



Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 06:23 AM JST

PDB ID : 7VOR
EMDB ID : EMD-32058
Title : The structure of dimeric photosynthetic RC-LH1 supercomplex in Class-1
Authors : Cao, P.; Li, M.; Liu, L.N.
Deposited on : 2021-10-14
Resolution : 2.74 Å(reported)

This is a Full wwPDB EM Validation 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:

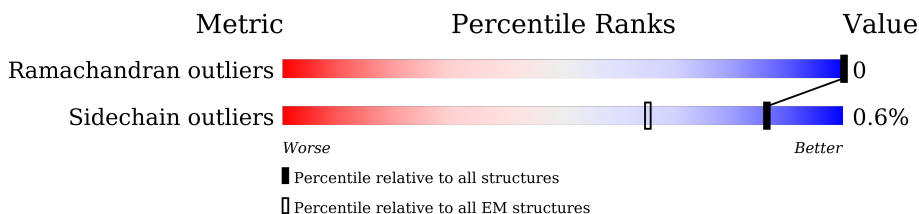
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 2.74 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) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | L | 282 | |
| 1 | l | 282 | |
| 2 | M | 308 | |
| 2 | m | 308 | |
| 3 | H | 260 | |
| 3 | h | 260 | |
| 4 | 1 | 58 | |
| 4 | 3 | 58 | |
| 4 | 5 | 58 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | 6 | 58 | 83% 17% |
| 4 | 7 | 58 | 83% 17% |
| 4 | 9 | 58 | 95% 5% |
| 4 | A | 58 | 95% 5% |
| 4 | D | 58 | 95% 5% |
| 4 | F | 58 | 95% 5% |
| 4 | I | 58 | 93% 7% |
| 4 | K | 58 | 93% 7% |
| 4 | O | 58 | 7% 91% 7% |
| 4 | Q | 58 | 7% 95% 5% |
| 4 | S | 58 | 5% 95% 5% |
| 4 | U | 58 | 5% 91% 9% |
| 4 | W | 58 | 26% 93% 7% |
| 4 | a | 58 | 95% 5% |
| 4 | b1 | 58 | 66% 81% 19% |
| 4 | b9 | 58 | 95% 5% |
| 4 | d | 58 | 95% 5% |
| 4 | f | 58 | 95% 5% |
| 4 | i | 58 | 93% 7% |
| 4 | k | 58 | 93% 7% |
| 4 | o | 58 | 7% 91% 7% |
| 4 | q | 58 | 7% 95% 5% |
| 4 | s | 58 | 5% 95% 5% |
| 4 | u | 58 | 5% 91% 9% |
| 4 | w | 58 | 26% 93% 7% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5 | 0 | 49 | 90% 10% |
| 5 | 2 | 49 | 67% 78% 22% |
| 5 | 4 | 49 | 67% 78% 22% |
| 5 | 8 | 49 | 90% 10% |
| 5 | B | 49 | 90% 10% |
| 5 | C | 49 | 41% 86% 14% |
| 5 | E | 49 | 88% 12% |
| 5 | G | 49 | 90% 10% |
| 5 | J | 49 | 88% 12% |
| 5 | N | 49 | 8% 86% 14% |
| 5 | P | 49 | 6% 88% 12% |
| 5 | R | 49 | 10% 88% 12% |
| 5 | T | 49 | 84% 14% 1% |
| 5 | V | 49 | 16% 86% 14% |
| 5 | Z | 49 | 69% 84% 14% 1% |
| 5 | b | 49 | 90% 10% |
| 5 | b0 | 49 | 90% 10% |
| 5 | b8 | 49 | 90% 10% |
| 5 | c | 49 | 41% 86% 14% |
| 5 | e | 49 | 88% 12% |
| 5 | g | 49 | 90% 10% |
| 5 | j | 49 | 88% 12% |
| 5 | n | 49 | 8% 86% 14% |
| 5 | p | 49 | 6% 88% 12% |
| 5 | r | 49 | 10% 88% 12% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------|
| 5 | t | 49 | <p>84% 14%</p> |
| 5 | v | 49 | <p>16% 86% 14%</p> |
| 5 | z | 49 | <p>73% 84% 14%</p> |
| 6 | X | 82 | <p>6% 83% 17%</p> |
| 6 | x | 82 | <p>6% 83% 17%</p> |
| 7 | Y | 53 | <p>92% 8%</p> |
| 7 | y | 53 | <p>83% 92% 8%</p> |

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 44980 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 Reaction center protein L chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | L | 281 | Total | C | N | O | S | 0 | 0 |
| | | | 2232 | 1507 | 355 | 362 | 8 | | |
| 1 | l | 281 | Total | C | N | O | S | 0 | 0 |
| | | | 2232 | 1507 | 355 | 362 | 8 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | M | 307 | Total | C | N | O | S | 0 | 0 |
| | | | 2445 | 1630 | 400 | 404 | 11 | | |
| 2 | m | 307 | Total | C | N | O | S | 0 | 0 |
| | | | 2445 | 1630 | 400 | 404 | 11 | | |

- Molecule 3 is a protein called Reaction center protein H chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | H | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1973 | 1264 | 335 | 363 | 11 | | |
| 3 | h | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 1973 | 1264 | 335 | 363 | 11 | | |

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | A | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 460 | 313 | 74 | 70 | 3 | | |
| 4 | D | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 460 | 313 | 74 | 70 | 3 | | |
| 4 | F | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 460 | 313 | 74 | 70 | 3 | | |
| 4 | I | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 455 | 310 | 73 | 69 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | K | 54 | 452 | 308 | 73 | 69 | 2 | 0 | 0 |
| 4 | O | 54 | 455 | 310 | 73 | 69 | 3 | 0 | 0 |
| 4 | Q | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | S | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | U | 53 | 447 | 305 | 72 | 68 | 2 | 0 | 0 |
| 4 | W | 54 | 452 | 308 | 73 | 69 | 2 | 0 | 0 |
| 4 | 3 | 52 | 437 | 299 | 70 | 66 | 2 | 0 | 0 |
| 4 | 1 | 47 | 392 | 266 | 64 | 60 | 2 | 0 | 0 |
| 4 | 7 | 48 | 403 | 277 | 62 | 61 | 3 | 0 | 0 |
| 4 | 9 | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | a | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | d | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | f | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | i | 54 | 455 | 310 | 73 | 69 | 3 | 0 | 0 |
| 4 | k | 54 | 452 | 308 | 73 | 69 | 2 | 0 | 0 |
| 4 | o | 54 | 455 | 310 | 73 | 69 | 3 | 0 | 0 |
| 4 | q | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | s | 55 | 460 | 313 | 74 | 70 | 3 | 0 | 0 |
| 4 | u | 53 | 447 | 305 | 72 | 68 | 2 | 0 | 0 |
| 4 | w | 54 | 452 | 308 | 73 | 69 | 2 | 0 | 0 |
| 4 | 5 | 52 | 437 | 299 | 70 | 66 | 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4 | b1 | 47 | Total | C | N | O | S | 0 | 0 |
| | | | 392 | 266 | 64 | 60 | 2 | | |
| 4 | 6 | 48 | Total | C | N | O | S | 0 | 0 |
| | | | 403 | 277 | 62 | 61 | 3 | | |
| 4 | b9 | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 460 | 313 | 74 | 70 | 3 | | |

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5 | B | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |
| 5 | E | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |
| 5 | G | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |
| 5 | J | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |
| 5 | N | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | P | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |
| 5 | R | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |
| 5 | T | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | V | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | C | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | Z | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | 2 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 309 | 206 | 50 | 52 | 1 | | |
| 5 | 8 | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |
| 5 | 0 | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |
| 5 | b | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |
| 5 | e | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5 | g | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |
| 5 | j | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |
| 5 | n | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | p | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |
| 5 | r | 43 | Total | C | N | O | S | 0 | 0 |
| | | | 352 | 236 | 55 | 60 | 1 | | |
| 5 | t | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | v | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | c | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | z | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 344 | 230 | 54 | 59 | 1 | | |
| 5 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 309 | 206 | 50 | 52 | 1 | | |
| 5 | b8 | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |
| 5 | b0 | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 360 | 240 | 56 | 63 | 1 | | |

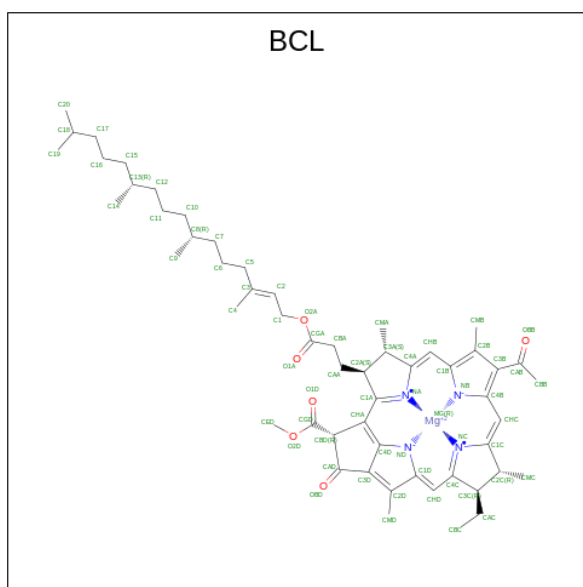
- Molecule 6 is a protein called Intrinsic membrane protein PufX.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6 | X | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 529 | 345 | 93 | 88 | 3 | | |
| 6 | x | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 529 | 345 | 93 | 88 | 3 | | |

- Molecule 7 is a protein called Rsp_7571 Protein-Y PufY.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | Y | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 361 | 248 | 55 | 55 | 3 | | |
| 7 | y | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 361 | 248 | 55 | 55 | 3 | | |

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|
| | | | Total | C | Mg | N | O | |
| 8 | L | 1 | Total 129 | C 107 | Mg 2 | N 8 | O 12 | 0 |
| 8 | L | 1 | Total 129 | C 107 | Mg 2 | N 8 | O 12 | 0 |
| 8 | M | 1 | Total 132 | C 110 | Mg 2 | N 8 | O 12 | 0 |
| 8 | M | 1 | Total 132 | C 110 | Mg 2 | N 8 | O 12 | 0 |
| 8 | A | 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 | D | 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 | F | 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 | I | 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 | K | 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 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|
| | | | Total | C | Mg | N | O | |
| 8 | O | 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 | 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 | S | 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 | U | 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 | W | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | C | 1 | Total 61 | C 50 | Mg 1 | N 4 | O 6 | 0 |
| 8 | 3 | 1 | Total 51 | C 40 | Mg 1 | N 4 | O 6 | 0 |
| 8 | Z | 1 | Total 56 | C 45 | Mg 1 | N 4 | O 6 | 0 |
| 8 | 1 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 8 | 2 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 8 | 7 | 1 | Total 122 | C 100 | Mg 2 | N 8 | O 12 | 0 |
| 8 | 7 | 1 | Total 122 | C 100 | Mg 2 | N 8 | O 12 | 0 |
| 8 | 9 | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | 0 | 1 | Total 61 | C 50 | Mg 1 | N 4 | O 6 | 0 |
| 8 | l | 1 | Total 129 | C 107 | Mg 2 | N 8 | O 12 | 0 |
| 8 | l | 1 | Total 129 | C 107 | Mg 2 | N 8 | O 12 | 0 |
| 8 | m | 1 | Total 132 | C 110 | Mg 2 | N 8 | O 12 | 0 |

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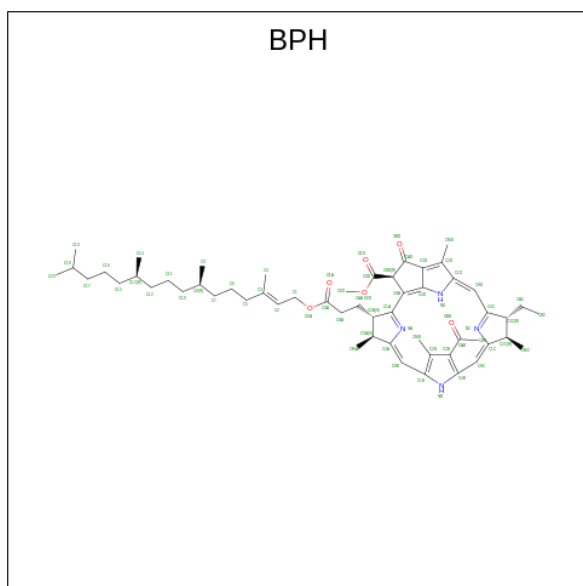
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|--------------|----------|---------|--------|---------|---------|
| | | | Total | C | Mg | N | O | |
| 8 | m | 1 | Total 132 | C 110 | Mg 2 | N 8 | O 12 | 0 |
| 8 | a | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | b | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | d | 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 | f | 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 | i | 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 | k | 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 | o | 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 | 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 | s | 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 | u | 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 | w | 1 | Total 66 | C 55 | Mg 1 | N 4 | O 6 | 0 |
| 8 | c | 1 | Total 61 | C 50 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | |
|-----|-------|----------|-------|-----|----|---|---------|---|
| 8 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 8 | z | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 45 | 1 | 4 | 6 | |
| 8 | b1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 8 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 8 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 122 | 100 | 2 | 8 | 12 | |
| 8 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 122 | 100 | 2 | 8 | 12 | |
| 8 | b9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 8 | b0 | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 50 | 1 | 4 | 6 | |

