



## wwPDB EM Validation Summary Report ⓘ

Dec 29, 2024 – 10:47 AM EST

PDB ID : 7O0X  
EMDB ID : EMD-12682  
Title : Cryo-EM structure (model\_2b) of the RC-dLH complex from Gemmatimonas phototrophica at 2.44 Å  
Authors : Qian, P.; Koblizek, M.  
Deposited on : 2021-03-28  
Resolution : 2.44 Å (reported)  
Based on initial models : 1LGH, 6ET5, 5Y5S

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

The types of validation reports are described at

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

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

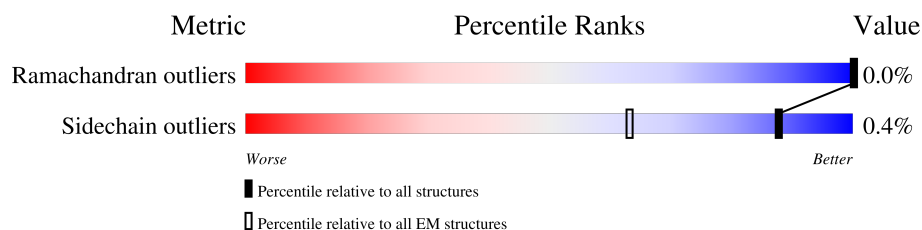
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.44 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.













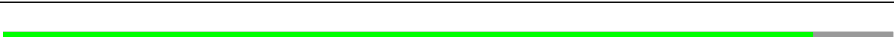


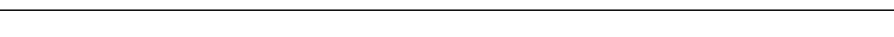
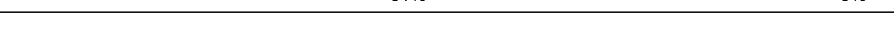
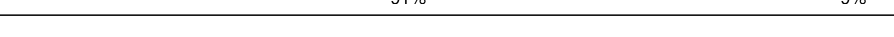



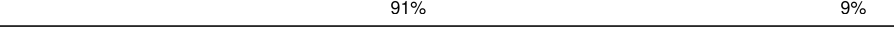





| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894          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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AA    | 54     | 89% 9%           |
| 1   | AB    | 54     | 89% 9%           |
| 1   | AC    | 54     | 87% 11%          |
| 1   | AD    | 54     | 87% 11%          |
| 1   | AE    | 54     | 89% 9%           |
| 1   | AF    | 54     | 89% 9%           |
| 1   | AG    | 54     | 89% 9%           |
| 1   | AH    | 54     | 89% 9%           |
| 1   | AI    | 54     | 89% 9%           |









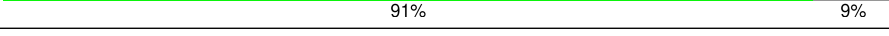

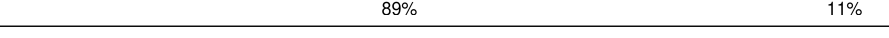
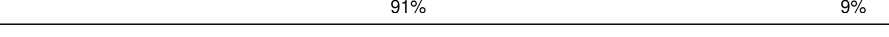
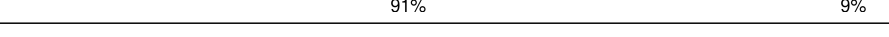
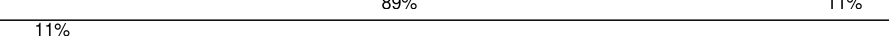


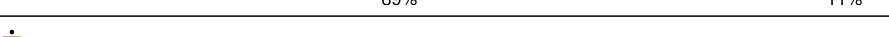

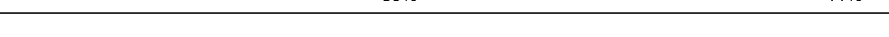






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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | AJ    | 54     |  89% 9%    |
| 1   | AK    | 54     |  89% 9%    |
| 1   | AL    | 54     |  89% 9%    |
| 1   | AM    | 54     |  89% 9%    |
| 1   | AN    | 54     |  89% 9%    |
| 1   | AO    | 54     |  91% 9%    |
| 1   | AP    | 54     |  89% 9%    |
| 1   | AQ    | 54     |  89% 9%    |
| 1   | AR    | 54     |  89% 9%    |
| 1   | AS    | 54     |  89% 9%    |
| 1   | AT    | 54     |  91% 9%    |
| 1   | AU    | 54     |  91% 9%    |
| 1   | AV    | 54     |  89% 9%  |
| 1   | AW    | 54     |  91% 9%  |
| 1   | AX    | 54     |  91% 9%  |
| 2   | BA    | 44     |  89% 11% |
| 2   | BB    | 44     |  91% 9%  |
| 2   | BC    | 44     |  89% 11% |
| 2   | BD    | 44     |  91% 9%  |
| 2   | BE    | 44     |  91% 9%  |
| 2   | BF    | 44     |  89% 11% |
| 2   | BG    | 44     |  89% 11% |
| 2   | BH    | 44     |  86% 11% |
| 2   | BI    | 44     |  91% 9%  |
| 2   | BJ    | 44     |  89% 11% |

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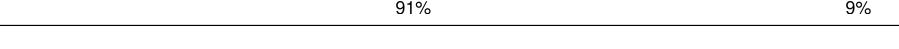
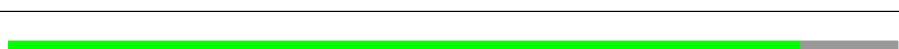

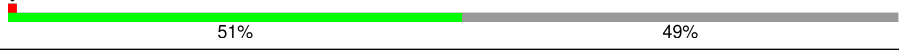

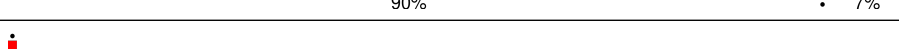



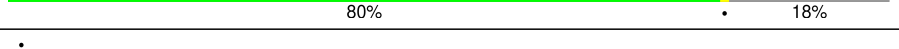

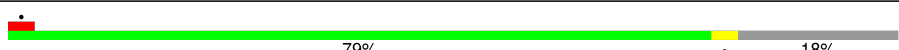


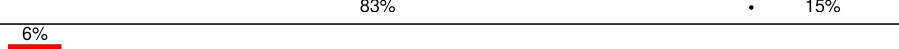







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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | BK    | 44     |    |
| 2   | BL    | 44     |    |
| 2   | BM    | 44     |    |
| 2   | BN    | 44     |    |
| 2   | BO    | 44     |    |
| 2   | BP    | 44     |    |
| 2   | BQ    | 44     |    |
| 2   | BR    | 44     |    |
| 2   | BS    | 44     |    |
| 2   | BT    | 44     |    |
| 2   | BU    | 44     |    |
| 2   | BV    | 44     |   |
| 2   | BW    | 44     |  |
| 2   | BX    | 44     |  |
| 2   | ba    | 44     |  |
| 2   | bb    | 44     |  |
| 2   | bc    | 44     |  |
| 2   | bd    | 44     |  |
| 2   | be    | 44     |  |
| 2   | bf    | 44     |  |
| 2   | bg    | 44     |  |
| 2   | bh    | 44     |  |
| 2   | bi    | 44     |  |
| 2   | bj    | 44     |  |
| 2   | bk    | 44     |  |

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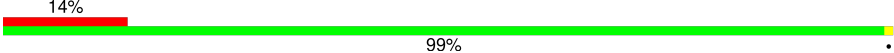

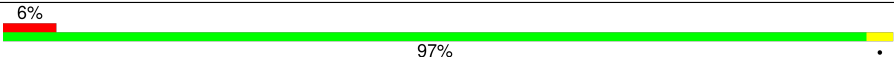
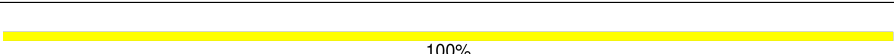
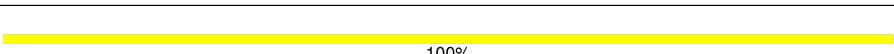


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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | bl    | 44     |    |
| 2   | bm    | 44     |    |
| 2   | bn    | 44     |    |
| 2   | bo    | 44     |    |
| 2   | bp    | 44     |    |
| 3   | C     | 354    |    |
| 4   | C1    | 202    |    |
| 5   | C2    | 125    |    |
| 6   | H1    | 67     |    |
| 7   | H2    | 181    |   |
| 8   | L     | 274    |  |
| 9   | M     | 367    |  |
| 10  | aa    | 71     |  |
| 11  | ab    | 71     |  |
| 11  | ac    | 71     |  |
| 11  | ad    | 71     |  |
| 11  | ae    | 71     |  |
| 11  | af    | 71     |  |
| 11  | ag    | 71     |  |
| 11  | ah    | 71     |  |
| 11  | ai    | 71     |  |
| 11  | aj    | 71     |  |
| 11  | ak    | 71     |  |
| 11  | al    | 71     |  |
| 11  | am    | 71     |  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 11  | an    | 71     |  14% 99%    |
| 11  | ao    | 71     |  6% 83% 15% |
| 11  | ap    | 71     |  6% 97%     |
| 12  | CG    | 2      |  100%       |
| 12  | MG    | 2      |  100%       |

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 56446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called LHH-alpha.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | AA    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AB    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AC    | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 384   | 256 | 64 | 60 | 4 |         |       |
| 1   | AD    | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 384   | 256 | 64 | 60 | 4 |         |       |
| 1   | AE    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AF    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AG    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AH    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AI    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AJ    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AK    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AL    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AM    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AN    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AO    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AP    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AQ    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | AR    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AS    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AT    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AU    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AV    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AW    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |
| 1   | AX    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 261 | 65 | 61 | 4 |         |       |

- Molecule 2 is a protein called Light-harvesting protein B:885 subunit beta.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | BA    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | BB    | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 327   | 215 | 56 | 54 | 2 |         |       |
| 2   | BC    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | BD    | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 327   | 215 | 56 | 54 | 2 |         |       |
| 2   | BE    | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 327   | 215 | 56 | 54 | 2 |         |       |
| 2   | BF    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | BG    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | BH    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | BI    | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 327   | 215 | 56 | 54 | 2 |         |       |
| 2   | BJ    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | BK    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | BL    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |

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| Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 2   | BM    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | BN    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | BO    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | BP    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | BQ    | 40       | Total<br>327 | C<br>215 | N<br>56 | O<br>54 | S<br>2 | 0       | 0     |
| 2   | BR    | 40       | Total<br>327 | C<br>215 | N<br>56 | O<br>54 | S<br>2 | 0       | 0     |
| 2   | BS    | 40       | Total<br>327 | C<br>215 | N<br>56 | O<br>54 | S<br>2 | 0       | 0     |
| 2   | BT    | 40       | Total<br>327 | C<br>215 | N<br>56 | O<br>54 | S<br>2 | 0       | 0     |
| 2   | BU    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | BV    | 40       | Total<br>327 | C<br>215 | N<br>56 | O<br>54 | S<br>2 | 0       | 0     |
| 2   | BW    | 40       | Total<br>327 | C<br>215 | N<br>56 | O<br>54 | S<br>2 | 0       | 0     |
| 2   | BX    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | ba    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | bb    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | bc    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | bd    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | be    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | bf    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | bg    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | bh    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |
| 2   | bi    | 39       | Total<br>323 | C<br>213 | N<br>55 | O<br>53 | S<br>2 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | bj    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | bk    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | bl    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | bm    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | bn    | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 327   | 215 | 56 | 54 | 2 |         |       |
| 2   | bo    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |
| 2   | bp    | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 323   | 213 | 55 | 53 | 2 |         |       |

- Molecule 3 is a protein called MULTIHEME\_CYTC domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2325  | 1464 | 419 | 423 | 19 |         |       |

- Molecule 4 is a protein called RC-S.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | C1    | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 806   | 506 | 151 | 145 | 4 |         |       |

- Molecule 5 is a protein called RC-U.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | C2    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 766   | 483 | 148 | 132 | 3 |         |       |

- Molecule 6 is a protein called PRCH domain-containing protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | H1    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 522   | 343 | 89 | 88 | 2 |         |       |

- Molecule 7 is a protein called RC-Hc.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H2    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1404  | 894 | 239 | 267 | 4 |         |       |

- Molecule 8 is a protein called Photosynthetic reaction center L subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | L     | 273      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2165  | 1457 | 351 | 347 | 10 |         |       |

- Molecule 9 is a protein called RC-M.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | M     | 335      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2694  | 1789 | 442 | 453 | 10 |         |       |

- Molecule 10 is a protein called LHC domain-containing protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | aa    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 433   | 284 | 76 | 71 | 2 |         |       |

- Molecule 11 is a protein called LHC domain-containing protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | ab    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 298 | 79 | 75 | 3 |         |       |
| 11  | ac    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 443   | 290 | 77 | 73 | 3 |         |       |
| 11  | ad    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 304 | 81 | 77 | 3 |         |       |
| 11  | ae    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 298 | 79 | 75 | 3 |         |       |
| 11  | af    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 298 | 79 | 75 | 3 |         |       |
| 11  | ag    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 298 | 79 | 75 | 3 |         |       |
| 11  | ah    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 304 | 81 | 77 | 3 |         |       |
| 11  | ai    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 304 | 81 | 77 | 3 |         |       |
| 11  | aj    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 304 | 81 | 77 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | ak    | 71       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 542   | 352 | 95 | 91 | 4 |         |       |
| 11  | al    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 304 | 81 | 77 | 3 |         |       |
| 11  | am    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 304 | 81 | 77 | 3 |         |       |
| 11  | an    | 71       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 542   | 352 | 95 | 91 | 4 |         |       |
| 11  | ao    | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 465   | 304 | 81 | 77 | 3 |         |       |
| 11  | ap    | 71       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 543   | 352 | 95 | 92 | 4 |         |       |

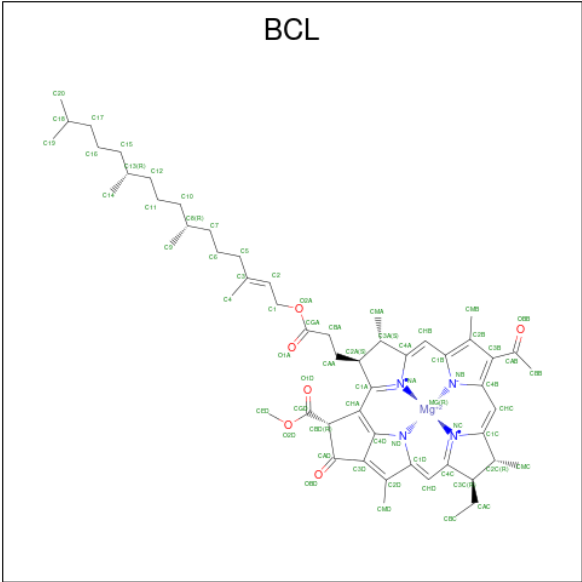
- Molecule 12 is an oligosaccharide called alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose.



| Mol | Chain | Residues | Atoms |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|---------|-------|
| 12  | MG    | 2        | Total | C  | O | 0       | 0     |
|     |       |          | 21    | 12 | 9 |         |       |
| 12  | CG    | 2        | Total | C  | O | 0       | 0     |
|     |       |          | 21    | 12 | 9 |         |       |

- Molecule 13 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | AA    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AA    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AB    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AB    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AC    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AC    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AD    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AD    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AE    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AE    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AF    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AF    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AG    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AG    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | AH    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AH    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AI    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AI    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AJ    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AJ    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AK    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AK    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AL    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AL    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AM    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AM    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AN    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AN    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AO    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AO    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AP    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AP    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AQ    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AQ    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AQ    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | AR    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AS    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AS    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AS    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AT    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AU    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AU    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AV    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AV    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AW    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AW    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AW    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | AX    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BA    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BB    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BC    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BD    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BE    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BF    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BG    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BH    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | BI    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BJ    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BK    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BL    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BM    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BN    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BO    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BP    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BQ    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BR    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BS    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BT    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BU    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BV    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BW    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | BX    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | aa    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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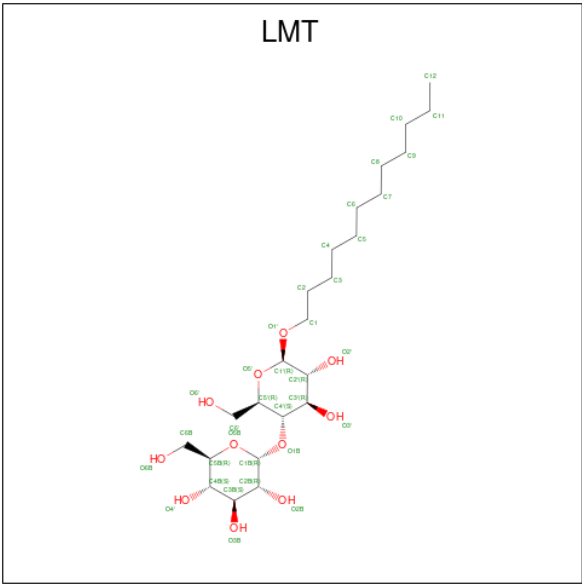
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | ab    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ac    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ad    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ae    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | af    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ag    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ah    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ai    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | aj    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ak    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | al    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | am    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | an    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ao    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ap    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | ba    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | bb    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | bc    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | bd    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | be    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 13  | bf    | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 13  | bg    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bh    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bi    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bj    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bk    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bl    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bm    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bn    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bo    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 13  | bp    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

- Molecule 14 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 14  | AA    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 14  | AB    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AB    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AD    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AD    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AF    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AG    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AH    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AH    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AH    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AI    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AJ    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AK    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AL    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AN    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AN    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AO    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AP    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AR    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AS    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AT    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AU    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 14  | AV    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | AW    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BA    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BA    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BA    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BA    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BB    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BB    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BC    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BC    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BD    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BD    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BD    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BD    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BE    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BE    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BE    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BE    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BF    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BF    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BF    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 14  | BG    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BG    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BH    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BH    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BH    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BI    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BI    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BI    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BI    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BJ    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BJ    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BK    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BK    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BK    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BK    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BL    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BL    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BL    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BM    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BM    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BN    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 14  | BN    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BN    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BN    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BO    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BO    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BP    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BP    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BP    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BP    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BQ    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BQ    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BR    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BR    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BR    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BR    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BS    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BS    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BS    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BT    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BT    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | BT    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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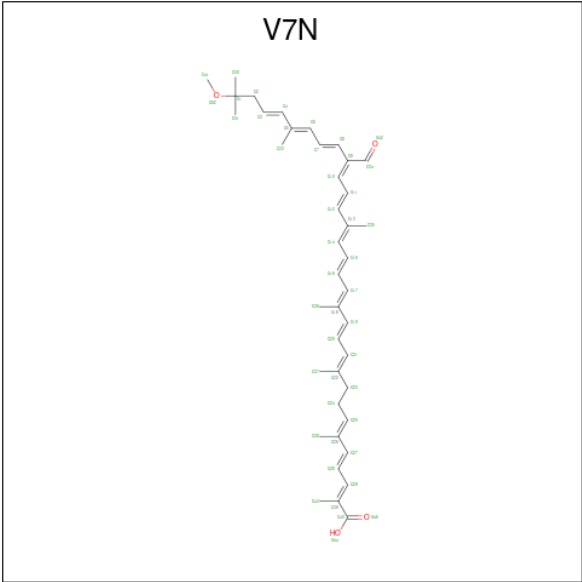
| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 14  | BU    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BU    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BU    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BV    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BV    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BW    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BW    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BW    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BW    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BW    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BX    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | BX    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | L     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | L     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | L     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | L     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | L     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | M     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | ac    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | bb    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | bc    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 14  | bd    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 14  | bf    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bf    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bg    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bh    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bh    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bj    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bk    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bl    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bl    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bm    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bn    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bo    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 14  | bp    | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 15 is (2 {E},4 {E},6 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {Z},24 {E},26 {E},28 {E})-23-methanoyl-31-methoxy-2,6,10,14,19,27,31-heptamethyl-dotriaconta-2,4,6,10,12,14,16,18,20,22,24,26,28-tridecaenoic acid (three-letter code: V7N) (formula: C<sub>41</sub>H<sub>54</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 15  | AE    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | AH    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | AT    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BA    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BB    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BC    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BD    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BE    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BG    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BH    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BJ    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BK    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BL    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | BM    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |

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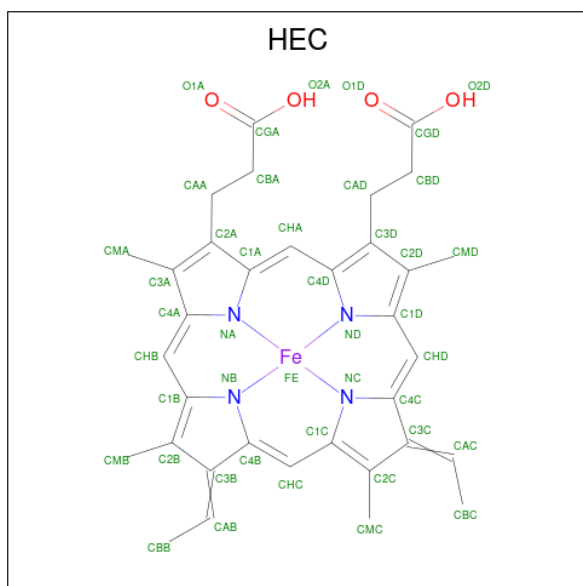
| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 15  | BN    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BO    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BP    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BQ    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BR    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BS    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BT    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BV    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BW    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | BX    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | ba    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bb    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bc    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bd    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | be    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bf    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bg    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bh    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bi    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bj    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |
| 15  | bk    | 1        | Total<br>45 | C<br>41 | O<br>4 | 0       |

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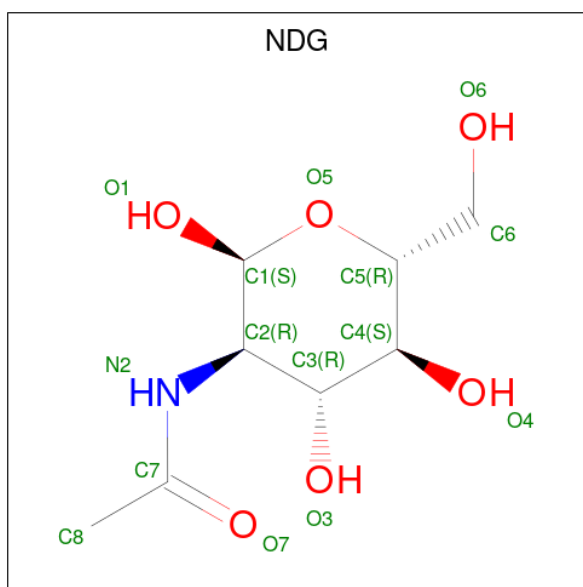
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 15  | bl    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | bm    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | bn    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | bo    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |
| 15  | bp    | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 41 | 4 |         |

- Molecule 16 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



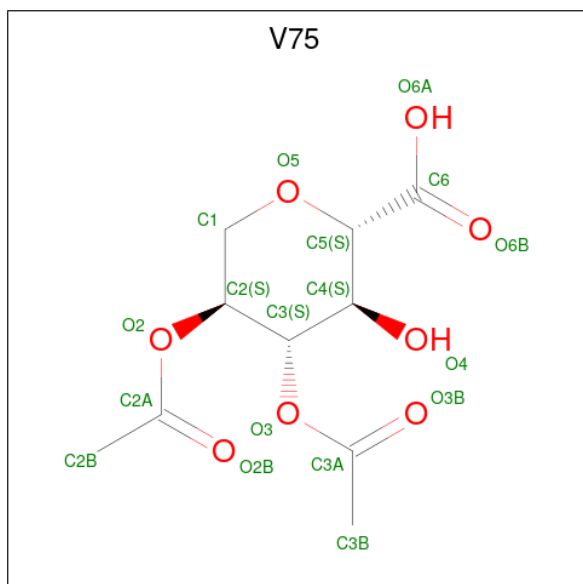
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 16  | C     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 16  | C     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 16  | C     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 16  | C     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 17 is 2-acetamido-2-deoxy- $\alpha$ -D-glucopyranose (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 17  | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 17  | C1    | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

- Molecule 18 is (2 {S},3 {S},4 {S},5 {S})-4,5-diacetyloxy-3-oxidanyl-oxane-2-carboxylic acid (three-letter code: V75) (formula:  $C_{10}H_{14}O_8$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 18  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 10 | 8 |         |

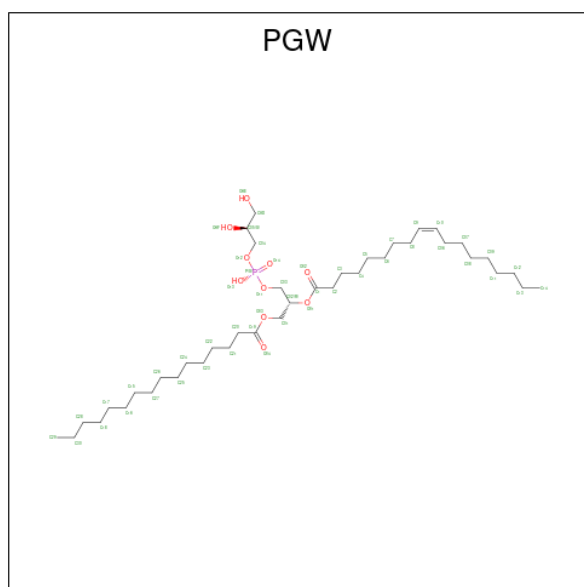
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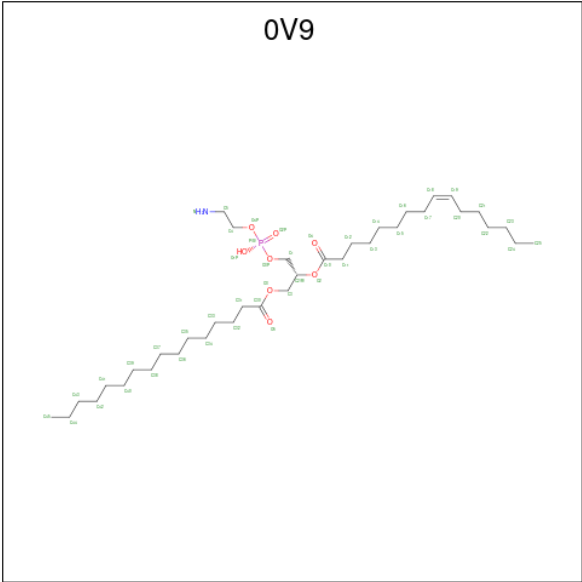
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 18  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 10 | 8 |         |

- Molecule 19 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula:  $C_{40}H_{77}O_{10}P$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 19  | H1    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |

- Molecule 20 is (19R,22S)-25-amino-22-hydroxy-22-oxido-16-oxo-17,21,23-trioxa-22lambda da 5 -phosphapentacosan-19-yl (9Z)-hexadec-9-enoate (three-letter code: OV9) (formula:  $C_{37}H_{72}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



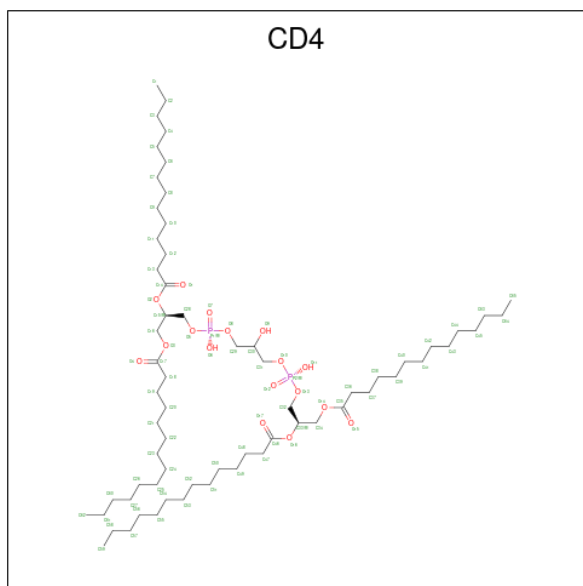
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 20  | H1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | aj    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | ba    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | ba    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bb    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bc    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | be    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | be    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bf    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bg    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bh    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bi    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bj    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 20  | bk    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bk    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bl    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bm    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bn    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 20  | bo    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |

- Molecule 21 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (three-letter code: CD4) (formula:  $C_{65}H_{126}O_{17}P_2$ ).



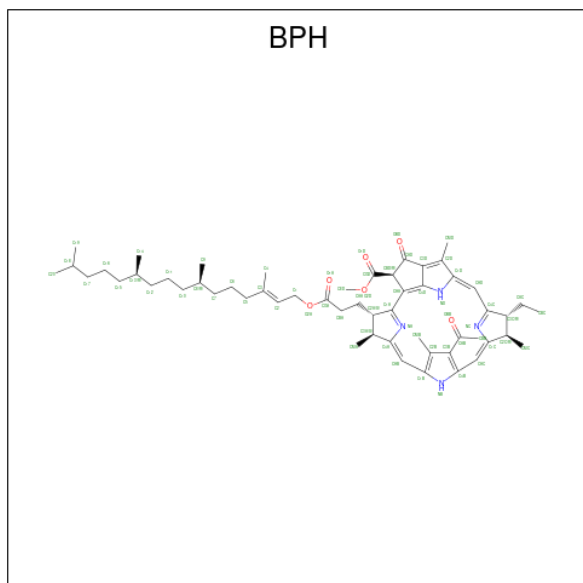
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 21  | H1    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 84    | 65 | 17 | 2 |         |
| 21  | M     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 84    | 65 | 17 | 2 |         |
| 21  | ad    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 84    | 65 | 17 | 2 |         |
| 21  | af    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 84    | 65 | 17 | 2 |         |

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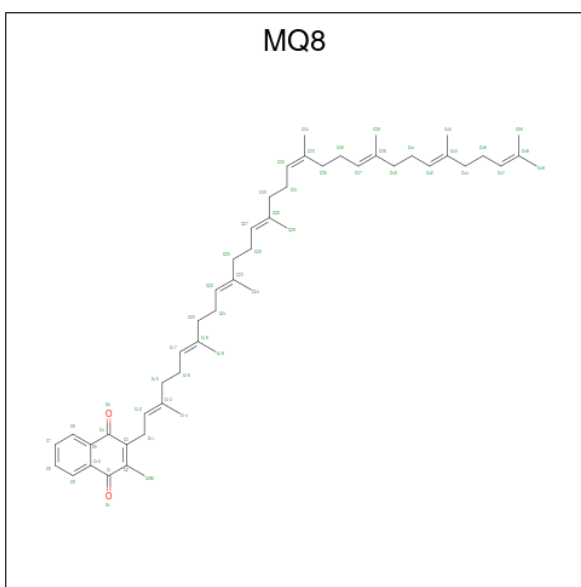
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 21  | af    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 84    | 65 | 17 | 2 |         |
| 21  | ai    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 84    | 65 | 17 | 2 |         |

- Molecule 22 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 22  | L     | 1        | Total | C  | N | O | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |
| 22  | M     | 1        | Total | C  | N | O | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |

- Molecule 23 is MENAQUINONE 8 (three-letter code: MQ8) (formula:  $C_{51}H_{72}O_2$ ).

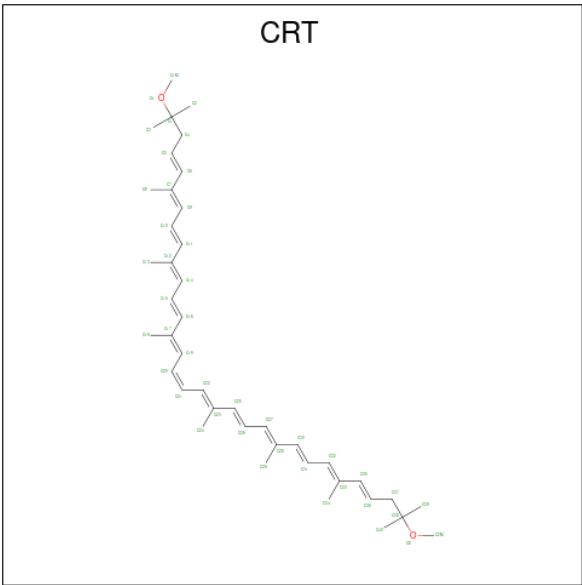


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 23  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 51 | 2 |         |
| 23  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 51 | 2 |         |
| 23  | an    | 1        | Total | C  | O | 0       |
|     |       |          | 53    | 51 | 2 |         |

- Molecule 24 is FE (III) ION (three-letter code: FE) (formula: Fe).

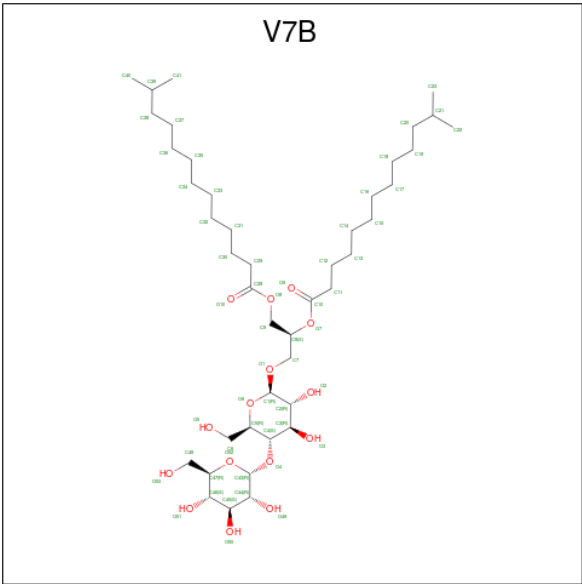
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | M     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 25 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 42 | 2 |         |

- Molecule 26 is [(2 {S})-3-[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-5-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]oxy-2-(12-methyltridecanoyloxy)propyl] 12-methyltridecanoate (three-letter code: V7B) (formula: C<sub>43</sub>H<sub>80</sub>O<sub>15</sub>) (labeled as "Ligand of Interest" by depositor).



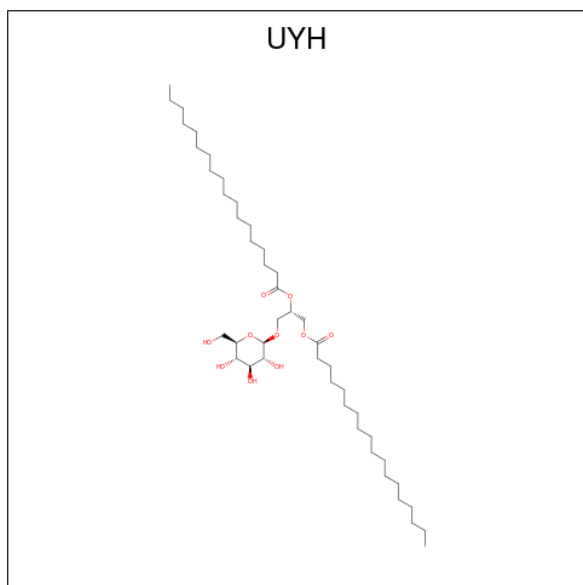
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 26  | af    | 1        | Total | C  | O  | 0       |
|     |       |          | 58    | 43 | 15 |         |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 26  | ag    | 1        | Total | C  | O  | 0       |
|     |       |          | 58    | 43 | 15 |         |

- Molecule 27 is [(2 {S})-3-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-2-octadecanoyloxy-propyl] octadecanoate (three-letter code: UYH) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 27  | ai    | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |

- Molecule 28 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 28  | AA    | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 28  | AB    | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 28  | AC    | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 28  | AD    | 5        | Total | O | 0       |
|     |       |          | 5     | 5 |         |
| 28  | AG    | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 28  | AH    | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 28  | AI    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | AJ    | 6        | Total<br>6  | O<br>6  | 0       |
| 28  | AK    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | AL    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | AM    | 4        | Total<br>4  | O<br>4  | 0       |
| 28  | AN    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | AO    | 2        | Total<br>2  | O<br>2  | 0       |
| 28  | AP    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | AQ    | 5        | Total<br>5  | O<br>5  | 0       |
| 28  | AR    | 2        | Total<br>2  | O<br>2  | 0       |
| 28  | AS    | 5        | Total<br>5  | O<br>5  | 0       |
| 28  | AT    | 7        | Total<br>7  | O<br>7  | 0       |
| 28  | AV    | 6        | Total<br>6  | O<br>6  | 0       |
| 28  | AW    | 6        | Total<br>6  | O<br>6  | 0       |
| 28  | AX    | 5        | Total<br>5  | O<br>5  | 0       |
| 28  | BD    | 1        | Total<br>1  | O<br>1  | 0       |
| 28  | BE    | 1        | Total<br>1  | O<br>1  | 0       |
| 28  | BF    | 1        | Total<br>1  | O<br>1  | 0       |
| 28  | BO    | 1        | Total<br>1  | O<br>1  | 0       |
| 28  | BW    | 1        | Total<br>1  | O<br>1  | 0       |
| 28  | C     | 98       | Total<br>98 | O<br>98 | 0       |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 28  | C1    | 48       | Total<br>48 | O<br>48 | 0       |
| 28  | C2    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | H1    | 9        | Total<br>9  | O<br>9  | 0       |
| 28  | H2    | 35       | Total<br>35 | O<br>35 | 0       |
| 28  | L     | 53       | Total<br>53 | O<br>53 | 0       |
| 28  | M     | 59       | Total<br>59 | O<br>59 | 0       |
| 28  | aa    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | ab    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | ac    | 4        | Total<br>4  | O<br>4  | 0       |
| 28  | ad    | 9        | Total<br>9  | O<br>9  | 0       |
| 28  | ae    | 7        | Total<br>7  | O<br>7  | 0       |
| 28  | af    | 7        | Total<br>7  | O<br>7  | 0       |
| 28  | ag    | 7        | Total<br>7  | O<br>7  | 0       |
| 28  | ah    | 6        | Total<br>6  | O<br>6  | 0       |
| 28  | ai    | 3        | Total<br>3  | O<br>3  | 0       |
| 28  | aj    | 6        | Total<br>6  | O<br>6  | 0       |
| 28  | ak    | 14       | Total<br>14 | O<br>14 | 0       |
| 28  | al    | 8        | Total<br>8  | O<br>8  | 0       |
| 28  | am    | 8        | Total<br>8  | O<br>8  | 0       |
| 28  | an    | 5        | Total<br>5  | O<br>5  | 0       |
| 28  | ao    | 2        | Total<br>2  | O<br>2  | 0       |

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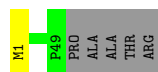
| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 28  | ap    | 8        | Total<br>8 | O<br>8 | 0       |
| 28  | bb    | 2        | Total<br>2 | O<br>2 | 0       |
| 28  | bc    | 2        | Total<br>2 | O<br>2 | 0       |
| 28  | bd    | 1        | Total<br>1 | O<br>1 | 0       |
| 28  | be    | 1        | Total<br>1 | O<br>1 | 0       |
| 28  | bf    | 1        | Total<br>1 | O<br>1 | 0       |
| 28  | bg    | 1        | Total<br>1 | O<br>1 | 0       |
| 28  | bh    | 2        | Total<br>2 | O<br>2 | 0       |
| 28  | bi    | 3        | Total<br>3 | O<br>3 | 0       |
| 28  | bk    | 4        | Total<br>4 | O<br>4 | 0       |
| 28  | bl    | 3        | Total<br>3 | O<br>3 | 0       |
| 28  | bm    | 4        | Total<br>4 | O<br>4 | 0       |
| 28  | bn    | 3        | Total<br>3 | O<br>3 | 0       |
| 28  | bo    | 2        | Total<br>2 | O<br>2 | 0       |
| 28  | bp    | 1        | Total<br>1 | O<br>1 | 0       |

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

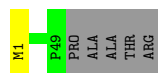
- Molecule 1: LHh-alpha

Chain AA:  89% • 9%



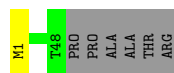
- Molecule 1: LHh-alpha

Chain AB:  89% • 9%



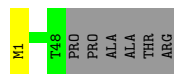
- Molecule 1: LHh-alpha

Chain AC:  87% • 11%



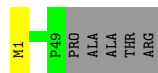
- Molecule 1: LHh-alpha

Chain AD:  87% • 11%



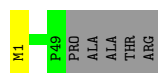
- Molecule 1: LHh-alpha

Chain AE:  89% • 9%



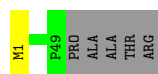
- Molecule 1: LHh-alpha

Chain AF:  89% • 9%



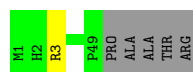
- Molecule 1: LHh-alpha

Chain AG:  89% • 9%




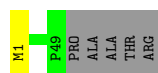
- Molecule 1: LHh-alpha

Chain AH:  89% • 9%



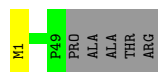
- Molecule 1: LHh-alpha

Chain AI:  89% • 9%



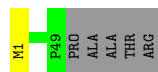
- Molecule 1: LHh-alpha

Chain AJ:  89% • 9%



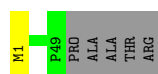
- Molecule 1: LHh-alpha

Chain AK:  89% • 9%



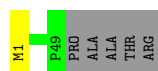
- Molecule 1: LHh-alpha

Chain AL:  89% • 9%



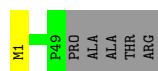
- Molecule 1: LHh-alpha

Chain AM:  89% 9%



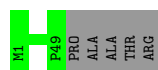
- Molecule 1: LHh-alpha

Chain AN:  89% 9%



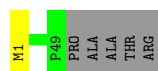
- Molecule 1: LHh-alpha

Chain AO:  91% 9%



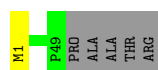
- Molecule 1: LHh-alpha

Chain AP:  89% 9%



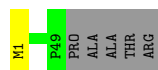
- Molecule 1: LHh-alpha

Chain AQ:  89% 9%




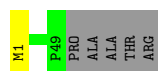
- Molecule 1: LHh-alpha

Chain AR:  89% 9%



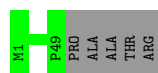
- Molecule 1: LHh-alpha

Chain AS:  89% 9%



- Molecule 1: LHh-alpha

Chain AT:  91% 9%



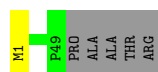
- Molecule 1: LHh-alpha

Chain AU:  91% 9%



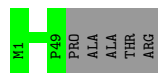
- Molecule 1: LHh-alpha

Chain AV:  89% 9%



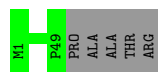
- Molecule 1: LHh-alpha

Chain AW:  91% 9%



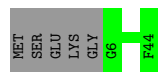
- Molecule 1: LHh-alpha

Chain AX:  91% 9%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BA:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BB:  91% 9%



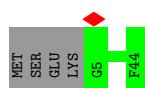
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BC:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BD:  91% 9%



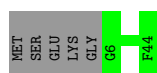
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BE:  91% 9%



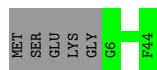
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BF:  89% 11%




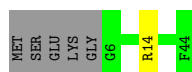
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BG:  89% 11%



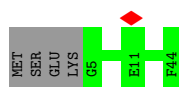
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BH:  86% 11%



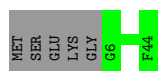
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BI:  91% 9%




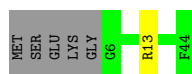
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BJ:  89% 11%



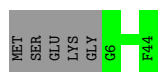
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BK:  86% 11%



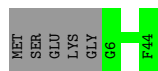
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BL:  89% 11%



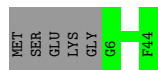
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BM:  89% 11%



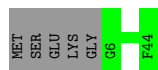
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BN:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BO:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

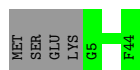
Chain BP:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta



Chain BQ:  91% 9%



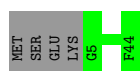
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BR:  91% 9%



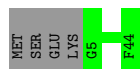
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BS:  91% 9%



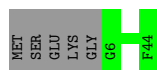
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BT:  91% 9%



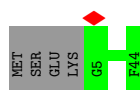
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BU:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BV:  91% 9%



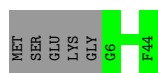
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BW:  91% 9%



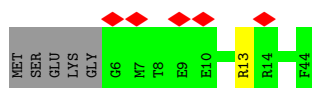
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain BX:  89% 11%




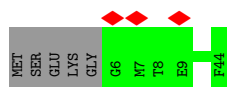
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain ba:  11% 86% 11%




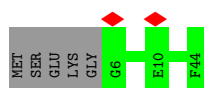
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bb:  7% 89% 11%




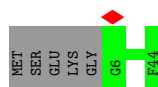
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bc:  5% 89% 11%




- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bd:  1% 89% 11%




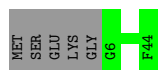
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain be:  89% 11%



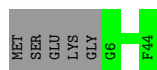
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bf:  89% 11%



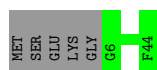
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bg:  89% 11%




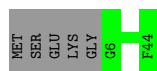
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bh:  89% 11%




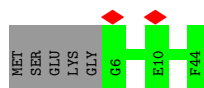
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bi:  89% 11%




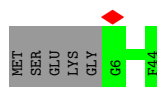
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bj:  5% 89% 11%




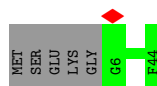
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bk:  5% 89% 11%



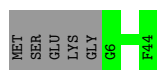
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bl:  5% 89% 11%

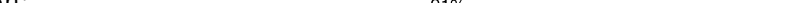


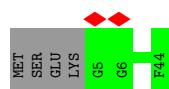
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bm:  89% 11%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bn:  5% 91% 9%



- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bo:  86% • 11%



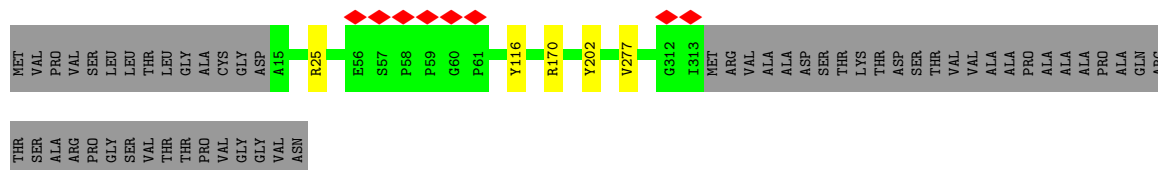
- Molecule 2: Light-harvesting protein B:885 subunit beta

Chain bp:  89% 11%



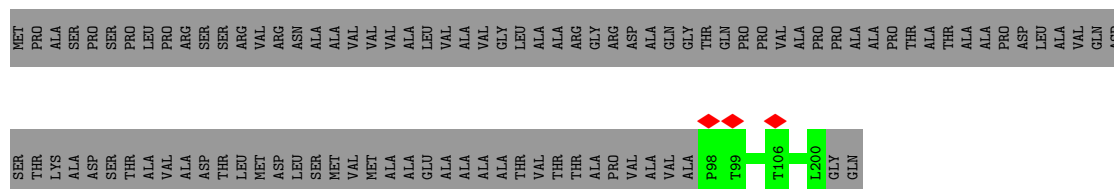
- Molecule 3: MULTHEME\_CYTC domain-containing protein

Chain C:  83% 16%




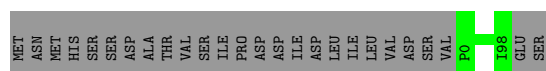
- Molecule 4: RC-S

Chain C1:  51% 49%



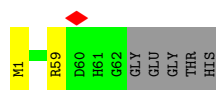
- Molecule 5: RC-U

Chain C2:  79% 21%

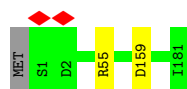


- Molecule 6: PRCH domain-containing protein

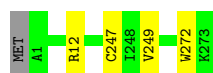
Chain H1:  90% 7%



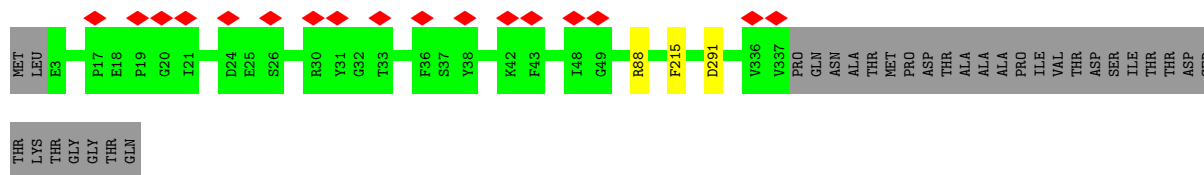
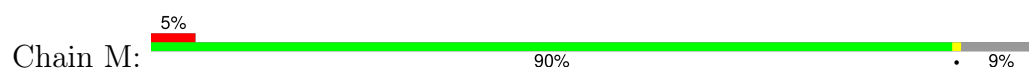
- Molecule 7: RC-Hc



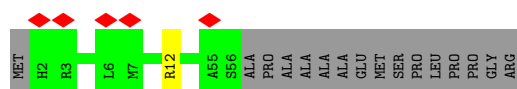
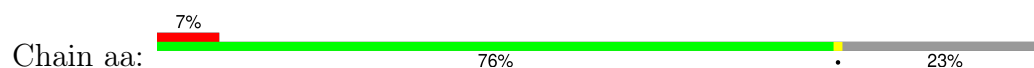
- Molecule 8: Photosynthetic reaction center L subunit



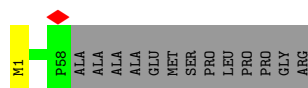
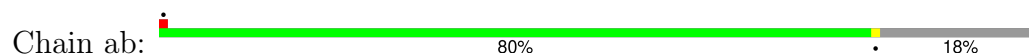
- Molecule 9: RC-M



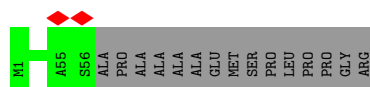
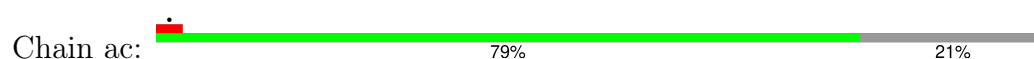
- Molecule 10: LHC domain-containing protein



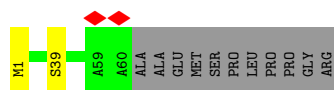
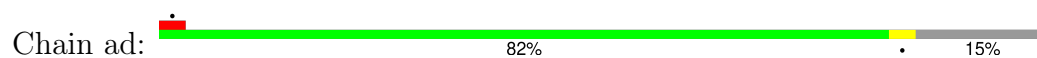
- Molecule 11: LHC domain-containing protein



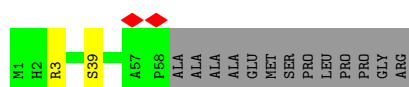
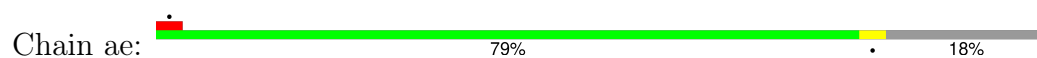
- Molecule 11: LHC domain-containing protein



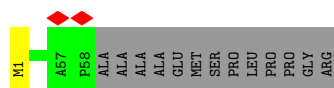
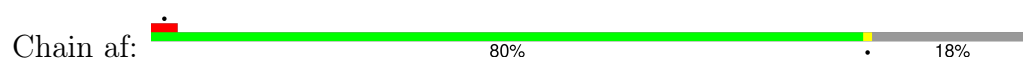
- Molecule 11: LHC domain-containing protein



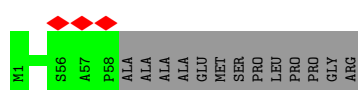
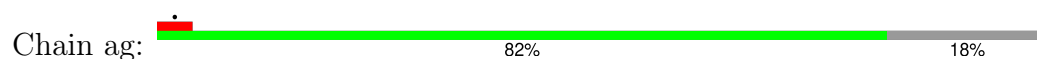
- Molecule 11: LHC domain-containing protein



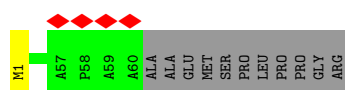
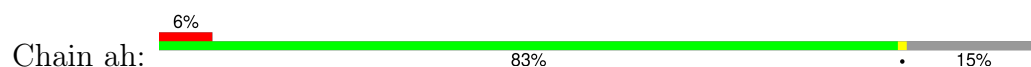
- Molecule 11: LHC domain-containing protein



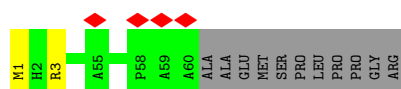
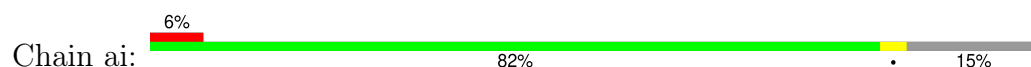
- Molecule 11: LHC domain-containing protein



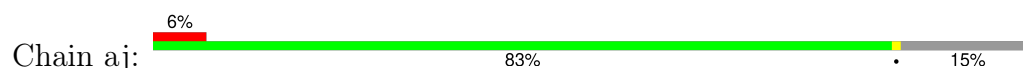
- Molecule 11: LHC domain-containing protein

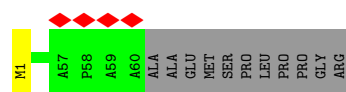


- Molecule 11: LHC domain-containing protein

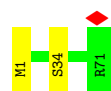


- Molecule 11: LHC domain-containing protein

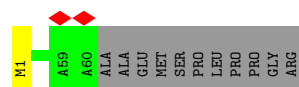
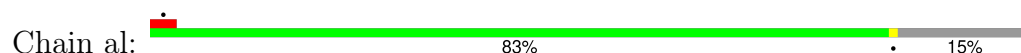




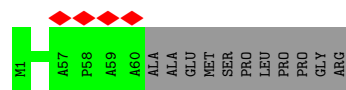
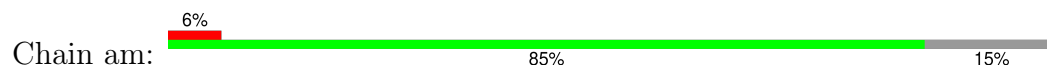
- Molecule 11: LHC domain-containing protein



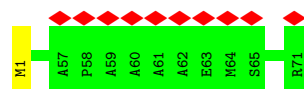
- Molecule 11: LHC domain-containing protein



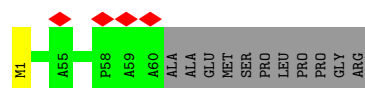
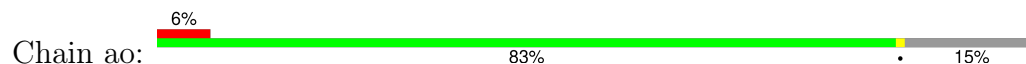
- Molecule 11: LHC domain-containing protein



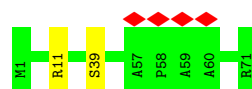
- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein



- Molecule 11: LHC domain-containing protein



- Molecule 12: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain MG:  100%

MAN1  
RAM2

- Molecule 12: alpha-L-rhamnopyranose-(1-4)-alpha-D-mannopyranose

Chain CG:  100%

MAN1  
RAM2



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 73853                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 24.8                                    | Depositor |
| Minimum defocus (nm)                 | -800                                    | Depositor |
| Maximum defocus (nm)                 | -2400                                   | Depositor |
| Magnification                        | 120000                                  | Depositor |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.204                                   | Depositor |
| Minimum map value                    | -0.061                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.0292                                  | Depositor |
| Map size (Å)                         | 399.784, 399.784, 399.784               | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.99946, 0.99946, 0.99946               | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0V9, MAN, BCL, MQ8, NDG, V7B, FME, V7N, PGW, BPH, FE, V75, LMT, HEC, CRT, UYH, RAM, CD4

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   | AA    | 0.24         | 0/396       | 0.49        | 0/541       |
| 1   | AB    | 0.24         | 0/396       | 0.50        | 0/541       |
| 1   | AC    | 0.25         | 0/388       | 0.53        | 0/529       |
| 1   | AD    | 0.25         | 0/388       | 0.52        | 0/529       |
| 1   | AE    | 0.24         | 0/396       | 0.52        | 0/541       |
| 1   | AF    | 0.24         | 0/396       | 0.50        | 0/541       |
| 1   | AG    | 0.25         | 0/396       | 0.50        | 0/541       |
| 1   | AH    | 0.24         | 0/396       | 0.51        | 0/541       |
| 1   | AI    | 0.24         | 0/396       | 0.50        | 0/541       |
| 1   | AJ    | 0.24         | 0/396       | 0.52        | 0/541       |
| 1   | AK    | 0.25         | 0/396       | 0.51        | 0/541       |
| 1   | AL    | 0.24         | 0/396       | 0.52        | 0/541       |
| 1   | AM    | 0.24         | 0/396       | 0.48        | 0/541       |
| 1   | AN    | 0.24         | 0/396       | 0.53        | 0/541       |
| 1   | AO    | 0.23         | 0/396       | 0.50        | 0/541       |
| 1   | AP    | 0.24         | 0/396       | 0.49        | 0/541       |
| 1   | AQ    | 0.24         | 0/396       | 0.51        | 0/541       |
| 1   | AR    | 0.24         | 0/396       | 0.50        | 0/541       |
| 1   | AS    | 0.24         | 0/396       | 0.53        | 0/541       |
| 1   | AT    | 0.24         | 0/396       | 0.52        | 0/541       |
| 1   | AU    | 0.24         | 0/396       | 0.50        | 0/541       |
| 1   | AV    | 0.24         | 0/396       | 0.51        | 0/541       |
| 1   | AW    | 0.24         | 0/396       | 0.53        | 0/541       |
| 1   | AX    | 0.24         | 0/396       | 0.51        | 0/541       |
| 2   | BA    | 0.24         | 0/336       | 0.50        | 0/456       |
| 2   | BB    | 0.25         | 0/340       | 0.49        | 0/461       |
| 2   | BC    | 0.24         | 0/336       | 0.49        | 0/456       |
| 2   | BD    | 0.25         | 0/340       | 0.50        | 0/461       |
| 2   | BE    | 0.25         | 0/340       | 0.49        | 0/461       |
| 2   | BF    | 0.24         | 0/336       | 0.50        | 0/456       |
| 2   | BG    | 0.24         | 0/336       | 0.49        | 0/456       |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 2   | BH    | 0.24         | 0/336   | 0.48        | 0/456   |
| 2   | BI    | 0.25         | 0/340   | 0.49        | 0/461   |
| 2   | BJ    | 0.24         | 0/336   | 0.49        | 0/456   |
| 2   | BK    | 0.24         | 0/336   | 0.50        | 0/456   |
| 2   | BL    | 0.25         | 0/336   | 0.54        | 0/456   |
| 2   | BM    | 0.25         | 0/336   | 0.51        | 0/456   |
| 2   | BN    | 0.25         | 0/336   | 0.51        | 0/456   |
| 2   | BO    | 0.24         | 0/336   | 0.51        | 0/456   |
| 2   | BP    | 0.24         | 0/336   | 0.51        | 0/456   |
| 2   | BQ    | 0.24         | 0/340   | 0.50        | 0/461   |
| 2   | BR    | 0.26         | 0/340   | 0.52        | 0/461   |
| 2   | BS    | 0.24         | 0/340   | 0.49        | 0/461   |
| 2   | BT    | 0.24         | 0/340   | 0.52        | 0/461   |
| 2   | BU    | 0.24         | 0/336   | 0.50        | 0/456   |
| 2   | BV    | 0.24         | 0/340   | 0.50        | 0/461   |
| 2   | BW    | 0.24         | 0/340   | 0.49        | 0/461   |
| 2   | BX    | 0.24         | 0/336   | 0.48        | 0/456   |
| 2   | ba    | 0.25         | 0/336   | 0.53        | 0/456   |
| 2   | bb    | 0.24         | 0/336   | 0.49        | 0/456   |
| 2   | bc    | 0.25         | 0/336   | 0.51        | 0/456   |
| 2   | bd    | 0.26         | 0/336   | 0.49        | 0/456   |
| 2   | be    | 0.26         | 0/336   | 0.53        | 0/456   |
| 2   | bf    | 0.24         | 0/336   | 0.48        | 0/456   |
| 2   | bg    | 0.26         | 0/336   | 0.51        | 0/456   |
| 2   | bh    | 0.24         | 0/336   | 0.49        | 0/456   |
| 2   | bi    | 0.27         | 0/336   | 0.51        | 0/456   |
| 2   | bj    | 0.27         | 0/336   | 0.52        | 0/456   |
| 2   | bk    | 0.26         | 0/336   | 0.52        | 0/456   |
| 2   | bl    | 0.25         | 0/336   | 0.49        | 0/456   |
| 2   | bm    | 0.26         | 0/336   | 0.50        | 0/456   |
| 2   | bn    | 0.25         | 0/340   | 0.50        | 0/461   |
| 2   | bo    | 0.25         | 0/336   | 0.49        | 0/456   |
| 2   | bp    | 0.25         | 0/336   | 0.49        | 0/456   |
| 3   | C     | 0.27         | 0/2392  | 0.55        | 0/3263  |
| 4   | C1    | 0.24         | 0/826   | 0.58        | 0/1128  |
| 5   | C2    | 0.24         | 0/787   | 0.56        | 0/1075  |
| 6   | H1    | 0.27         | 0/531   | 0.52        | 0/717   |
| 7   | H2    | 0.25         | 0/1443  | 0.55        | 0/1970  |
| 8   | L     | 0.25         | 0/2252  | 0.51        | 0/3081  |
| 9   | M     | 0.26         | 0/2795  | 0.54        | 0/3824  |
| 10  | aa    | 0.24         | 0/444   | 0.54        | 0/605   |
| 11  | ab    | 0.25         | 0/457   | 0.51        | 0/624   |
| 11  | ac    | 0.26         | 0/444   | 0.55        | 0/605   |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 11  | ad    | 0.25         | 0/467   | 0.54        | 0/638   |
| 11  | ae    | 0.26         | 0/457   | 0.53        | 0/624   |
| 11  | af    | 0.25         | 0/457   | 0.52        | 0/624   |
| 11  | ag    | 0.25         | 0/457   | 0.56        | 0/624   |
| 11  | ah    | 0.26         | 0/467   | 0.54        | 0/638   |
| 11  | ai    | 0.25         | 0/467   | 0.53        | 0/638   |
| 11  | aj    | 0.25         | 0/467   | 0.55        | 0/638   |
| 11  | ak    | 0.27         | 0/547   | 0.53        | 0/748   |
| 11  | al    | 0.26         | 0/467   | 0.54        | 0/638   |
| 11  | am    | 0.26         | 0/467   | 0.53        | 0/638   |
| 11  | an    | 0.26         | 0/547   | 0.55        | 0/748   |
| 11  | ao    | 0.26         | 0/467   | 0.55        | 0/638   |
| 11  | ap    | 0.25         | 0/548   | 0.55        | 0/748   |
| All | All   | 0.25         | 0/41625 | 0.52        | 0/56729 |

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   | AH    | 0                   | 1                   |
| 2   | BH    | 0                   | 1                   |
| 2   | bo    | 0                   | 1                   |
| 3   | C     | 0                   | 1                   |
| 6   | H1    | 0                   | 1                   |
| 7   | H2    | 0                   | 1                   |
| 8   | L     | 0                   | 1                   |
| 9   | M     | 0                   | 1                   |
| 11  | ae    | 0                   | 1                   |
| 11  | ai    | 0                   | 1                   |
| All | All   | 0                   | 10                  |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AH    | 3   | ARG  | Sidechain |
| 2   | BH    | 14  | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | C     | 170 | ARG  | Sidechain |
| 6   | H1    | 59  | ARG  | Sidechain |
| 7   | H2    | 55  | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed    | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 1   | AA    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AB    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AC    | 46/54 (85%) | 46 (100%) | 0       | 0        | 100         | 100 |
| 1   | AD    | 46/54 (85%) | 46 (100%) | 0       | 0        | 100         | 100 |
| 1   | AE    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AF    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AG    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AH    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AI    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AJ    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AK    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AL    | 47/54 (87%) | 46 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | AM    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AN    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AO    | 47/54 (87%) | 46 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | AP    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed    | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 1   | AQ    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AR    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AS    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AT    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AU    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AV    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 1   | AW    | 47/54 (87%) | 46 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 1   | AX    | 47/54 (87%) | 47 (100%) | 0       | 0        | 100         | 100 |
| 2   | BA    | 37/44 (84%) | 36 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 2   | BB    | 38/44 (86%) | 37 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 2   | BC    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BD    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BE    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BF    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BG    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BH    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BI    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BJ    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BK    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BL    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BM    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BN    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BO    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BP    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BQ    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BR    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BS    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BT    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BU    | 37/44 (84%) | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | BV    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |
| 2   | BW    | 38/44 (86%) | 38 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | BX    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | ba    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bb    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bc    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bd    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | be    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bf    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bg    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bh    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bi    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bj    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bk    | 37/44 (84%)   | 36 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 2   | bl    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bm    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 2   | bn    | 38/44 (86%)   | 37 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 2   | bo    | 37/44 (84%)   | 36 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 2   | bp    | 37/44 (84%)   | 37 (100%) | 0       | 0        | 100         | 100 |
| 3   | C     | 297/354 (84%) | 283 (95%) | 13 (4%) | 1 (0%)   | 37          | 44  |
| 4   | C1    | 101/202 (50%) | 97 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 5   | C2    | 97/125 (78%)  | 96 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 6   | H1    | 60/67 (90%)   | 60 (100%) | 0       | 0        | 100         | 100 |
| 7   | H2    | 178/181 (98%) | 173 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 8   | L     | 271/274 (99%) | 263 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 9   | M     | 333/367 (91%) | 324 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 10  | aa    | 53/71 (75%)   | 53 (100%) | 0       | 0        | 100         | 100 |
| 11  | ab    | 56/71 (79%)   | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 11  | ac    | 54/71 (76%)   | 52 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 11  | ad    | 58/71 (82%)   | 57 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 11  | ae    | 56/71 (79%)   | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 11  | af    | 56/71 (79%)   | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 11  | ag    | 56/71 (79%)   | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 11  | ah    | 58/71 (82%)     | 58 (100%)  | 0       | 0        | 100         | 100 |
| 11  | ai    | 58/71 (82%)     | 56 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 11  | aj    | 58/71 (82%)     | 57 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 11  | ak    | 69/71 (97%)     | 66 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 11  | al    | 58/71 (82%)     | 57 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 11  | am    | 58/71 (82%)     | 57 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 11  | an    | 69/71 (97%)     | 64 (93%)   | 5 (7%)  | 0        | 100         | 100 |
| 11  | ao    | 58/71 (82%)     | 57 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 11  | ap    | 69/71 (97%)     | 69 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 4898/5762 (85%) | 4828 (99%) | 69 (1%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 25  | ARG  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed    | Rotameric | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1   | AA    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AB    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AC    | 37/41 (90%) | 37 (100%) | 0        | 100         | 100 |
| 1   | AD    | 37/41 (90%) | 37 (100%) | 0        | 100         | 100 |
| 1   | AE    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AF    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AG    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AH    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AI    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed    | Rotameric | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 1   | AJ    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AK    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AL    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AM    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AN    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AO    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AP    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AQ    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AR    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AS    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AT    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AU    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AV    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AW    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 1   | AX    | 38/41 (93%) | 38 (100%) | 0        | 100         | 100 |
| 2   | BA    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BB    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BC    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BD    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BE    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BF    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BG    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BH    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BI    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BJ    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BK    | 31/35 (89%) | 30 (97%)  | 1 (3%)   | 34          | 45  |
| 2   | BL    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BM    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BN    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BO    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |
| 2   | BP    | 31/35 (89%) | 31 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 2   | BQ    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | BR    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | BS    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | BT    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | BU    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | BV    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | BW    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | BX    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | ba    | 31/35 (89%)    | 30 (97%)  | 1 (3%)   | 34          | 45  |
| 2   | bb    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bc    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bd    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | be    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bf    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bg    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bh    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bi    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bj    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bk    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bl    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bm    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bn    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bo    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 2   | bp    | 31/35 (89%)    | 31 (100%) | 0        | 100         | 100 |
| 3   | C     | 245/285 (86%)  | 242 (99%) | 3 (1%)   | 67          | 79  |
| 4   | C1    | 88/156 (56%)   | 88 (100%) | 0        | 100         | 100 |
| 5   | C2    | 70/95 (74%)    | 70 (100%) | 0        | 100         | 100 |
| 6   | H1    | 50/53 (94%)    | 50 (100%) | 0        | 100         | 100 |
| 7   | H2    | 150/151 (99%)  | 149 (99%) | 1 (1%)   | 81          | 89  |
| 8   | L     | 215/216 (100%) | 212 (99%) | 3 (1%)   | 62          | 75  |
| 9   | M     | 273/299 (91%)  | 271 (99%) | 2 (1%)   | 81          | 89  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 10  | aa    | 45/55 (82%)     | 44 (98%)    | 1 (2%)   | 47          | 60  |
| 11  | ab    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | ac    | 45/54 (83%)     | 45 (100%)   | 0        | 100         | 100 |
| 11  | ad    | 46/54 (85%)     | 45 (98%)    | 1 (2%)   | 47          | 60  |
| 11  | ae    | 46/54 (85%)     | 45 (98%)    | 1 (2%)   | 47          | 60  |
| 11  | af    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | ag    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | ah    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | ai    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | aj    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | ak    | 54/54 (100%)    | 53 (98%)    | 1 (2%)   | 52          | 65  |
| 11  | al    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | am    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | an    | 54/54 (100%)    | 54 (100%)   | 0        | 100         | 100 |
| 11  | ao    | 46/54 (85%)     | 46 (100%)   | 0        | 100         | 100 |
| 11  | ap    | 54/54 (100%)    | 52 (96%)    | 2 (4%)   | 29          | 40  |
| All | All   | 3999/4504 (89%) | 3982 (100%) | 17 (0%)  | 88          | 94  |

5 of 17 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | ap    | 11  | ARG  |
| 2   | ba    | 13  | ARG  |
| 8   | L     | 272 | TRP  |
| 9   | M     | 215 | PHE  |
| 9   | M     | 291 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | L     | 116 | HIS  |
| 9   | M     | 110 | ASN  |
| 5   | C2    | 24  | HIS  |
| 7   | H2    | 12  | ASN  |
| 7   | H2    | 119 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

40 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  | AT    | 1   | 1    | 8,9,10       | 0.97 | 0           | 8,9,11      | 0.84 | 0           |
| 11  | FME  | af    | 1   | 11   | 8,9,10       | 0.94 | 0           | 8,9,11      | 1.22 | 1 (12%)     |
| 1   | FME  | AP    | 1   | 1    | 8,9,10       | 0.94 | 0           | 8,9,11      | 0.98 | 1 (12%)     |
| 11  | FME  | ao    | 1   | 11   | 8,9,10       | 0.97 | 0           | 8,9,11      | 0.98 | 1 (12%)     |
| 6   | FME  | H1    | 1   | 6    | 8,9,10       | 0.96 | 0           | 8,9,11      | 1.01 | 1 (12%)     |
| 11  | FME  | an    | 1   | 11   | 8,9,10       | 0.99 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 1   | FME  | AG    | 1   | 1    | 8,9,10       | 0.92 | 0           | 8,9,11      | 1.15 | 1 (12%)     |
| 11  | FME  | ak    | 1   | 11   | 8,9,10       | 0.97 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 1   | FME  | AS    | 1   | 1    | 8,9,10       | 0.96 | 0           | 8,9,11      | 1.07 | 1 (12%)     |
| 1   | FME  | AD    | 1   | 1    | 8,9,10       | 0.95 | 0           | 8,9,11      | 1.04 | 1 (12%)     |
| 1   | FME  | AK    | 1   | 1    | 8,9,10       | 0.96 | 0           | 8,9,11      | 1.05 | 1 (12%)     |
| 1   | FME  | AA    | 1   | 1    | 8,9,10       | 0.96 | 0           | 8,9,11      | 1.03 | 1 (12%)     |
| 1   | FME  | AJ    | 1   | 1    | 8,9,10       | 0.96 | 0           | 8,9,11      | 0.97 | 1 (12%)     |
| 1   | FME  | AX    | 1   | 1    | 8,9,10       | 1.00 | 0           | 8,9,11      | 0.82 | 0           |
| 1   | FME  | AV    | 1   | 1    | 8,9,10       | 0.99 | 0           | 8,9,11      | 0.94 | 1 (12%)     |
| 11  | FME  | al    | 1   | 11   | 8,9,10       | 0.97 | 0           | 8,9,11      | 1.11 | 1 (12%)     |
| 1   | FME  | AL    | 1   | 1    | 8,9,10       | 0.95 | 0           | 8,9,11      | 1.01 | 1 (12%)     |
| 1   | FME  | AU    | 1   | 1    | 8,9,10       | 0.98 | 0           | 8,9,11      | 0.88 | 0           |
| 11  | FME  | ai    | 1   | 11   | 8,9,10       | 0.98 | 0           | 8,9,11      | 1.14 | 1 (12%)     |
| 1   | FME  | AW    | 1   | 1    | 8,9,10       | 0.92 | 0           | 8,9,11      | 0.88 | 0           |
| 1   | FME  | AF    | 1   | 1    | 8,9,10       | 0.94 | 0           | 8,9,11      | 1.23 | 2 (25%)     |
| 11  | FME  | aj    | 1   | 11   | 8,9,10       | 0.95 | 0           | 8,9,11      | 1.09 | 1 (12%)     |
| 1   | FME  | AO    | 1   | 1    | 8,9,10       | 0.97 | 0           | 8,9,11      | 0.86 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | FME  | ae    | 1   | 11   | 8,9,10       | 0.95 | 0        | 8,9,11      | 0.82 | 0        |
| 11  | FME  | ah    | 1   | 11   | 8,9,10       | 0.95 | 0        | 8,9,11      | 1.15 | 1 (12%)  |
| 11  | FME  | ab    | 1   | 11   | 8,9,10       | 0.94 | 0        | 8,9,11      | 1.20 | 1 (12%)  |
| 1   | FME  | AB    | 1   | 1    | 8,9,10       | 0.94 | 0        | 8,9,11      | 1.00 | 1 (12%)  |
| 1   | FME  | AM    | 1   | 1    | 8,9,10       | 0.96 | 0        | 8,9,11      | 0.96 | 1 (12%)  |
| 1   | FME  | AQ    | 1   | 1    | 8,9,10       | 0.94 | 0        | 8,9,11      | 1.14 | 1 (12%)  |
| 1   | FME  | AH    | 1   | 1    | 8,9,10       | 0.96 | 0        | 8,9,11      | 0.93 | 0        |
| 11  | FME  | am    | 1   | 11   | 8,9,10       | 0.96 | 0        | 8,9,11      | 0.73 | 0        |
| 1   | FME  | AE    | 1   | 1    | 8,9,10       | 0.96 | 0        | 8,9,11      | 1.04 | 1 (12%)  |
| 1   | FME  | AR    | 1   | 1    | 8,9,10       | 0.96 | 0        | 8,9,11      | 0.92 | 1 (12%)  |
| 1   | FME  | AI    | 1   | 1    | 8,9,10       | 0.98 | 0        | 8,9,11      | 0.93 | 1 (12%)  |
| 11  | FME  | ac    | 1   | 11   | 8,9,10       | 0.98 | 0        | 8,9,11      | 1.06 | 0        |
| 11  | FME  | ag    | 1   | 11   | 8,9,10       | 0.93 | 0        | 8,9,11      | 0.94 | 0        |
| 1   | FME  | AN    | 1   | 1    | 8,9,10       | 0.93 | 0        | 8,9,11      | 1.04 | 1 (12%)  |
| 11  | FME  | ad    | 1   | 11   | 8,9,10       | 0.93 | 0        | 8,9,11      | 1.20 | 1 (12%)  |
| 11  | FME  | ap    | 1   | 11   | 8,9,10       | 0.95 | 0        | 8,9,11      | 0.91 | 0        |
| 1   | FME  | AC    | 1   | 1    | 8,9,10       | 0.94 | 0        | 8,9,11      | 1.26 | 2 (25%)  |

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  | AT    | 1   | 1    | -       | 1/7/9/11 | -     |
| 11  | FME  | af    | 1   | 11   | -       | 0/7/9/11 | -     |
| 1   | FME  | AP    | 1   | 1    | -       | 1/7/9/11 | -     |
| 11  | FME  | ao    | 1   | 11   | -       | 0/7/9/11 | -     |
| 6   | FME  | H1    | 1   | 6    | -       | 2/7/9/11 | -     |
| 11  | FME  | an    | 1   | 11   | -       | 0/7/9/11 | -     |
| 1   | FME  | AG    | 1   | 1    | -       | 1/7/9/11 | -     |
| 11  | FME  | ak    | 1   | 11   | -       | 1/7/9/11 | -     |
| 1   | FME  | AS    | 1   | 1    | -       | 1/7/9/11 | -     |
| 1   | FME  | AD    | 1   | 1    | -       | 1/7/9/11 | -     |
| 1   | FME  | AK    | 1   | 1    | -       | 1/7/9/11 | -     |
| 1   | FME  | AA    | 1   | 1    | -       | 1/7/9/11 | -     |
| 1   | FME  | AJ    | 1   | 1    | -       | 0/7/9/11 | -     |
| 1   | FME  | AX    | 1   | 1    | -       | 1/7/9/11 | -     |
| 1   | FME  | AV    | 1   | 1    | -       | 0/7/9/11 | -     |
| 11  | FME  | al    | 1   | 11   | -       | 0/7/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | FME  | AL    | 1   | 1    | -       | 0/7/9/11 | -     |
| 1   | FME  | AU    | 1   | 1    | -       | 0/7/9/11 | -     |
| 11  | FME  | ai    | 1   | 11   | -       | 0/7/9/11 | -     |
| 1   | FME  | AW    | 1   | 1    | -       | 3/7/9/11 | -     |
| 1   | FME  | AF    | 1   | 1    | -       | 1/7/9/11 | -     |
| 11  | FME  | aj    | 1   | 11   | -       | 0/7/9/11 | -     |
| 1   | FME  | AO    | 1   | 1    | -       | 0/7/9/11 | -     |
| 11  | FME  | ae    | 1   | 11   | -       | 0/7/9/11 | -     |
| 11  | FME  | ah    | 1   | 11   | -       | 1/7/9/11 | -     |
| 11  | FME  | ab    | 1   | 11   | -       | 0/7/9/11 | -     |
| 1   | FME  | AB    | 1   | 1    | -       | 2/7/9/11 | -     |
| 1   | FME  | AM    | 1   | 1    | -       | 2/7/9/11 | -     |
| 1   | FME  | AQ    | 1   | 1    | -       | 1/7/9/11 | -     |
| 1   | FME  | AH    | 1   | 1    | -       | 0/7/9/11 | -     |
| 11  | FME  | am    | 1   | 11   | -       | 1/7/9/11 | -     |
| 1   | FME  | AE    | 1   | 1    | -       | 0/7/9/11 | -     |
| 1   | FME  | AR    | 1   | 1    | -       | 0/7/9/11 | -     |
| 1   | FME  | AI    | 1   | 1    | -       | 0/7/9/11 | -     |
| 11  | FME  | ac    | 1   | 11   | -       | 1/7/9/11 | -     |
| 11  | FME  | ag    | 1   | 11   | -       | 1/7/9/11 | -     |
| 1   | FME  | AN    | 1   | 1    | -       | 2/7/9/11 | -     |
| 11  | FME  | ad    | 1   | 11   | -       | 2/7/9/11 | -     |
| 11  | FME  | ap    | 1   | 11   | -       | 1/7/9/11 | -     |
| 1   | FME  | AC    | 1   | 1    | -       | 0/7/9/11 | -     |

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 11  | ad    | 1   | FME  | C-CA-N | 2.79 | 114.88      | 109.50   |
| 11  | af    | 1   | FME  | C-CA-N | 2.78 | 114.87      | 109.50   |
| 11  | ab    | 1   | FME  | C-CA-N | 2.71 | 114.72      | 109.50   |
| 11  | ah    | 1   | FME  | C-CA-N | 2.59 | 114.49      | 109.50   |
| 1   | AC    | 1   | FME  | C-CA-N | 2.54 | 114.39      | 109.50   |

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms     |
|-----|-------|-----|------|-----------|
| 11  | ah    | 1   | FME  | O-C-CA-CB |

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| Mol | Chain | Res | Type | Atoms     |
|-----|-------|-----|------|-----------|
| 1   | AB    | 1   | FME  | O-C-CA-CB |
| 1   | AK    | 1   | FME  | O-C-CA-CB |
| 1   | AM    | 1   | FME  | O-C-CA-CB |
| 1   | AN    | 1   | FME  | O-C-CA-CB |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

4 monosaccharides 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$ |
| 12  | MAN  | CG    | 1   | 12,3,18 | 11,11,12     | 0.78 | 1 (9%)      | 15,15,17    | 1.00 | 1 (6%)      |
| 12  | RAM  | CG    | 2   | 12      | 10,10,11     | 1.71 | 3 (30%)     | 14,14,16    | 0.77 | 0           |
| 12  | MAN  | MG    | 1   | 12,18,9 | 11,11,12     | 0.89 | 0           | 15,15,17    | 1.14 | 1 (6%)      |
| 12  | RAM  | MG    | 2   | 12      | 10,10,11     | 1.79 | 3 (30%)     | 14,14,16    | 2.14 | 4 (28%)     |

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

| Mol | Type | Chain | Res | Link    | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|---------|---------|-----------|---------|
| 12  | MAN  | CG    | 1   | 12,3,18 | -       | 2/2/19/22 | 0/1/1/1 |
| 12  | RAM  | CG    | 2   | 12      | -       | -         | 0/1/1/1 |
| 12  | MAN  | MG    | 1   | 12,18,9 | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | RAM  | MG    | 2   | 12      | -       | -         | 0/1/1/1 |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 12  | MG    | 2   | RAM  | O5-C1 | 4.22  | 1.50        | 1.43     |
| 12  | CG    | 2   | RAM  | O5-C1 | 4.14  | 1.50        | 1.43     |
| 12  | MG    | 2   | RAM  | C2-C3 | -2.54 | 1.48        | 1.52     |
| 12  | CG    | 2   | RAM  | C2-C3 | -2.27 | 1.49        | 1.52     |
| 12  | MG    | 2   | RAM  | O5-C5 | 2.19  | 1.47        | 1.43     |

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 12  | MG    | 2   | RAM  | C6-C5-C4 | -4.17 | 105.45      | 113.08   |
| 12  | MG    | 2   | RAM  | O5-C5-C4 | 4.12  | 116.97      | 109.55   |
| 12  | MG    | 2   | RAM  | C3-C4-C5 | 3.91  | 115.76      | 109.81   |
| 12  | MG    | 1   | MAN  | C1-O5-C5 | 3.41  | 116.76      | 112.19   |
| 12  | CG    | 1   | MAN  | C1-O5-C5 | 2.45  | 115.47      | 112.19   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

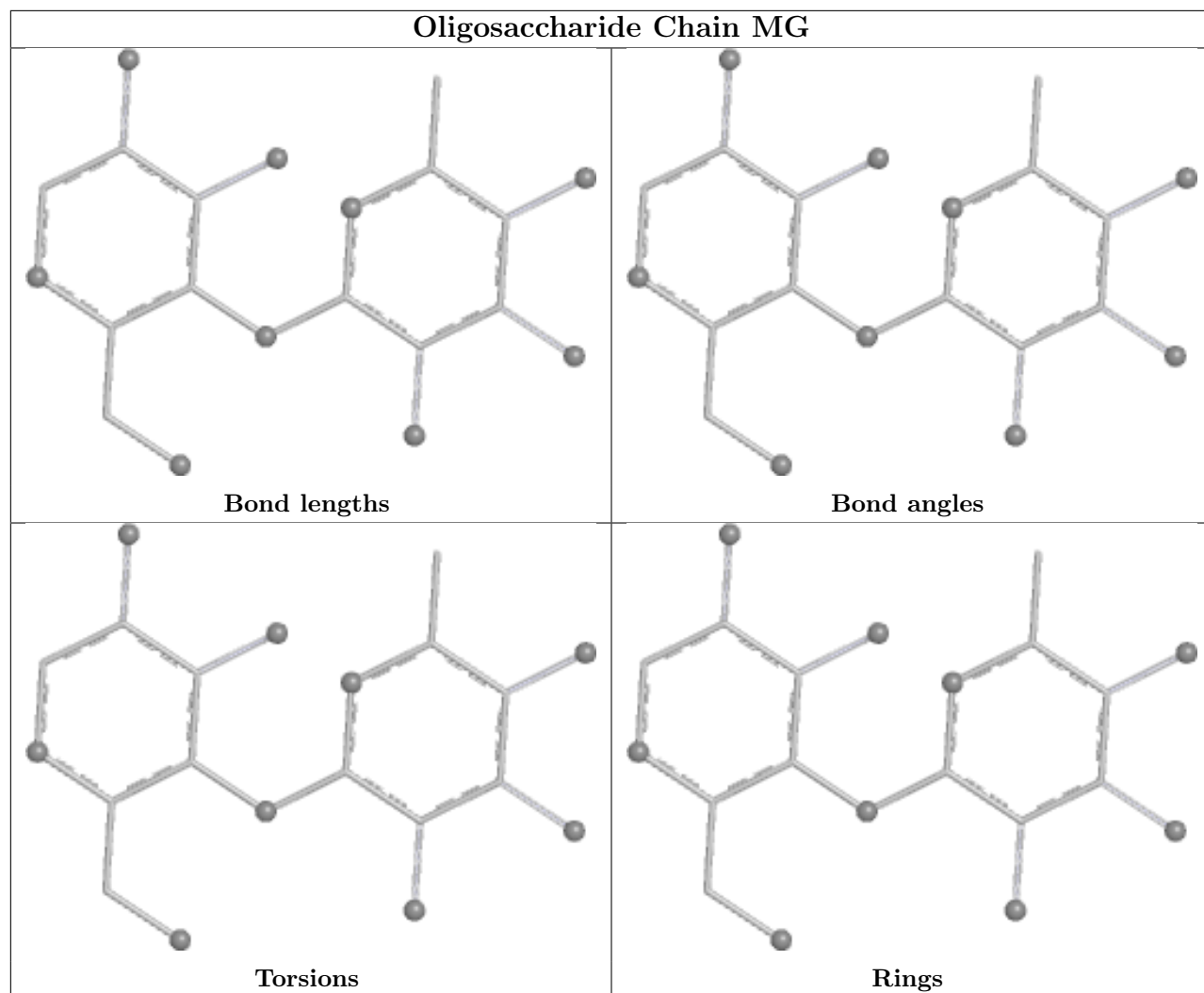
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 12  | CG    | 1   | MAN  | O5-C5-C6-O6 |
| 12  | CG    | 1   | MAN  | C4-C5-C6-O6 |

