



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:58 PM UTC

PDB ID : 1V54 / pdb\_00001v54  
Title : Bovine heart cytochrome c oxidase at the fully oxidized state  
Authors : Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.  
Deposited on : 2003-11-21  
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](mailto: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                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtrriage (Phenix)              | : | <b>NOT EXECUTED</b>                                              |
| EDS                            | : | <b>NOT EXECUTED</b>                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

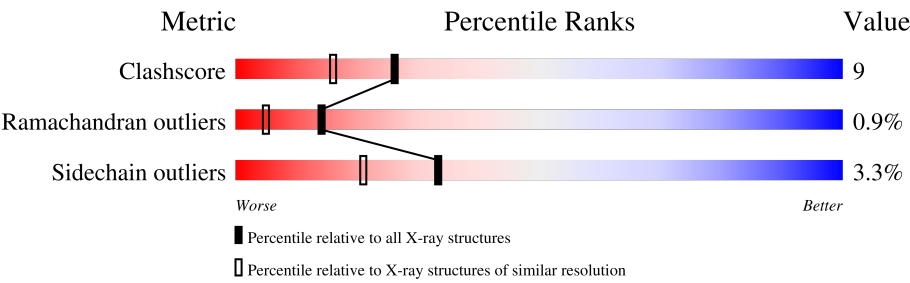
# 1 Overall quality at a glance

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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 8479 (1.80-1.80)                                      |
| Ramachandran outliers | 187476                      | 8391 (1.80-1.80)                                      |
| Sidechain outliers    | 187428                      | 8390 (1.80-1.80)                                      |

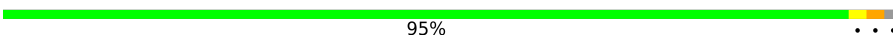
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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    | <div><div>81%17%.</div></div>  |
| 1   | N     | 514    | <div><div>79%19%.</div></div>  |
| 2   | B     | 227    | <div><div>78%17%.</div></div>  |
| 2   | O     | 227    | <div><div>70%26%..</div></div> |
| 3   | C     | 261    | <div><div>87%12%.</div></div>  |
| 3   | P     | 261    | <div><div>85%14%.</div></div>  |
| 4   | D     | 147    | <div><div>87%11%.</div></div>  |
| 4   | Q     | 147    | <div><div>74%23%..</div></div> |

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  | TGL  | L     | 3522 | -         | -        | X       | -                |
| 21  | CHD  | C     | 3271 | X         | -        | -       | -                |
| 21  | CHD  | J     | 3060 | X         | -        | -       | -                |
| 21  | CHD  | P     | 4271 | X         | -        | -       | -                |
| 21  | CHD  | W     | 4060 | X         | -        | -       | -                |
| 25  | PSC  | O     | 4230 | -         | -        | X       | -                |
| 27  | DMU  | M     | 3526 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 27  | DMU  | Z     | 4526 | X         | -        | -       | -                |

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32636 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 polypeptide I.

| 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 polypeptide II.

| 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 polypeptide III.

| 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 IV 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 polypeptide VIb.

| 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 (CCD ID: 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  |         |         |

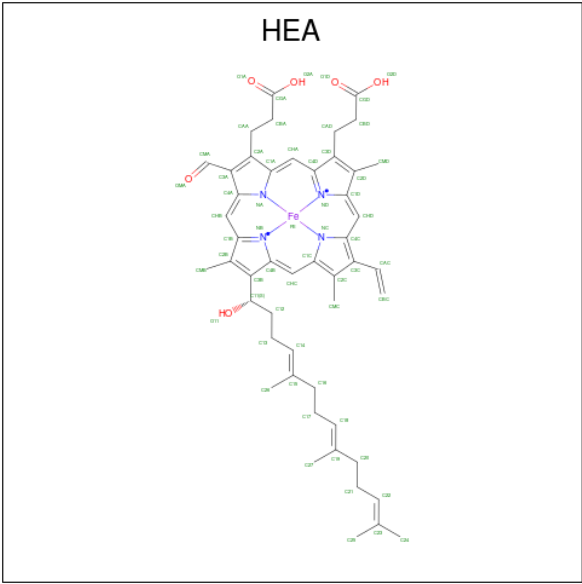
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| 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 (CCD ID: NA) (formula: Na).

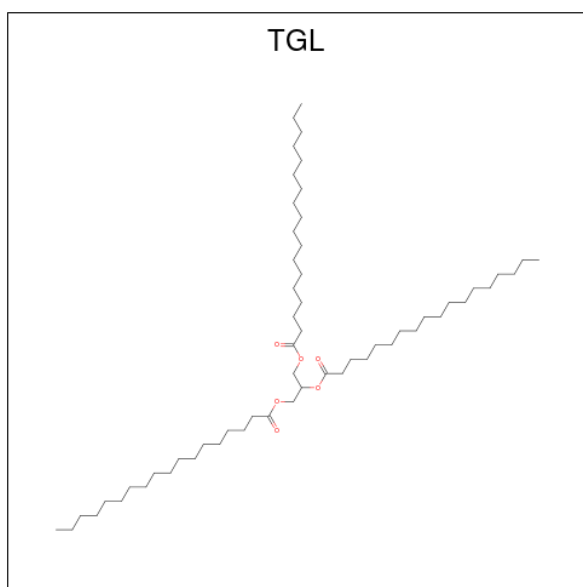
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | N     | 1        | Total | Na | 0       | 0       |
|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

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



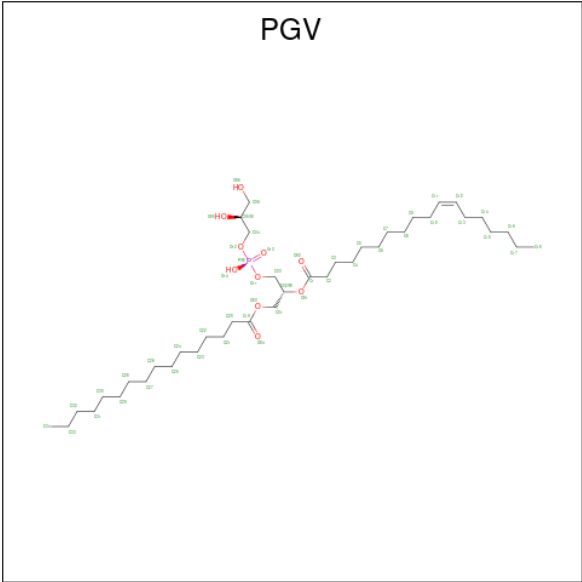
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |
| 17  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |
| 17  | N     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |
| 17  | N     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |         |

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



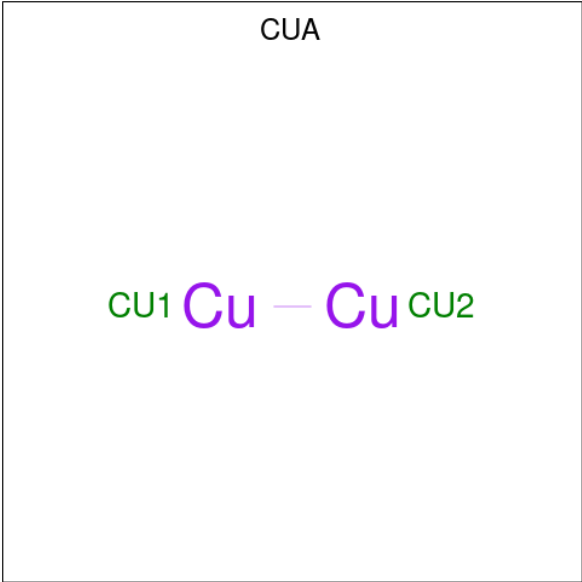
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 18  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 63    | 57 | 6 |         |         |
| 18  | D     | 1        | Total | C  | O | 0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

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



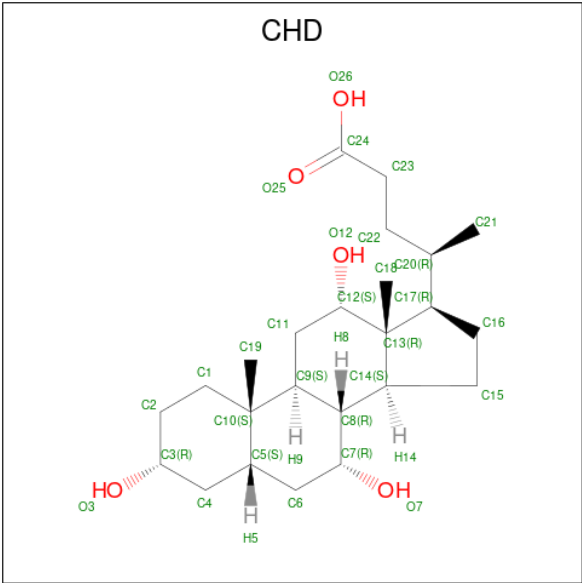
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 19  | A     | 1       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

- Molecule 20 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 20  | B     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 20  | O     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 21 is CHOLIC ACID (CCD ID: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



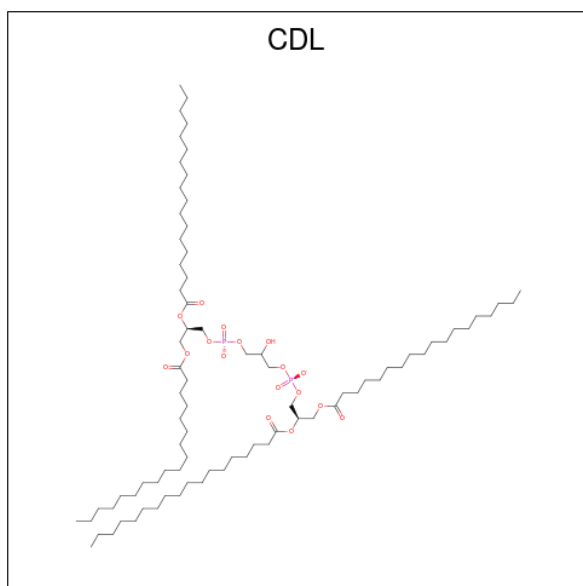
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |
| 21  | W     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 24 | 5 |         |         |

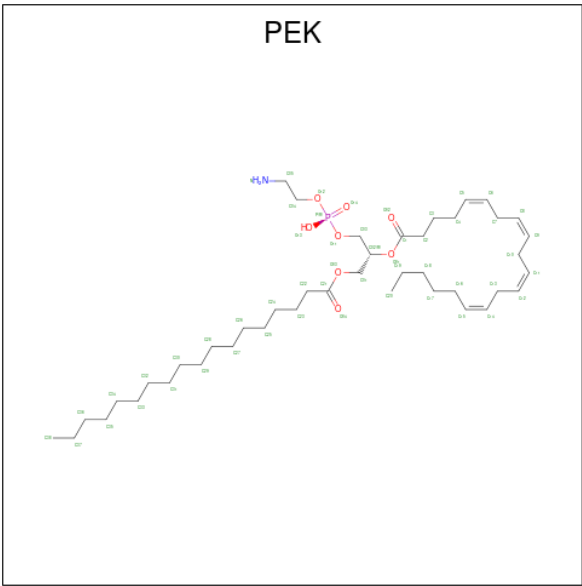
- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 22  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 22  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 22  | P     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 22  | T     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE

(CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).

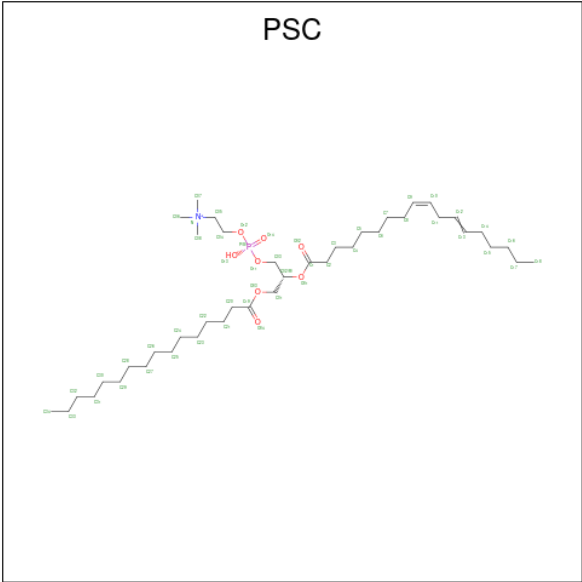


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 23  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |
| 23  | T     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |         |

- Molecule 24 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 24  | C     | 1        | Total | X | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 24  | P     | 1        | Total | X | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 25 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).

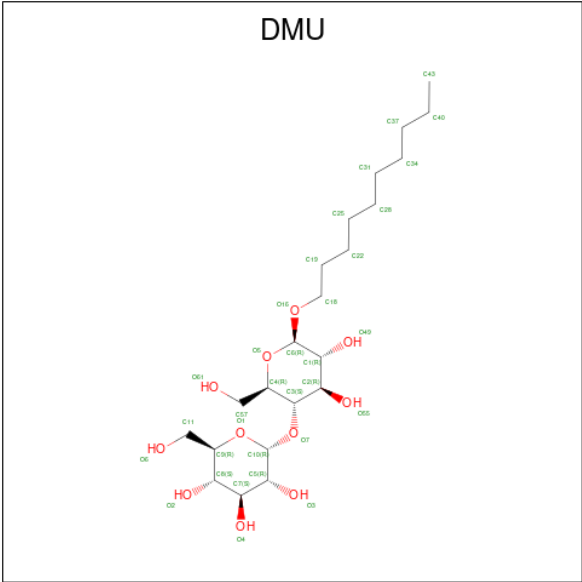


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 25  | E     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |
| 25  | O     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |         |

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 26  | F     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 26  | S     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 27  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 27  | Z     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |

- Molecule 28 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 28  | A     | 227      | Total | O   | 0       | 0       |
|     |       |          | 227   | 227 |         |         |
| 28  | B     | 180      | Total | O   | 0       | 0       |
|     |       |          | 180   | 180 |         |         |
| 28  | C     | 116      | Total | O   | 0       | 0       |
|     |       |          | 116   | 116 |         |         |
| 28  | D     | 109      | Total | O   | 0       | 0       |
|     |       |          | 109   | 109 |         |         |
| 28  | E     | 68       | Total | O   | 0       | 0       |
|     |       |          | 68    | 68  |         |         |
| 28  | F     | 80       | Total | O   | 0       | 0       |
|     |       |          | 80    | 80  |         |         |
| 28  | G     | 59       | Total | O   | 0       | 0       |
|     |       |          | 59    | 59  |         |         |
| 28  | H     | 71       | Total | O   | 0       | 0       |
|     |       |          | 71    | 71  |         |         |
| 28  | I     | 61       | Total | O   | 0       | 0       |
|     |       |          | 61    | 61  |         |         |
| 28  | J     | 21       | Total | O   | 0       | 0       |
|     |       |          | 21    | 21  |         |         |

Continued on next page...

*Continued from previous page...*

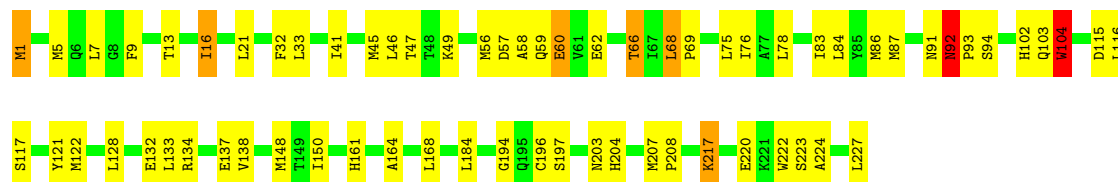
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 28  | K     | 37       | Total<br>37  | O<br>37  | 0       | 0       |
| 28  | L     | 23       | Total<br>23  | O<br>23  | 0       | 0       |
| 28  | M     | 32       | Total<br>32  | O<br>32  | 0       | 0       |
| 28  | N     | 217      | Total<br>217 | O<br>217 | 0       | 0       |
| 28  | O     | 146      | Total<br>146 | O<br>146 | 0       | 0       |
| 28  | P     | 120      | Total<br>120 | O<br>120 | 0       | 0       |
| 28  | Q     | 73       | Total<br>73  | O<br>73  | 0       | 0       |
| 28  | R     | 32       | Total<br>32  | O<br>32  | 0       | 0       |
| 28  | S     | 54       | Total<br>54  | O<br>54  | 0       | 0       |
| 28  | T     | 58       | Total<br>58  | O<br>58  | 0       | 0       |
| 28  | U     | 65       | Total<br>65  | O<br>65  | 0       | 0       |
| 28  | V     | 36       | Total<br>36  | O<br>36  | 0       | 0       |
| 28  | W     | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 28  | X     | 29       | Total<br>29  | O<br>29  | 0       | 0       |
| 28  | Y     | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 28  | Z     | 18       | Total<br>18  | O<br>18  | 0       | 0       |





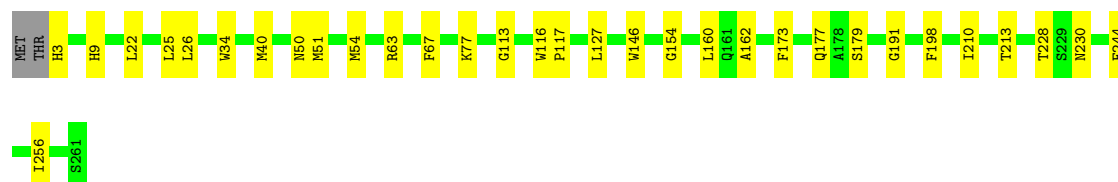
• Molecule 2: Cytochrome c oxidase polypeptide II

Chain O: 70% 26% ..



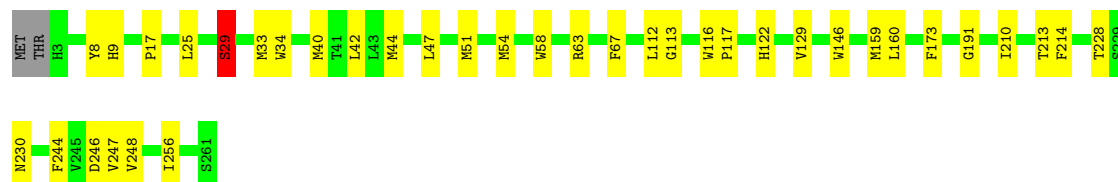
• Molecule 3: Cytochrome c oxidase polypeptide III

Chain C: 87% 12% .



• Molecule 3: Cytochrome c oxidase polypeptide III

Chain P: 85% 14% .



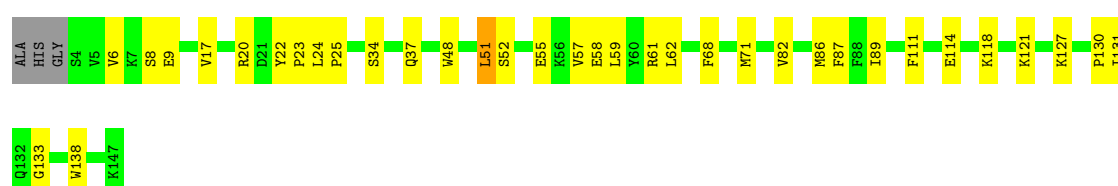
• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

Chain D: 87% 11% .



• Molecule 4: Cytochrome c oxidase subunit IV isoform 1

Chain Q: 74% 23% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:  85% 11% .



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  74% 21% ..



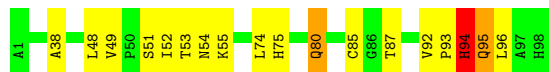
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  74% 21% ..



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  82% 15% ..



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  69% 20% 9% .



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  73% 19% 7% .



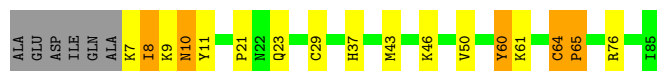
- Molecule 8: Cytochrome c oxidase polypeptide VIIb

Chain H:  76% 14% . 7%



- Molecule 8: Cytochrome c oxidase polypeptide VIIb

Chain U:  73% 14% 6% 7%



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  79% 19% .



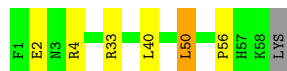
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  79% 21%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  88% 8% . .



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  95% . . .



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  79% 9% 12%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  75% 11% . 12%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  83% 9% 6% .



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  79% 17% ..



