



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:30 AM UTC

PDB ID : 9JPB / pdb_00009jpb
EMDB ID : EMD-61695
Title : Cryo-EM structure of a tri-heme cytochrome-associated RC-LH1 complex from a marine photoheterotrophic bacterium, purified with EDTA-containing solutions
Authors : Chen, J.H.; Zheng, Q.; Zhang, X.; Wang, W.; Liu, Y.; Gu, J.
Deposited on : 2024-09-25
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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

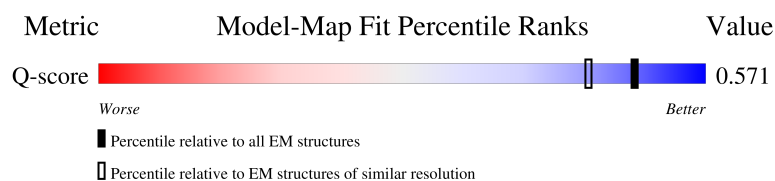
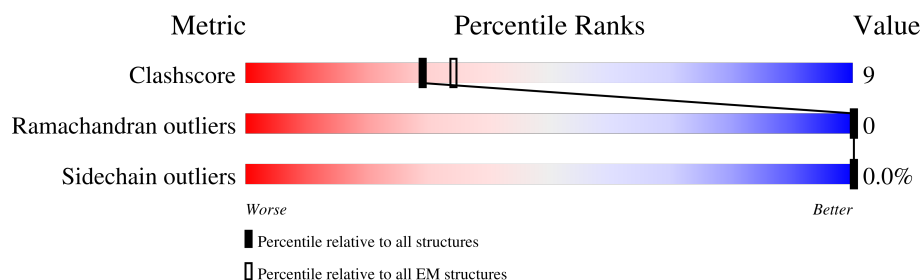
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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














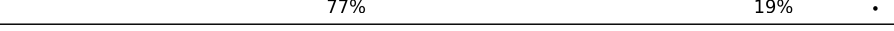







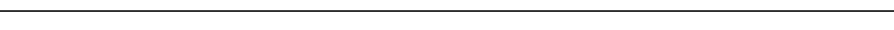

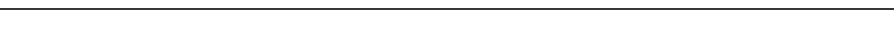
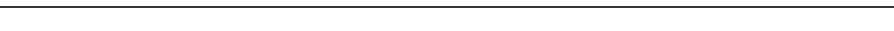


| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 11806 (2.30 - 3.30) |

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 ≥ 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 | 1 | 53 | 79% 15% 6% |
| 1 | A | 53 | 72% 25% . |
| 1 | B | 53 | 85% 11% . |
| 1 | D | 53 | 81% 15% . |











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 1 | E | 53 |  70% 26% . |
| 1 | F | 53 |  83% 13% . |
| 1 | G | 53 |  81% 15% . |
| 1 | I | 53 |  85% 11% . |
| 1 | J | 53 |  79% 15% 6% |
| 1 | K | 53 |  87% 9% . |
| 1 | N | 53 |  81% 15% . |
| 1 | P | 53 |  75% 21% . |
| 1 | Q | 53 |  79% 17% . |
| 1 | R | 53 |  74% 23% . |
| 1 | S | 53 |  81% 15% . |
| 1 | T | 53 |  77% 19% . |
| 1 | V | 53 |  91% 6% . |
| 2 | O | 239 |  20% . 78% |
| 3 | 2 | 49 |  82% 8% 10% |
| 3 | a | 49 |  69% 20% 10% |
| 3 | b | 49 |  82% 8% 10% |
| 3 | d | 49 |  71% 18% 10% |
| 3 | e | 49 |  80% 10% 10% |
| 3 | f | 49 |  76% 14% 10% |
| 3 | g | 49 |  76% 14% 10% |
| 3 | i | 49 |  71% 16% 12% |
| 3 | j | 49 |  76% 12% 12% |
| 3 | k | 49 |  73% 14% 12% |
| 3 | n | 49 |  73% 16% 10% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3 | p | 49 |  |
| 3 | q | 49 |  |
| 3 | r | 49 |  |
| 3 | s | 49 |  |
| 3 | t | 49 |  |
| 3 | v | 49 |  |
| 4 | M | 330 |  |
| 5 | L | 279 |  |
| 6 | H | 256 |  |
| 7 | C | 360 |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 9 | SPN | 2 | 102 | - | X | - | - |
| 9 | SPN | 2 | 103 | - | X | - | - |
| 9 | SPN | D | 102 | - | X | - | - |
| 9 | SPN | D | 103 | - | X | - | - |
| 9 | SPN | E | 102 | - | X | - | - |
| 9 | SPN | F | 102 | - | X | - | - |
| 9 | SPN | G | 103 | - | X | - | - |
| 9 | SPN | G | 104 | - | X | - | - |
| 9 | SPN | I | 101 | - | X | - | - |
| 9 | SPN | K | 102 | - | X | - | - |
| 9 | SPN | M | 404 | - | X | - | - |
| 9 | SPN | Q | 102 | - | X | - | - |
| 9 | SPN | R | 102 | - | X | - | - |
| 9 | SPN | S | 101 | - | X | - | - |
| 9 | SPN | S | 102 | - | X | - | - |
| 9 | SPN | V | 102 | - | X | - | - |
| 9 | SPN | a | 101 | - | X | - | - |
| 9 | SPN | a | 103 | - | X | - | - |
| 9 | SPN | a | 104 | - | X | - | - |
| 9 | SPN | b | 102 | - | X | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 9 | SPN | e | 102 | - | X | - | - |
| 9 | SPN | f | 102 | - | X | - | - |
| 9 | SPN | i | 101 | - | X | - | - |
| 9 | SPN | i | 103 | - | X | - | - |
| 9 | SPN | j | 102 | - | X | - | - |
| 9 | SPN | k | 101 | - | X | - | - |
| 9 | SPN | k | 103 | - | X | - | - |
| 9 | SPN | n | 102 | - | X | - | - |
| 9 | SPN | p | 101 | - | X | - | - |
| 9 | SPN | p | 102 | - | X | - | - |
| 9 | SPN | q | 101 | - | X | - | - |
| 9 | SPN | r | 101 | - | X | - | - |
| 9 | SPN | r | 103 | - | X | - | - |
| 9 | SPN | t | 102 | - | X | - | - |
| 9 | SPN | v | 102 | - | X | - | - |

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28258 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 Antenna pigment protein alpha chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1 | P | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 425 | 291 | 68 | 64 | 2 | | |
| 1 | V | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | S | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | T | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | Q | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | R | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | 1 | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 417 | 286 | 67 | 63 | 1 | | |
| 1 | N | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | K | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | J | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 417 | 286 | 67 | 63 | 1 | | |
| 1 | I | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | G | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | F | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | E | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | D | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | B | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |
| 1 | A | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 289 | 68 | 64 | 1 | | |

- Molecule 2 is a protein called Reaction center protein O chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2 | O | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 371 | 249 | 56 | 59 | 7 | | |

- Molecule 3 is a protein called Antenna pigment protein beta chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 | v | 40 | Total | C | N | O | S | 0 | 0 |
| | | | 321 | 215 | 52 | 53 | 1 | | |
| 3 | t | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 346 | 233 | 55 | 57 | 1 | | |
| 3 | s | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | r | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 350 | 235 | 55 | 59 | 1 | | |
| 3 | q | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | p | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | 2 | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | n | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | k | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 346 | 233 | 55 | 57 | 1 | | |
| 3 | j | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 346 | 233 | 55 | 57 | 1 | | |
| 3 | i | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 346 | 233 | 55 | 57 | 1 | | |
| 3 | g | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | f | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | e | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | d | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 354 | 237 | 56 | 60 | 1 | | |
| 3 | b | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 358 | 239 | 56 | 62 | 1 | | |
| 3 | a | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 358 | 239 | 56 | 62 | 1 | | |

- Molecule 4 is a protein called Reaction center protein M chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | M | 325 | Total | C | N | O | S | 0 | 0 |
| | | | 2633 | 1752 | 421 | 452 | 8 | | |

- Molecule 5 is a protein called Reaction center protein L chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | L | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1469 | 346 | 354 | 9 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| L | 278 | ASP | GLY | conflict | UNP A8LQ16 |
| L | 279 | CYS | LEU | conflict | UNP A8LQ16 |

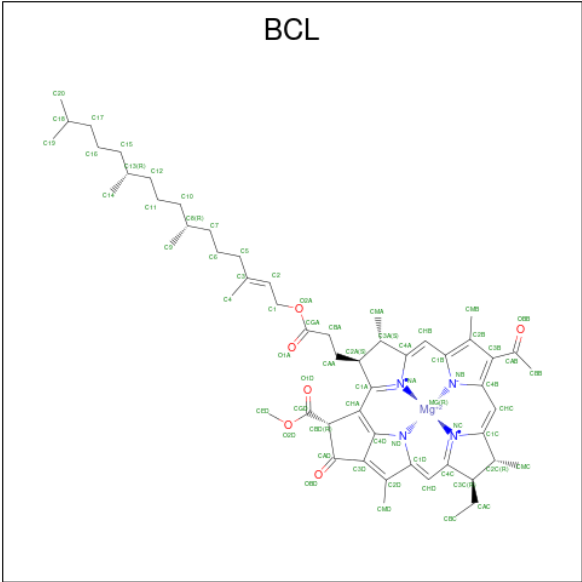
- Molecule 6 is a protein called Reaction center protein H chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | H | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 2022 | 1283 | 345 | 385 | 9 | | |

- Molecule 7 is a protein called Photosynthetic reaction center cytochrome c subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | C | 352 | Total | C | N | O | S | 0 | 0 |
| | | | 2740 | 1731 | 455 | 540 | 14 | | |

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 8 | P | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | V | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | v | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | t | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | T | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | s | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | Q | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | r | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | R | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | R | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | q | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | p | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | 2 | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | 1 | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |

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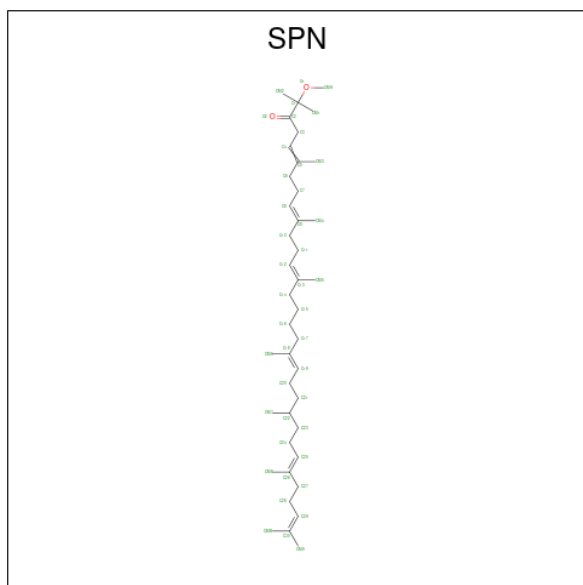
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 8 | n | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | N | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | k | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | K | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | j | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | J | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | i | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | I | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | G | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | G | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | f | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | F | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | e | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | E | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | d | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | D | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | b | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | B | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | a | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | A | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | M | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 8 | M | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 8 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 8 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 9 | V | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | v | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | S | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | S | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | t | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | Q | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | r | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | r | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |

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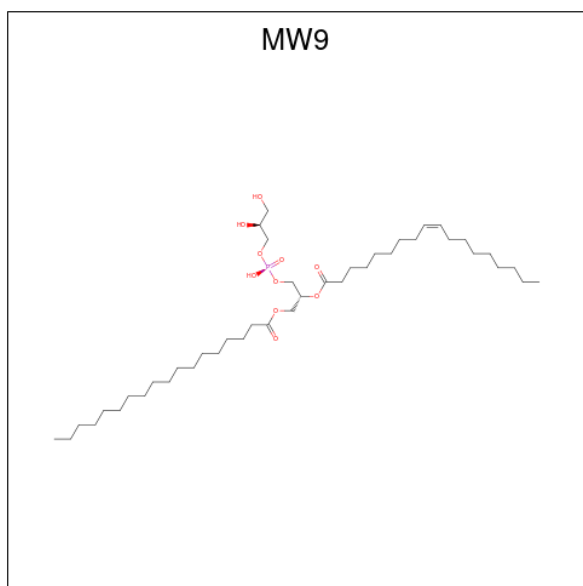
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 9 | R | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | q | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | p | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | p | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | 2 | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | 2 | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | n | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | k | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | k | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | K | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | j | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | i | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | i | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | I | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | G | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | G | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | f | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | F | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | e | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | E | 1 | Total 43 | C 41 | O 2 | 0 |
| 9 | D | 1 | Total 43 | C 41 | O 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 9 | D | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | b | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | a | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | a | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | a | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |
| 9 | M | 1 | Total | C | O | 0 |
| | | | 43 | 41 | 2 | |

- Molecule 10 is (21R,24R,27S)-24,27,28-trihydroxy-18,24-dioxo-19,23,25-trioxa-24lambda 5 -phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (CCD ID: MW9) (formula: C₄₂H₈₁O₁₀P).



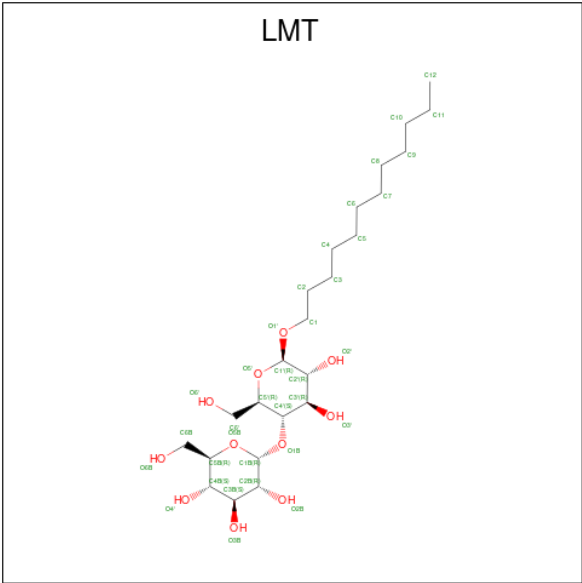
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 10 | Q | 1 | Total | C | O | P | 0 |
| | | | 45 | 34 | 10 | 1 | |
| 10 | I | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 10 | G | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 10 | F | 1 | Total | C | O | P | 0 |
| | | | 43 | 32 | 10 | 1 | |
| 10 | F | 1 | Total | C | O | P | 0 |
| | | | 48 | 37 | 10 | 1 | |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 10 | D | 1 | Total | C | O | 0 |
| | | | 27 | 22 | 5 | |
| 10 | B | 1 | Total | C | O | P |
| | | | 53 | 42 | 10 | 1 |
| 10 | M | 1 | Total | C | O | P |
| | | | 49 | 38 | 10 | 1 |
| 10 | M | 1 | Total | C | O | P |
| | | | 53 | 42 | 10 | 1 |
| 10 | L | 1 | Total | C | O | P |
| | | | 37 | 26 | 10 | 1 |
| 10 | L | 1 | Total | C | O | P |
| | | | 36 | 25 | 10 | 1 |
| 10 | H | 1 | Total | C | O | P |
| | | | 37 | 28 | 8 | 1 |

- Molecule 11 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 11 | E | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 11 | L | 1 | Total | C | O | 0 |
| | | | 24 | 18 | 6 | |
| 11 | L | 1 | Total | C | O | 0 |
| | | | 24 | 19 | 5 | |
| 11 | H | 1 | Total | C | O | 0 |
| | | | 24 | 18 | 6 | |

Continued on next page...

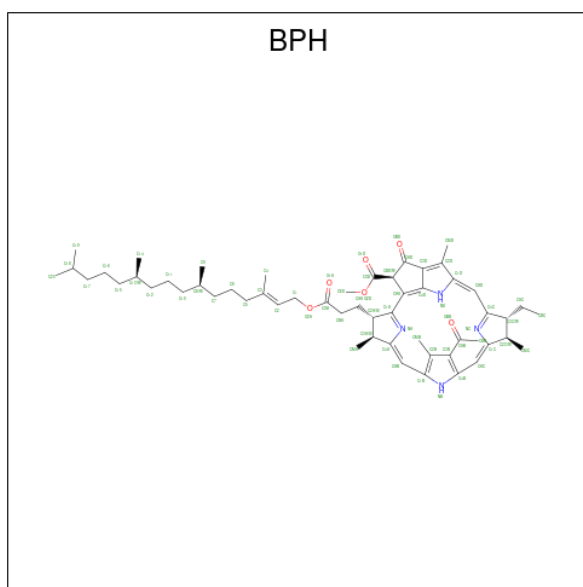
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 11 | C | 1 | Total | C | O | 0 |
| | | | 24 | 18 | 6 | |

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

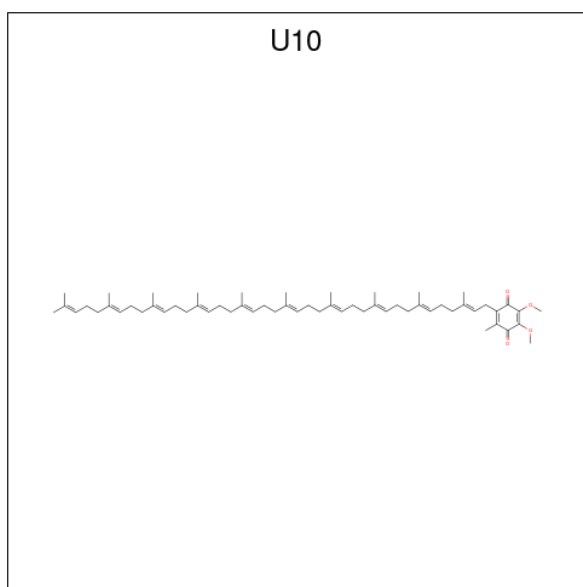
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 12 | M | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



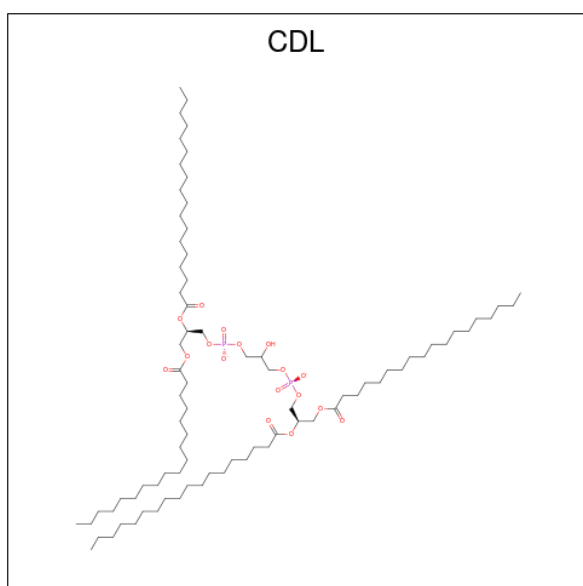
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 13 | M | 1 | Total | C | N | O | 0 |
| | | | 65 | 55 | 4 | 6 | |
| 13 | L | 1 | Total | C | N | O | 0 |
| | | | 65 | 55 | 4 | 6 | |

- Molecule 14 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



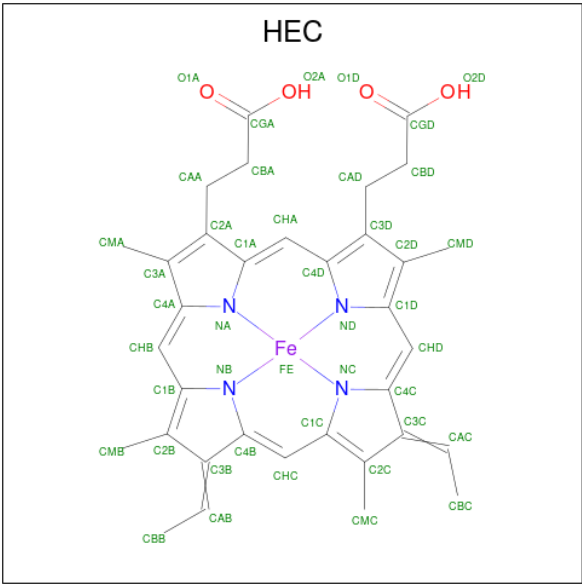
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 14 | M | 1 | Total | C | O | 0 |
| | | | 63 | 59 | 4 | |
| 14 | L | 1 | Total | C | O | 0 |
| | | | 48 | 44 | 4 | |

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 15 | H | 1 | Total | C | O | P | 0 |
| | | | 91 | 72 | 17 | 2 | |
| 15 | H | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |

- Molecule 16 is HEME C (CCD ID: 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 | |

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.

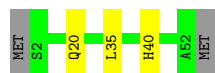
- Molecule 1: Antenna pigment protein alpha chain

Chain P: 




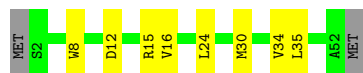
- Molecule 1: Antenna pigment protein alpha chain

Chain V: 




- Molecule 1: Antenna pigment protein alpha chain

Chain S: 




- Molecule 1: Antenna pigment protein alpha chain

Chain T: 



- Molecule 1: Antenna pigment protein alpha chain

Chain Q: 




- Molecule 1: Antenna pigment protein alpha chain

Chain R:  74% 23% .




- Molecule 1: Antenna pigment protein alpha chain

Chain 1:  79% 15% 6%




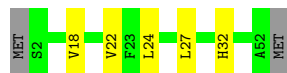
- Molecule 1: Antenna pigment protein alpha chain

Chain N:  81% 15% .




- Molecule 1: Antenna pigment protein alpha chain

Chain K:  87% 9% .




- Molecule 1: Antenna pigment protein alpha chain

Chain J:  79% 15% 6%




- Molecule 1: Antenna pigment protein alpha chain

Chain I:  85% 11% .




- Molecule 1: Antenna pigment protein alpha chain

Chain G:  81% 15% .



- Molecule 1: Antenna pigment protein alpha chain

Chain F:  83% 13% .




- Molecule 1: Antenna pigment protein alpha chain

Chain E:  70% 26% .




- Molecule 1: Antenna pigment protein alpha chain

Chain D:  81% 15% .



- Molecule 1: Antenna pigment protein alpha chain

Chain B:  85% 11% .



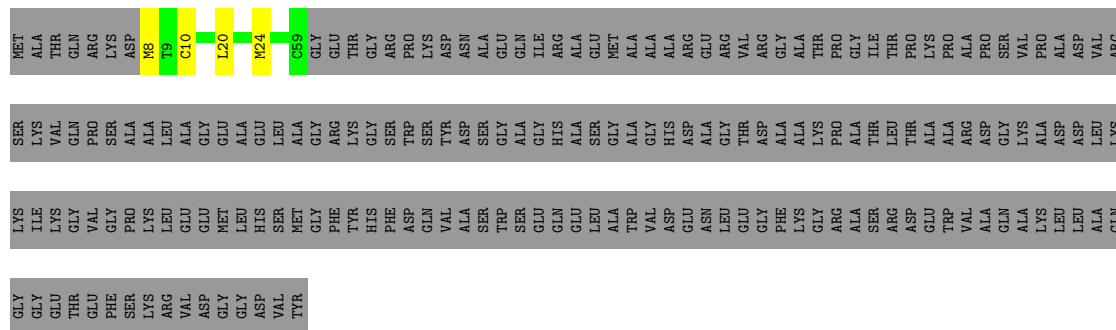
- Molecule 1: Antenna pigment protein alpha chain

Chain A:  72% 25% .




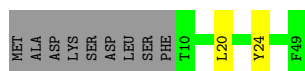
- Molecule 2: Reaction center protein O chain

Chain O:  20% 78% .



- Molecule 3: Antenna pigment protein beta chain

Chain v:  78% 18%




- Molecule 3: Antenna pigment protein beta chain

Chain t:  71% 16% 12%




- Molecule 3: Antenna pigment protein beta chain

Chain s:  84% 6% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain r:  78% 10% 12%



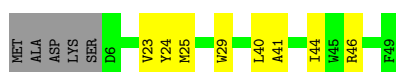
- Molecule 3: Antenna pigment protein beta chain

Chain q:  80% 10% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain p:  73% 16% 10%



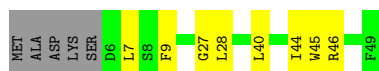
- Molecule 3: Antenna pigment protein beta chain

Chain 2:  82% 8% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain n:  73% 16% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain k:  73% 14% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain j:  76% 12% 12%




- Molecule 3: Antenna pigment protein beta chain

Chain i:  71% 16% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain g:  76% 14% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain f:  76% 14% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain e:  80% 10% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain d:  71% 18% 10%

MET
ALA
ASP
LYS
SER
D6
E19
L20
H21
S22
V23
Y24
M25
T42
R46
P47
W48
F49

- Molecule 3: Antenna pigment protein beta chain

Chain b:  82% 8% 10%


MET
ALA
ASP
LYS
SER
D6
T13
Q16
Y24
A38
F49

- Molecule 3: Antenna pigment protein beta chain

Chain a:  69% 20% 10%

MET
ALA
ASP
LYS
SER
D6
L7
S8
F9
Q16
E19
L20
H21
M25
S32
A33
V36
V37
F49

- Molecule 4: Reaction center protein M chain


Chain M:  79% 19% .

MET
P2
E3
Y4
Q5
N6
V11
E30
G50
Y53
W56
F57
W68
M76
L77
L91
L94
A95
P99
P108
P109
L110
G114
A119
S129
R133
L137
K145
A148
L157
F158
L159
V160
L161
G162
L163
F164
L168
P182

H183
L184
D185
F202
H203
I207
V208
S213
F217
T228
R229
F230
D241
R242
A245
S246
E247
L251
T256
M257
G258
F259
W260
A261
W269
A270
A274
V275
L276
T277
P278
L279
T280
L286
N294
L297
Q310
D311
Y312
G313
Y314
R326
GLU
GLU

GLY
ASN


- Molecule 5: Reaction center protein L chain

Chain L:  83% 15% .

MET
A2
E7
R8
K9
F23
Y31
V37
L44
W52
L76
P80
L81
M82
E83
R104
R110
I126
V130
L132
T131
V133
V134
F135
R136
P137
W143
L166
H167
F168
H169
I176
T179
L188
A189
L190
L194
E206
E213

F217
R218
D219
Y223
S224
L225
R232
V233
G234
A246
N265
E269
S275
GLN
VAL
ASP
CYS

- Molecule 6: Reaction center protein H chain

Chain H:  88% 12%

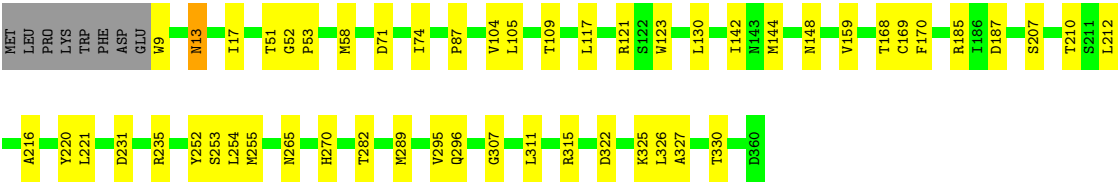
M1
E2
F5
D10
E33
N34
M35
R36
E42
K64
D78
V79
Q80
R81
R82
D83
N84
P100
G108
V109
G110
P111
A112
S113
R117
P133
G145
W168
Y178
R200
L231
K235
L236
M237
A238
G242
L256

- Molecule 7: Photosynthetic reaction center cytochrome c subunit

Chain C:

83%

14%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 230375 | 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 ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 1.280 | Depositor |
| Minimum map value | -0.705 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.042 | Depositor |
| Recommended contour level | 0.103 | Depositor |
| Map size (Å) | 307.2, 307.2, 307.2 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.2, 1.2, 1.2 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MW9, CDL, BPH, LMT, FE, SPN, BCL, HEC, U10

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 | 1 | 0.15 | 0/431 | 0.37 | 0/585 |
| 1 | A | 0.13 | 0/436 | 0.27 | 0/592 |
| 1 | B | 0.12 | 0/436 | 0.23 | 0/592 |
| 1 | D | 0.15 | 0/436 | 0.33 | 0/592 |
| 1 | E | 0.16 | 0/436 | 0.29 | 0/592 |
| 1 | F | 0.17 | 0/436 | 0.30 | 0/592 |
| 1 | G | 0.15 | 0/436 | 0.30 | 0/592 |
| 1 | I | 0.14 | 0/436 | 0.28 | 0/592 |
| 1 | J | 0.13 | 0/431 | 0.29 | 0/585 |
| 1 | K | 0.13 | 0/436 | 0.29 | 0/592 |
| 1 | N | 0.15 | 0/436 | 0.32 | 0/592 |
| 1 | P | 0.14 | 0/439 | 0.31 | 0/595 |
| 1 | Q | 0.13 | 0/436 | 0.29 | 0/592 |
| 1 | R | 0.14 | 0/436 | 0.24 | 0/592 |
| 1 | S | 0.15 | 0/436 | 0.32 | 0/592 |
| 1 | T | 0.12 | 0/436 | 0.27 | 0/592 |
| 1 | V | 0.12 | 0/436 | 0.28 | 0/592 |
| 2 | O | 0.13 | 0/378 | 0.26 | 0/516 |
| 3 | 2 | 0.10 | 0/367 | 0.21 | 0/503 |
| 3 | a | 0.14 | 0/371 | 0.31 | 0/508 |
| 3 | b | 0.12 | 0/371 | 0.24 | 0/508 |
| 3 | d | 0.15 | 0/367 | 0.28 | 0/503 |
| 3 | e | 0.13 | 0/367 | 0.21 | 0/503 |
| 3 | f | 0.13 | 0/367 | 0.21 | 0/503 |
| 3 | g | 0.14 | 0/367 | 0.22 | 0/503 |
| 3 | i | 0.13 | 0/359 | 0.21 | 0/492 |
| 3 | j | 0.12 | 0/359 | 0.29 | 0/492 |
| 3 | k | 0.14 | 0/359 | 0.28 | 0/492 |
| 3 | n | 0.13 | 0/367 | 0.26 | 0/503 |
| 3 | p | 0.13 | 0/367 | 0.27 | 0/503 |
| 3 | q | 0.11 | 0/367 | 0.21 | 0/503 |
| 3 | r | 0.11 | 0/363 | 0.20 | 0/497 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 3 | s | 0.12 | 0/367 | 0.25 | 0/503 |
| 3 | t | 0.12 | 0/359 | 0.23 | 0/492 |
| 3 | v | 0.11 | 0/333 | 0.23 | 0/457 |
| 4 | M | 0.16 | 0/2731 | 0.30 | 0/3735 |
| 5 | L | 0.17 | 0/2267 | 0.34 | 0/3105 |
| 6 | H | 0.13 | 0/2072 | 0.24 | 0/2804 |
| 7 | C | 0.14 | 0/2818 | 0.30 | 0/3868 |
| All | All | 0.14 | 0/23848 | 0.28 | 0/32546 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1 | 417 | 0 | 421 | 8 | 0 |
| 1 | A | 422 | 0 | 426 | 17 | 0 |
| 1 | B | 422 | 0 | 426 | 7 | 0 |
| 1 | D | 422 | 0 | 426 | 7 | 0 |
| 1 | E | 422 | 0 | 426 | 13 | 0 |
| 1 | F | 422 | 0 | 426 | 8 | 0 |
| 1 | G | 422 | 0 | 426 | 7 | 0 |
| 1 | I | 422 | 0 | 426 | 5 | 0 |
| 1 | J | 417 | 0 | 421 | 9 | 0 |
| 1 | K | 422 | 0 | 426 | 4 | 0 |
| 1 | N | 422 | 0 | 426 | 8 | 0 |
| 1 | P | 425 | 0 | 433 | 9 | 0 |
| 1 | Q | 422 | 0 | 426 | 9 | 0 |
| 1 | R | 422 | 0 | 426 | 9 | 0 |
| 1 | S | 422 | 0 | 426 | 5 | 0 |
| 1 | T | 422 | 0 | 426 | 9 | 0 |
| 1 | V | 422 | 0 | 426 | 3 | 0 |
| 2 | O | 371 | 0 | 393 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 2 | 354 | 0 | 334 | 5 | 0 |
| 3 | a | 358 | 0 | 338 | 7 | 0 |
| 3 | b | 358 | 0 | 338 | 3 | 0 |
| 3 | d | 354 | 0 | 334 | 9 | 0 |
| 3 | e | 354 | 0 | 334 | 4 | 0 |
| 3 | f | 354 | 0 | 334 | 6 | 0 |
| 3 | g | 354 | 0 | 334 | 7 | 0 |
| 3 | i | 346 | 0 | 330 | 7 | 0 |
| 3 | j | 346 | 0 | 330 | 5 | 0 |
| 3 | k | 346 | 0 | 330 | 5 | 0 |
| 3 | n | 354 | 0 | 334 | 10 | 0 |
| 3 | p | 354 | 0 | 334 | 9 | 0 |
| 3 | q | 354 | 0 | 334 | 4 | 0 |
| 3 | r | 350 | 0 | 334 | 5 | 0 |
| 3 | s | 354 | 0 | 334 | 3 | 0 |
| 3 | t | 346 | 0 | 330 | 9 | 0 |
| 3 | v | 321 | 0 | 305 | 3 | 0 |
| 4 | M | 2633 | 0 | 2524 | 61 | 0 |
| 5 | L | 2178 | 0 | 2118 | 45 | 0 |
| 6 | H | 2022 | 0 | 1971 | 23 | 0 |
| 7 | C | 2740 | 0 | 2581 | 45 | 0 |
| 8 | 1 | 66 | 0 | 74 | 3 | 0 |
| 8 | 2 | 66 | 0 | 74 | 2 | 0 |
| 8 | A | 66 | 0 | 74 | 6 | 0 |
| 8 | B | 66 | 0 | 74 | 3 | 0 |
| 8 | D | 66 | 0 | 74 | 2 | 0 |
| 8 | E | 66 | 0 | 74 | 4 | 0 |
| 8 | F | 66 | 0 | 74 | 4 | 0 |
| 8 | G | 132 | 0 | 146 | 8 | 0 |
| 8 | I | 66 | 0 | 74 | 7 | 0 |
| 8 | J | 66 | 0 | 74 | 7 | 0 |
| 8 | K | 66 | 0 | 74 | 4 | 0 |
| 8 | L | 132 | 0 | 144 | 9 | 0 |
| 8 | M | 132 | 0 | 144 | 7 | 0 |
| 8 | N | 66 | 0 | 74 | 4 | 0 |
| 8 | P | 66 | 0 | 74 | 4 | 0 |
| 8 | Q | 66 | 0 | 74 | 5 | 0 |
| 8 | R | 132 | 0 | 145 | 6 | 0 |
| 8 | T | 66 | 0 | 74 | 5 | 0 |
| 8 | V | 66 | 0 | 72 | 5 | 0 |
| 8 | a | 66 | 0 | 74 | 3 | 0 |
| 8 | b | 66 | 0 | 74 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8 | d | 66 | 0 | 74 | 8 | 0 |
| 8 | e | 66 | 0 | 74 | 7 | 0 |
| 8 | f | 66 | 0 | 74 | 9 | 0 |
| 8 | i | 66 | 0 | 74 | 6 | 0 |
| 8 | j | 66 | 0 | 74 | 10 | 0 |
| 8 | k | 66 | 0 | 74 | 4 | 0 |
| 8 | n | 66 | 0 | 74 | 3 | 0 |
| 8 | p | 66 | 0 | 74 | 2 | 0 |
| 8 | q | 66 | 0 | 74 | 5 | 0 |
| 8 | r | 66 | 0 | 74 | 4 | 0 |
| 8 | s | 66 | 0 | 74 | 2 | 0 |
| 8 | t | 66 | 0 | 73 | 9 | 0 |
| 8 | v | 66 | 0 | 74 | 5 | 0 |
| 9 | 2 | 86 | 0 | 134 | 8 | 0 |
| 9 | D | 86 | 0 | 136 | 6 | 0 |
| 9 | E | 43 | 0 | 68 | 4 | 0 |
| 9 | F | 43 | 0 | 68 | 4 | 0 |
| 9 | G | 86 | 0 | 136 | 8 | 0 |
| 9 | I | 43 | 0 | 65 | 9 | 0 |
| 9 | K | 43 | 0 | 68 | 8 | 0 |
| 9 | M | 43 | 0 | 68 | 3 | 0 |
| 9 | Q | 43 | 0 | 68 | 3 | 0 |
| 9 | R | 43 | 0 | 68 | 10 | 0 |
| 9 | S | 86 | 0 | 131 | 10 | 0 |
| 9 | V | 43 | 0 | 68 | 9 | 0 |
| 9 | a | 129 | 0 | 197 | 11 | 0 |
| 9 | b | 43 | 0 | 66 | 12 | 0 |
| 9 | e | 43 | 0 | 65 | 4 | 0 |
| 9 | f | 43 | 0 | 68 | 1 | 0 |
| 9 | i | 86 | 0 | 133 | 8 | 0 |
| 9 | j | 43 | 0 | 68 | 4 | 0 |
| 9 | k | 86 | 0 | 131 | 3 | 0 |
| 9 | n | 43 | 0 | 68 | 8 | 0 |
| 9 | p | 86 | 0 | 132 | 15 | 0 |
| 9 | q | 43 | 0 | 65 | 2 | 0 |
| 9 | r | 86 | 0 | 134 | 5 | 0 |
| 9 | t | 43 | 0 | 63 | 3 | 0 |
| 9 | v | 43 | 0 | 68 | 6 | 0 |
| 10 | B | 53 | 0 | 0 | 0 | 0 |
| 10 | D | 27 | 0 | 0 | 0 | 0 |
| 10 | F | 91 | 0 | 0 | 0 | 0 |
| 10 | G | 49 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10 | H | 37 | 0 | 0 | 0 | 0 |
| 10 | I | 40 | 0 | 0 | 0 | 0 |
| 10 | L | 73 | 0 | 0 | 0 | 0 |
| 10 | M | 102 | 0 | 0 | 0 | 0 |
| 10 | Q | 45 | 0 | 0 | 0 | 0 |
| 11 | C | 24 | 0 | 34 | 0 | 0 |
| 11 | E | 35 | 0 | 46 | 4 | 0 |
| 11 | H | 24 | 0 | 34 | 0 | 0 |
| 11 | L | 48 | 0 | 65 | 1 | 0 |
| 12 | M | 1 | 0 | 0 | 0 | 0 |
| 13 | L | 65 | 0 | 76 | 2 | 0 |
| 13 | M | 65 | 0 | 73 | 2 | 0 |
| 14 | L | 48 | 0 | 63 | 7 | 0 |
| 14 | M | 63 | 0 | 90 | 6 | 0 |
| 15 | H | 158 | 0 | 213 | 6 | 0 |
| 16 | C | 129 | 0 | 89 | 10 | 0 |
| All | All | 28258 | 0 | 28382 | 526 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 526 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:C:144:MET:SD | 16:C:401:HEC:NC | 2.17 | 1.18 |
| 7:C:144:MET:SD | 16:C:401:HEC:FE | 1.52 | 1.00 |
| 7:C:144:MET:SD | 16:C:401:HEC:NB | 2.51 | 0.84 |
| 5:L:131:THR:HA | 5:L:135:PHE:HB2 | 1.61 | 0.83 |
| 4:M:270:ALA:HB1 | 5:L:188:LEU:HD11 | 1.61 | 0.82 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 1 | 48/53 (91%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 1 | A | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | B | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | D | 49/53 (92%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 1 | E | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | F | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | G | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | I | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | J | 48/53 (91%) | 48 (100%) | 0 | 0 | 100 | 100 |
| 1 | K | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | N | 49/53 (92%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 1 | P | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | Q | 49/53 (92%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 1 | R | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | S | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | T | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 1 | V | 49/53 (92%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 2 | O | 50/239 (21%) | 48 (96%) | 2 (4%) | 0 | 100 | 100 |
| 3 | 2 | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 3 | a | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | b | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 3 | d | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | e | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 3 | f | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 3 | g | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 3 | i | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 3 | j | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 3 | k | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 3 | n | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | p | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 3 | q | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 3 | r | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 3 | s | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 3 | t | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 3 | v | 38/49 (78%) | 38 (100%) | 0 | 0 | 100 | 100 |
| 4 | M | 323/330 (98%) | 313 (97%) | 10 (3%) | 0 | 100 | 100 |
| 5 | L | 272/279 (98%) | 261 (96%) | 11 (4%) | 0 | 100 | 100 |
| 6 | H | 254/256 (99%) | 246 (97%) | 8 (3%) | 0 | 100 | 100 |
| 7 | C | 350/360 (97%) | 337 (96%) | 13 (4%) | 0 | 100 | 100 |
| All | All | 2785/3198 (87%) | 2732 (98%) | 53 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