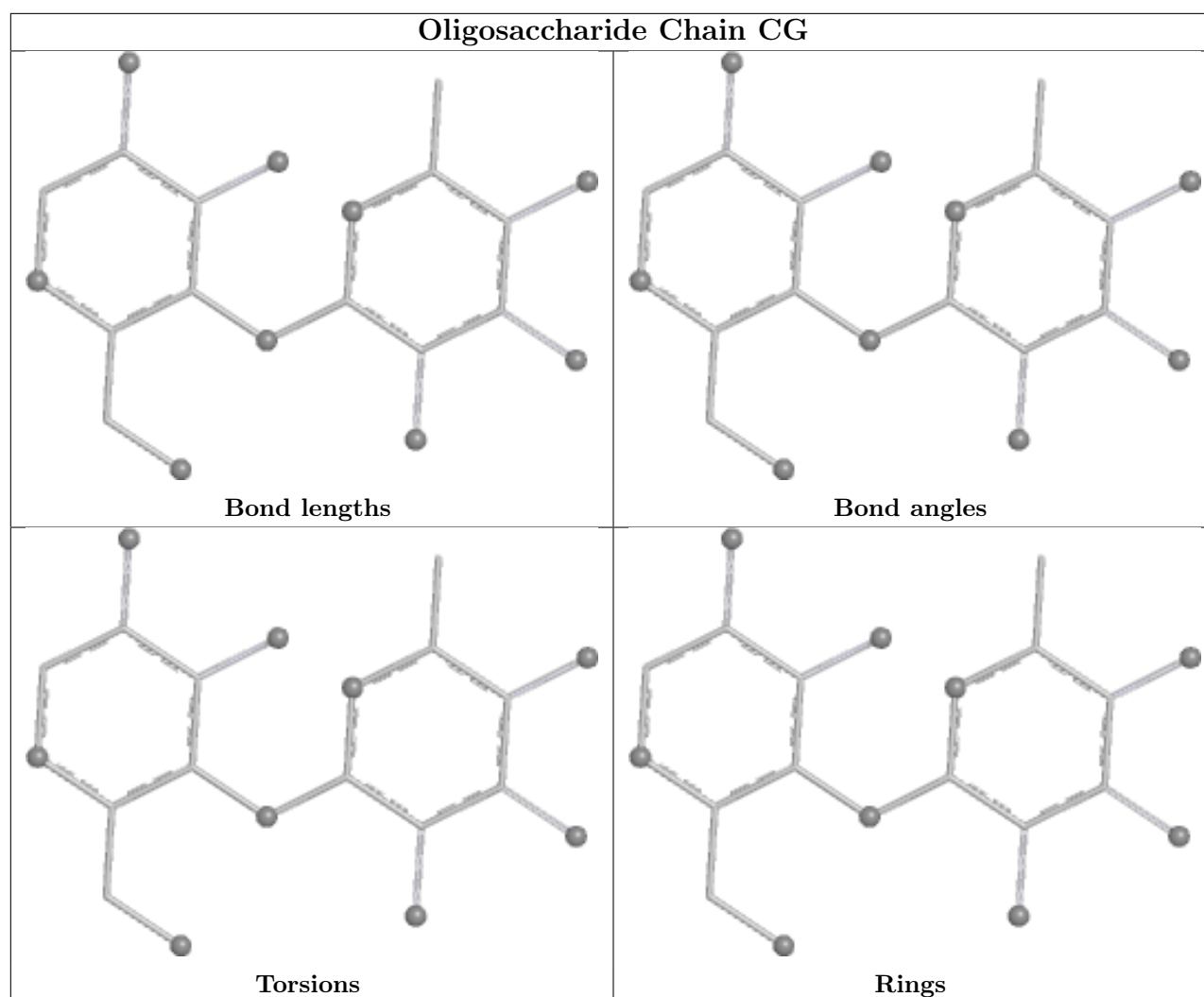
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 1 is monoatomic - leaving 311 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 14  | LMT  | BW    | 1002 | -    | 36,36,36     | 1.05 | 4 (11%)     | 47,47,47    | 0.93 | 1 (2%)      |
| 20  | 0V9  | be    | 103  | -    | 44,44,46     | 0.76 | 1 (2%)      | 47,49,51    | 0.83 | 0           |
| 26  | V7B  | ag    | 1002 | -    | 59,59,59     | 0.93 | 5 (8%)      | 75,75,75    | 1.29 | 8 (10%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | BCL  | bf    | 105  | -    | 64,74,74     | 1.70 | 6 (9%)   | 74,115,115  | 1.40 | 10 (13%) |
| 14  | LMT  | bo    | 103  | -    | 36,36,36     | 1.05 | 3 (8%)   | 47,47,47    | 0.89 | 1 (2%)   |
| 14  | LMT  | bm    | 104  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.97 | 2 (4%)   |
| 13  | BCL  | BH    | 1003 | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.52 | 12 (16%) |
| 14  | LMT  | BP    | 1002 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.92 | 1 (2%)   |
| 15  | V7N  | ba    | 101  | -    | 44,44,44     | 1.69 | 7 (15%)  | 48,54,54    | 1.54 | 11 (22%) |
| 16  | HEC  | C     | 1002 | 3    | 32,50,50     | 1.92 | 3 (9%)   | 30,82,82    | 2.20 | 6 (20%)  |
| 13  | BCL  | BQ    | 1003 | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.43 | 9 (12%)  |
| 13  | BCL  | AE    | 1001 | -    | 64,74,74     | 1.66 | 7 (10%)  | 74,115,115  | 1.44 | 10 (13%) |
| 14  | LMT  | BE    | 105  | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.89 | 2 (4%)   |
| 14  | LMT  | BH    | 1004 | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.92 | 1 (2%)   |
| 13  | BCL  | aj    | 102  | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.55 | 12 (16%) |
| 14  | LMT  | BO    | 1003 | -    | 36,36,36     | 1.03 | 4 (11%)  | 47,47,47    | 0.94 | 2 (4%)   |
| 14  | LMT  | BU    | 1002 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.86 | 1 (2%)   |
| 13  | BCL  | AX    | 101  | -    | 64,74,74     | 1.63 | 7 (10%)  | 74,115,115  | 1.47 | 9 (12%)  |
| 13  | BCL  | ao    | 1001 | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.46 | 9 (12%)  |
| 13  | BCL  | BC    | 103  | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.43 | 10 (13%) |
| 13  | BCL  | AF    | 1001 | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.49 | 11 (14%) |
| 14  | LMT  | BS    | 1003 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.89 | 0        |
| 13  | BCL  | AI    | 103  | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.42 | 9 (12%)  |
| 23  | MQ8  | L     | 309  | -    | 54,54,54     | 0.64 | 0        | 67,69,69    | 0.77 | 2 (2%)   |
| 13  | BCL  | AW    | 101  | 28   | 64,74,74     | 1.70 | 6 (9%)   | 74,115,115  | 1.49 | 12 (16%) |
| 14  | LMT  | AU    | 101  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.84 | 0        |
| 13  | BCL  | bl    | 105  | -    | 64,74,74     | 1.69 | 7 (10%)  | 74,115,115  | 1.40 | 10 (13%) |
| 13  | BCL  | AW    | 103  | -    | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.45 | 9 (12%)  |
| 13  | BCL  | AA    | 1001 | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.47 | 10 (13%) |
| 13  | BCL  | AO    | 102  | -    | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.43 | 9 (12%)  |
| 13  | BCL  | ai    | 102  | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.51 | 12 (16%) |
| 14  | LMT  | BC    | 102  | -    | 36,36,36     | 1.05 | 3 (8%)   | 47,47,47    | 0.91 | 1 (2%)   |
| 14  | LMT  | BF    | 101  | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 1.11 | 3 (6%)   |
| 13  | BCL  | AQ    | 102  | 28   | 64,74,74     | 1.72 | 6 (9%)   | 74,115,115  | 1.46 | 11 (14%) |
| 14  | LMT  | BG    | 1003 | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.85 | 1 (2%)   |
| 15  | V7N  | bi    | 101  | -    | 44,44,44     | 1.67 | 8 (18%)  | 48,54,54    | 1.60 | 11 (22%) |
| 14  | LMT  | M     | 402  | -    | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.93 | 2 (4%)   |
| 13  | BCL  | af    | 102  | -    | 64,74,74     | 1.70 | 6 (9%)   | 74,115,115  | 1.45 | 10 (13%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | V7N  | bb    | 101  | -    | 44,44,44     | 1.68 | 7 (15%)  | 48,54,54    | 1.76 | 12 (25%) |
| 14  | LMT  | BU    | 1001 | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.90 | 1 (2%)   |
| 15  | V7N  | BM    | 1001 | -    | 44,44,44     | 1.65 | 8 (18%)  | 48,54,54    | 1.76 | 11 (22%) |
| 22  | BPH  | M     | 406  | -    | 51,70,70     | 0.87 | 1 (1%)   | 52,101,101  | 1.05 | 6 (11%)  |
| 14  | LMT  | bg    | 103  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 14  | LMT  | BQ    | 1002 | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.93 | 3 (6%)   |
| 14  | LMT  | BA    | 106  | -    | 36,36,36     | 1.03 | 4 (11%)  | 47,47,47    | 1.03 | 3 (6%)   |
| 15  | V7N  | bc    | 104  | -    | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.63 | 12 (25%) |
| 14  | LMT  | bl    | 104  | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.91 | 2 (4%)   |
| 13  | BCL  | ad    | 102  | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.47 | 9 (12%)  |
| 14  | LMT  | BA    | 105  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.94 | 3 (6%)   |
| 13  | BCL  | BE    | 104  | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.58 | 13 (17%) |
| 14  | LMT  | BM    | 1002 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.87 | 1 (2%)   |
| 14  | LMT  | BI    | 105  | -    | 36,36,36     | 1.07 | 5 (13%)  | 47,47,47    | 0.91 | 1 (2%)   |
| 15  | V7N  | BO    | 1001 | -    | 44,44,44     | 1.66 | 7 (15%)  | 48,54,54    | 1.52 | 8 (16%)  |
| 13  | BCL  | AO    | 101  | -    | 64,74,74     | 1.72 | 6 (9%)   | 74,115,115  | 1.44 | 10 (13%) |
| 15  | V7N  | BD    | 101  | -    | 44,44,44     | 1.65 | 8 (18%)  | 48,54,54    | 1.71 | 12 (25%) |
| 13  | BCL  | AC    | 1001 | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.41 | 9 (12%)  |
| 14  | LMT  | AG    | 101  | -    | 36,36,36     | 1.10 | 4 (11%)  | 47,47,47    | 1.11 | 2 (4%)   |
| 20  | 0V9  | bg    | 102  | -    | 44,44,46     | 0.75 | 1 (2%)   | 47,49,51    | 0.83 | 3 (6%)   |
| 15  | V7N  | bm    | 101  | -    | 44,44,44     | 1.66 | 7 (15%)  | 48,54,54    | 1.61 | 12 (25%) |
| 14  | LMT  | BI    | 101  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.92 | 1 (2%)   |
| 14  | LMT  | BJ    | 1003 | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.81 | 1 (2%)   |
| 15  | V7N  | bh    | 102  | -    | 44,44,44     | 1.65 | 7 (15%)  | 48,54,54    | 1.63 | 9 (18%)  |
| 15  | V7N  | BA    | 101  | -    | 44,44,44     | 1.67 | 6 (13%)  | 48,54,54    | 1.62 | 10 (20%) |
| 14  | LMT  | AB    | 104  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.98 | 2 (4%)   |
| 13  | BCL  | AQ    | 103  | -    | 64,74,74     | 1.72 | 6 (9%)   | 74,115,115  | 1.74 | 13 (17%) |
| 14  | LMT  | BO    | 1002 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.88 | 1 (2%)   |
| 13  | BCL  | BL    | 1004 | -    | 64,74,74     | 1.63 | 6 (9%)   | 74,115,115  | 1.44 | 10 (13%) |
| 21  | CD4  | M     | 404  | -    | 83,83,83     | 0.47 | 0        | 89,95,95    | 1.07 | 5 (5%)   |
| 15  | V7N  | bp    | 102  | -    | 44,44,44     | 1.69 | 7 (15%)  | 48,54,54    | 1.60 | 11 (22%) |
| 14  | LMT  | BL    | 1005 | -    | 36,36,36     | 1.03 | 4 (11%)  | 47,47,47    | 1.01 | 2 (4%)   |
| 20  | 0V9  | H1    | 1002 | -    | 44,44,46     | 0.77 | 1 (2%)   | 47,49,51    | 0.83 | 2 (4%)   |
| 14  | LMT  | BQ    | 1004 | -    | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.90 | 2 (4%)   |
| 13  | BCL  | AG    | 102  | -    | 64,74,74     | 1.66 | 5 (7%)   | 74,115,115  | 1.51 | 11 (14%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | LMT  | AK    | 101  | -    | 36,36,36     | 1.07 | 5 (13%)  | 47,47,47    | 0.97 | 1 (2%)   |
| 14  | LMT  | BH    | 1002 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.88 | 0        |
| 14  | LMT  | BA    | 103  | -    | 36,36,36     | 1.03 | 4 (11%)  | 47,47,47    | 0.94 | 2 (4%)   |
| 13  | BCL  | BX    | 1004 | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.43 | 11 (14%) |
| 15  | V7N  | bg    | 101  | -    | 44,44,44     | 1.69 | 8 (18%)  | 48,54,54    | 1.65 | 11 (22%) |
| 14  | LMT  | BF    | 102  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 1.00 | 2 (4%)   |
| 15  | V7N  | BT    | 1001 | -    | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.59 | 11 (22%) |
| 13  | BCL  | AW    | 104  | -    | 64,74,74     | 1.69 | 5 (7%)   | 74,115,115  | 1.59 | 14 (18%) |
| 14  | LMT  | BI    | 103  | -    | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.90 | 1 (2%)   |
| 14  | LMT  | AJ    | 103  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.86 | 1 (2%)   |
| 14  | LMT  | bf    | 104  | -    | 36,36,36     | 1.08 | 5 (13%)  | 47,47,47    | 0.86 | 2 (4%)   |
| 25  | CRT  | M     | 408  | -    | 43,43,43     | 0.59 | 0        | 48,54,54    | 0.70 | 0        |
| 20  | OV9  | bh    | 104  | -    | 44,44,46     | 0.74 | 1 (2%)   | 47,49,51    | 0.84 | 2 (4%)   |
| 13  | BCL  | BP    | 1004 | -    | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.51 | 12 (16%) |
| 15  | V7N  | bj    | 101  | -    | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.59 | 11 (22%) |
| 13  | BCL  | bk    | 105  | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.54 | 12 (16%) |
| 14  | LMT  | L     | 307  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.96 | 2 (4%)   |
| 20  | OV9  | bc    | 102  | -    | 44,44,46     | 0.75 | 1 (2%)   | 47,49,51    | 0.90 | 3 (6%)   |
| 15  | V7N  | BR    | 1001 | -    | 44,44,44     | 1.65 | 7 (15%)  | 48,54,54    | 1.77 | 13 (27%) |
| 14  | LMT  | BT    | 1005 | -    | 36,36,36     | 1.03 | 4 (11%)  | 47,47,47    | 0.99 | 2 (4%)   |
| 14  | LMT  | bh    | 103  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.99 | 1 (2%)   |
| 15  | V7N  | BB    | 101  | -    | 44,44,44     | 1.65 | 8 (18%)  | 48,54,54    | 1.65 | 13 (27%) |
| 13  | BCL  | bi    | 103  | -    | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.43 | 12 (16%) |
| 14  | LMT  | BA    | 102  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.94 | 2 (4%)   |
| 15  | V7N  | BV    | 1001 | -    | 44,44,44     | 1.68 | 7 (15%)  | 48,54,54    | 1.57 | 12 (25%) |
| 15  | V7N  | BW    | 1001 | -    | 44,44,44     | 1.65 | 6 (13%)  | 48,54,54    | 1.62 | 11 (22%) |
| 16  | HEC  | C     | 1003 | 3    | 32,50,50     | 1.89 | 3 (9%)   | 30,82,82    | 2.16 | 6 (20%)  |
| 23  | MQ8  | M     | 407  | -    | 54,54,54     | 0.65 | 0        | 67,69,69    | 0.64 | 1 (1%)   |
| 15  | V7N  | BQ    | 1001 | -    | 44,44,44     | 1.65 | 6 (13%)  | 48,54,54    | 1.61 | 12 (25%) |
| 14  | LMT  | BG    | 1002 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.83 | 0        |
| 13  | BCL  | AN    | 102  | 28   | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.49 | 11 (14%) |
| 13  | BCL  | BB    | 104  | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.51 | 12 (16%) |
| 20  | OV9  | L     | 310  | -    | 44,44,46     | 0.75 | 1 (2%)   | 47,49,51    | 0.83 | 1 (2%)   |
| 22  | BPH  | L     | 301  | -    | 51,70,70     | 0.88 | 1 (1%)   | 52,101,101  | 1.12 | 7 (13%)  |
| 13  | BCL  | BK    | 1003 | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.46 | 9 (12%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | LMT  | BX    | 1002 | -     | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.88 | 2 (4%)   |
| 20  | 0V9  | bj    | 103  | -     | 44,44,46     | 0.78 | 1 (2%)   | 47,49,51    | 0.94 | 2 (4%)   |
| 14  | LMT  | BX    | 1003 | -     | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.94 | 2 (4%)   |
| 14  | LMT  | L     | 305  | -     | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.84 | 0        |
| 13  | BCL  | be    | 104  | -     | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.39 | 10 (13%) |
| 13  | BCL  | al    | 1001 | -     | 64,74,74     | 1.70 | 6 (9%)   | 74,115,115  | 1.49 | 11 (14%) |
| 20  | 0V9  | ba    | 104  | -     | 44,44,46     | 0.76 | 1 (2%)   | 47,49,51    | 0.91 | 1 (2%)   |
| 13  | BCL  | AN    | 104  | -     | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.44 | 9 (12%)  |
| 14  | LMT  | BN    | 1002 | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.97 | 2 (4%)   |
| 13  | BCL  | bd    | 103  | -     | 64,74,74     | 1.67 | 7 (10%)  | 74,115,115  | 1.45 | 10 (13%) |
| 14  | LMT  | BN    | 1004 | -     | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.87 | 0        |
| 15  | V7N  | BX    | 1001 | -     | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.61 | 11 (22%) |
| 13  | BCL  | AB    | 101  | -     | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.53 | 12 (16%) |
| 15  | V7N  | BK    | 1001 | -     | 44,44,44     | 1.66 | 6 (13%)  | 48,54,54    | 1.59 | 12 (25%) |
| 16  | HEC  | C     | 1001 | 3     | 32,50,50     | 1.89 | 3 (9%)   | 30,82,82    | 2.34 | 8 (26%)  |
| 13  | BCL  | AV    | 102  | -     | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.41 | 9 (12%)  |
| 15  | V7N  | BN    | 1001 | -     | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.85 | 11 (22%) |
| 14  | LMT  | L     | 304  | -     | 36,36,36     | 1.01 | 4 (11%)  | 47,47,47    | 0.94 | 1 (2%)   |
| 14  | LMT  | bn    | 102  | -     | 36,36,36     | 1.06 | 5 (13%)  | 47,47,47    | 0.87 | 1 (2%)   |
| 15  | V7N  | BE    | 101  | -     | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.55 | 11 (22%) |
| 14  | LMT  | BR    | 1005 | -     | 36,36,36     | 1.07 | 5 (13%)  | 47,47,47    | 0.91 | 0        |
| 20  | 0V9  | aj    | 101  | -     | 44,44,46     | 0.76 | 1 (2%)   | 47,49,51    | 0.86 | 3 (6%)   |
| 15  | V7N  | BP    | 1001 | -     | 44,44,44     | 1.65 | 8 (18%)  | 48,54,54    | 1.74 | 13 (27%) |
| 14  | LMT  | BD    | 102  | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.93 | 2 (4%)   |
| 18  | V75  | C     | 1006 | 12,17 | 18,18,18     | 1.59 | 4 (22%)  | 21,25,25    | 1.73 | 2 (9%)   |
| 14  | LMT  | BP    | 1005 | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.83 | 1 (2%)   |
| 13  | BCL  | AT    | 102  | -     | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.46 | 9 (12%)  |
| 14  | LMT  | AH    | 106  | -     | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 1.08 | 5 (10%)  |
| 15  | V7N  | BS    | 1001 | -     | 44,44,44     | 1.65 | 7 (15%)  | 48,54,54    | 1.69 | 12 (25%) |
| 14  | LMT  | BV    | 1002 | -     | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.89 | 2 (4%)   |
| 15  | V7N  | BH    | 1001 | -     | 44,44,44     | 1.66 | 7 (15%)  | 48,54,54    | 1.68 | 12 (25%) |
| 20  | 0V9  | bk    | 104  | -     | 44,44,46     | 0.74 | 1 (2%)   | 47,49,51    | 0.99 | 3 (6%)   |
| 17  | NDG  | C1    | 301  | 18    | 14,14,15     | 0.69 | 1 (7%)   | 17,19,21    | 0.88 | 1 (5%)   |
| 14  | LMT  | BR    | 1002 | -     | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.92 | 1 (2%)   |
| 13  | BCL  | AM    | 102  | -     | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.43 | 9 (12%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | BCL  | AH    | 102  | -    | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.44 | 9 (12%)  |
| 15  | V7N  | AT    | 103  | -    | 44,44,44     | 1.71 | 8 (18%)  | 48,54,54    | 1.67 | 13 (27%) |
| 13  | BCL  | ae    | 1001 | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.47 | 9 (12%)  |
| 13  | BCL  | AB    | 103  | 28   | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.60 | 13 (17%) |
| 14  | LMT  | AT    | 101  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.87 | 2 (4%)   |
| 13  | BCL  | AA    | 1002 | 28   | 64,74,74     | 1.68 | 5 (7%)   | 74,115,115  | 1.53 | 12 (16%) |
| 14  | LMT  | BN    | 1003 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.99 | 2 (4%)   |
| 21  | CD4  | af    | 104  | -    | 83,83,83     | 0.49 | 0        | 89,95,95    | 1.06 | 5 (5%)   |
| 14  | LMT  | BS    | 1004 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.89 | 1 (2%)   |
| 13  | BCL  | AU    | 103  | -    | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.43 | 9 (12%)  |
| 14  | LMT  | bd    | 102  | -    | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.87 | 1 (2%)   |
| 23  | MQ8  | an    | 101  | -    | 54,54,54     | 0.65 | 0        | 67,69,69    | 1.17 | 6 (8%)   |
| 14  | LMT  | BH    | 1005 | -    | 36,36,36     | 1.09 | 4 (11%)  | 47,47,47    | 0.91 | 2 (4%)   |
| 14  | LMT  | AB    | 102  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.83 | 2 (4%)   |
| 14  | LMT  | AN    | 101  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 1.01 | 3 (6%)   |
| 14  | LMT  | BC    | 104  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.90 | 1 (2%)   |
| 13  | BCL  | BW    | 1003 | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.49 | 11 (14%) |
| 14  | LMT  | BE    | 102  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.91 | 2 (4%)   |
| 14  | LMT  | BF    | 103  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.92 | 1 (2%)   |
| 15  | V7N  | BG    | 1001 | -    | 44,44,44     | 1.68 | 7 (15%)  | 48,54,54    | 1.68 | 12 (25%) |
| 14  | LMT  | BD    | 105  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.92 | 2 (4%)   |
| 14  | LMT  | BP    | 1003 | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.87 | 1 (2%)   |
| 13  | BCL  | AP    | 101  | -    | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.43 | 10 (13%) |
| 26  | V7B  | af    | 101  | -    | 59,59,59     | 0.88 | 3 (5%)   | 75,75,75    | 1.13 | 5 (6%)   |
| 13  | BCL  | AM    | 101  | 28   | 64,74,74     | 1.73 | 6 (9%)   | 74,115,115  | 1.57 | 13 (17%) |
| 13  | BCL  | AH    | 101  | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.53 | 12 (16%) |
| 15  | V7N  | AH    | 105  | -    | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.51 | 9 (18%)  |
| 20  | 0V9  | ba    | 102  | -    | 44,44,46     | 0.76 | 1 (2%)   | 47,49,51    | 0.88 | 1 (2%)   |
| 20  | 0V9  | bk    | 102  | -    | 44,44,46     | 0.77 | 1 (2%)   | 47,49,51    | 0.81 | 1 (2%)   |
| 13  | BCL  | bn    | 103  | -    | 64,74,74     | 1.66 | 7 (10%)  | 74,115,115  | 1.40 | 10 (13%) |
| 21  | CD4  | af    | 103  | -    | 83,83,83     | 0.49 | 0        | 89,95,95    | 1.08 | 6 (6%)   |
| 20  | 0V9  | bm    | 102  | -    | 44,44,46     | 0.75 | 1 (2%)   | 47,49,51    | 0.92 | 1 (2%)   |
| 14  | LMT  | AW    | 102  | -    | 36,36,36     | 1.05 | 3 (8%)   | 47,47,47    | 0.96 | 3 (6%)   |
| 15  | V7N  | BJ    | 1001 | -    | 44,44,44     | 1.66 | 6 (13%)  | 48,54,54    | 1.65 | 12 (25%) |
| 14  | LMT  | AN    | 103  | -    | 36,36,36     | 1.01 | 4 (11%)  | 47,47,47    | 0.98 | 2 (4%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | 0V9  | bn    | 104  | -    | 44,44,46     | 0.75 | 1 (2%)   | 47,49,51    | 0.93 | 2 (4%)   |
| 14  | LMT  | bc    | 101  | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 1.06 | 4 (8%)   |
| 14  | LMT  | AL    | 102  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.83 | 0        |
| 15  | V7N  | bl    | 102  | -    | 44,44,44     | 1.68 | 7 (15%)  | 48,54,54    | 1.58 | 11 (22%) |
| 13  | BCL  | L     | 308  | -    | 64,74,74     | 1.56 | 6 (9%)   | 74,115,115  | 1.40 | 10 (13%) |
| 13  | BCL  | AG    | 103  | -    | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.44 | 9 (12%)  |
| 14  | LMT  | BK    | 1005 | -    | 36,36,36     | 1.08 | 4 (11%)  | 47,47,47    | 0.97 | 2 (4%)   |
| 13  | BCL  | AL    | 103  | -    | 64,74,74     | 1.71 | 6 (9%)   | 74,115,115  | 1.63 | 13 (17%) |
| 14  | LMT  | BL    | 1003 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.95 | 3 (6%)   |
| 13  | BCL  | BI    | 104  | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.48 | 10 (13%) |
| 13  | BCL  | BV    | 1004 | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.45 | 11 (14%) |
| 14  | LMT  | AV    | 101  | -    | 36,36,36     | 1.09 | 4 (11%)  | 47,47,47    | 1.04 | 3 (6%)   |
| 13  | BCL  | AP    | 103  | 28   | 64,74,74     | 1.72 | 6 (9%)   | 74,115,115  | 1.52 | 11 (14%) |
| 21  | CD4  | H1    | 1003 | -    | 83,83,83     | 0.46 | 0        | 89,95,95    | 0.95 | 4 (4%)   |
| 13  | BCL  | bo    | 102  | -    | 64,74,74     | 1.69 | 7 (10%)  | 74,115,115  | 1.39 | 10 (13%) |
| 13  | BCL  | ab    | 1001 | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.47 | 12 (16%) |
| 13  | BCL  | bm    | 103  | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.44 | 10 (13%) |
| 17  | NDG  | C     | 1005 | 18   | 14,14,15     | 0.68 | 0        | 17,19,21    | 1.07 | 2 (11%)  |
| 20  | 0V9  | bo    | 104  | -    | 44,44,46     | 0.75 | 1 (2%)   | 47,49,51    | 0.83 | 1 (2%)   |
| 14  | LMT  | bh    | 101  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 1.02 | 3 (6%)   |
| 13  | BCL  | AK    | 103  | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.46 | 11 (14%) |
| 20  | 0V9  | bi    | 102  | -    | 44,44,46     | 0.76 | 1 (2%)   | 47,49,51    | 0.82 | 3 (6%)   |
| 14  | LMT  | bl    | 101  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 1.07 | 5 (10%)  |
| 13  | BCL  | BA    | 104  | -    | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.68 | 12 (16%) |
| 13  | BCL  | bj    | 104  | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.43 | 11 (14%) |
| 13  | BCL  | AR    | 101  | -    | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.41 | 9 (12%)  |
| 13  | BCL  | bg    | 104  | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.40 | 11 (14%) |
| 14  | LMT  | BU    | 1003 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 1.04 | 3 (6%)   |
| 14  | LMT  | BS    | 1002 | -    | 36,36,36     | 1.07 | 5 (13%)  | 47,47,47    | 0.93 | 2 (4%)   |
| 14  | LMT  | L     | 306  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.86 | 1 (2%)   |
| 14  | LMT  | bp    | 101  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 1.11 | 3 (6%)   |
| 21  | CD4  | ad    | 101  | -    | 83,83,83     | 0.47 | 0        | 89,95,95    | 1.09 | 5 (5%)   |
| 13  | BCL  | ba    | 103  | -    | 64,74,74     | 1.70 | 6 (9%)   | 74,115,115  | 1.43 | 10 (13%) |
| 13  | BCL  | AS    | 102  | 28   | 64,74,74     | 1.70 | 6 (9%)   | 74,115,115  | 1.53 | 10 (13%) |
| 13  | BCL  | AJ    | 102  | 28   | 64,74,74     | 1.69 | 5 (7%)   | 74,115,115  | 1.64 | 14 (18%) |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | BCL  | bp    | 103  | -    | 64,74,74     | 1.70 | 7 (10%)  | 74,115,115  | 1.44 | 11 (14%) |
| 13  | BCL  | ap    | 1001 | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.44 | 9 (12%)  |
| 14  | LMT  | BE    | 106  | -    | 36,36,36     | 1.08 | 5 (13%)  | 47,47,47    | 0.94 | 2 (4%)   |
| 13  | BCL  | am    | 1001 | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.45 | 9 (12%)  |
| 13  | BCL  | AF    | 1002 | -    | 64,74,74     | 1.68 | 5 (7%)   | 74,115,115  | 1.49 | 11 (14%) |
| 13  | BCL  | ak    | 1001 | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.46 | 10 (13%) |
| 14  | LMT  | AA    | 1003 | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 1.00 | 1 (2%)   |
| 13  | BCL  | BT    | 1004 | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.54 | 14 (18%) |
| 13  | BCL  | AD    | 1001 | 28   | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.50 | 11 (14%) |
| 14  | LMT  | bf    | 101  | -    | 36,36,36     | 1.11 | 4 (11%)  | 47,47,47    | 0.93 | 2 (4%)   |
| 13  | BCL  | BR    | 1003 | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.42 | 10 (13%) |
| 15  | V7N  | AE    | 1003 | -    | 44,44,44     | 1.67 | 7 (15%)  | 48,54,54    | 1.57 | 10 (20%) |
| 14  | LMT  | BL    | 1002 | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 1.09 | 3 (6%)   |
| 13  | BCL  | BF    | 104  | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.40 | 10 (13%) |
| 13  | BCL  | AS    | 101  | -    | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.42 | 9 (12%)  |
| 14  | LMT  | BW    | 1005 | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 1.41 | 4 (8%)   |
| 15  | V7N  | bo    | 101  | -    | 44,44,44     | 1.67 | 8 (18%)  | 48,54,54    | 1.58 | 10 (20%) |
| 20  | 0V9  | be    | 102  | -    | 44,44,46     | 0.77 | 1 (2%)   | 47,49,51    | 0.96 | 3 (6%)   |
| 13  | BCL  | ag    | 1001 | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.47 | 10 (13%) |
| 13  | BCL  | BD    | 106  | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.46 | 11 (14%) |
| 14  | LMT  | AP    | 102  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.92 | 1 (2%)   |
| 14  | LMT  | bk    | 101  | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.98 | 2 (4%)   |
| 13  | BCL  | AE    | 1002 | -    | 64,74,74     | 1.65 | 7 (10%)  | 74,115,115  | 1.42 | 9 (12%)  |
| 14  | LMT  | bb    | 102  | -    | 36,36,36     | 1.10 | 5 (13%)  | 47,47,47    | 0.94 | 3 (6%)   |
| 15  | V7N  | bk    | 103  | -    | 44,44,44     | 1.70 | 8 (18%)  | 48,54,54    | 1.49 | 9 (18%)  |
| 14  | LMT  | BJ    | 1002 | -    | 36,36,36     | 1.02 | 4 (11%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 13  | BCL  | ah    | 1001 | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.44 | 9 (12%)  |
| 14  | LMT  | BM    | 1003 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.86 | 1 (2%)   |
| 13  | BCL  | BN    | 1006 | -    | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.52 | 11 (14%) |
| 14  | LMT  | BK    | 1004 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 1.12 | 3 (6%)   |
| 13  | BCL  | an    | 102  | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.45 | 10 (13%) |
| 14  | LMT  | AH    | 104  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.82 | 0        |
| 14  | LMT  | L     | 302  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.97 | 1 (2%)   |
| 14  | LMT  | AF    | 1003 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.89 | 1 (2%)   |
| 14  | LMT  | BE    | 103  | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.86 | 1 (2%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | 0V9  | bb    | 104  | -    | 44,44,46     | 0.77 | 1 (2%)   | 47,49,51    | 0.87 | 1 (2%)   |
| 14  | LMT  | BB    | 103  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.99 | 3 (6%)   |
| 20  | 0V9  | bl    | 103  | -    | 44,44,46     | 0.76 | 1 (2%)   | 47,49,51    | 0.86 | 0        |
| 14  | LMT  | BK    | 1006 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 1.01 | 2 (4%)   |
| 14  | LMT  | ac    | 101  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.86 | 1 (2%)   |
| 13  | BCL  | BM    | 1004 | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.54 | 12 (16%) |
| 13  | BCL  | BG    | 1004 | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.50 | 11 (14%) |
| 13  | BCL  | AD    | 1002 | -    | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.47 | 10 (13%) |
| 14  | LMT  | AD    | 1004 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.87 | 2 (4%)   |
| 14  | LMT  | AO    | 103  | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.93 | 0        |
| 14  | LMT  | bj    | 102  | -    | 36,36,36     | 1.07 | 4 (11%)  | 47,47,47    | 0.91 | 2 (4%)   |
| 15  | V7N  | bd    | 101  | -    | 44,44,44     | 1.66 | 7 (15%)  | 48,54,54    | 1.58 | 10 (20%) |
| 14  | LMT  | BT    | 1002 | -    | 36,36,36     | 1.09 | 5 (13%)  | 47,47,47    | 0.91 | 1 (2%)   |
| 14  | LMT  | BW    | 1004 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.89 | 0        |
| 13  | BCL  | AC    | 1002 | -    | 64,74,74     | 1.70 | 6 (9%)   | 74,115,115  | 1.47 | 11 (14%) |
| 14  | LMT  | BR    | 1006 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 14  | LMT  | BV    | 1003 | -    | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.89 | 2 (4%)   |
| 13  | BCL  | BJ    | 1004 | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.53 | 13 (17%) |
| 14  | LMT  | AS    | 103  | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.95 | 2 (4%)   |
| 13  | BCL  | AQ    | 101  | -    | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.45 | 9 (12%)  |
| 14  | LMT  | BK    | 1002 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.94 | 2 (4%)   |
| 20  | 0V9  | bf    | 103  | -    | 44,44,46     | 0.76 | 1 (2%)   | 47,49,51    | 0.89 | 3 (6%)   |
| 14  | LMT  | AR    | 102  | -    | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 1.08 | 3 (6%)   |
| 15  | V7N  | BC    | 101  | -    | 44,44,44     | 1.67 | 6 (13%)  | 48,54,54    | 1.64 | 12 (25%) |
| 13  | BCL  | M     | 403  | -    | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.42 | 11 (14%) |
| 16  | HEC  | C     | 1004 | 3    | 32,50,50     | 1.92 | 3 (9%)   | 30,82,82    | 2.29 | 8 (26%)  |
| 13  | BCL  | aa    | 1001 | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.47 | 10 (13%) |
| 15  | V7N  | BL    | 1001 | -    | 44,44,44     | 1.68 | 6 (13%)  | 48,54,54    | 1.59 | 12 (25%) |
| 13  | BCL  | ac    | 102  | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.46 | 10 (13%) |
| 27  | UYH  | ai    | 101  | -    | 55,55,55     | 2.18 | 14 (25%) | 63,63,63    | 1.01 | 3 (4%)   |
| 13  | BCL  | AL    | 101  | -    | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.43 | 9 (12%)  |
| 13  | BCL  | bc    | 103  | -    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.43 | 12 (16%) |
| 13  | BCL  | L     | 303  | -    | 64,74,74     | 1.67 | 7 (10%)  | 74,115,115  | 1.39 | 10 (13%) |
| 13  | BCL  | AU    | 102  | -    | 64,74,74     | 1.68 | 6 (9%)   | 74,115,115  | 1.61 | 13 (17%) |
| 21  | CD4  | ai    | 103  | -    | 83,83,83     | 0.49 | 0        | 89,95,95    | 1.07 | 7 (7%)   |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | LMT  | BP    | 1006 | -     | 36,36,36     | 1.03 | 4 (11%)  | 47,47,47    | 1.00 | 2 (4%)   |
| 13  | BCL  | AI    | 102  | -     | 64,74,74     | 1.72 | 6 (9%)   | 74,115,115  | 1.48 | 9 (12%)  |
| 13  | BCL  | BO    | 1004 | -     | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.44 | 11 (14%) |
| 14  | LMT  | BB    | 102  | -     | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.85 | 2 (4%)   |
| 15  | V7N  | bf    | 102  | -     | 44,44,44     | 1.68 | 7 (15%)  | 48,54,54    | 1.58 | 10 (20%) |
| 14  | LMT  | BD    | 103  | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.88 | 1 (2%)   |
| 19  | PGW  | H1    | 1001 | -     | 50,50,50     | 0.45 | 0        | 53,56,56    | 1.06 | 3 (5%)   |
| 14  | LMT  | BT    | 1003 | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.86 | 1 (2%)   |
| 13  | BCL  | bh    | 105  | -     | 64,74,74     | 1.64 | 6 (9%)   | 74,115,115  | 1.40 | 11 (14%) |
| 14  | LMT  | AD    | 1003 | -     | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 0.97 | 3 (6%)   |
| 13  | BCL  | AJ    | 101  | -     | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.42 | 9 (12%)  |
| 14  | LMT  | BD    | 104  | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.87 | 1 (2%)   |
| 15  | V7N  | bn    | 101  | -     | 44,44,44     | 1.68 | 7 (15%)  | 48,54,54    | 1.57 | 12 (25%) |
| 13  | BCL  | BS    | 1005 | -     | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.51 | 11 (14%) |
| 13  | BCL  | AS    | 104  | 28    | 64,74,74     | 1.69 | 6 (9%)   | 74,115,115  | 1.64 | 14 (18%) |
| 13  | BCL  | M     | 405  | -     | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.51 | 9 (12%)  |
| 15  | V7N  | be    | 101  | -     | 44,44,44     | 1.64 | 6 (13%)  | 48,54,54    | 1.66 | 10 (20%) |
| 14  | LMT  | BW    | 1006 | -     | 36,36,36     | 1.04 | 4 (11%)  | 47,47,47    | 1.17 | 5 (10%)  |
| 14  | LMT  | BI    | 102  | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.83 | 1 (2%)   |
| 14  | LMT  | BN    | 1005 | -     | 36,36,36     | 1.05 | 4 (11%)  | 47,47,47    | 0.94 | 2 (4%)   |
| 13  | BCL  | BU    | 1004 | -     | 64,74,74     | 1.65 | 6 (9%)   | 74,115,115  | 1.46 | 10 (13%) |
| 14  | LMT  | AH    | 103  | -     | 36,36,36     | 1.09 | 4 (11%)  | 47,47,47    | 0.81 | 0        |
| 13  | BCL  | bb    | 103  | -     | 64,74,74     | 1.66 | 6 (9%)   | 74,115,115  | 1.39 | 11 (14%) |
| 18  | V75  | M     | 409  | 12,17 | 18,18,18     | 1.64 | 5 (27%)  | 21,25,25    | 1.75 | 2 (9%)   |
| 13  | BCL  | AV    | 103  | 28    | 64,74,74     | 1.66 | 7 (10%)  | 74,115,115  | 1.49 | 11 (14%) |
| 14  | LMT  | AI    | 101  | -     | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 0.83 | 0        |
| 13  | BCL  | AK    | 102  | -     | 64,74,74     | 1.67 | 6 (9%)   | 74,115,115  | 1.43 | 9 (12%)  |
| 14  | LMT  | BR    | 1004 | -     | 36,36,36     | 1.04 | 3 (8%)   | 47,47,47    | 1.00 | 2 (4%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 14  | LMT  | BW    | 1002 | -    | -       | 3/21/61/61 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 20  | 0V9  | be    | 103  | -    | -       | 11/48/48/50  | -       |
| 26  | V7B  | ag    | 1002 | -    | -       | 14/48/88/88  | 0/2/2/2 |
| 13  | BCL  | bf    | 105  | -    | -       | 3/37/137/137 | -       |
| 14  | LMT  | bo    | 103  | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 14  | LMT  | bm    | 104  | -    | -       | 8/21/61/61   | 0/2/2/2 |
| 13  | BCL  | BH    | 1003 | -    | -       | 8/37/137/137 | -       |
| 14  | LMT  | BP    | 1002 | -    | -       | 5/21/61/61   | 0/2/2/2 |
| 15  | V7N  | ba    | 101  | -    | -       | 7/53/53/53   | -       |
| 16  | HEC  | C     | 1002 | 3    | -       | 4/10/54/54   | -       |
| 13  | BCL  | BQ    | 1003 | -    | -       | 5/37/137/137 | -       |
| 13  | BCL  | AE    | 1001 | -    | -       | 9/37/137/137 | -       |
| 14  | LMT  | BE    | 105  | -    | -       | 1/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BH    | 1004 | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 13  | BCL  | aj    | 102  | -    | -       | 5/37/137/137 | -       |
| 14  | LMT  | BO    | 1003 | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BU    | 1002 | -    | -       | 1/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AX    | 101  | -    | -       | 4/37/137/137 | -       |
| 13  | BCL  | ao    | 1001 | -    | -       | 7/37/137/137 | -       |
| 13  | BCL  | BC    | 103  | -    | -       | 3/37/137/137 | -       |
| 13  | BCL  | AF    | 1001 | -    | -       | 5/37/137/137 | -       |
| 14  | LMT  | BS    | 1003 | -    | -       | 6/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AI    | 103  | -    | -       | 6/37/137/137 | -       |
| 23  | MQ8  | L     | 309  | -    | -       | 9/47/67/67   | 0/2/2/2 |
| 13  | BCL  | AW    | 101  | 28   | -       | 8/37/137/137 | -       |
| 14  | LMT  | AU    | 101  | -    | -       | 5/21/61/61   | 0/2/2/2 |
| 13  | BCL  | bl    | 105  | -    | -       | 7/37/137/137 | -       |
| 13  | BCL  | AW    | 103  | -    | -       | 4/37/137/137 | -       |
| 13  | BCL  | AA    | 1001 | -    | -       | 2/37/137/137 | -       |
| 13  | BCL  | AO    | 102  | -    | -       | 1/37/137/137 | -       |
| 13  | BCL  | ai    | 102  | -    | -       | 6/37/137/137 | -       |
| 14  | LMT  | BC    | 102  | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BF    | 101  | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AQ    | 102  | 28   | -       | 6/37/137/137 | -       |
| 14  | LMT  | BG    | 1003 | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 15  | V7N  | bi    | 101  | -    | -       | 4/53/53/53   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 14  | LMT  | M     | 402  | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 13  | BCL  | af    | 102  | -    | -       | 3/37/137/137  | -       |
| 15  | V7N  | bb    | 101  | -    | -       | 16/53/53/53   | -       |
| 14  | LMT  | BU    | 1001 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 15  | V7N  | BM    | 1001 | -    | -       | 7/53/53/53    | -       |
| 22  | BPH  | M     | 406  | -    | -       | 3/37/105/105  | 0/5/6/6 |
| 14  | LMT  | bg    | 103  | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 14  | LMT  | BQ    | 1002 | -    | -       | 1/21/61/61    | 0/2/2/2 |
| 14  | LMT  | BA    | 106  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 15  | V7N  | bc    | 104  | -    | -       | 9/53/53/53    | -       |
| 14  | LMT  | bl    | 104  | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 13  | BCL  | ad    | 102  | -    | -       | 4/37/137/137  | -       |
| 14  | LMT  | BA    | 105  | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BE    | 104  | -    | -       | 2/37/137/137  | -       |
| 14  | LMT  | BM    | 1002 | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 14  | LMT  | BI    | 105  | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 15  | V7N  | BO    | 1001 | -    | -       | 6/53/53/53    | -       |
| 13  | BCL  | AO    | 101  | -    | -       | 9/37/137/137  | -       |
| 15  | V7N  | BD    | 101  | -    | -       | 4/53/53/53    | -       |
| 13  | BCL  | AC    | 1001 | -    | -       | 6/37/137/137  | -       |
| 14  | LMT  | AG    | 101  | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 20  | 0V9  | bg    | 102  | -    | -       | 15/48/48/50   | -       |
| 15  | V7N  | bm    | 101  | -    | -       | 4/53/53/53    | -       |
| 14  | LMT  | BI    | 101  | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 14  | LMT  | BJ    | 1003 | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 15  | V7N  | bh    | 102  | -    | -       | 6/53/53/53    | -       |
| 15  | V7N  | BA    | 101  | -    | -       | 6/53/53/53    | -       |
| 14  | LMT  | AB    | 104  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 13  | BCL  | AQ    | 103  | -    | -       | 10/37/137/137 | -       |
| 14  | LMT  | BO    | 1002 | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BL    | 1004 | -    | -       | 6/37/137/137  | -       |
| 21  | CD4  | M     | 404  | -    | -       | 20/94/94/94   | -       |
| 15  | V7N  | bp    | 102  | -    | -       | 6/53/53/53    | -       |
| 14  | LMT  | BL    | 1005 | -    | -       | 5/21/61/61    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 20  | 0V9  | H1    | 1002 | -    | -       | 9/48/48/50    | -       |
| 14  | LMT  | BQ    | 1004 | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 13  | BCL  | AG    | 102  | -    | -       | 11/37/137/137 | -       |
| 14  | LMT  | AK    | 101  | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 14  | LMT  | BH    | 1002 | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 14  | LMT  | BA    | 103  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BX    | 1004 | -    | -       | 4/37/137/137  | -       |
| 15  | V7N  | bg    | 101  | -    | -       | 7/53/53/53    | -       |
| 14  | LMT  | BF    | 102  | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 15  | V7N  | BT    | 1001 | -    | -       | 4/53/53/53    | -       |
| 13  | BCL  | AW    | 104  | -    | -       | 12/37/137/137 | -       |
| 14  | LMT  | BI    | 103  | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 14  | LMT  | AJ    | 103  | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 14  | LMT  | bf    | 104  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 25  | CRT  | M     | 408  | -    | -       | 3/51/51/51    | -       |
| 20  | 0V9  | bh    | 104  | -    | -       | 11/48/48/50   | -       |
| 13  | BCL  | BP    | 1004 | -    | -       | 5/37/137/137  | -       |
| 15  | V7N  | bj    | 101  | -    | -       | 3/53/53/53    | -       |
| 13  | BCL  | bk    | 105  | -    | -       | 8/37/137/137  | -       |
| 14  | LMT  | L     | 307  | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 20  | 0V9  | bc    | 102  | -    | -       | 15/48/48/50   | -       |
| 15  | V7N  | BR    | 1001 | -    | -       | 6/53/53/53    | -       |
| 14  | LMT  | BT    | 1005 | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 14  | LMT  | bh    | 103  | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 15  | V7N  | BB    | 101  | -    | -       | 4/53/53/53    | -       |
| 13  | BCL  | bi    | 103  | -    | -       | 5/37/137/137  | -       |
| 14  | LMT  | BA    | 102  | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 15  | V7N  | BV    | 1001 | -    | -       | 5/53/53/53    | -       |
| 15  | V7N  | BW    | 1001 | -    | -       | 6/53/53/53    | -       |
| 16  | HEC  | C     | 1003 | 3    | -       | 2/10/54/54    | -       |
| 23  | MQ8  | M     | 407  | -    | -       | 0/47/67/67    | 0/2/2/2 |
| 15  | V7N  | BQ    | 1001 | -    | -       | 4/53/53/53    | -       |
| 14  | LMT  | BG    | 1002 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 13  | BCL  | AN    | 102  | 28   | -       | 4/37/137/137  | -       |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions     | Rings   |
|-----|------|-------|------|-------|---------|--------------|---------|
| 13  | BCL  | BB    | 104  | -     | -       | 5/37/137/137 | -       |
| 20  | 0V9  | L     | 310  | -     | -       | 9/48/48/50   | -       |
| 22  | BPH  | L     | 301  | -     | -       | 2/37/105/105 | 0/5/6/6 |
| 13  | BCL  | BK    | 1003 | -     | -       | 9/37/137/137 | -       |
| 14  | LMT  | BX    | 1002 | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 20  | 0V9  | bj    | 103  | -     | -       | 6/48/48/50   | -       |
| 14  | LMT  | BX    | 1003 | -     | -       | 8/21/61/61   | 0/2/2/2 |
| 14  | LMT  | L     | 305  | -     | -       | 7/21/61/61   | 0/2/2/2 |
| 13  | BCL  | be    | 104  | -     | -       | 6/37/137/137 | -       |
| 13  | BCL  | al    | 1001 | -     | -       | 5/37/137/137 | -       |
| 20  | 0V9  | ba    | 104  | -     | -       | 11/48/48/50  | -       |
| 13  | BCL  | AN    | 104  | -     | -       | 1/37/137/137 | -       |
| 14  | LMT  | BN    | 1002 | -     | -       | 8/21/61/61   | 0/2/2/2 |
| 13  | BCL  | bd    | 103  | -     | -       | 4/37/137/137 | -       |
| 14  | LMT  | BN    | 1004 | -     | -       | 4/21/61/61   | 0/2/2/2 |
| 15  | V7N  | BX    | 1001 | -     | -       | 5/53/53/53   | -       |
| 13  | BCL  | AB    | 101  | -     | -       | 2/37/137/137 | -       |
| 15  | V7N  | BK    | 1001 | -     | -       | 4/53/53/53   | -       |
| 16  | HEC  | C     | 1001 | 3     | -       | 5/10/54/54   | -       |
| 13  | BCL  | AV    | 102  | -     | -       | 3/37/137/137 | -       |
| 15  | V7N  | BN    | 1001 | -     | -       | 10/53/53/53  | -       |
| 14  | LMT  | L     | 304  | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 14  | LMT  | bn    | 102  | -     | -       | 2/21/61/61   | 0/2/2/2 |
| 15  | V7N  | BE    | 101  | -     | -       | 4/53/53/53   | -       |
| 14  | LMT  | BR    | 1005 | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 20  | 0V9  | aj    | 101  | -     | -       | 15/48/48/50  | -       |
| 15  | V7N  | BP    | 1001 | -     | -       | 5/53/53/53   | -       |
| 14  | LMT  | BD    | 102  | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 18  | V75  | C     | 1006 | 12,17 | -       | 1/12/29/29   | 0/1/1/1 |
| 14  | LMT  | BP    | 1005 | -     | -       | 4/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AT    | 102  | -     | -       | 1/37/137/137 | -       |
| 14  | LMT  | AH    | 106  | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 15  | V7N  | BS    | 1001 | -     | -       | 7/53/53/53   | -       |
| 14  | LMT  | BV    | 1002 | -     | -       | 2/21/61/61   | 0/2/2/2 |
| 15  | V7N  | BH    | 1001 | -     | -       | 5/53/53/53   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 20  | 0V9  | bk    | 104  | -    | -       | 11/48/48/50  | -       |
| 17  | NDG  | C1    | 301  | 18   | -       | 0/6/23/26    | 0/1/1/1 |
| 14  | LMT  | BR    | 1002 | -    | -       | 6/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AM    | 102  | -    | -       | 4/37/137/137 | -       |
| 13  | BCL  | AH    | 102  | -    | -       | 0/37/137/137 | -       |
| 15  | V7N  | AT    | 103  | -    | -       | 6/53/53/53   | -       |
| 13  | BCL  | ae    | 1001 | -    | -       | 7/37/137/137 | -       |
| 13  | BCL  | AB    | 103  | 28   | -       | 5/37/137/137 | -       |
| 14  | LMT  | AT    | 101  | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AA    | 1002 | 28   | -       | 9/37/137/137 | -       |
| 14  | LMT  | BN    | 1003 | -    | -       | 6/21/61/61   | 0/2/2/2 |
| 21  | CD4  | af    | 104  | -    | -       | 17/94/94/94  | -       |
| 14  | LMT  | BS    | 1004 | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AU    | 103  | -    | -       | 2/37/137/137 | -       |
| 14  | LMT  | bd    | 102  | -    | -       | 8/21/61/61   | 0/2/2/2 |
| 23  | MQ8  | an    | 101  | -    | -       | 5/47/67/67   | 0/2/2/2 |
| 14  | LMT  | BH    | 1005 | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 14  | LMT  | AB    | 102  | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 14  | LMT  | AN    | 101  | -    | -       | 2/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BC    | 104  | -    | -       | 6/21/61/61   | 0/2/2/2 |
| 13  | BCL  | BW    | 1003 | -    | -       | 2/37/137/137 | -       |
| 14  | LMT  | BE    | 102  | -    | -       | 5/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BF    | 103  | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 15  | V7N  | BG    | 1001 | -    | -       | 6/53/53/53   | -       |
| 14  | LMT  | BD    | 105  | -    | -       | 8/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BP    | 1003 | -    | -       | 6/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AP    | 101  | -    | -       | 4/37/137/137 | -       |
| 26  | V7B  | af    | 101  | -    | -       | 14/48/88/88  | 0/2/2/2 |
| 13  | BCL  | AM    | 101  | 28   | -       | 7/37/137/137 | -       |
| 13  | BCL  | AH    | 101  | -    | -       | 8/37/137/137 | -       |
| 15  | V7N  | AH    | 105  | -    | -       | 7/53/53/53   | -       |
| 20  | 0V9  | ba    | 102  | -    | -       | 6/48/48/50   | -       |
| 20  | 0V9  | bk    | 102  | -    | -       | 11/48/48/50  | -       |
| 13  | BCL  | bn    | 103  | -    | -       | 5/37/137/137 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 21  | CD4  | af    | 103  | -    | -       | 29/94/94/94   | -       |
| 20  | 0V9  | bm    | 102  | -    | -       | 11/48/48/50   | -       |
| 14  | LMT  | AW    | 102  | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 15  | V7N  | BJ    | 1001 | -    | -       | 5/53/53/53    | -       |
| 14  | LMT  | AN    | 103  | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 20  | 0V9  | bn    | 104  | -    | -       | 11/48/48/50   | -       |
| 14  | LMT  | bc    | 101  | -    | -       | 11/21/61/61   | 0/2/2/2 |
| 14  | LMT  | AL    | 102  | -    | -       | 5/21/61/61    | 0/2/2/2 |
| 15  | V7N  | bl    | 102  | -    | -       | 9/53/53/53    | -       |
| 13  | BCL  | L     | 308  | -    | -       | 0/37/137/137  | -       |
| 13  | BCL  | AG    | 103  | -    | -       | 4/37/137/137  | -       |
| 14  | LMT  | BK    | 1005 | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 13  | BCL  | AL    | 103  | -    | -       | 8/37/137/137  | -       |
| 14  | LMT  | BL    | 1003 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BI    | 104  | -    | -       | 10/37/137/137 | -       |
| 13  | BCL  | BV    | 1004 | -    | -       | 9/37/137/137  | -       |
| 14  | LMT  | AV    | 101  | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 13  | BCL  | AP    | 103  | 28   | -       | 6/37/137/137  | -       |
| 21  | CD4  | H1    | 1003 | -    | -       | 17/94/94/94   | -       |
| 13  | BCL  | bo    | 102  | -    | -       | 4/37/137/137  | -       |
| 13  | BCL  | ab    | 1001 | -    | -       | 4/37/137/137  | -       |
| 13  | BCL  | bm    | 103  | -    | -       | 7/37/137/137  | -       |
| 17  | NDG  | C     | 1005 | 18   | -       | 0/6/23/26     | 0/1/1/1 |
| 20  | 0V9  | bo    | 104  | -    | -       | 7/48/48/50    | -       |
| 14  | LMT  | bh    | 101  | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 13  | BCL  | AK    | 103  | -    | -       | 12/37/137/137 | -       |
| 20  | 0V9  | bi    | 102  | -    | -       | 6/48/48/50    | -       |
| 14  | LMT  | bl    | 101  | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BA    | 104  | -    | -       | 7/37/137/137  | -       |
| 13  | BCL  | bj    | 104  | -    | -       | 11/37/137/137 | -       |
| 13  | BCL  | AR    | 101  | -    | -       | 3/37/137/137  | -       |
| 13  | BCL  | bg    | 104  | -    | -       | 8/37/137/137  | -       |
| 14  | LMT  | BU    | 1003 | -    | -       | 4/21/61/61    | 0/2/2/2 |
| 14  | LMT  | BS    | 1002 | -    | -       | 3/21/61/61    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 14  | LMT  | L     | 306  | -    | -       | 3/21/61/61    | 0/2/2/2 |
| 14  | LMT  | bp    | 101  | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 21  | CD4  | ad    | 101  | -    | -       | 20/94/94/94   | -       |
| 13  | BCL  | ba    | 103  | -    | -       | 8/37/137/137  | -       |
| 13  | BCL  | AS    | 102  | 28   | -       | 6/37/137/137  | -       |
| 13  | BCL  | AJ    | 102  | 28   | -       | 7/37/137/137  | -       |
| 13  | BCL  | bp    | 103  | -    | -       | 7/37/137/137  | -       |
| 13  | BCL  | ap    | 1001 | -    | -       | 10/37/137/137 | -       |
| 14  | LMT  | BE    | 106  | -    | -       | 2/21/61/61    | 0/2/2/2 |
| 13  | BCL  | am    | 1001 | -    | -       | 2/37/137/137  | -       |
| 13  | BCL  | AF    | 1002 | -    | -       | 8/37/137/137  | -       |
| 13  | BCL  | ak    | 1001 | -    | -       | 6/37/137/137  | -       |
| 14  | LMT  | AA    | 1003 | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BT    | 1004 | -    | -       | 5/37/137/137  | -       |
| 13  | BCL  | AD    | 1001 | 28   | -       | 3/37/137/137  | -       |
| 14  | LMT  | bf    | 101  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BR    | 1003 | -    | -       | 5/37/137/137  | -       |
| 15  | V7N  | AE    | 1003 | -    | -       | 4/53/53/53    | -       |
| 14  | LMT  | BL    | 1002 | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 13  | BCL  | BF    | 104  | -    | -       | 4/37/137/137  | -       |
| 13  | BCL  | AS    | 101  | -    | -       | 7/37/137/137  | -       |
| 14  | LMT  | BW    | 1005 | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 15  | V7N  | bo    | 101  | -    | -       | 4/53/53/53    | -       |
| 20  | 0V9  | be    | 102  | -    | -       | 16/48/48/50   | -       |
| 13  | BCL  | ag    | 1001 | -    | -       | 4/37/137/137  | -       |
| 13  | BCL  | BD    | 106  | -    | -       | 4/37/137/137  | -       |
| 14  | LMT  | AP    | 102  | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 14  | LMT  | bk    | 101  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 13  | BCL  | AE    | 1002 | -    | -       | 1/37/137/137  | -       |
| 14  | LMT  | bb    | 102  | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 15  | V7N  | bk    | 103  | -    | -       | 10/53/53/53   | -       |
| 14  | LMT  | BJ    | 1002 | -    | -       | 6/21/61/61    | 0/2/2/2 |
| 13  | BCL  | ah    | 1001 | -    | -       | 7/37/137/137  | -       |
| 14  | LMT  | BM    | 1003 | -    | -       | 2/21/61/61    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 13  | BCL  | BN    | 1006 | -    | -       | 8/37/137/137 | -       |
| 14  | LMT  | BK    | 1004 | -    | -       | 7/21/61/61   | 0/2/2/2 |
| 13  | BCL  | an    | 102  | -    | -       | 3/37/137/137 | -       |
| 14  | LMT  | AH    | 104  | -    | -       | 2/21/61/61   | 0/2/2/2 |
| 14  | LMT  | L     | 302  | -    | -       | 6/21/61/61   | 0/2/2/2 |
| 14  | LMT  | AF    | 1003 | -    | -       | 5/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BE    | 103  | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 20  | 0V9  | bb    | 104  | -    | -       | 10/48/48/50  | -       |
| 14  | LMT  | BB    | 103  | -    | -       | 6/21/61/61   | 0/2/2/2 |
| 20  | 0V9  | bl    | 103  | -    | -       | 11/48/48/50  | -       |
| 14  | LMT  | BK    | 1006 | -    | -       | 3/21/61/61   | 0/2/2/2 |
| 14  | LMT  | ac    | 101  | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 13  | BCL  | BM    | 1004 | -    | -       | 2/37/137/137 | -       |
| 13  | BCL  | BG    | 1004 | -    | -       | 9/37/137/137 | -       |
| 13  | BCL  | AD    | 1002 | -    | -       | 0/37/137/137 | -       |
| 14  | LMT  | AD    | 1004 | -    | -       | 1/21/61/61   | 0/2/2/2 |
| 14  | LMT  | AO    | 103  | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 14  | LMT  | bj    | 102  | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 15  | V7N  | bd    | 101  | -    | -       | 6/53/53/53   | -       |
| 14  | LMT  | BT    | 1002 | -    | -       | 5/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BW    | 1004 | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AC    | 1002 | -    | -       | 8/37/137/137 | -       |
| 14  | LMT  | BR    | 1006 | -    | -       | 2/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BV    | 1003 | -    | -       | 1/21/61/61   | 0/2/2/2 |
| 13  | BCL  | BJ    | 1004 | -    | -       | 5/37/137/137 | -       |
| 14  | LMT  | AS    | 103  | -    | -       | 8/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AQ    | 101  | -    | -       | 2/37/137/137 | -       |
| 14  | LMT  | BK    | 1002 | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 20  | 0V9  | bf    | 103  | -    | -       | 10/48/48/50  | -       |
| 14  | LMT  | AR    | 102  | -    | -       | 11/21/61/61  | 0/2/2/2 |
| 15  | V7N  | BC    | 101  | -    | -       | 4/53/53/53   | -       |
| 13  | BCL  | M     | 403  | -    | -       | 5/37/137/137 | -       |
| 16  | HEC  | C     | 1004 | 3    | -       | 0/10/54/54   | -       |
| 13  | BCL  | aa    | 1001 | -    | -       | 3/37/137/137 | -       |
| 15  | V7N  | BL    | 1001 | -    | -       | 7/53/53/53   | -       |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions     | Rings   |
|-----|------|-------|------|-------|---------|--------------|---------|
| 13  | BCL  | ac    | 102  | -     | -       | 2/37/137/137 | -       |
| 27  | UYH  | ai    | 101  | -     | -       | 9/50/70/70   | 0/1/1/1 |
| 13  | BCL  | AL    | 101  | -     | -       | 1/37/137/137 | -       |
| 13  | BCL  | bc    | 103  | -     | -       | 5/37/137/137 | -       |
| 13  | BCL  | L     | 303  | -     | -       | 1/37/137/137 | -       |
| 13  | BCL  | AU    | 102  | -     | -       | 7/37/137/137 | -       |
| 21  | CD4  | ai    | 103  | -     | -       | 17/94/94/94  | -       |
| 14  | LMT  | BP    | 1006 | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AI    | 102  | -     | -       | 3/37/137/137 | -       |
| 13  | BCL  | BO    | 1004 | -     | -       | 8/37/137/137 | -       |
| 14  | LMT  | BB    | 102  | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 15  | V7N  | bf    | 102  | -     | -       | 4/53/53/53   | -       |
| 14  | LMT  | BD    | 103  | -     | -       | 4/21/61/61   | 0/2/2/2 |
| 19  | PGW  | H1    | 1001 | -     | -       | 15/55/55/55  | -       |
| 14  | LMT  | BT    | 1003 | -     | -       | 4/21/61/61   | 0/2/2/2 |
| 13  | BCL  | bh    | 105  | -     | -       | 7/37/137/137 | -       |
| 14  | LMT  | AD    | 1003 | -     | -       | 6/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AJ    | 101  | -     | -       | 0/37/137/137 | -       |
| 14  | LMT  | BD    | 104  | -     | -       | 2/21/61/61   | 0/2/2/2 |
| 15  | V7N  | bn    | 101  | -     | -       | 6/53/53/53   | -       |
| 13  | BCL  | BS    | 1005 | -     | -       | 7/37/137/137 | -       |
| 13  | BCL  | AS    | 104  | 28    | -       | 7/37/137/137 | -       |
| 13  | BCL  | M     | 405  | -     | -       | 3/37/137/137 | -       |
| 15  | V7N  | be    | 101  | -     | -       | 6/53/53/53   | -       |
| 14  | LMT  | BW    | 1006 | -     | -       | 8/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BI    | 102  | -     | -       | 4/21/61/61   | 0/2/2/2 |
| 14  | LMT  | BN    | 1005 | -     | -       | 1/21/61/61   | 0/2/2/2 |
| 13  | BCL  | BU    | 1004 | -     | -       | 9/37/137/137 | -       |
| 14  | LMT  | AH    | 103  | -     | -       | 3/21/61/61   | 0/2/2/2 |
| 13  | BCL  | bb    | 103  | -     | -       | 5/37/137/137 | -       |
| 18  | V75  | M     | 409  | 12,17 | -       | 0/12/29/29   | 0/1/1/1 |
| 13  | BCL  | AV    | 103  | 28    | -       | 6/37/137/137 | -       |
| 14  | LMT  | AI    | 101  | -     | -       | 4/21/61/61   | 0/2/2/2 |
| 13  | BCL  | AK    | 102  | -     | -       | 1/37/137/137 | -       |
| 14  | LMT  | BR    | 1004 | -     | -       | 7/21/61/61   | 0/2/2/2 |

The worst 5 of 1481 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 13  | AO    | 101  | BCL  | CHC-C1C | 8.78 | 1.41        | 1.33     |
| 13  | ag    | 1001 | BCL  | CHC-C1C | 8.75 | 1.41        | 1.33     |
| 13  | bf    | 105  | BCL  | CHC-C1C | 8.72 | 1.41        | 1.33     |
| 13  | ba    | 103  | BCL  | CHC-C1C | 8.69 | 1.41        | 1.33     |
| 13  | AK    | 102  | BCL  | CHC-C1C | 8.68 | 1.41        | 1.33     |

The worst 5 of 1937 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | AQ    | 103  | BCL  | C1-O2A-CGA  | 6.93  | 133.42      | 116.65   |
| 13  | BA    | 104  | BCL  | C1-C2-C3    | 6.85  | 137.41      | 126.20   |
| 15  | bb    | 101  | V7N  | C28-C27-C26 | -6.59 | 108.29      | 126.36   |
| 15  | BG    | 1001 | V7N  | C28-C27-C26 | -6.49 | 108.57      | 126.36   |
| 15  | BN    | 1001 | V7N  | C28-C27-C26 | -5.94 | 110.08      | 126.36   |

There are no chirality outliers.

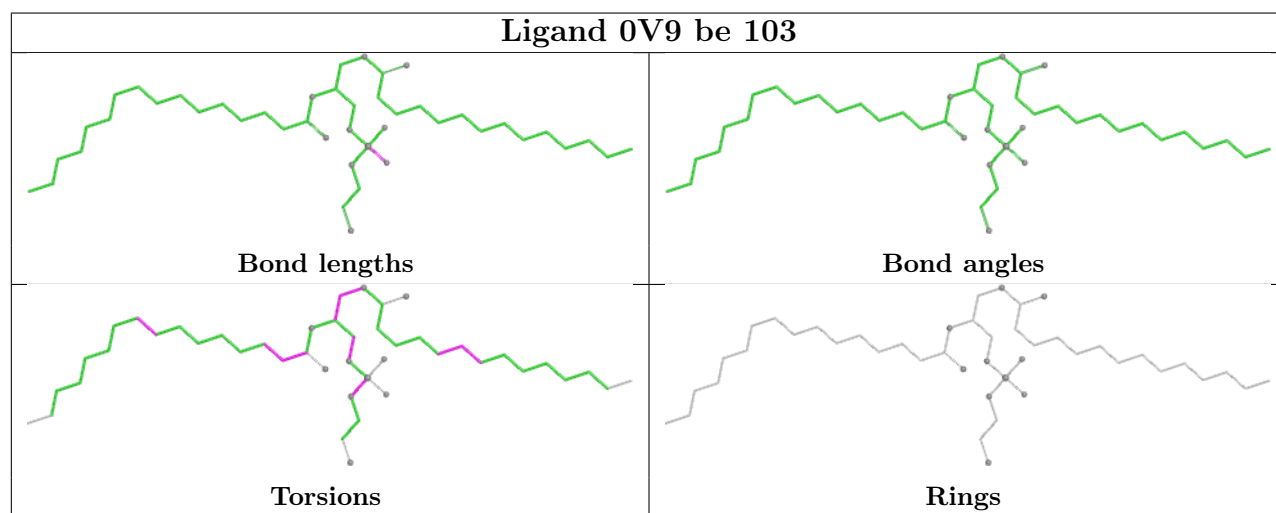
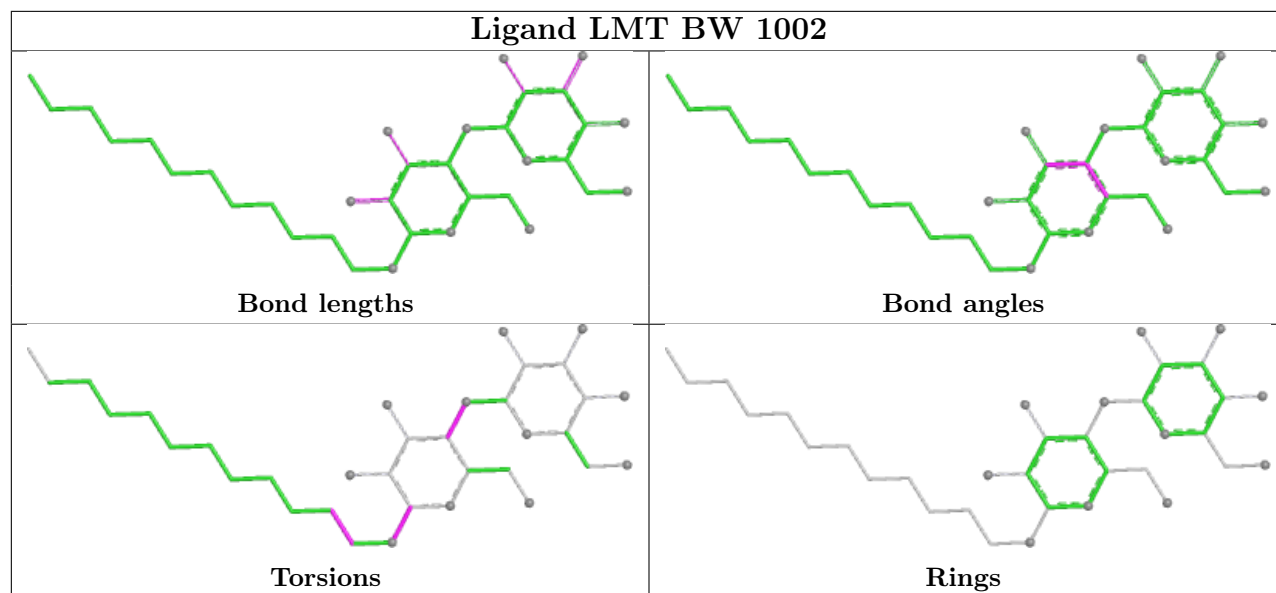
5 of 1760 torsion outliers are listed below:

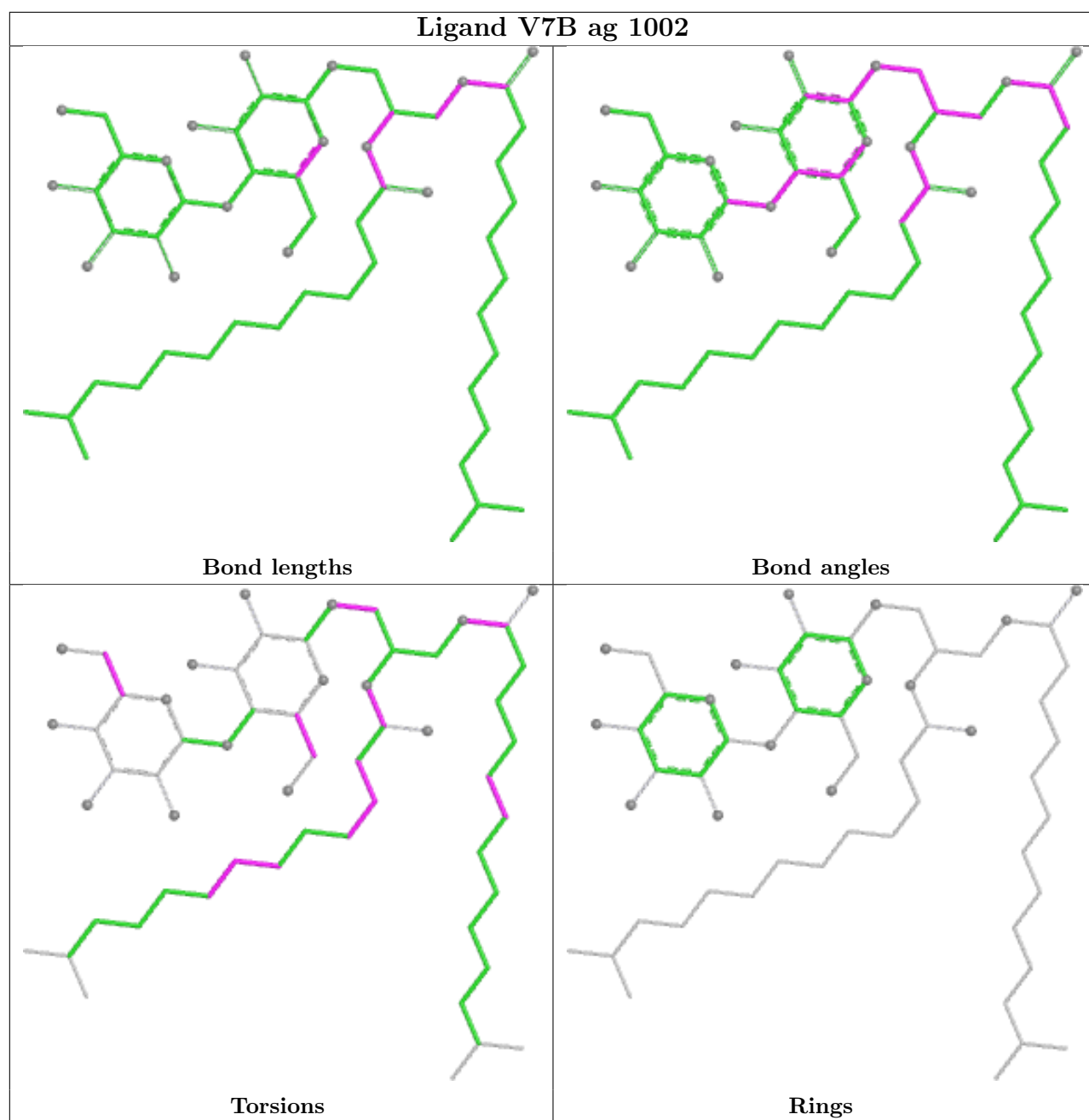
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | AB    | 103  | BCL  | C1A-C2A-CAA-CBA |
| 13  | AB    | 103  | BCL  | C3A-C2A-CAA-CBA |
| 13  | AD    | 1001 | BCL  | C3A-C2A-CAA-CBA |
| 13  | AF    | 1002 | BCL  | C1A-C2A-CAA-CBA |
| 13  | AG    | 102  | BCL  | C1A-C2A-CAA-CBA |

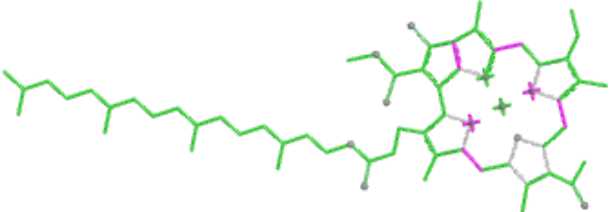
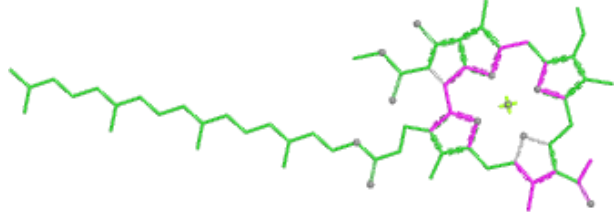
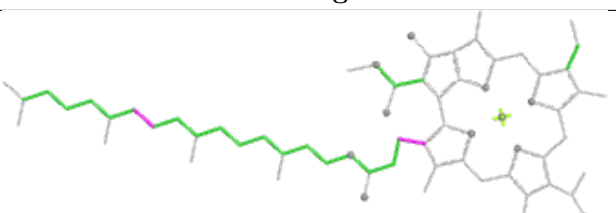
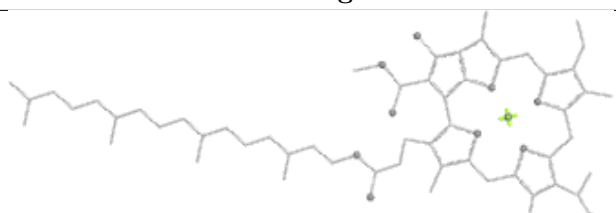
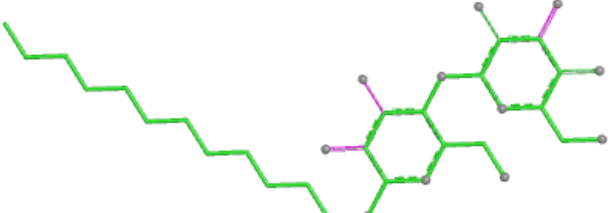
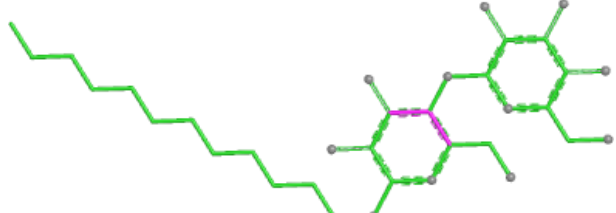
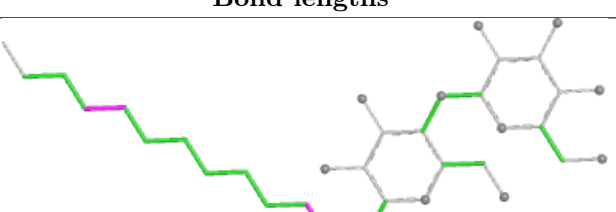
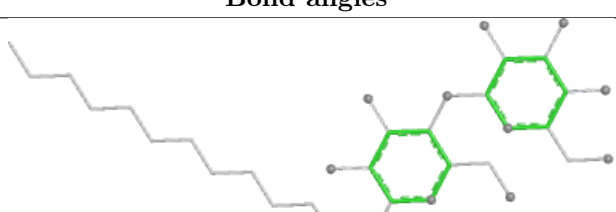
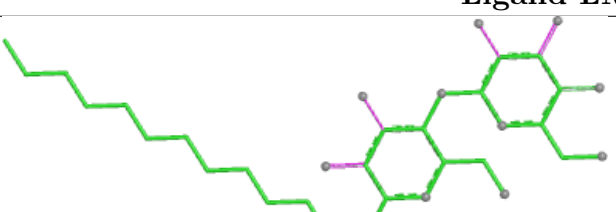
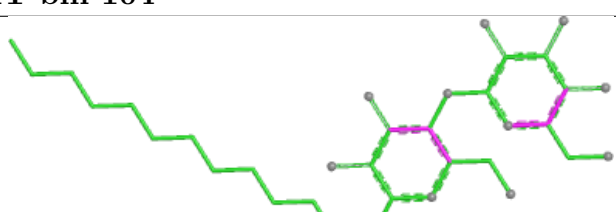
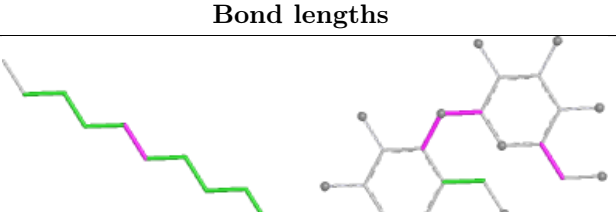
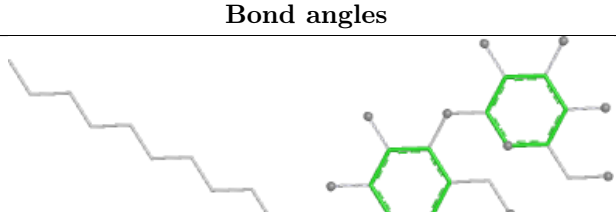
There are no ring outliers.

No monomer is involved in short contacts.

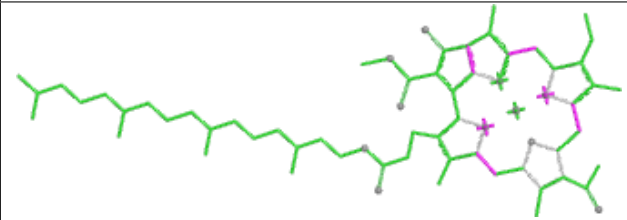
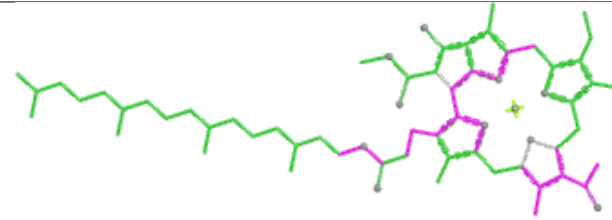
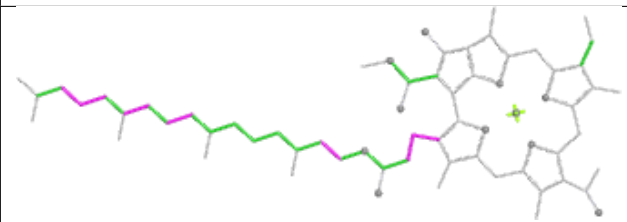
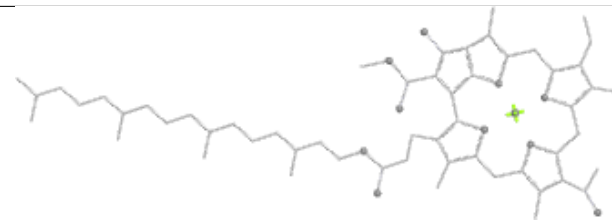
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

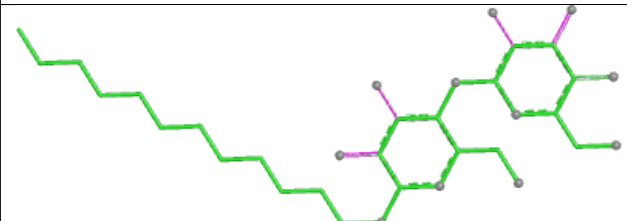
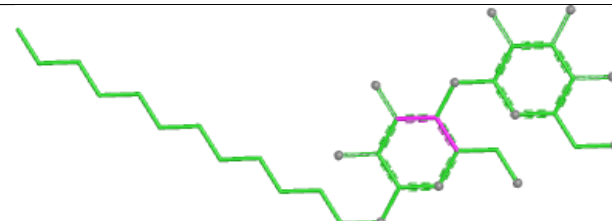
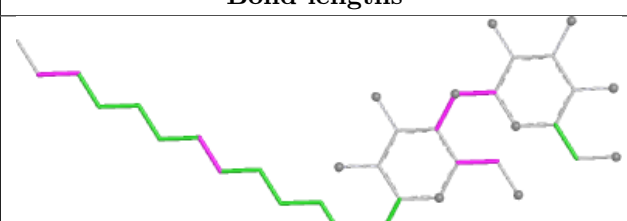
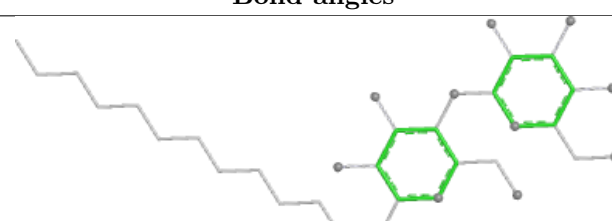


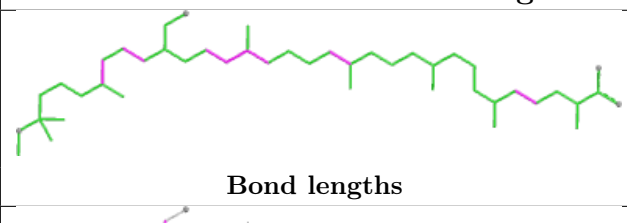
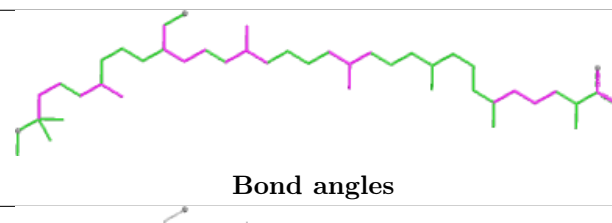




| Ligand BCL bf 105   |   |
|---|---|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMT bo 103   |   |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand LMT bm 104   |   |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

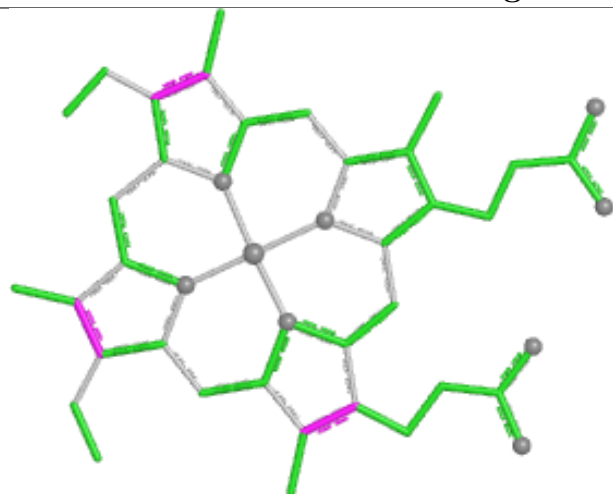


| Ligand BCL BH 1003  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

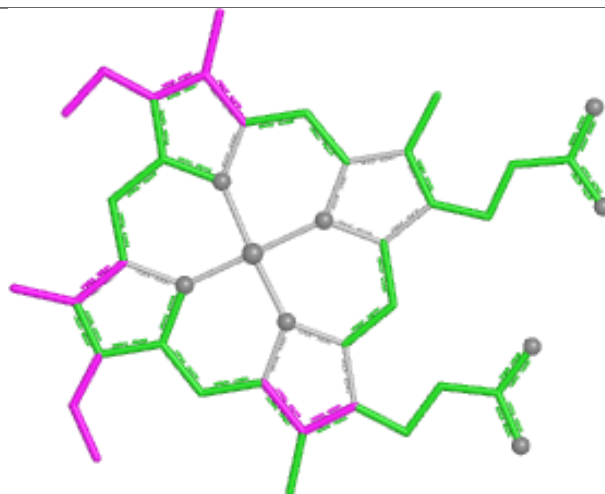
| Ligand LMT BP 1002  |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand V7N ba 101   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

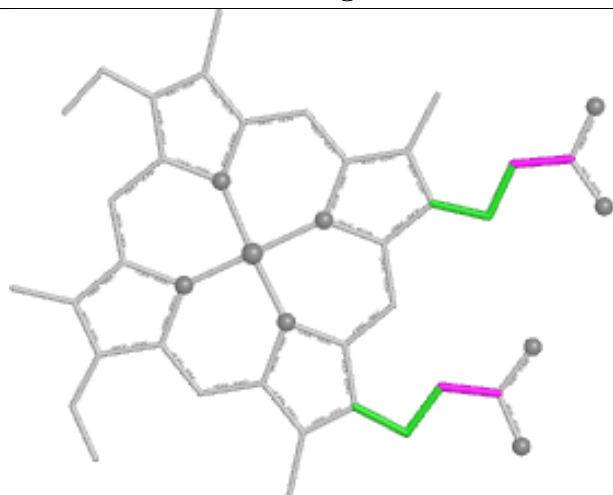
## Ligand HEC C 1002



Bond lengths



Bond angles

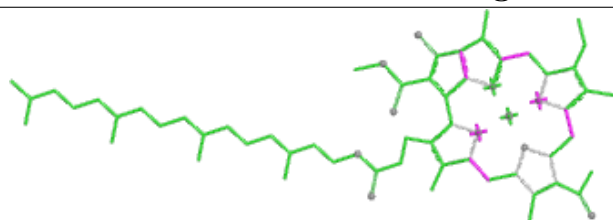


Torsions

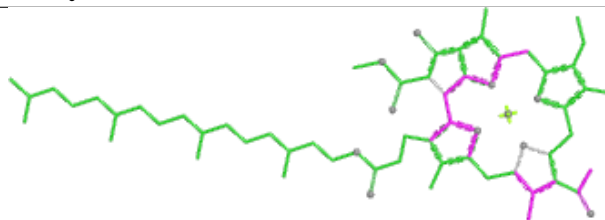


Rings

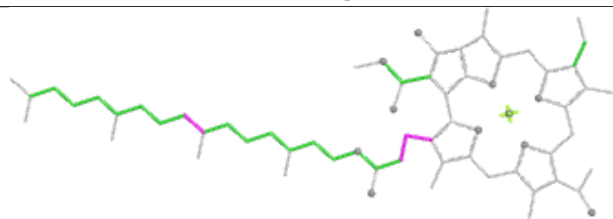
## Ligand BCL BQ 1003



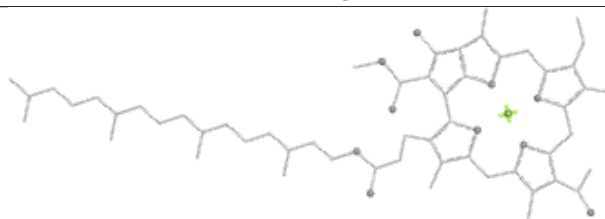
Bond lengths



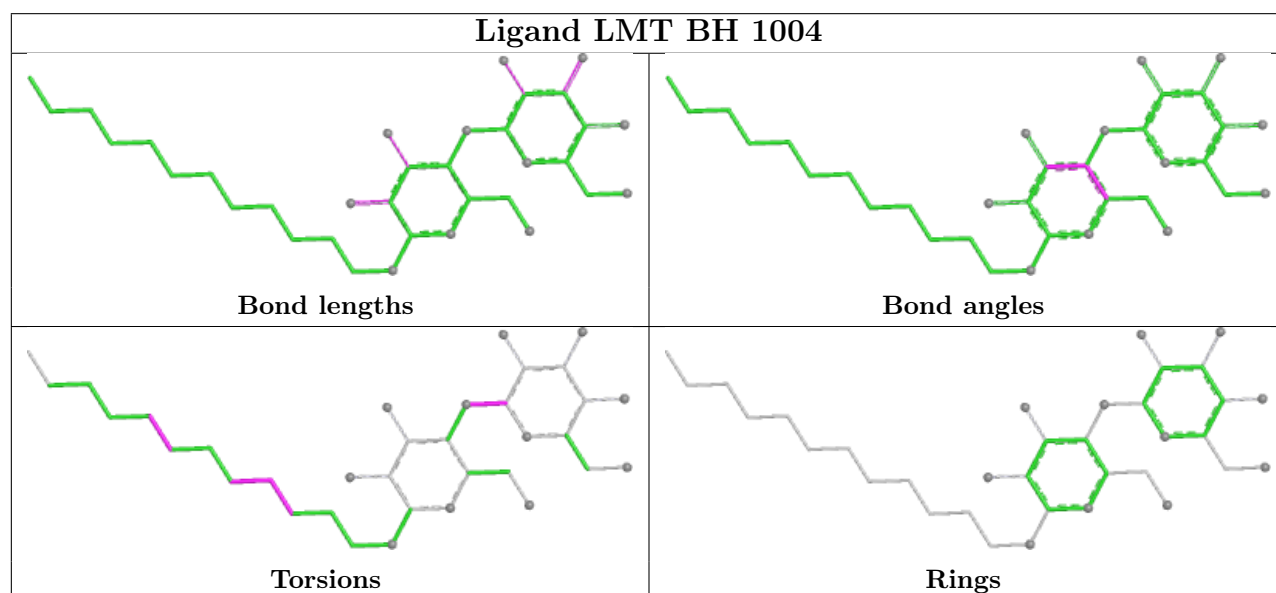
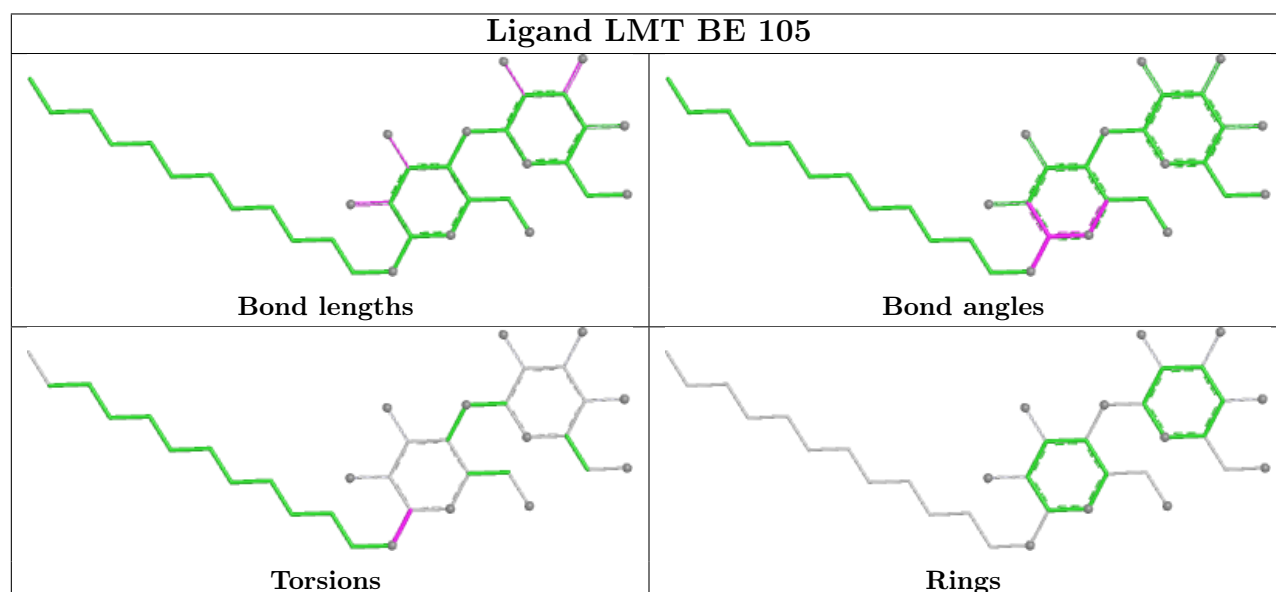
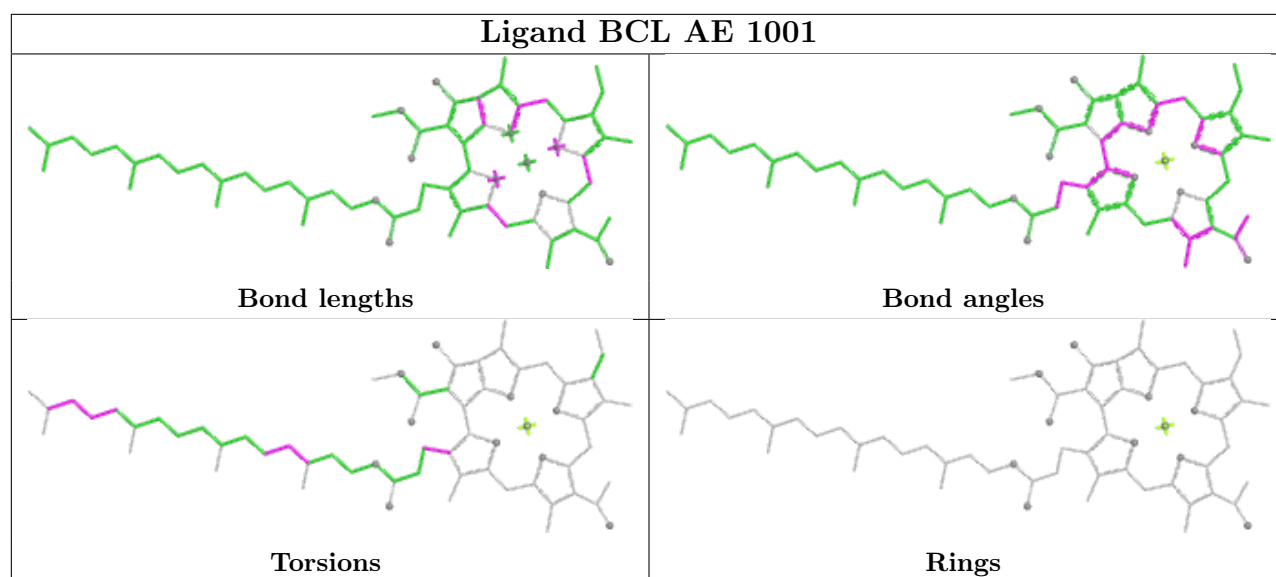
Bond angles