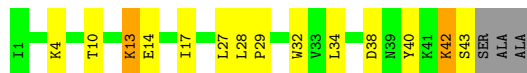
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  74% 17% . 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  63% 26% . 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<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 182.59Å 205.14Å 178.25Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 40.00 – 1.80                                    | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (40.00-1.80)                    | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | X-PLOR                                          | Depositor |
| R, $R_{free}$                                            | 0.202 , 0.227                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 32636                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 36.0                                            | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.67         | 4/4156 (0.1%)  | 1.07        | 30/5678 (0.5%)   |
| 1   | N     | 0.64         | 1/4156 (0.0%)  | 1.05        | 26/5678 (0.5%)   |
| 2   | B     | 0.59         | 0/1860         | 1.06        | 8/2534 (0.3%)    |
| 2   | O     | 0.62         | 0/1860         | 1.09        | 9/2534 (0.4%)    |
| 3   | C     | 0.58         | 0/2197         | 0.90        | 5/3005 (0.2%)    |
| 3   | P     | 0.56         | 0/2197         | 0.94        | 8/3005 (0.3%)    |
| 4   | D     | 0.56         | 0/1229         | 1.00        | 1/1658 (0.1%)    |
| 4   | Q     | 0.59         | 0/1229         | 1.00        | 4/1658 (0.2%)    |
| 5   | E     | 0.58         | 0/871          | 0.96        | 1/1182 (0.1%)    |
| 5   | R     | 0.57         | 0/871          | 1.06        | 4/1182 (0.3%)    |
| 6   | F     | 0.62         | 0/765          | 1.18        | 8/1038 (0.8%)    |
| 6   | S     | 0.66         | 0/765          | 1.15        | 5/1038 (0.5%)    |
| 7   | G     | 0.60         | 0/690          | 1.00        | 1/937 (0.1%)     |
| 7   | T     | 0.65         | 1/690 (0.1%)   | 1.03        | 1/937 (0.1%)     |
| 8   | H     | 0.58         | 0/682          | 1.02        | 5/921 (0.5%)     |
| 8   | U     | 0.57         | 0/682          | 1.03        | 3/921 (0.3%)     |
| 9   | I     | 0.57         | 0/605          | 0.89        | 1/802 (0.1%)     |
| 9   | V     | 0.56         | 0/605          | 0.86        | 1/802 (0.1%)     |
| 10  | J     | 0.54         | 0/471          | 0.93        | 0/636            |
| 10  | W     | 0.52         | 0/471          | 0.98        | 0/636            |
| 11  | K     | 0.60         | 0/398          | 1.13        | 3/546 (0.5%)     |
| 11  | X     | 0.58         | 0/398          | 1.06        | 1/546 (0.2%)     |
| 12  | L     | 0.53         | 0/393          | 0.90        | 3/526 (0.6%)     |
| 12  | Y     | 0.54         | 0/393          | 0.94        | 2/526 (0.4%)     |
| 13  | M     | 0.56         | 0/345          | 0.95        | 1/470 (0.2%)     |
| 13  | Z     | 0.51         | 0/345          | 0.98        | 1/470 (0.2%)     |
| All | All   | 0.60         | 6/29324 (0.0%) | 1.02        | 132/39866 (0.3%) |

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                   | 2                   |
| 1   | N     | 0                   | 2                   |
| 8   | U     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | A     | 61  | HIS  | CD2-NE2 | 5.92 | 1.44        | 1.37     |
| 7   | T     | 5   | LYS  | CA-C    | 5.55 | 1.56        | 1.53     |
| 1   | A     | 376 | HIS  | ND1-CE1 | 5.33 | 1.37        | 1.32     |
| 1   | A     | 80  | ASN  | CG-OD1  | 5.29 | 1.33        | 1.23     |
| 1   | A     | 130 | PRO  | CA-C    | 5.16 | 1.56        | 1.52     |

The worst 5 of 132 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | D     | 133 | GLY  | N-CA-C    | 12.65 | 127.17      | 112.50   |
| 4   | Q     | 133 | GLY  | N-CA-C    | 12.22 | 126.67      | 112.50   |
| 6   | F     | 93  | PRO  | N-CA-C    | 10.89 | 126.90      | 111.33   |
| 1   | A     | 61  | HIS  | CB-CG-CD2 | -9.24 | 119.19      | 131.20   |
| 1   | A     | 125 | GLY  | N-CA-C    | -9.20 | 101.35      | 112.48   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 19  | TYR  | Sidechain |
| 1   | A     | 240 | HIS  | Sidechain |
| 1   | N     | 240 | HIS  | Sidechain |
| 1   | N     | 304 | TYR  | Sidechain |
| 8   | U     | 11  | 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     | 69      | 0            |
| 1   | N     | 4027  | 0        | 4001     | 75      | 0            |
| 2   | B     | 1824  | 0        | 1833     | 37      | 0            |
| 2   | O     | 1824  | 0        | 1833     | 53      | 0            |
| 3   | C     | 2110  | 0        | 2027     | 22      | 0            |
| 3   | P     | 2110  | 0        | 2027     | 28      | 0            |
| 4   | D     | 1195  | 0        | 1183     | 15      | 0            |
| 4   | Q     | 1195  | 0        | 1183     | 26      | 0            |
| 5   | E     | 852   | 0        | 845      | 6       | 0            |
| 5   | R     | 852   | 0        | 845      | 12      | 0            |
| 6   | F     | 748   | 0        | 728      | 16      | 0            |
| 6   | S     | 748   | 0        | 728      | 12      | 0            |
| 7   | G     | 675   | 0        | 644      | 26      | 0            |
| 7   | T     | 675   | 0        | 644      | 21      | 0            |
| 8   | H     | 662   | 0        | 623      | 7       | 0            |
| 8   | U     | 662   | 0        | 623      | 11      | 0            |
| 9   | I     | 601   | 0        | 613      | 9       | 0            |
| 9   | V     | 601   | 0        | 613      | 11      | 0            |
| 10  | J     | 460   | 0        | 459      | 5       | 0            |
| 10  | W     | 460   | 0        | 459      | 2       | 0            |
| 11  | K     | 384   | 0        | 366      | 2       | 0            |
| 11  | X     | 384   | 0        | 366      | 8       | 0            |
| 12  | L     | 380   | 0        | 380      | 15      | 0            |
| 12  | Y     | 380   | 0        | 380      | 11      | 0            |
| 13  | M     | 335   | 0        | 352      | 5       | 0            |
| 13  | Z     | 335   | 0        | 352      | 6       | 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     | 120   | 0        | 108      | 3       | 0            |
| 17  | N     | 120   | 0        | 108      | 3       | 0            |
| 18  | A     | 63    | 0        | 110      | 11      | 0            |
| 18  | D     | 63    | 0        | 110      | 15      | 0            |
| 18  | L     | 63    | 0        | 110      | 25      | 0            |
| 18  | N     | 126   | 0        | 220      | 39      | 0            |
| 18  | Q     | 63    | 0        | 110      | 15      | 0            |
| 19  | A     | 102   | 0        | 152      | 7       | 0            |
| 19  | C     | 102   | 0        | 152      | 8       | 0            |
| 19  | N     | 102   | 0        | 152      | 5       | 0            |
| 19  | P     | 102   | 0        | 152      | 9       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | B     | 2     | 0        | 0        | 0       | 0            |
| 20  | O     | 2     | 0        | 0        | 0       | 0            |
| 21  | B     | 29    | 0        | 39       | 1       | 0            |
| 21  | C     | 58    | 0        | 78       | 3       | 0            |
| 21  | J     | 29    | 0        | 39       | 2       | 0            |
| 21  | O     | 29    | 0        | 39       | 1       | 0            |
| 21  | P     | 58    | 0        | 78       | 2       | 0            |
| 21  | W     | 29    | 0        | 39       | 2       | 0            |
| 22  | C     | 100   | 0        | 156      | 14      | 0            |
| 22  | G     | 100   | 0        | 156      | 14      | 0            |
| 22  | P     | 100   | 0        | 156      | 19      | 0            |
| 22  | T     | 100   | 0        | 156      | 15      | 0            |
| 23  | C     | 106   | 0        | 154      | 7       | 0            |
| 23  | G     | 53    | 0        | 77       | 10      | 0            |
| 23  | P     | 106   | 0        | 154      | 6       | 0            |
| 23  | T     | 53    | 0        | 77       | 9       | 0            |
| 24  | C     | 1     | 0        | 0        | 0       | 0            |
| 24  | P     | 1     | 0        | 0        | 0       | 0            |
| 25  | E     | 52    | 0        | 80       | 13      | 0            |
| 25  | O     | 52    | 0        | 80       | 21      | 0            |
| 26  | F     | 1     | 0        | 0        | 0       | 0            |
| 26  | S     | 1     | 0        | 0        | 0       | 0            |
| 27  | M     | 33    | 0        | 36       | 0       | 0            |
| 27  | Z     | 33    | 0        | 36       | 0       | 0            |
| 28  | A     | 227   | 0        | 0        | 2       | 0            |
| 28  | B     | 180   | 0        | 0        | 8       | 0            |
| 28  | C     | 116   | 0        | 0        | 1       | 0            |
| 28  | D     | 109   | 0        | 0        | 3       | 0            |
| 28  | E     | 68    | 0        | 0        | 2       | 0            |
| 28  | F     | 80    | 0        | 0        | 2       | 0            |
| 28  | G     | 59    | 0        | 0        | 4       | 0            |
| 28  | H     | 71    | 0        | 0        | 1       | 0            |
| 28  | I     | 61    | 0        | 0        | 2       | 0            |
| 28  | J     | 21    | 0        | 0        | 0       | 0            |
| 28  | K     | 37    | 0        | 0        | 0       | 0            |
| 28  | L     | 23    | 0        | 0        | 1       | 0            |
| 28  | M     | 32    | 0        | 0        | 0       | 0            |
| 28  | N     | 217   | 0        | 0        | 5       | 0            |
| 28  | O     | 146   | 0        | 0        | 1       | 0            |
| 28  | P     | 120   | 0        | 0        | 1       | 0            |
| 28  | Q     | 73    | 0        | 0        | 5       | 0            |
| 28  | R     | 32    | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | S     | 54    | 0        | 0        | 3       | 0            |
| 28  | T     | 58    | 0        | 0        | 2       | 0            |
| 28  | U     | 65    | 0        | 0        | 1       | 0            |
| 28  | V     | 36    | 0        | 0        | 2       | 0            |
| 28  | W     | 13    | 0        | 0        | 0       | 0            |
| 28  | X     | 29    | 0        | 0        | 1       | 0            |
| 28  | Y     | 25    | 0        | 0        | 1       | 0            |
| 28  | Z     | 18    | 0        | 0        | 0       | 0            |
| All | All   | 32636 | 0        | 31222    | 580     | 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 9.

The worst 5 of 580 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:84:LYS:H       | 7:G:84:LYS:HD2     | 1.14                     | 1.08              |
| 22:C:3270:CDL:H662 | 19:C:3267:PGV:H182 | 1.41                     | 1.03              |
| 3:P:63:ARG:HE      | 22:P:4270:CDL:HA22 | 1.24                     | 1.03              |
| 7:T:84:LYS:HD2     | 7:T:84:LYS:H       | 1.23                     | 1.02              |
| 3:C:63:ARG:HE      | 22:C:3270:CDL:HA22 | 1.23                     | 1.01              |

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%) | 496 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | N     | 512/514 (100%) | 500 (98%) | 12 (2%) | 0        | 100         | 100 |
| 2   | B     | 225/227 (99%)  | 208 (92%) | 14 (6%) | 3 (1%)   | 9           | 3   |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | O     | 225/227 (99%)   | 206 (92%)  | 16 (7%)  | 3 (1%)   | 9           | 3   |
| 3   | C     | 257/261 (98%)   | 252 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 3   | P     | 257/261 (98%)   | 252 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 4   | D     | 142/147 (97%)   | 138 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 4   | Q     | 142/147 (97%)   | 138 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 5   | E     | 103/109 (94%)   | 103 (100%) | 0        | 0        | 100         | 100 |
| 5   | R     | 103/109 (94%)   | 102 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 6   | F     | 96/98 (98%)     | 89 (93%)   | 4 (4%)   | 3 (3%)   | 3           | 0   |
| 6   | S     | 96/98 (98%)     | 89 (93%)   | 4 (4%)   | 3 (3%)   | 3           | 0   |
| 7   | G     | 81/85 (95%)     | 68 (84%)   | 6 (7%)   | 7 (9%)   | 0           | 0   |
| 7   | T     | 81/85 (95%)     | 65 (80%)   | 9 (11%)  | 7 (9%)   | 0           | 0   |
| 8   | H     | 77/85 (91%)     | 70 (91%)   | 5 (6%)   | 2 (3%)   | 4           | 0   |
| 8   | U     | 77/85 (91%)     | 70 (91%)   | 5 (6%)   | 2 (3%)   | 4           | 0   |
| 9   | I     | 71/73 (97%)     | 67 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 9   | V     | 71/73 (97%)     | 67 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 10  | J     | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 10  | W     | 56/59 (95%)     | 55 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 11  | K     | 47/56 (84%)     | 46 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 11  | X     | 47/56 (84%)     | 46 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 12  | L     | 44/47 (94%)     | 43 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 12  | Y     | 44/47 (94%)     | 43 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 13  | M     | 41/46 (89%)     | 41 (100%)  | 0        | 0        | 100         | 100 |
| 13  | Z     | 41/46 (89%)     | 41 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 3504/3614 (97%) | 3350 (96%) | 124 (4%) | 30 (1%)  | 14          | 5   |

5 of 30 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 95  | GLN  |
| 7   | G     | 4   | ALA  |
| 7   | G     | 7   | ASP  |
| 7   | G     | 8   | HIS  |
| 7   | G     | 39  | SER  |

### 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%) | 421 (99%) | 5 (1%)   | 63          | 57  |
| 1   | N     | 426/426 (100%) | 416 (98%) | 10 (2%)  | 44          | 33  |
| 2   | B     | 210/210 (100%) | 200 (95%) | 10 (5%)  | 23          | 11  |
| 2   | O     | 210/210 (100%) | 198 (94%) | 12 (6%)  | 18          | 8   |
| 3   | C     | 224/226 (99%)  | 220 (98%) | 4 (2%)   | 51          | 43  |
| 3   | P     | 224/226 (99%)  | 219 (98%) | 5 (2%)   | 45          | 34  |
| 4   | D     | 128/129 (99%)  | 126 (98%) | 2 (2%)   | 55          | 47  |
| 4   | Q     | 128/129 (99%)  | 124 (97%) | 4 (3%)   | 35          | 23  |
| 5   | E     | 92/95 (97%)    | 90 (98%)  | 2 (2%)   | 45          | 34  |
| 5   | R     | 92/95 (97%)    | 89 (97%)  | 3 (3%)   | 33          | 21  |
| 6   | F     | 81/81 (100%)   | 78 (96%)  | 3 (4%)   | 30          | 18  |
| 6   | S     | 81/81 (100%)   | 77 (95%)  | 4 (5%)   | 22          | 10  |
| 7   | G     | 67/68 (98%)    | 63 (94%)  | 4 (6%)   | 17          | 7   |
| 7   | T     | 67/68 (98%)    | 64 (96%)  | 3 (4%)   | 24          | 12  |
| 8   | H     | 71/75 (95%)    | 68 (96%)  | 3 (4%)   | 26          | 14  |
| 8   | U     | 71/75 (95%)    | 67 (94%)  | 4 (6%)   | 19          | 8   |
| 9   | I     | 57/57 (100%)   | 53 (93%)  | 4 (7%)   | 14          | 4   |
| 9   | V     | 57/57 (100%)   | 53 (93%)  | 4 (7%)   | 14          | 4   |
| 10  | J     | 49/50 (98%)    | 48 (98%)  | 1 (2%)   | 48          | 38  |
| 10  | W     | 49/50 (98%)    | 48 (98%)  | 1 (2%)   | 48          | 38  |
| 11  | K     | 39/46 (85%)    | 39 (100%) | 0        | 100         | 100 |
| 11  | X     | 39/46 (85%)    | 38 (97%)  | 1 (3%)   | 40          | 28  |
| 12  | L     | 39/40 (98%)    | 38 (97%)  | 1 (3%)   | 40          | 28  |
| 12  | Y     | 39/40 (98%)    | 38 (97%)  | 1 (3%)   | 40          | 28  |
| 13  | M     | 37/38 (97%)    | 32 (86%)  | 5 (14%)  | 4           | 1   |
| 13  | Z     | 37/38 (97%)    | 33 (89%)  | 4 (11%)  | 6           | 1   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| All | All   | 3040/3082 (99%) | 2940 (97%) | 100 (3%) | 33          | 21 |

5 of 100 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 66  | THR  |
| 4   | Q     | 8   | SER  |
| 13  | Z     | 42  | LYS  |
| 2   | O     | 75  | LEU  |
| 2   | O     | 217 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 170 | ASN  |
| 3   | P     | 3   | HIS  |
| 10  | W     | 57  | HIS  |
| 1   | N     | 178 | GLN  |
| 1   | N     | 503 | HIS  |

### 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 | $\# Z  > 2$ |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 0.66 | 0           | 8,9,11      | 1.08 | 1 (12%)     |
| 2   | FME  | B     | 1   | 2    | 8,9,10       | 0.77 | 0           | 8,9,11      | 2.30 | 2 (25%)     |

| 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        | 2.55 | 2 (28%)  | 7,9,11      | 1.72 | 2 (28%)  |
| 9   | SAC  | V     | 1   | 9    | 7,8,9        | 2.64 | 2 (28%)  | 7,9,11      | 2.00 | 3 (42%)  |
| 1   | FME  | N     | 1   | 1    | 8,9,10       | 0.79 | 0        | 8,9,11      | 1.82 | 2 (25%)  |
| 2   | FME  | O     | 1   | 2    | 8,9,10       | 0.67 | 0        | 8,9,11      | 1.73 | 2 (25%)  |
| 7   | TPO  | G     | 11  | 7    | 8,10,11      | 1.43 | 2 (25%)  | 10,14,16    | 1.15 | 1 (10%)  |
| 7   | TPO  | T     | 11  | 7    | 8,10,11      | 1.37 | 1 (12%)  | 10,14,16    | 1.16 | 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  | A     | 1   | 1    | -       | 3/7/9/11  | -     |
| 2   | FME  | B     | 1   | 2    | -       | 1/7/9/11  | -     |
| 9   | SAC  | I     | 1   | 9    | -       | 3/7/8/10  | -     |
| 9   | SAC  | V     | 1   | 9    | -       | 3/7/8/10  | -     |
| 1   | FME  | N     | 1   | 1    | -       | 3/7/9/11  | -     |
| 2   | FME  | O     | 1   | 2    | -       | 1/7/9/11  | -     |
| 7   | TPO  | G     | 11  | 7    | -       | 4/9/11/13 | -     |
| 7   | TPO  | T     | 11  | 7    | -       | 4/9/11/13 | -     |

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 | 5.27 | 1.35        | 1.23     |
| 9   | I     | 1   | SAC  | OAC-C1A | 5.19 | 1.34        | 1.23     |
| 9   | V     | 1   | SAC  | CA-N    | 4.15 | 1.52        | 1.46     |
| 9   | I     | 1   | SAC  | CA-N    | 4.05 | 1.52        | 1.46     |
| 7   | T     | 11  | TPO  | CB-CA   | 2.80 | 1.59        | 1.53     |

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

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 1   | FME  | CA-N-CN | -4.79 | 115.46      | 122.82   |
| 1   | N     | 1   | FME  | CA-N-CN | -4.24 | 116.30      | 122.82   |
| 2   | B     | 1   | FME  | C-CA-N  | 4.11  | 117.43      | 109.50   |
| 2   | O     | 1   | FME  | C-CA-N  | 3.57  | 116.38      | 109.50   |
| 9   | I     | 1   | SAC  | C-CA-N  | -3.18 | 103.36      | 109.50   |

There are no chirality outliers.

5 of 22 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.