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



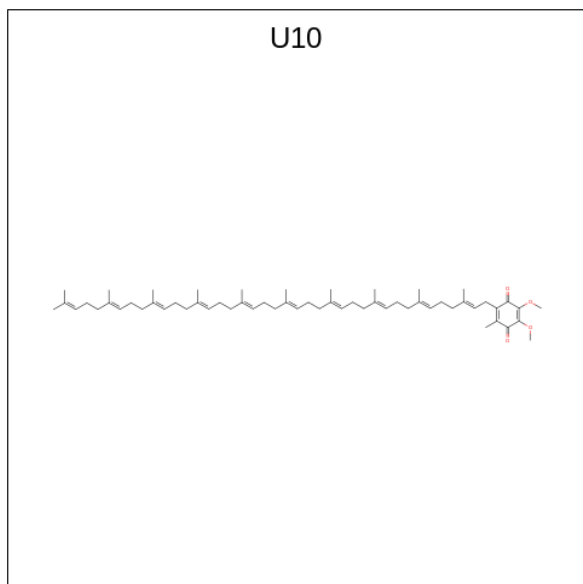
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 9 | L | 1 | Total | C | N | O | 0 |
| | | | 65 | 55 | 4 | 6 | |
| 9 | M | 1 | Total | C | N | O | 0 |
| | | | 55 | 45 | 4 | 6 | |
| 9 | l | 1 | Total | C | N | O | 0 |
| | | | 65 | 55 | 4 | 6 | |

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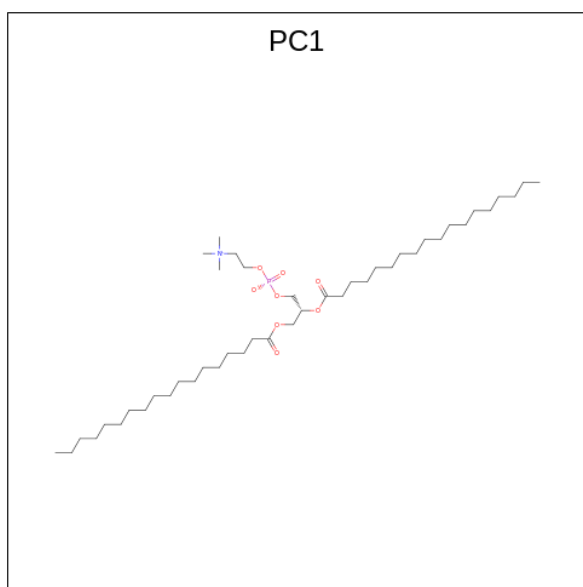
| Mol | Chain | Residues | Atoms | | | AltConf | |
|-----|-------|----------|-------|----|---|---------|---|
| | | | Total | C | N | | O |
| 9 | m | 1 | 55 | 45 | 4 | 6 | 0 |

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| | | | Total | C | O | |
| 10 | L | 1 | 81 | 73 | 8 | 0 |
| 10 | L | 1 | 81 | 73 | 8 | 0 |
| 10 | M | 1 | 48 | 44 | 4 | 0 |
| 10 | l | 1 | 81 | 73 | 8 | 0 |
| 10 | l | 1 | 81 | 73 | 8 | 0 |
| 10 | m | 1 | 48 | 44 | 4 | 0 |

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 11 | L | 1 | 79 | 59 | 2 | 16 | 2 | 0 |
| 11 | L | 1 | 79 | 59 | 2 | 16 | 2 | 0 |
| 11 | H | 1 | 77 | 57 | 2 | 16 | 2 | 0 |
| 11 | H | 1 | 77 | 57 | 2 | 16 | 2 | 0 |
| 11 | A | 1 | 114 | 84 | 3 | 24 | 3 | 0 |
| 11 | A | 1 | 114 | 84 | 3 | 24 | 3 | 0 |
| 11 | A | 1 | 114 | 84 | 3 | 24 | 3 | 0 |
| 11 | D | 1 | 39 | 29 | 1 | 8 | 1 | 0 |
| 11 | l | 1 | 79 | 59 | 2 | 16 | 2 | 0 |
| 11 | l | 1 | 79 | 59 | 2 | 16 | 2 | 0 |
| 11 | h | 1 | 77 | 57 | 2 | 16 | 2 | 0 |
| 11 | h | 1 | 77 | 57 | 2 | 16 | 2 | 0 |
| 11 | a | 1 | 114 | 84 | 3 | 24 | 3 | 0 |
| 11 | a | 1 | 114 | 84 | 3 | 24 | 3 | 0 |

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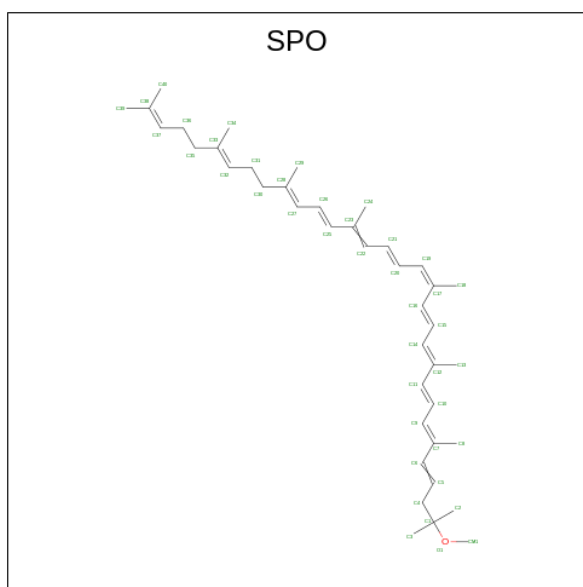
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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 11 | a | 1 | 114 | 84 | 3 | 24 | 3 | 0 |
| 11 | d | 1 | 39 | 29 | 1 | 8 | 1 | 0 |

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| | | | Total | C | O | |
| 13 | M | 1 | 42 | 41 | 1 | 0 |
| 13 | A | 1 | 42 | 41 | 1 | 0 |
| 13 | B | 1 | 42 | 41 | 1 | 0 |
| 13 | D | 1 | 42 | 41 | 1 | 0 |
| 13 | E | 1 | 84 | 82 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|-----|---|---------|
| 13 | E | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | G | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | G | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | I | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | J | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | N | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | O | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | P | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | Q | 1 | Total | C | O | 0 |
| | | | 126 | 123 | 3 | |
| 13 | Q | 1 | Total | C | O | 0 |
| | | | 126 | 123 | 3 | |
| 13 | Q | 1 | Total | C | O | 0 |
| | | | 126 | 123 | 3 | |
| 13 | S | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | S | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | U | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | U | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | C | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | 3 | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | 3 | 1 | Total | C | O | 0 |
| | | | 84 | 82 | 2 | |
| 13 | 9 | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | 0 | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |
| 13 | X | 1 | Total | C | O | 0 |
| | | | 42 | 41 | 1 | |

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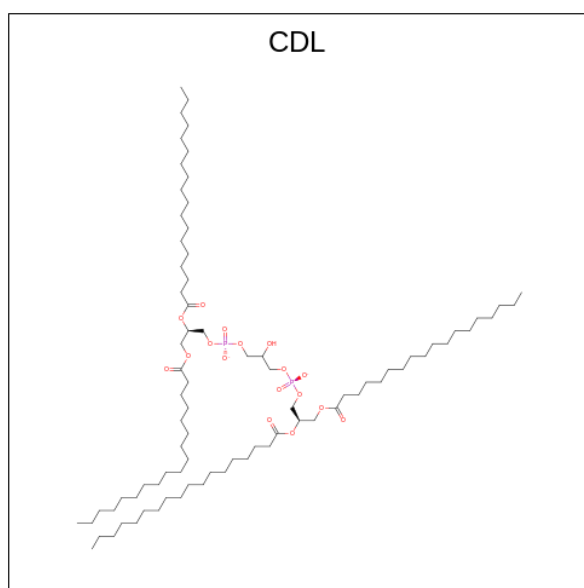
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|-----|---|---------|
| | | | Total | C | O | |
| 13 | m | 1 | 42 | 41 | 1 | 0 |
| 13 | a | 1 | 42 | 41 | 1 | 0 |
| 13 | b | 1 | 42 | 41 | 1 | 0 |
| 13 | d | 1 | 42 | 41 | 1 | 0 |
| 13 | e | 1 | 84 | 82 | 2 | 0 |
| 13 | e | 1 | 84 | 82 | 2 | 0 |
| 13 | g | 1 | 84 | 82 | 2 | 0 |
| 13 | g | 1 | 84 | 82 | 2 | 0 |
| 13 | i | 1 | 42 | 41 | 1 | 0 |
| 13 | j | 1 | 42 | 41 | 1 | 0 |
| 13 | n | 1 | 42 | 41 | 1 | 0 |
| 13 | o | 1 | 42 | 41 | 1 | 0 |
| 13 | p | 1 | 42 | 41 | 1 | 0 |
| 13 | q | 1 | 126 | 123 | 3 | 0 |
| 13 | q | 1 | 126 | 123 | 3 | 0 |
| 13 | q | 1 | 126 | 123 | 3 | 0 |
| 13 | s | 1 | 84 | 82 | 2 | 0 |
| 13 | s | 1 | 84 | 82 | 2 | 0 |
| 13 | u | 1 | 84 | 82 | 2 | 0 |
| 13 | u | 1 | 84 | 82 | 2 | 0 |
| 13 | c | 1 | 42 | 41 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| | | | Total | C | O | |
| 13 | 5 | 1 | 84 | 82 | 2 | 0 |
| 13 | 5 | 1 | 84 | 82 | 2 | 0 |
| 13 | b9 | 1 | 42 | 41 | 1 | 0 |
| 13 | b0 | 1 | 42 | 41 | 1 | 0 |
| 13 | x | 1 | 42 | 41 | 1 | 0 |

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| | | | Total | C | O | P | |
| 14 | M | 1 | 82 | 63 | 17 | 2 | 0 |
| 14 | F | 1 | 63 | 44 | 17 | 2 | 0 |
| 14 | m | 1 | 82 | 63 | 17 | 2 | 0 |
| 14 | f | 1 | 63 | 44 | 17 | 2 | 0 |

3 Residue-property plots

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.

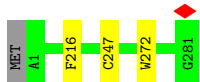
- Molecule 1: Reaction center protein L chain

Chain L:  99%



- Molecule 1: Reaction center protein L chain

Chain l:  99%



- Molecule 2: Reaction center protein M chain

Chain M:  99%



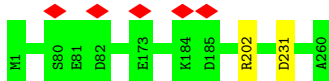
- Molecule 2: Reaction center protein M chain

Chain m:  99%



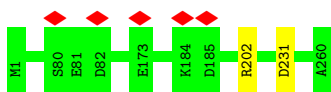
- Molecule 3: Reaction center protein H chain

Chain H:  99%



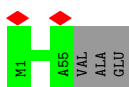
- Molecule 3: Reaction center protein H chain

Chain h:  99%



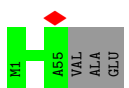
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain A:  95%



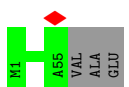
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain D:  95%

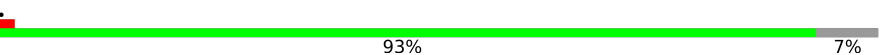


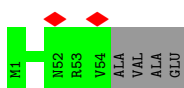
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F:  95%



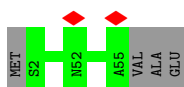
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I:  93%

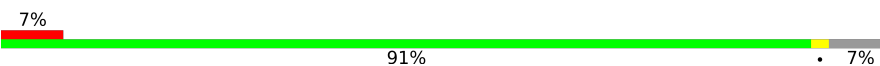


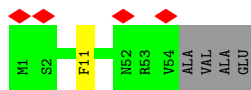
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:  93%

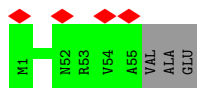


- Molecule 4: Light-harvesting protein B-875 alpha chain

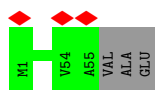
Chain O:  91%



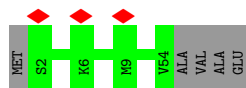
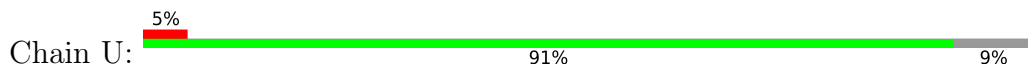
- Molecule 4: Light-harvesting protein B-875 alpha chain



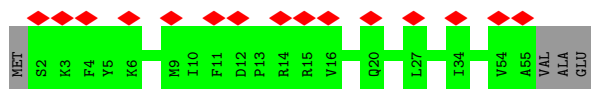
- Molecule 4: Light-harvesting protein B-875 alpha chain



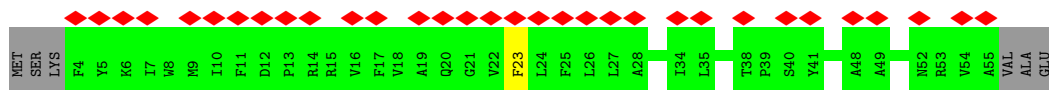
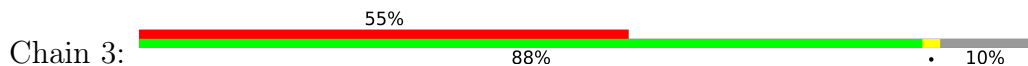
- Molecule 4: Light-harvesting protein B-875 alpha chain