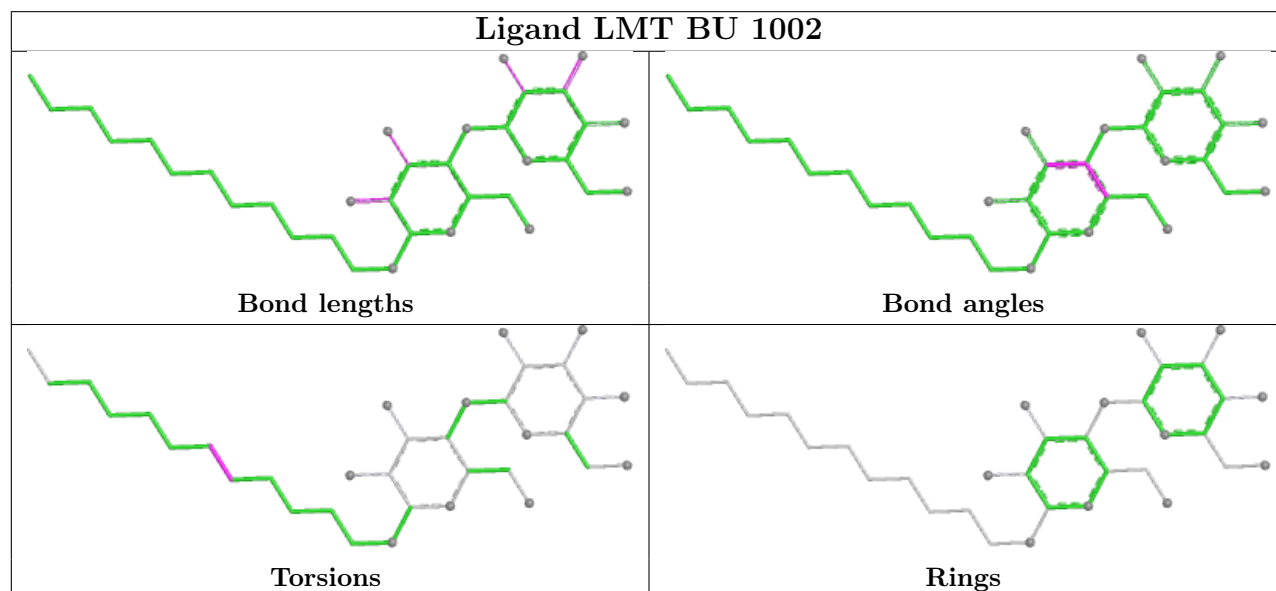
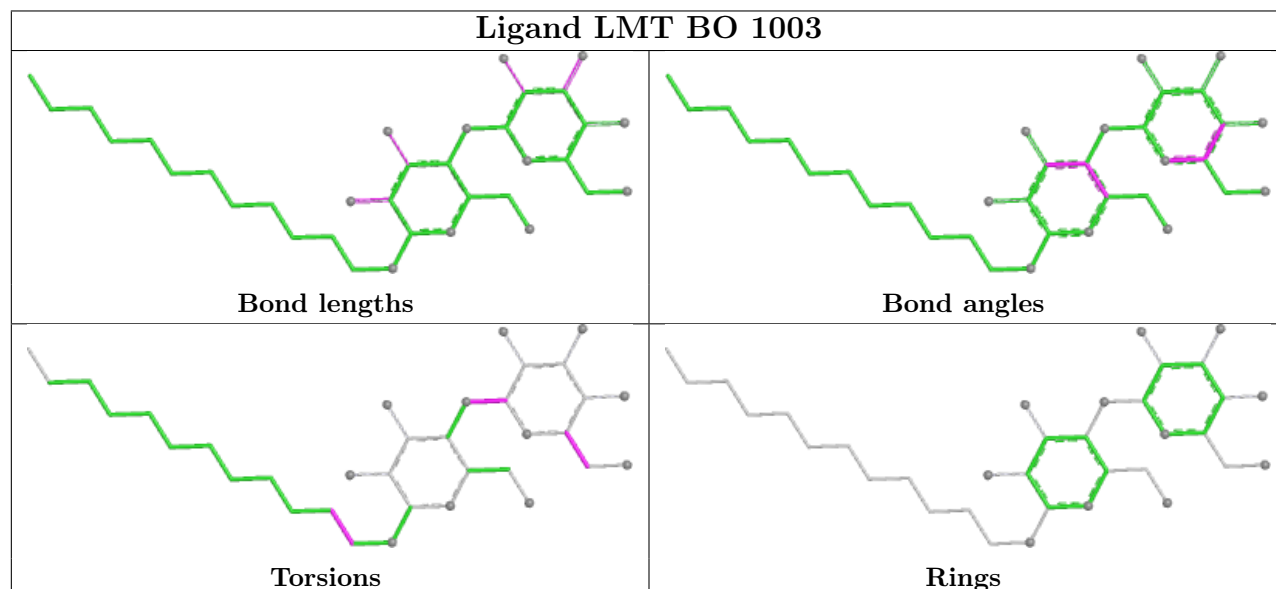
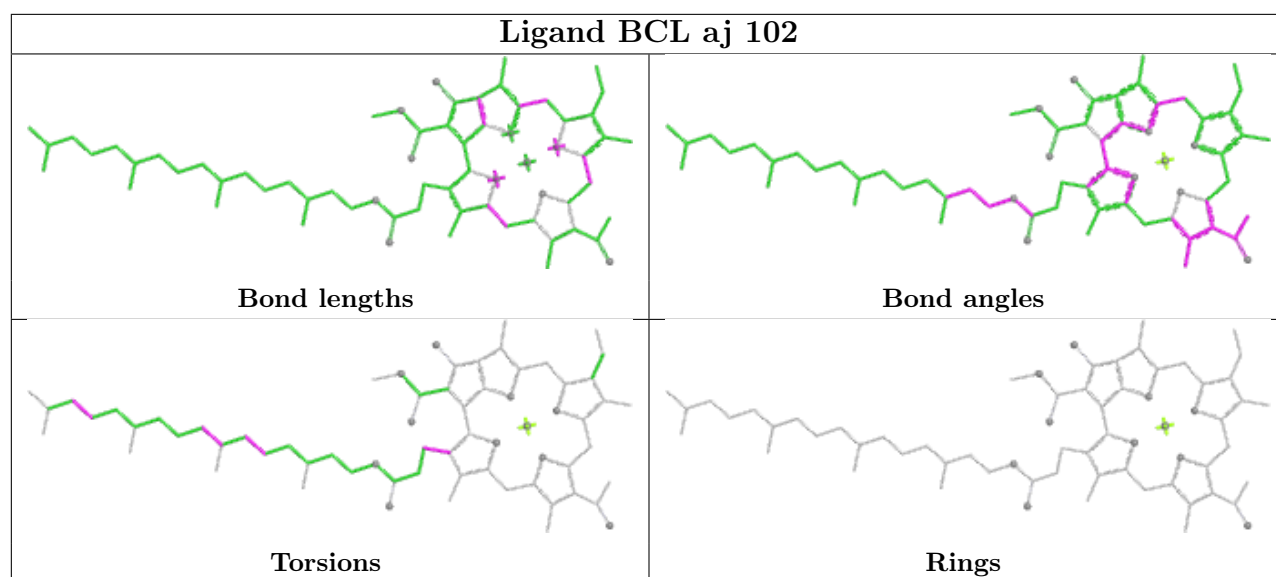


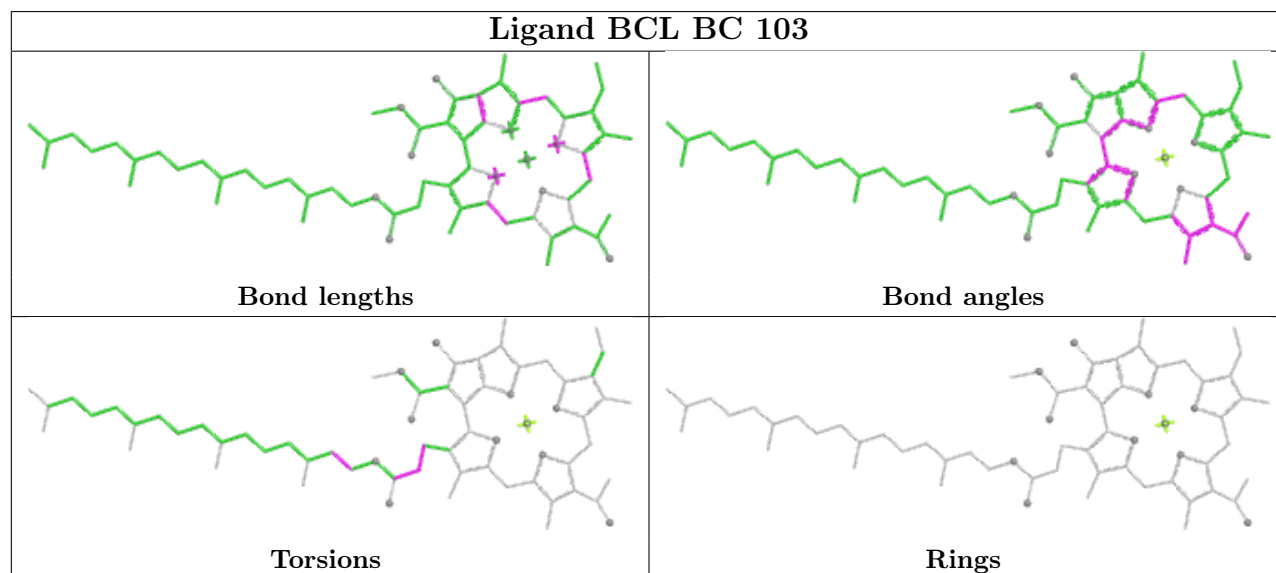
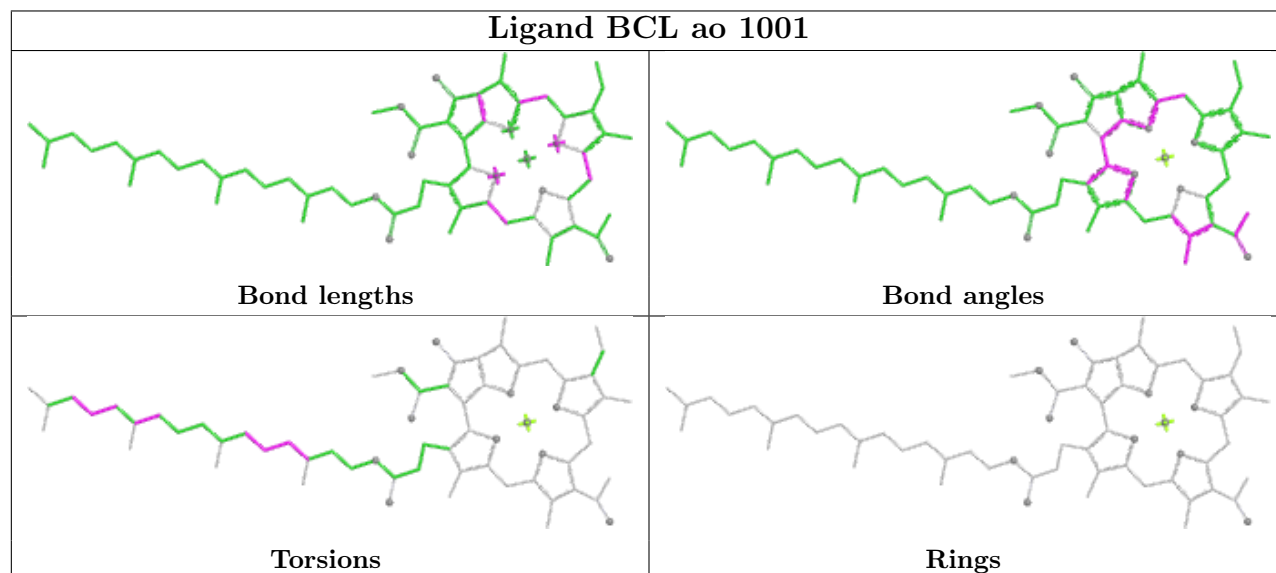
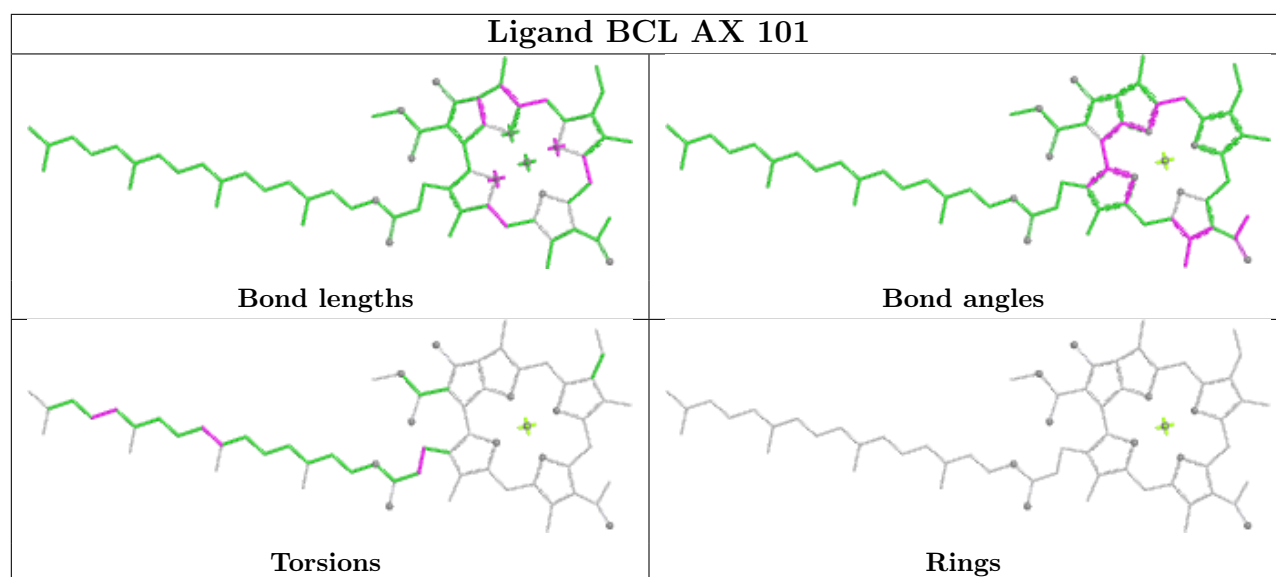
Torsions

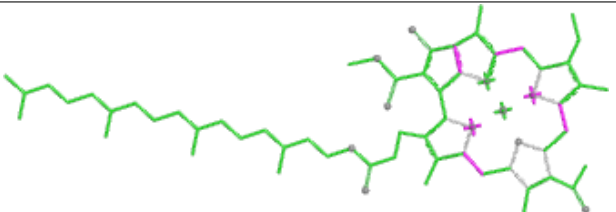
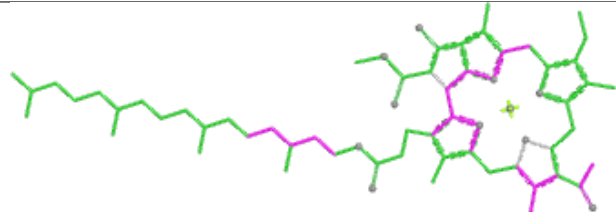
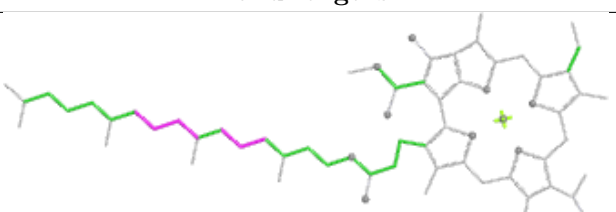
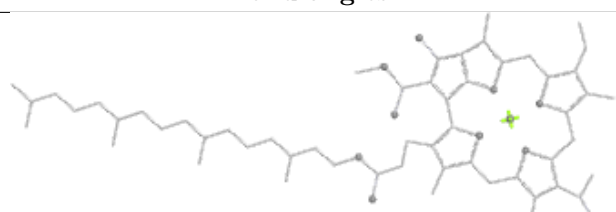


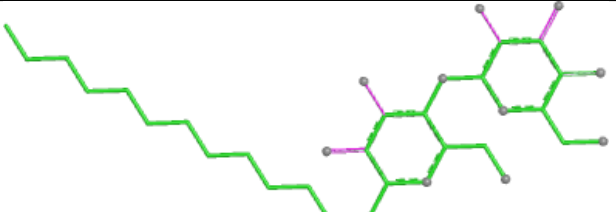
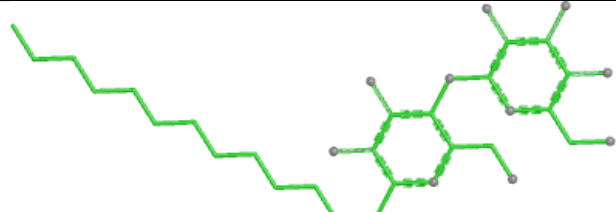
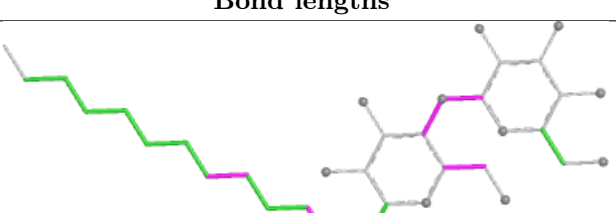
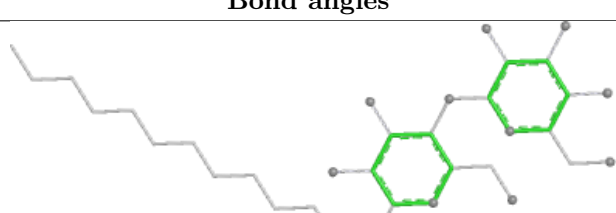
Rings

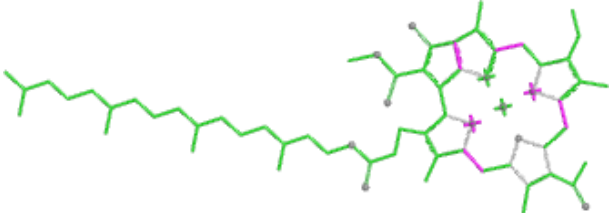
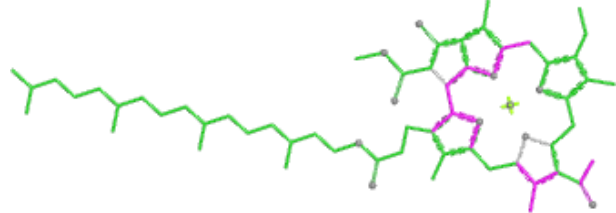
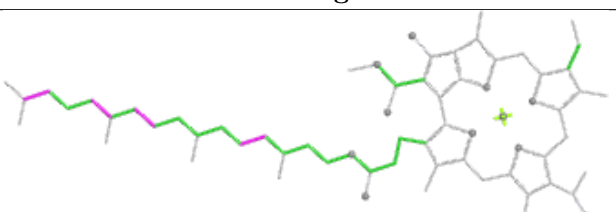
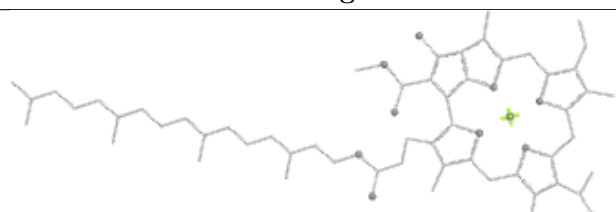


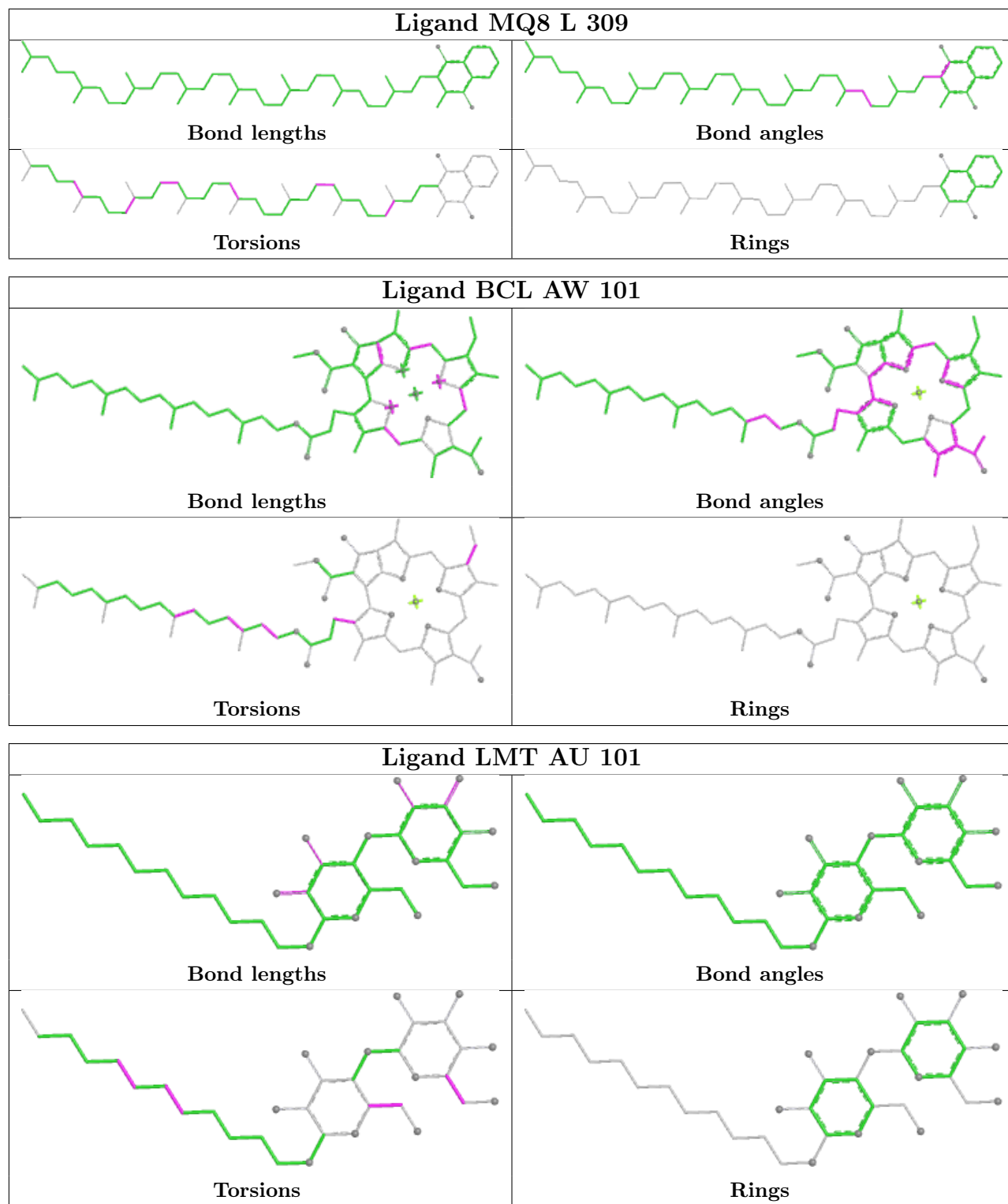


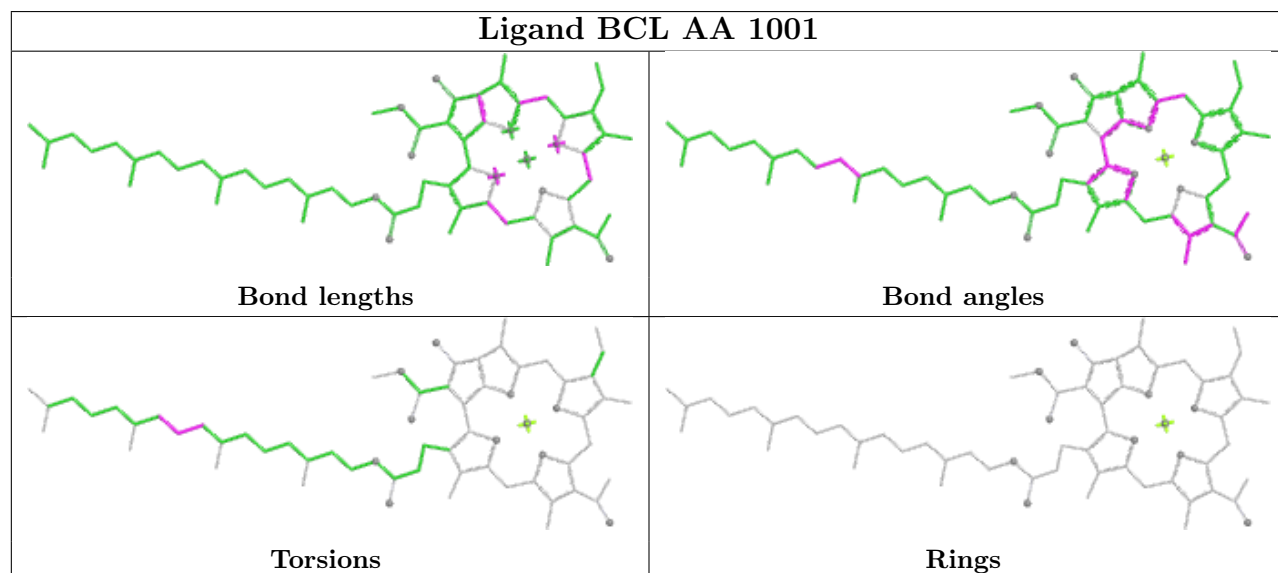
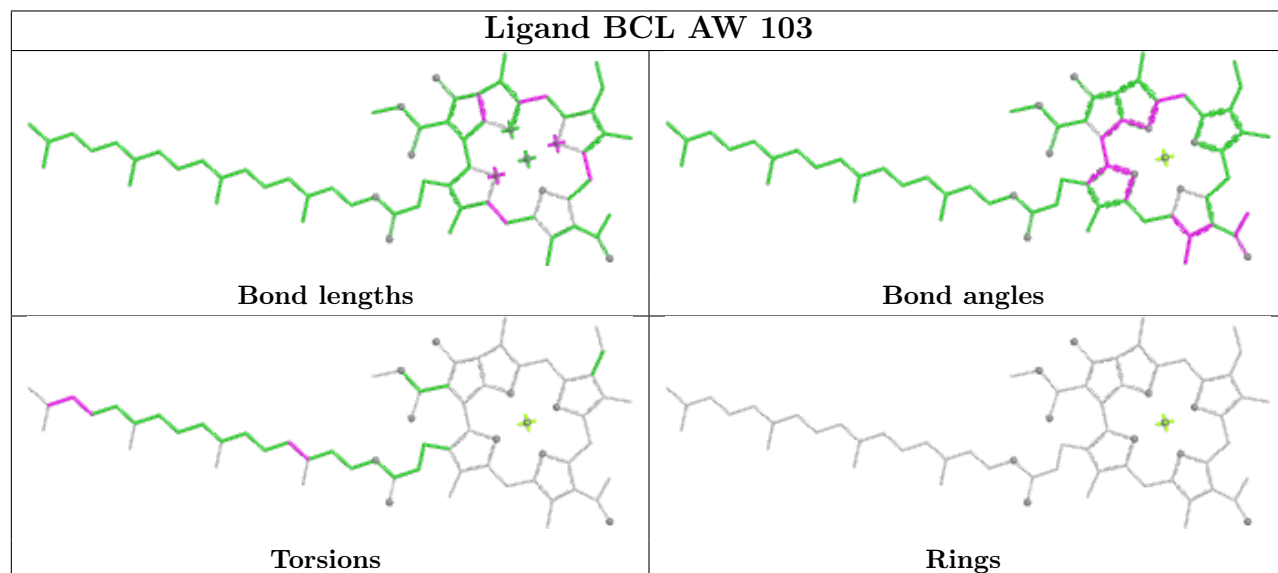
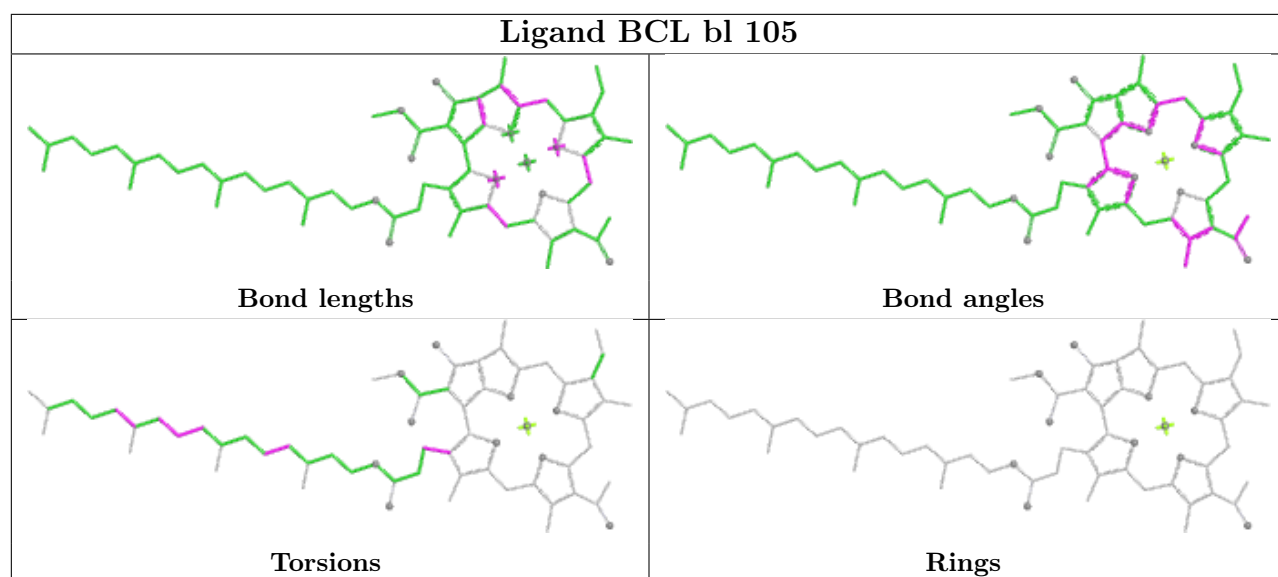


| Ligand BCL AF 1001  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

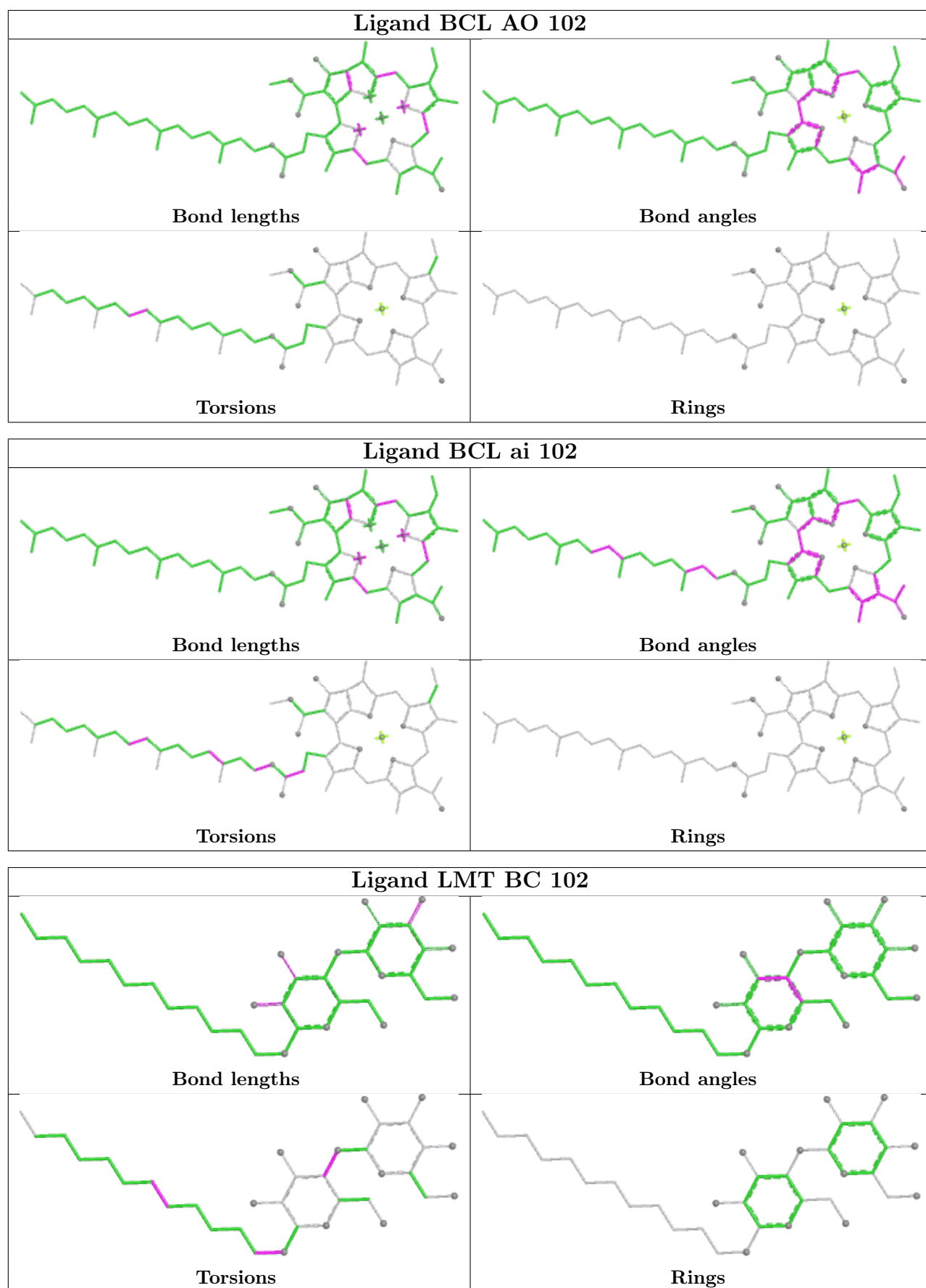
| Ligand LMT BS 1003  |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

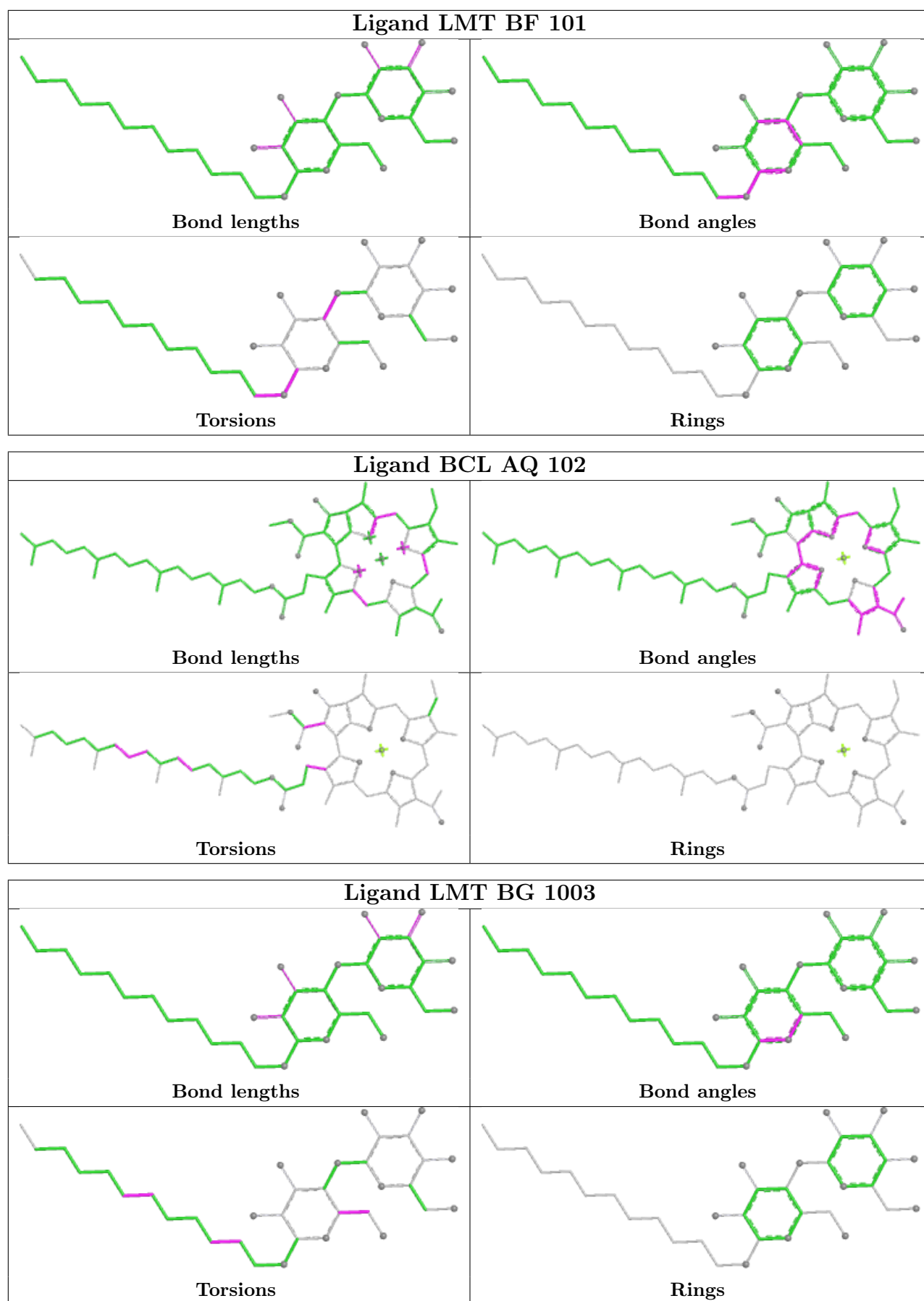
| Ligand BCL AI 103   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

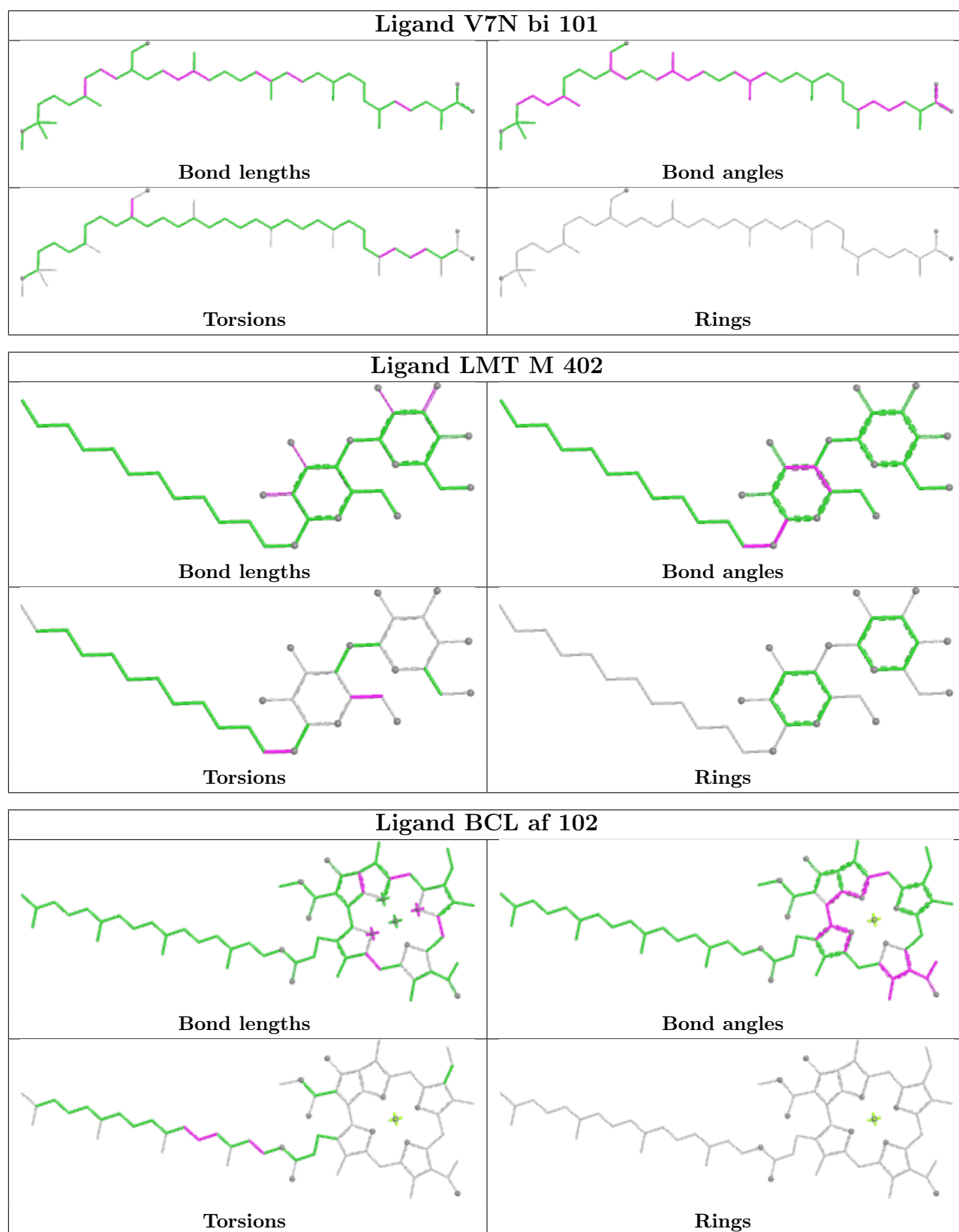


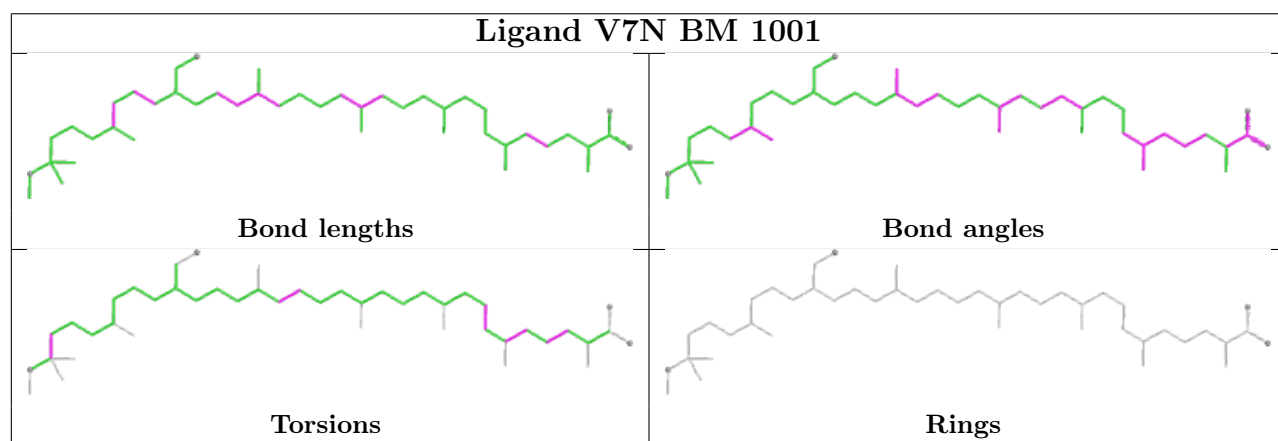
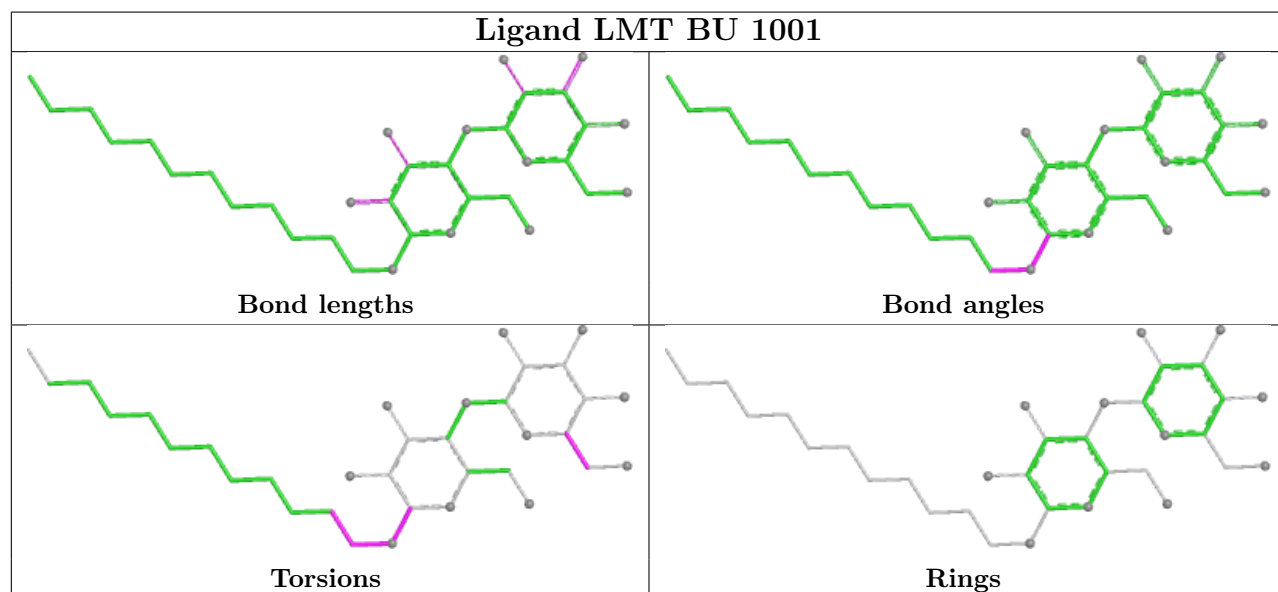
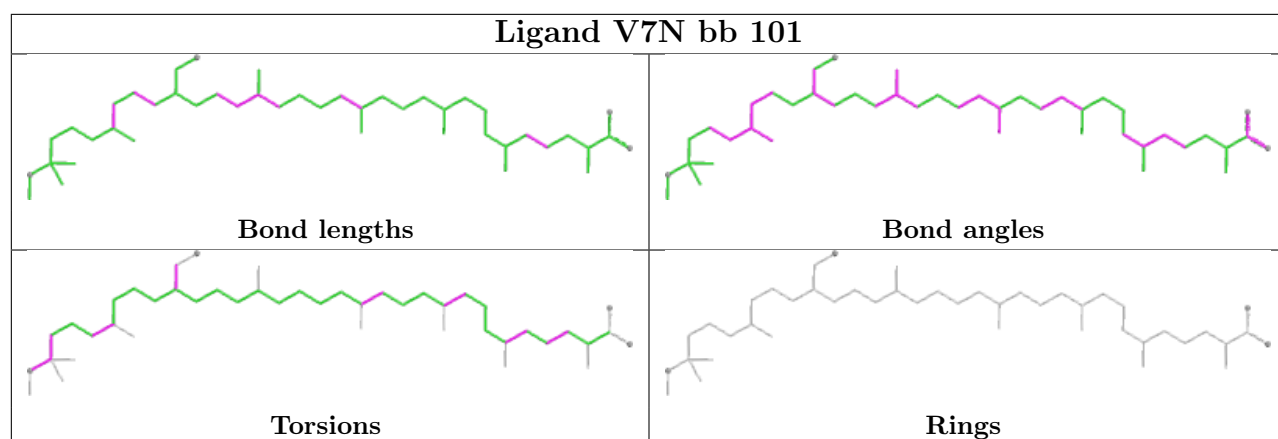


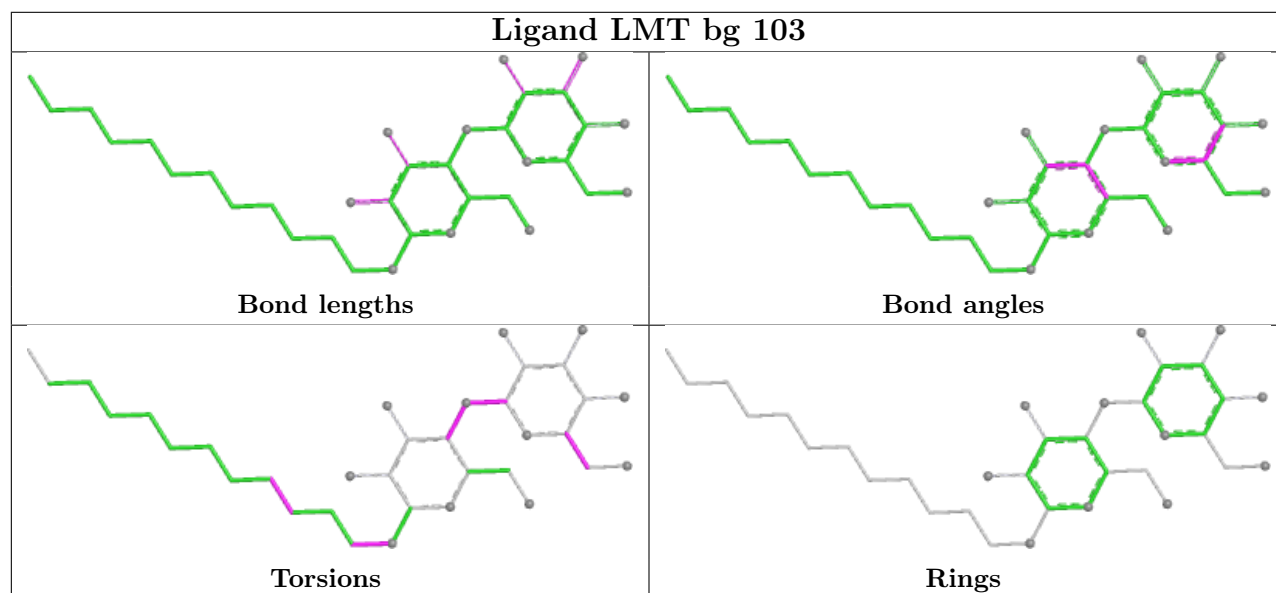
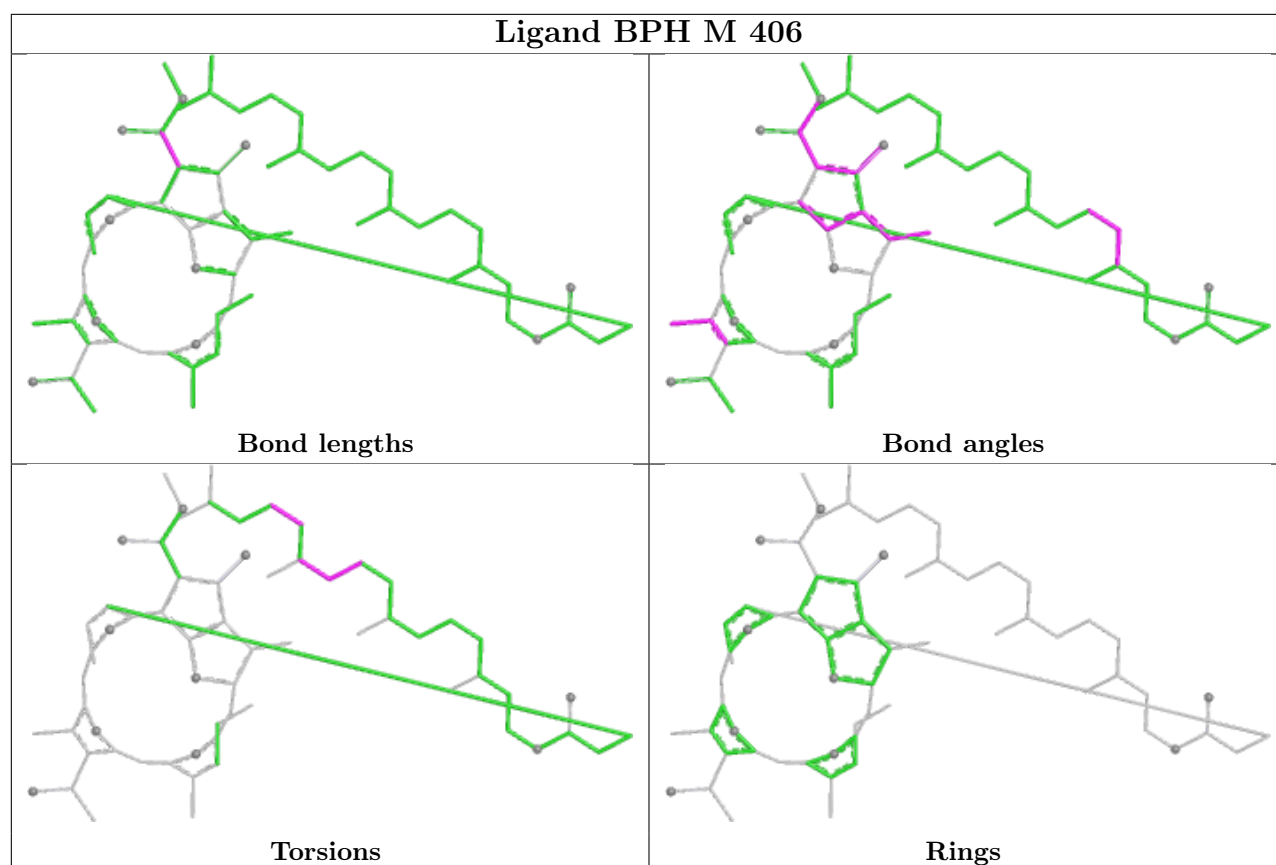


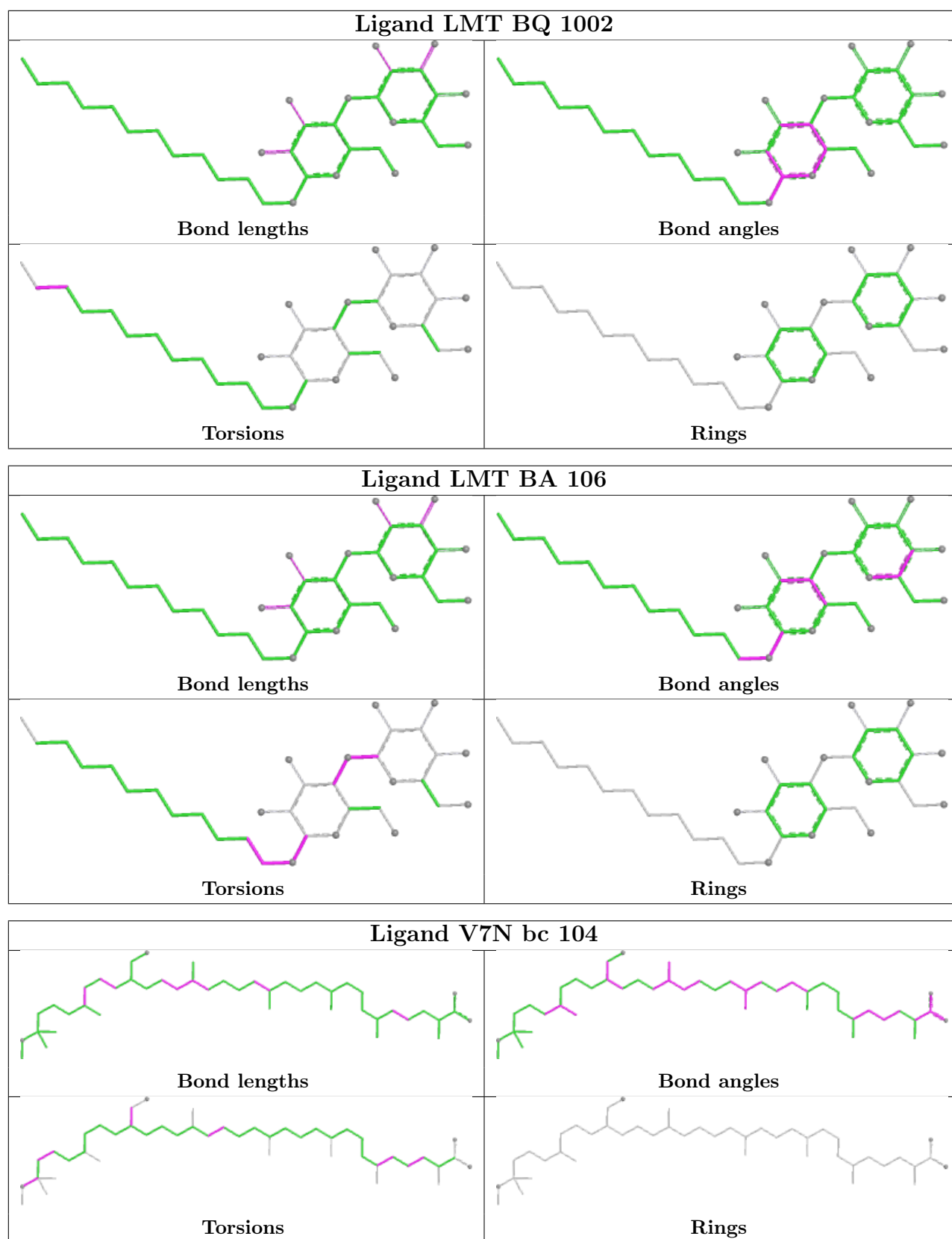


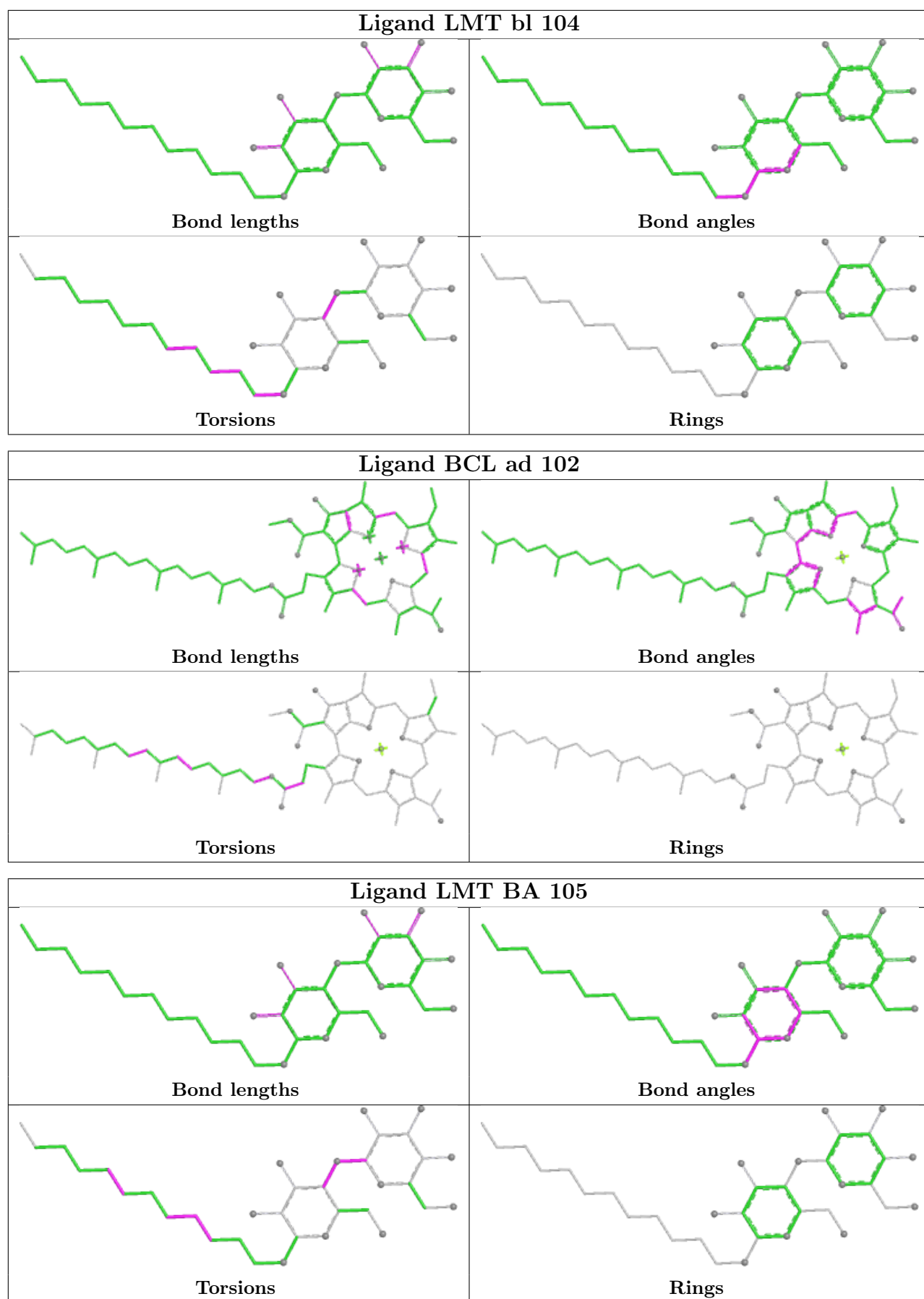


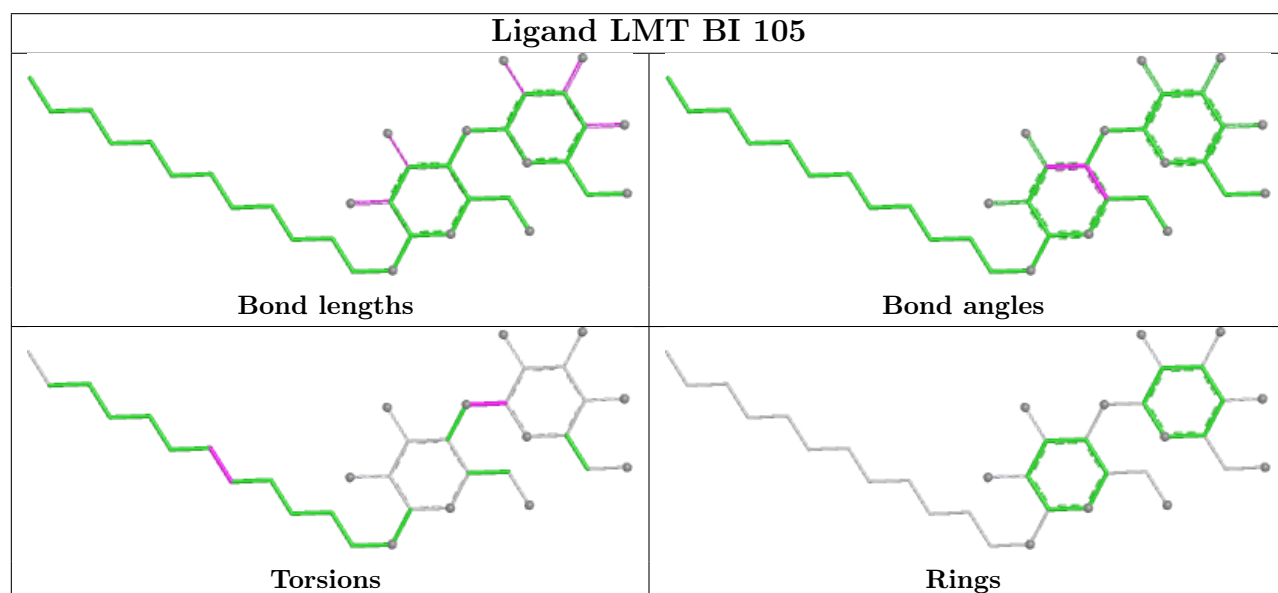
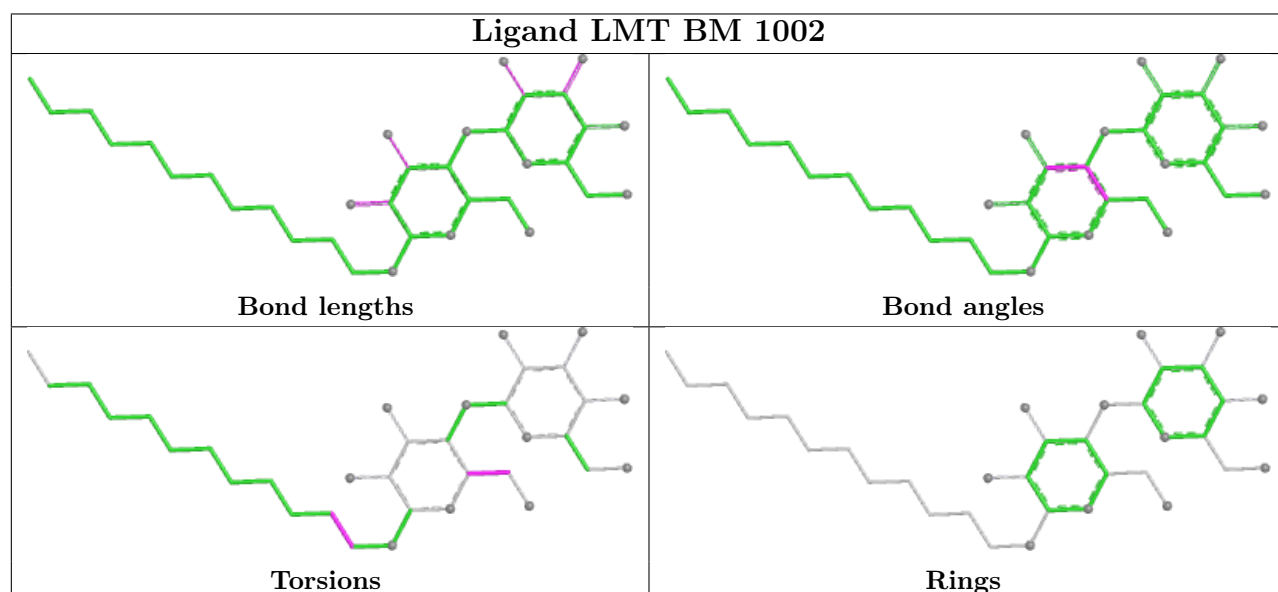
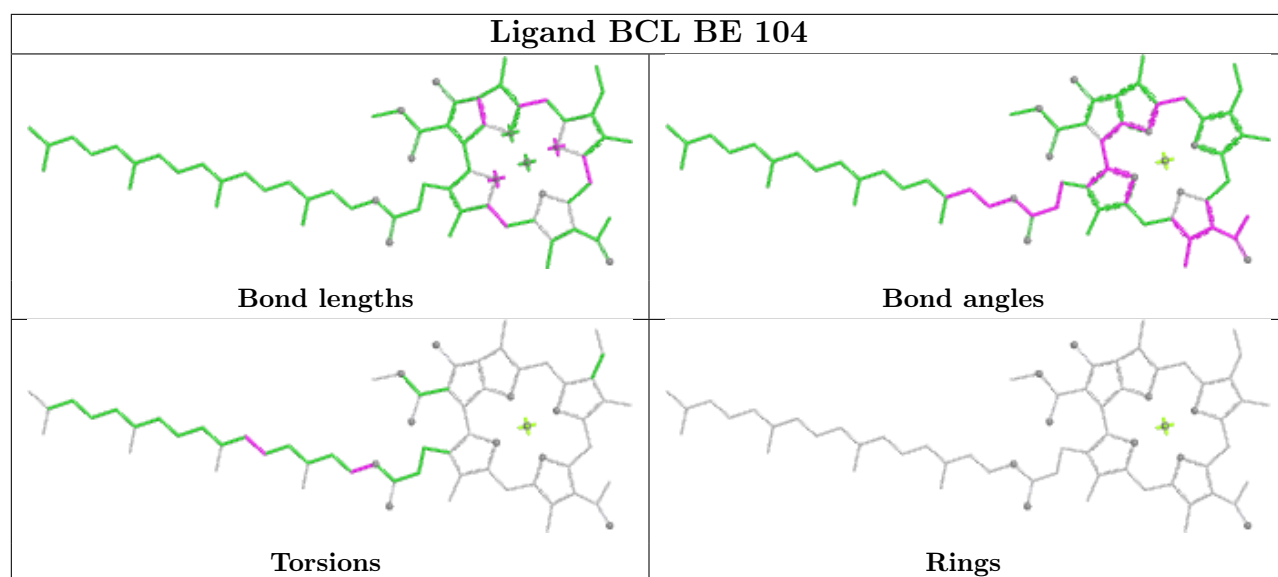




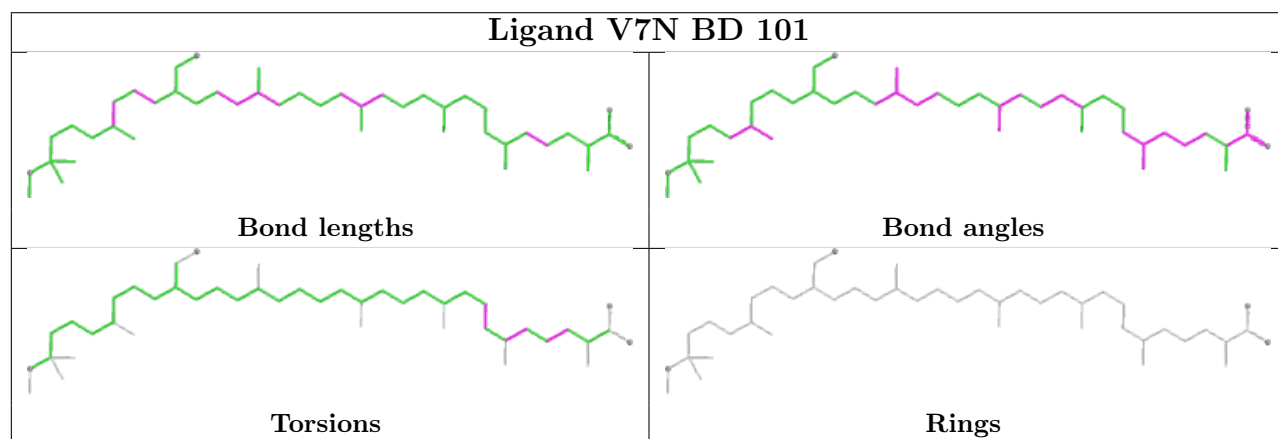
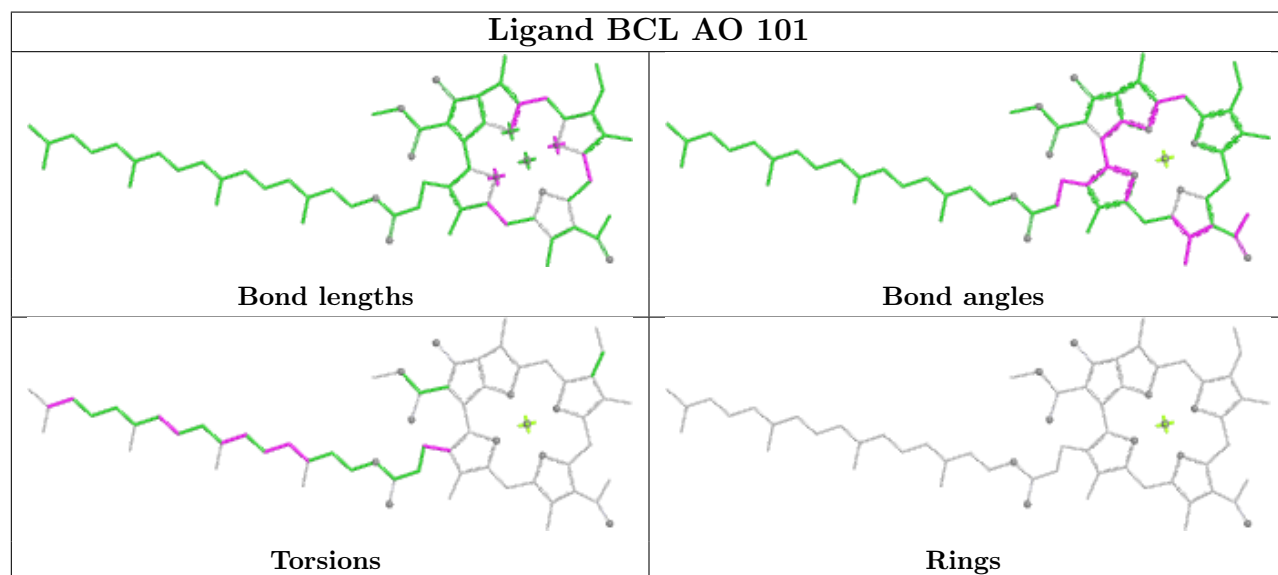
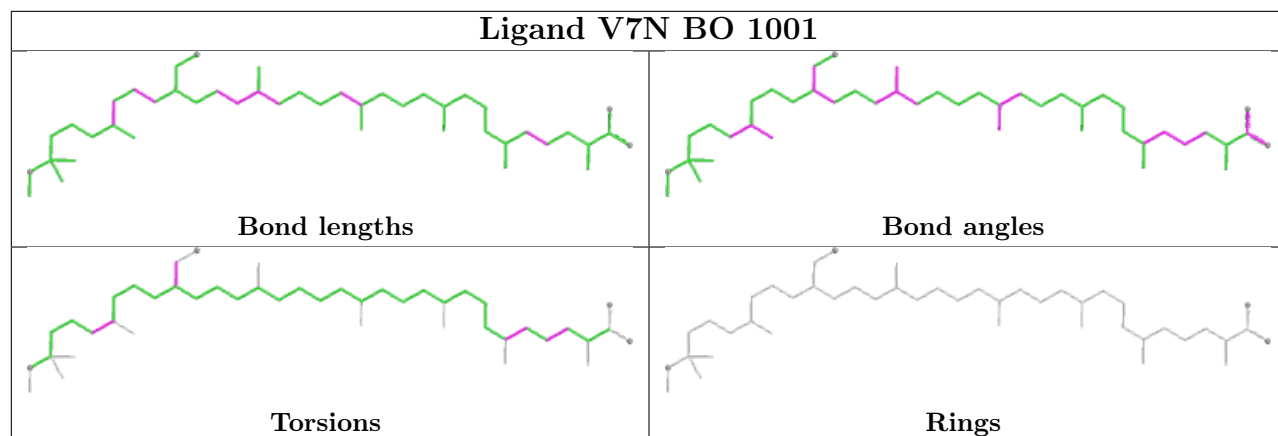


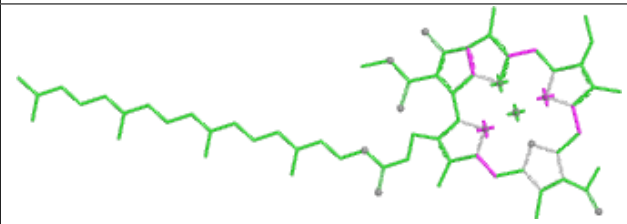
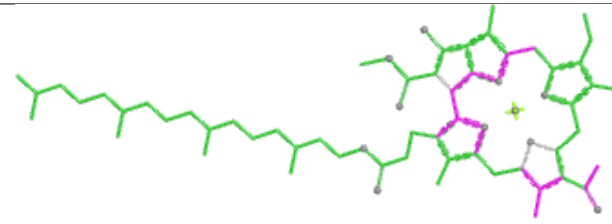
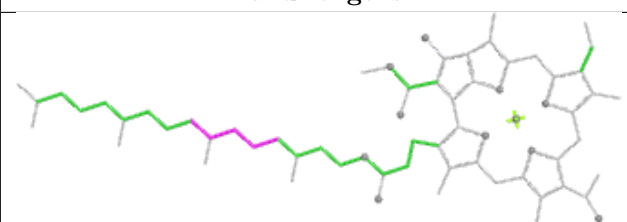
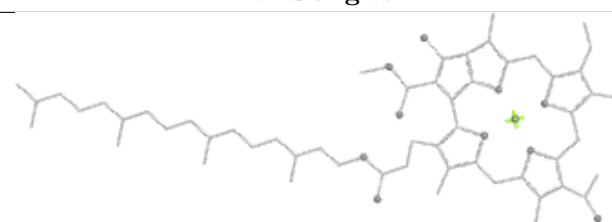


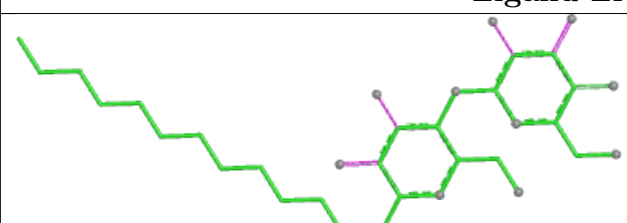
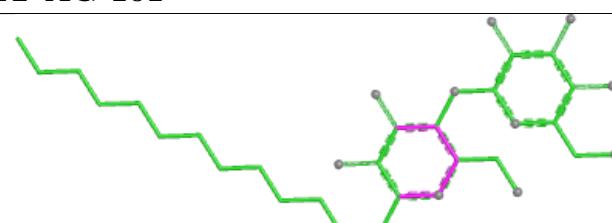
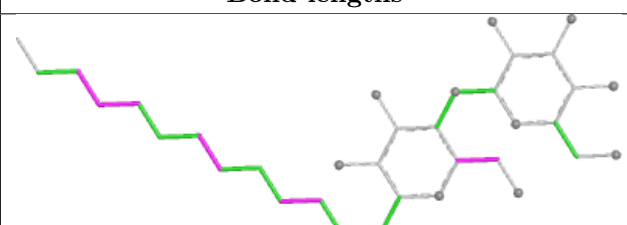
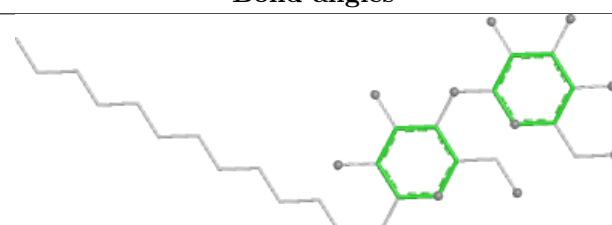


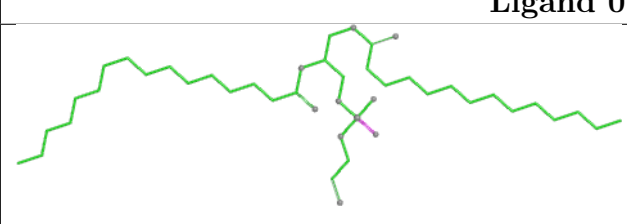
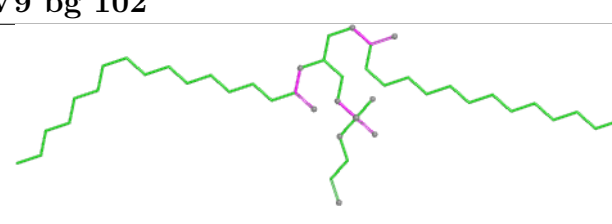
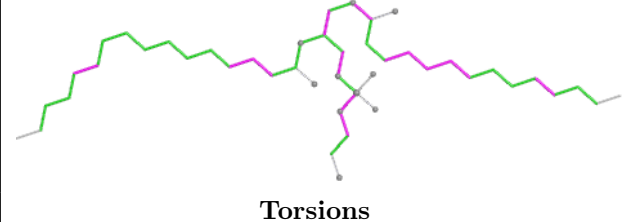
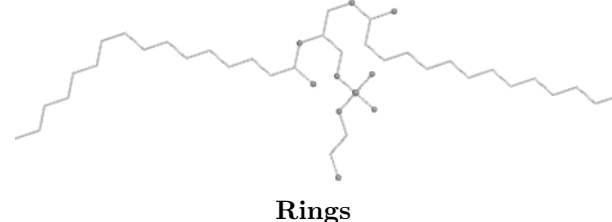


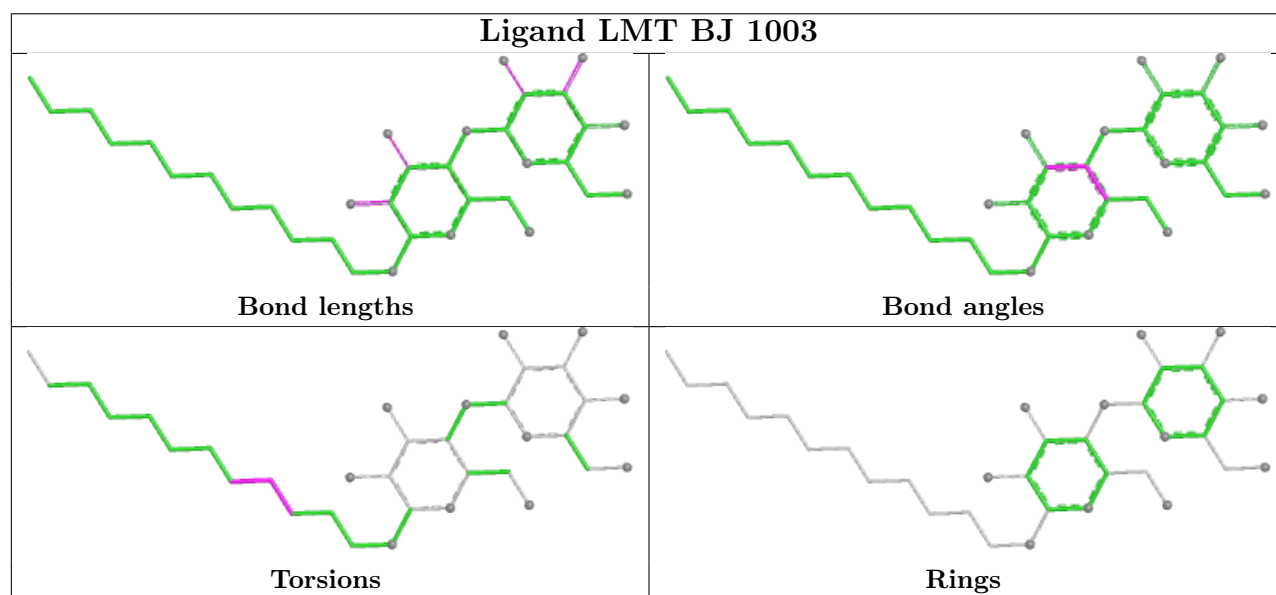
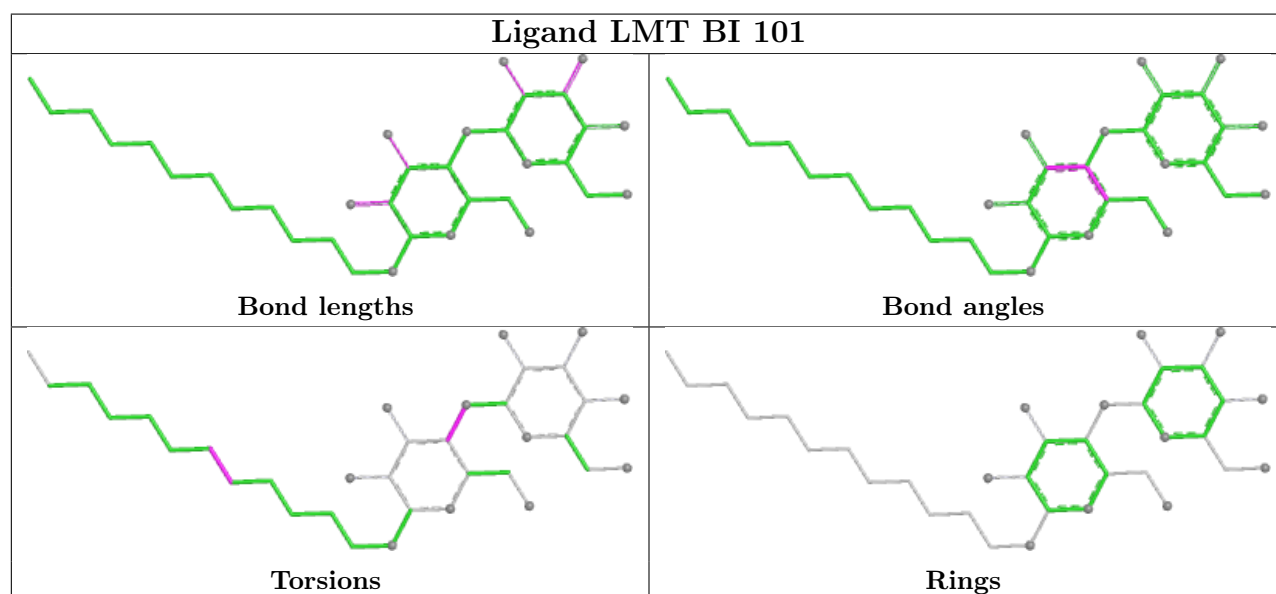
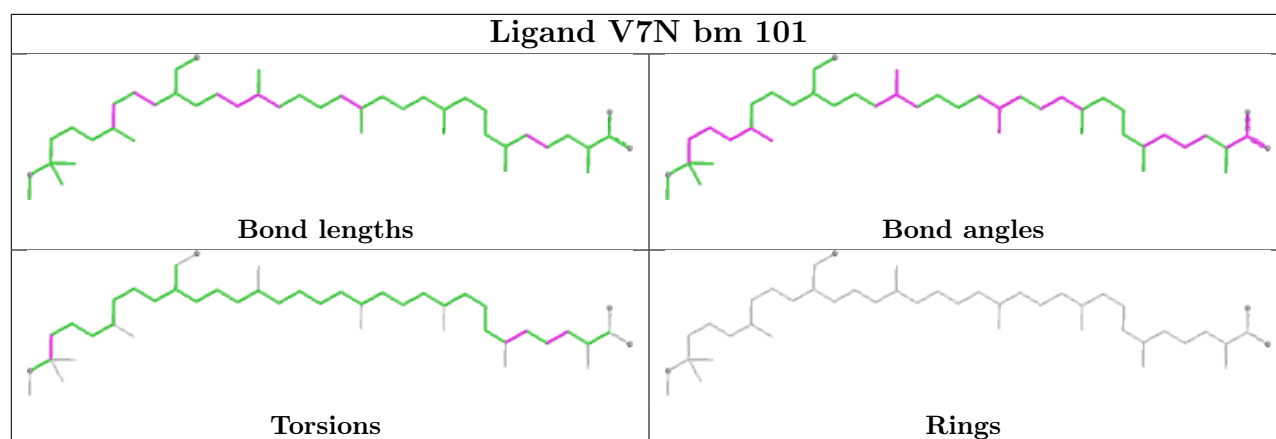


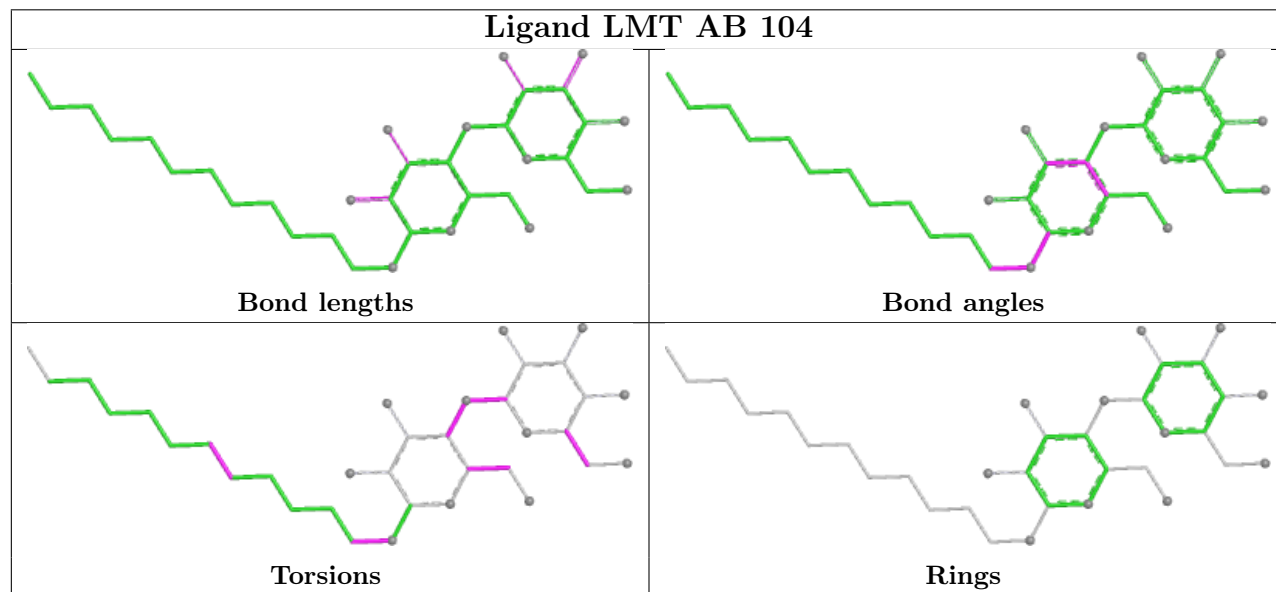
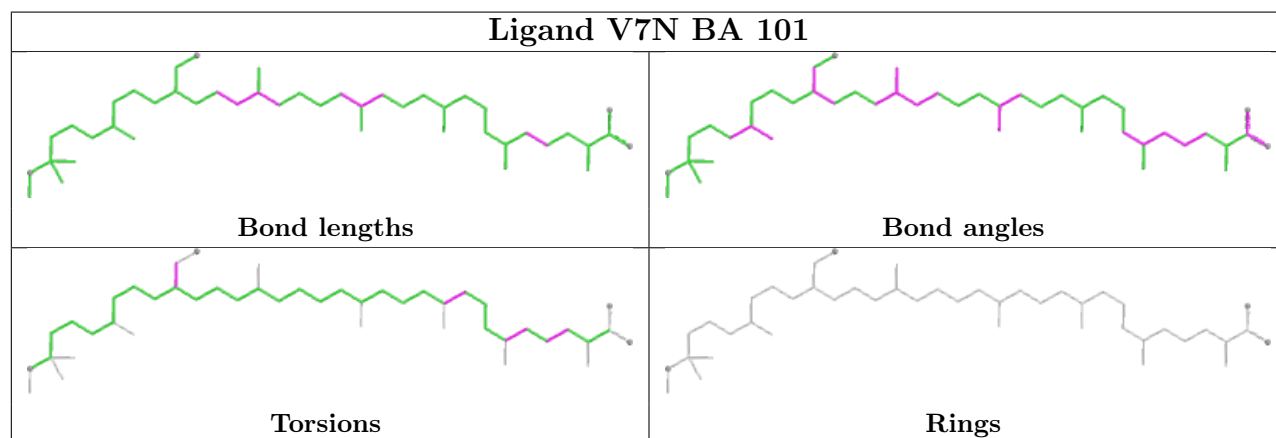
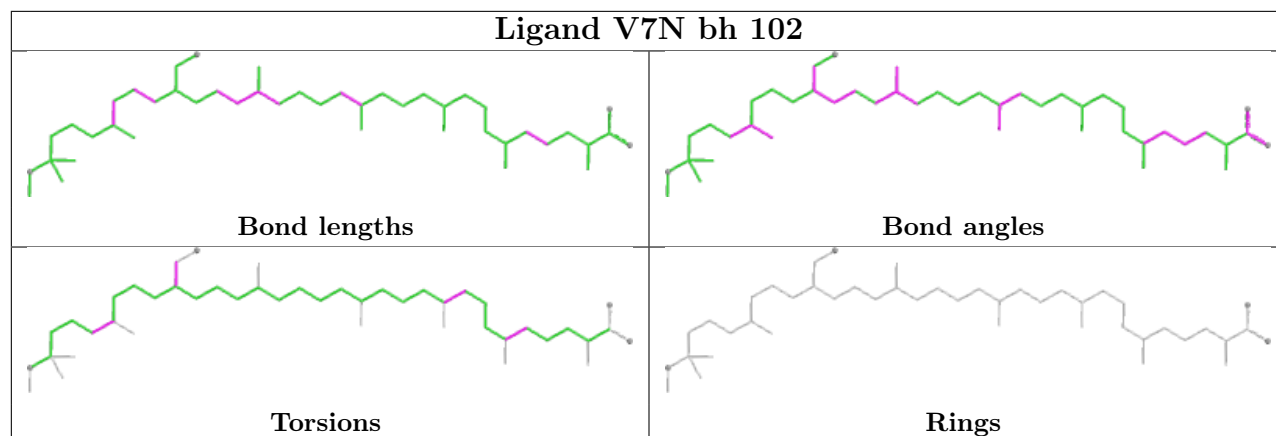


