | 1.93 | 23 (37%) |
| 23 | CHD | C | 306 | - | 32,32,32 | 0.63 | 0 | 51,51,51 | 1.18 | 6 (11%) |

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 |
|-----|------|-------|-----|------|----------|----------------|---------|
| 14 | HEA | A | 601 | 1 | 3/3/7/16 | 6/32/76/76 | - |
| 21 | EDO | B | 303 | - | - | 0/1/1/1 | - |
| 21 | EDO | N | 614 | - | - | 1/1/1/1 | - |
| 21 | EDO | N | 613 | - | - | 0/1/1/1 | - |
| 21 | EDO | A | 612 | - | - | 0/1/1/1 | - |
| 20 | PGV | N | 609 | - | - | 8/55/55/55 | - |
| 19 | TGL | L | 101 | - | - | 29/65/65/65 | - |
| 21 | EDO | S | 104 | - | - | 0/1/1/1 | - |
| 25 | CDL | P | 305 | - | - | 58/110/110/110 | - |
| 27 | PSC | R | 201 | - | - | 23/55/55/55 | - |
| 20 | PGV | A | 608 | - | - | 8/55/55/55 | - |
| 21 | EDO | O | 306 | - | - | 0/1/1/1 | - |
| 21 | EDO | Q | 203 | - | - | 0/1/1/1 | - |
| 23 | CHD | C | 301 | - | - | 1/9/74/74 | 0/4/4/4 |
| 24 | PEK | T | 102 | - | - | 25/56/56/56 | - |
| 21 | EDO | A | 610 | - | - | 0/1/1/1 | - |
| 26 | DMU | P | 307 | - | - | 10/19/59/59 | 0/2/2/2 |
| 21 | EDO | A | 613 | - | - | 0/1/1/1 | - |
| 21 | EDO | O | 305 | - | - | 0/1/1/1 | - |
| 19 | TGL | A | 607 | - | - | 33/65/65/65 | - |
| 21 | EDO | N | 611 | - | - | 0/1/1/1 | - |
| 14 | HEA | N | 601 | 1 | 3/3/7/16 | 5/32/76/76 | - |
| 23 | CHD | P | 301 | - | - | 2/9/74/74 | 0/4/4/4 |
| 21 | EDO | N | 615 | - | - | 0/1/1/1 | - |
| 20 | PGV | P | 303 | - | - | 9/55/55/55 | - |
| 21 | EDO | S | 102 | - | - | 0/1/1/1 | - |
| 25 | CDL | G | 102 | - | - | 50/110/110/110 | - |
| 19 | TGL | D | 201 | - | - | 30/65/65/65 | - |
| 24 | PEK | G | 101 | - | - | 25/51/51/56 | - |
| 19 | TGL | O | 303 | - | - | 33/65/65/65 | - |
| 24 | PEK | T | 101 | - | - | 36/56/56/56 | - |
| 21 | EDO | A | 611 | - | - | 0/1/1/1 | - |
| 14 | HEA | N | 602 | 15,1 | 3/3/7/16 | 4/32/76/76 | - |
| 20 | PGV | P | 304 | - | - | 18/55/55/55 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|----------|----------------|---------|
| 25 | CDL | T | 103 | - | - | 48/110/110/110 | - |
| 21 | EDO | F | 102 | - | - | 0/1/1/1 | - |
| 24 | PEK | P | 302 | - | - | 19/56/56/56 | - |
| 23 | CHD | O | 302 | - | - | 2/9/74/74 | 0/4/4/4 |
| 24 | PEK | G | 103 | - | - | 24/56/56/56 | - |
| 19 | TGL | Q | 201 | - | - | 26/65/65/65 | - |
| 26 | DMU | W | 102 | - | - | 5/18/58/59 | 0/2/2/2 |
| 26 | DMU | C | 307 | - | - | 7/19/59/59 | 0/2/2/2 |
| 21 | EDO | S | 103 | - | - | 0/1/1/1 | - |
| 21 | EDO | P | 308 | - | - | 1/1/1/1 | - |
| 23 | CHD | P | 306 | - | - | 2/9/74/74 | 0/4/4/4 |
| 19 | TGL | N | 607 | - | - | 33/65/65/65 | - |
| 21 | EDO | C | 308 | - | - | 1/1/1/1 | - |
| 20 | PGV | C | 304 | - | - | 15/55/55/55 | - |
| 23 | CHD | W | 101 | - | - | 6/9/74/74 | 0/4/4/4 |
| 20 | PGV | N | 608 | - | - | 20/47/47/55 | - |
| 20 | PGV | C | 303 | - | - | 6/55/55/55 | - |
| 21 | EDO | N | 610 | - | - | 0/1/1/1 | - |
| 21 | EDO | N | 612 | - | - | 0/1/1/1 | - |
| 26 | DMU | M | 101 | - | - | 6/19/59/59 | 0/2/2/2 |
| 26 | DMU | O | 304 | - | - | 6/13/33/59 | 0/1/1/2 |
| 21 | EDO | P | 309 | - | - | 0/1/1/1 | - |
| 23 | CHD | J | 101 | - | - | 5/9/74/74 | 0/4/4/4 |
| 21 | EDO | Q | 202 | - | - | 1/1/1/1 | - |
| 24 | PEK | C | 302 | - | - | 15/56/56/56 | - |
| 26 | DMU | Z | 101 | - | - | 5/19/59/59 | 0/2/2/2 |
| 27 | PSC | E | 201 | - | - | 32/55/55/55 | - |
| 23 | CHD | B | 302 | - | - | 2/9/74/74 | 0/4/4/4 |
| 25 | CDL | C | 305 | - | - | 48/110/110/110 | - |
| 20 | PGV | A | 609 | - | - | 19/55/55/55 | - |
| 14 | HEA | A | 602 | 15,1 | 3/3/7/16 | 5/32/76/76 | - |
| 23 | CHD | C | 306 | - | - | 4/9/74/74 | 0/4/4/4 |

The worst 5 of 161 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 19 | N | 607 | TGL | OG2-CB1 | 5.33 | 1.49 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 19 | L | 101 | TGL | OG2-CB1 | 5.22 | 1.49 | 1.34 |
| 24 | T | 101 | PEK | O03-C21 | 5.15 | 1.48 | 1.33 |
| 20 | P | 304 | PGV | O01-C1 | 5.11 | 1.48 | 1.34 |
| 24 | G | 101 | PEK | O03-C21 | 4.82 | 1.47 | 1.33 |

The worst 5 of 377 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | P | 302 | PEK | C2-C3-C4 | 9.28 | 129.78 | 113.23 |
| 26 | P | 307 | DMU | C18-O16-C6 | 8.01 | 127.12 | 113.84 |
| 14 | A | 601 | HEA | C13-C12-C11 | -7.40 | 103.24 | 114.35 |
| 25 | C | 305 | CDL | CB4-OB6-CB5 | -6.83 | 100.98 | 117.79 |
| 25 | P | 305 | CDL | CB4-OB6-CB5 | -6.70 | 101.29 | 117.79 |

5 of 12 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14 | A | 601 | HEA | NB |
| 14 | A | 601 | HEA | ND |
| 14 | A | 601 | HEA | NA |
| 14 | A | 602 | HEA | NB |
| 14 | A | 602 | HEA | ND |

5 of 777 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 19 | A | 607 | TGL | OG1-CG1-CG2-OG2 |
| 19 | N | 607 | TGL | CB2-CB1-OG2-CG2 |
| 20 | A | 609 | PGV | C03-O11-P-O13 |
| 20 | A | 609 | PGV | C04-O12-P-O11 |
| 20 | A | 609 | PGV | C2-C1-O01-C02 |

There are no ring outliers.

44 monomers are involved in 220 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14 | A | 601 | HEA | 3 | 0 |
| 21 | N | 614 | EDO | 1 | 0 |
| 19 | L | 101 | TGL | 8 | 0 |
| 25 | P | 305 | CDL | 19 | 0 |
| 27 | R | 201 | PSC | 10 | 0 |

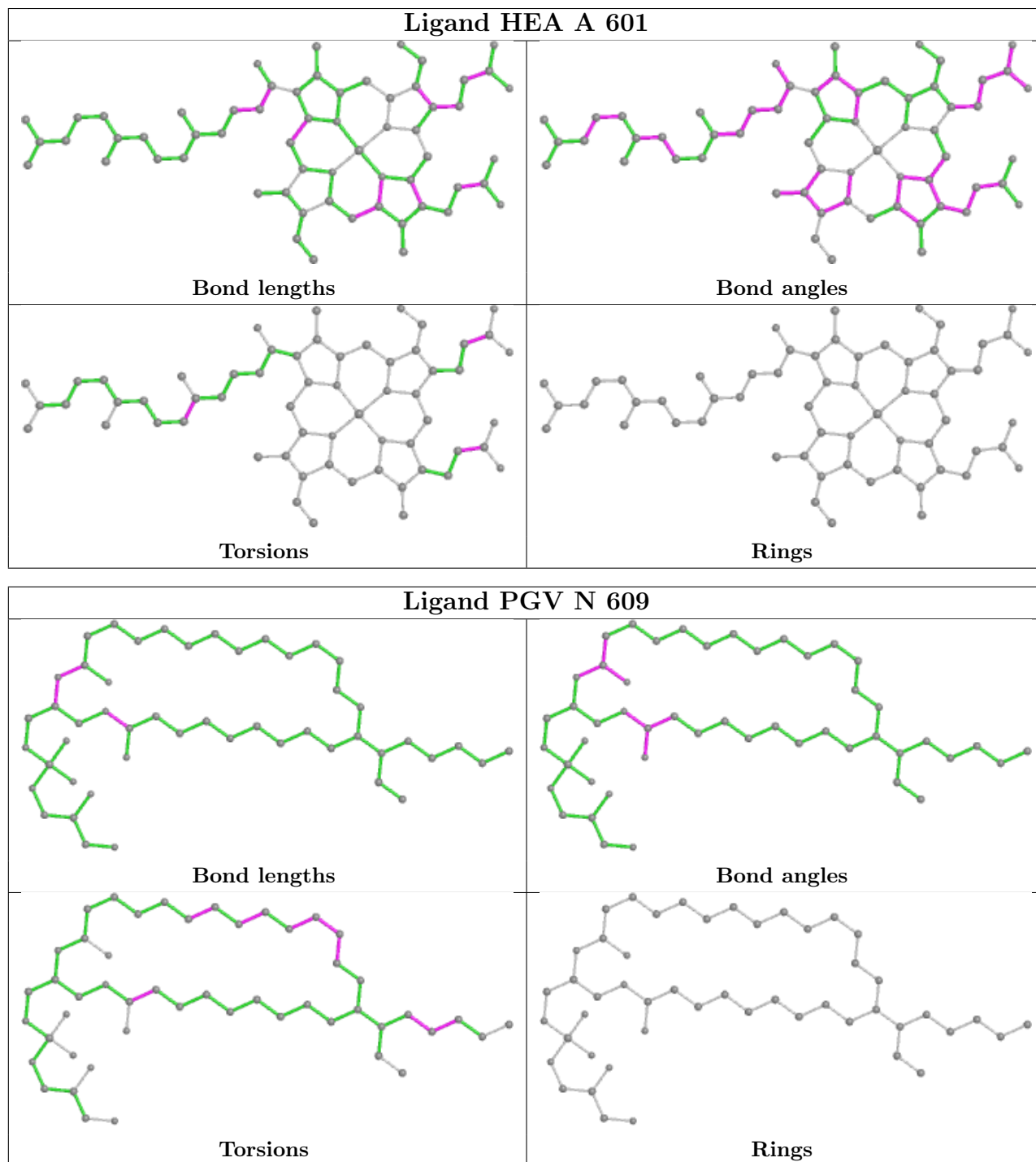
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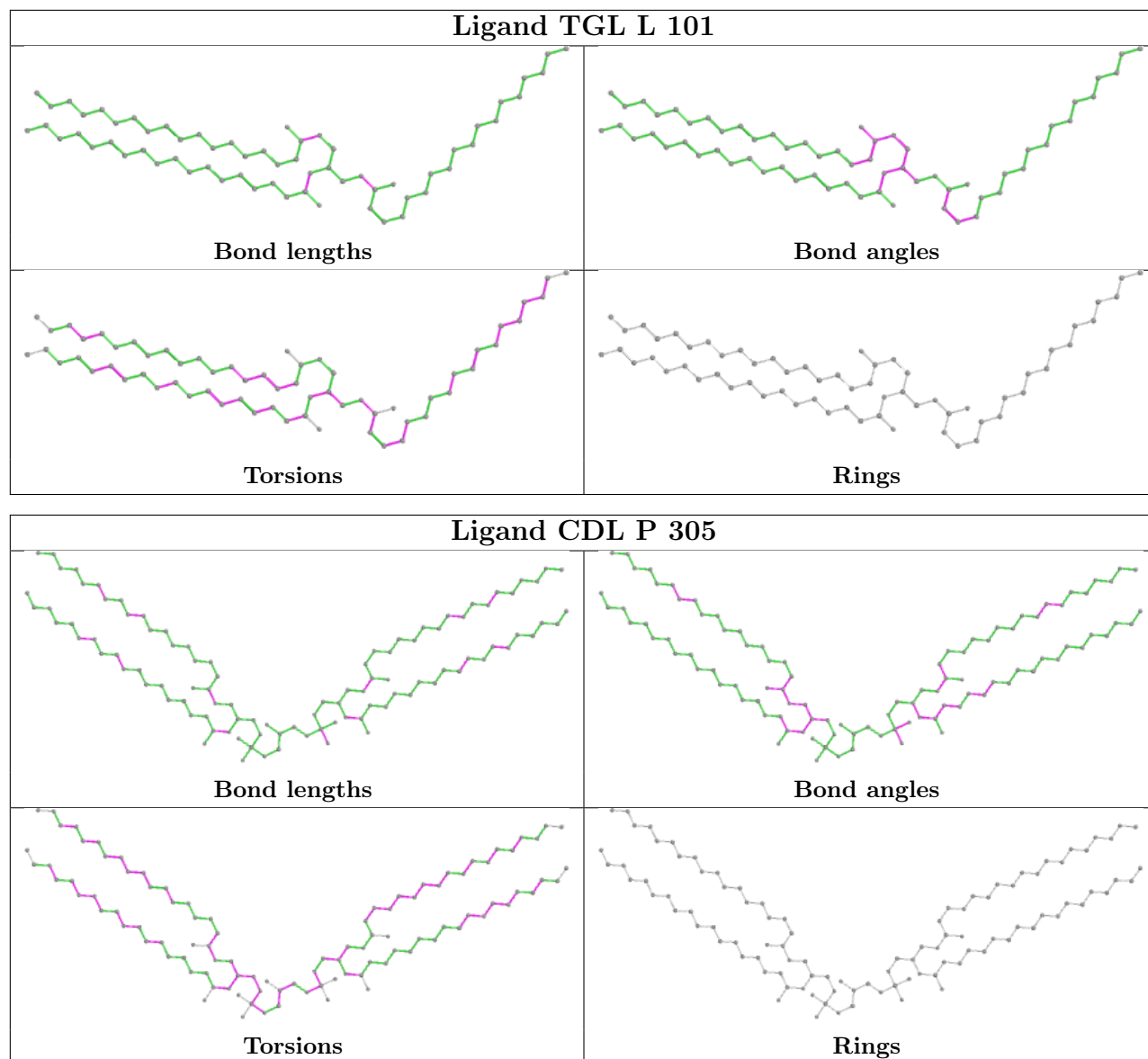
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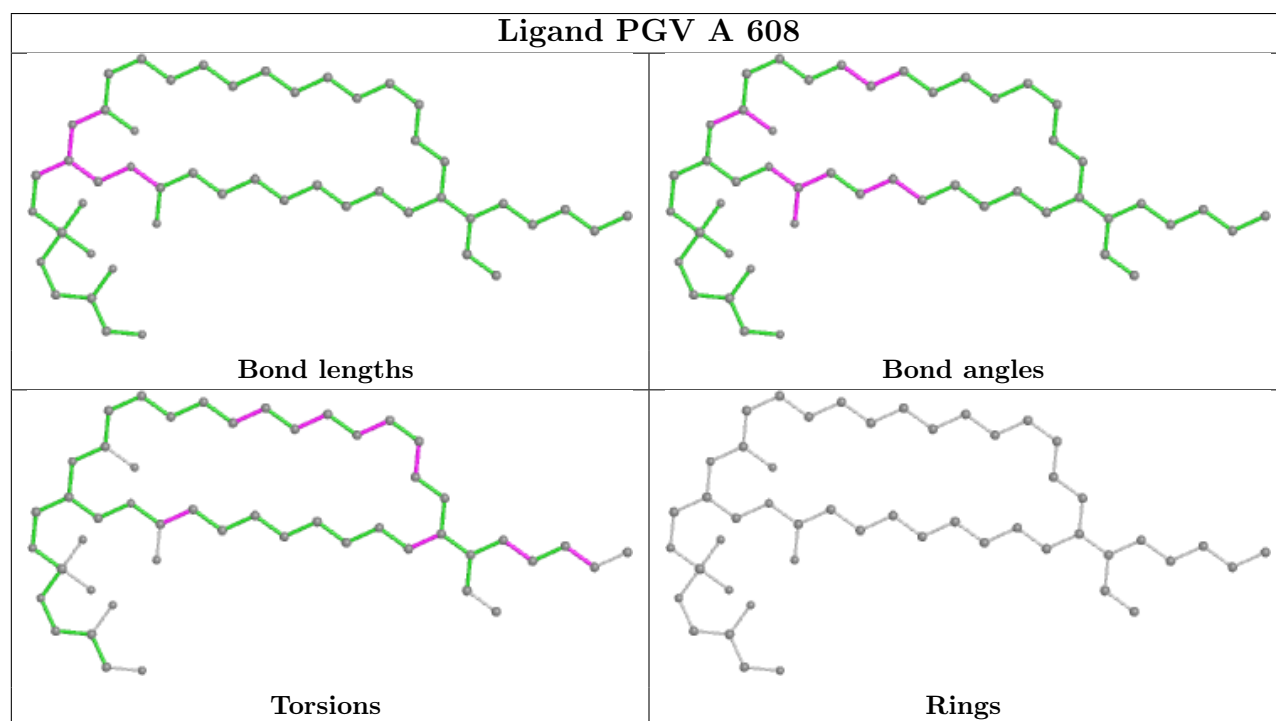
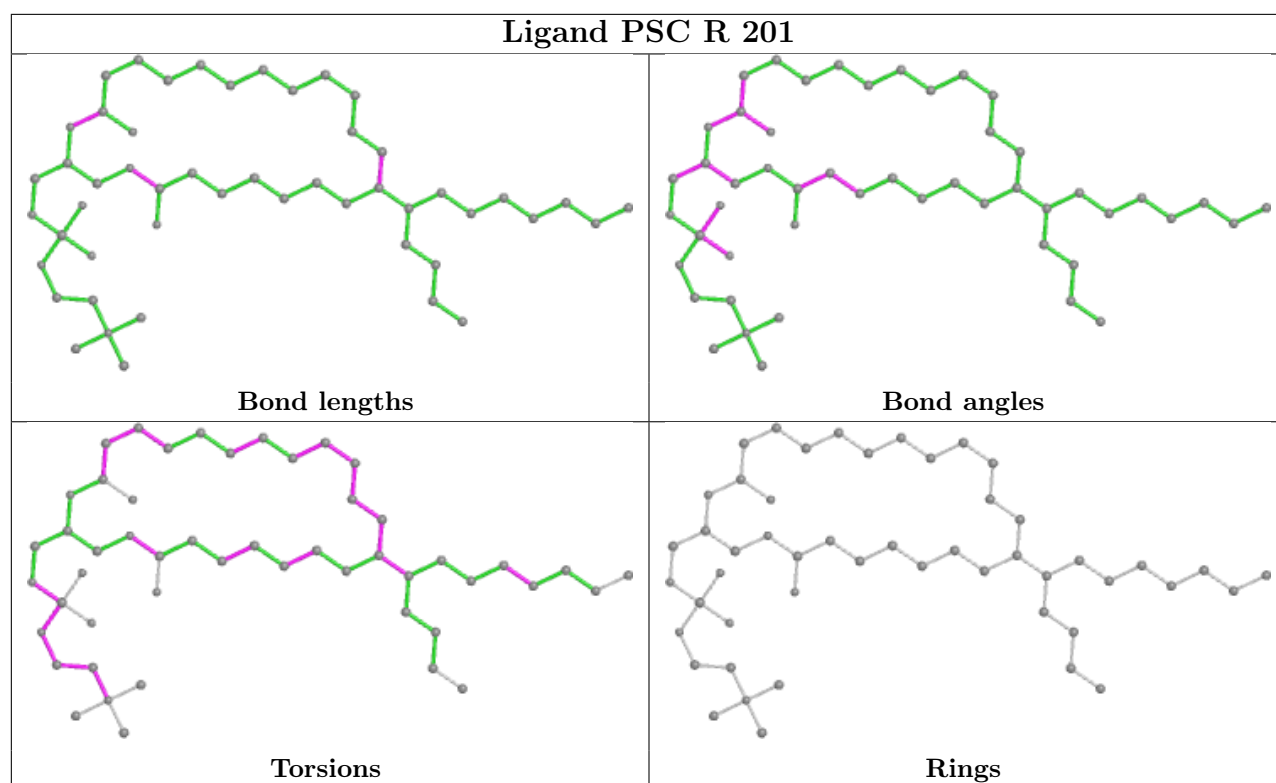
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | C | 301 | CHD | 1 | 0 |
| 24 | T | 102 | PEK | 6 | 0 |
| 26 | P | 307 | DMU | 8 | 0 |
| 21 | A | 613 | EDO | 1 | 0 |
| 19 | A | 607 | TGL | 3 | 0 |
| 14 | N | 601 | HEA | 3 | 0 |
| 21 | N | 615 | EDO | 1 | 0 |
| 20 | P | 303 | PGV | 3 | 0 |
| 25 | G | 102 | CDL | 23 | 0 |
| 19 | D | 201 | TGL | 8 | 0 |
| 24 | G | 101 | PEK | 1 | 0 |
| 24 | T | 101 | PEK | 4 | 0 |
| 14 | N | 602 | HEA | 5 | 0 |
| 20 | P | 304 | PGV | 3 | 0 |
| 25 | T | 103 | CDL | 14 | 0 |
| 24 | P | 302 | PEK | 6 | 0 |
| 23 | O | 302 | CHD | 2 | 0 |
| 24 | G | 103 | PEK | 4 | 0 |
| 19 | Q | 201 | TGL | 9 | 0 |
| 26 | W | 102 | DMU | 4 | 0 |
| 26 | C | 307 | DMU | 2 | 0 |
| 21 | P | 308 | EDO | 1 | 0 |
| 23 | P | 306 | CHD | 1 | 0 |
| 19 | N | 607 | TGL | 8 | 0 |
| 20 | C | 304 | PGV | 4 | 0 |
| 23 | W | 101 | CHD | 1 | 0 |
| 20 | N | 608 | PGV | 5 | 0 |
| 20 | C | 303 | PGV | 4 | 0 |
| 26 | M | 101 | DMU | 1 | 0 |
| 26 | O | 304 | DMU | 1 | 0 |
| 23 | J | 101 | CHD | 2 | 0 |
| 24 | C | 302 | PEK | 6 | 0 |
| 26 | Z | 101 | DMU | 1 | 0 |
| 27 | E | 201 | PSC | 12 | 0 |
| 23 | B | 302 | CHD | 1 | 0 |
| 25 | C | 305 | CDL | 14 | 0 |
| 20 | A | 609 | PGV | 4 | 0 |
| 14 | A | 602 | HEA | 5 | 0 |
| 23 | C | 306 | CHD | 2 | 0 |

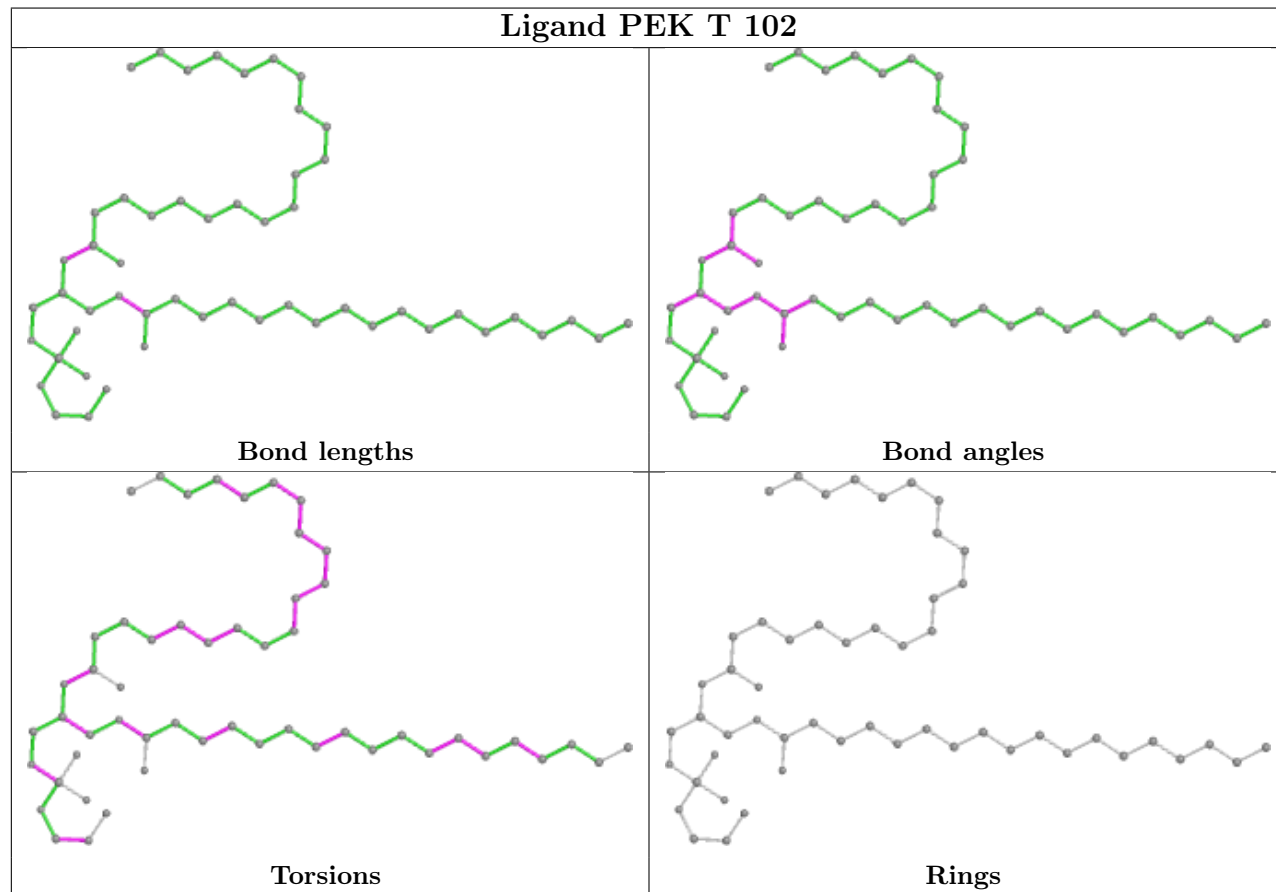
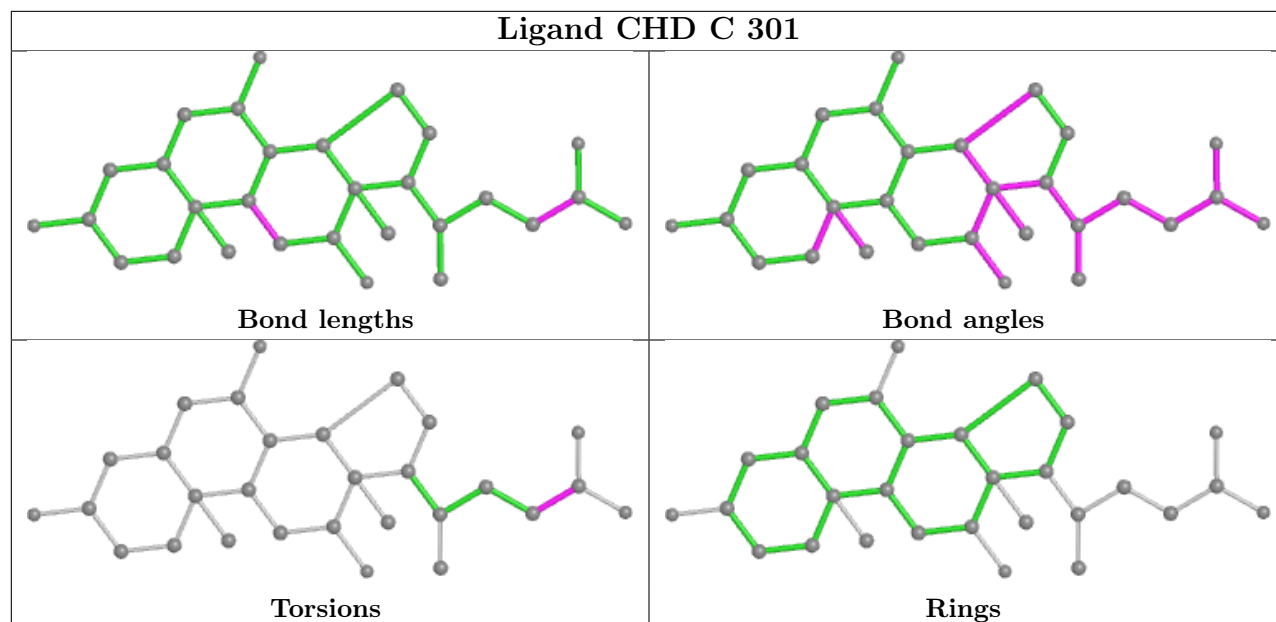
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

