



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:13 am BST

PDB ID : 2EIM
Title : Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully reduced state
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2007-03-13
Resolution : 2.60 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 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) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

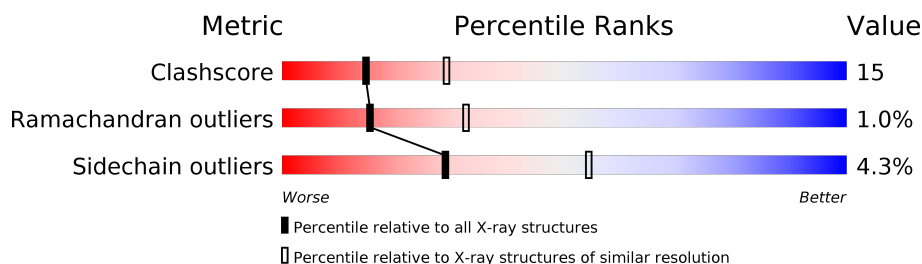
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 3518 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |












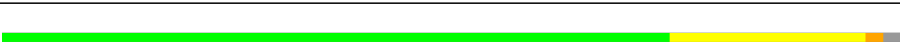




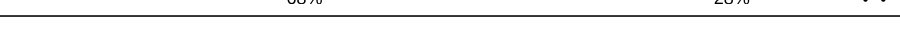

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 514 | |
| 1 | N | 514 | |
| 2 | B | 227 | |
| 2 | O | 227 | |
| 3 | C | 261 | |
| 3 | P | 261 | |
| 4 | D | 147 | |
| 4 | Q | 147 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | E | 109 |  |
| 5 | R | 109 |  |
| 6 | F | 98 |  |
| 6 | S | 98 |  |
| 7 | G | 85 |  |
| 7 | T | 85 |  |
| 8 | H | 85 |  |
| 8 | U | 85 |  |
| 9 | I | 73 |  |
| 9 | V | 73 |  |
| 10 | J | 59 |  |
| 10 | W | 59 |  |
| 11 | K | 56 |  |
| 11 | X | 56 |  |
| 12 | L | 47 |  |
| 12 | Y | 47 |  |
| 13 | M | 46 |  |
| 13 | Z | 46 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 18 | HEA | A | 515 | X | - | - | - |
| 18 | HEA | A | 516 | X | - | - | - |
| 18 | HEA | N | 515 | X | - | - | - |
| 18 | HEA | N | 516 | X | - | - | - |
| 20 | CHD | C | 271 | X | - | - | - |
| 20 | CHD | J | 60 | X | - | - | - |
| 20 | CHD | W | 1060 | X | - | - | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 20 | CHD | W | 1271 | X | - | - | - |
| 22 | TGL | L | 522 | - | - | X | - |
| 24 | DMU | C | 272 | X | - | - | - |
| 24 | DMU | M | 526 | X | - | - | - |
| 24 | DMU | P | 1272 | X | - | - | - |
| 24 | DMU | Z | 1526 | X | - | - | - |
| 26 | CDL | G | 269 | - | - | X | - |
| 26 | CDL | T | 1269 | - | - | X | - |
| 9 | SAC | V | 1 | - | X | - | - |

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 31961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4027 | 2691 | 623 | 678 | 35 | | | |
| 1 | N | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4027 | 2691 | 623 | 678 | 35 | | | |

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

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

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

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

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

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

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

| 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 polypeptide Vb.

| 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 polypeptide VIa-heart.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 84 | Total | C | N | O | P | S | 0 | 0 |
| | | | 675 | 431 | 129 | 113 | 1 | 1 | | |
| 7 | T | 84 | Total | C | N | O | P | S | 0 | 0 |
| | | | 675 | 431 | 129 | 113 | 1 | 1 | | |

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

| 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 polypeptide VIc.

| 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 polypeptide VIIa-heart.

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

Continued on next page...

Continued from previous page...

| 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 polypeptide VIIb.

| 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 polypeptide VIIc.

| 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 polypeptide VIII-heart.

| 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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | N | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

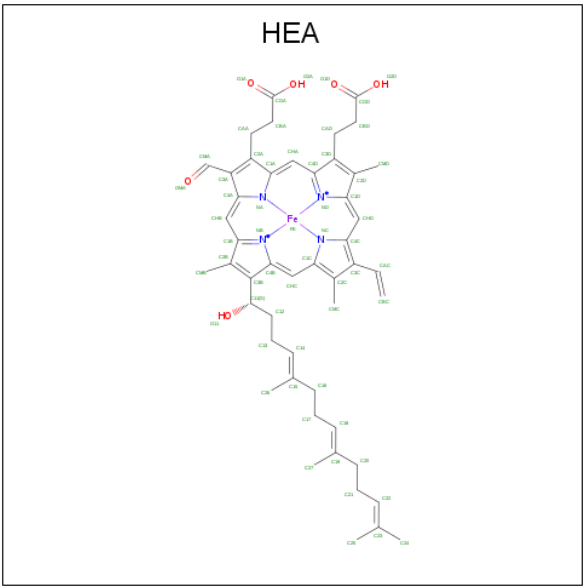
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



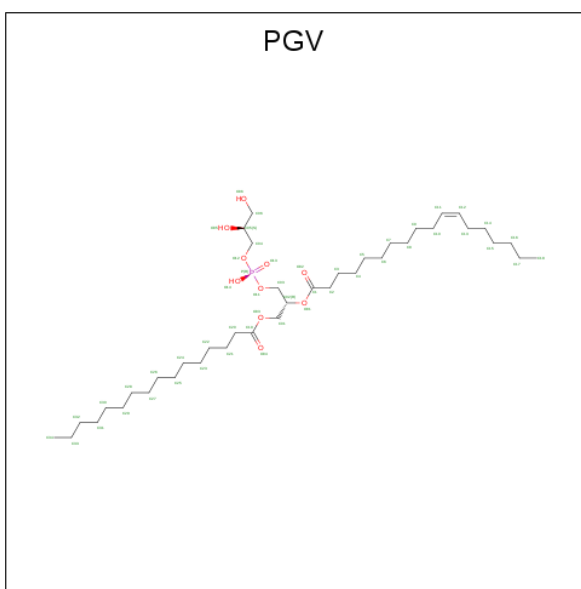
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 18 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 18 | A | 1 | Total | C | Fe | N | O | |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 18 | N | 1 | Total | C | Fe | N | O | |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 18 | N | 1 | Total | C | Fe | N | O | |
| | | | 60 | 49 | 1 | 4 | 6 | |

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



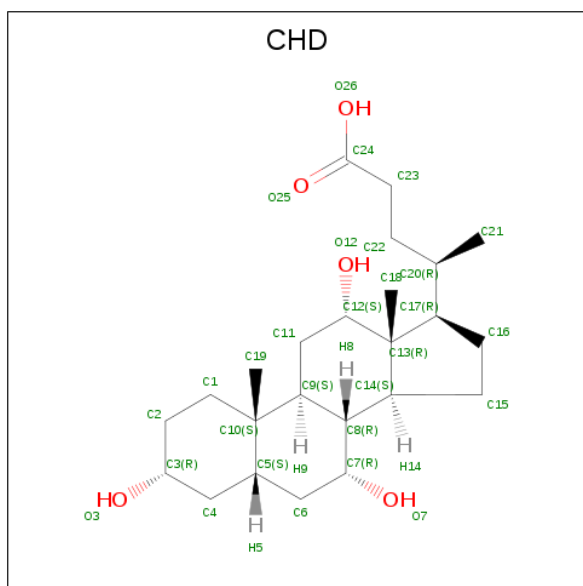
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19 | A | 1 | Total | C | O | P | | |
| | | | 51 | 40 | 10 | 1 | 0 | 0 |
| 19 | C | 1 | Total | C | O | P | | |
| | | | 51 | 40 | 10 | 1 | 0 | 0 |
| 19 | C | 1 | Total | C | O | P | | |
| | | | 51 | 40 | 10 | 1 | 0 | 0 |
| 19 | C | 1 | Total | C | O | P | | |
| | | | 51 | 40 | 10 | 1 | 0 | 0 |
| 19 | N | 1 | Total | C | O | P | | |
| | | | 51 | 40 | 10 | 1 | 0 | 0 |
| 19 | P | 1 | Total | C | O | P | | |
| | | | 51 | 40 | 10 | 1 | 0 | 0 |
| 19 | P | 1 | Total | C | O | P | | |
| | | | 51 | 40 | 10 | 1 | 0 | 0 |

Continued on next page...

Continued from previous page...

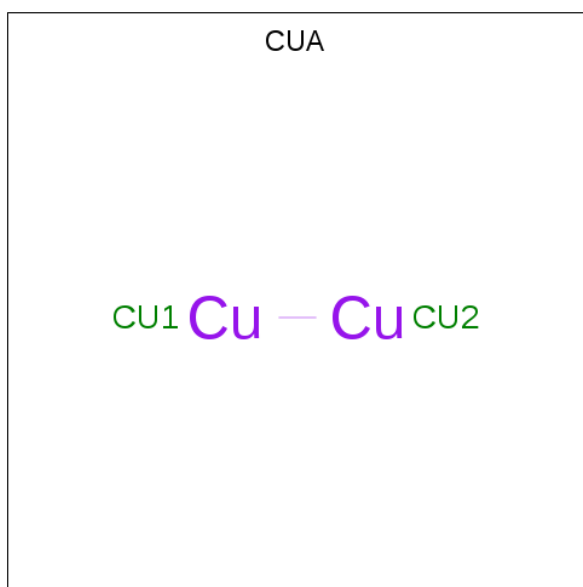
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |

- Molecule 20 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



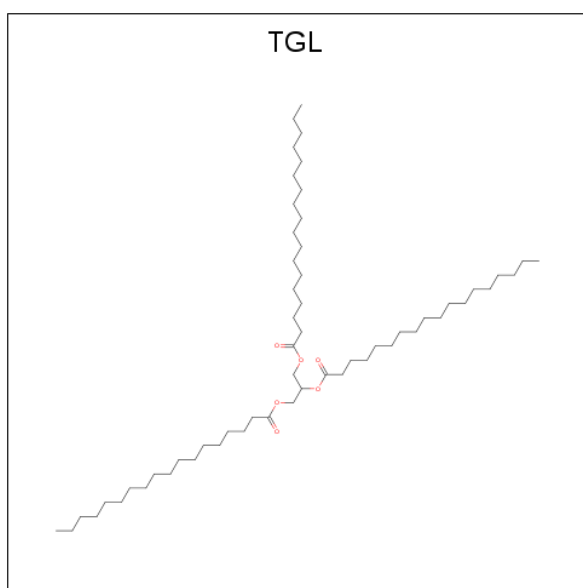
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 20 | A | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 20 | B | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 20 | C | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 20 | J | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 20 | N | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 20 | P | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 20 | W | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 20 | W | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|--|---------|---------|
| 21 | B | 1 | Total | Cu | | 0 | 0 |
| | | | 2 | 2 | | | |
| 21 | O | 1 | Total | Cu | | 0 | 0 |
| | | | 2 | 2 | | | |

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



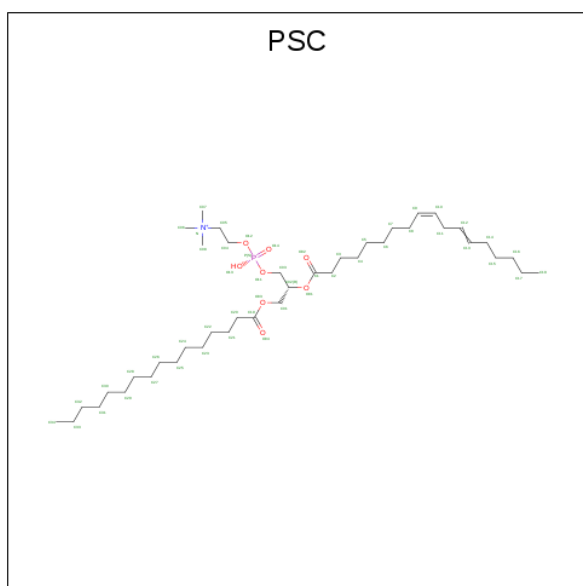
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 22 | B | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 22 | D | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

Continued on next page...

Continued from previous page...

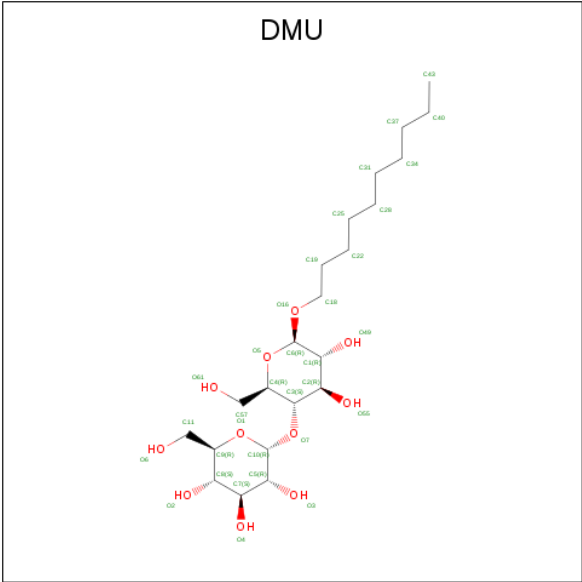
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 22 | L | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 22 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 22 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 22 | O | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

- Molecule 23 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: $C_{42}H_{81}NO_8P$).



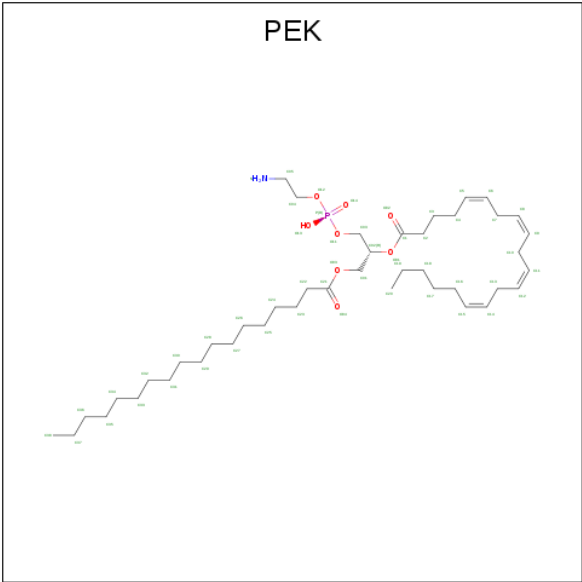
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 23 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |
| 23 | O | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



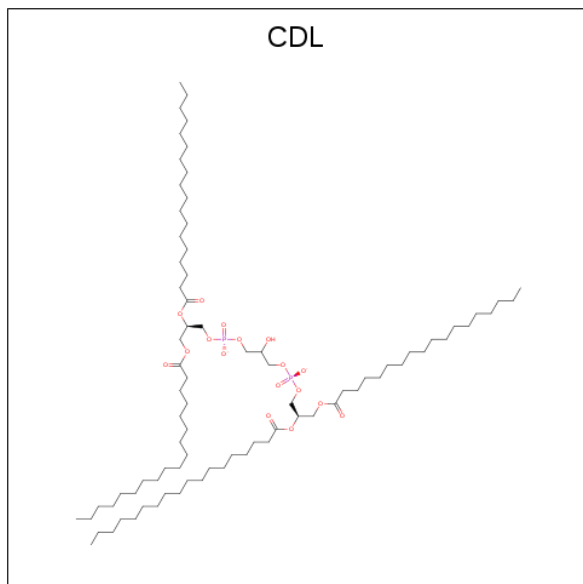
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 24 | C | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 24 | M | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 24 | P | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |
| 24 | Z | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 22 | 11 | | |

- Molecule 25 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 |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 25 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 26 | G | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 26 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 26 | T | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |

- Molecule 27 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 27 | A | 182 | Total 182 | O 182 | 0 | 0 |
| 27 | B | 96 | Total 96 | O 96 | 0 | 0 |
| 27 | C | 82 | Total 82 | O 82 | 0 | 0 |
| 27 | D | 61 | Total 61 | O 61 | 0 | 0 |
| 27 | E | 43 | Total 43 | O 43 | 0 | 0 |
| 27 | F | 52 | Total 52 | O 52 | 0 | 0 |
| 27 | G | 37 | Total 37 | O 37 | 0 | 0 |
| 27 | H | 35 | Total 35 | O 35 | 0 | 0 |
| 27 | I | 22 | Total 22 | O 22 | 0 | 0 |
| 27 | J | 12 | Total 12 | O 12 | 0 | 0 |
| 27 | K | 12 | Total 12 | O 12 | 0 | 0 |
| 27 | L | 13 | Total 13 | O 13 | 0 | 0 |
| 27 | M | 13 | Total 13 | O 13 | 0 | 0 |
| 27 | N | 171 | Total 171 | O 171 | 0 | 0 |
| 27 | O | 79 | Total 79 | O 79 | 0 | 0 |
| 27 | P | 73 | Total 73 | O 73 | 0 | 0 |
| 27 | Q | 42 | Total 42 | O 42 | 0 | 0 |
| 27 | R | 30 | Total 30 | O 30 | 0 | 0 |
| 27 | S | 42 | Total 42 | O 42 | 0 | 0 |
| 27 | T | 30 | Total 30 | O 30 | 0 | 0 |
| 27 | U | 30 | Total 30 | O 30 | 0 | 0 |
| 27 | V | 19 | Total 19 | O 19 | 0 | 0 |

Continued on next page...

Continued from previous page...

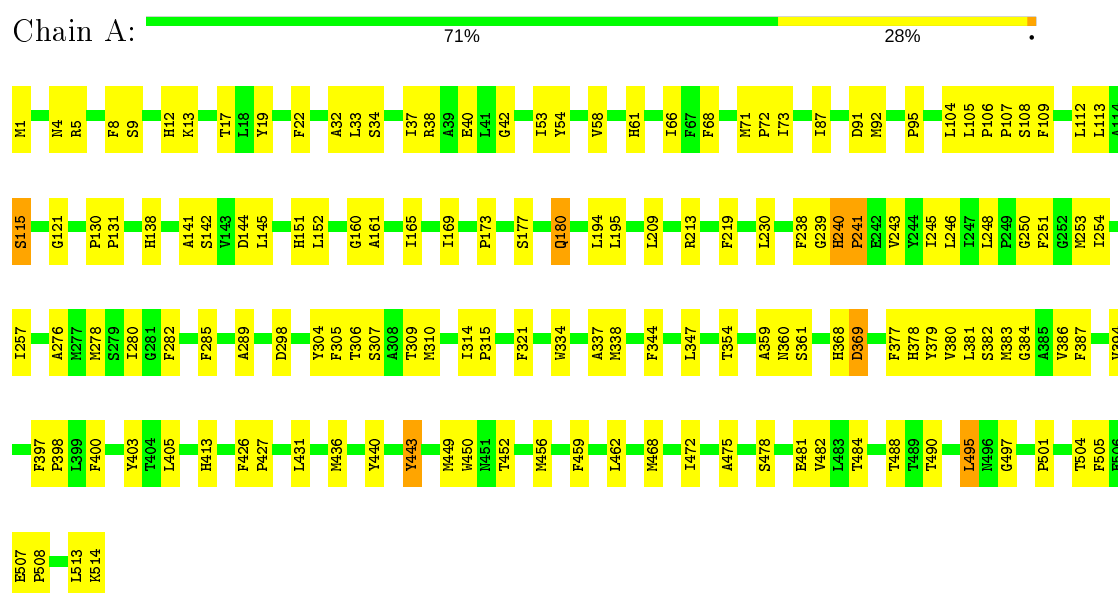
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 27 | W | 8 | Total 8 | O 8 | 0 | 0 |
| 27 | X | 18 | Total 18 | O 18 | 0 | 0 |
| 27 | Y | 14 | Total 14 | O 14 | 0 | 0 |
| 27 | Z | 11 | Total 11 | O 11 | 0 | 0 |

3 Residue-property plots [i](#)

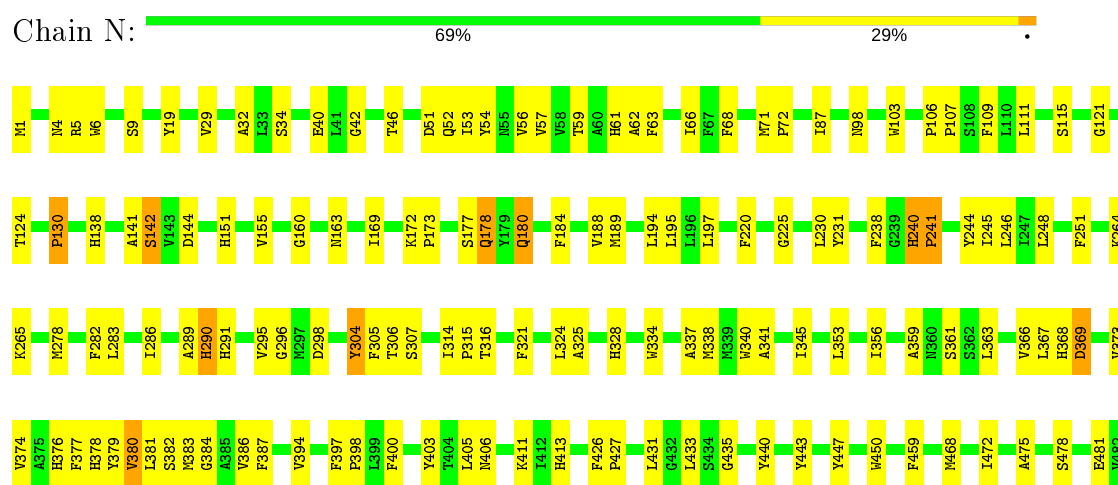
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Cytochrome c oxidase subunit 1



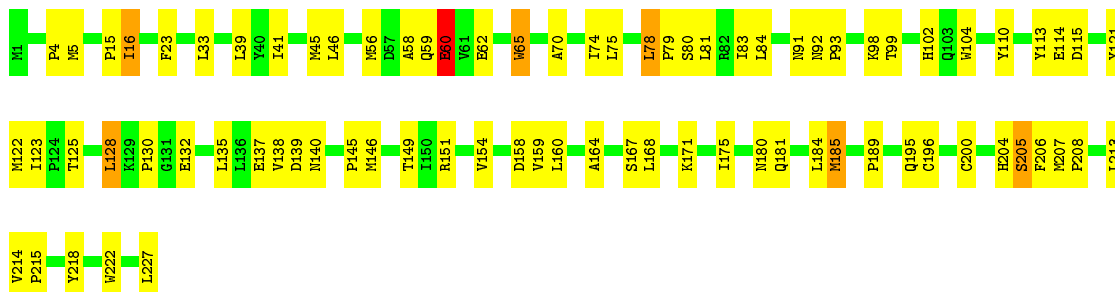
• Molecule 1: Cytochrome c oxidase subunit 1





• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 65% 32%



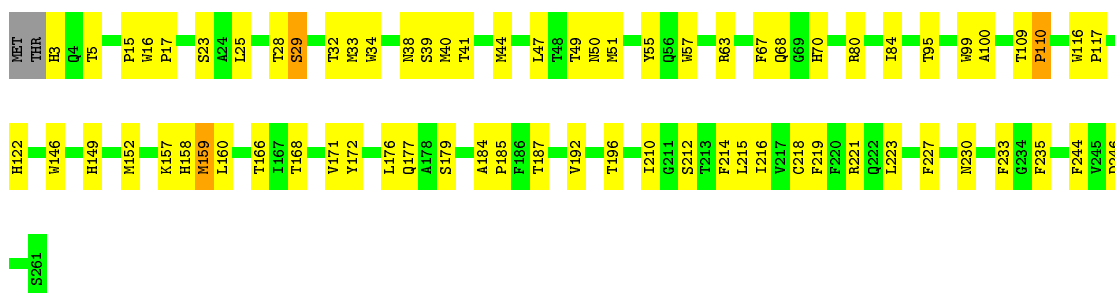
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 63% 34%



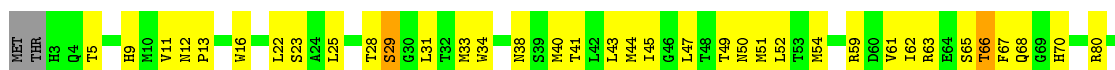
• Molecule 3: Cytochrome c oxidase subunit 3

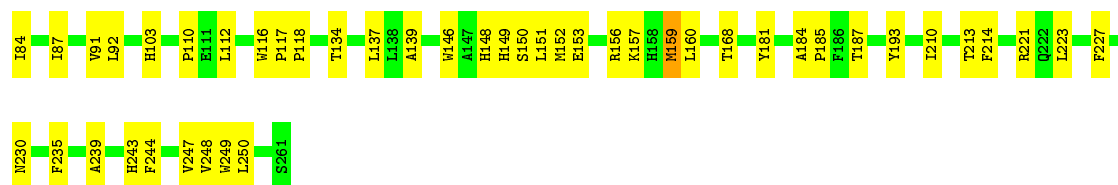
Chain C: 72% 26%



• Molecule 3: Cytochrome c oxidase subunit 3

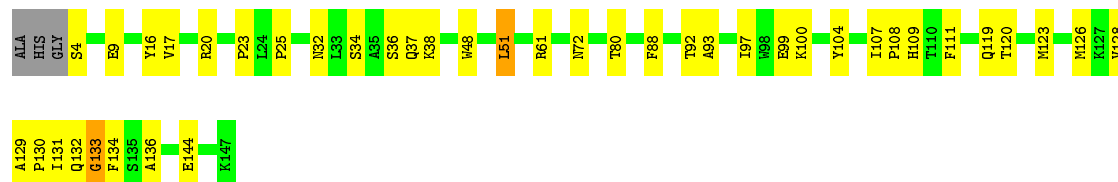
Chain P: 68% 30%





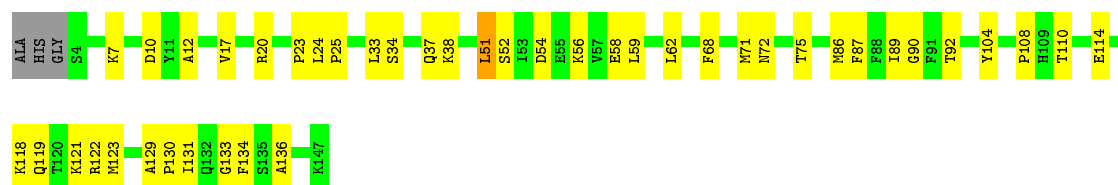
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 70% 27% ..



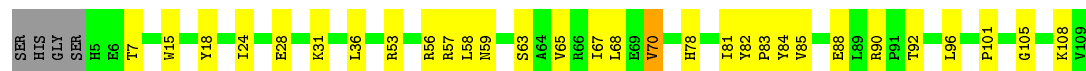
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 69% 29% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E: 69% 27% . .



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R: 81% 16% .




- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F: 67% 29% ..



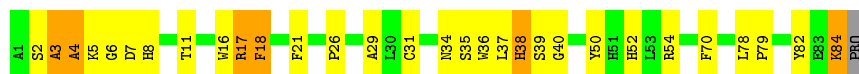
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  77% 18% . .



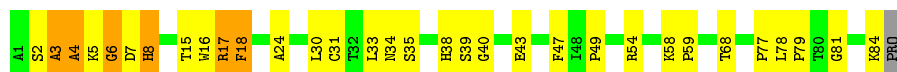
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  64% 28% 7% .




- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  61% 31% 7% .



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  79% 11% 7% .




- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  73% 20% 7% .




- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  78% 19% .




- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  77% 22% .



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  78% 20% .



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  75% 22% ..



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  66% 21% 13%



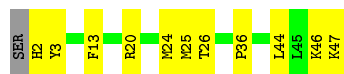
- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  63% 25% 13%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  74% 23% .



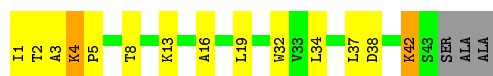
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  68% 28% ..



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  63% 26% . 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:

67%

22%

•

7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 183.91Å 206.72Å 178.34Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 2.60 | Depositor |
| % Data completeness (in resolution range) | (Not available) (40.00-2.60) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | X-PLOR 3.851 | Depositor |
| R, R_{free} | 0.204 , 0.256 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 31961 | wwPDB-VP |
| Average B, all atoms (Å ²) | 48.0 | wwPDB-VP |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.70 | 0/4156 | 0.78 | 1/5678 (0.0%) |
| 1 | N | 0.64 | 0/4156 | 0.76 | 2/5678 (0.0%) |
| 2 | B | 0.60 | 0/1860 | 0.83 | 1/2534 (0.0%) |
| 2 | O | 0.59 | 0/1860 | 0.83 | 0/2534 |
| 3 | C | 0.68 | 0/2197 | 0.70 | 0/3005 |
| 3 | P | 0.63 | 0/2197 | 0.72 | 0/3005 |
| 4 | D | 0.60 | 0/1229 | 0.73 | 1/1658 (0.1%) |
| 4 | Q | 0.64 | 0/1229 | 0.71 | 0/1658 |
| 5 | E | 0.62 | 0/871 | 0.73 | 0/1182 |
| 5 | R | 0.61 | 0/871 | 0.75 | 0/1182 |
| 6 | F | 0.60 | 0/765 | 0.86 | 2/1038 (0.2%) |
| 6 | S | 0.59 | 0/765 | 0.86 | 2/1038 (0.2%) |
| 7 | G | 0.61 | 0/690 | 0.77 | 1/937 (0.1%) |
| 7 | T | 0.63 | 0/690 | 0.81 | 2/937 (0.2%) |
| 8 | H | 0.64 | 0/682 | 0.71 | 0/921 |
| 8 | U | 0.57 | 0/682 | 0.72 | 0/921 |
| 9 | I | 0.62 | 0/605 | 0.70 | 0/802 |
| 9 | V | 0.60 | 0/605 | 0.68 | 0/802 |
| 10 | J | 0.59 | 0/471 | 0.74 | 0/636 |
| 10 | W | 0.59 | 0/471 | 0.73 | 0/636 |
| 11 | K | 0.71 | 0/398 | 0.75 | 0/546 |
| 11 | X | 0.59 | 0/398 | 0.74 | 0/546 |
| 12 | L | 0.63 | 0/393 | 0.69 | 0/526 |
| 12 | Y | 0.62 | 0/393 | 0.67 | 0/526 |
| 13 | M | 0.57 | 0/345 | 0.70 | 0/470 |
| 13 | Z | 0.60 | 0/345 | 0.70 | 0/470 |
| All | All | 0.63 | 0/29324 | 0.76 | 12/39866 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 3 |
| 1 | N | 0 | 5 |
| 2 | B | 0 | 1 |
| 2 | O | 0 | 1 |
| All | All | 0 | 10 |

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 6 | S | 94 | HIS | N-CA-C | 6.74 | 129.20 | 111.00 |
| 6 | F | 94 | HIS | N-CA-C | 6.46 | 128.43 | 111.00 |
| 2 | B | 128 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 6 | S | 93 | PRO | N-CA-C | 5.74 | 127.02 | 112.10 |
| 7 | T | 33 | LEU | CA-CB-CG | 5.72 | 128.47 | 115.30 |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 19 | TYR | Sidechain |
| 1 | A | 240 | HIS | Sidechain |
| 1 | A | 443 | TYR | Sidechain |
| 2 | B | 218 | TYR | Sidechain |
| 1 | N | 19 | TYR | Sidechain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4027 | 0 | 4001 | 130 | 0 |
| 1 | N | 4027 | 0 | 4001 | 145 | 0 |
| 2 | B | 1824 | 0 | 1833 | 66 | 0 |
| 2 | O | 1824 | 0 | 1833 | 85 | 0 |
| 3 | C | 2110 | 0 | 2027 | 66 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | P | 2110 | 0 | 2027 | 76 | 0 |
| 4 | D | 1195 | 0 | 1183 | 34 | 0 |
| 4 | Q | 1195 | 0 | 1183 | 37 | 0 |
| 5 | E | 852 | 0 | 845 | 23 | 0 |
| 5 | R | 852 | 0 | 845 | 11 | 0 |
| 6 | F | 748 | 0 | 728 | 24 | 0 |
| 6 | S | 748 | 0 | 728 | 16 | 0 |
| 7 | G | 675 | 0 | 644 | 35 | 0 |
| 7 | T | 675 | 0 | 644 | 40 | 0 |
| 8 | H | 662 | 0 | 623 | 8 | 0 |
| 8 | U | 662 | 0 | 623 | 14 | 0 |
| 9 | I | 601 | 0 | 613 | 14 | 0 |
| 9 | V | 601 | 0 | 613 | 16 | 0 |
| 10 | J | 460 | 0 | 459 | 12 | 0 |
| 10 | W | 460 | 0 | 459 | 11 | 0 |
| 11 | K | 384 | 0 | 366 | 8 | 0 |
| 11 | X | 384 | 0 | 366 | 9 | 0 |
| 12 | L | 380 | 0 | 380 | 21 | 0 |
| 12 | Y | 380 | 0 | 380 | 14 | 0 |
| 13 | M | 335 | 0 | 352 | 10 | 0 |
| 13 | Z | 335 | 0 | 352 | 11 | 0 |
| 14 | A | 1 | 0 | 0 | 0 | 0 |
| 14 | N | 1 | 0 | 0 | 0 | 0 |
| 15 | A | 1 | 0 | 0 | 0 | 0 |
| 15 | N | 1 | 0 | 0 | 0 | 0 |
| 16 | A | 1 | 0 | 0 | 0 | 0 |
| 16 | N | 1 | 0 | 0 | 0 | 0 |
| 17 | A | 1 | 0 | 0 | 0 | 0 |
| 17 | C | 1 | 0 | 0 | 0 | 0 |
| 17 | F | 1 | 0 | 0 | 0 | 0 |
| 17 | N | 1 | 0 | 0 | 0 | 0 |
| 17 | P | 1 | 0 | 0 | 0 | 0 |
| 17 | S | 1 | 0 | 0 | 0 | 0 |
| 18 | A | 120 | 0 | 108 | 9 | 0 |
| 18 | N | 120 | 0 | 108 | 12 | 0 |
| 19 | A | 51 | 0 | 76 | 7 | 0 |
| 19 | C | 153 | 0 | 228 | 12 | 0 |
| 19 | N | 51 | 0 | 76 | 10 | 0 |
| 19 | P | 153 | 0 | 228 | 11 | 0 |
| 20 | A | 29 | 0 | 39 | 1 | 0 |
| 20 | B | 29 | 0 | 39 | 1 | 0 |
| 20 | C | 29 | 0 | 39 | 2 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20 | J | 29 | 0 | 37 | 5 | 0 |
| 20 | N | 29 | 0 | 39 | 2 | 0 |
| 20 | P | 29 | 0 | 39 | 2 | 0 |
| 20 | W | 58 | 0 | 76 | 5 | 0 |
| 21 | B | 2 | 0 | 0 | 0 | 0 |
| 21 | O | 2 | 0 | 0 | 0 | 0 |
| 22 | B | 63 | 0 | 110 | 6 | 0 |
| 22 | D | 63 | 0 | 110 | 5 | 0 |
| 22 | L | 63 | 0 | 110 | 27 | 0 |
| 22 | N | 126 | 0 | 220 | 22 | 0 |
| 22 | O | 63 | 0 | 110 | 8 | 0 |
| 23 | B | 52 | 0 | 80 | 19 | 0 |
| 23 | O | 52 | 0 | 80 | 18 | 0 |
| 24 | C | 33 | 0 | 36 | 3 | 0 |
| 24 | M | 33 | 0 | 38 | 1 | 0 |
| 24 | P | 33 | 0 | 37 | 4 | 0 |
| 24 | Z | 33 | 0 | 38 | 0 | 0 |
| 25 | C | 106 | 0 | 154 | 17 | 0 |
| 25 | G | 53 | 0 | 77 | 9 | 0 |
| 25 | P | 106 | 0 | 154 | 18 | 0 |
| 25 | T | 53 | 0 | 77 | 14 | 0 |
| 26 | C | 100 | 0 | 156 | 19 | 0 |
| 26 | G | 100 | 0 | 156 | 22 | 0 |
| 26 | P | 100 | 0 | 156 | 13 | 0 |
| 26 | T | 100 | 0 | 156 | 23 | 0 |
| 27 | A | 182 | 0 | 0 | 9 | 0 |
| 27 | B | 96 | 0 | 0 | 2 | 0 |
| 27 | C | 82 | 0 | 0 | 5 | 0 |
| 27 | D | 61 | 0 | 0 | 7 | 0 |
| 27 | E | 43 | 0 | 0 | 4 | 0 |
| 27 | F | 52 | 0 | 0 | 5 | 0 |
| 27 | G | 37 | 0 | 0 | 1 | 0 |
| 27 | H | 35 | 0 | 0 | 1 | 0 |
| 27 | I | 22 | 0 | 0 | 2 | 0 |
| 27 | J | 12 | 0 | 0 | 1 | 0 |
| 27 | K | 12 | 0 | 0 | 2 | 0 |
| 27 | L | 13 | 0 | 0 | 0 | 0 |
| 27 | M | 13 | 0 | 0 | 2 | 0 |
| 27 | N | 171 | 0 | 0 | 14 | 0 |
| 27 | O | 79 | 0 | 0 | 4 | 0 |
| 27 | P | 73 | 0 | 0 | 0 | 0 |
| 27 | Q | 42 | 0 | 0 | 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27 | R | 30 | 0 | 0 | 2 | 0 |
| 27 | S | 42 | 0 | 0 | 0 | 0 |
| 27 | T | 30 | 0 | 0 | 3 | 0 |
| 27 | U | 30 | 0 | 0 | 0 | 0 |
| 27 | V | 19 | 0 | 0 | 3 | 0 |
| 27 | W | 8 | 0 | 0 | 0 | 0 |
| 27 | X | 18 | 0 | 0 | 1 | 0 |
| 27 | Y | 14 | 0 | 0 | 0 | 0 |
| 27 | Z | 11 | 0 | 0 | 2 | 0 |
| All | All | 31961 | 0 | 31295 | 945 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 945 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:W:33:ARG:HG2 | 20:W:1060:CHD:H152 | 1.29 | 1.14 |
| 3:C:63:ARG:HE | 26:C:270:CDL:HA22 | 1.19 | 1.07 |
| 3:P:63:ARG:HE | 26:P:1270:CDL:HA22 | 1.30 | 0.97 |
| 23:O:1230:PSC:H142 | 23:O:1230:PSC:H343 | 1.46 | 0.97 |
| 7:T:5:LYS:HB2 | 25:T:263:PEK:H362 | 1.49 | 0.95 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | A | 512/514 (100%) | 488 (95%) | 24 (5%) | 0 | 100 | 100 |
| 1 | N | 512/514 (100%) | 484 (94%) | 27 (5%) | 1 (0%) | 47 | 71 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2 | B | 225/227 (99%) | 210 (93%) | 10 (4%) | 5 (2%) | 6 | 12 |
| 2 | O | 225/227 (99%) | 206 (92%) | 16 (7%) | 3 (1%) | 12 | 24 |
| 3 | C | 257/261 (98%) | 249 (97%) | 7 (3%) | 1 (0%) | 34 | 57 |
| 3 | P | 257/261 (98%) | 249 (97%) | 7 (3%) | 1 (0%) | 34 | 57 |
| 4 | D | 142/147 (97%) | 137 (96%) | 5 (4%) | 0 | 100 | 100 |
| 4 | Q | 142/147 (97%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 5 | E | 103/109 (94%) | 97 (94%) | 6 (6%) | 0 | 100 | 100 |
| 5 | R | 103/109 (94%) | 94 (91%) | 9 (9%) | 0 | 100 | 100 |
| 6 | F | 96/98 (98%) | 85 (88%) | 8 (8%) | 3 (3%) | 4 | 6 |
| 6 | S | 96/98 (98%) | 85 (88%) | 7 (7%) | 4 (4%) | 3 | 3 |
| 7 | G | 81/85 (95%) | 65 (80%) | 9 (11%) | 7 (9%) | 1 | 0 |
| 7 | T | 81/85 (95%) | 65 (80%) | 10 (12%) | 6 (7%) | 1 | 1 |
| 8 | H | 77/85 (91%) | 69 (90%) | 7 (9%) | 1 (1%) | 12 | 24 |
| 8 | U | 77/85 (91%) | 69 (90%) | 7 (9%) | 1 (1%) | 12 | 24 |
| 9 | I | 71/73 (97%) | 66 (93%) | 4 (6%) | 1 (1%) | 11 | 22 |
| 9 | V | 71/73 (97%) | 66 (93%) | 4 (6%) | 1 (1%) | 11 | 22 |
| 10 | J | 56/59 (95%) | 54 (96%) | 1 (2%) | 1 (2%) | 8 | 16 |
| 10 | W | 56/59 (95%) | 52 (93%) | 4 (7%) | 0 | 100 | 100 |
| 11 | K | 47/56 (84%) | 44 (94%) | 3 (6%) | 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%) | 39 (95%) | 2 (5%) | 0 | 100 | 100 |
| 13 | Z | 41/46 (89%) | 38 (93%) | 3 (7%) | 0 | 100 | 100 |
| All | All | 3504/3614 (97%) | 3279 (94%) | 189 (5%) | 36 (1%) | 15 | 32 |

5 of 36 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 94 | HIS |
| 7 | G | 4 | ALA |
| 7 | G | 7 | ASP |
| 7 | G | 39 | SER |
| 6 | S | 94 | HIS |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1 | A | 426/426 (100%) | 413 (97%) | 13 (3%) | 40 | 66 |
| 1 | N | 426/426 (100%) | 411 (96%) | 15 (4%) | 36 | 62 |
| 2 | B | 210/210 (100%) | 196 (93%) | 14 (7%) | 16 | 33 |
| 2 | O | 210/210 (100%) | 200 (95%) | 10 (5%) | 25 | 49 |
| 3 | C | 224/226 (99%) | 213 (95%) | 11 (5%) | 25 | 48 |
| 3 | P | 224/226 (99%) | 216 (96%) | 8 (4%) | 35 | 61 |
| 4 | D | 128/129 (99%) | 125 (98%) | 3 (2%) | 50 | 75 |
| 4 | Q | 128/129 (99%) | 124 (97%) | 4 (3%) | 40 | 66 |
| 5 | E | 92/95 (97%) | 89 (97%) | 3 (3%) | 38 | 64 |
| 5 | R | 92/95 (97%) | 91 (99%) | 1 (1%) | 73 | 88 |
| 6 | F | 81/81 (100%) | 78 (96%) | 3 (4%) | 34 | 60 |
| 6 | S | 81/81 (100%) | 75 (93%) | 6 (7%) | 13 | 28 |
| 7 | G | 67/68 (98%) | 60 (90%) | 7 (10%) | 7 | 13 |
| 7 | T | 67/68 (98%) | 62 (92%) | 5 (8%) | 13 | 27 |
| 8 | H | 71/75 (95%) | 67 (94%) | 4 (6%) | 21 | 42 |
| 8 | U | 71/75 (95%) | 70 (99%) | 1 (1%) | 67 | 85 |
| 9 | I | 57/57 (100%) | 55 (96%) | 2 (4%) | 36 | 62 |
| 9 | V | 57/57 (100%) | 56 (98%) | 1 (2%) | 59 | 80 |
| 10 | J | 49/50 (98%) | 49 (100%) | 0 | 100 | 100 |
| 10 | W | 49/50 (98%) | 48 (98%) | 1 (2%) | 55 | 78 |
| 11 | K | 39/46 (85%) | 38 (97%) | 1 (3%) | 46 | 72 |
| 11 | X | 39/46 (85%) | 36 (92%) | 3 (8%) | 13 | 25 |
| 12 | L | 39/40 (98%) | 37 (95%) | 2 (5%) | 24 | 46 |
| 12 | Y | 39/40 (98%) | 38 (97%) | 1 (3%) | 46 | 72 |
| 13 | M | 37/38 (97%) | 30 (81%) | 7 (19%) | 1 | 2 |
| 13 | Z | 37/38 (97%) | 33 (89%) | 4 (11%) | 6 | 12 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All | 3040/3082 (99%) | 2910 (96%) | 130 (4%) | 29 54 |