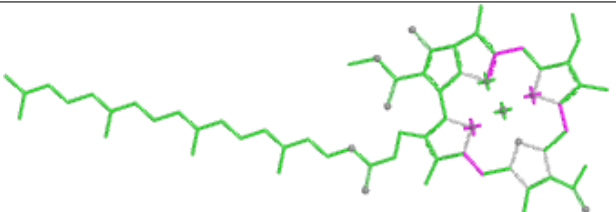
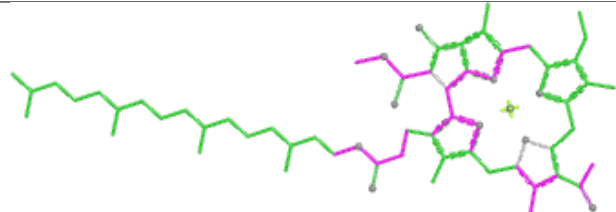
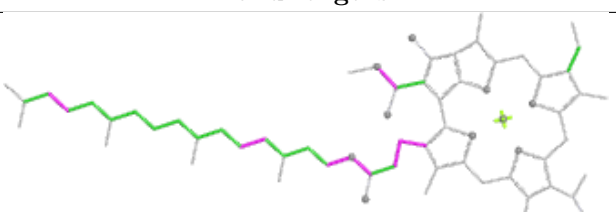
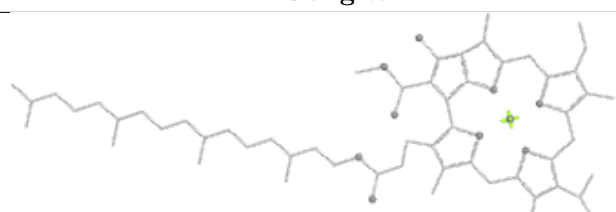
| Ligand BCL AC 1001  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

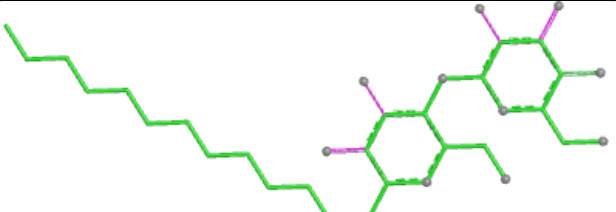
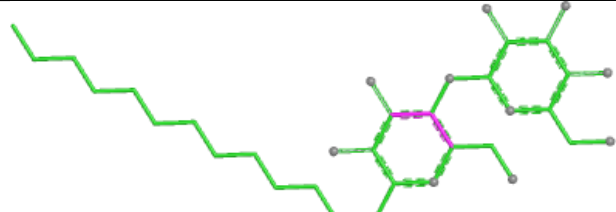
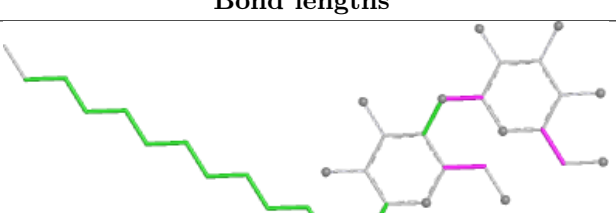
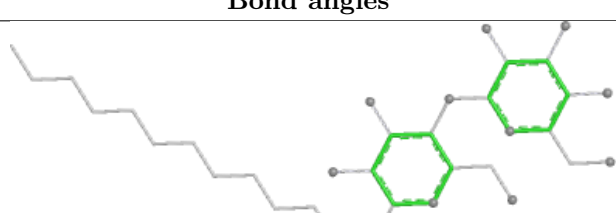
| Ligand LMT AG 101   |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

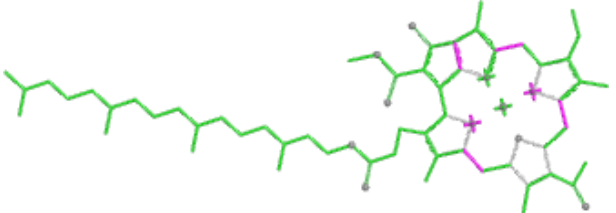
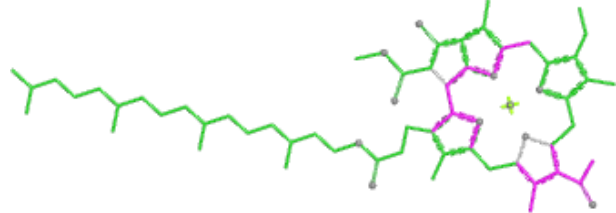
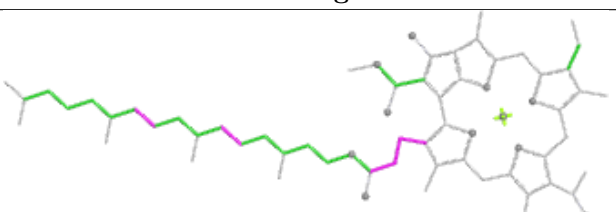
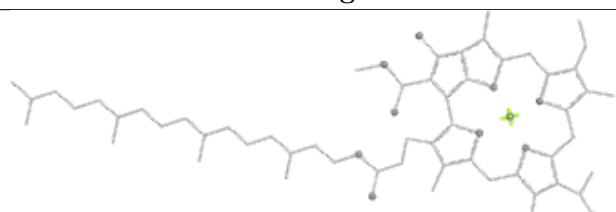
| Ligand 0V9 bg 102   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

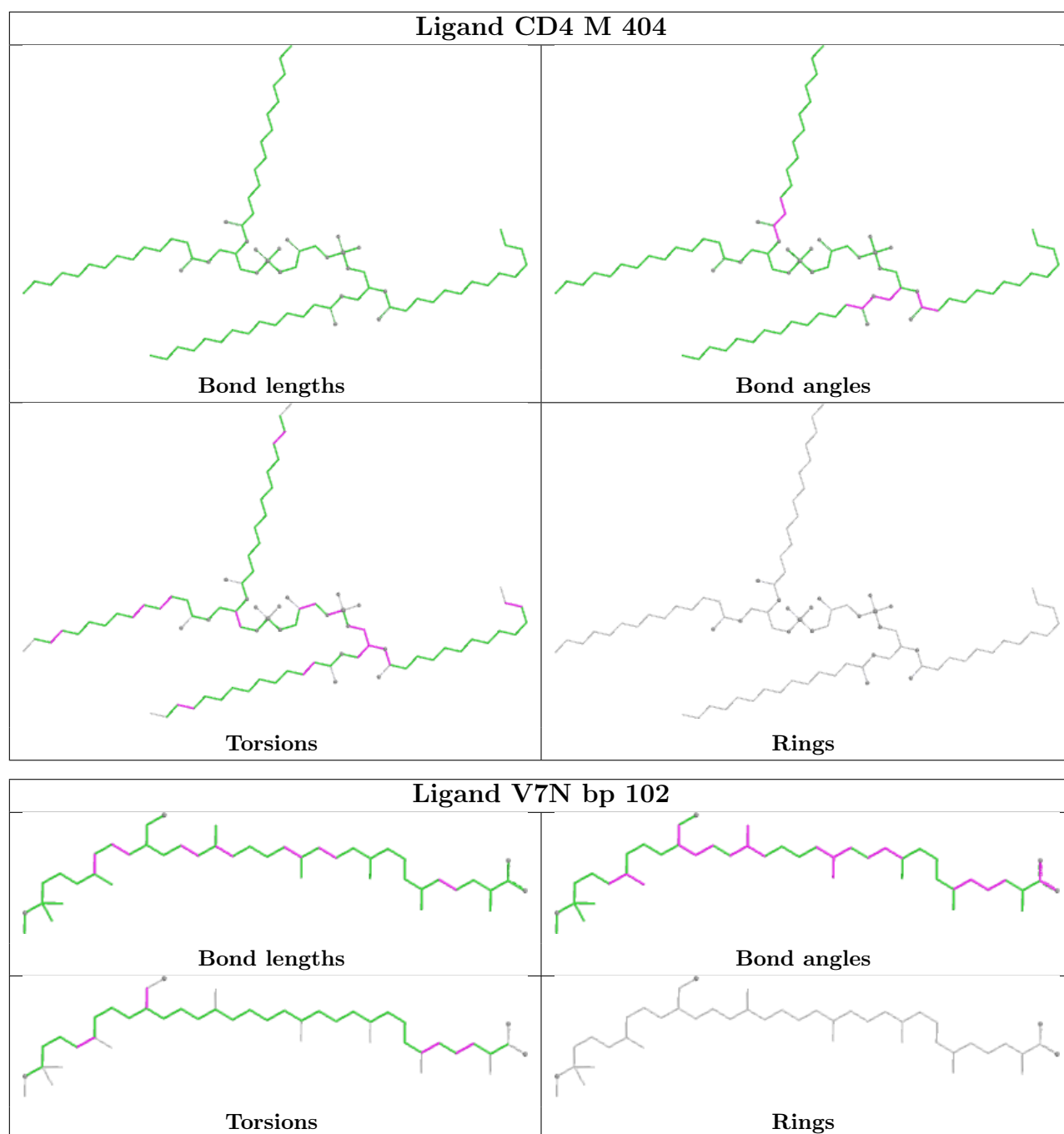


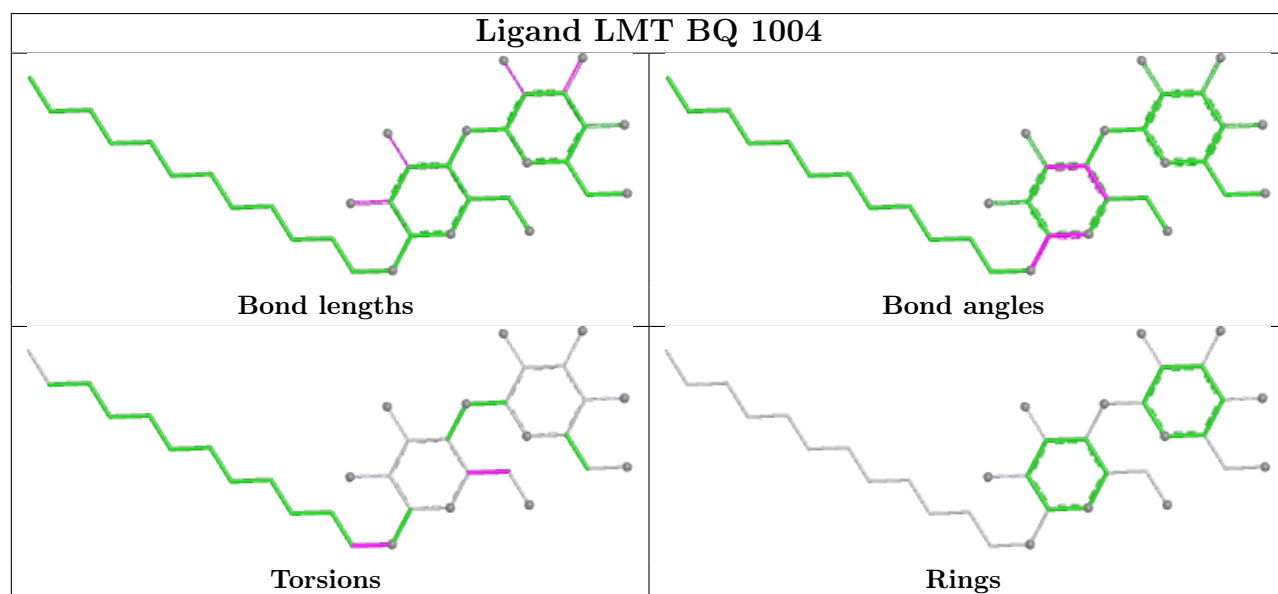
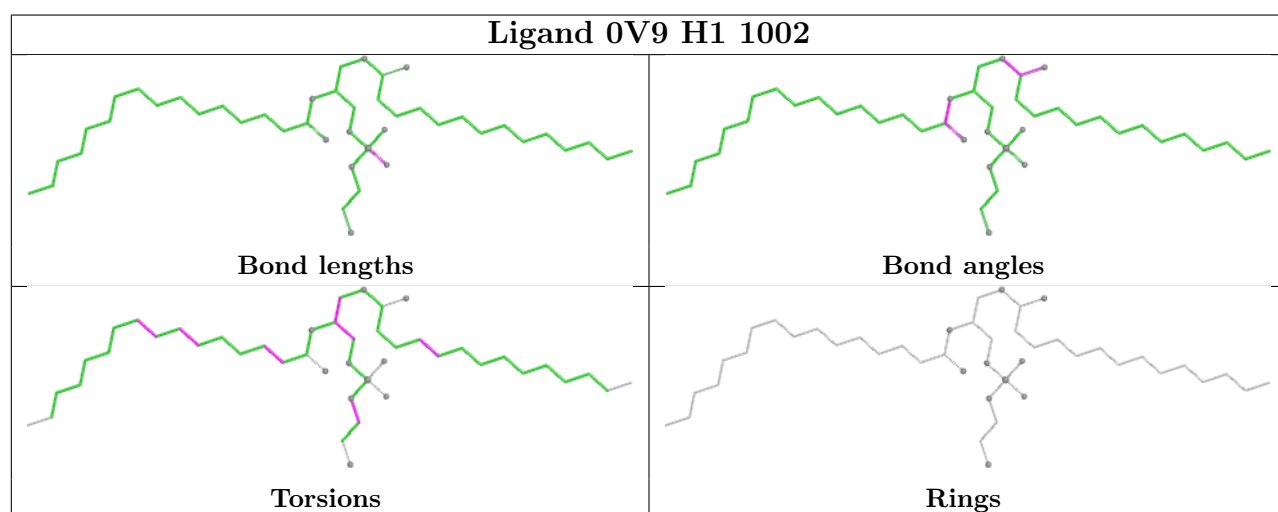
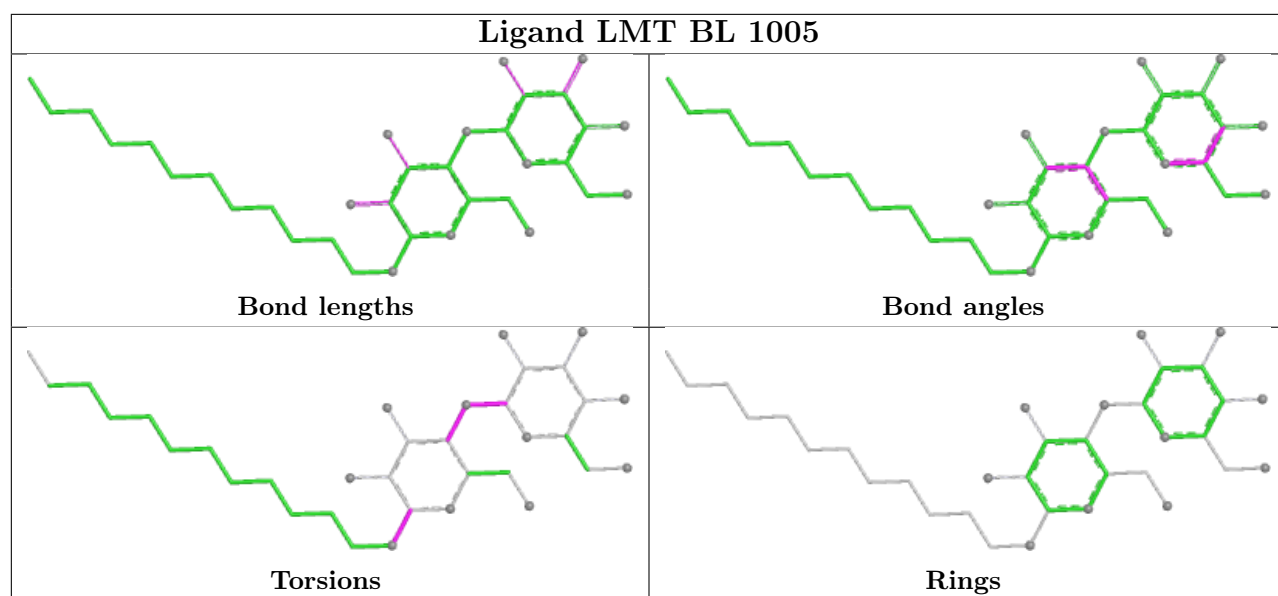


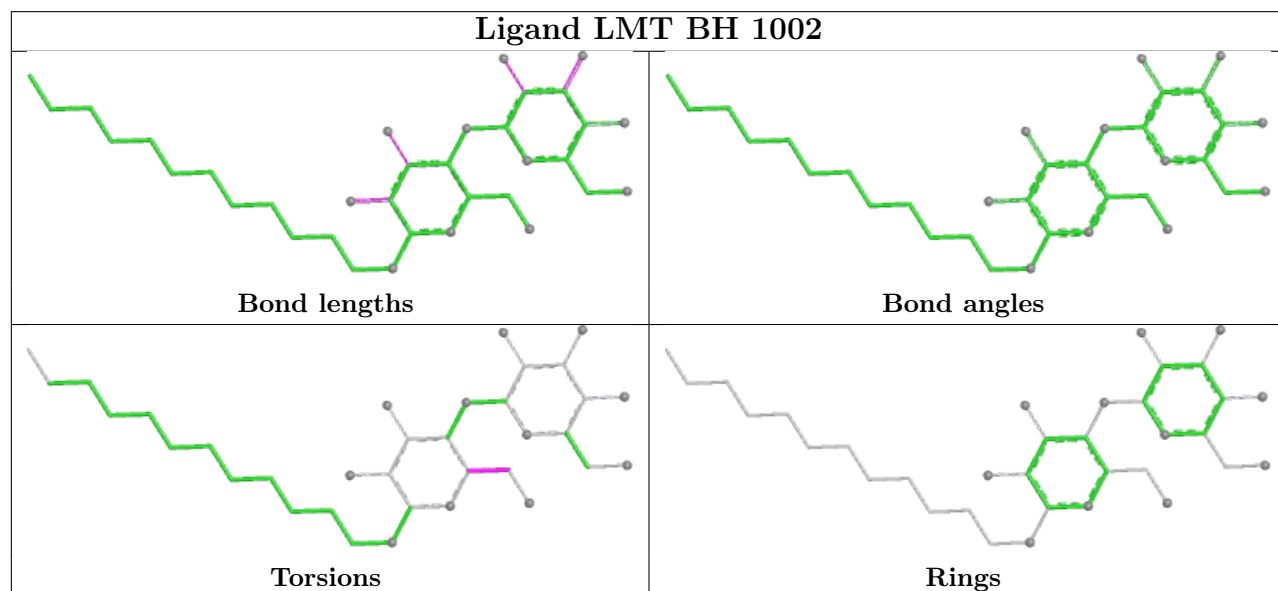
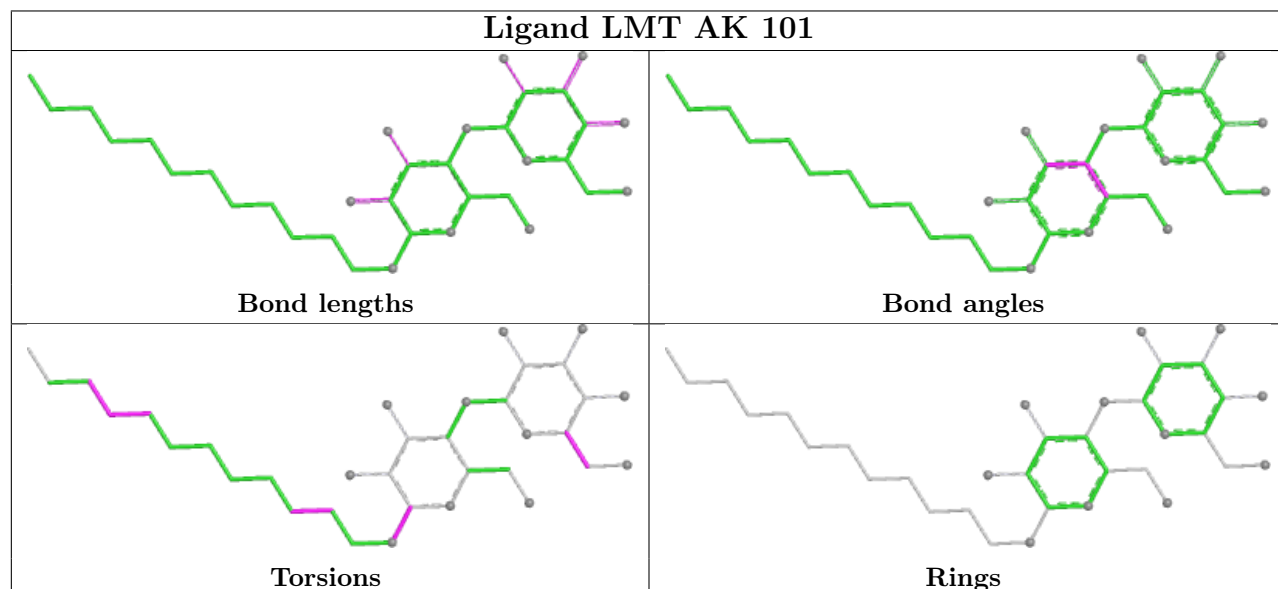
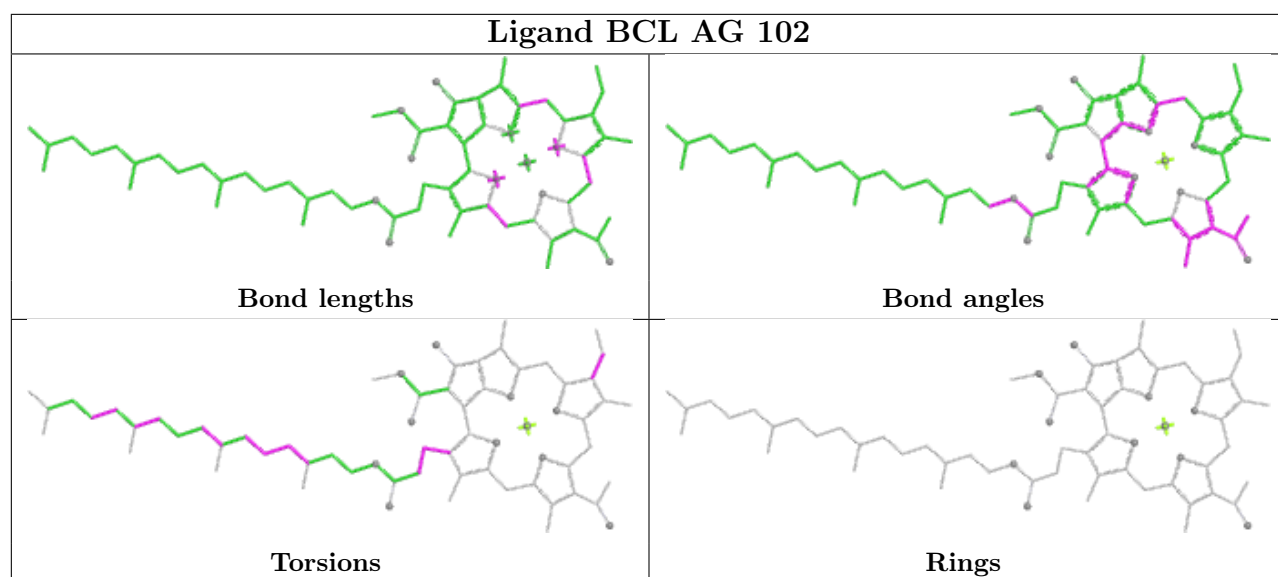
| Ligand BCL AQ 103   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand LMT BO 1002  |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

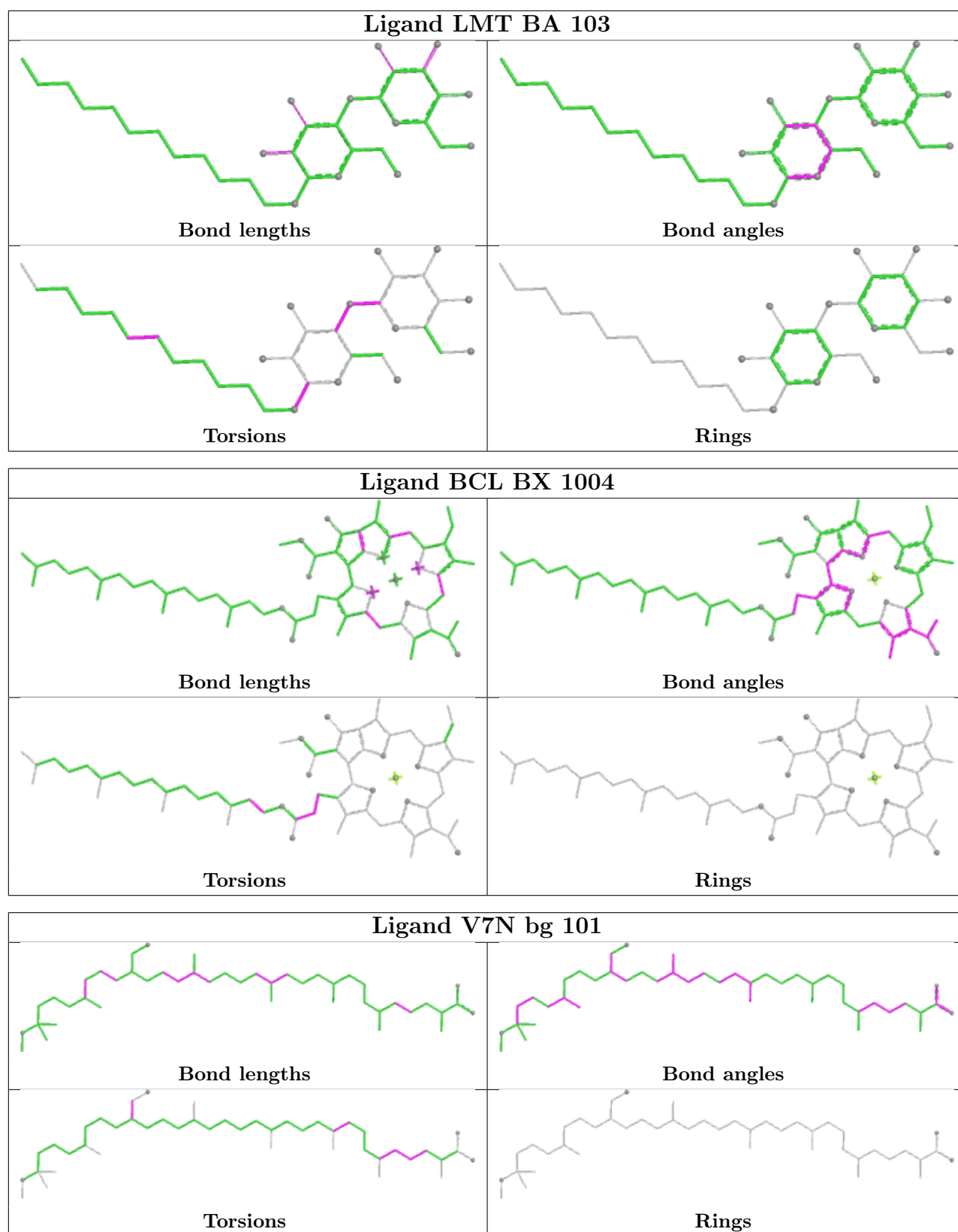
| Ligand BCL BL 1004  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

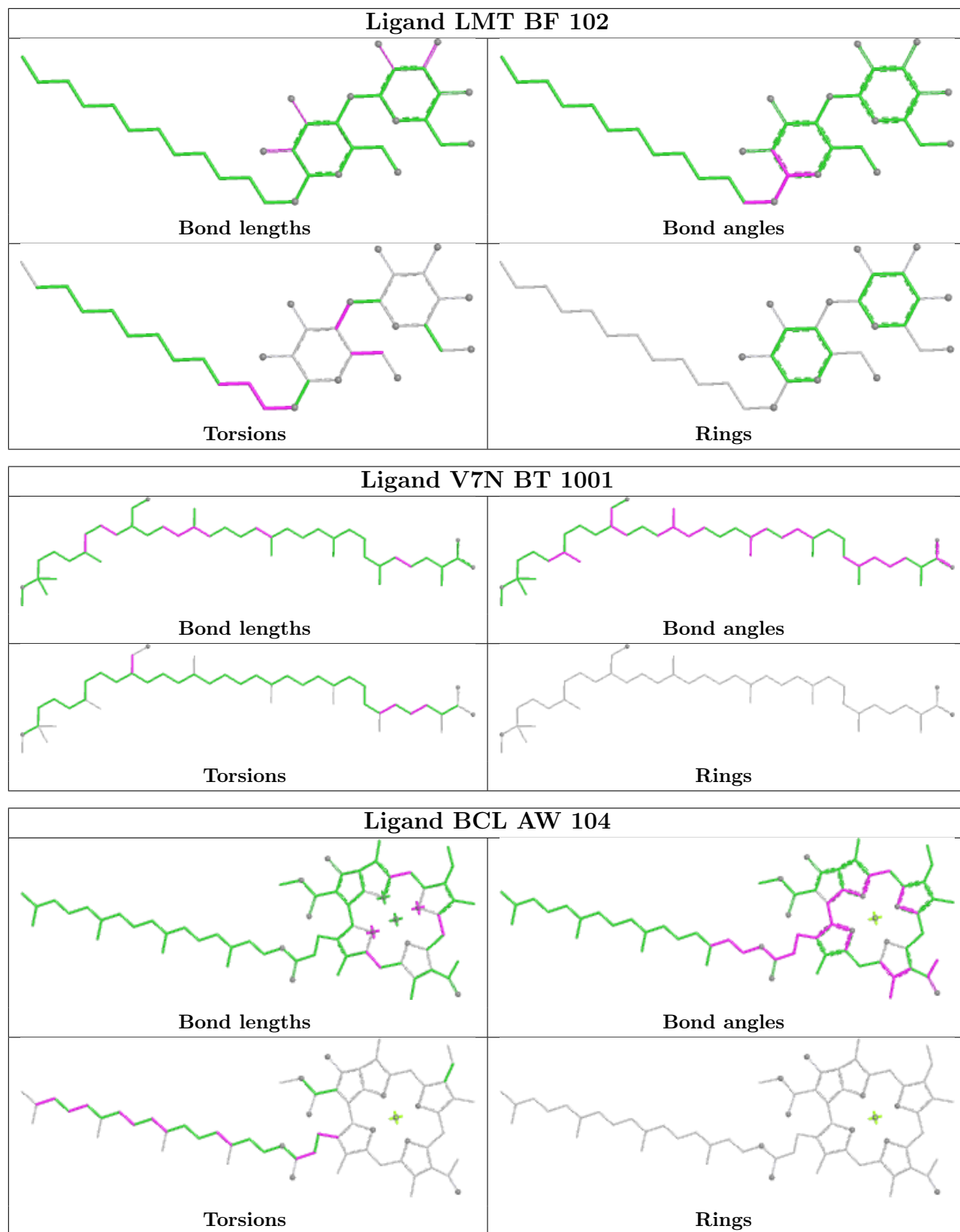


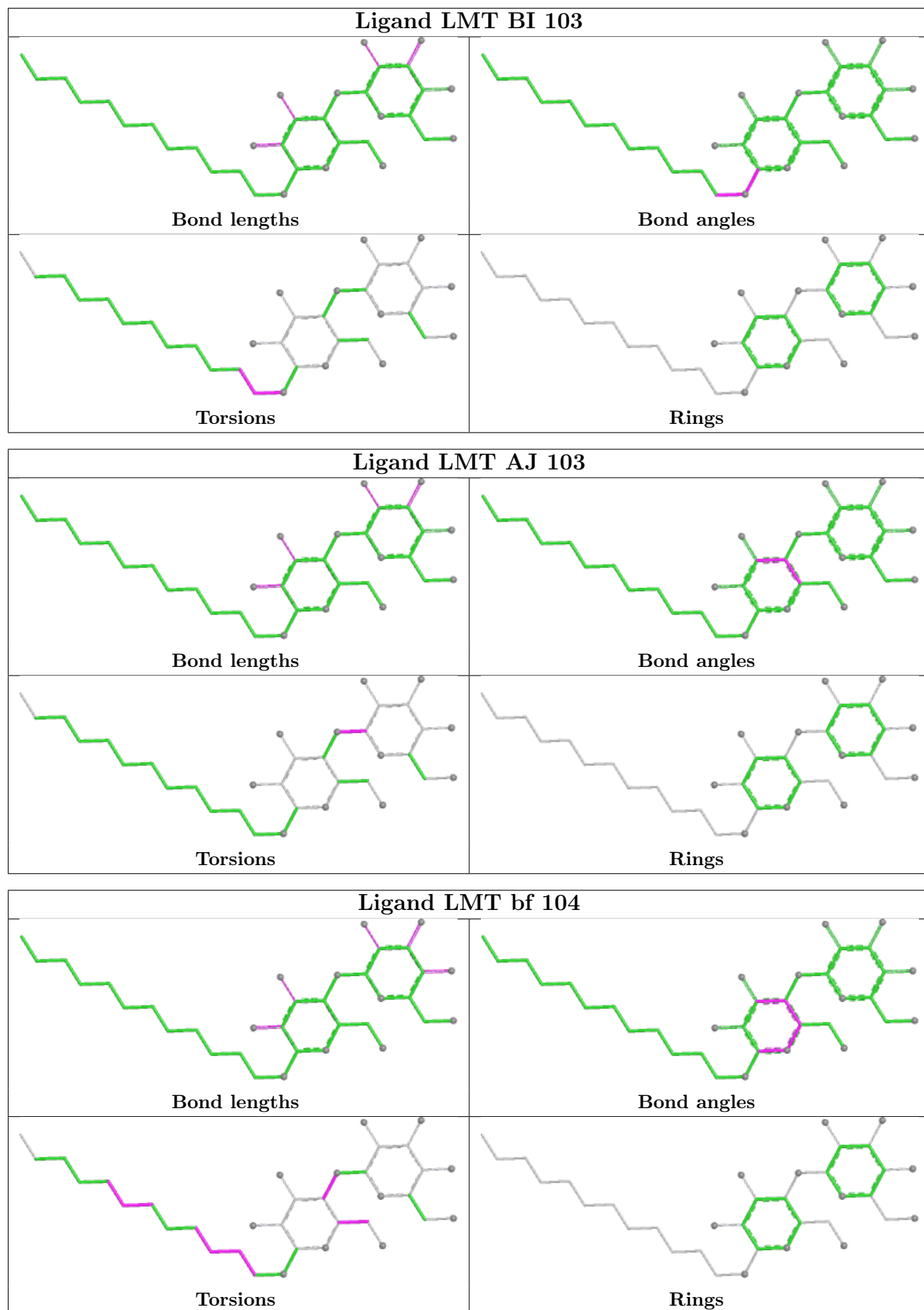


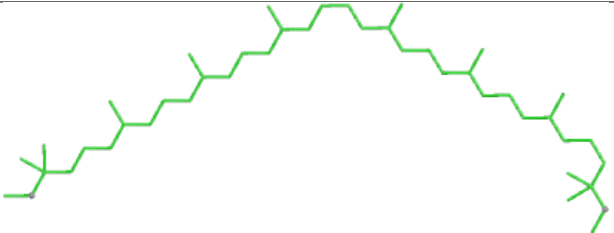
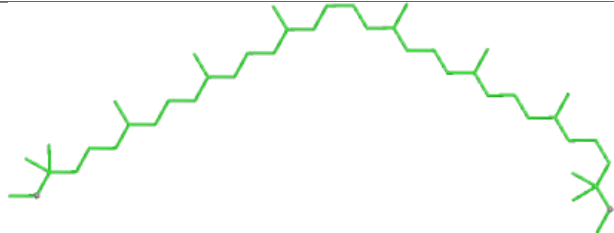
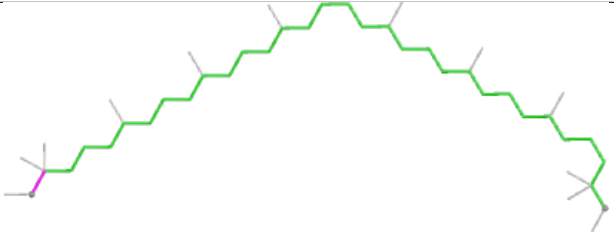



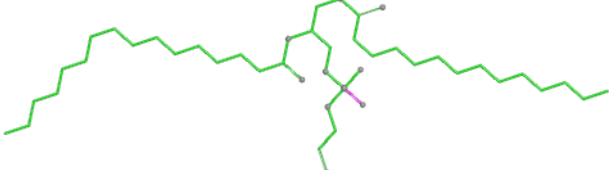

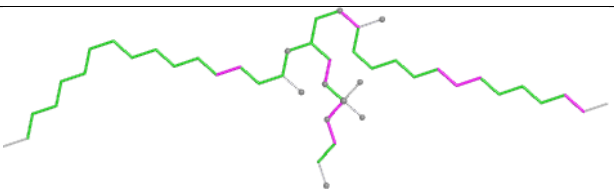
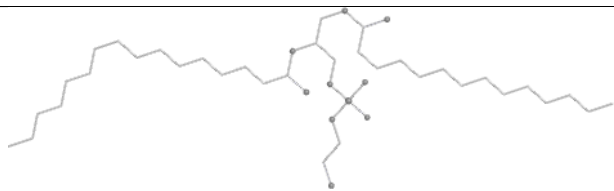


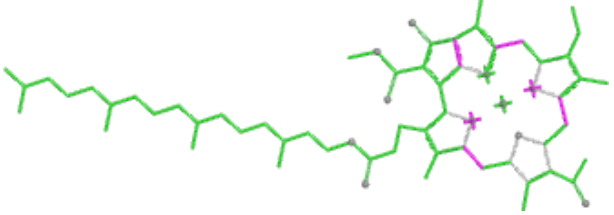
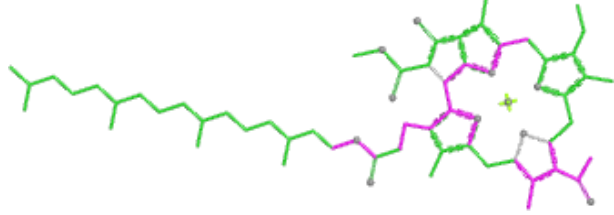
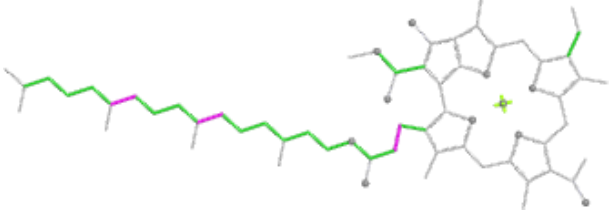
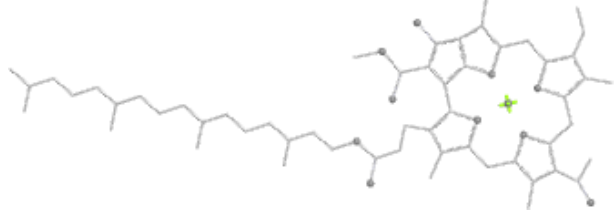


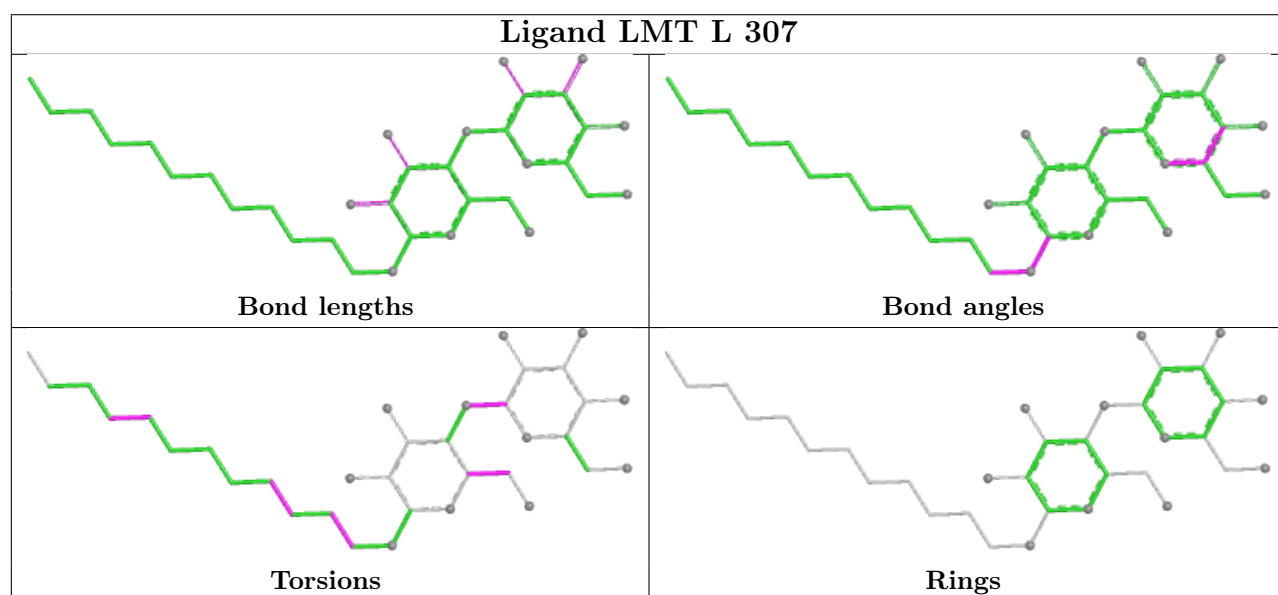
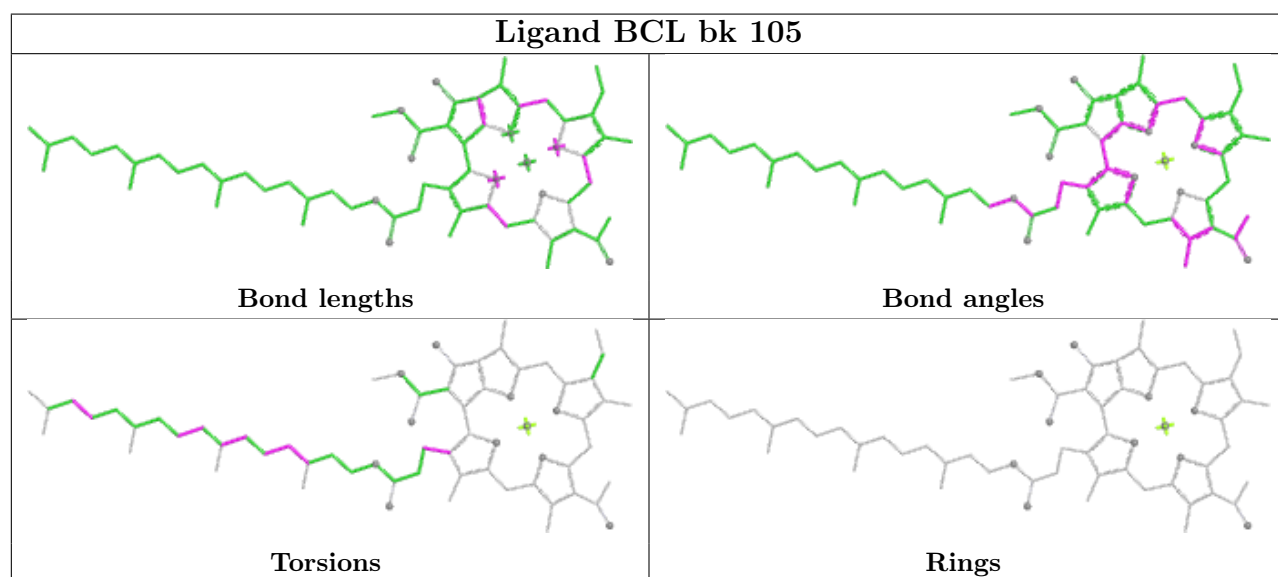
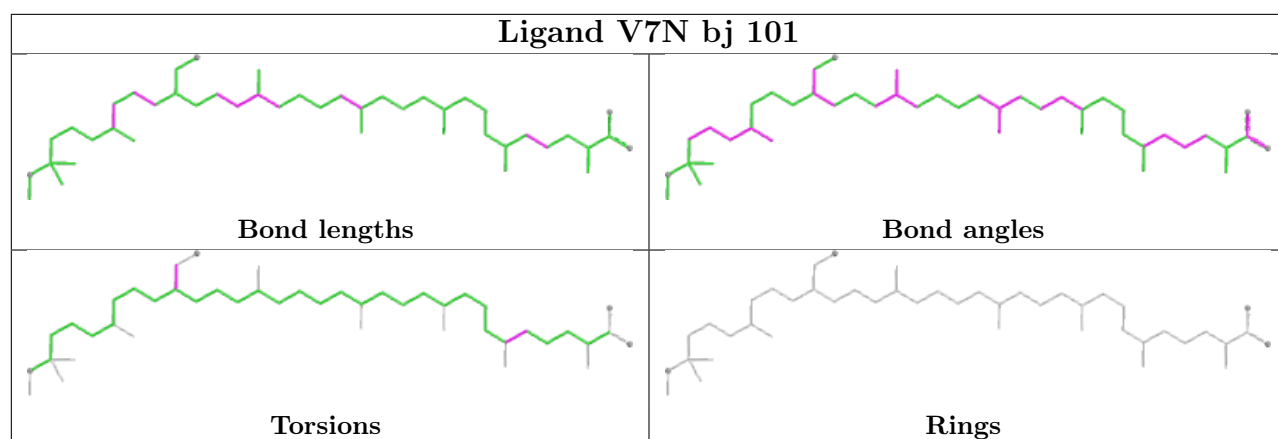


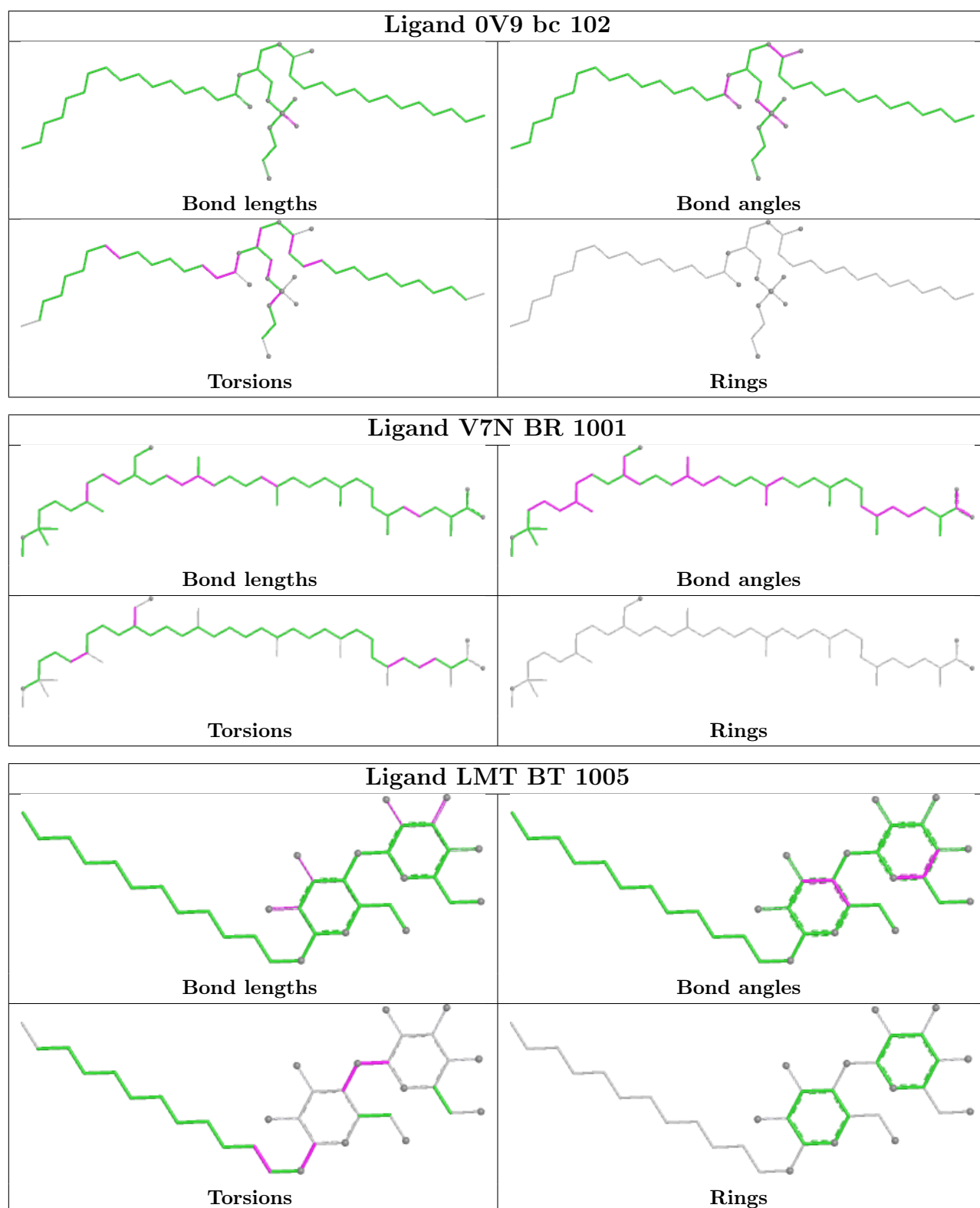


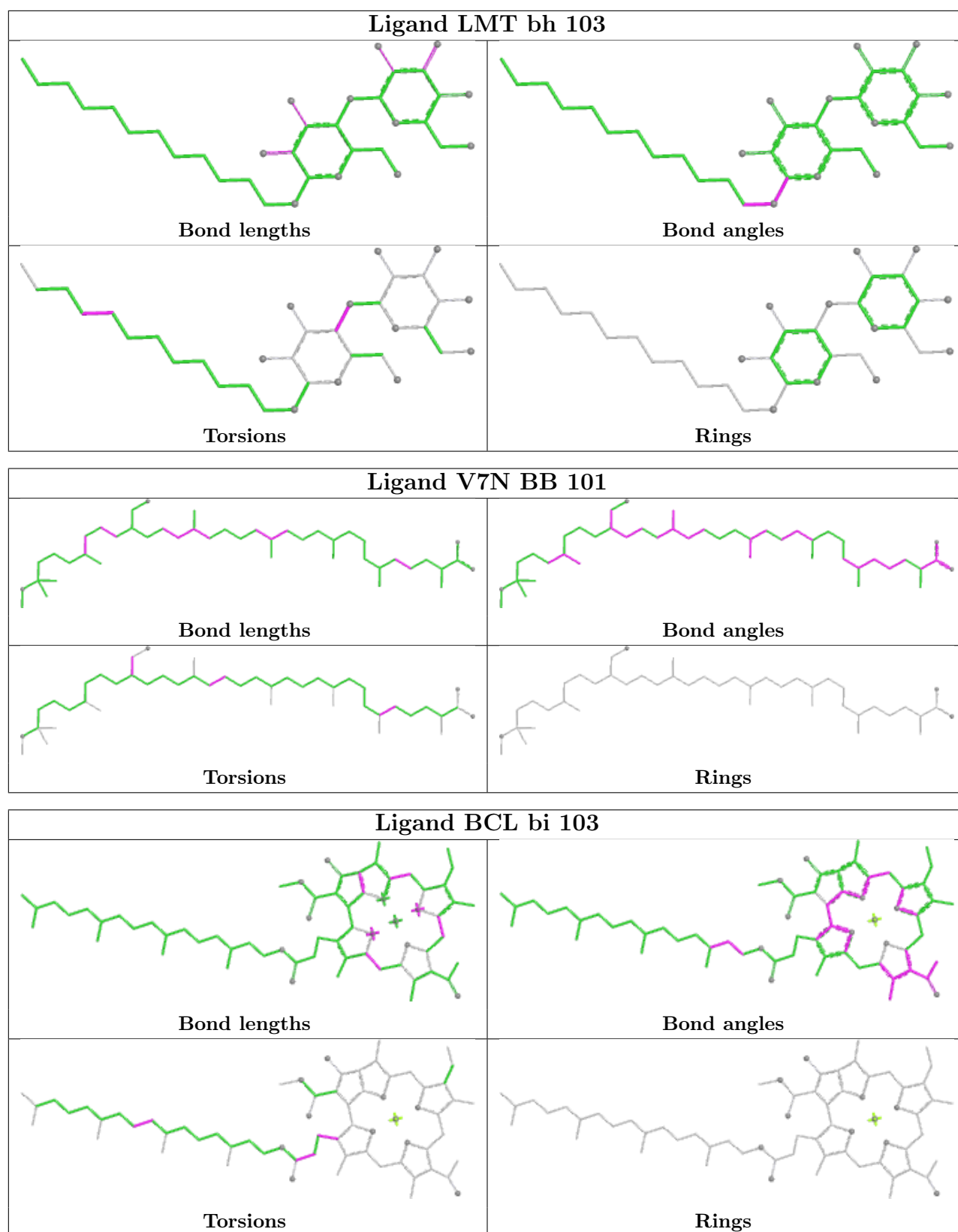
| Ligand CRT M 408  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

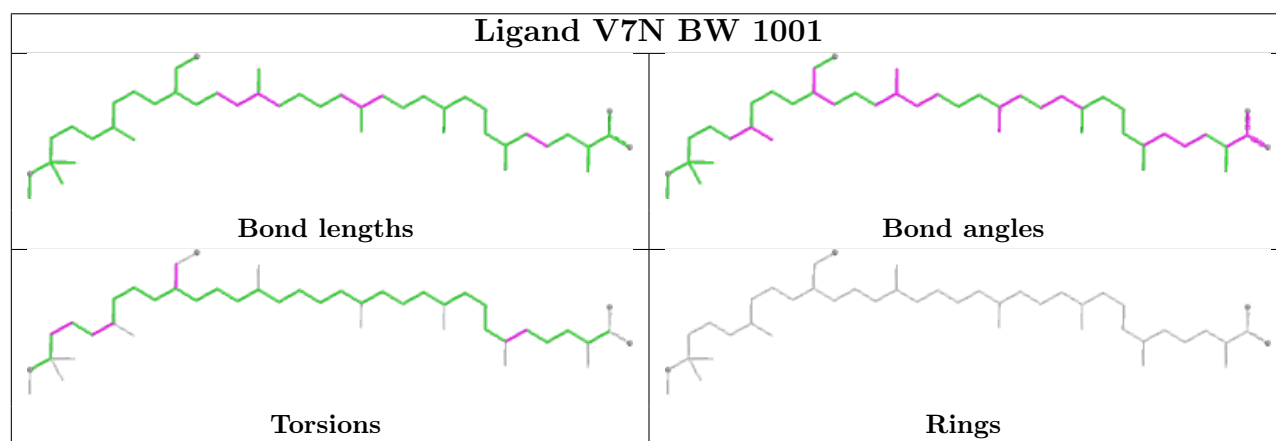
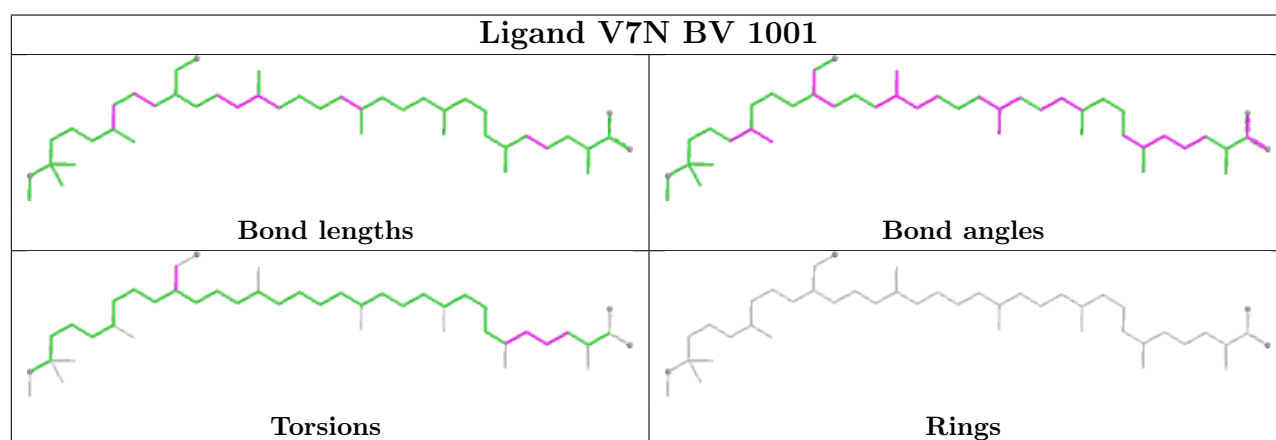
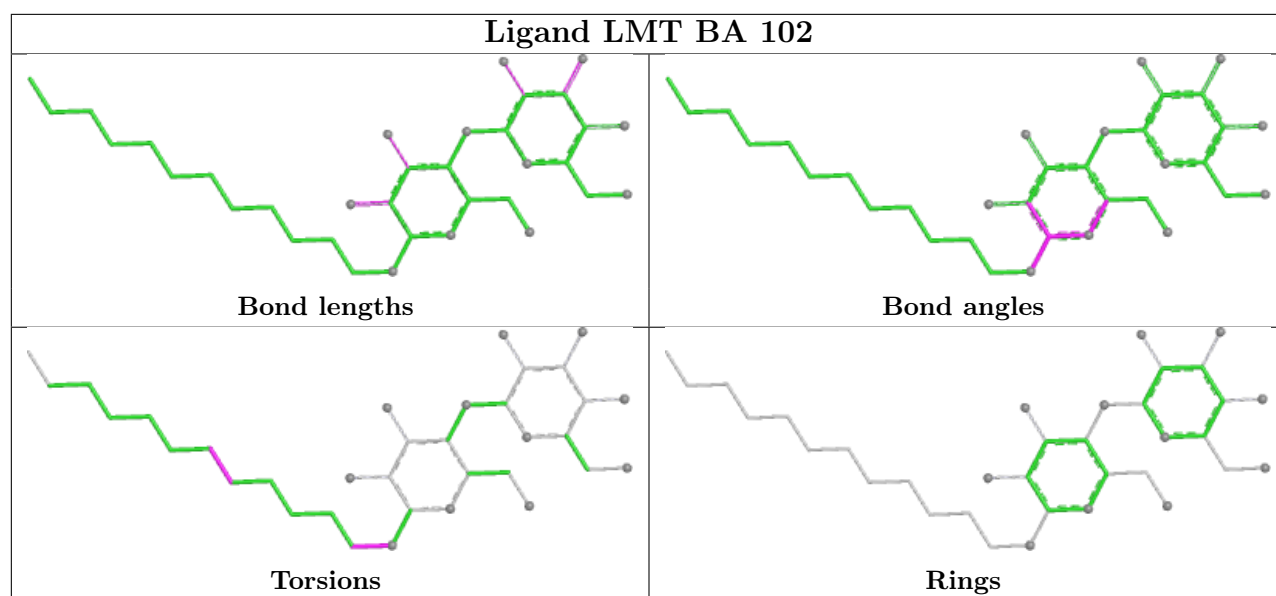
| Ligand 0V9 bh 104   |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand BCL BP 1004  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

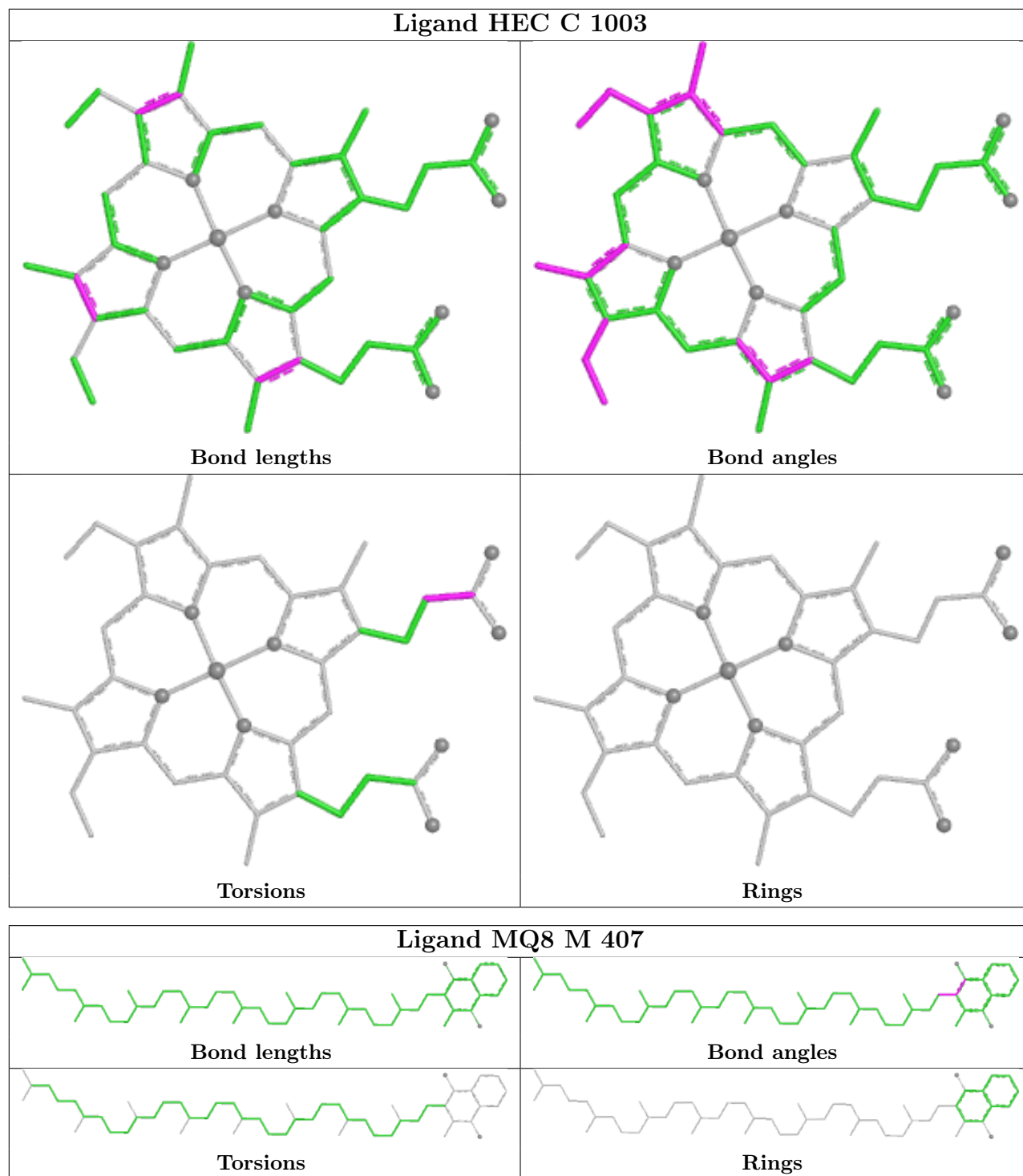


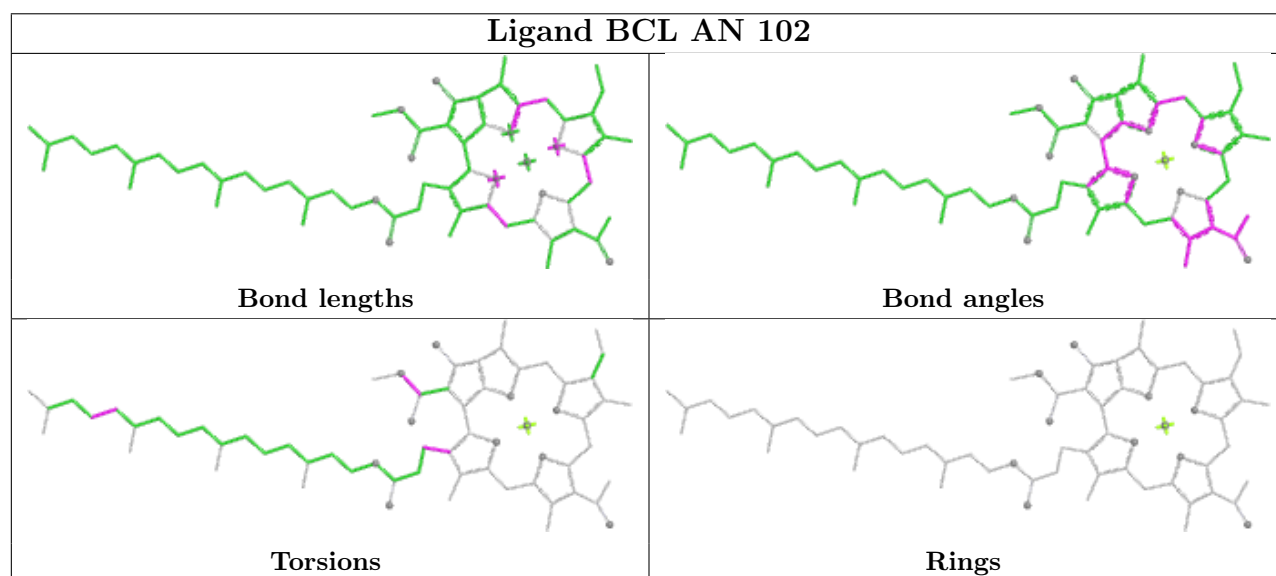
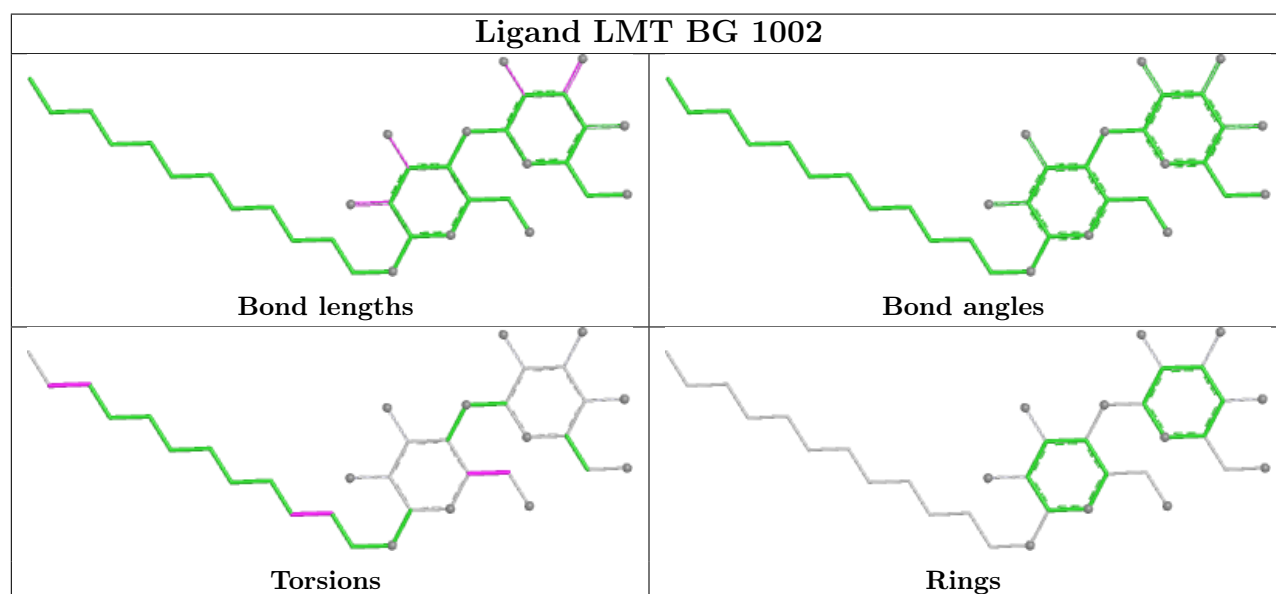
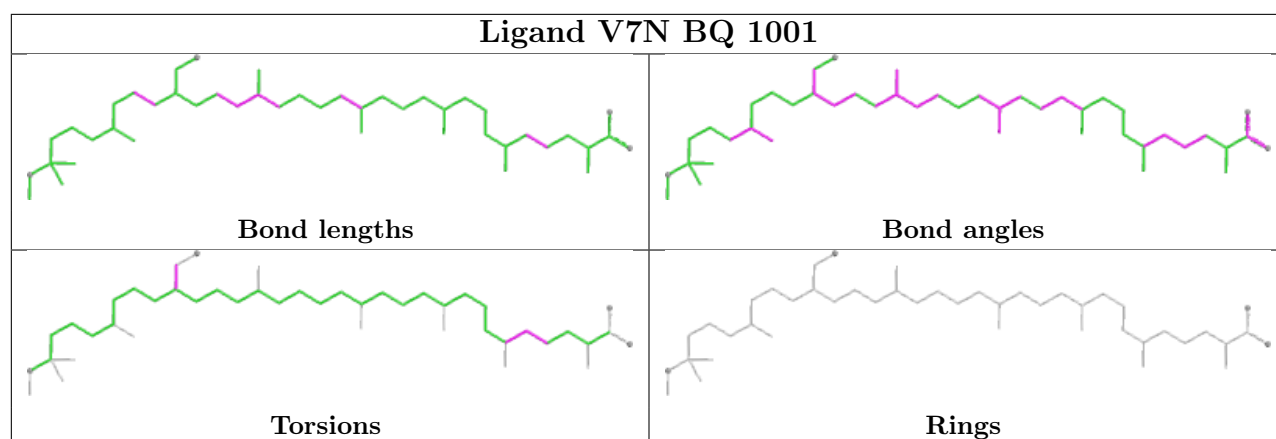


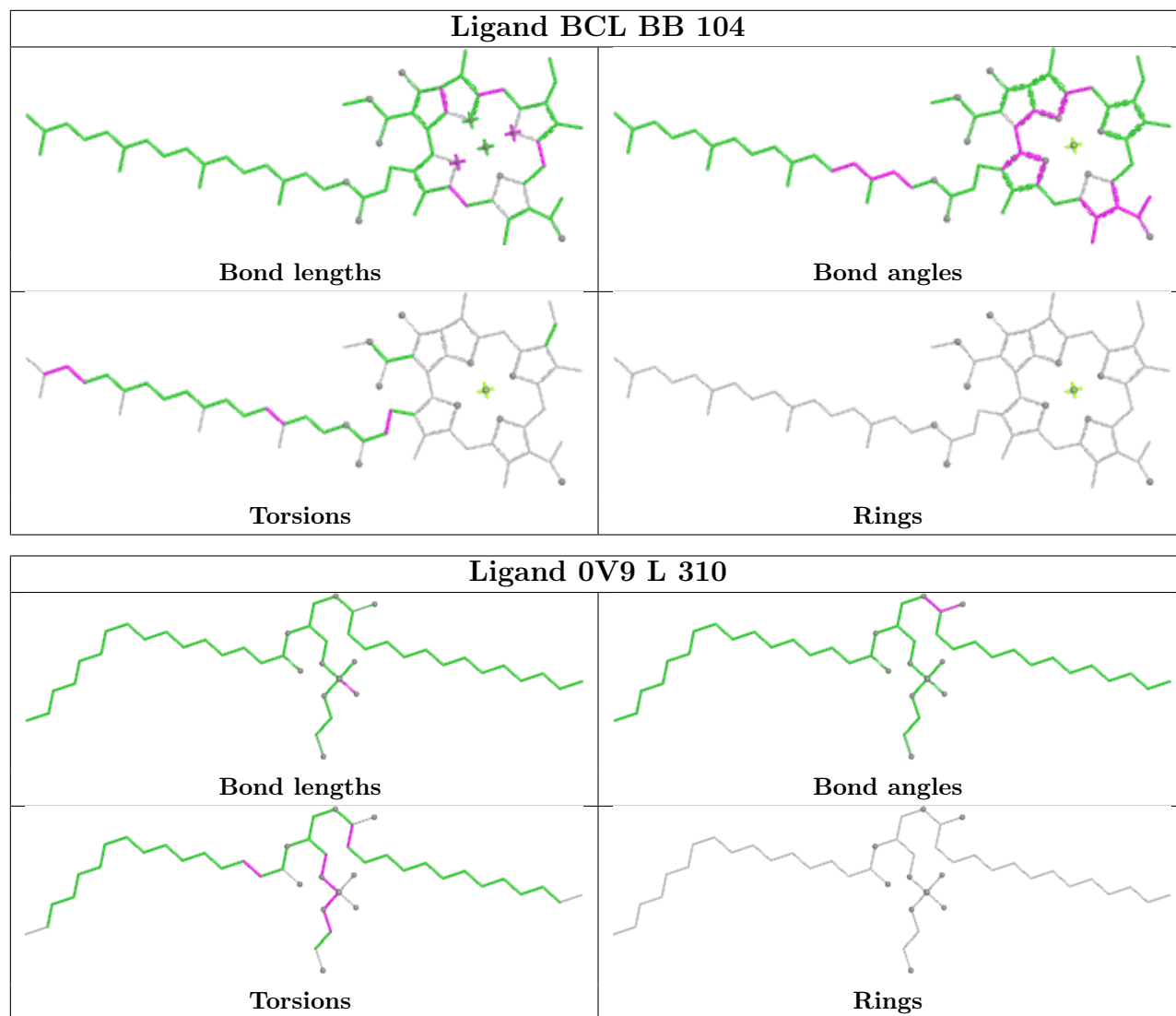




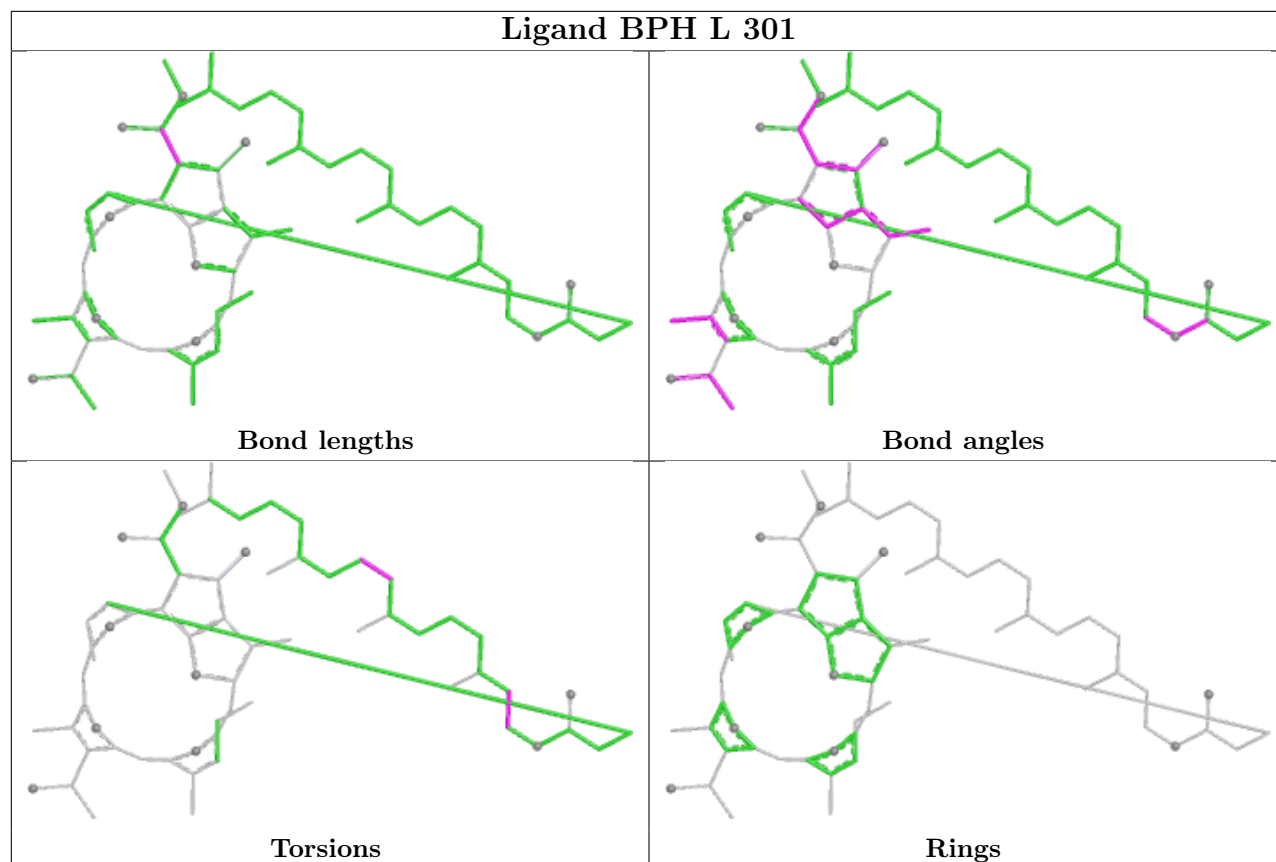




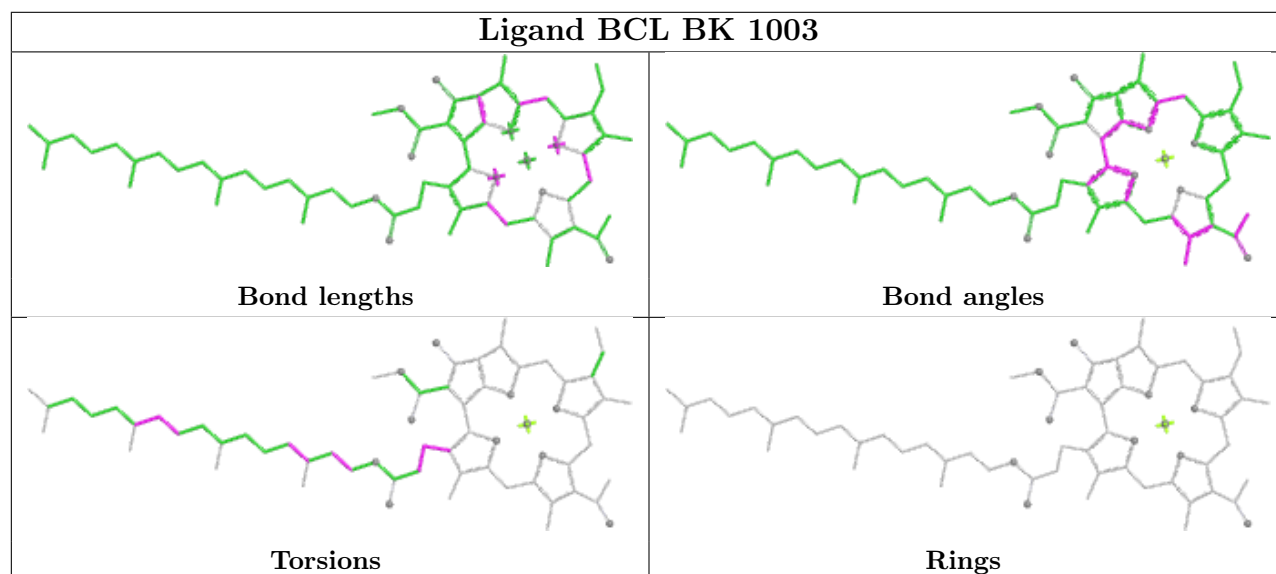


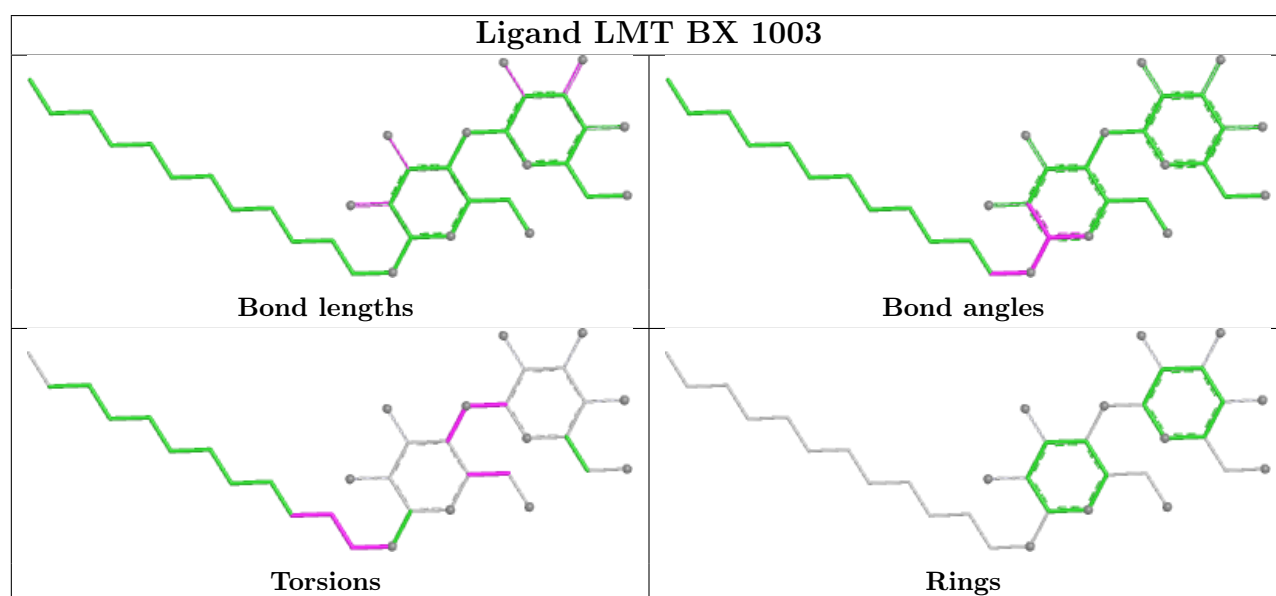
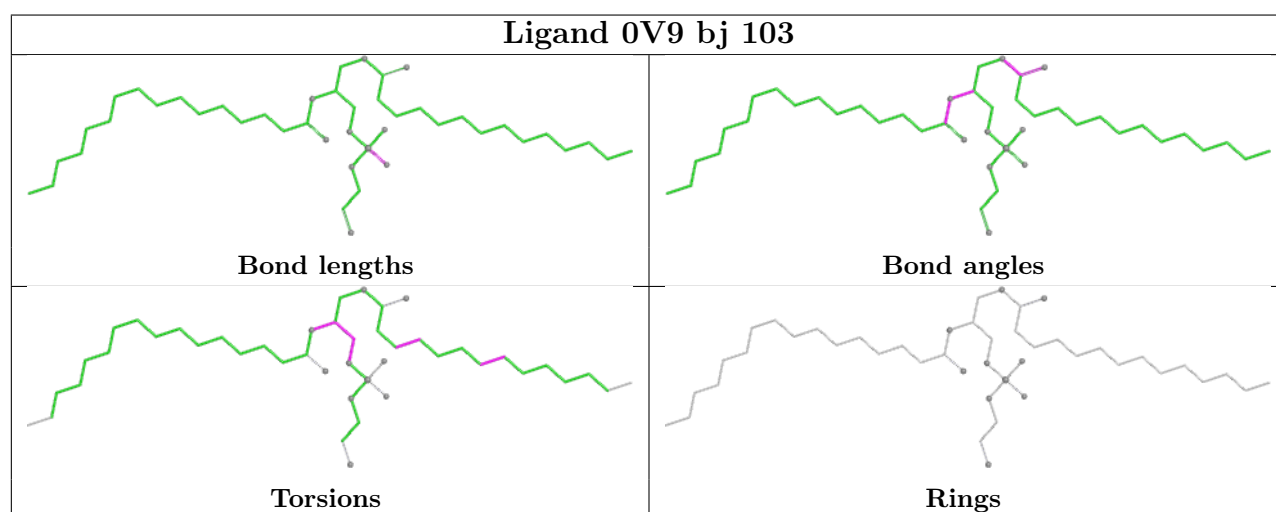
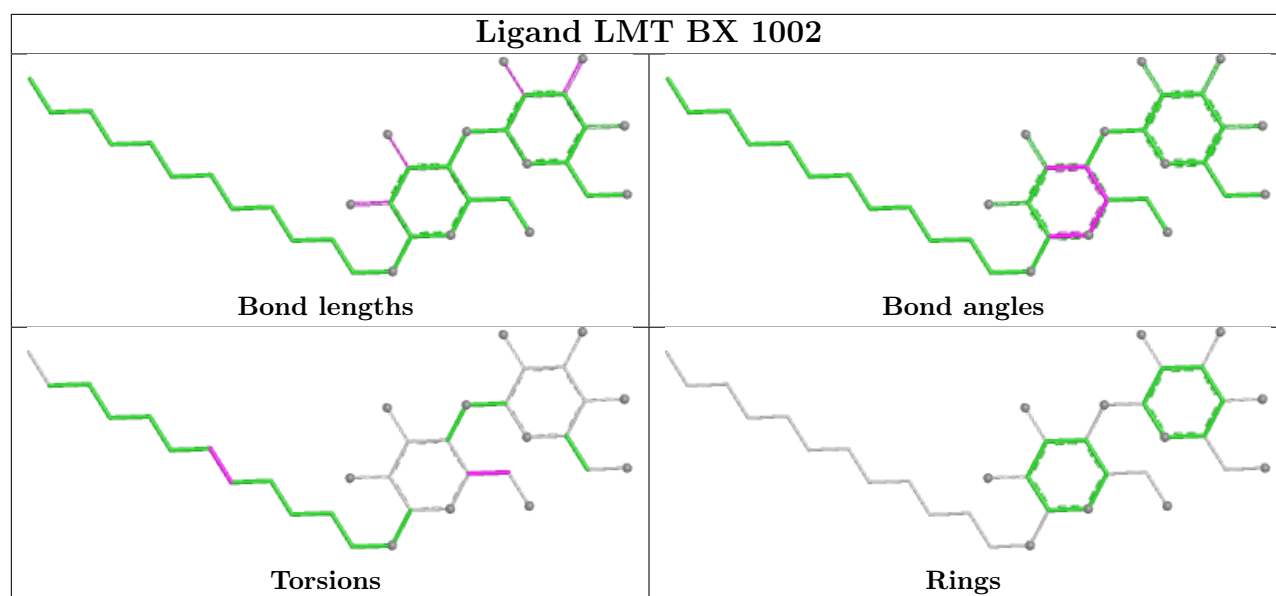


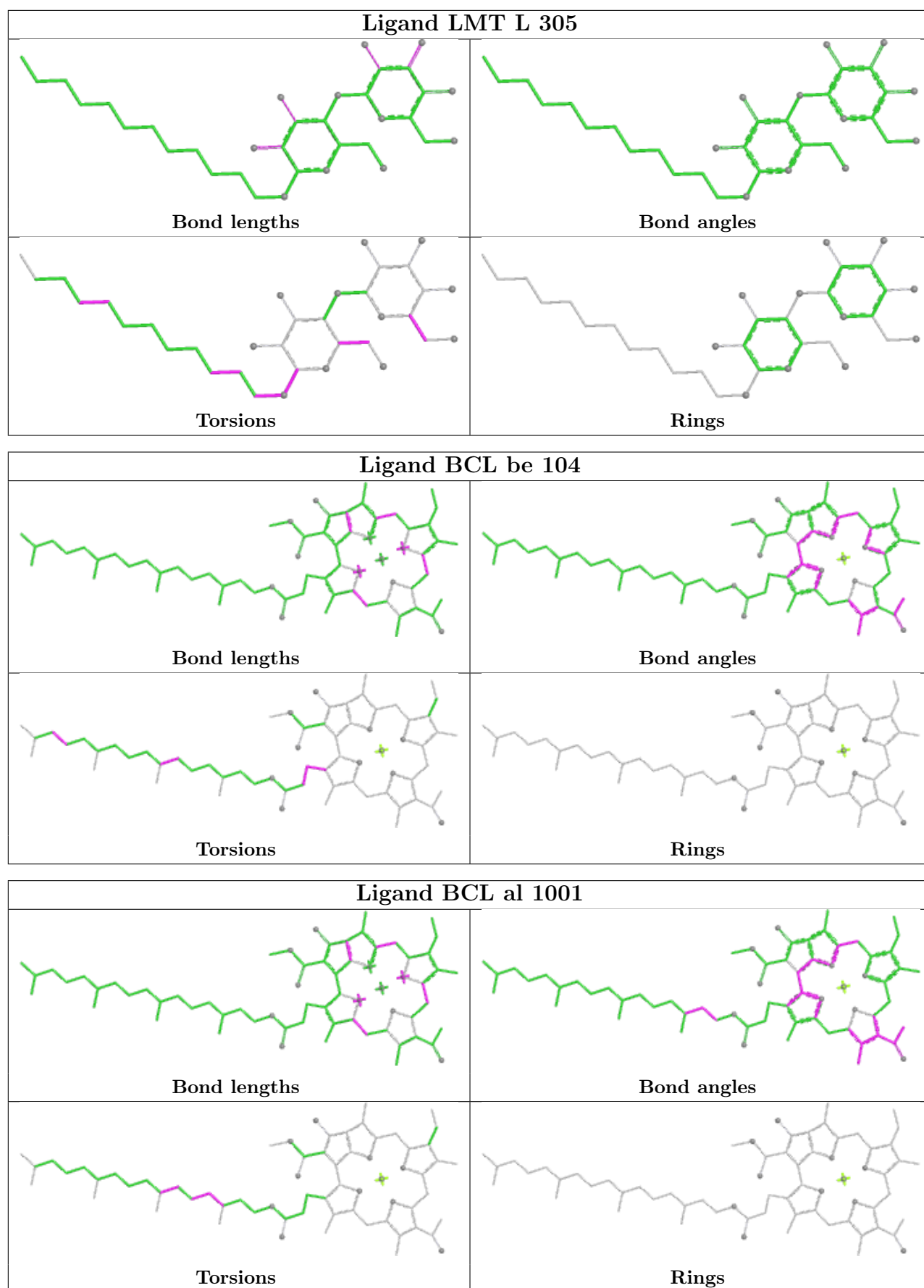
## Ligand BPH L 301

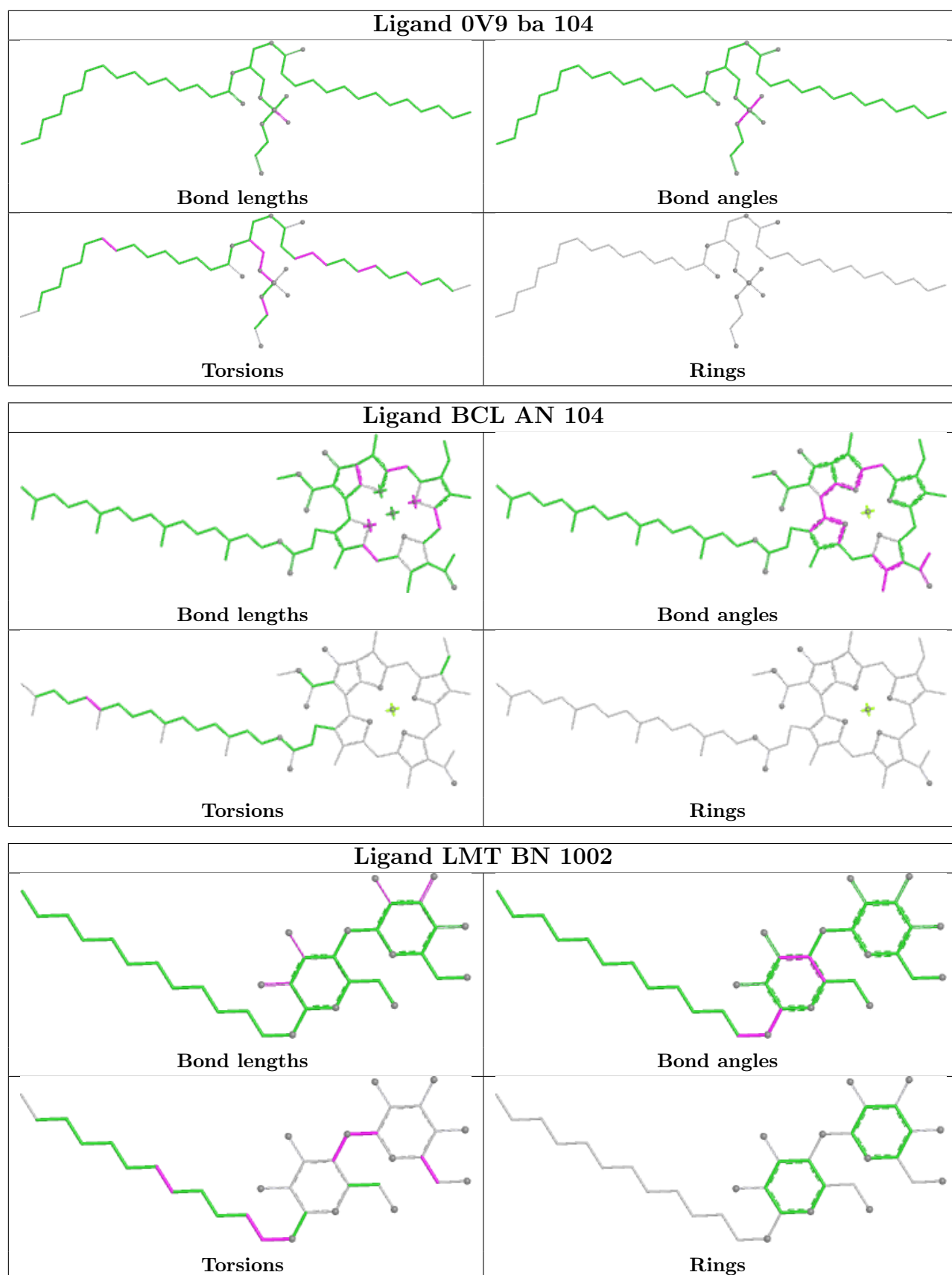


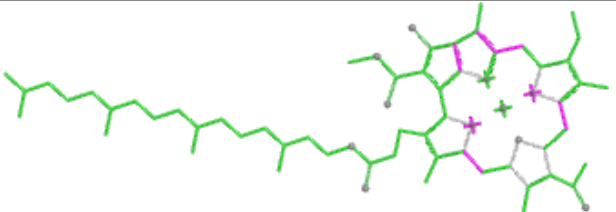
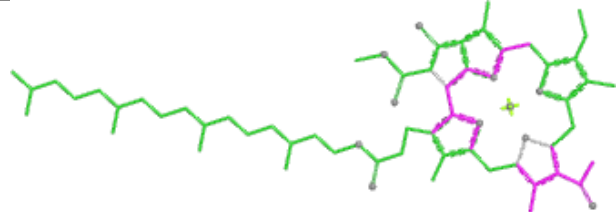
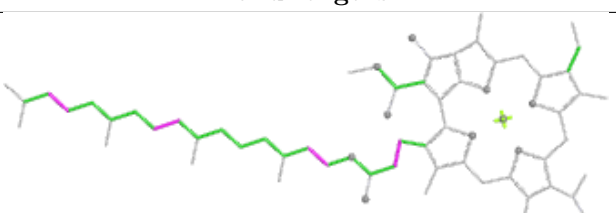
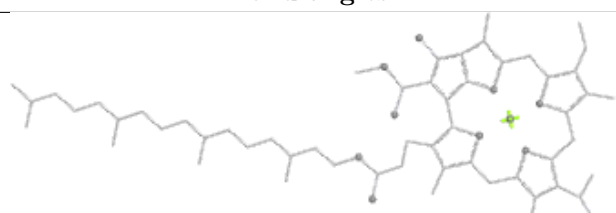
## Ligand BCL BK 1003