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 | 1 | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | A | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | B | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | D | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | E | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | F | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | G | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | I | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | J | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | K | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | N | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | P | 43/44 (98%) | 43 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1 | Q | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | R | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | S | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | T | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 1 | V | 42/44 (96%) | 42 (100%) | 0 | 100 | 100 |
| 2 | O | 39/174 (22%) | 39 (100%) | 0 | 100 | 100 |
| 3 | 2 | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | a | 37/41 (90%) | 37 (100%) | 0 | 100 | 100 |
| 3 | b | 37/41 (90%) | 37 (100%) | 0 | 100 | 100 |
| 3 | d | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | e | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | f | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | g | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | i | 35/41 (85%) | 35 (100%) | 0 | 100 | 100 |
| 3 | j | 35/41 (85%) | 35 (100%) | 0 | 100 | 100 |
| 3 | k | 35/41 (85%) | 35 (100%) | 0 | 100 | 100 |
| 3 | n | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | p | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | q | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | r | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | s | 36/41 (88%) | 36 (100%) | 0 | 100 | 100 |
| 3 | t | 35/41 (85%) | 35 (100%) | 0 | 100 | 100 |
| 3 | v | 32/41 (78%) | 32 (100%) | 0 | 100 | 100 |
| 4 | M | 266/270 (98%) | 266 (100%) | 0 | 100 | 100 |
| 5 | L | 218/223 (98%) | 218 (100%) | 0 | 100 | 100 |
| 6 | H | 214/214 (100%) | 214 (100%) | 0 | 100 | 100 |
| 7 | C | 298/307 (97%) | 297 (100%) | 1 (0%) | 86 | 95 |
| All | All | 2356/2633 (90%) | 2355 (100%) | 1 (0%) | 100 | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | C | 13 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M | 260 | ASN |
| 6 | H | 34 | ASN |
| 7 | C | 148 | ASN |
| 5 | L | 265 | ASN |
| 6 | H | 67 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 1 is monoatomic - leaving 99 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 | $\# Z > 2$ |
| 13 | BPH | M | 403 | 8 | 59,70,70 | 1.38 | 4 (6%) | 59,101,101 | 0.88 | 5 (8%) |
| 9 | SPN | b | 102 | - | 42,42,42 | 4.19 | 16 (38%) | 50,52,52 | 4.54 | 24 (48%) |
| 9 | SPN | M | 404 | - | 42,42,42 | 4.14 | 14 (33%) | 50,52,52 | 4.53 | 25 (50%) |
| 16 | HEC | C | 403 | 7 | 46,50,50 | 1.92 | 10 (21%) | 58,82,82 | 1.82 | 7 (12%) |
| 9 | SPN | I | 101 | - | 42,42,42 | 4.16 | 14 (33%) | 50,52,52 | 4.60 | 25 (50%) |
| 8 | BCL | T | 101 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.08 | 27 (34%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 9 | SPN | E | 102 | - | 42,42,42 | 4.15 | 15 (35%) | 50,52,52 | 4.52 | 25 (50%) |
| 10 | MW9 | M | 407 | - | 48,48,52 | 1.52 | 6 (12%) | 51,54,58 | 1.53 | 5 (9%) |
| 14 | U10 | L | 303 | - | 48,48,63 | 0.17 | 0 | 60,61,79 | 0.46 | 1 (1%) |
| 9 | SPN | k | 101 | - | 42,42,42 | 4.15 | 14 (33%) | 50,52,52 | 4.48 | 25 (50%) |
| 16 | HEC | C | 402 | 7 | 46,50,50 | 1.89 | 7 (15%) | 58,82,82 | 1.86 | 7 (12%) |
| 8 | BCL | G | 102 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.13 | 27 (34%) |
| 9 | SPN | i | 103 | - | 42,42,42 | 4.14 | 15 (35%) | 50,52,52 | 4.56 | 25 (50%) |
| 8 | BCL | G | 101 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.04 | 26 (32%) |
| 9 | SPN | q | 101 | - | 42,42,42 | 4.14 | 14 (33%) | 50,52,52 | 4.56 | 25 (50%) |
| 11 | LMT | C | 404 | - | 24,24,36 | 1.01 | 2 (8%) | 29,29,47 | 1.07 | 1 (3%) |
| 11 | LMT | L | 306 | - | 24,24,36 | 1.03 | 3 (12%) | 29,29,47 | 1.19 | 2 (6%) |
| 9 | SPN | F | 102 | - | 42,42,42 | 4.15 | 15 (35%) | 50,52,52 | 4.53 | 25 (50%) |
| 10 | MW9 | F | 103 | - | 42,42,52 | 1.48 | 6 (14%) | 45,48,58 | 1.53 | 4 (8%) |
| 11 | LMT | H | 301 | - | 24,24,36 | 1.02 | 3 (12%) | 29,29,47 | 1.07 | 1 (3%) |
| 9 | SPN | Q | 102 | - | 42,42,42 | 4.16 | 15 (35%) | 50,52,52 | 4.59 | 25 (50%) |
| 10 | MW9 | Q | 103 | - | 44,44,52 | 1.48 | 5 (11%) | 47,50,58 | 1.53 | 5 (10%) |
| 8 | BCL | k | 102 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.07 | 27 (34%) |
| 8 | BCL | f | 101 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.05 | 26 (32%) |
| 9 | SPN | a | 104 | - | 42,42,42 | 4.16 | 14 (33%) | 50,52,52 | 4.61 | 25 (50%) |
| 9 | SPN | p | 101 | - | 42,42,42 | 4.17 | 14 (33%) | 50,52,52 | 4.48 | 25 (50%) |
| 8 | BCL | v | 101 | - | 69,74,74 | 1.70 | 14 (20%) | 79,115,115 | 2.05 | 26 (32%) |
| 11 | LMT | L | 305 | - | 24,24,36 | 1.03 | 2 (8%) | 29,29,47 | 1.11 | 2 (6%) |
| 9 | SPN | k | 103 | - | 42,42,42 | 4.15 | 15 (35%) | 50,52,52 | 4.55 | 25 (50%) |
| 8 | BCL | l | 101 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.14 | 28 (35%) |
| 8 | BCL | M | 402 | 13 | 69,74,74 | 1.70 | 14 (20%) | 79,115,115 | 2.06 | 23 (29%) |
| 8 | BCL | J | 101 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.11 | 27 (34%) |
| 16 | HEC | C | 401 | 7 | 46,50,50 | 1.92 | 9 (19%) | 58,82,82 | 1.82 | 7 (12%) |
| 8 | BCL | E | 101 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.13 | 28 (35%) |
| 8 | BCL | r | 102 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.05 | 28 (35%) |
| 8 | BCL | A | 101 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.04 | 27 (34%) |
| 9 | SPN | v | 102 | - | 42,42,42 | 4.18 | 15 (35%) | 50,52,52 | 4.52 | 25 (50%) |
| 8 | BCL | M | 405 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.01 | 27 (34%) |
| 8 | BCL | R | 103 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.05 | 27 (34%) |
| 9 | SPN | G | 104 | - | 42,42,42 | 4.14 | 15 (35%) | 50,52,52 | 4.62 | 25 (50%) |
| 10 | MW9 | L | 307 | - | 36,36,52 | 1.51 | 5 (13%) | 39,42,58 | 1.61 | 4 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 8 | BCL | e | 101 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.04 | 27 (34%) |
| 8 | BCL | N | 101 | - | 69,74,74 | 1.72 | 15 (21%) | 79,115,115 | 2.11 | 27 (34%) |
| 8 | BCL | I | 102 | - | 69,74,74 | 1.73 | 14 (20%) | 79,115,115 | 2.15 | 27 (34%) |
| 9 | SPN | a | 103 | - | 42,42,42 | 4.18 | 16 (38%) | 50,52,52 | 4.46 | 25 (50%) |
| 8 | BCL | L | 304 | 8 | 69,74,74 | 1.69 | 14 (20%) | 79,115,115 | 2.15 | 27 (34%) |
| 8 | BCL | i | 102 | - | 69,74,74 | 1.73 | 13 (18%) | 79,115,115 | 2.13 | 27 (34%) |
| 9 | SPN | D | 102 | - | 42,42,42 | 4.16 | 15 (35%) | 50,52,52 | 4.47 | 25 (50%) |
| 14 | U10 | M | 406 | - | 63,63,63 | 0.15 | 0 | 78,79,79 | 0.42 | 1 (1%) |
| 8 | BCL | Q | 101 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.03 | 26 (32%) |
| 8 | BCL | j | 101 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.08 | 28 (35%) |
| 8 | BCL | B | 101 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.05 | 25 (31%) |
| 9 | SPN | 2 | 103 | - | 42,42,42 | 4.15 | 14 (33%) | 50,52,52 | 4.53 | 25 (50%) |
| 9 | SPN | f | 102 | - | 42,42,42 | 4.14 | 15 (35%) | 50,52,52 | 4.57 | 25 (50%) |
| 15 | CDL | H | 303 | - | 90,90,99 | 0.92 | 8 (8%) | 96,102,111 | 1.14 | 4 (4%) |
| 8 | BCL | D | 101 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.04 | 26 (32%) |
| 9 | SPN | p | 102 | - | 42,42,42 | 4.16 | 14 (33%) | 50,52,52 | 4.56 | 25 (50%) |
| 9 | SPN | G | 103 | - | 42,42,42 | 4.15 | 14 (33%) | 50,52,52 | 4.52 | 25 (50%) |
| 10 | MW9 | L | 308 | - | 35,35,52 | 1.27 | 3 (8%) | 38,41,58 | 1.13 | 2 (5%) |
| 9 | SPN | e | 102 | - | 42,42,42 | 4.14 | 15 (35%) | 50,52,52 | 4.57 | 25 (50%) |
| 9 | SPN | j | 102 | - | 42,42,42 | 4.15 | 14 (33%) | 50,52,52 | 4.56 | 25 (50%) |
| 10 | MW9 | H | 302 | - | 36,36,52 | 1.61 | 7 (19%) | 39,41,58 | 1.88 | 5 (12%) |
| 9 | SPN | S | 101 | - | 42,42,42 | 4.20 | 17 (40%) | 50,52,52 | 4.56 | 25 (50%) |
| 9 | SPN | i | 101 | - | 42,42,42 | 4.16 | 15 (35%) | 50,52,52 | 4.64 | 25 (50%) |
| 8 | BCL | b | 101 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.06 | 28 (35%) |
| 9 | SPN | R | 102 | - | 42,42,42 | 4.16 | 15 (35%) | 50,52,52 | 4.54 | 25 (50%) |
| 9 | SPN | D | 103 | - | 42,42,42 | 4.16 | 15 (35%) | 50,52,52 | 4.49 | 25 (50%) |
| 8 | BCL | L | 301 | 8 | 69,74,74 | 1.69 | 15 (21%) | 79,115,115 | 2.16 | 27 (34%) |
| 9 | SPN | r | 103 | - | 42,42,42 | 4.17 | 14 (33%) | 50,52,52 | 4.54 | 25 (50%) |
| 15 | CDL | H | 304 | - | 66,66,99 | 1.06 | 8 (12%) | 72,78,111 | 1.16 | 4 (5%) |
| 9 | SPN | S | 102 | 9 | 42,42,42 | 4.17 | 15 (35%) | 50,52,52 | 4.58 | 24 (48%) |
| 8 | BCL | q | 102 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.06 | 28 (35%) |
| 8 | BCL | P | 101 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.04 | 26 (32%) |
| 8 | BCL | p | 103 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.07 | 26 (32%) |
| 8 | BCL | s | 101 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.07 | 28 (35%) |
| 9 | SPN | K | 102 | - | 42,42,42 | 4.15 | 14 (33%) | 50,52,52 | 4.60 | 25 (50%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 10 | MW9 | F | 104 | - | 47,47,52 | 1.44 | 6 (12%) | 50,53,58 | 1.49 | 3 (6%) |
| 8 | BCL | a | 102 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.07 | 28 (35%) |
| 11 | LMT | E | 103 | - | 36,36,36 | 1.13 | 4 (11%) | 47,47,47 | 0.99 | 2 (4%) |
| 9 | SPN | t | 102 | 9 | 42,42,42 | 4.16 | 15 (35%) | 50,52,52 | 4.56 | 25 (50%) |
| 8 | BCL | V | 101 | 8 | 69,74,74 | 1.70 | 12 (17%) | 79,115,115 | 2.03 | 28 (35%) |
| 9 | SPN | n | 102 | - | 42,42,42 | 4.15 | 15 (35%) | 50,52,52 | 4.44 | 25 (50%) |
| 10 | MW9 | G | 105 | - | 48,48,52 | 1.52 | 6 (12%) | 51,54,58 | 1.50 | 4 (7%) |
| 9 | SPN | V | 102 | - | 42,42,42 | 4.18 | 14 (33%) | 50,52,52 | 4.58 | 25 (50%) |
| 13 | BPH | L | 302 | - | 59,70,70 | 1.06 | 2 (3%) | 59,101,101 | 0.86 | 4 (6%) |
| 10 | MW9 | D | 104 | - | 26,26,52 | 1.48 | 4 (15%) | 28,28,58 | 1.30 | 2 (7%) |
| 9 | SPN | a | 101 | - | 42,42,42 | 4.14 | 15 (35%) | 50,52,52 | 4.57 | 25 (50%) |
| 8 | BCL | F | 101 | - | 69,74,74 | 1.72 | 14 (20%) | 79,115,115 | 2.12 | 28 (35%) |
| 10 | MW9 | M | 408 | - | 52,52,52 | 1.48 | 6 (11%) | 55,58,58 | 1.49 | 5 (9%) |
| 8 | BCL | 2 | 101 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.10 | 26 (32%) |
| 8 | BCL | d | 101 | - | 69,74,74 | 1.73 | 11 (15%) | 79,115,115 | 2.07 | 26 (32%) |
| 10 | MW9 | I | 103 | - | 39,39,52 | 1.46 | 5 (12%) | 42,45,58 | 1.17 | 3 (7%) |
| 8 | BCL | n | 101 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.05 | 27 (34%) |
| 8 | BCL | K | 101 | - | 69,74,74 | 1.71 | 14 (20%) | 79,115,115 | 2.09 | 25 (31%) |
| 8 | BCL | t | 101 | 8 | 69,74,74 | 1.73 | 13 (18%) | 79,115,115 | 1.98 | 25 (31%) |
| 8 | BCL | R | 101 | - | 69,74,74 | 1.71 | 13 (18%) | 79,115,115 | 2.02 | 26 (32%) |
| 9 | SPN | 2 | 102 | - | 42,42,42 | 4.15 | 14 (33%) | 50,52,52 | 4.58 | 25 (50%) |
| 9 | SPN | r | 101 | - | 42,42,42 | 4.15 | 15 (35%) | 50,52,52 | 4.53 | 25 (50%) |
| 10 | MW9 | B | 102 | - | 52,52,52 | 1.48 | 6 (11%) | 55,58,58 | 1.48 | 4 (7%) |

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 |
|-----|------|-------|-----|------|---------|---------------|---------|
| 13 | BPH | M | 403 | 8 | - | 12/37/105/105 | 0/5/6/6 |
| 9 | SPN | b | 102 | - | - | 27/50/51/51 | - |
| 9 | SPN | M | 404 | - | - | 28/50/51/51 | - |
| 16 | HEC | C | 403 | 7 | - | 6/14/54/54 | - |
| 9 | SPN | I | 101 | - | - | 26/50/51/51 | - |
| 8 | BCL | T | 101 | - | - | 11/41/137/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|---------------|---------|
| 9 | SPN | E | 102 | - | - | 28/50/51/51 | - |
| 10 | MW9 | M | 407 | - | - | 27/53/53/57 | - |
| 14 | U10 | L | 303 | - | - | 10/45/69/87 | 0/1/1/1 |
| 9 | SPN | k | 101 | - | - | 32/50/51/51 | - |
| 16 | HEC | C | 402 | 7 | - | 5/14/54/54 | - |
| 8 | BCL | G | 102 | - | - | 10/41/137/137 | - |
| 9 | SPN | i | 103 | - | - | 22/50/51/51 | - |
| 8 | BCL | G | 101 | - | - | 16/41/137/137 | - |
| 9 | SPN | q | 101 | - | - | 27/50/51/51 | - |
| 11 | LMT | C | 404 | - | - | 4/15/35/61 | 0/1/1/2 |
| 11 | LMT | L | 306 | - | - | 7/15/35/61 | 0/1/1/2 |
| 9 | SPN | F | 102 | - | - | 28/50/51/51 | - |
| 10 | MW9 | F | 103 | - | - | 27/47/47/57 | - |
| 11 | LMT | H | 301 | - | - | 6/15/35/61 | 0/1/1/2 |
| 9 | SPN | Q | 102 | - | - | 30/50/51/51 | - |
| 10 | MW9 | Q | 103 | - | - | 31/49/49/57 | - |
| 8 | BCL | k | 102 | - | - | 12/41/137/137 | - |
| 8 | BCL | f | 101 | - | - | 17/41/137/137 | - |
| 9 | SPN | a | 104 | - | - | 27/50/51/51 | - |
| 9 | SPN | p | 101 | - | - | 31/50/51/51 | - |
| 8 | BCL | v | 101 | - | - | 20/41/137/137 | - |
| 11 | LMT | L | 305 | - | - | 5/15/35/61 | 0/1/1/2 |
| 9 | SPN | k | 103 | - | - | 33/50/51/51 | - |
| 8 | BCL | l | 101 | - | - | 12/41/137/137 | - |
| 8 | BCL | M | 402 | 13 | - | 14/41/137/137 | - |
| 8 | BCL | J | 101 | - | - | 10/41/137/137 | - |
| 16 | HEC | C | 401 | 7 | - | 6/14/54/54 | - |
| 8 | BCL | E | 101 | - | - | 10/41/137/137 | - |
| 8 | BCL | r | 102 | - | - | 12/41/137/137 | - |
| 8 | BCL | A | 101 | - | - | 14/41/137/137 | - |
| 9 | SPN | v | 102 | - | - | 28/50/51/51 | - |
| 8 | BCL | M | 405 | - | - | 12/41/137/137 | - |
| 8 | BCL | R | 103 | - | - | 9/41/137/137 | - |
| 9 | SPN | G | 104 | - | - | 26/50/51/51 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 10 | MW9 | L | 307 | - | - | 19/41/41/57 | - |
| 8 | BCL | e | 101 | - | - | 12/41/137/137 | - |
| 8 | BCL | N | 101 | - | - | 12/41/137/137 | - |
| 8 | BCL | I | 102 | - | - | 15/41/137/137 | - |
| 9 | SPN | a | 103 | - | - | 29/50/51/51 | - |
| 8 | BCL | L | 304 | 8 | - | 18/41/137/137 | - |
| 8 | BCL | i | 102 | - | - | 15/41/137/137 | - |
| 9 | SPN | D | 102 | - | - | 27/50/51/51 | - |
| 14 | U10 | M | 406 | - | - | 8/63/87/87 | 0/1/1/1 |
| 8 | BCL | Q | 101 | - | - | 14/41/137/137 | - |
| 8 | BCL | j | 101 | - | - | 12/41/137/137 | - |
| 8 | BCL | B | 101 | - | - | 16/41/137/137 | - |
| 9 | SPN | 2 | 103 | - | - | 26/50/51/51 | - |
| 9 | SPN | f | 102 | - | - | 26/50/51/51 | - |
| 15 | CDL | H | 303 | - | - | 43/101/101/110 | - |
| 8 | BCL | D | 101 | - | - | 13/41/137/137 | - |
| 9 | SPN | p | 102 | - | - | 27/50/51/51 | - |
| 9 | SPN | G | 103 | - | - | 29/50/51/51 | - |
| 10 | MW9 | L | 308 | - | - | 16/40/40/57 | - |
| 9 | SPN | e | 102 | - | - | 30/50/51/51 | - |
| 9 | SPN | j | 102 | - | - | 28/50/51/51 | - |
| 10 | MW9 | H | 302 | - | - | 24/38/38/57 | - |
| 9 | SPN | S | 101 | - | - | 25/50/51/51 | - |
| 9 | SPN | i | 101 | - | - | 25/50/51/51 | - |
| 8 | BCL | b | 101 | - | - | 9/41/137/137 | - |
| 9 | SPN | R | 102 | - | - | 29/50/51/51 | - |
| 9 | SPN | D | 103 | - | - | 28/50/51/51 | - |
| 8 | BCL | L | 301 | 8 | - | 14/41/137/137 | - |
| 9 | SPN | r | 103 | - | - | 34/50/51/51 | - |
| 15 | CDL | H | 304 | - | - | 41/77/77/110 | - |
| 9 | SPN | S | 102 | 9 | - | 30/50/51/51 | - |
| 8 | BCL | q | 102 | - | - | 15/41/137/137 | - |
| 8 | BCL | P | 101 | - | - | 12/41/137/137 | - |
| 8 | BCL | p | 103 | - | - | 14/41/137/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|---------------|---------|
| 8 | BCL | s | 101 | - | - | 17/41/137/137 | - |
| 9 | SPN | K | 102 | - | - | 23/50/51/51 | - |
| 10 | MW9 | F | 104 | - | - | 29/52/52/57 | - |
| 8 | BCL | a | 102 | - | - | 15/41/137/137 | - |
| 11 | LMT | E | 103 | - | - | 8/21/61/61 | 0/2/2/2 |
| 9 | SPN | t | 102 | 9 | - | 31/50/51/51 | - |
| 8 | BCL | V | 101 | 8 | - | 10/41/137/137 | - |
| 9 | SPN | n | 102 | - | - | 26/50/51/51 | - |
| 10 | MW9 | G | 105 | - | - | 26/53/53/57 | - |
| 9 | SPN | V | 102 | - | - | 29/50/51/51 | - |
| 13 | BPH | L | 302 | - | - | 6/37/105/105 | 0/5/6/6 |
| 10 | MW9 | D | 104 | - | - | 13/28/28/57 | - |
| 9 | SPN | a | 101 | - | - | 25/50/51/51 | - |
| 8 | BCL | F | 101 | - | - | 9/41/137/137 | - |
| 10 | MW9 | M | 408 | - | - | 38/57/57/57 | - |
| 8 | BCL | 2 | 101 | - | - | 18/41/137/137 | - |
| 8 | BCL | d | 101 | - | - | 18/41/137/137 | - |
| 10 | MW9 | I | 103 | - | - | 30/44/44/57 | - |
| 8 | BCL | n | 101 | - | - | 9/41/137/137 | - |
| 8 | BCL | K | 101 | - | - | 9/41/137/137 | - |
| 8 | BCL | t | 101 | 8 | - | 9/41/137/137 | - |
| 8 | BCL | R | 101 | - | - | 9/41/137/137 | - |
| 9 | SPN | 2 | 102 | - | - | 28/50/51/51 | - |
| 9 | SPN | r | 101 | - | - | 27/50/51/51 | - |
| 10 | MW9 | B | 102 | - | - | 33/57/57/57 | - |

The worst 5 of 1160 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 9 | q | 101 | SPN | C3-C4 | -10.26 | 1.34 | 1.50 |
| 9 | G | 103 | SPN | C3-C4 | -10.23 | 1.34 | 1.50 |
| 9 | p | 101 | SPN | C3-C4 | -10.22 | 1.34 | 1.50 |
| 9 | v | 102 | SPN | C3-C4 | -10.16 | 1.34 | 1.50 |
| 9 | S | 102 | SPN | C3-C4 | -10.15 | 1.34 | 1.50 |

The worst 5 of 1983 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9 | K | 102 | SPN | C3-C4-C5 | 15.81 | 154.07 | 126.83 |
| 9 | V | 102 | SPN | C3-C4-C5 | 15.66 | 153.80 | 126.83 |
| 9 | G | 104 | SPN | C3-C4-C5 | 15.57 | 153.65 | 126.83 |
| 9 | i | 103 | SPN | C3-C4-C5 | 15.40 | 153.35 | 126.83 |
| 9 | a | 101 | SPN | C3-C4-C5 | 15.27 | 153.15 | 126.83 |

There are no chirality outliers.

5 of 1948 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 8 | P | 101 | BCL | C3A-C2A-CAA-CBA |
| 8 | P | 101 | BCL | C2C-C3C-CAC-CBC |
| 8 | P | 101 | BCL | C4C-C3C-CAC-CBC |
| 8 | V | 101 | BCL | C2C-C3C-CAC-CBC |
| 8 | V | 101 | BCL | C4C-C3C-CAC-CBC |

There are no ring outliers.