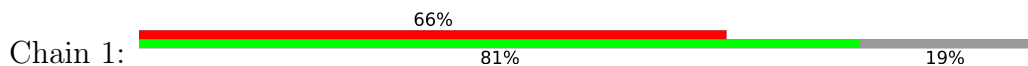
- Molecule 4: Light-harvesting protein B-875 alpha chain




- Molecule 4: Light-harvesting protein B-875 alpha chain

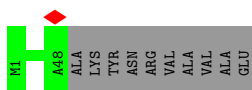


- Molecule 4: Light-harvesting protein B-875 alpha chain



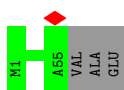
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 7:  83% 17%



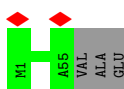
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 9:  95% 5%



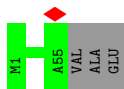
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain a:  95% 5%



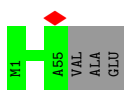
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain d:  95% 5%



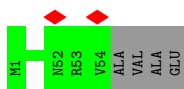
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain f:  95% 5%



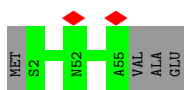
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain i:  93% 7%

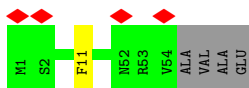
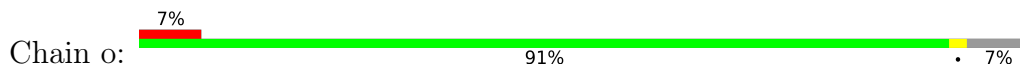


- Molecule 4: Light-harvesting protein B-875 alpha chain

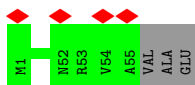
Chain k:  93% 7%



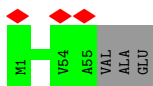
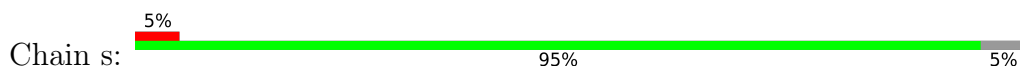
- Molecule 4: Light-harvesting protein B-875 alpha chain



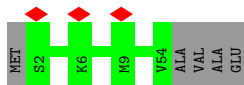
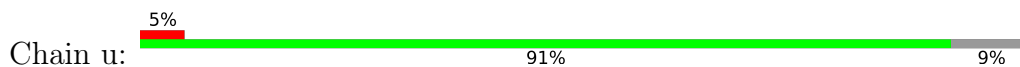
- Molecule 4: Light-harvesting protein B-875 alpha chain



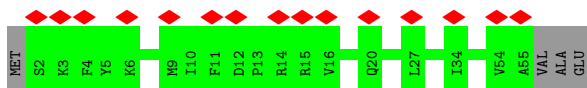
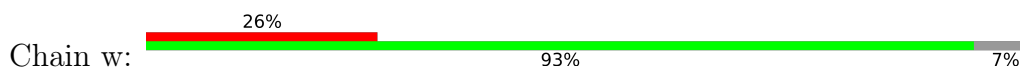
- Molecule 4: Light-harvesting protein B-875 alpha chain



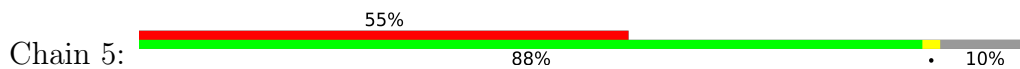
- Molecule 4: Light-harvesting protein B-875 alpha chain



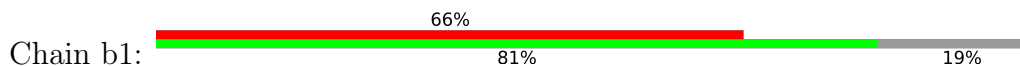
- Molecule 4: Light-harvesting protein B-875 alpha chain



- Molecule 4: Light-harvesting protein B-875 alpha chain

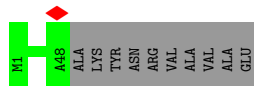
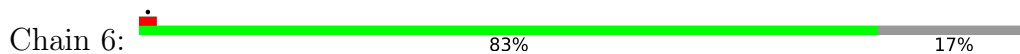


- Molecule 4: Light-harvesting protein B-875 alpha chain

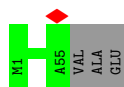




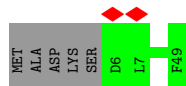
• Molecule 4: Light-harvesting protein B-875 alpha chain



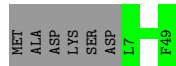
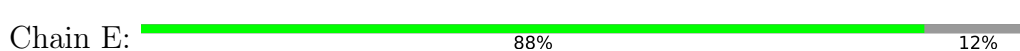
• Molecule 4: Light-harvesting protein B-875 alpha chain



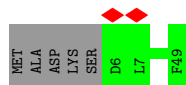
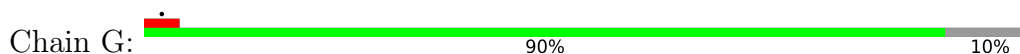
• Molecule 5: Light-harvesting protein B-875 beta chain



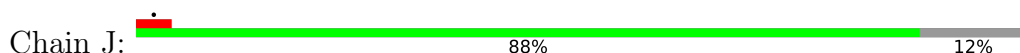
• Molecule 5: Light-harvesting protein B-875 beta chain



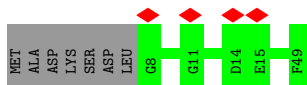
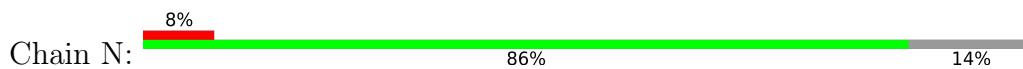
• Molecule 5: Light-harvesting protein B-875 beta chain



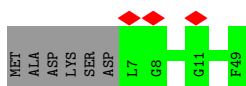
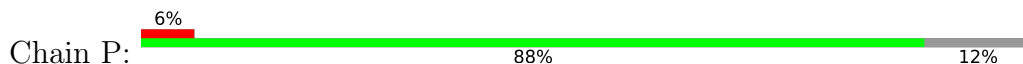
• Molecule 5: Light-harvesting protein B-875 beta chain



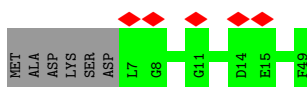
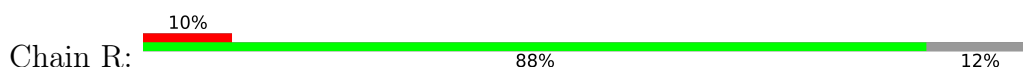
• Molecule 5: Light-harvesting protein B-875 beta chain



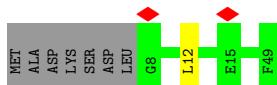
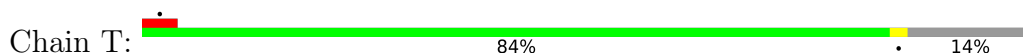
- Molecule 5: Light-harvesting protein B-875 beta chain



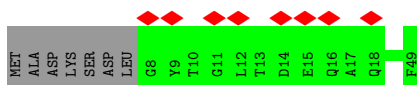
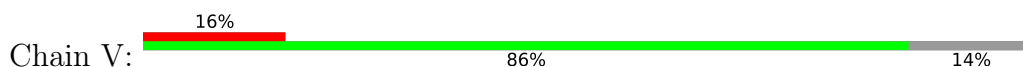
- Molecule 5: Light-harvesting protein B-875 beta chain



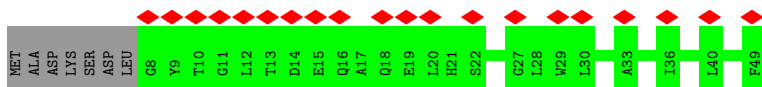
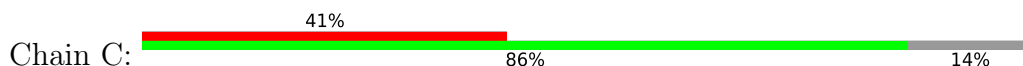
- Molecule 5: Light-harvesting protein B-875 beta chain



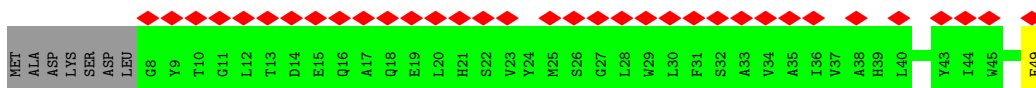
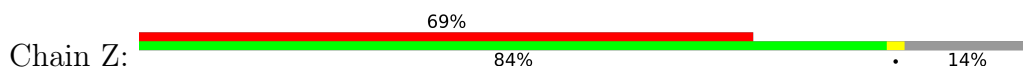
- Molecule 5: Light-harvesting protein B-875 beta chain



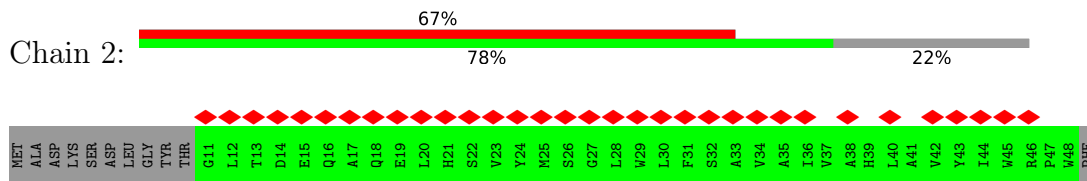
- Molecule 5: Light-harvesting protein B-875 beta chain



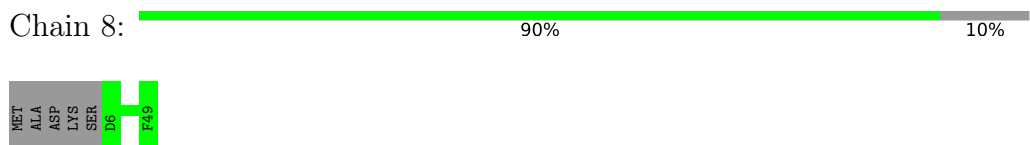
- Molecule 5: Light-harvesting protein B-875 beta chain



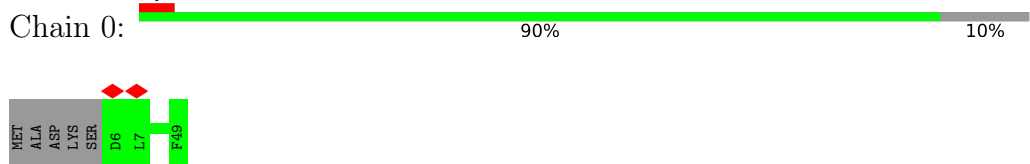
- Molecule 5: Light-harvesting protein B-875 beta chain



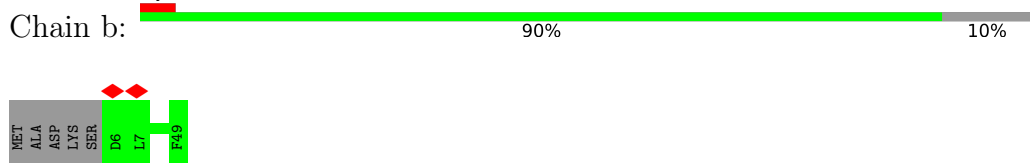
- Molecule 5: Light-harvesting protein B-875 beta chain



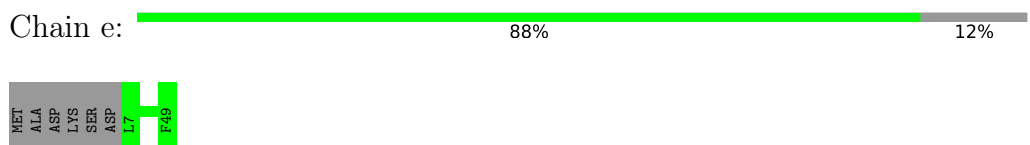
- Molecule 5: Light-harvesting protein B-875 beta chain



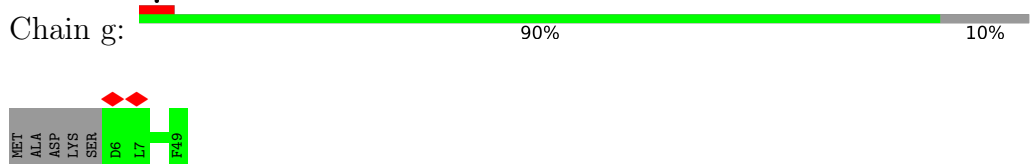
- Molecule 5: Light-harvesting protein B-875 beta chain



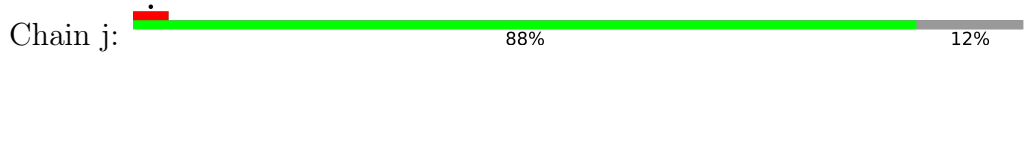
- Molecule 5: Light-harvesting protein B-875 beta chain