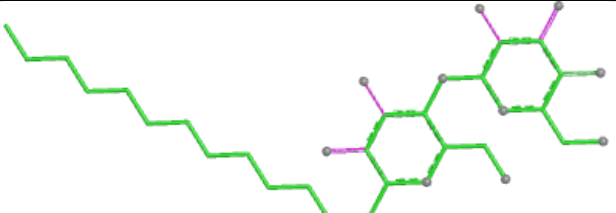
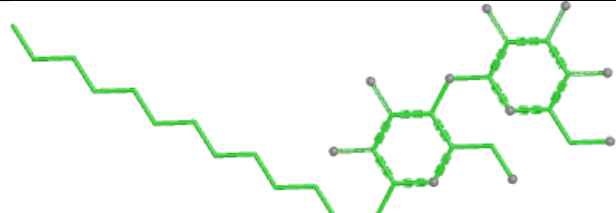
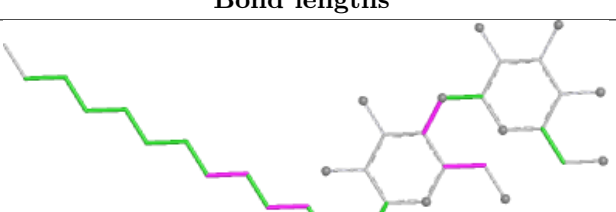
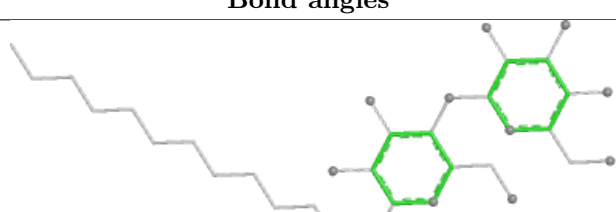


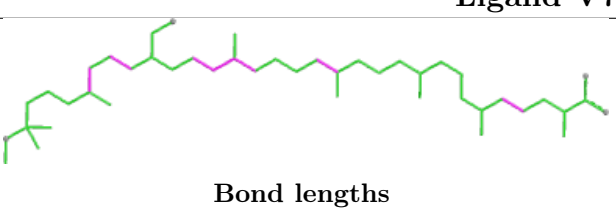
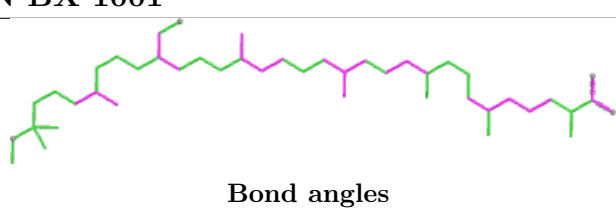
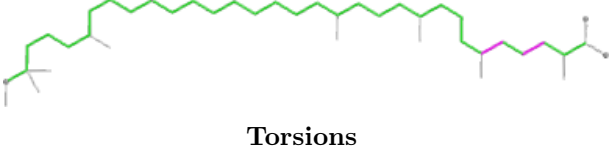





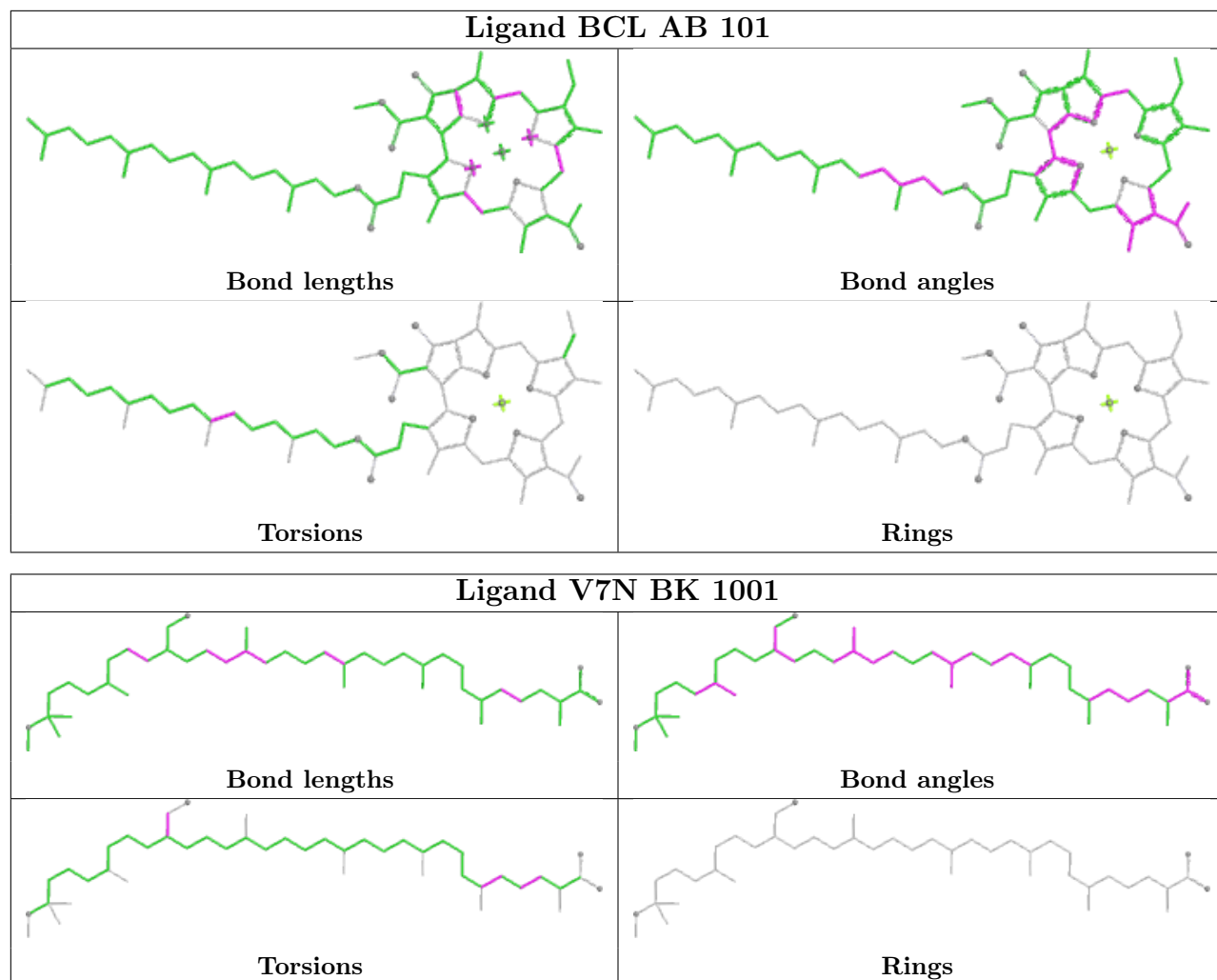


| Ligand BCL bd 103   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

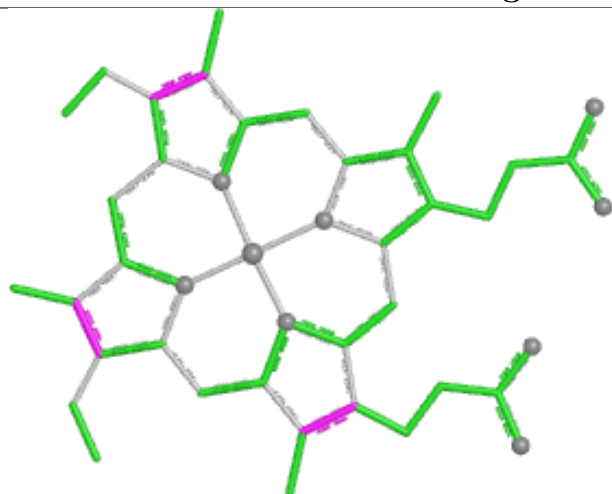
| Ligand LMT BN 1004  |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand V7N BX 1001  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

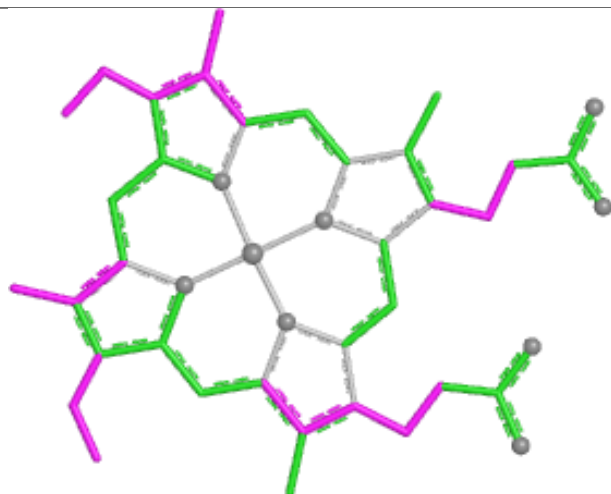




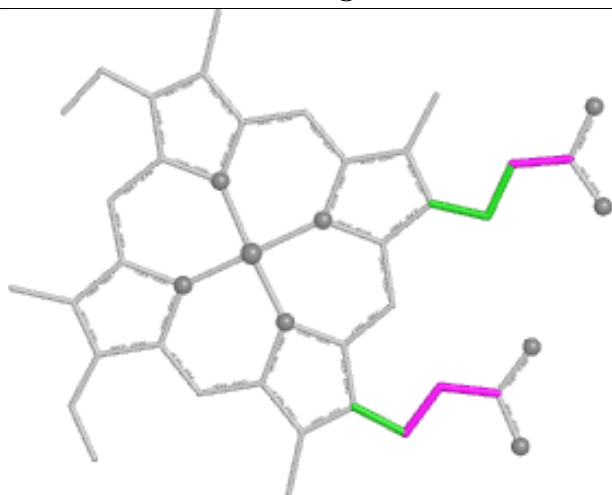
## Ligand HEC C 1001



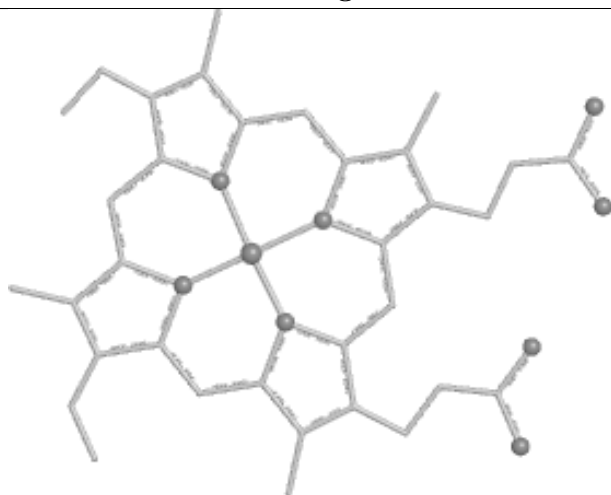
Bond lengths



Bond angles

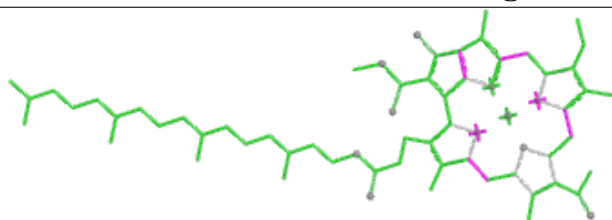


Torsions

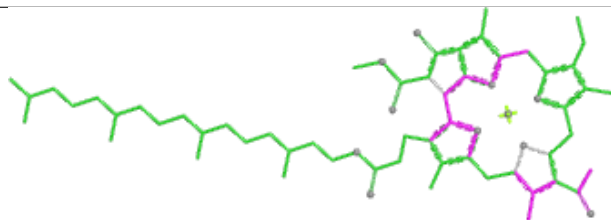


Rings

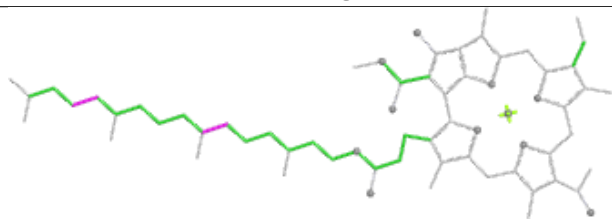
## Ligand BCL AV 102



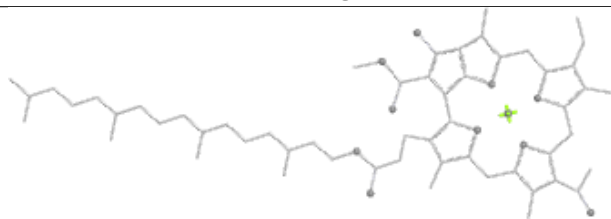
Bond lengths



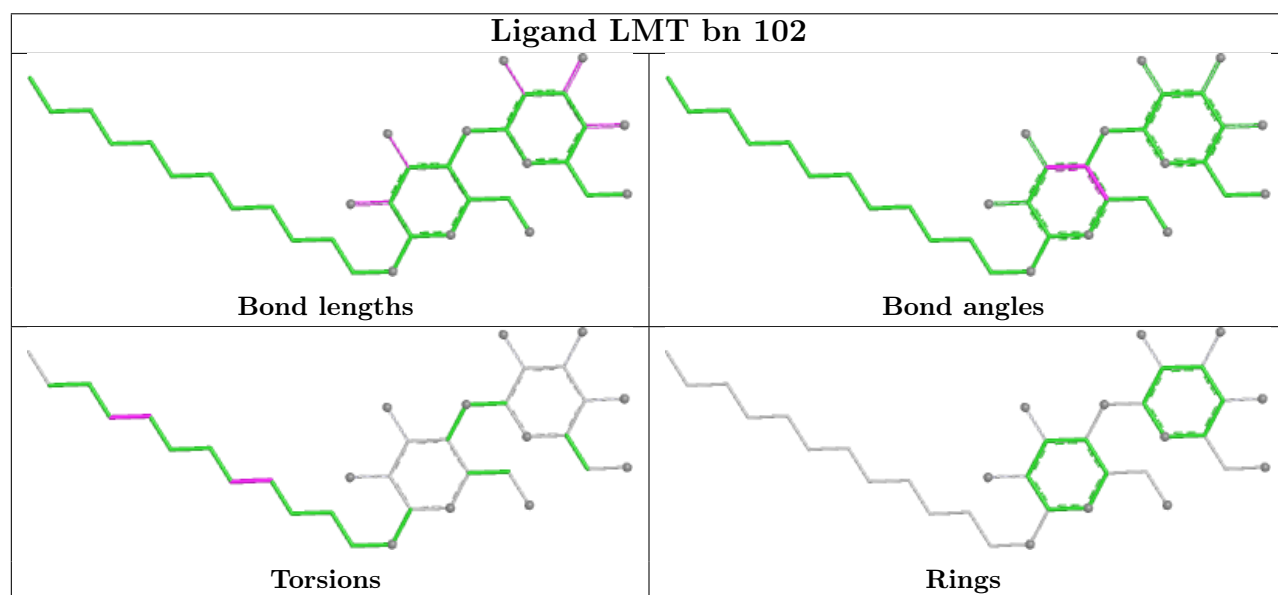
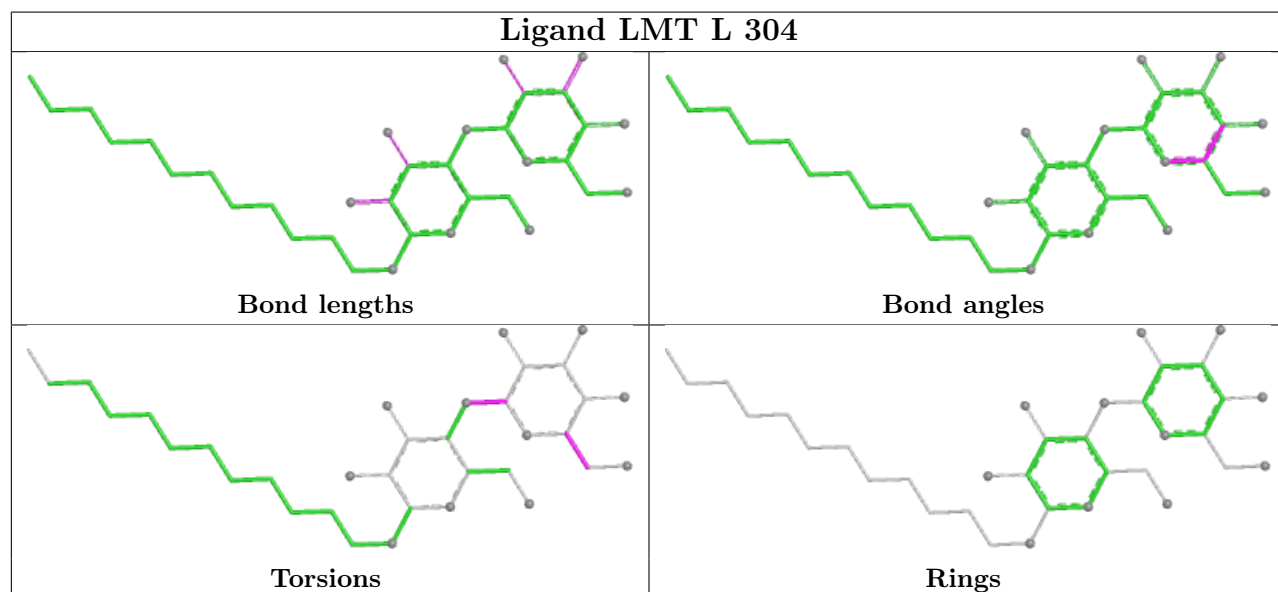
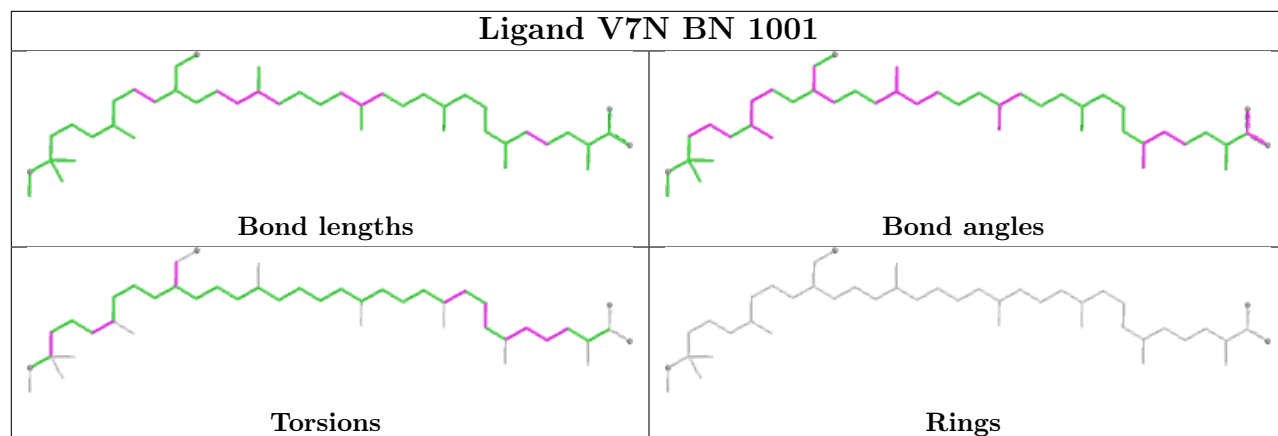
Bond angles

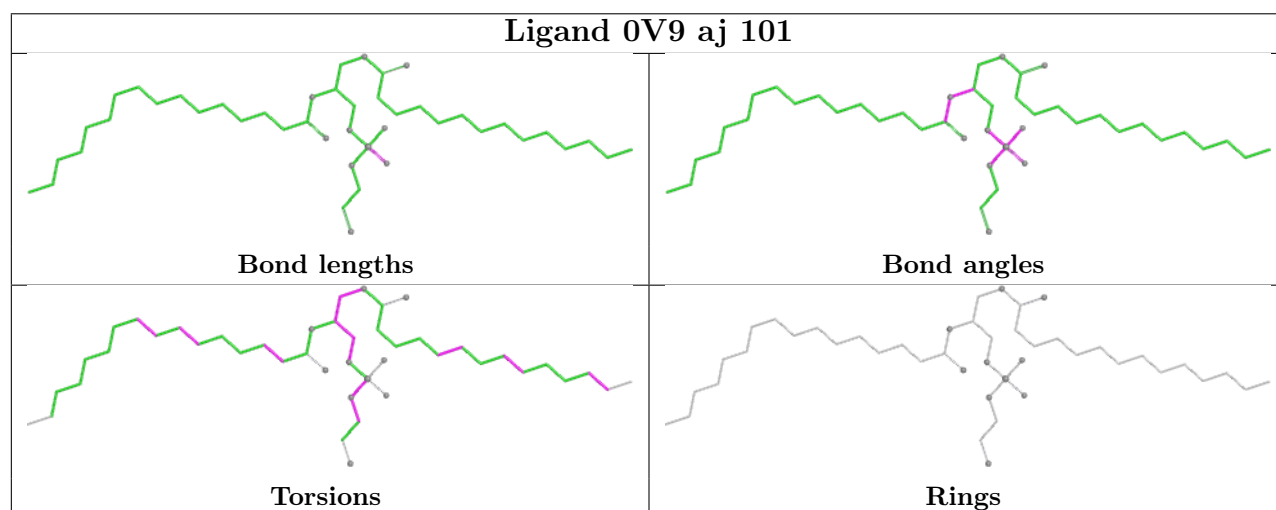
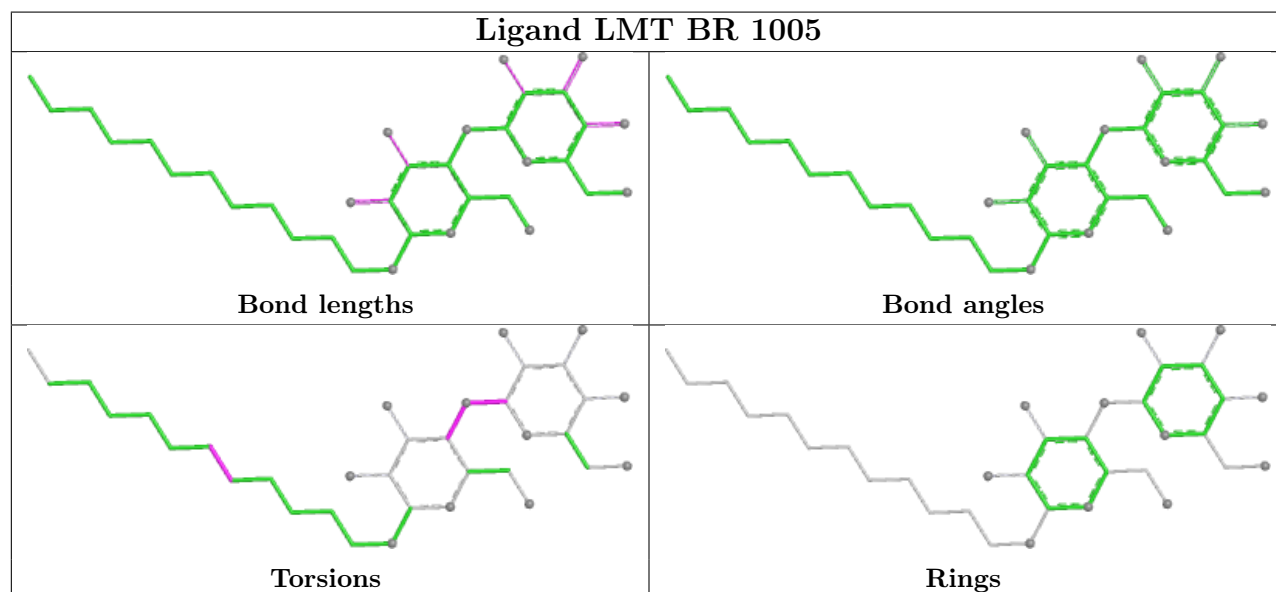
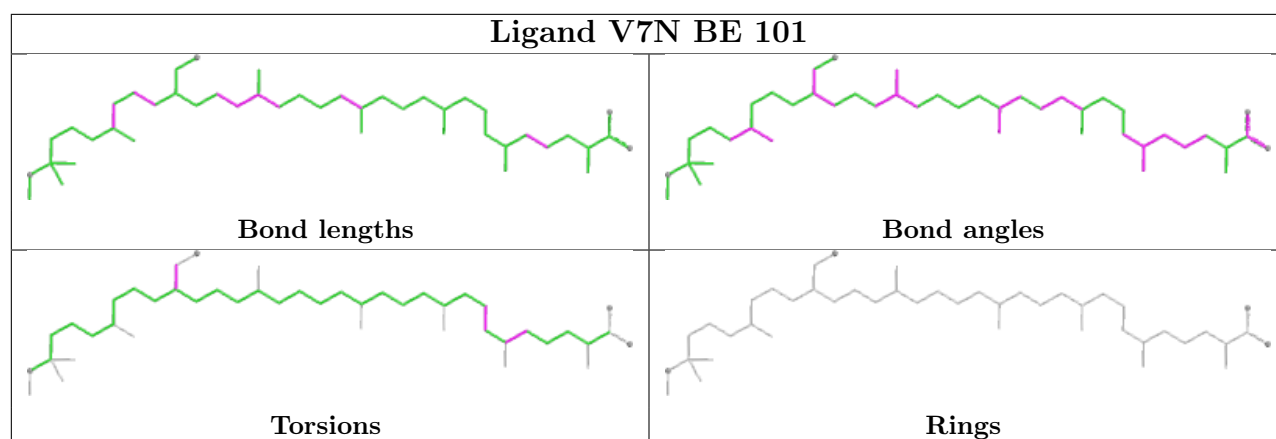


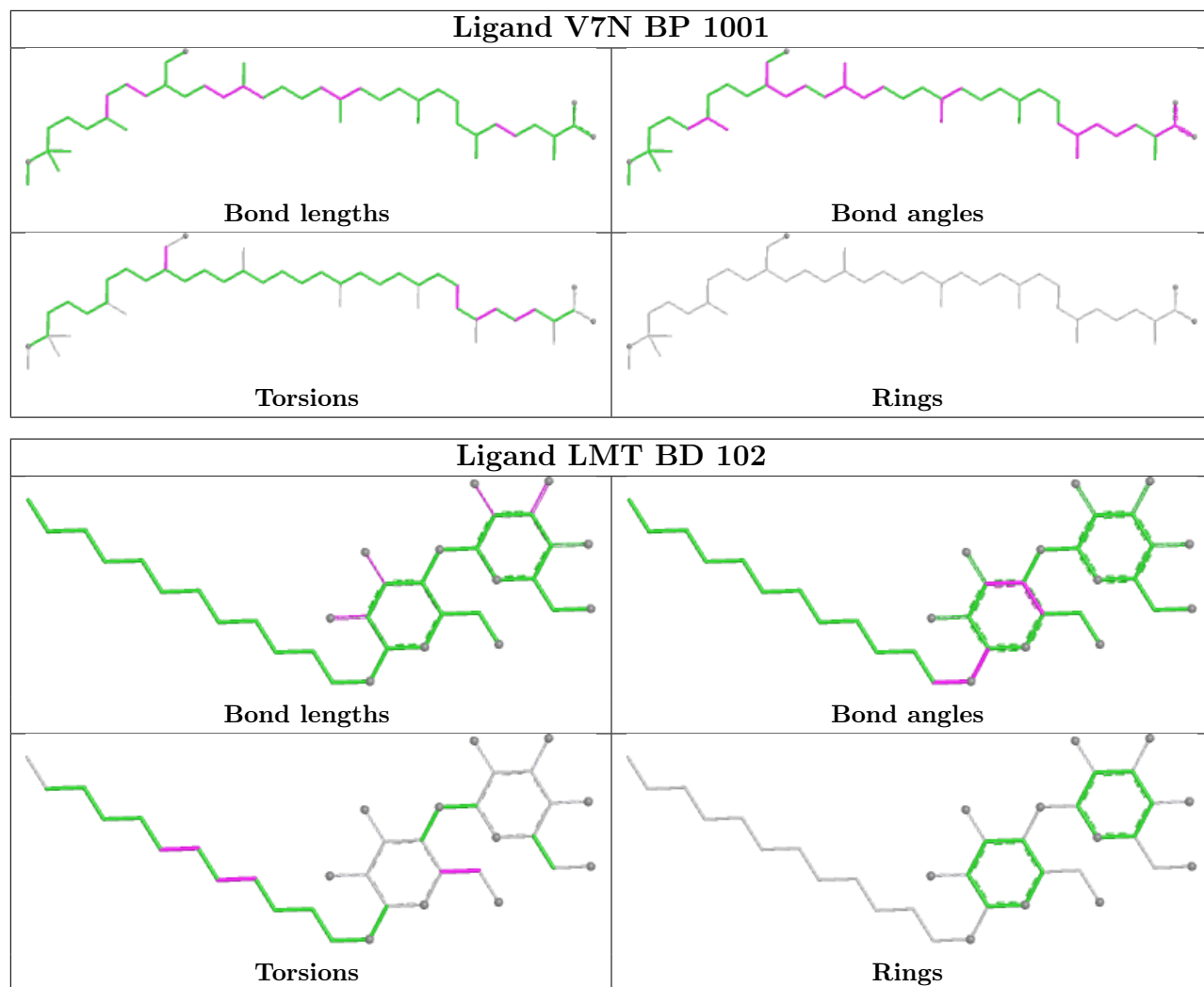
Torsions

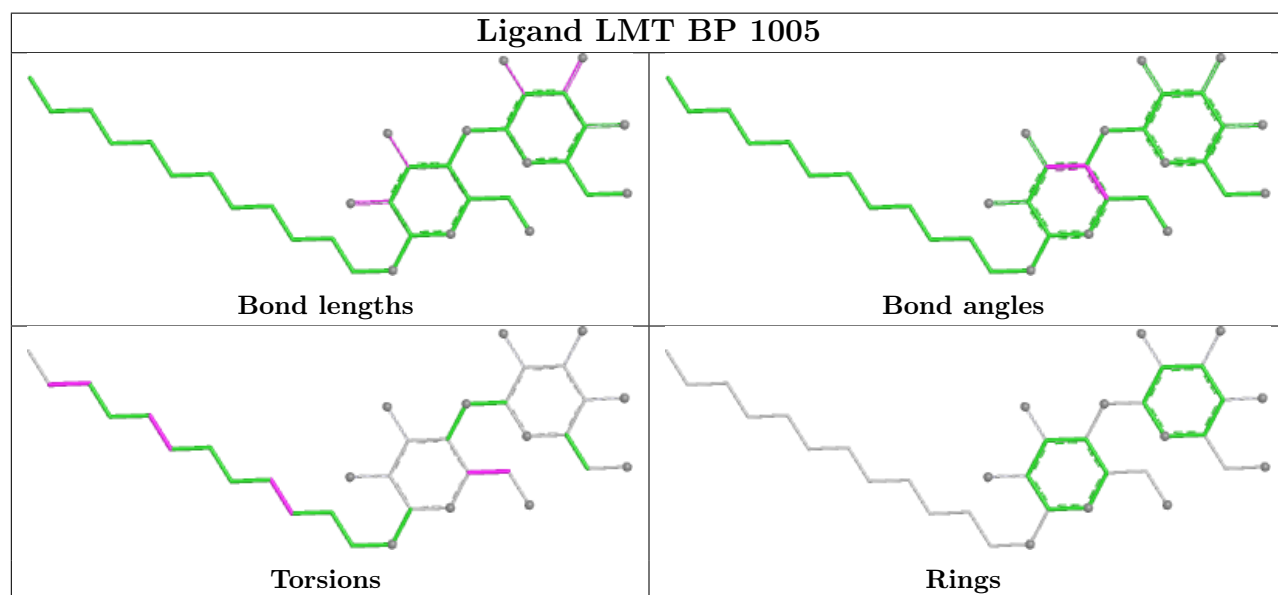
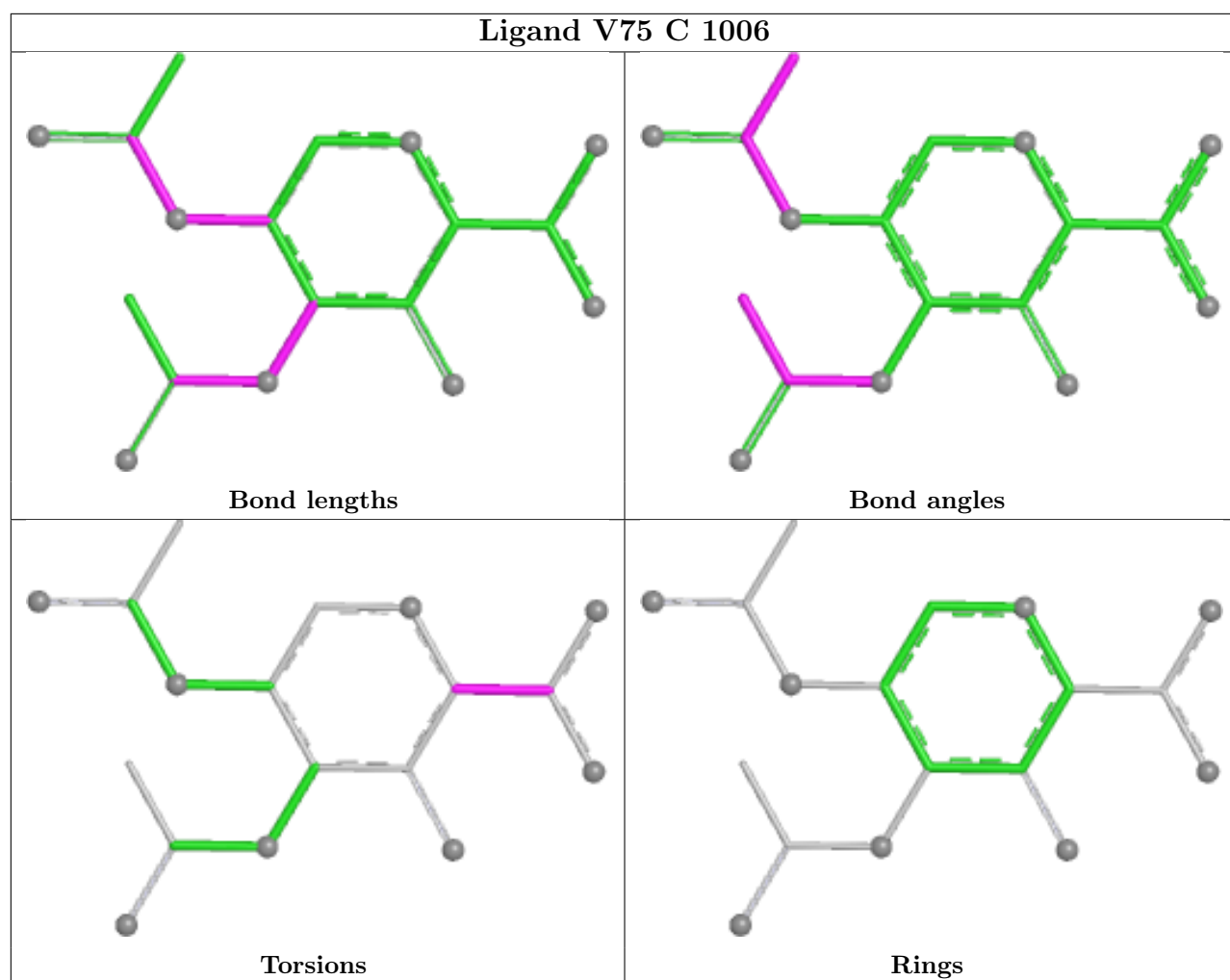


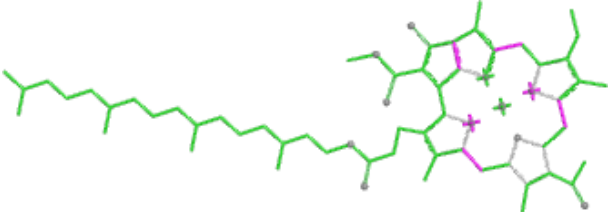
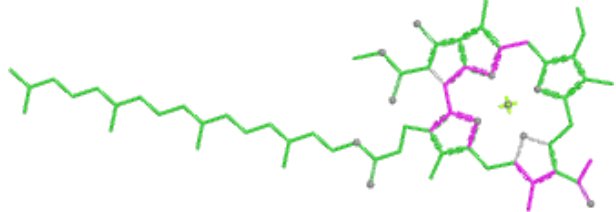
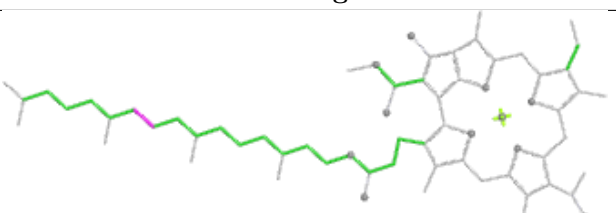
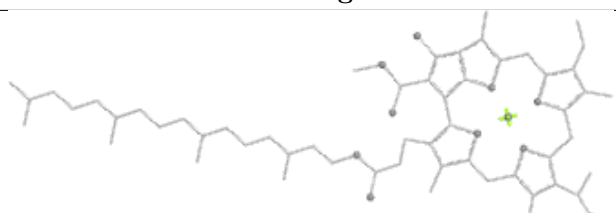
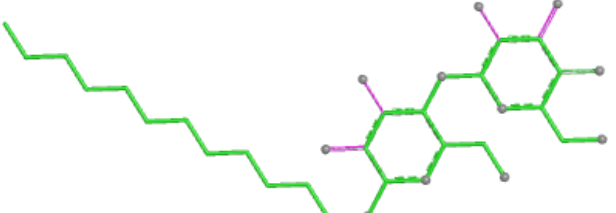
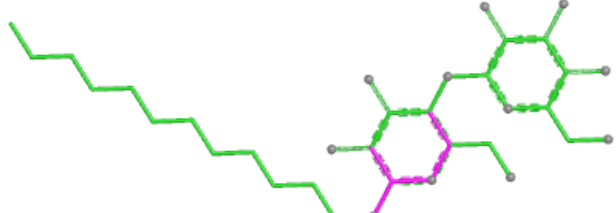
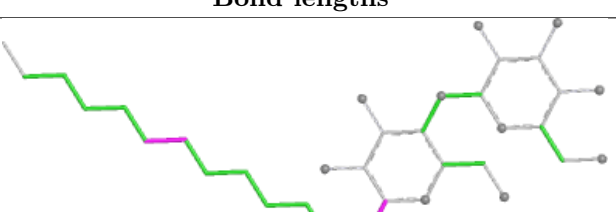
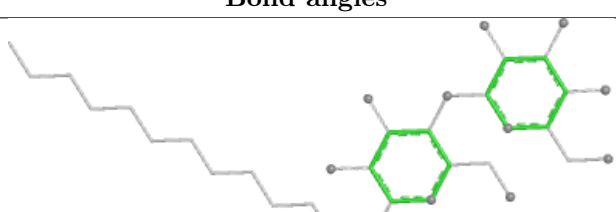
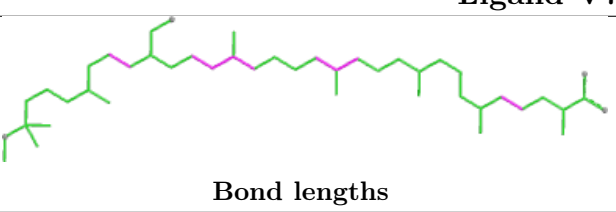
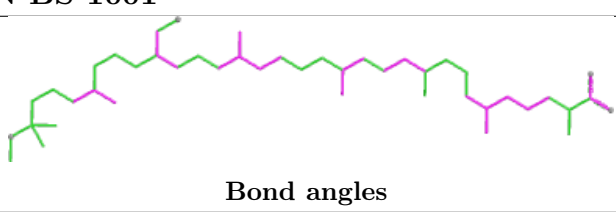
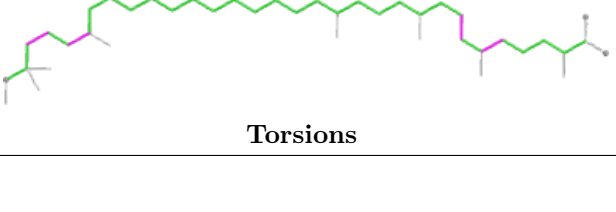
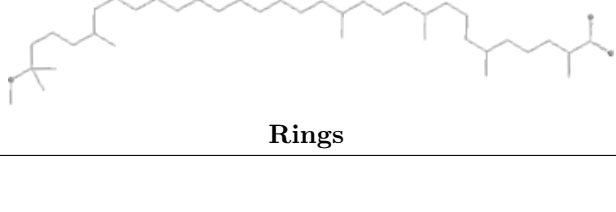
Rings

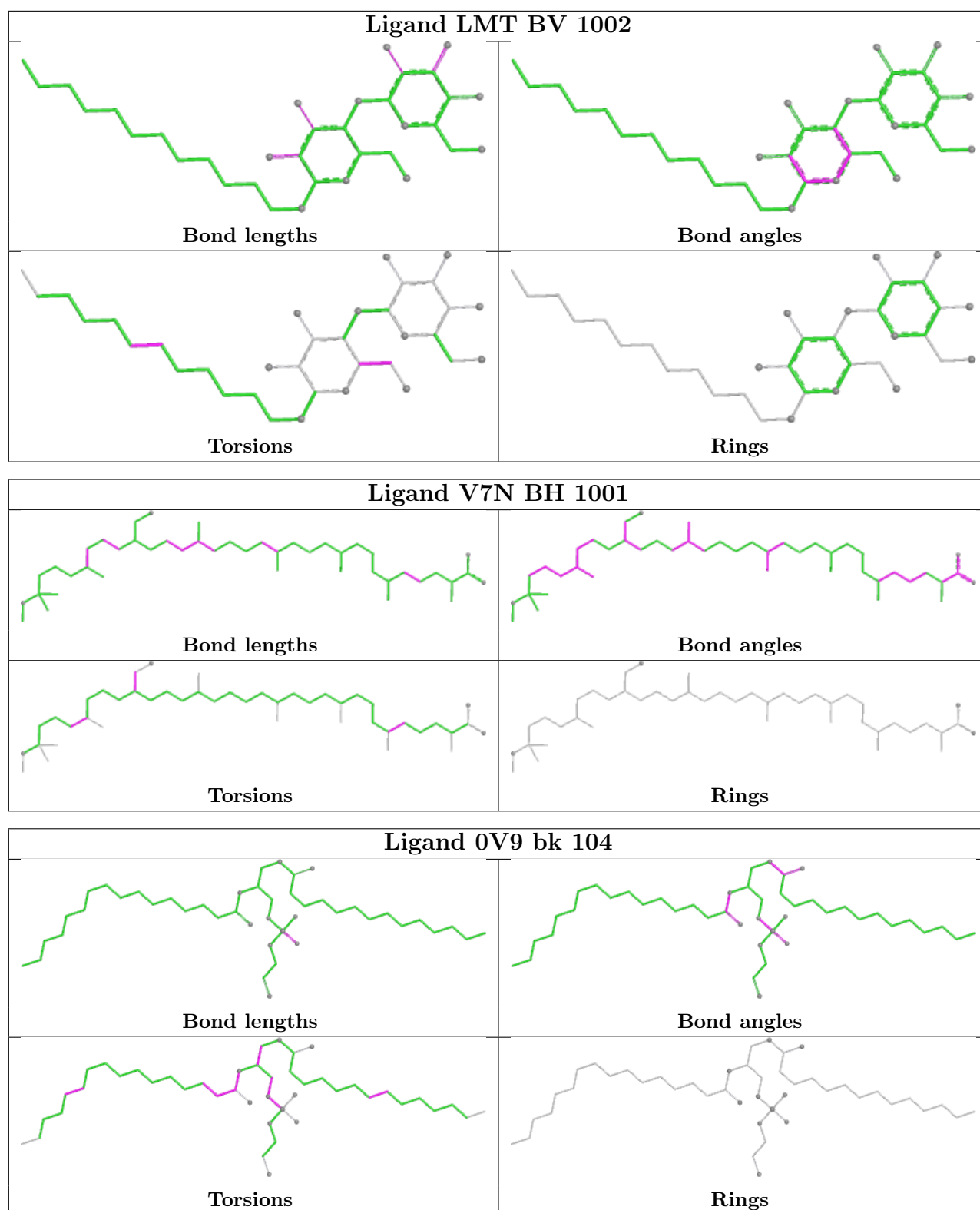




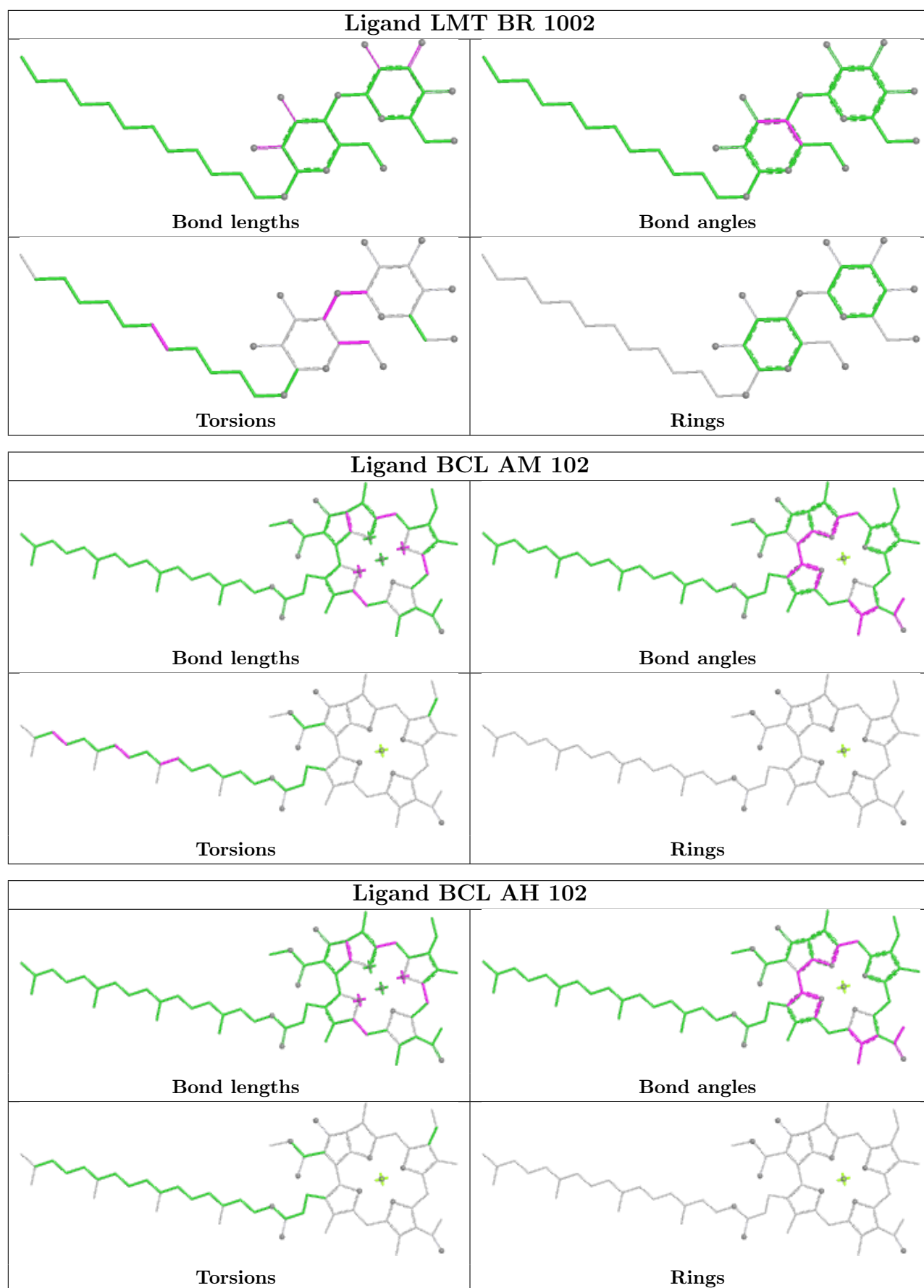


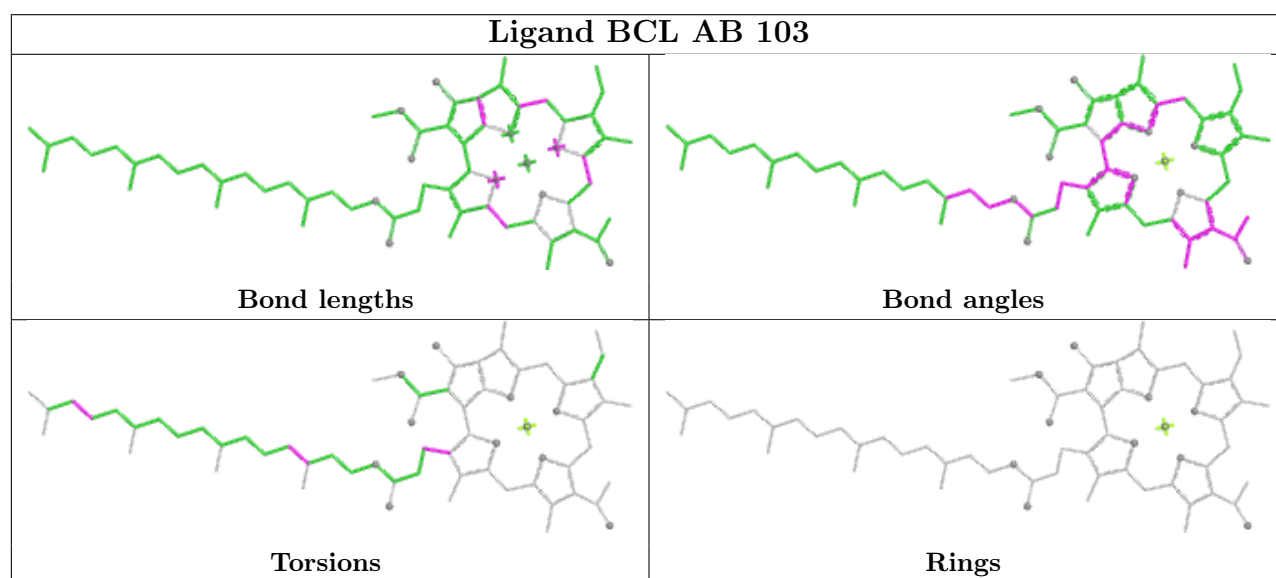
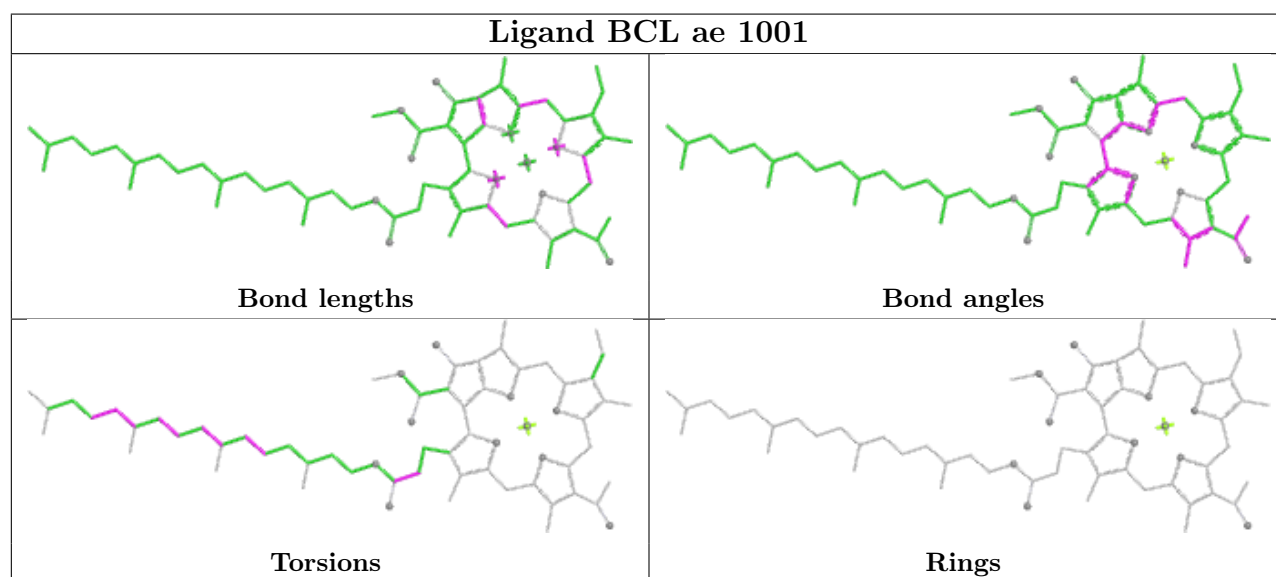
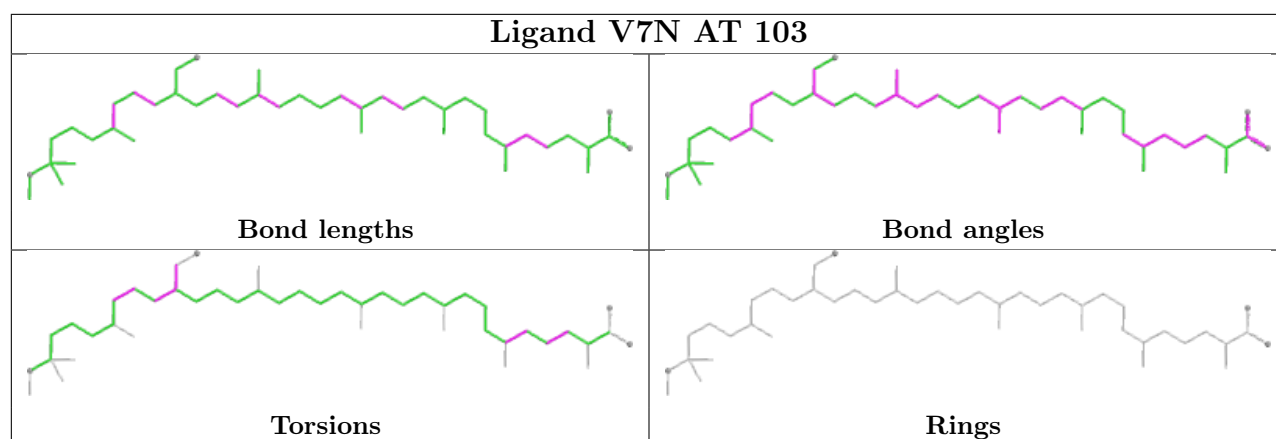


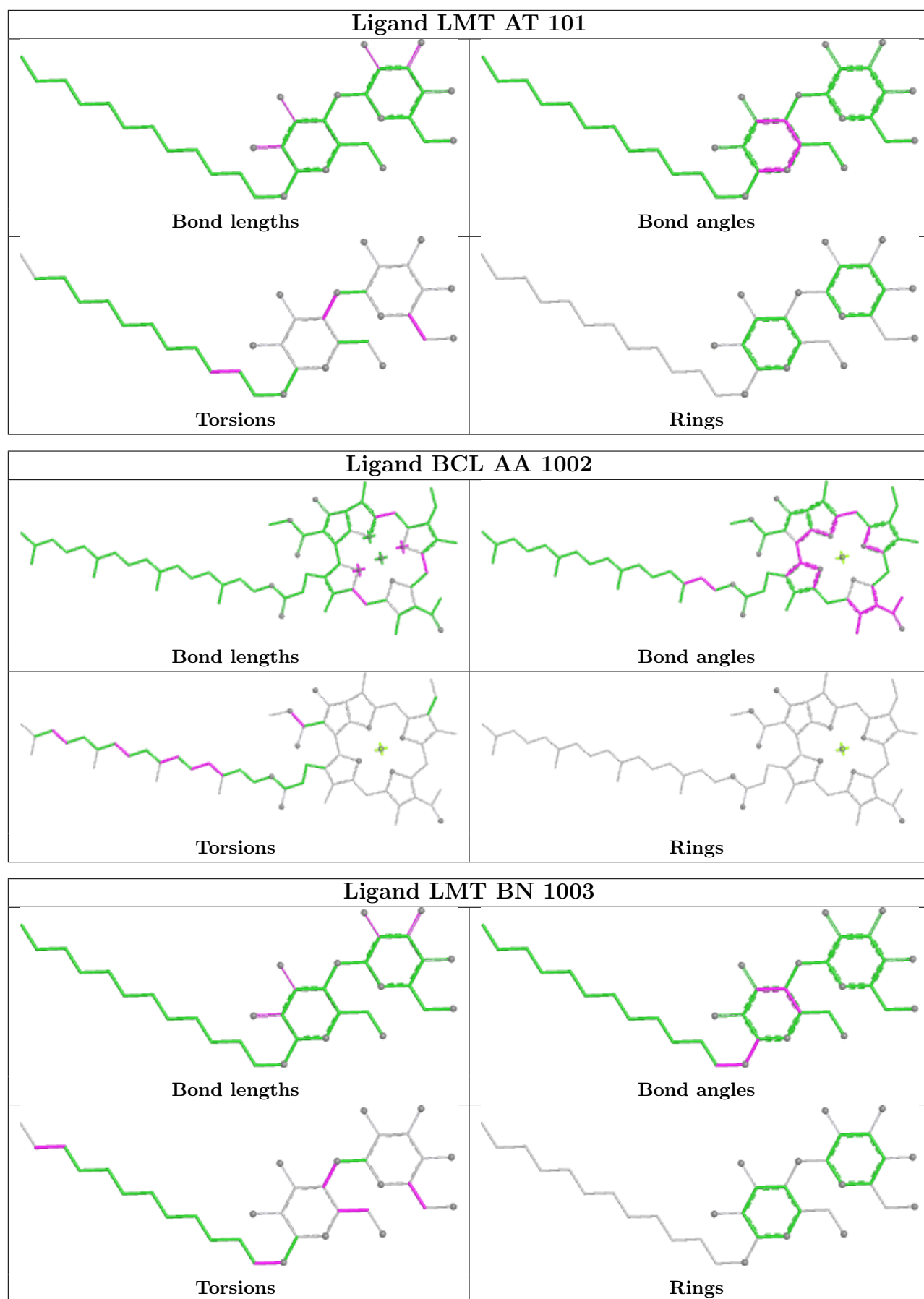
| Ligand BCL AT 102   |   |
|---|---|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand LMT AH 106   |   |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand V7N BS 1001  |   |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

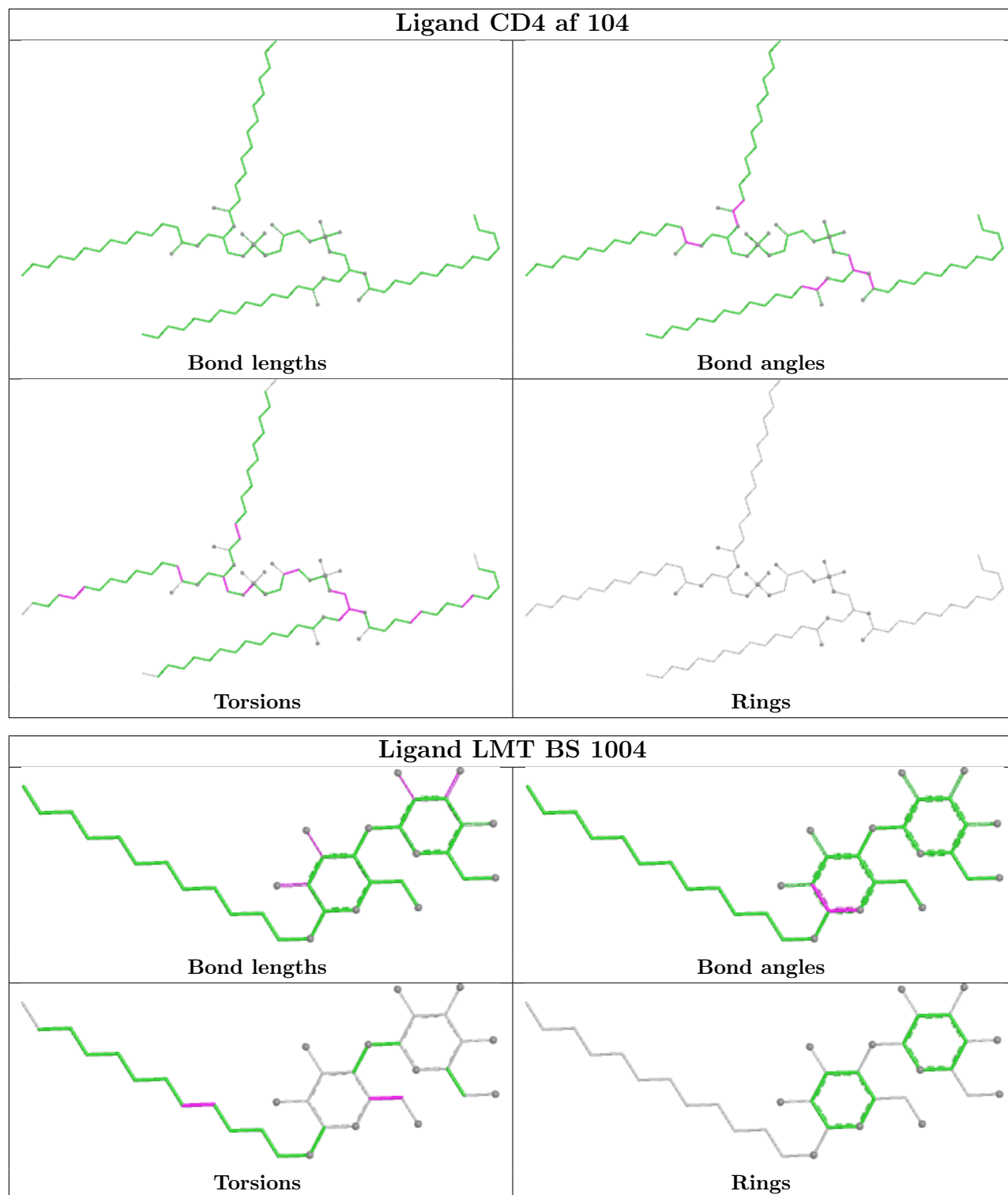


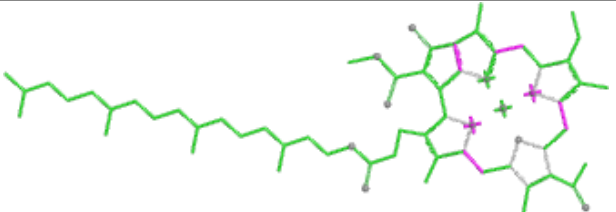
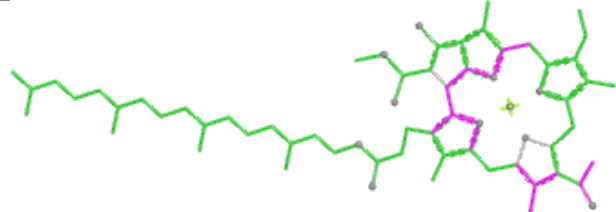
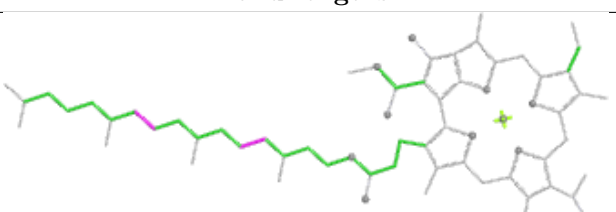
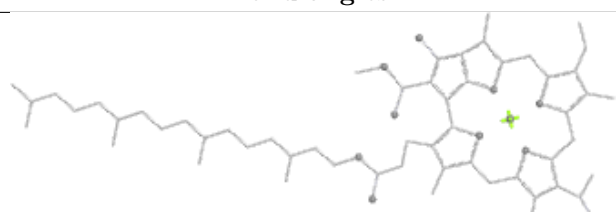


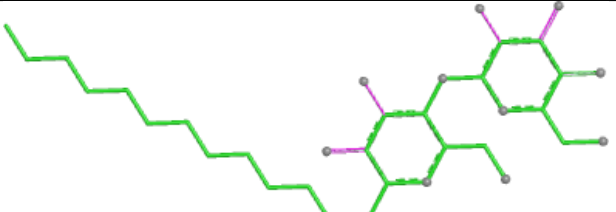
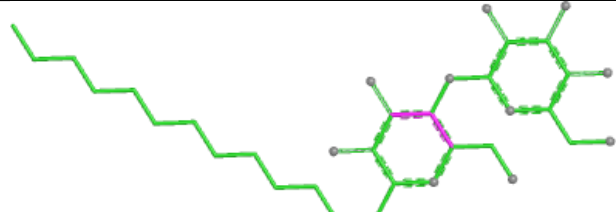
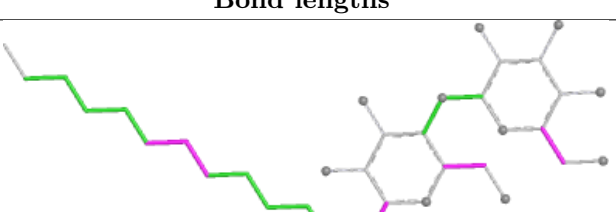
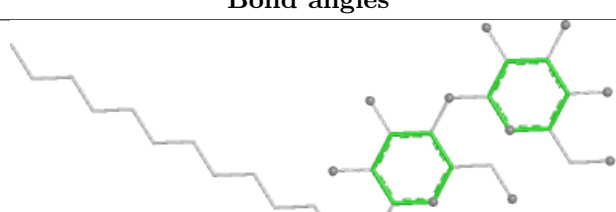




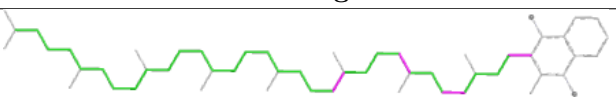
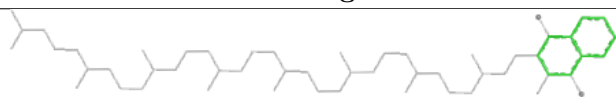


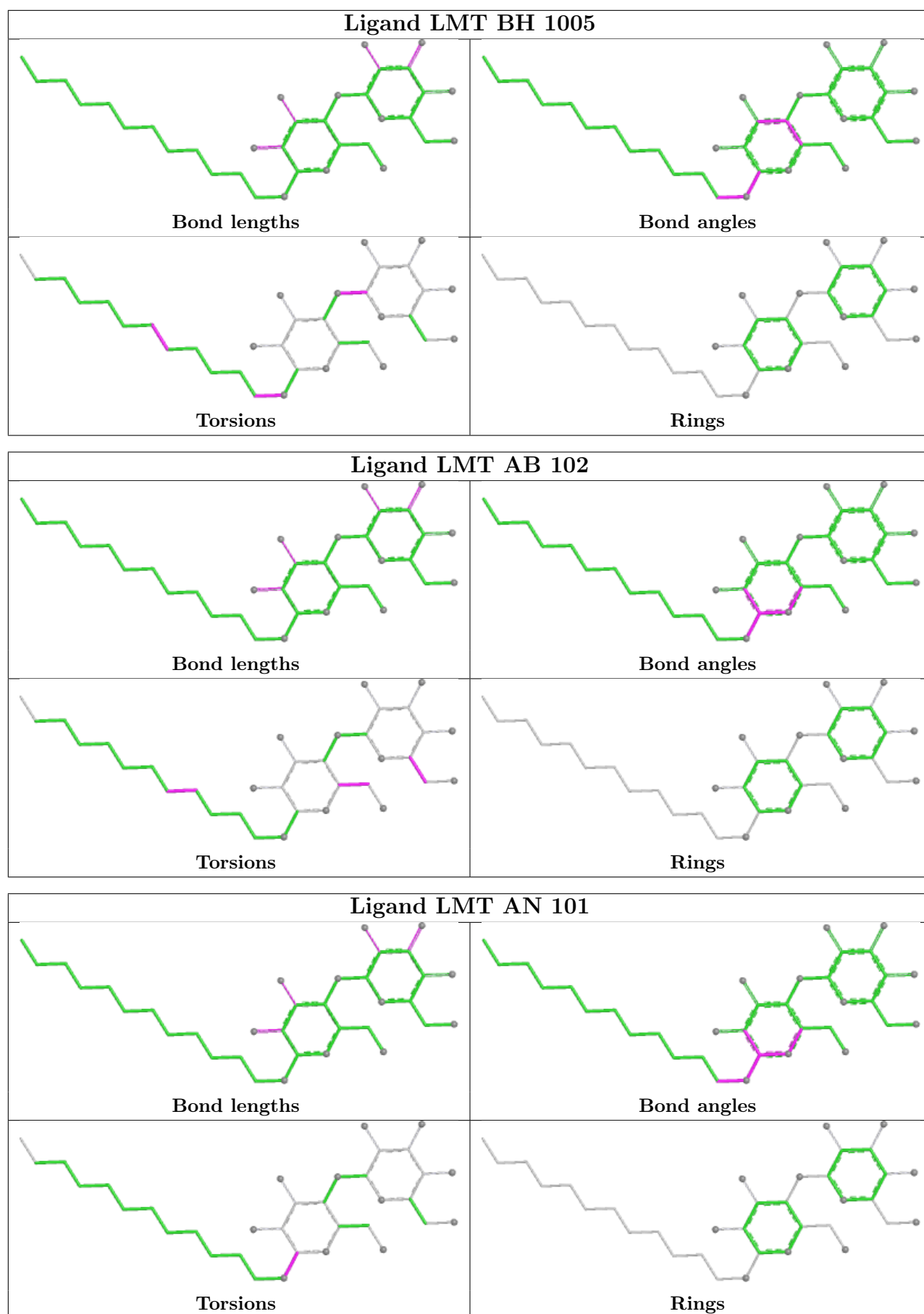


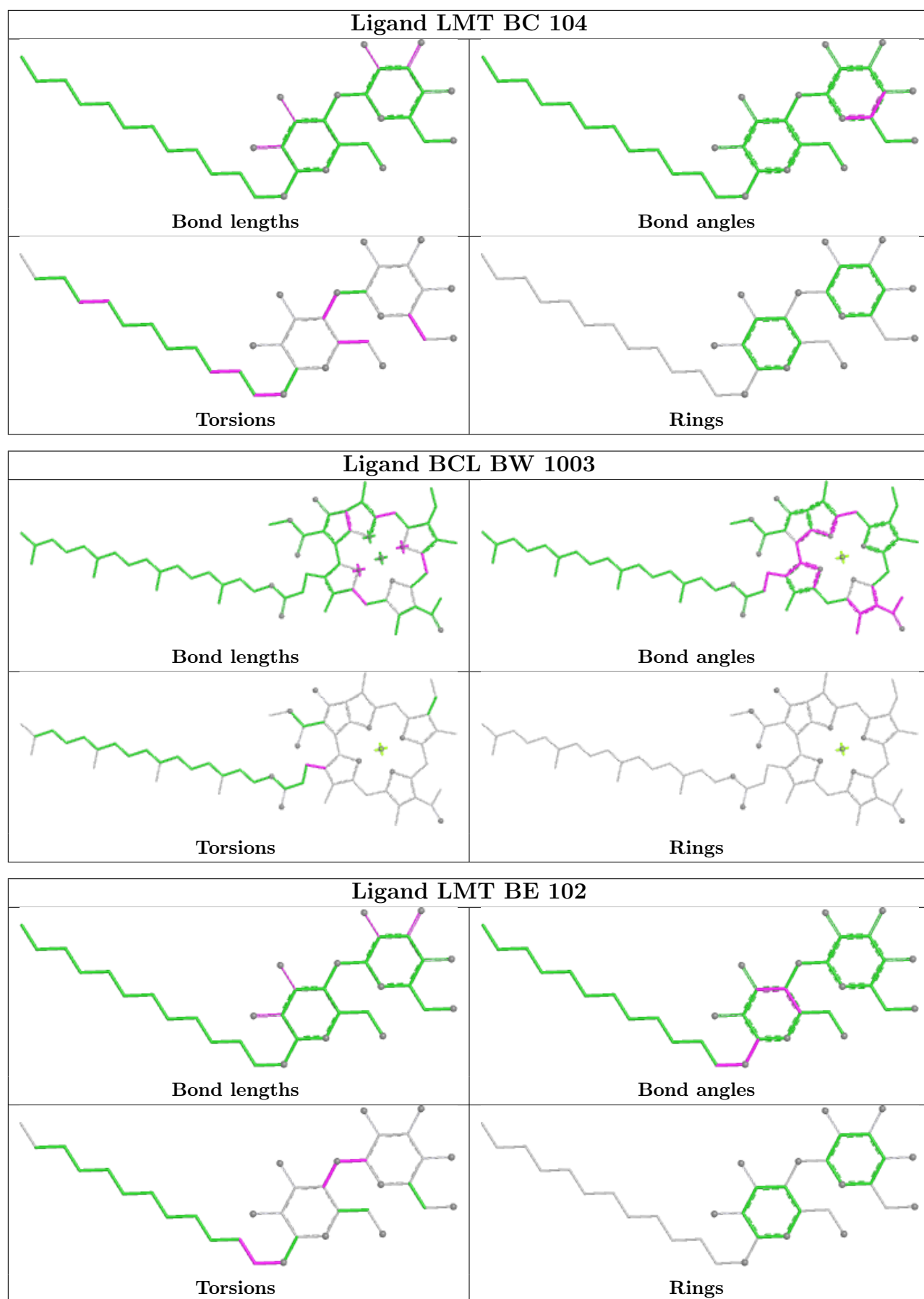


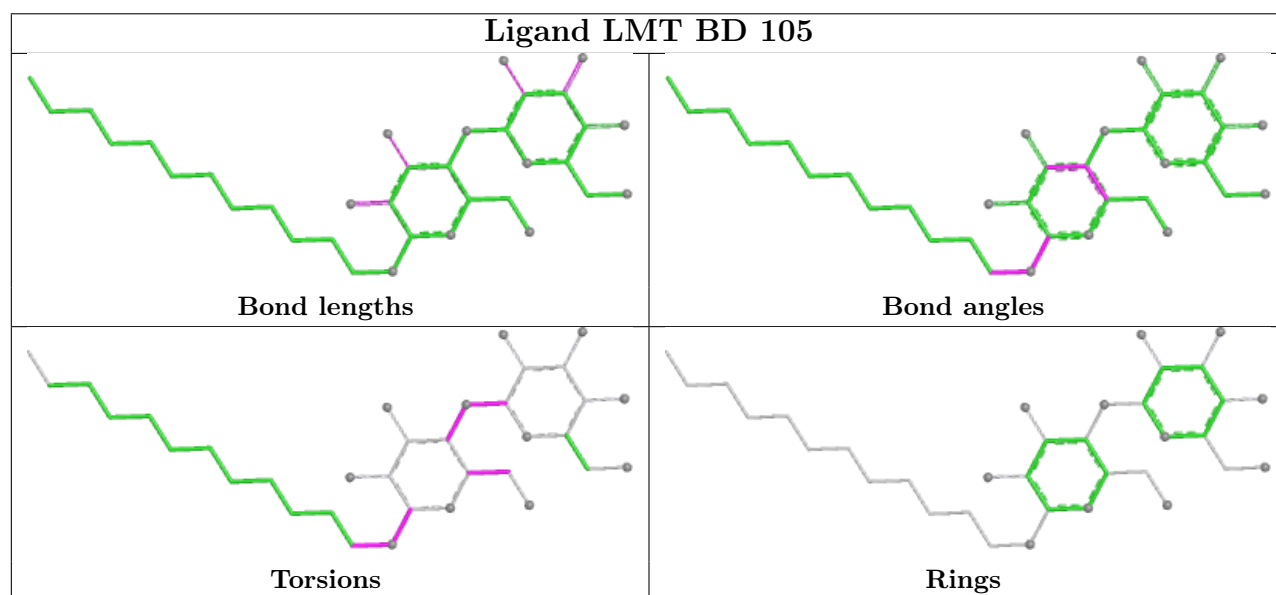
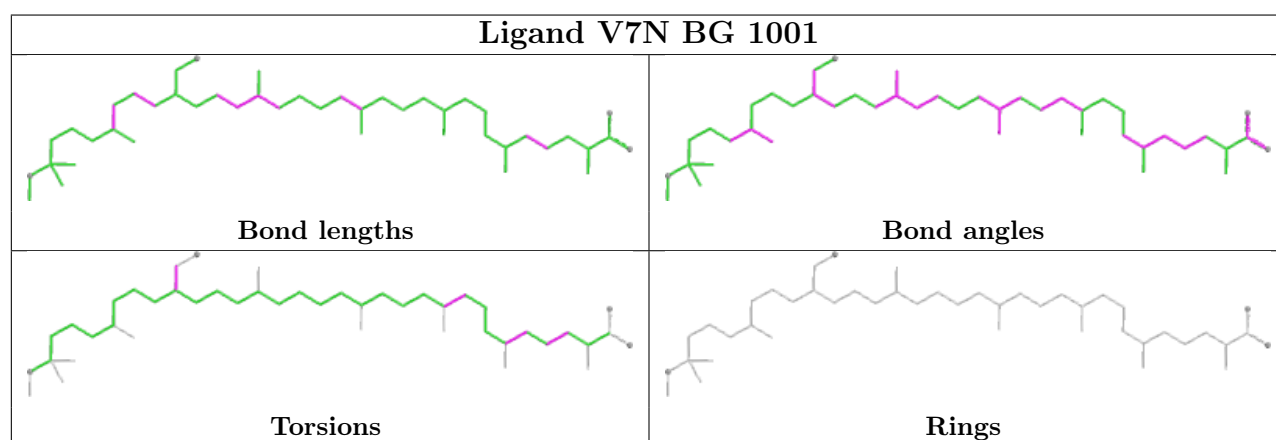
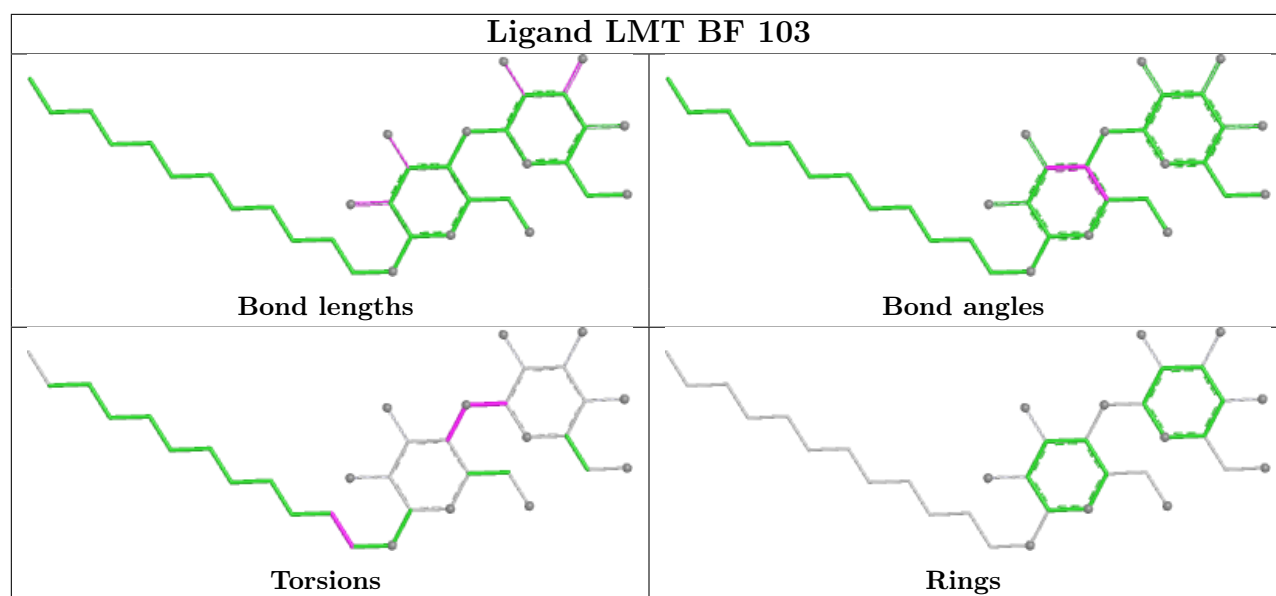
| Ligand BCL AU 103   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand LMT bd 102   |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

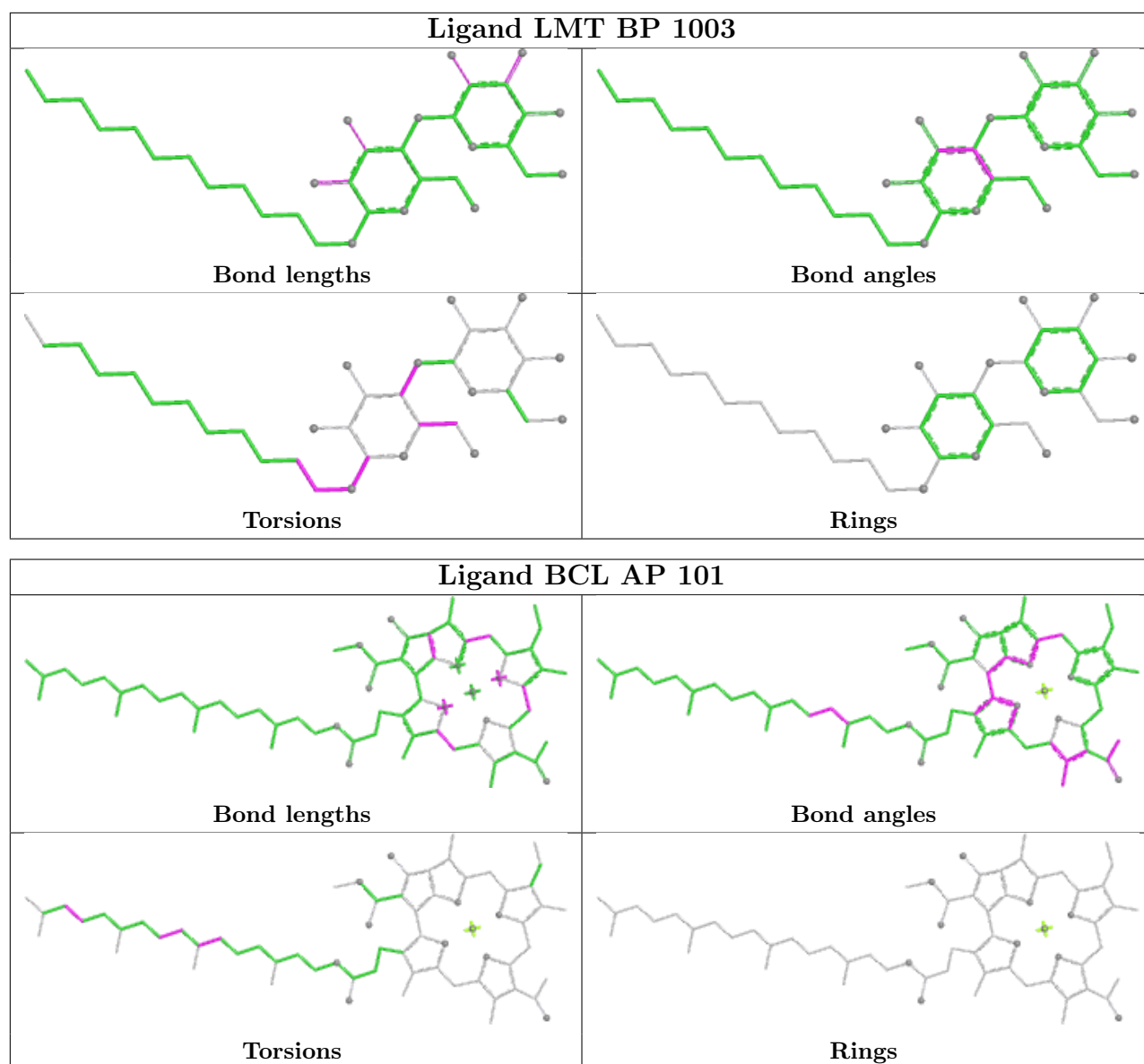
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|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

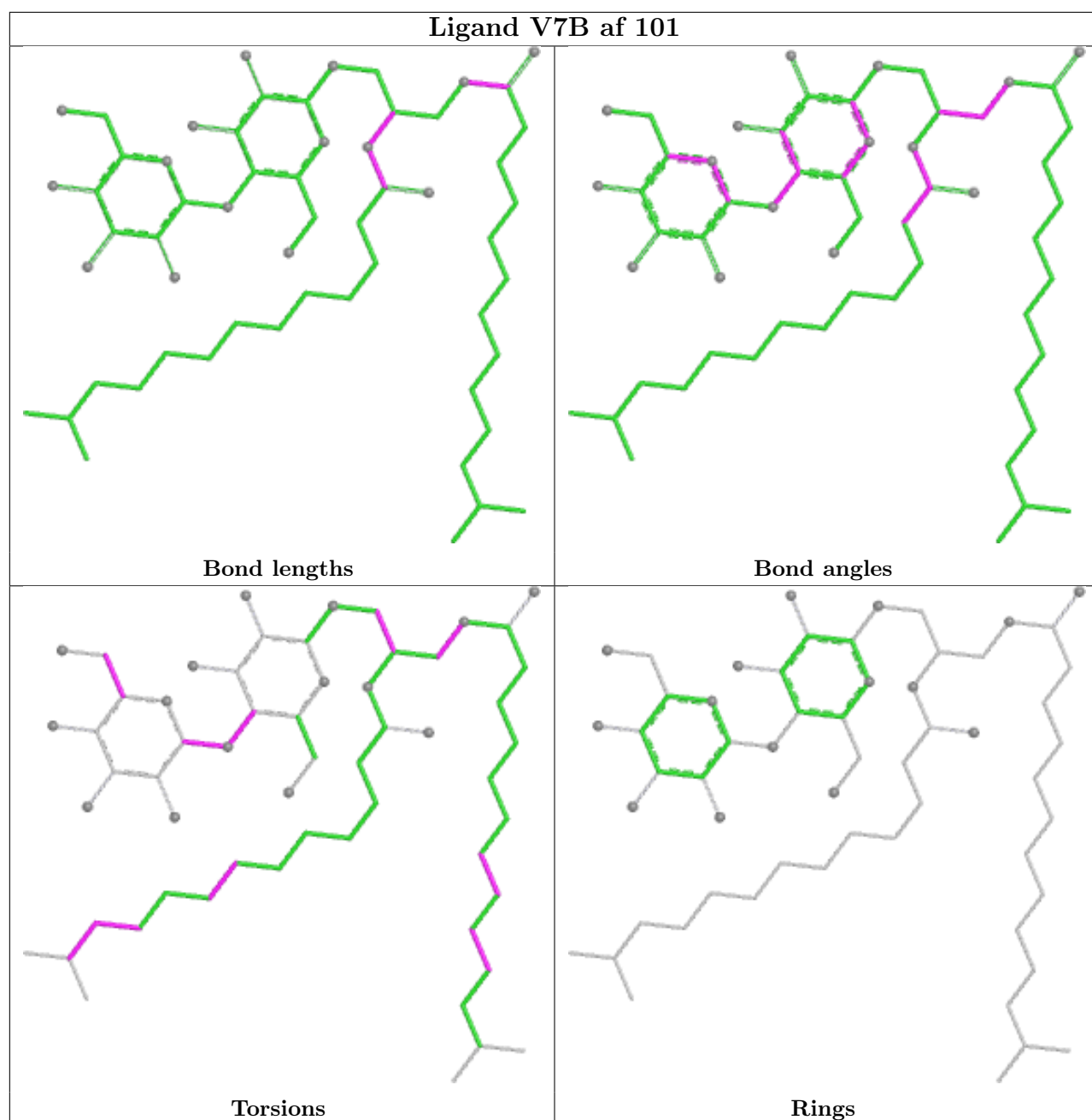


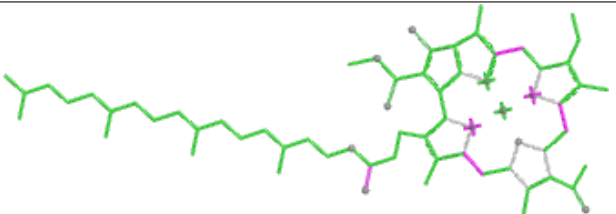
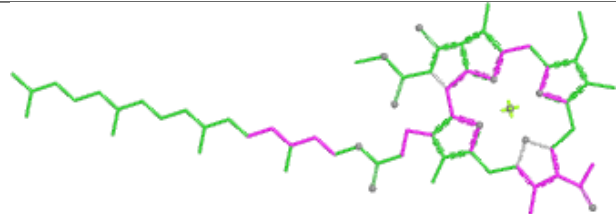
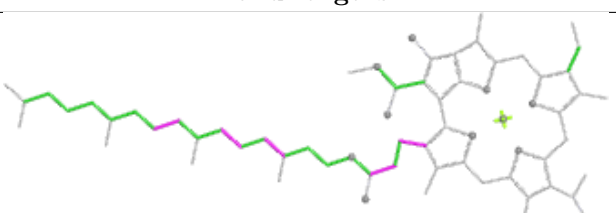
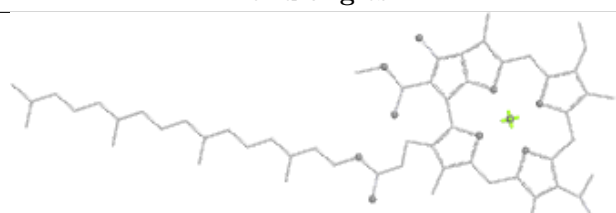