84 monomers are involved in 316 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13 | M | 403 | BPH | 2 | 0 |
| 9 | b | 102 | SPN | 12 | 0 |
| 9 | M | 404 | SPN | 3 | 0 |
| 16 | C | 403 | HEC | 1 | 0 |
| 9 | I | 101 | SPN | 9 | 0 |
| 8 | T | 101 | BCL | 5 | 0 |
| 9 | E | 102 | SPN | 4 | 0 |
| 14 | L | 303 | U10 | 7 | 0 |
| 9 | k | 101 | SPN | 1 | 0 |
| 16 | C | 402 | HEC | 3 | 0 |
| 8 | G | 102 | BCL | 3 | 0 |
| 9 | i | 103 | SPN | 3 | 0 |
| 8 | G | 101 | BCL | 6 | 0 |
| 9 | q | 101 | SPN | 2 | 0 |
| 9 | F | 102 | SPN | 4 | 0 |
| 9 | Q | 102 | SPN | 3 | 0 |
| 8 | k | 102 | BCL | 4 | 0 |
| 8 | f | 101 | BCL | 9 | 0 |
| 9 | a | 104 | SPN | 7 | 0 |
| 9 | p | 101 | SPN | 10 | 0 |
| 8 | v | 101 | BCL | 5 | 0 |
| 11 | L | 305 | LMT | 1 | 0 |

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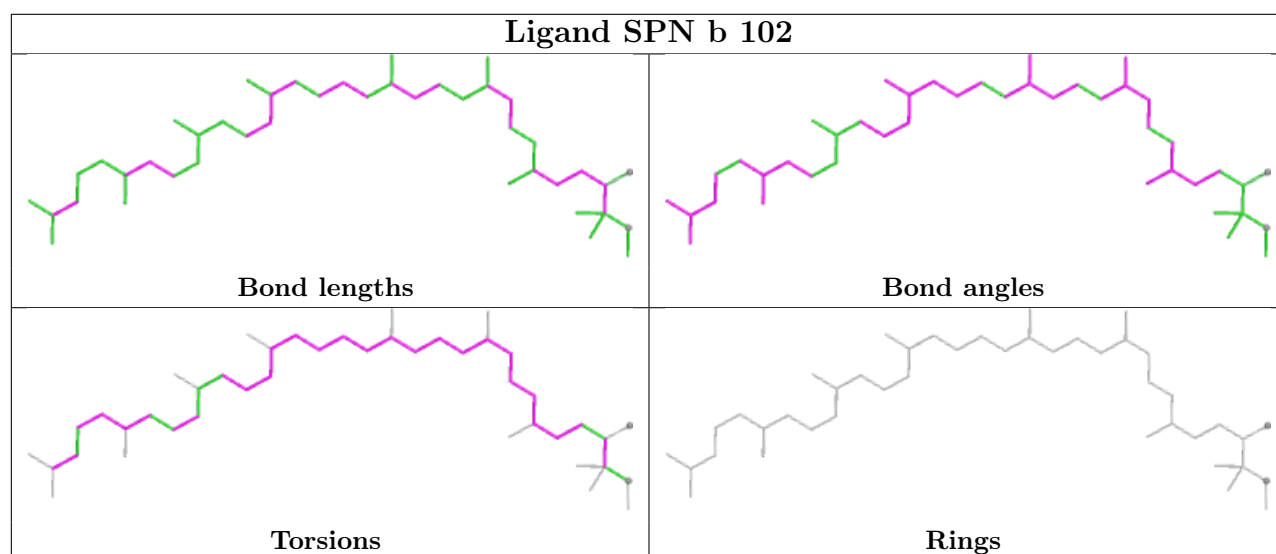
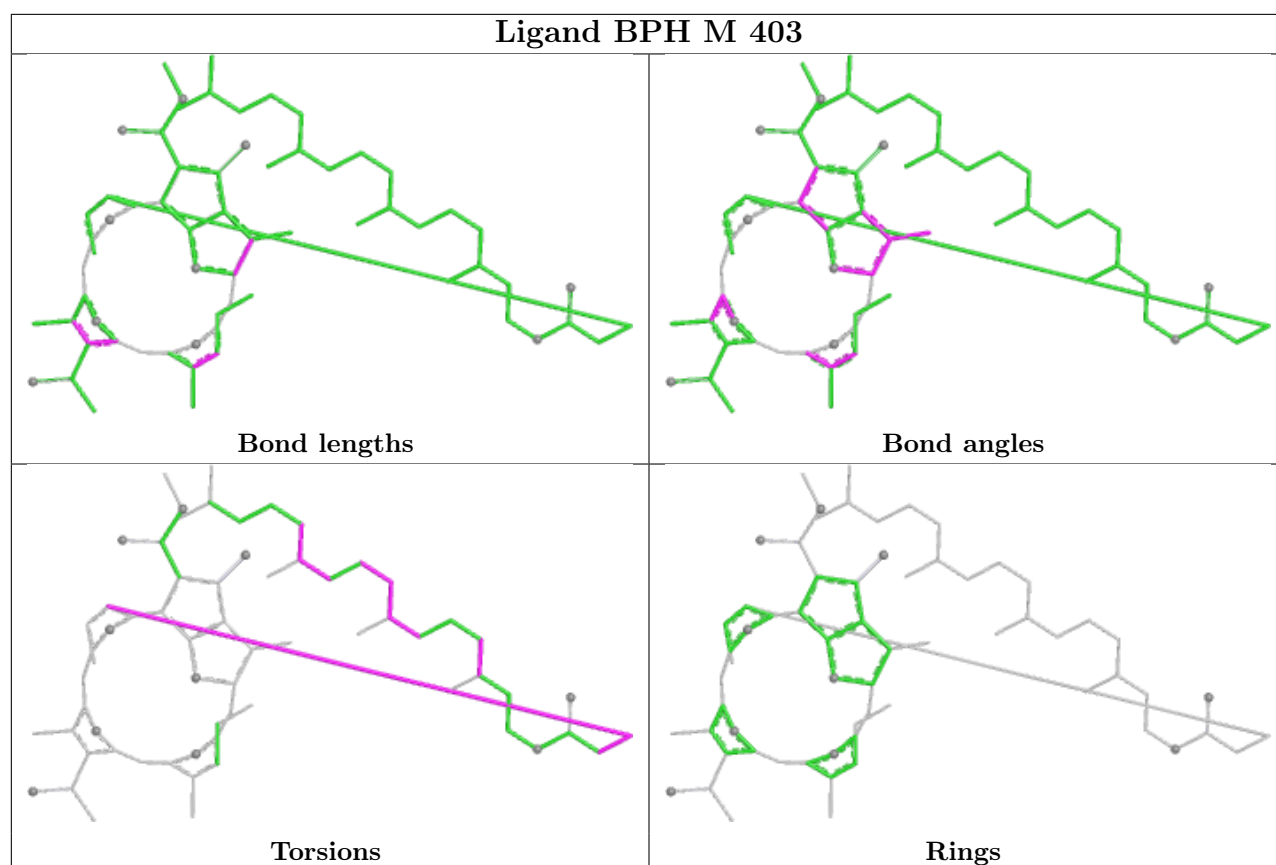
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9 | k | 103 | SPN | 2 | 0 |
| 8 | l | 101 | BCL | 3 | 0 |
| 8 | M | 402 | BCL | 4 | 0 |
| 8 | J | 101 | BCL | 7 | 0 |
| 16 | C | 401 | HEC | 6 | 0 |
| 8 | E | 101 | BCL | 4 | 0 |
| 8 | r | 102 | BCL | 4 | 0 |
| 8 | A | 101 | BCL | 6 | 0 |
| 9 | v | 102 | SPN | 6 | 0 |
| 8 | M | 405 | BCL | 4 | 0 |
| 8 | R | 103 | BCL | 4 | 0 |
| 9 | G | 104 | SPN | 3 | 0 |
| 8 | e | 101 | BCL | 7 | 0 |
| 8 | N | 101 | BCL | 4 | 0 |
| 8 | I | 102 | BCL | 7 | 0 |
| 9 | a | 103 | SPN | 2 | 0 |
| 8 | L | 304 | BCL | 7 | 0 |
| 8 | i | 102 | BCL | 6 | 0 |
| 9 | D | 102 | SPN | 3 | 0 |
| 14 | M | 406 | U10 | 6 | 0 |
| 8 | Q | 101 | BCL | 5 | 0 |
| 8 | j | 101 | BCL | 10 | 0 |
| 8 | B | 101 | BCL | 3 | 0 |
| 9 | 2 | 103 | SPN | 6 | 0 |
| 9 | f | 102 | SPN | 1 | 0 |
| 15 | H | 303 | CDL | 4 | 0 |
| 8 | D | 101 | BCL | 2 | 0 |
| 9 | p | 102 | SPN | 5 | 0 |
| 9 | G | 103 | SPN | 5 | 0 |
| 9 | e | 102 | SPN | 4 | 0 |
| 9 | j | 102 | SPN | 4 | 0 |
| 9 | S | 101 | SPN | 6 | 0 |
| 9 | i | 101 | SPN | 5 | 0 |
| 8 | b | 101 | BCL | 3 | 0 |
| 9 | R | 102 | SPN | 10 | 0 |
| 9 | D | 103 | SPN | 3 | 0 |
| 8 | L | 301 | BCL | 3 | 0 |
| 9 | r | 103 | SPN | 1 | 0 |
| 15 | H | 304 | CDL | 2 | 0 |
| 9 | S | 102 | SPN | 4 | 0 |
| 8 | q | 102 | BCL | 5 | 0 |
| 8 | P | 101 | BCL | 4 | 0 |

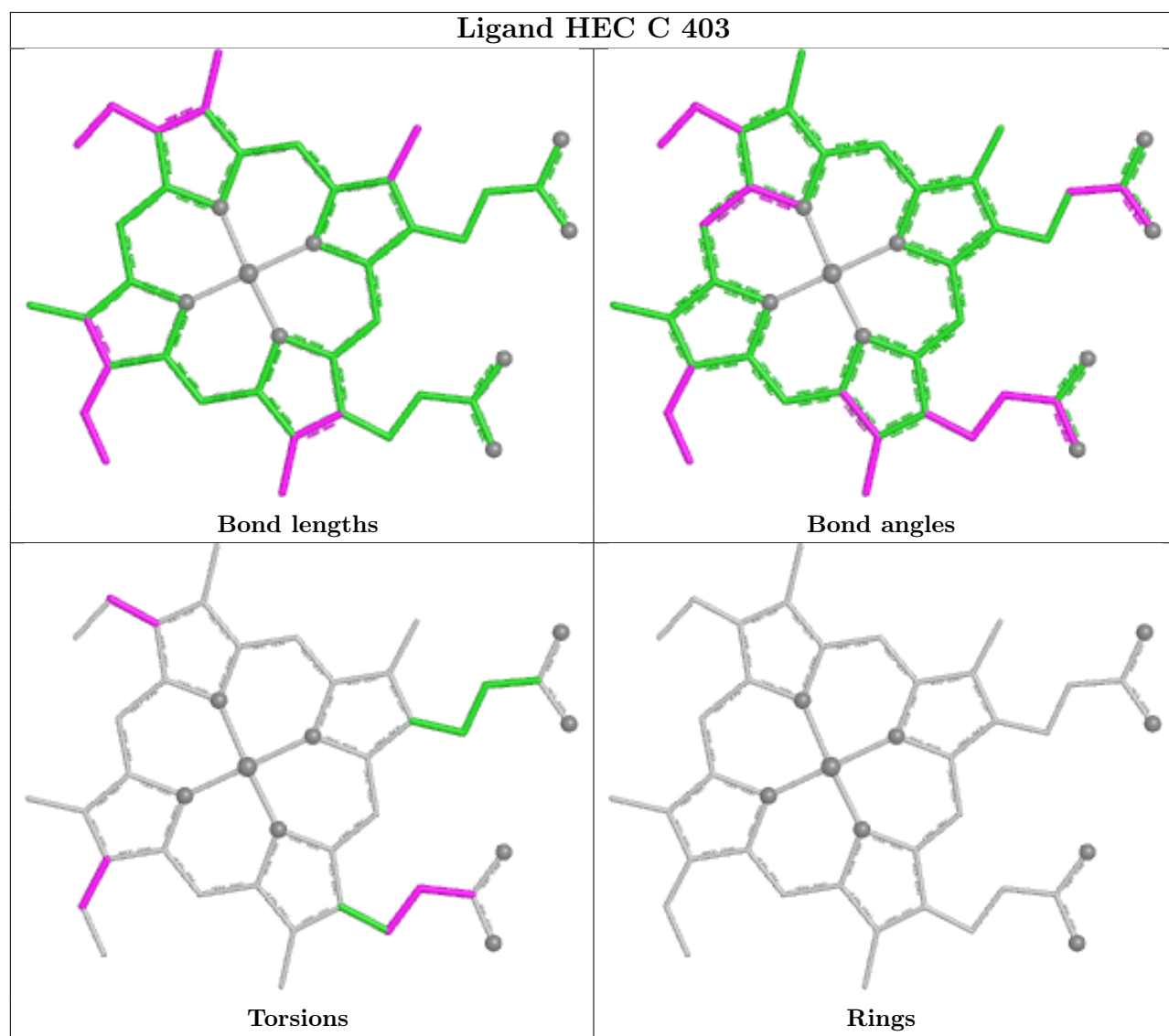
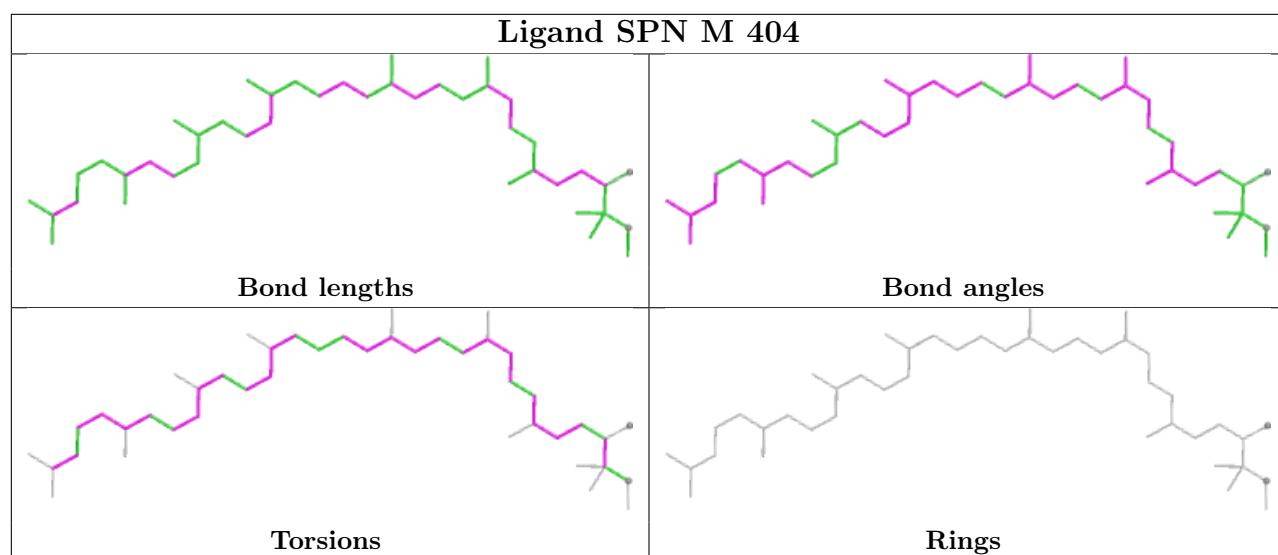
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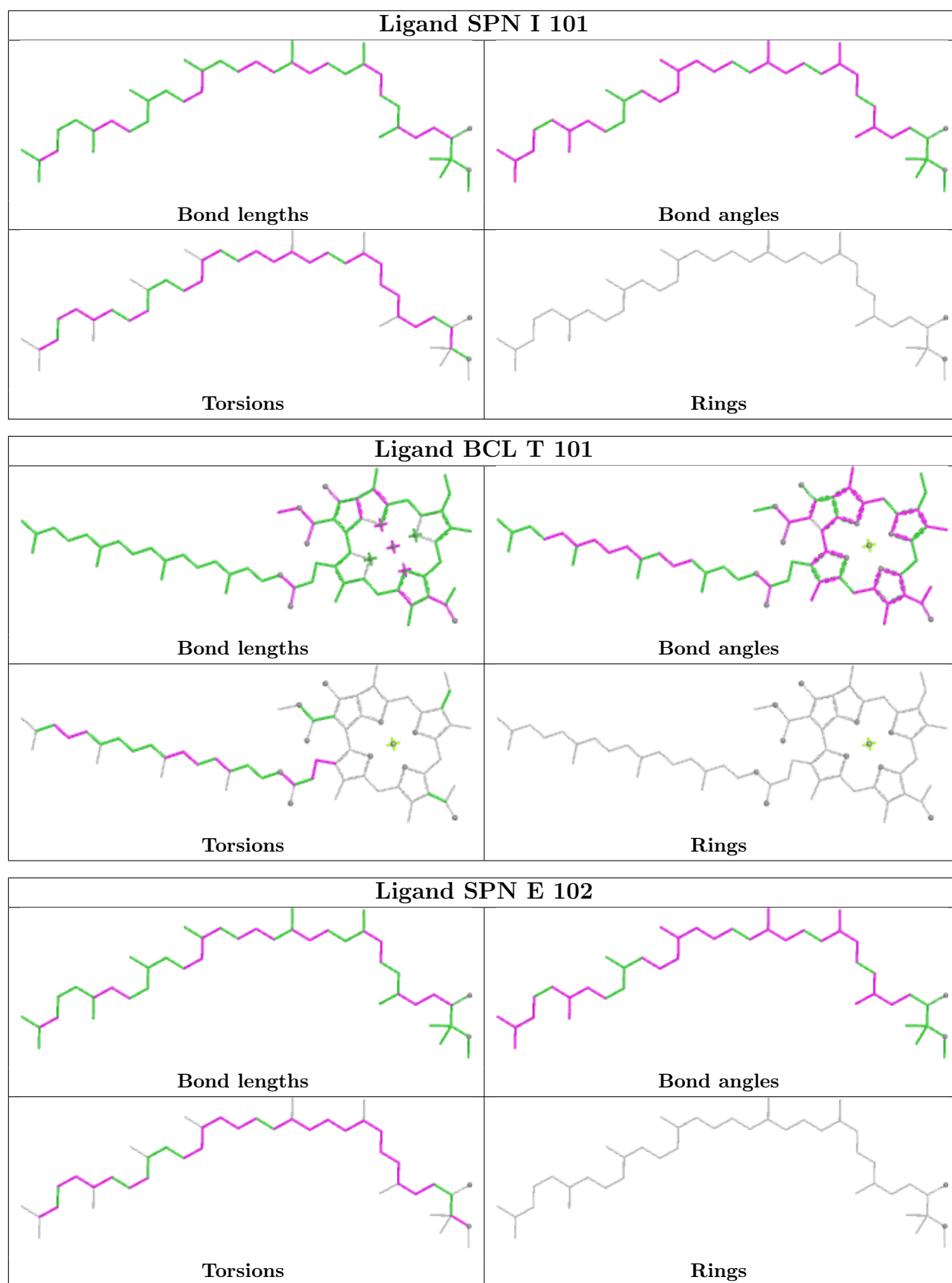
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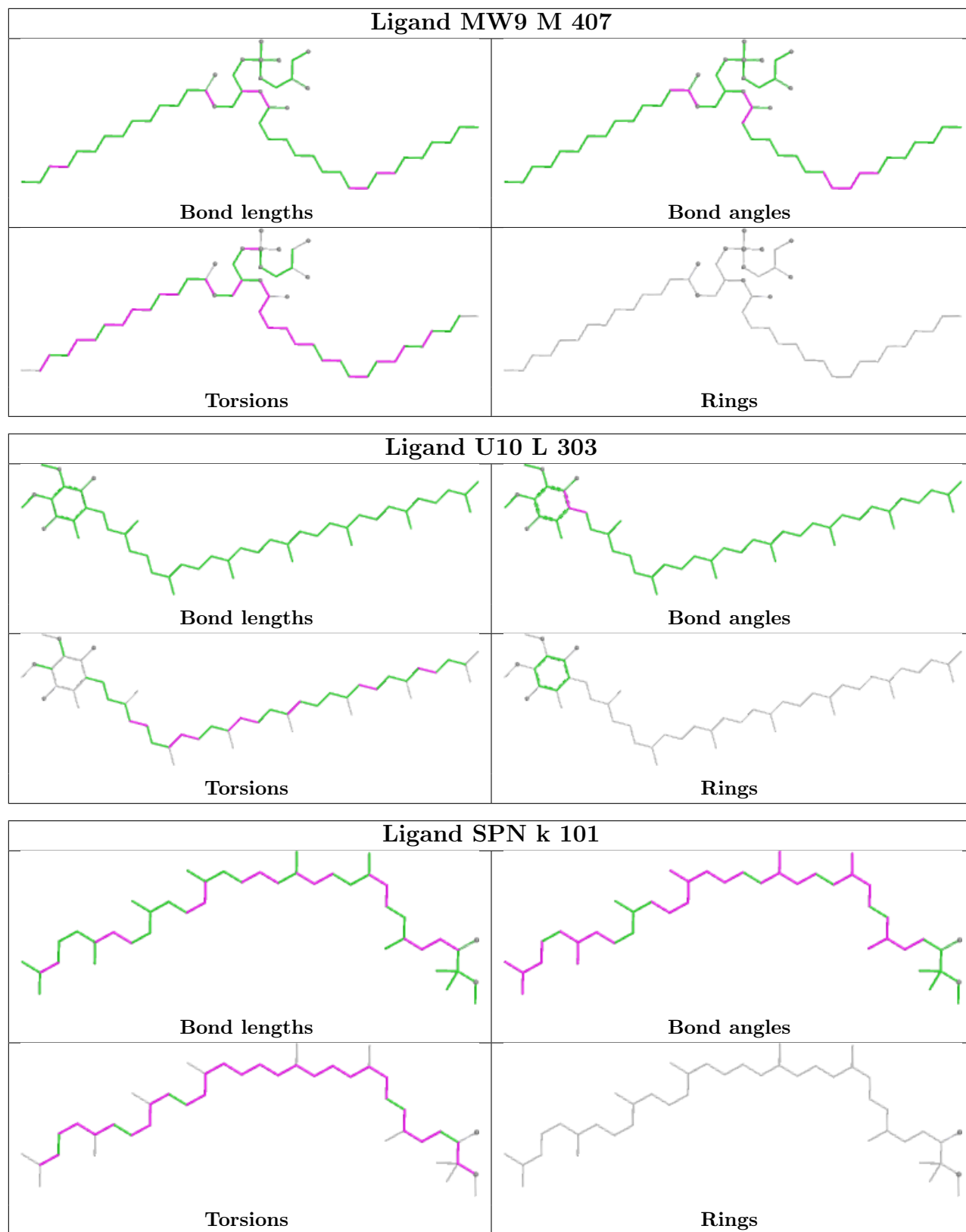
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 8 | p | 103 | BCL | 2 | 0 |
| 8 | s | 101 | BCL | 2 | 0 |
| 9 | K | 102 | SPN | 8 | 0 |
| 8 | a | 102 | BCL | 3 | 0 |
| 11 | E | 103 | LMT | 4 | 0 |
| 9 | t | 102 | SPN | 3 | 0 |
| 8 | V | 101 | BCL | 5 | 0 |
| 9 | n | 102 | SPN | 8 | 0 |
| 9 | V | 102 | SPN | 9 | 0 |
| 13 | L | 302 | BPH | 2 | 0 |
| 9 | a | 101 | SPN | 2 | 0 |
| 8 | F | 101 | BCL | 4 | 0 |
| 8 | 2 | 101 | BCL | 2 | 0 |
| 8 | d | 101 | BCL | 8 | 0 |
| 8 | n | 101 | BCL | 3 | 0 |
| 8 | K | 101 | BCL | 4 | 0 |
| 8 | t | 101 | BCL | 9 | 0 |
| 8 | R | 101 | BCL | 2 | 0 |
| 9 | 2 | 102 | SPN | 2 | 0 |
| 9 | r | 101 | SPN | 4 | 0 |

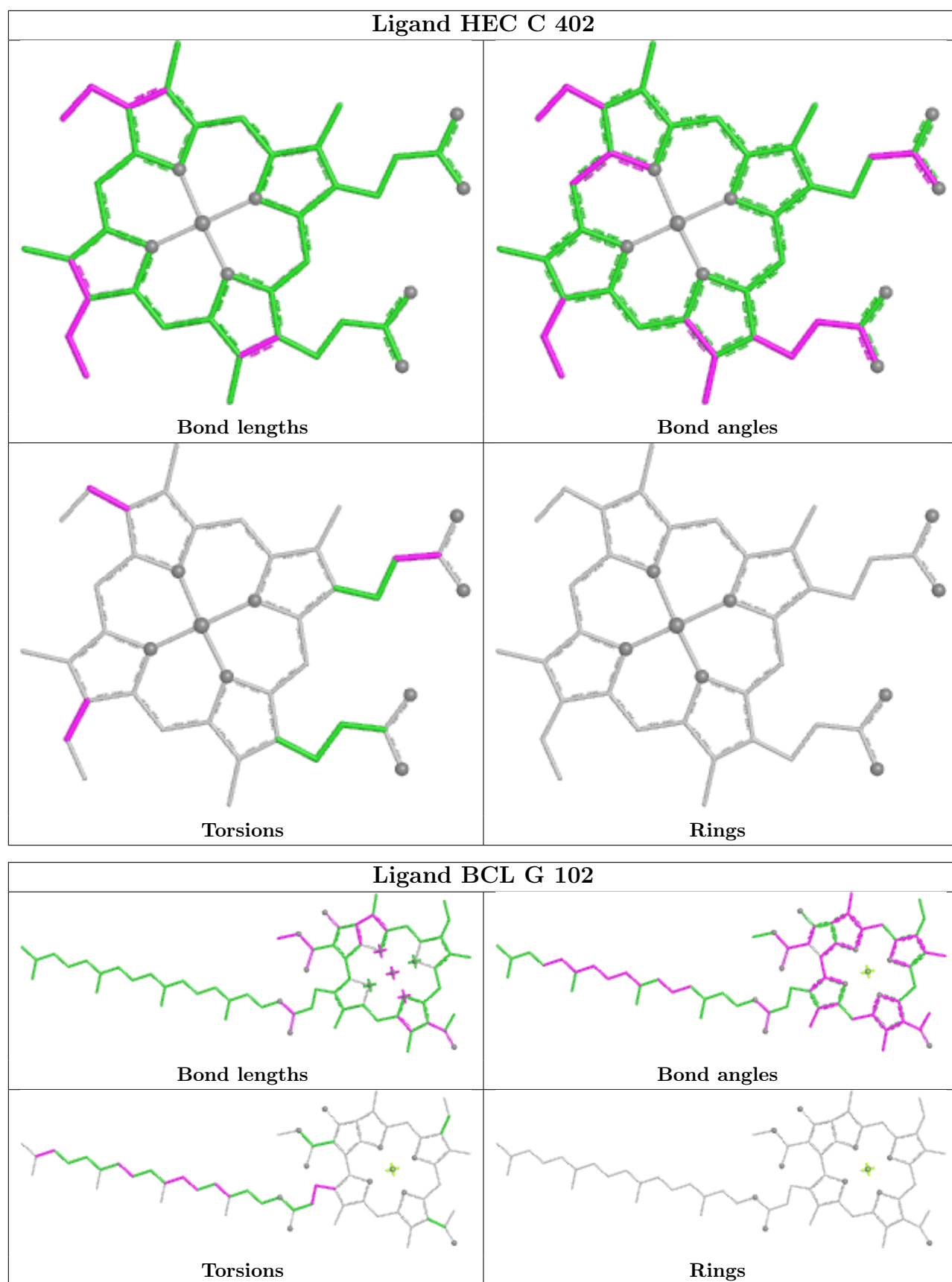
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

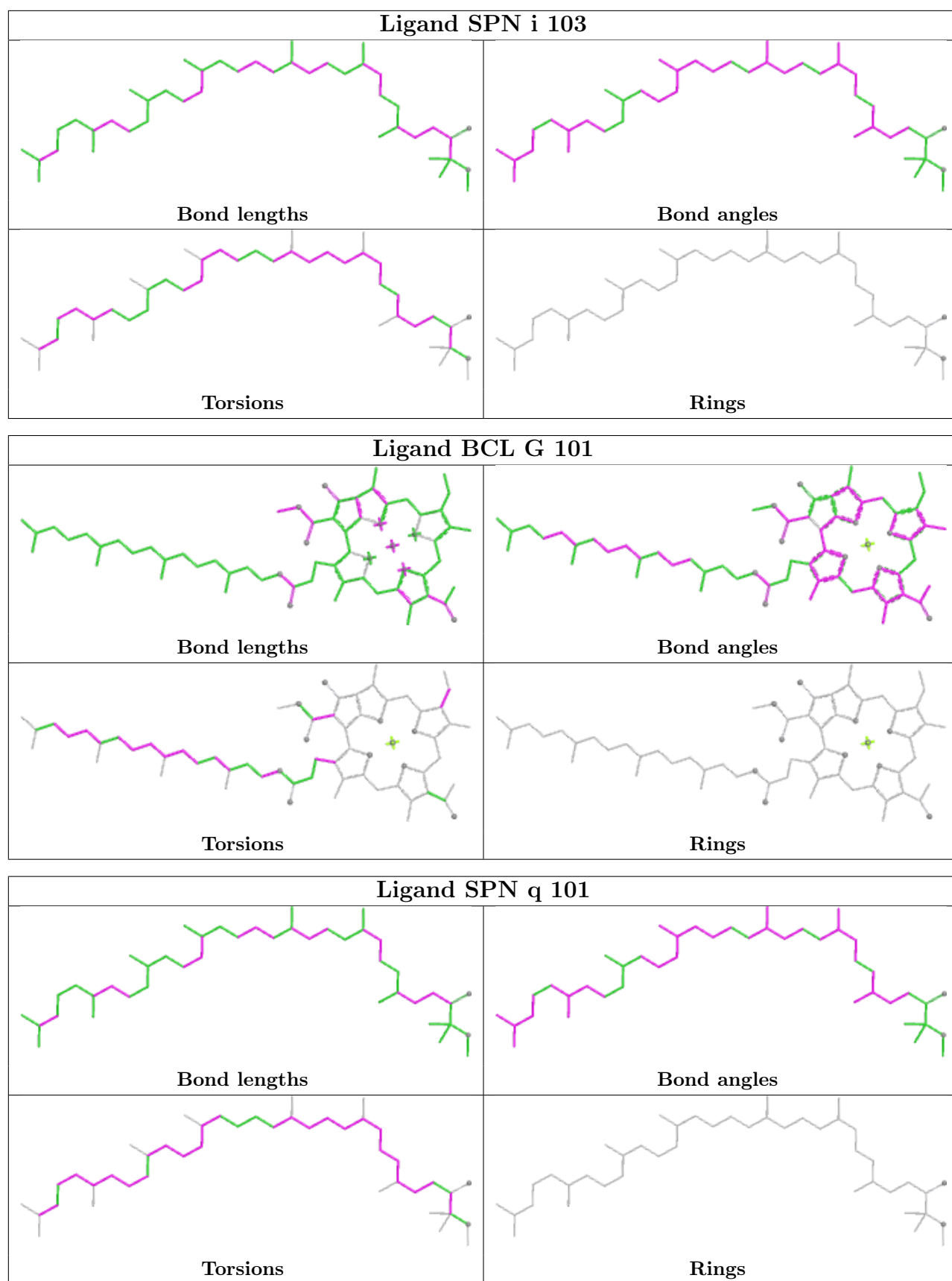


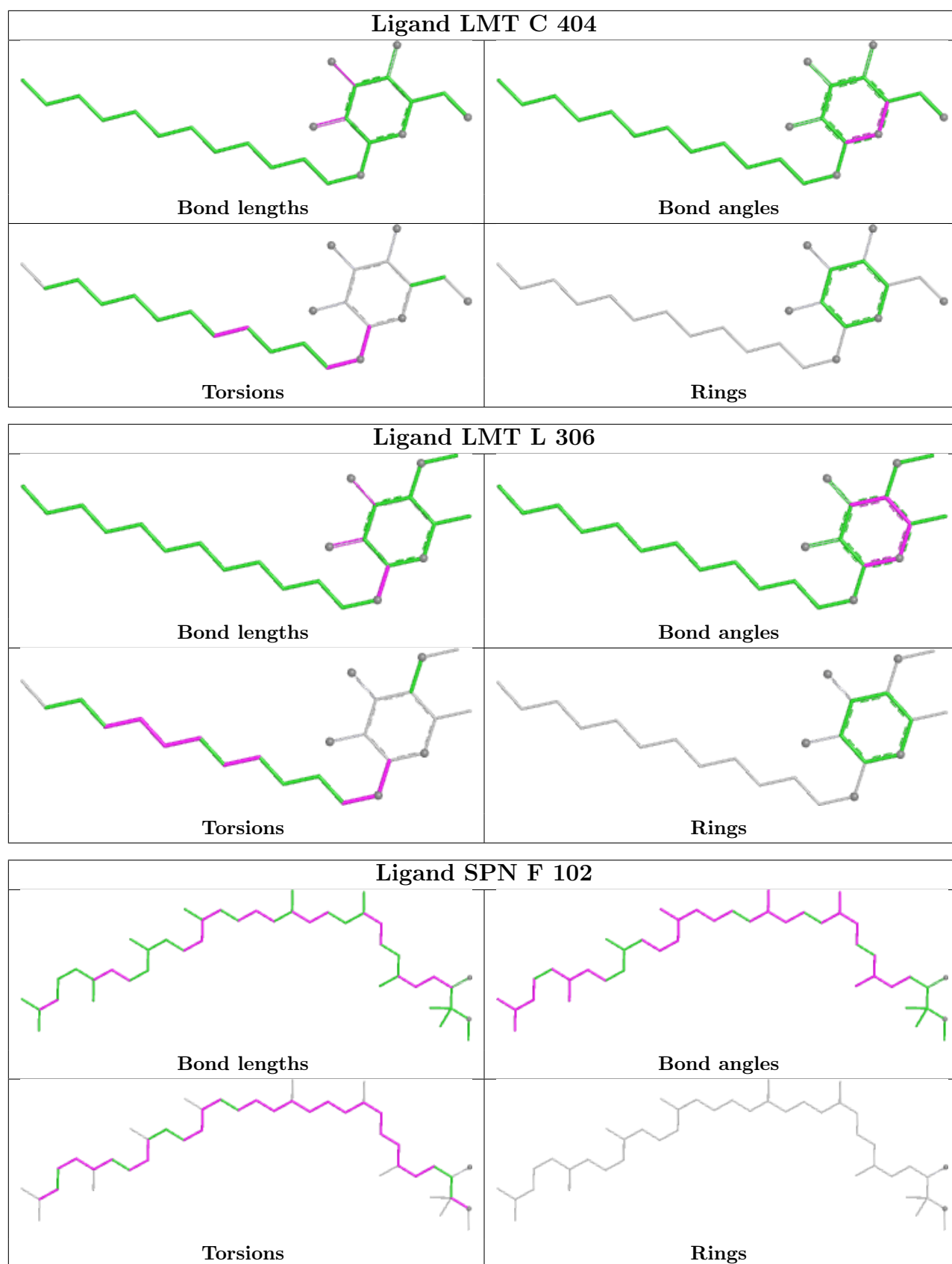


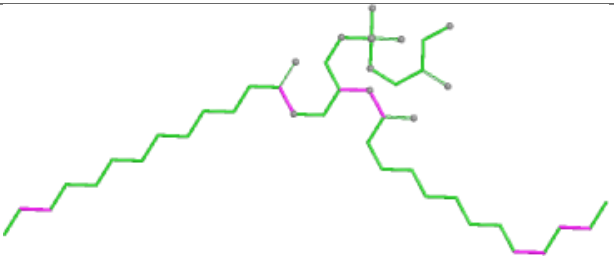
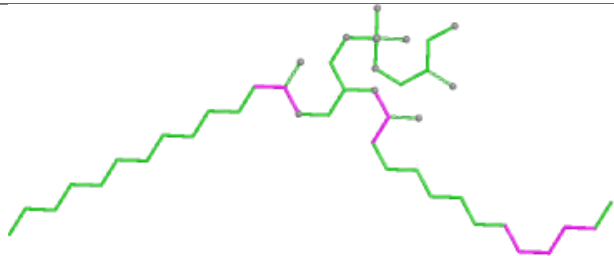
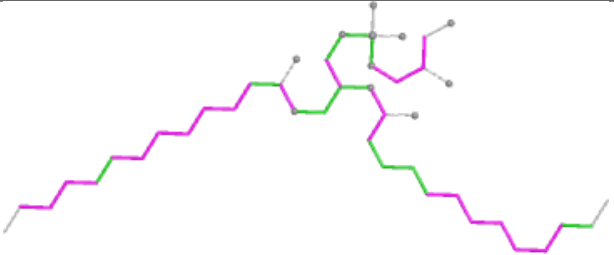
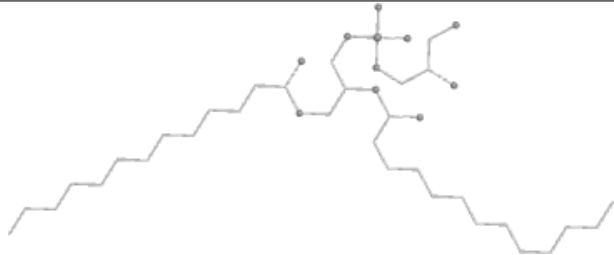


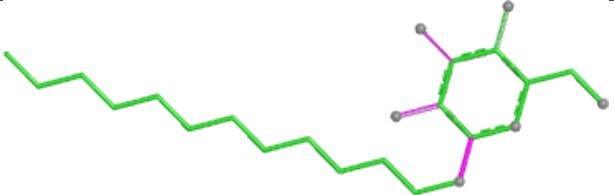
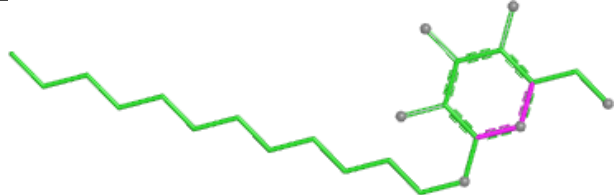
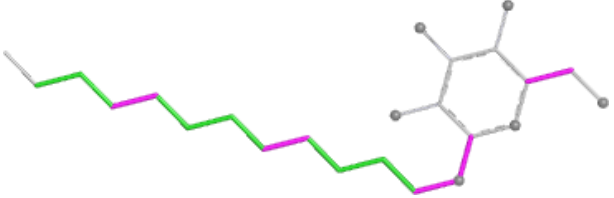



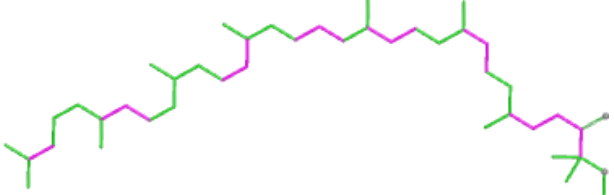
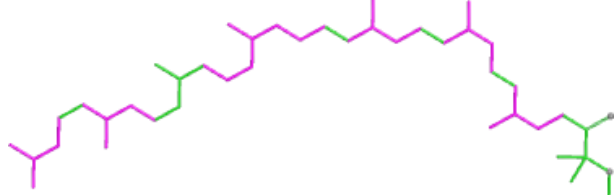
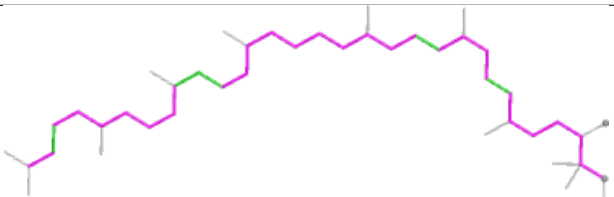
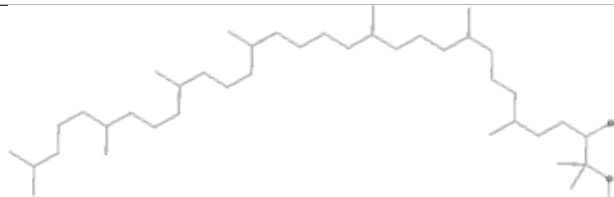