5 of 130 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 8 | GLN |
| 1 | N | 178 | GLN |
| 9 | V | 8 | GLN |
| 11 | K | 54 | ARG |
| 13 | M | 34 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 94 | ASN |
| 11 | K | 41 | ASN |
| 5 | R | 78 | HIS |
| 7 | G | 34 | ASN |
| 8 | H | 31 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 |
| 9 | SAC | I | 1 | 9 | 7,8,9 | 2.53 | 2 (28%) | 8,9,11 | 2.92 | 3 (37%) |
| 1 | FME | A | 1 | 1 | 8,9,10 | 0.76 | 0 | 7,9,11 | 1.25 | 1 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 7 | TPO | T | 11 | 7 | 8,10,11 | 1.39 | 1 (12%) | 10,14,16 | 1.03 | 0 |
| 2 | FME | B | 1 | 2 | 8,9,10 | 1.01 | 0 | 7,9,11 | 1.66 | 2 (28%) |
| 1 | FME | N | 1 | 1 | 8,9,10 | 0.87 | 0 | 7,9,11 | 1.26 | 1 (14%) |
| 2 | FME | O | 1 | 2 | 8,9,10 | 0.72 | 0 | 7,9,11 | 2.28 | 2 (28%) |
| 7 | TPO | G | 11 | 7 | 8,10,11 | 1.68 | 2 (25%) | 10,14,16 | 0.95 | 0 |
| 9 | SAC | V | 1 | 9 | 7,8,9 | 2.86 | 2 (28%) | 8,9,11 | 3.22 | 5 (62%) |

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 9 | SAC | I | 1 | 9 | - | 3/7/8/10 | - |
| 1 | FME | A | 1 | 1 | - | 3/7/9/11 | - |
| 7 | TPO | T | 11 | 7 | - | 5/9/11/13 | - |
| 2 | FME | B | 1 | 2 | - | 2/7/9/11 | - |
| 1 | FME | N | 1 | 1 | - | 3/7/9/11 | - |
| 2 | FME | O | 1 | 2 | - | 2/7/9/11 | - |
| 7 | TPO | G | 11 | 7 | - | 4/9/11/13 | - |
| 9 | SAC | V | 1 | 9 | - | 3/7/8/10 | - |

The worst 5 of 7 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 9 | V | 1 | SAC | OAC-C1A | 5.46 | 1.35 | 1.23 |
| 9 | I | 1 | SAC | OAC-C1A | 5.21 | 1.35 | 1.23 |
| 9 | V | 1 | SAC | CA-N | 4.51 | 1.52 | 1.46 |
| 9 | I | 1 | SAC | CA-N | 3.85 | 1.51 | 1.46 |
| 7 | G | 11 | TPO | CB-CA | 3.04 | 1.60 | 1.53 |

The worst 5 of 14 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9 | V | 1 | SAC | CA-N-C1A | -7.18 | 109.91 | 123.15 |
| 9 | I | 1 | SAC | CA-N-C1A | -6.40 | 111.34 | 123.15 |
| 2 | O | 1 | FME | C-CA-N | 4.73 | 118.27 | 109.73 |
| 2 | O | 1 | FME | CA-N-CN | -3.50 | 117.45 | 122.82 |
| 9 | I | 1 | SAC | CB-CA-N | 3.19 | 117.71 | 110.55 |

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 9 | I | 1 | SAC | C2A-C1A-N-CA |
| 9 | I | 1 | SAC | OAC-C1A-N-CA |
| 9 | I | 1 | SAC | CB-CA-N-C1A |
| 1 | A | 1 | FME | O1-CN-N-CA |
| 1 | A | 1 | FME | N-CA-CB-CG |

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 1 | FME | 2 | 0 |
| 1 | N | 1 | FME | 1 | 0 |
| 7 | G | 11 | TPO | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 12 are monoatomic - leaving 44 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 | $\# Z > 2$ |
| 19 | PGV | C | 267 | - | 50,50,50 | 1.04 | 3 (6%) | 53,56,56 | 1.05 | 5 (9%) |
| 26 | CDL | C | 270 | - | 99,99,99 | 1.07 | 8 (8%) | 105,111,111 | 1.09 | 9 (8%) |
| 20 | CHD | J | 60 | - | 29,32,32 | 1.95 | 10 (34%) | 48,51,51 | 4.08 | 28 (58%) |
| 22 | TGL | B | 521 | - | 62,62,62 | 1.08 | 3 (4%) | 65,65,65 | 1.46 | 8 (12%) |
| 19 | PGV | N | 1524 | - | 50,50,50 | 1.23 | 5 (10%) | 53,56,56 | 0.89 | 1 (1%) |
| 19 | PGV | C | 266 | - | 50,50,50 | 1.17 | 5 (10%) | 53,56,56 | 0.95 | 2 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 20 | CHD | W | 1060 | - | 29,32,32 | 2.09 | 8 (27%) | 48,51,51 | 4.13 | 28 (58%) |
| 24 | DMU | Z | 1526 | - | 34,34,34 | 3.25 | 8 (23%) | 45,45,45 | 3.95 | 20 (44%) |
| 19 | PGV | A | 524 | - | 50,50,50 | 1.26 | 5 (10%) | 53,56,56 | 0.82 | 1 (1%) |
| 18 | HEA | A | 516 | 1 | 44,67,67 | 1.51 | 7 (15%) | 37,103,103 | 1.37 | 6 (16%) |
| 25 | PEK | C | 264 | - | 52,52,52 | 1.45 | 6 (11%) | 55,57,57 | 1.24 | 3 (5%) |
| 23 | PSC | B | 230 | - | 51,51,51 | 1.40 | 6 (11%) | 57,59,59 | 1.00 | 2 (3%) |
| 23 | PSC | O | 1230 | - | 51,51,51 | 1.52 | 7 (13%) | 57,59,59 | 0.98 | 1 (1%) |
| 19 | PGV | P | 1268 | - | 50,50,50 | 1.43 | 5 (10%) | 53,56,56 | 0.87 | 1 (1%) |
| 22 | TGL | O | 1521 | - | 62,62,62 | 1.11 | 5 (8%) | 65,65,65 | 1.46 | 8 (12%) |
| 21 | CUA | O | 228 | 2 | 0,1,1 | 0.00 | - | - | | |
| 20 | CHD | N | 1604 | - | 29,32,32 | 0.96 | 2 (6%) | 48,51,51 | 2.47 | 17 (35%) |
| 25 | PEK | P | 1264 | - | 52,52,52 | 1.65 | 8 (15%) | 55,57,57 | 1.37 | 7 (12%) |
| 24 | DMU | P | 1272 | - | 34,34,34 | 2.70 | 15 (44%) | 45,45,45 | 3.95 | 17 (37%) |
| 25 | PEK | C | 265 | - | 52,52,52 | 1.75 | 11 (21%) | 55,57,57 | 1.21 | 7 (12%) |
| 18 | HEA | N | 516 | 1 | 44,67,67 | 1.42 | 7 (15%) | 37,103,103 | 1.42 | 6 (16%) |
| 19 | PGV | P | 1266 | - | 50,50,50 | 1.36 | 6 (12%) | 53,56,56 | 1.04 | 4 (7%) |
| 19 | PGV | C | 268 | - | 50,50,50 | 1.45 | 7 (14%) | 53,56,56 | 0.90 | 0 |
| 25 | PEK | P | 1265 | - | 52,52,52 | 1.78 | 11 (21%) | 55,57,57 | 1.19 | 7 (12%) |
| 20 | CHD | A | 525 | - | 29,32,32 | 0.95 | 1 (3%) | 48,51,51 | 2.55 | 18 (37%) |
| 22 | TGL | L | 522 | - | 62,62,62 | 1.35 | 5 (8%) | 65,65,65 | 1.68 | 12 (18%) |
| 18 | HEA | A | 515 | 1 | 44,67,67 | 2.25 | 7 (15%) | 37,103,103 | 1.81 | 12 (32%) |
| 18 | HEA | N | 515 | 1 | 44,67,67 | 2.00 | 5 (11%) | 37,103,103 | 1.94 | 14 (37%) |
| 24 | DMU | M | 526 | - | 34,34,34 | 3.36 | 9 (26%) | 45,45,45 | 3.94 | 21 (46%) |
| 20 | CHD | P | 1525 | - | 29,32,32 | 0.98 | 2 (6%) | 48,51,51 | 2.67 | 23 (47%) |
| 22 | TGL | N | 1523 | - | 62,62,62 | 0.96 | 3 (4%) | 65,65,65 | 1.25 | 7 (10%) |
| 26 | CDL | T | 1269 | - | 99,99,99 | 1.25 | 11 (11%) | 105,111,111 | 0.99 | 7 (6%) |
| 25 | PEK | G | 1263 | - | 52,52,52 | 2.08 | 11 (21%) | 55,57,57 | 1.29 | 4 (7%) |
| 26 | CDL | G | 269 | - | 99,99,99 | 1.25 | 9 (9%) | 105,111,111 | 0.98 | 8 (7%) |
| 25 | PEK | T | 263 | - | 52,52,52 | 2.12 | 12 (23%) | 55,57,57 | 1.32 | 4 (7%) |
| 26 | CDL | P | 1270 | - | 99,99,99 | 1.21 | 9 (9%) | 105,111,111 | 1.09 | 5 (4%) |
| 24 | DMU | C | 272 | - | 34,34,34 | 2.64 | 16 (47%) | 45,45,45 | 3.99 | 18 (40%) |
| 20 | CHD | C | 271 | - | 29,32,32 | 1.38 | 3 (10%) | 48,51,51 | 3.72 | 24 (50%) |
| 22 | TGL | N | 1522 | - | 62,62,62 | 1.49 | 6 (9%) | 65,65,65 | 1.64 | 10 (15%) |
| 19 | PGV | P | 1267 | - | 50,50,50 | 0.96 | 3 (6%) | 53,56,56 | 1.02 | 4 (7%) |
| 20 | CHD | B | 1086 | - | 29,32,32 | 0.82 | 0 | 48,51,51 | 2.52 | 20 (41%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | TGL | D | 523 | - | 62,62,62 | 1.01 | 3 (4%) | 65,65,65 | 1.30 | 9 (13%) |
| 21 | CUA | B | 228 | 2 | 0,1,1 | 0.00 | - | - | | |
| 20 | CHD | W | 1271 | - | 29,32,32 | 1.31 | 4 (13%) | 48,51,51 | 3.63 | 25 (52%) |

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 |
|-----|------|-------|------|------|-----------|----------------|---------|
| 19 | PGV | C | 267 | - | - | 17/55/55/55 | - |
| 26 | CDL | C | 270 | - | - | 68/110/110/110 | - |
| 20 | CHD | J | 60 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |
| 22 | TGL | B | 521 | - | - | 14/65/65/65 | - |
| 19 | PGV | N | 1524 | - | - | 35/55/55/55 | - |
| 19 | PGV | C | 266 | - | - | 16/55/55/55 | - |
| 20 | CHD | W | 1060 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |
| 24 | DMU | Z | 1526 | - | 5/5/10/10 | 8/19/59/59 | 0/2/2/2 |
| 18 | HEA | N | 515 | 1 | 3/3/7/16 | 2/24/76/76 | - |
| 18 | HEA | A | 516 | 1 | 3/3/7/16 | 1/24/76/76 | - |
| 25 | PEK | C | 264 | - | - | 23/56/56/56 | - |
| 23 | PSC | B | 230 | - | - | 37/55/55/55 | - |
| 23 | PSC | O | 1230 | - | - | 37/55/55/55 | - |
| 19 | PGV | P | 1268 | - | - | 35/55/55/55 | - |
| 22 | TGL | O | 1521 | - | - | 14/65/65/65 | - |
| 20 | CHD | N | 1604 | - | - | 1/7/74/74 | 0/4/4/4 |
| 25 | PEK | P | 1264 | - | - | 24/56/56/56 | - |
| 24 | DMU | P | 1272 | - | 6/6/10/10 | 11/19/59/59 | 0/2/2/2 |
| 25 | PEK | C | 265 | - | - | 21/56/56/56 | - |
| 18 | HEA | N | 516 | 1 | 3/3/7/16 | 1/24/76/76 | - |
| 19 | PGV | P | 1266 | - | - | 15/55/55/55 | - |
| 19 | PGV | C | 268 | - | - | 34/55/55/55 | - |
| 25 | PEK | P | 1265 | - | - | 20/56/56/56 | - |
| 20 | CHD | A | 525 | - | - | 0/7/74/74 | 0/4/4/4 |
| 22 | TGL | L | 522 | - | - | 19/65/65/65 | - |
| 18 | HEA | A | 515 | 1 | 3/3/7/16 | 2/24/76/76 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|----------------|---------|
| 19 | PGV | A | 524 | - | - | 35/55/55/55 | - |
| 24 | DMU | M | 526 | - | 5/5/10/10 | 8/19/59/59 | 0/2/2/2 |
| 20 | CHD | P | 1525 | - | - | 0/7/74/74 | 0/4/4/4 |
| 22 | TGL | N | 1523 | - | - | 15/65/65/65 | - |
| 26 | CDL | T | 1269 | - | - | 62/110/110/110 | - |
| 25 | PEK | G | 1263 | - | - | 29/56/56/56 | - |
| 26 | CDL | G | 269 | - | - | 62/110/110/110 | - |
| 25 | PEK | T | 263 | - | - | 29/56/56/56 | - |
| 26 | CDL | P | 1270 | - | - | 69/110/110/110 | - |
| 24 | DMU | C | 272 | - | 6/6/10/10 | 10/19/59/59 | 0/2/2/2 |
| 20 | CHD | C | 271 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |
| 22 | TGL | N | 1522 | - | - | 19/65/65/65 | - |
| 19 | PGV | P | 1267 | - | - | 17/55/55/55 | - |
| 20 | CHD | B | 1086 | - | - | 0/7/74/74 | 0/4/4/4 |
| 22 | TGL | D | 523 | - | - | 15/65/65/65 | - |
| 20 | CHD | W | 1271 | - | 5/5/12/12 | 6/7/74/74 | 0/4/4/4 |

The worst 5 of 277 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 18 | A | 515 | HEA | C3B-C11 | -12.57 | 1.43 | 1.52 |
| 18 | N | 515 | HEA | C3B-C11 | -10.46 | 1.44 | 1.52 |
| 24 | M | 526 | DMU | O7-C3 | -8.58 | 1.21 | 1.43 |
| 24 | M | 526 | DMU | O16-C6 | -7.92 | 1.26 | 1.40 |
| 24 | Z | 1526 | DMU | O7-C3 | -7.78 | 1.23 | 1.43 |

The worst 5 of 433 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 24 | P | 1272 | DMU | O16-C6-C1 | 11.86 | 126.82 | 108.30 |
| 24 | C | 272 | DMU | O16-C6-C1 | 10.72 | 125.04 | 108.30 |
| 24 | M | 526 | DMU | C1-C2-C3 | 9.86 | 132.19 | 109.68 |
| 24 | Z | 1526 | DMU | C1-C2-C3 | 9.75 | 131.95 | 109.68 |
| 20 | C | 271 | CHD | C10-C9-C8 | 9.68 | 122.21 | 111.82 |

5 of 54 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 20 | J | 60 | CHD | C12 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 20 | J | 60 | CHD | C8 |
| 20 | J | 60 | CHD | C9 |
| 20 | J | 60 | CHD | C14 |
| 20 | J | 60 | CHD | C17 |

5 of 849 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 25 | P | 1265 | PEK | C03-O11-P-O13 |
| 25 | P | 1265 | PEK | C04-O12-P-O13 |
| 25 | P | 1265 | PEK | C04-O12-P-O14 |
| 26 | C | 270 | CDL | CA2-C1-CB2-OB2 |
| 26 | C | 270 | CDL | CA2-OA2-PA1-OA3 |

There are no ring outliers.

41 monomers are involved in 312 short contacts:

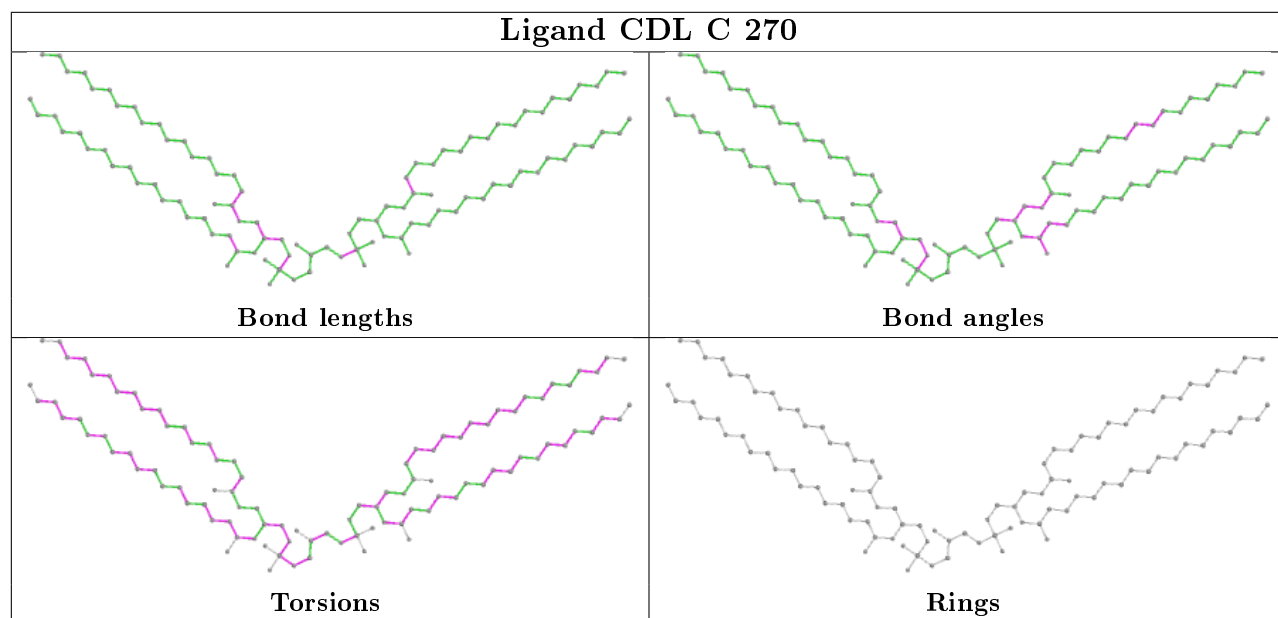
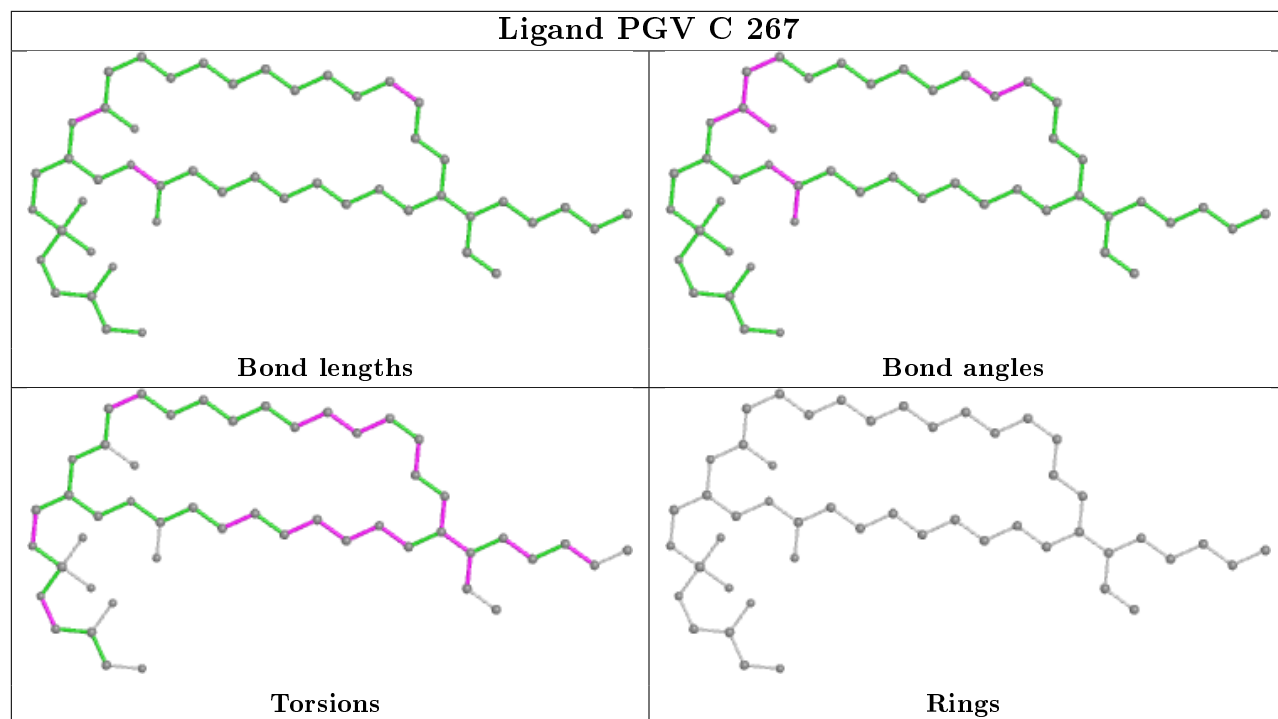
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 19 | C | 267 | PGV | 7 | 0 |
| 26 | C | 270 | CDL | 19 | 0 |
| 20 | J | 60 | CHD | 5 | 0 |
| 22 | B | 521 | TGL | 6 | 0 |
| 19 | N | 1524 | PGV | 10 | 0 |
| 19 | C | 266 | PGV | 3 | 0 |
| 20 | W | 1060 | CHD | 3 | 0 |
| 19 | A | 524 | PGV | 7 | 0 |
| 18 | A | 516 | HEA | 5 | 0 |
| 25 | C | 264 | PEK | 6 | 0 |
| 23 | B | 230 | PSC | 19 | 0 |
| 23 | O | 1230 | PSC | 18 | 0 |
| 19 | P | 1268 | PGV | 1 | 0 |
| 22 | O | 1521 | TGL | 8 | 0 |
| 20 | N | 1604 | CHD | 2 | 0 |
| 25 | P | 1264 | PEK | 9 | 0 |
| 24 | P | 1272 | DMU | 4 | 0 |
| 25 | C | 265 | PEK | 11 | 0 |
| 18 | N | 516 | HEA | 8 | 0 |
| 19 | P | 1266 | PGV | 2 | 0 |
| 19 | C | 268 | PGV | 2 | 0 |
| 25 | P | 1265 | PEK | 9 | 0 |
| 20 | A | 525 | CHD | 1 | 0 |
| 22 | L | 522 | TGL | 27 | 0 |

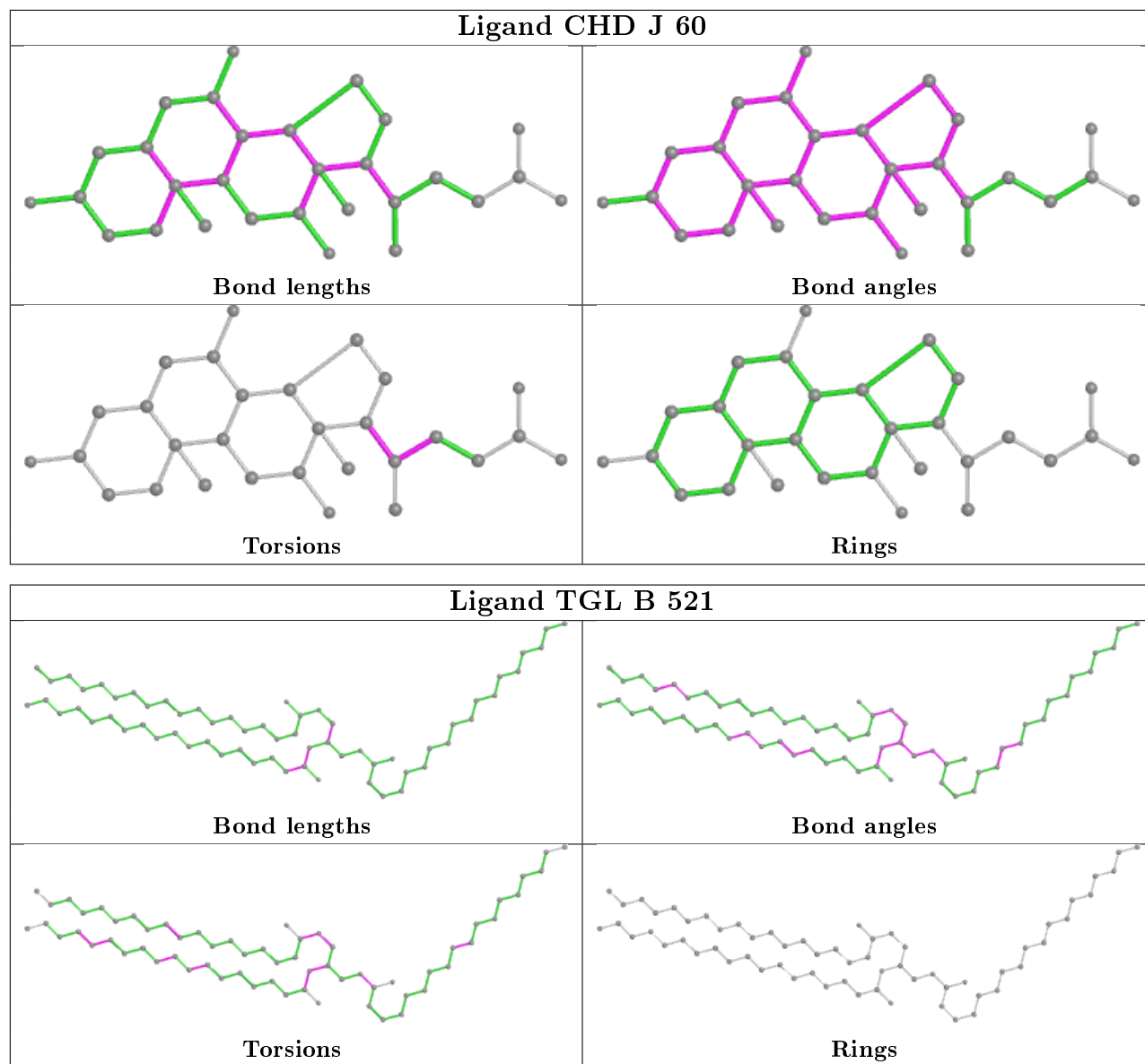
Continued on next page...