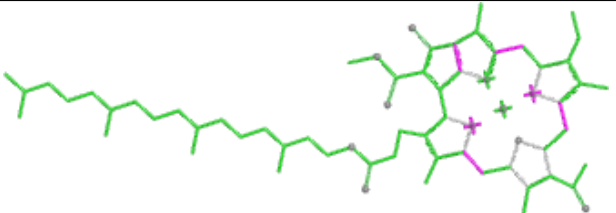
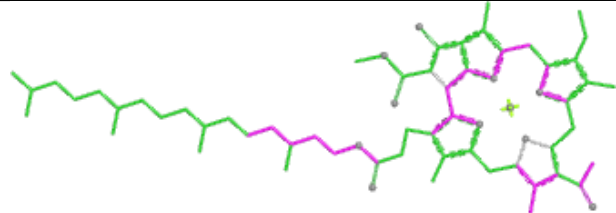
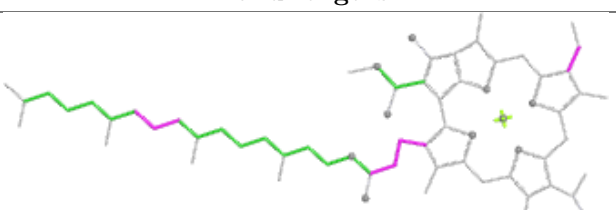
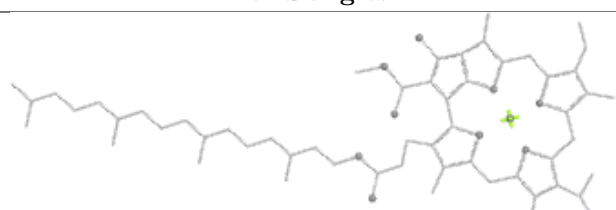


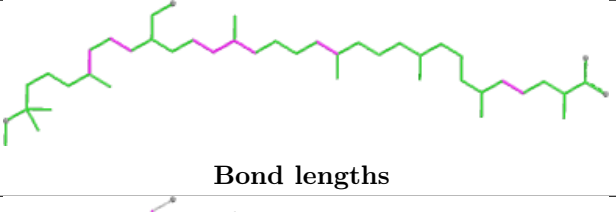
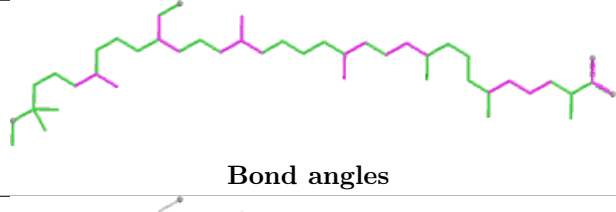




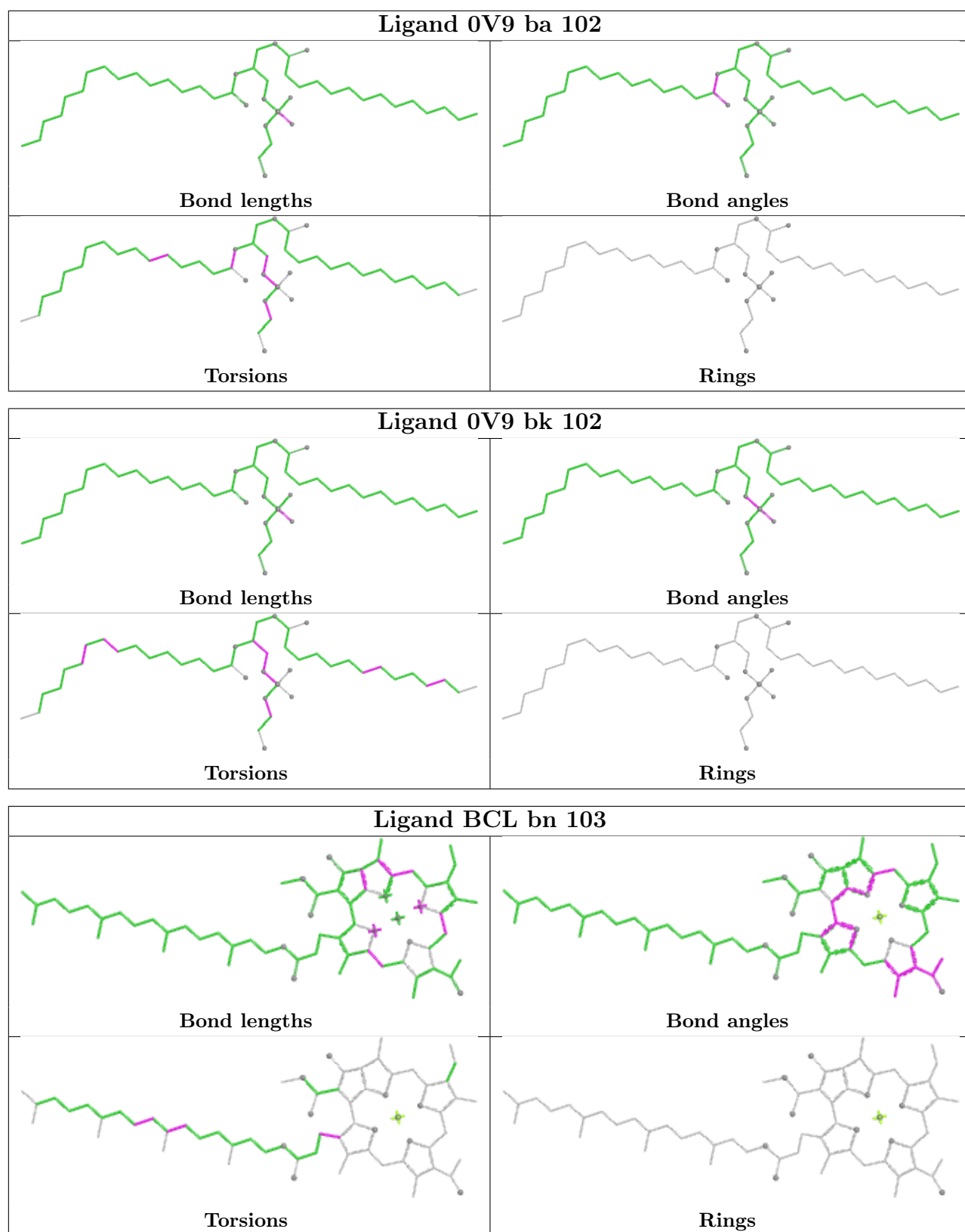


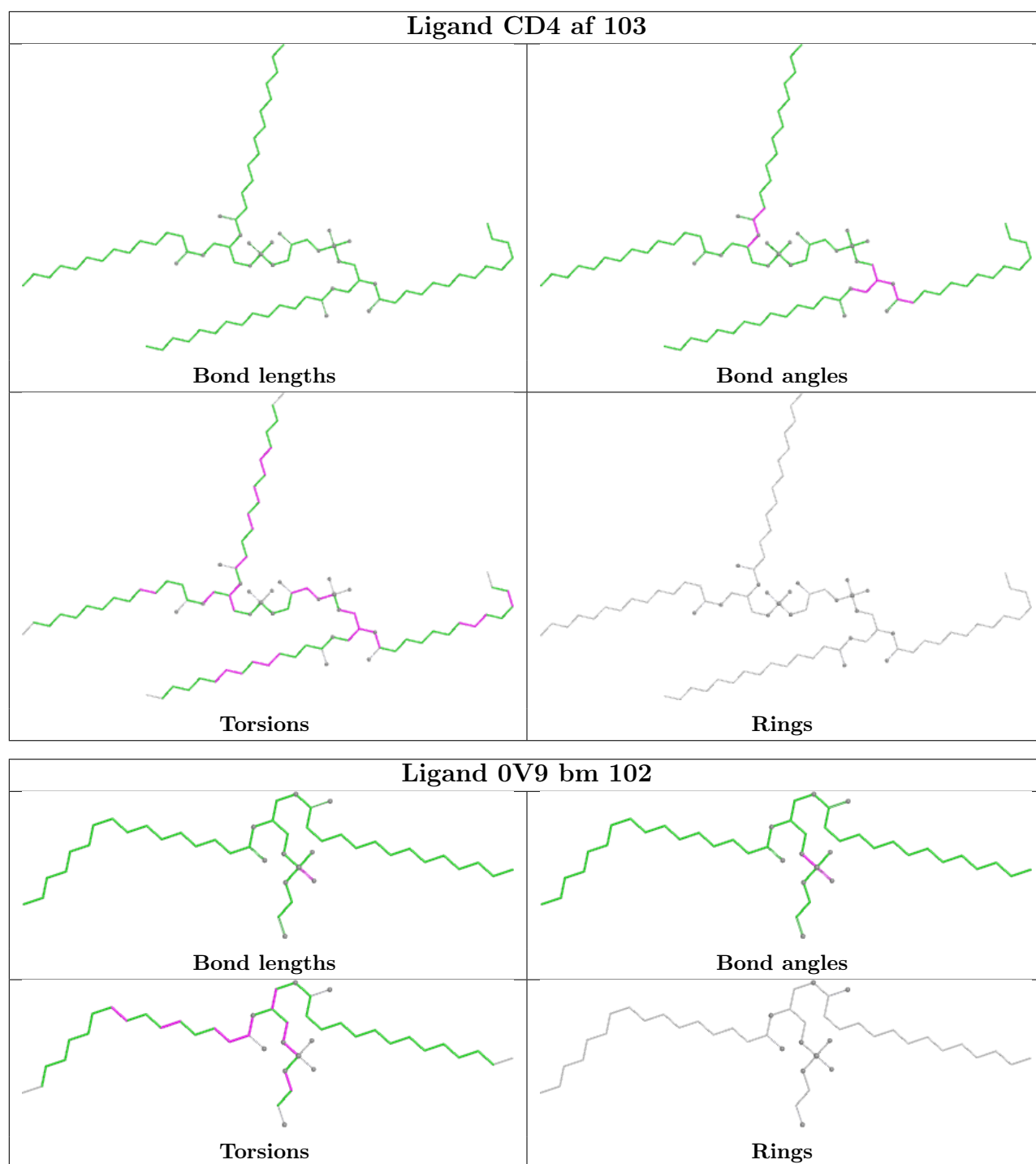


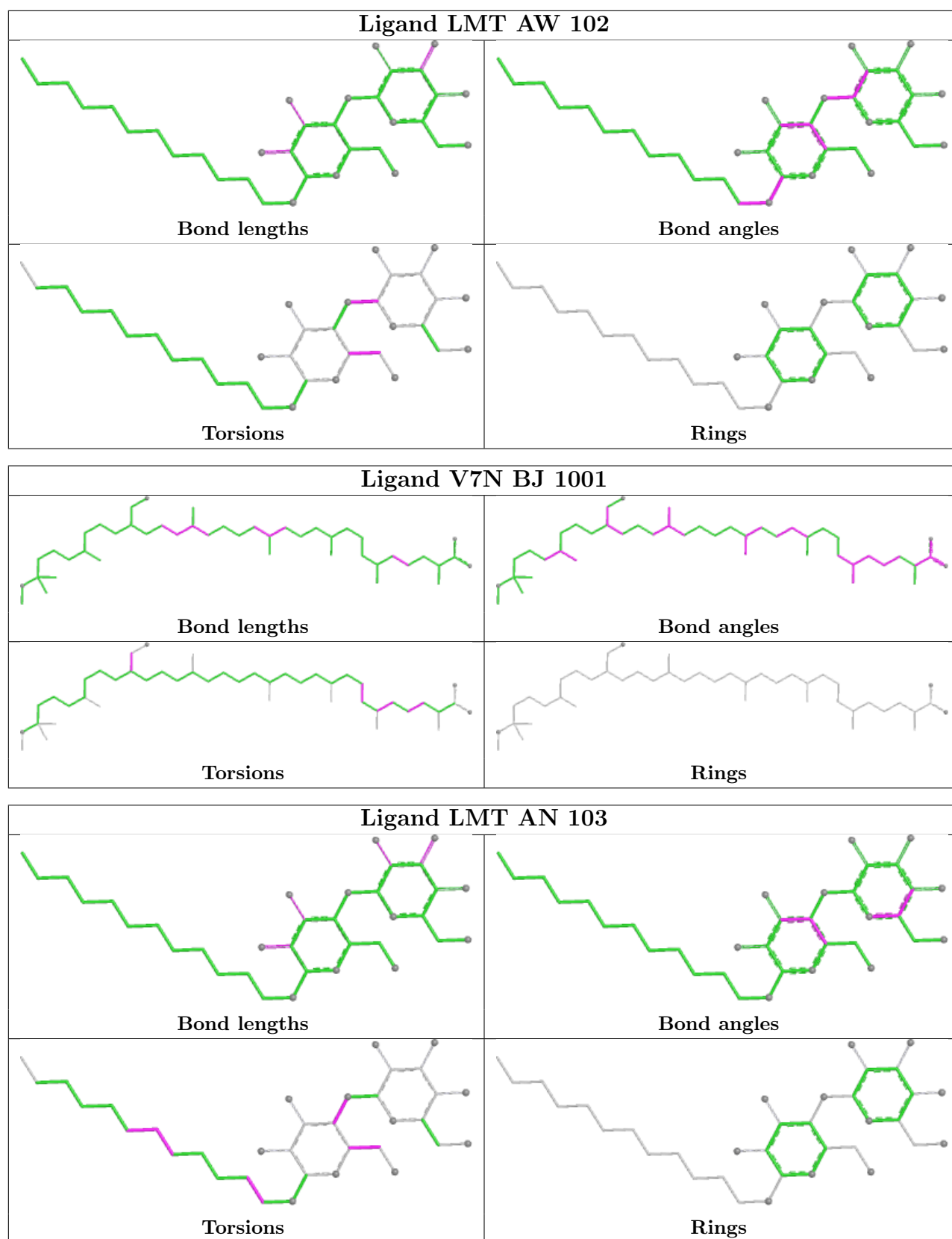
| Ligand BCL AM 101   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

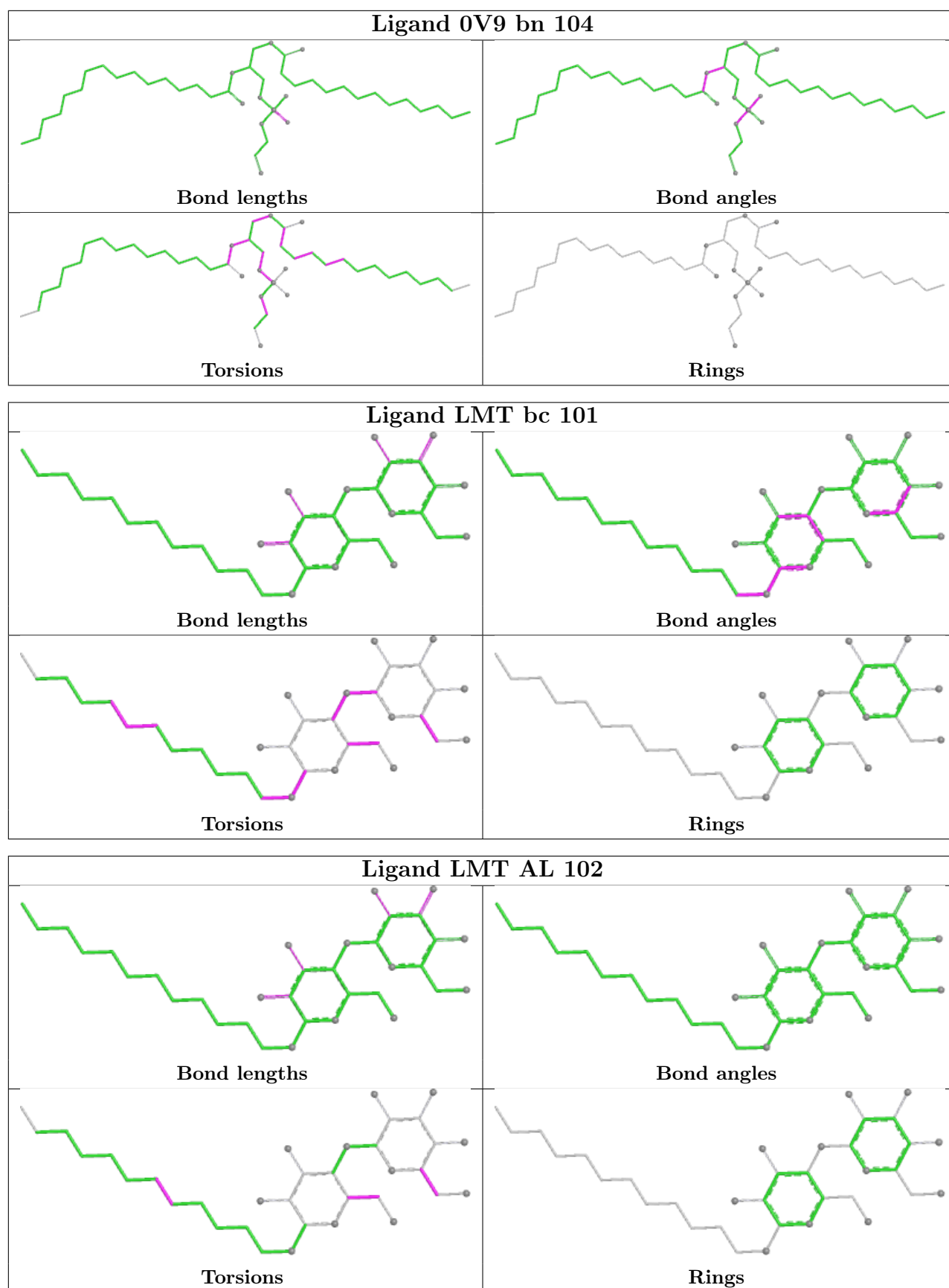
| Ligand BCL AH 101   |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

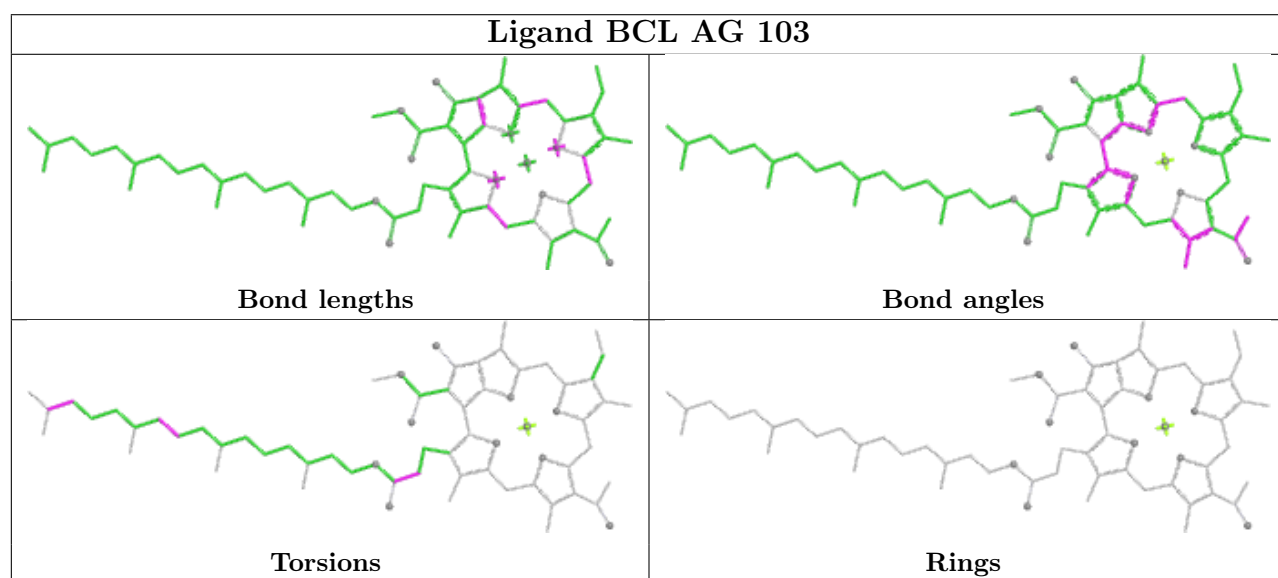
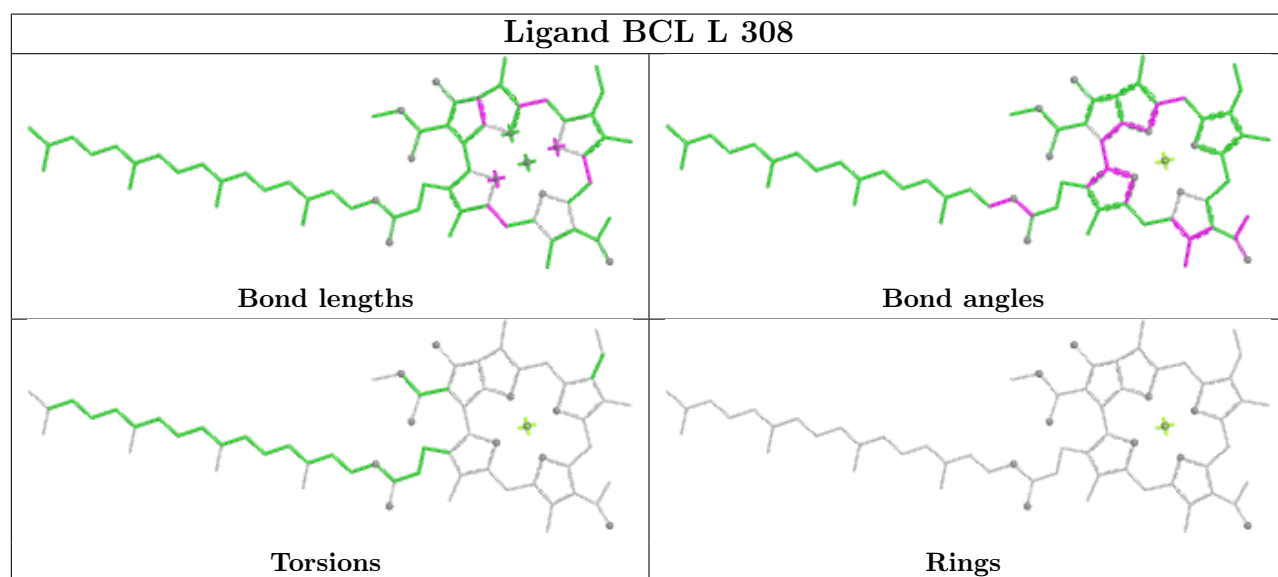
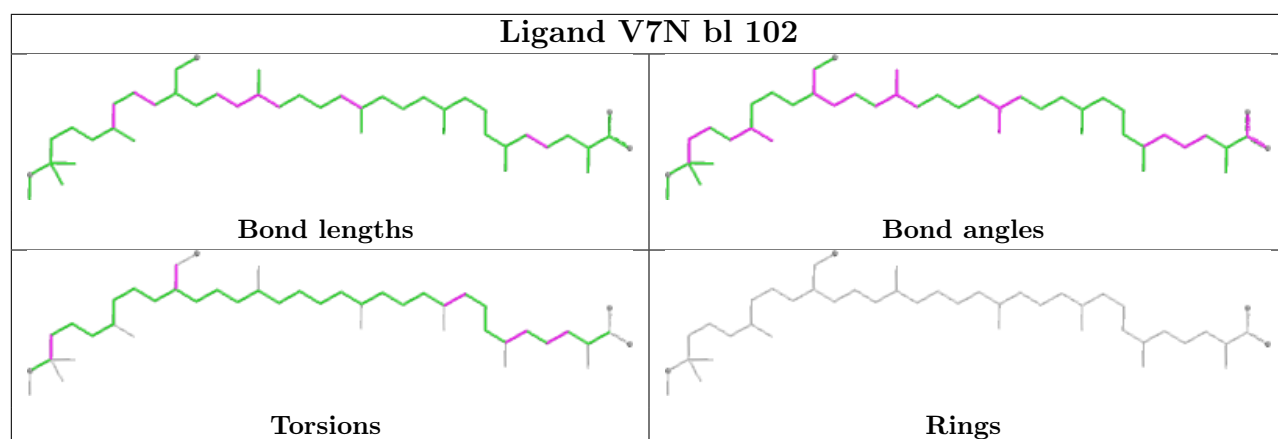
| Ligand V7N AH 105   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |



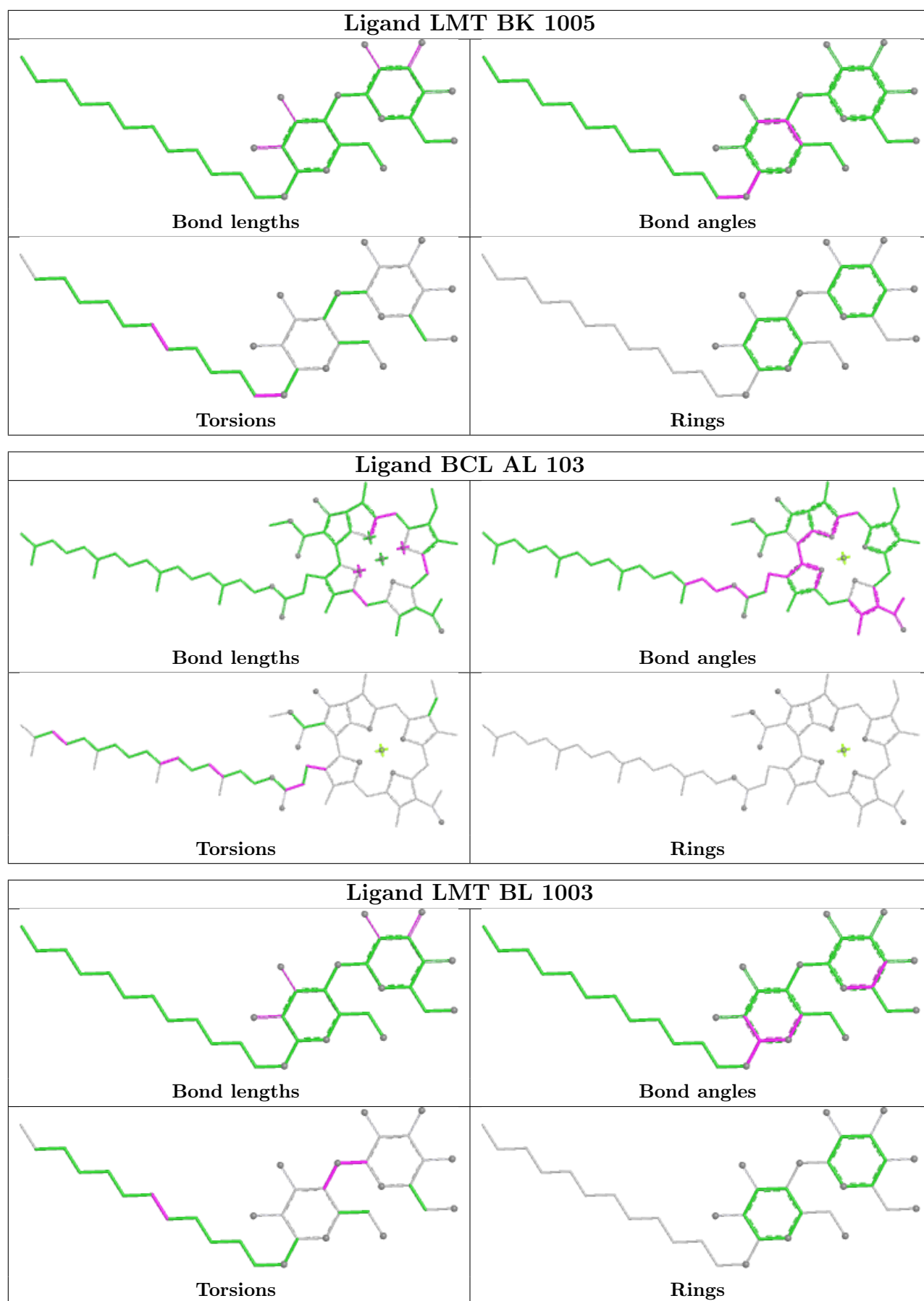


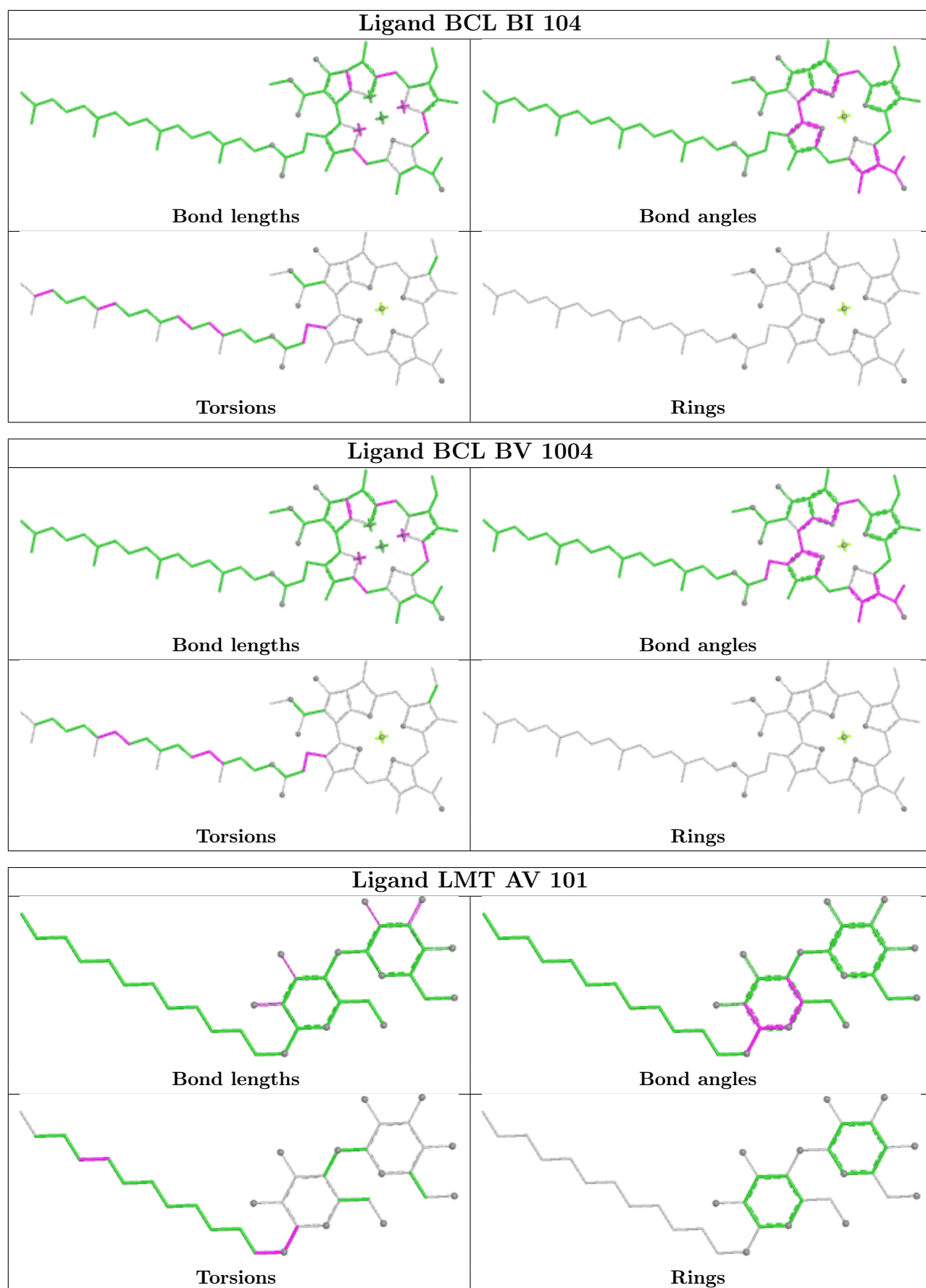


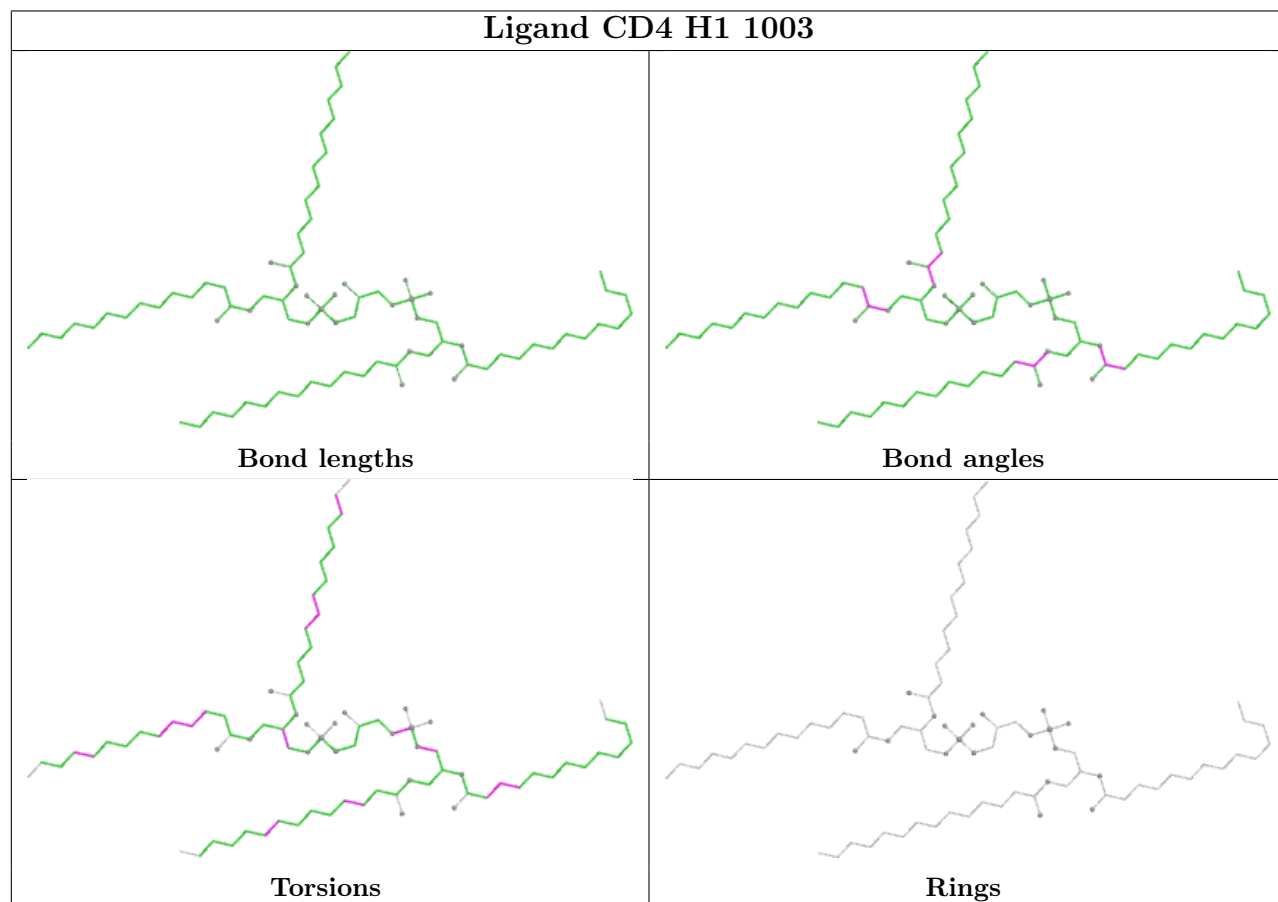
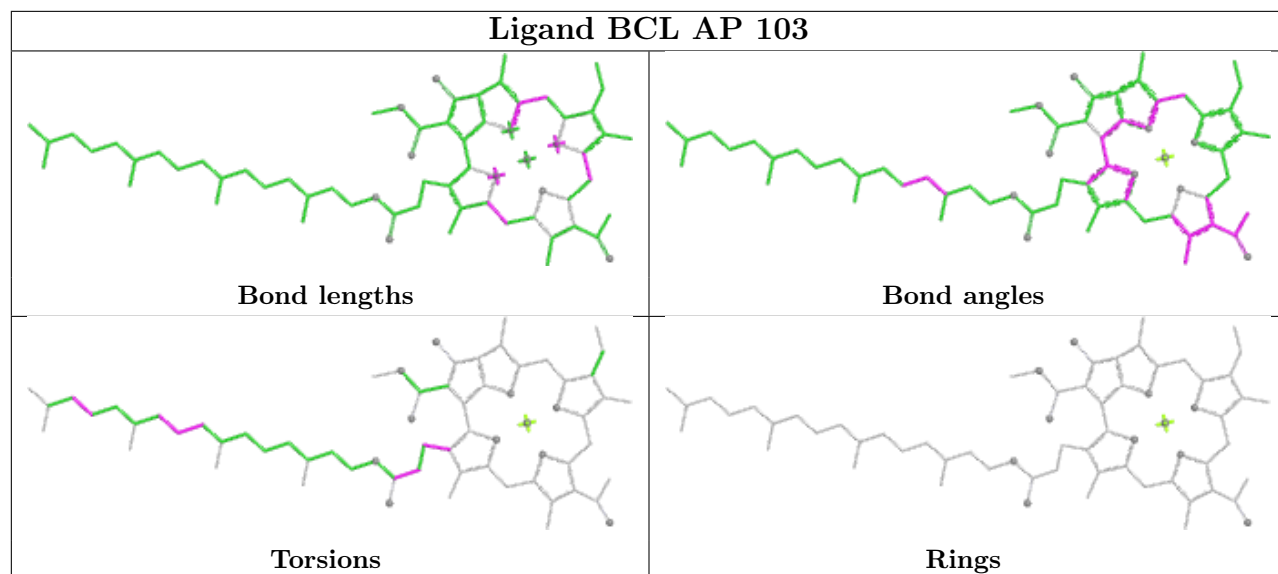


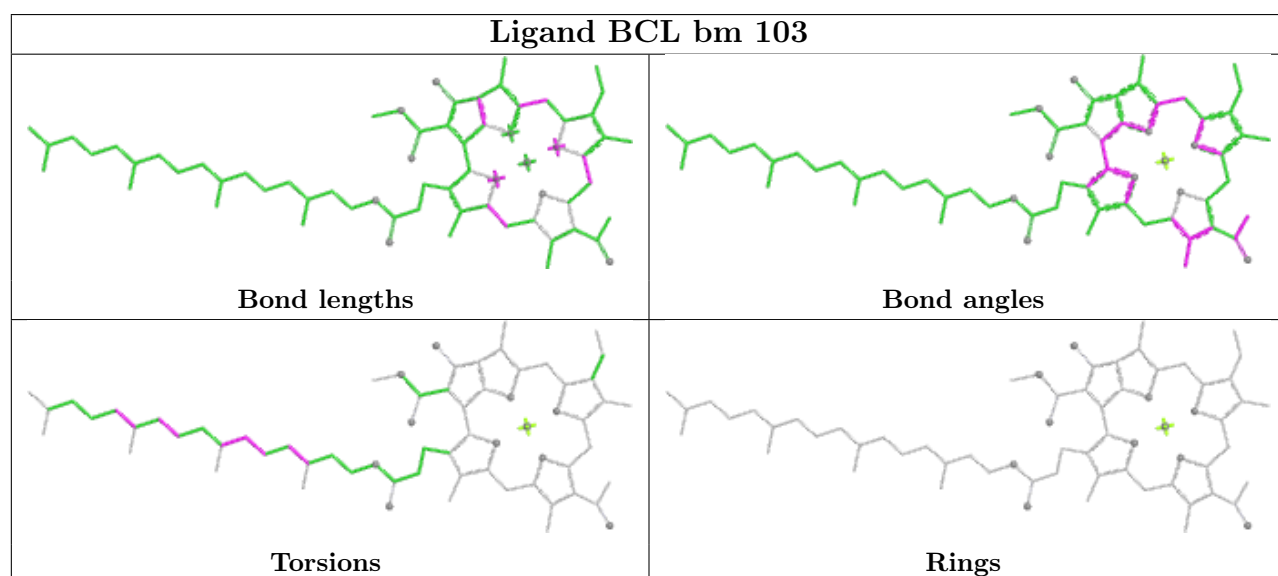
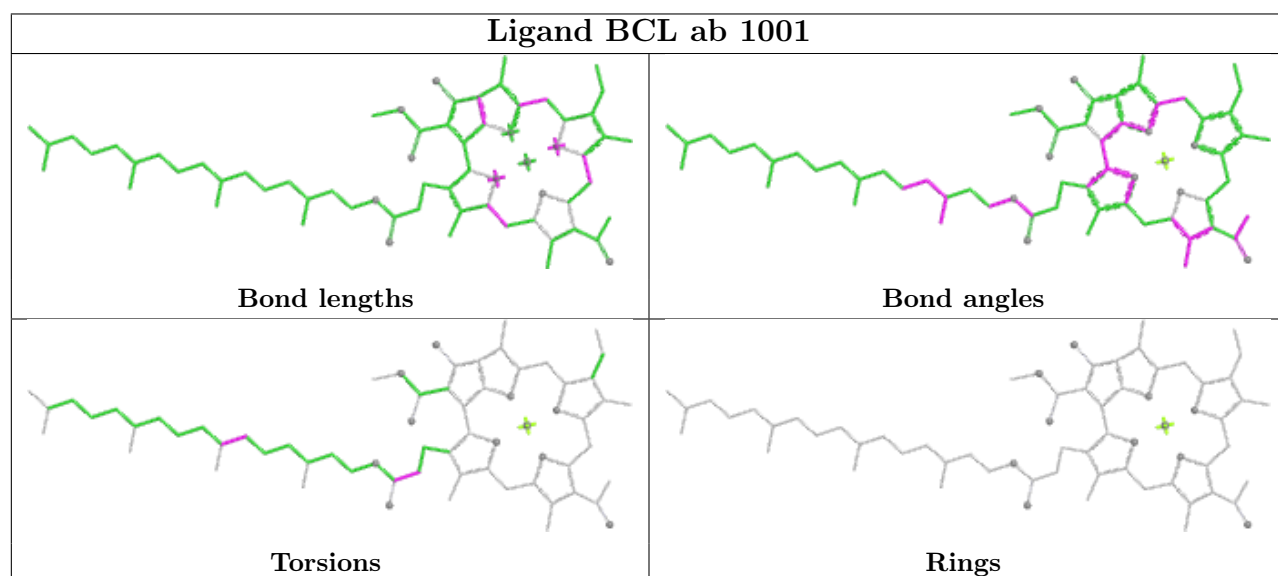
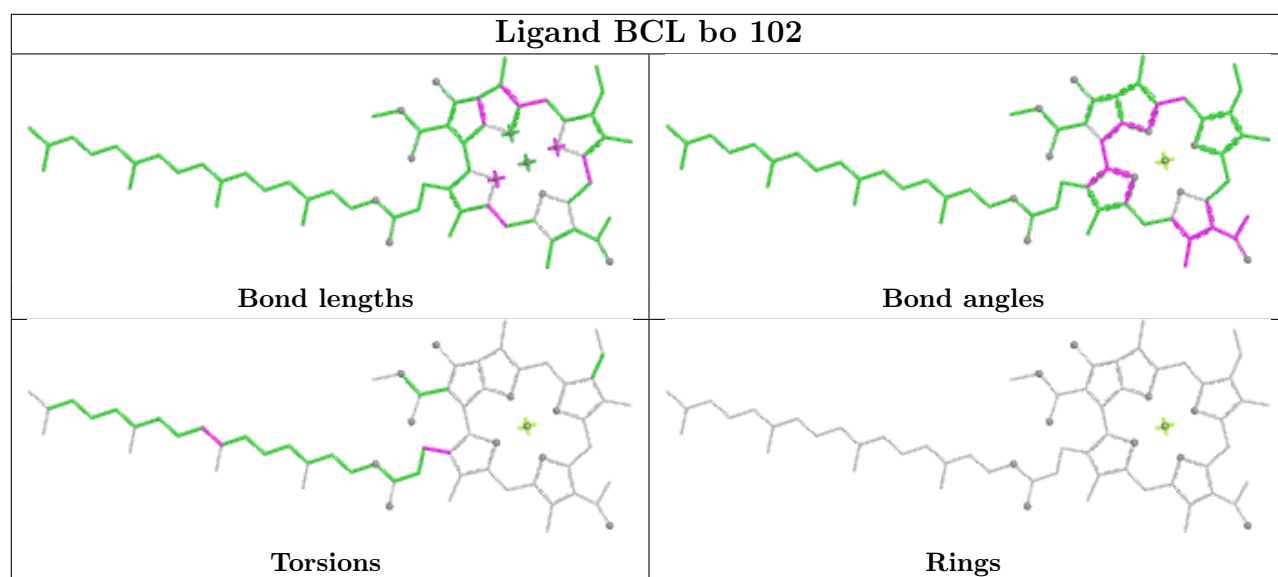


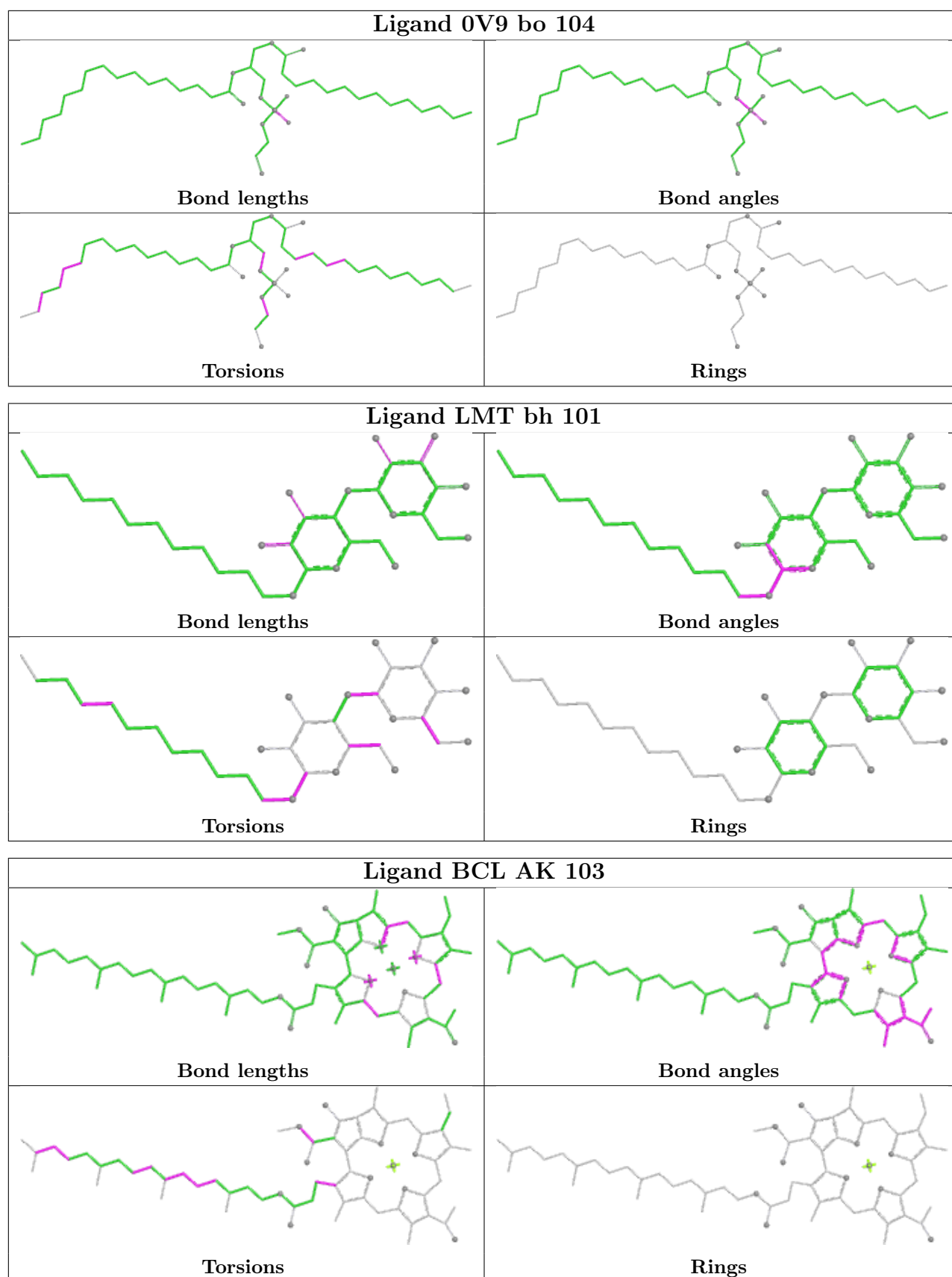


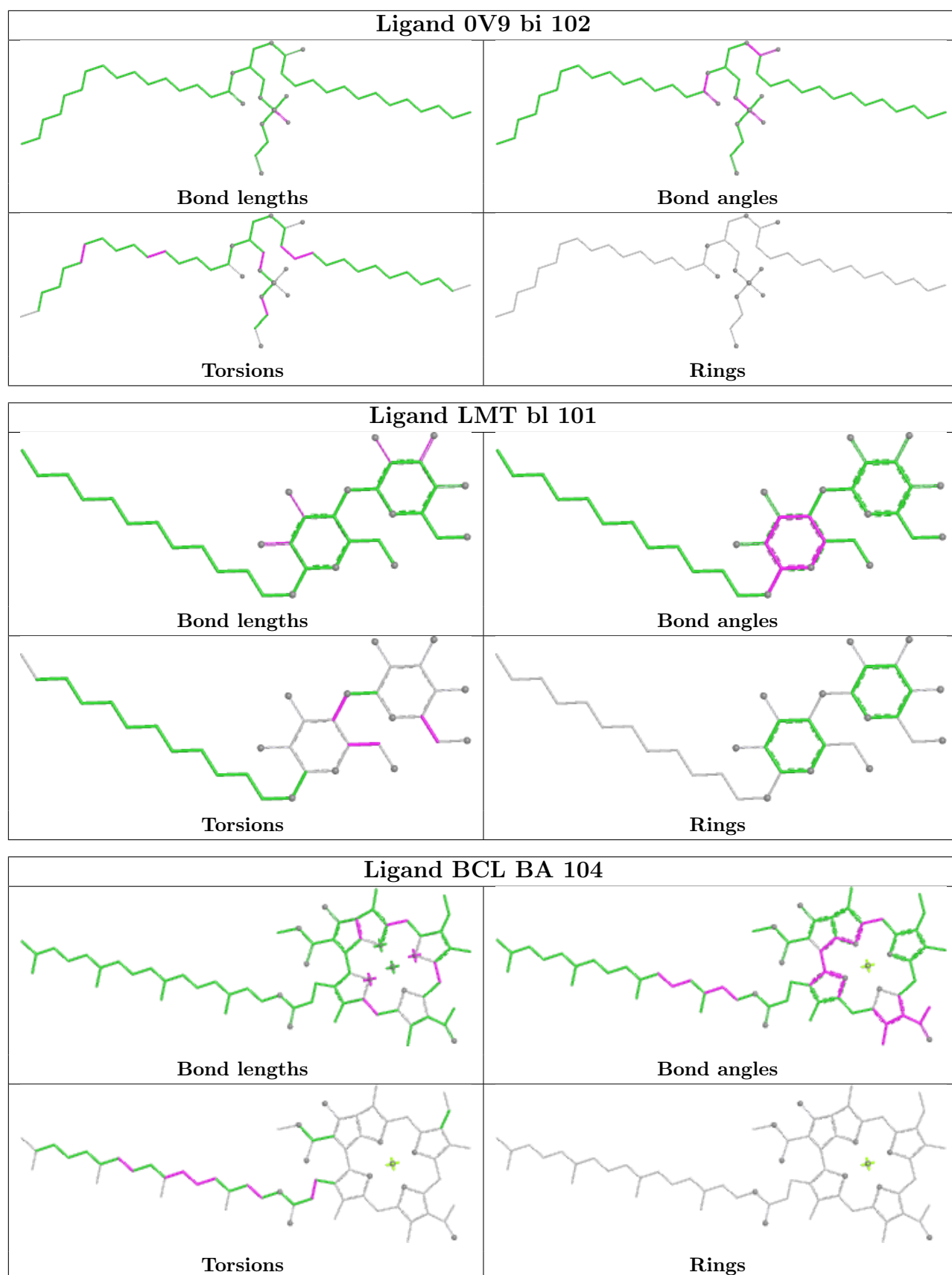


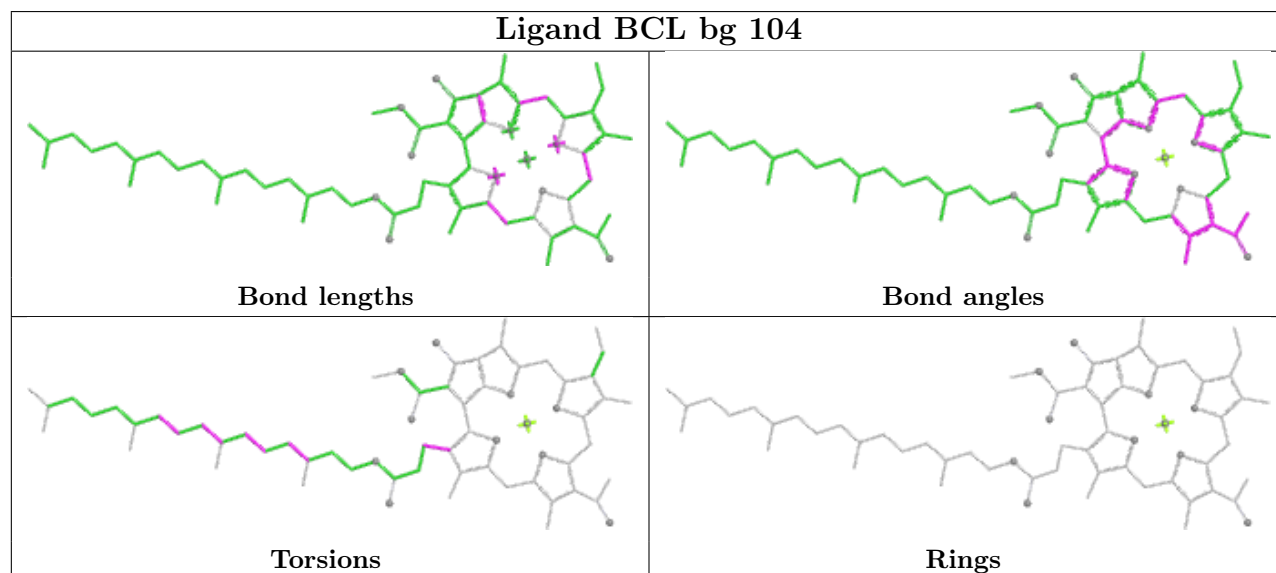
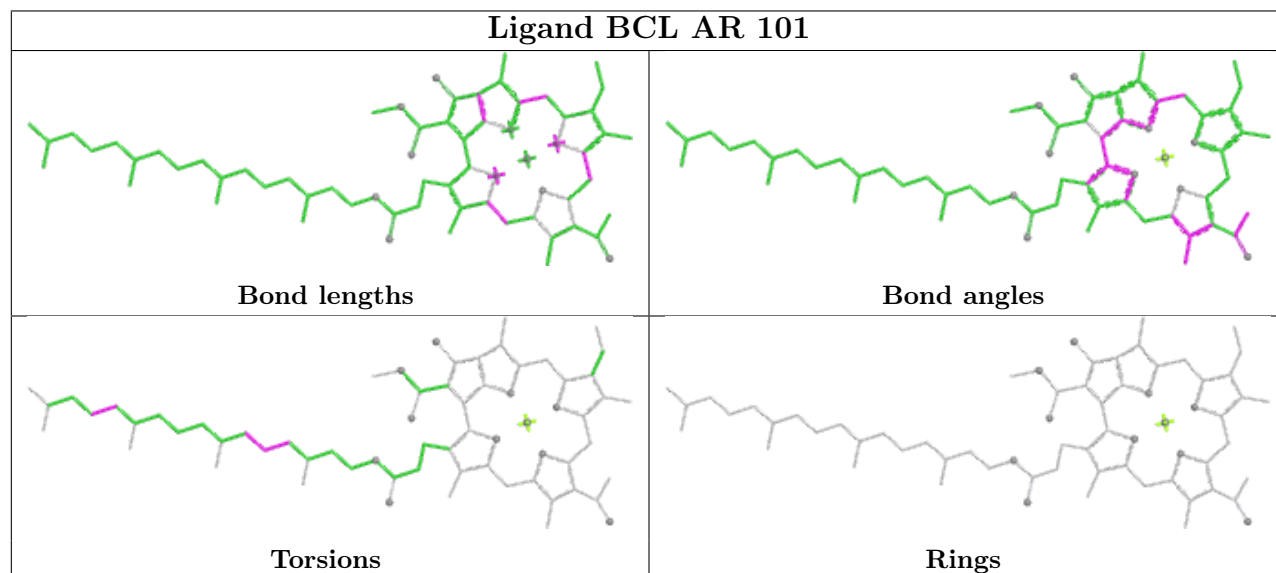
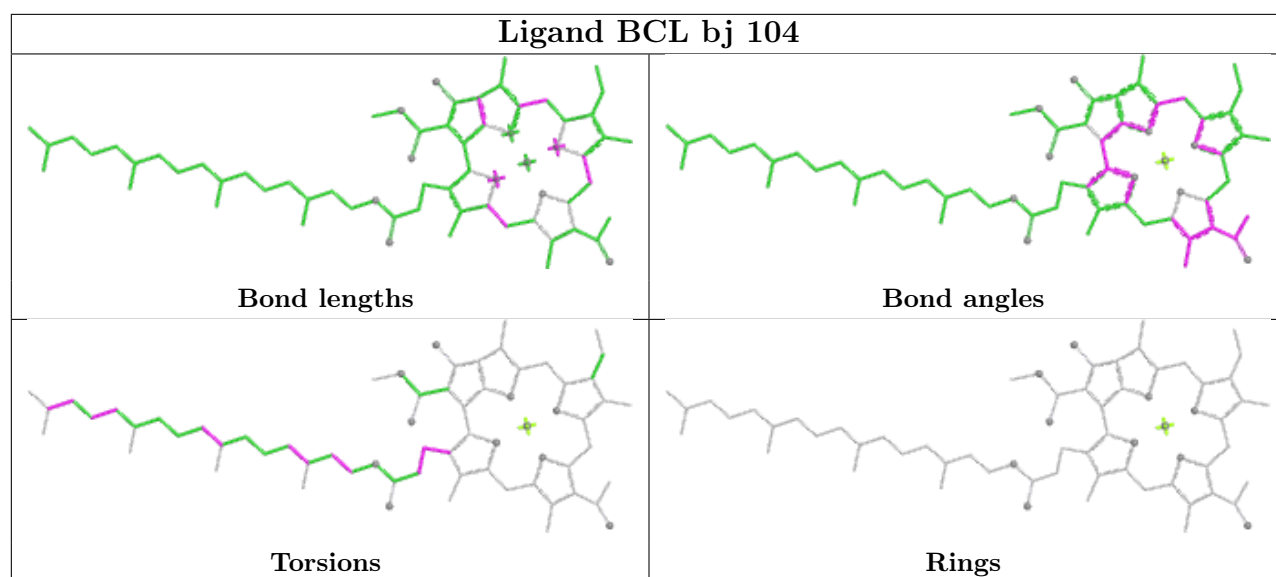


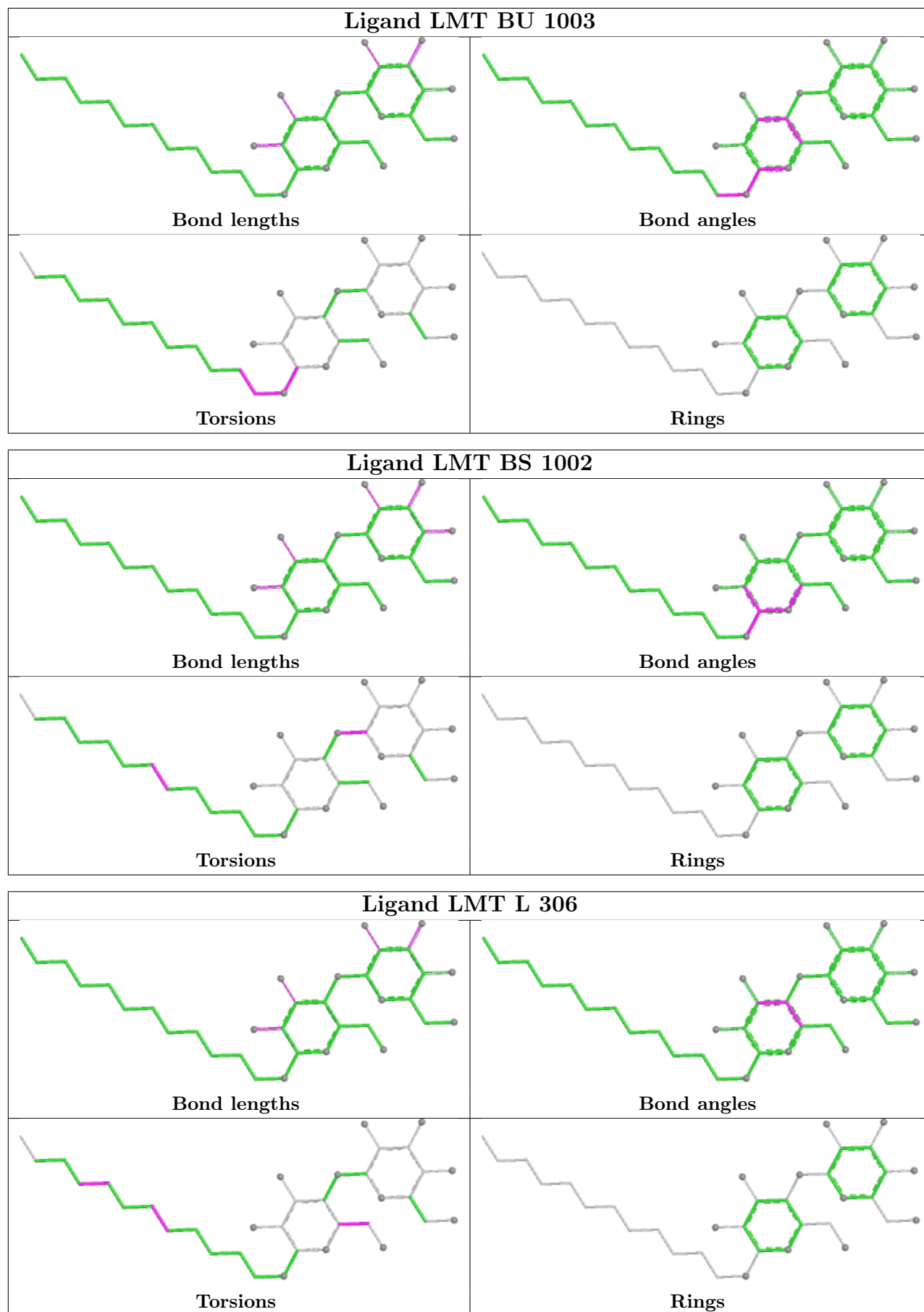




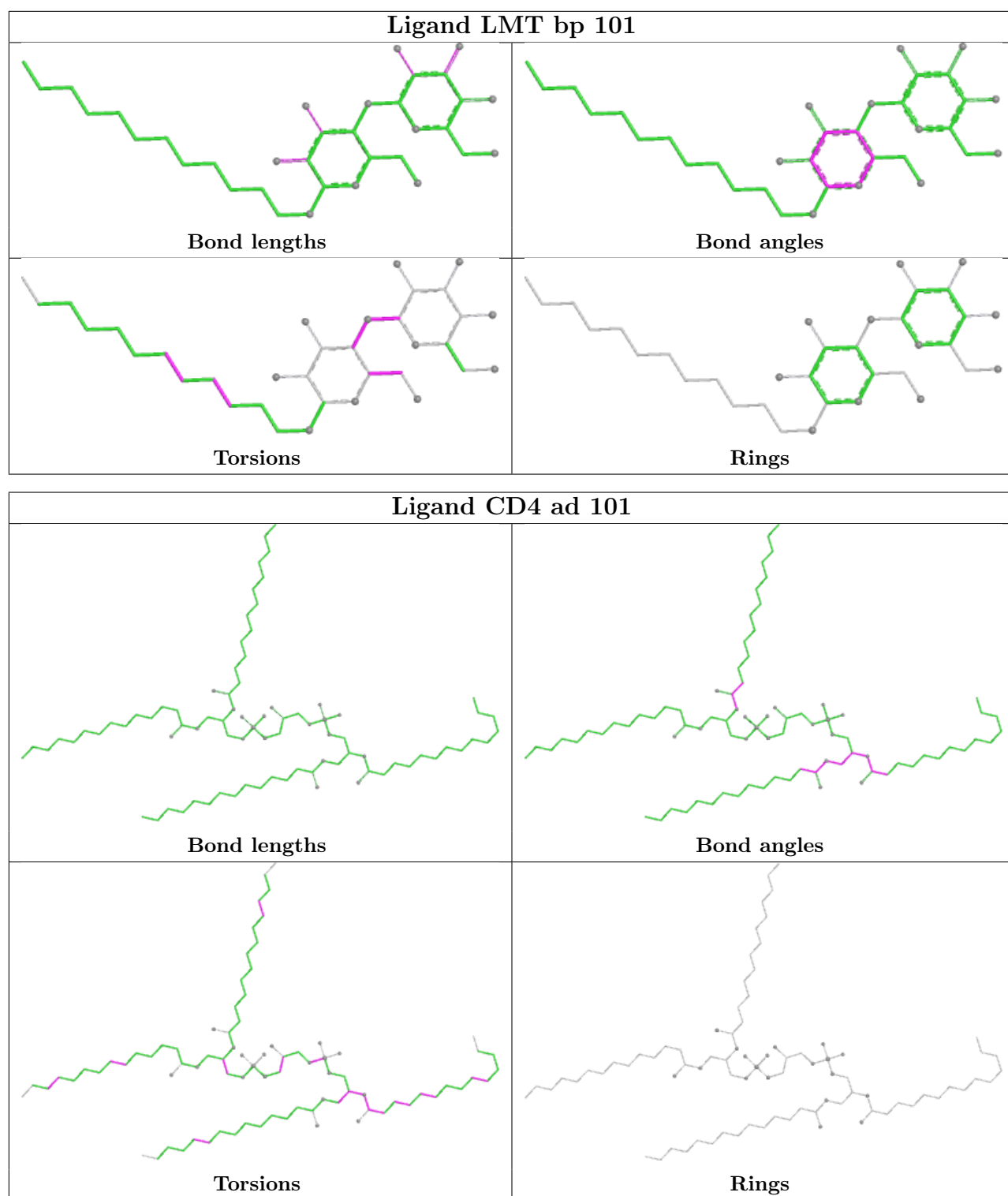


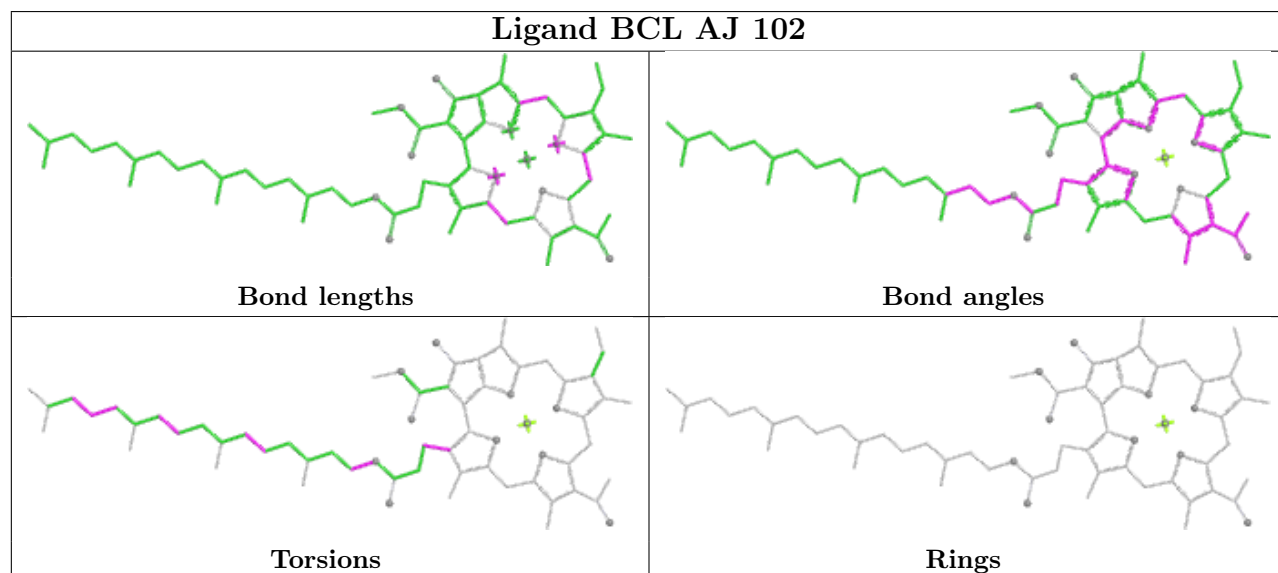
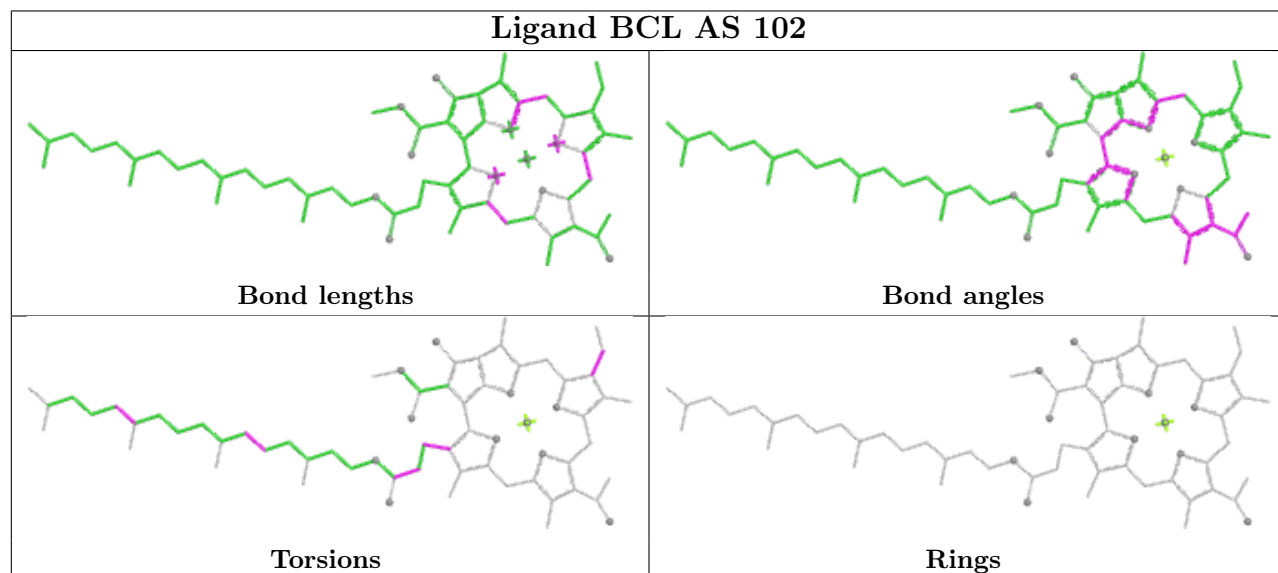
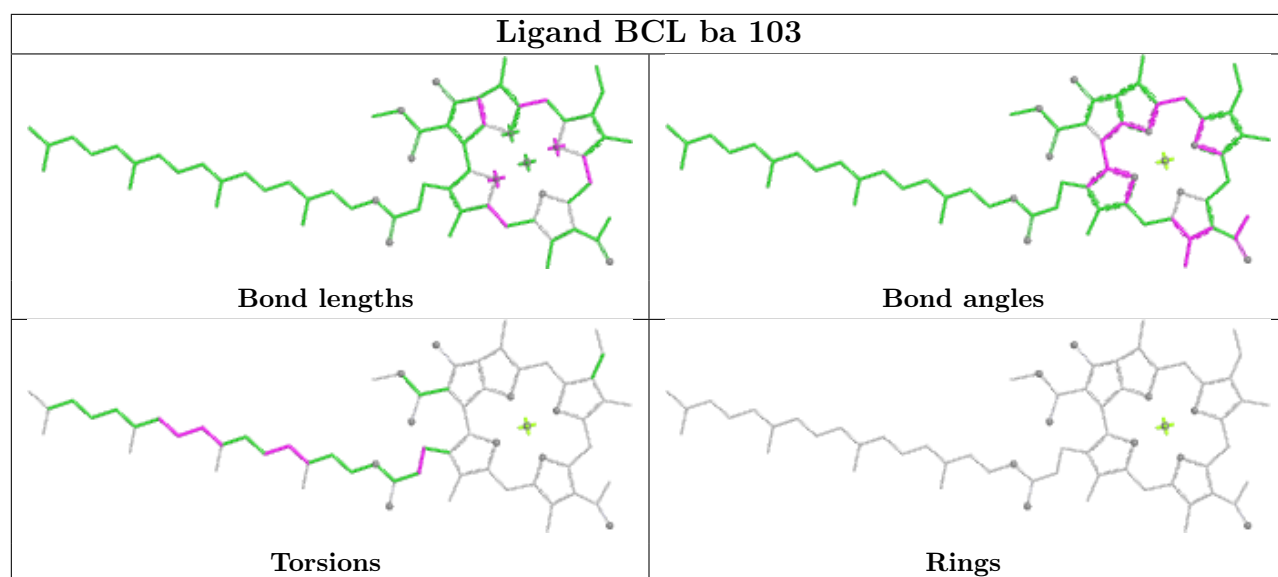


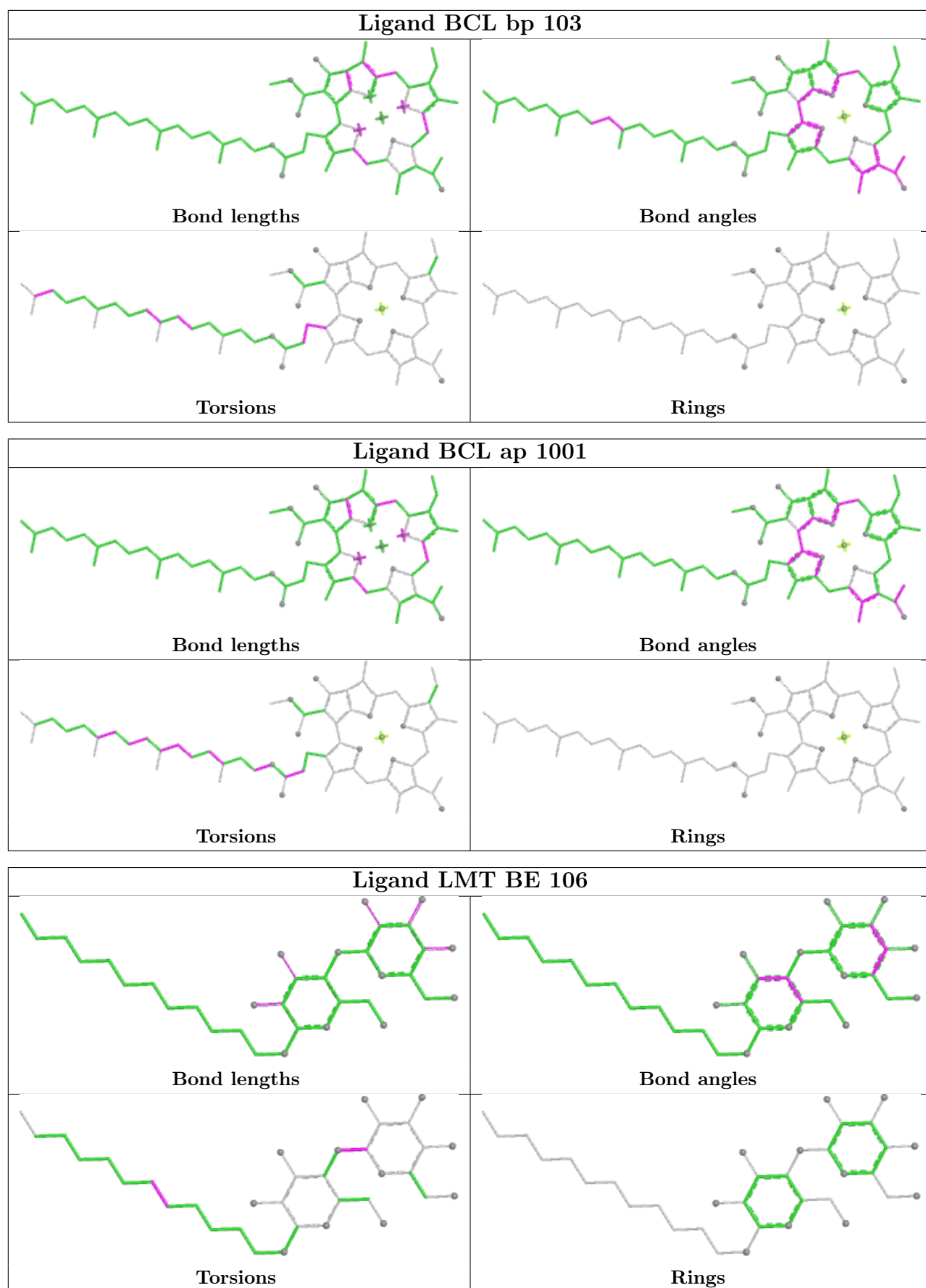


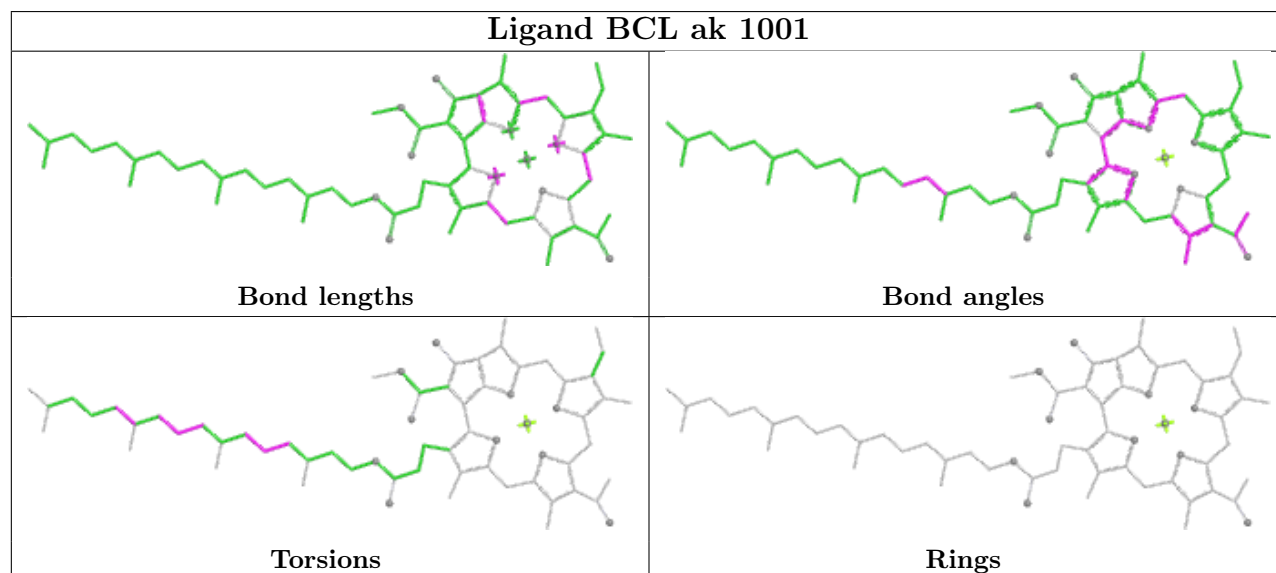
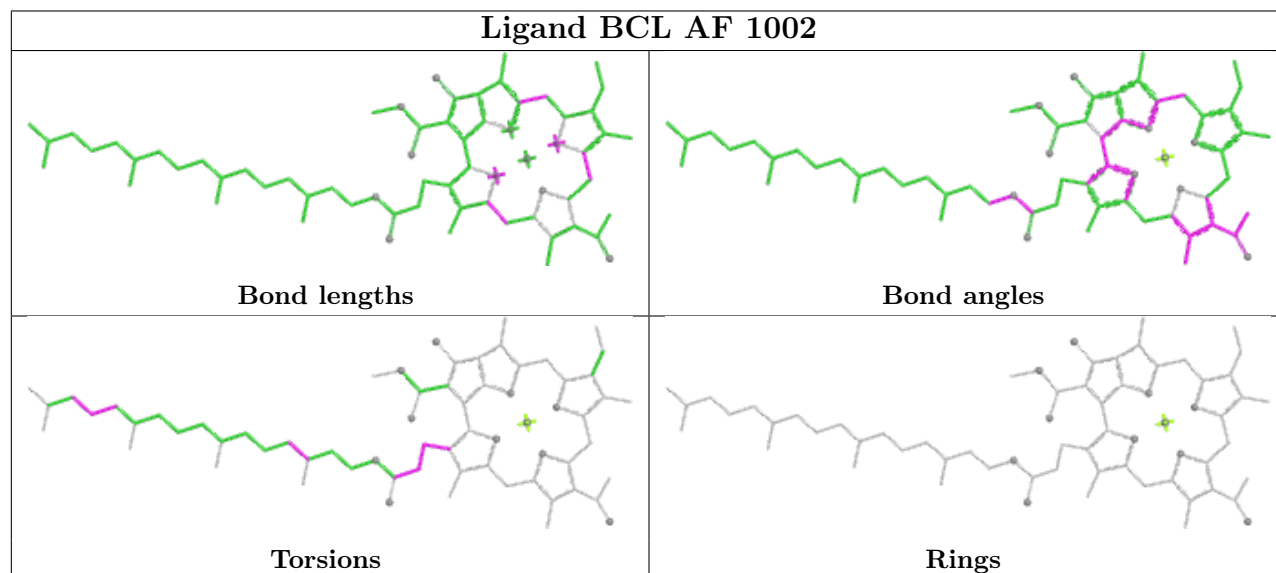
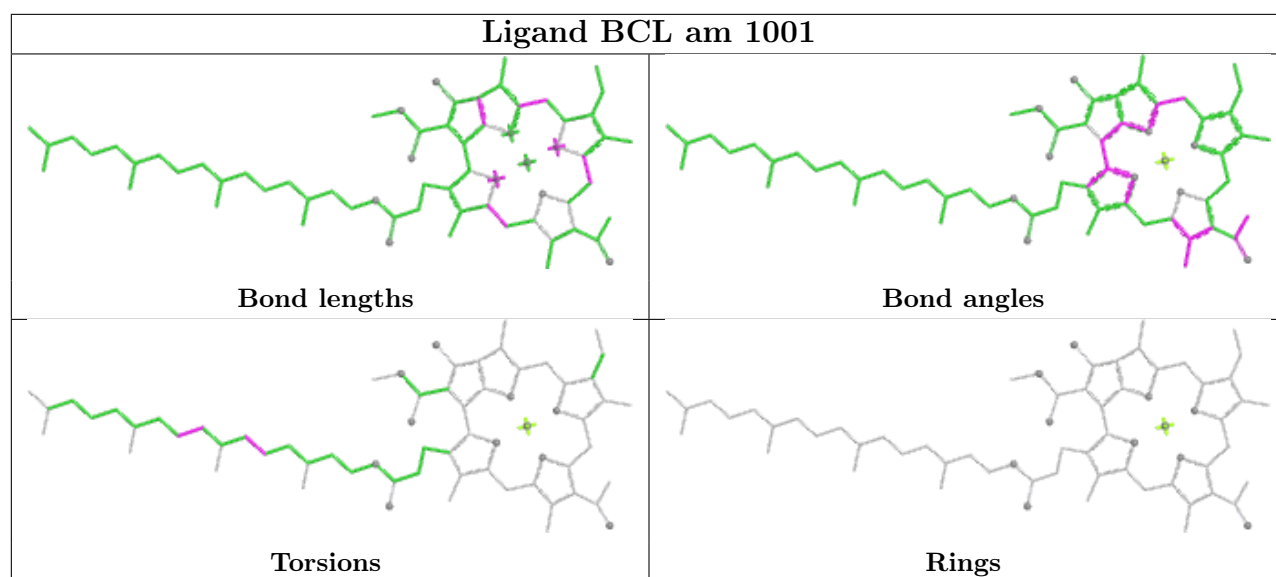