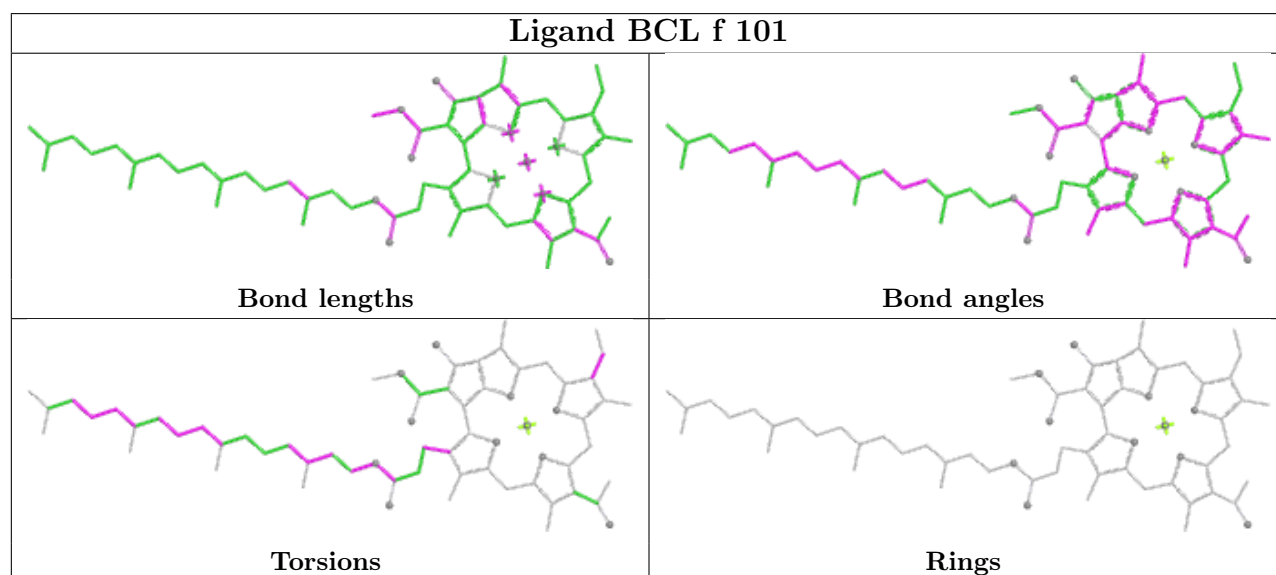
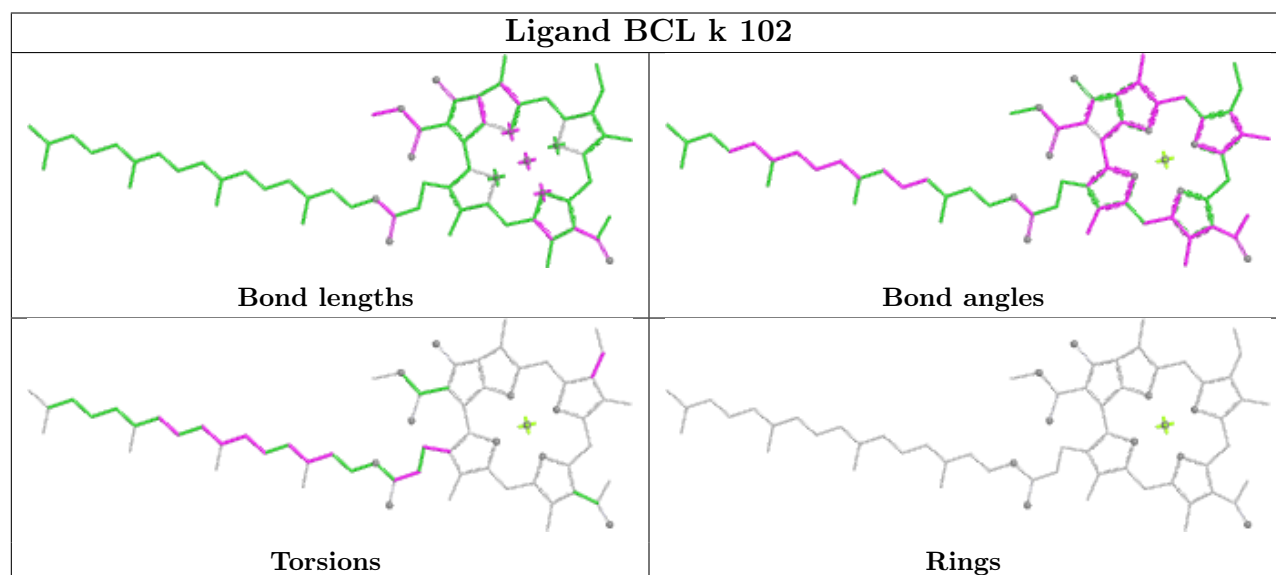
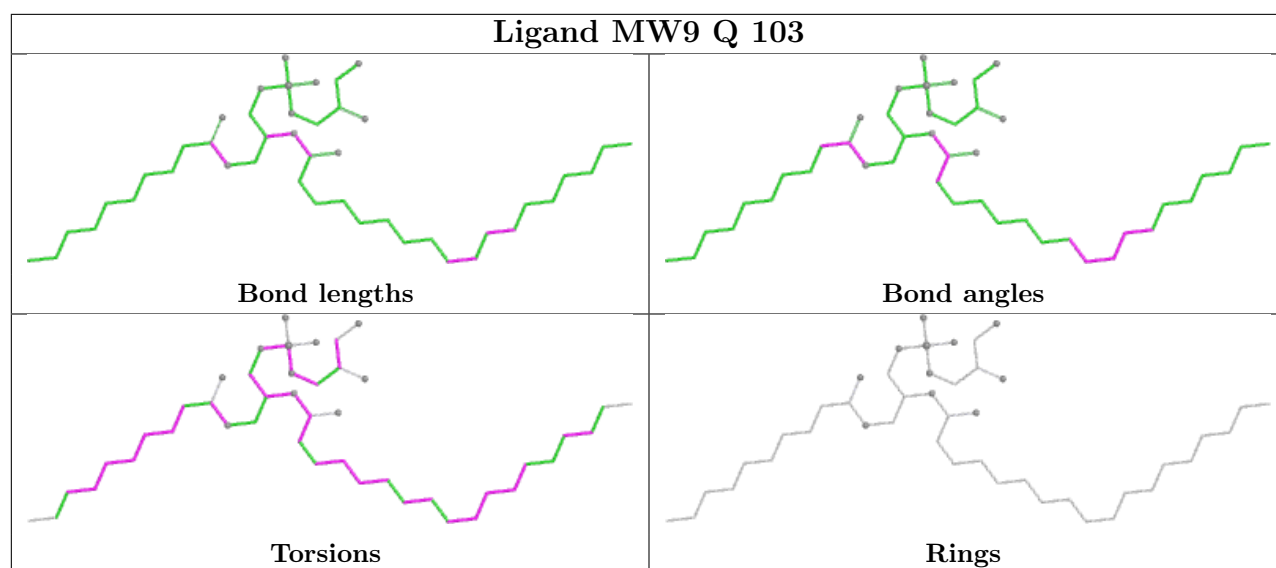


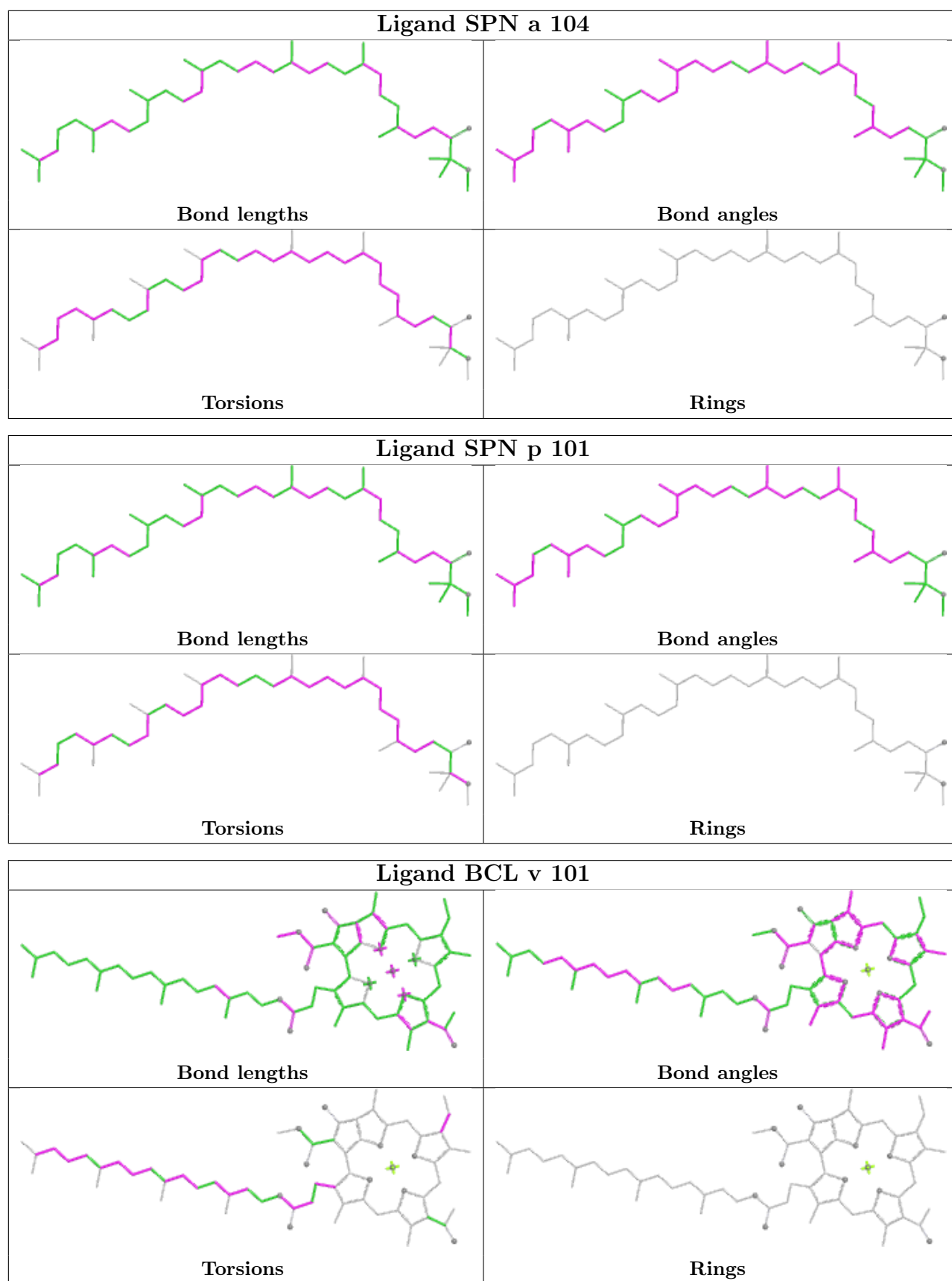


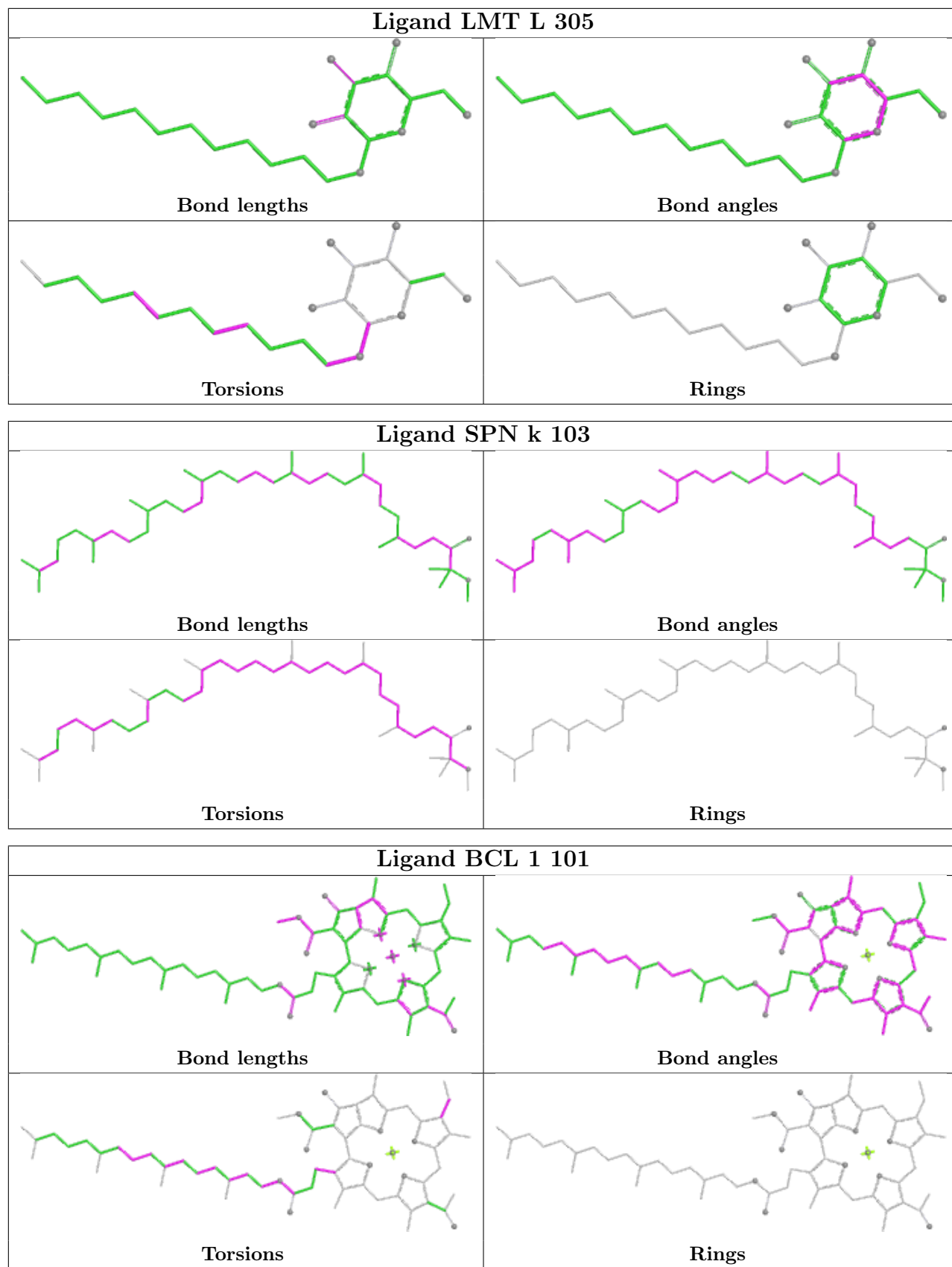
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|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

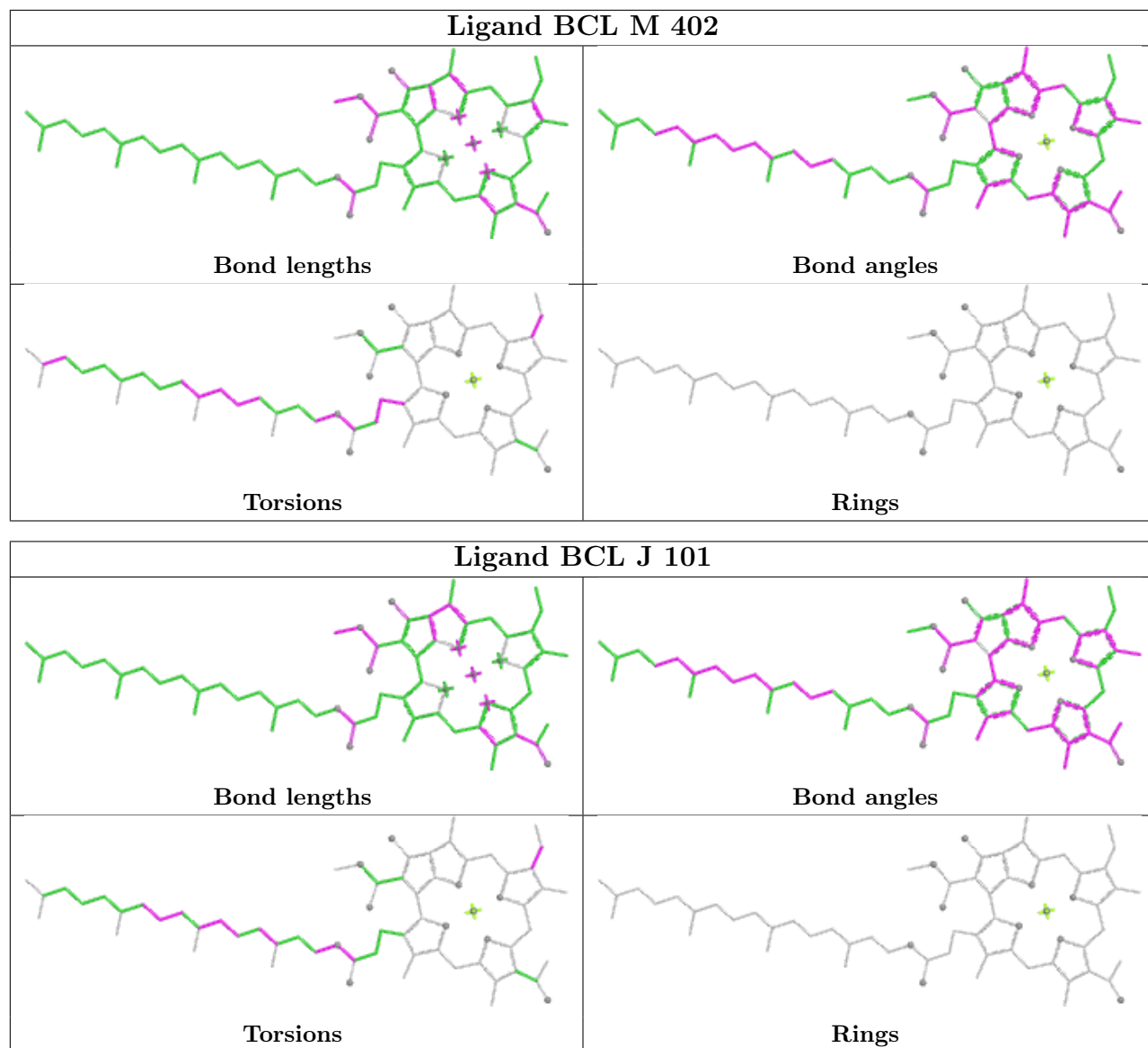
| Ligand LMT H 301 | |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

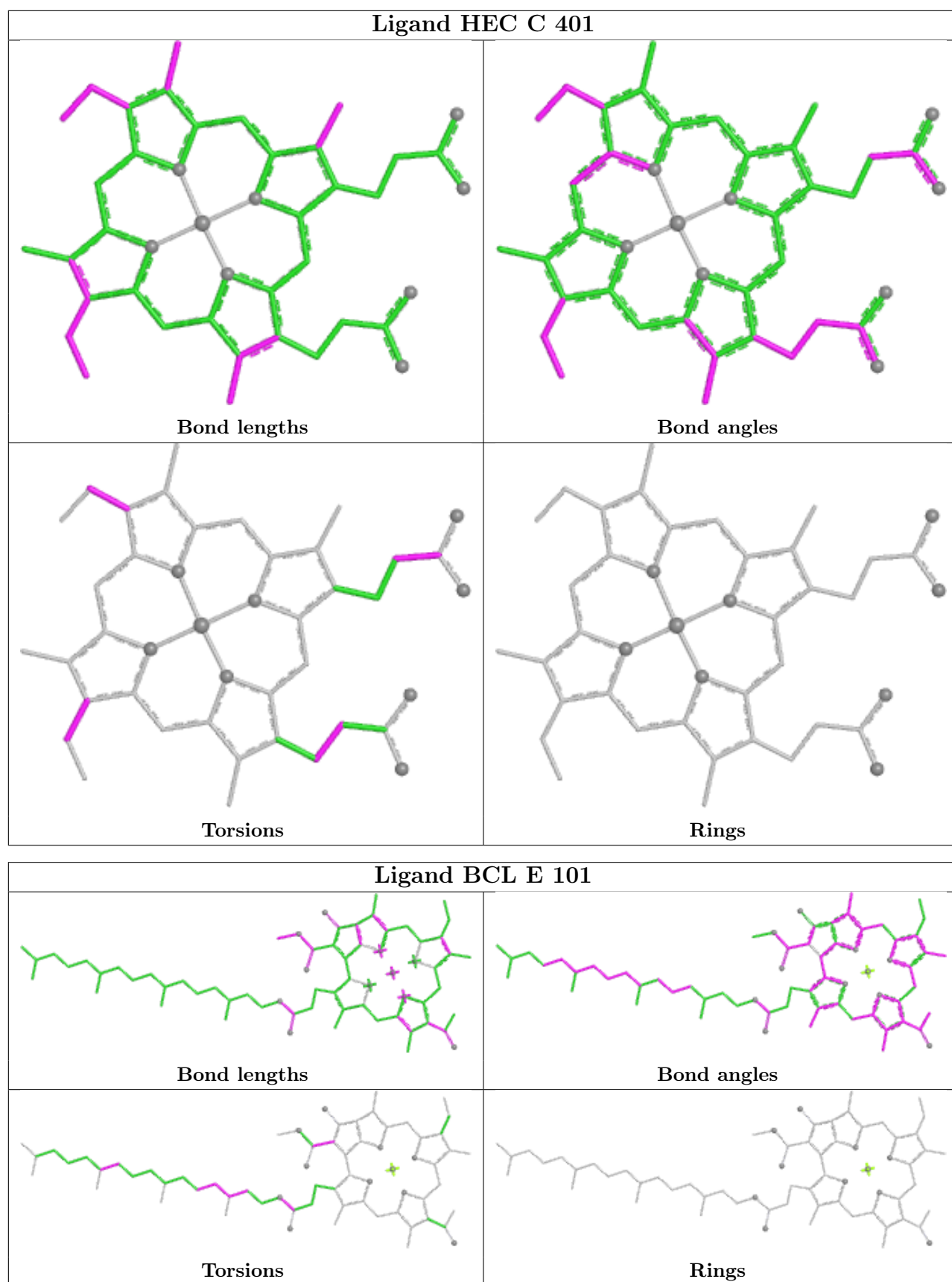
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|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

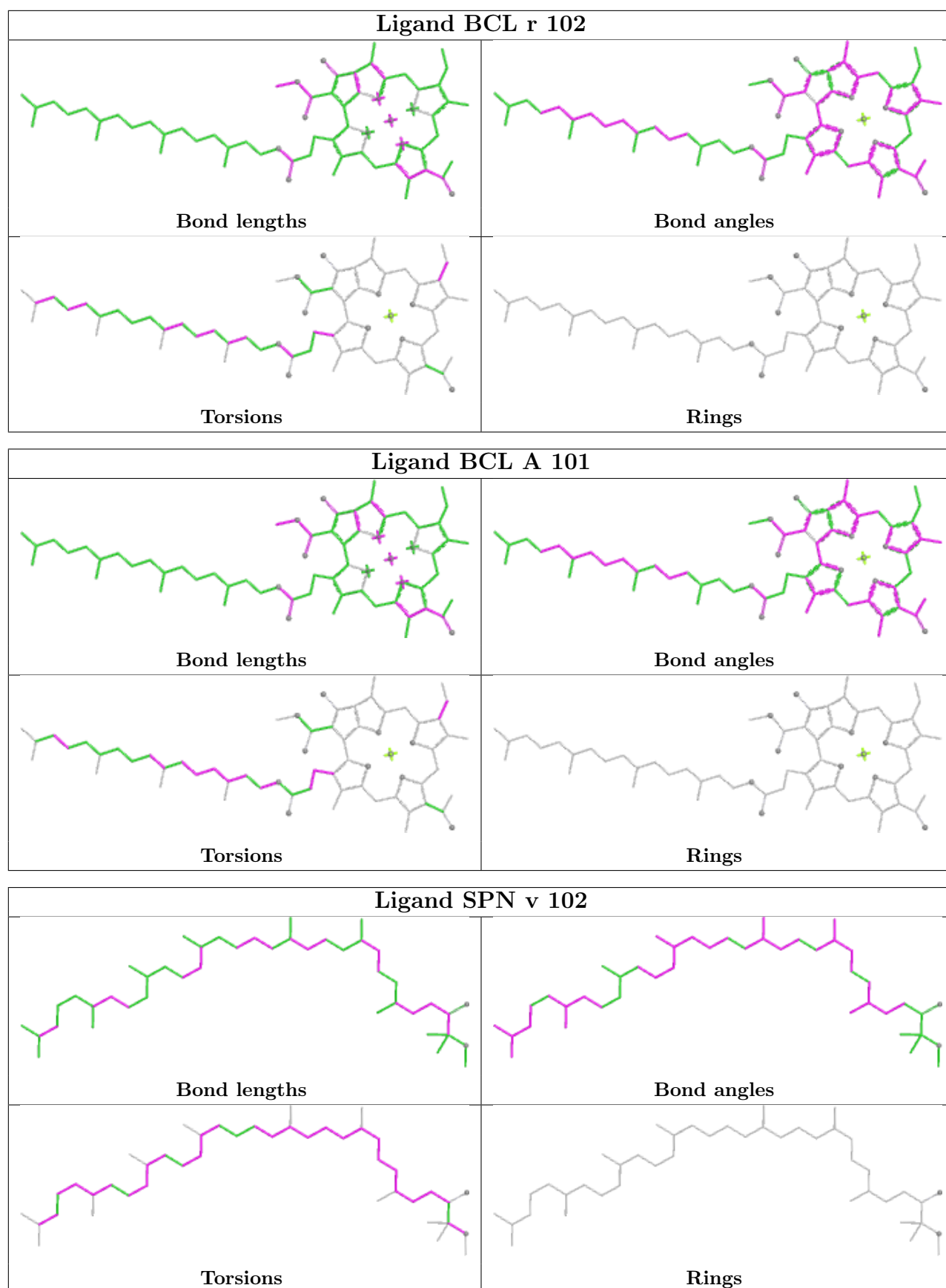


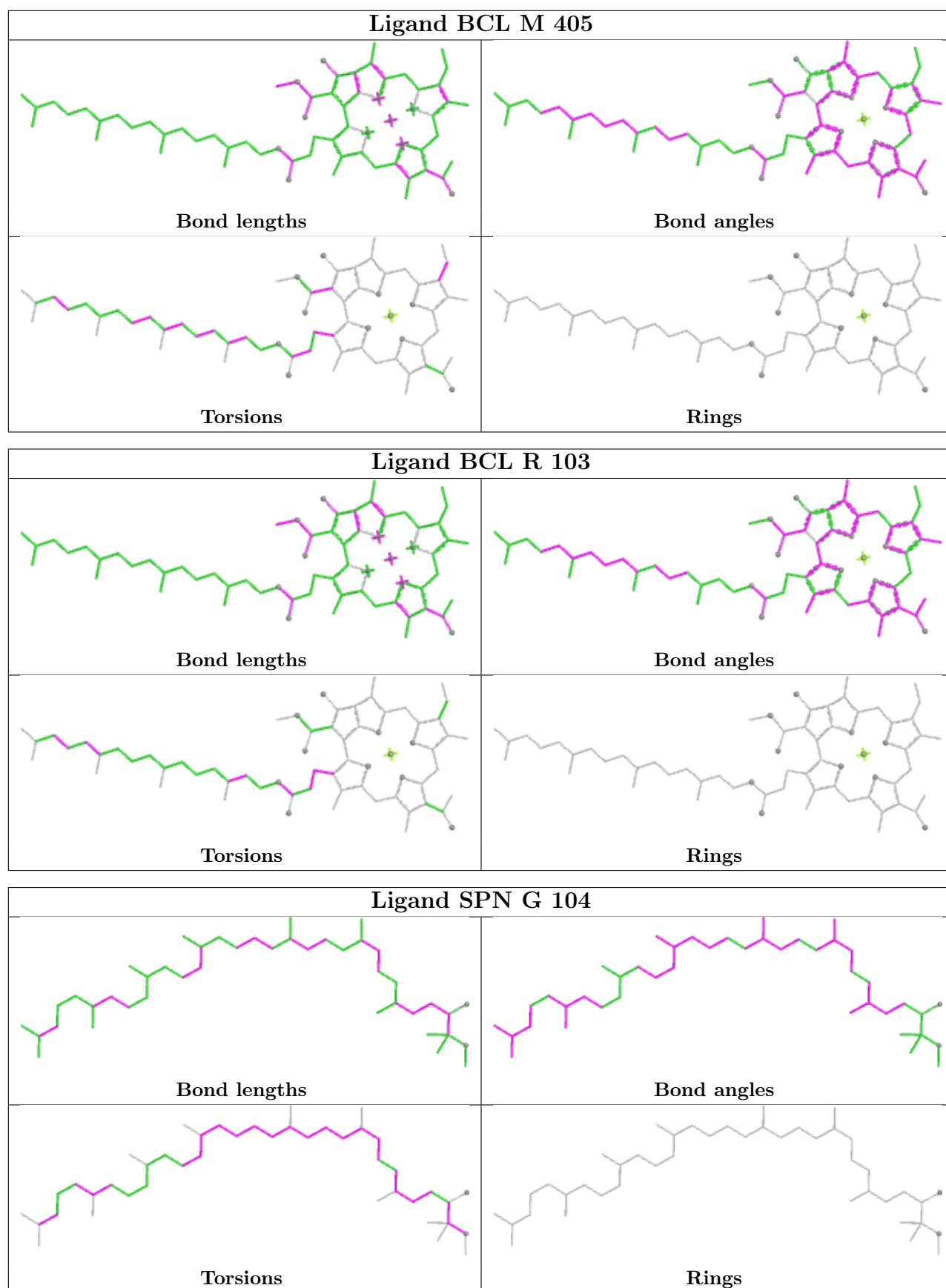


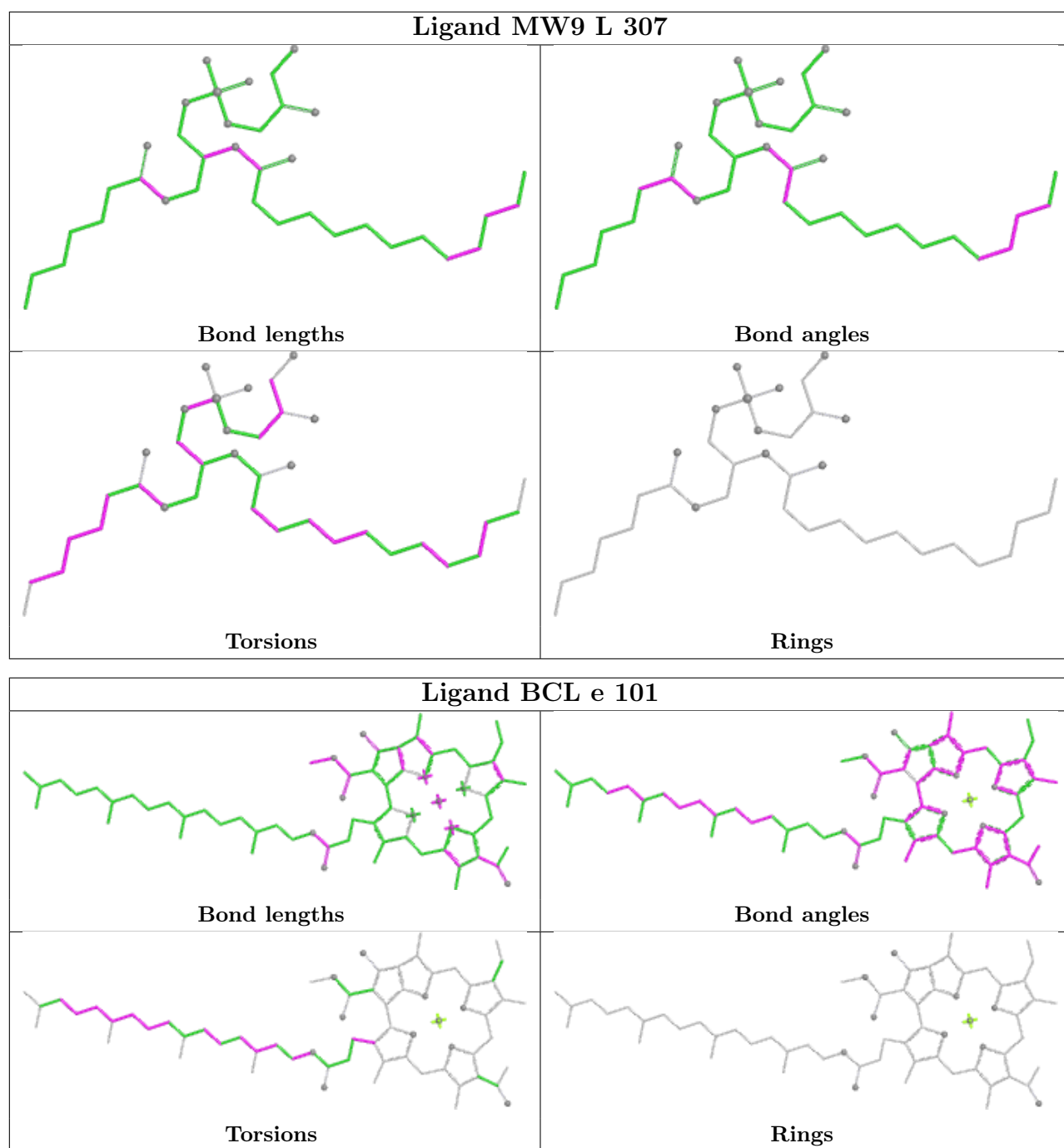


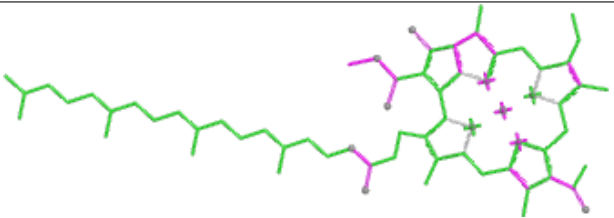
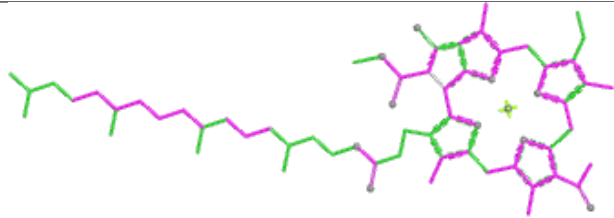
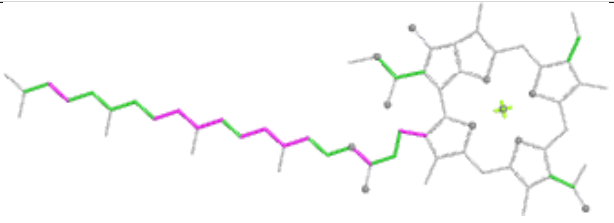
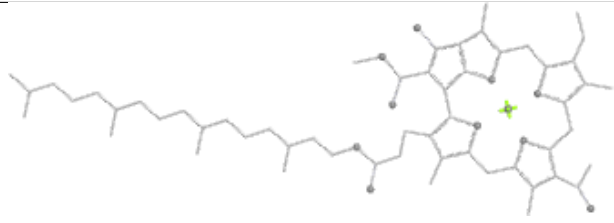