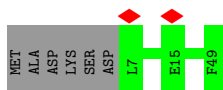


- Molecule 5: Light-harvesting protein B-875 beta chain

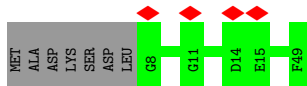
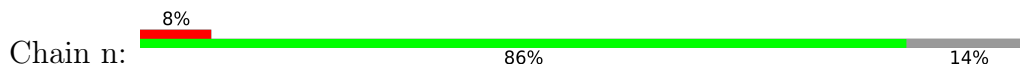


- Molecule 5: Light-harvesting protein B-875 beta chain

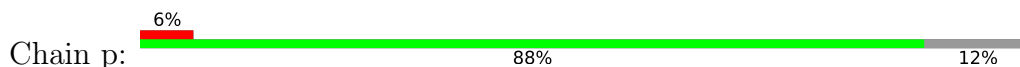




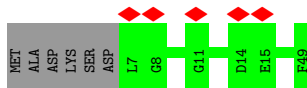
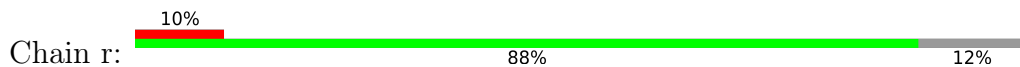
• Molecule 5: Light-harvesting protein B-875 beta chain



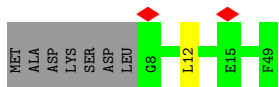
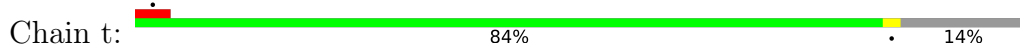
• Molecule 5: Light-harvesting protein B-875 beta chain



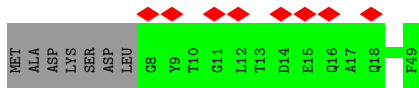
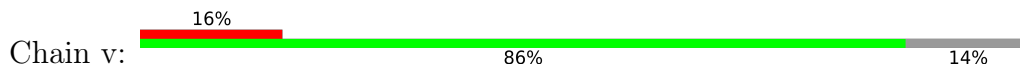
• Molecule 5: Light-harvesting protein B-875 beta chain



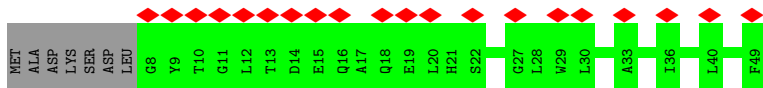
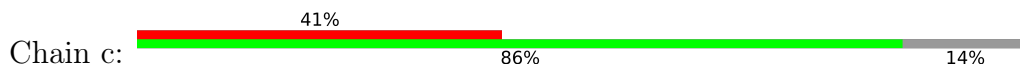
• Molecule 5: Light-harvesting protein B-875 beta chain



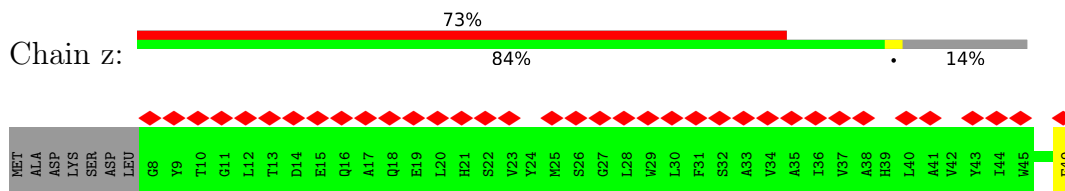
• Molecule 5: Light-harvesting protein B-875 beta chain



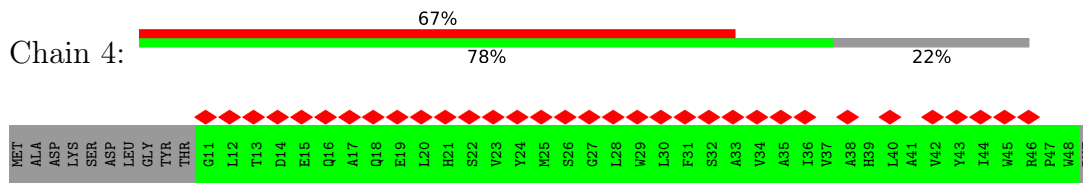
• Molecule 5: Light-harvesting protein B-875 beta chain



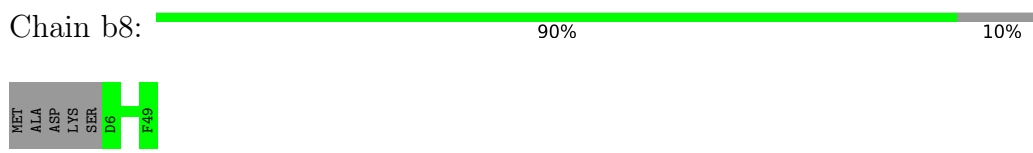
• Molecule 5: Light-harvesting protein B-875 beta chain



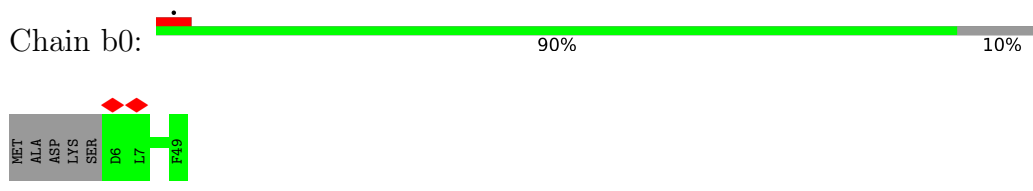
• Molecule 5: Light-harvesting protein B-875 beta chain



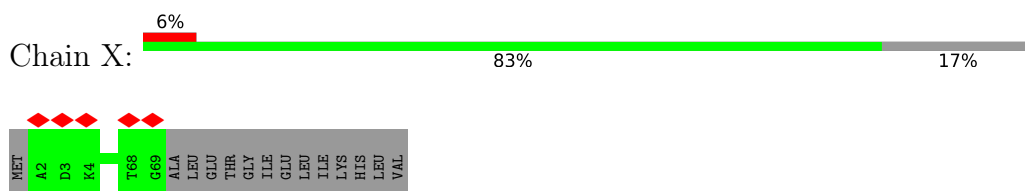
• Molecule 5: Light-harvesting protein B-875 beta chain



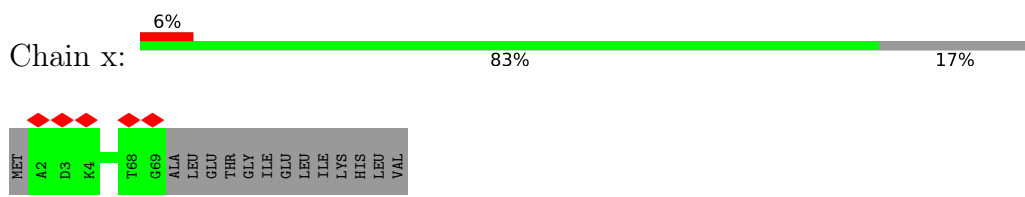
• Molecule 5: Light-harvesting protein B-875 beta chain



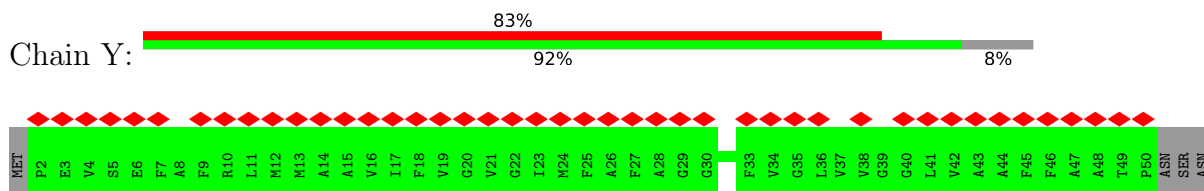
• Molecule 6: Intrinsic membrane protein PufX



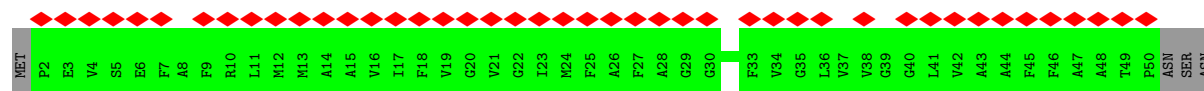
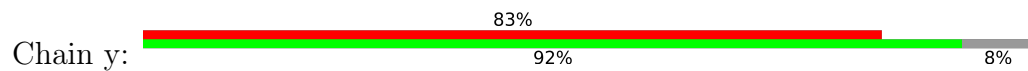
• Molecule 6: Intrinsic membrane protein PufX



• Molecule 7: Rsp_7571 Protein-Y PufY



• Molecule 7: Rsp_7571 Protein-Y PufY



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 145392 | 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 ($e^-/\text{\AA}^2$) | 60 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.196 | Depositor |
| Minimum map value | -0.092 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.02 | Depositor |
| Map size (\AA) | 432.63998, 432.63998, 432.63998 | wwPDB |
| Map dimensions | 416, 416, 416 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.04, 1.04, 1.04 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: U10, PC1, BCL, CDL, SPO, FE2, BPH

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 | L | 0.38 | 0/2320 | 0.45 | 0/3175 |
| 1 | l | 0.38 | 0/2320 | 0.45 | 0/3175 |
| 2 | M | 0.38 | 0/2538 | 0.45 | 0/3464 |
| 2 | m | 0.38 | 0/2538 | 0.45 | 0/3464 |
| 3 | H | 0.28 | 0/2024 | 0.46 | 0/2752 |
| 3 | h | 0.28 | 0/2024 | 0.46 | 0/2752 |
| 4 | 1 | 0.24 | 0/404 | 0.40 | 0/550 |
| 4 | 3 | 0.24 | 0/451 | 0.42 | 0/613 |
| 4 | 5 | 0.24 | 0/451 | 0.42 | 0/613 |
| 4 | 6 | 0.36 | 0/416 | 0.42 | 0/564 |
| 4 | 7 | 0.36 | 0/416 | 0.42 | 0/564 |
| 4 | 9 | 0.36 | 0/474 | 0.44 | 0/642 |
| 4 | A | 0.35 | 0/474 | 0.45 | 0/642 |
| 4 | D | 0.36 | 0/474 | 0.45 | 0/642 |
| 4 | F | 0.34 | 0/474 | 0.43 | 0/642 |
| 4 | I | 0.33 | 0/469 | 0.44 | 0/635 |
| 4 | K | 0.32 | 0/466 | 0.42 | 0/632 |
| 4 | O | 0.31 | 0/469 | 0.42 | 0/635 |
| 4 | Q | 0.31 | 0/474 | 0.43 | 0/642 |
| 4 | S | 0.32 | 0/474 | 0.43 | 0/642 |
| 4 | U | 0.27 | 0/461 | 0.42 | 0/625 |
| 4 | W | 0.26 | 0/466 | 0.40 | 0/632 |
| 4 | a | 0.35 | 0/474 | 0.45 | 0/642 |
| 4 | b1 | 0.24 | 0/404 | 0.40 | 0/550 |
| 4 | b9 | 0.36 | 0/474 | 0.44 | 0/642 |
| 4 | d | 0.36 | 0/474 | 0.45 | 0/642 |
| 4 | f | 0.35 | 0/474 | 0.43 | 0/642 |
| 4 | i | 0.33 | 0/469 | 0.44 | 0/635 |
| 4 | k | 0.32 | 0/466 | 0.42 | 0/632 |
| 4 | o | 0.31 | 0/469 | 0.42 | 0/635 |
| 4 | q | 0.31 | 0/474 | 0.43 | 0/642 |
| 4 | s | 0.32 | 0/474 | 0.43 | 0/642 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 4 | u | 0.27 | 0/461 | 0.42 | 0/625 |
| 4 | w | 0.26 | 0/466 | 0.40 | 0/632 |
| 5 | 0 | 0.34 | 0/373 | 0.40 | 0/510 |
| 5 | 2 | 0.23 | 0/320 | 0.34 | 0/439 |
| 5 | 4 | 0.23 | 0/320 | 0.34 | 0/439 |
| 5 | 8 | 0.33 | 0/373 | 0.39 | 0/510 |
| 5 | B | 0.33 | 0/373 | 0.39 | 0/510 |
| 5 | C | 0.26 | 0/357 | 0.38 | 0/488 |
| 5 | E | 0.32 | 0/365 | 0.43 | 0/499 |
| 5 | G | 0.31 | 0/373 | 0.39 | 0/510 |
| 5 | J | 0.27 | 0/365 | 0.39 | 0/499 |
| 5 | N | 0.29 | 0/357 | 0.37 | 0/488 |
| 5 | P | 0.35 | 0/365 | 0.39 | 0/499 |
| 5 | R | 0.30 | 0/365 | 0.38 | 0/499 |
| 5 | T | 0.28 | 0/357 | 0.40 | 0/488 |
| 5 | V | 0.27 | 0/357 | 0.39 | 0/488 |
| 5 | Z | 0.24 | 0/357 | 0.36 | 0/488 |
| 5 | b | 0.33 | 0/373 | 0.39 | 0/510 |
| 5 | b0 | 0.34 | 0/373 | 0.40 | 0/510 |
| 5 | b8 | 0.33 | 0/373 | 0.39 | 0/510 |
| 5 | c | 0.26 | 0/357 | 0.38 | 0/488 |
| 5 | e | 0.32 | 0/365 | 0.43 | 0/499 |
| 5 | g | 0.31 | 0/373 | 0.39 | 0/510 |
| 5 | j | 0.27 | 0/365 | 0.39 | 0/499 |
| 5 | n | 0.29 | 0/357 | 0.37 | 0/488 |
| 5 | p | 0.35 | 0/365 | 0.39 | 0/499 |
| 5 | r | 0.30 | 0/365 | 0.38 | 0/499 |
| 5 | t | 0.28 | 0/357 | 0.40 | 0/488 |
| 5 | v | 0.27 | 0/357 | 0.39 | 0/488 |
| 5 | z | 0.24 | 0/357 | 0.36 | 0/488 |
| 6 | X | 0.27 | 0/543 | 0.42 | 0/736 |
| 6 | x | 0.27 | 0/543 | 0.42 | 0/736 |
| 7 | Y | 0.27 | 0/373 | 0.39 | 0/505 |
| 7 | y | 0.27 | 0/373 | 0.38 | 0/505 |
| All | All | 0.32 | 0/38602 | 0.43 | 0/52570 |