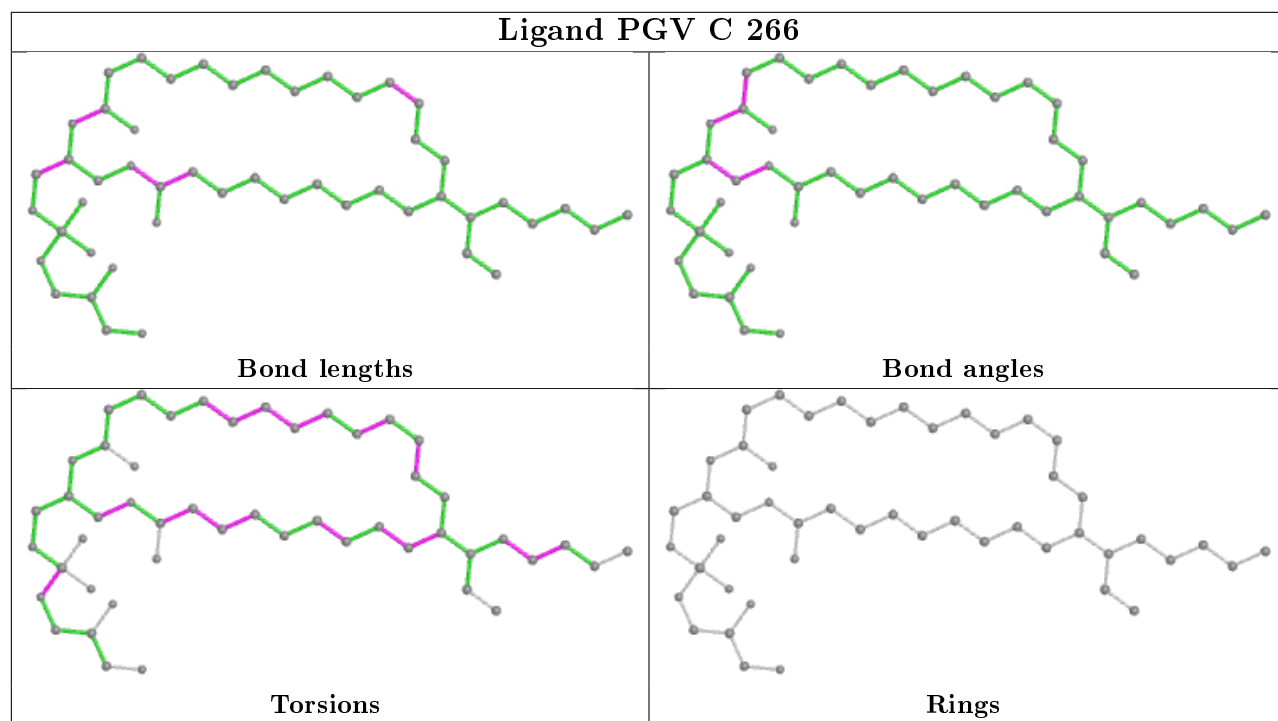
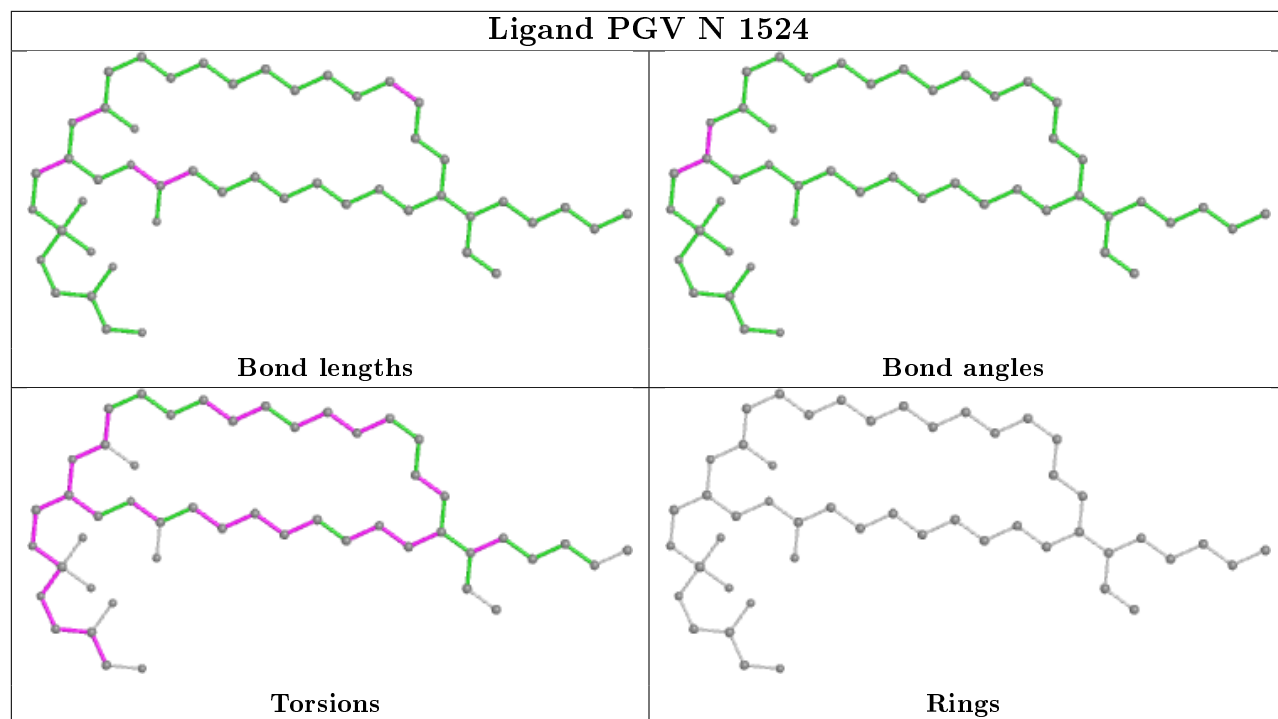
Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18 | A | 515 | HEA | 4 | 0 |
| 18 | N | 515 | HEA | 4 | 0 |
| 24 | M | 526 | DMU | 1 | 0 |
| 20 | P | 1525 | CHD | 2 | 0 |
| 22 | N | 1523 | TGL | 7 | 0 |
| 26 | T | 1269 | CDL | 23 | 0 |
| 25 | G | 1263 | PEK | 9 | 0 |
| 26 | G | 269 | CDL | 22 | 0 |
| 25 | T | 263 | PEK | 14 | 0 |
| 26 | P | 1270 | CDL | 13 | 0 |
| 24 | C | 272 | DMU | 3 | 0 |
| 20 | C | 271 | CHD | 2 | 0 |
| 22 | N | 1522 | TGL | 15 | 0 |
| 19 | P | 1267 | PGV | 8 | 0 |
| 20 | B | 1086 | CHD | 1 | 0 |
| 22 | D | 523 | TGL | 5 | 0 |
| 20 | W | 1271 | CHD | 2 | 0 |

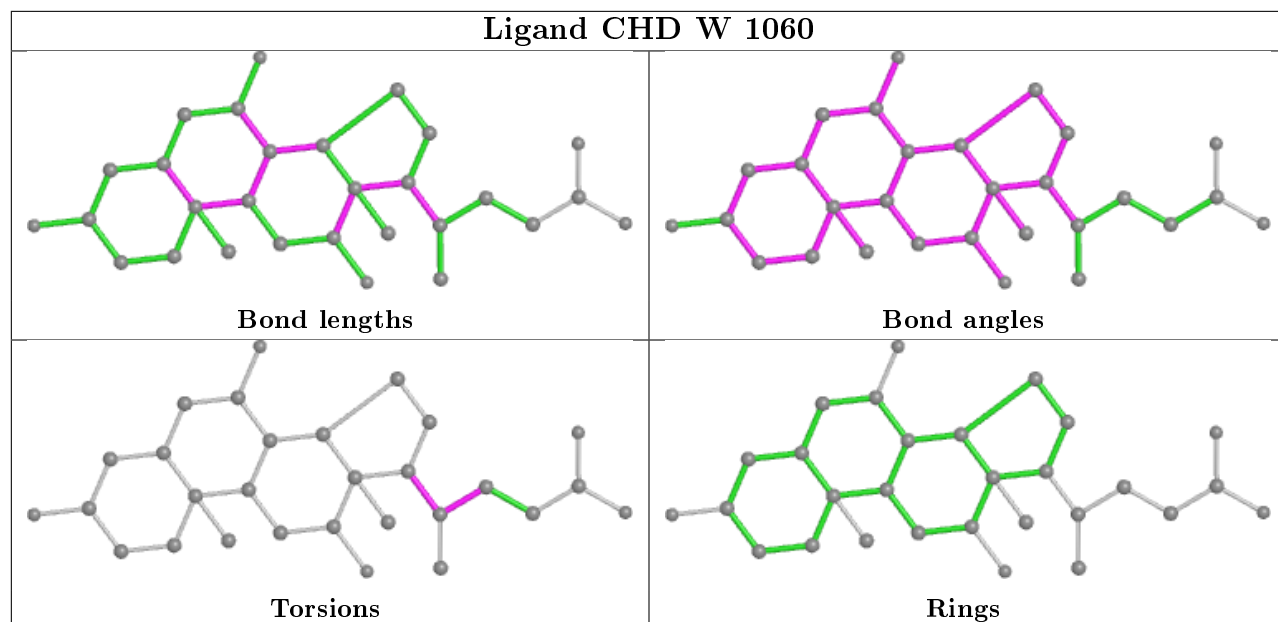
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



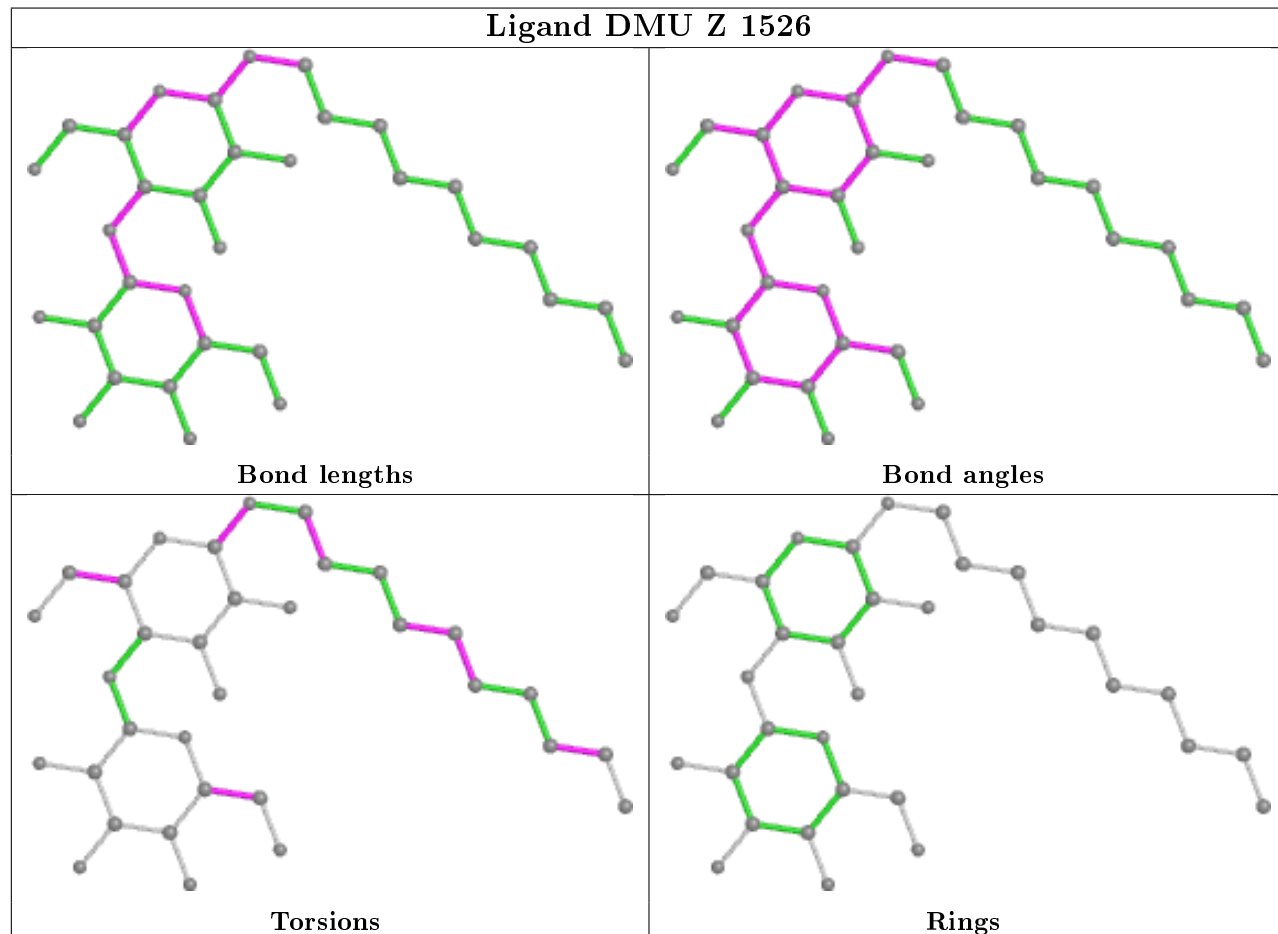


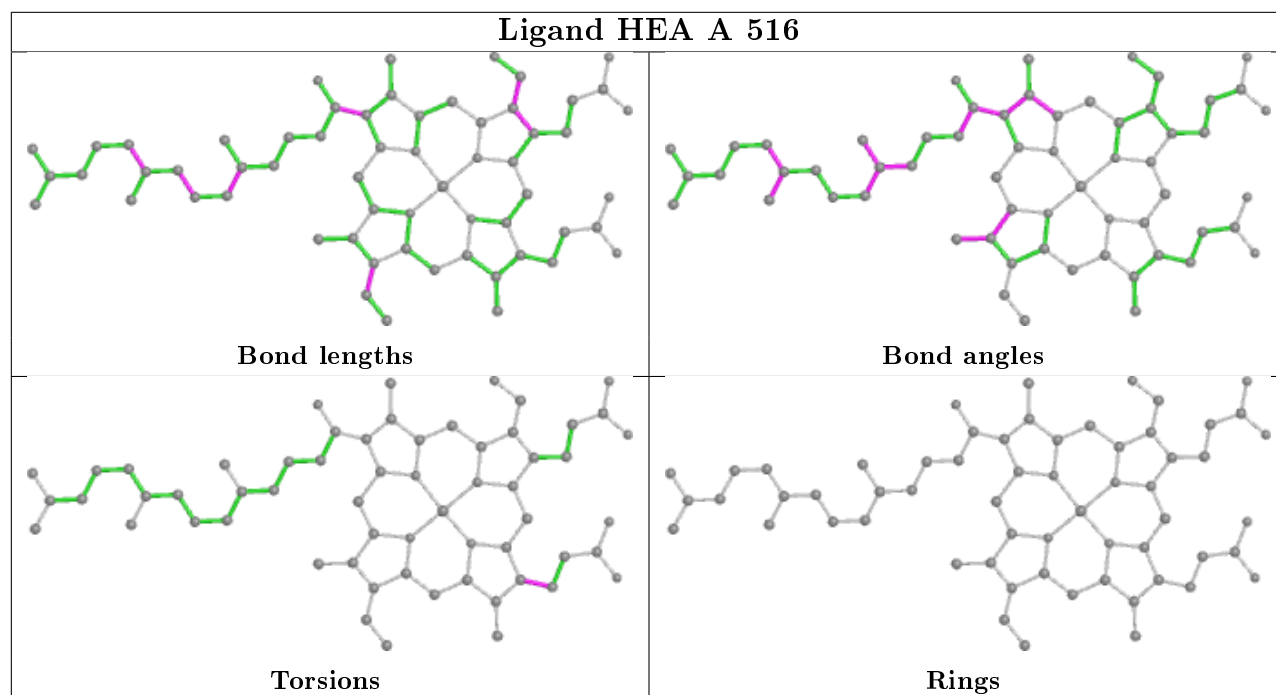
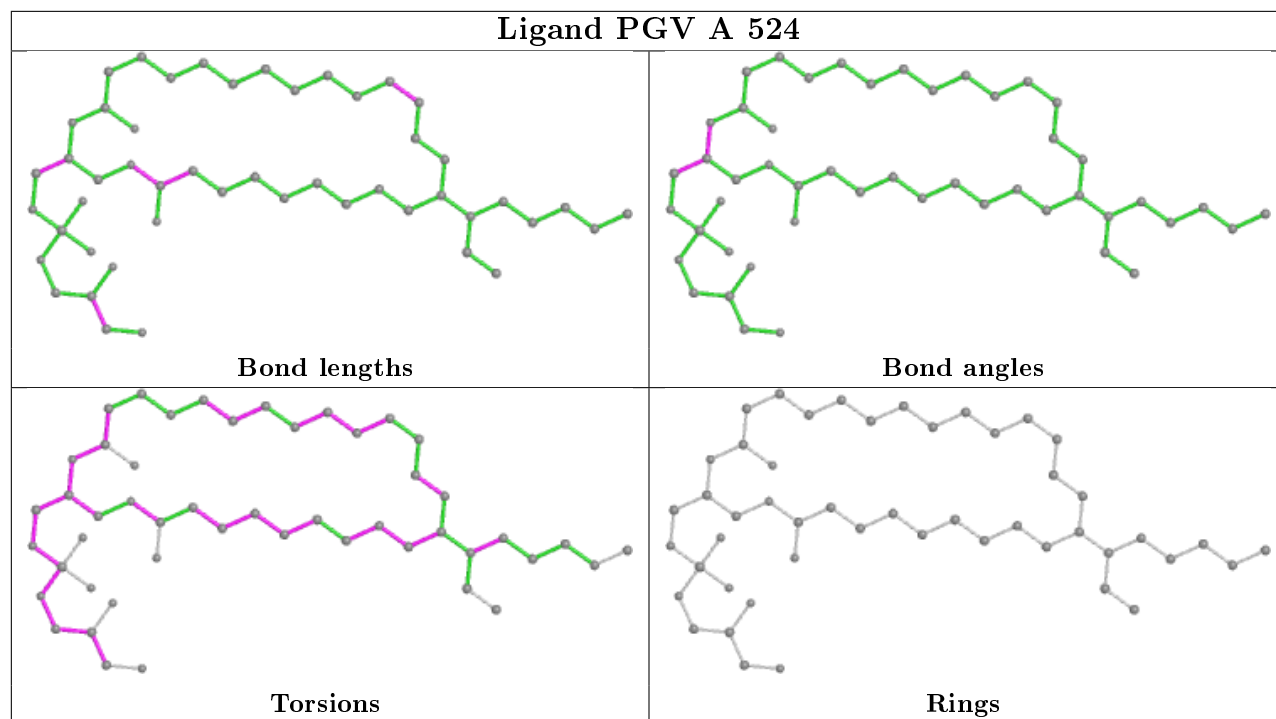