5 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | A     | 1   | FME  | 5       | 0            |
| 1   | N     | 1   | FME  | 1       | 0            |
| 2   | O     | 1   | FME  | 3       | 0            |
| 7   | G     | 11  | TPO  | 1       | 0            |
| 7   | T     | 11  | TPO  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 42 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 | $\# Z  > 2$ |
| 18  | TGL  | L     | 3522 | -    | 62,62,62     | 1.40 | 6 (9%)      | 65,65,65    | 1.23 | 6 (9%)      |
| 19  | PGV  | A     | 3266 | -    | 50,50,50     | 0.91 | 1 (2%)      | 53,56,56    | 0.78 | 2 (3%)      |
| 21  | CHD  | B     | 4085 | -    | 32,32,32     | 0.81 | 0           | 51,51,51    | 1.87 | 13 (25%)    |
| 23  | PEK  | P     | 4265 | -    | 52,52,52     | 1.71 | 12 (23%)    | 55,57,57    | 0.98 | 5 (9%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | CHD  | W     | 4060 | -    | 32,32,32     | 1.01 | 2 (6%)   | 51,51,51    | 3.20 | 26 (50%) |
| 22  | CDL  | G     | 3269 | -    | 99,99,99     | 0.99 | 5 (5%)   | 105,111,111 | 0.94 | 7 (6%)   |
| 19  | PGV  | N     | 4524 | -    | 50,50,50     | 1.13 | 3 (6%)   | 53,56,56    | 1.20 | 8 (15%)  |
| 19  | PGV  | A     | 3524 | -    | 50,50,50     | 1.13 | 7 (14%)  | 53,56,56    | 1.26 | 8 (15%)  |
| 21  | CHD  | J     | 3060 | -    | 32,32,32     | 0.93 | 1 (3%)   | 51,51,51    | 3.24 | 25 (49%) |
| 25  | PSC  | E     | 3230 | -    | 51,51,51     | 1.25 | 3 (5%)   | 57,59,59    | 1.02 | 4 (7%)   |
| 21  | CHD  | O     | 3085 | -    | 32,32,32     | 0.84 | 0        | 51,51,51    | 1.89 | 18 (35%) |
| 18  | TGL  | Q     | 4523 | -    | 62,62,62     | 1.16 | 3 (4%)   | 65,65,65    | 1.06 | 4 (6%)   |
| 17  | HEA  | A     | 515  | 1    | 67,67,67     | 0.99 | 2 (2%)   | 81,103,103  | 1.18 | 6 (7%)   |
| 19  | PGV  | P     | 4268 | -    | 50,50,50     | 1.12 | 3 (6%)   | 53,56,56    | 0.67 | 0        |
| 19  | PGV  | C     | 3267 | -    | 50,50,50     | 0.83 | 1 (2%)   | 53,56,56    | 0.94 | 4 (7%)   |
| 17  | HEA  | N     | 515  | 1    | 67,67,67     | 1.00 | 2 (2%)   | 81,103,103  | 1.17 | 8 (9%)   |
| 18  | TGL  | N     | 4522 | -    | 62,62,62     | 1.43 | 6 (9%)   | 65,65,65    | 1.14 | 6 (9%)   |
| 17  | HEA  | A     | 516  | 1    | 67,67,67     | 1.15 | 4 (5%)   | 81,103,103  | 1.03 | 3 (3%)   |
| 19  | PGV  | C     | 3268 | -    | 50,50,50     | 1.12 | 3 (6%)   | 53,56,56    | 0.66 | 0        |
| 20  | CUA  | B     | 228  | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 23  | PEK  | C     | 3264 | -    | 52,52,52     | 1.52 | 5 (9%)   | 55,57,57    | 1.29 | 7 (12%)  |
| 21  | CHD  | C     | 3271 | -    | 32,32,32     | 0.86 | 2 (6%)   | 51,51,51    | 3.61 | 22 (43%) |
| 18  | TGL  | N     | 4521 | -    | 62,62,62     | 1.02 | 4 (6%)   | 65,65,65    | 1.11 | 6 (9%)   |
| 18  | TGL  | D     | 3523 | -    | 62,62,62     | 1.17 | 3 (4%)   | 65,65,65    | 1.13 | 7 (10%)  |
| 23  | PEK  | T     | 3263 | -    | 52,52,52     | 1.70 | 11 (21%) | 55,57,57    | 1.00 | 3 (5%)   |
| 27  | DMU  | M     | 3526 | -    | 34,34,34     | 3.26 | 8 (23%)  | 45,45,45    | 4.36 | 19 (42%) |
| 20  | CUA  | O     | 228  | 2    | 0,1,1        | -    | -        | -           | -    | -        |
| 21  | CHD  | P     | 4525 | -    | 32,32,32     | 0.92 | 2 (6%)   | 51,51,51    | 1.65 | 9 (17%)  |
| 23  | PEK  | G     | 4263 | -    | 52,52,52     | 1.70 | 9 (17%)  | 55,57,57    | 1.01 | 3 (5%)   |
| 23  | PEK  | P     | 4264 | -    | 52,52,52     | 1.51 | 5 (9%)   | 55,57,57    | 1.35 | 10 (18%) |
| 18  | TGL  | A     | 3521 | -    | 62,62,62     | 1.00 | 4 (6%)   | 65,65,65    | 1.14 | 6 (9%)   |
| 17  | HEA  | N     | 516  | 1    | 67,67,67     | 1.14 | 6 (8%)   | 81,103,103  | 1.10 | 2 (2%)   |
| 19  | PGV  | N     | 4266 | -    | 50,50,50     | 1.04 | 3 (6%)   | 53,56,56    | 1.00 | 3 (5%)   |
| 21  | CHD  | P     | 4271 | -    | 32,32,32     | 0.83 | 0        | 51,51,51    | 3.54 | 22 (43%) |
| 22  | CDL  | C     | 3270 | -    | 99,99,99     | 0.80 | 3 (3%)   | 105,111,111 | 0.91 | 5 (4%)   |
| 22  | CDL  | P     | 4270 | -    | 99,99,99     | 0.83 | 4 (4%)   | 105,111,111 | 0.89 | 5 (4%)   |
| 25  | PSC  | O     | 4230 | -    | 51,51,51     | 1.21 | 3 (5%)   | 57,59,59    | 1.03 | 4 (7%)   |
| 27  | DMU  | Z     | 4526 | -    | 34,34,34     | 3.24 | 8 (23%)  | 45,45,45    | 4.32 | 19 (42%) |
| 21  | CHD  | C     | 3525 | -    | 32,32,32     | 0.87 | 1 (3%)   | 51,51,51    | 1.60 | 12 (23%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | PGV  | P     | 4267 | -    | 50,50,50     | 1.01 | 2 (4%)   | 53,56,56    | 1.06 | 3 (5%)   |
| 23  | PEK  | C     | 3265 | -    | 52,52,52     | 1.67 | 11 (21%) | 55,57,57    | 1.00 | 4 (7%)   |
| 22  | CDL  | T     | 4269 | -    | 99,99,99     | 0.95 | 4 (4%)   | 105,111,111 | 0.96 | 9 (8%)   |

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   |
|-----|------|-------|------|------|-----------|----------------|---------|
| 18  | TGL  | L     | 3522 | -    | -         | 33/65/65/65    | -       |
| 19  | PGV  | A     | 3266 | -    | -         | 12/55/55/55    | -       |
| 21  | CHD  | B     | 4085 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 23  | PEK  | P     | 4265 | -    | -         | 24/56/56/56    | -       |
| 21  | CHD  | W     | 4060 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 22  | CDL  | G     | 3269 | -    | -         | 68/110/110/110 | -       |
| 19  | PGV  | N     | 4524 | -    | -         | 29/55/55/55    | -       |
| 21  | CHD  | J     | 3060 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 19  | PGV  | A     | 3524 | -    | -         | 29/55/55/55    | -       |
| 25  | PSC  | E     | 3230 | -    | -         | 35/55/55/55    | -       |
| 21  | CHD  | O     | 3085 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 18  | TGL  | Q     | 4523 | -    | -         | 27/65/65/65    | -       |
| 17  | HEA  | A     | 515  | 1    | -         | 6/36/76/76     | -       |
| 19  | PGV  | P     | 4268 | -    | -         | 33/55/55/55    | -       |
| 19  | PGV  | C     | 3267 | -    | -         | 18/55/55/55    | -       |
| 17  | HEA  | N     | 515  | 1    | -         | 7/36/76/76     | -       |
| 18  | TGL  | N     | 4522 | -    | -         | 35/65/65/65    | -       |
| 17  | HEA  | A     | 516  | 1    | -         | 7/36/76/76     | -       |
| 19  | PGV  | C     | 3268 | -    | -         | 33/55/55/55    | -       |
| 23  | PEK  | C     | 3264 | -    | -         | 16/56/56/56    | -       |
| 21  | CHD  | C     | 3271 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 18  | TGL  | N     | 4521 | -    | -         | 32/65/65/65    | -       |
| 18  | TGL  | D     | 3523 | -    | -         | 29/65/65/65    | -       |
| 23  | PEK  | T     | 3263 | -    | -         | 23/56/56/56    | -       |
| 27  | DMU  | M     | 3526 | -    | 5/5/10/10 | 6/19/59/59     | 0/2/2/2 |
| 21  | CHD  | P     | 4525 | -    | -         | 2/9/74/74      | 0/4/4/4 |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions       | Rings   |
|-----|------|-------|------|------|-----------|----------------|---------|
| 27  | DMU  | Z     | 4526 | -    | 5/5/10/10 | 6/19/59/59     | 0/2/2/2 |
| 23  | PEK  | G     | 4263 | -    | -         | 22/56/56/56    | -       |
| 18  | TGL  | A     | 3521 | -    | -         | 31/65/65/65    | -       |
| 21  | CHD  | P     | 4271 | -    | 5/5/12/12 | 8/9/74/74      | 0/4/4/4 |
| 17  | HEA  | N     | 516  | 1    | -         | 7/36/76/76     | -       |
| 19  | PGV  | N     | 4266 | -    | -         | 15/55/55/55    | -       |
| 22  | CDL  | C     | 3270 | -    | -         | 71/110/110/110 | -       |
| 22  | CDL  | P     | 4270 | -    | -         | 72/110/110/110 | -       |
| 23  | PEK  | P     | 4264 | -    | -         | 17/56/56/56    | -       |
| 25  | PSC  | O     | 4230 | -    | -         | 38/55/55/55    | -       |
| 21  | CHD  | C     | 3525 | -    | -         | 2/9/74/74      | 0/4/4/4 |
| 19  | PGV  | P     | 4267 | -    | -         | 15/55/55/55    | -       |
| 23  | PEK  | C     | 3265 | -    | -         | 24/56/56/56    | -       |
| 22  | CDL  | T     | 4269 | -    | -         | 67/110/110/110 | -       |

The worst 5 of 162 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 27  | M     | 3526 | DMU  | O7-C3  | -8.46 | 1.22        | 1.43     |
| 27  | Z     | 4526 | DMU  | O7-C3  | -8.26 | 1.22        | 1.43     |
| 27  | Z     | 4526 | DMU  | O16-C6 | -7.80 | 1.27        | 1.40     |
| 27  | M     | 3526 | DMU  | O16-C6 | -7.35 | 1.28        | 1.40     |
| 27  | M     | 3526 | DMU  | O1-C9  | -7.05 | 1.27        | 1.44     |

The worst 5 of 333 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 21  | C     | 3271 | CHD  | C17-C13-C14 | 10.50  | 110.64      | 100.11   |
| 27  | M     | 3526 | DMU  | C10-C5-C7   | 10.43  | 131.95      | 110.01   |
| 27  | Z     | 4526 | DMU  | C10-C5-C7   | 10.33  | 131.73      | 110.01   |
| 21  | C     | 3271 | CHD  | C17-C13-C12 | -10.12 | 108.56      | 117.67   |
| 21  | P     | 4271 | CHD  | C17-C13-C14 | 10.08  | 110.22      | 100.11   |

5 of 30 chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 21  | C     | 3271 | CHD  | C14  |
| 21  | C     | 3271 | CHD  | C8   |
| 21  | C     | 3271 | CHD  | C3   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 21  | C     | 3271 | CHD  | C9   |
| 21  | C     | 3271 | CHD  | C12  |

5 of 927 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | A     | 3521 | TGL  | CB2-CB1-OG2-CG2 |
| 18  | A     | 3521 | TGL  | OB1-CB1-OG2-CG2 |
| 18  | A     | 3521 | TGL  | OG1-CG1-CG2-OG2 |
| 18  | D     | 3523 | TGL  | CB2-CB1-OG2-CG2 |
| 18  | D     | 3523 | TGL  | OB1-CB1-OG2-CG2 |

There are no ring outliers.

32 monomers are involved in 270 short contacts:

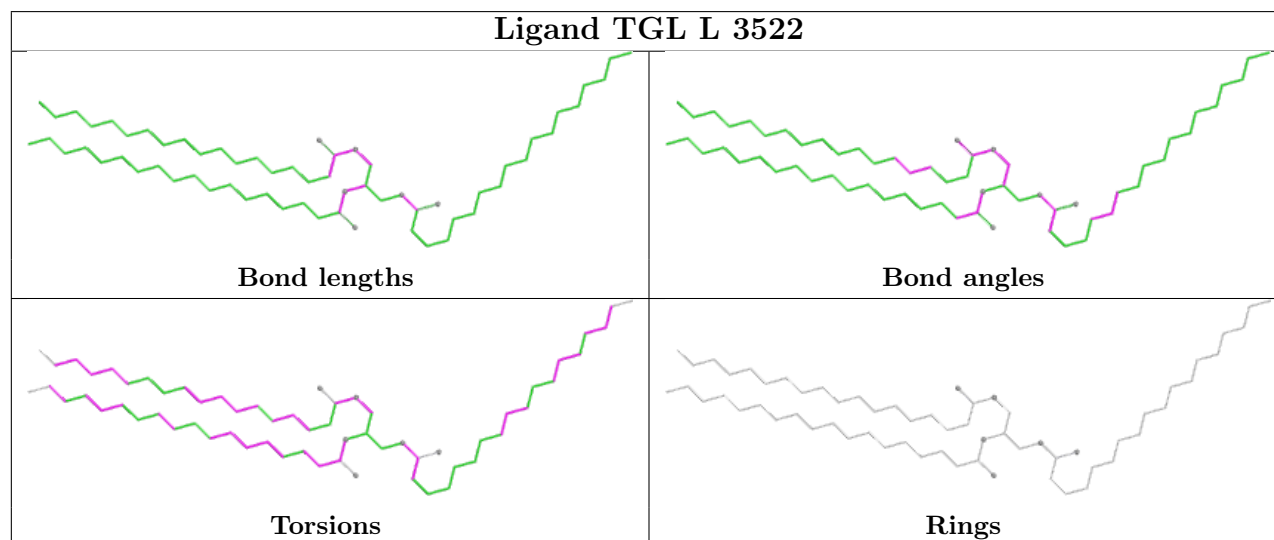
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18  | L     | 3522 | TGL  | 25      | 0            |
| 21  | B     | 4085 | CHD  | 1       | 0            |
| 23  | P     | 4265 | PEK  | 2       | 0            |
| 21  | W     | 4060 | CHD  | 2       | 0            |
| 22  | G     | 3269 | CDL  | 14      | 0            |
| 19  | N     | 4524 | PGV  | 5       | 0            |
| 19  | A     | 3524 | PGV  | 7       | 0            |
| 21  | J     | 3060 | CHD  | 2       | 0            |
| 25  | E     | 3230 | PSC  | 13      | 0            |
| 21  | O     | 3085 | CHD  | 1       | 0            |
| 18  | Q     | 4523 | TGL  | 15      | 0            |
| 17  | A     | 515  | HEA  | 2       | 0            |
| 19  | C     | 3267 | PGV  | 7       | 0            |
| 17  | N     | 515  | HEA  | 3       | 0            |
| 18  | N     | 4522 | TGL  | 20      | 0            |
| 17  | A     | 516  | HEA  | 1       | 0            |
| 19  | C     | 3268 | PGV  | 1       | 0            |
| 23  | C     | 3264 | PEK  | 4       | 0            |
| 21  | C     | 3271 | CHD  | 3       | 0            |
| 18  | N     | 4521 | TGL  | 19      | 0            |
| 18  | D     | 3523 | TGL  | 15      | 0            |
| 23  | T     | 3263 | PEK  | 9       | 0            |
| 23  | G     | 4263 | PEK  | 10      | 0            |
| 23  | P     | 4264 | PEK  | 4       | 0            |
| 18  | A     | 3521 | TGL  | 11      | 0            |
| 21  | P     | 4271 | CHD  | 2       | 0            |

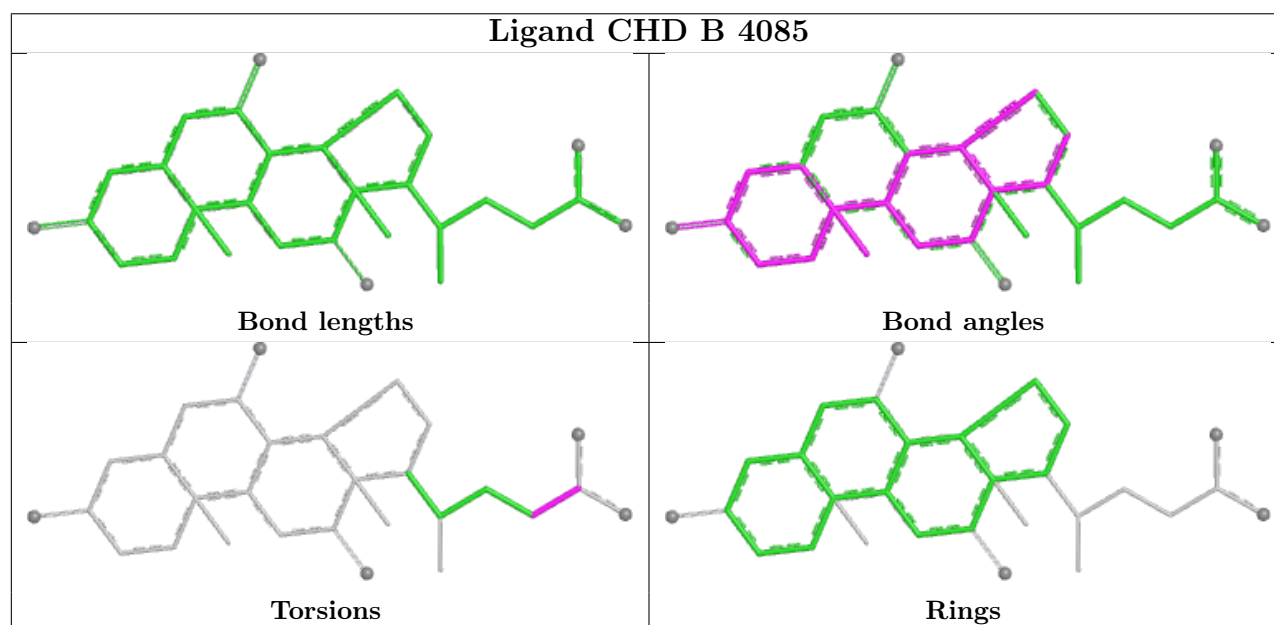
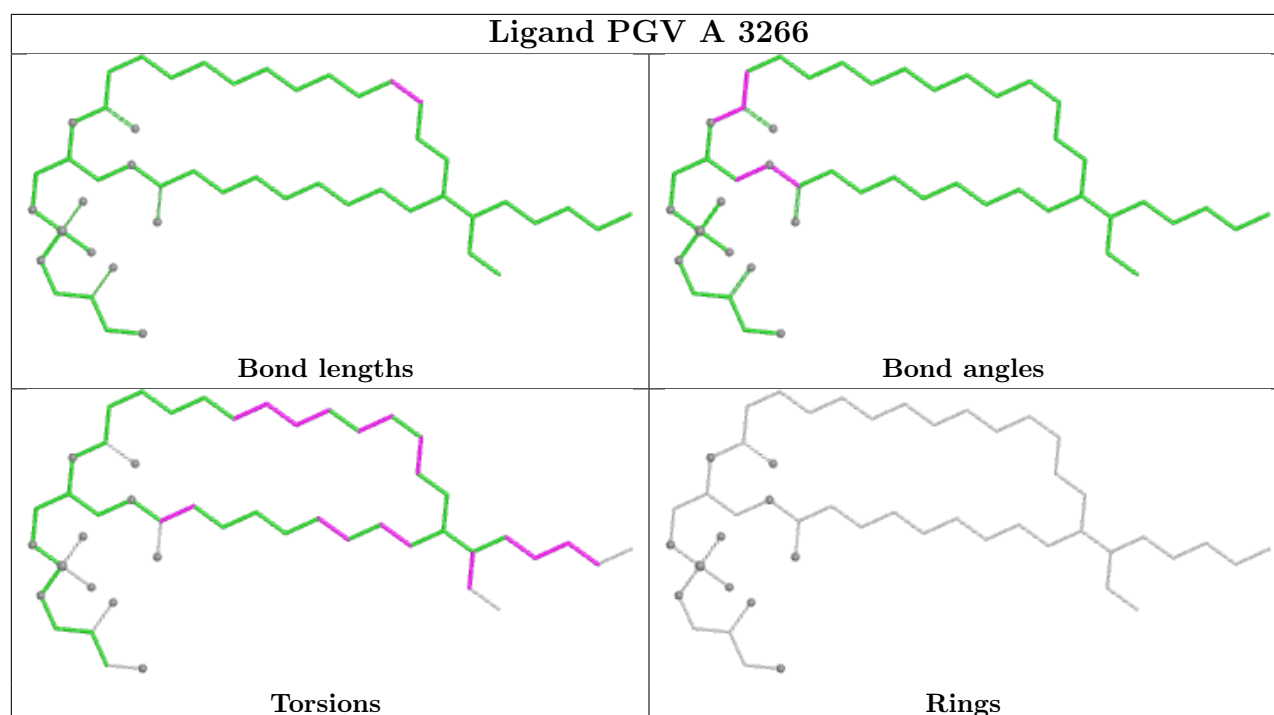
*Continued on next page...*