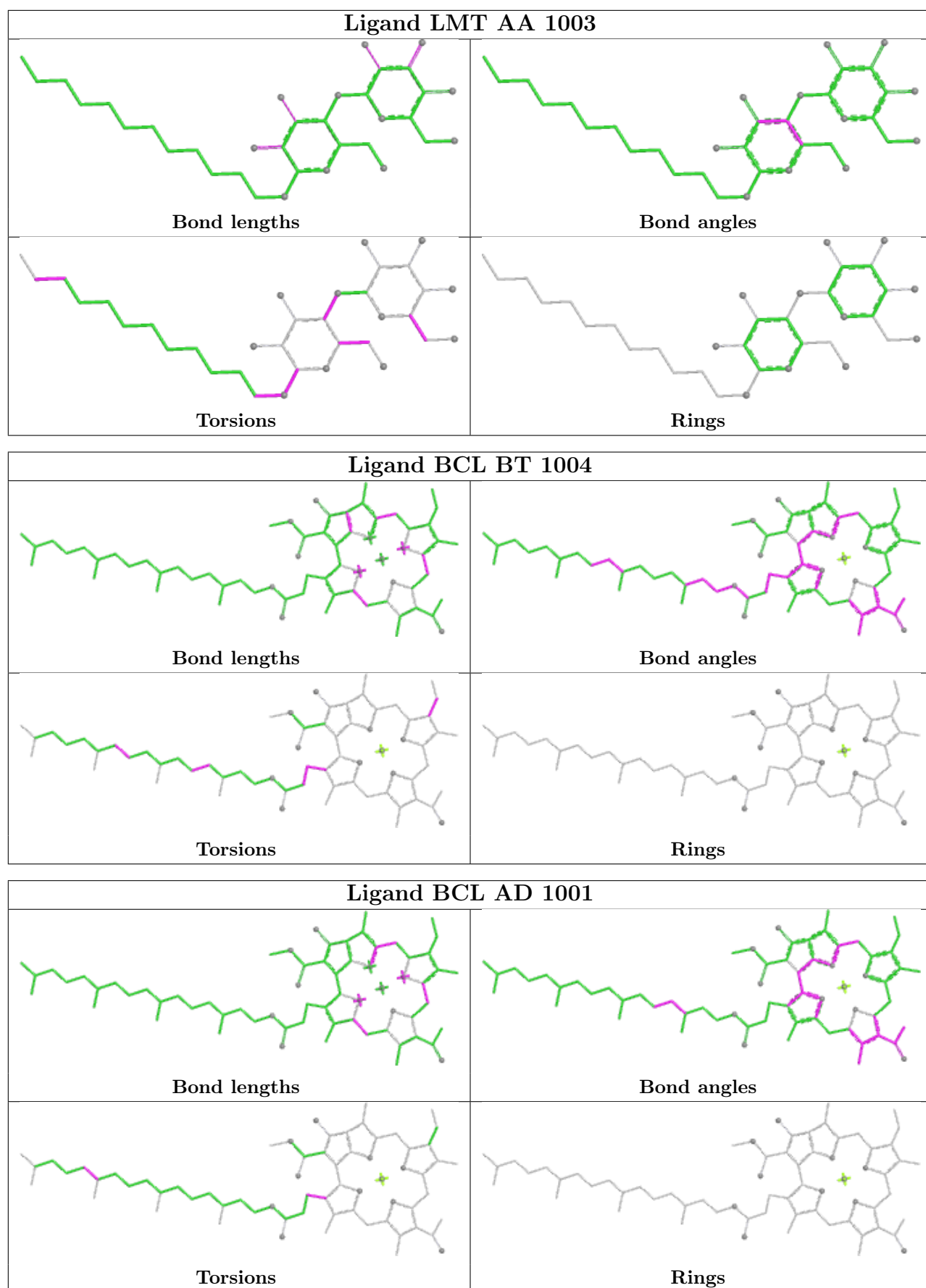


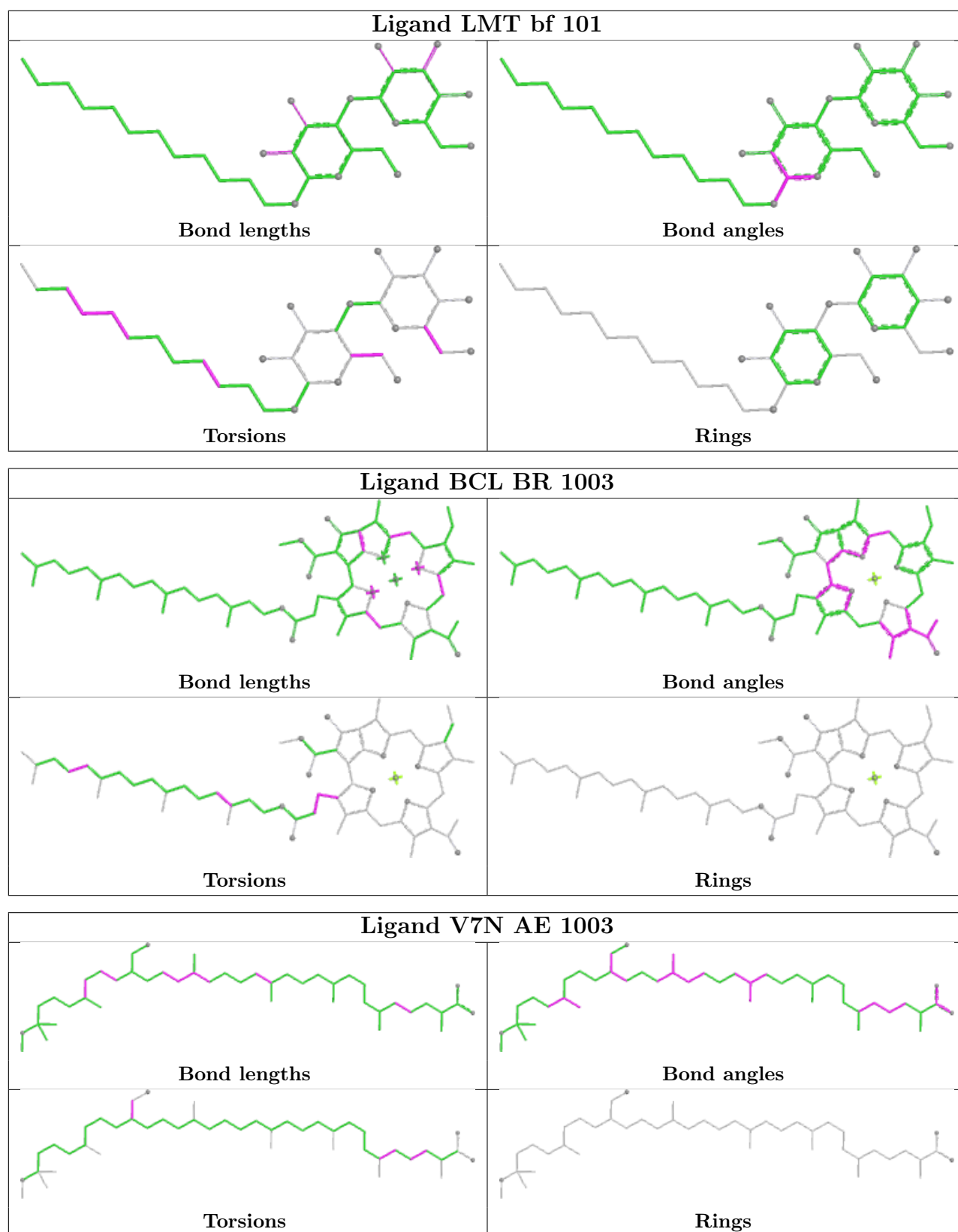


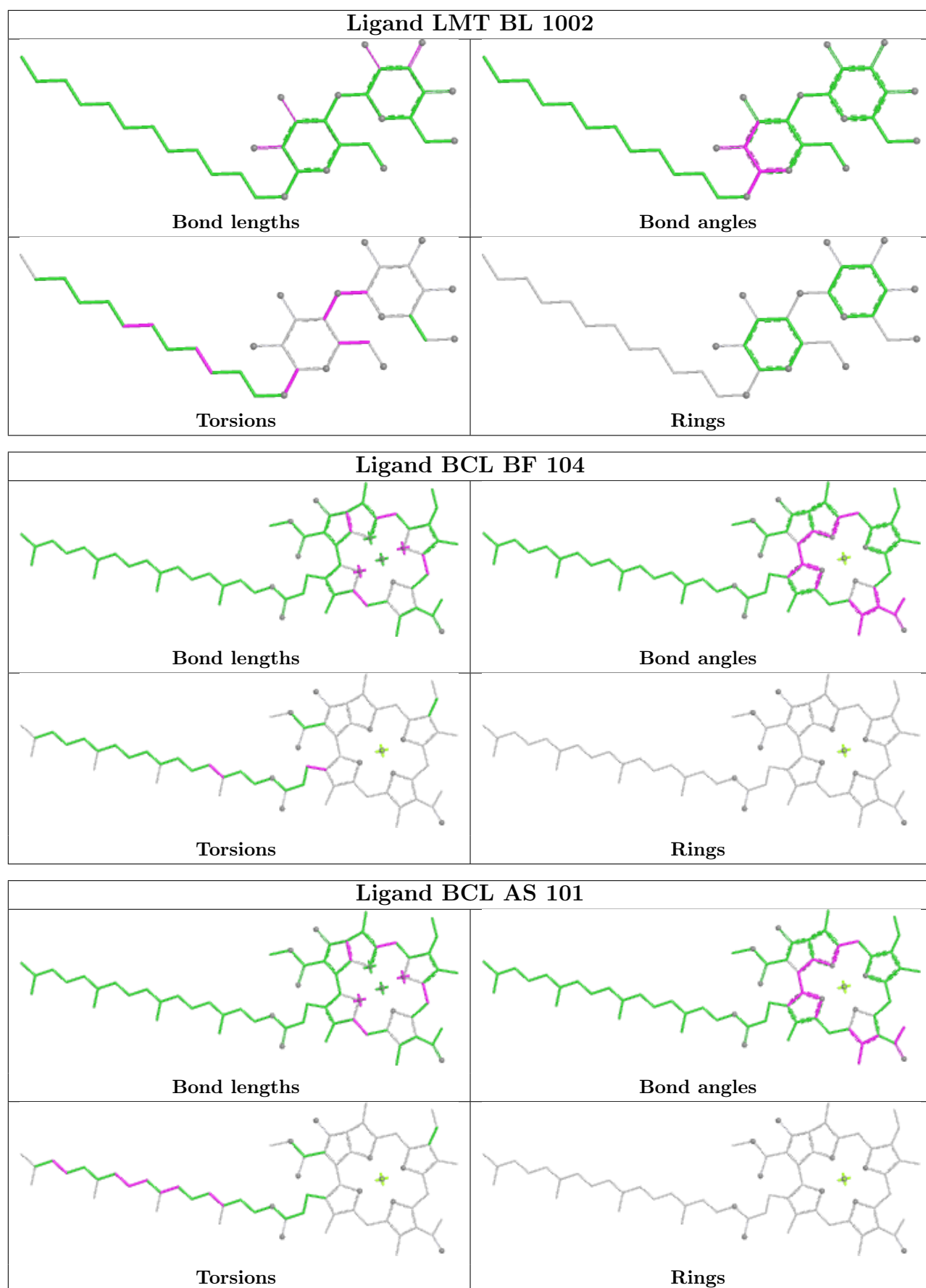


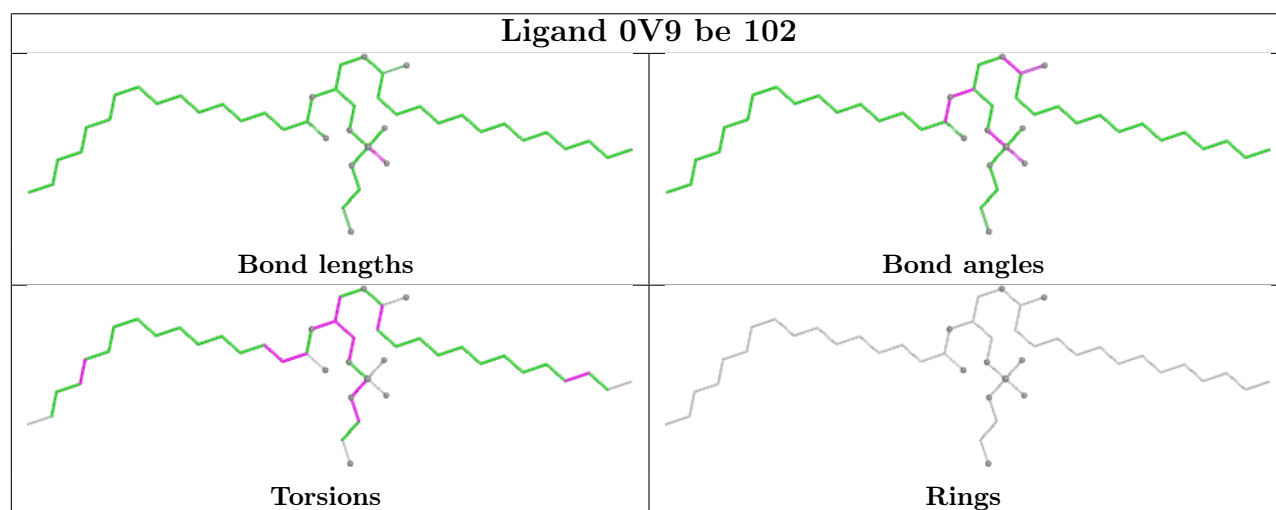
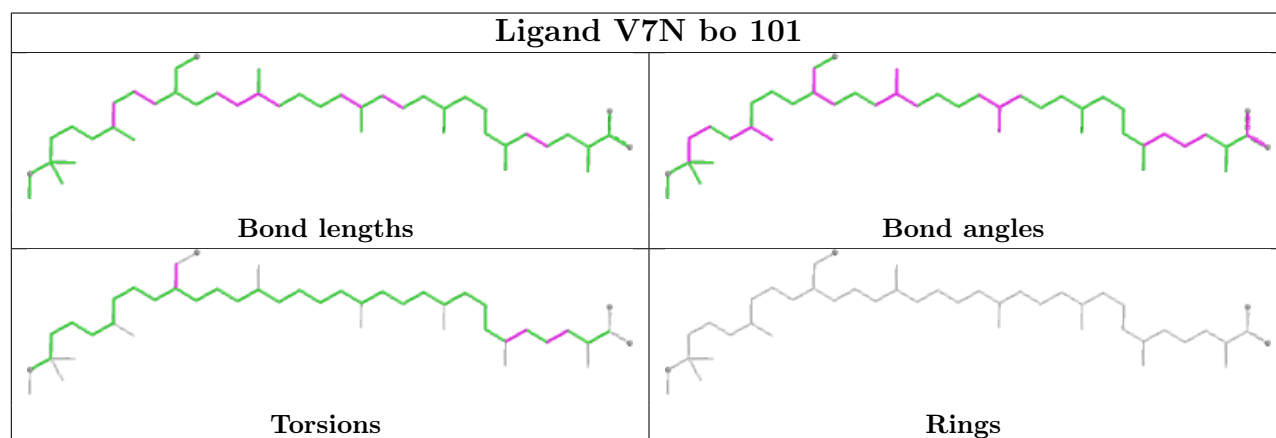
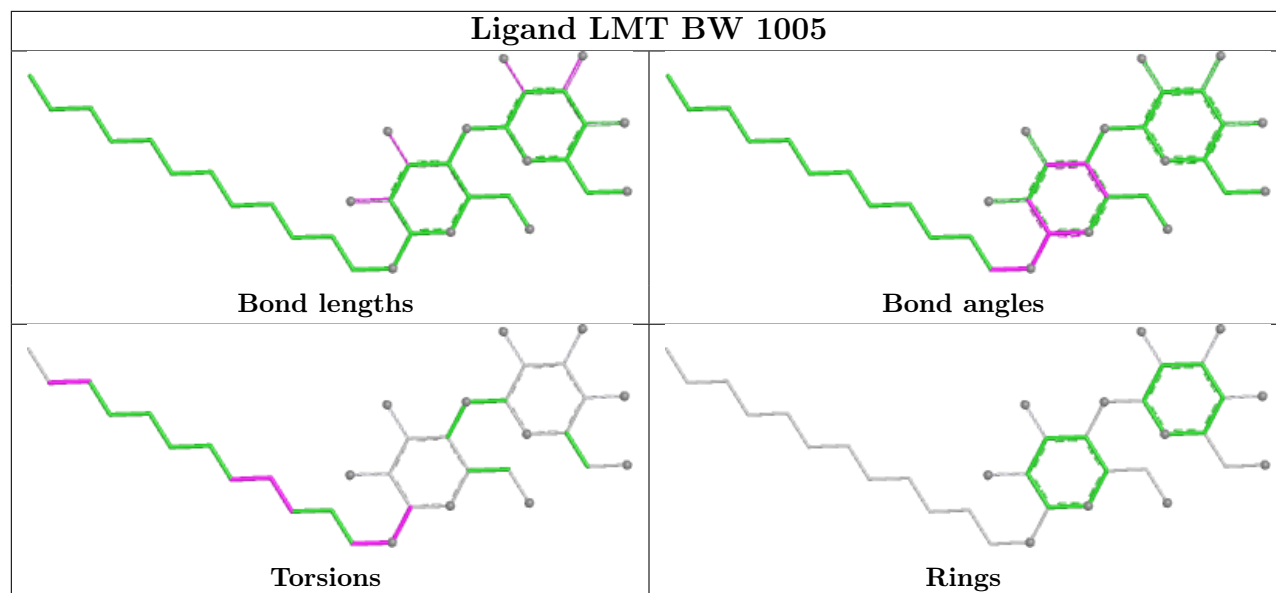




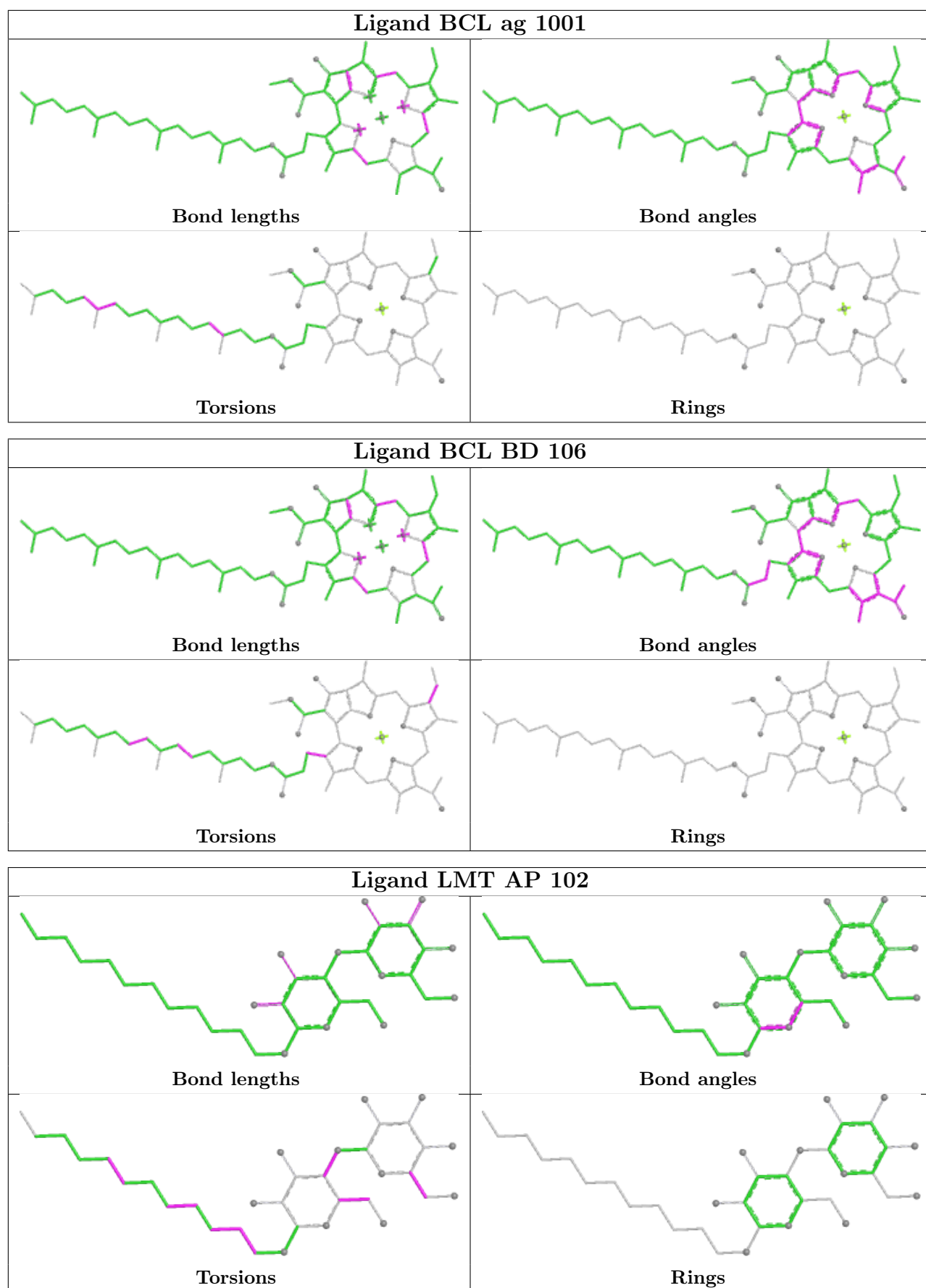


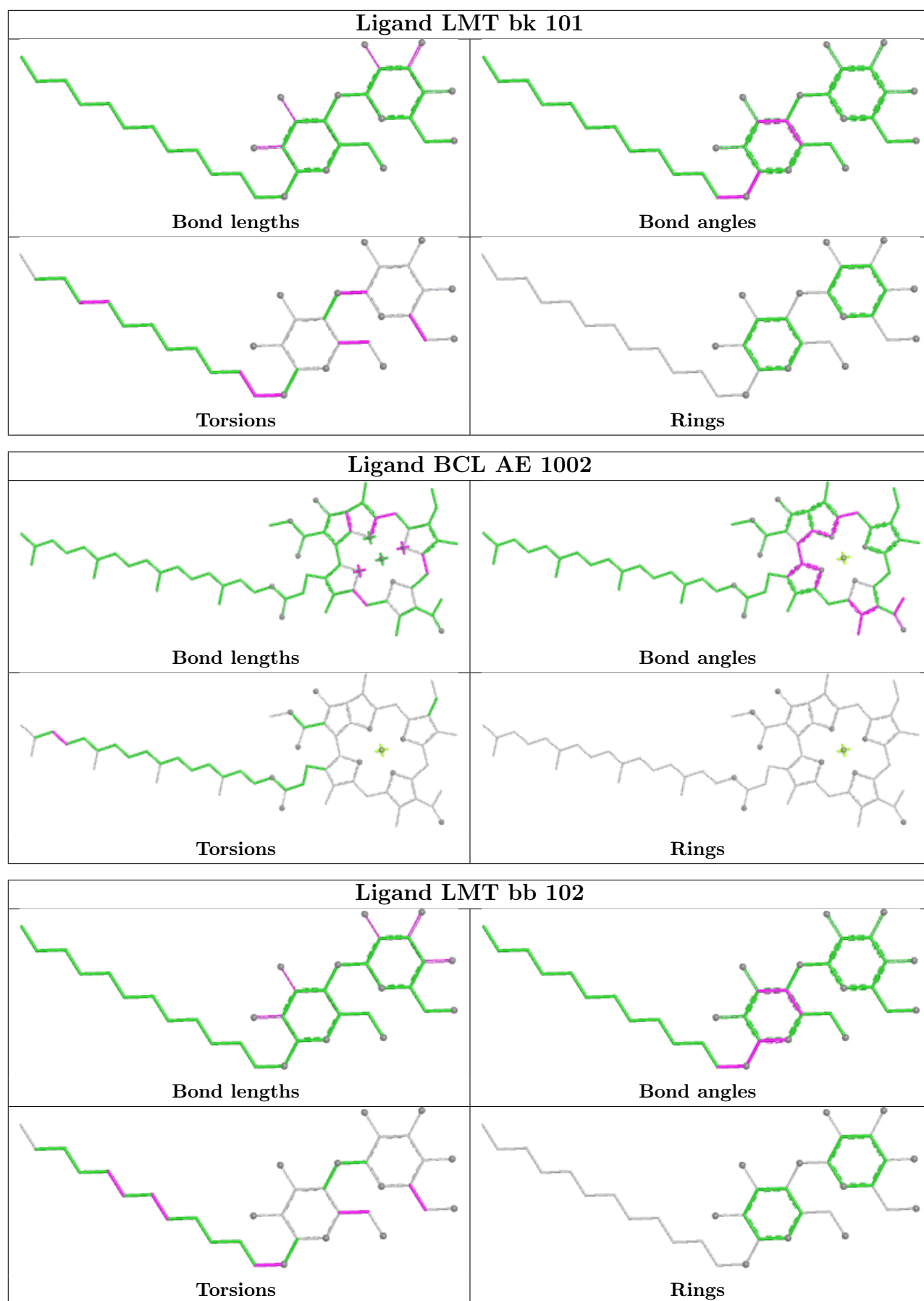


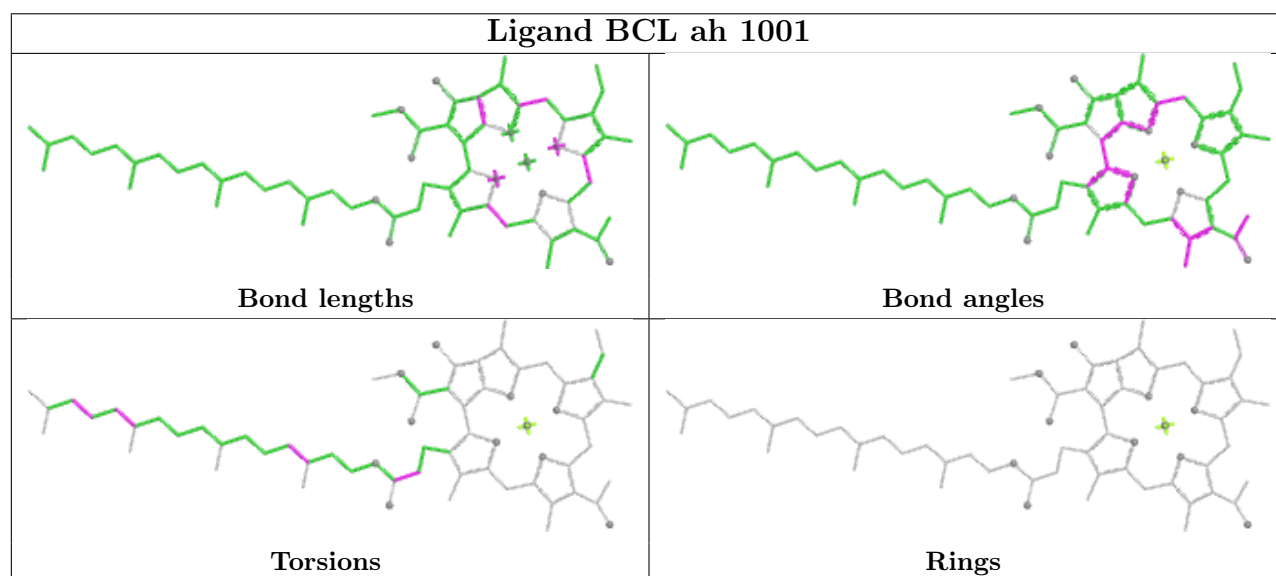
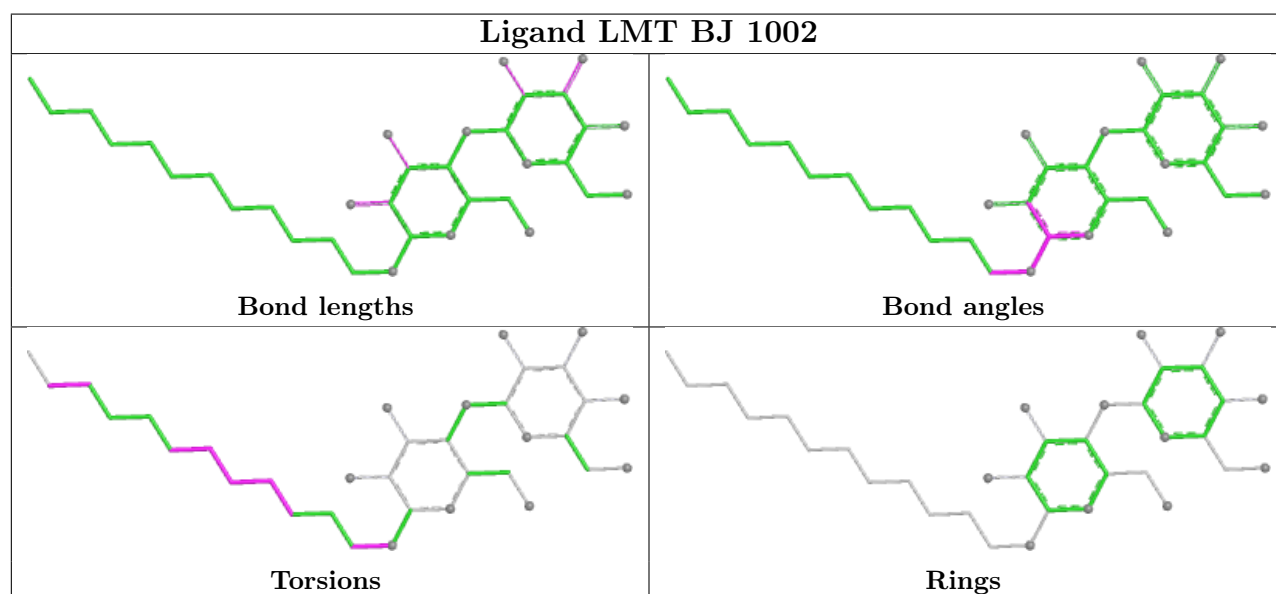
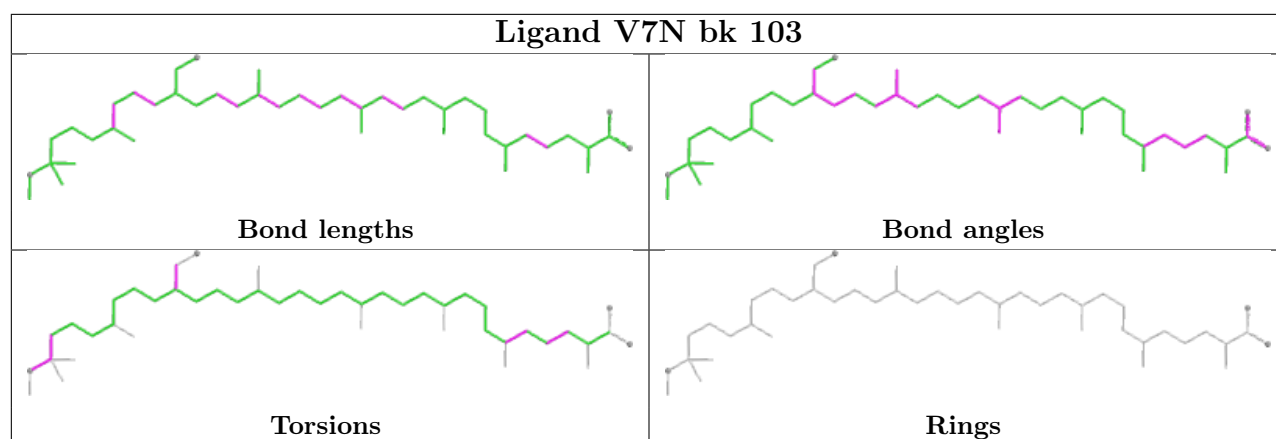


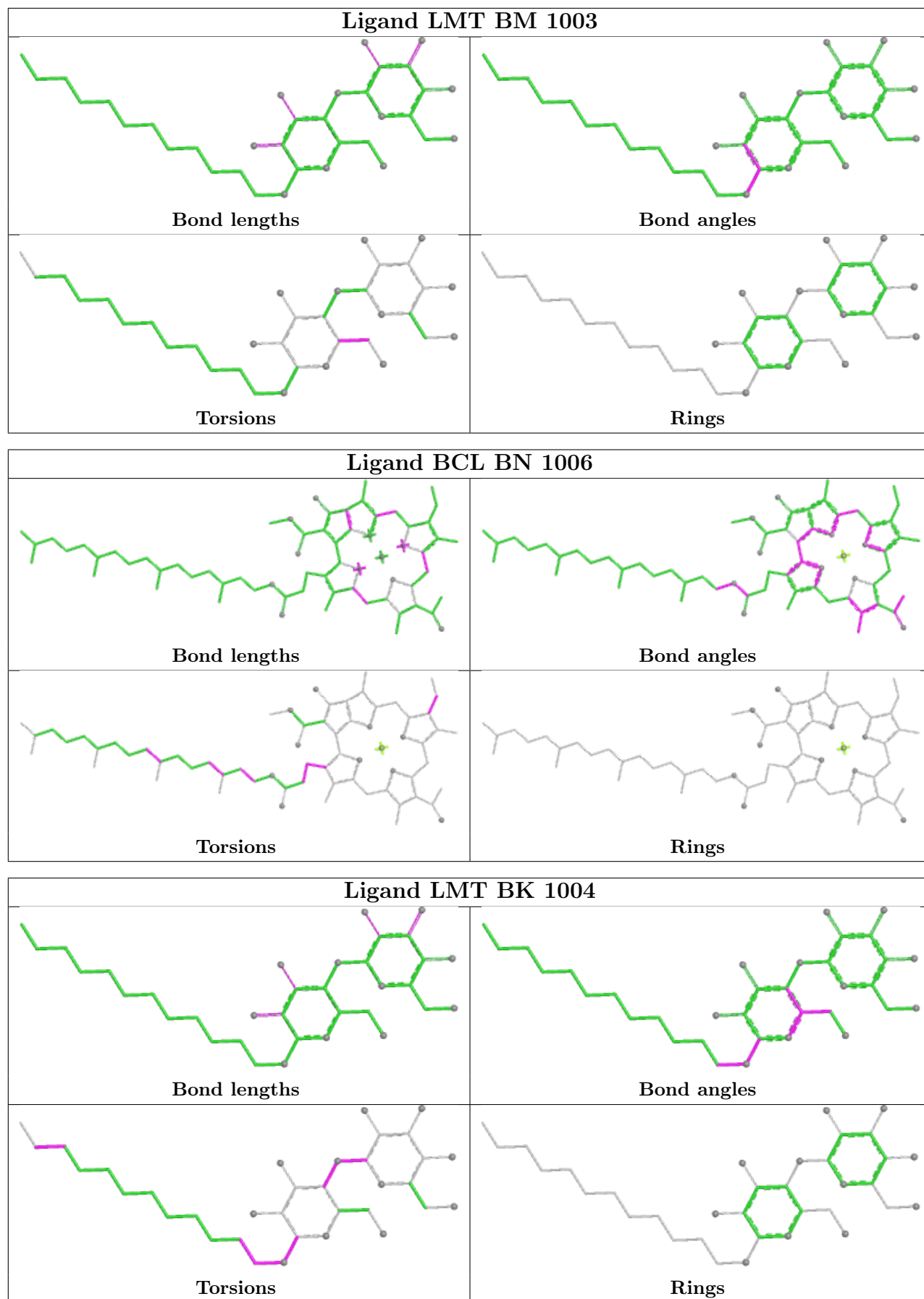


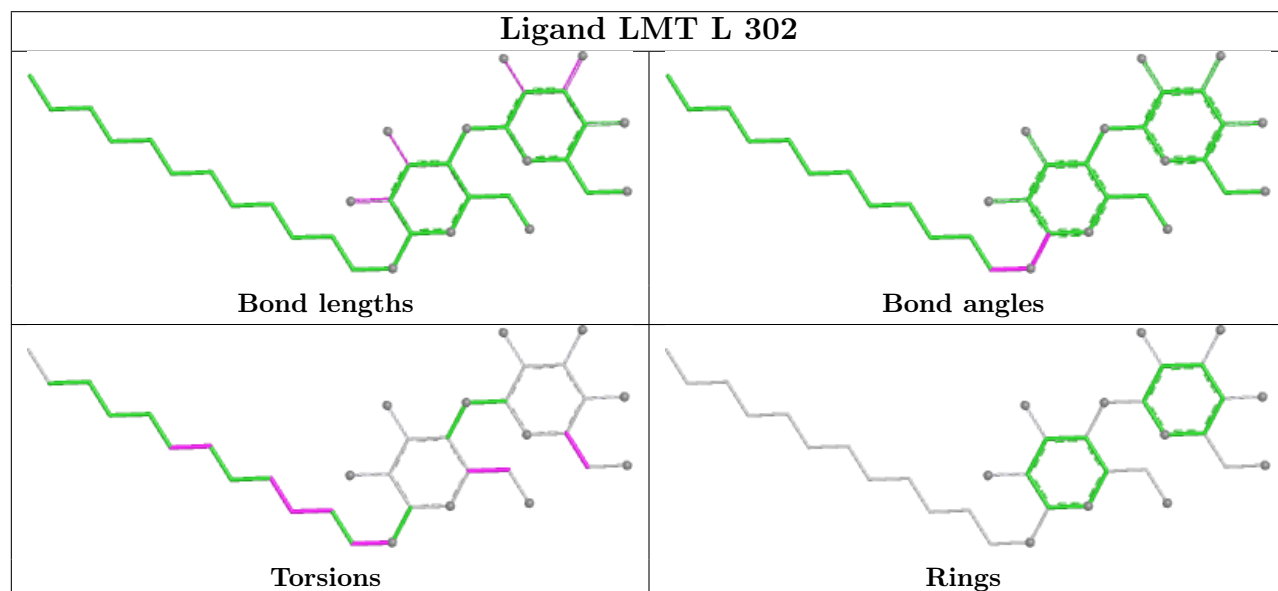
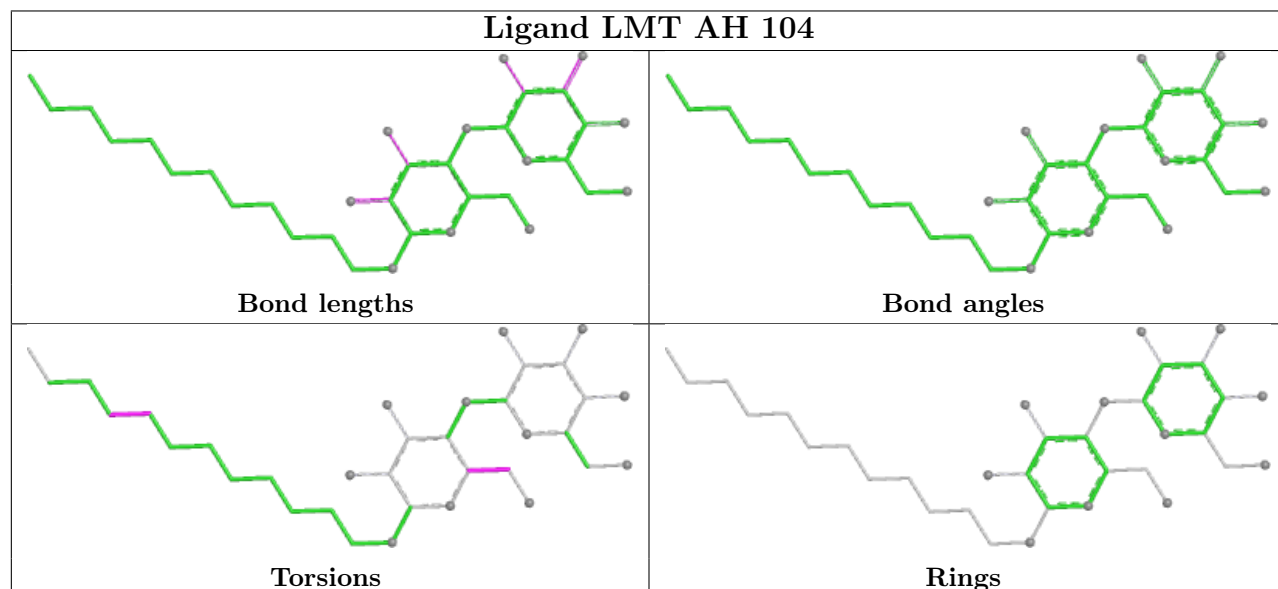
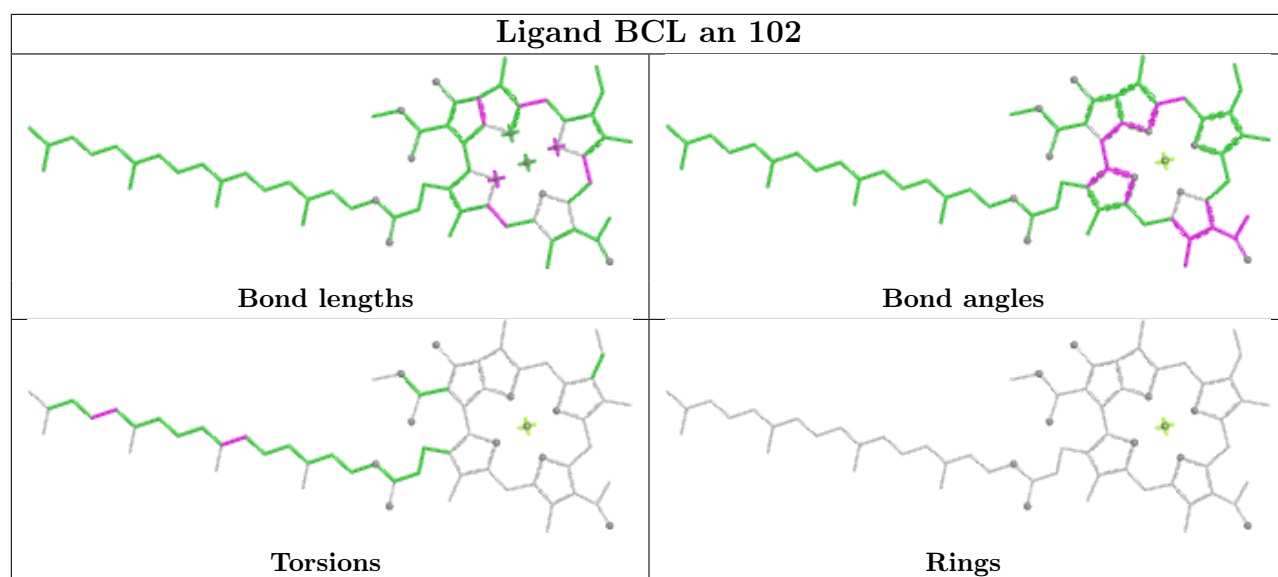


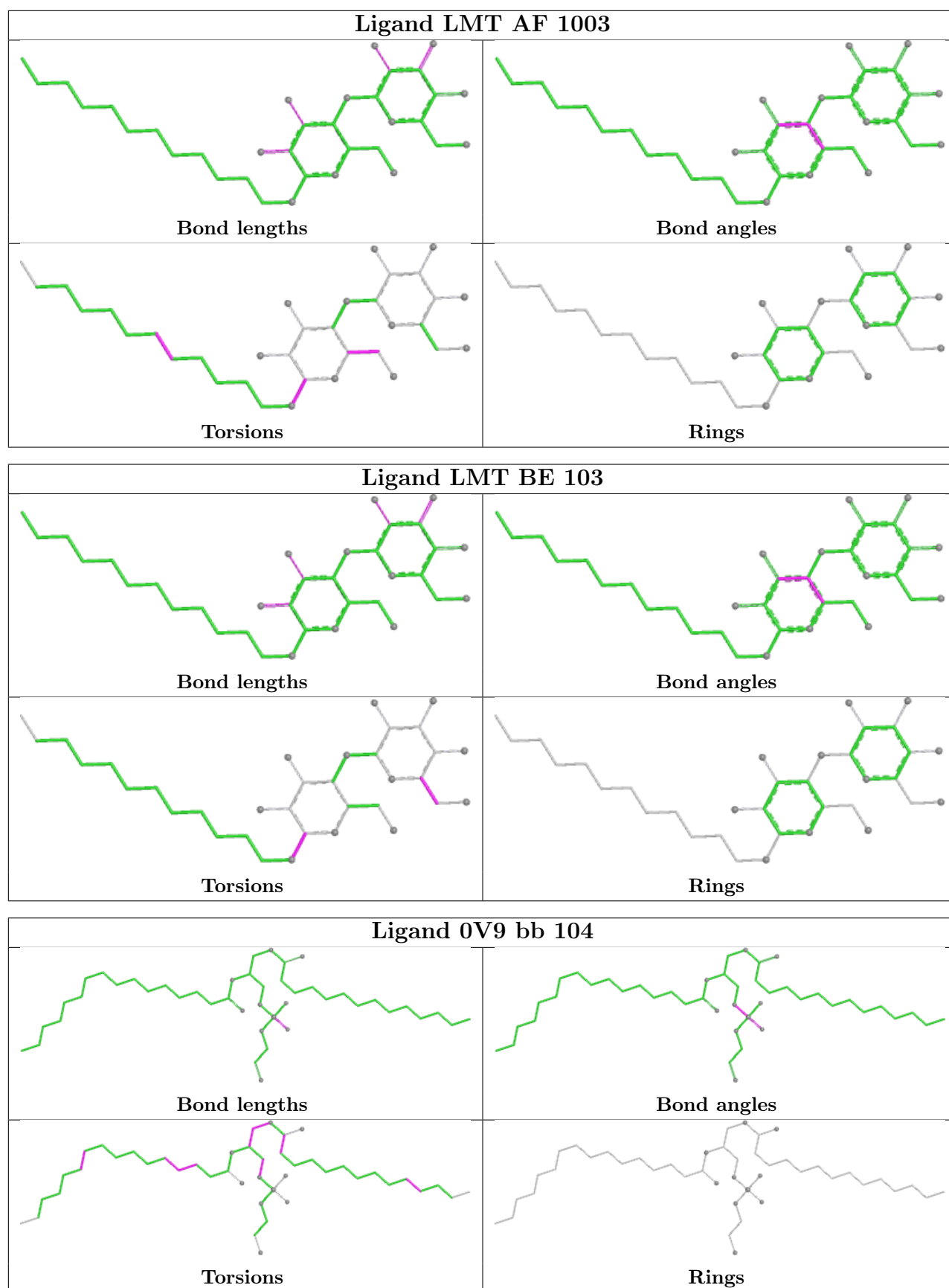


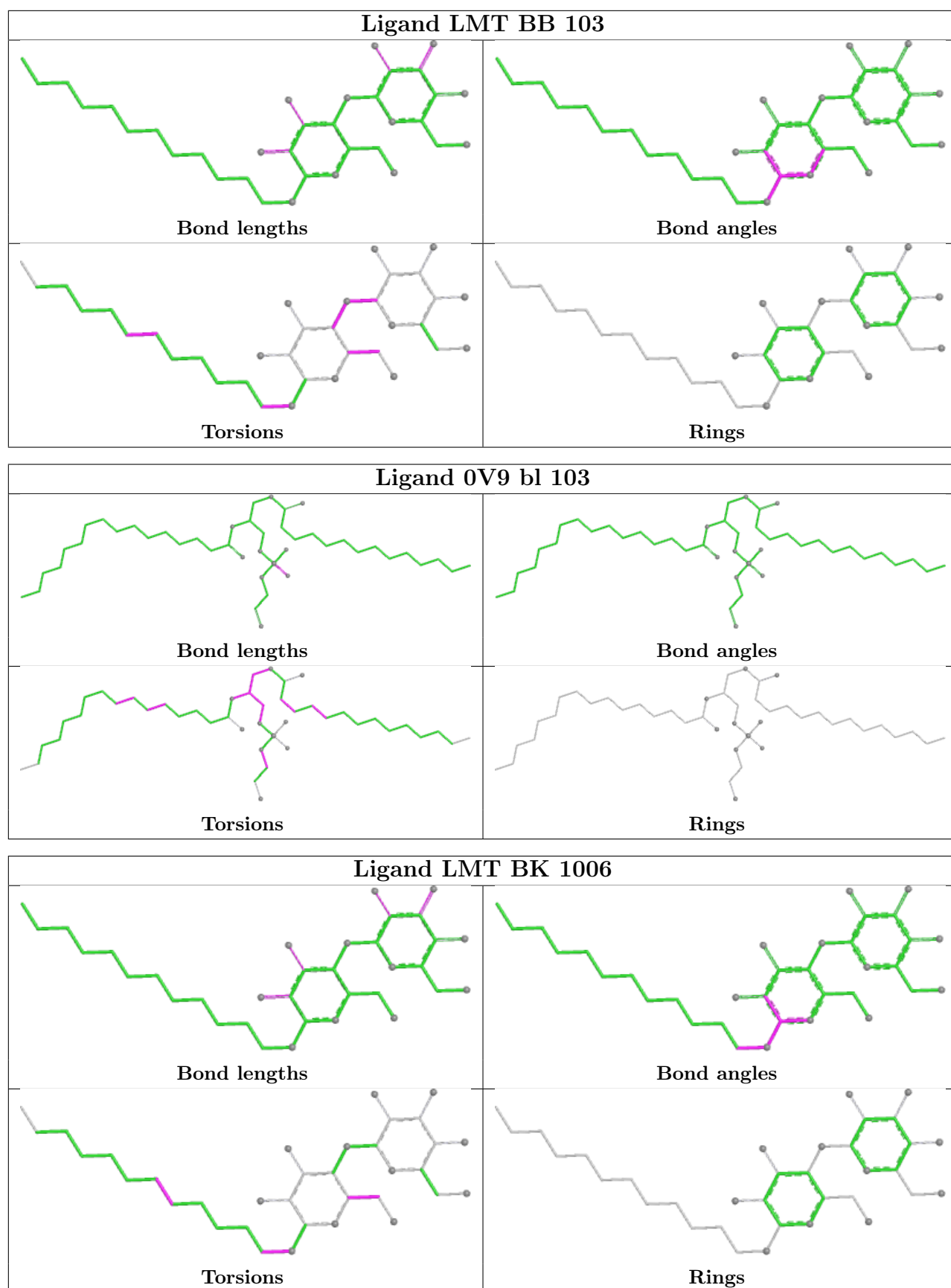


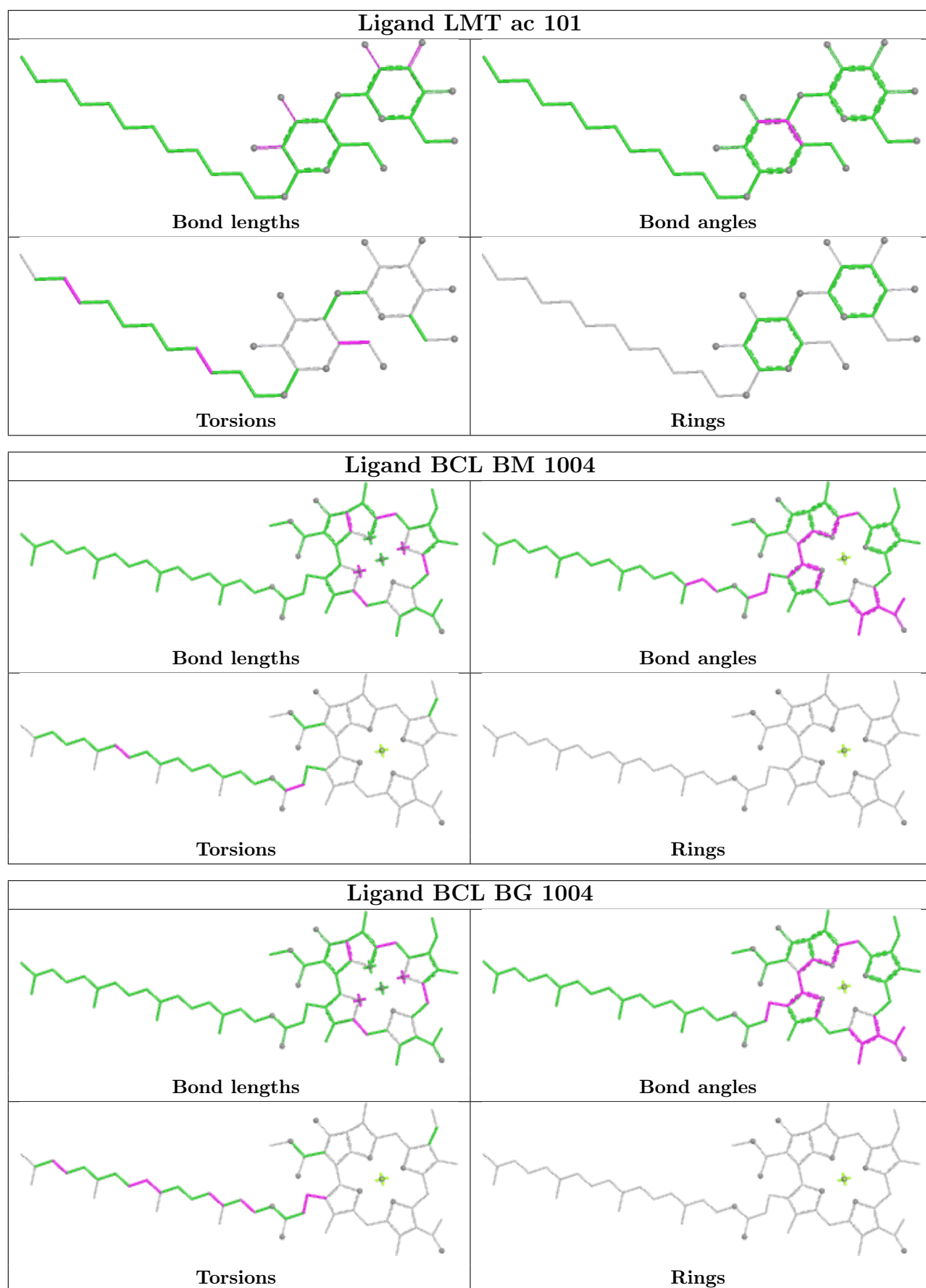




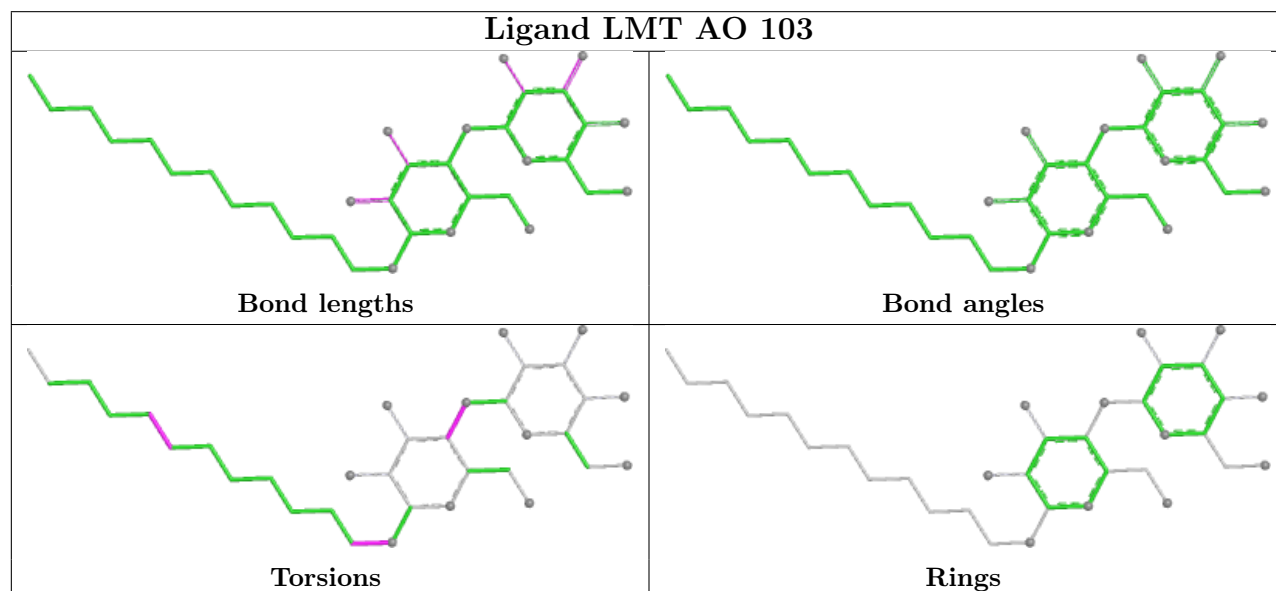
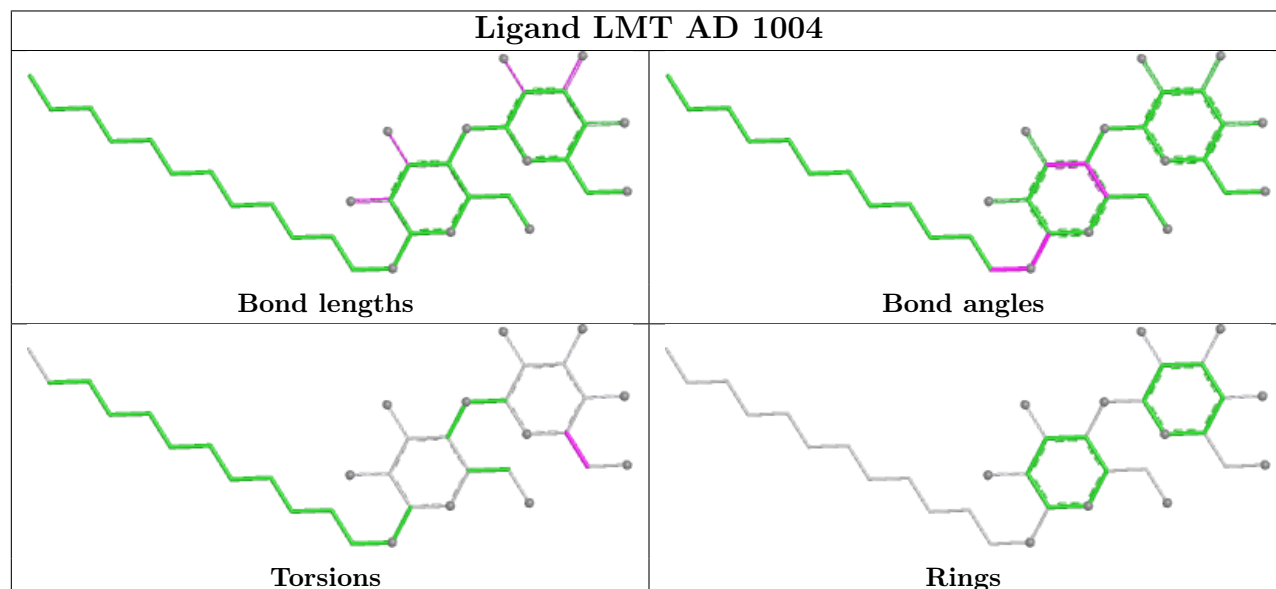
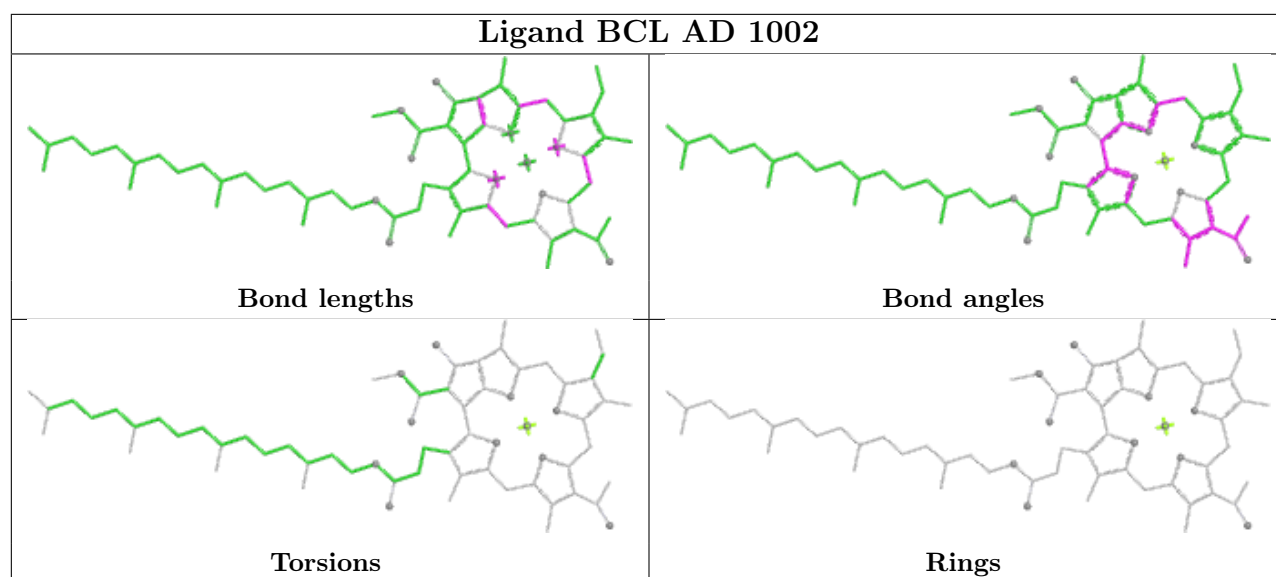


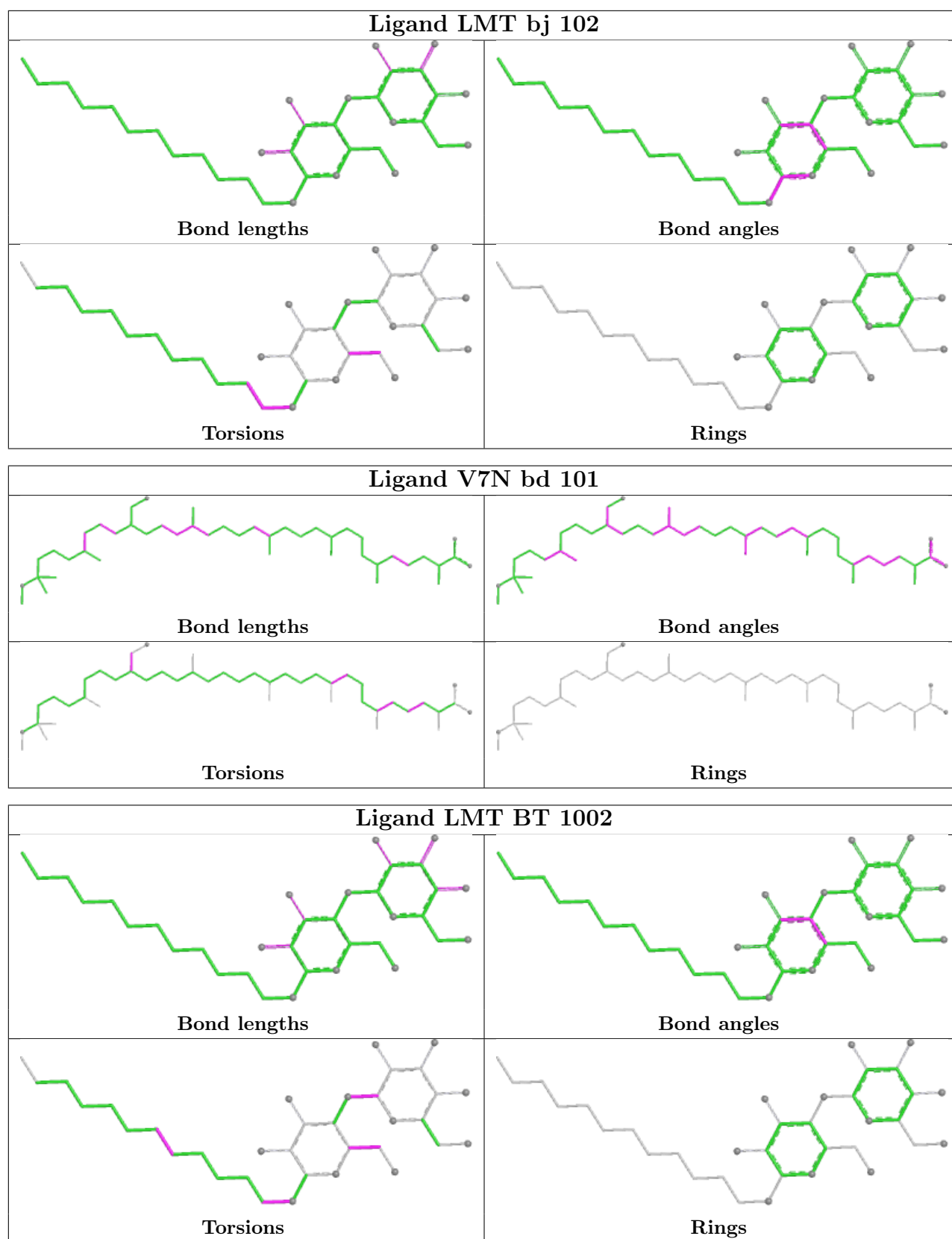


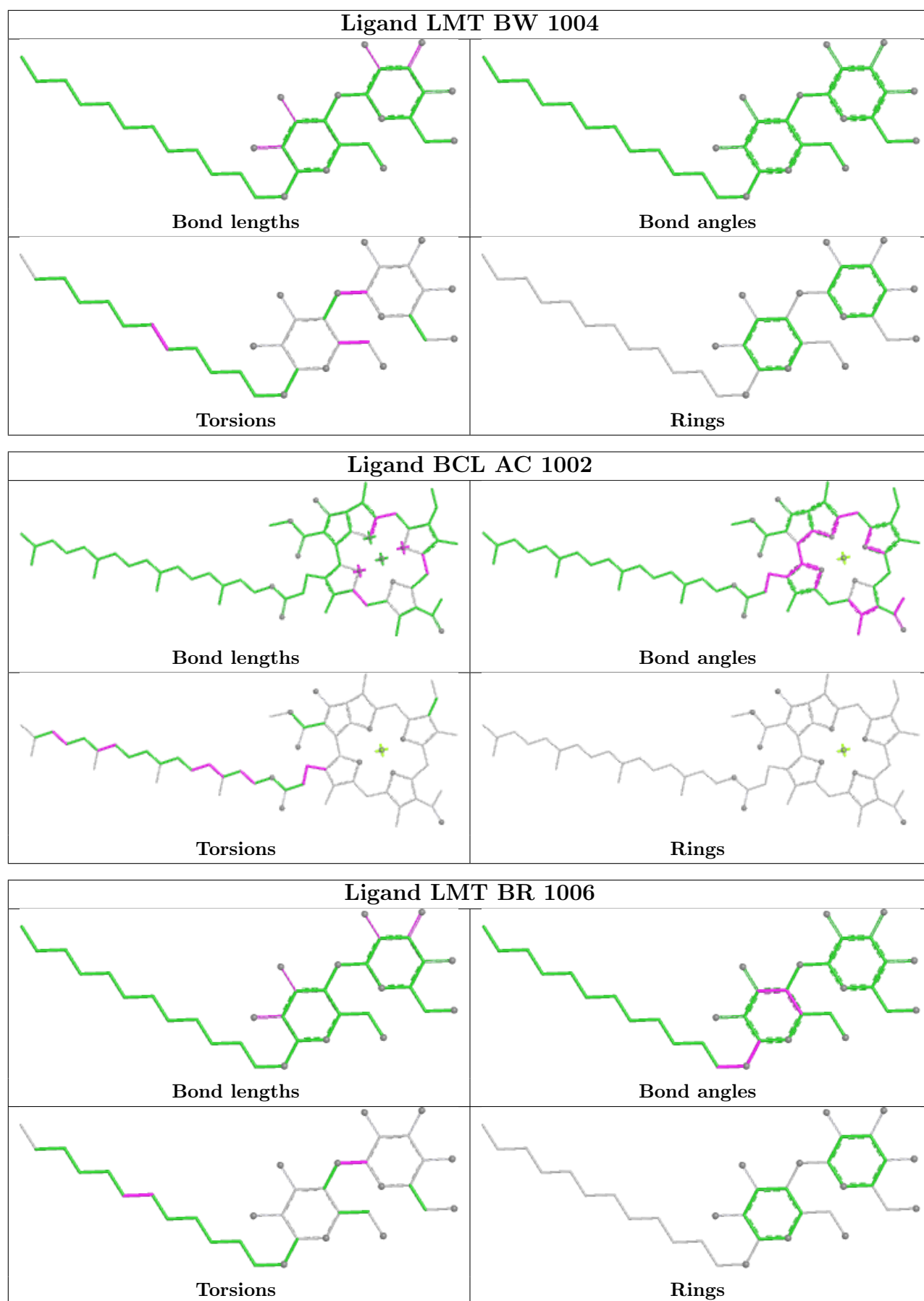


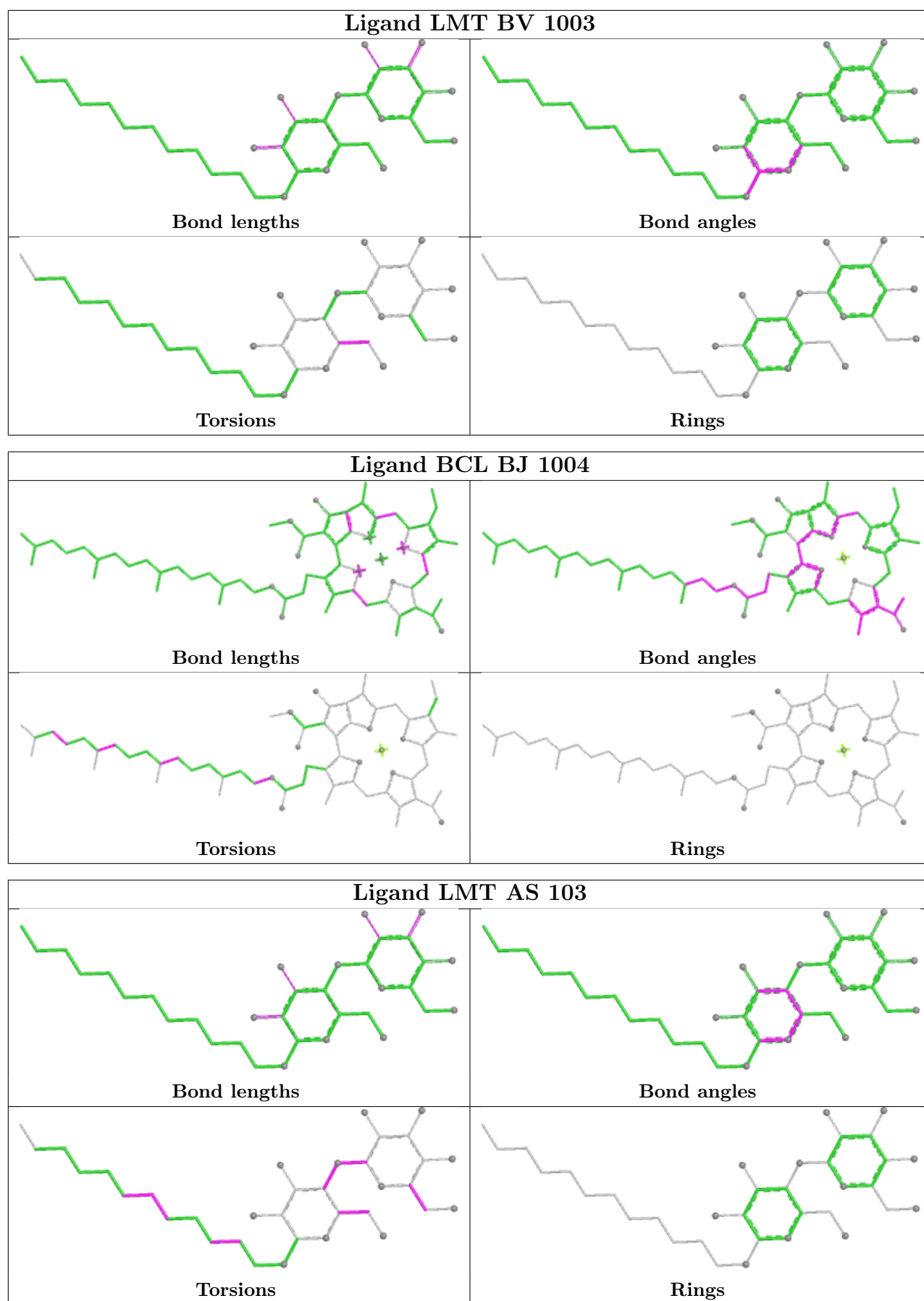


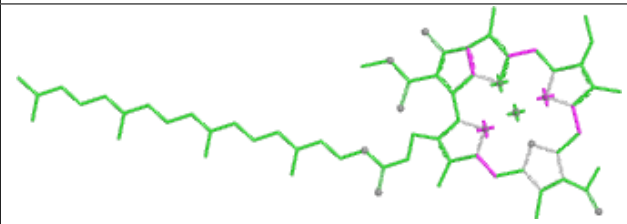
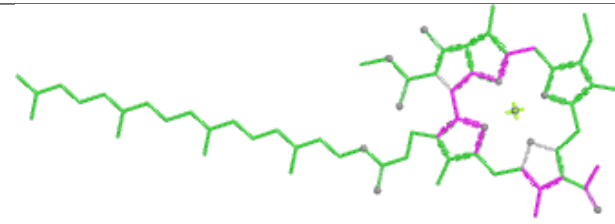
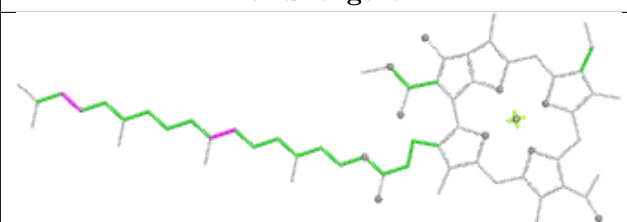
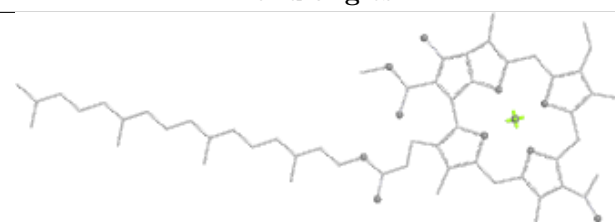


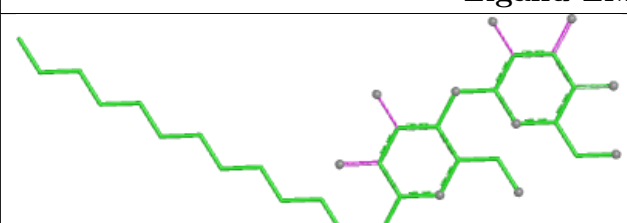

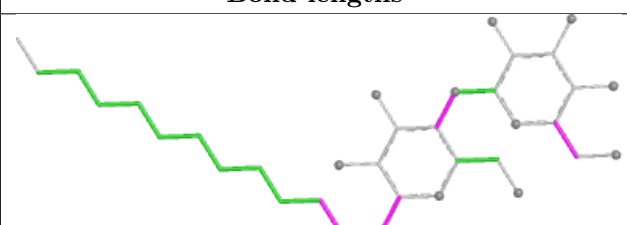
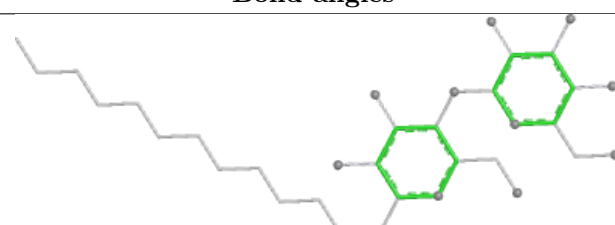


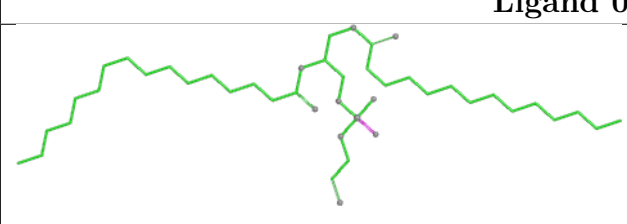
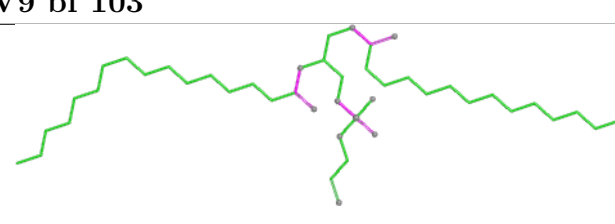
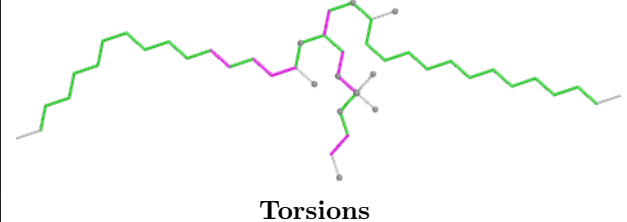
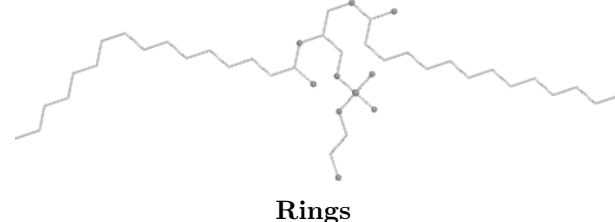


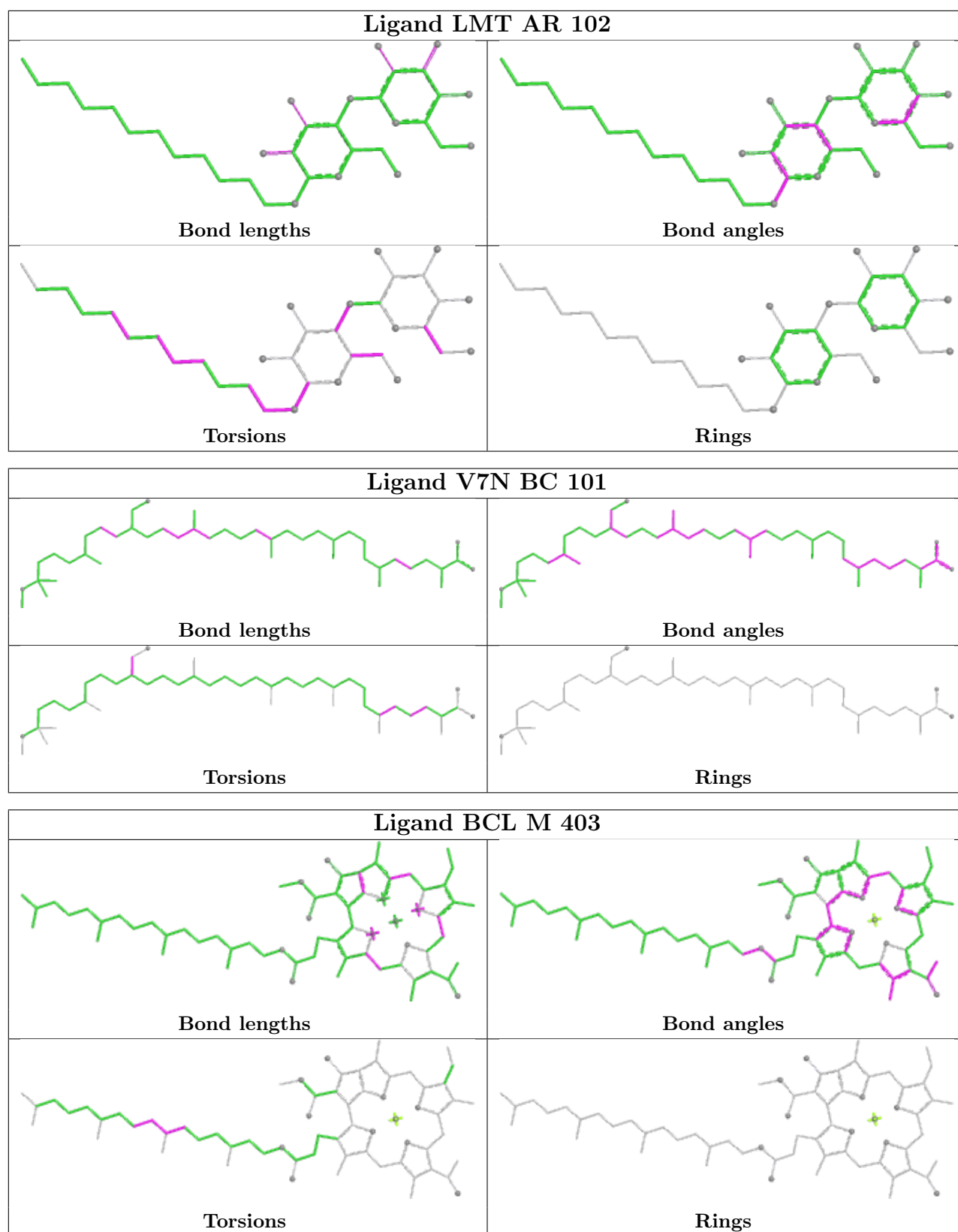




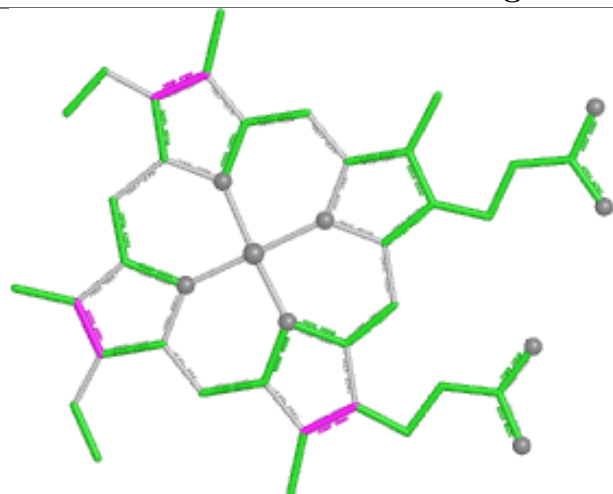
| Ligand BCL AQ 101   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand LMT BK 1002  |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

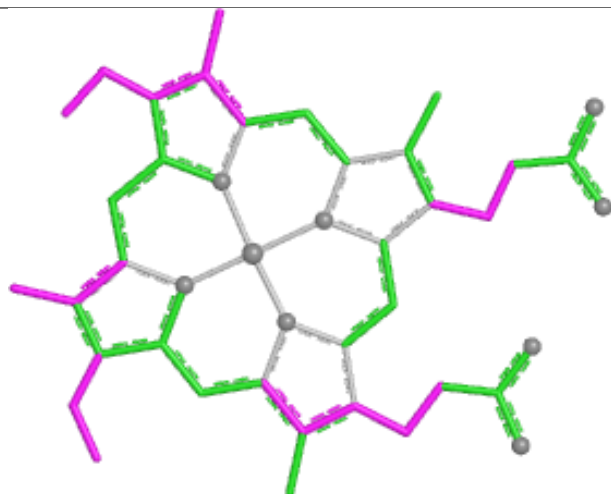
| Ligand OV9 bf 103   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |



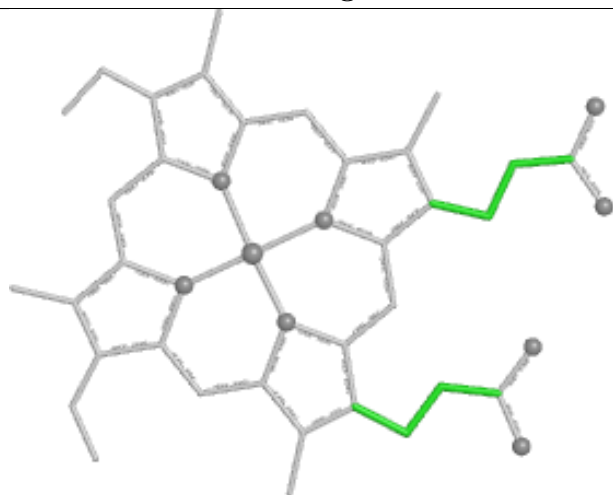
## Ligand HEC C 1004



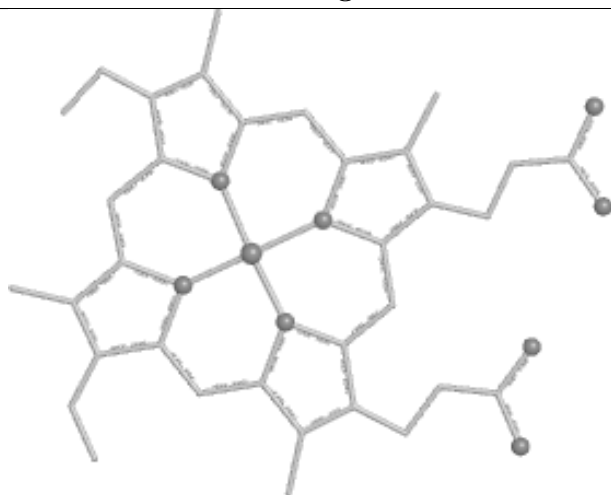
Bond lengths



Bond angles

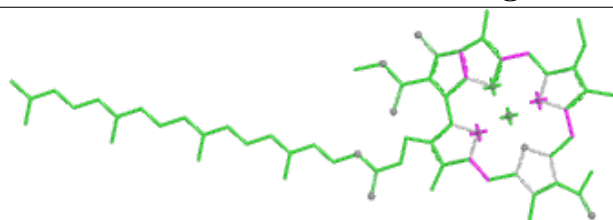


Torsions

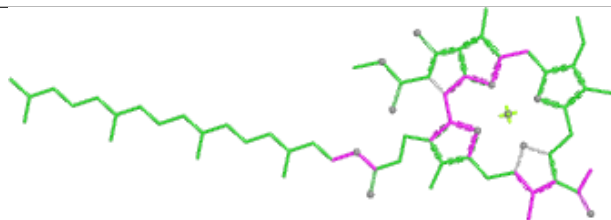


Rings

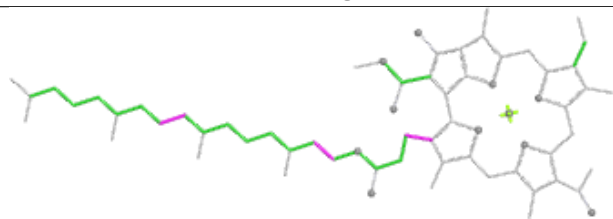
## Ligand BCL aa 1001



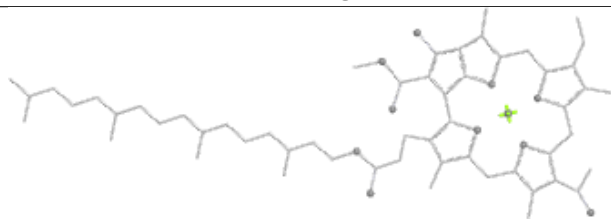
Bond lengths



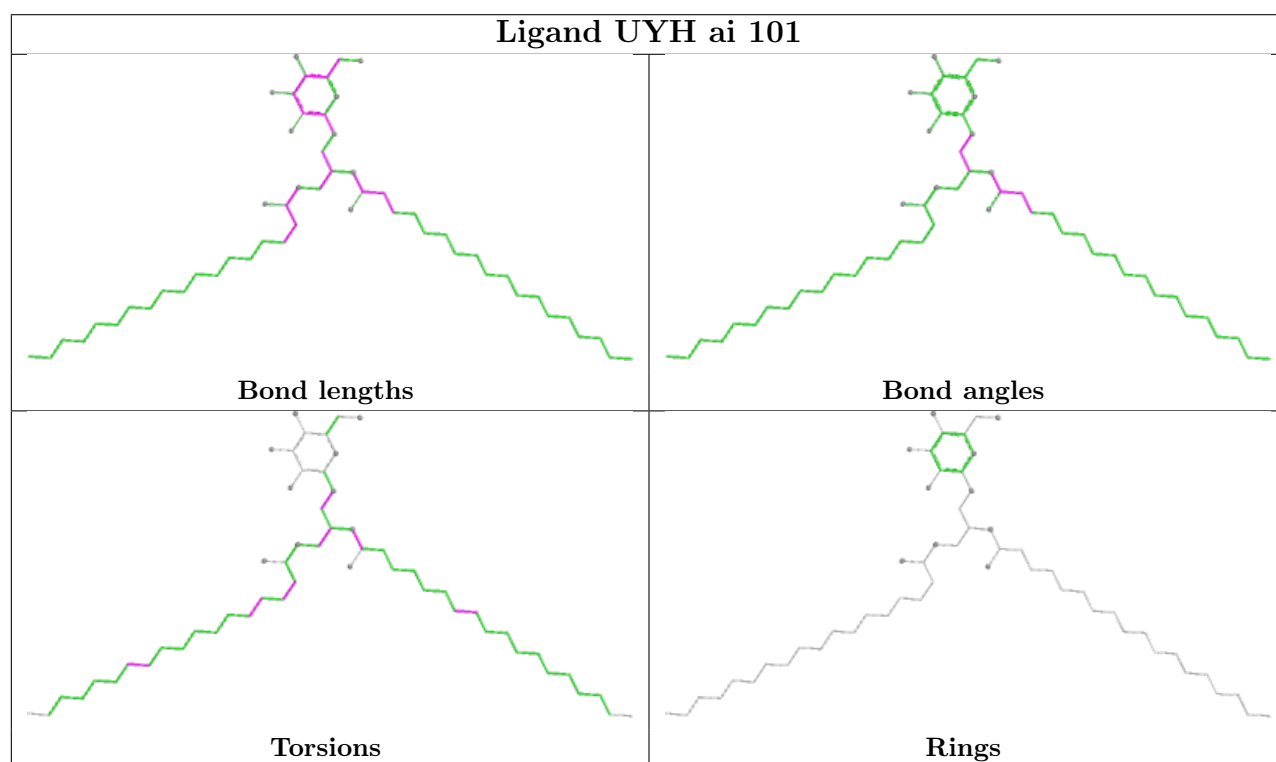
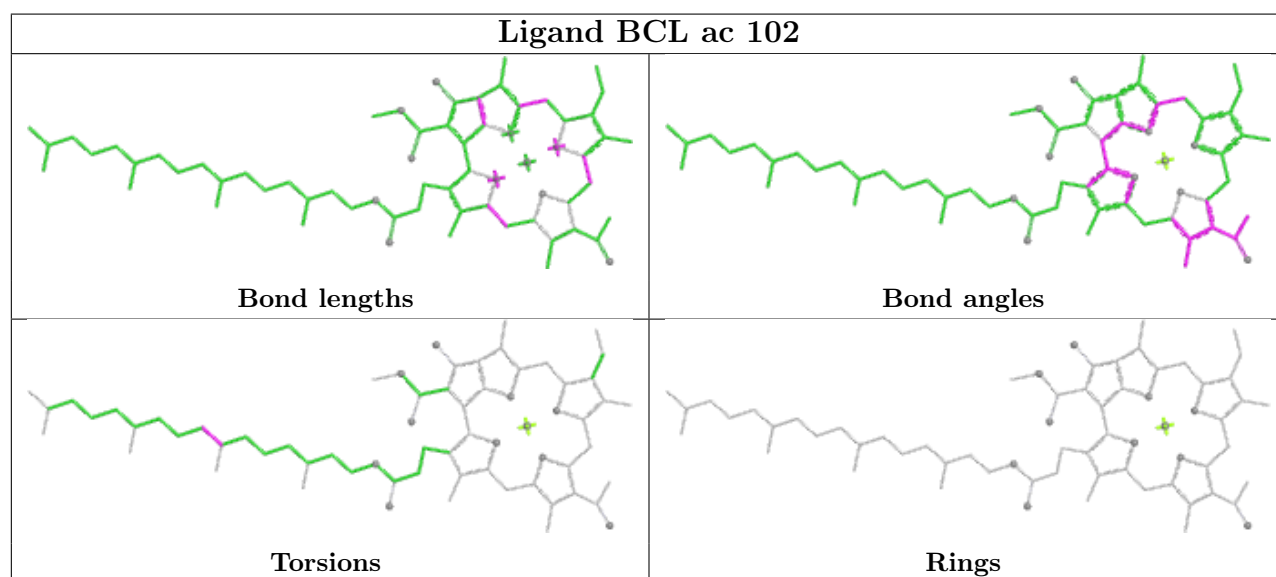
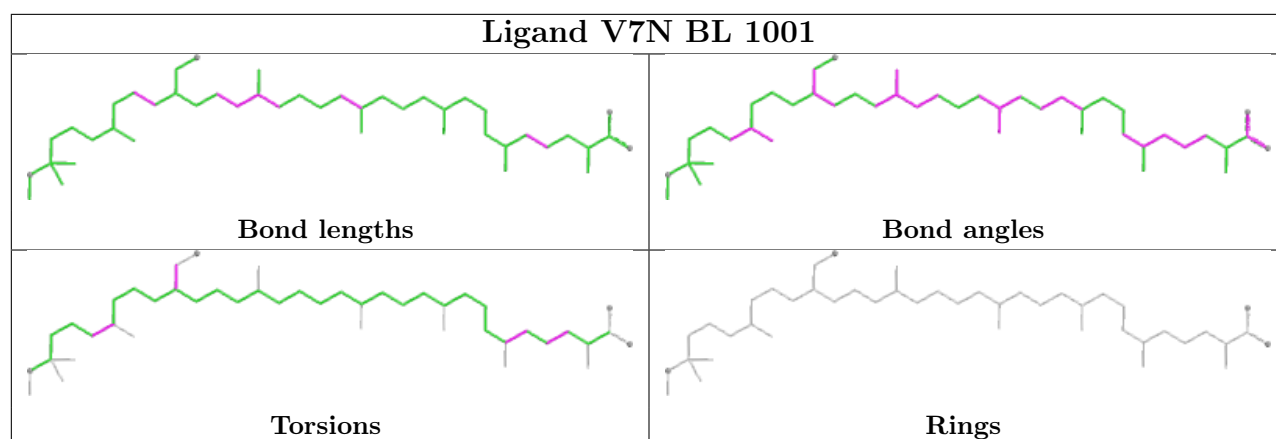
Bond angles