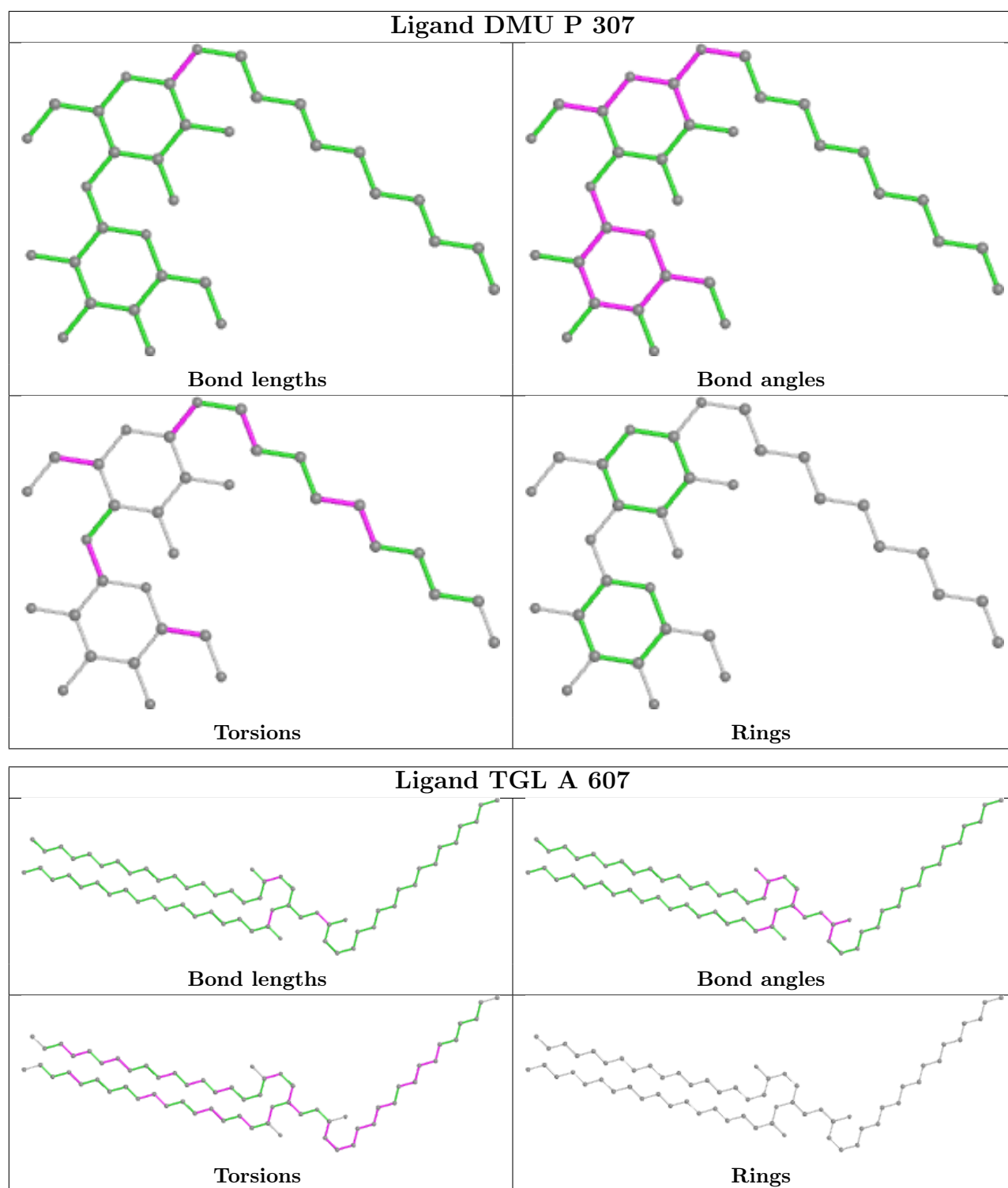
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

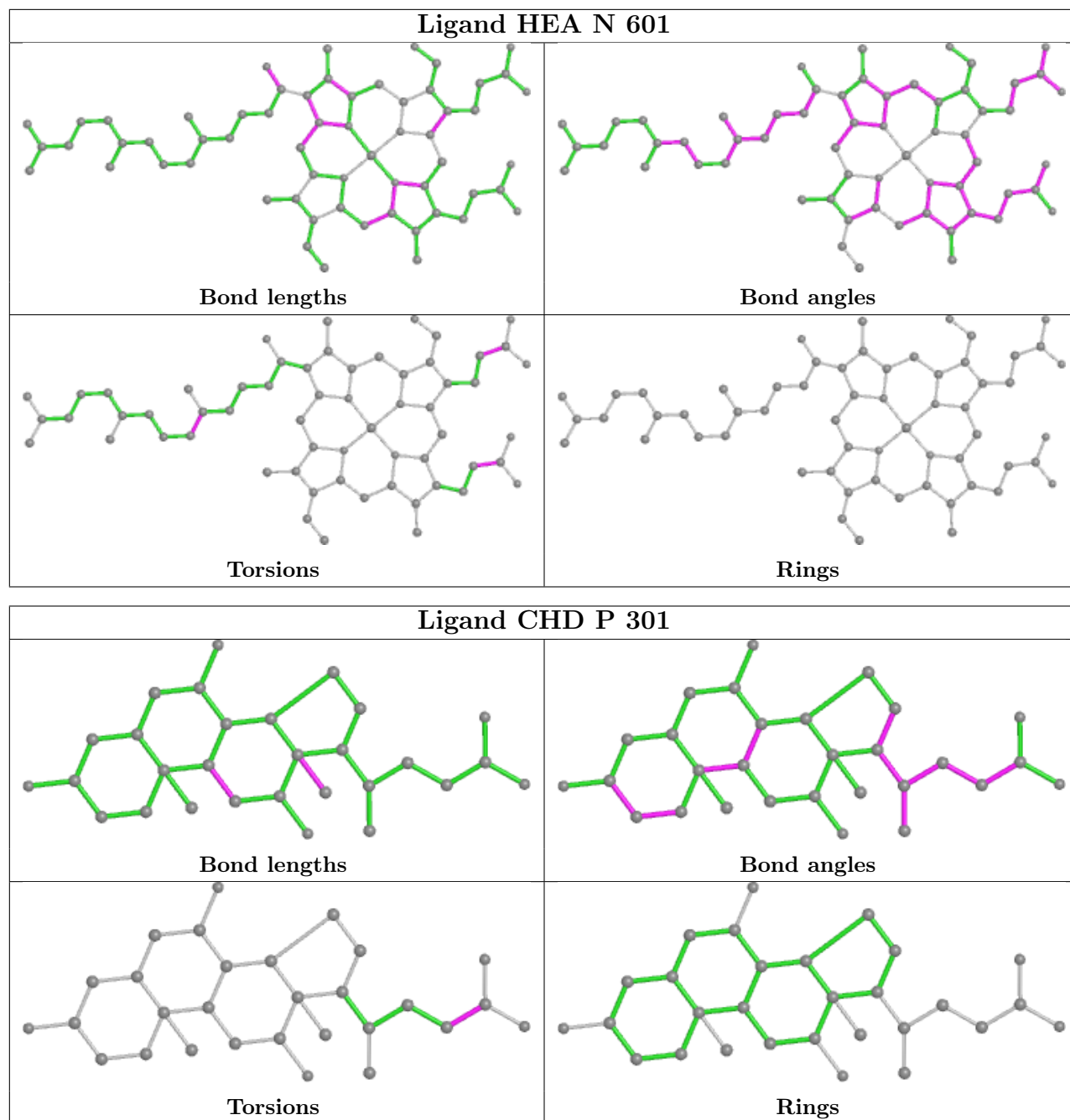


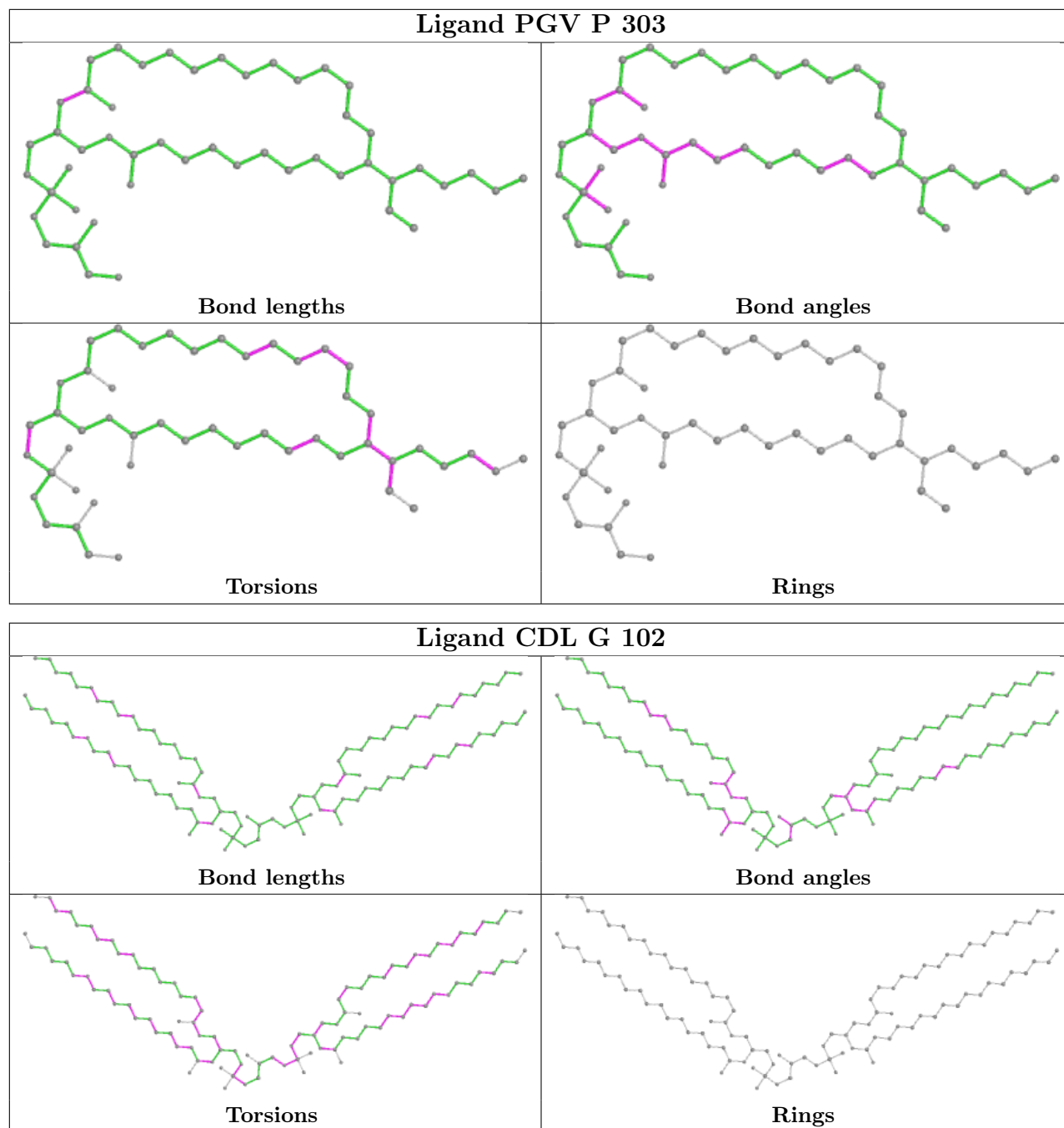


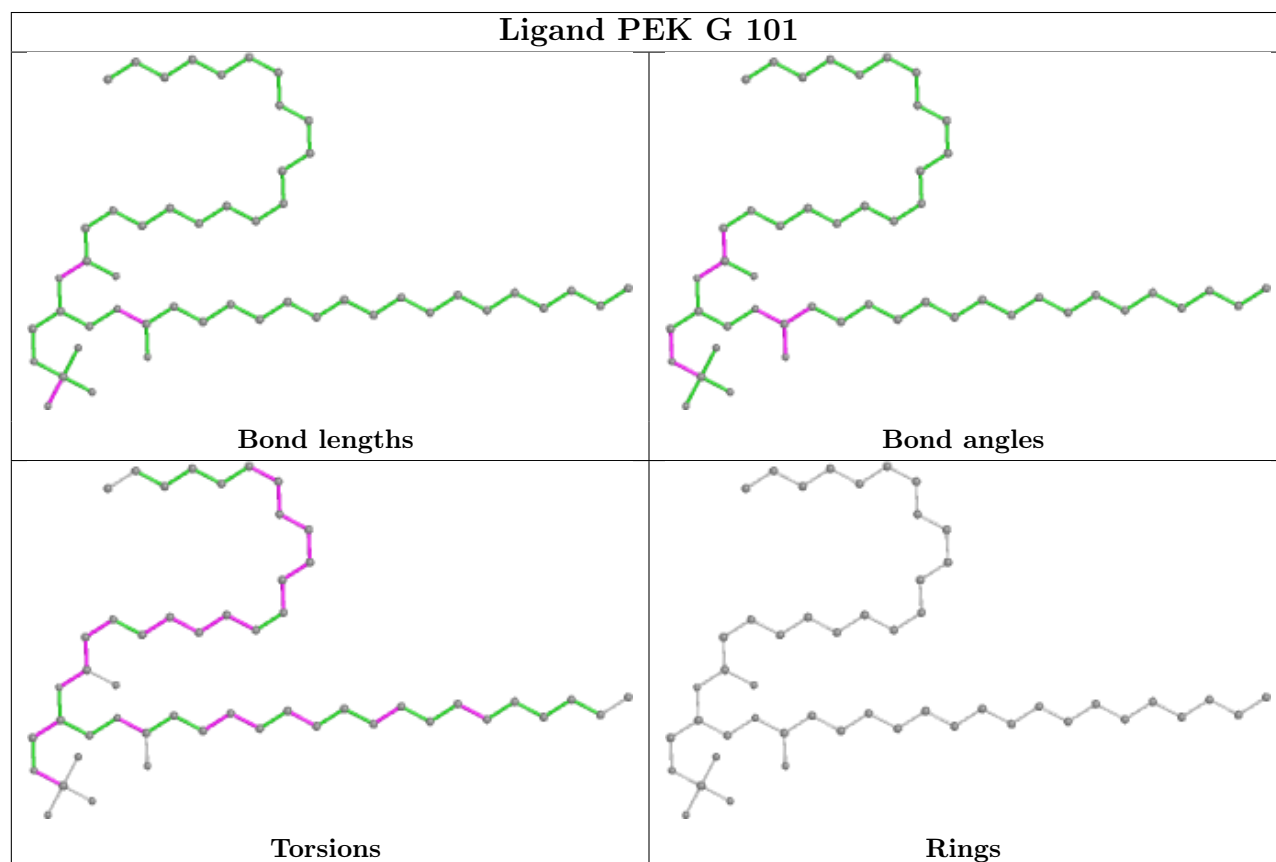
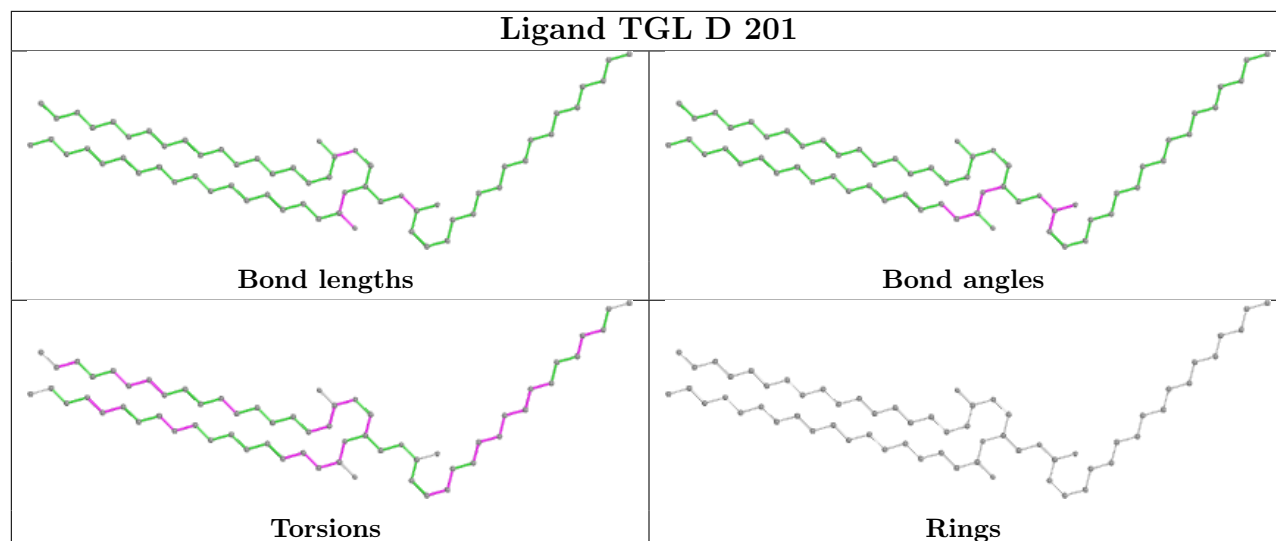


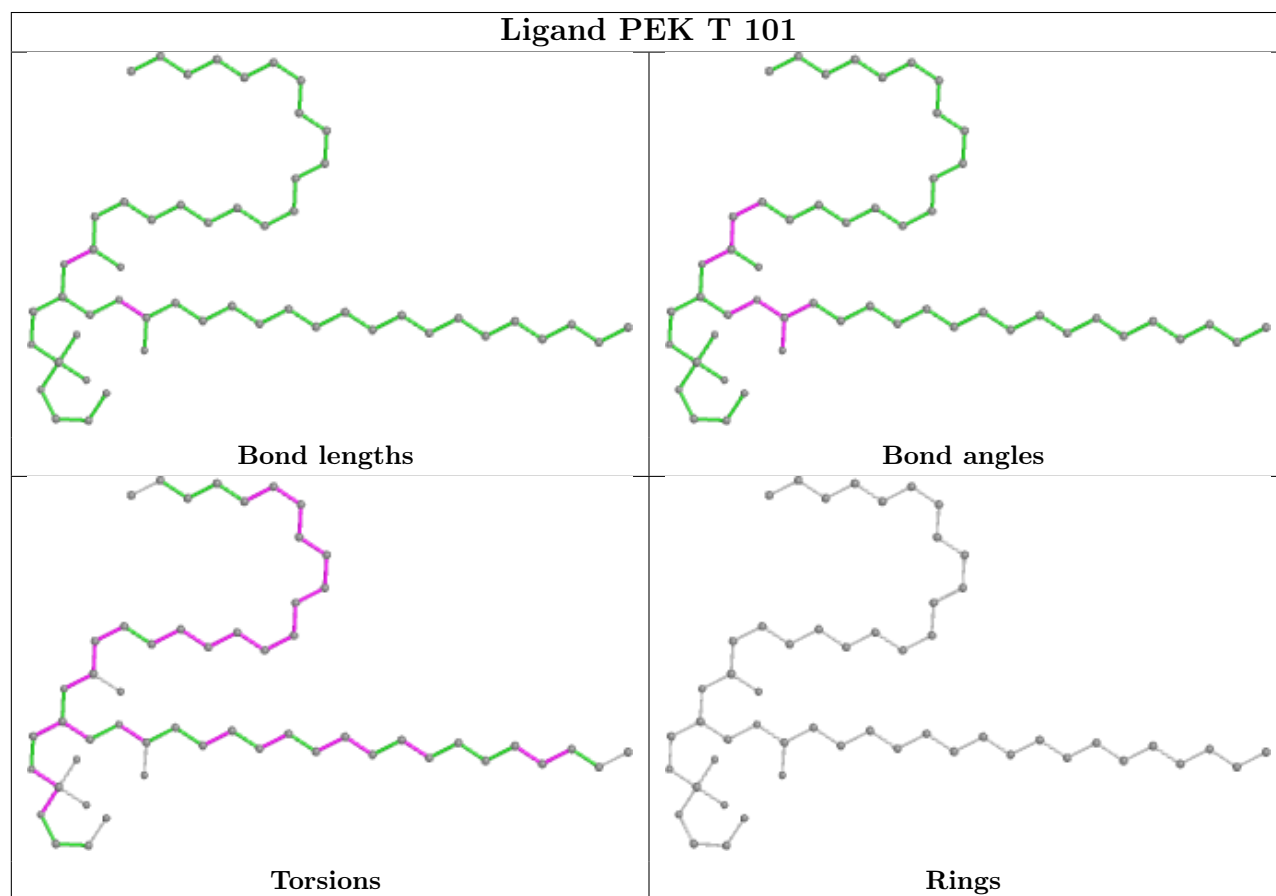
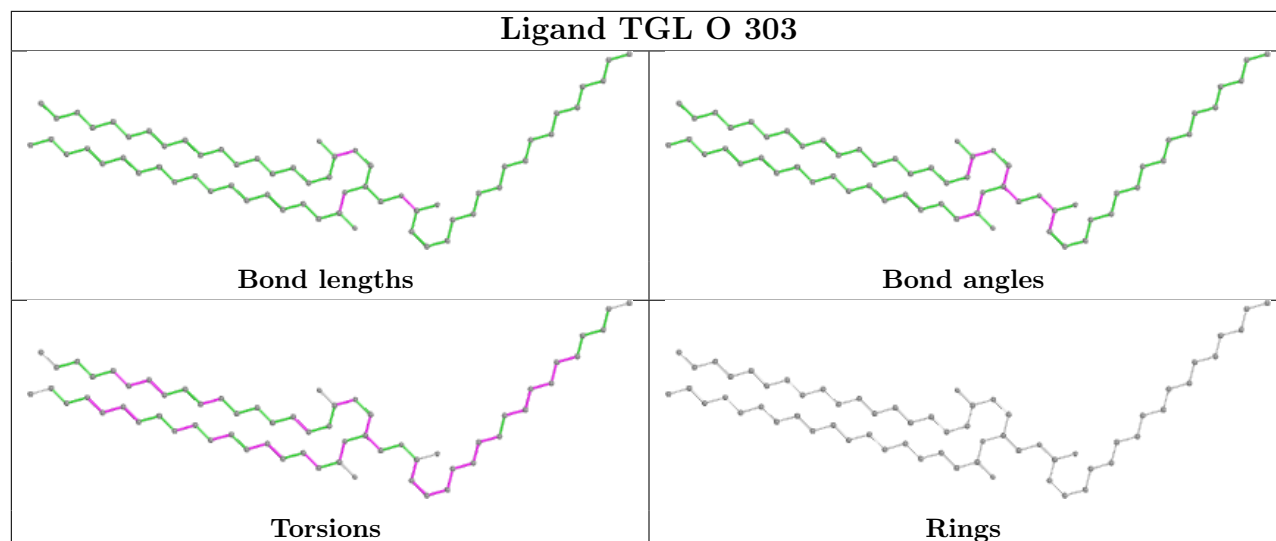


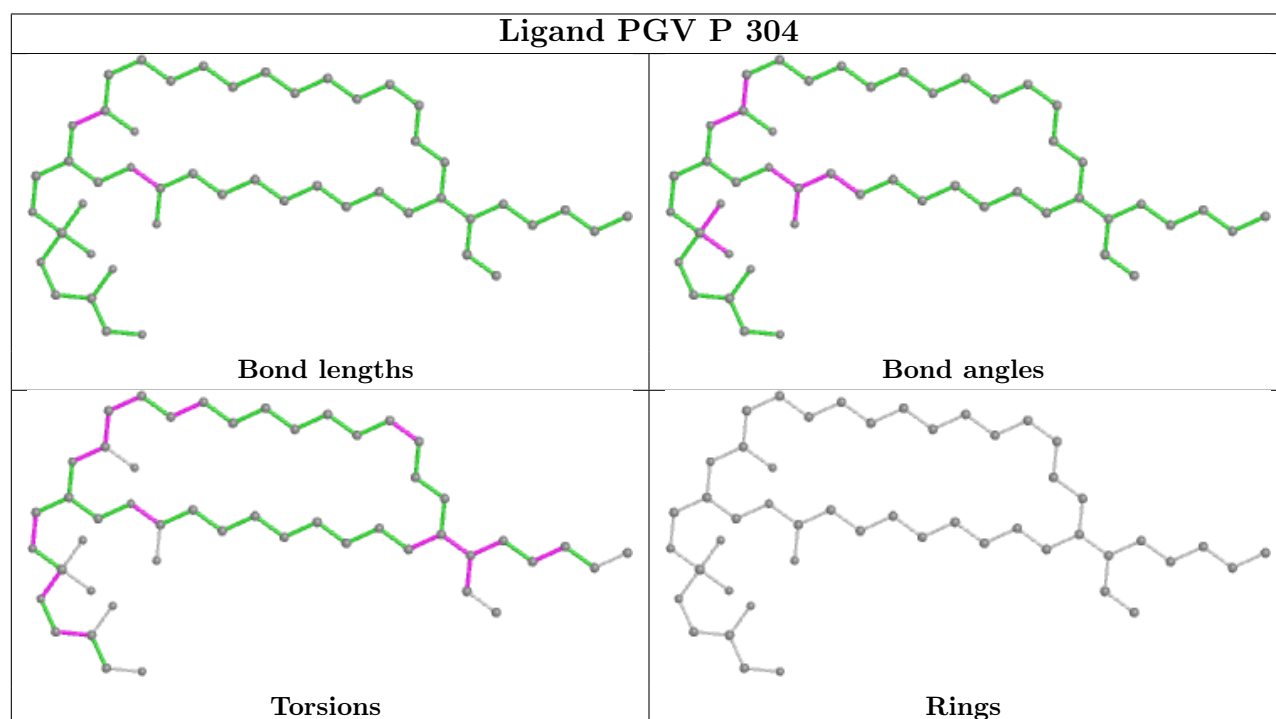
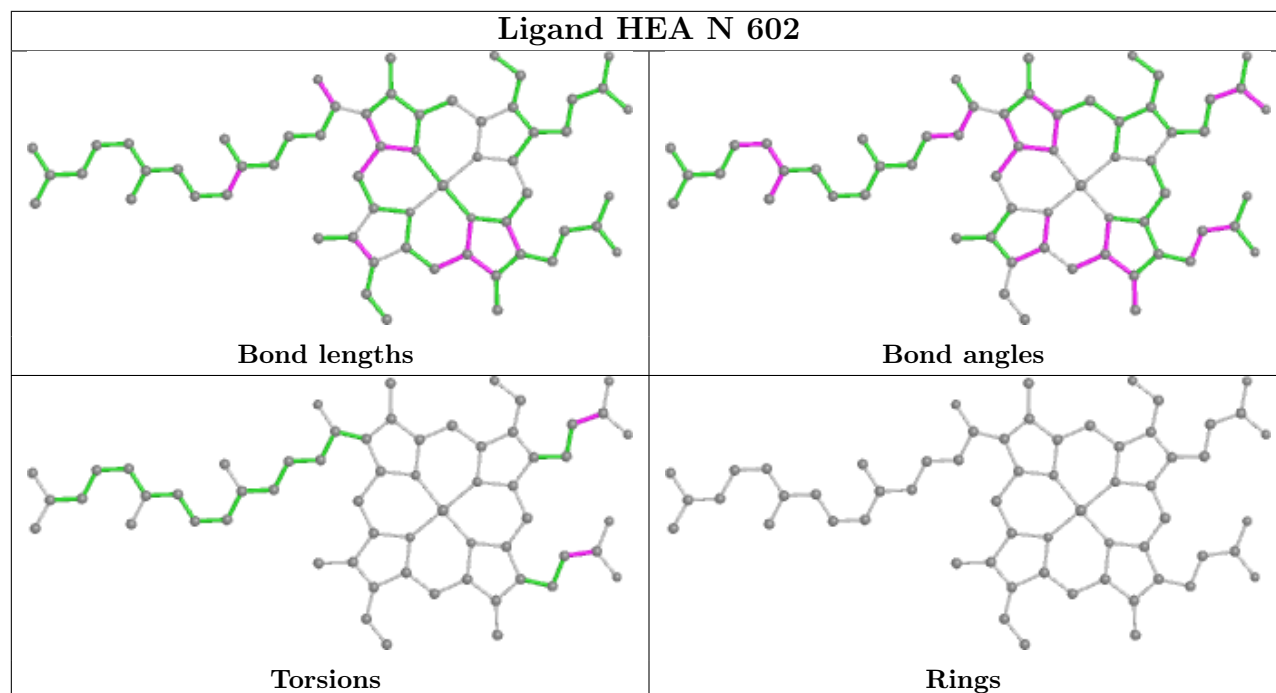