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](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | L | 279/282 (99%) | 272 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | l | 279/282 (99%) | 272 (98%) | 7 (2%) | 0 | 100 | 100 |
| 2 | M | 305/308 (99%) | 299 (98%) | 6 (2%) | 0 | 100 | 100 |
| 2 | m | 305/308 (99%) | 299 (98%) | 6 (2%) | 0 | 100 | 100 |
| 3 | H | 258/260 (99%) | 252 (98%) | 6 (2%) | 0 | 100 | 100 |
| 3 | h | 258/260 (99%) | 252 (98%) | 6 (2%) | 0 | 100 | 100 |
| 4 | 1 | 45/58 (78%) | 45 (100%) | 0 | 0 | 100 | 100 |
| 4 | 3 | 50/58 (86%) | 49 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | 5 | 50/58 (86%) | 49 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | 6 | 46/58 (79%) | 44 (96%) | 2 (4%) | 0 | 100 | 100 |
| 4 | 7 | 46/58 (79%) | 44 (96%) | 2 (4%) | 0 | 100 | 100 |
| 4 | 9 | 53/58 (91%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | A | 53/58 (91%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | D | 53/58 (91%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | F | 53/58 (91%) | 51 (96%) | 2 (4%) | 0 | 100 | 100 |
| 4 | I | 52/58 (90%) | 51 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | K | 52/58 (90%) | 52 (100%) | 0 | 0 | 100 | 100 |
| 4 | O | 52/58 (90%) | 52 (100%) | 0 | 0 | 100 | 100 |
| 4 | Q | 53/58 (91%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |
| 4 | S | 53/58 (91%) | 53 (100%) | 0 | 0 | 100 | 100 |
| 4 | U | 51/58 (88%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 4 | W | 52/58 (90%) | 50 (96%) | 2 (4%) | 0 | 100 | 100 |
| 4 | a | 53/58 (91%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | b1 | 45/58 (78%) | 45 (100%) | 0 | 0 | 100 | 100 |
| 4 | b9 | 53/58 (91%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | d | 53/58 (91%) | 52 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | f | 53/58 (91%) | 51 (96%) | 2 (4%) | 0 | 100 | 100 |
| 4 | i | 52/58 (90%) | 51 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | k | 52/58 (90%) | 52 (100%) | 0 | 0 | 100 | 100 |
| 4 | o | 52/58 (90%) | 52 (100%) | 0 | 0 | 100 | 100 |
| 4 | q | 53/58 (91%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |
| 4 | s | 53/58 (91%) | 53 (100%) | 0 | 0 | 100 | 100 |
| 4 | u | 51/58 (88%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | w | 52/58 (90%) | 50 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | 0 | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | 2 | 36/49 (74%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 5 | 4 | 36/49 (74%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 5 | 8 | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 5 | B | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | C | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | E | 41/49 (84%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | G | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 5 | J | 41/49 (84%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | N | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | P | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 5 | R | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 5 | T | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | V | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | Z | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | b | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | b0 | 42/49 (86%) | 41 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | b8 | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 5 | c | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | e | 41/49 (84%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | g | 42/49 (86%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 5 | j | 41/49 (84%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| 5 | n | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | p | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 5 | r | 41/49 (84%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 5 | t | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | v | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 5 | z | 40/49 (82%) | 40 (100%) | 0 | 0 | 100 | 100 |
| 6 | X | 66/82 (80%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 6 | x | 66/82 (80%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 7 | Y | 47/53 (89%) | 47 (100%) | 0 | 0 | 100 | 100 |
| 7 | y | 47/53 (89%) | 47 (100%) | 0 | 0 | 100 | 100 |
| All | All | 4482/4966 (90%) | 4402 (98%) | 80 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | L | 220/221 (100%) | 217 (99%) | 3 (1%) | 67 | 80 |
| 1 | l | 220/221 (100%) | 217 (99%) | 3 (1%) | 67 | 80 |
| 2 | M | 240/241 (100%) | 237 (99%) | 3 (1%) | 69 | 82 |
| 2 | m | 240/241 (100%) | 237 (99%) | 3 (1%) | 69 | 82 |
| 3 | H | 208/208 (100%) | 206 (99%) | 2 (1%) | 76 | 85 |
| 3 | h | 208/208 (100%) | 206 (99%) | 2 (1%) | 76 | 85 |
| 4 | 1 | 42/51 (82%) | 42 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------|-----------|----------|-------------|-----|
| 4 | 3 | 46/51 (90%) | 45 (98%) | 1 (2%) | 52 | 71 |
| 4 | 5 | 46/51 (90%) | 45 (98%) | 1 (2%) | 52 | 71 |
| 4 | 6 | 44/51 (86%) | 44 (100%) | 0 | 100 | 100 |
| 4 | 7 | 44/51 (86%) | 44 (100%) | 0 | 100 | 100 |
| 4 | 9 | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | A | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | D | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | F | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | I | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | K | 48/51 (94%) | 48 (100%) | 0 | 100 | 100 |
| 4 | O | 49/51 (96%) | 48 (98%) | 1 (2%) | 55 | 72 |
| 4 | Q | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | S | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | U | 48/51 (94%) | 48 (100%) | 0 | 100 | 100 |
| 4 | W | 48/51 (94%) | 48 (100%) | 0 | 100 | 100 |
| 4 | a | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | b1 | 42/51 (82%) | 42 (100%) | 0 | 100 | 100 |
| 4 | b9 | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | d | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | f | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | i | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | k | 48/51 (94%) | 48 (100%) | 0 | 100 | 100 |
| 4 | o | 49/51 (96%) | 48 (98%) | 1 (2%) | 55 | 72 |
| 4 | q | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | s | 49/51 (96%) | 49 (100%) | 0 | 100 | 100 |
| 4 | u | 48/51 (94%) | 48 (100%) | 0 | 100 | 100 |
| 4 | w | 48/51 (94%) | 48 (100%) | 0 | 100 | 100 |
| 5 | 0 | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |
| 5 | 2 | 31/40 (78%) | 31 (100%) | 0 | 100 | 100 |
| 5 | 4 | 31/40 (78%) | 31 (100%) | 0 | 100 | 100 |
| 5 | 8 | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 5 | B | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |
| 5 | C | 34/40 (85%) | 34 (100%) | 0 | 100 | 100 |
| 5 | E | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | G | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |
| 5 | J | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | N | 34/40 (85%) | 34 (100%) | 0 | 100 | 100 |
| 5 | P | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | R | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | T | 34/40 (85%) | 33 (97%) | 1 (3%) | 42 | 62 |
| 5 | V | 34/40 (85%) | 34 (100%) | 0 | 100 | 100 |
| 5 | Z | 34/40 (85%) | 33 (97%) | 1 (3%) | 42 | 62 |
| 5 | b | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |
| 5 | b0 | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |
| 5 | b8 | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |
| 5 | c | 34/40 (85%) | 34 (100%) | 0 | 100 | 100 |
| 5 | e | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | g | 36/40 (90%) | 36 (100%) | 0 | 100 | 100 |
| 5 | j | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | n | 34/40 (85%) | 34 (100%) | 0 | 100 | 100 |
| 5 | p | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | r | 35/40 (88%) | 35 (100%) | 0 | 100 | 100 |
| 5 | t | 34/40 (85%) | 33 (97%) | 1 (3%) | 42 | 62 |
| 5 | v | 34/40 (85%) | 34 (100%) | 0 | 100 | 100 |
| 5 | z | 34/40 (85%) | 33 (97%) | 1 (3%) | 42 | 62 |
| 6 | X | 54/66 (82%) | 54 (100%) | 0 | 100 | 100 |
| 6 | x | 54/66 (82%) | 54 (100%) | 0 | 100 | 100 |
| 7 | Y | 33/37 (89%) | 33 (100%) | 0 | 100 | 100 |
| 7 | y | 33/37 (89%) | 33 (100%) | 0 | 100 | 100 |
| All | All | 3816/4094 (93%) | 3792 (99%) | 24 (1%) | 86 | 91 |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 216 | PHE |
| 1 | L | 247 | CYS |
| 1 | L | 272 | TRP |
| 2 | M | 197 | PHE |
| 2 | M | 214 | LEU |
| 2 | M | 216 | PHE |
| 3 | H | 202 | ARG |
| 3 | H | 231 | ASP |
| 4 | O | 11 | PHE |
| 5 | T | 12 | LEU |
| 4 | 3 | 23 | PHE |
| 5 | Z | 49 | PHE |
| 1 | l | 216 | PHE |
| 1 | l | 247 | CYS |
| 1 | l | 272 | TRP |
| 2 | m | 197 | PHE |
| 2 | m | 214 | LEU |
| 2 | m | 216 | PHE |
| 3 | h | 202 | ARG |
| 3 | h | 231 | ASP |
| 4 | o | 11 | PHE |
| 5 | t | 12 | LEU |
| 4 | 5 | 23 | PHE |
| 5 | z | 49 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | M | 307 | ASN |
| 3 | H | 35 | ASN |
| 2 | m | 299 | GLN |
| 2 | m | 307 | ASN |
| 3 | h | 35 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 148 ligands modelled in this entry, 2 are monoatomic - leaving 146 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 |
| 8 | BCL | T | 101 | - | 58,74,74 | 1.20 | 3 (5%) | 69,115,115 | 1.39 | 12 (17%) |
| 8 | BCL | g | 102 | - | 58,74,74 | 1.21 | 3 (5%) | 69,115,115 | 1.45 | 11 (15%) |
| 8 | BCL | 1 | 101 | - | 38,54,74 | 1.47 | 4 (10%) | 45,91,115 | 1.58 | 9 (20%) |
| 8 | BCL | 3 | 101 | - | 43,59,74 | 1.46 | 5 (11%) | 51,97,115 | 1.61 | 11 (21%) |
| 13 | SPO | g | 101 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.29 | 0 |
| 13 | SPO | q | 104 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.31 | 0 |
| 13 | SPO | g | 103 | - | 40,41,41 | 0.18 | 0 | 47,50,50 | 0.39 | 0 |
| 8 | BCL | L | 302 | - | 55,71,74 | 1.21 | 4 (7%) | 65,111,115 | 1.40 | 10 (15%) |
| 8 | BCL | c | 101 | - | 53,69,74 | 1.26 | 3 (5%) | 63,109,115 | 1.36 | 10 (15%) |
| 11 | PC1 | d | 101 | - | 38,38,53 | 1.18 | 4 (10%) | 44,46,61 | 1.19 | 3 (6%) |
| 11 | PC1 | A | 104 | - | 30,30,53 | 1.31 | 4 (13%) | 36,38,61 | 1.19 | 3 (8%) |
| 13 | SPO | E | 101 | - | 40,41,41 | 0.29 | 0 | 47,50,50 | 0.28 | 0 |
| 8 | BCL | 6 | 101 | - | 53,69,74 | 1.22 | 3 (5%) | 63,109,115 | 1.52 | 13 (20%) |
| 13 | SPO | u | 103 | - | 40,41,41 | 0.17 | 0 | 47,50,50 | 0.39 | 0 |
| 10 | U10 | l | 304 | - | 38,38,63 | 2.63 | 12 (31%) | 46,49,79 | 1.74 | 12 (26%) |
| 13 | SPO | o | 102 | - | 40,41,41 | 0.27 | 0 | 47,50,50 | 0.43 | 0 |
| 13 | SPO | A | 102 | - | 40,41,41 | 0.30 | 0 | 47,50,50 | 0.34 | 0 |