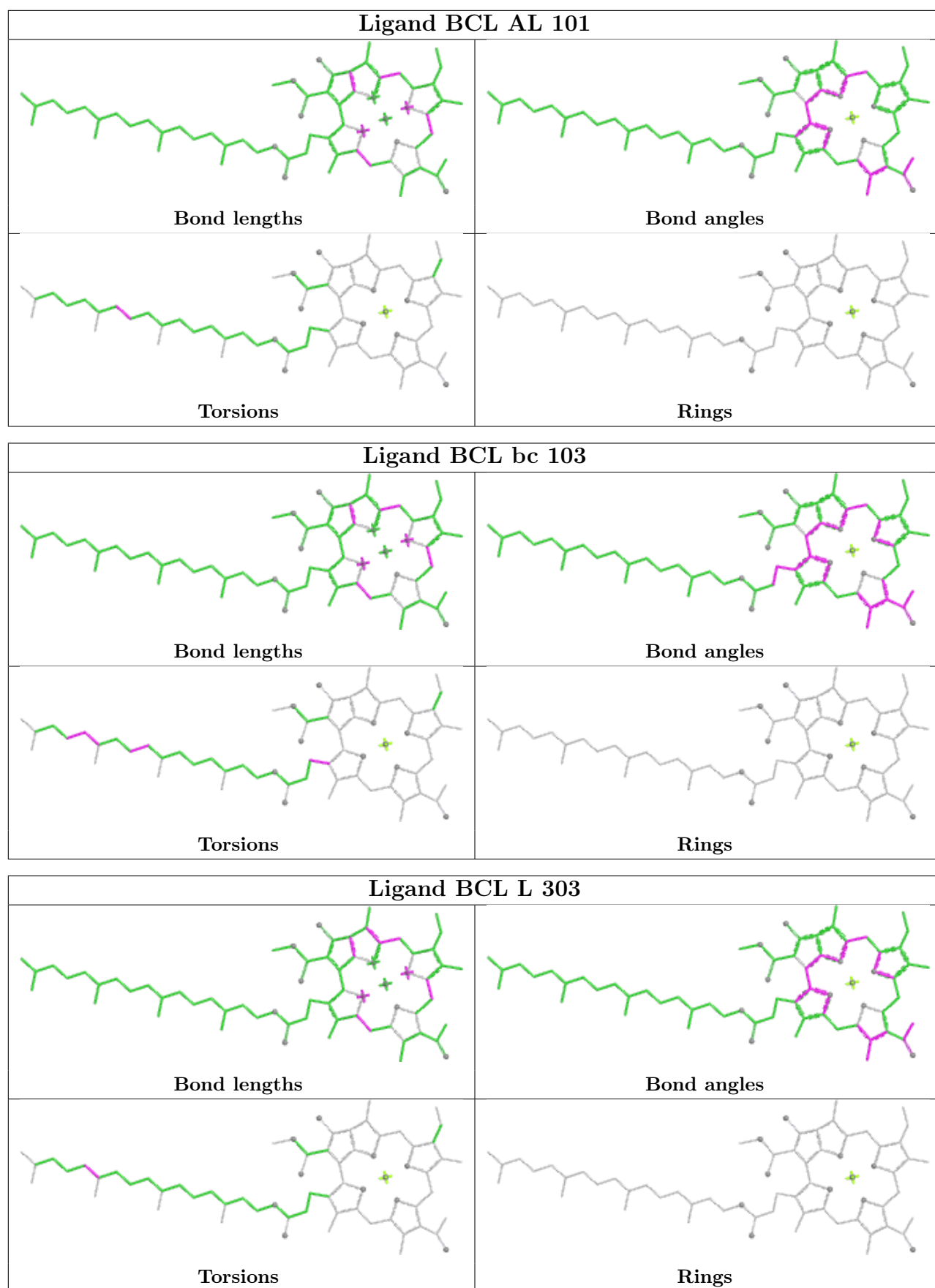
Torsions

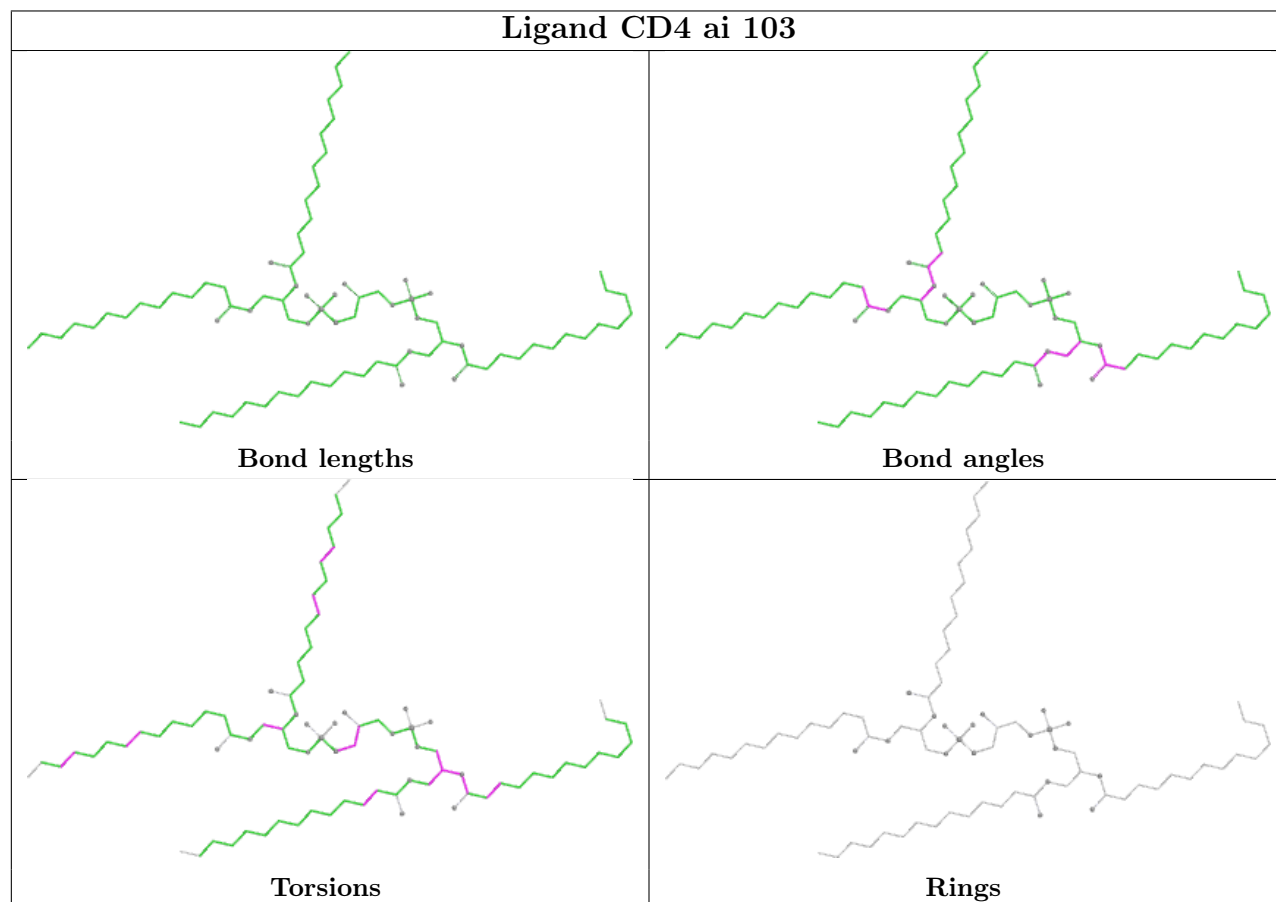
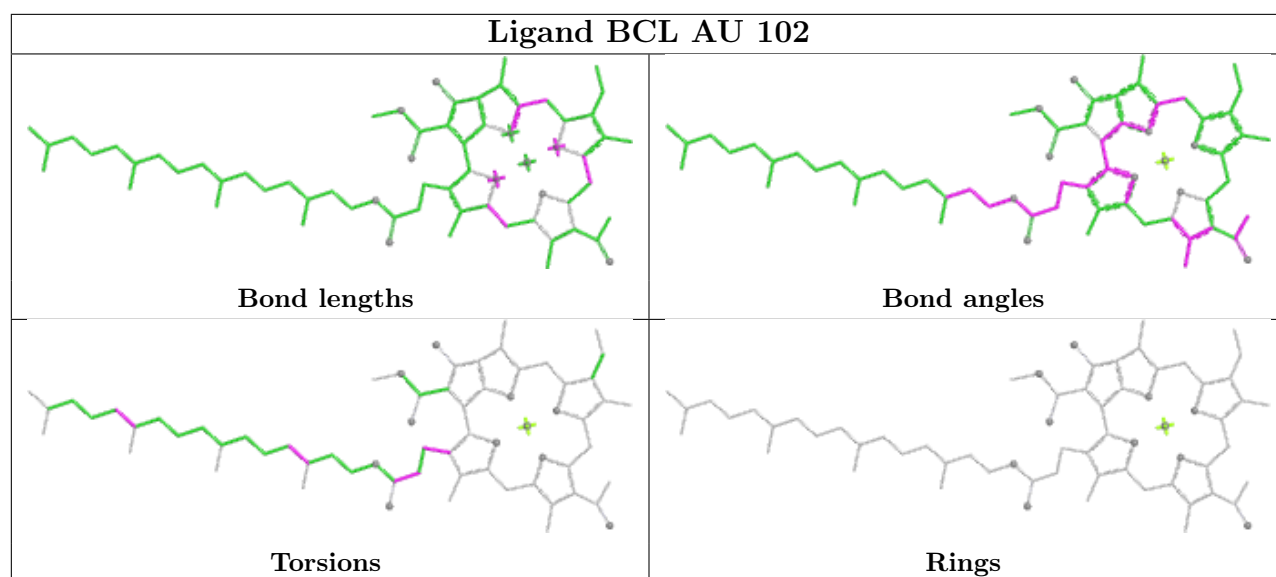


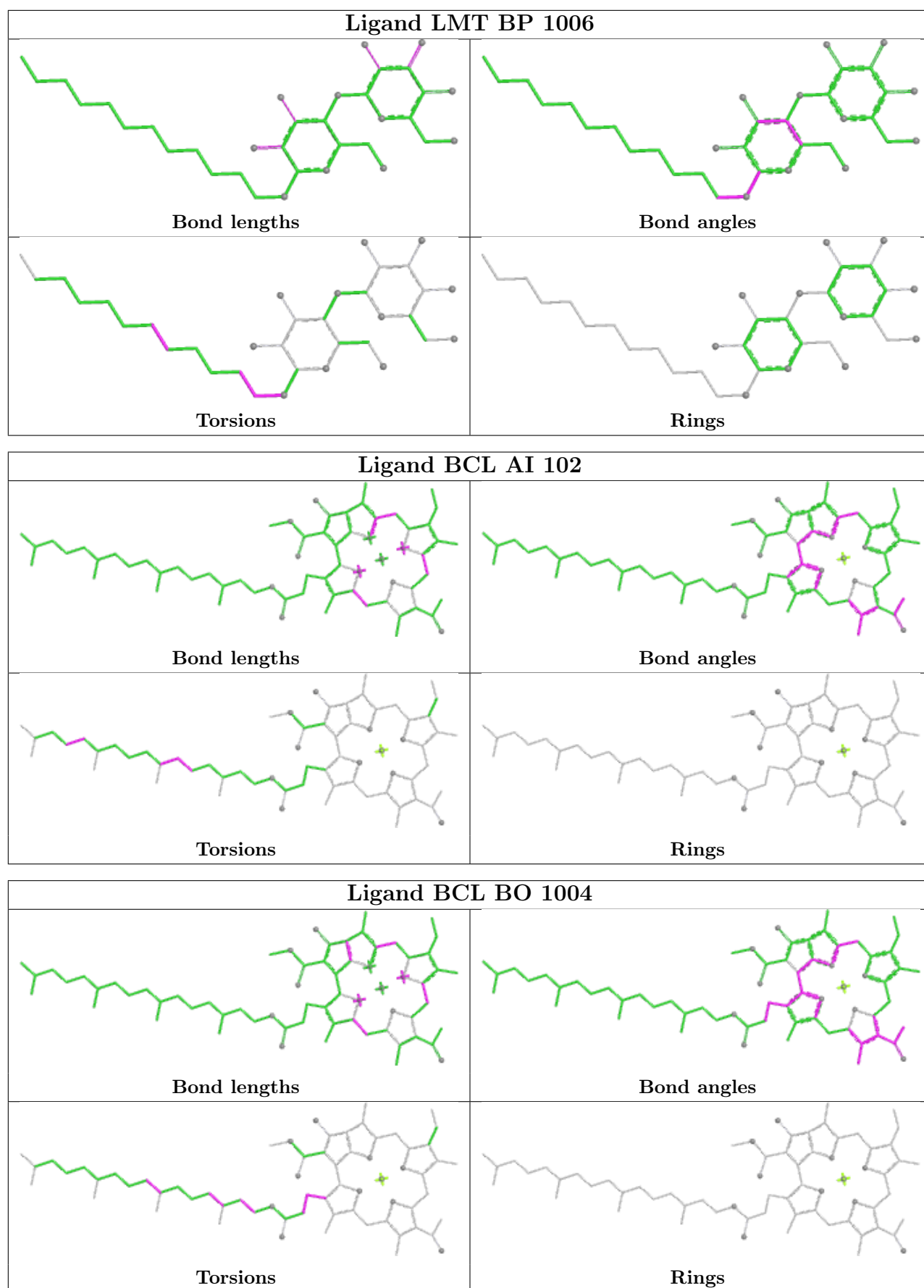
Rings

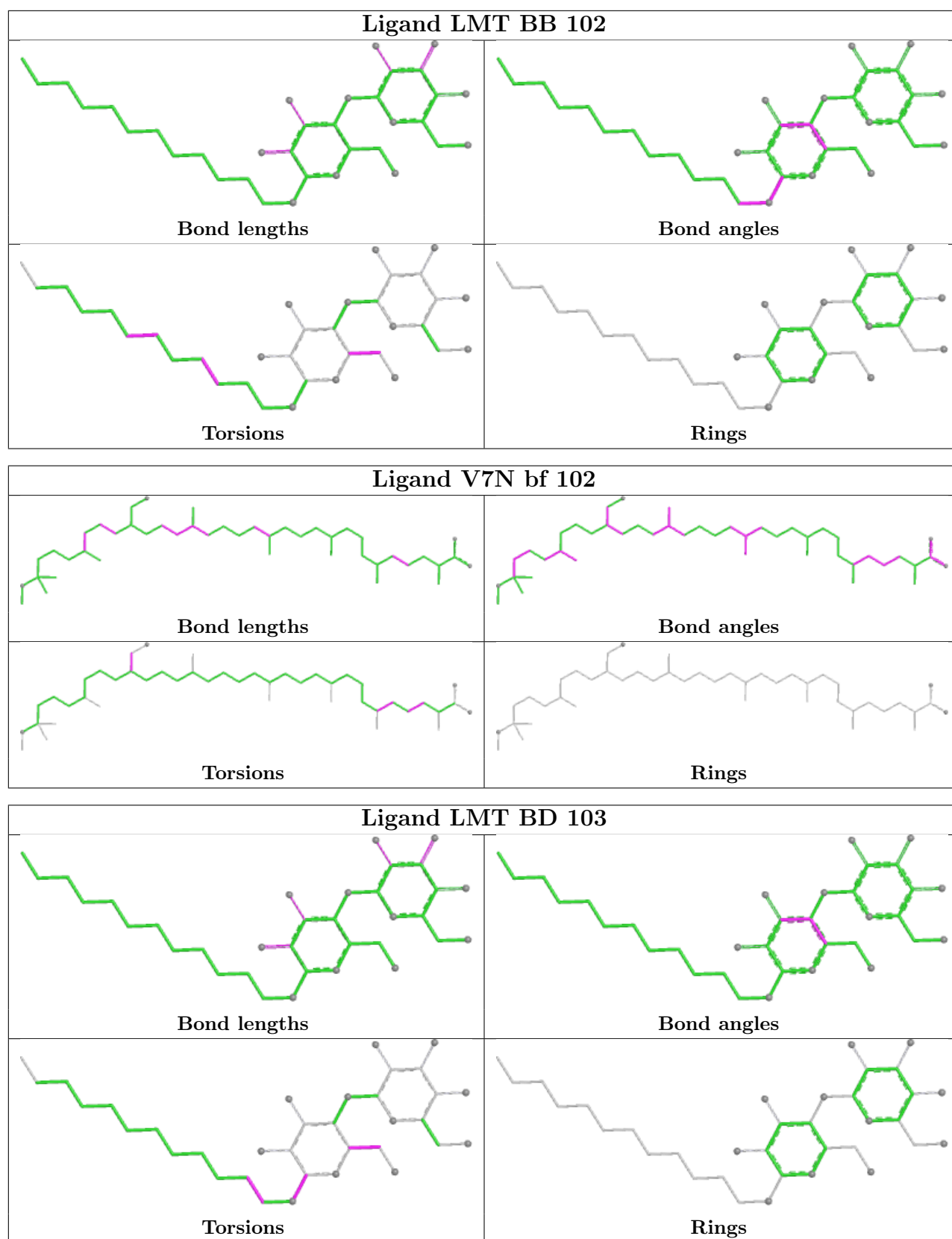


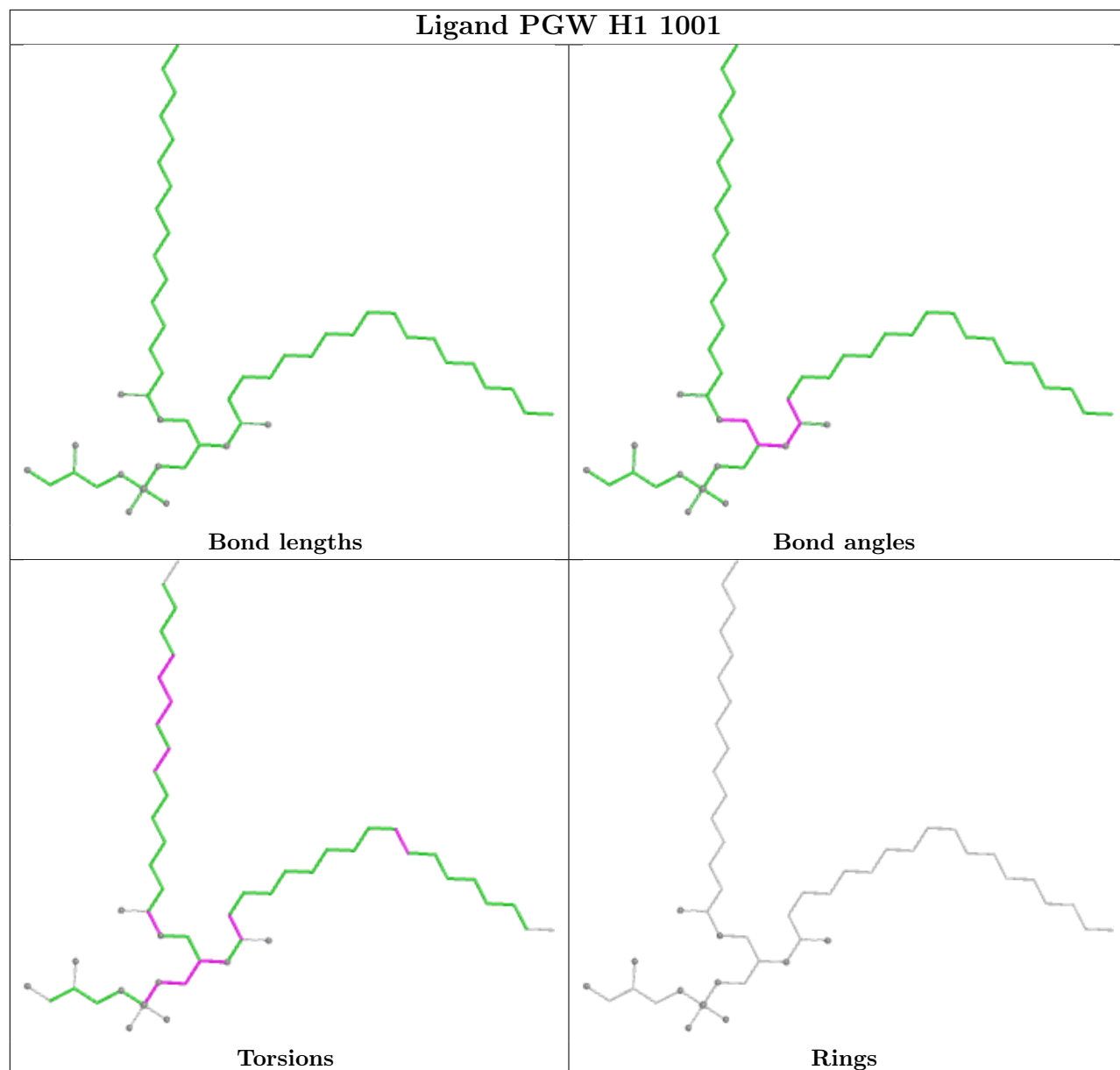


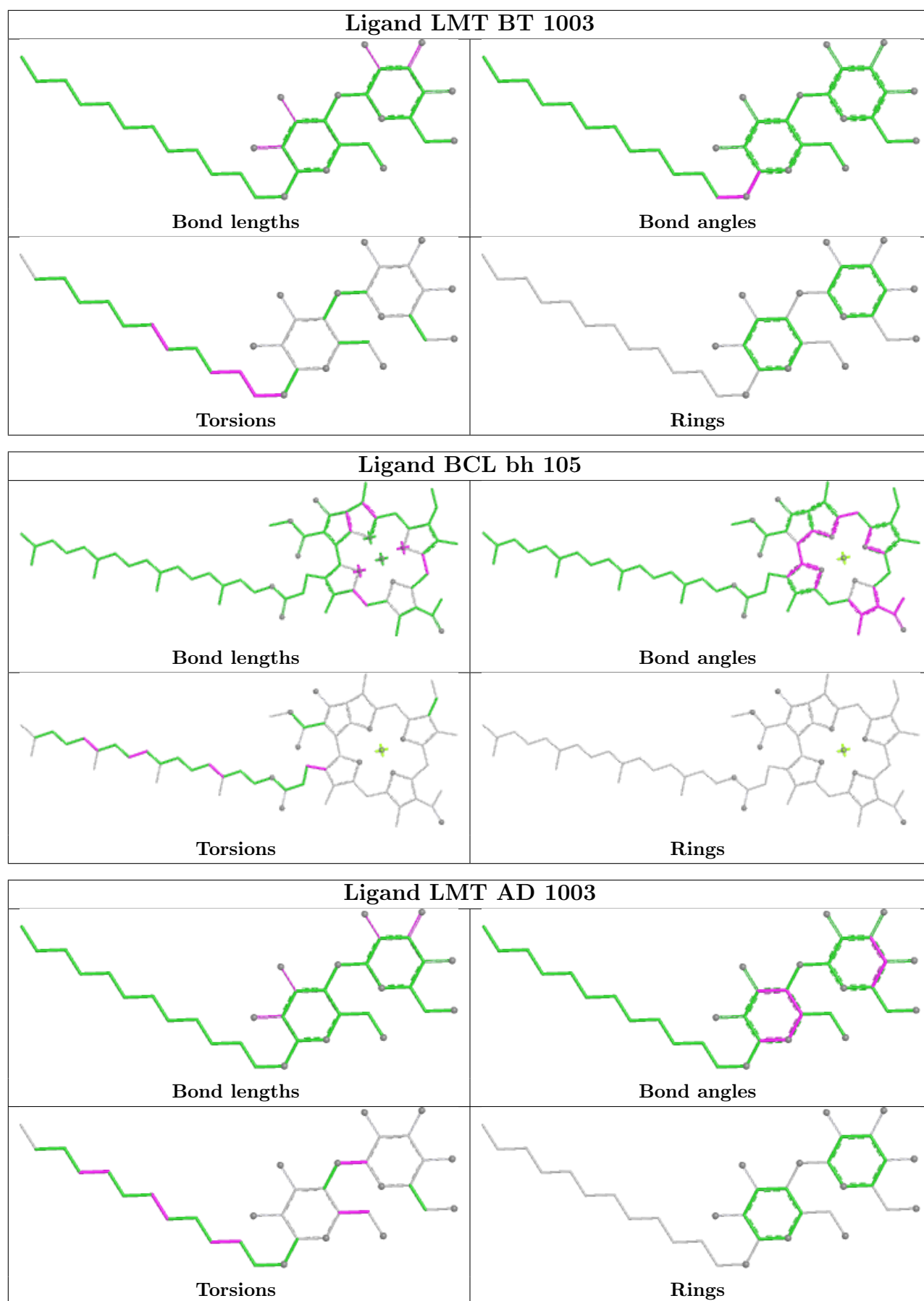


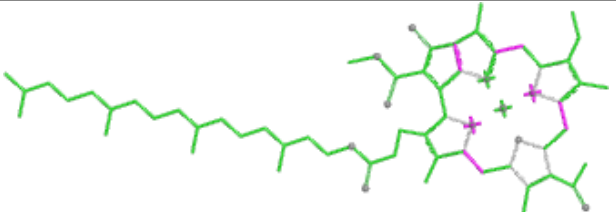
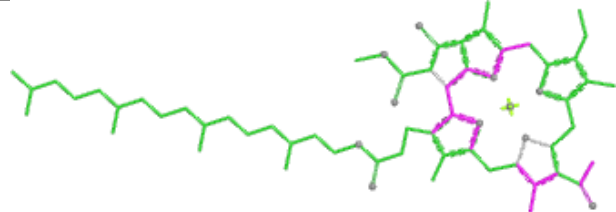
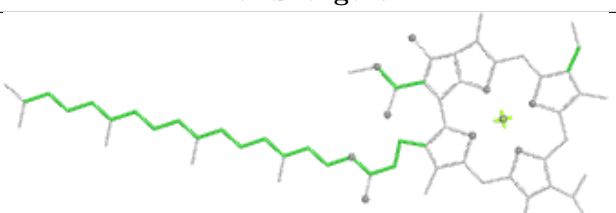
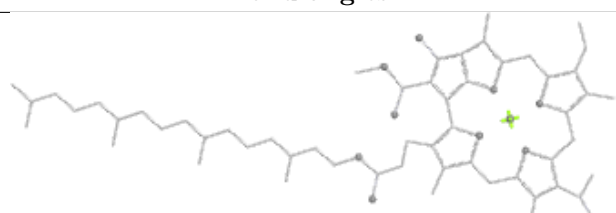


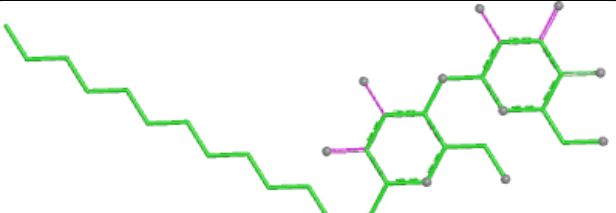
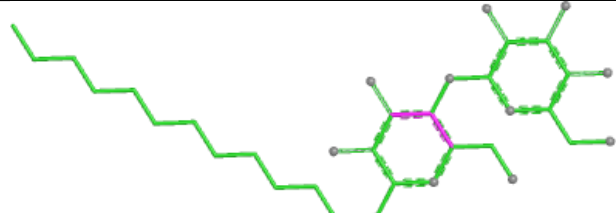
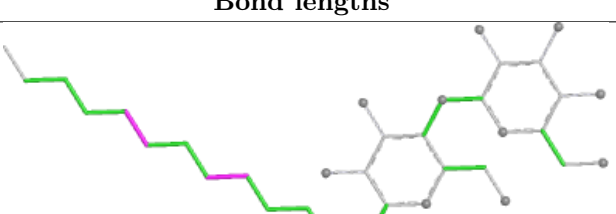
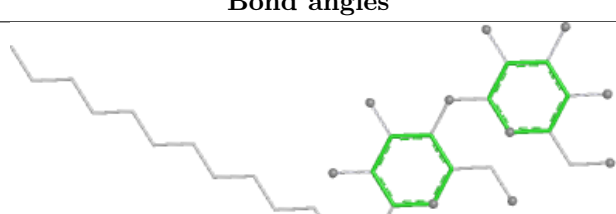


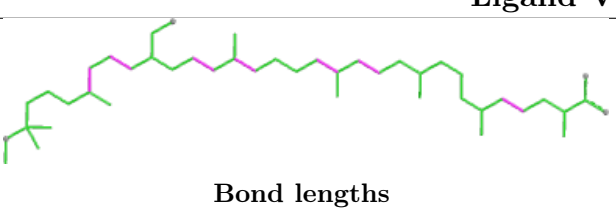
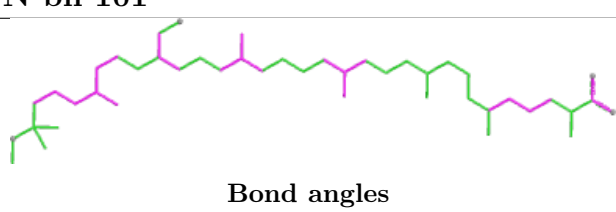
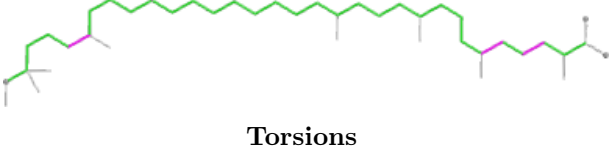



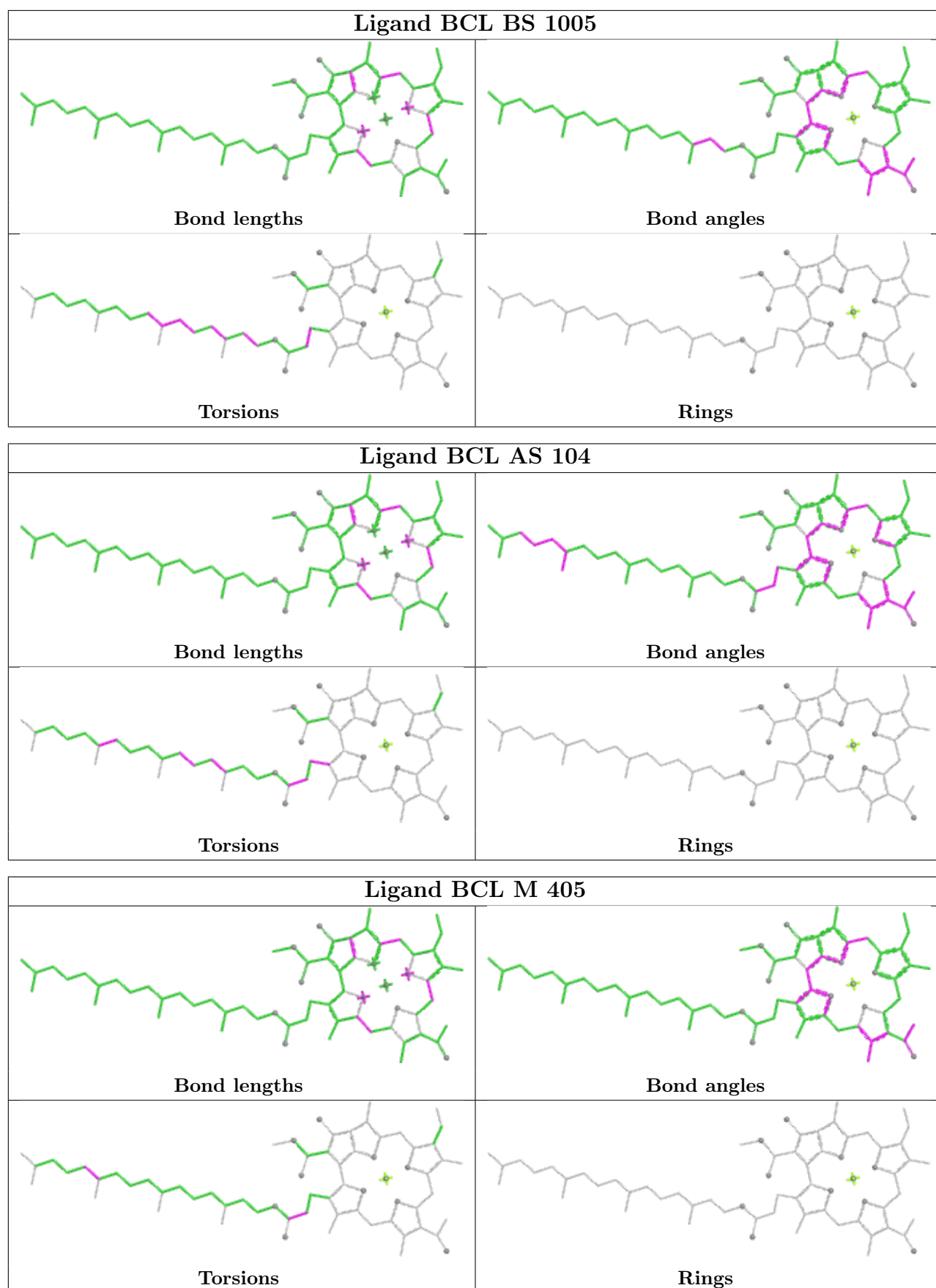




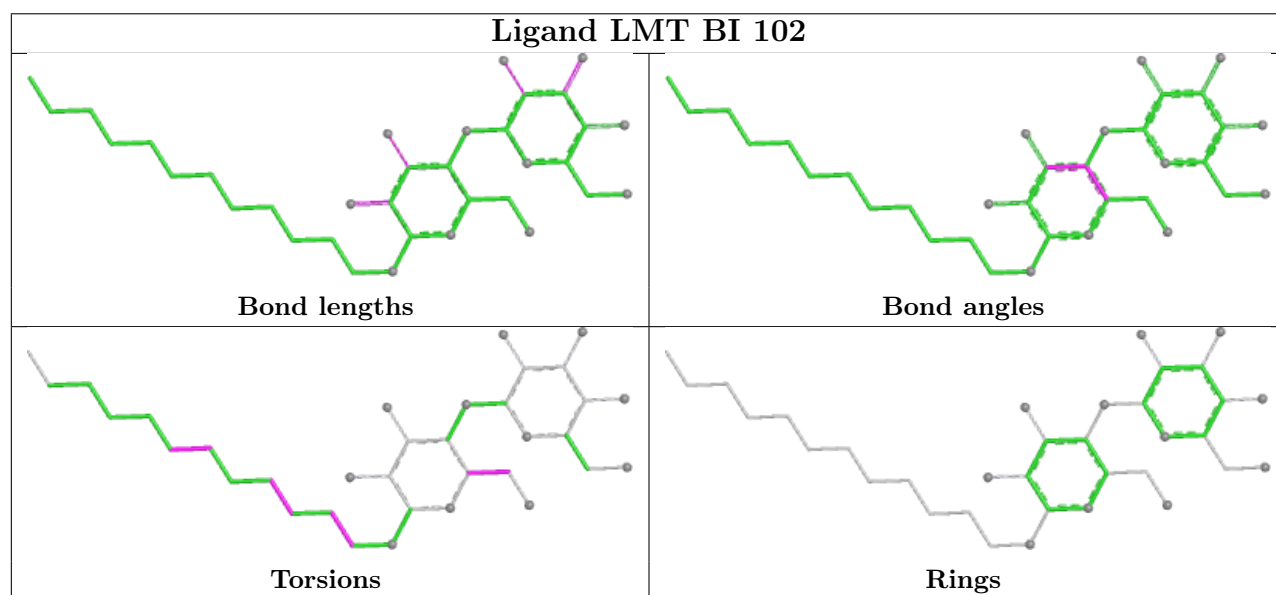
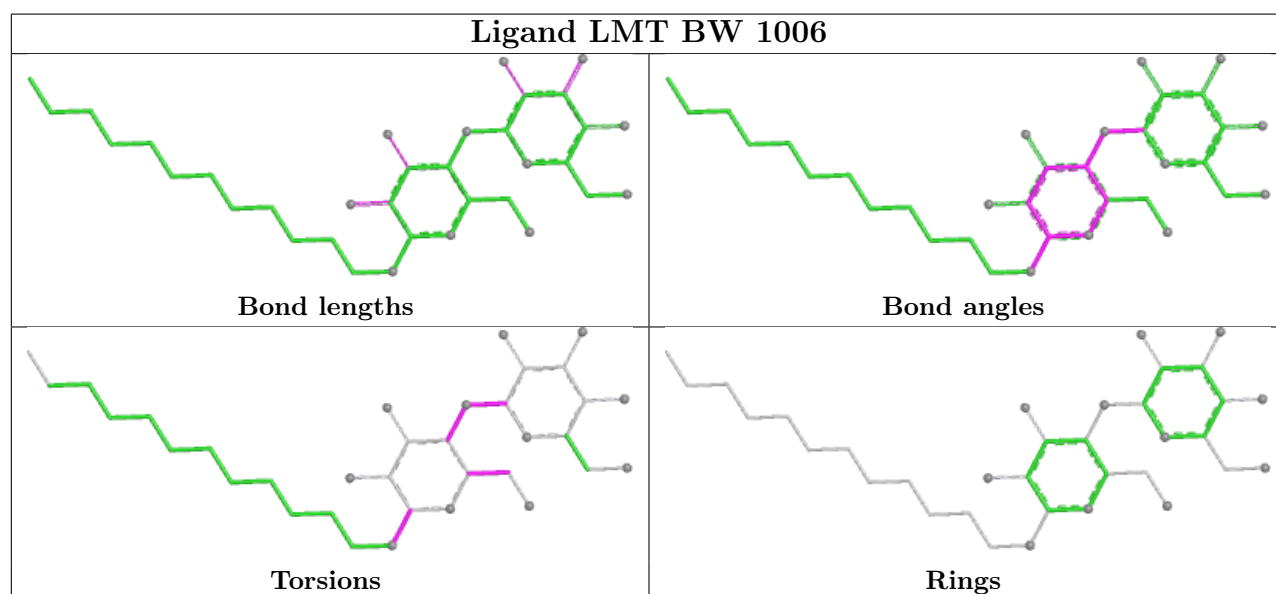
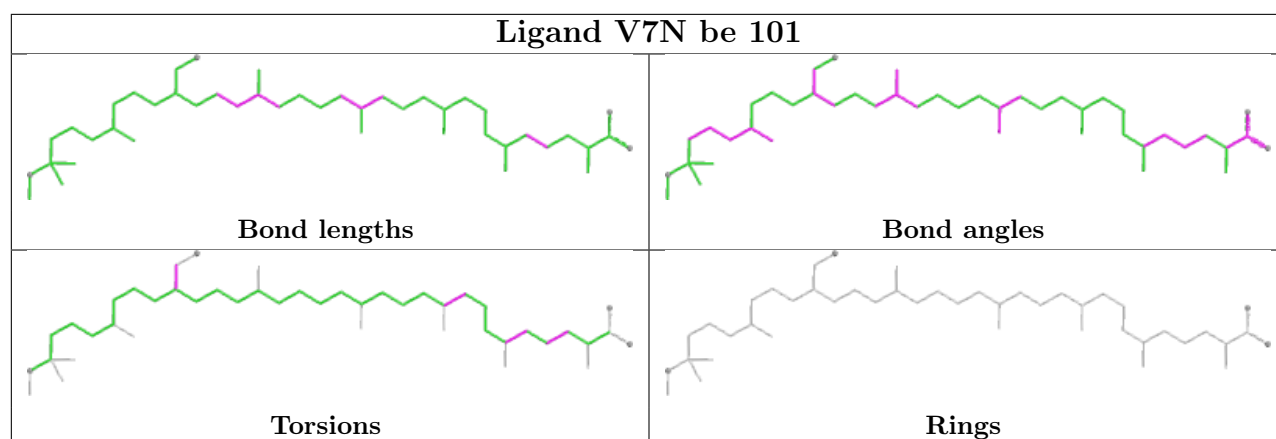
| Ligand BCL AJ 101   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

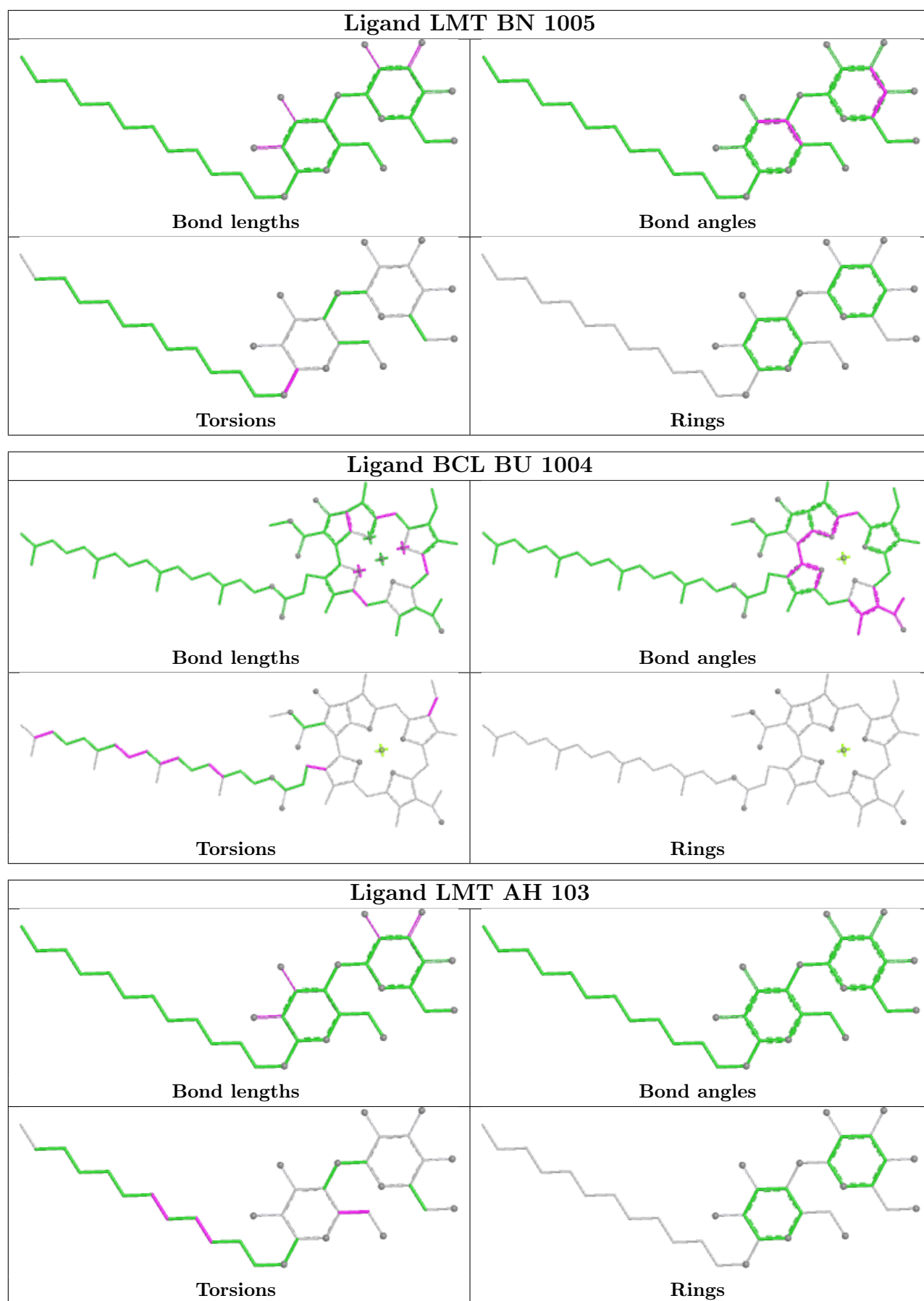
| Ligand LMT BD 104   |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

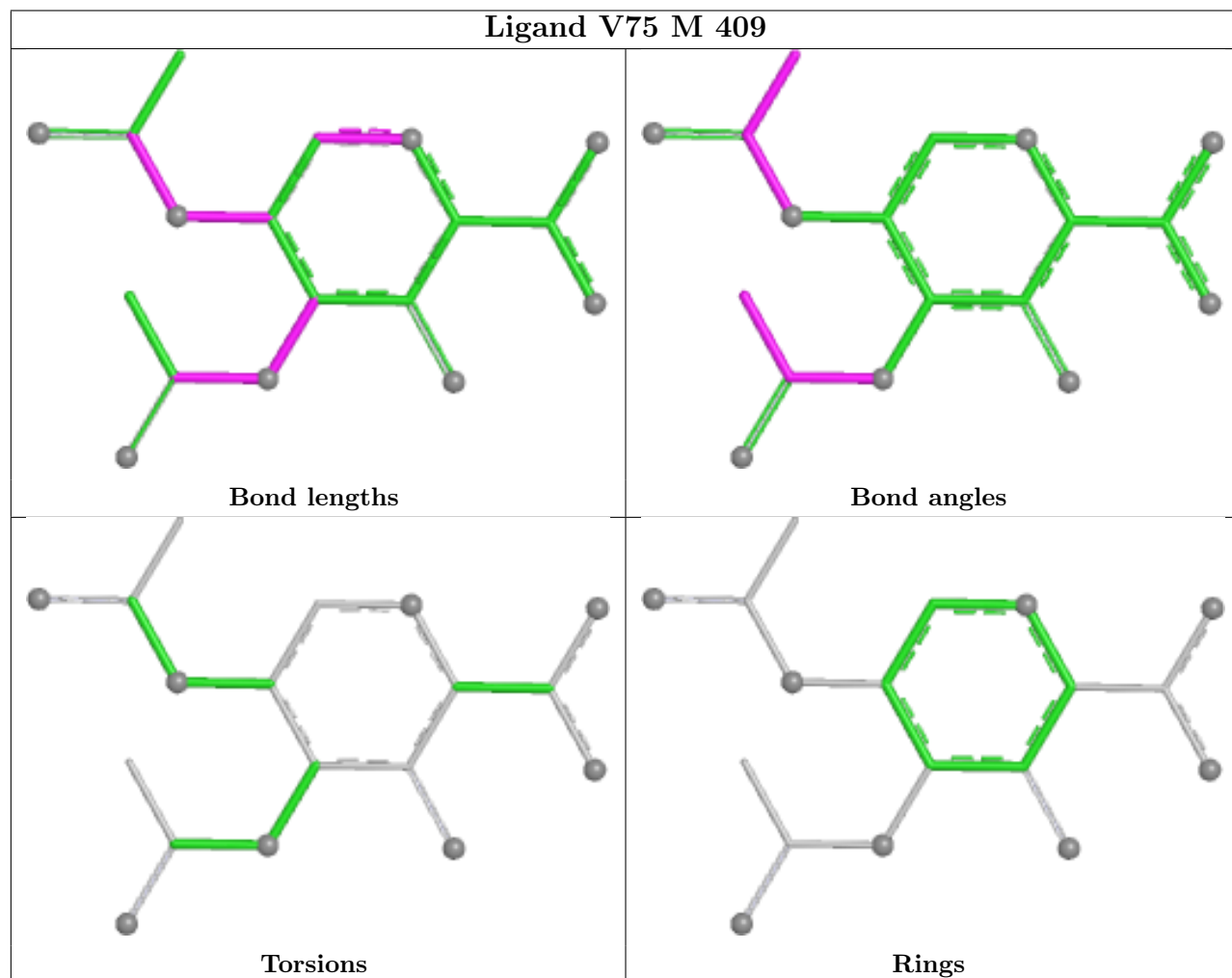
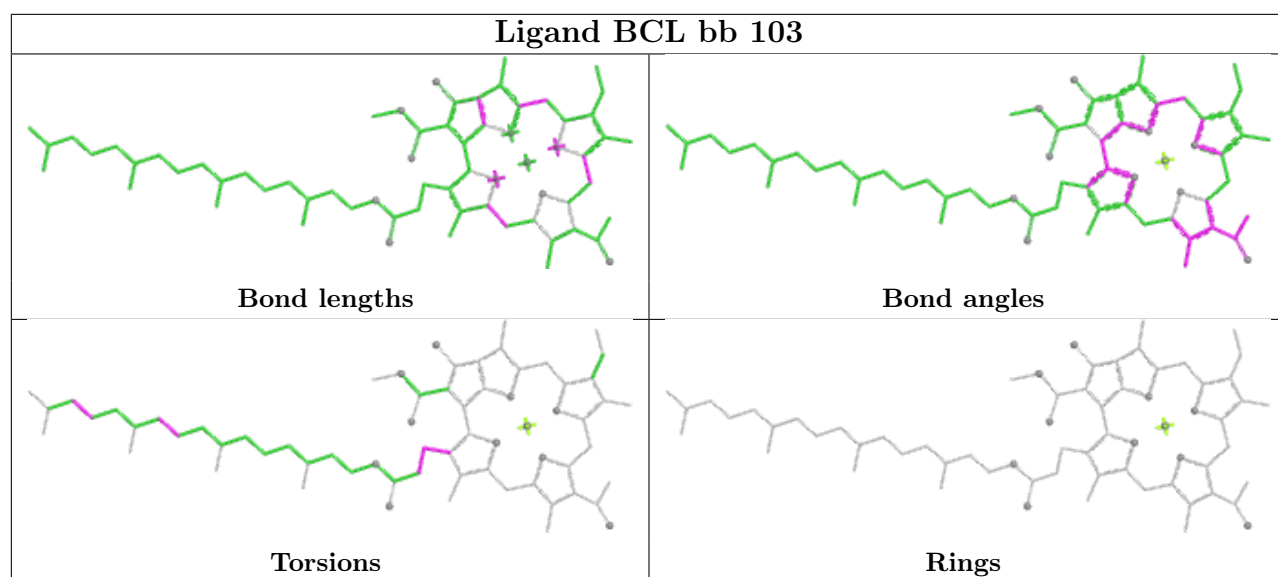
| Ligand V7N bn 101   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

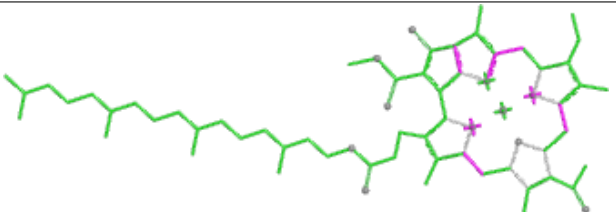
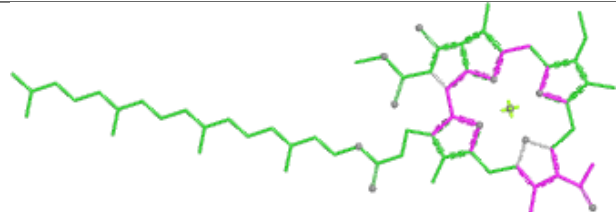
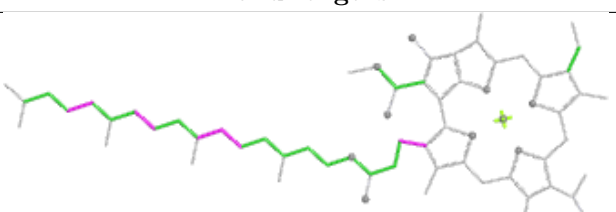
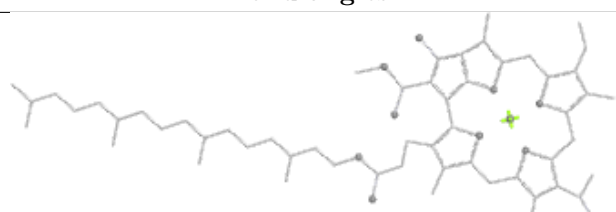


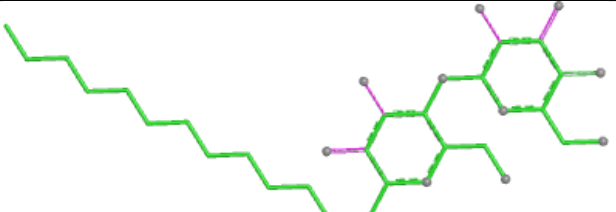
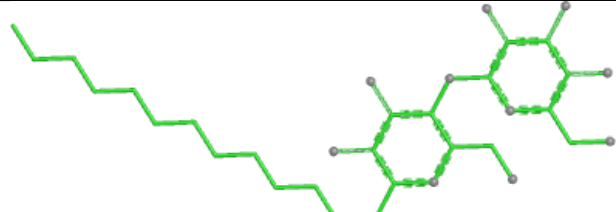
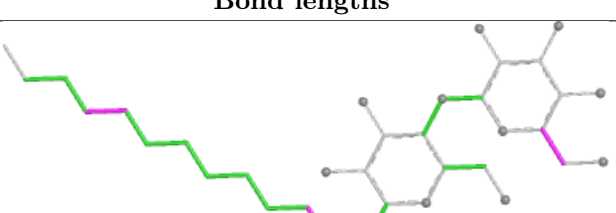
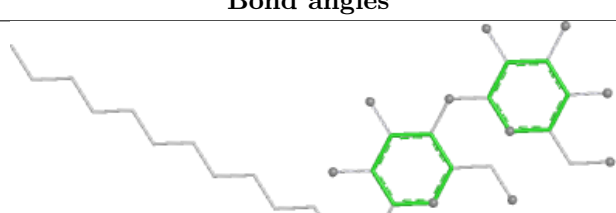


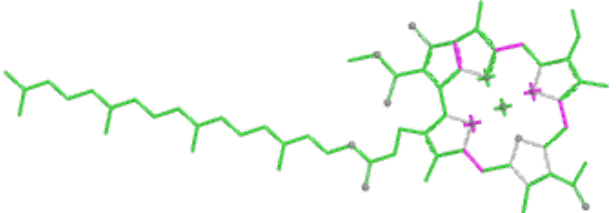
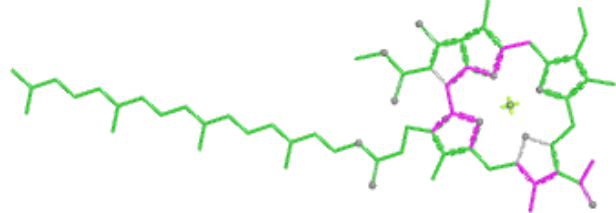
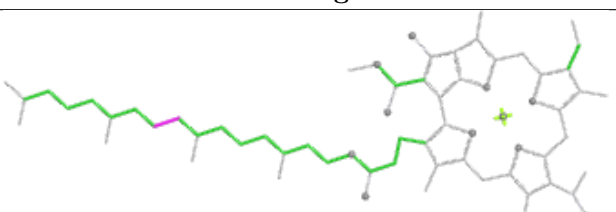
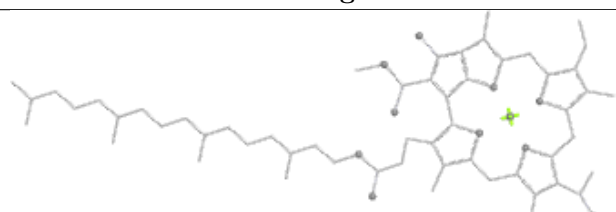


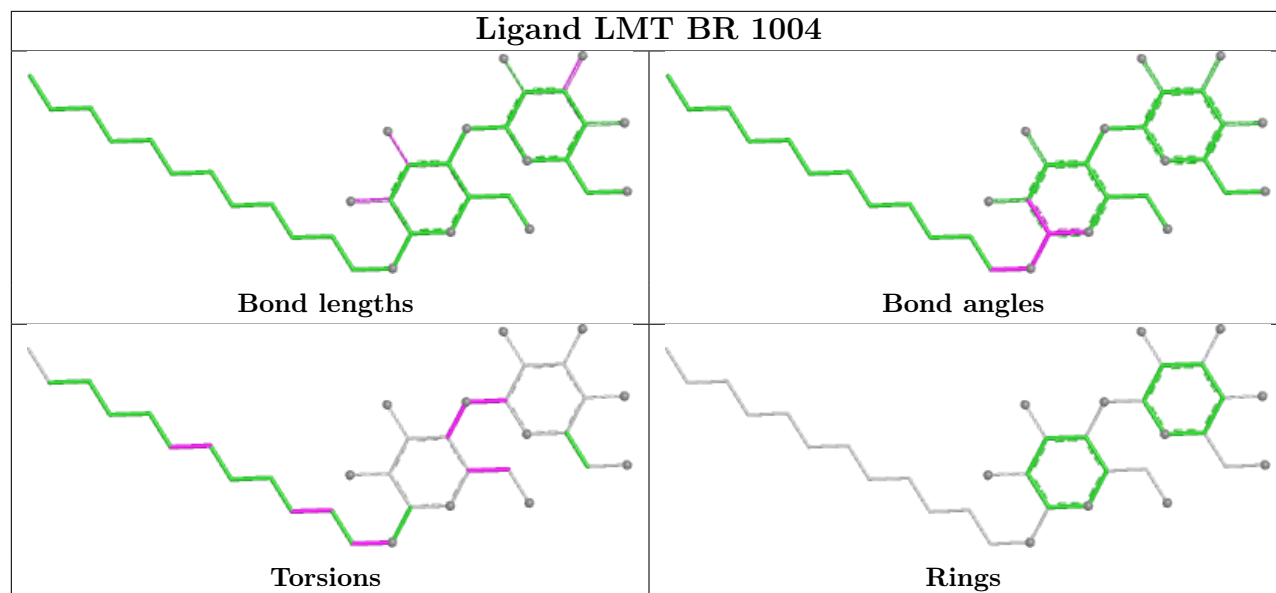




| Ligand BCL AV 103   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand LMT AI 101   |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand BCL AK 102   |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

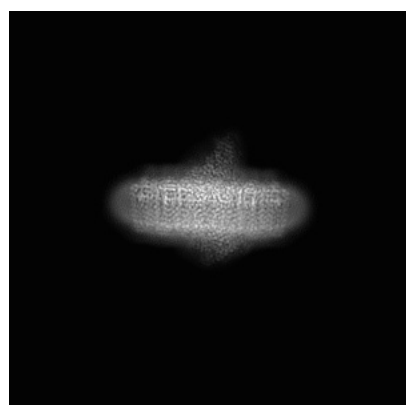
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12682. These allow visual inspection of the internal detail of the map and identification of artifacts.

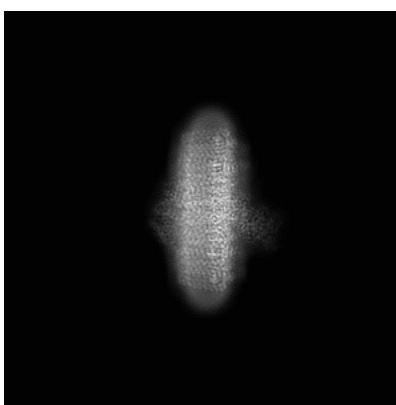
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

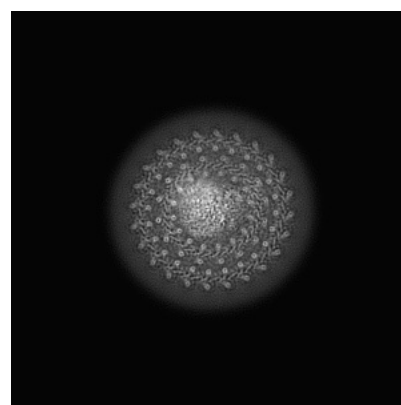
#### 6.1.1 Primary map



X



Y

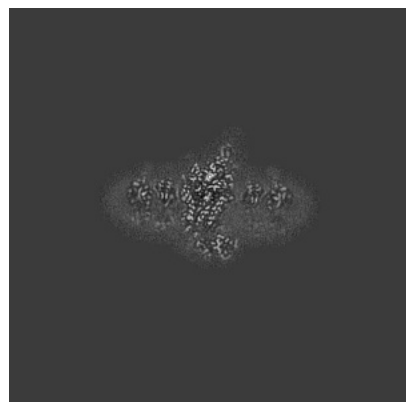


Z

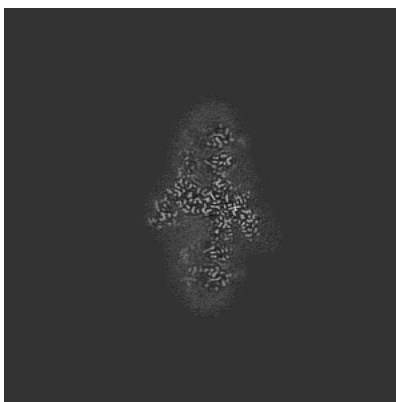
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

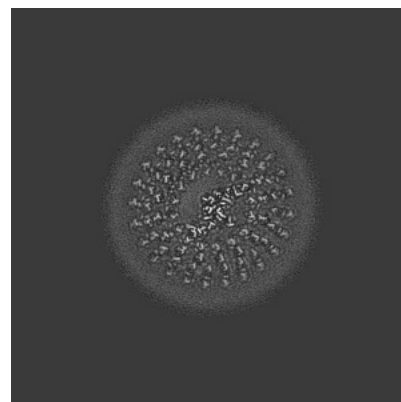
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

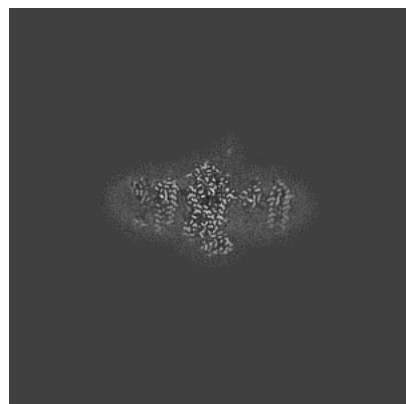


Z Index: 200

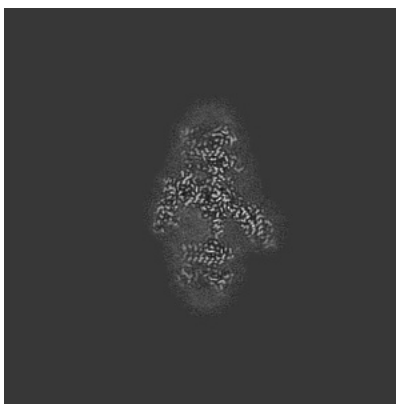
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

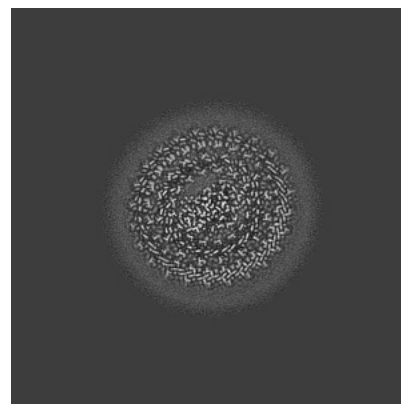
### 6.3.1 Primary map



X Index: 206



Y Index: 210

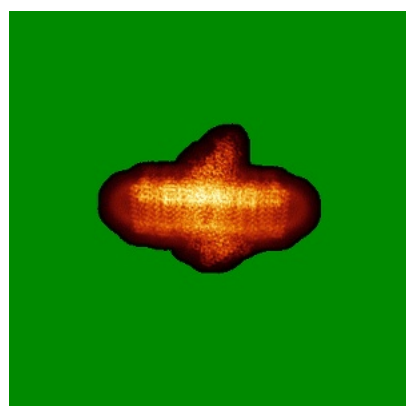


Z Index: 214

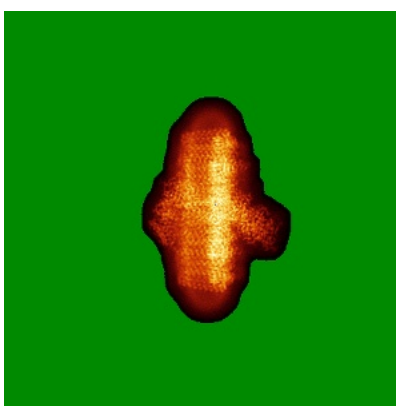
The images above show the largest variance slices of the map in three orthogonal directions.

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

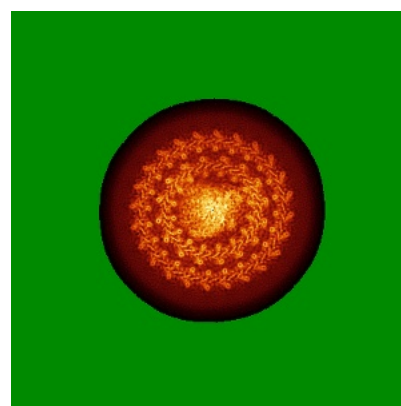
### 6.4.1 Primary map



X



Y

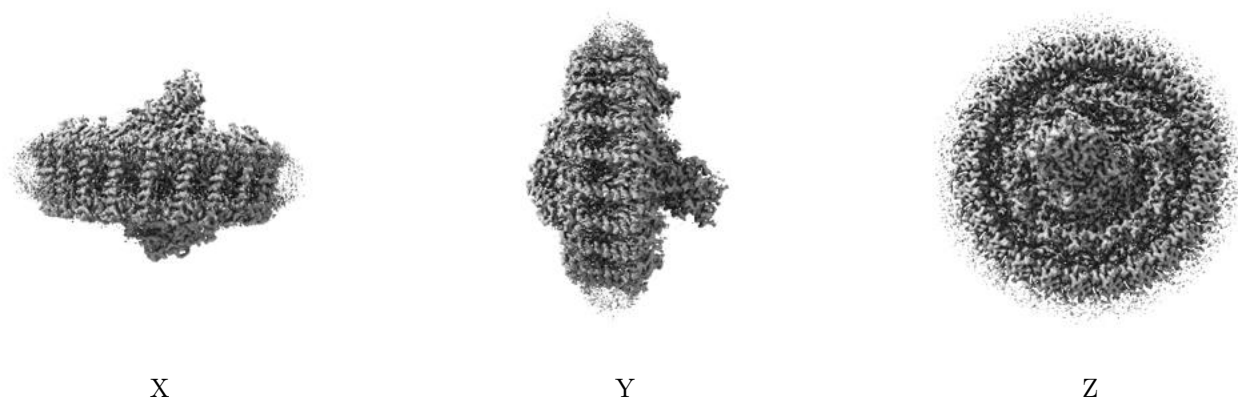


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

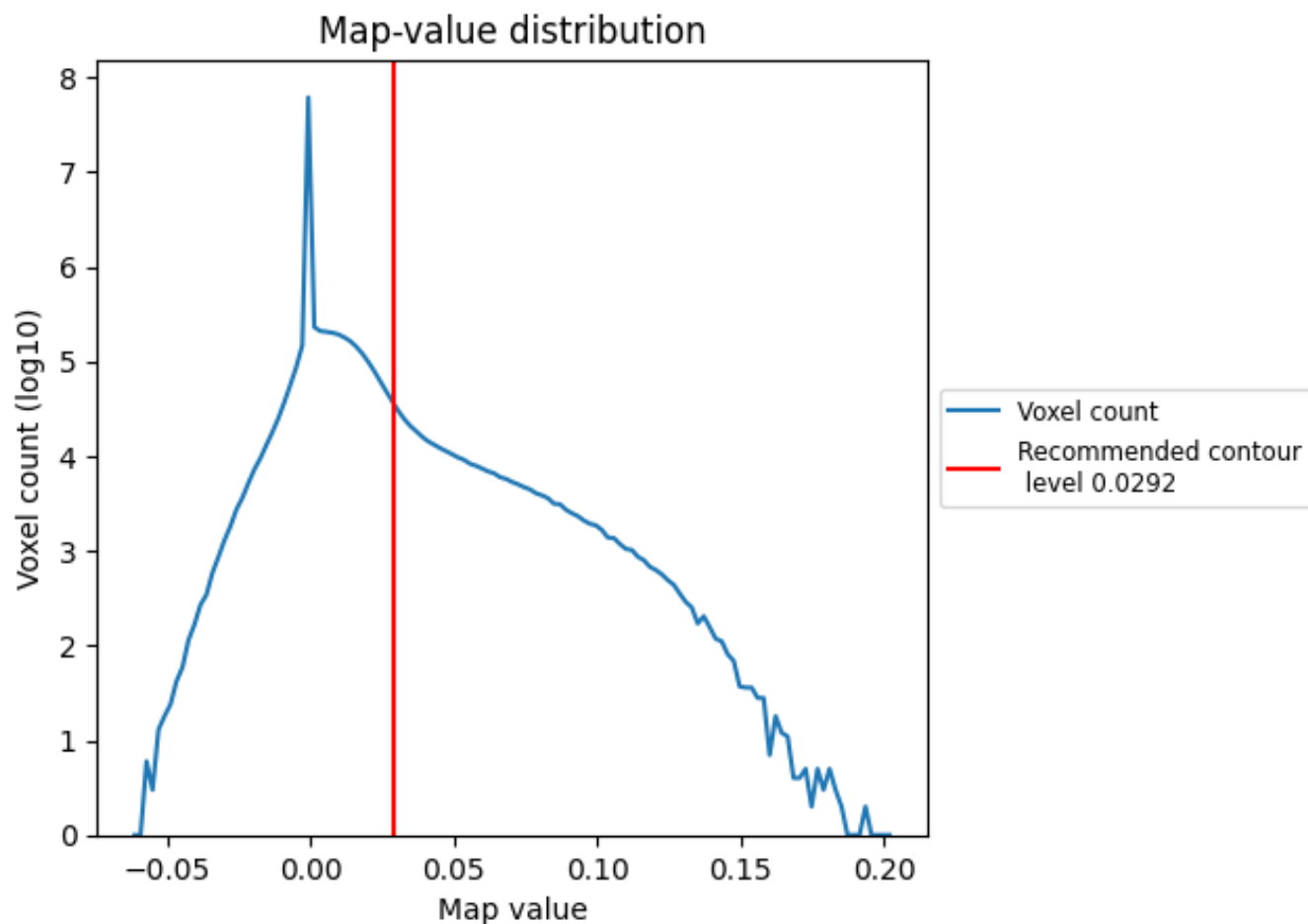
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

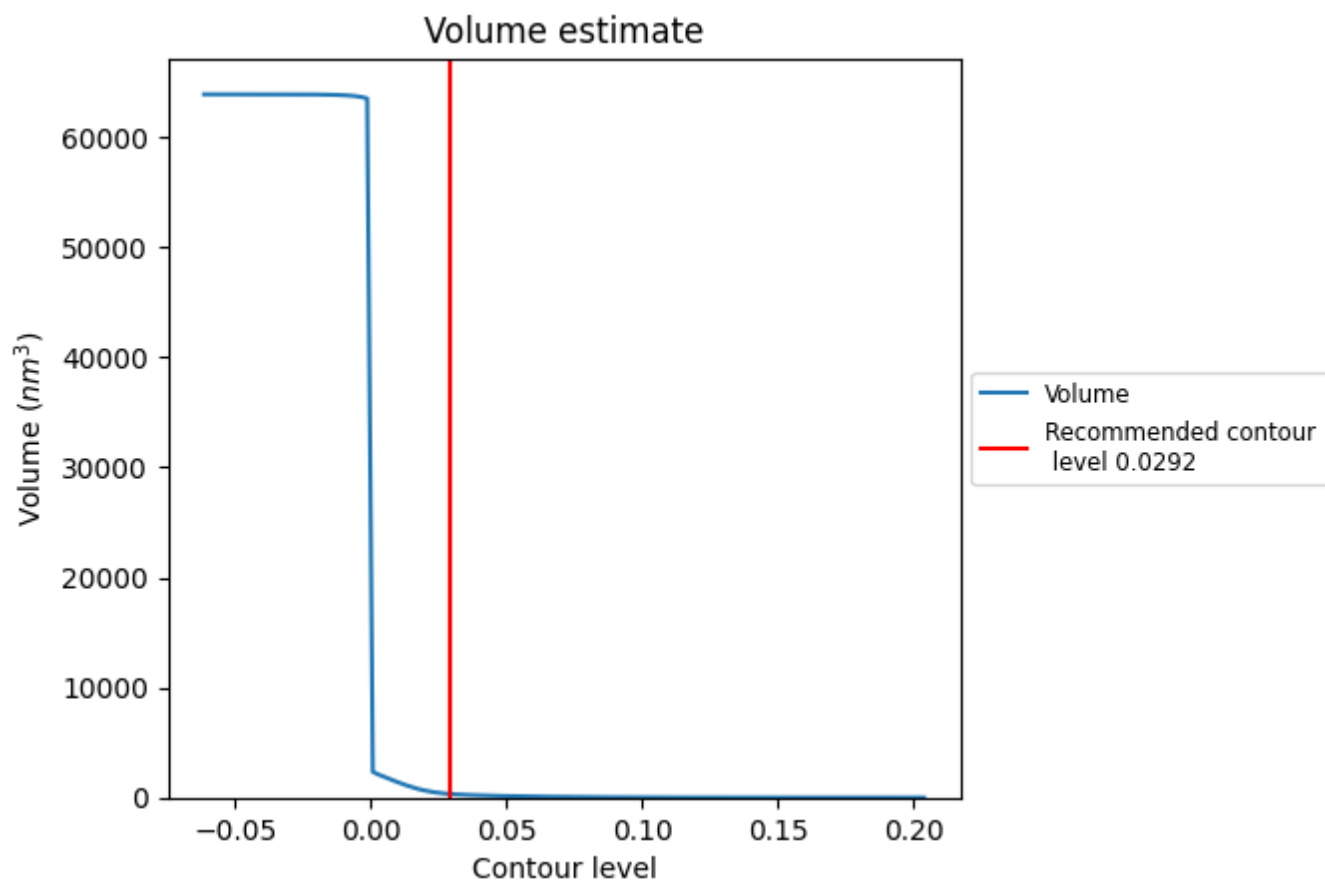
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

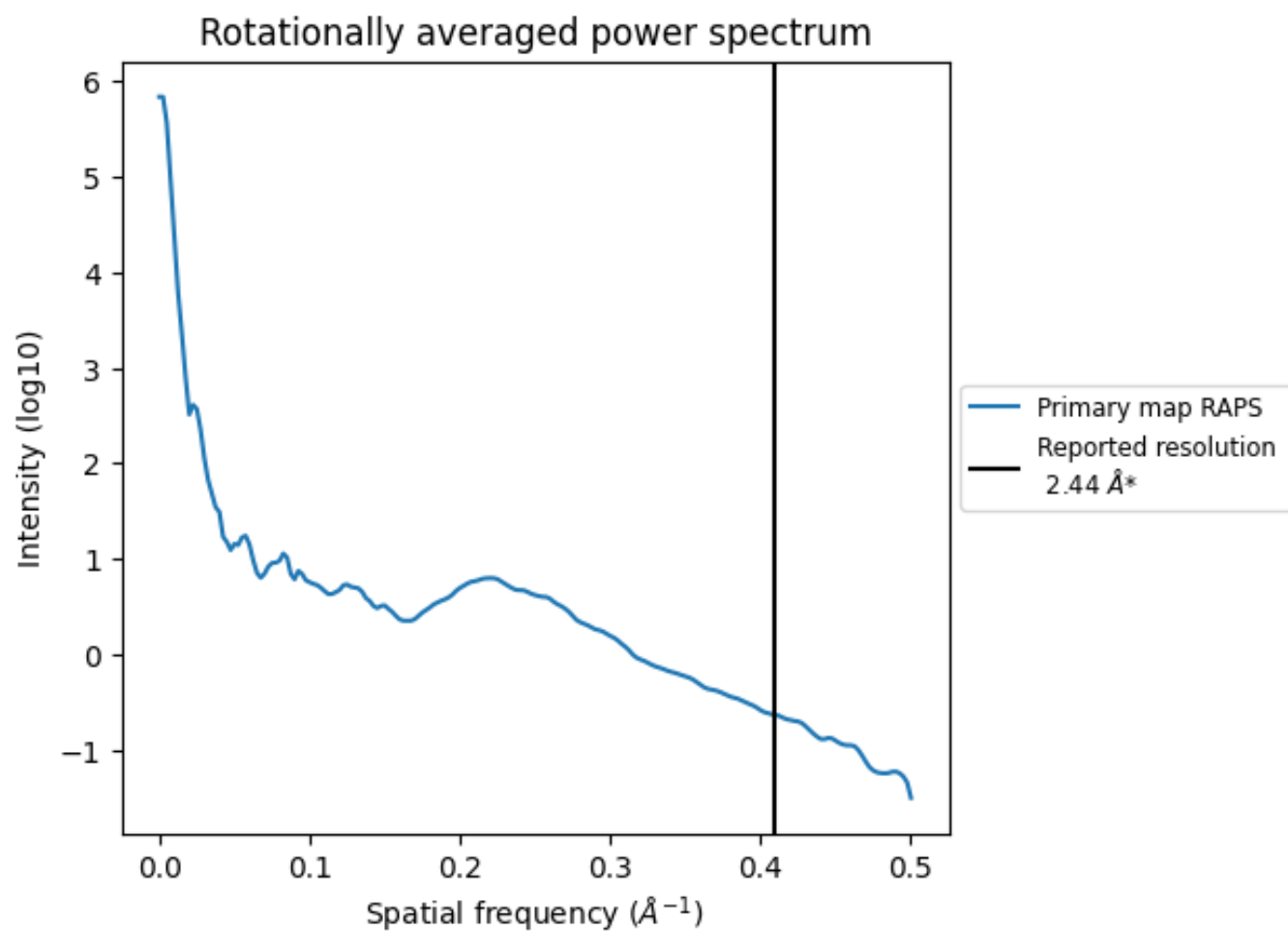
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327  $\text{nm}^3$ ; this corresponds to an approximate mass of 296 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

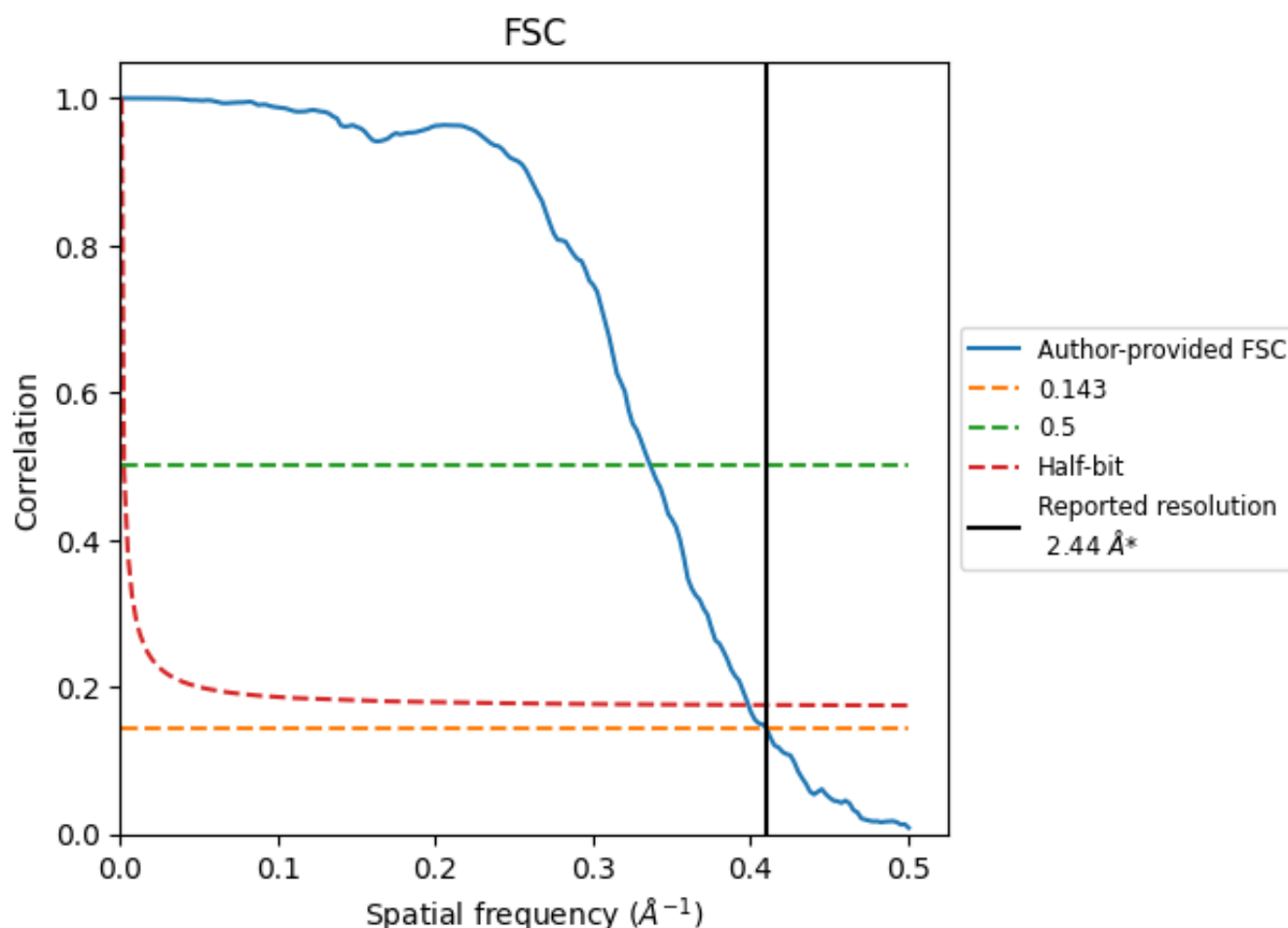


\*Reported resolution corresponds to spatial frequency of 0.410 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.410 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

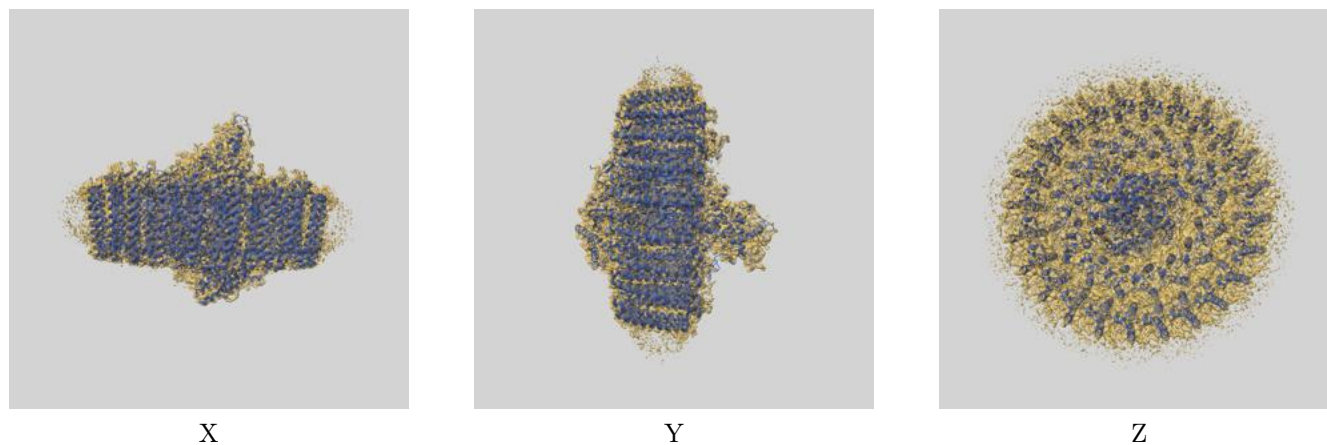
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.44                               | -    | -        |
| Author-provided FSC curve | 2.44                               | 2.97 | 2.51     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

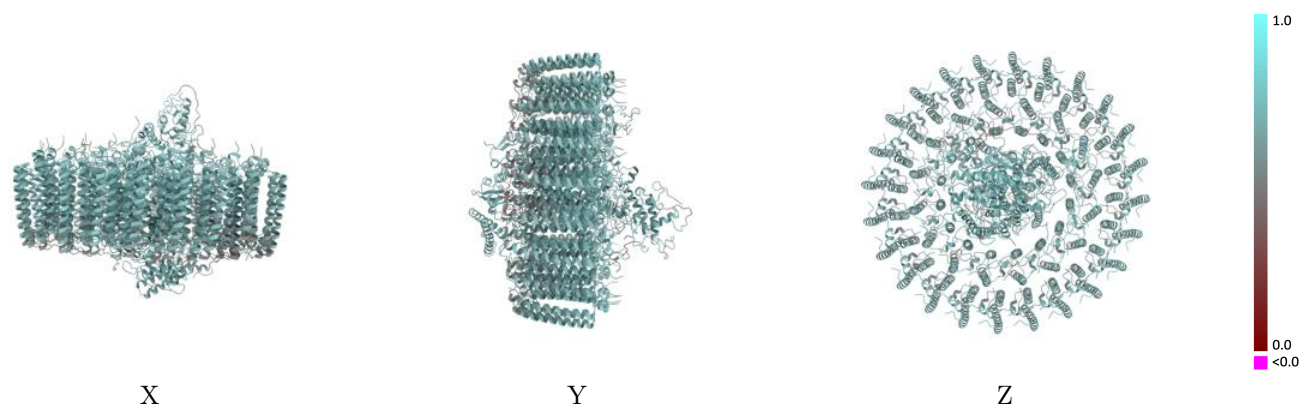
This section contains information regarding the fit between EMDB map EMD-12682 and PDB model 7O0X. Per-residue inclusion information can be found in section [3](#) on page [39](#).

### 9.1 Map-model overlay [i](#)



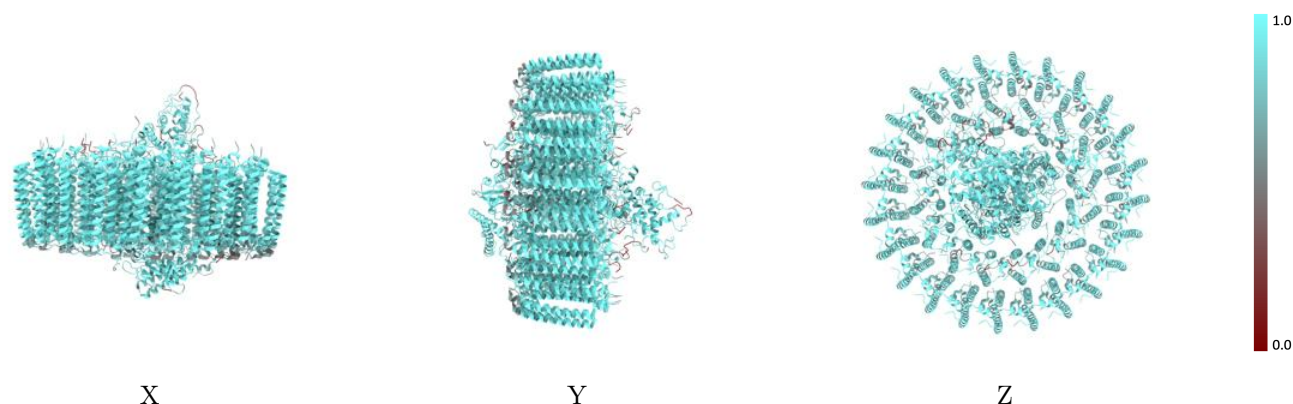
The images above show the 3D surface view of the map at the recommended contour level 0.0292 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



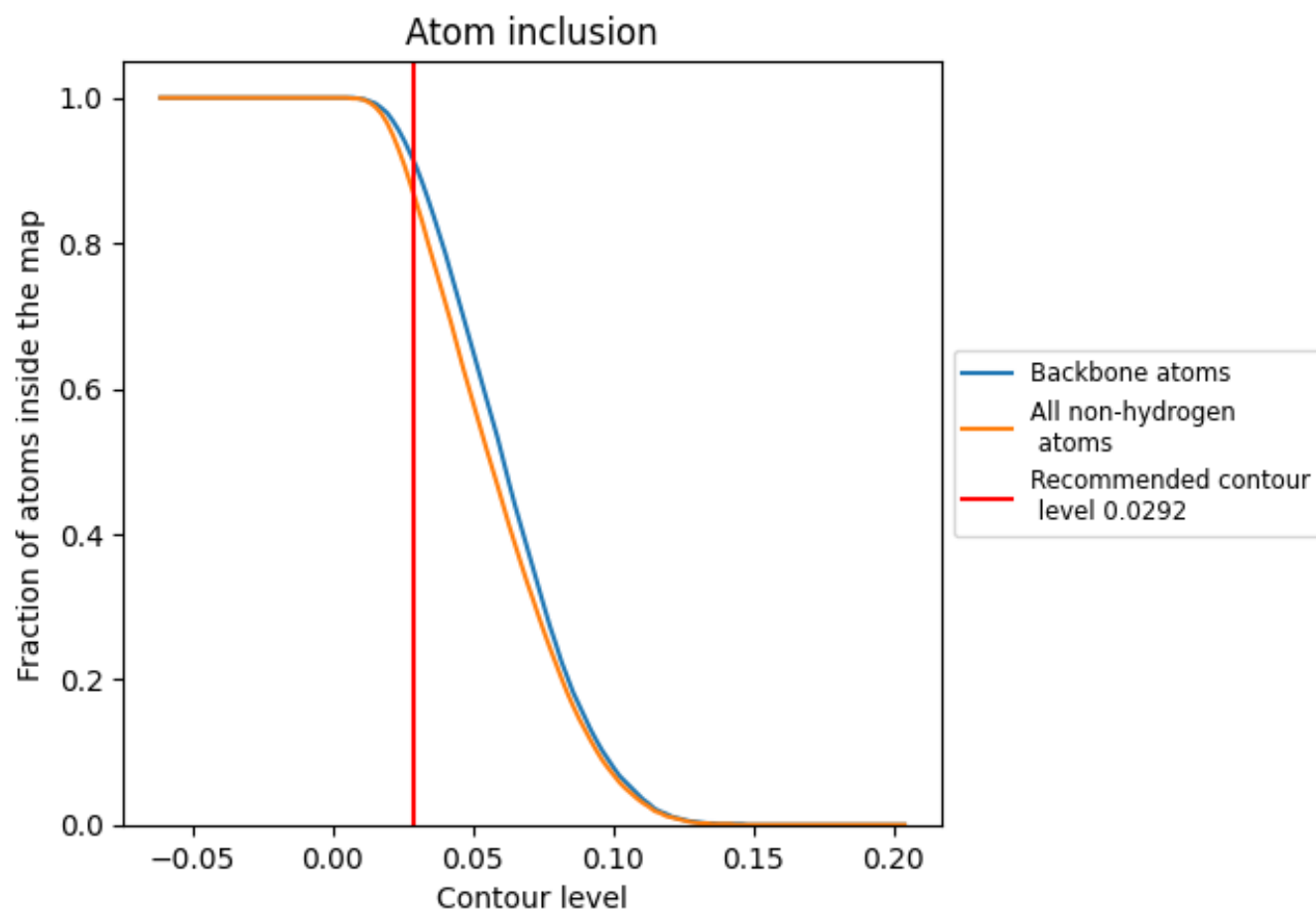
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0292).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0292) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8640   |  0.6290   |
| AA    |  0.9120   |  0.6400   |
| AB    |  0.8220   |  0.6000   |
| AC    |  0.7940   |  0.5860   |
| AD    |  0.8440   |  0.6100   |
| AE    |  0.8500   |  0.6240   |
| AF    |  0.7610   |  0.5730   |
| AG    |  0.8890   |  0.6320   |
| AH    |  0.8500   |  0.6170   |
| AI    |  0.8360   |  0.6050   |
| AJ    |  0.9230   |  0.6450   |
| AK    |  0.8820   |  0.6330   |
| AL    |  0.8470   |  0.6130   |
| AM    |  0.9270   |  0.6520   |
| AN    |  0.8480  |  0.6170  |
| AO    |  0.8290 |  0.6020 |
| AP    |  0.9060 |  0.6410 |
| AQ    |  0.8190 |  0.6140 |
| AR    |  0.9110 |  0.6350 |
| AS    |  0.8760 |  0.6310 |
| AT    |  0.9470 |  0.6510 |
| AU    |  0.8750 |  0.6240 |
| AV    |  0.9240 |  0.6460 |
| AW    |  0.7900 |  0.6050 |
| AX    |  0.9440 |  0.6460 |
| BA    |  0.7690 |  0.5840 |
| BB    |  0.7810 |  0.5860 |
| BC    |  0.7670 |  0.5800 |
| BD    |  0.7370 |  0.5680 |
| BE    |  0.7440 |  0.5700 |
| BF    |  0.7350 |  0.5540 |
| BG    |  0.8200 |  0.6110 |
| BH    |  0.8000 |  0.5990 |
| BI    |  0.7610 |  0.5750 |
| BJ    |  0.8360 |  0.6130 |





























*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| BK    |  0.7910   |  0.6010   |
| BL    |  0.7730   |  0.5990   |
| BM    |  0.8200   |  0.6030   |
| BN    |  0.7850   |  0.5910   |
| BO    |  0.8020   |  0.5910   |
| BP    |  0.7820   |  0.5940   |
| BQ    |  0.8030   |  0.5910   |
| BR    |  0.7780   |  0.5860   |
| BS    |  0.7940   |  0.5980   |
| BT    |  0.7900   |  0.5950   |
| BU    |  0.7850   |  0.5830   |
| BV    |  0.8280   |  0.6060   |
| BW    |  0.7920   |  0.5970   |
| BX    |  0.8160   |  0.6060   |
| C     |  0.9290   |  0.6680   |
| C1    |  0.9220   |  0.6700   |
| C2    |  0.9240   |  0.6370   |
| CG    |  0.7620  |  0.5010  |
| H1    |  0.8990 |  0.6520 |
| H2    |  0.9290 |  0.6570 |
| L     |  0.9570 |  0.6870 |
| M     |  0.9240 |  0.6800 |
| MG    |  0.9520 |  0.6080 |
| aa    |  0.8220 |  0.6010 |
| ab    |  0.8630 |  0.6280 |
| ac    |  0.8640 |  0.6250 |
| ad    |  0.9280 |  0.6630 |
| ae    |  0.9390 |  0.6700 |
| af    |  0.8540 |  0.6360 |
| ag    |  0.8790 |  0.6330 |
| ah    |  0.8990 |  0.6420 |
| ai    |  0.8320 |  0.6150 |
| aj    |  0.9110 |  0.6490 |
| ak    |  0.9560 |  0.6680 |
| al    |  0.9200 |  0.6600 |
| am    |  0.8780 |  0.6420 |
| an    |  0.8070 |  0.6170 |
| ao    |  0.9150 |  0.6620 |
| ap    |  0.9050 |  0.6340 |
| ba    |  0.8050 |  0.5900 |
| bb    |  0.7840 |  0.6010 |
| bc    |  0.8660 |  0.6240 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| bd    |  0.8920 |  0.6470 |
| be    |  0.9020 |  0.6340 |
| bf    |  0.8970 |  0.6450 |
| bg    |  0.8900 |  0.6310 |
| bh    |  0.8730 |  0.6250 |
| bi    |  0.8900 |  0.6280 |
| bj    |  0.8920 |  0.6420 |
| bk    |  0.8710 |  0.6220 |
| bl    |  0.8460 |  0.6190 |
| bm    |  0.8700 |  0.6320 |
| bn    |  0.8690 |  0.6320 |
| bo    |  0.9040 |  0.6370 |
| bp    |  0.8720 |  0.6360 |