Ligand CHD W 1060

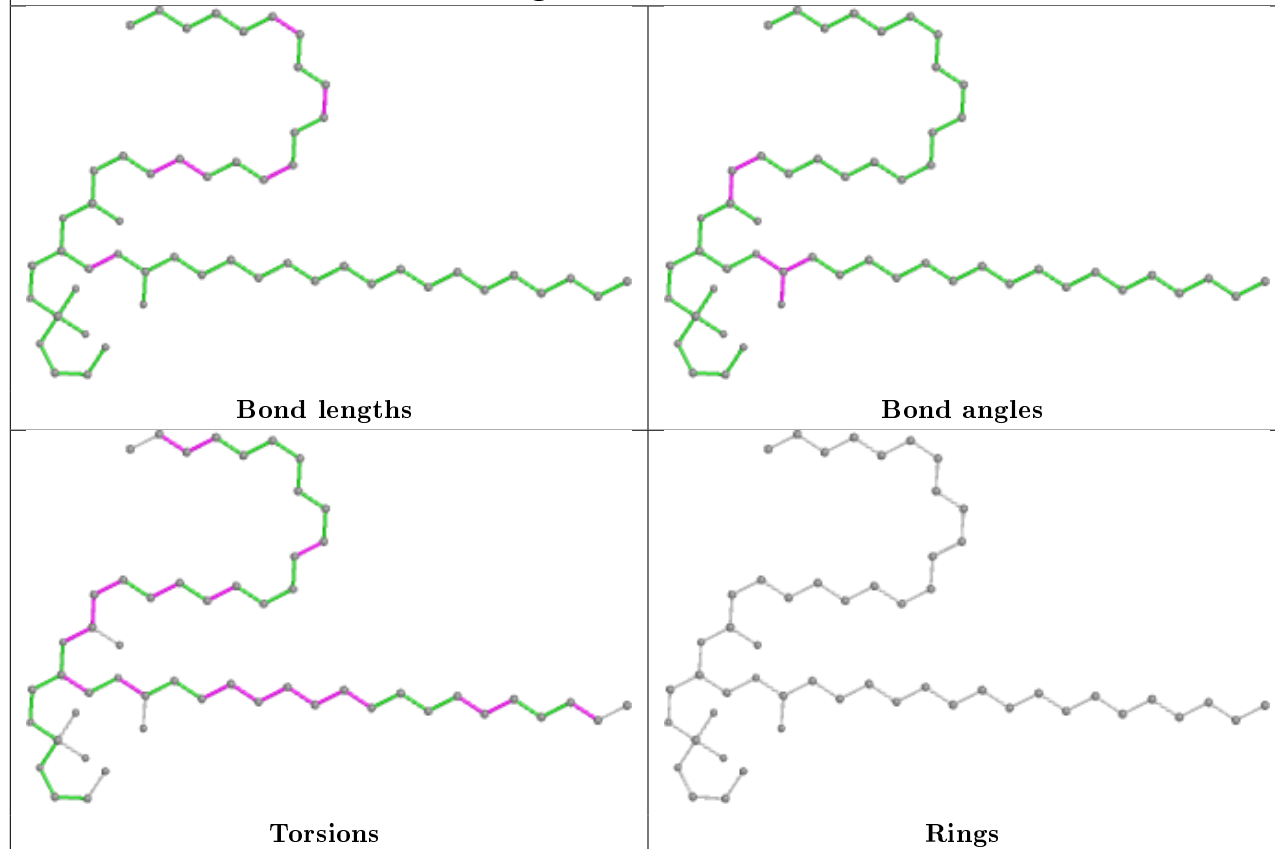


Ligand DMU Z 1526

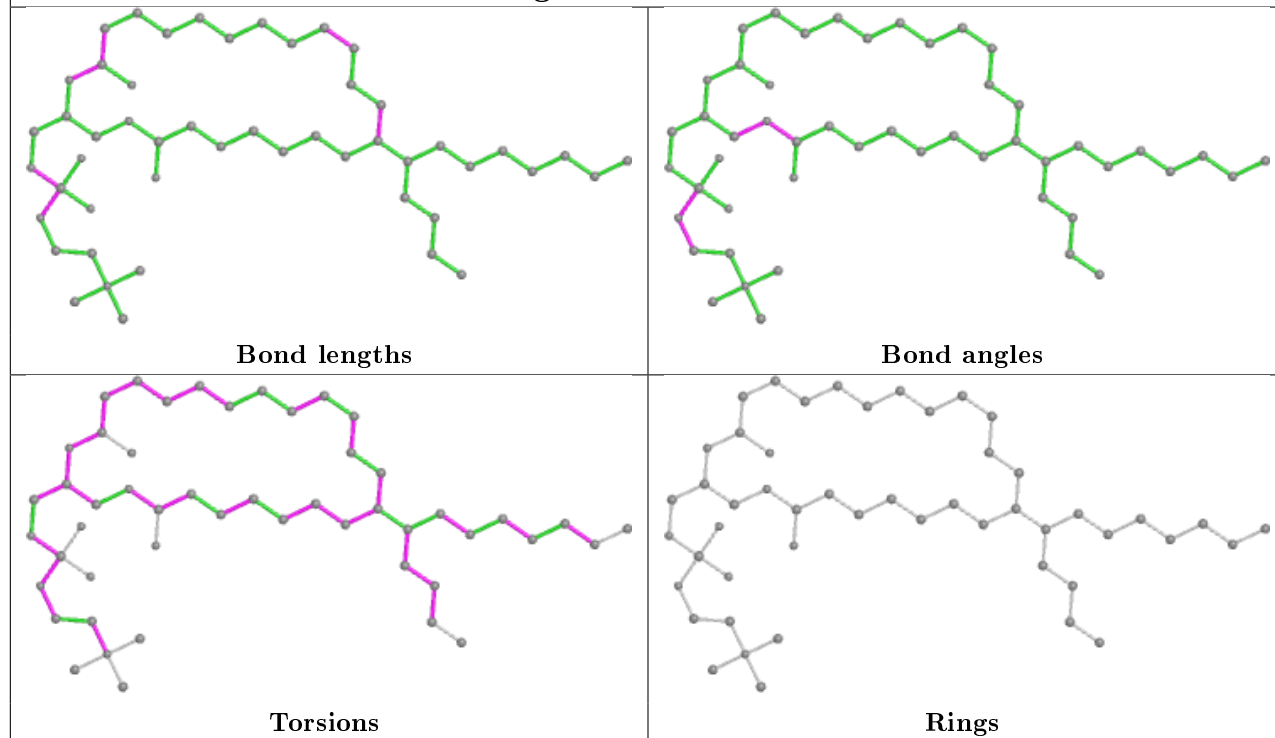


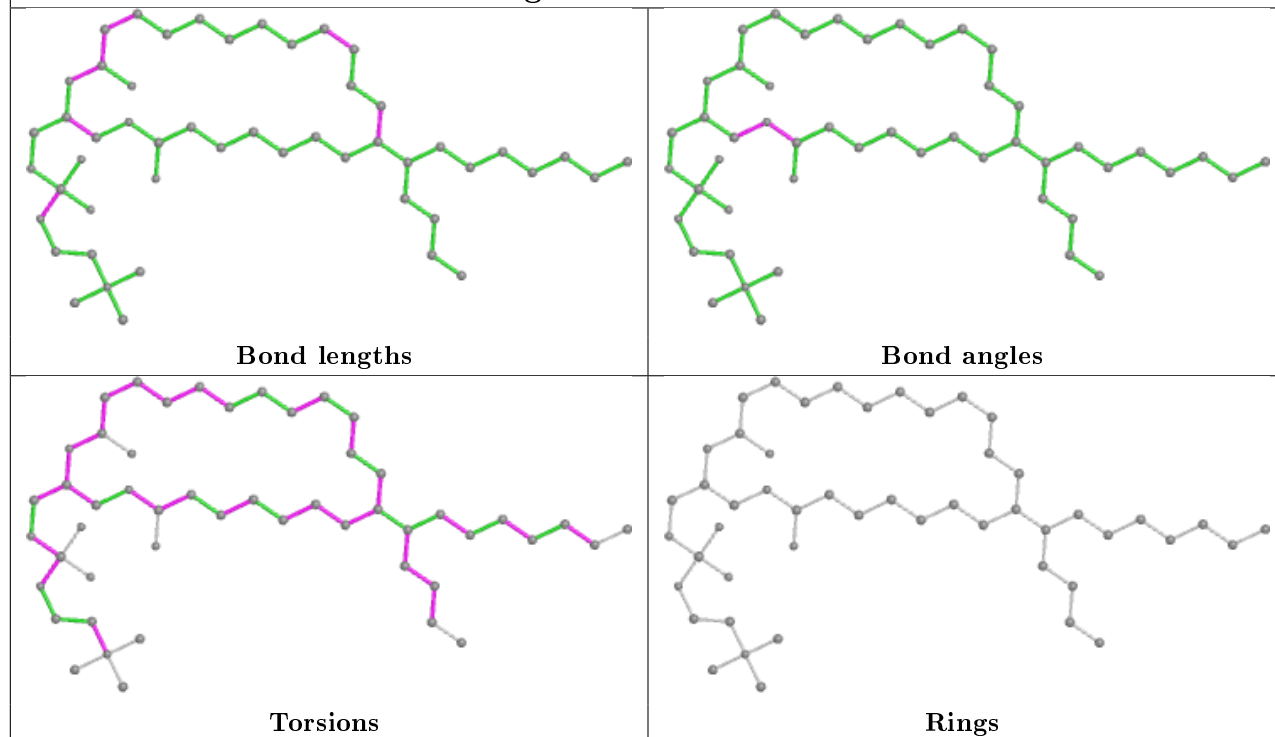
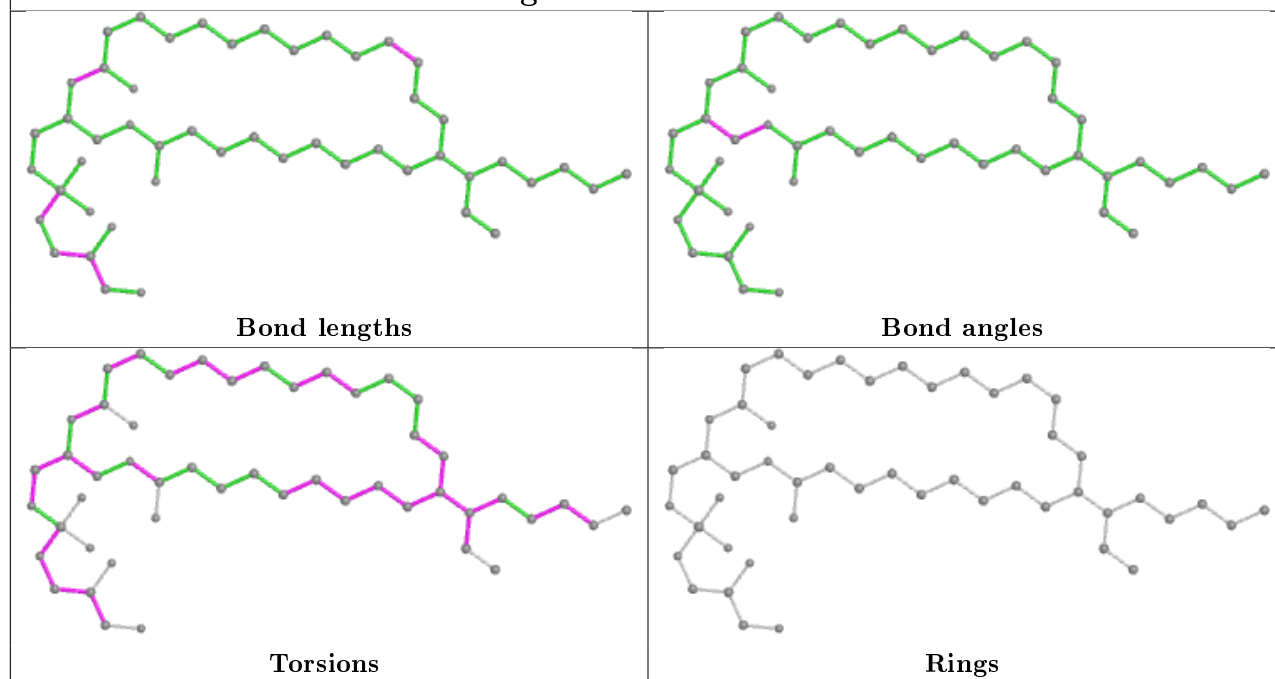


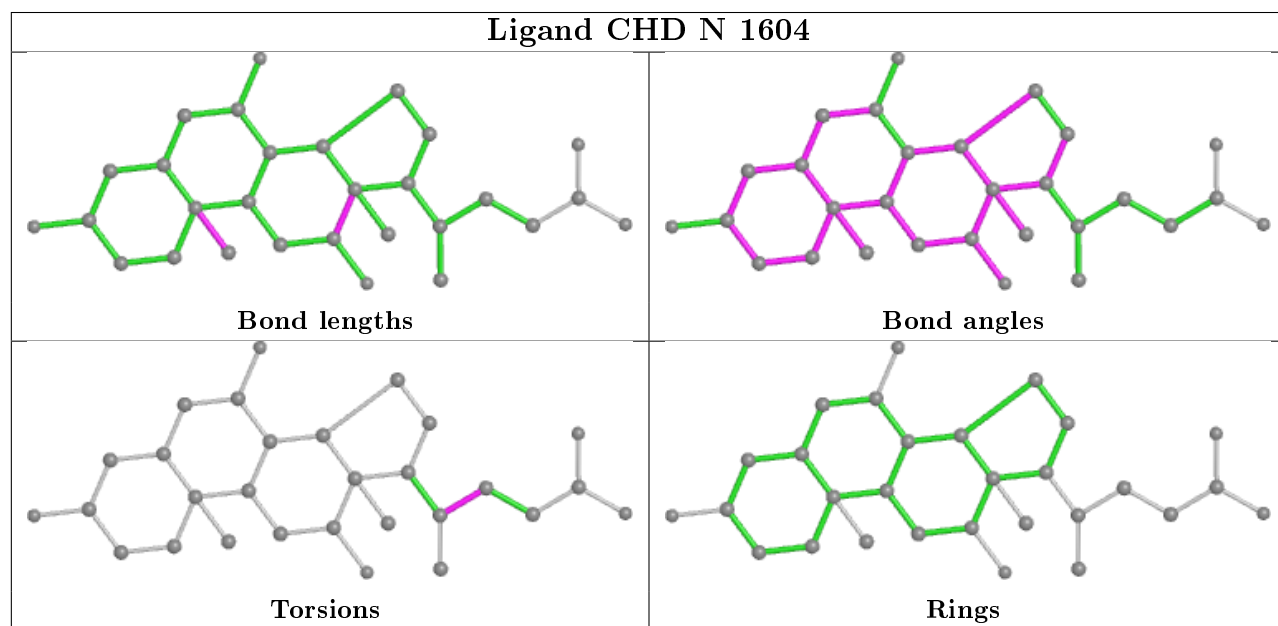
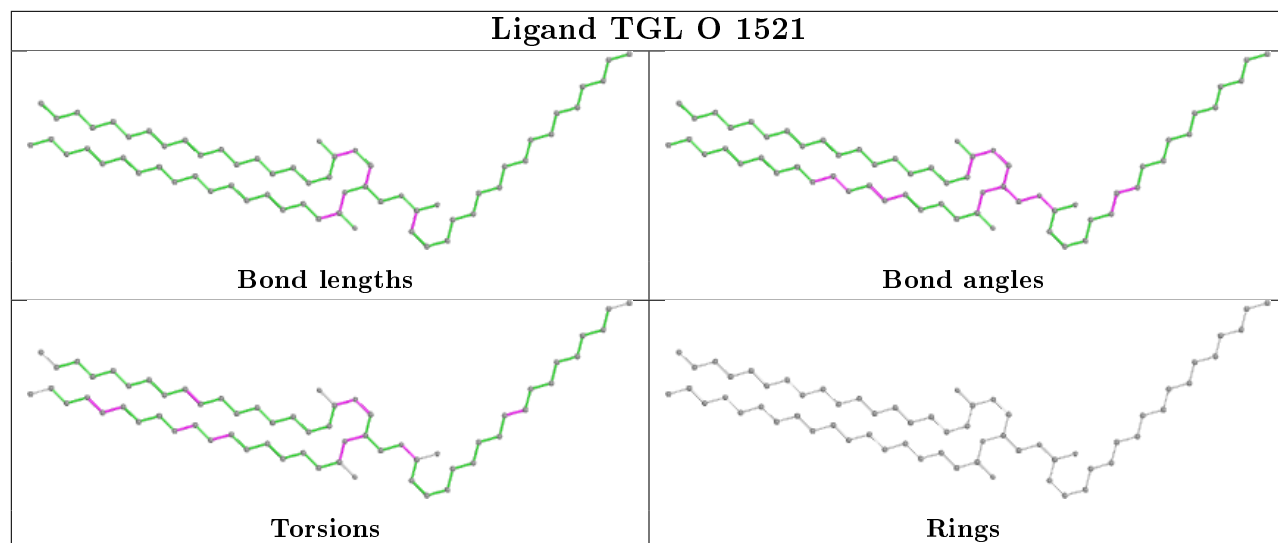
Ligand PEK C 264