| 8 | BCL | U | 101 | - | 58,74,74 | 1.21 | 3 (5%) | 69,115,115 | 1.41 | 11 (15%) |
| 10 | U10 | L | 304 | - | 38,38,63 | 2.63 | 12 (31%) | 46,49,79 | 1.74 | 12 (26%) |
| 8 | BCL | I | 101 | - | 58,74,74 | 1.17 | 4 (6%) | 69,115,115 | 1.45 | 10 (14%) |
| 8 | BCL | Z | 101 | - | 48,64,74 | 1.35 | 3 (6%) | 57,103,115 | 1.37 | 8 (14%) |
| 9 | BPH | L | 303 | - | 51,70,70 | 0.95 | 1 (1%) | 52,101,101 | 1.28 | 6 (11%) |
| 8 | BCL | G | 102 | - | 58,74,74 | 1.21 | 3 (5%) | 69,115,115 | 1.45 | 12 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 13 | SPO | G | 101 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.29 | 0 |
| 11 | PC1 | D | 101 | - | 38,38,53 | 1.18 | 4 (10%) | 44,46,61 | 1.19 | 3 (6%) |
| 8 | BCL | m | 403 | - | 58,74,74 | 1.20 | 6 (10%) | 69,115,115 | 1.47 | 10 (14%) |
| 13 | SPO | s | 102 | - | 40,41,41 | 0.23 | 0 | 47,50,50 | 0.30 | 0 |
| 13 | SPO | G | 103 | - | 40,41,41 | 0.18 | 0 | 47,50,50 | 0.39 | 0 |
| 8 | BCL | s | 101 | - | 58,74,74 | 1.21 | 4 (6%) | 69,115,115 | 1.48 | 12 (17%) |
| 8 | BCL | K | 101 | - | 58,74,74 | 1.20 | 4 (6%) | 69,115,115 | 1.43 | 12 (17%) |
| 13 | SPO | C | 102 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.44 | 0 |
| 13 | SPO | x | 101 | - | 40,41,41 | 0.28 | 0 | 47,50,50 | 0.44 | 0 |
| 13 | SPO | S | 103 | - | 40,41,41 | 0.26 | 0 | 47,50,50 | 0.35 | 0 |
| 8 | BCL | a | 101 | - | 58,74,74 | 1.18 | 4 (6%) | 69,115,115 | 1.47 | 11 (15%) |
| 8 | BCL | L | 301 | - | 58,74,74 | 1.20 | 4 (6%) | 69,115,115 | 1.45 | 11 (15%) |
| 8 | BCL | M | 402 | - | 58,74,74 | 1.17 | 3 (5%) | 69,115,115 | 1.42 | 10 (14%) |
| 13 | SPO | U | 102 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.42 | 0 |
| 13 | SPO | P | 101 | - | 40,41,41 | 0.19 | 0 | 47,50,50 | 0.32 | 0 |
| 8 | BCL | n | 102 | - | 58,74,74 | 1.20 | 3 (5%) | 69,115,115 | 1.41 | 11 (15%) |
| 13 | SPO | D | 103 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.32 | 0 |
| 8 | BCL | 2 | 101 | - | 38,54,74 | 1.47 | 4 (10%) | 45,91,115 | 1.50 | 8 (17%) |
| 13 | SPO | 5 | 103 | - | 40,41,41 | 0.17 | 0 | 47,50,50 | 0.32 | 0 |
| 8 | BCL | q | 101 | - | 58,74,74 | 1.20 | 3 (5%) | 69,115,115 | 1.51 | 13 (18%) |
| 8 | BCL | o | 101 | - | 58,74,74 | 1.17 | 3 (5%) | 69,115,115 | 1.41 | 11 (15%) |
| 13 | SPO | p | 101 | - | 40,41,41 | 0.19 | 0 | 47,50,50 | 0.33 | 0 |
| 8 | BCL | W | 101 | - | 58,74,74 | 1.17 | 3 (5%) | 69,115,115 | 1.42 | 11 (15%) |
| 8 | BCL | z | 101 | - | 48,64,74 | 1.35 | 3 (6%) | 57,103,115 | 1.37 | 8 (14%) |
| 8 | BCL | 5 | 101 | - | 43,59,74 | 1.46 | 5 (11%) | 51,97,115 | 1.61 | 11 (21%) |
| 13 | SPO | m | 406 | - | 40,41,41 | 0.29 | 0 | 47,50,50 | 0.48 | 1 (2%) |
| 11 | PC1 | A | 105 | - | 37,37,53 | 0.57 | 0 | 43,45,61 | 0.60 | 1 (2%) |
| 11 | PC1 | a | 104 | - | 30,30,53 | 1.32 | 4 (13%) | 36,38,61 | 1.19 | 3 (8%) |
| 13 | SPO | B | 102 | - | 40,41,41 | 0.27 | 0 | 47,50,50 | 0.30 | 0 |
| 13 | SPO | b0 | 102 | - | 40,41,41 | 0.25 | 0 | 47,50,50 | 0.33 | 0 |
| 8 | BCL | b0 | 101 | - | 53,69,74 | 1.22 | 3 (5%) | 63,109,115 | 1.63 | 13 (20%) |
| 13 | SPO | n | 101 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.32 | 0 |
| 8 | BCL | E | 102 | - | 58,74,74 | 1.19 | 3 (5%) | 69,115,115 | 1.43 | 13 (18%) |
| 8 | BCL | B | 101 | - | 58,74,74 | 1.18 | 3 (5%) | 69,115,115 | 1.54 | 12 (17%) |
| 13 | SPO | u | 102 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.42 | 0 |
| 13 | SPO | e | 101 | - | 40,41,41 | 0.29 | 0 | 47,50,50 | 0.28 | 0 |
| 8 | BCL | l | 302 | - | 55,71,74 | 1.21 | 4 (7%) | 65,111,115 | 1.40 | 10 (15%) |
| 13 | SPO | Q | 103 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.50 | 1 (2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 8 | BCL | D | 102 | - | 58,74,74 | 1.21 | 4 (6%) | 69,115,115 | 1.46 | 11 (15%) |
| 14 | CDL | f | 102 | - | 62,62,99 | 1.14 | 8 (12%) | 68,74,111 | 1.25 | 6 (8%) |
| 8 | BCL | m | 402 | - | 58,74,74 | 1.17 | 3 (5%) | 69,115,115 | 1.42 | 10 (14%) |
| 8 | BCL | 6 | 102 | - | 53,69,74 | 1.20 | 3 (5%) | 63,109,115 | 1.55 | 12 (19%) |
| 8 | BCL | 4 | 101 | - | 38,54,74 | 1.47 | 4 (10%) | 45,91,115 | 1.50 | 8 (17%) |
| 13 | SPO | S | 102 | - | 40,41,41 | 0.23 | 0 | 47,50,50 | 0.30 | 0 |
| 8 | BCL | 0 | 101 | - | 53,69,74 | 1.22 | 3 (5%) | 63,109,115 | 1.63 | 13 (20%) |
| 10 | U10 | M | 405 | - | 48,48,63 | 2.65 | 14 (29%) | 58,61,79 | 1.73 | 15 (25%) |
| 8 | BCL | r | 101 | - | 58,74,74 | 1.18 | 3 (5%) | 69,115,115 | 1.33 | 10 (14%) |
| 8 | BCL | b1 | 101 | - | 38,54,74 | 1.47 | 4 (10%) | 45,91,115 | 1.59 | 9 (20%) |
| 13 | SPO | e | 103 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.38 | 0 |
| 8 | BCL | u | 101 | - | 58,74,74 | 1.21 | 3 (5%) | 69,115,115 | 1.41 | 11 (15%) |
| 13 | SPO | X | 101 | - | 40,41,41 | 0.28 | 0 | 47,50,50 | 0.44 | 0 |
| 13 | SPO | b9 | 102 | - | 40,41,41 | 0.31 | 0 | 47,50,50 | 0.35 | 0 |
| 11 | PC1 | h | 302 | - | 33,33,53 | 1.26 | 4 (12%) | 39,41,61 | 1.09 | 3 (7%) |
| 13 | SPO | O | 102 | - | 40,41,41 | 0.27 | 0 | 47,50,50 | 0.43 | 0 |
| 13 | SPO | b | 102 | - | 40,41,41 | 0.27 | 0 | 47,50,50 | 0.30 | 0 |
| 13 | SPO | E | 103 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.38 | 0 |
| 13 | SPO | 9 | 102 | - | 40,41,41 | 0.31 | 0 | 47,50,50 | 0.35 | 0 |
| 8 | BCL | 7 | 102 | - | 53,69,74 | 1.20 | 3 (5%) | 63,109,115 | 1.55 | 12 (19%) |
| 11 | PC1 | a | 105 | - | 37,37,53 | 0.57 | 0 | 43,45,61 | 0.60 | 1 (2%) |
| 14 | CDL | m | 407 | - | 81,81,99 | 1.02 | 9 (11%) | 87,93,111 | 1.19 | 6 (6%) |
| 8 | BCL | t | 101 | - | 58,74,74 | 1.20 | 3 (5%) | 69,115,115 | 1.39 | 12 (17%) |
| 13 | SPO | s | 103 | - | 40,41,41 | 0.26 | 0 | 47,50,50 | 0.35 | 0 |
| 13 | SPO | d | 103 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.32 | 0 |
| 8 | BCL | M | 403 | - | 58,74,74 | 1.20 | 6 (10%) | 69,115,115 | 1.47 | 10 (14%) |
| 8 | BCL | C | 101 | - | 53,69,74 | 1.26 | 3 (5%) | 63,109,115 | 1.36 | 10 (15%) |
| 8 | BCL | w | 101 | - | 58,74,74 | 1.17 | 3 (5%) | 69,115,115 | 1.42 | 11 (15%) |
| 14 | CDL | M | 407 | - | 81,81,99 | 1.02 | 9 (11%) | 87,93,111 | 1.19 | 6 (6%) |
| 8 | BCL | V | 101 | - | 58,74,74 | 1.21 | 3 (5%) | 69,115,115 | 1.42 | 12 (17%) |
| 9 | BPH | l | 303 | - | 51,70,70 | 0.95 | 1 (1%) | 52,101,101 | 1.28 | 6 (11%) |
| 13 | SPO | j | 102 | - | 40,41,41 | 0.16 | 0 | 47,50,50 | 0.30 | 0 |
| 8 | BCL | O | 101 | - | 58,74,74 | 1.17 | 3 (5%) | 69,115,115 | 1.41 | 11 (15%) |
| 8 | BCL | R | 101 | - | 58,74,74 | 1.18 | 3 (5%) | 69,115,115 | 1.33 | 10 (14%) |
| 11 | PC1 | h | 301 | - | 42,42,53 | 1.12 | 5 (11%) | 48,50,61 | 1.16 | 3 (6%) |
| 8 | BCL | p | 102 | - | 58,74,74 | 1.19 | 3 (5%) | 69,115,115 | 1.42 | 11 (15%) |
| 10 | U10 | m | 405 | - | 48,48,63 | 2.65 | 14 (29%) | 58,61,79 | 1.73 | 15 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 13 | SPO | 3 | 103 | - | 40,41,41 | 0.17 | 0 | 47,50,50 | 0.32 | 0 |
| 8 | BCL | i | 101 | - | 58,74,74 | 1.18 | 4 (6%) | 69,115,115 | 1.45 | 10 (14%) |
| 8 | BCL | f | 101 | - | 58,74,74 | 1.21 | 3 (5%) | 69,115,115 | 1.47 | 11 (15%) |
| 13 | SPO | 0 | 102 | - | 40,41,41 | 0.25 | 0 | 47,50,50 | 0.33 | 0 |
| 11 | PC1 | A | 103 | - | 44,44,53 | 1.09 | 4 (9%) | 50,52,61 | 1.20 | 3 (6%) |
| 13 | SPO | I | 102 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.33 | 0 |
| 8 | BCL | J | 101 | - | 58,74,74 | 1.19 | 3 (5%) | 69,115,115 | 1.38 | 10 (14%) |
| 8 | BCL | k | 101 | - | 58,74,74 | 1.20 | 4 (6%) | 69,115,115 | 1.43 | 12 (17%) |
| 13 | SPO | Q | 102 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.31 | 0 |
| 8 | BCL | Q | 101 | - | 58,74,74 | 1.20 | 3 (5%) | 69,115,115 | 1.51 | 13 (18%) |
| 13 | SPO | J | 102 | - | 40,41,41 | 0.16 | 0 | 47,50,50 | 0.30 | 0 |
| 13 | SPO | 3 | 102 | - | 40,41,41 | 0.17 | 0 | 47,50,50 | 0.37 | 0 |
| 13 | SPO | Q | 104 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.31 | 0 |
| 9 | BPH | m | 404 | - | 41,60,70 | 1.08 | 3 (7%) | 40,89,101 | 1.16 | 4 (10%) |
| 13 | SPO | a | 102 | - | 40,41,41 | 0.30 | 0 | 47,50,50 | 0.34 | 0 |
| 8 | BCL | v | 101 | - | 58,74,74 | 1.20 | 3 (5%) | 69,115,115 | 1.42 | 12 (17%) |
| 8 | BCL | b | 101 | - | 58,74,74 | 1.18 | 3 (5%) | 69,115,115 | 1.54 | 12 (17%) |
| 13 | SPO | M | 406 | - | 40,41,41 | 0.29 | 0 | 47,50,50 | 0.48 | 1 (2%) |
| 8 | BCL | 7 | 101 | - | 53,69,74 | 1.22 | 3 (5%) | 63,109,115 | 1.53 | 13 (20%) |
| 13 | SPO | q | 103 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.50 | 1 (2%) |
| 8 | BCL | e | 102 | - | 58,74,74 | 1.19 | 3 (5%) | 69,115,115 | 1.43 | 13 (18%) |
| 8 | BCL | S | 101 | - | 58,74,74 | 1.21 | 4 (6%) | 69,115,115 | 1.48 | 12 (17%) |
| 9 | BPH | M | 404 | - | 41,60,70 | 1.08 | 3 (7%) | 40,89,101 | 1.16 | 4 (10%) |
| 8 | BCL | F | 101 | - | 58,74,74 | 1.21 | 3 (5%) | 69,115,115 | 1.47 | 11 (15%) |
| 11 | PC1 | L | 307 | - | 39,39,53 | 1.13 | 4 (10%) | 45,47,61 | 1.12 | 3 (6%) |
| 13 | SPO | i | 102 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.33 | 0 |
| 8 | BCL | A | 101 | - | 58,74,74 | 1.18 | 4 (6%) | 69,115,115 | 1.47 | 11 (15%) |
| 13 | SPO | q | 102 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.31 | 0 |
| 8 | BCL | l | 301 | - | 58,74,74 | 1.20 | 4 (6%) | 69,115,115 | 1.45 | 11 (15%) |
| 8 | BCL | P | 102 | - | 58,74,74 | 1.19 | 3 (5%) | 69,115,115 | 1.42 | 11 (15%) |
| 13 | SPO | N | 101 | - | 40,41,41 | 0.20 | 0 | 47,50,50 | 0.32 | 0 |
| 8 | BCL | j | 101 | - | 58,74,74 | 1.19 | 3 (5%) | 69,115,115 | 1.38 | 10 (14%) |
| 8 | BCL | b9 | 101 | - | 58,74,74 | 1.18 | 4 (6%) | 69,115,115 | 1.48 | 11 (15%) |
| 11 | PC1 | H | 302 | - | 33,33,53 | 1.26 | 4 (12%) | 39,41,61 | 1.09 | 3 (7%) |
| 8 | BCL | N | 102 | - | 58,74,74 | 1.20 | 3 (5%) | 69,115,115 | 1.41 | 11 (15%) |
| 8 | BCL | d | 102 | - | 58,74,74 | 1.21 | 4 (6%) | 69,115,115 | 1.46 | 11 (15%) |
| 13 | SPO | 5 | 102 | - | 40,41,41 | 0.17 | 0 | 47,50,50 | 0.37 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 10 | U10 | L | 305 | - | 43,43,63 | 2.68 | 13 (30%) | 52,55,79 | 1.76 | 13 (25%) |
| 14 | CDL | F | 102 | - | 62,62,99 | 1.14 | 8 (12%) | 68,74,111 | 1.26 | 6 (8%) |
| 11 | PC1 | H | 301 | - | 42,42,53 | 1.12 | 5 (11%) | 48,50,61 | 1.16 | 3 (6%) |
| 11 | PC1 | l | 306 | - | 38,38,53 | 1.15 | 4 (10%) | 44,46,61 | 1.19 | 3 (6%) |
| 13 | SPO | U | 103 | - | 40,41,41 | 0.17 | 0 | 47,50,50 | 0.39 | 0 |
| 8 | BCL | 9 | 101 | - | 58,74,74 | 1.18 | 4 (6%) | 69,115,115 | 1.48 | 11 (15%) |
| 11 | PC1 | l | 307 | - | 39,39,53 | 1.14 | 4 (10%) | 45,47,61 | 1.12 | 3 (6%) |
| 10 | U10 | l | 305 | - | 43,43,63 | 2.68 | 13 (30%) | 52,55,79 | 1.76 | 13 (25%) |
| 11 | PC1 | L | 306 | - | 38,38,53 | 1.15 | 4 (10%) | 44,46,61 | 1.19 | 3 (6%) |
| 13 | SPO | c | 102 | - | 40,41,41 | 0.22 | 0 | 47,50,50 | 0.44 | 0 |
| 11 | PC1 | a | 103 | - | 44,44,53 | 1.09 | 4 (9%) | 50,52,61 | 1.20 | 3 (6%) |