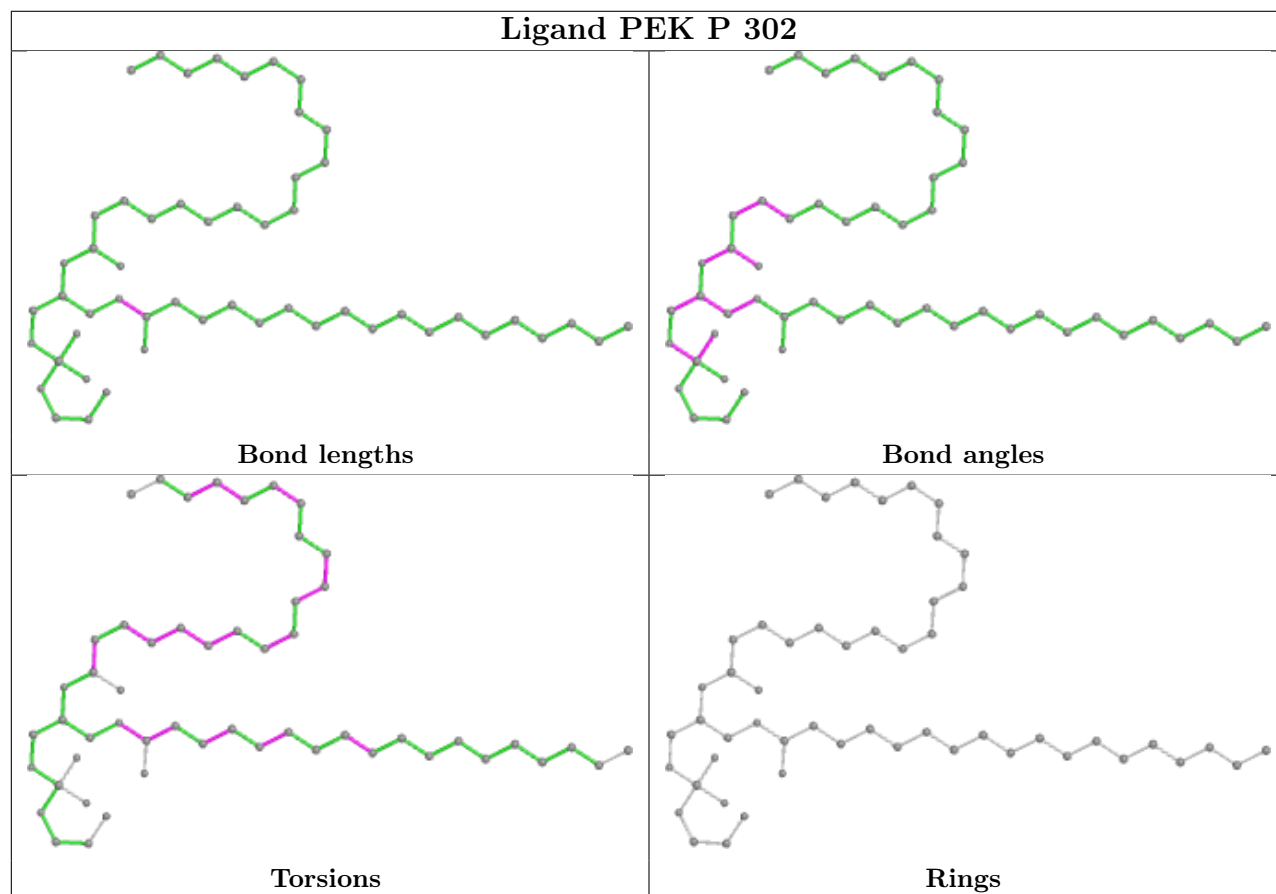
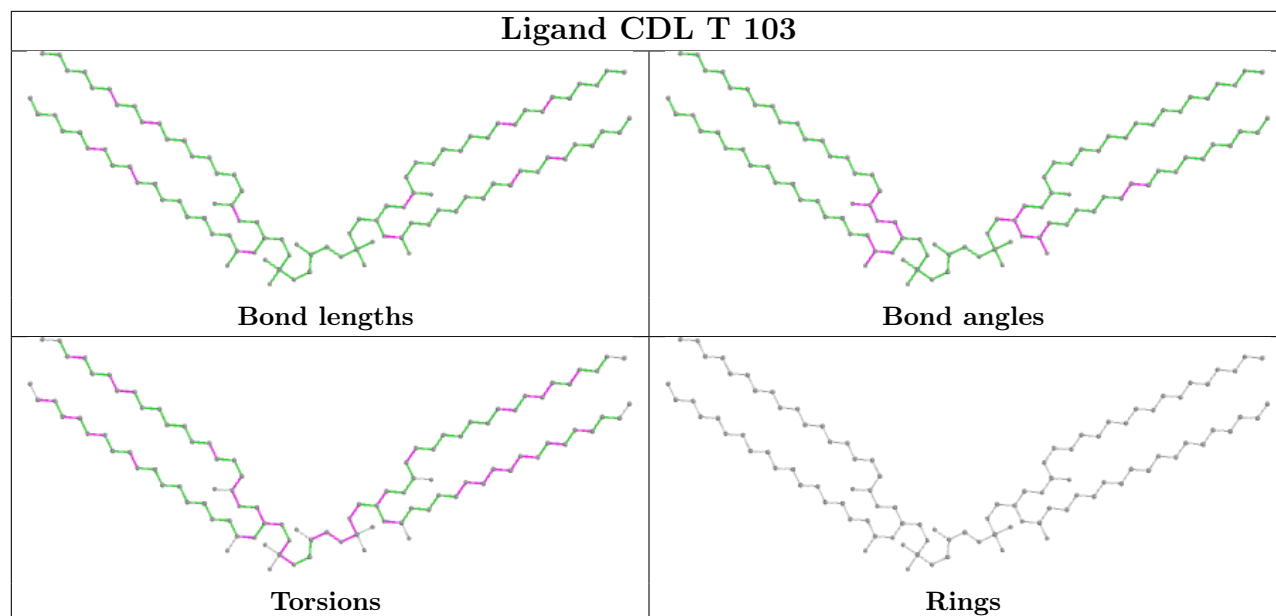


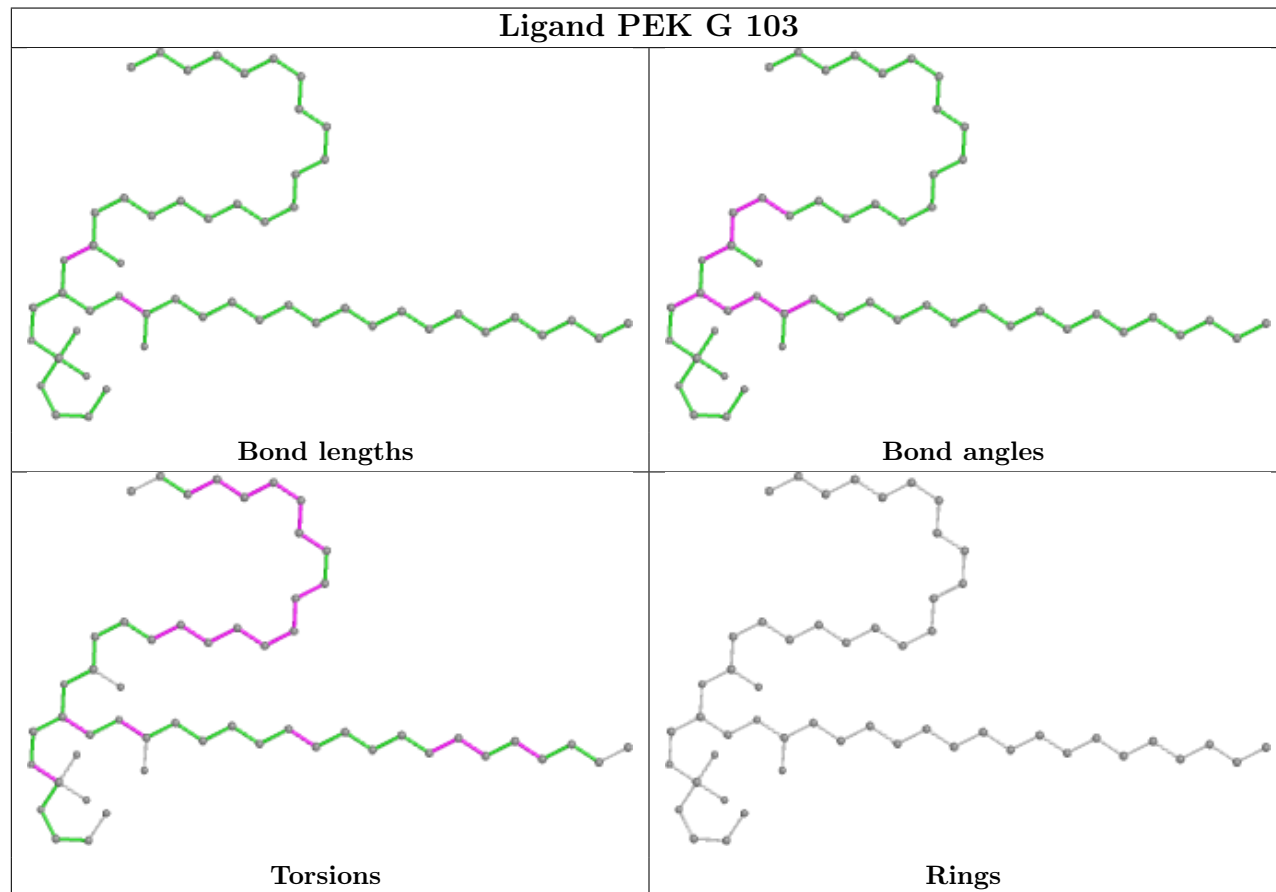
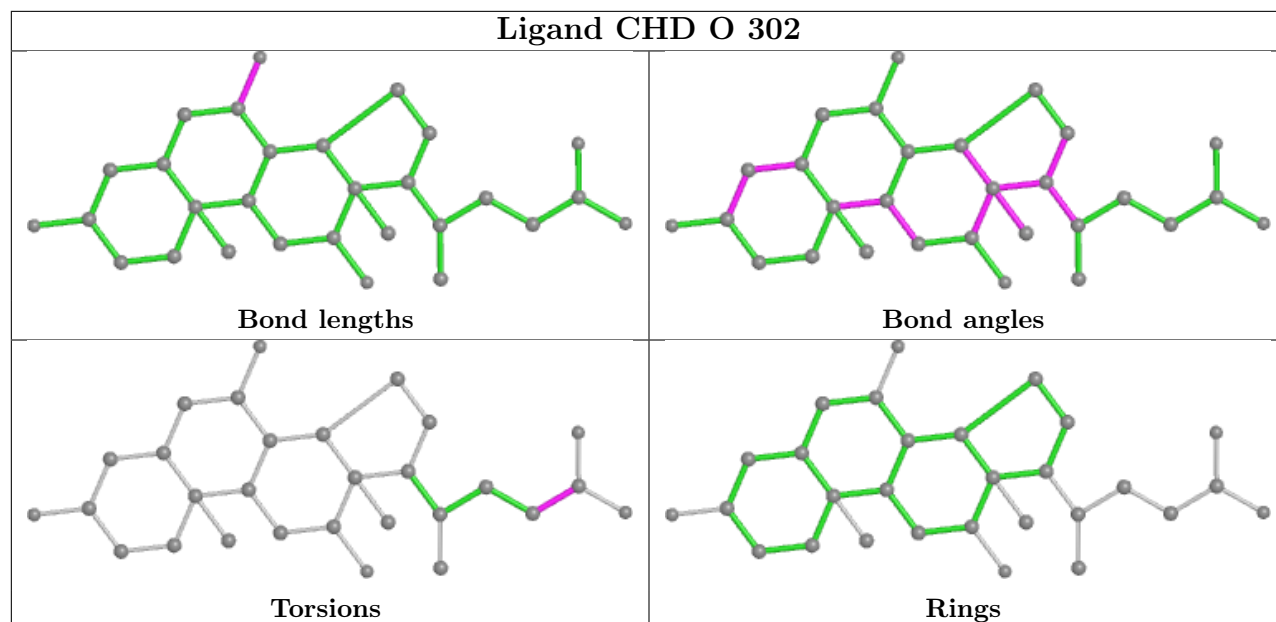


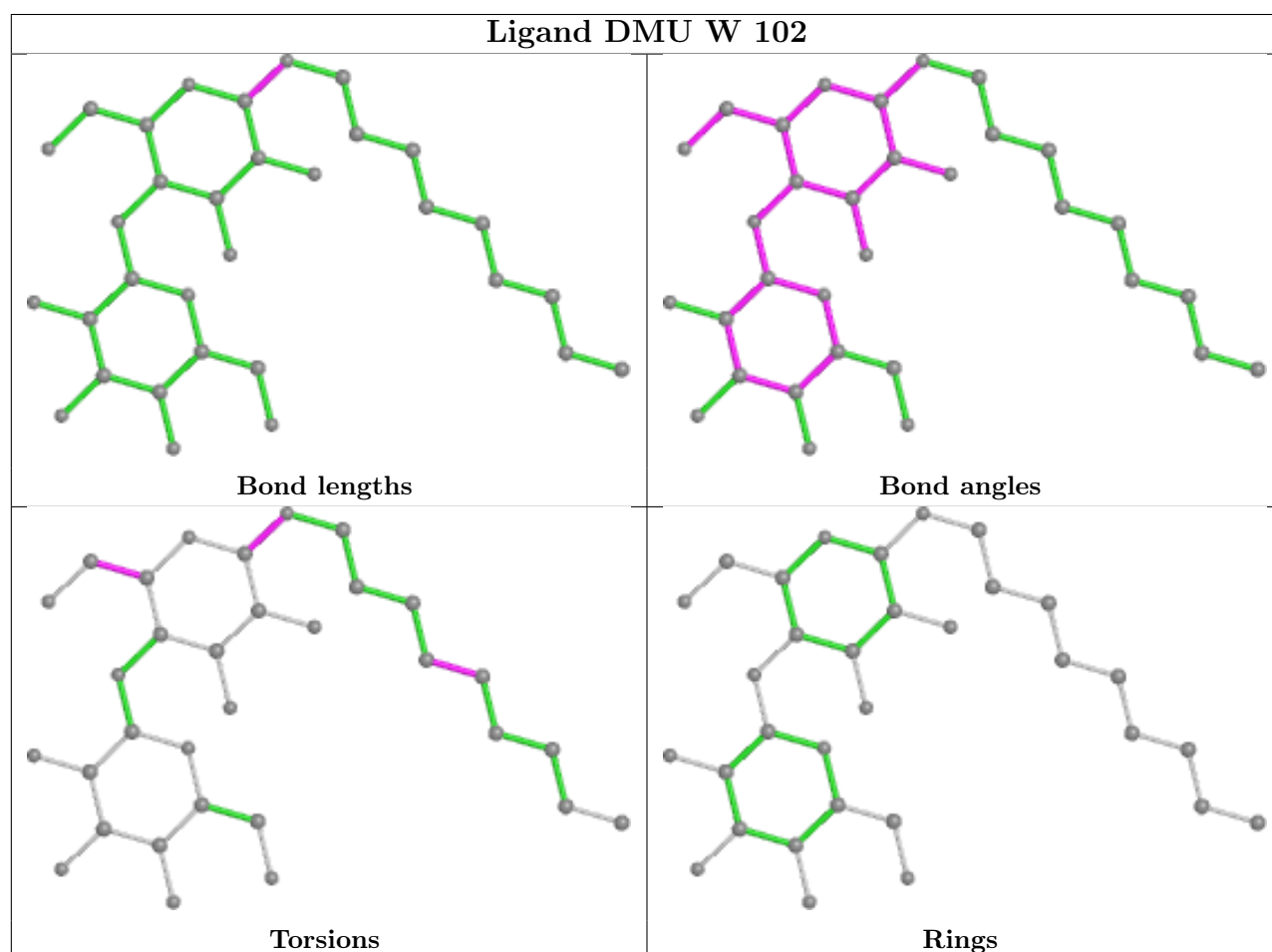
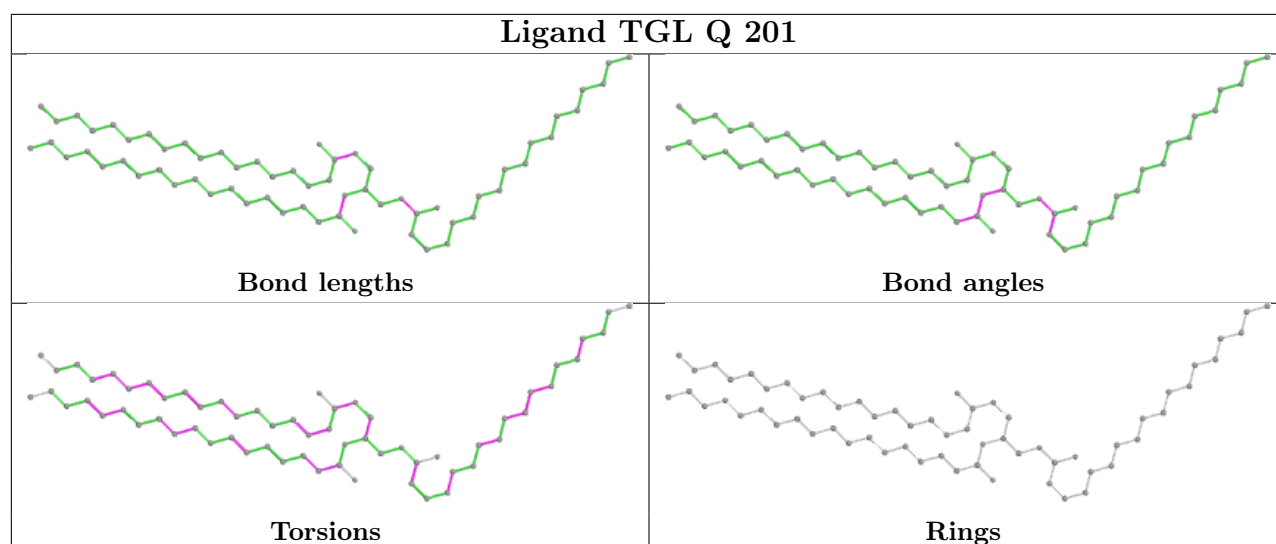


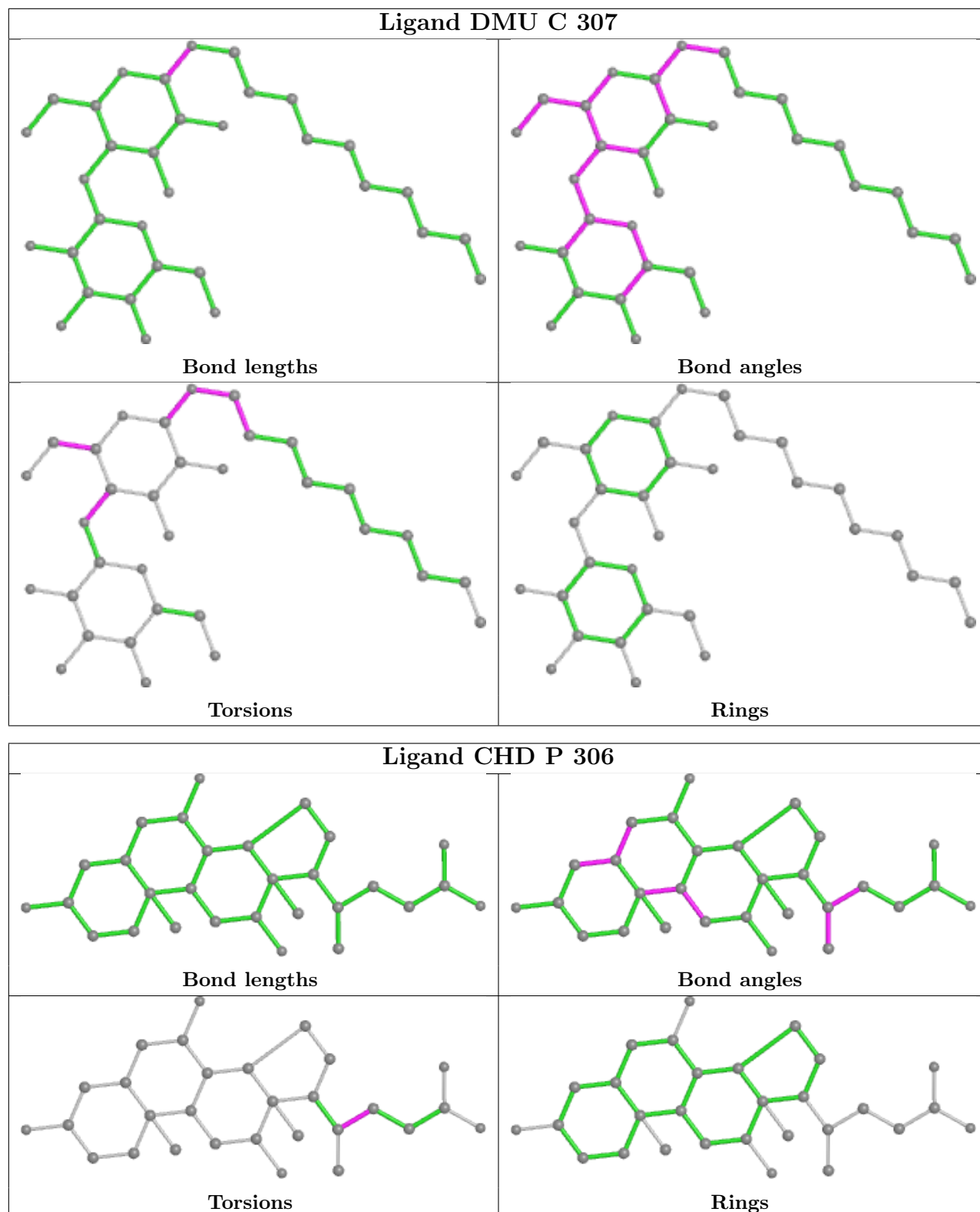


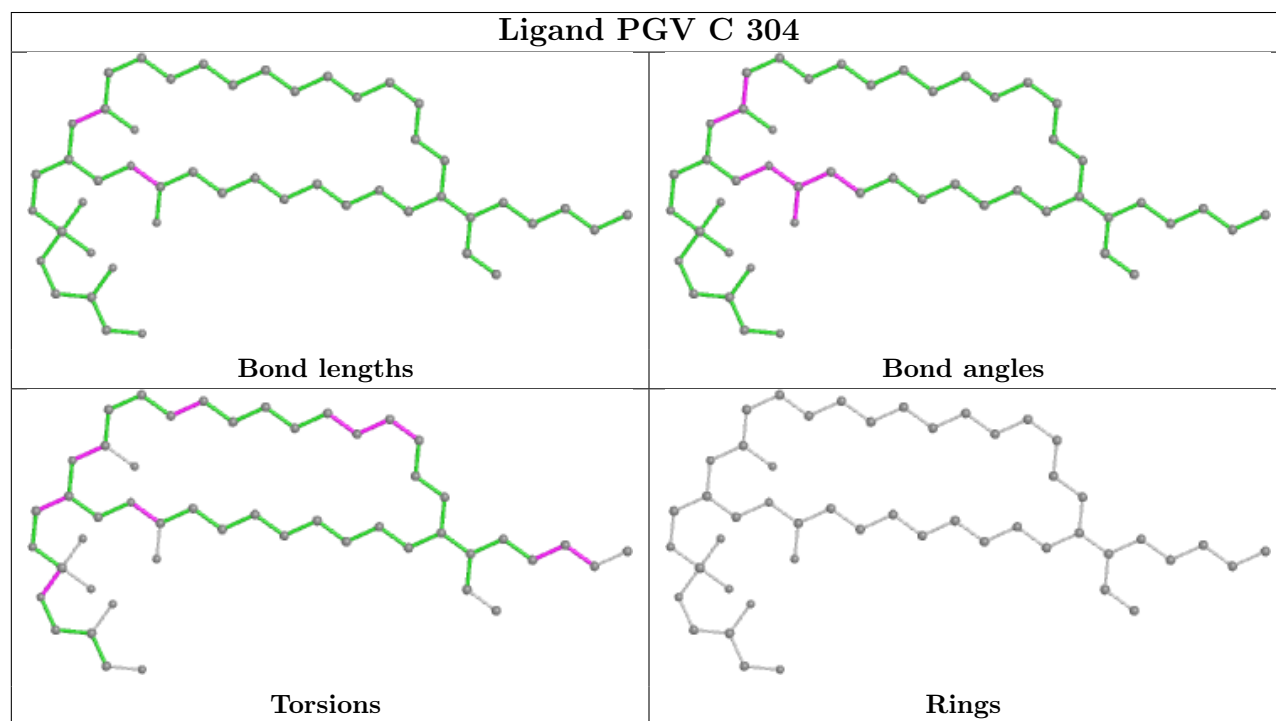
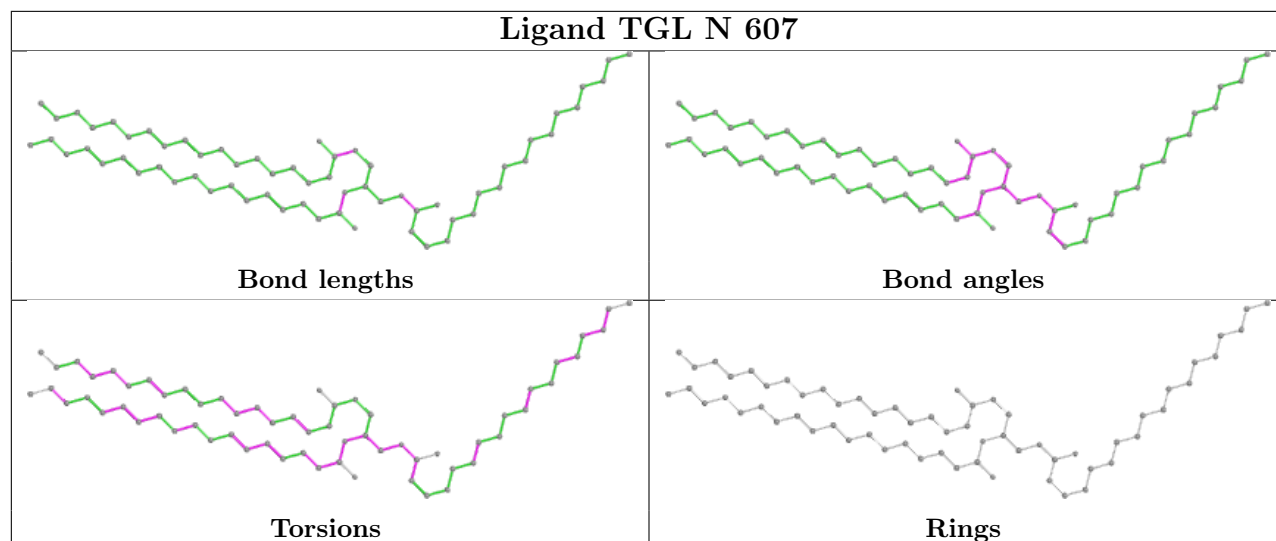