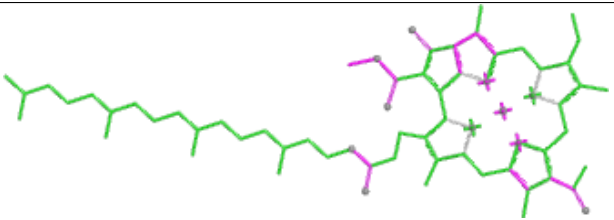
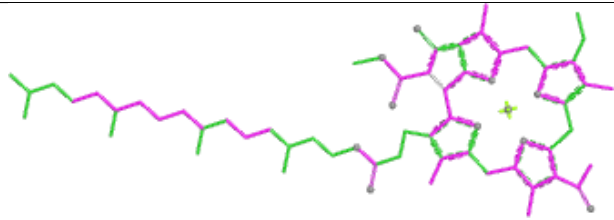
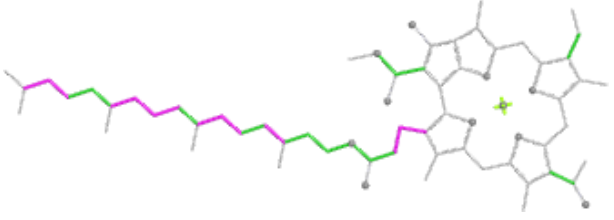
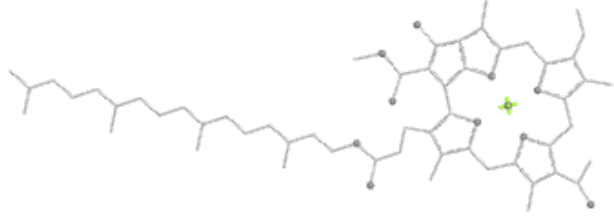


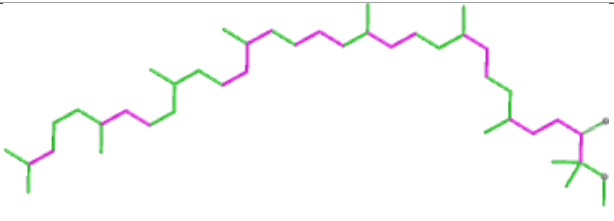
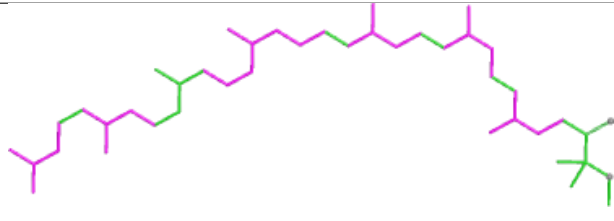
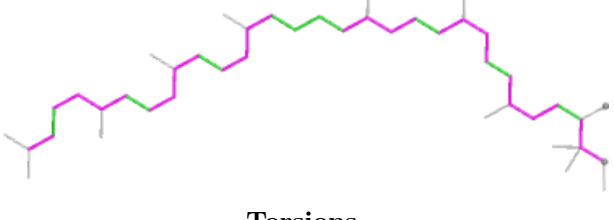
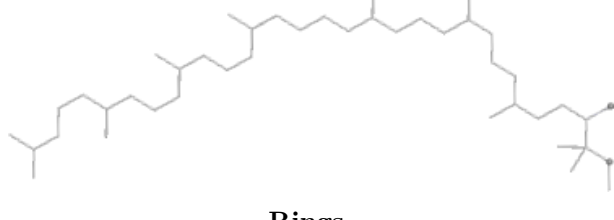


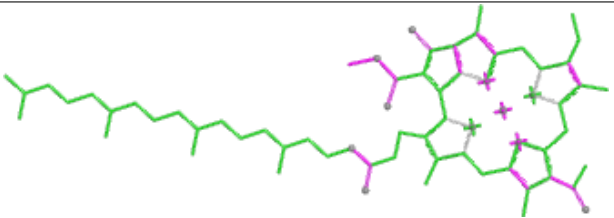
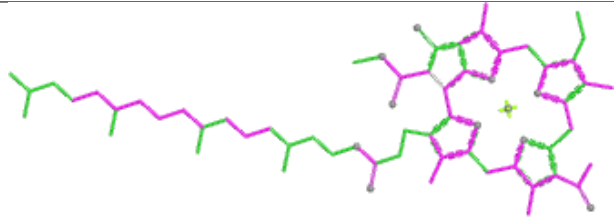
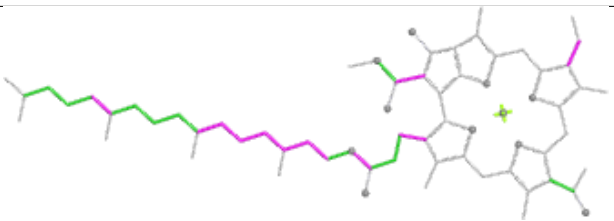
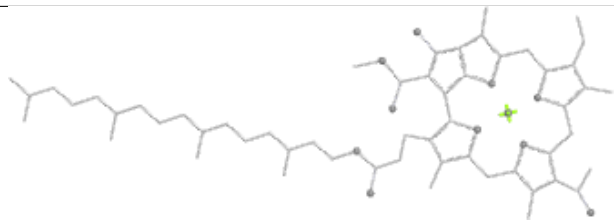


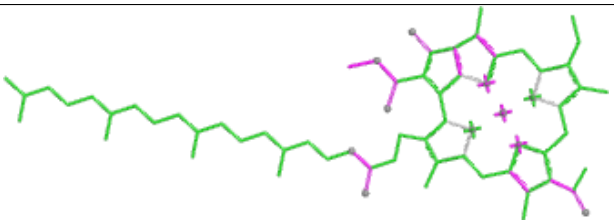
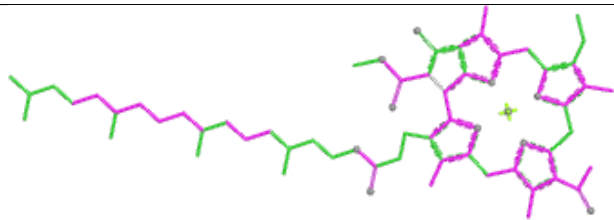
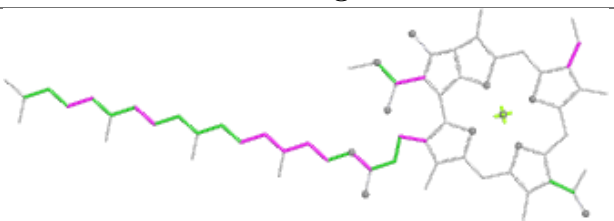
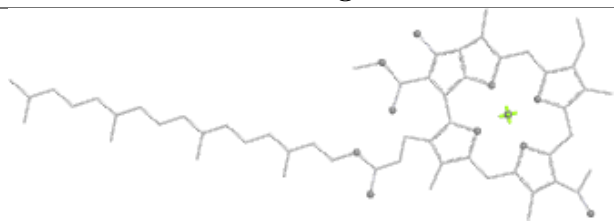


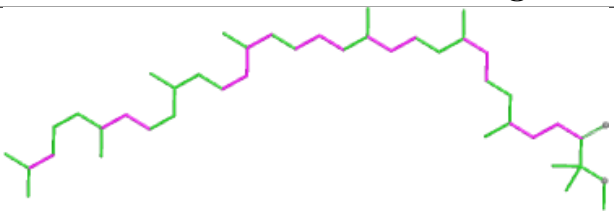
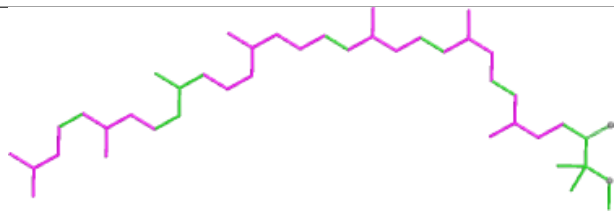
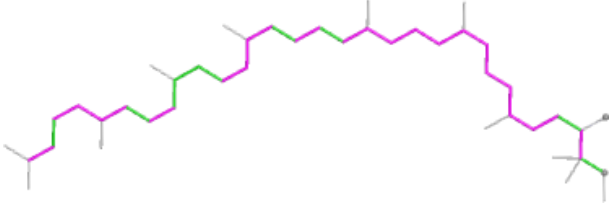
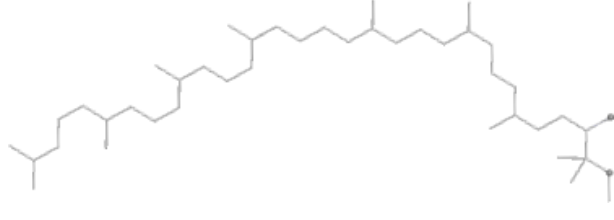
| Ligand BCL N 101 | |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

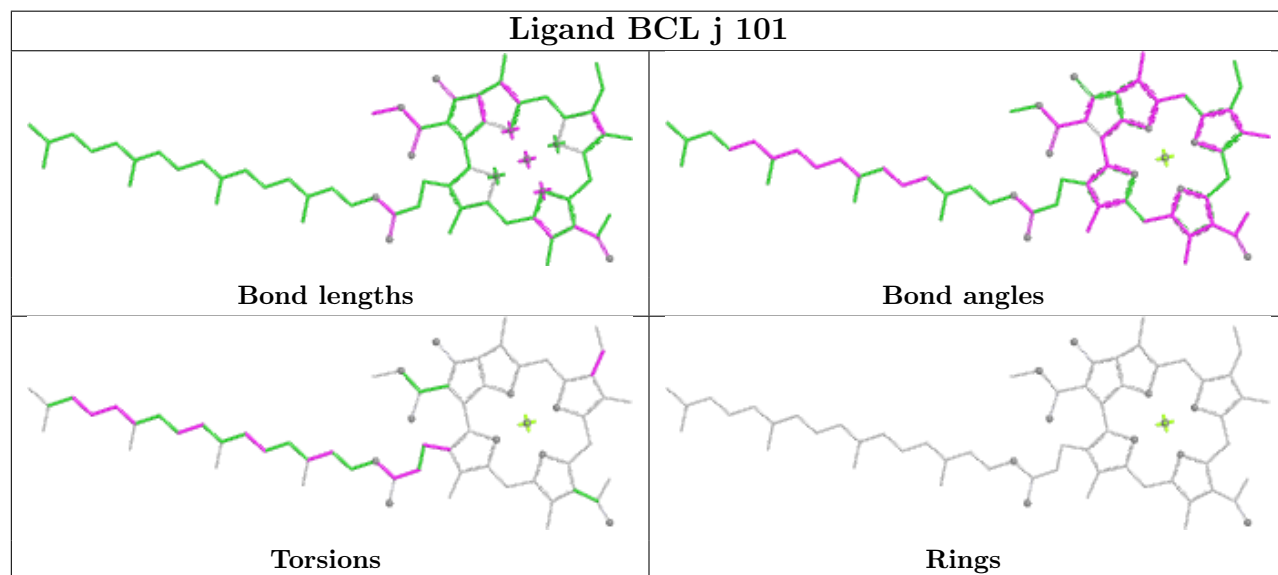
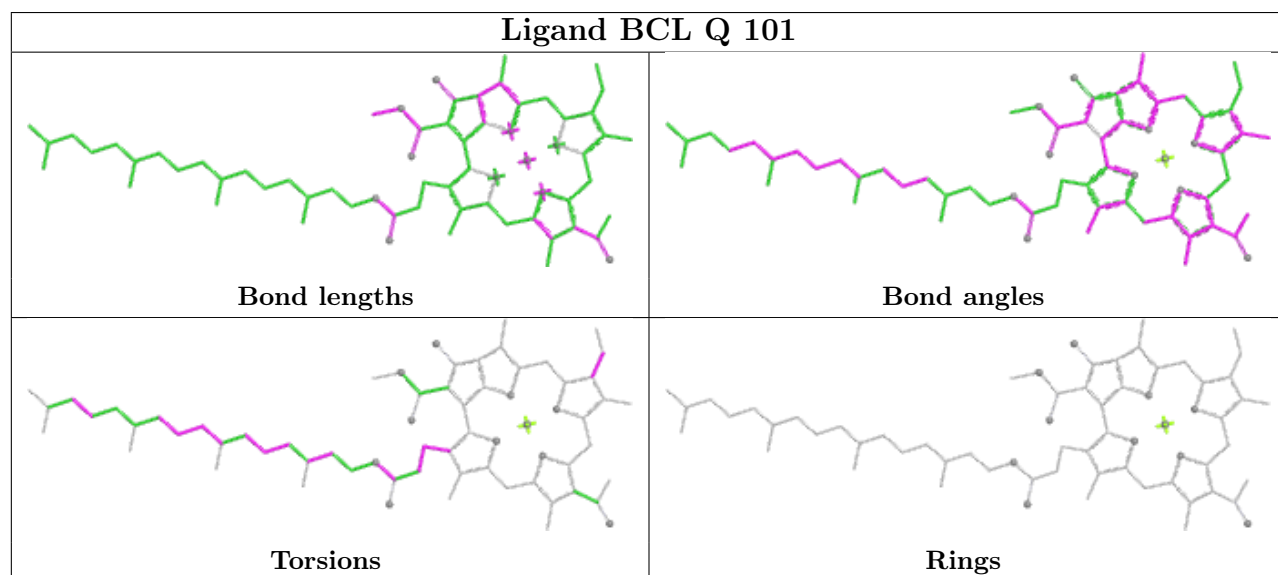
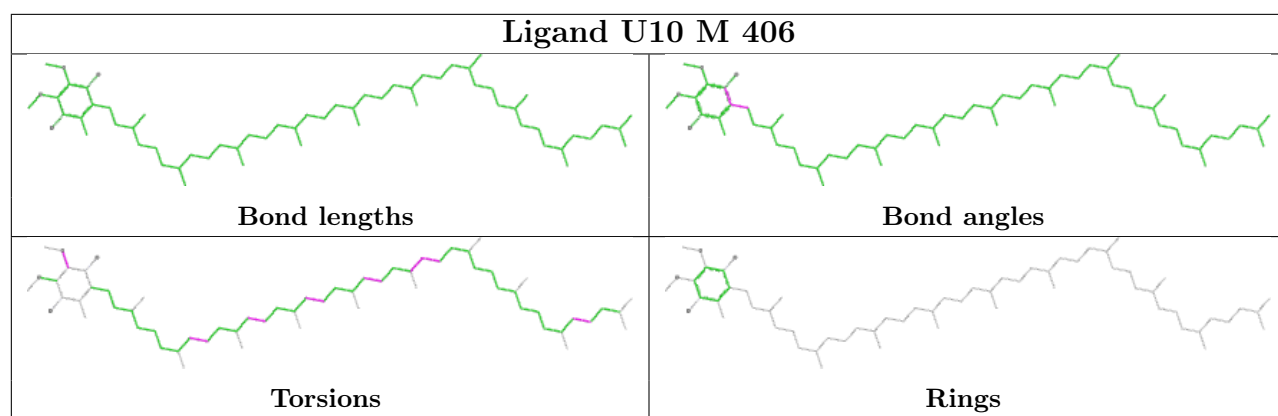
| Ligand BCL I 102 | |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

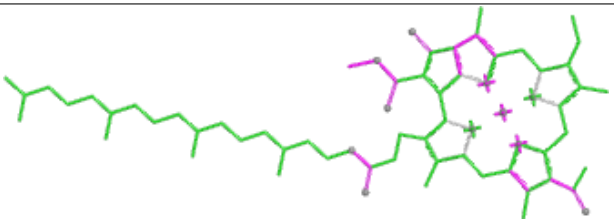
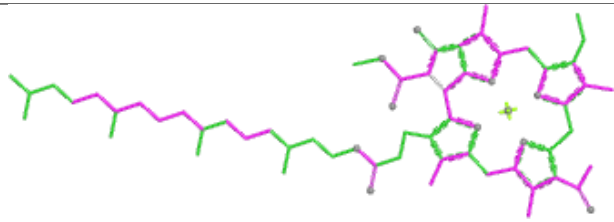
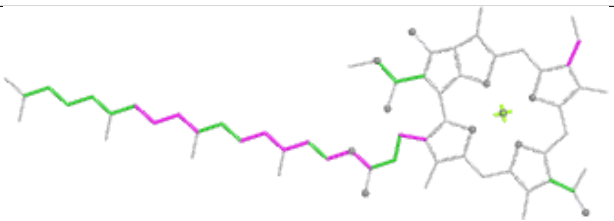
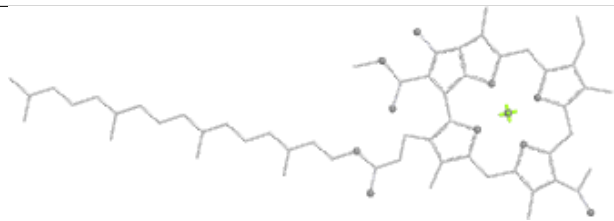
| Ligand SPN a 103 | |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

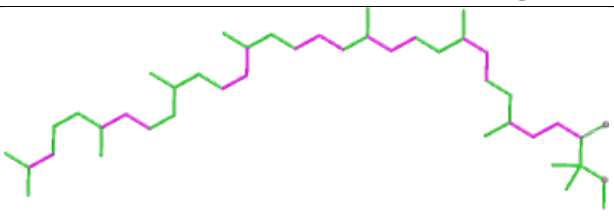
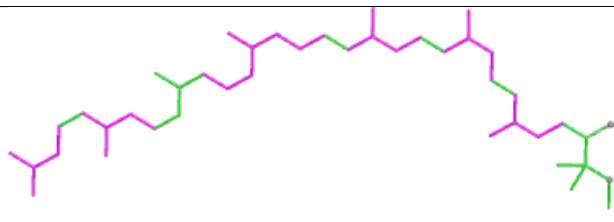
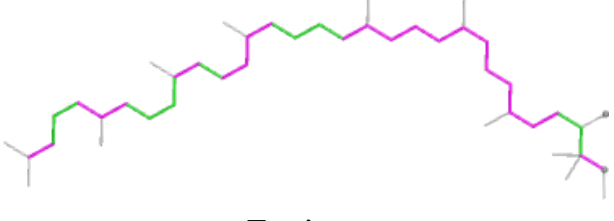
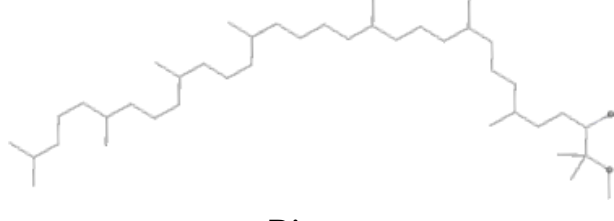
| Ligand BCL L 304 | |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

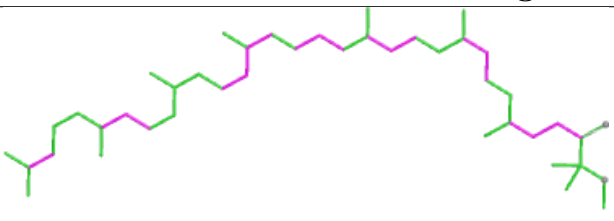
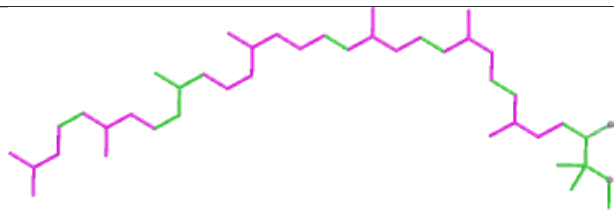
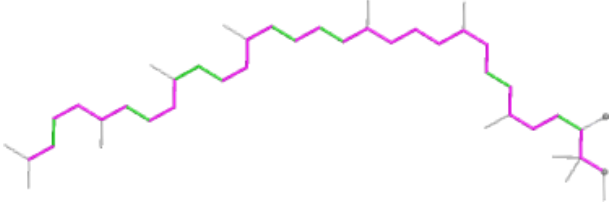
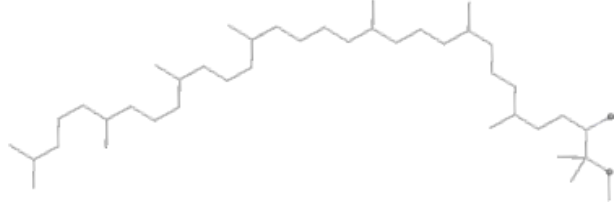
| Ligand BCL i 102 | |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

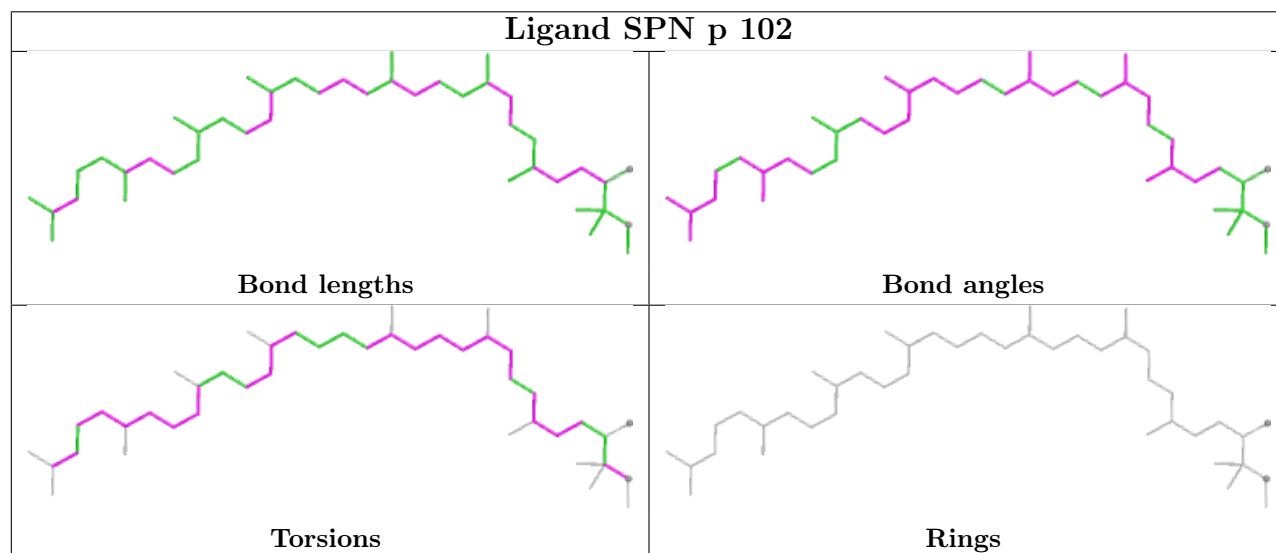
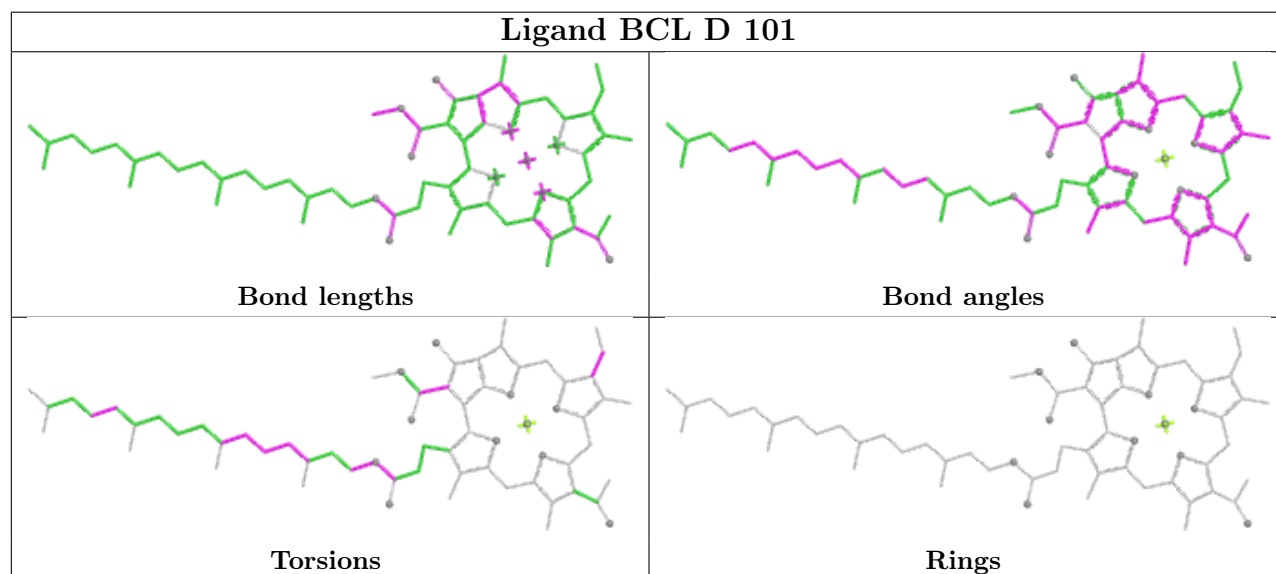
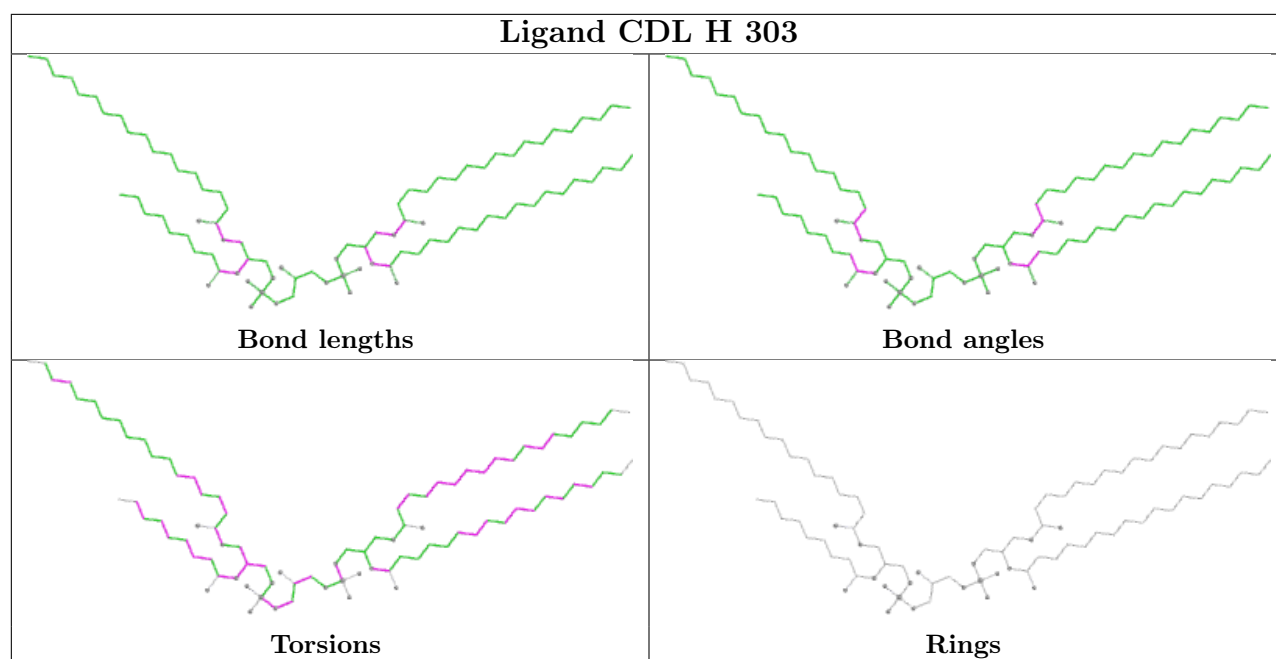
| Ligand SPN D 102 | |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

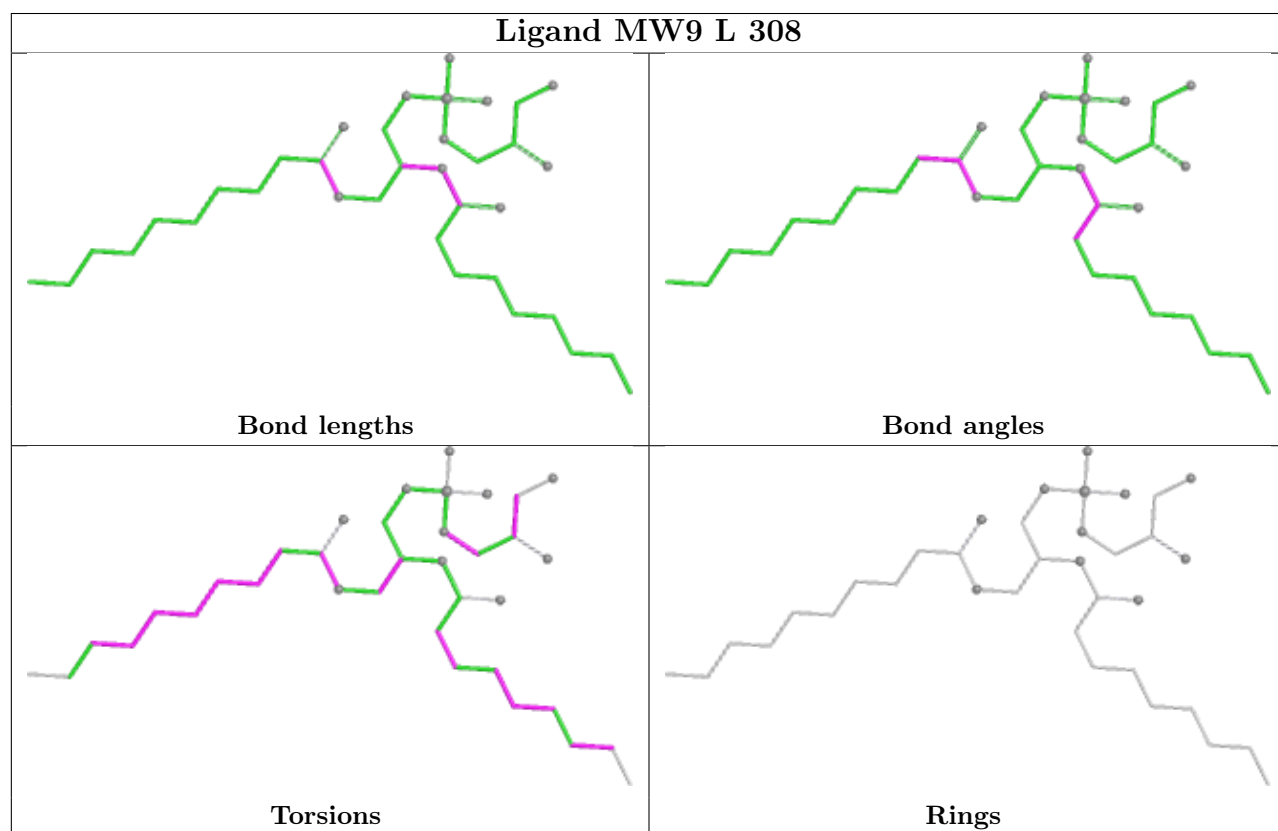
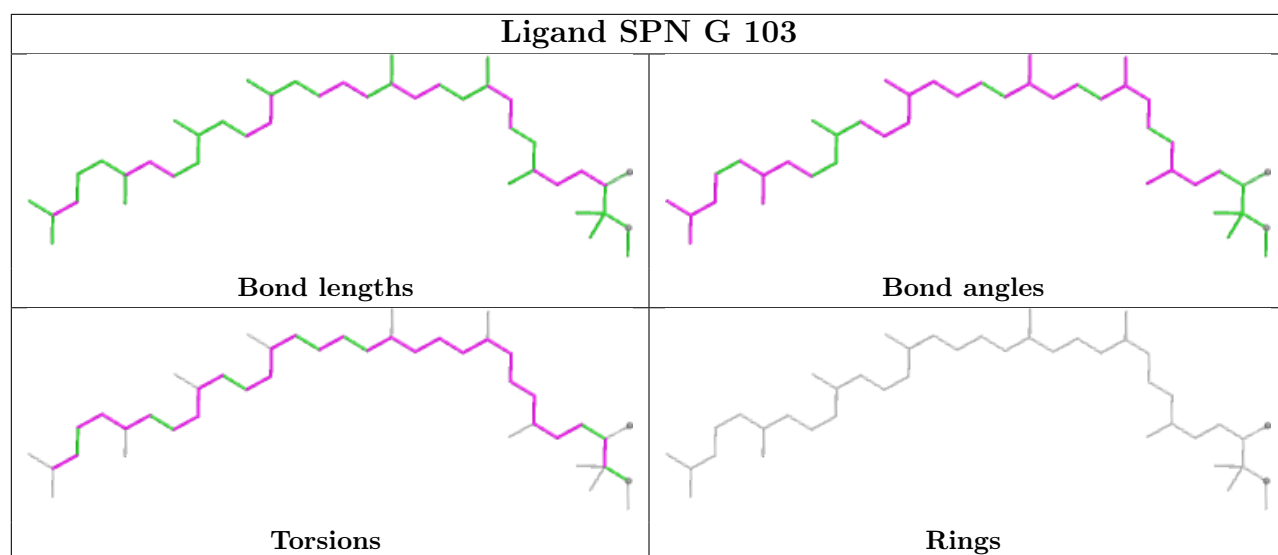