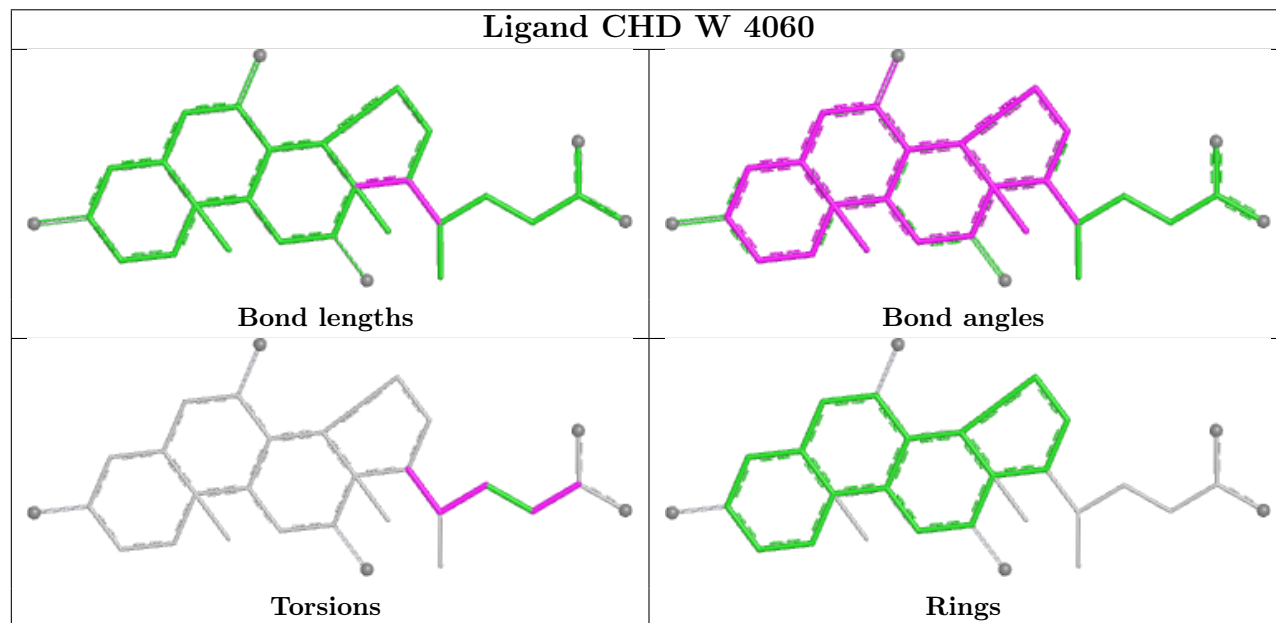
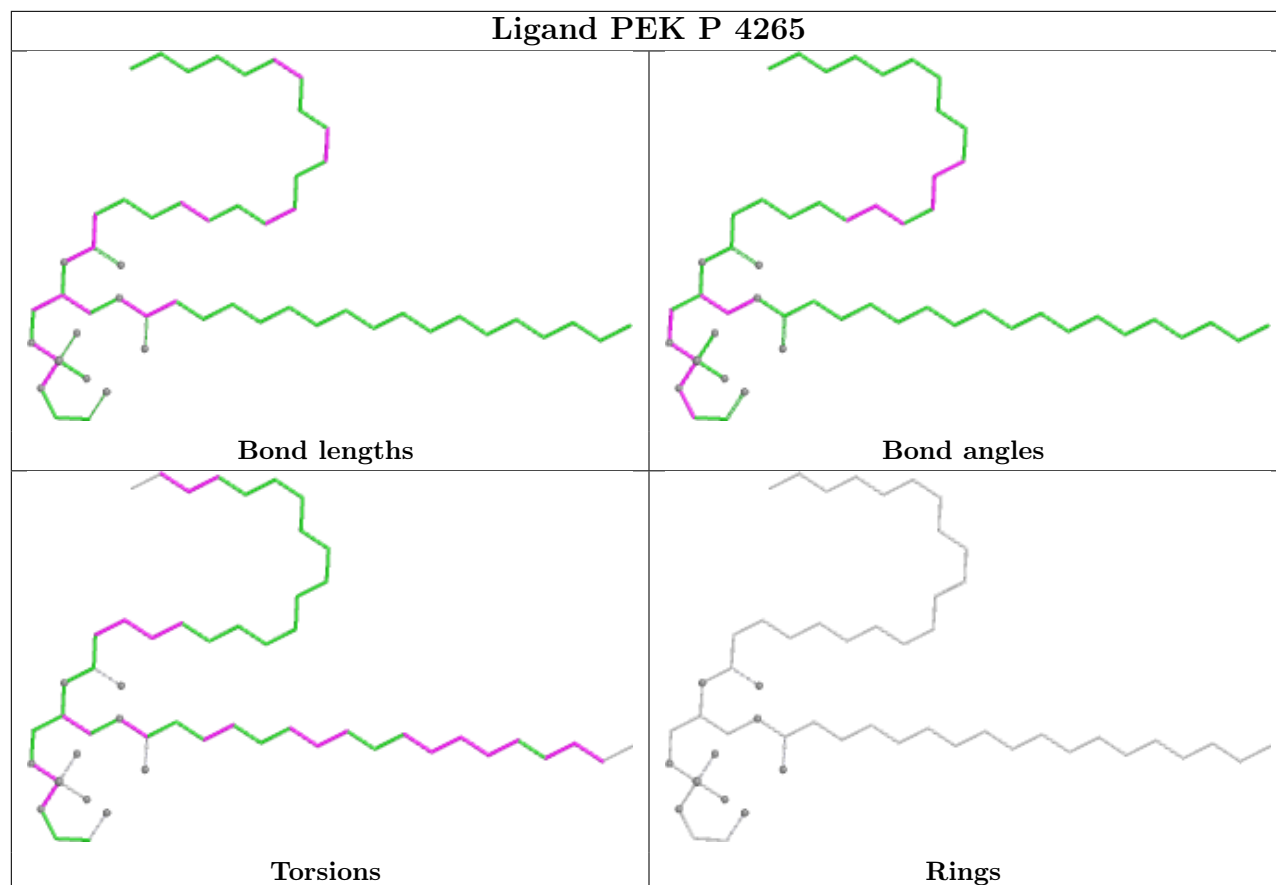
*Continued from previous page...*

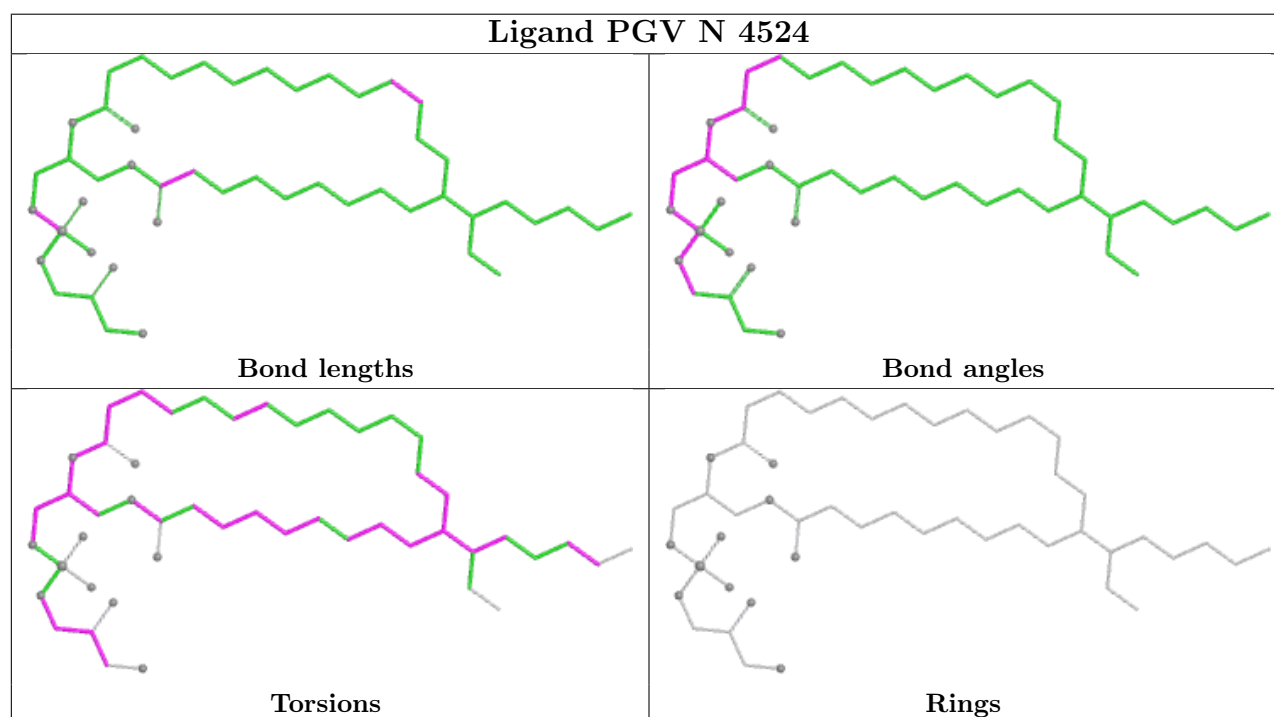
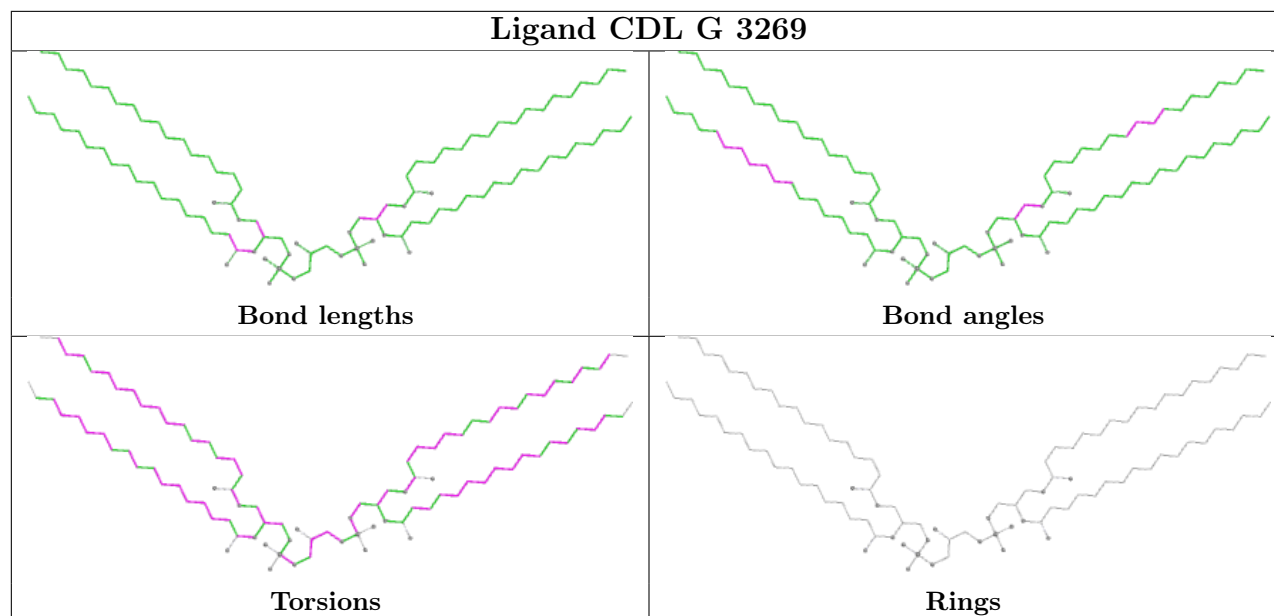
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | C     | 3270 | CDL  | 14      | 0            |
| 22  | P     | 4270 | CDL  | 19      | 0            |
| 25  | O     | 4230 | PSC  | 21      | 0            |
| 19  | P     | 4267 | PGV  | 9       | 0            |
| 23  | C     | 3265 | PEK  | 3       | 0            |
| 22  | T     | 4269 | CDL  | 15      | 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.