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 |
|-----|------|-------|-----|------|---------|--------------|---------|
| 8 | BCL | T | 101 | - | - | 4/37/137/137 | - |
| 8 | BCL | g | 102 | - | - | 1/37/137/137 | - |
| 8 | BCL | l | 101 | - | - | 2/13/113/137 | - |
| 8 | BCL | 3 | 101 | - | - | 0/19/119/137 | - |
| 13 | SPO | g | 101 | - | - | 12/47/47/47 | - |
| 13 | SPO | q | 104 | - | - | 12/47/47/47 | - |
| 13 | SPO | g | 103 | - | - | 11/47/47/47 | - |
| 8 | BCL | L | 302 | - | - | 0/34/134/137 | - |
| 8 | BCL | c | 101 | - | - | 4/31/131/137 | - |
| 11 | PC1 | d | 101 | - | - | 13/42/42/57 | - |
| 11 | PC1 | A | 104 | - | - | 17/34/34/57 | - |
| 13 | SPO | E | 101 | - | - | 11/47/47/47 | - |
| 8 | BCL | 6 | 101 | - | - | 6/31/131/137 | - |
| 13 | SPO | u | 103 | - | - | 9/47/47/47 | - |
| 10 | U10 | l | 304 | - | - | 14/33/57/87 | 0/1/1/1 |
| 13 | SPO | o | 102 | - | - | 15/47/47/47 | - |
| 13 | SPO | A | 102 | - | - | 12/47/47/47 | - |
| 8 | BCL | U | 101 | - | - | 0/37/137/137 | - |
| 10 | U10 | L | 304 | - | - | 14/33/57/87 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|---------|
| 8 | BCL | I | 101 | - | - | 2/37/137/137 | - |
| 8 | BCL | Z | 101 | - | - | 4/25/125/137 | - |
| 9 | BPH | L | 303 | - | - | 2/37/105/105 | 0/5/6/6 |
| 8 | BCL | G | 102 | - | - | 1/37/137/137 | - |
| 13 | SPO | G | 101 | - | - | 12/47/47/47 | - |
| 11 | PC1 | D | 101 | - | - | 13/42/42/57 | - |
| 8 | BCL | m | 403 | - | - | 1/37/137/137 | - |
| 13 | SPO | s | 102 | - | - | 14/47/47/47 | - |
| 13 | SPO | G | 103 | - | - | 11/47/47/47 | - |
| 8 | BCL | s | 101 | - | - | 0/37/137/137 | - |
| 8 | BCL | K | 101 | - | - | 1/37/137/137 | - |
| 13 | SPO | C | 102 | - | - | 16/47/47/47 | - |
| 13 | SPO | x | 101 | - | - | 9/47/47/47 | - |
| 13 | SPO | S | 103 | - | - | 9/47/47/47 | - |
| 8 | BCL | a | 101 | - | - | 3/37/137/137 | - |
| 8 | BCL | L | 301 | - | - | 0/37/137/137 | - |
| 8 | BCL | M | 402 | - | - | 4/37/137/137 | - |
| 13 | SPO | U | 102 | - | - | 7/47/47/47 | - |
| 13 | SPO | P | 101 | - | - | 12/47/47/47 | - |
| 8 | BCL | n | 102 | - | - | 5/37/137/137 | - |
| 13 | SPO | D | 103 | - | - | 15/47/47/47 | - |
| 8 | BCL | 2 | 101 | - | - | 2/13/113/137 | - |
| 13 | SPO | 5 | 103 | - | - | 13/47/47/47 | - |
| 8 | BCL | q | 101 | - | - | 4/37/137/137 | - |
| 8 | BCL | o | 101 | - | - | 0/37/137/137 | - |
| 13 | SPO | p | 101 | - | - | 12/47/47/47 | - |
| 8 | BCL | W | 101 | - | - | 0/37/137/137 | - |
| 8 | BCL | z | 101 | - | - | 4/25/125/137 | - |
| 8 | BCL | 5 | 101 | - | - | 0/19/119/137 | - |
| 13 | SPO | m | 406 | - | - | 9/47/47/47 | - |
| 11 | PC1 | A | 105 | - | - | 18/41/41/57 | - |
| 11 | PC1 | a | 104 | - | - | 17/34/34/57 | - |
| 13 | SPO | B | 102 | - | - | 14/47/47/47 | - |
| 13 | SPO | b0 | 102 | - | - | 14/47/47/47 | - |
| 8 | BCL | b0 | 101 | - | - | 3/31/131/137 | - |
| 13 | SPO | n | 101 | - | - | 10/47/47/47 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|---------|
| 8 | BCL | E | 102 | - | - | 6/37/137/137 | - |
| 8 | BCL | B | 101 | - | - | 5/37/137/137 | - |
| 13 | SPO | u | 102 | - | - | 7/47/47/47 | - |
| 13 | SPO | e | 101 | - | - | 11/47/47/47 | - |
| 8 | BCL | l | 302 | - | - | 0/34/134/137 | - |
| 13 | SPO | Q | 103 | - | - | 12/47/47/47 | - |
| 8 | BCL | D | 102 | - | - | 3/37/137/137 | - |
| 14 | CDL | f | 102 | - | - | 29/73/73/110 | - |
| 8 | BCL | m | 402 | - | - | 4/37/137/137 | - |
| 8 | BCL | 6 | 102 | - | - | 7/31/131/137 | - |
| 8 | BCL | 4 | 101 | - | - | 2/13/113/137 | - |
| 13 | SPO | S | 102 | - | - | 14/47/47/47 | - |
| 8 | BCL | 0 | 101 | - | - | 3/31/131/137 | - |
| 10 | U10 | M | 405 | - | - | 10/45/69/87 | 0/1/1/1 |
| 8 | BCL | r | 101 | - | - | 5/37/137/137 | - |
| 8 | BCL | b1 | 101 | - | - | 2/13/113/137 | - |
| 13 | SPO | e | 103 | - | - | 16/47/47/47 | - |
| 8 | BCL | u | 101 | - | - | 0/37/137/137 | - |
| 13 | SPO | X | 101 | - | - | 9/47/47/47 | - |
| 13 | SPO | b9 | 102 | - | - | 14/47/47/47 | - |
| 11 | PC1 | h | 302 | - | - | 13/37/37/57 | - |
| 13 | SPO | O | 102 | - | - | 15/47/47/47 | - |
| 13 | SPO | b | 102 | - | - | 14/47/47/47 | - |
| 13 | SPO | E | 103 | - | - | 16/47/47/47 | - |
| 13 | SPO | 9 | 102 | - | - | 14/47/47/47 | - |
| 8 | BCL | 7 | 102 | - | - | 7/31/131/137 | - |
| 11 | PC1 | a | 105 | - | - | 18/41/41/57 | - |
| 14 | CDL | m | 407 | - | - | 27/92/92/110 | - |
| 8 | BCL | t | 101 | - | - | 4/37/137/137 | - |
| 13 | SPO | s | 103 | - | - | 9/47/47/47 | - |
| 13 | SPO | d | 103 | - | - | 15/47/47/47 | - |
| 8 | BCL | M | 403 | - | - | 1/37/137/137 | - |
| 8 | BCL | C | 101 | - | - | 4/31/131/137 | - |
| 8 | BCL | w | 101 | - | - | 0/37/137/137 | - |
| 14 | CDL | M | 407 | - | - | 27/92/92/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|---------|
| 8 | BCL | V | 101 | - | - | 4/37/137/137 | - |
| 9 | BPH | l | 303 | - | - | 2/37/105/105 | 0/5/6/6 |
| 13 | SPO | j | 102 | - | - | 13/47/47/47 | - |
| 8 | BCL | O | 101 | - | - | 0/37/137/137 | - |
| 8 | BCL | R | 101 | - | - | 4/37/137/137 | - |
| 11 | PC1 | h | 301 | - | - | 12/46/46/57 | - |
| 8 | BCL | p | 102 | - | - | 4/37/137/137 | - |
| 10 | U10 | m | 405 | - | - | 10/45/69/87 | 0/1/1/1 |
| 13 | SPO | 3 | 103 | - | - | 13/47/47/47 | - |
| 8 | BCL | i | 101 | - | - | 2/37/137/137 | - |
| 8 | BCL | f | 101 | - | - | 2/37/137/137 | - |
| 13 | SPO | 0 | 102 | - | - | 14/47/47/47 | - |
| 11 | PC1 | A | 103 | - | - | 17/48/48/57 | - |
| 13 | SPO | I | 102 | - | - | 13/47/47/47 | - |
| 8 | BCL | J | 101 | - | - | 5/37/137/137 | - |
| 8 | BCL | k | 101 | - | - | 1/37/137/137 | - |
| 13 | SPO | Q | 102 | - | - | 8/47/47/47 | - |
| 8 | BCL | Q | 101 | - | - | 4/37/137/137 | - |
| 13 | SPO | J | 102 | - | - | 13/47/47/47 | - |
| 13 | SPO | 3 | 102 | - | - | 13/47/47/47 | - |
| 13 | SPO | Q | 104 | - | - | 12/47/47/47 | - |
| 9 | BPH | m | 404 | - | - | 4/25/93/105 | 0/5/6/6 |
| 13 | SPO | a | 102 | - | - | 12/47/47/47 | - |
| 8 | BCL | v | 101 | - | - | 4/37/137/137 | - |
| 8 | BCL | b | 101 | - | - | 5/37/137/137 | - |
| 13 | SPO | M | 406 | - | - | 9/47/47/47 | - |
| 8 | BCL | 7 | 101 | - | - | 6/31/131/137 | - |
| 13 | SPO | q | 103 | - | - | 12/47/47/47 | - |
| 8 | BCL | e | 102 | - | - | 6/37/137/137 | - |
| 8 | BCL | S | 101 | - | - | 0/37/137/137 | - |
| 9 | BPH | M | 404 | - | - | 4/25/93/105 | 0/5/6/6 |
| 8 | BCL | F | 101 | - | - | 2/37/137/137 | - |
| 11 | PC1 | L | 307 | - | - | 19/43/43/57 | - |
| 13 | SPO | i | 102 | - | - | 13/47/47/47 | - |
| 8 | BCL | A | 101 | - | - | 3/37/137/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|---------|
| 13 | SPO | q | 102 | - | - | 8/47/47/47 | - |
| 8 | BCL | l | 301 | - | - | 0/37/137/137 | - |
| 8 | BCL | P | 102 | - | - | 4/37/137/137 | - |
| 13 | SPO | N | 101 | - | - | 10/47/47/47 | - |
| 8 | BCL | j | 101 | - | - | 5/37/137/137 | - |
| 8 | BCL | b9 | 101 | - | - | 3/37/137/137 | - |
| 11 | PC1 | H | 302 | - | - | 13/37/37/57 | - |
| 8 | BCL | N | 102 | - | - | 5/37/137/137 | - |
| 8 | BCL | d | 102 | - | - | 3/37/137/137 | - |
| 13 | SPO | 5 | 102 | - | - | 13/47/47/47 | - |
| 10 | U10 | L | 305 | - | - | 10/39/63/87 | 0/1/1/1 |
| 14 | CDL | F | 102 | - | - | 29/73/73/110 | - |
| 11 | PC1 | H | 301 | - | - | 12/46/46/57 | - |
| 11 | PC1 | l | 306 | - | - | 12/42/42/57 | - |
| 13 | SPO | U | 103 | - | - | 9/47/47/47 | - |
| 8 | BCL | 9 | 101 | - | - | 3/37/137/137 | - |
| 11 | PC1 | l | 307 | - | - | 19/43/43/57 | - |
| 10 | U10 | l | 305 | - | - | 10/39/63/87 | 0/1/1/1 |
| 11 | PC1 | L | 306 | - | - | 12/42/42/57 | - |
| 13 | SPO | c | 102 | - | - | 16/47/47/47 | - |
| 11 | PC1 | a | 103 | - | - | 17/48/48/57 | - |