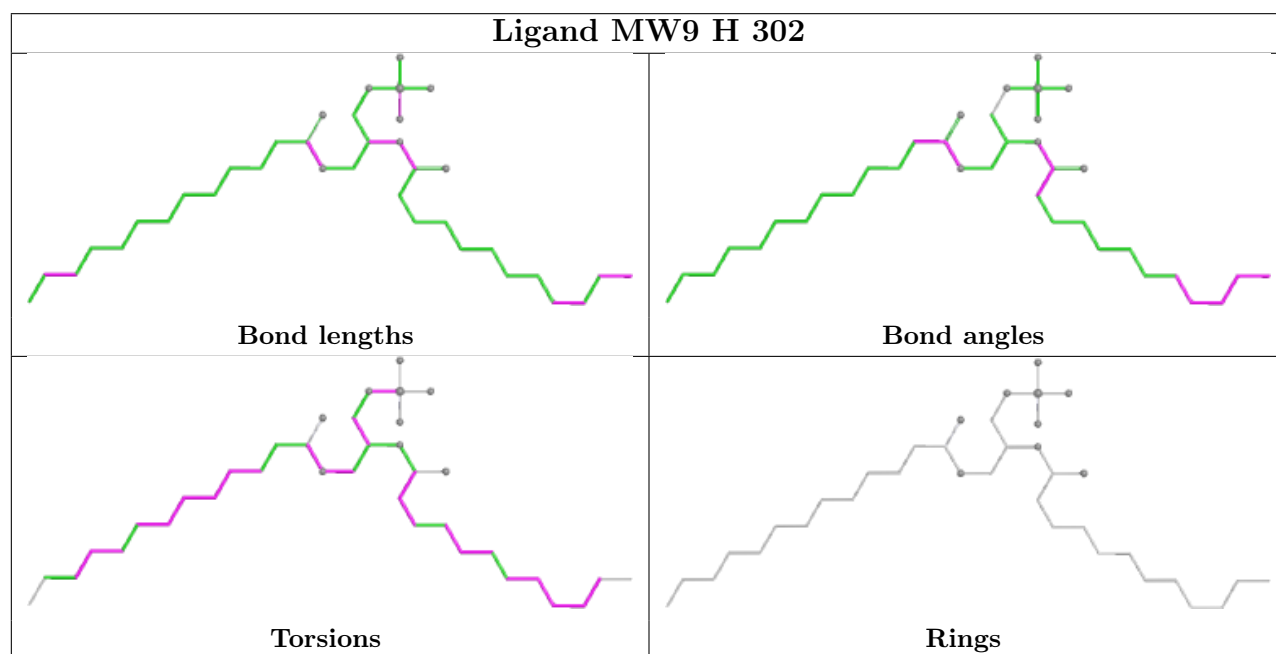
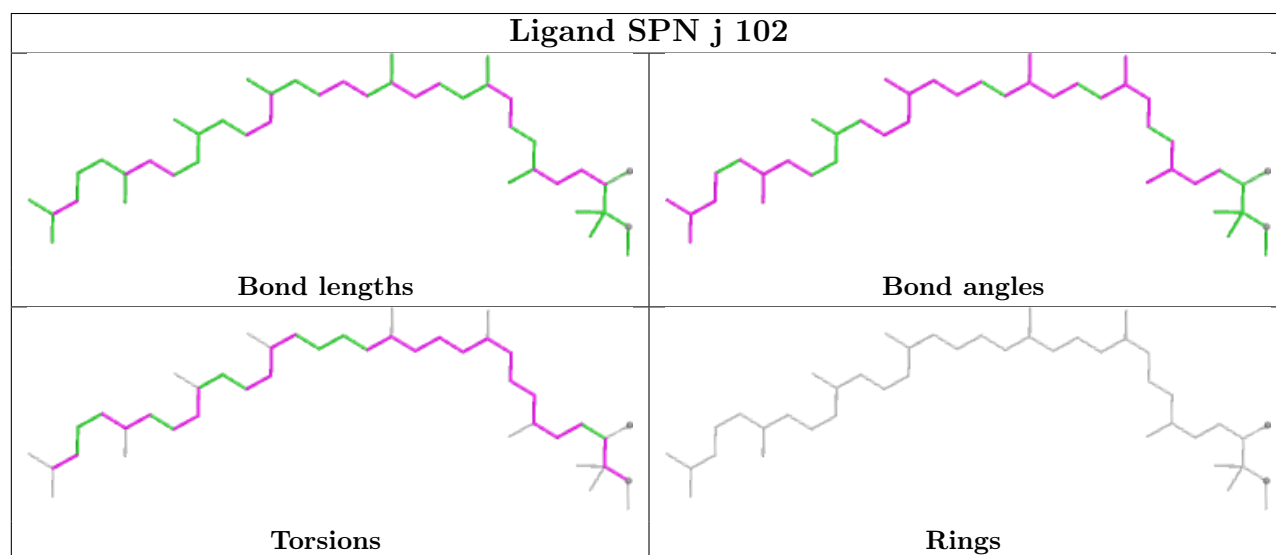
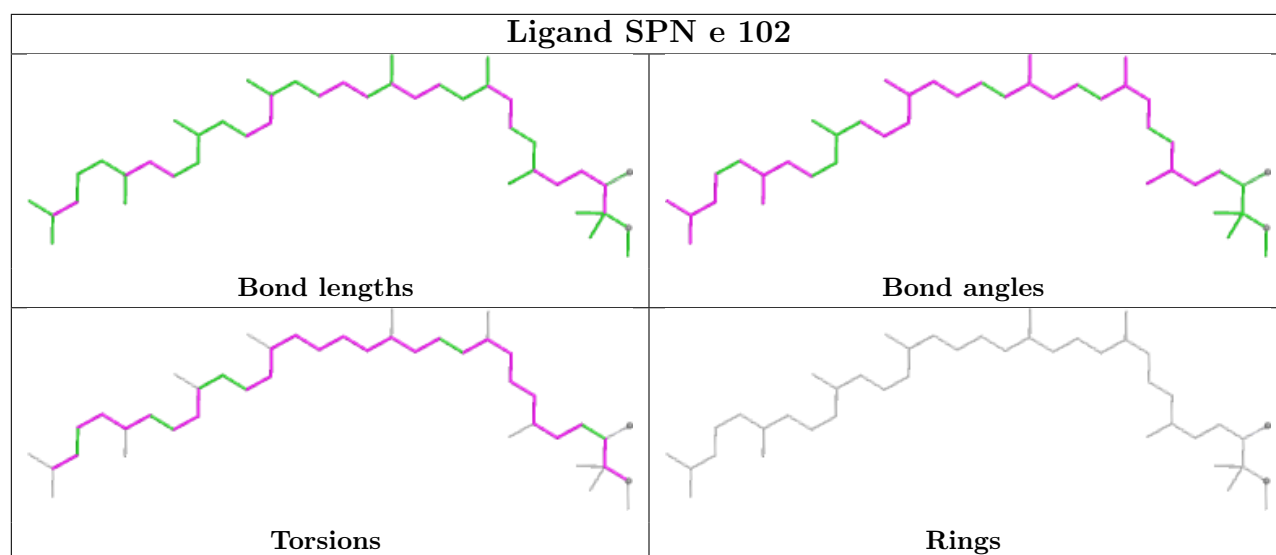
| Ligand BCL B 101 | |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

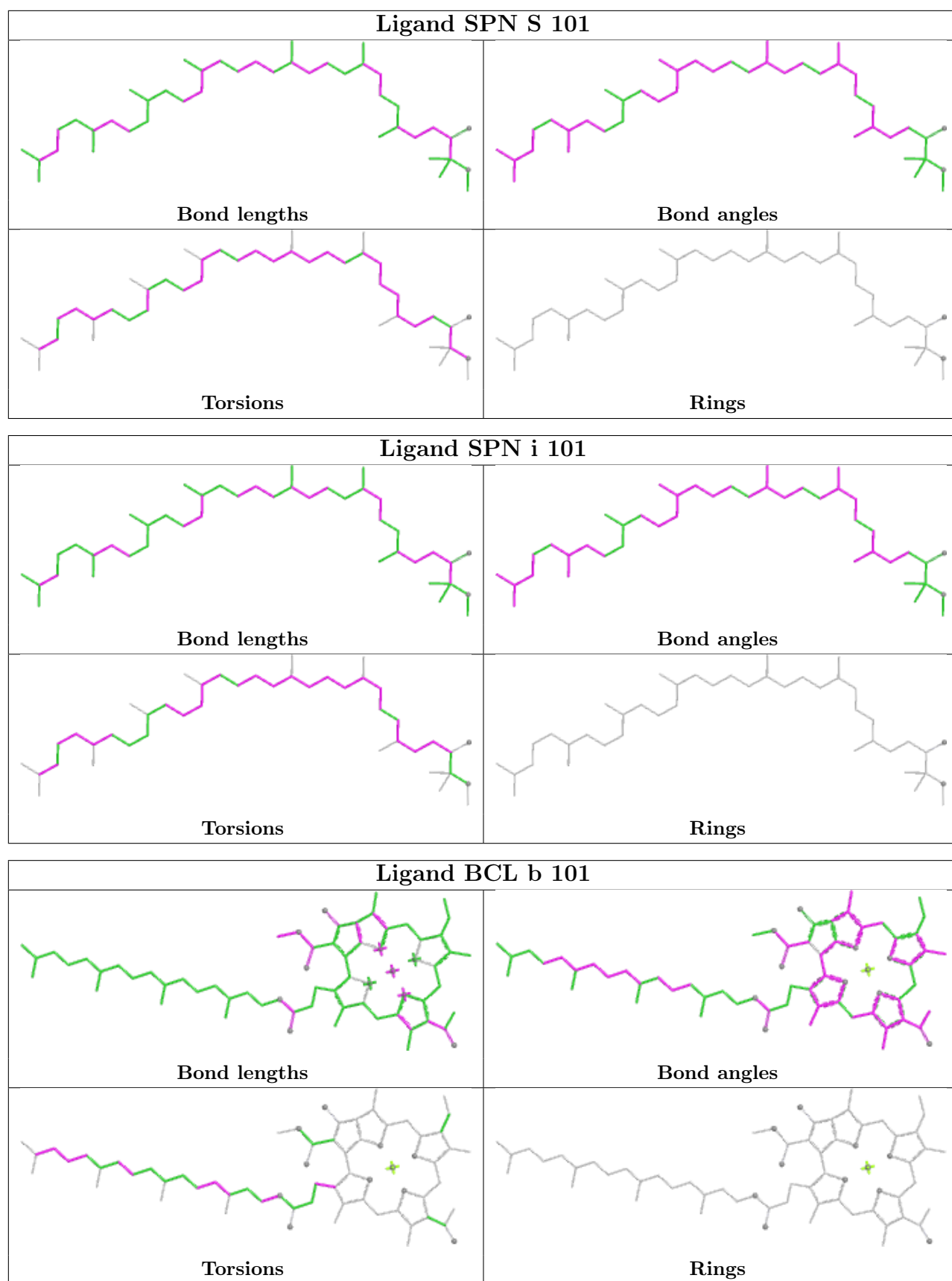
| Ligand SPN 2 103 | |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

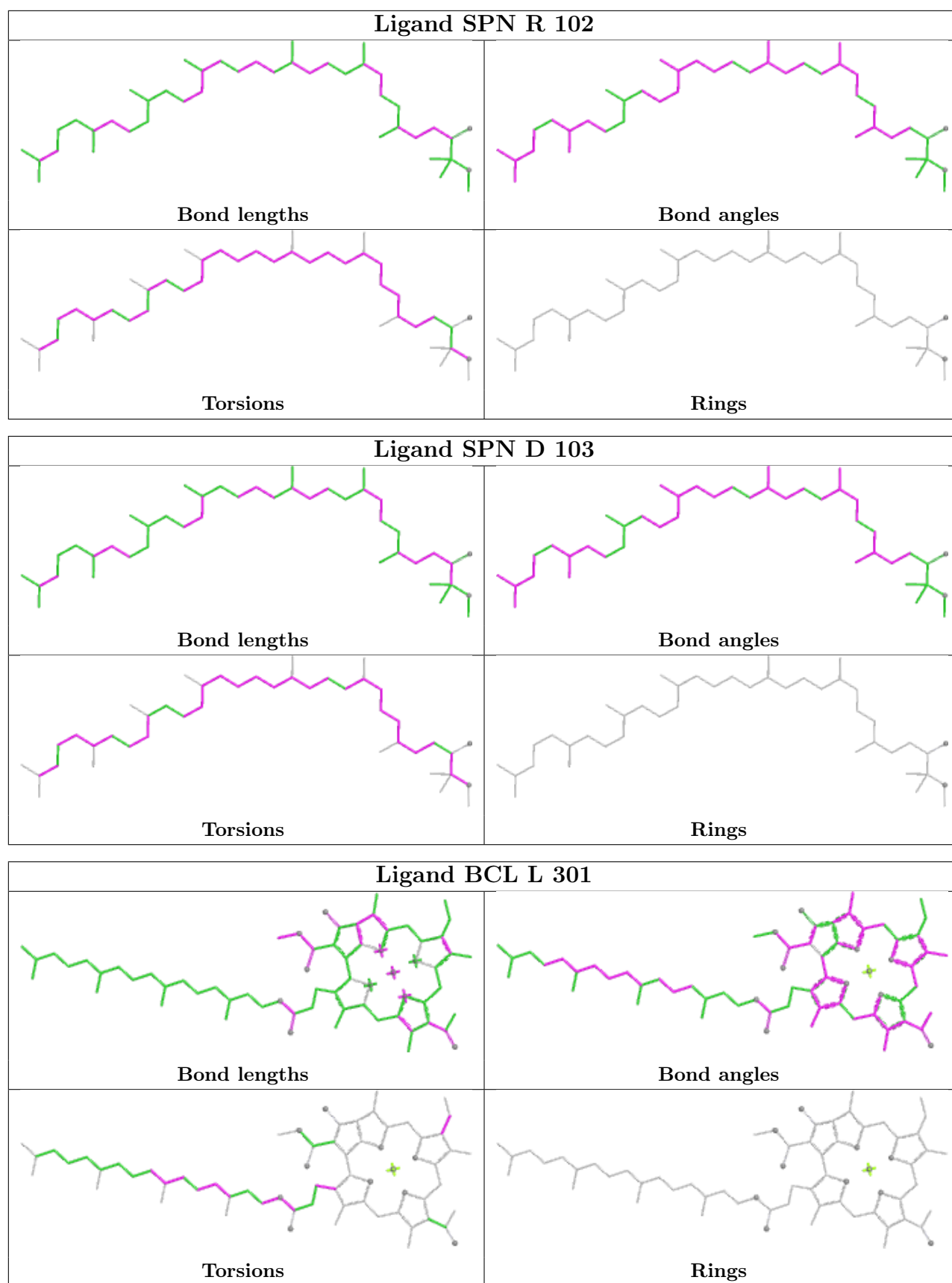
| Ligand SPN f 102 | |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

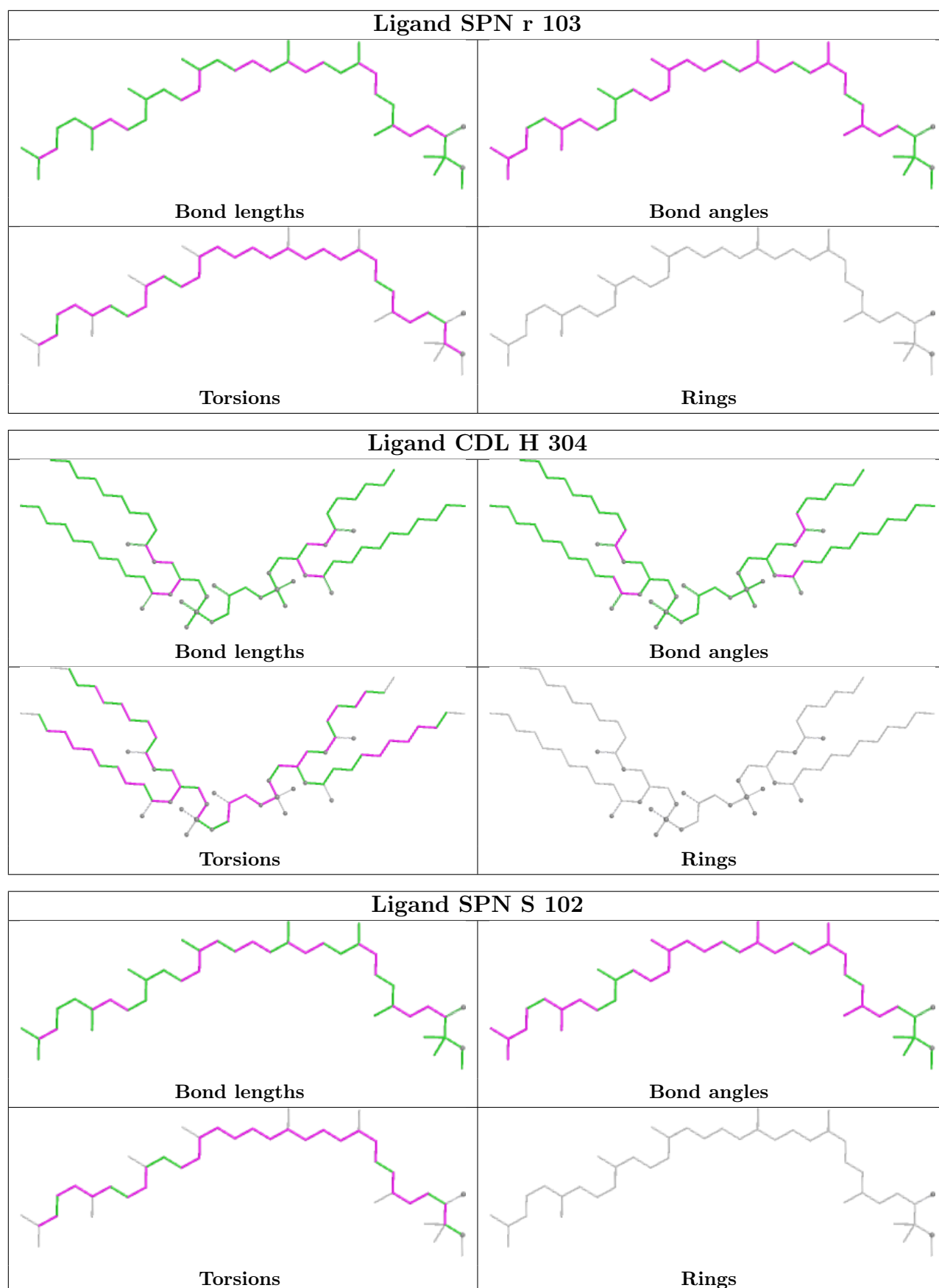


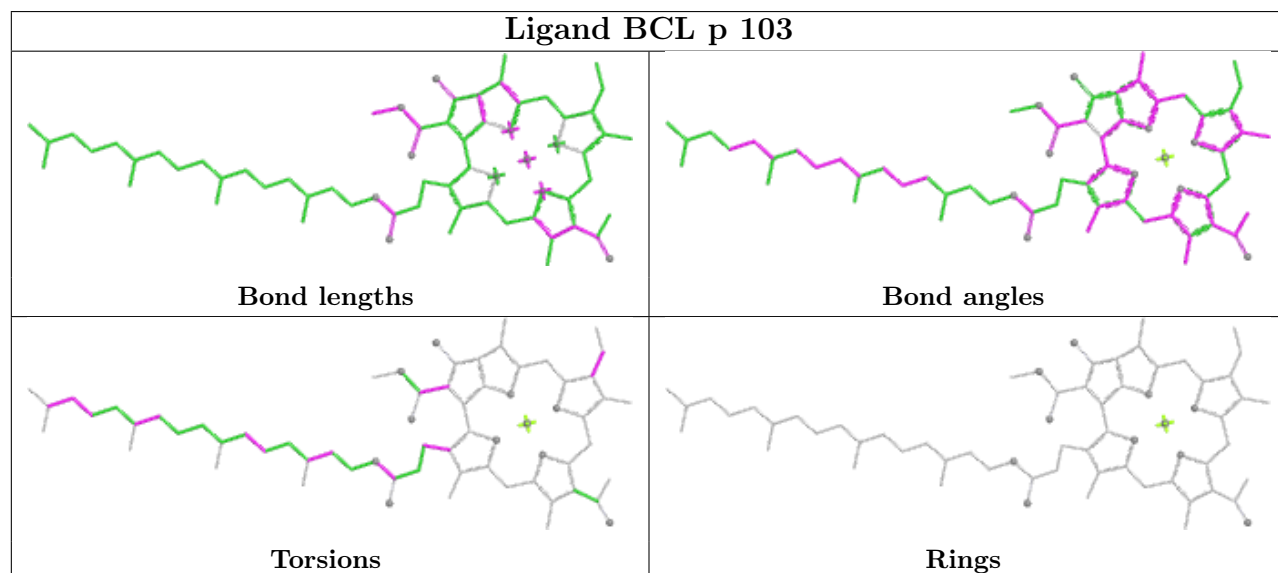
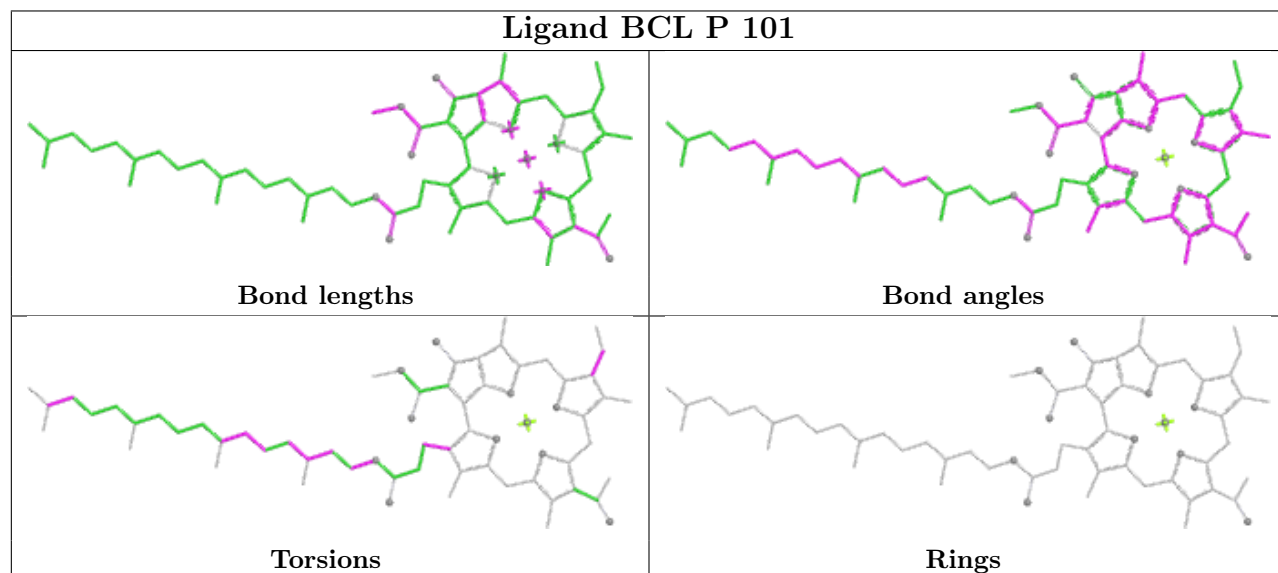
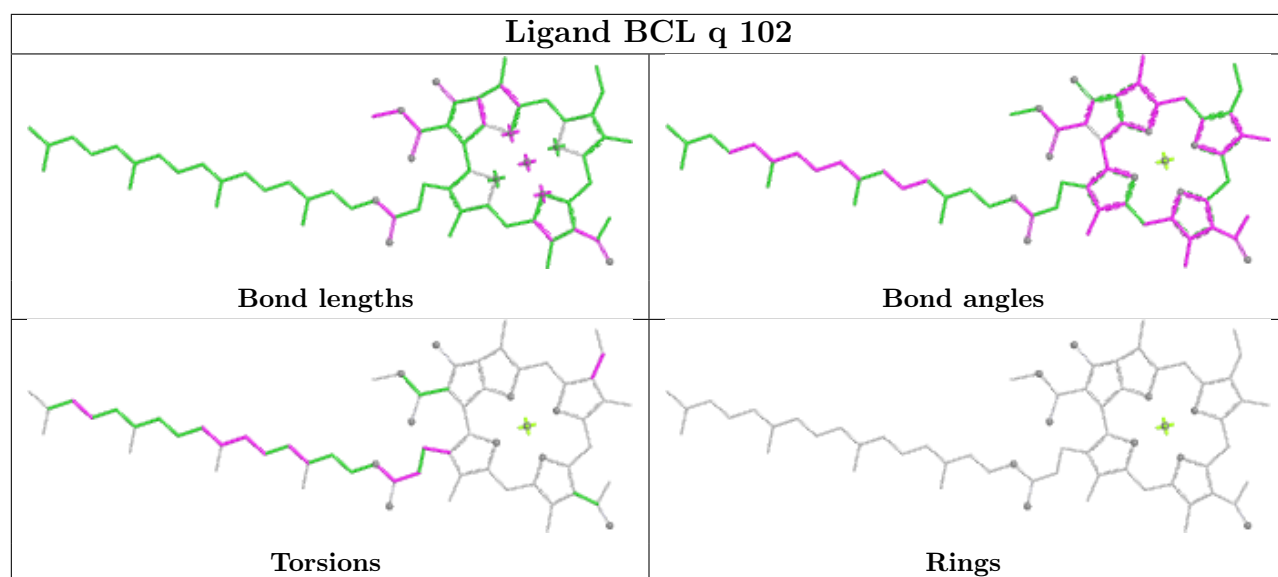


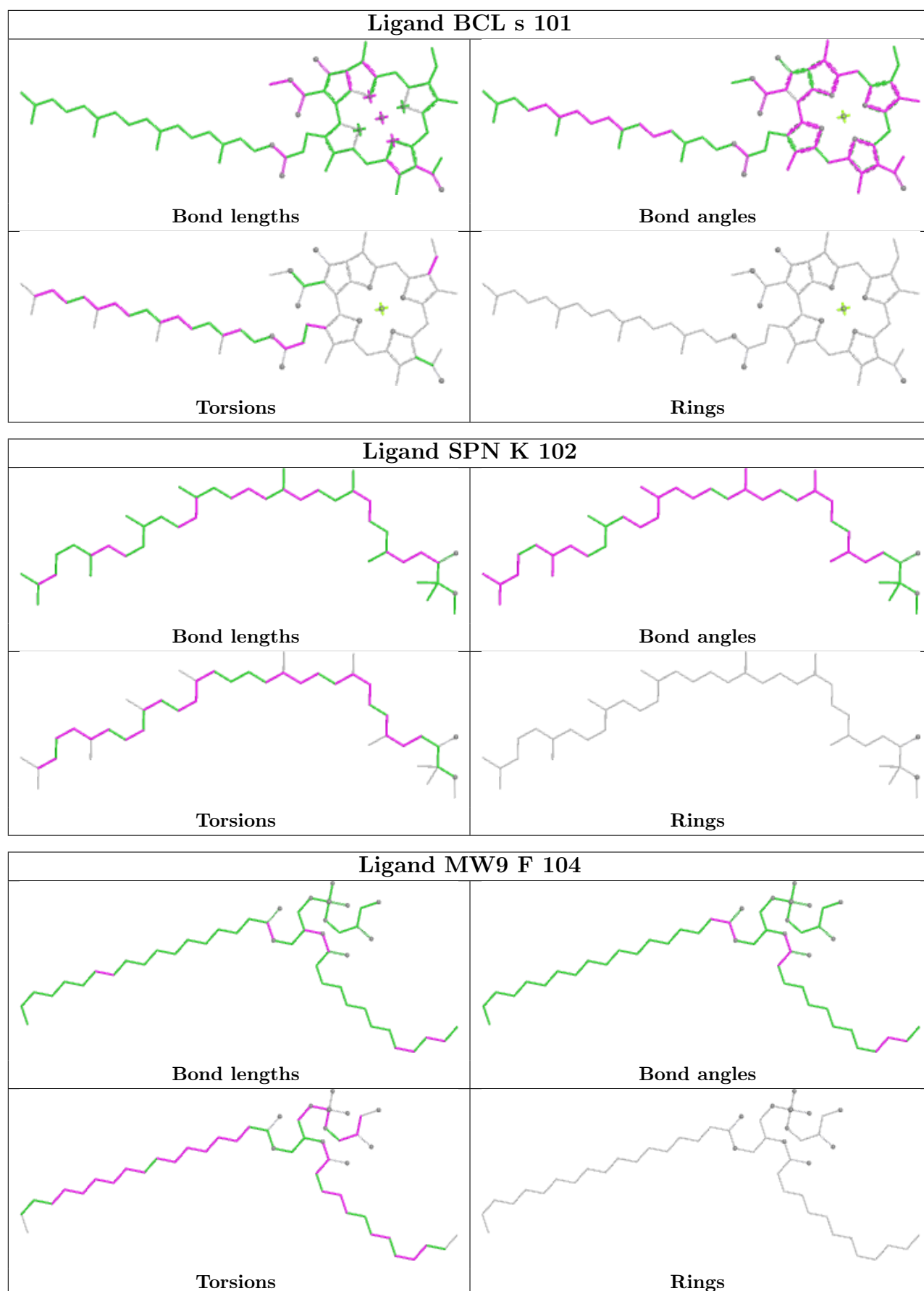


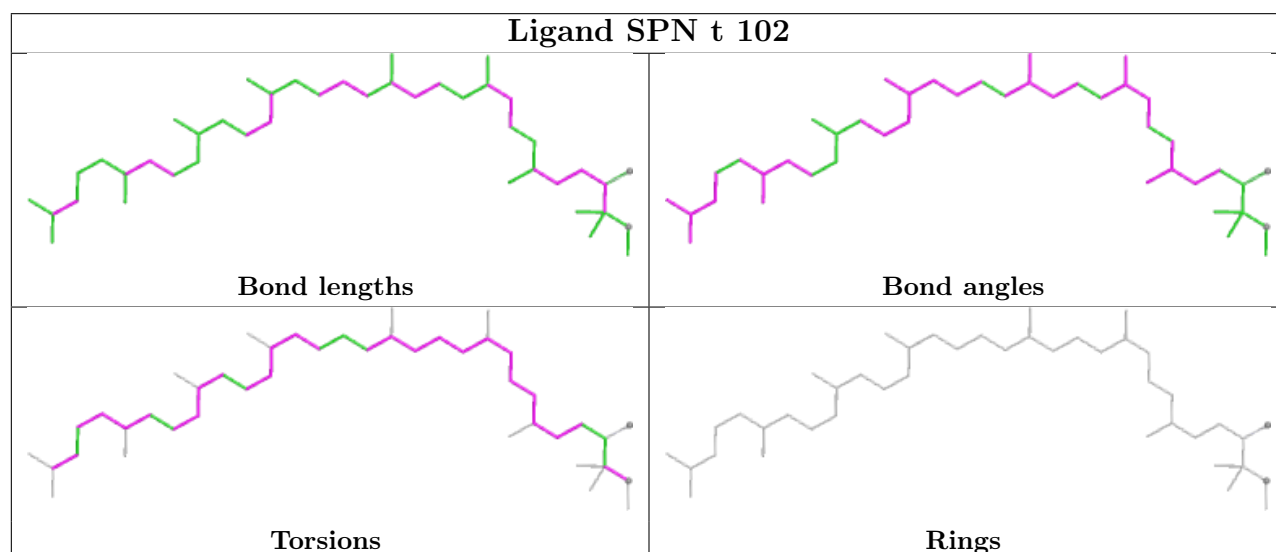
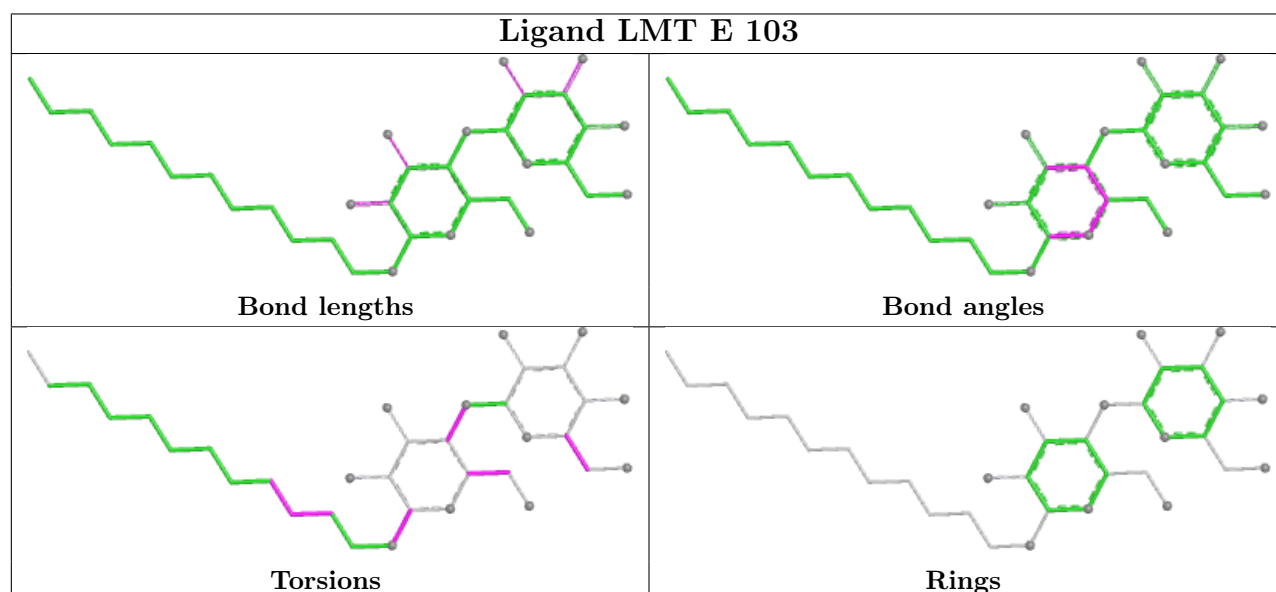
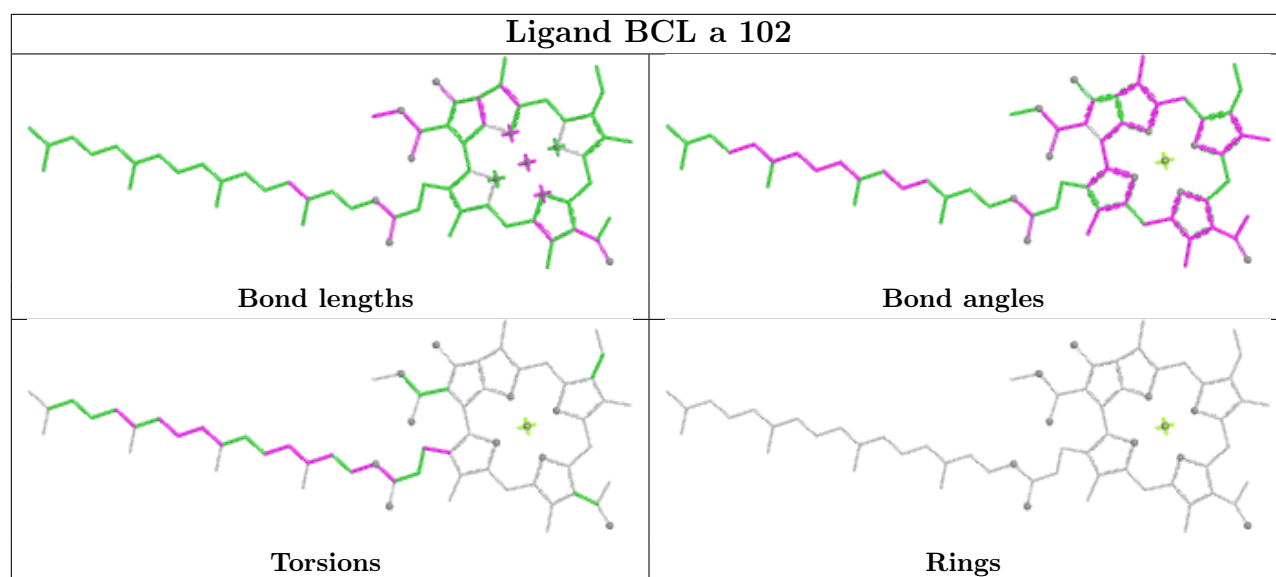