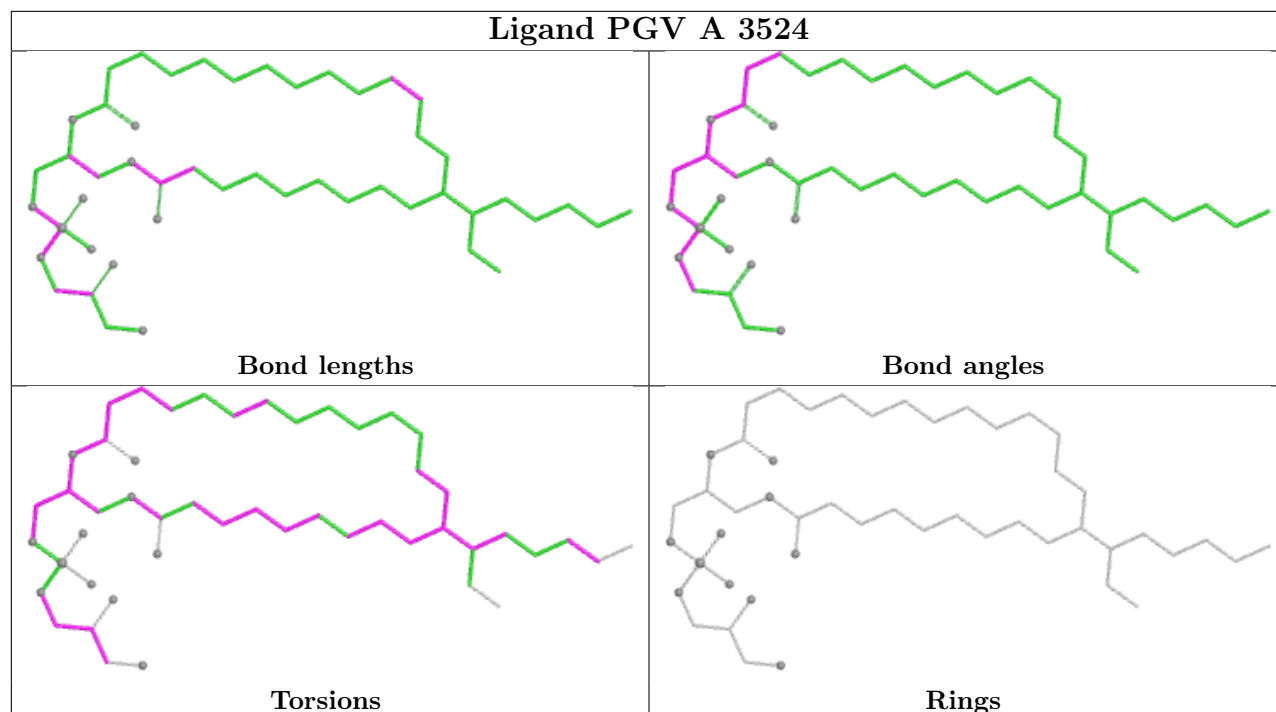




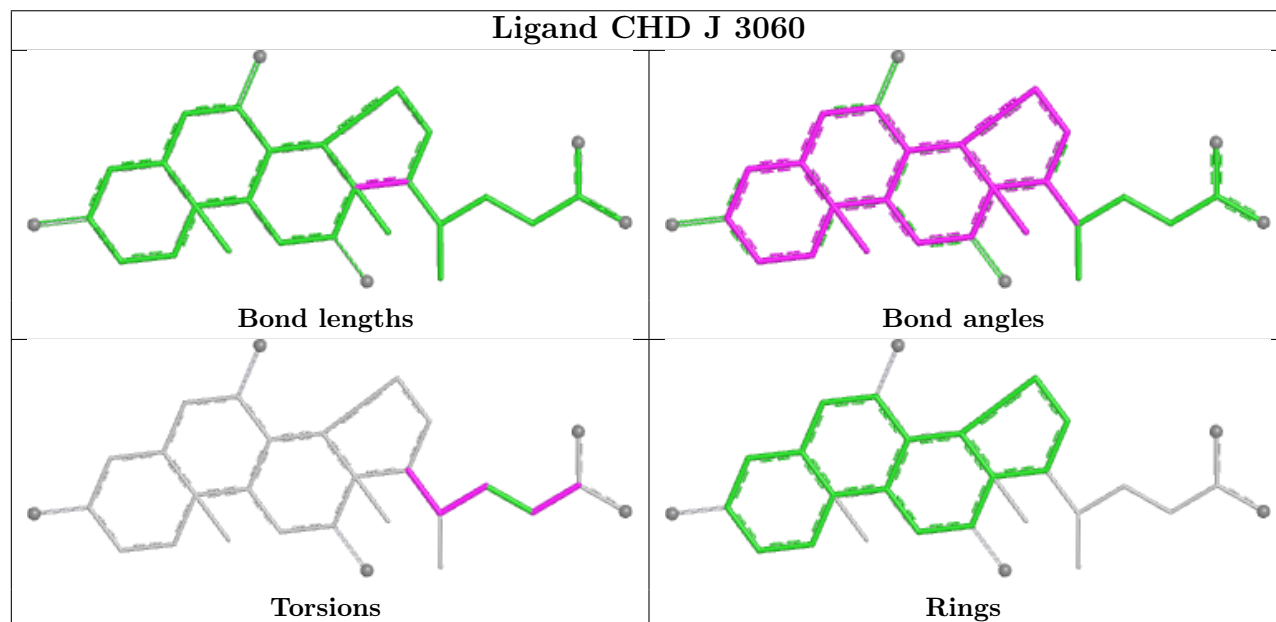


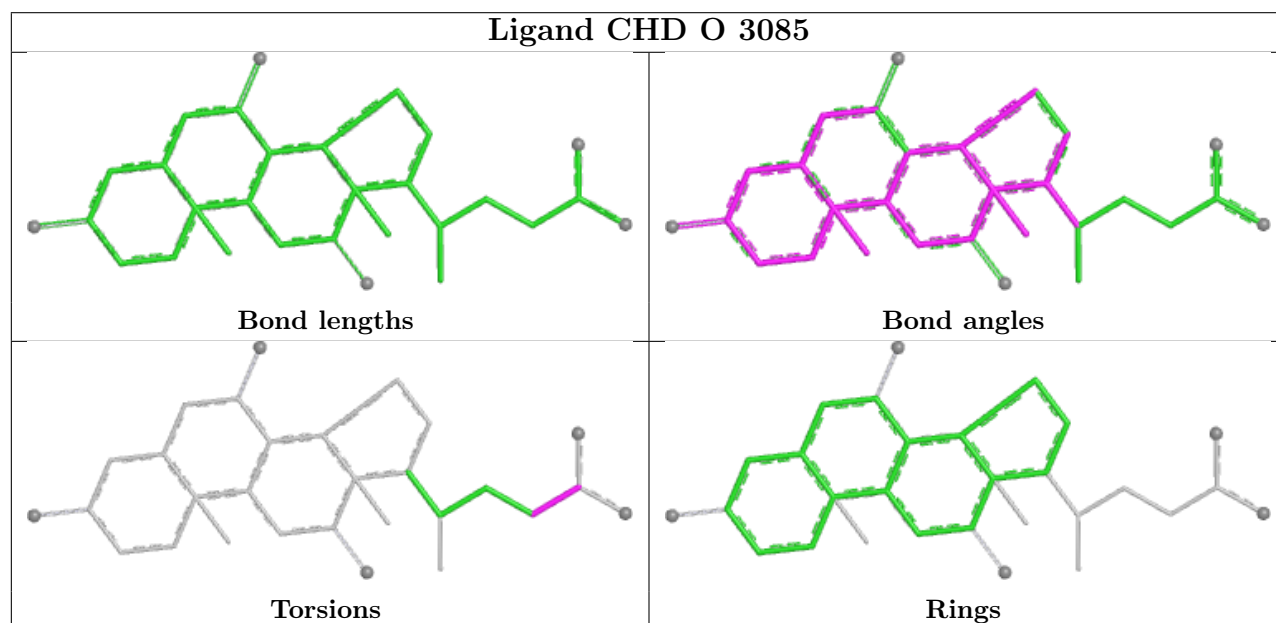
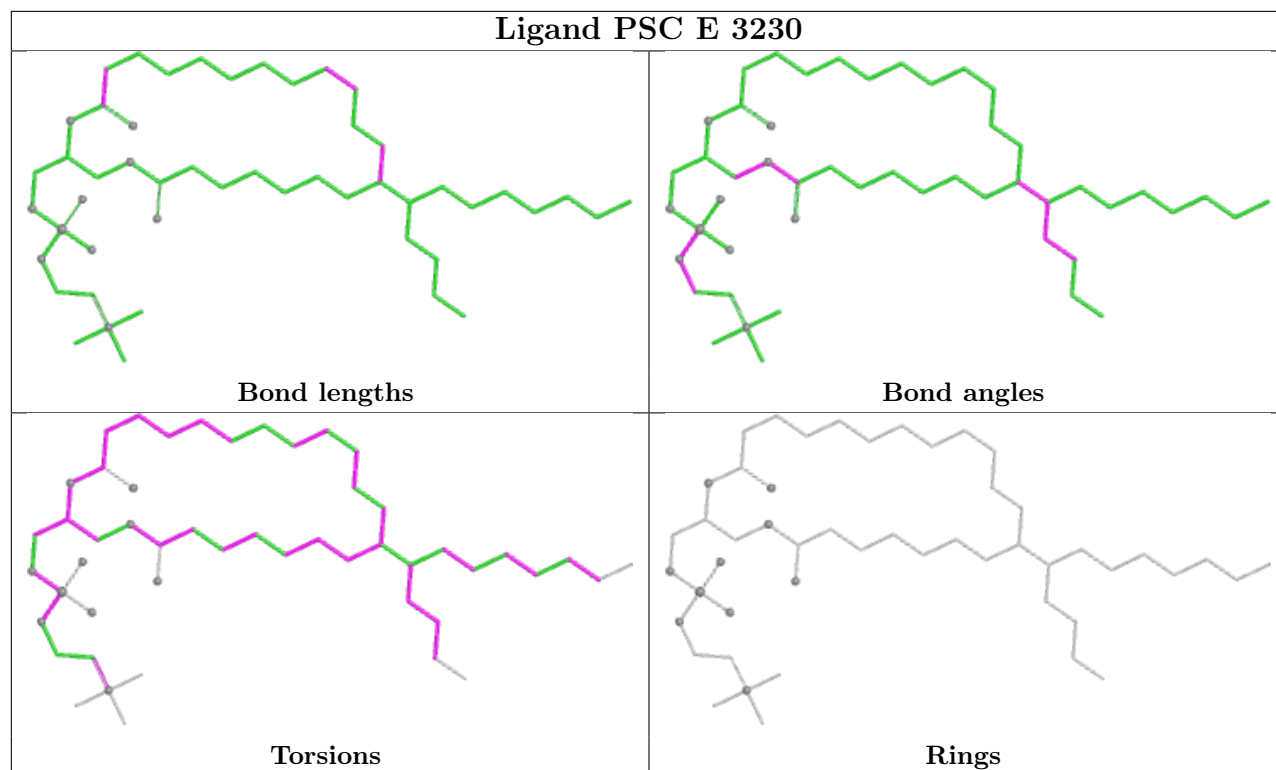


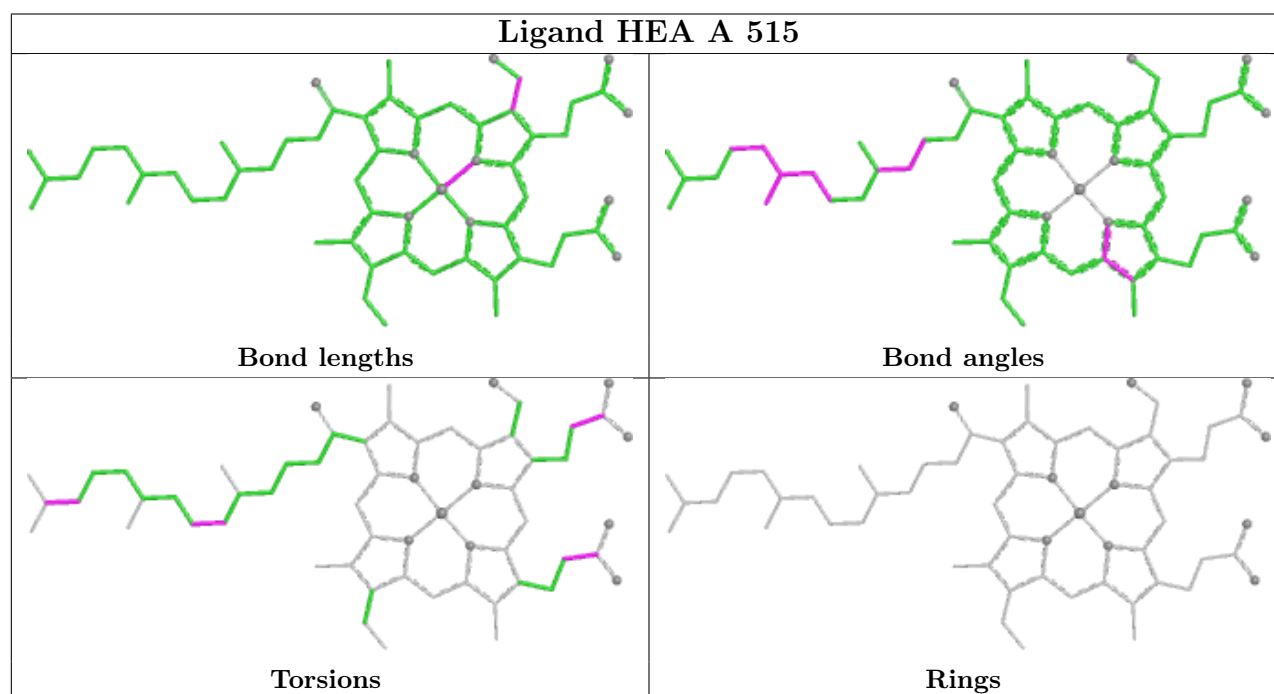
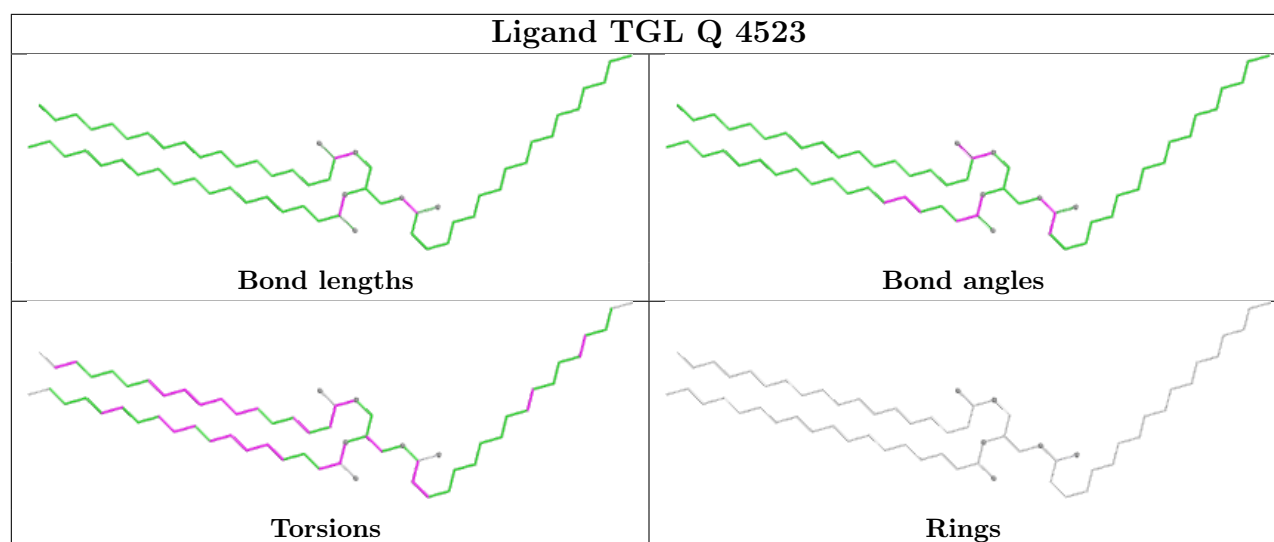
## Ligand PGV A 3524

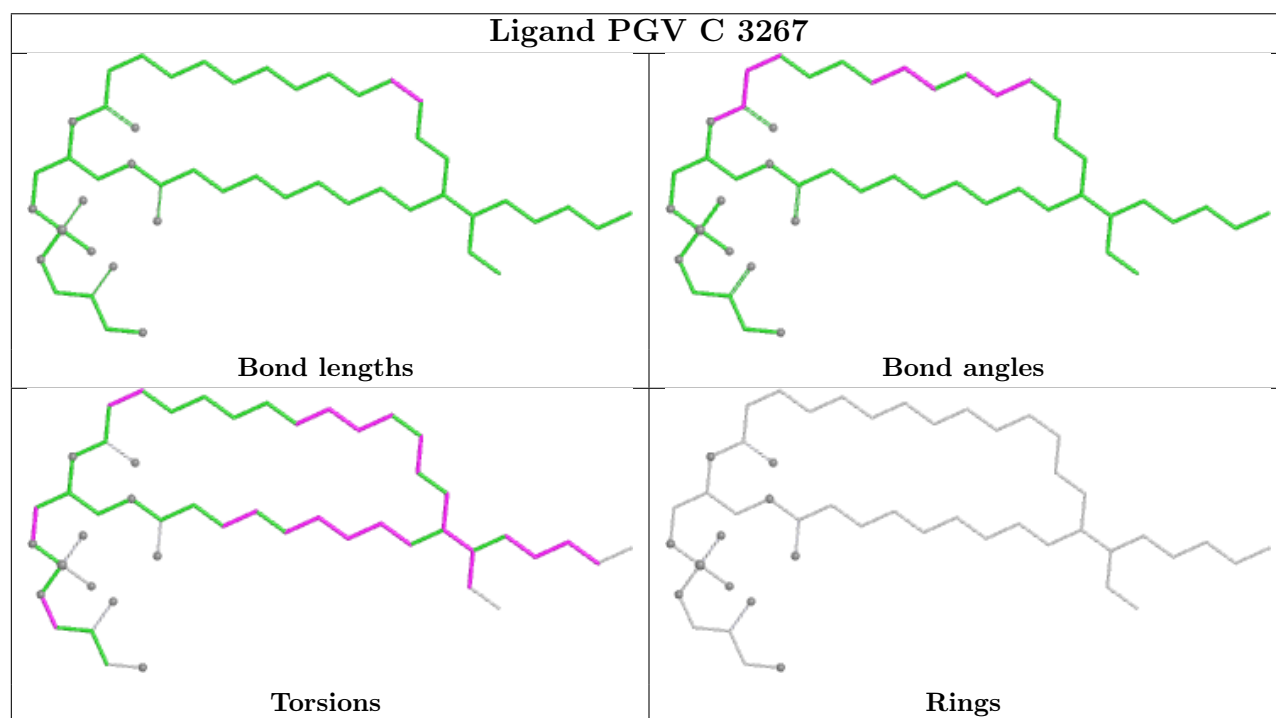
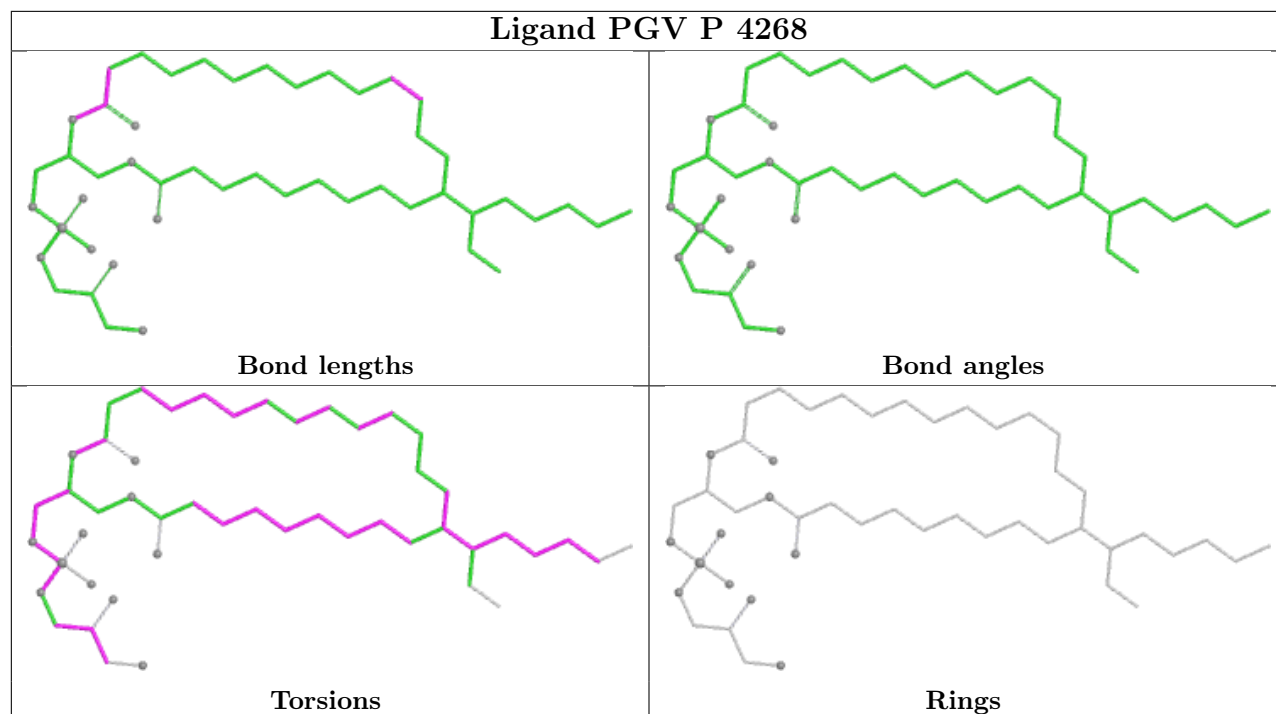