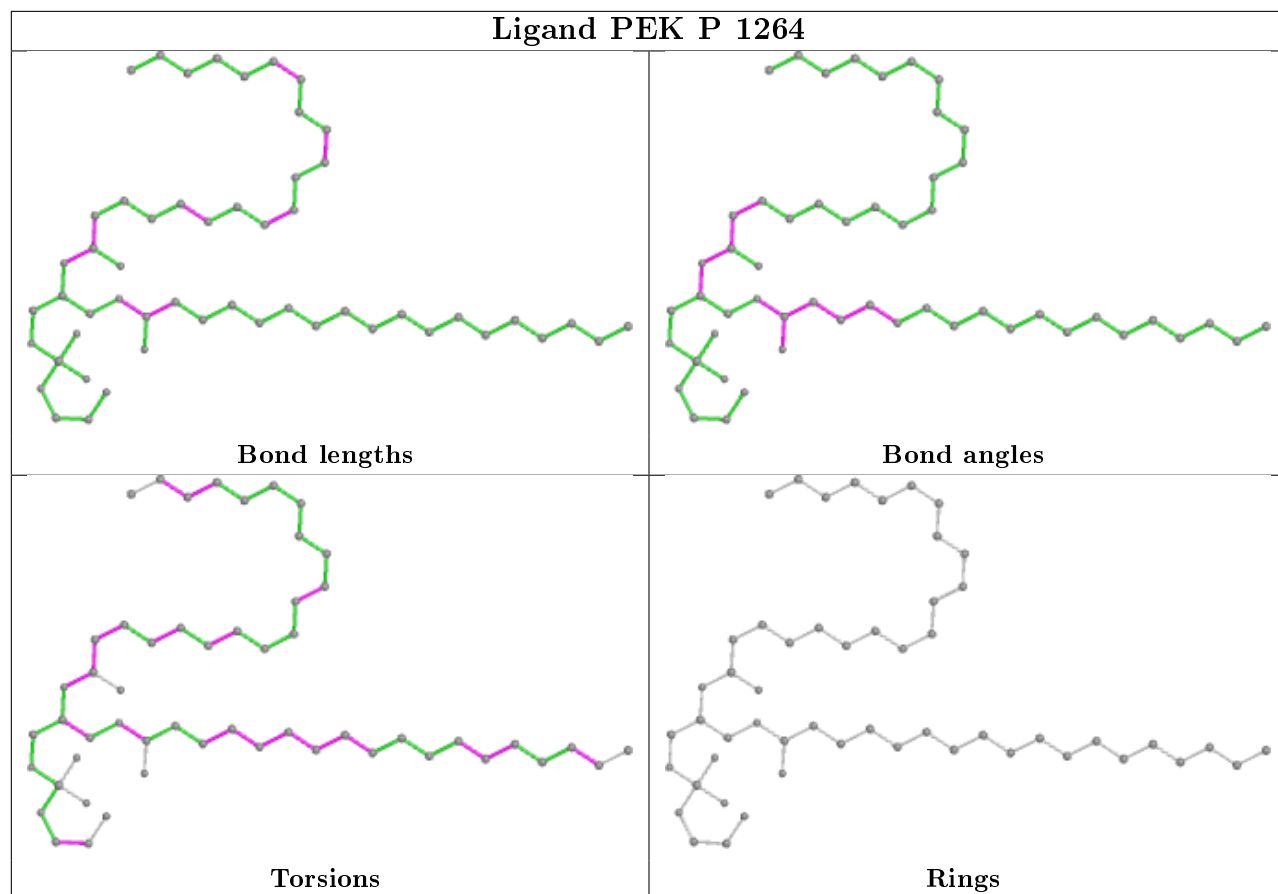


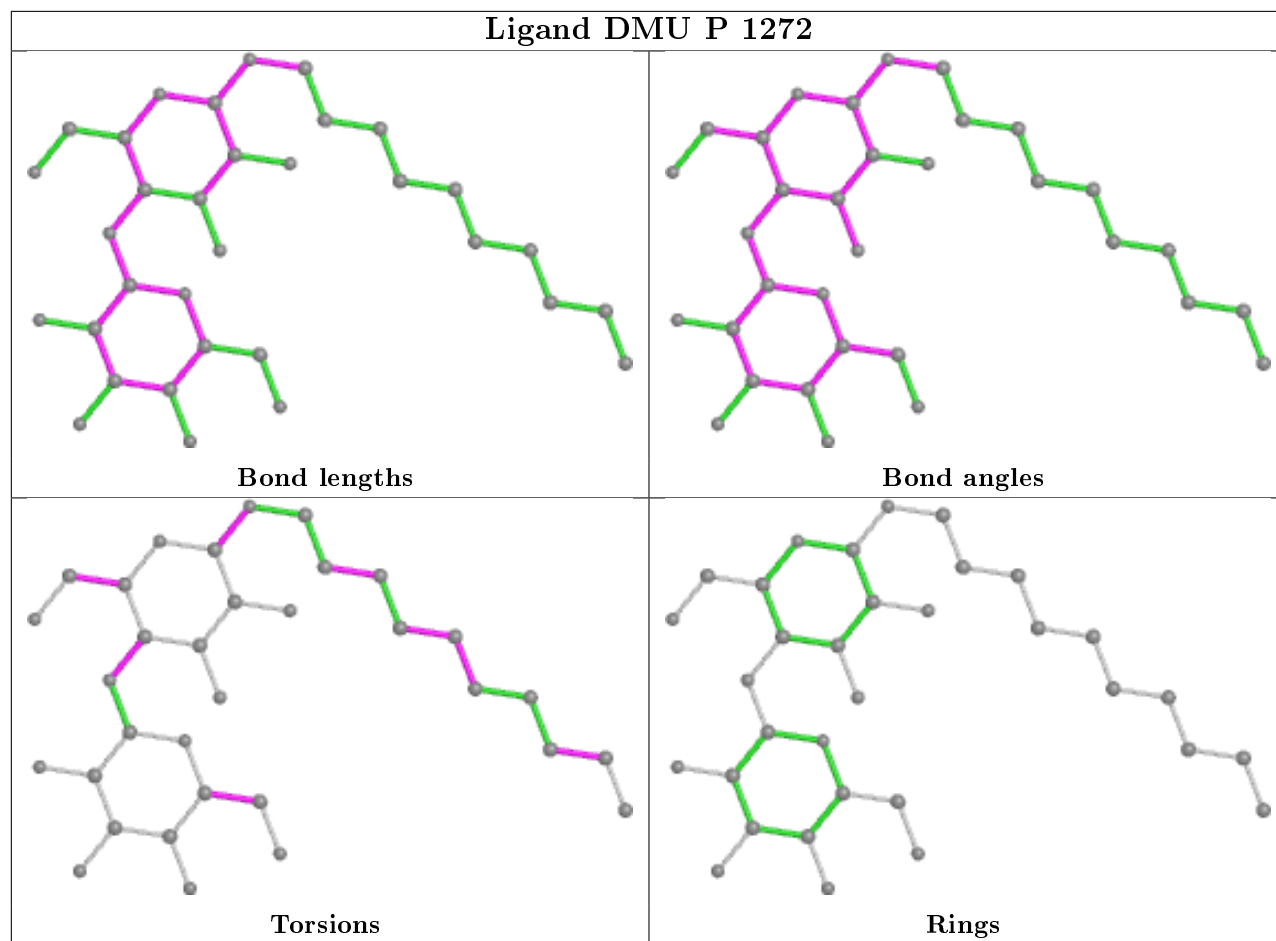
Ligand PSC B 230

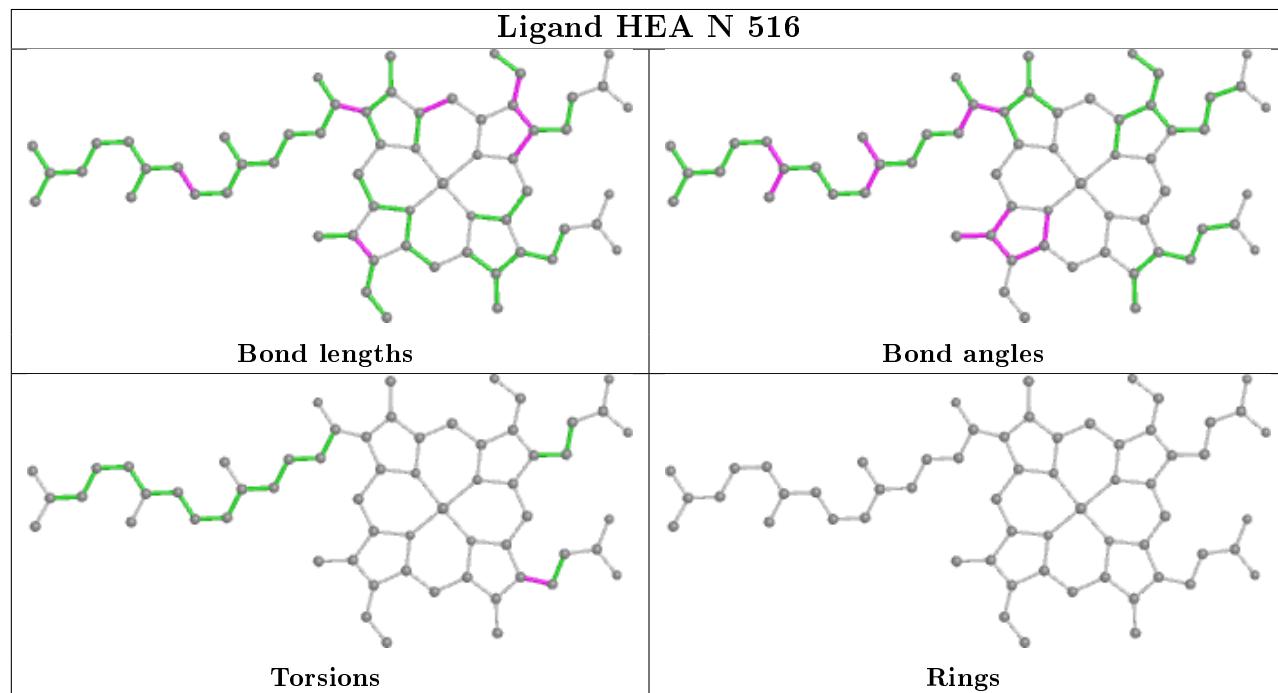
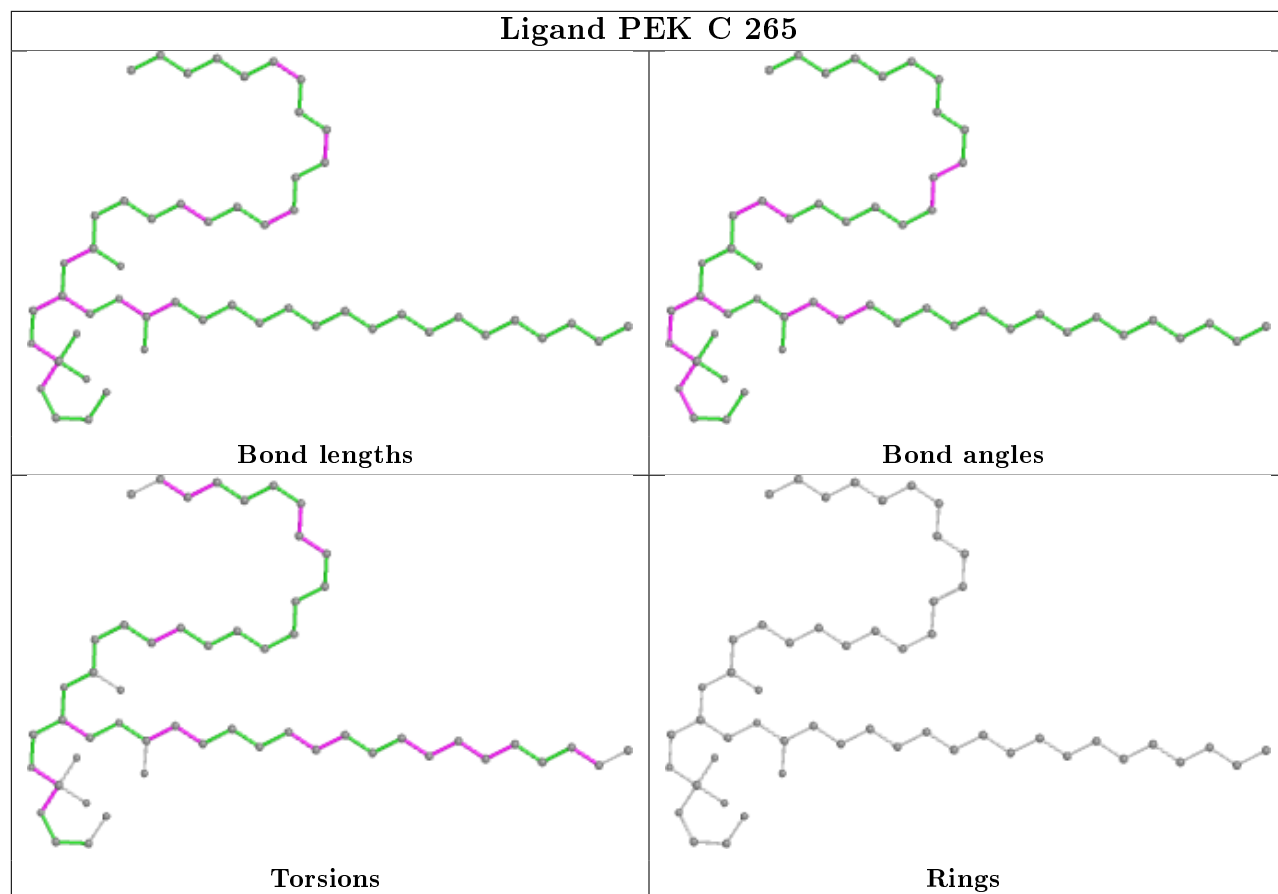


Ligand PSC O 1230**Ligand PGV P 1268**

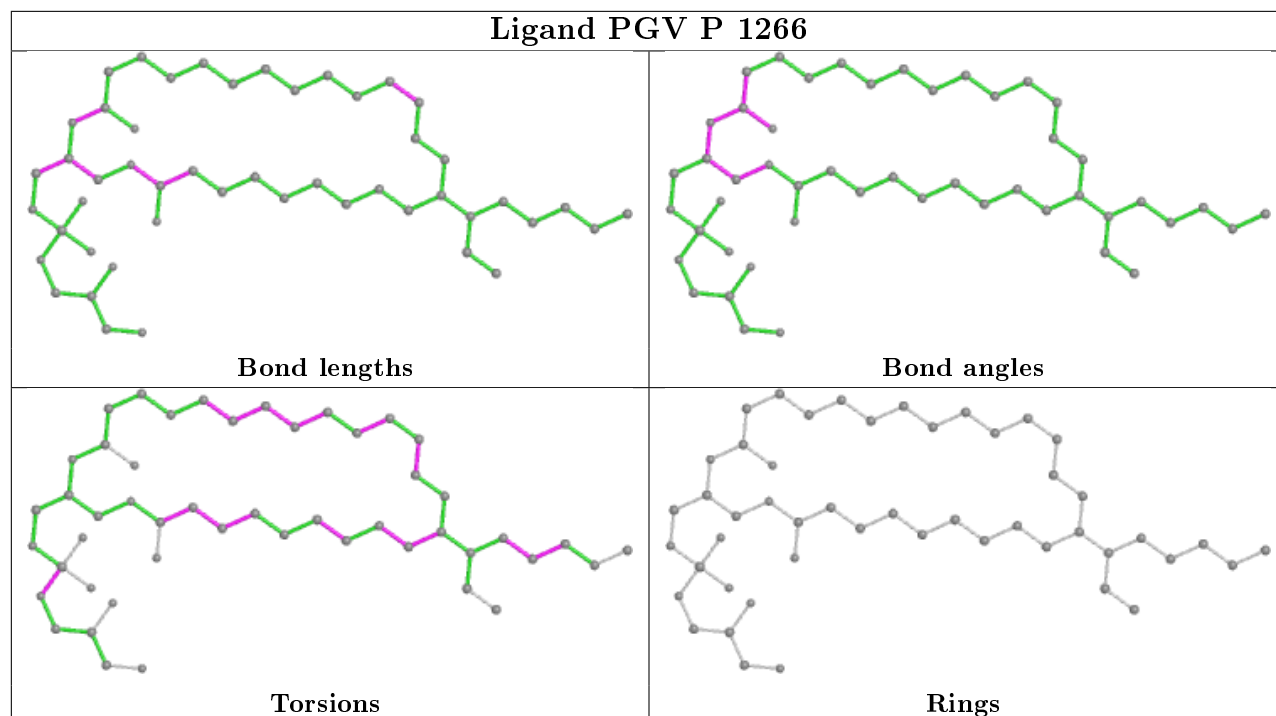




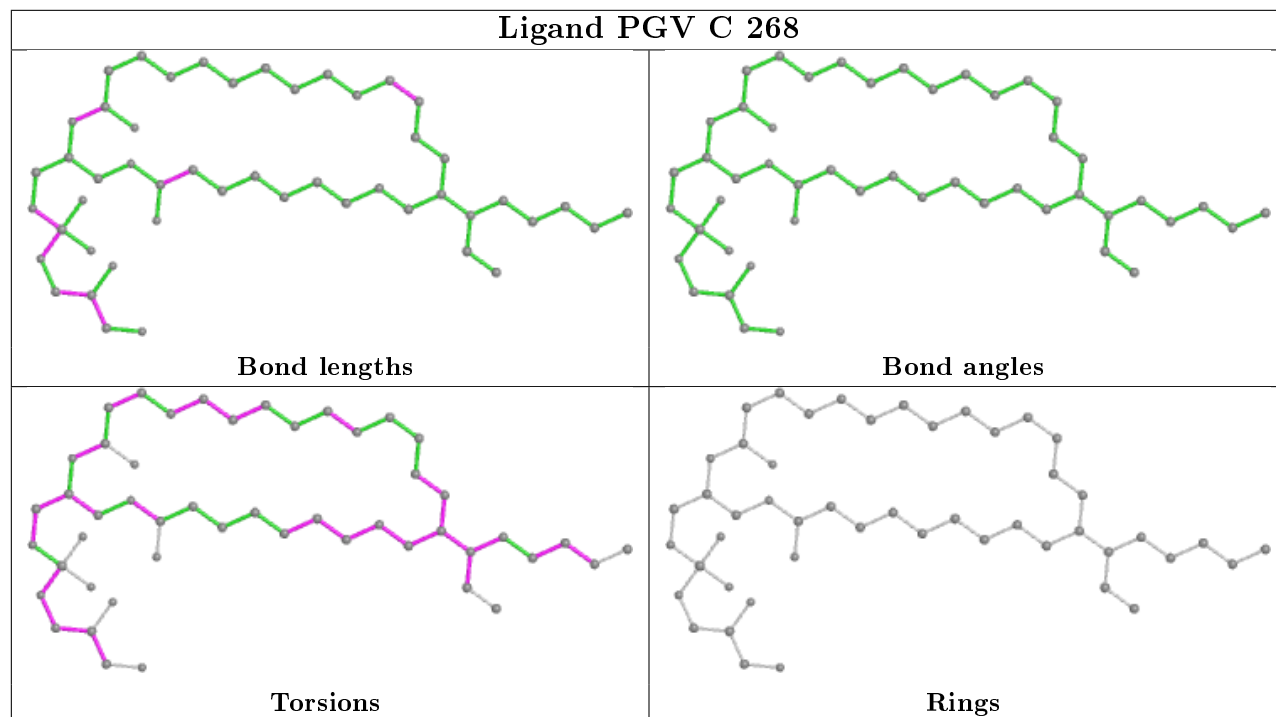


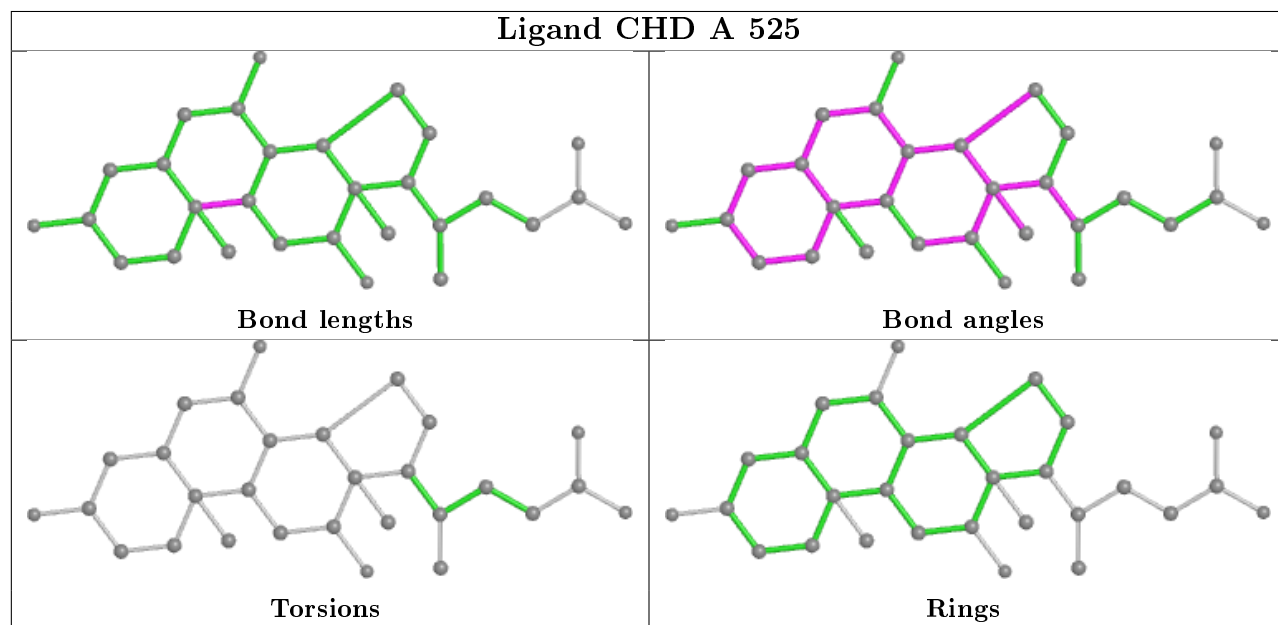
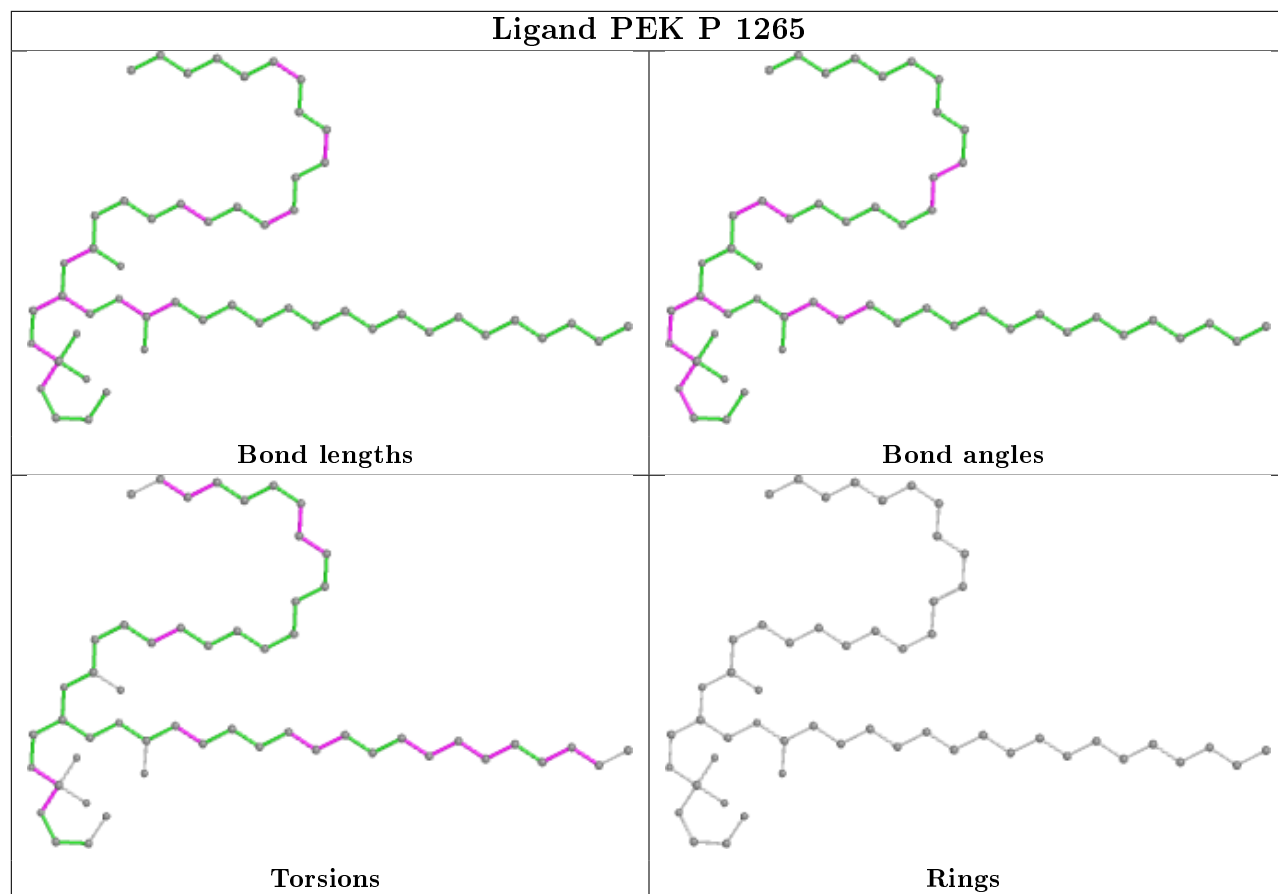