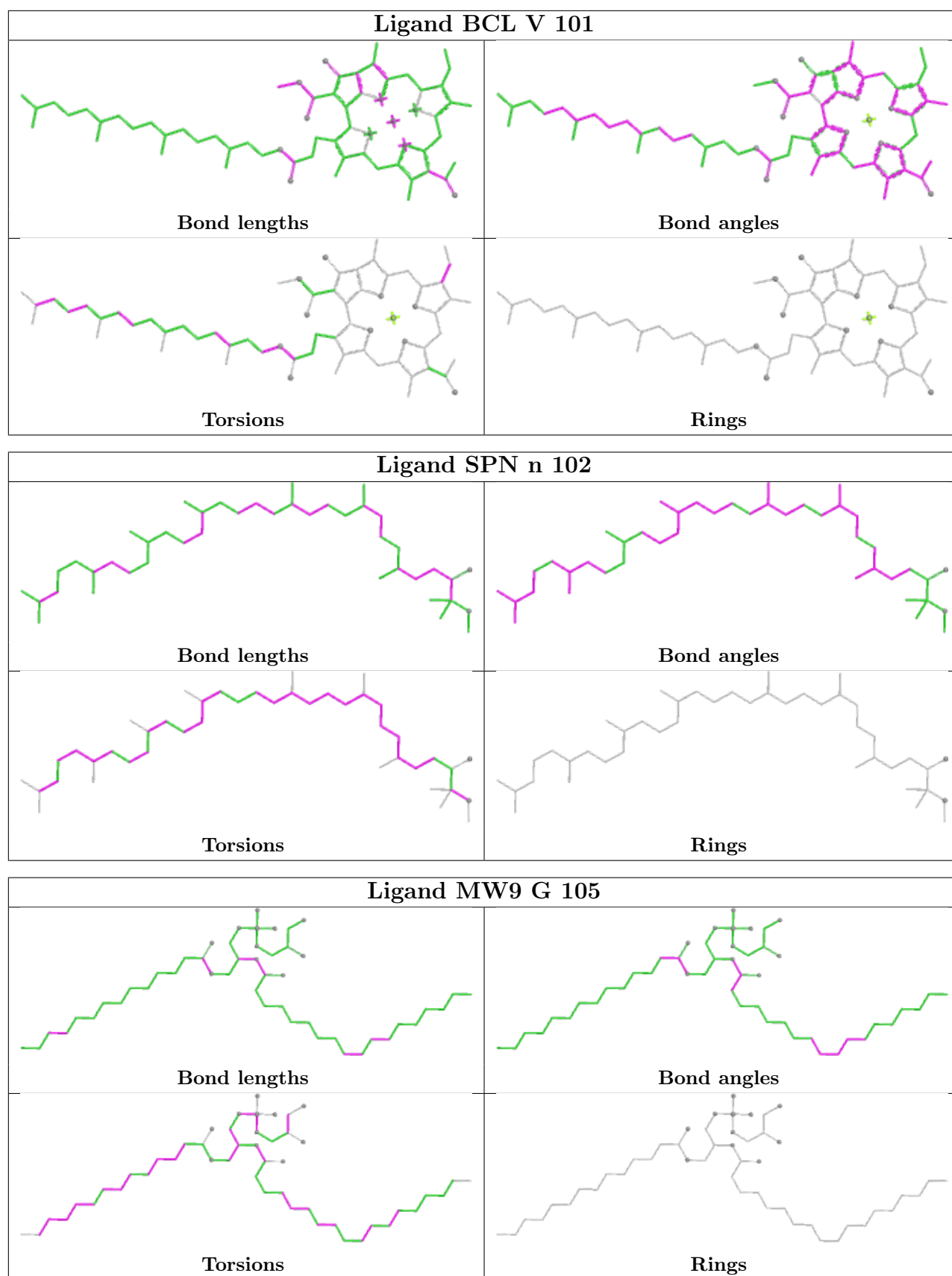


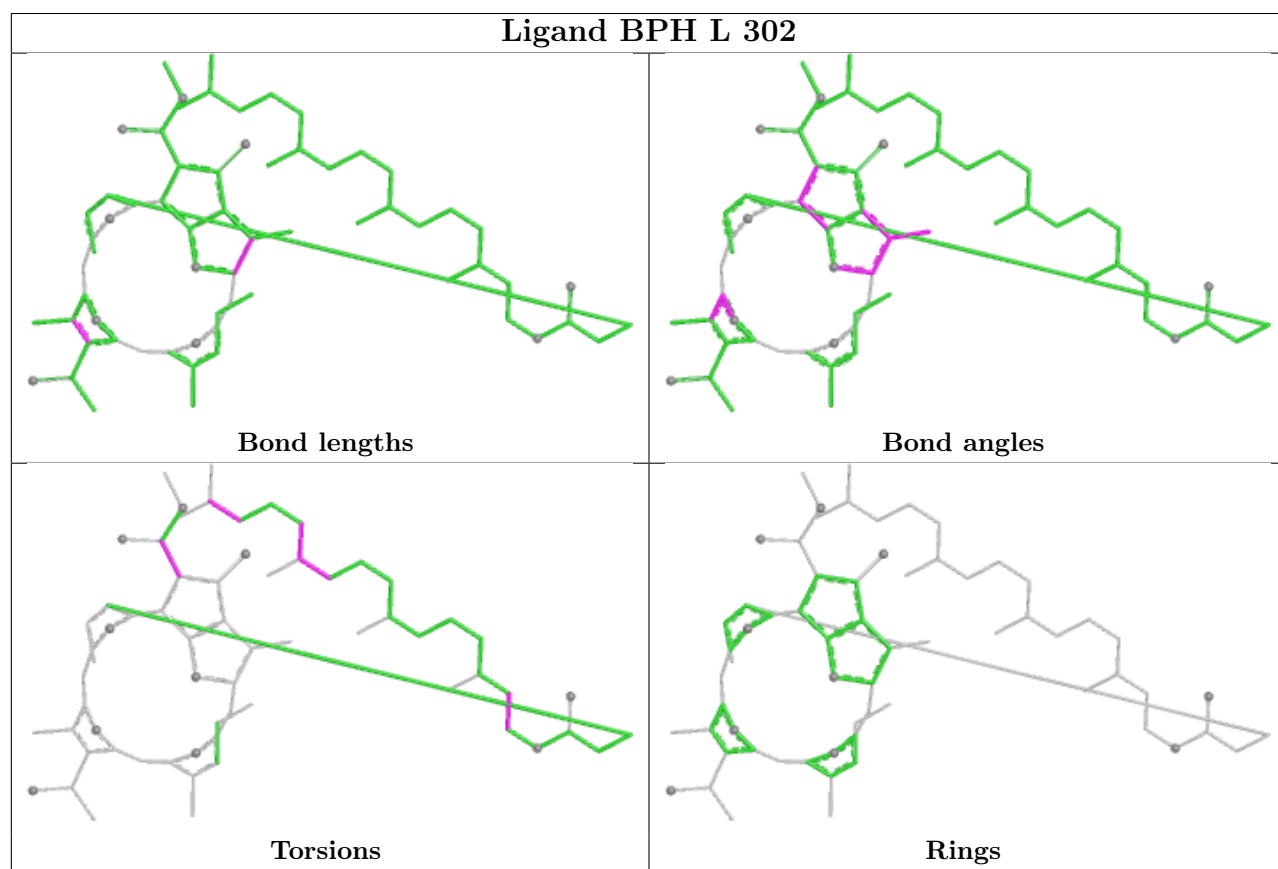
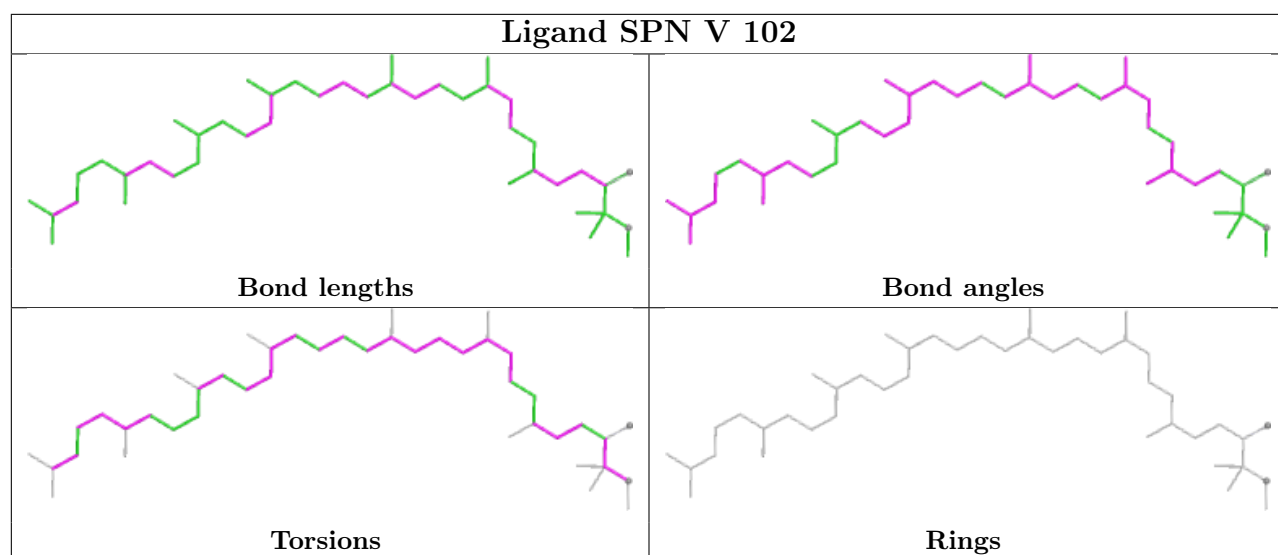


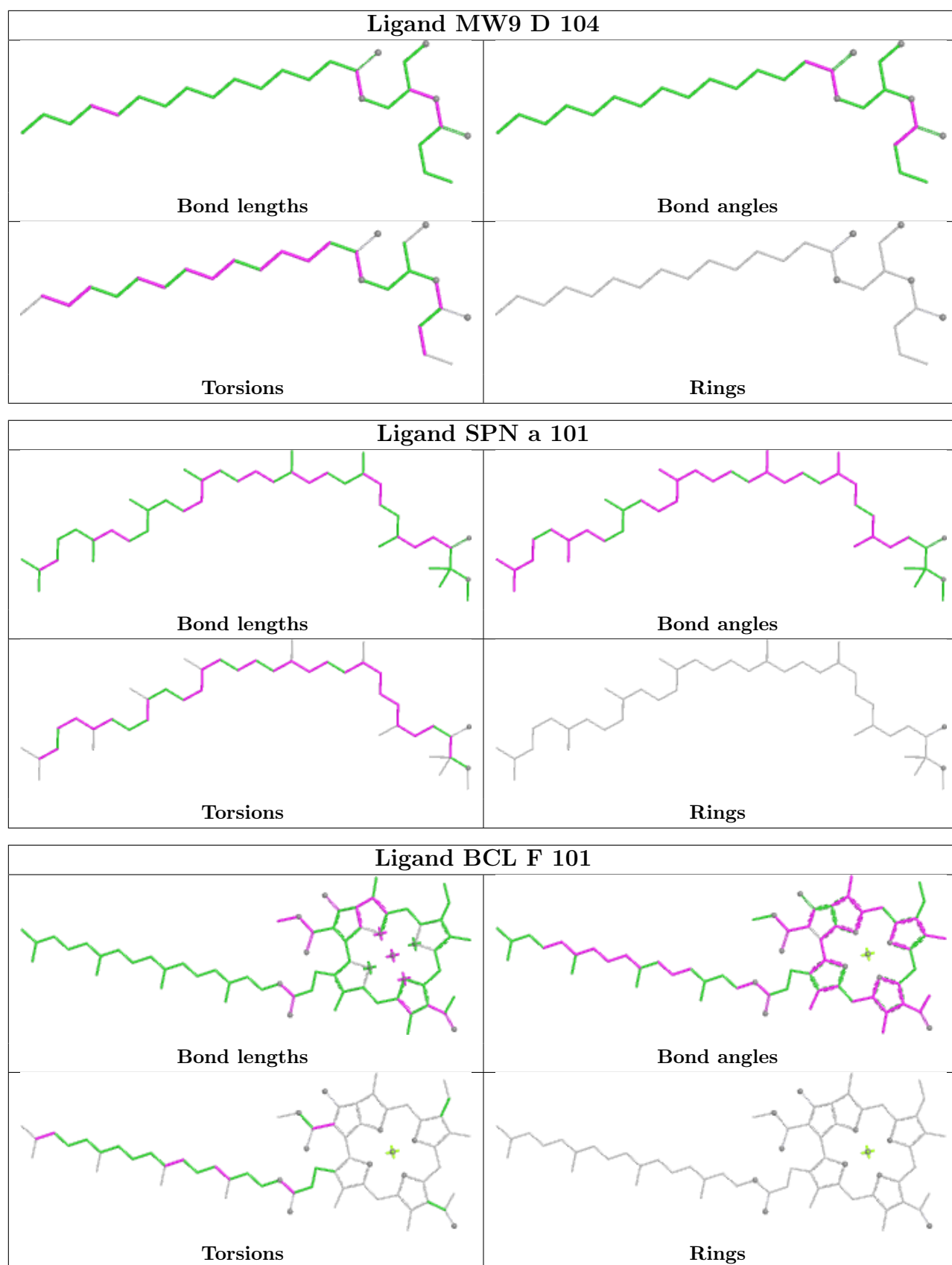


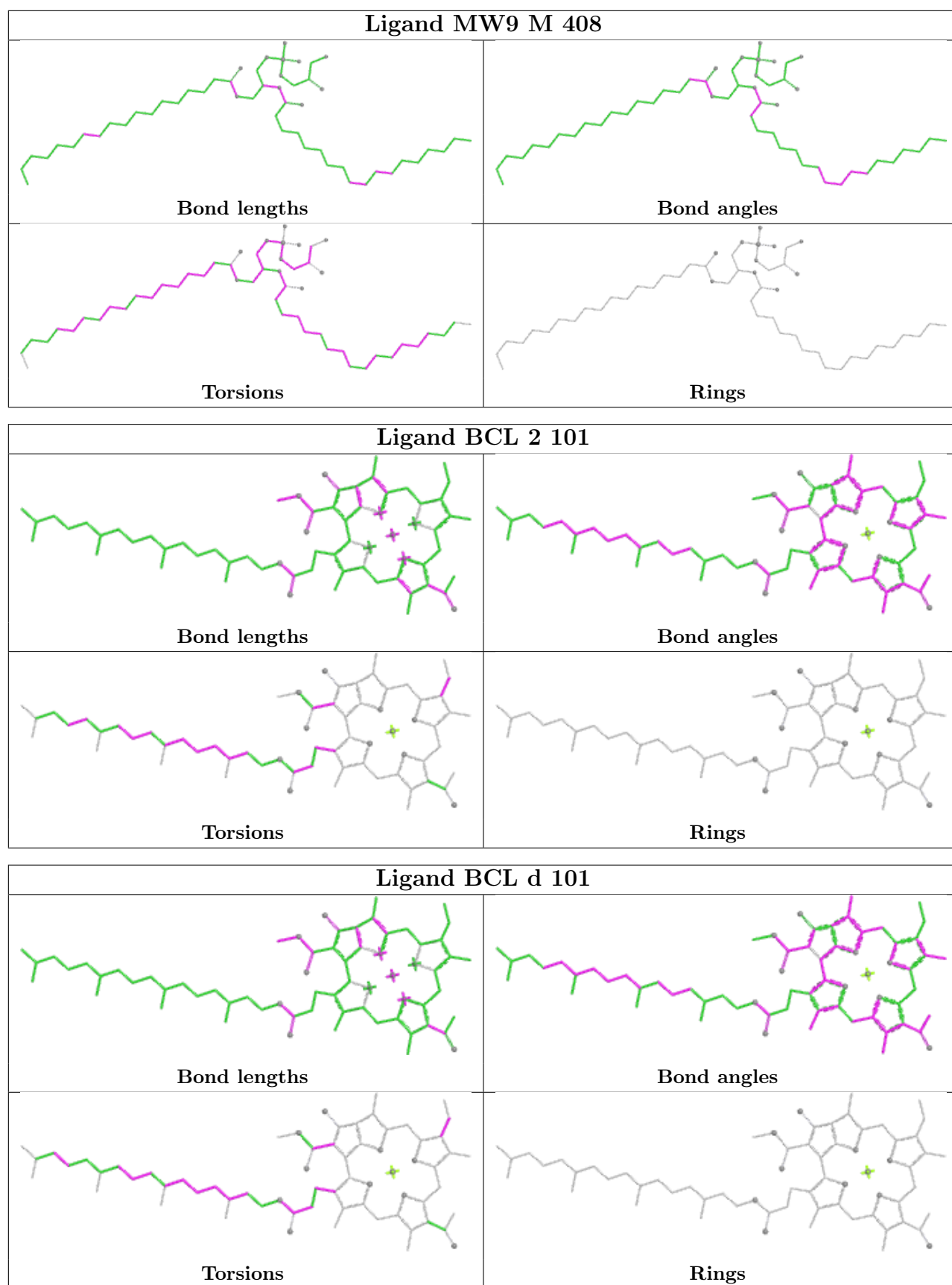


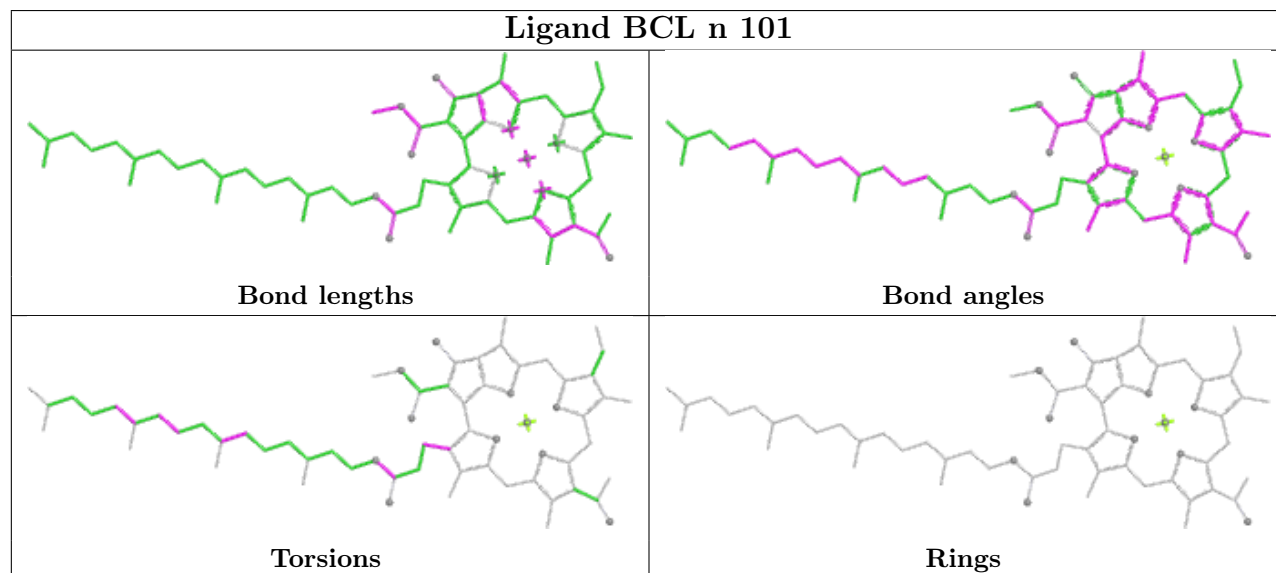
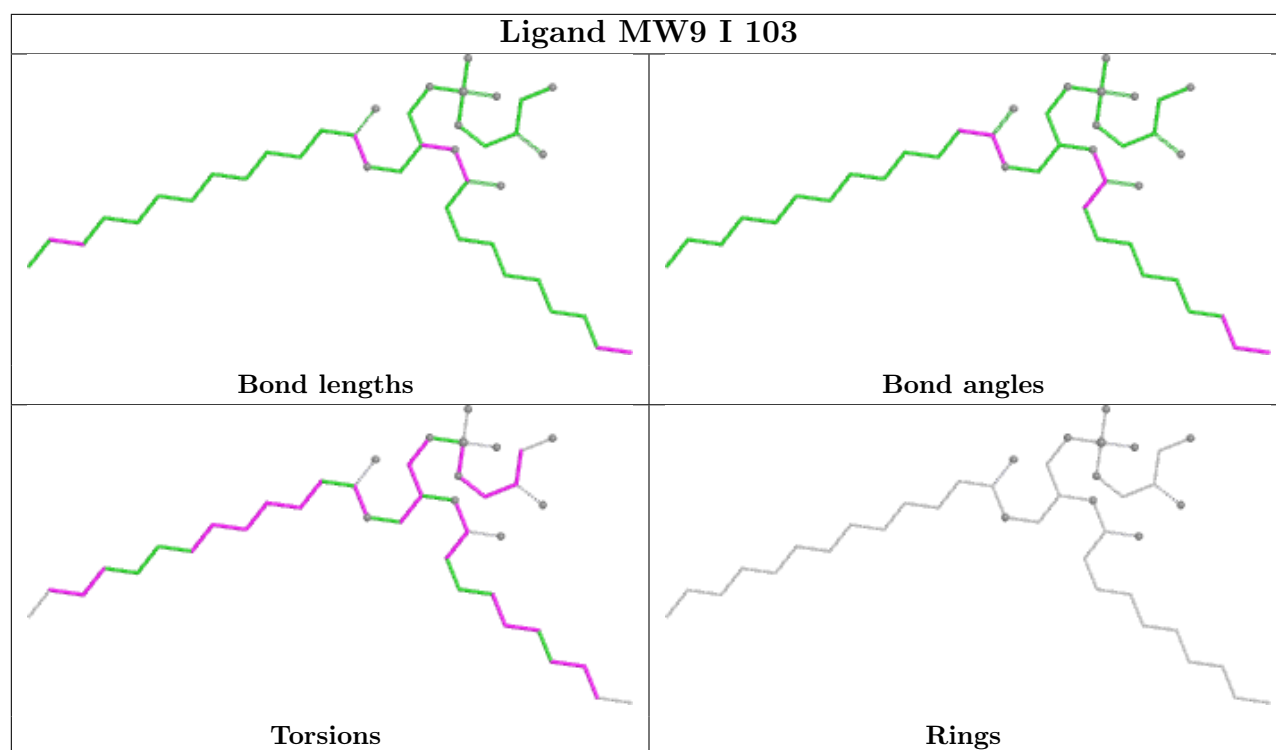


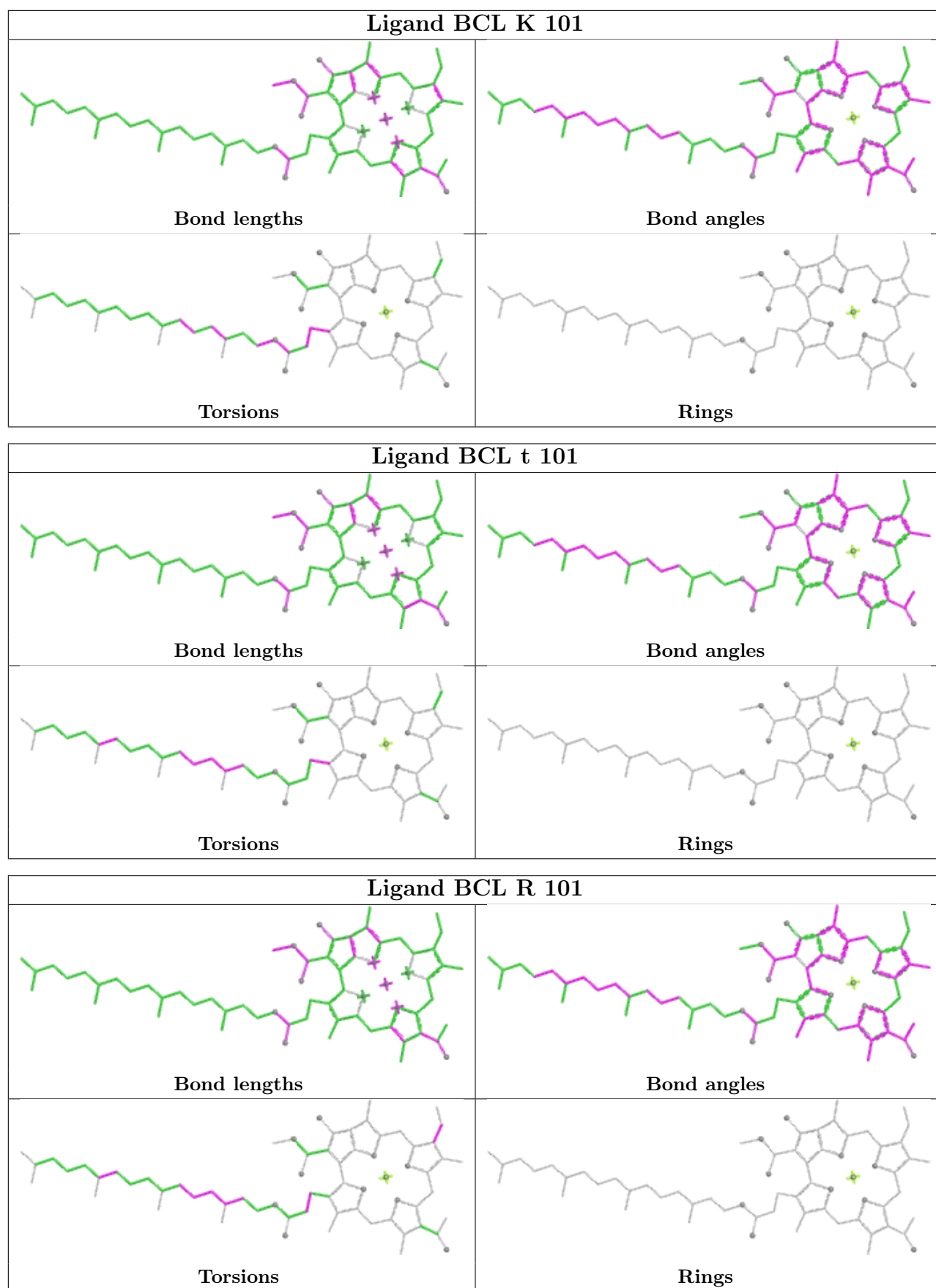


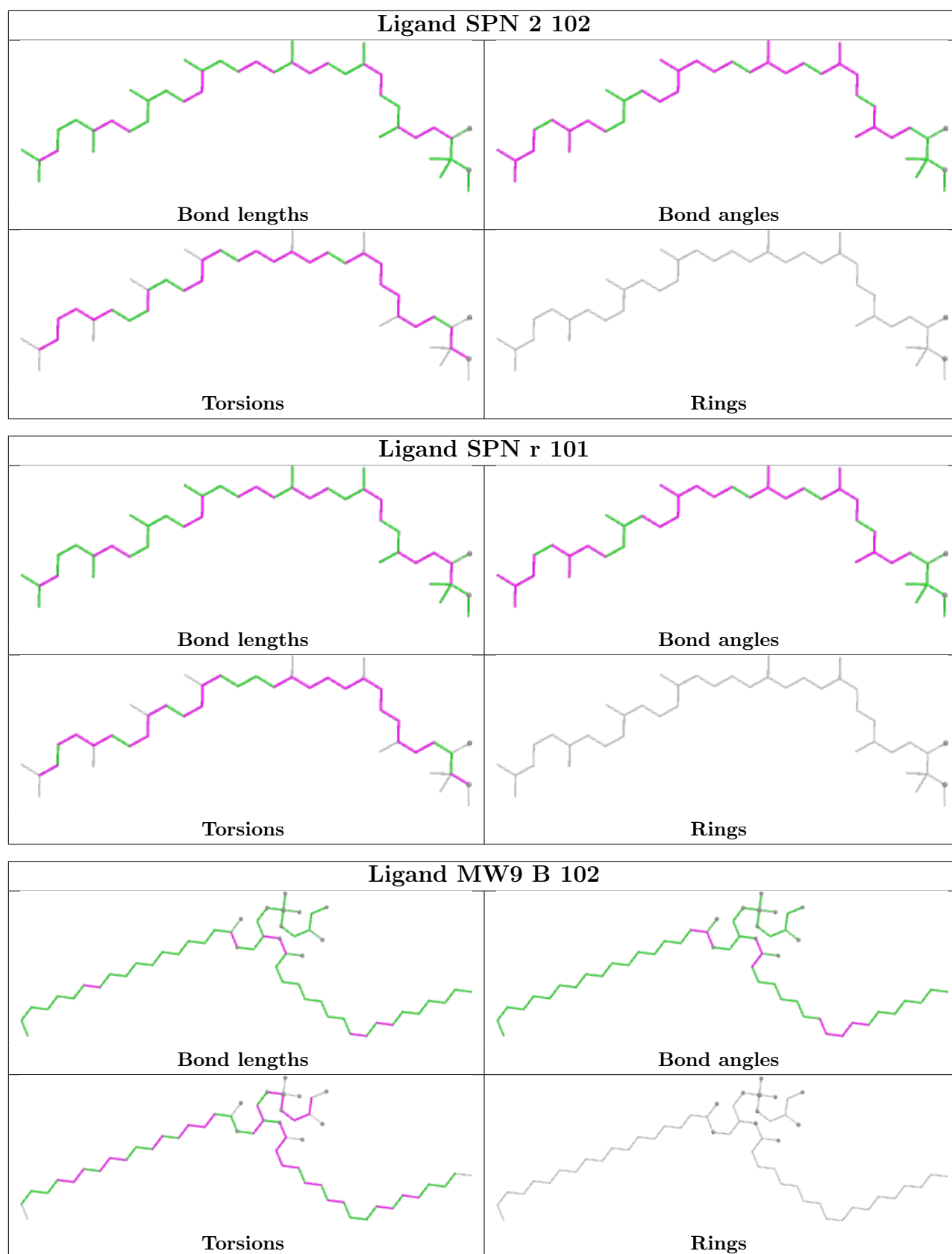












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

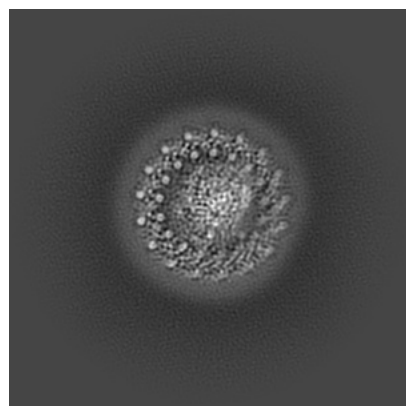
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61695. These allow visual inspection of the internal detail of the map and identification of artifacts.