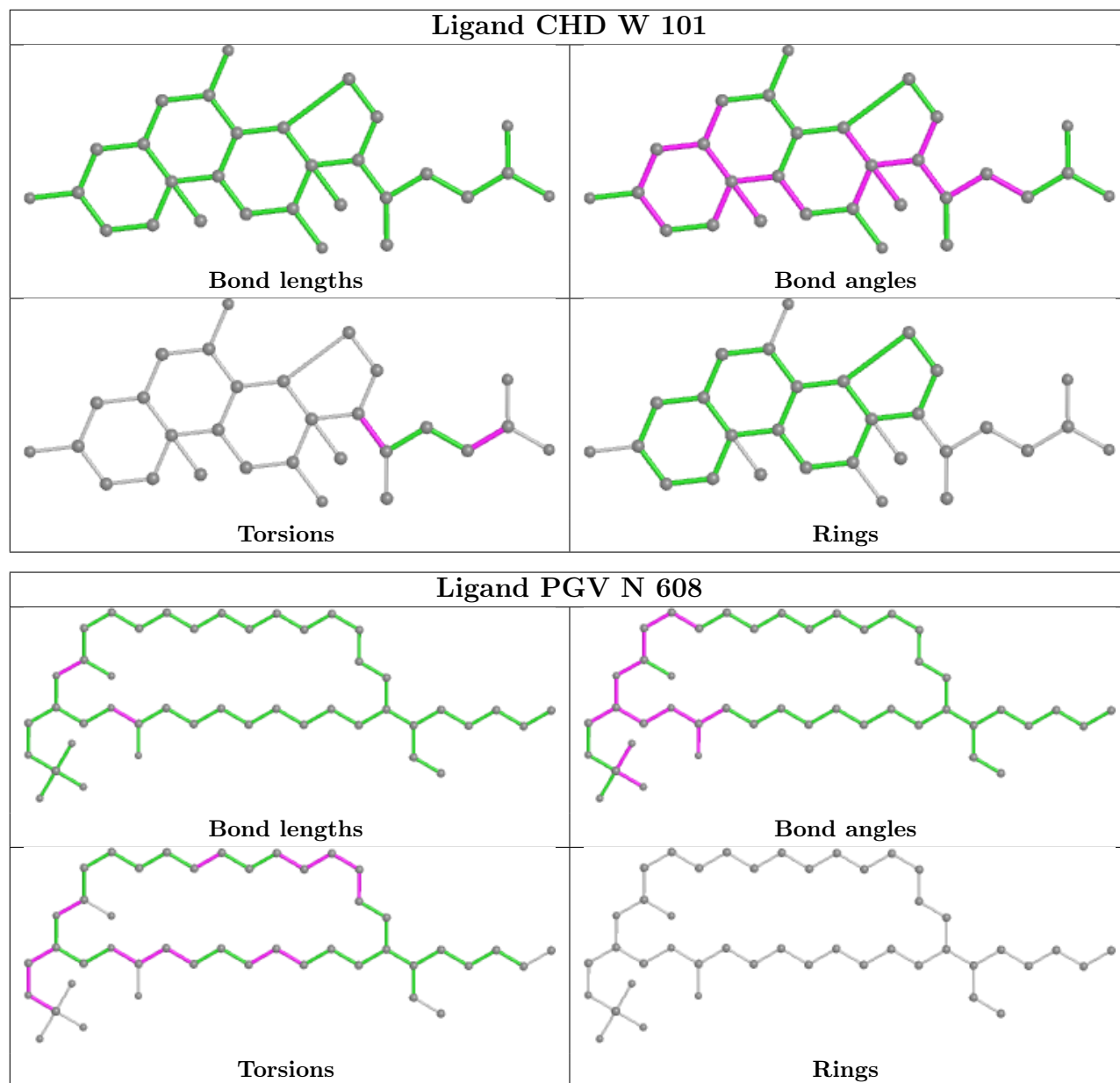


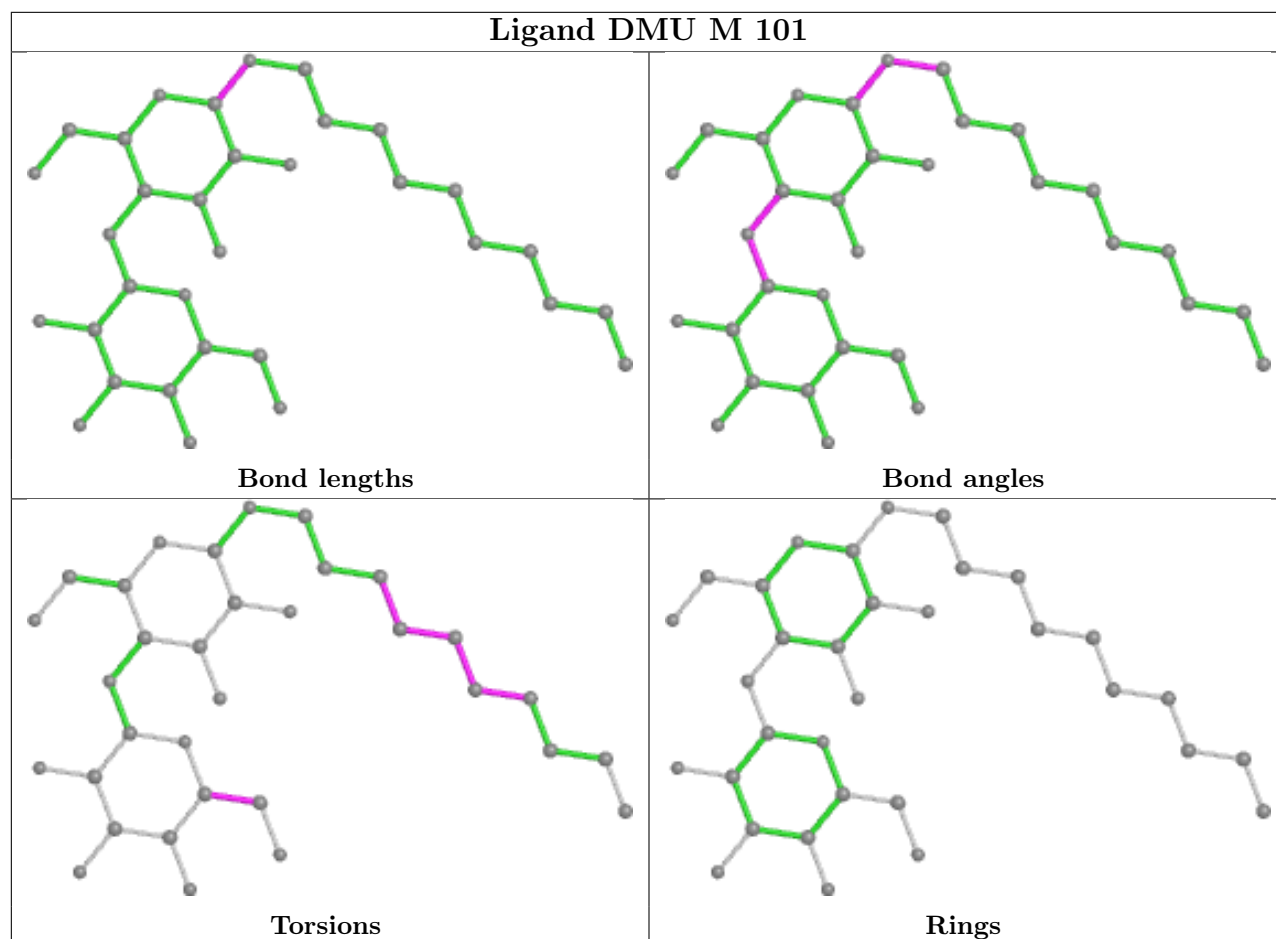
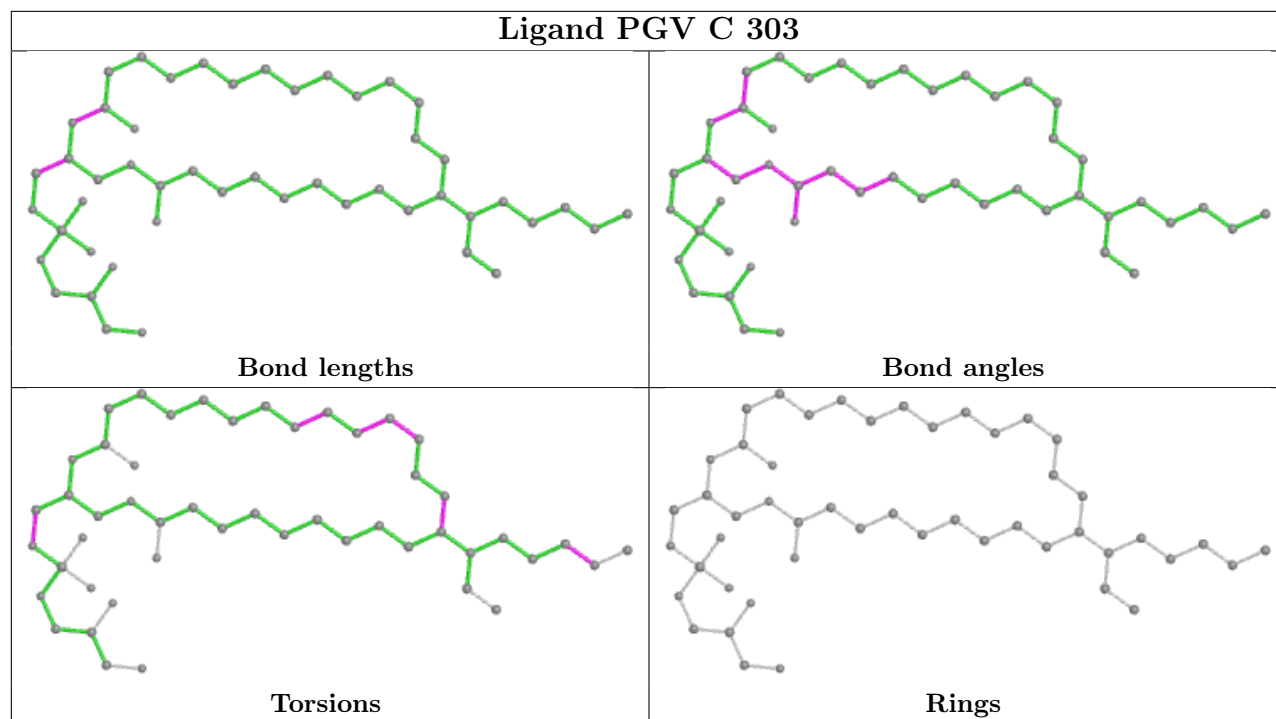


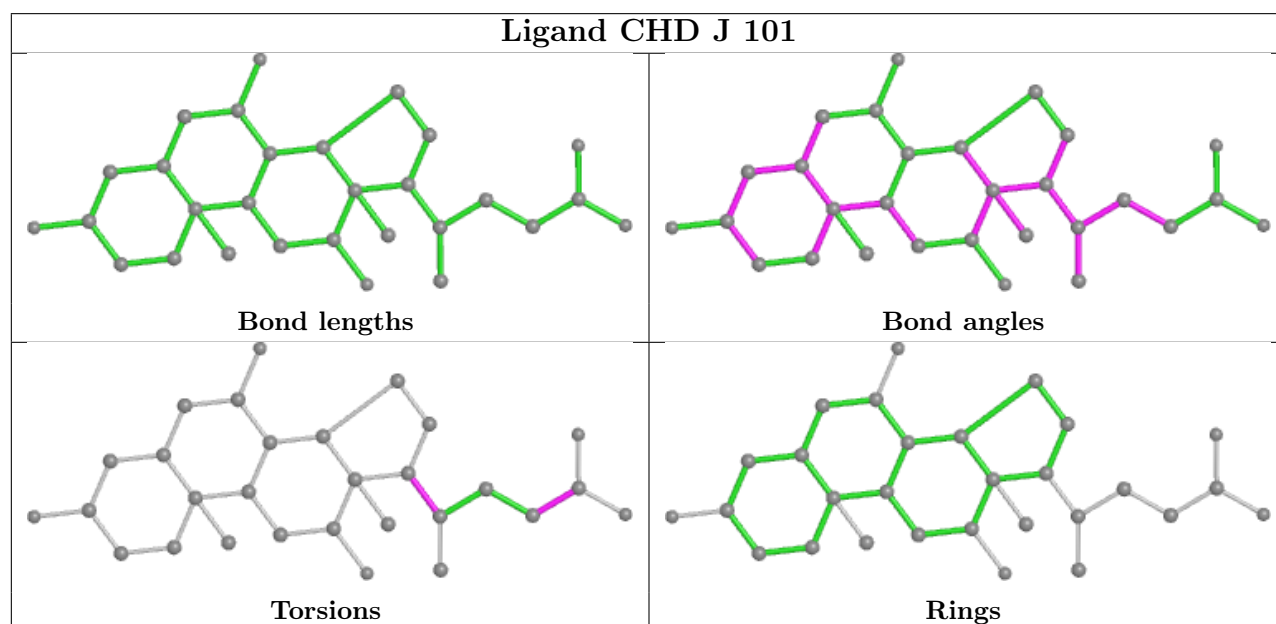
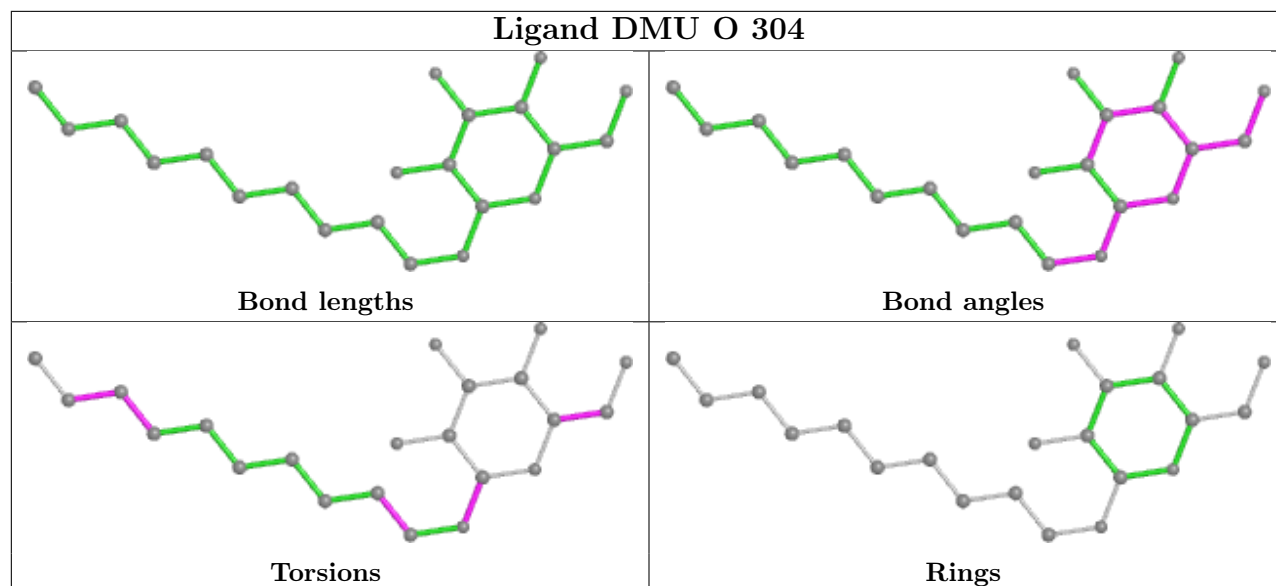


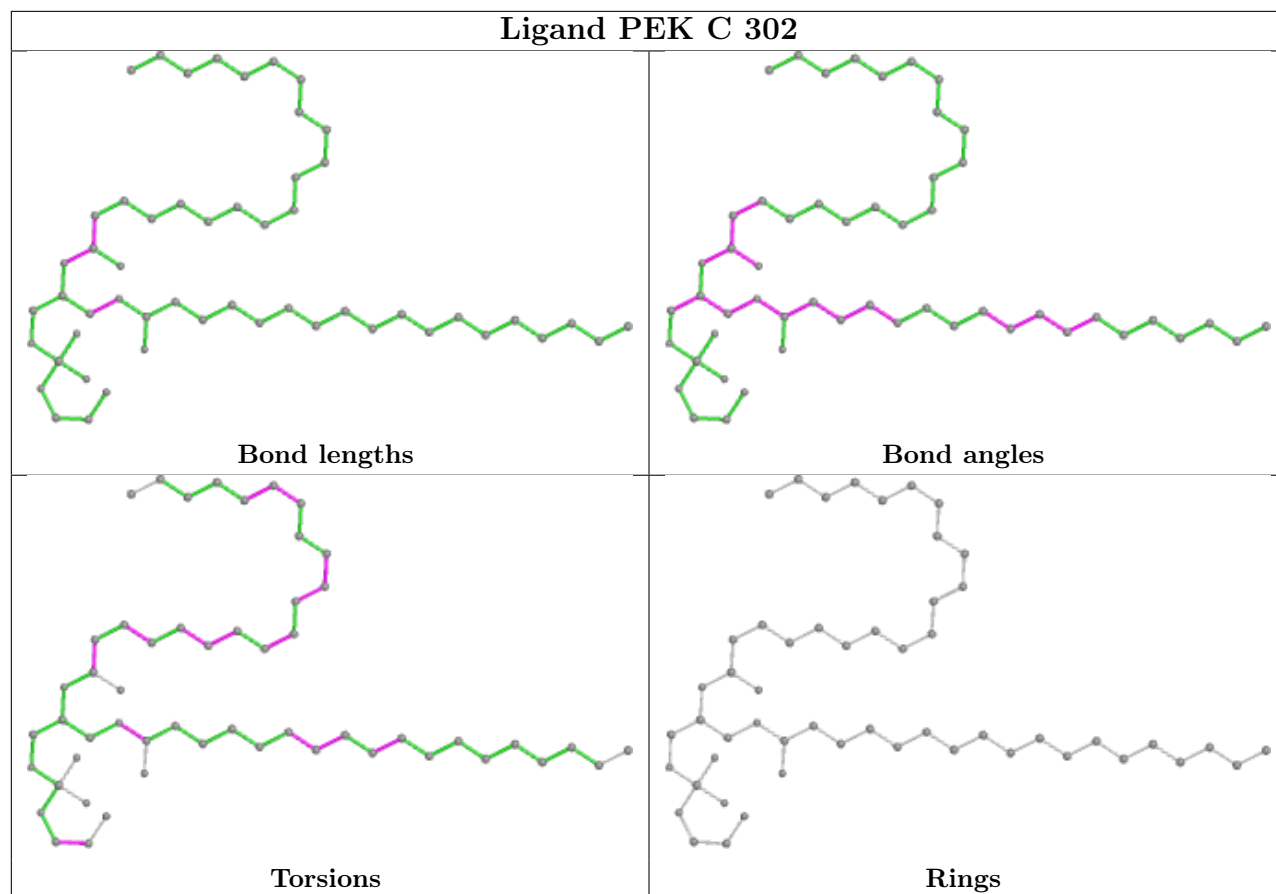


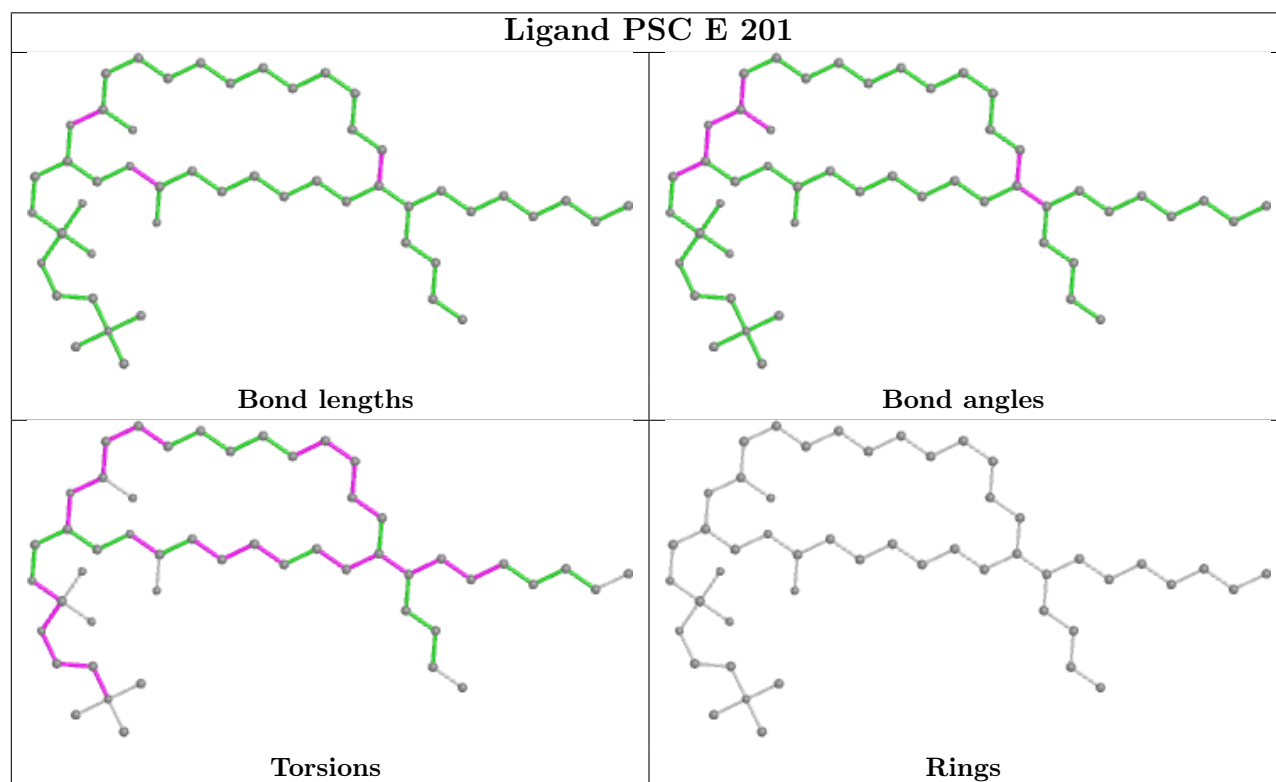
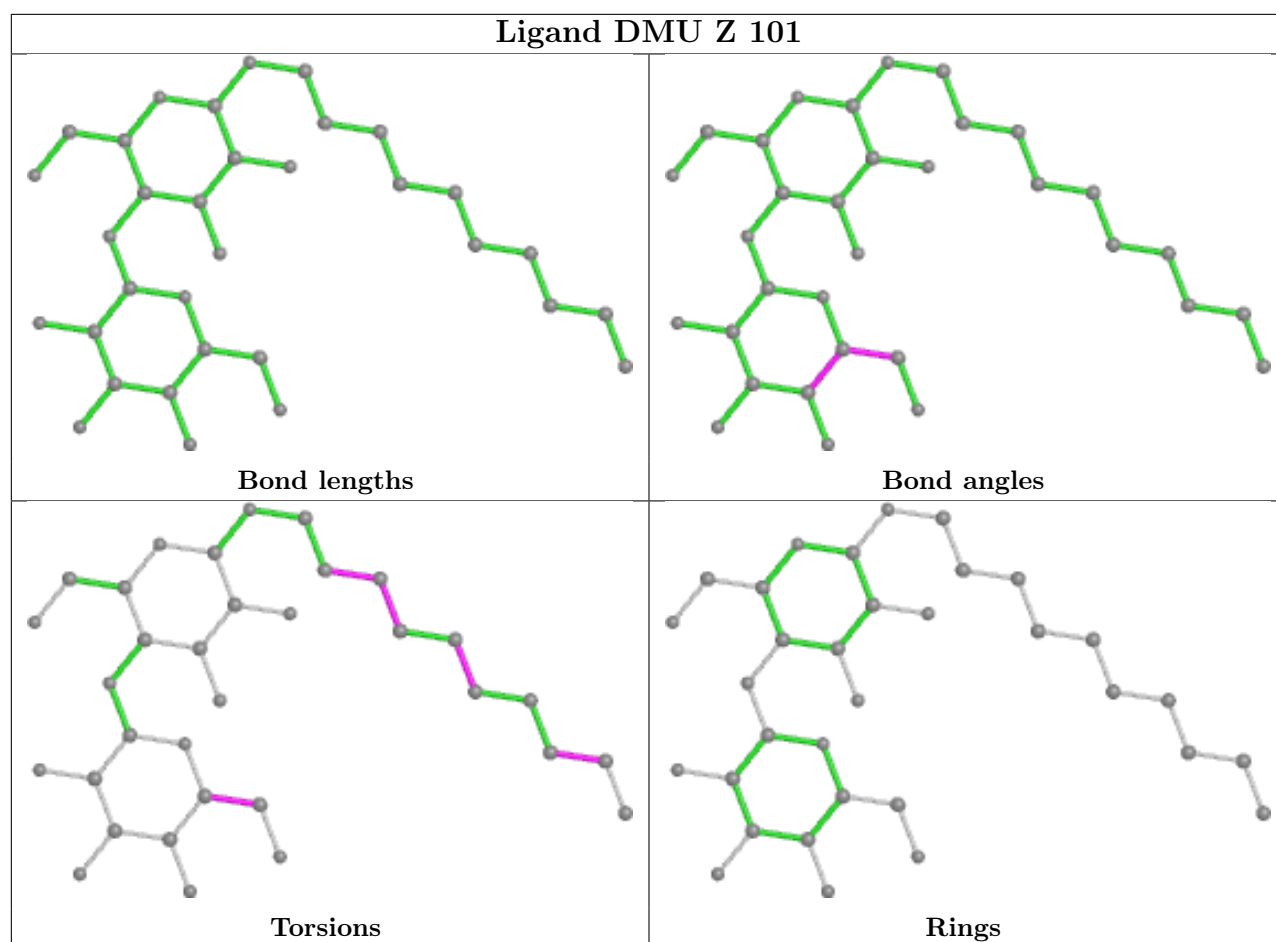