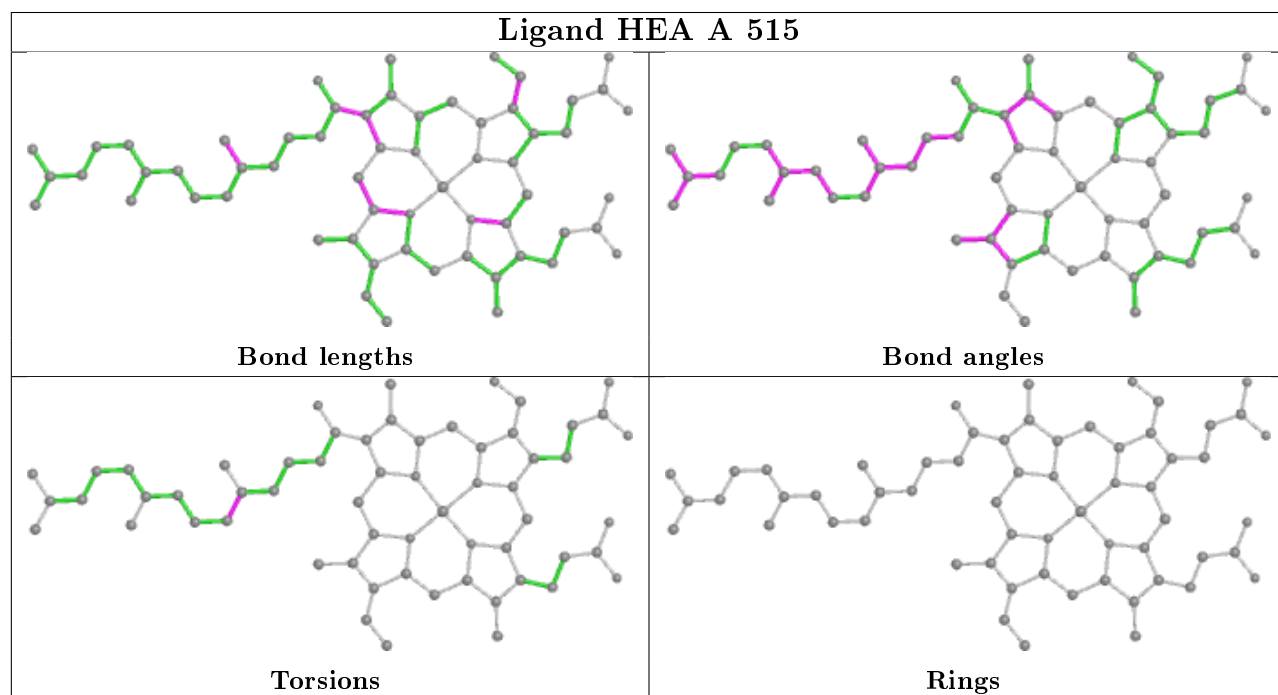
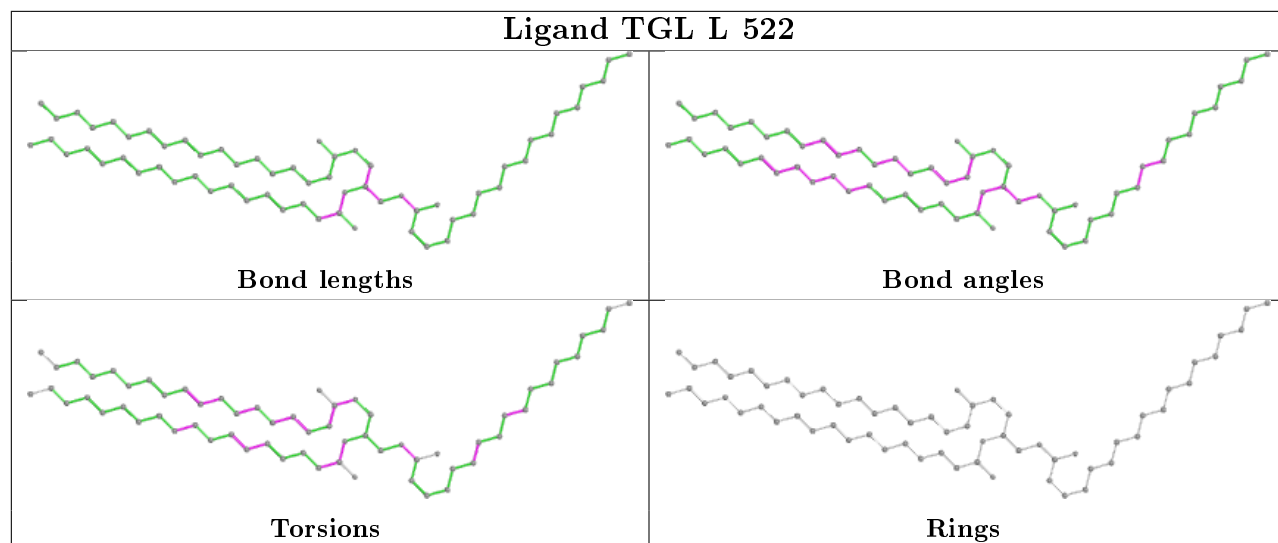
Ligand PGV P 1266

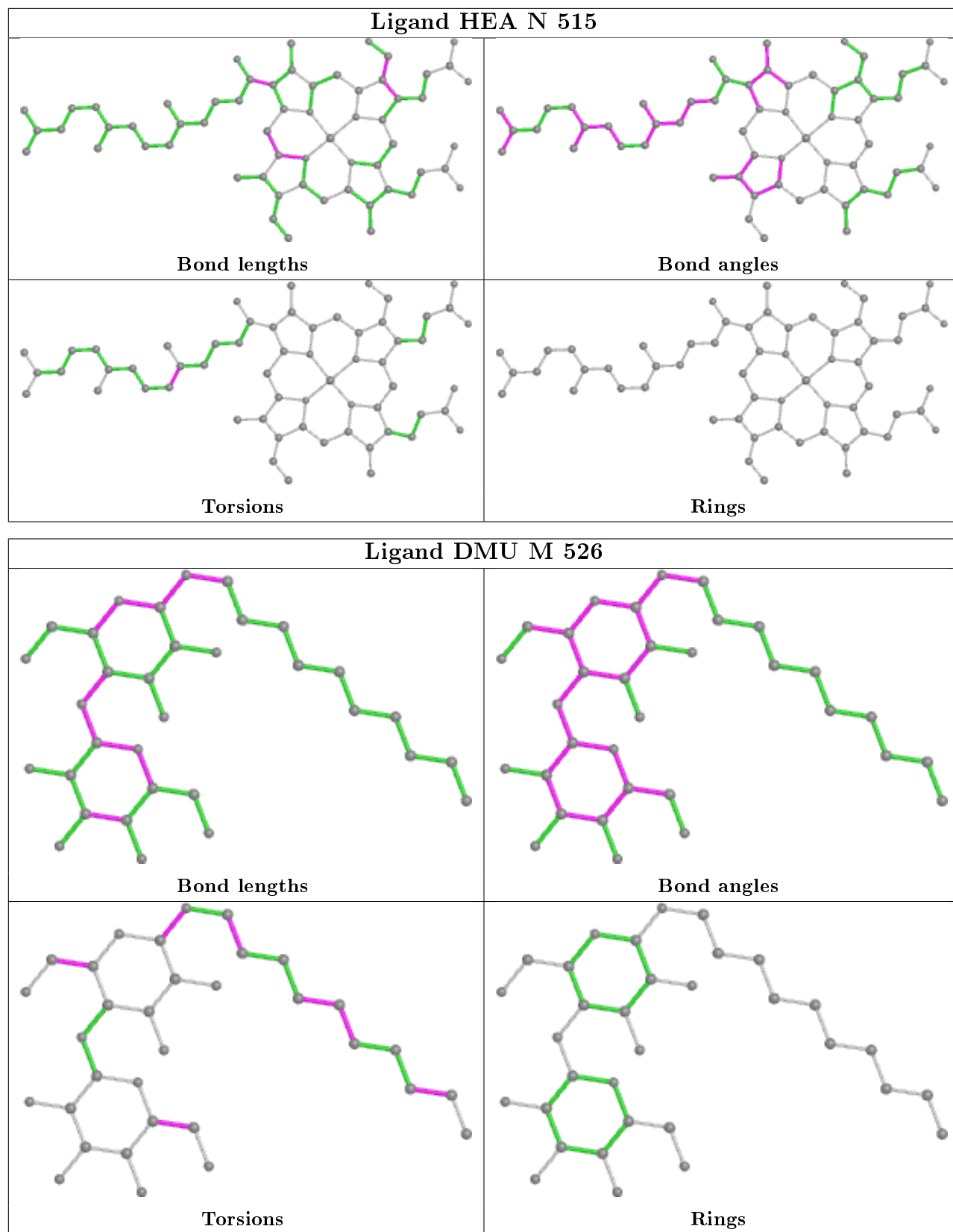


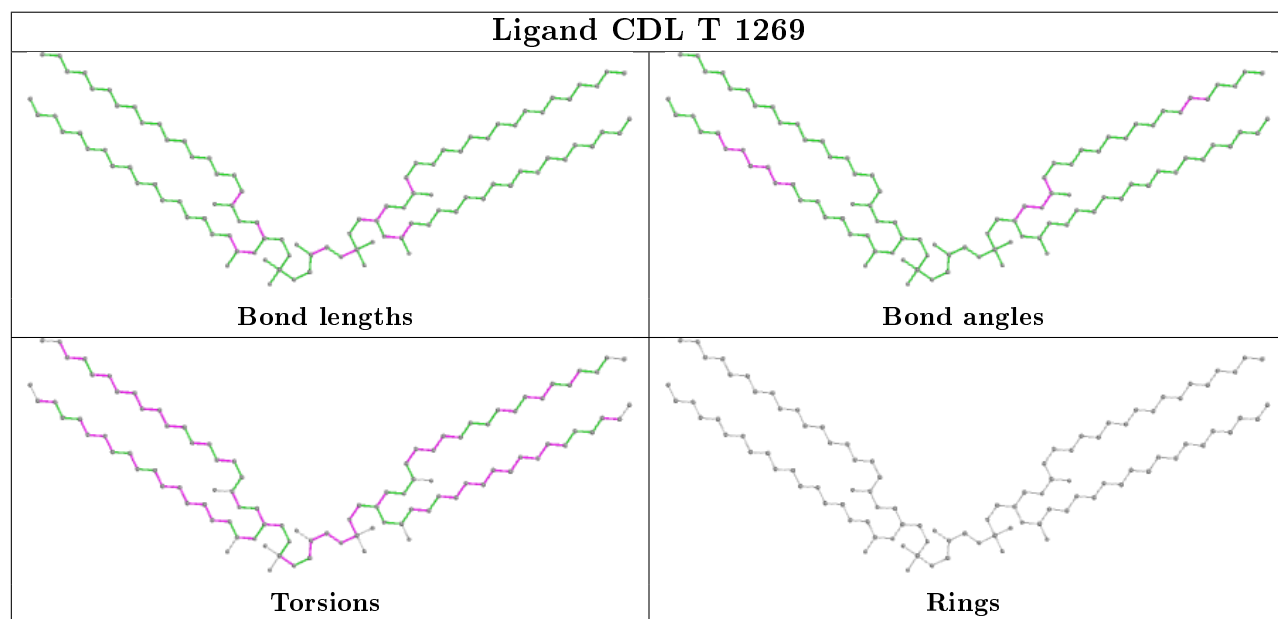
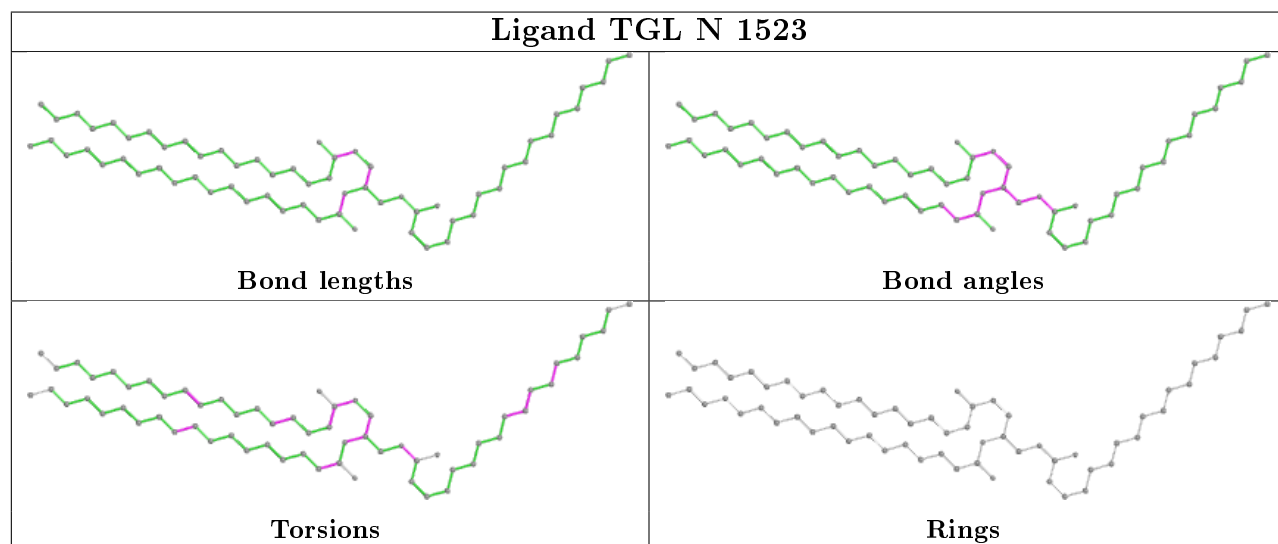
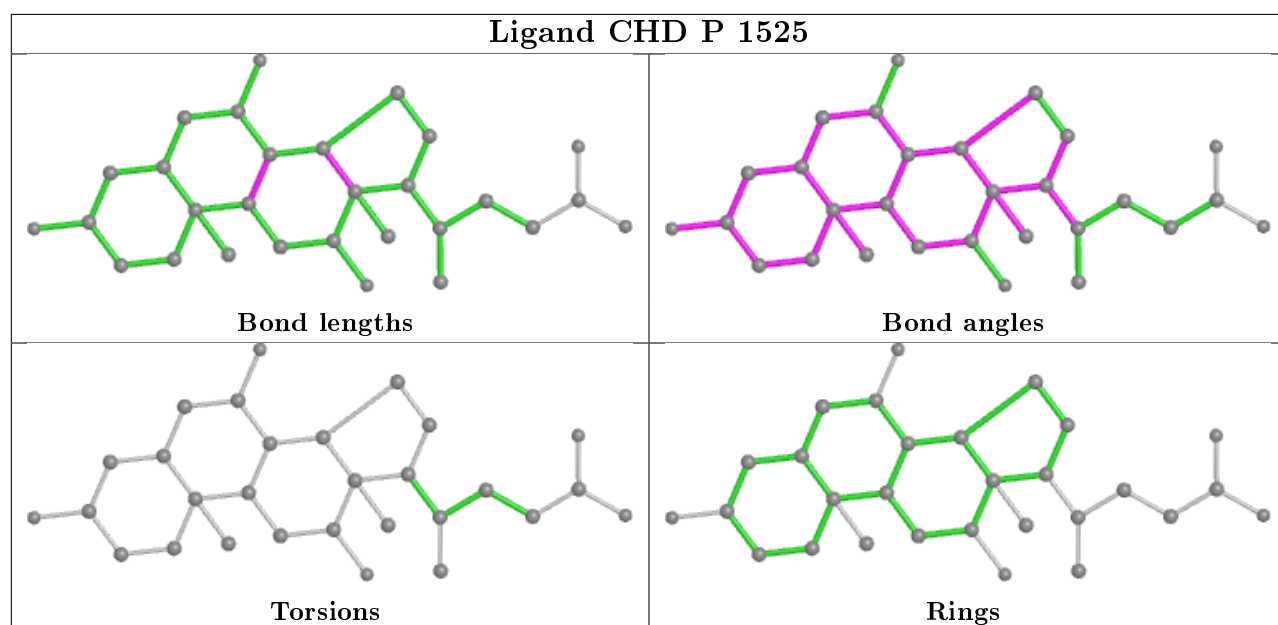
Ligand PGV C 268

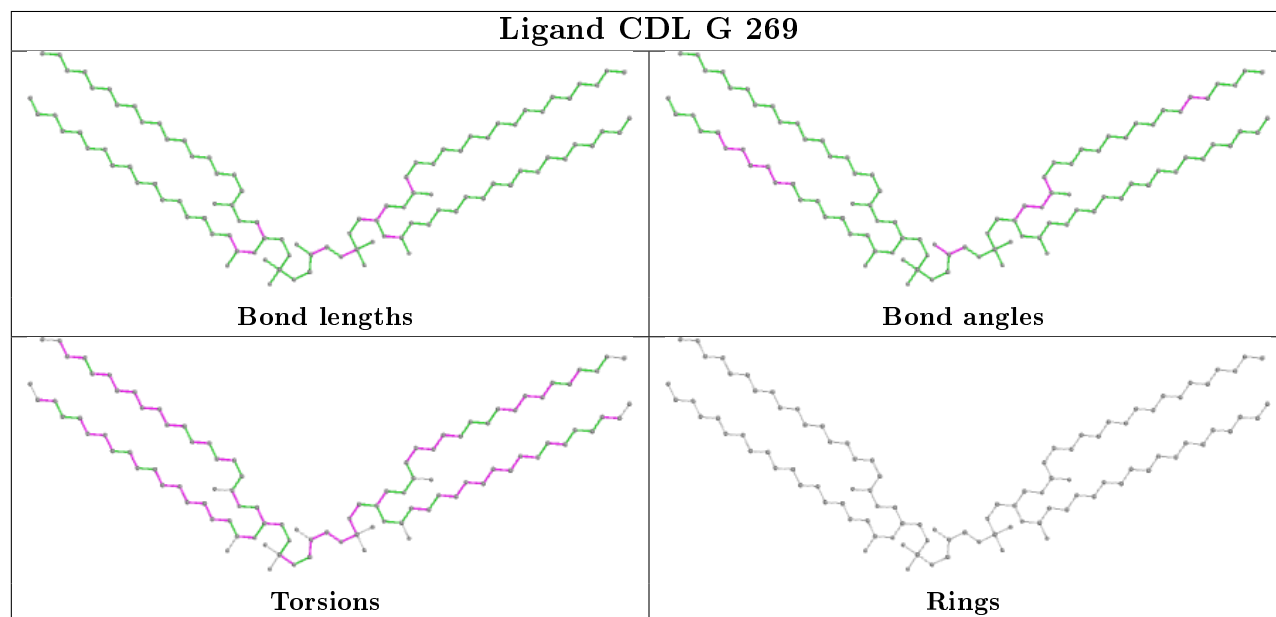
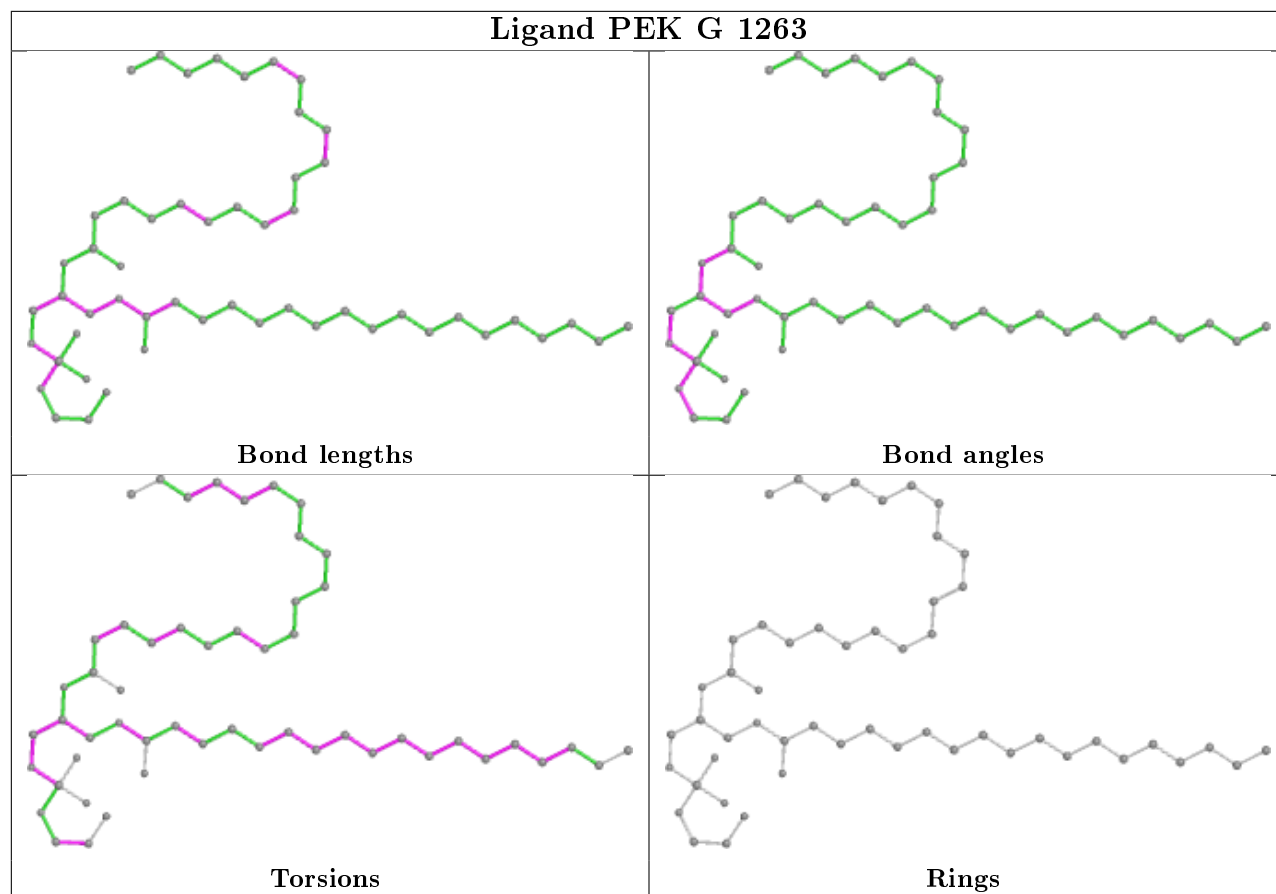