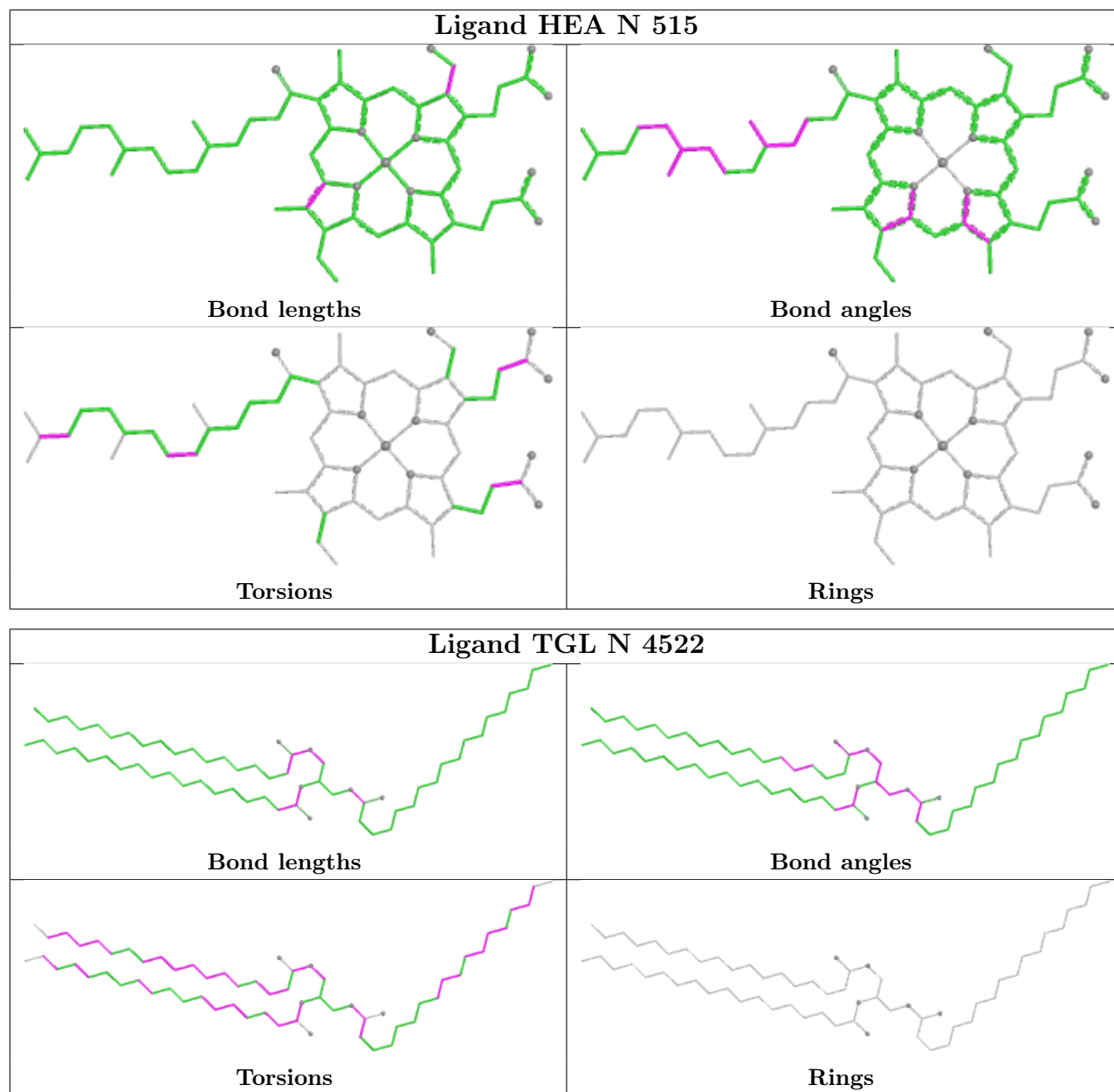
## Ligand CHD J 3060

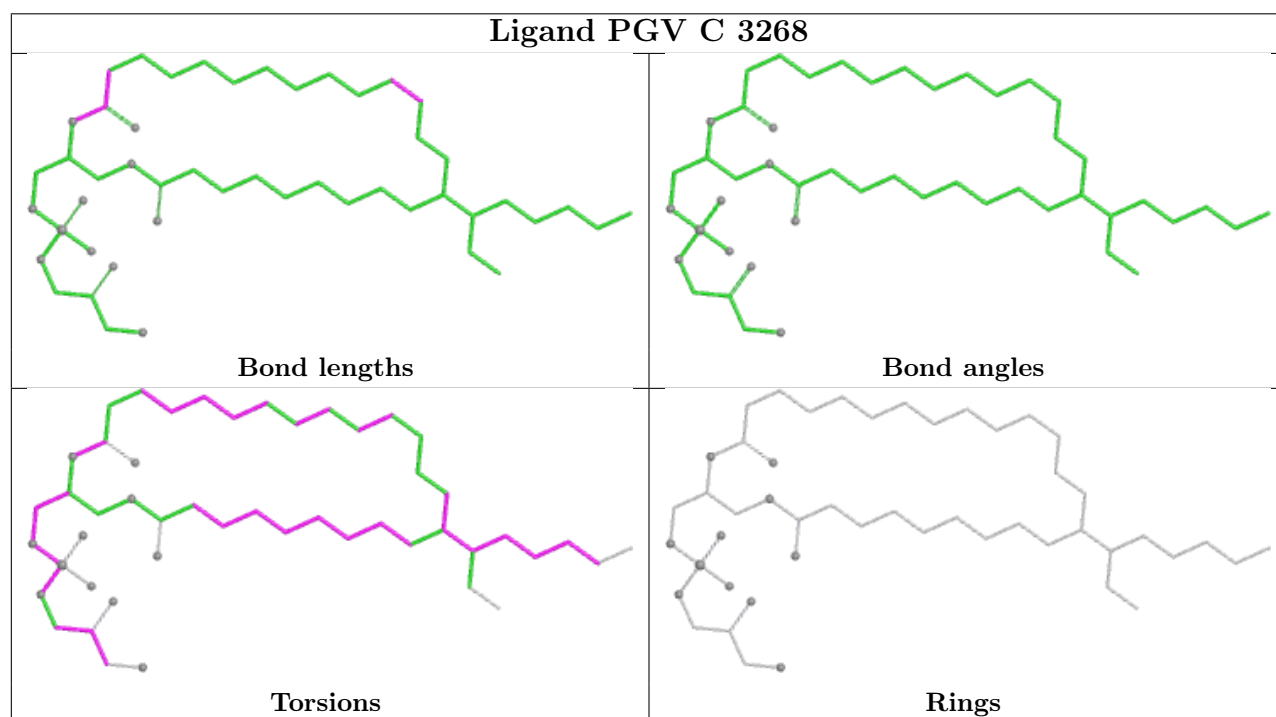
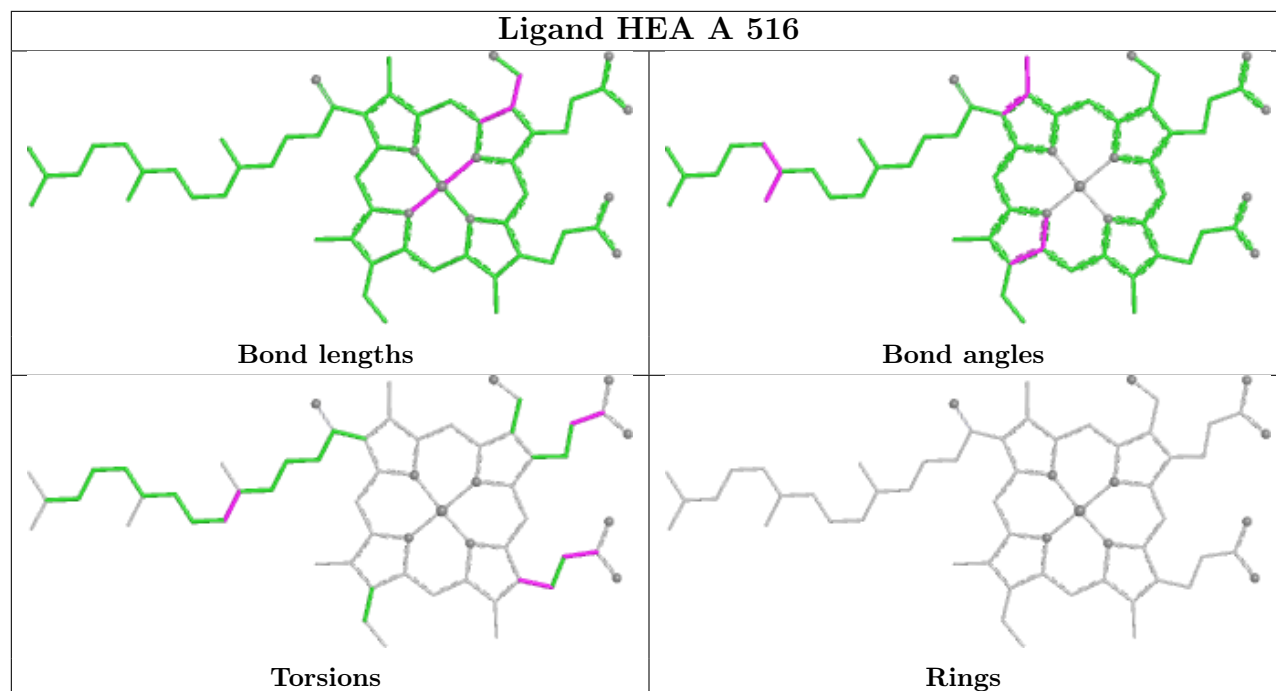




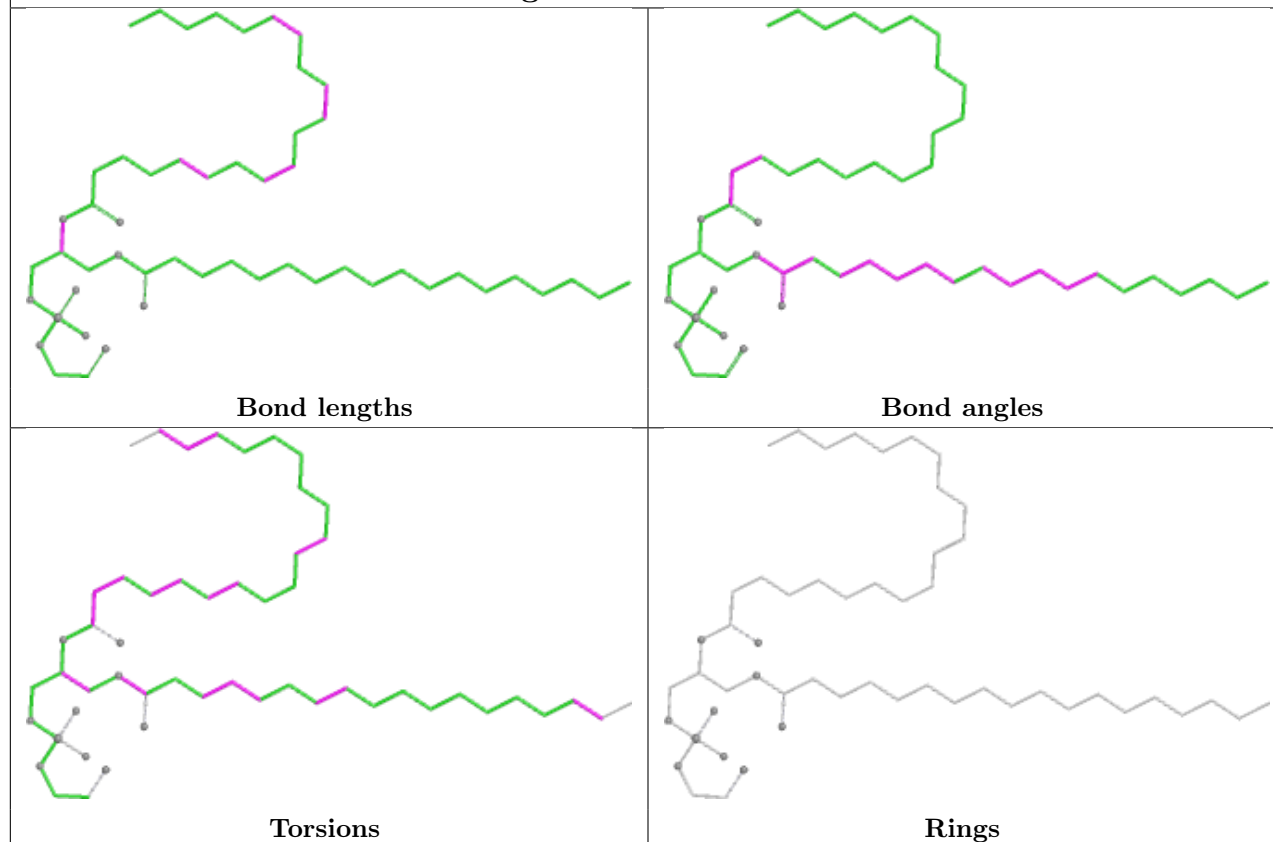




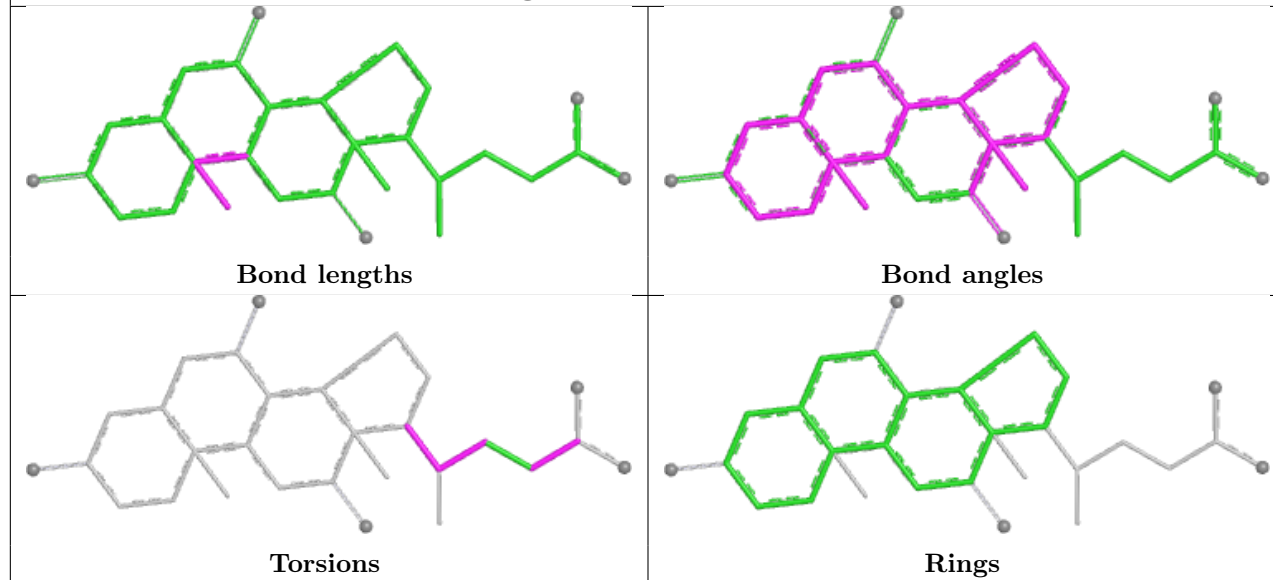


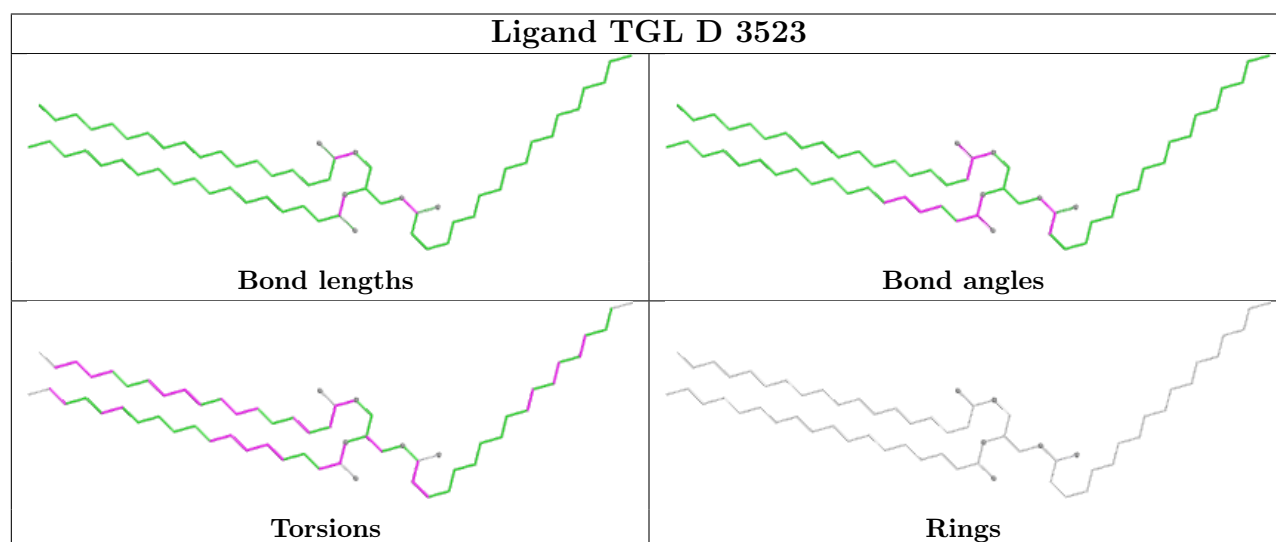
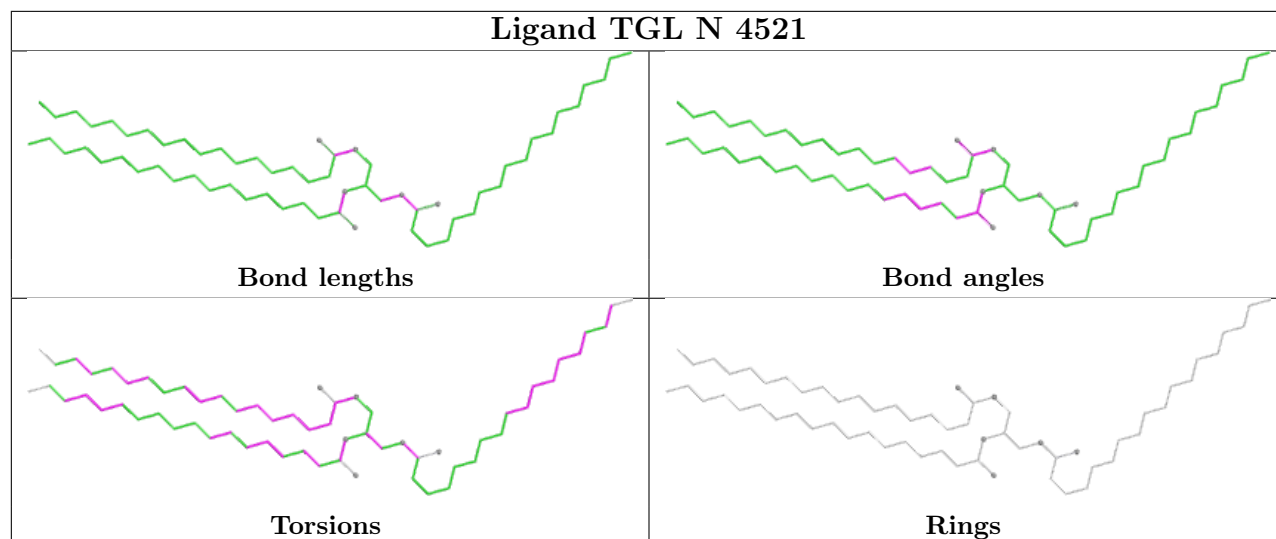