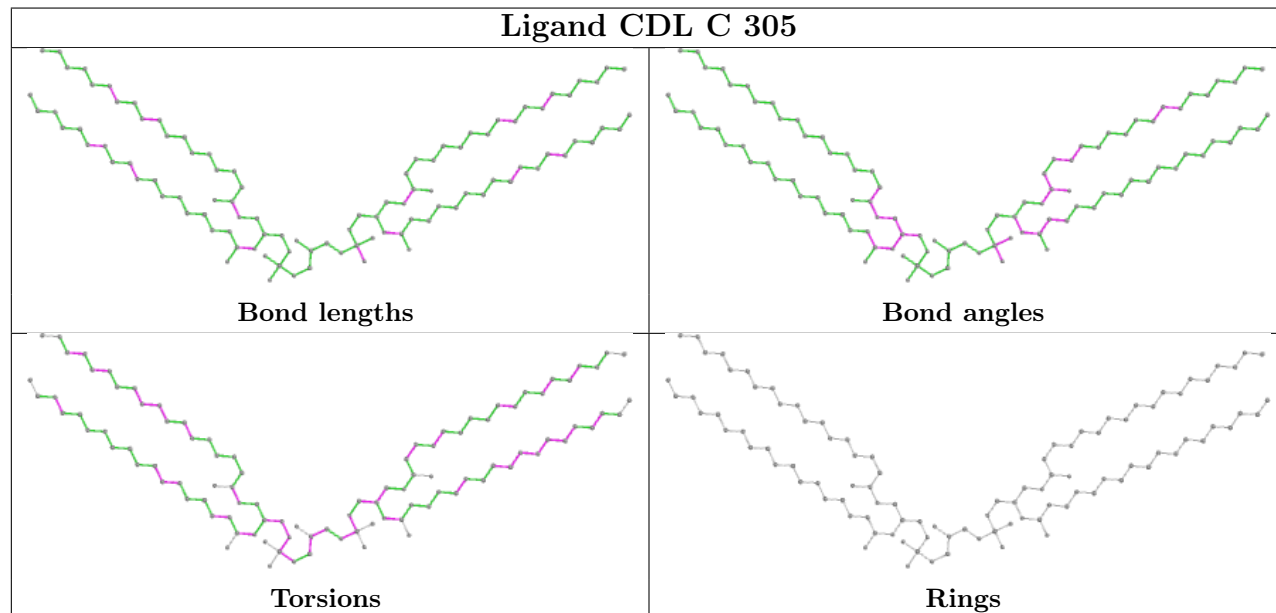
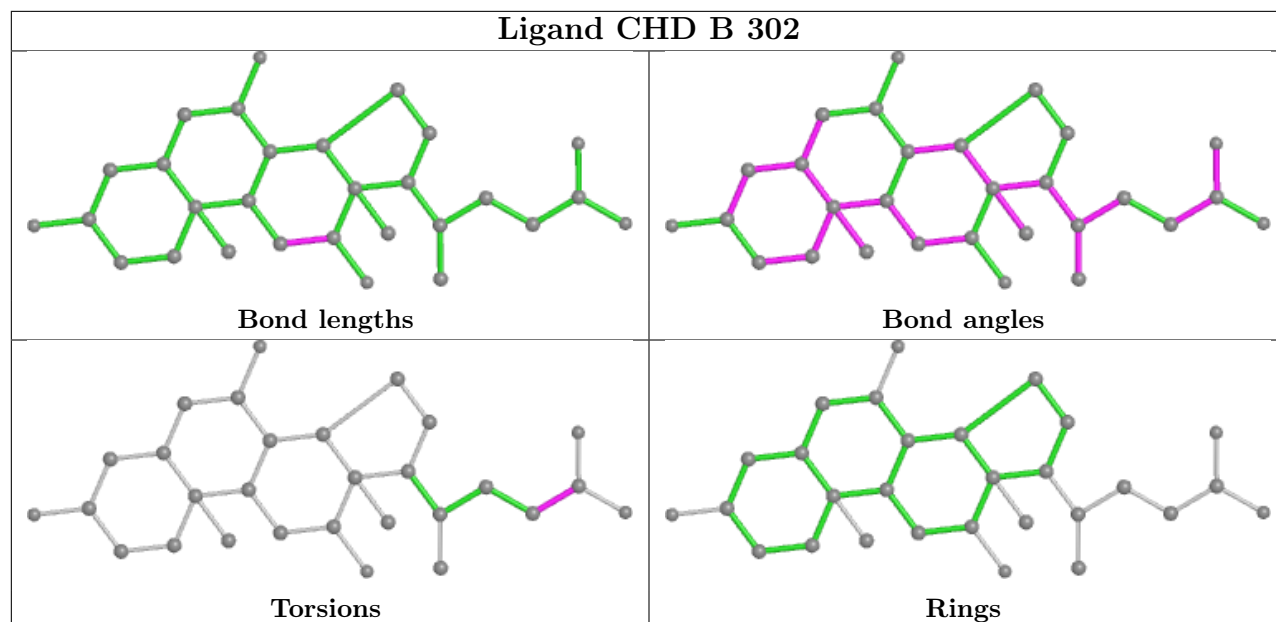


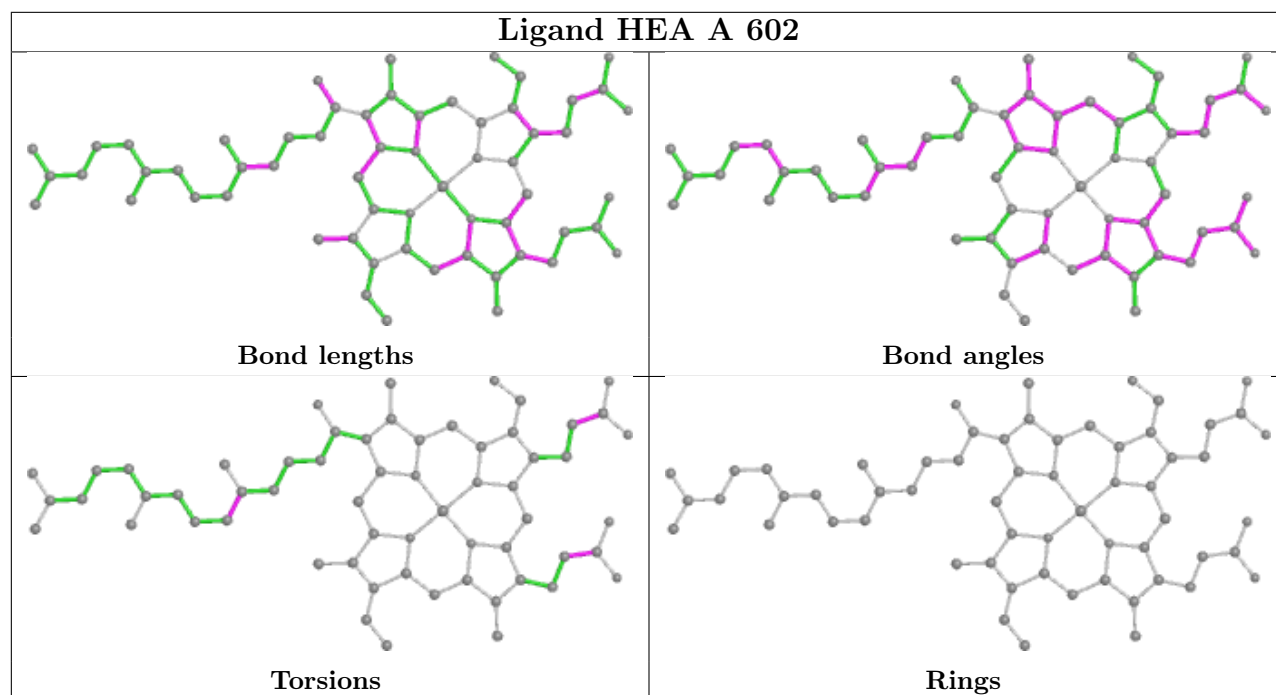
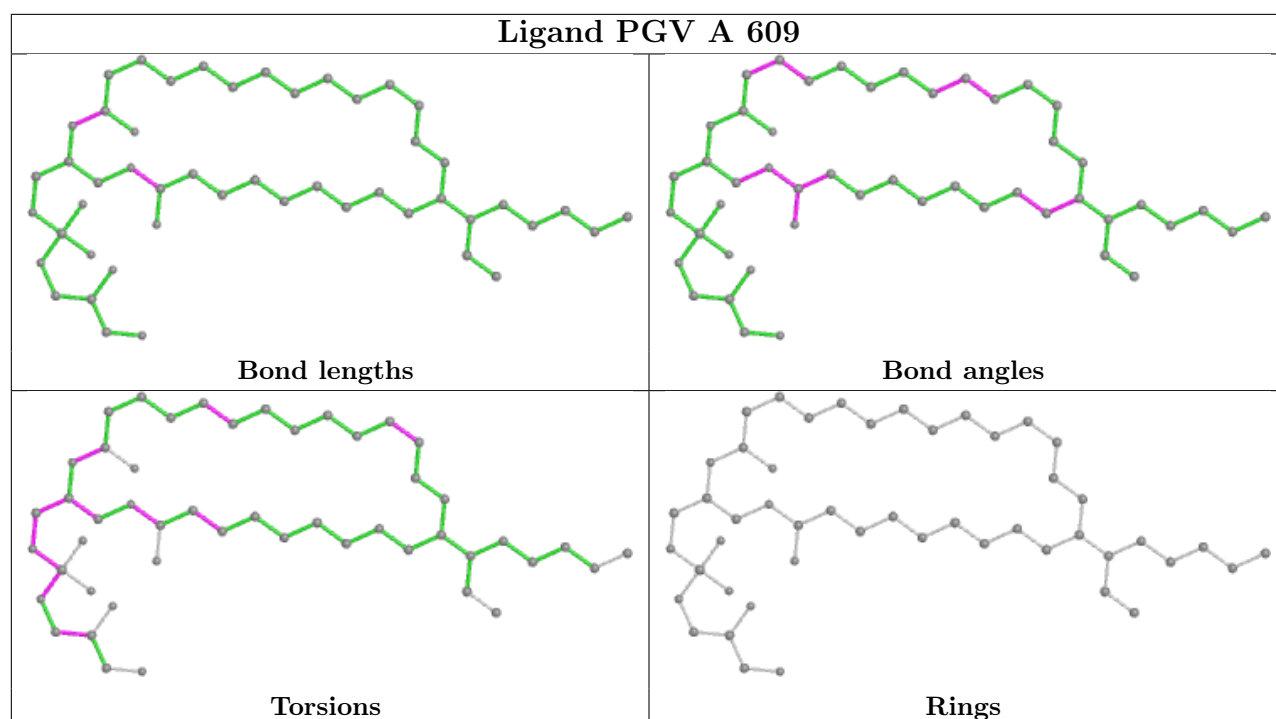


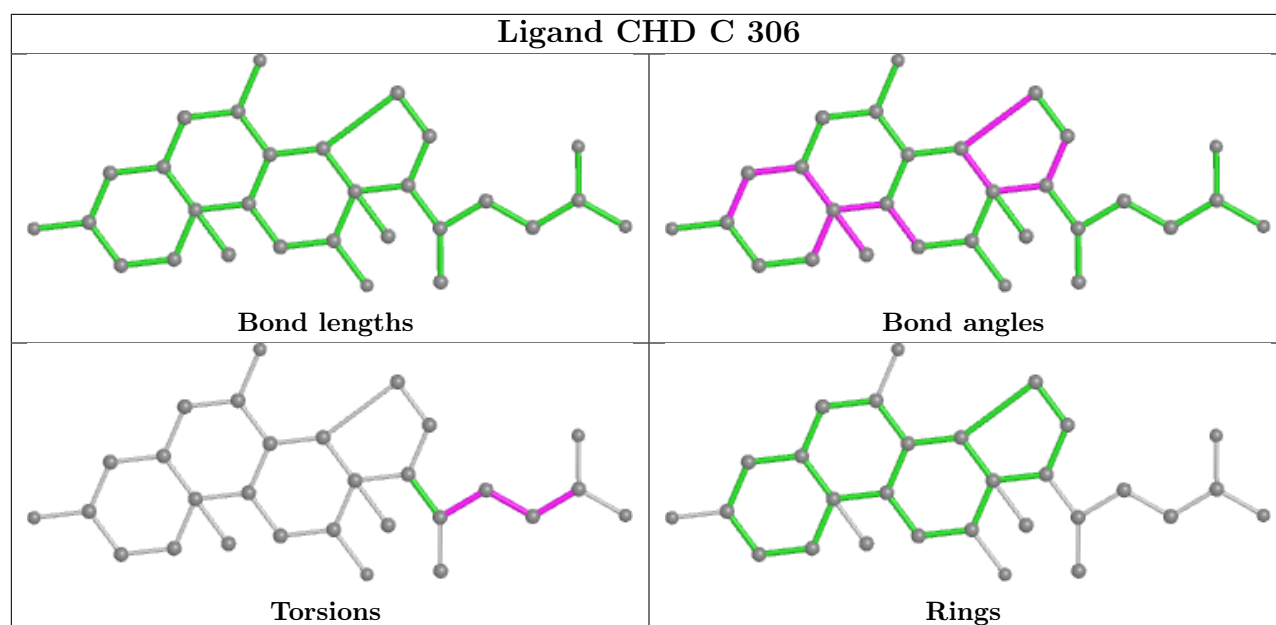












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%) | -0.18 | 0 100 100 | 19, 25, 35, 79 | 0 |
| 1 | N | 513/514 (99%) | -0.21 | 0 100 100 | 23, 30, 40, 78 | 0 |
| 2 | B | 226/227 (99%) | -0.37 | 3 (1%) 77 74 | 22, 32, 55, 85 | 0 |
| 2 | O | 226/227 (99%) | -0.38 | 5 (2%) 62 57 | 27, 38, 72, 110 | 0 |
| 3 | C | 259/261 (99%) | -0.45 | 1 (0%) 92 90 | 22, 29, 42, 77 | 0 |
| 3 | P | 259/261 (99%) | -0.41 | 3 (1%) 79 76 | 25, 31, 47, 70 | 0 |
| 4 | D | 144/147 (97%) | -0.42 | 1 (0%) 87 86 | 29, 39, 57, 86 | 0 |
| 4 | Q | 144/147 (97%) | 0.53 | 14 (9%) 7 6 | 35, 48, 83, 162 | 0 |
| 5 | E | 105/109 (96%) | -0.27 | 2 (1%) 66 63 | 32, 39, 69, 134 | 0 |
| 5 | R | 105/109 (96%) | 0.15 | 8 (7%) 13 10 | 34, 46, 73, 145 | 0 |
| 6 | F | 98/98 (100%) | 0.36 | 7 (7%) 16 12 | 26, 37, 120, 152 | 0 |
| 6 | S | 98/98 (100%) | 0.20 | 8 (8%) 11 9 | 26, 39, 118, 159 | 0 |
| 7 | G | 83/85 (97%) | 0.86 | 18 (21%) 0 0 | 26, 37, 109, 152 | 0 |
| 7 | T | 83/85 (97%) | 0.74 | 16 (19%) 1 0 | 27, 41, 112, 149 | 0 |
| 8 | H | 79/85 (92%) | 0.22 | 12 (15%) 2 1 | 28, 40, 91, 135 | 0 |
| 8 | U | 79/85 (92%) | 0.33 | 12 (15%) 2 1 | 33, 44, 115, 144 | 0 |
| 9 | I | 72/73 (98%) | 0.12 | 3 (4%) 36 30 | 32, 45, 68, 77 | 0 |
| 9 | V | 72/73 (98%) | 0.51 | 7 (9%) 7 6 | 33, 51, 74, 128 | 0 |
| 10 | J | 58/59 (98%) | 0.42 | 6 (10%) 6 5 | 29, 38, 68, 127 | 0 |
| 10 | W | 58/59 (98%) | 0.27 | 7 (12%) 4 3 | 33, 44, 76, 146 | 0 |
| 11 | K | 49/56 (87%) | 0.27 | 3 (6%) 21 16 | 32, 41, 62, 71 | 0 |
| 11 | X | 49/56 (87%) | 1.44 | 11 (22%) 0 0 | 40, 51, 75, 93 | 0 |
| 12 | L | 46/47 (97%) | -0.44 | 1 (2%) 62 57 | 26, 32, 54, 94 | 0 |
| 12 | Y | 46/47 (97%) | -0.49 | 0 100 100 | 33, 41, 68, 125 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | M | 43/46 (93%) | -0.12 | 4 (9%) 8 6 | 29, 34, 76, 123 | 0 |
| 13 | Z | 43/46 (93%) | 0.37 | 6 (13%) 2 2 | 37, 45, 98, 153 | 0 |
| All | All | 3550/3614 (98%) | -0.06 | 158 (4%) 33 27 | 19, 34, 70, 162 | 0 |

The worst 5 of 158 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | Q | 5 | VAL | 15.1 |
| 4 | Q | 4 | SER | 13.8 |
| 6 | S | 1 | ALA | 13.6 |
| 6 | S | 97 | ALA | 13.0 |
| 6 | F | 96 | LEU | 12.2 |

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 | 0.49 | 0.53 | 147,152,161,162 | 0 |
| 7 | TPO | T | 11 | 11/12 | 0.51 | 0.35 | 103,113,156,158 | 0 |
| 7 | TPO | G | 11 | 11/12 | 0.51 | 0.36 | 90,120,150,166 | 0 |
| 9 | SAC | I | 1 | 9/10 | 0.87 | 0.27 | 65,84,106,118 | 0 |
| 2 | FME | B | 1 | 10/11 | 0.96 | 0.13 | 17,34,75,76 | 0 |
| 1 | FME | N | 1 | 10/11 | 0.96 | 0.09 | 40,54,91,104 | 0 |
| 1 | FME | A | 1 | 10/11 | 0.97 | 0.11 | 36,39,76,103 | 0 |
| 2 | FME | O | 1 | 10/11 | 0.97 | 0.10 | 30,39,45,76 | 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 |
|-----|------|-------|-----|---------|------|------|----------------------------|-------|
| 26 | DMU | C | 307 | 33/33 | 0.43 | 0.36 | 58,102,122,124 | 0 |
| 26 | DMU | P | 307 | 33/33 | 0.47 | 0.38 | 60,110,126,129 | 0 |
| 26 | DMU | W | 102 | 32/33 | 0.50 | 0.42 | 50,80,104,115 | 0 |
| 24 | PEK | T | 102 | 53/53 | 0.58 | 0.32 | 47,94,128,138 | 0 |
| 27 | PSC | R | 201 | 52/52 | 0.59 | 0.33 | 44,94,141,175 | 0 |
| 24 | PEK | T | 101 | 53/53 | 0.60 | 0.30 | 40,80,124,154 | 0 |
| 24 | PEK | G | 103 | 53/53 | 0.60 | 0.38 | 46,95,133,145 | 0 |
| 24 | PEK | G | 101 | 50/53 | 0.61 | 0.30 | 46,82,118,145 | 0 |
| 25 | CDL | G | 102 | 100/100 | 0.65 | 0.26 | 46,88,122,152 | 0 |
| 27 | PSC | E | 201 | 52/52 | 0.66 | 0.34 | 42,95,144,175 | 0 |
| 25 | CDL | T | 103 | 100/100 | 0.66 | 0.27 | 52,88,125,150 | 0 |
| 23 | CHD | J | 101 | 29/29 | 0.67 | 0.42 | 73,104,110,113 | 0 |
| 21 | EDO | N | 615 | 4/4 | 0.71 | 0.29 | 46,68,84,87 | 0 |
| 19 | TGL | N | 607 | 63/63 | 0.72 | 0.27 | 45,69,101,121 | 0 |
| 19 | TGL | D | 201 | 63/63 | 0.73 | 0.22 | 41,71,103,117 | 0 |
| 25 | CDL | P | 305 | 100/100 | 0.73 | 0.30 | 41,90,124,138 | 0 |
| 19 | TGL | Q | 201 | 63/63 | 0.74 | 0.24 | 49,77,107,112 | 0 |
| 20 | PGV | P | 304 | 51/51 | 0.74 | 0.28 | 43,78,120,149 | 0 |
| 23 | CHD | W | 101 | 29/29 | 0.75 | 0.40 | 81,107,119,120 | 0 |
| 20 | PGV | C | 304 | 51/51 | 0.78 | 0.28 | 44,88,114,150 | 0 |
| 25 | CDL | C | 305 | 100/100 | 0.78 | 0.29 | 41,86,116,128 | 0 |
| 20 | PGV | N | 608 | 46/51 | 0.79 | 0.30 | 40,83,127,143 | 0 |
| 19 | TGL | L | 101 | 63/63 | 0.79 | 0.24 | 33,63,97,113 | 0 |
| 19 | TGL | O | 303 | 63/63 | 0.79 | 0.18 | 52,76,99,106 | 0 |
| 26 | DMU | Z | 101 | 33/33 | 0.80 | 0.25 | 46,58,88,96 | 0 |
| 26 | DMU | O | 304 | 22/33 | 0.81 | 0.26 | 43,69,95,113 | 0 |
| 20 | PGV | A | 609 | 51/51 | 0.81 | 0.27 | 43,77,132,157 | 0 |
| 21 | EDO | S | 103 | 4/4 | 0.83 | 0.20 | 40,50,56,68 | 0 |
| 21 | EDO | N | 610 | 4/4 | 0.83 | 0.18 | 39,45,49,55 | 0 |
| 19 | TGL | A | 607 | 63/63 | 0.83 | 0.17 | 47,73,96,105 | 0 |
| 21 | EDO | Q | 203 | 4/4 | 0.88 | 0.16 | 41,46,57,69 | 0 |
| 26 | DMU | M | 101 | 33/33 | 0.89 | 0.15 | 36,48,66,80 | 0 |
| 21 | EDO | A | 611 | 4/4 | 0.91 | 0.13 | 29,30,33,47 | 0 |
| 23 | CHD | C | 306 | 29/29 | 0.91 | 0.20 | 42,54,66,104 | 0 |
| 21 | EDO | P | 308 | 4/4 | 0.92 | 0.16 | 53,62,69,87 | 0 |
| 24 | PEK | P | 302 | 53/53 | 0.92 | 0.16 | 31,53,96,104 | 0 |
| 21 | EDO | P | 309 | 4/4 | 0.92 | 0.10 | 37,41,42,53 | 0 |
| 21 | EDO | Q | 202 | 4/4 | 0.92 | 0.17 | 35,43,43,59 | 0 |
| 21 | EDO | O | 306 | 4/4 | 0.93 | 0.16 | 43,43,53,53 | 0 |
| 23 | CHD | P | 306 | 29/29 | 0.93 | 0.22 | 46,57,72,86 | 0 |
| 24 | PEK | C | 302 | 53/53 | 0.94 | 0.14 | 26,46,92,97 | 0 |
| 20 | PGV | P | 303 | 51/51 | 0.94 | 0.13 | 24,36,88,99 | 0 |

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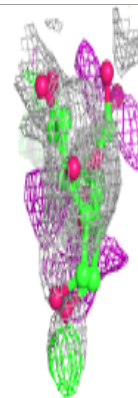
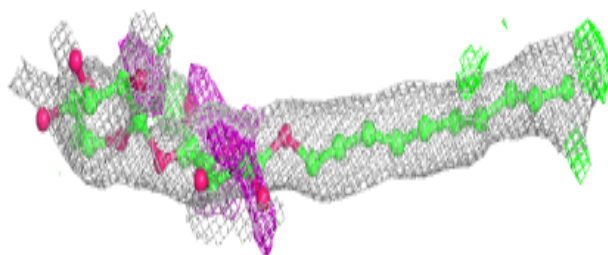
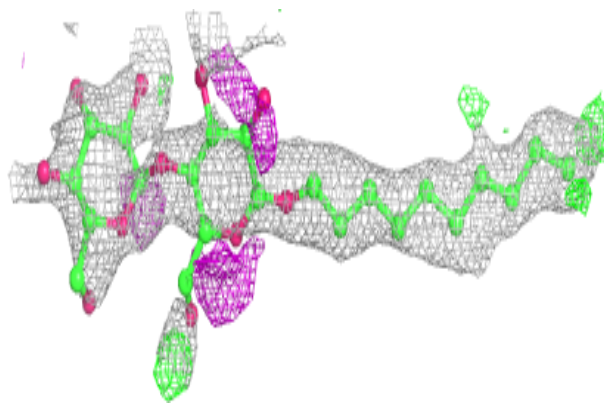
Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 21 | EDO | A | 613 | 4/4 | 0.94 | 0.08 | 34,42,61,62 | 0 |
| 20 | PGV | N | 609 | 51/51 | 0.95 | 0.14 | 23,35,75,81 | 0 |
| 23 | CHD | P | 301 | 29/29 | 0.95 | 0.11 | 24,31,35,37 | 0 |
| 20 | PGV | A | 608 | 51/51 | 0.96 | 0.11 | 20,31,73,85 | 0 |
| 21 | EDO | C | 308 | 4/4 | 0.96 | 0.08 | 34,40,48,56 | 0 |
| 20 | PGV | C | 303 | 51/51 | 0.96 | 0.11 | 20,33,83,93 | 0 |
| 21 | EDO | N | 611 | 4/4 | 0.96 | 0.10 | 31,32,32,40 | 0 |
| 21 | EDO | N | 612 | 4/4 | 0.96 | 0.14 | 33,47,64,72 | 0 |
| 21 | EDO | A | 612 | 4/4 | 0.97 | 0.11 | 31,38,51,57 | 0 |
| 21 | EDO | N | 613 | 4/4 | 0.97 | 0.07 | 40,47,52,58 | 0 |
| 23 | CHD | O | 302 | 29/29 | 0.97 | 0.09 | 24,28,36,41 | 0 |
| 21 | EDO | S | 102 | 4/4 | 0.97 | 0.11 | 26,27,29,30 | 0 |
| 21 | EDO | F | 102 | 4/4 | 0.97 | 0.09 | 25,25,26,27 | 0 |
| 21 | EDO | S | 104 | 4/4 | 0.97 | 0.07 | 40,40,47,58 | 0 |
| 23 | CHD | B | 302 | 29/29 | 0.97 | 0.08 | 24,28,35,40 | 0 |
| 23 | CHD | C | 301 | 29/29 | 0.97 | 0.12 | 24,29,35,38 | 0 |
| 14 | HEA | A | 601 | 60/60 | 0.98 | 0.10 | 16,22,37,41 | 0 |
| 21 | EDO | O | 305 | 4/4 | 0.98 | 0.07 | 32,33,36,36 | 0 |
| 14 | HEA | N | 601 | 60/60 | 0.98 | 0.09 | 21,27,44,47 | 0 |
| 21 | EDO | A | 610 | 4/4 | 0.98 | 0.15 | 24,24,26,29 | 0 |
| 18 | NA | N | 606 | 1/1 | 0.98 | 0.06 | 34,34,34,34 | 0 |
| 21 | EDO | N | 614 | 4/4 | 0.98 | 0.07 | 26,33,35,37 | 0 |
| 15 | NO | A | 603 | 2/2 | 0.99 | 0.10 | 20,20,20,25 | 0 |
| 17 | MG | A | 605 | 1/1 | 0.99 | 0.06 | 19,19,19,19 | 0 |
| 17 | MG | N | 605 | 1/1 | 0.99 | 0.02 | 24,24,24,24 | 0 |
| 18 | NA | A | 606 | 1/1 | 0.99 | 0.12 | 29,29,29,29 | 0 |
| 14 | HEA | A | 602 | 60/60 | 0.99 | 0.09 | 17,21,28,34 | 0 |
| 21 | EDO | B | 303 | 4/4 | 0.99 | 0.10 | 27,27,29,31 | 0 |
| 14 | HEA | N | 602 | 60/60 | 0.99 | 0.11 | 21,25,31,37 | 0 |
| 28 | ZN | F | 101 | 1/1 | 0.99 | 0.05 | 29,29,29,29 | 0 |
| 15 | NO | N | 603 | 2/2 | 1.00 | 0.09 | 26,26,26,27 | 0 |
| 22 | CUA | B | 301 | 2/2 | 1.00 | 0.09 | 23,23,23,23 | 0 |
| 22 | CUA | O | 301 | 2/2 | 1.00 | 0.07 | 28,28,28,28 | 0 |
| 16 | CU | A | 604 | 1/1 | 1.00 | 0.10 | 22,22,22,22 | 0 |
| 16 | CU | N | 604 | 1/1 | 1.00 | 0.11 | 24,24,24,24 | 0 |
| 28 | ZN | S | 101 | 1/1 | 1.00 | 0.07 | 31,31,31,31 | 0 |