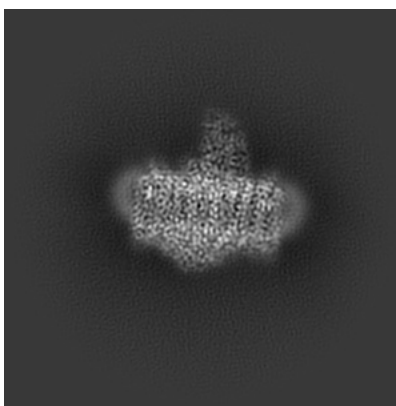
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

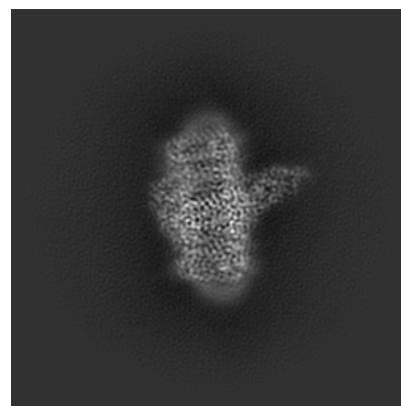
6.1.1 Primary map



X

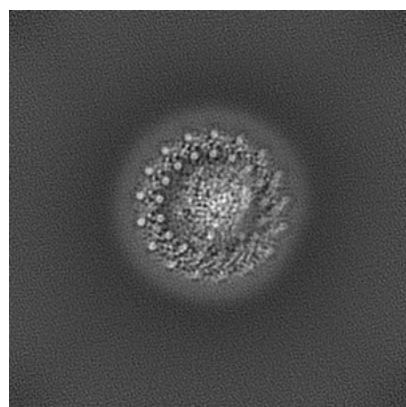


Y

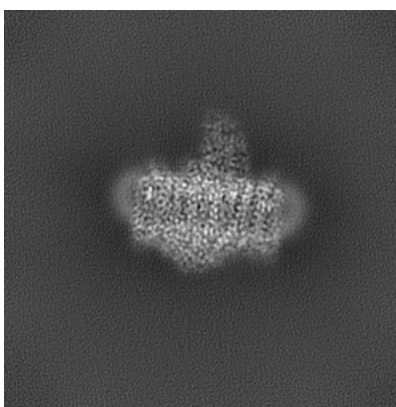


Z

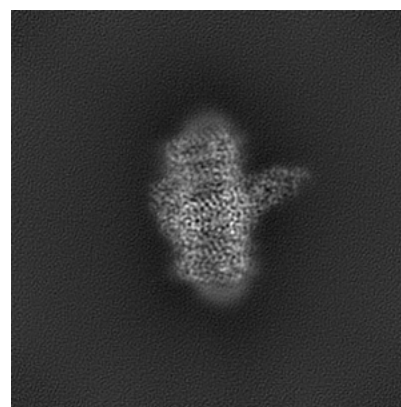
6.1.2 Raw map



X



Y

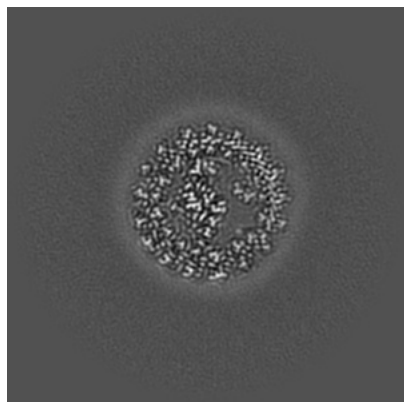


Z

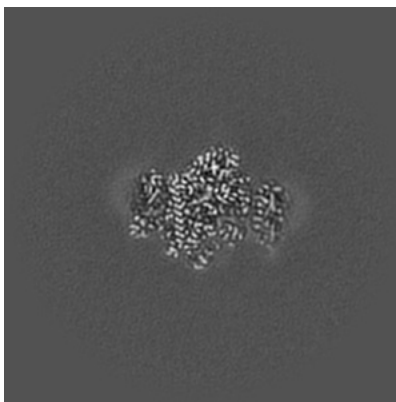
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

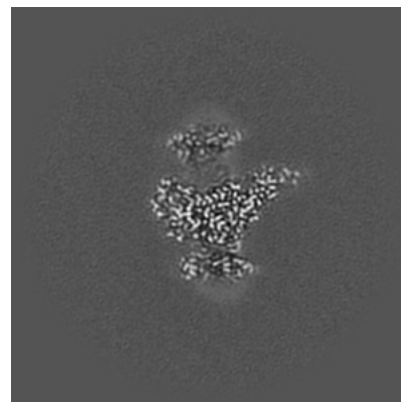
6.2.1 Primary map



X Index: 128

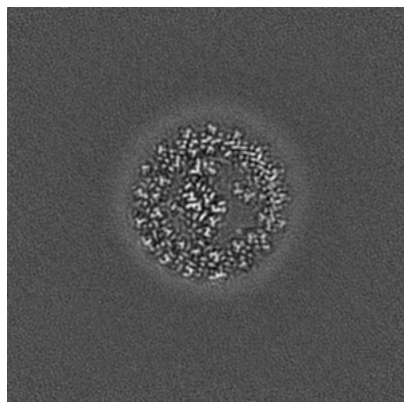


Y Index: 128

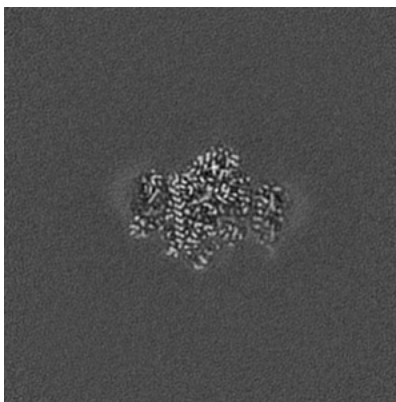


Z Index: 128

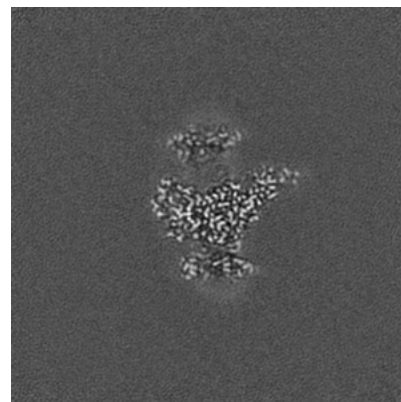
6.2.2 Raw map



X Index: 128



Y Index: 128

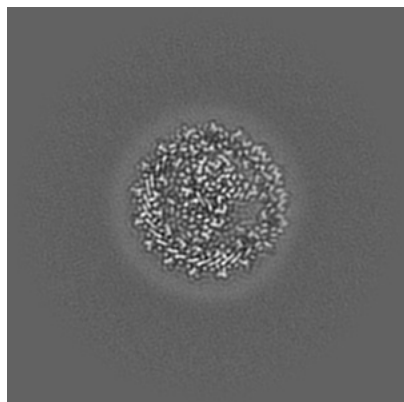


Z Index: 128

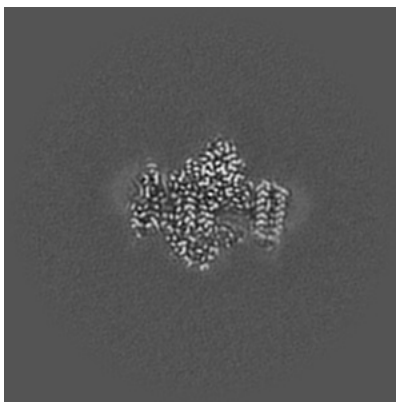
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

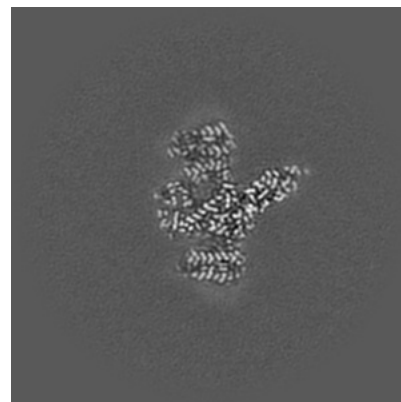
6.3.1 Primary map



X Index: 137

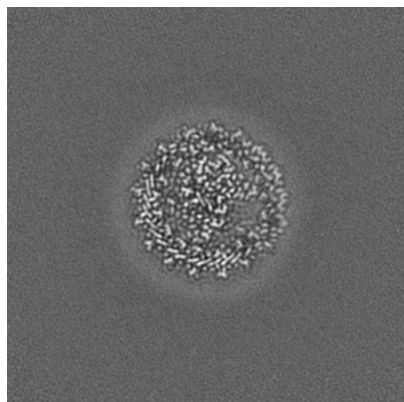


Y Index: 131

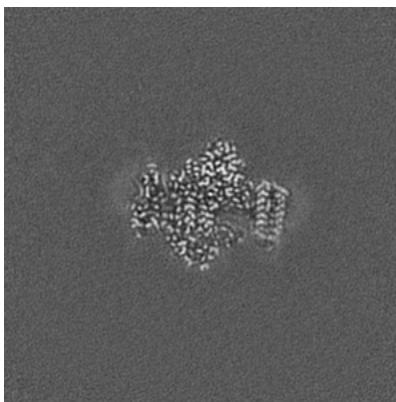


Z Index: 135

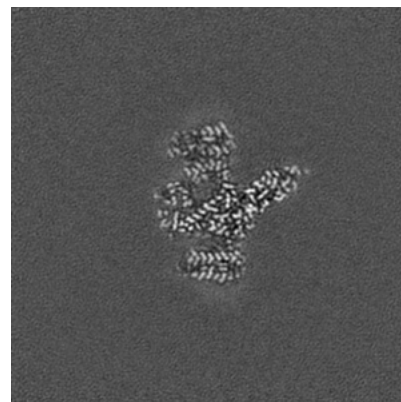
6.3.2 Raw map



X Index: 137



Y Index: 131

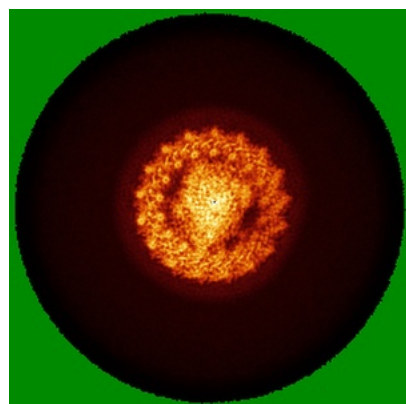


Z Index: 135

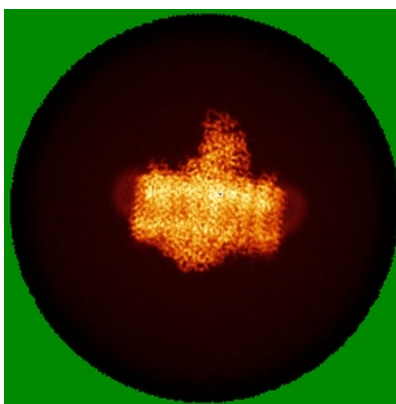
The images above show the largest variance slices of the map in three orthogonal directions.

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

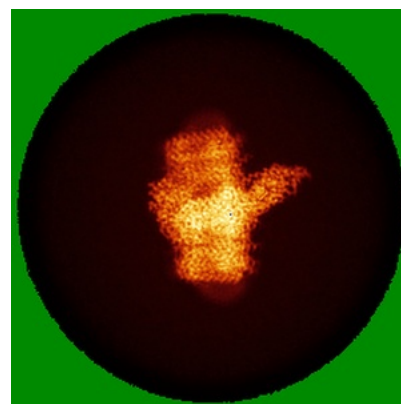
6.4.1 Primary map



X

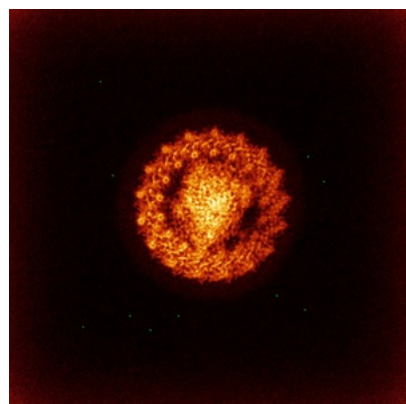


Y

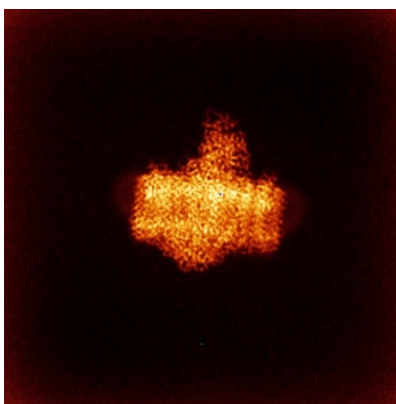


Z

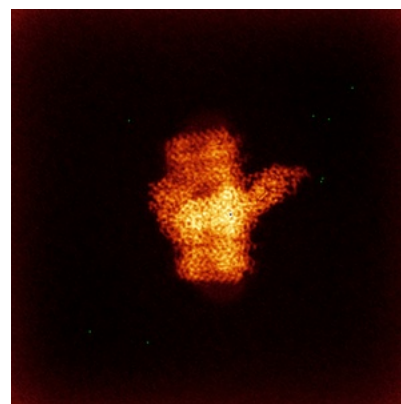
6.4.2 Raw map



X



Y

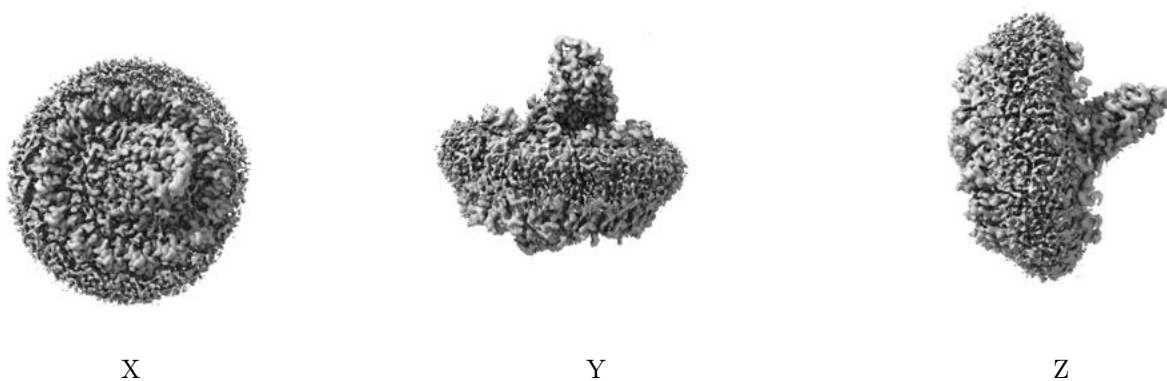


Z

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.

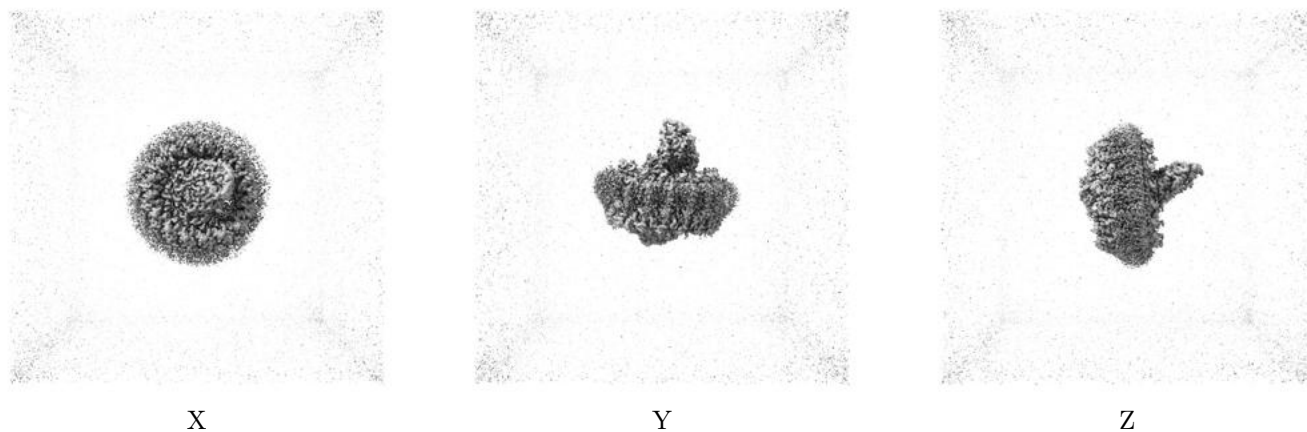
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.103. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

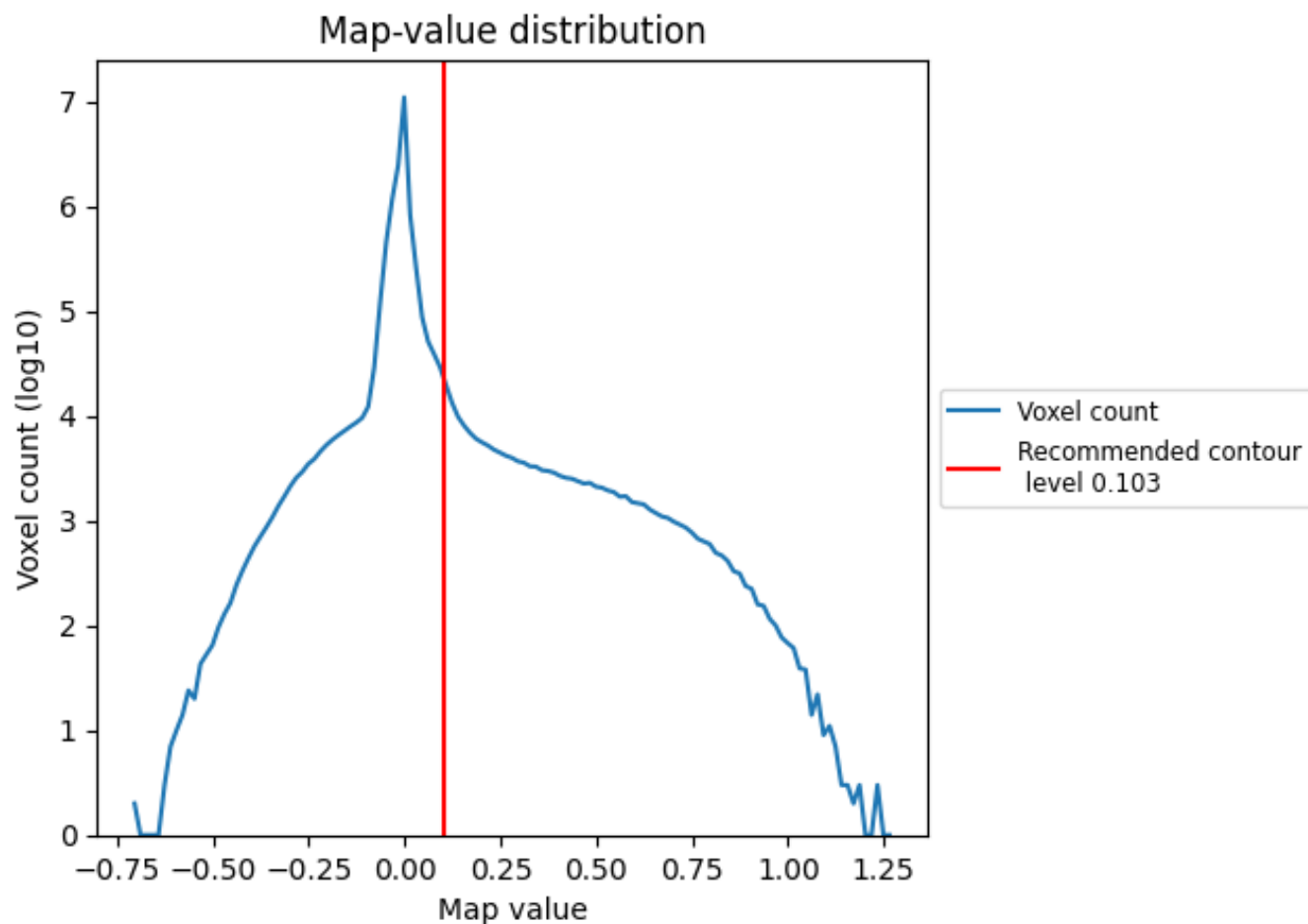
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

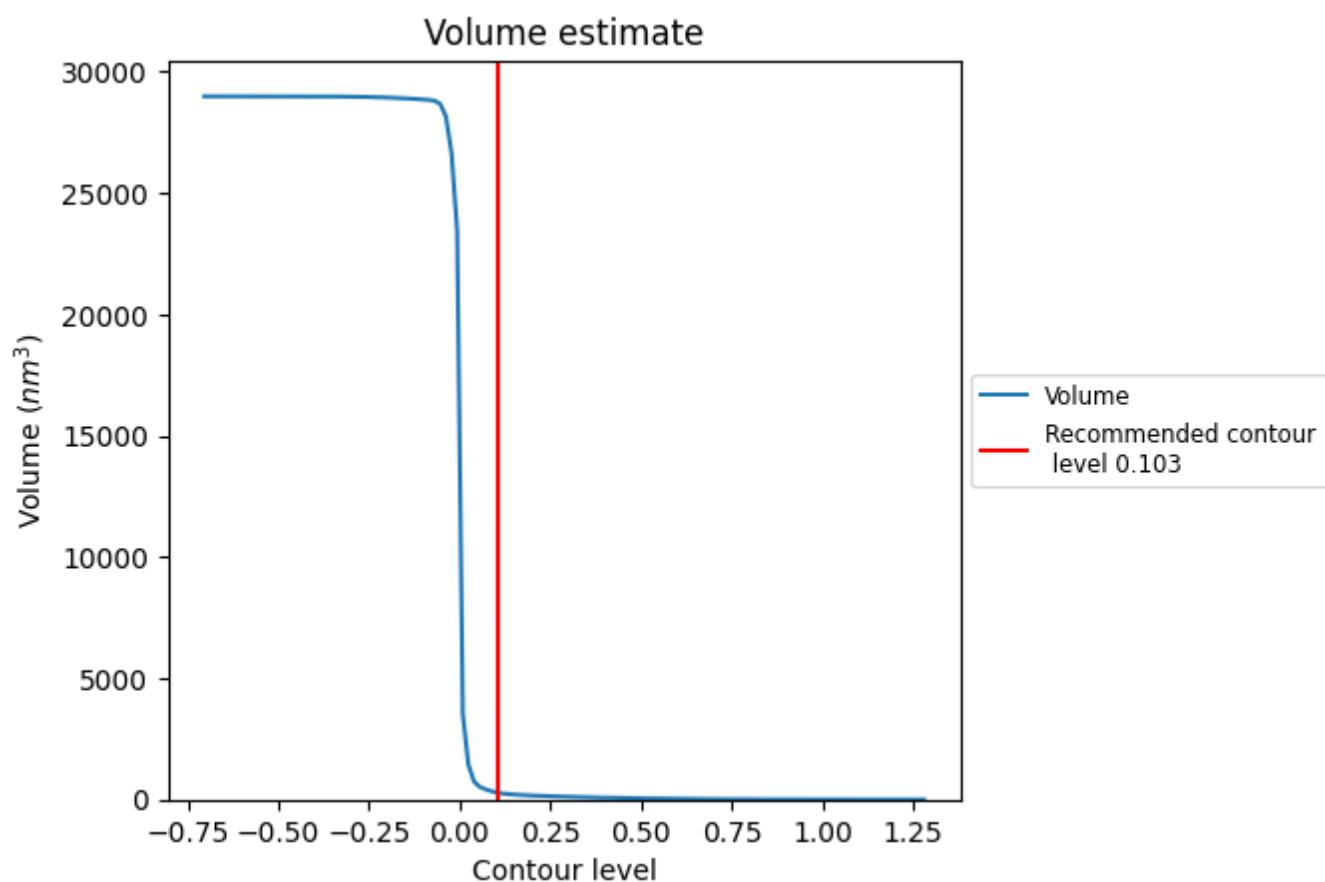
This section contains the results of statistical analysis of the map.

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.

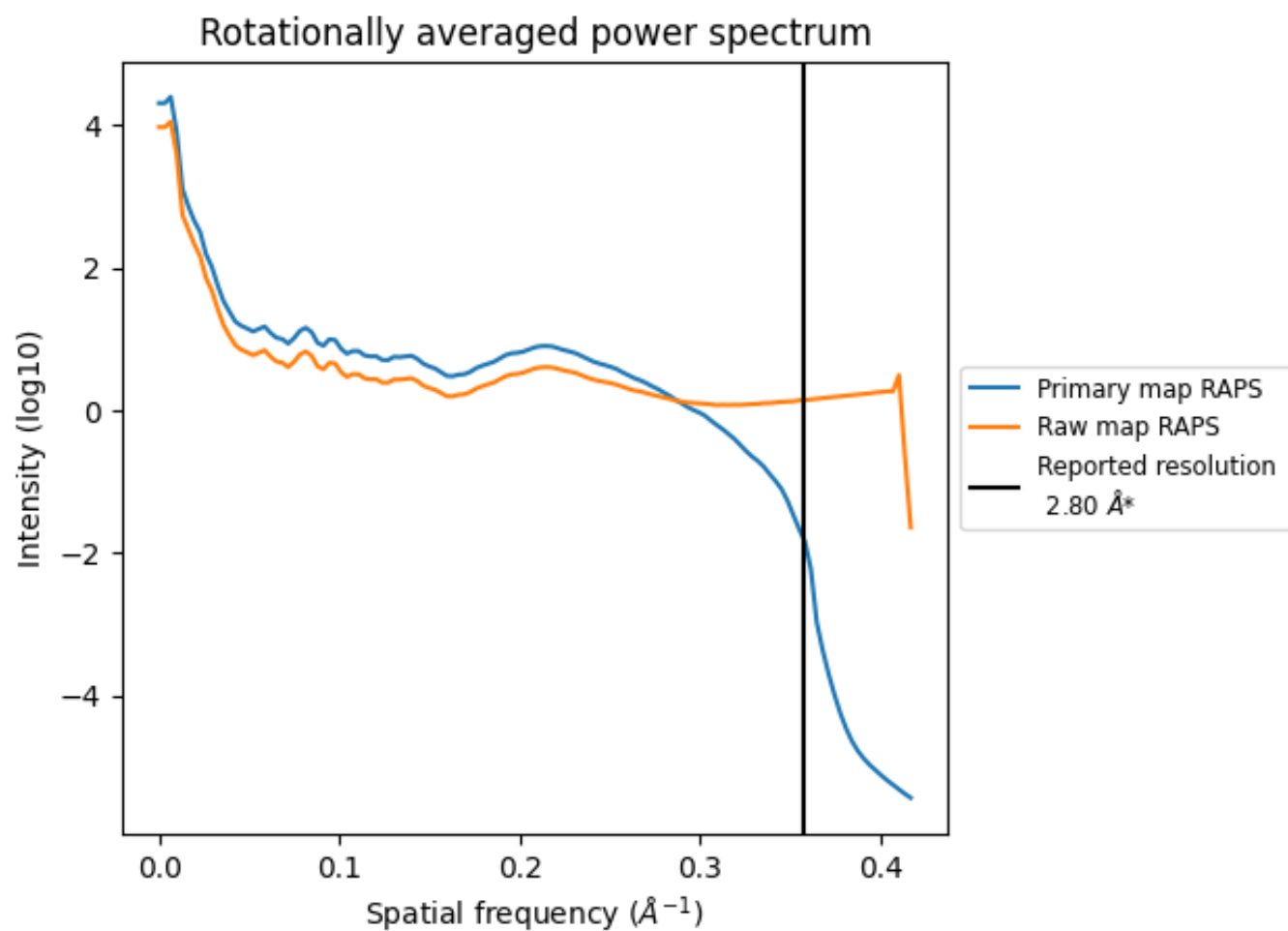
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm³; this corresponds to an approximate mass of 262 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 ⓘ

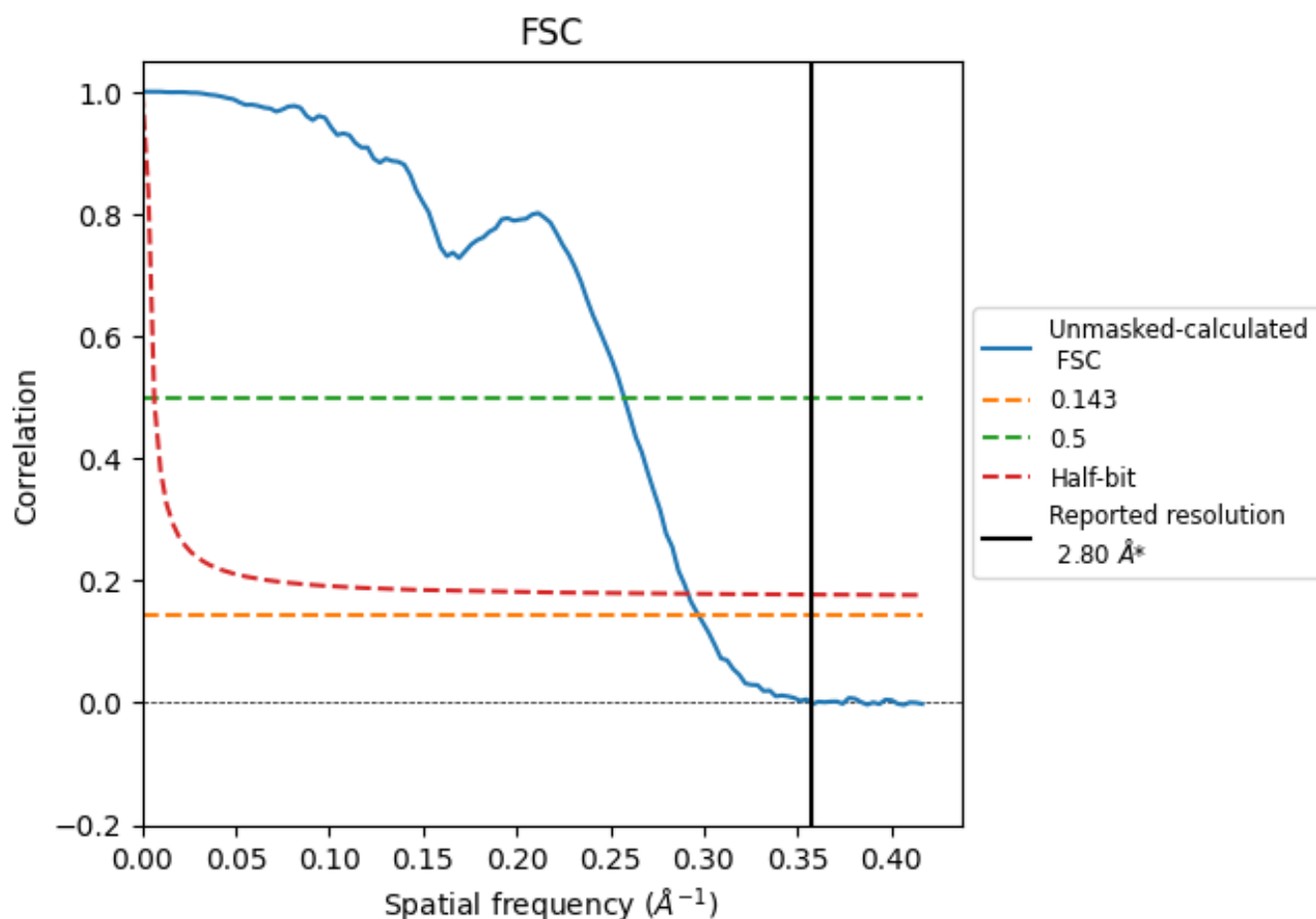


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.80 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.36 | 3.89 | 3.43 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 2.8 by more than 10 %

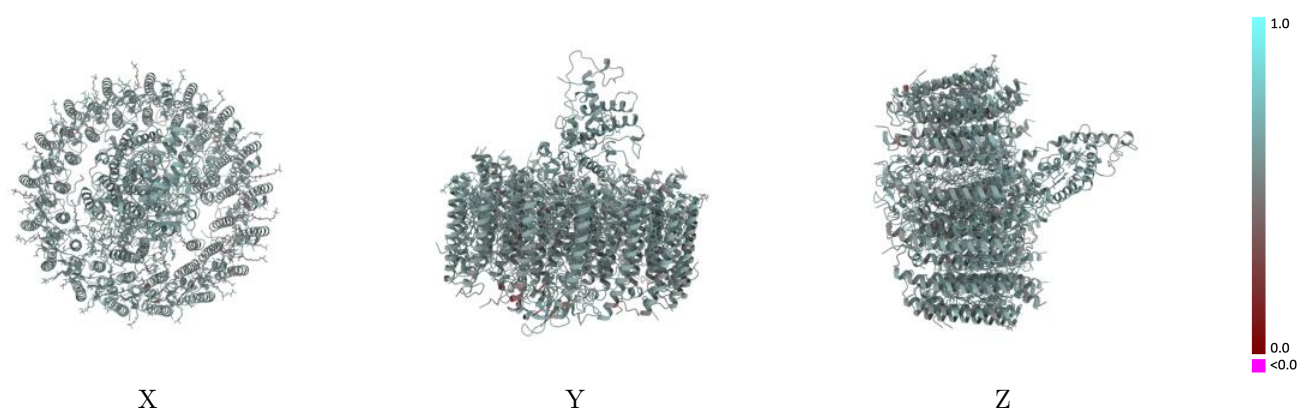
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61695 and PDB model 9JPB. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

This section was not generated.

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

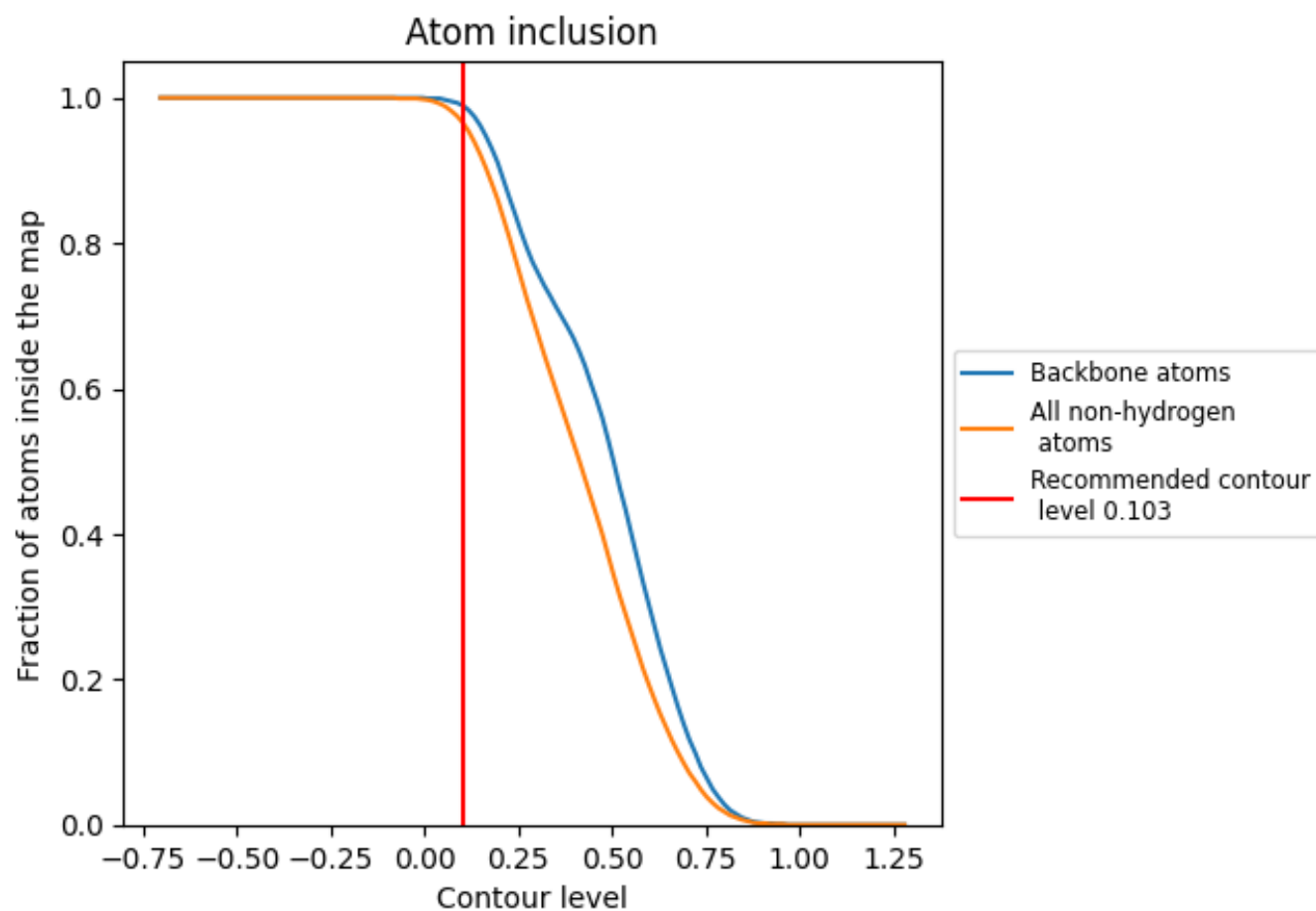


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.103) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All |  0.9650 |  0.5710 |
| 1 |  0.9620 |  0.5720 |
| 2 |  0.9620 |  0.5640 |
| A |  0.9430 |  0.5540 |
| B |  0.9450 |  0.5680 |
| C |  0.9730 |  0.5730 |
| D |  0.9760 |  0.5830 |
| E |  0.9680 |  0.5800 |
| F |  0.9790 |  0.5910 |
| G |  0.9660 |  0.5820 |
| H |  0.9760 |  0.5840 |
| I |  0.9820 |  0.5840 |
| J |  0.9700 |  0.5670 |
| K |  0.9640 |  0.5770 |
| L |  0.9790 |  0.5930 |
| M |  0.9760 |  0.5890 |
| N |  0.9670 |  0.5560 |
| O |  0.9650 |  0.5620 |
| P |  0.9520 |  0.5610 |
| Q |  0.9500 |  0.5670 |
| R |  0.9520 |  0.5590 |
| S |  0.9300 |  0.5580 |
| T |  0.9600 |  0.5500 |
| V |  0.8860 |  0.5220 |
| a |  0.9450 |  0.5430 |
| b |  0.9760 |  0.5600 |
| d |  0.9810 |  0.5720 |
| e |  0.9820 |  0.5830 |
| f |  0.9670 |  0.5820 |
| g |  0.9860 |  0.5720 |
| i |  0.9550 |  0.5620 |
| j |  0.9750 |  0.5640 |
| k |  0.9530 |  0.5560 |
| n |  0.9600 |  0.5620 |
| p |  0.9460 |  0.5350 |



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| Chain | Atom inclusion | Q-score |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| q |  0.9690 |  0.5640 |
| r |  0.9450 |  0.5600 |
| s |  0.9540 |  0.5470 |
| t |  0.9240 |  0.5260 |
| v |  0.9260 |  0.5060 |