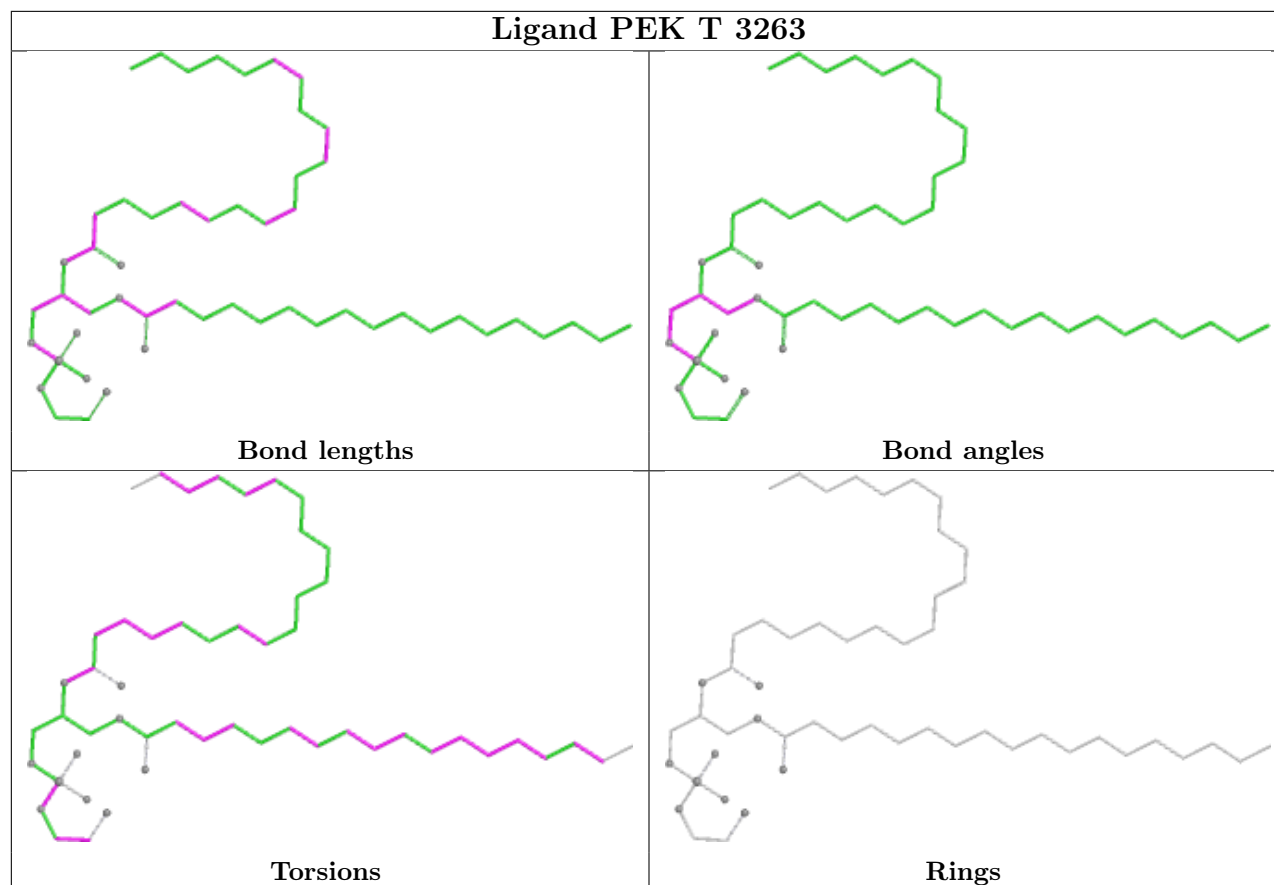
## Ligand PEK C 3264



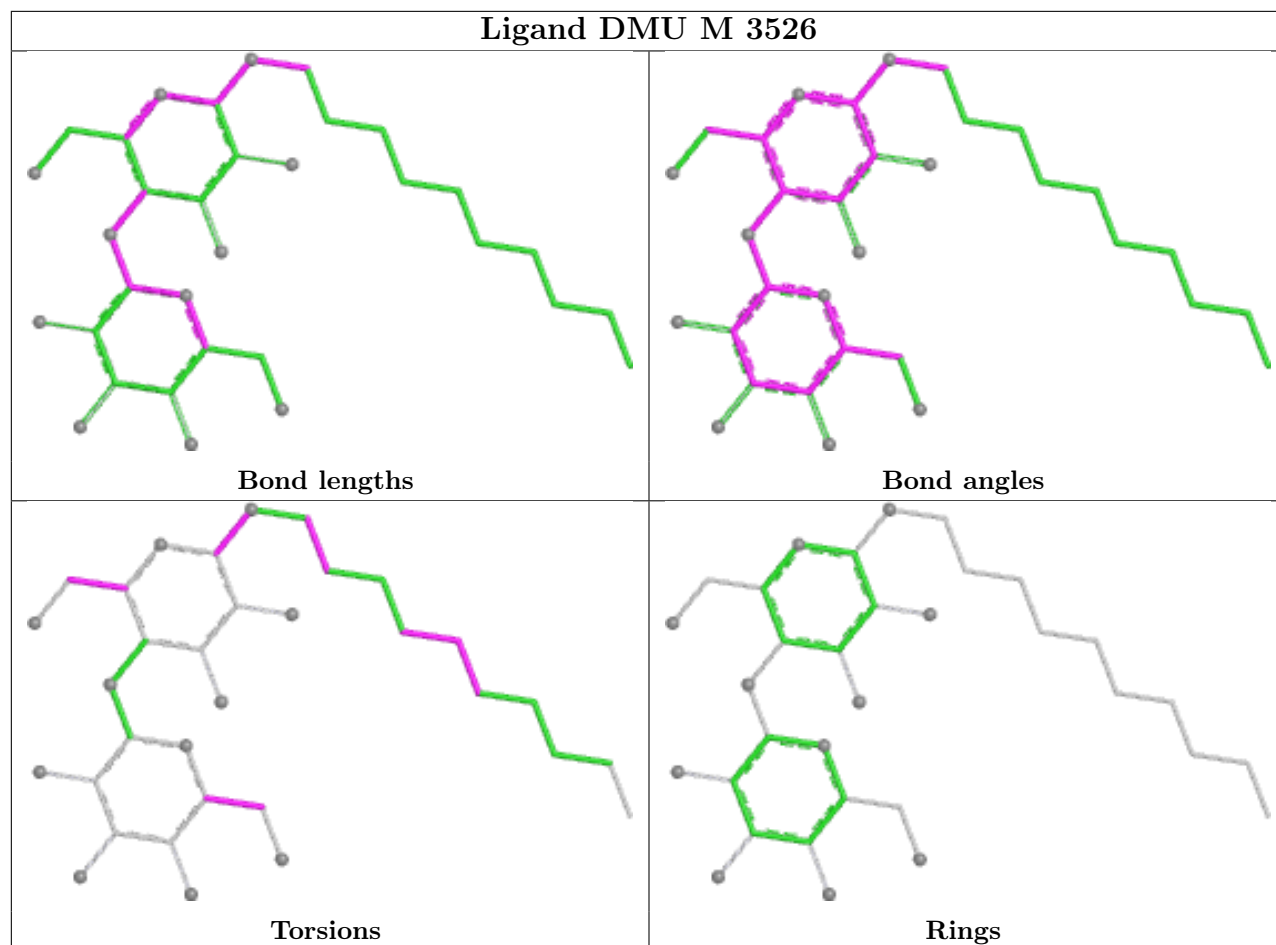
## Ligand CHD C 3271



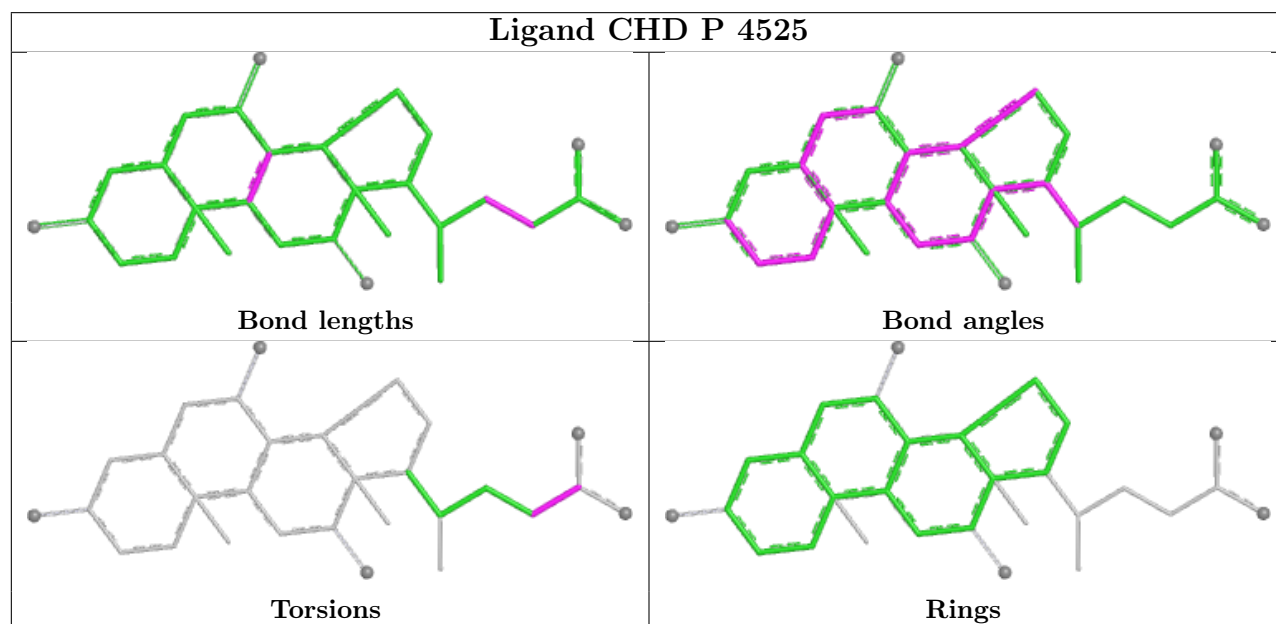




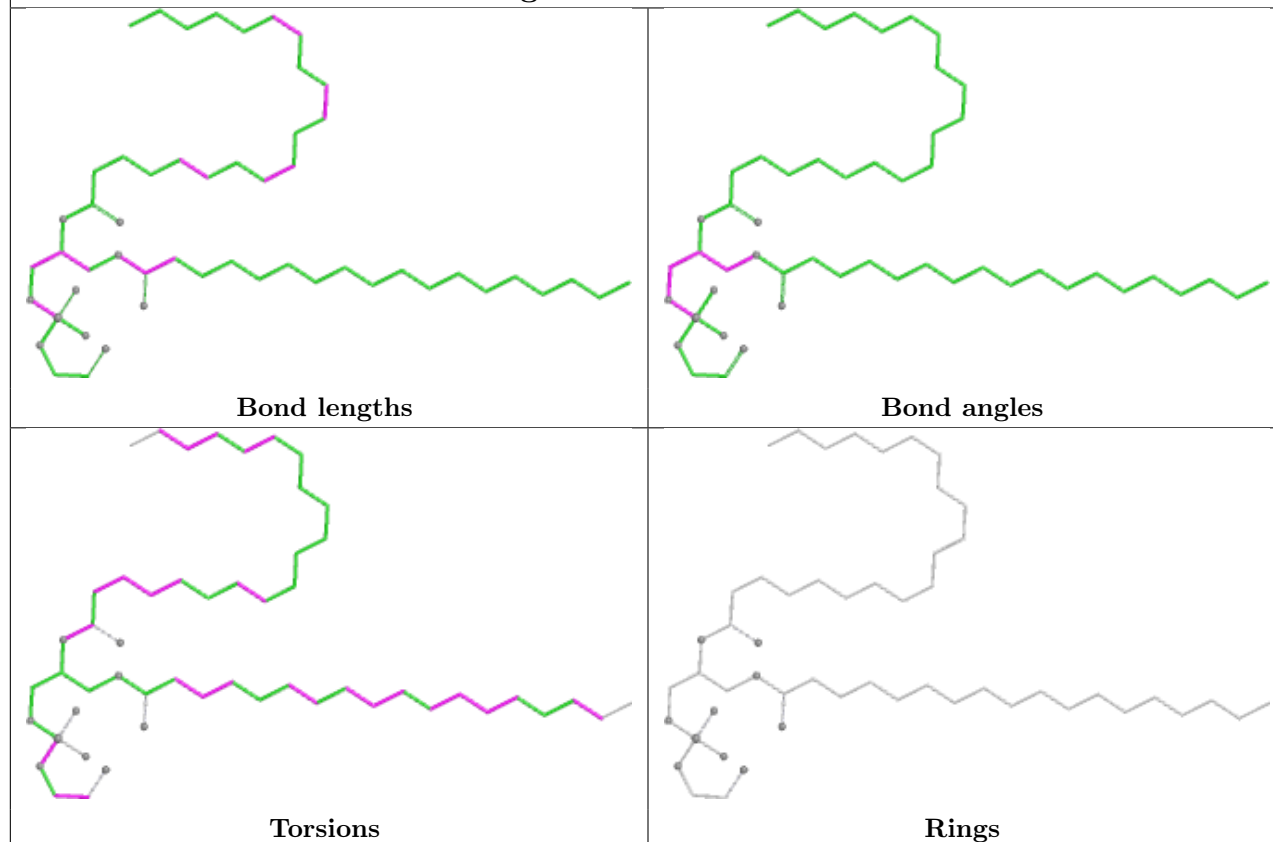
## Ligand DMU M 3526



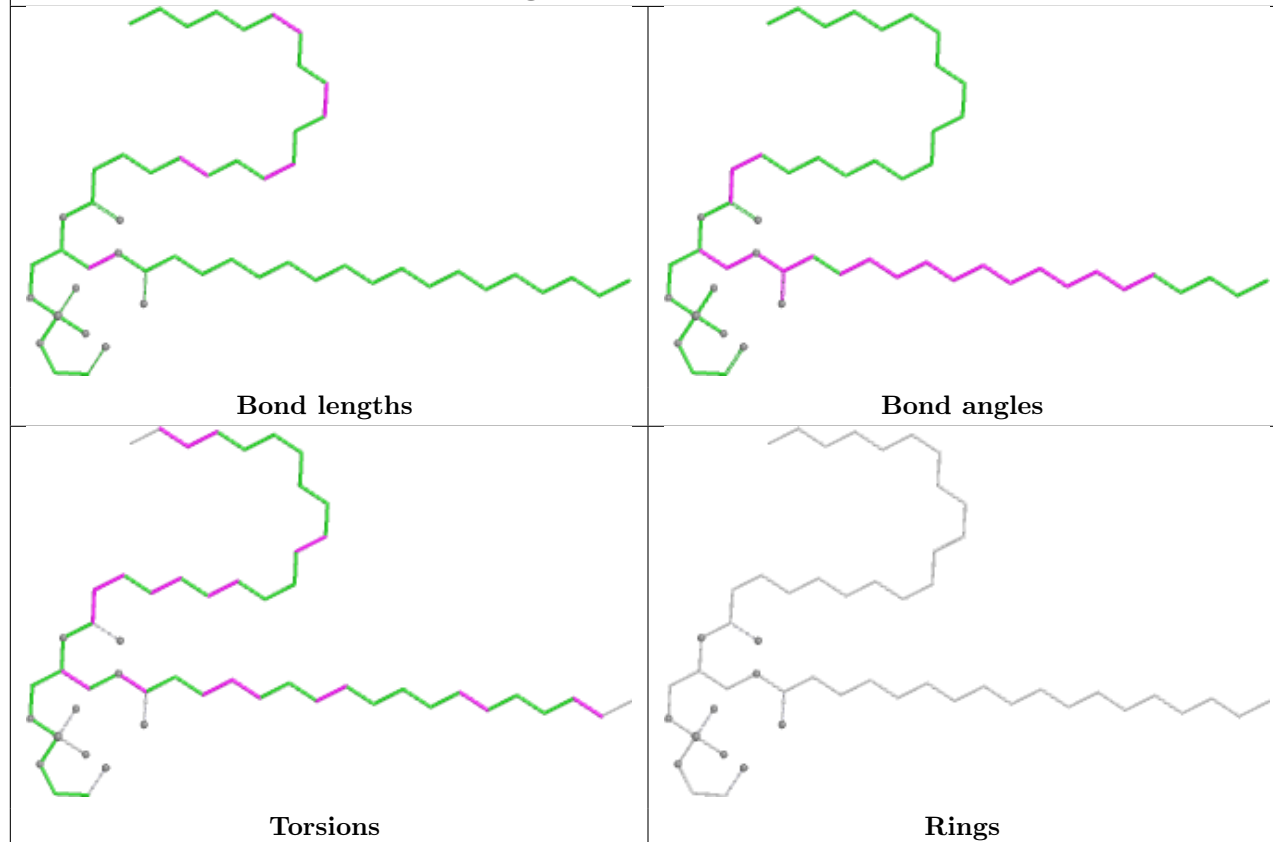
## Ligand CHD P 4525

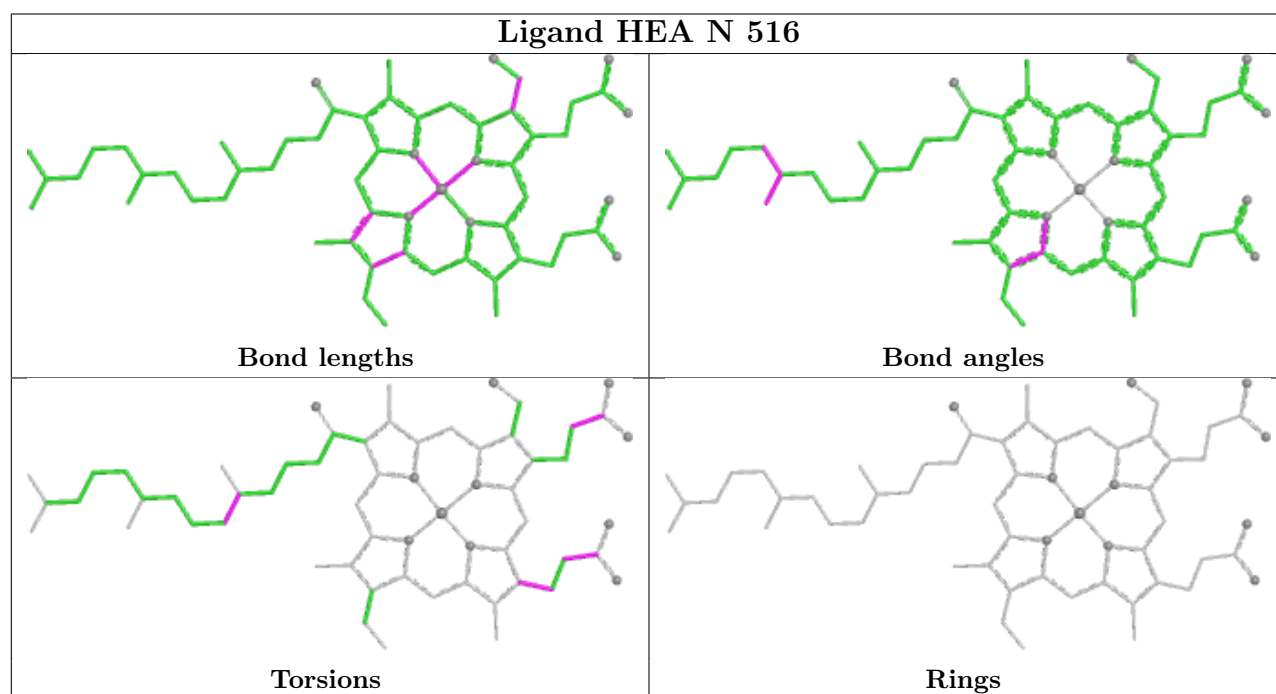
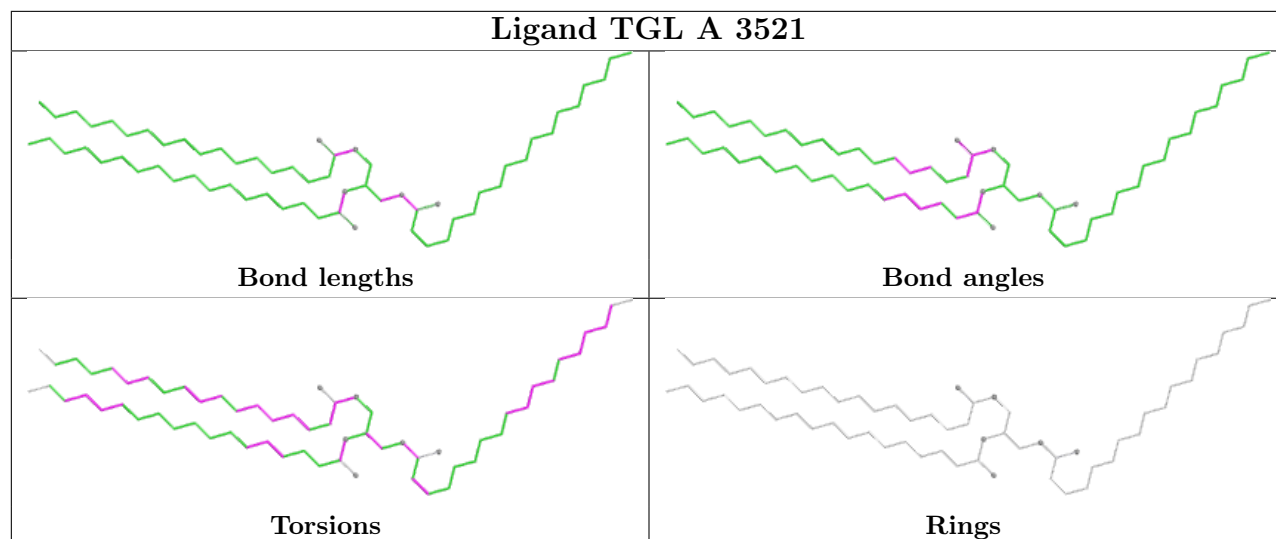