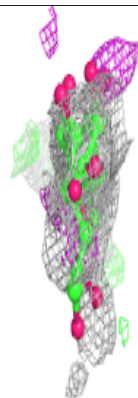
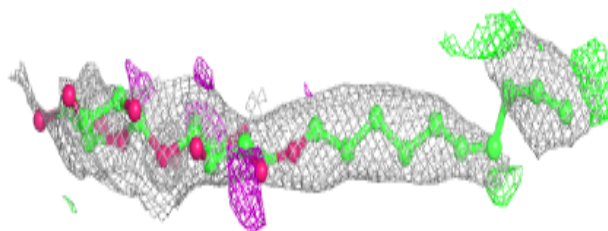
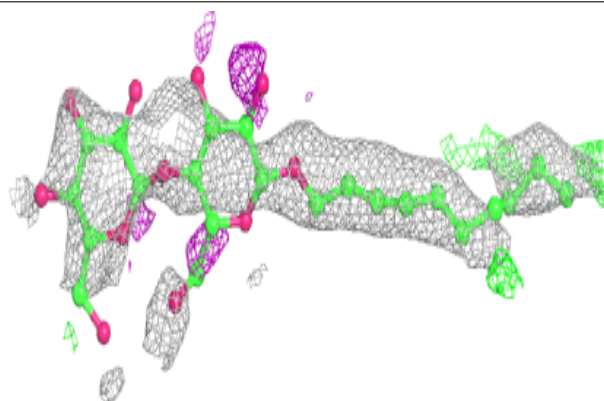
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU 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)

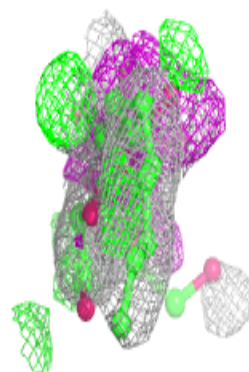
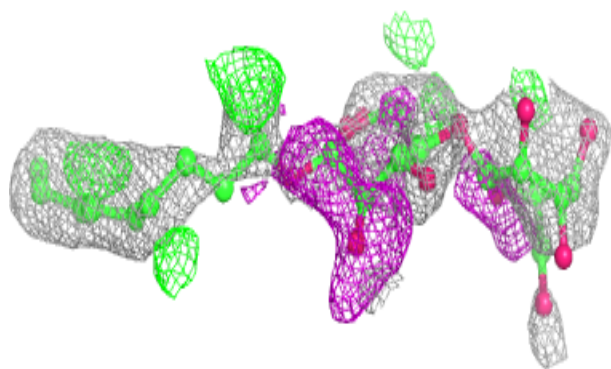
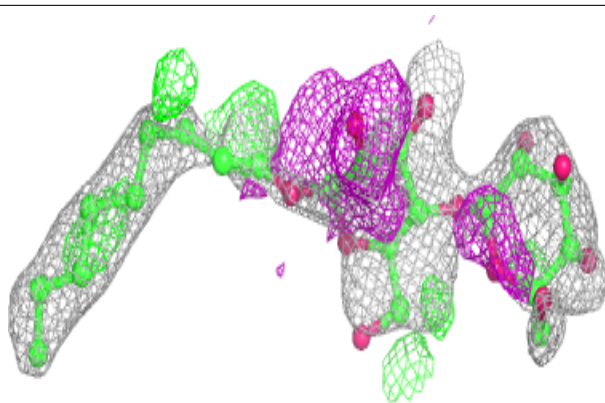
**Electron density around DMU P 307:**

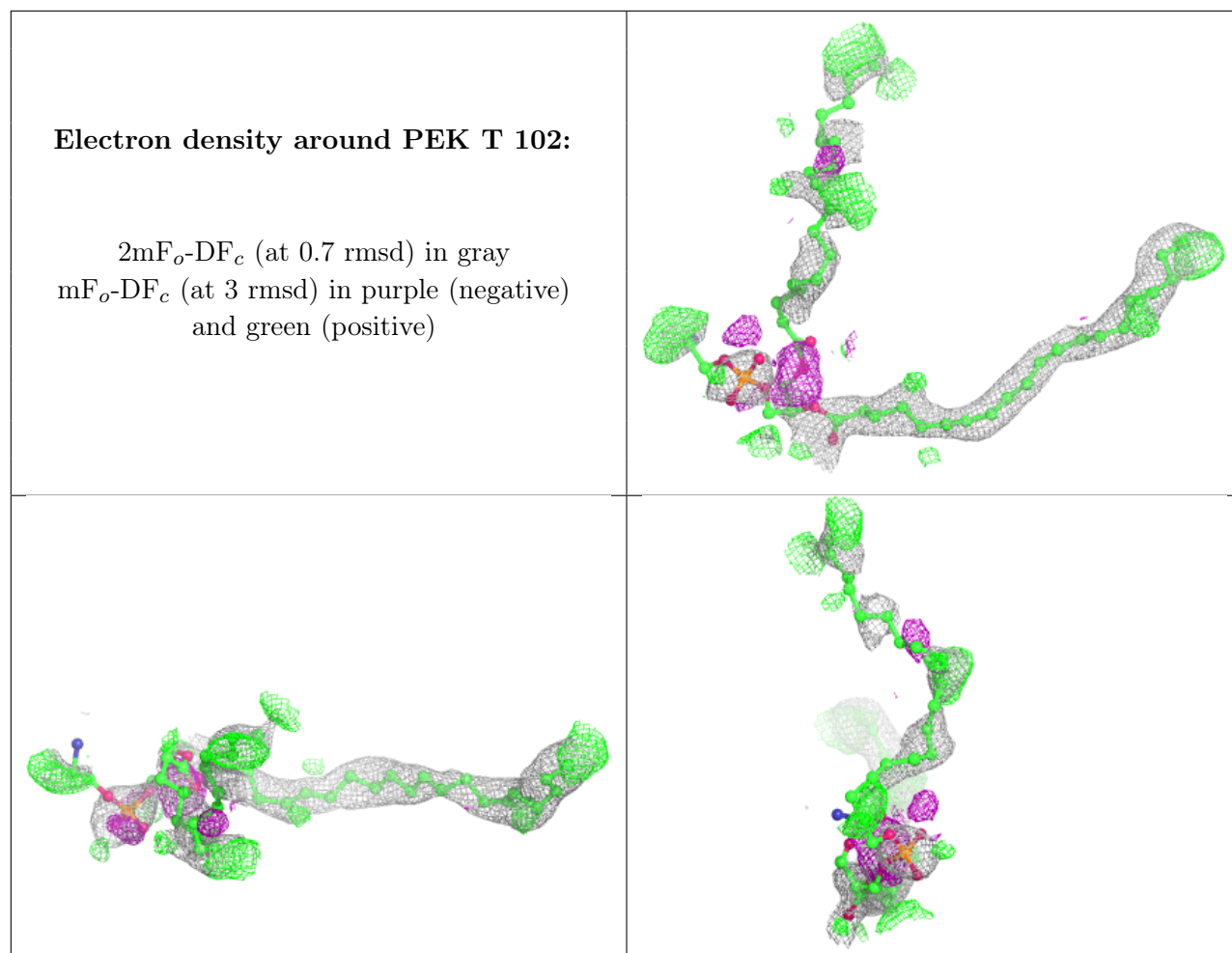
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DMU W 102:

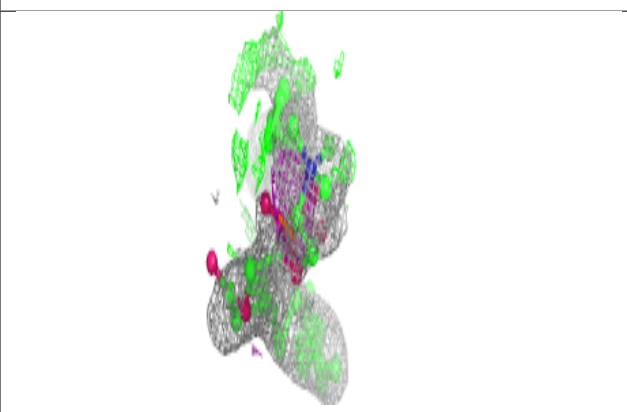
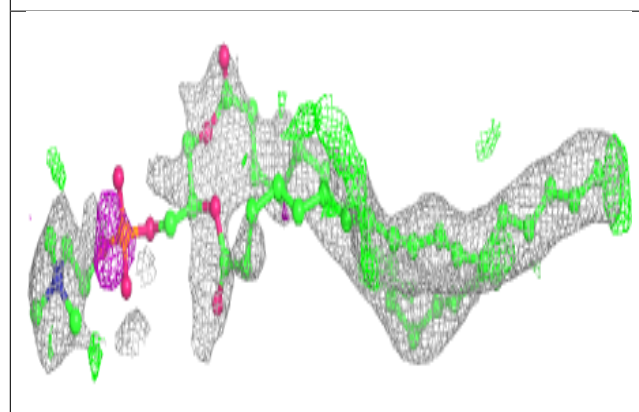
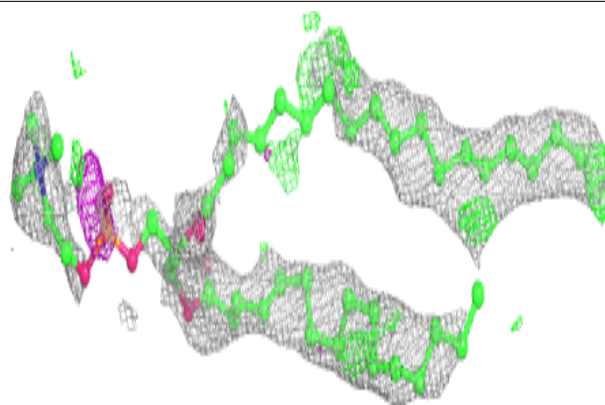
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



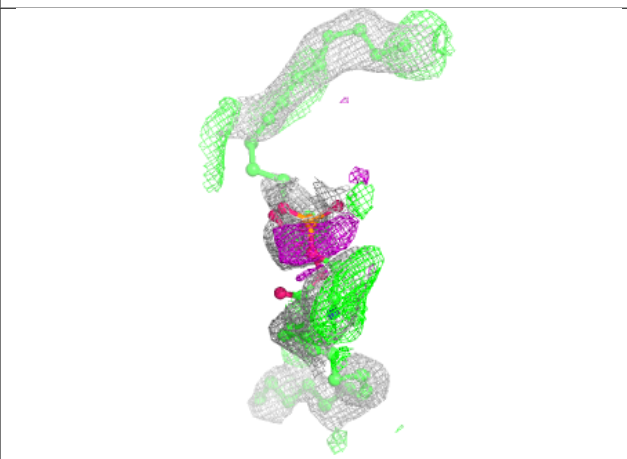
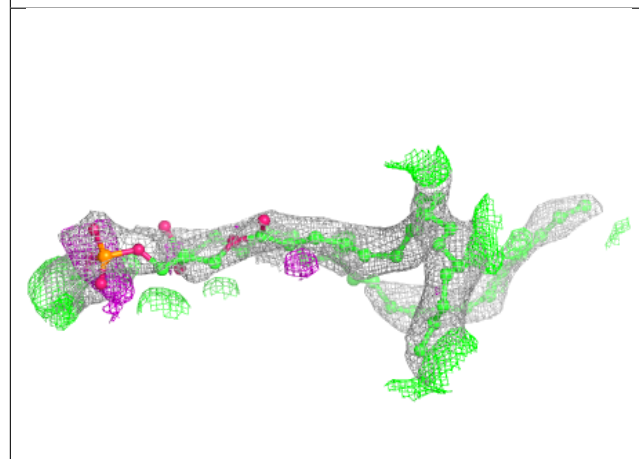
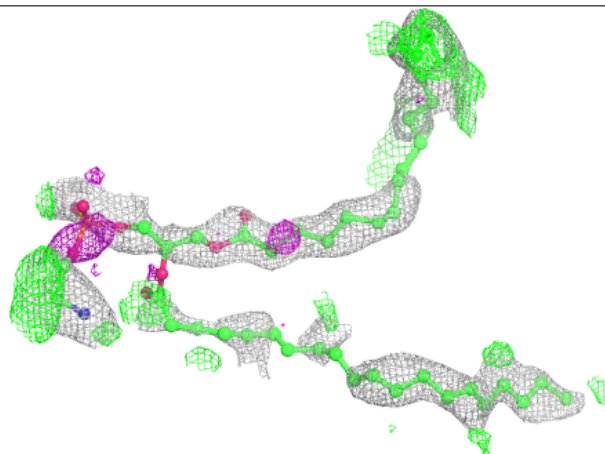


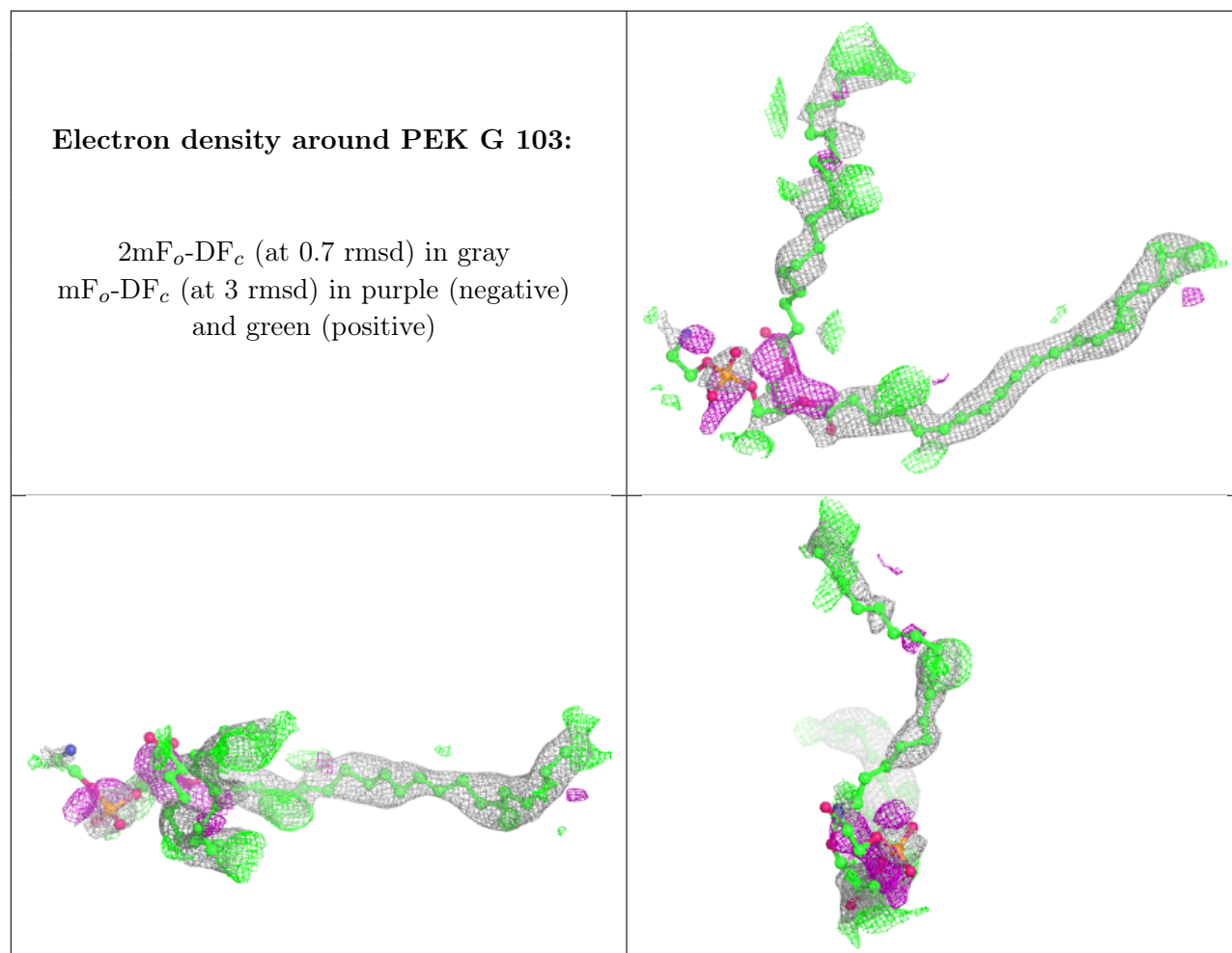
Electron density around PSC R 201:

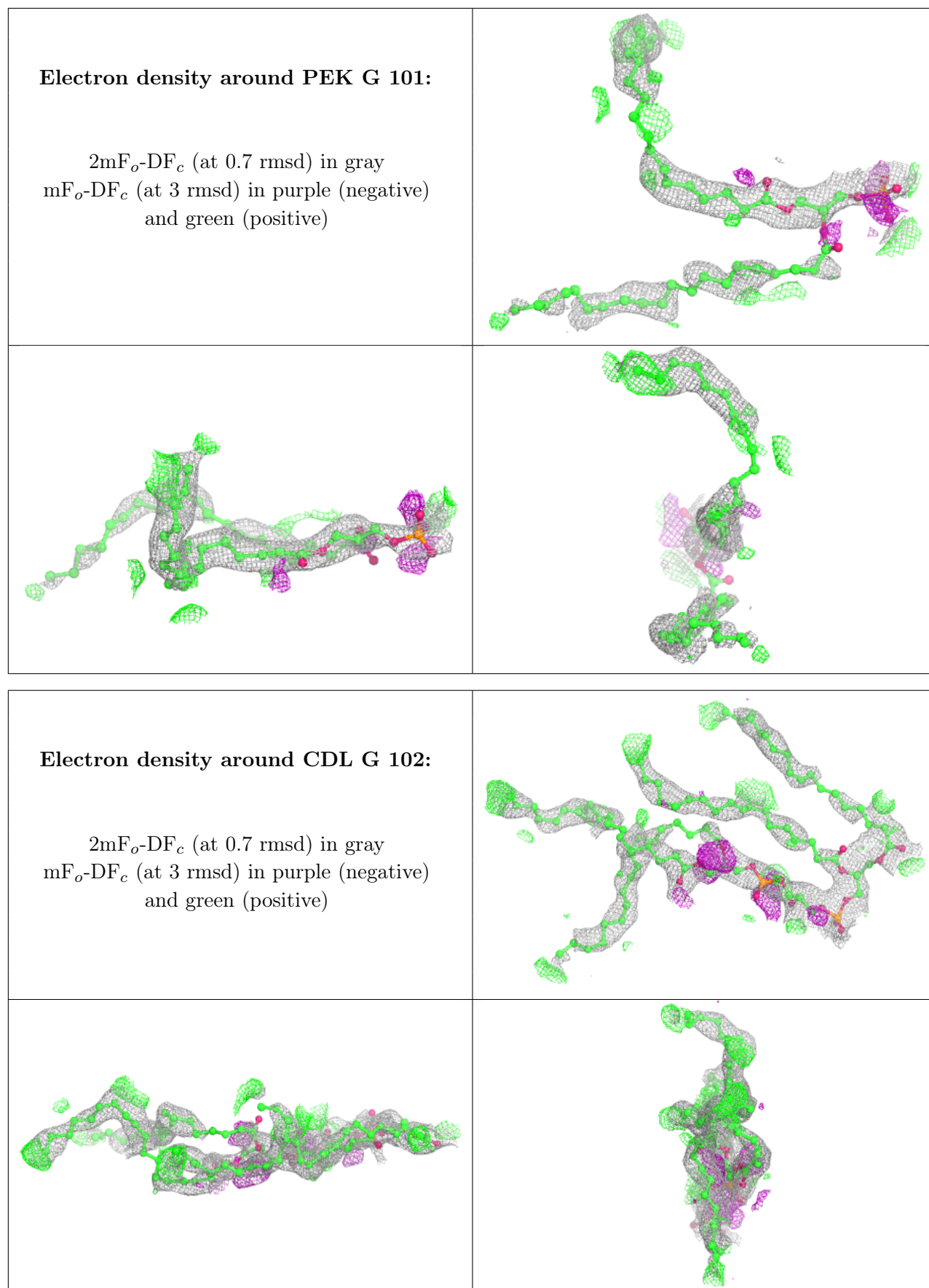
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 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)

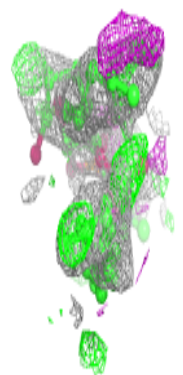
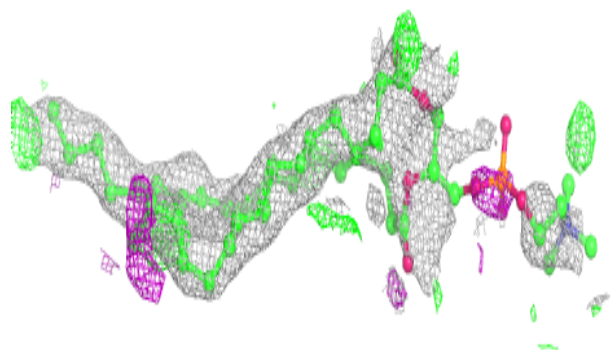
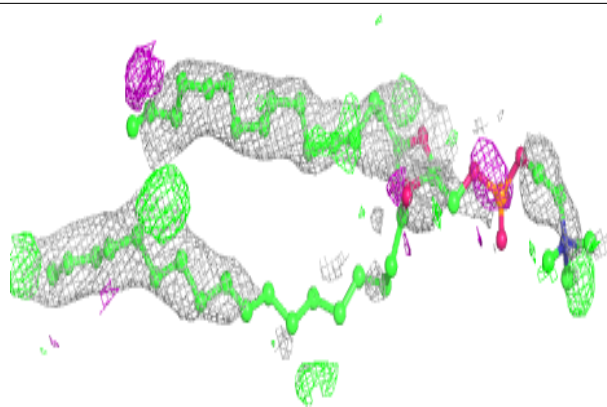




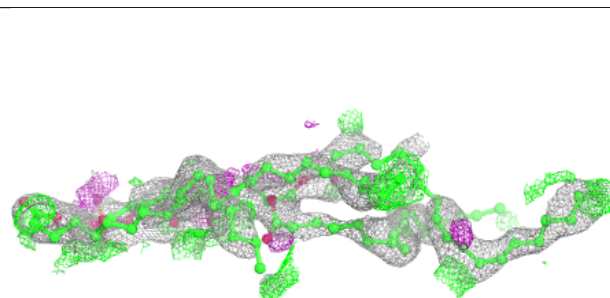
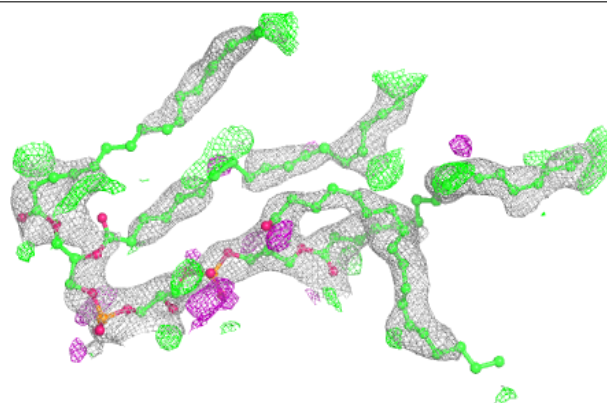


Electron density around PSC E 201:

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

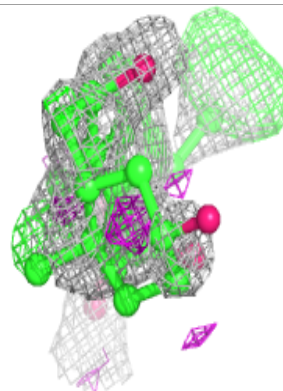
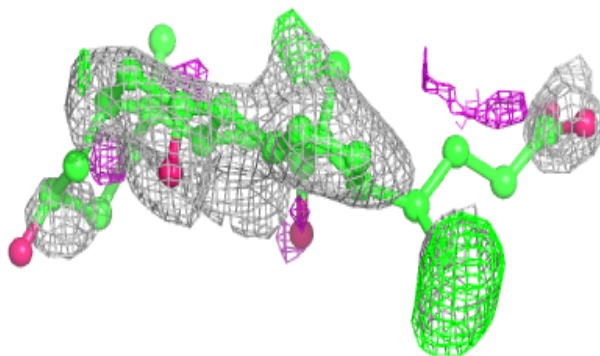
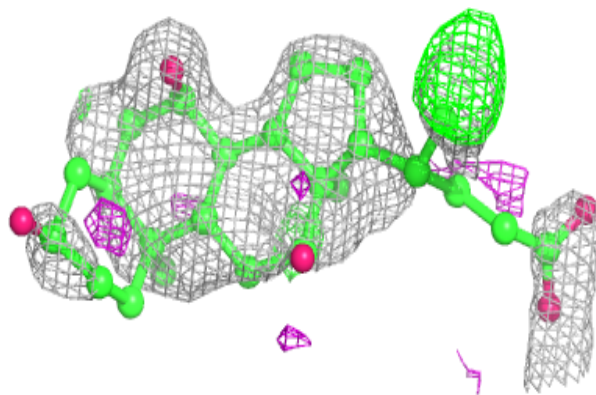
**Electron density around CDL T 103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

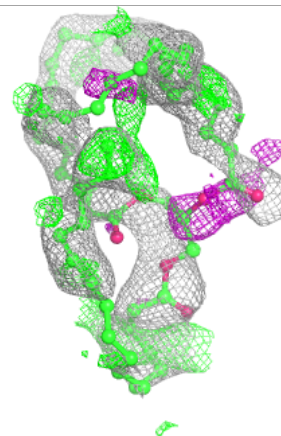
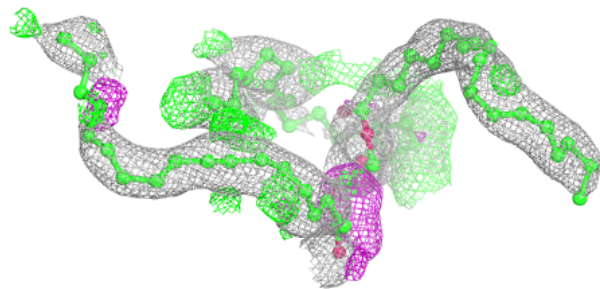
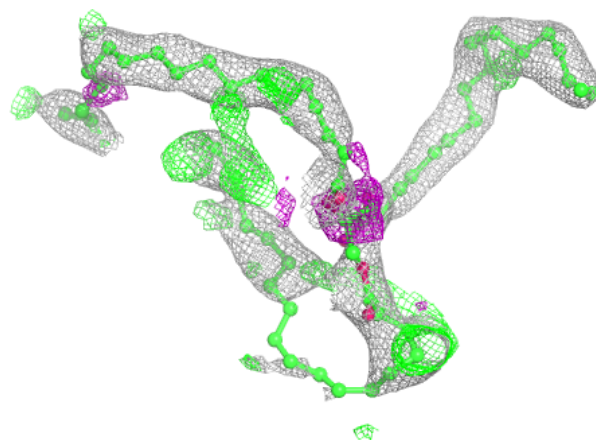