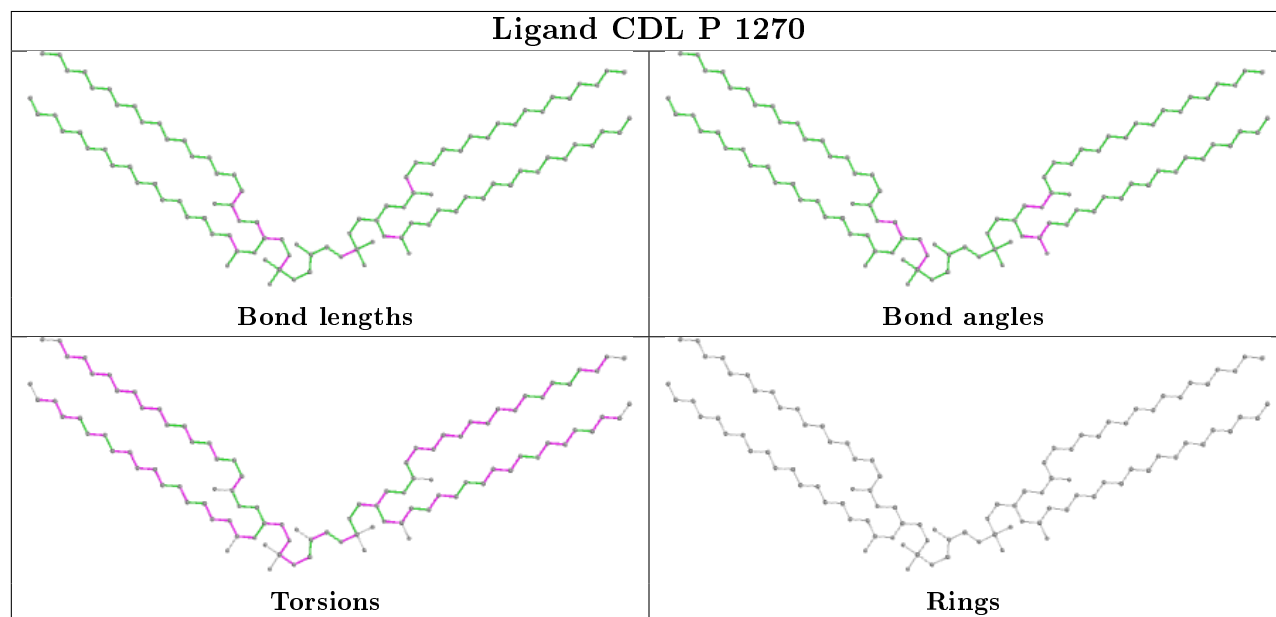
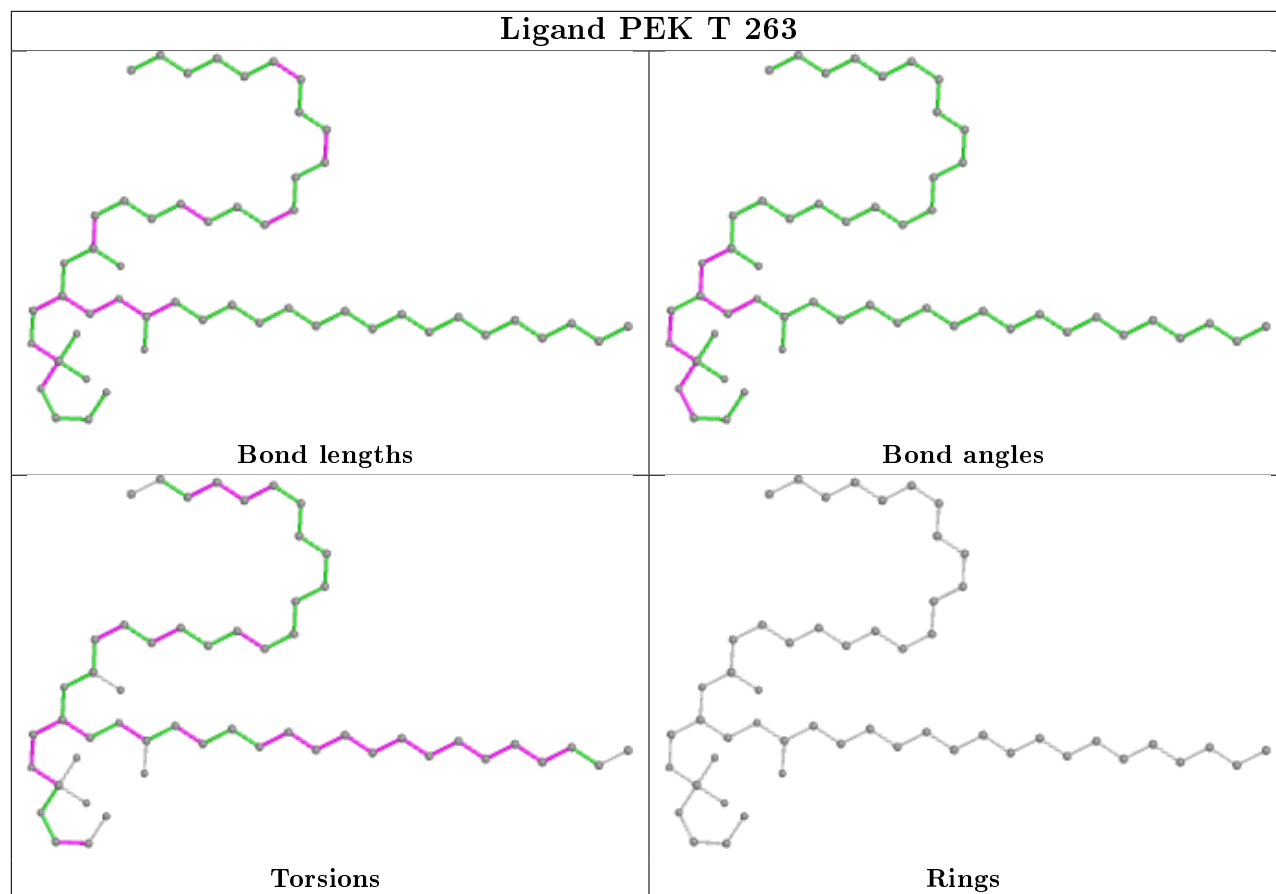




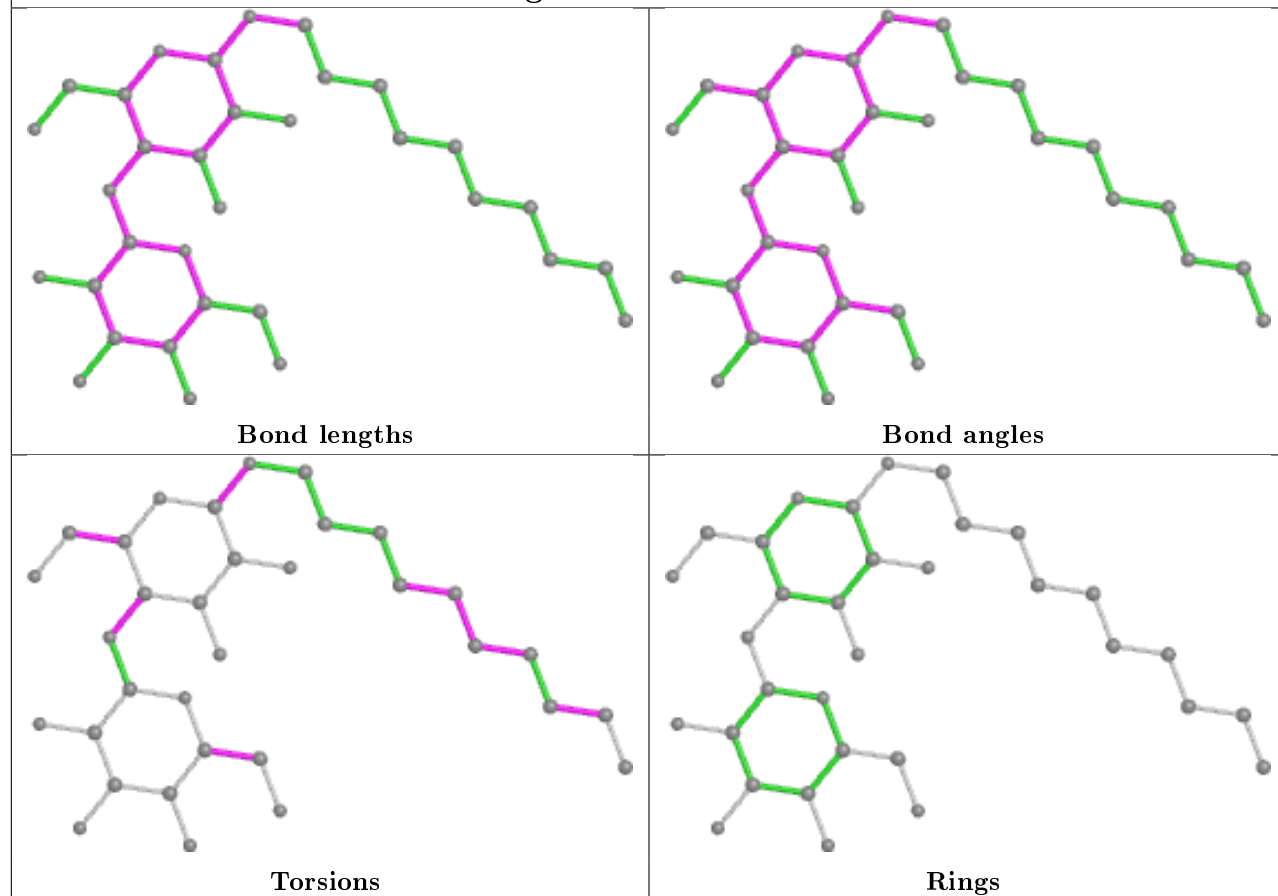




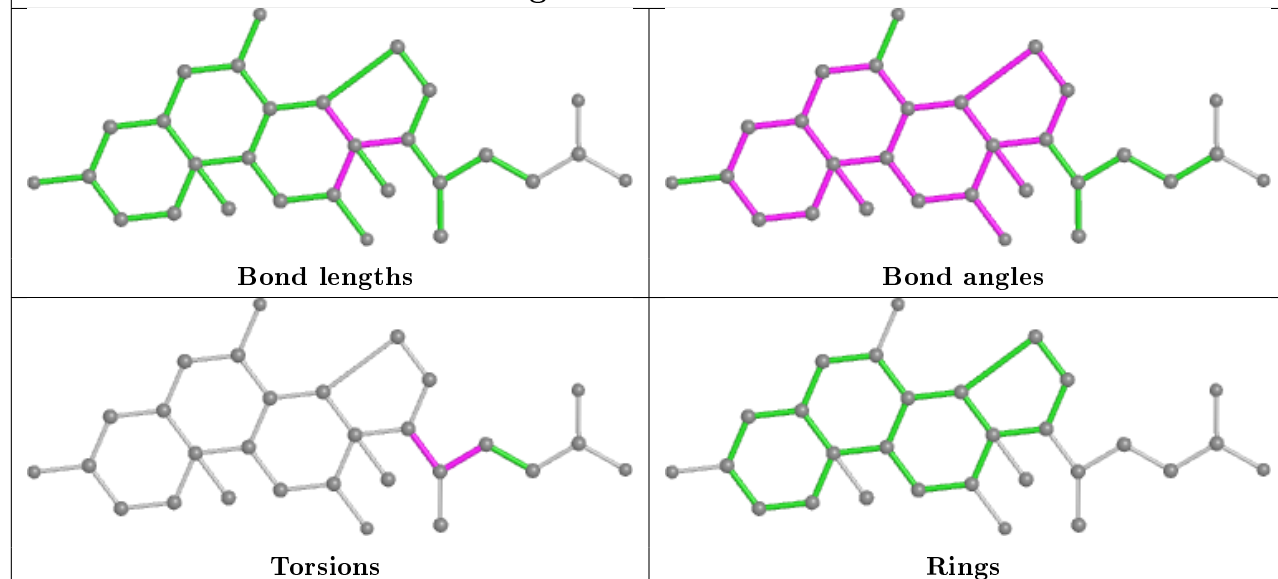


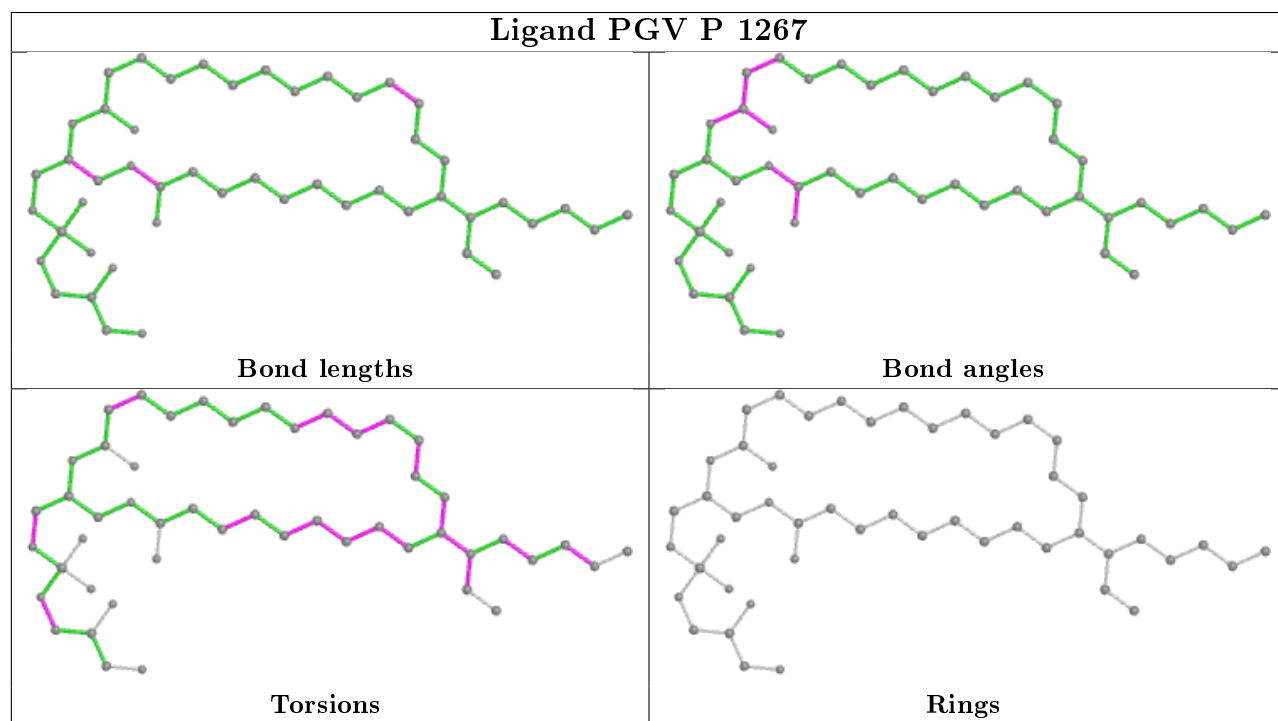
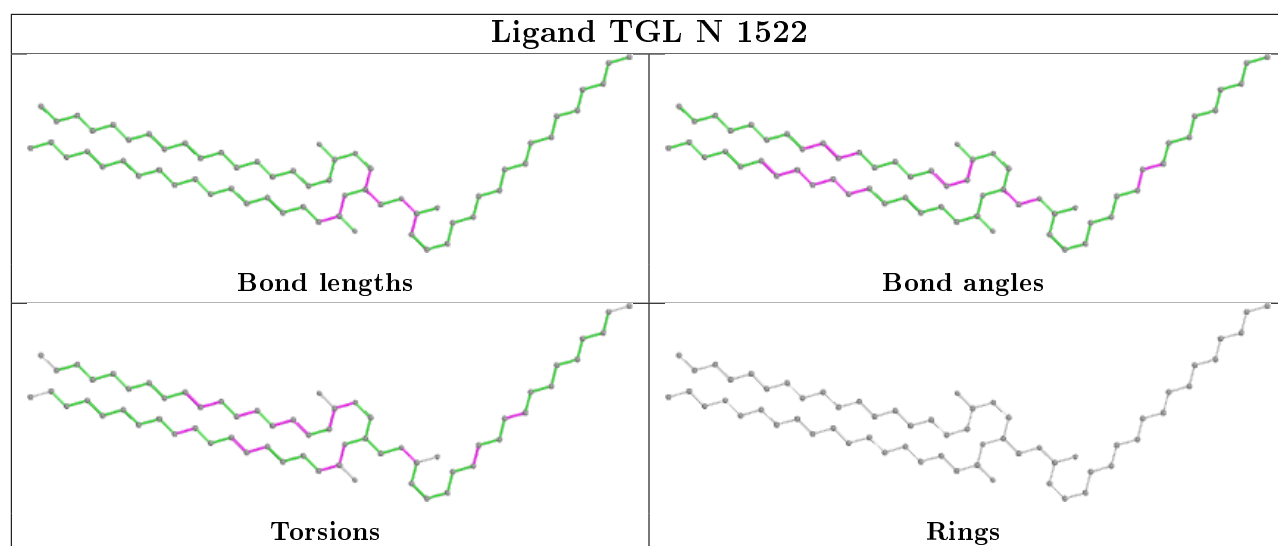


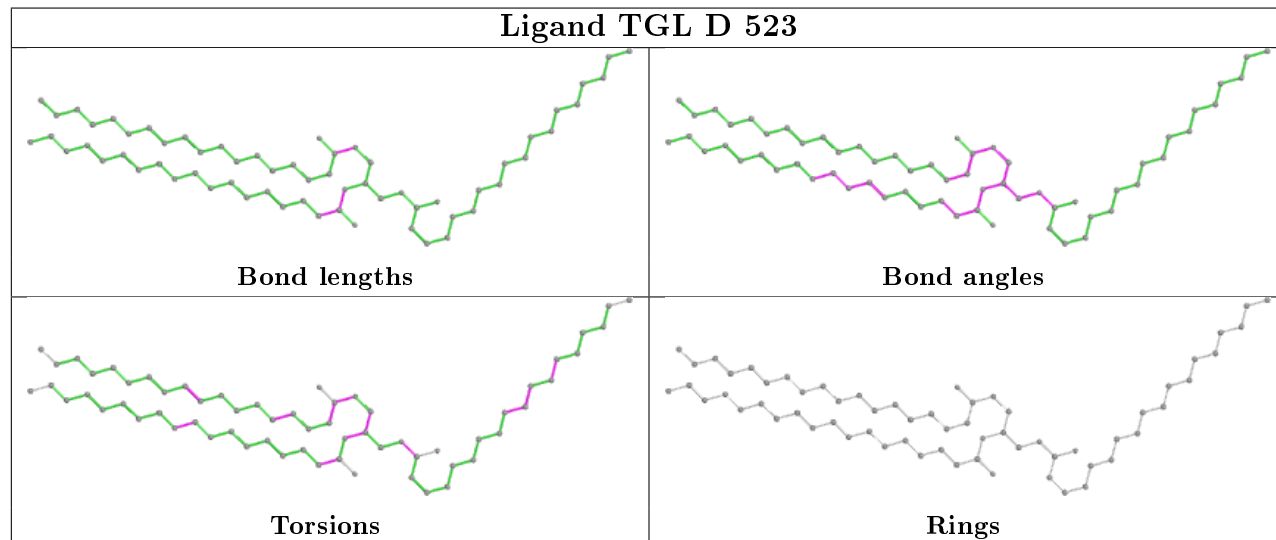
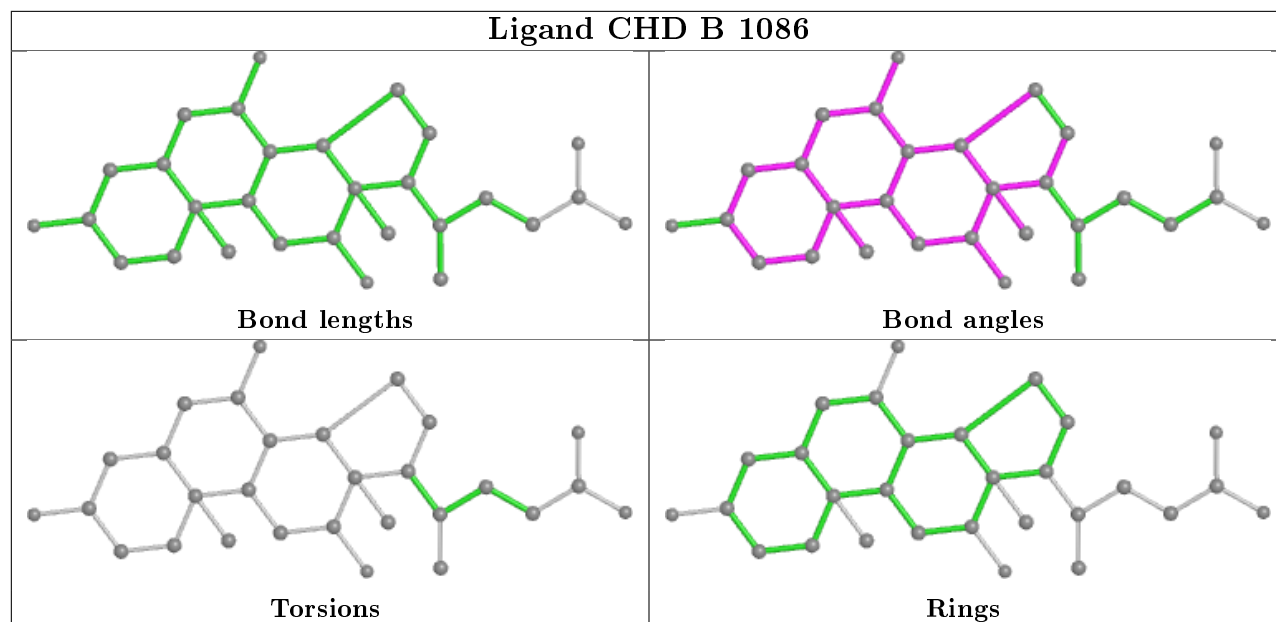
Ligand DMU C 272

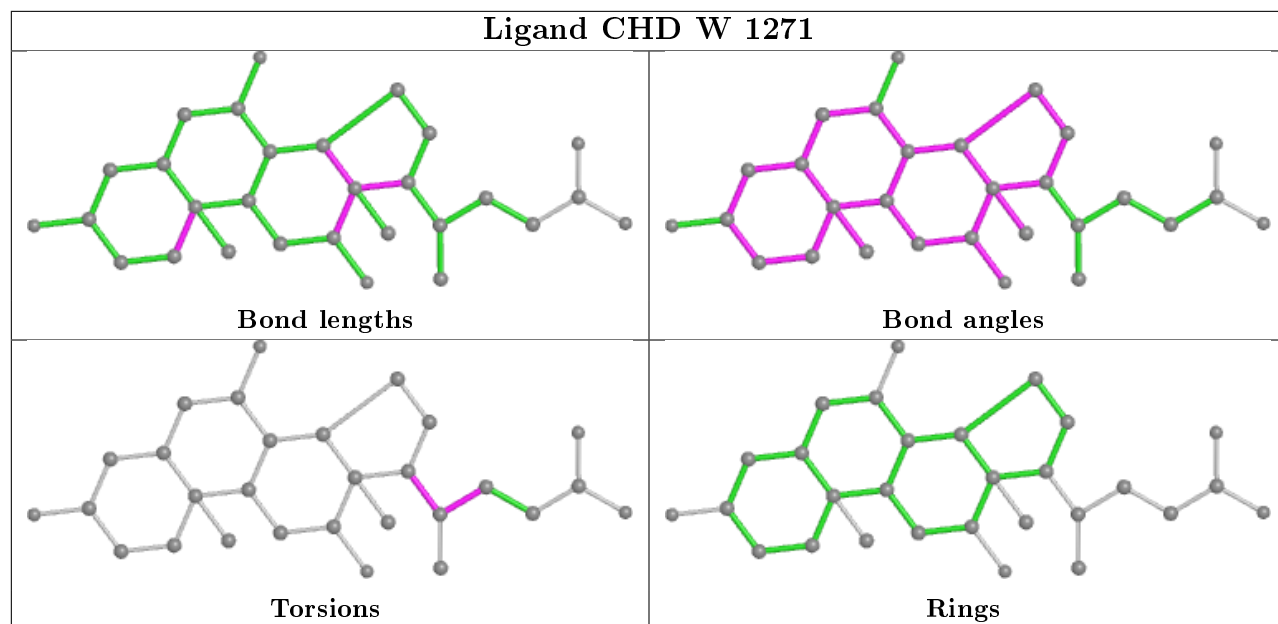


Ligand CHD C 271









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.