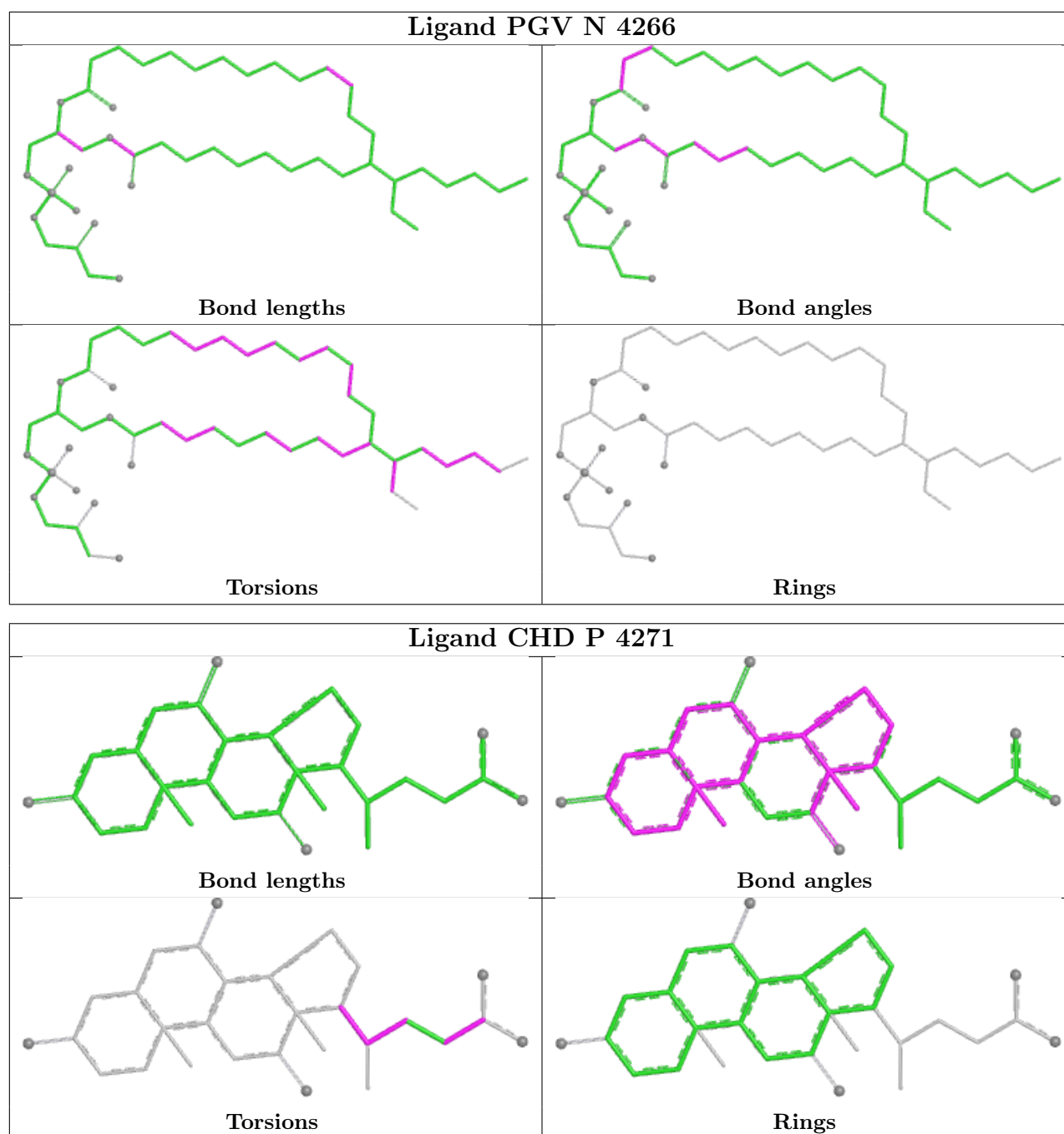
## Ligand PEK G 4263

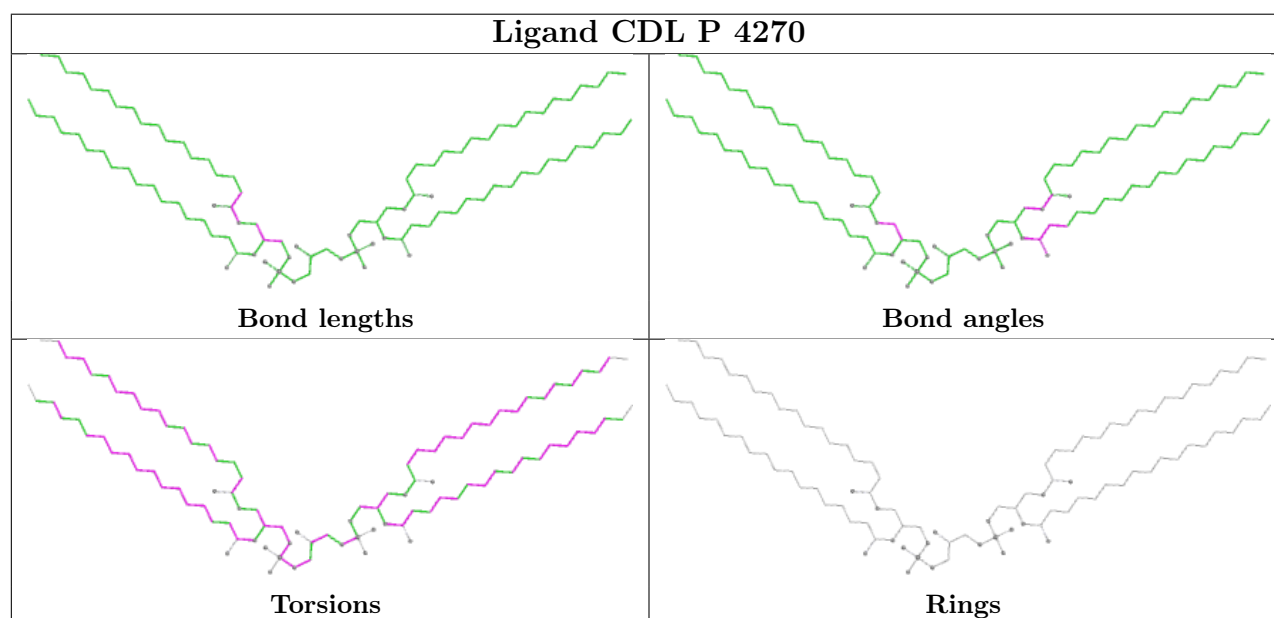
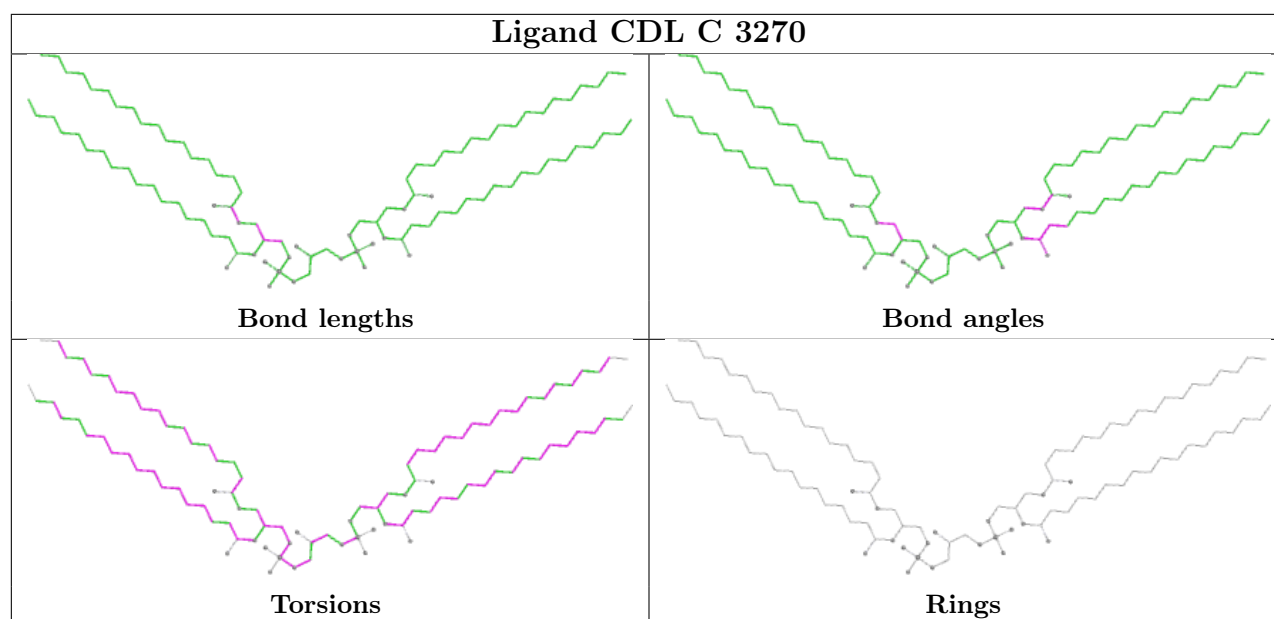


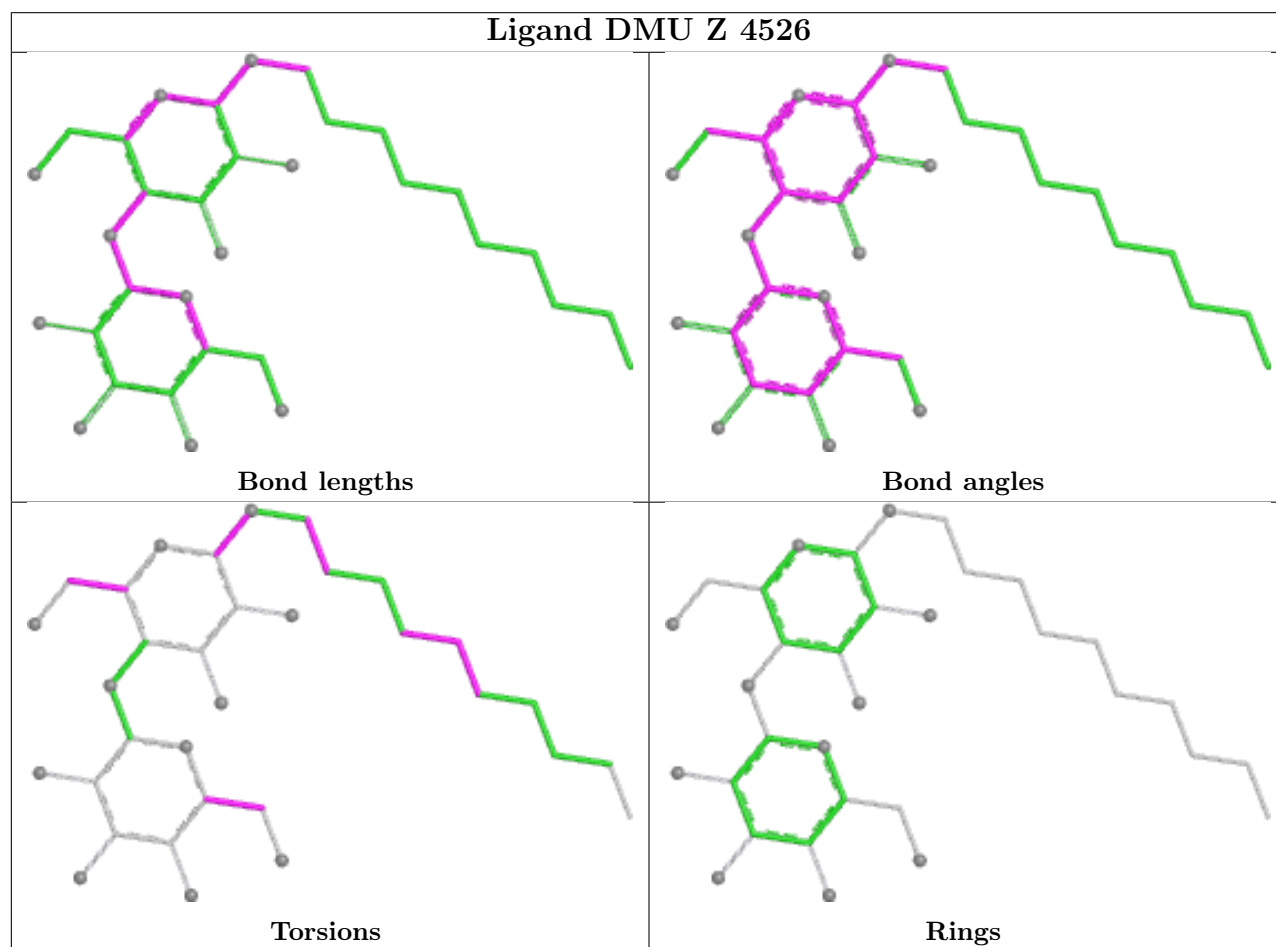
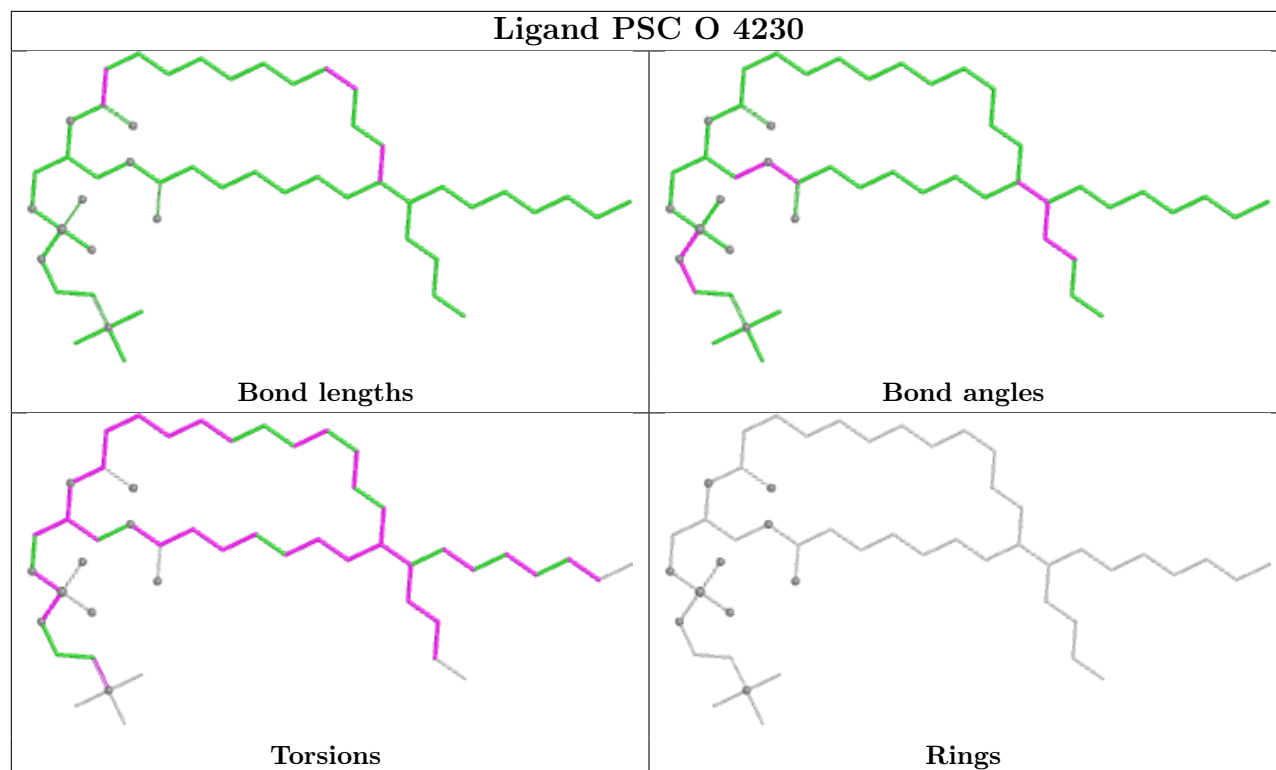
## Ligand PEK P 4264

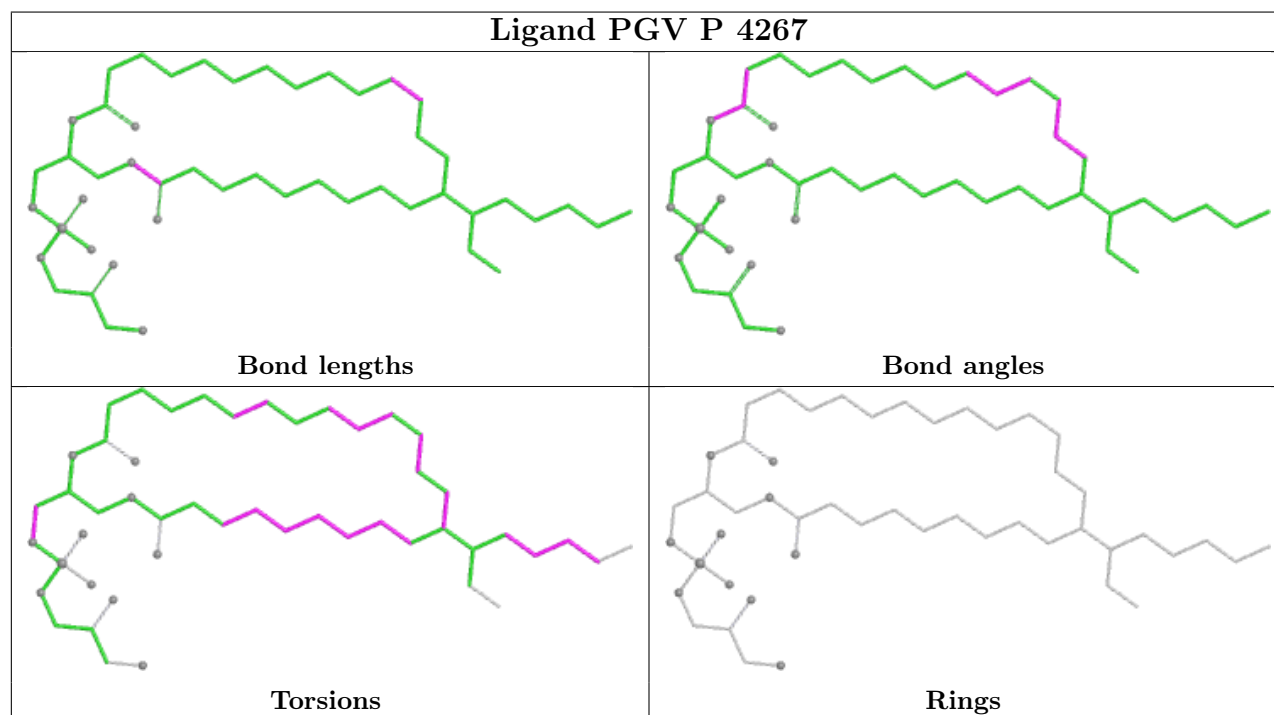
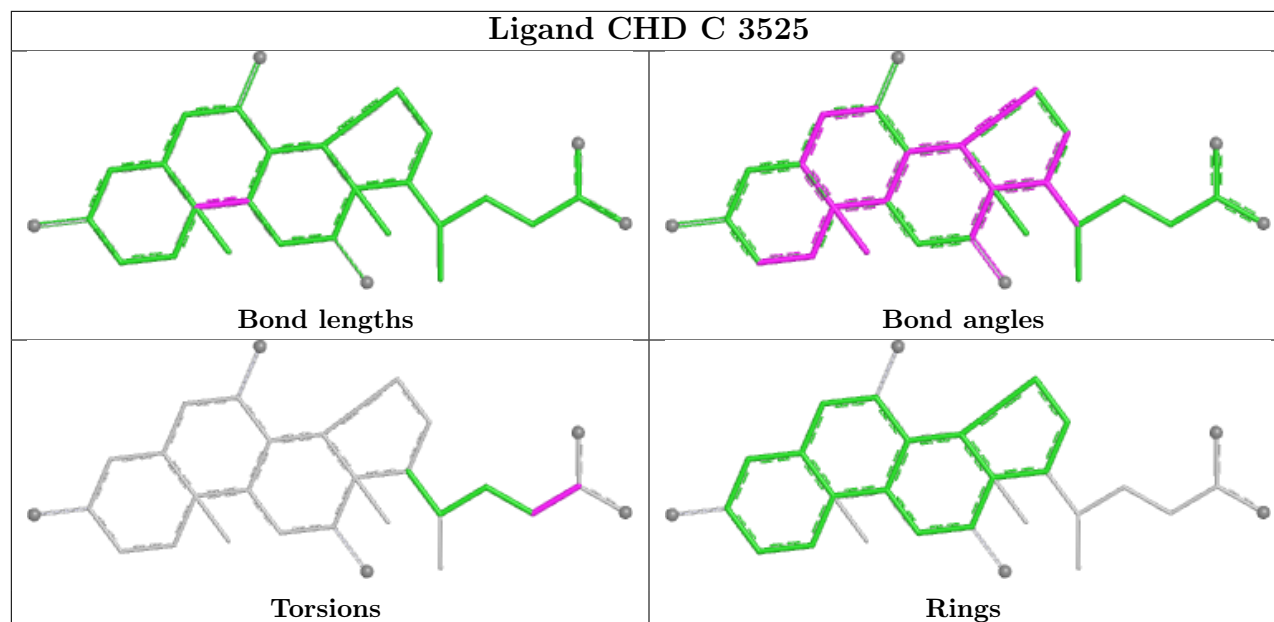


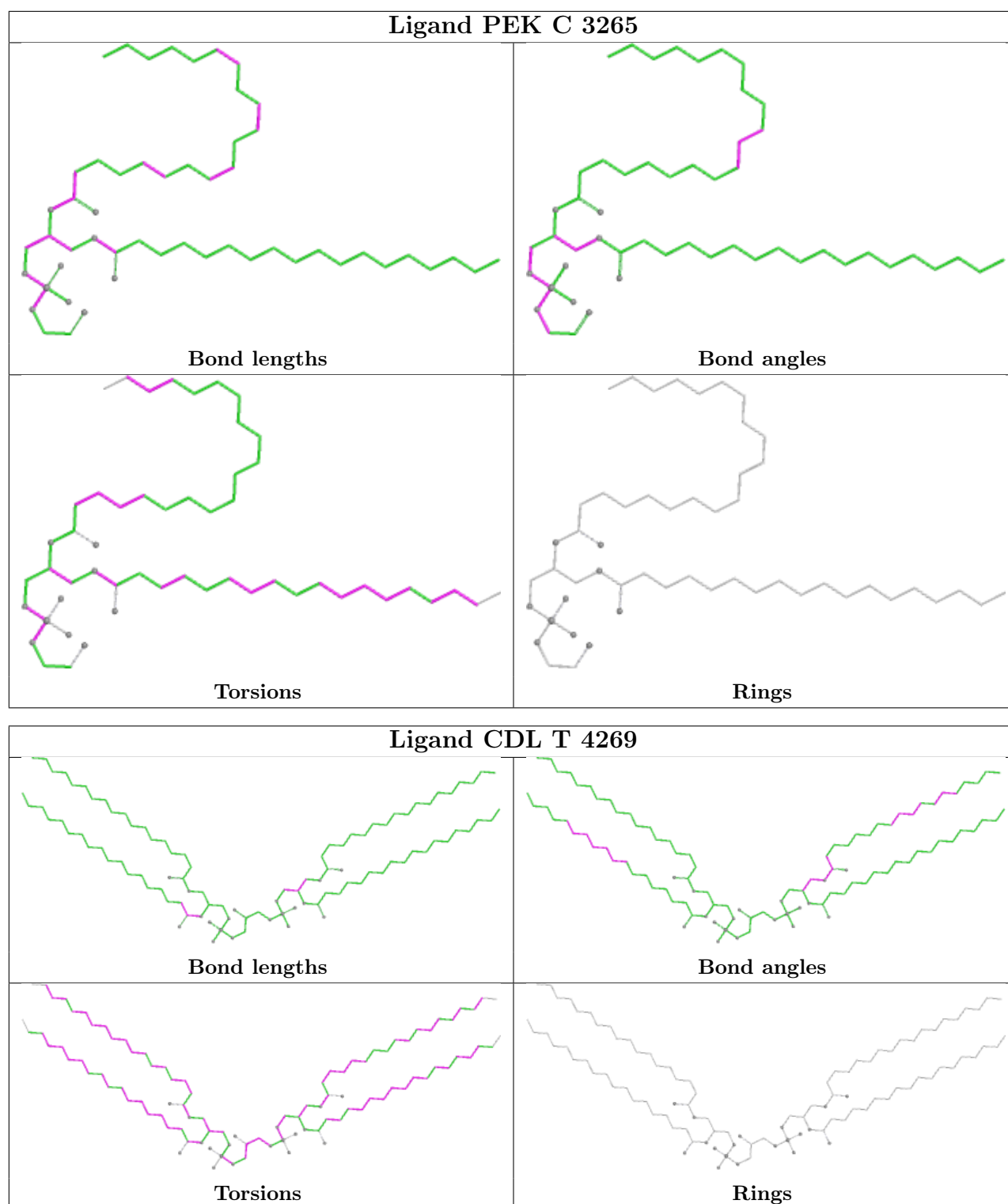












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.