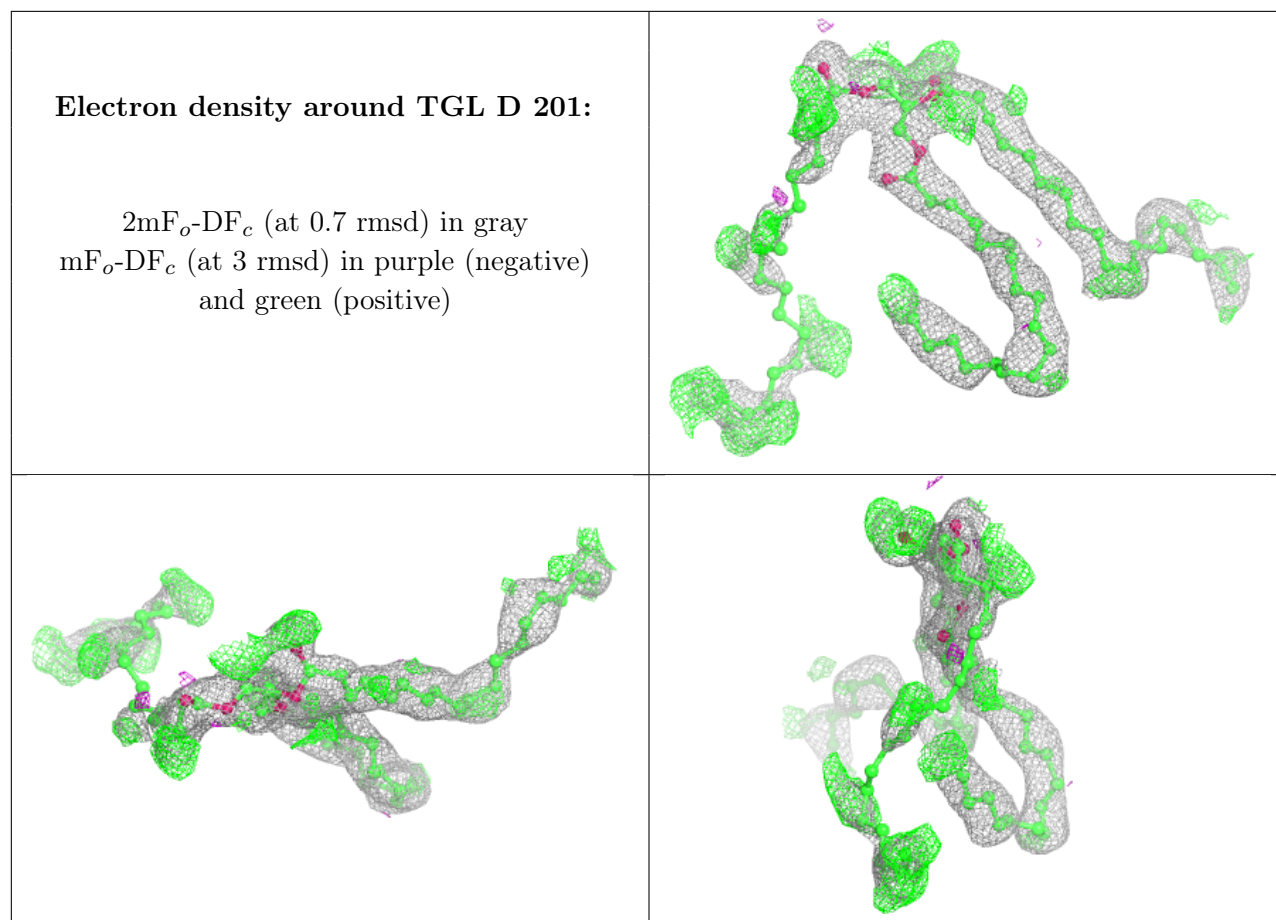
Electron density around CHD J 101:

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

**Electron density around TGL N 607:**

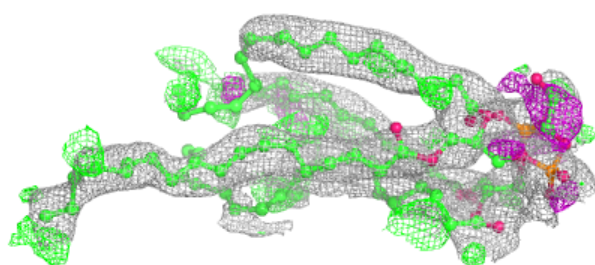
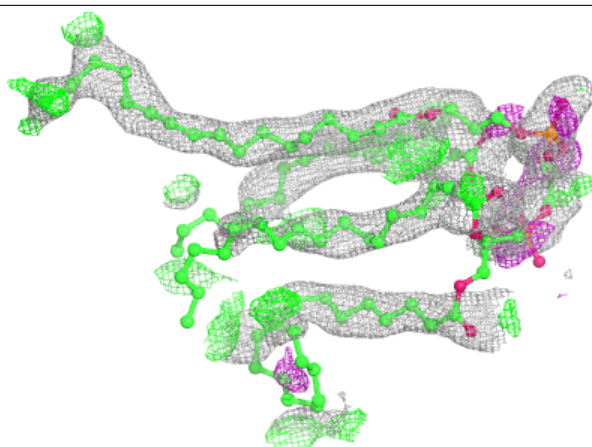
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



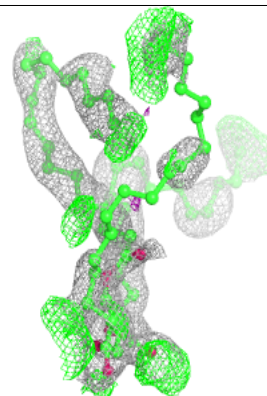
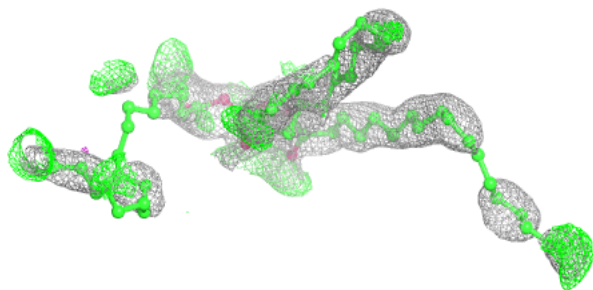
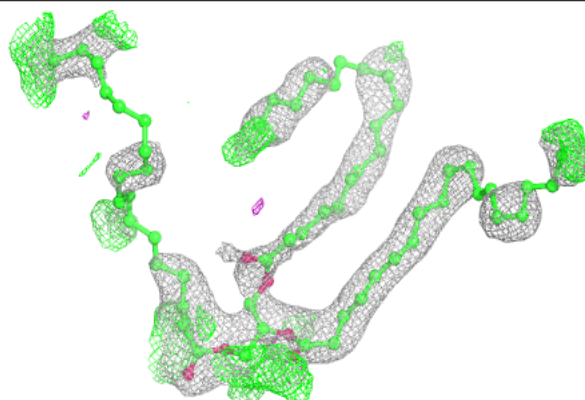


Electron density around CDL P 305:

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

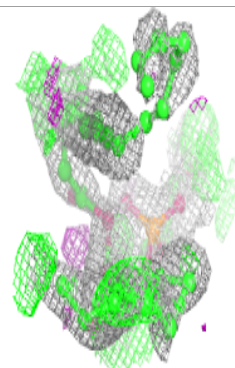
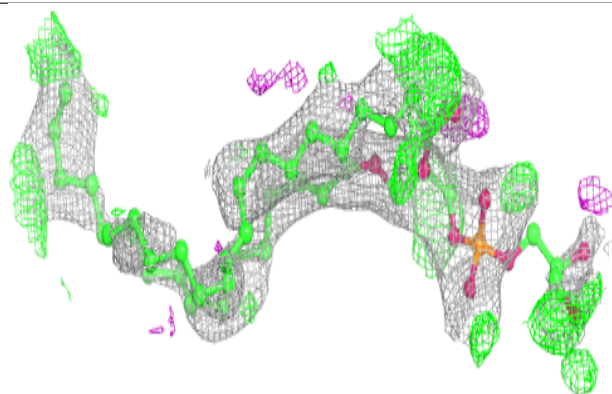
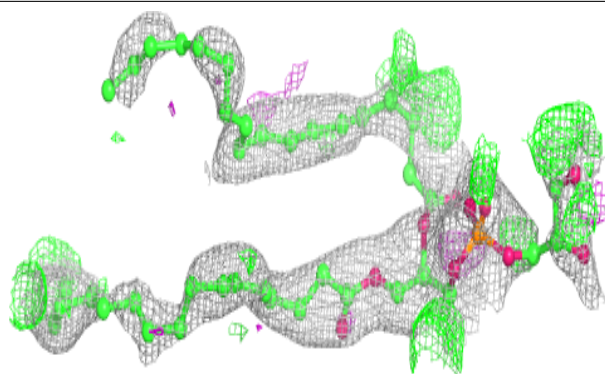
**Electron density around TGL Q 201:**

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

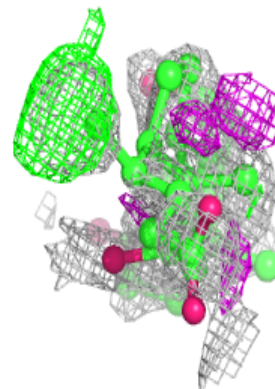
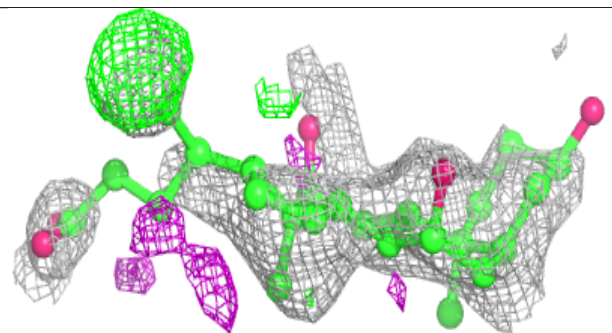
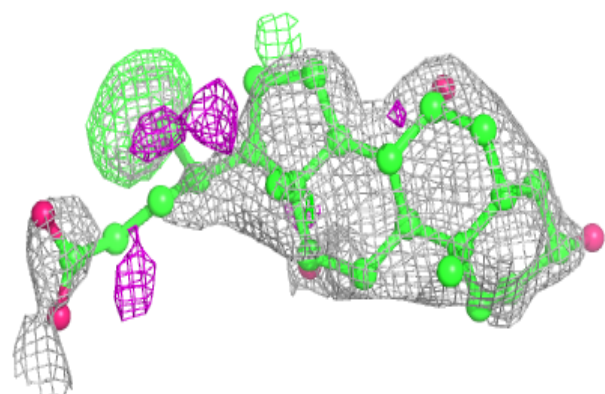


Electron density around PGV P 304:

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

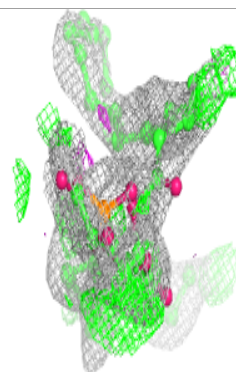
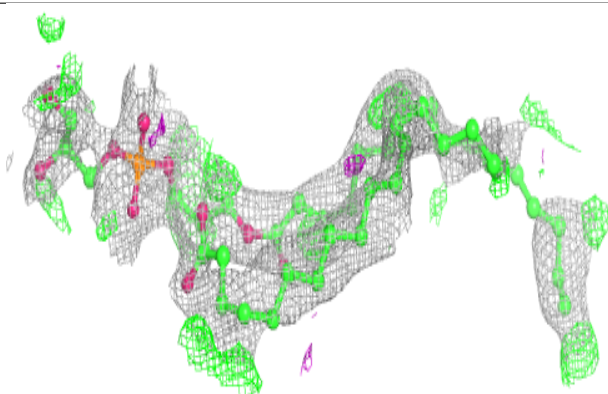
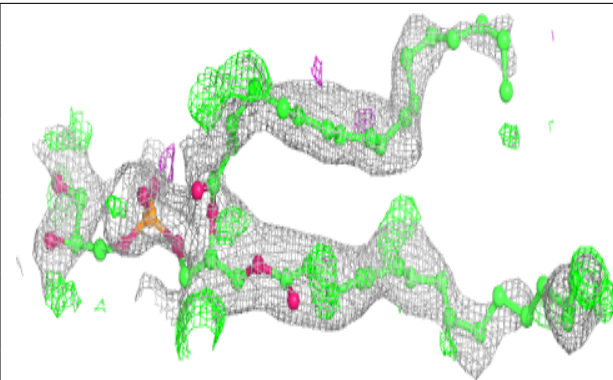
**Electron density around CHD W 101:**

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

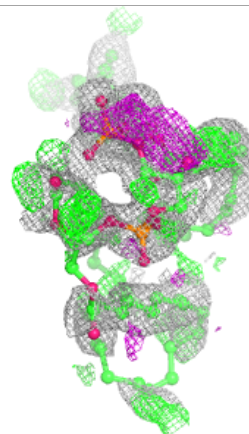
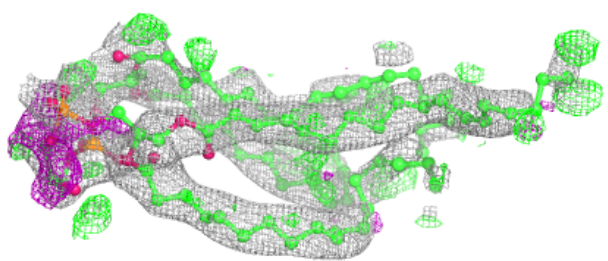
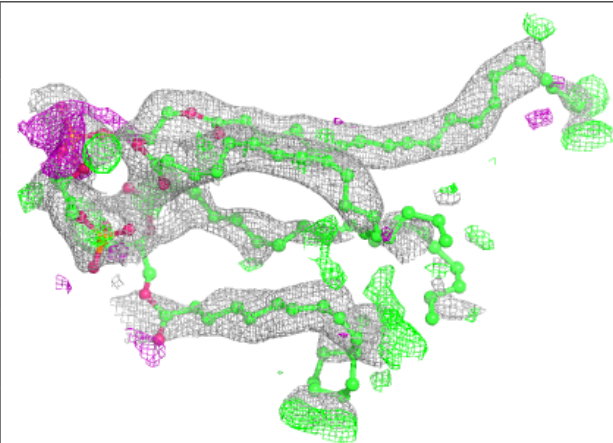


Electron density around PGV C 304:

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

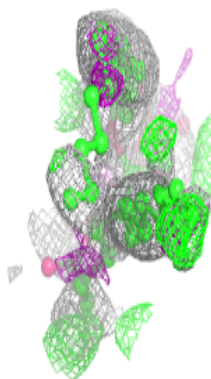
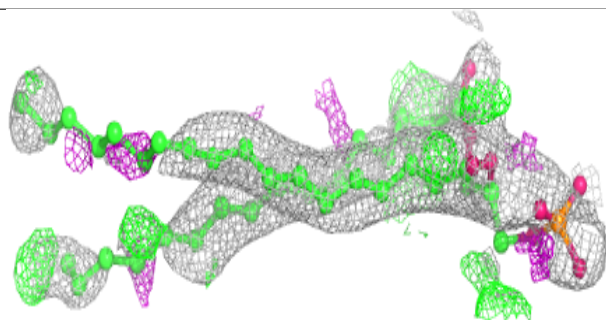
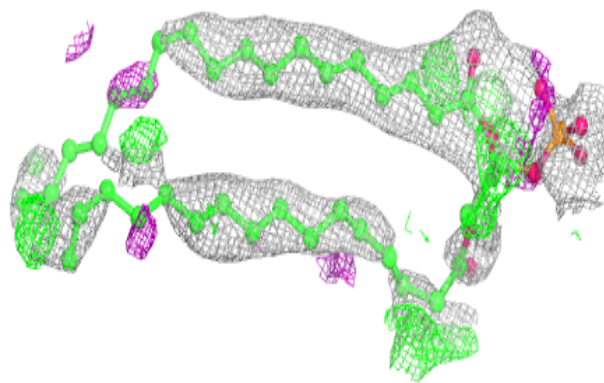
**Electron density around CDL C 305:**

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

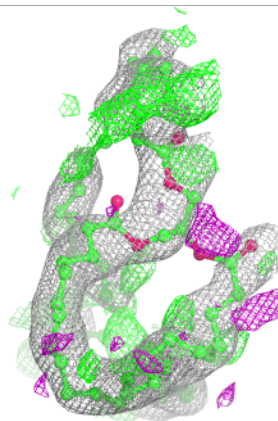
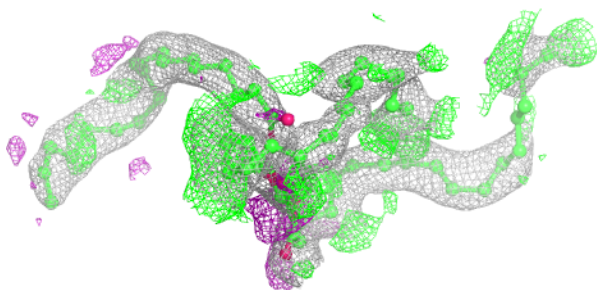
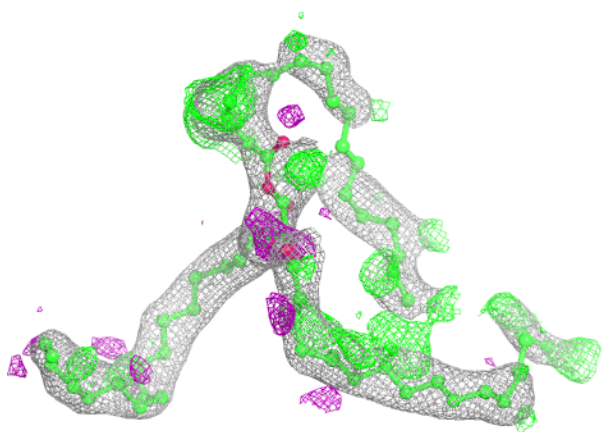


Electron density around PGV N 608:

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

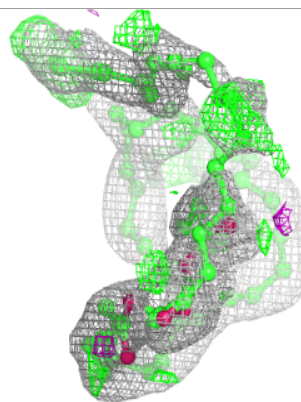
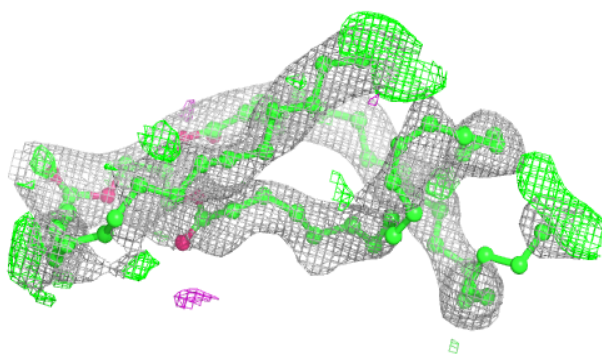
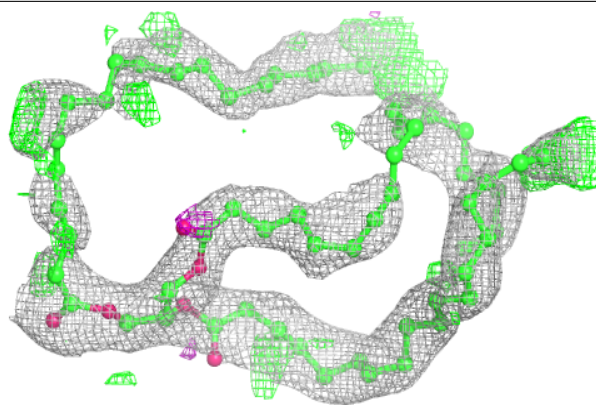
**Electron density around TGL L 101:**

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

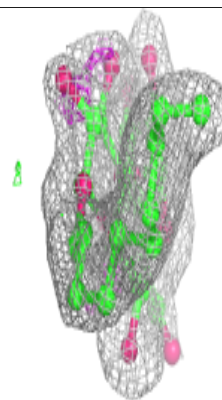
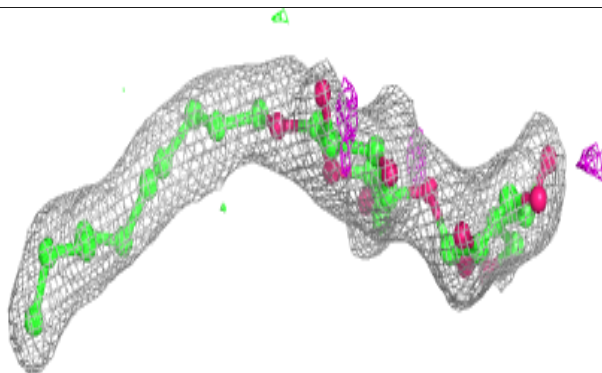
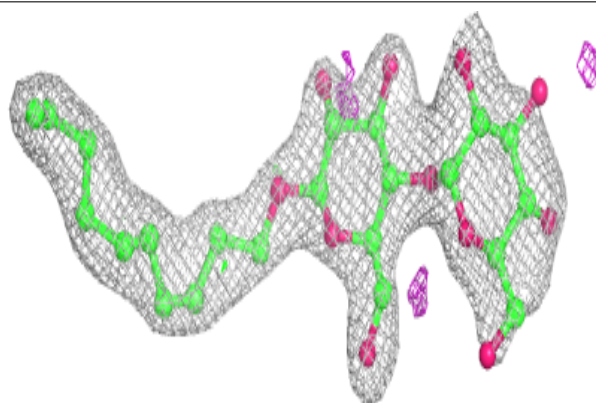


Electron density around TGL O 303:

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

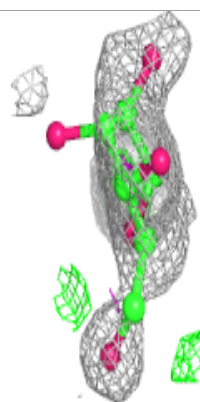
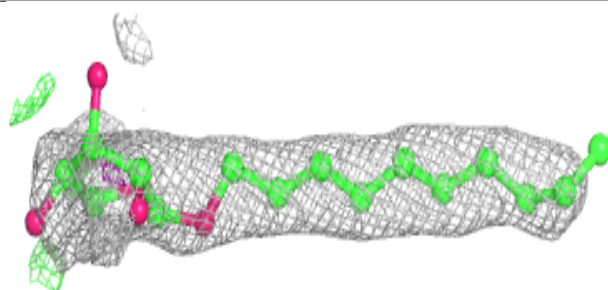
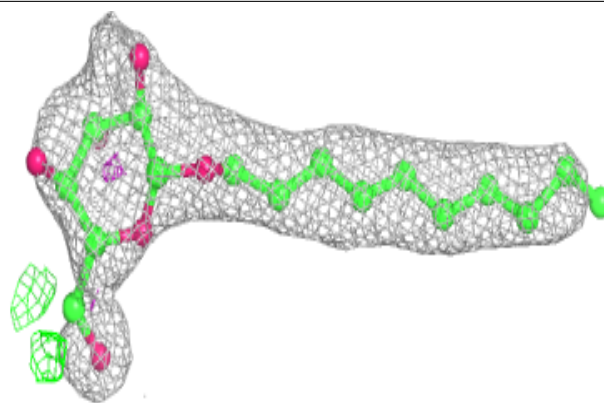
**Electron density around DMU Z 101:**

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

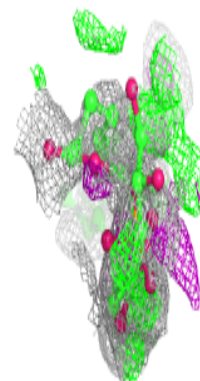
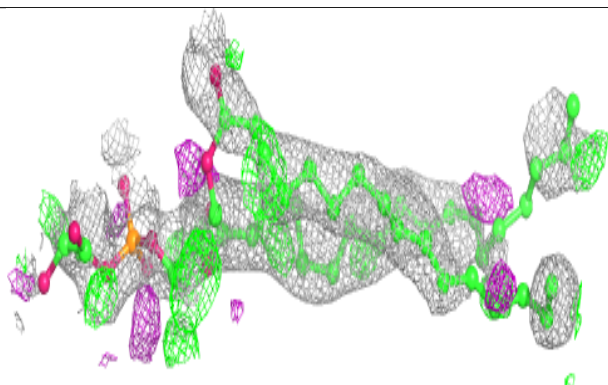
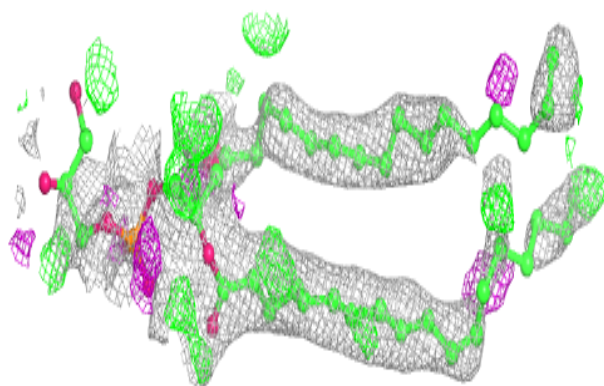


Electron density around DMU O 304:

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

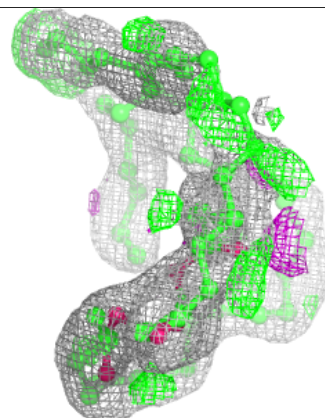
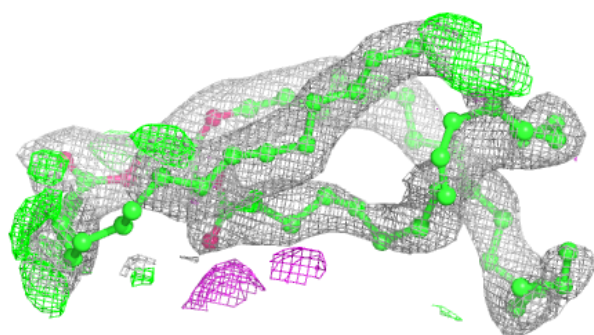
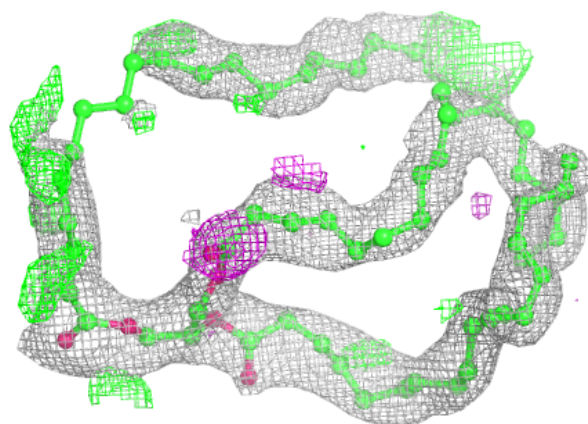
**Electron density around PGV A 609:**

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

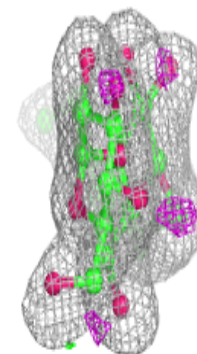
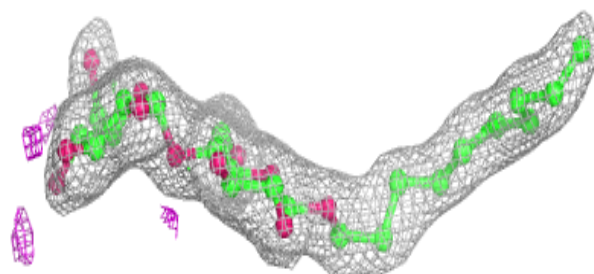
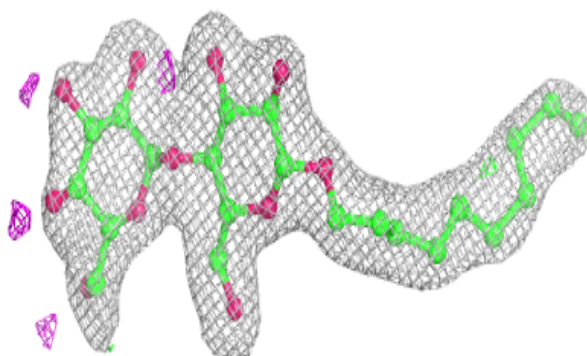


Electron density around TGL A 607:

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

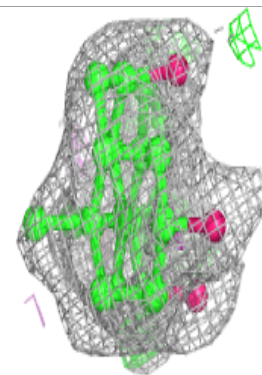
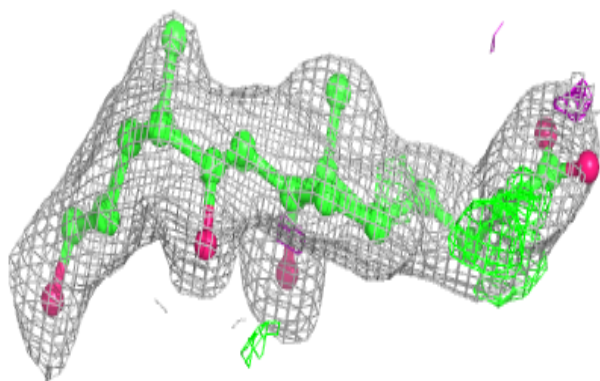
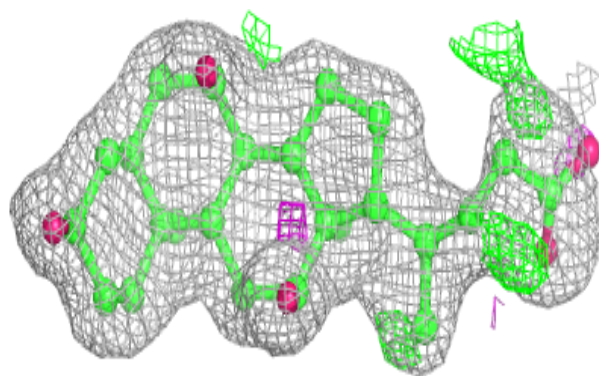
**Electron density around DMU M 101:**

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

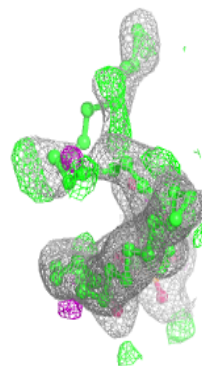
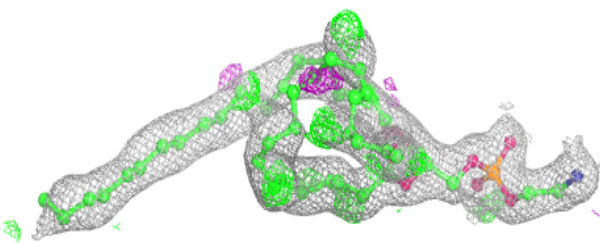
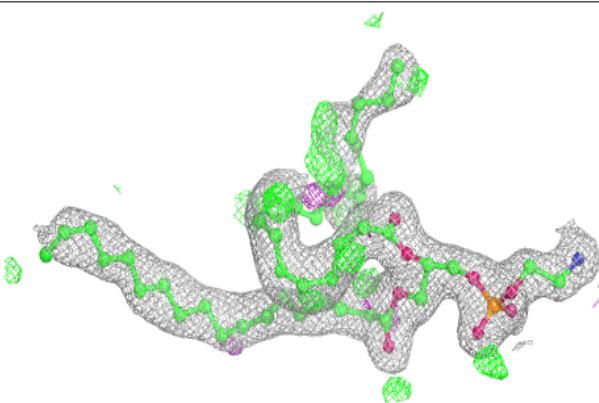


Electron density around CHD C 306:

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

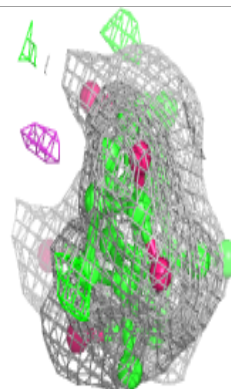
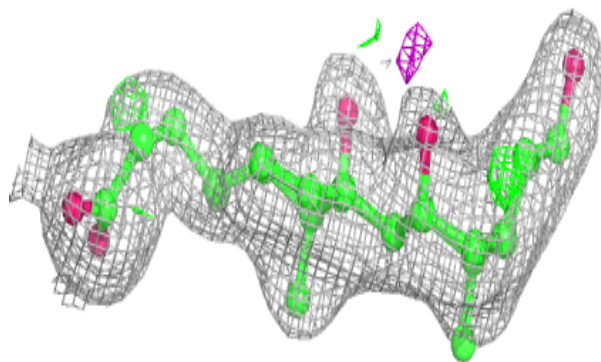
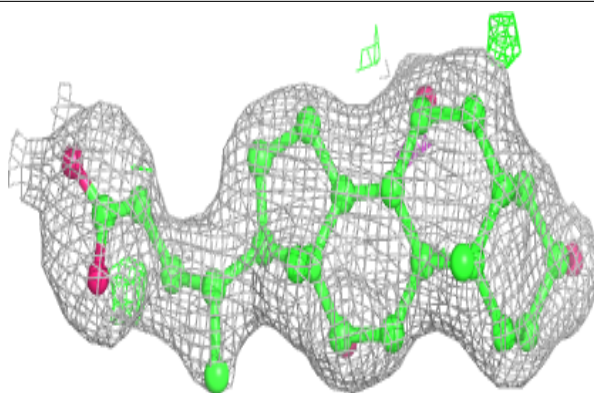
**Electron density around PEK P 302:**

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

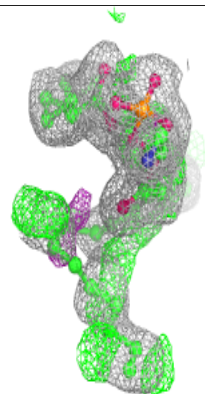
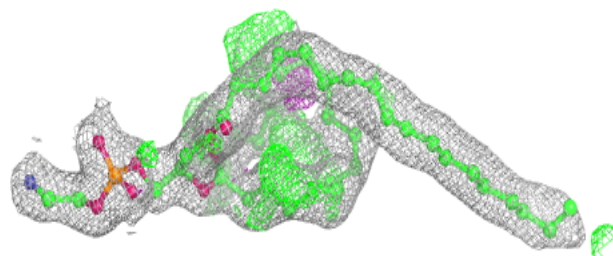
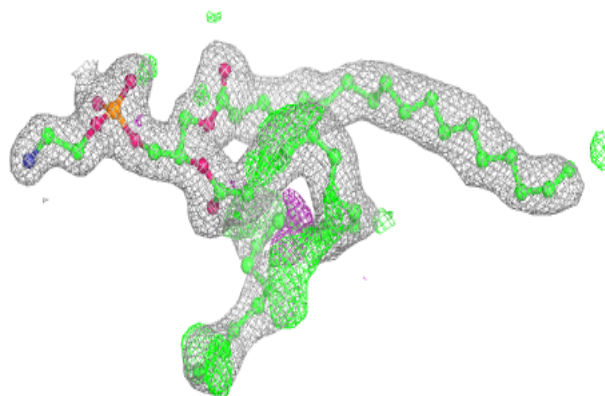


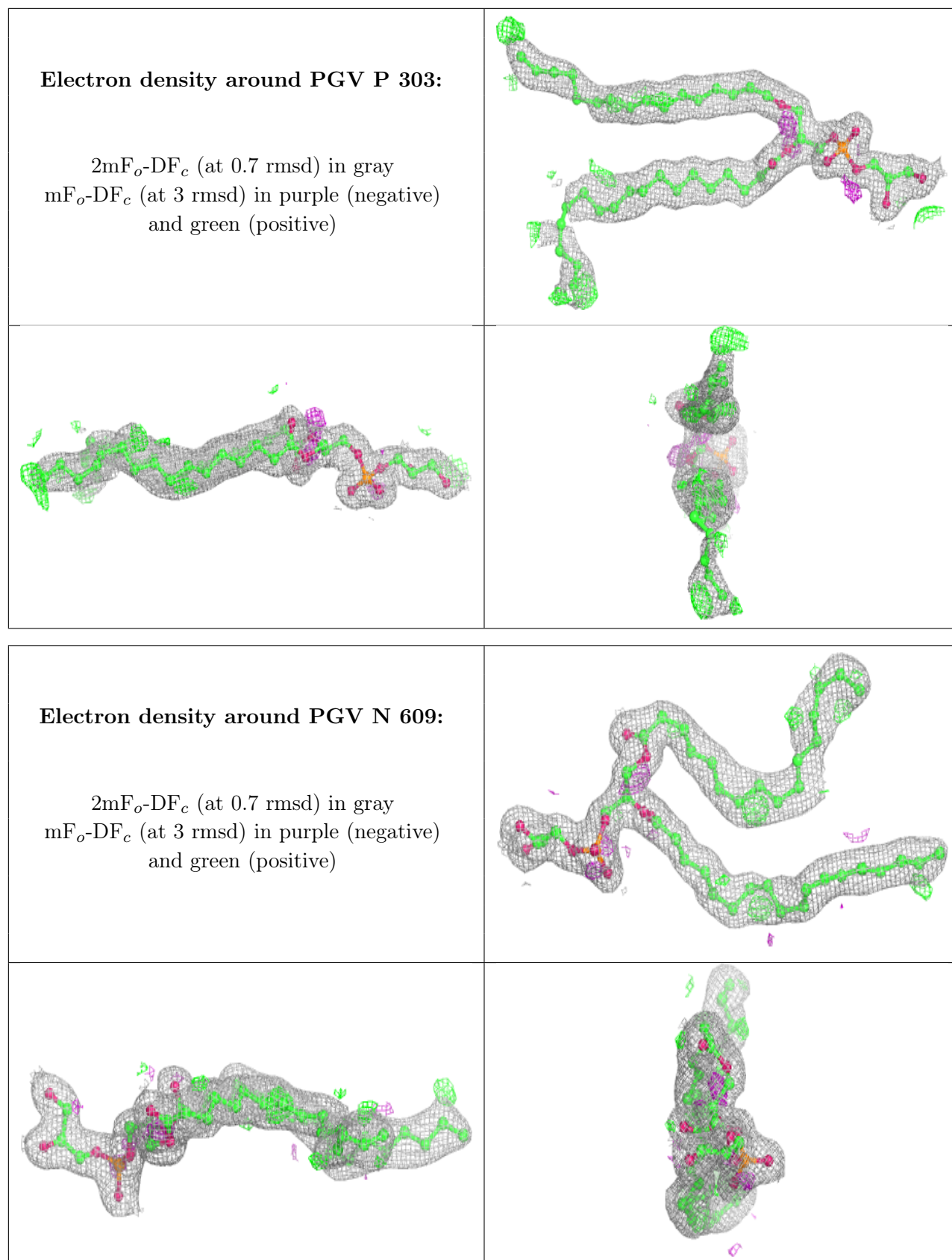
Electron density around CHD P 306:

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

**Electron density around PEK C 302:**

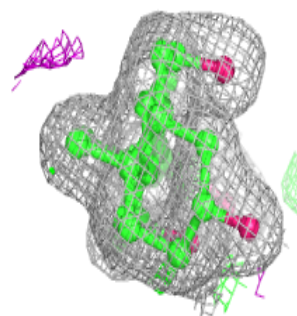
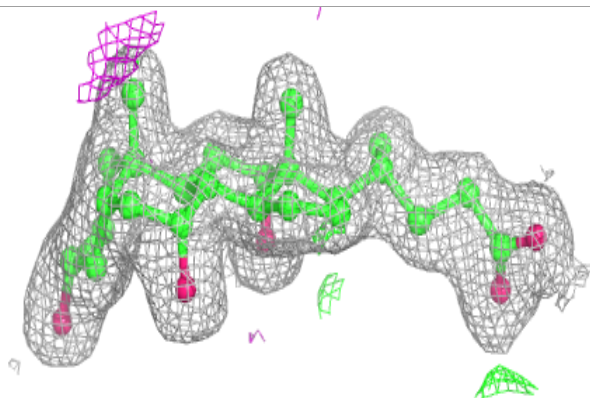
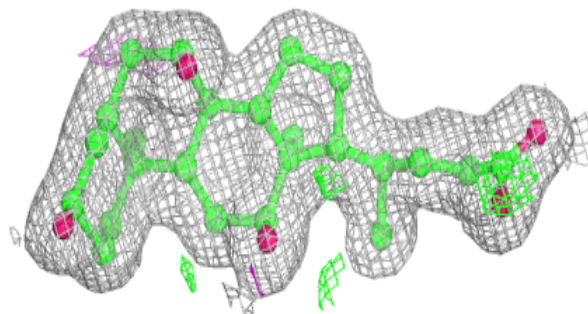
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



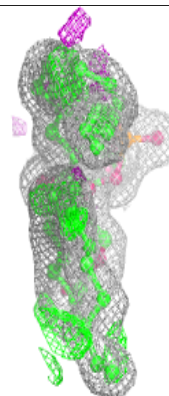
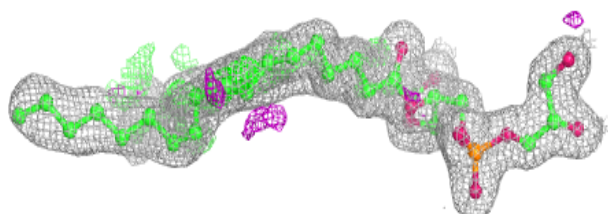
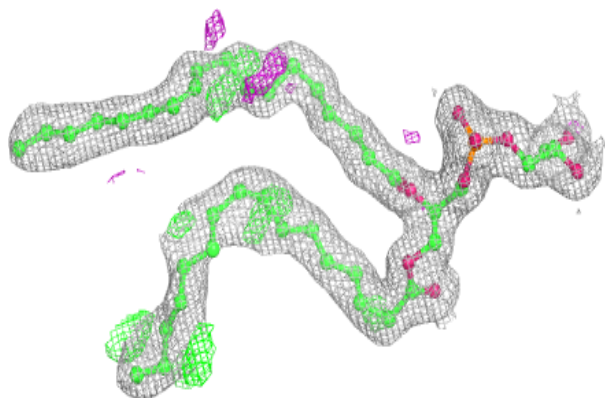


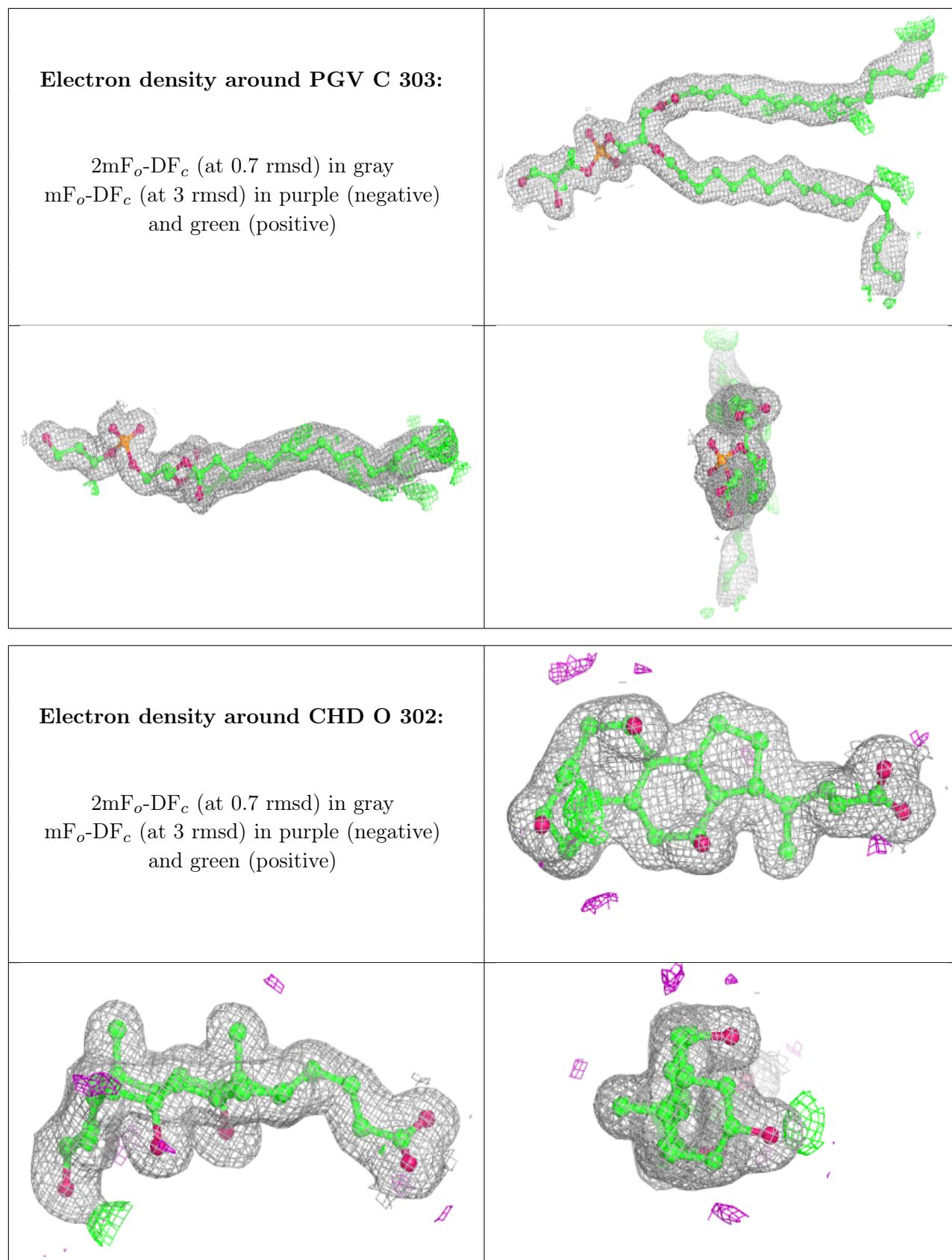
Electron density around CHD P 301:

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

**Electron density around PGV A 608:**

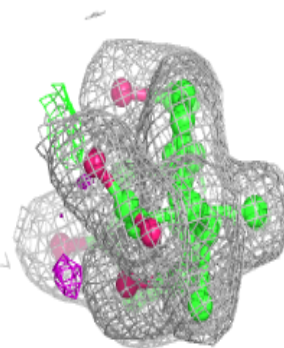
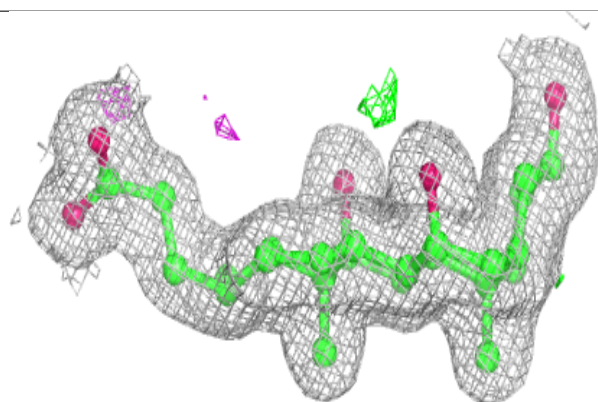
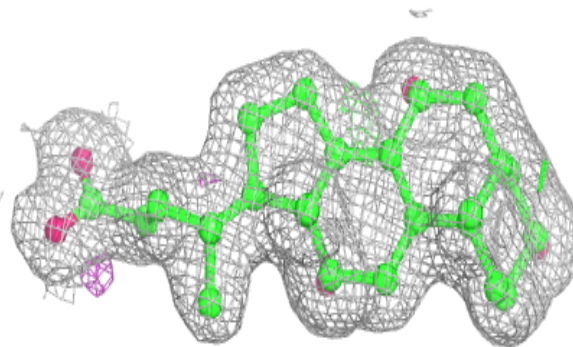
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



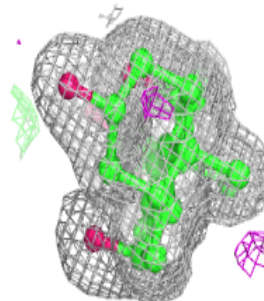
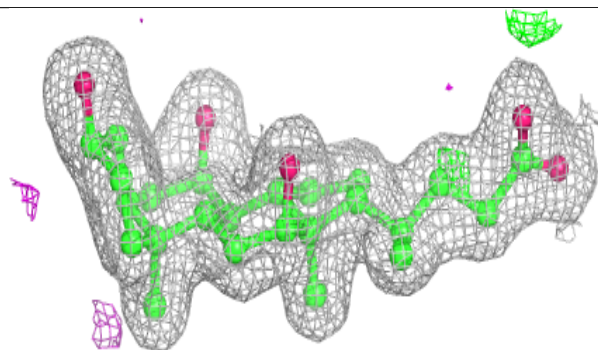
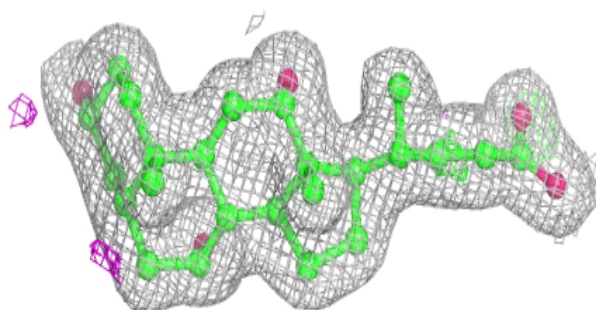


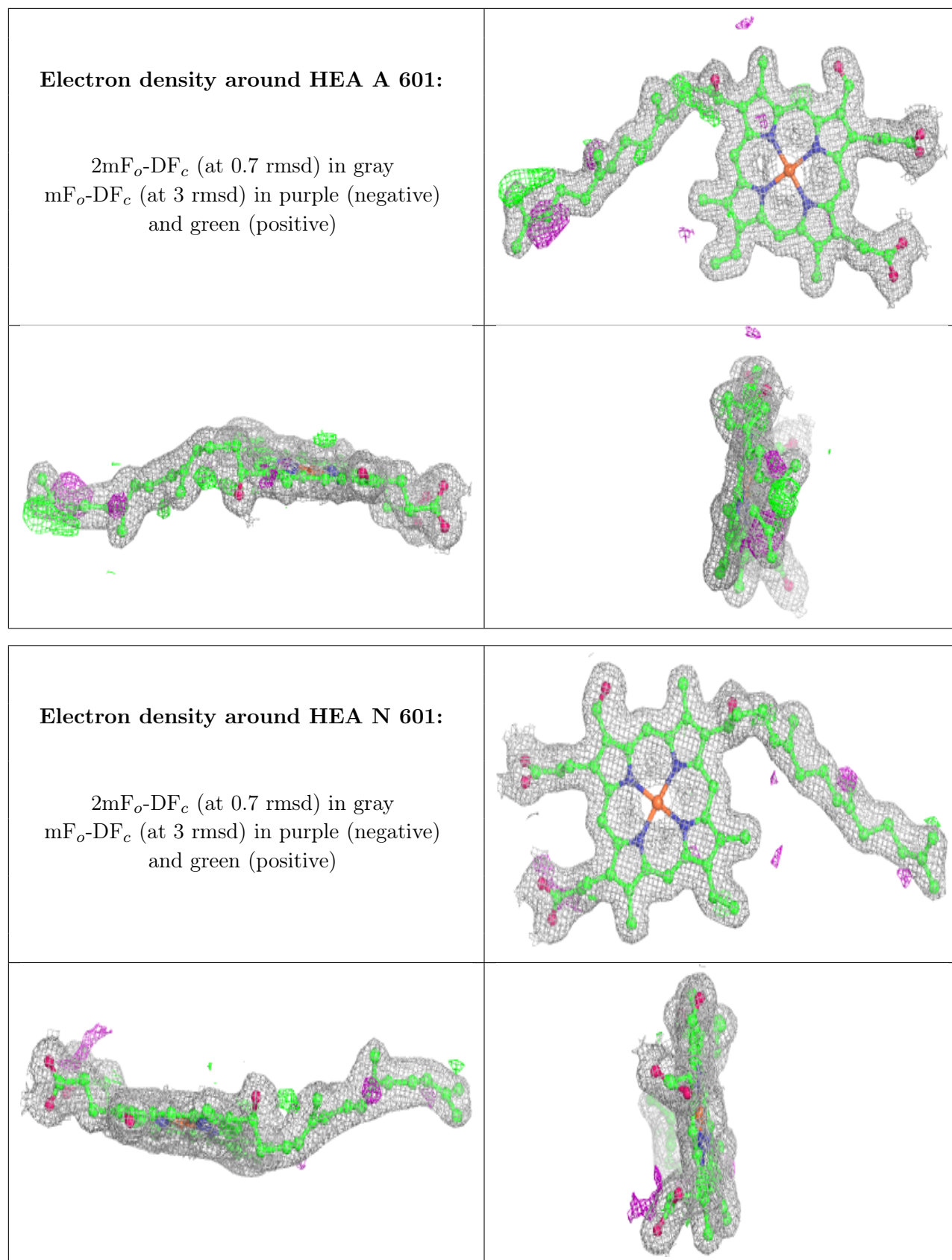
Electron density around CHD B 302:

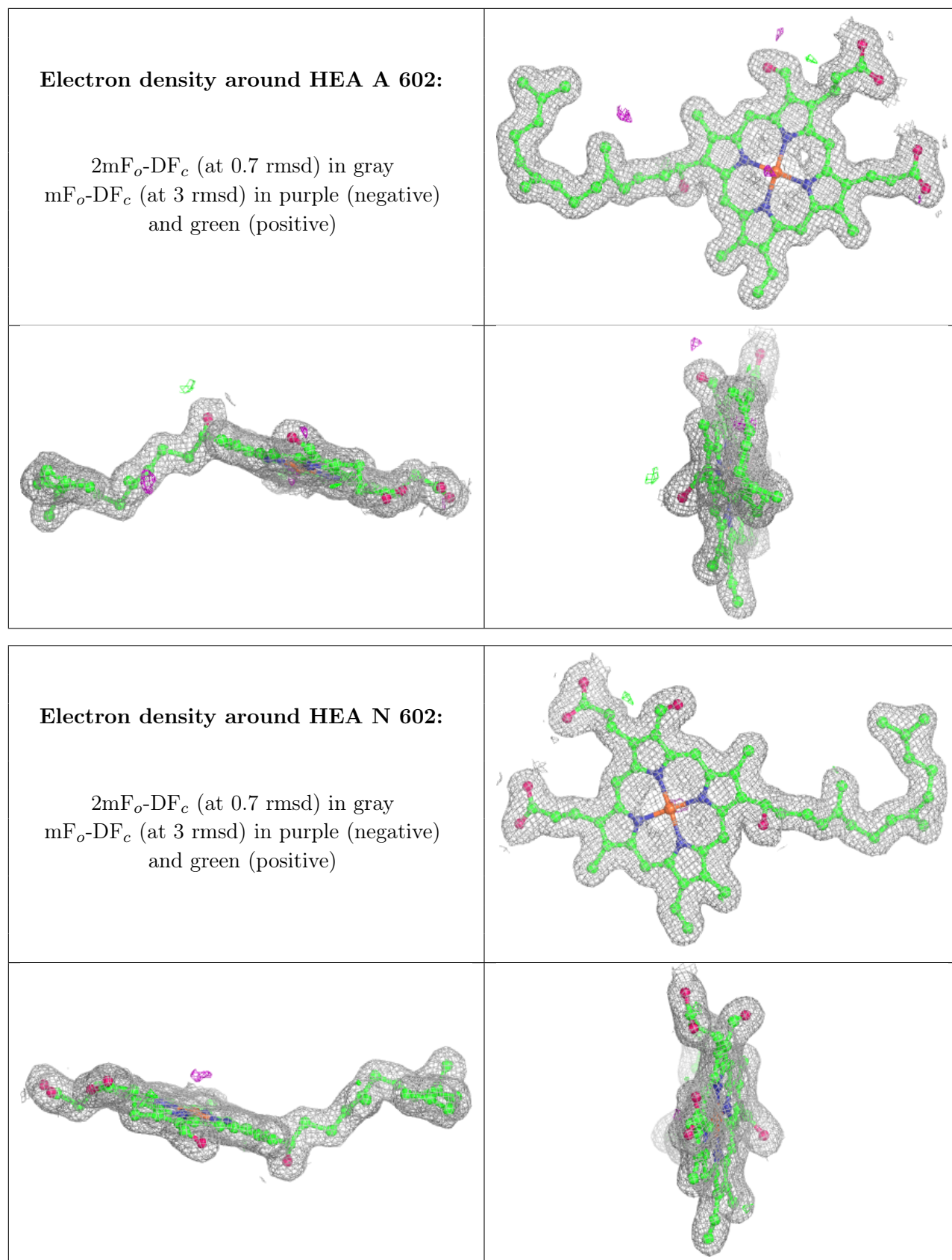
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 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)







6.5 Other polymers [i](#)

There are no such residues in this entry.