All (400) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 10 | L | 305 | U10 | C13-C14 | 6.05 | 1.47 | 1.33 |
| 10 | l | 305 | U10 | C13-C14 | 6.05 | 1.47 | 1.33 |
| 10 | L | 305 | U10 | C8-C9 | 6.00 | 1.47 | 1.33 |
| 10 | l | 305 | U10 | C8-C9 | 5.98 | 1.47 | 1.33 |
| 10 | L | 305 | U10 | C28-C29 | 5.97 | 1.47 | 1.33 |
| 10 | l | 305 | U10 | C28-C29 | 5.97 | 1.47 | 1.33 |
| 10 | L | 305 | U10 | C18-C19 | 5.91 | 1.47 | 1.33 |
| 10 | l | 305 | U10 | C18-C19 | 5.91 | 1.47 | 1.33 |
| 10 | L | 305 | U10 | C23-C24 | 5.91 | 1.47 | 1.33 |
| 10 | l | 305 | U10 | C23-C24 | 5.91 | 1.47 | 1.33 |
| 10 | L | 304 | U10 | C18-C19 | 5.88 | 1.47 | 1.33 |
| 10 | l | 304 | U10 | C18-C19 | 5.88 | 1.47 | 1.33 |
| 10 | L | 304 | U10 | C23-C24 | 5.84 | 1.47 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10 | l | 304 | U10 | C23-C24 | 5.84 | 1.47 | 1.33 |
| 10 | M | 405 | U10 | C33-C34 | 5.82 | 1.46 | 1.33 |
| 10 | m | 405 | U10 | C33-C34 | 5.82 | 1.46 | 1.33 |
| 10 | L | 304 | U10 | C8-C9 | 5.81 | 1.46 | 1.33 |
| 10 | l | 304 | U10 | C8-C9 | 5.81 | 1.46 | 1.33 |
| 10 | m | 405 | U10 | C28-C29 | 5.80 | 1.46 | 1.33 |
| 10 | L | 304 | U10 | C13-C14 | 5.80 | 1.46 | 1.33 |
| 10 | l | 304 | U10 | C13-C14 | 5.80 | 1.46 | 1.33 |
| 10 | M | 405 | U10 | C28-C29 | 5.80 | 1.46 | 1.33 |
| 10 | M | 405 | U10 | C13-C14 | 5.77 | 1.46 | 1.33 |
| 10 | m | 405 | U10 | C13-C14 | 5.77 | 1.46 | 1.33 |
| 10 | M | 405 | U10 | C23-C24 | 5.75 | 1.46 | 1.33 |
| 10 | m | 405 | U10 | C23-C24 | 5.75 | 1.46 | 1.33 |
| 10 | M | 405 | U10 | C18-C19 | 5.75 | 1.46 | 1.33 |
| 10 | m | 405 | U10 | C18-C19 | 5.75 | 1.46 | 1.33 |
| 10 | M | 405 | U10 | C8-C9 | 5.70 | 1.46 | 1.33 |
| 10 | m | 405 | U10 | C8-C9 | 5.70 | 1.46 | 1.33 |
| 10 | M | 405 | U10 | O3-C3 | -5.61 | 1.23 | 1.36 |
| 10 | m | 405 | U10 | O3-C3 | -5.61 | 1.23 | 1.36 |
| 10 | M | 405 | U10 | O4-C4 | -5.56 | 1.23 | 1.36 |
| 10 | m | 405 | U10 | O4-C4 | -5.56 | 1.23 | 1.36 |
| 10 | L | 305 | U10 | O3-C3 | -5.45 | 1.23 | 1.36 |
| 10 | l | 305 | U10 | O3-C3 | -5.45 | 1.23 | 1.36 |
| 10 | L | 305 | U10 | O4-C4 | -5.42 | 1.23 | 1.36 |
| 10 | l | 305 | U10 | O4-C4 | -5.42 | 1.23 | 1.36 |
| 10 | L | 304 | U10 | O4-C4 | -5.40 | 1.23 | 1.36 |
| 10 | l | 304 | U10 | O4-C4 | -5.40 | 1.23 | 1.36 |
| 10 | L | 304 | U10 | O3-C3 | -5.33 | 1.23 | 1.36 |
| 10 | l | 304 | U10 | O3-C3 | -5.33 | 1.23 | 1.36 |
| 10 | l | 304 | U10 | C28-C29 | 5.24 | 1.47 | 1.32 |
| 10 | L | 304 | U10 | C28-C29 | 5.22 | 1.47 | 1.32 |
| 10 | L | 305 | U10 | C33-C34 | 5.20 | 1.47 | 1.32 |
| 10 | l | 305 | U10 | C33-C34 | 5.20 | 1.47 | 1.32 |
| 10 | M | 405 | U10 | C38-C39 | 5.16 | 1.47 | 1.32 |
| 10 | m | 405 | U10 | C38-C39 | 5.16 | 1.47 | 1.32 |
| 8 | 3 | 101 | BCL | MG-NA | 4.95 | 2.18 | 2.06 |
| 8 | 5 | 101 | BCL | MG-NA | 4.95 | 2.18 | 2.06 |
| 8 | 5 | 101 | BCL | C1B-NB | 4.94 | 1.39 | 1.35 |
| 8 | 1 | 101 | BCL | C1B-NB | 4.91 | 1.39 | 1.35 |
| 8 | b1 | 101 | BCL | C1B-NB | 4.91 | 1.39 | 1.35 |
| 8 | Z | 101 | BCL | C1B-NB | 4.89 | 1.39 | 1.35 |
| 8 | z | 101 | BCL | C1B-NB | 4.89 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 8 | 3 | 101 | BCL | C1B-NB | 4.86 | 1.39 | 1.35 |
| 8 | z | 101 | BCL | MG-NA | 4.86 | 2.17 | 2.06 |
| 8 | Z | 101 | BCL | MG-NA | 4.85 | 2.17 | 2.06 |
| 8 | 2 | 101 | BCL | C1B-NB | 4.80 | 1.39 | 1.35 |
| 8 | 4 | 101 | BCL | C1B-NB | 4.80 | 1.39 | 1.35 |
| 8 | 2 | 101 | BCL | MG-NA | 4.76 | 2.17 | 2.06 |
| 8 | 4 | 101 | BCL | MG-NA | 4.76 | 2.17 | 2.06 |
| 8 | C | 101 | BCL | C1B-NB | 4.76 | 1.39 | 1.35 |
| 8 | c | 101 | BCL | C1B-NB | 4.76 | 1.39 | 1.35 |
| 8 | 1 | 101 | BCL | MG-NA | 4.76 | 2.17 | 2.06 |
| 8 | b1 | 101 | BCL | MG-NA | 4.76 | 2.17 | 2.06 |
| 8 | c | 101 | BCL | MG-NA | 4.72 | 2.17 | 2.06 |
| 8 | C | 101 | BCL | MG-NA | 4.71 | 2.17 | 2.06 |
| 8 | U | 101 | BCL | C1B-NB | 4.69 | 1.39 | 1.35 |
| 8 | u | 101 | BCL | C1B-NB | 4.69 | 1.39 | 1.35 |
| 8 | G | 102 | BCL | C1B-NB | 4.68 | 1.39 | 1.35 |
| 8 | g | 102 | BCL | C1B-NB | 4.68 | 1.39 | 1.35 |
| 8 | J | 101 | BCL | MG-NA | 4.67 | 2.17 | 2.06 |
| 8 | j | 101 | BCL | MG-NA | 4.67 | 2.17 | 2.06 |
| 8 | Q | 101 | BCL | MG-NA | 4.66 | 2.17 | 2.06 |
| 8 | q | 101 | BCL | MG-NA | 4.66 | 2.17 | 2.06 |
| 8 | g | 102 | BCL | MG-NA | 4.66 | 2.17 | 2.06 |
| 8 | T | 101 | BCL | C1B-NB | 4.65 | 1.39 | 1.35 |
| 8 | t | 101 | BCL | C1B-NB | 4.65 | 1.39 | 1.35 |
| 8 | G | 102 | BCL | MG-NA | 4.65 | 2.17 | 2.06 |
| 8 | P | 102 | BCL | MG-NA | 4.64 | 2.17 | 2.06 |
| 8 | p | 102 | BCL | MG-NA | 4.64 | 2.17 | 2.06 |
| 8 | S | 101 | BCL | MG-NA | 4.64 | 2.17 | 2.06 |
| 8 | s | 101 | BCL | MG-NA | 4.64 | 2.17 | 2.06 |
| 8 | W | 101 | BCL | MG-NA | 4.63 | 2.17 | 2.06 |
| 8 | w | 101 | BCL | MG-NA | 4.63 | 2.17 | 2.06 |
| 8 | n | 102 | BCL | MG-NA | 4.63 | 2.17 | 2.06 |
| 8 | J | 101 | BCL | C1B-NB | 4.63 | 1.39 | 1.35 |
| 8 | j | 101 | BCL | C1B-NB | 4.63 | 1.39 | 1.35 |
| 8 | R | 101 | BCL | MG-NA | 4.63 | 2.17 | 2.06 |
| 8 | r | 101 | BCL | MG-NA | 4.63 | 2.17 | 2.06 |
| 8 | N | 102 | BCL | MG-NA | 4.62 | 2.17 | 2.06 |
| 8 | T | 101 | BCL | MG-NA | 4.61 | 2.17 | 2.06 |
| 8 | t | 101 | BCL | MG-NA | 4.61 | 2.17 | 2.06 |
| 8 | U | 101 | BCL | MG-NA | 4.61 | 2.17 | 2.06 |
| 8 | u | 101 | BCL | MG-NA | 4.61 | 2.17 | 2.06 |
| 8 | V | 101 | BCL | C1B-NB | 4.59 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 8 | E | 102 | BCL | MG-NA | 4.59 | 2.17 | 2.06 |
| 8 | e | 102 | BCL | MG-NA | 4.59 | 2.17 | 2.06 |
| 8 | B | 101 | BCL | MG-NA | 4.58 | 2.17 | 2.06 |
| 8 | b | 101 | BCL | MG-NA | 4.58 | 2.17 | 2.06 |
| 8 | v | 101 | BCL | C1B-NB | 4.57 | 1.39 | 1.35 |
| 8 | V | 101 | BCL | MG-NA | 4.54 | 2.17 | 2.06 |
| 8 | v | 101 | BCL | MG-NA | 4.54 | 2.17 | 2.06 |
| 8 | W | 101 | BCL | C1B-NB | 4.54 | 1.39 | 1.35 |
| 8 | 0 | 101 | BCL | MG-NA | 4.53 | 2.17 | 2.06 |
| 8 | F | 101 | BCL | MG-NA | 4.52 | 2.17 | 2.06 |
| 8 | f | 101 | BCL | MG-NA | 4.52 | 2.17 | 2.06 |
| 8 | K | 101 | BCL | MG-NA | 4.51 | 2.17 | 2.06 |
| 8 | k | 101 | BCL | MG-NA | 4.51 | 2.17 | 2.06 |
| 8 | S | 101 | BCL | C1B-NB | 4.51 | 1.39 | 1.35 |
| 8 | s | 101 | BCL | C1B-NB | 4.51 | 1.39 | 1.35 |
| 8 | M | 403 | BCL | MG-NA | 4.51 | 2.17 | 2.06 |
| 8 | m | 403 | BCL | MG-NA | 4.51 | 2.17 | 2.06 |
| 8 | b0 | 101 | BCL | MG-NA | 4.49 | 2.16 | 2.06 |
| 8 | E | 102 | BCL | C1B-NB | 4.49 | 1.39 | 1.35 |
| 8 | N | 102 | BCL | C1B-NB | 4.48 | 1.39 | 1.35 |
| 8 | n | 102 | BCL | C1B-NB | 4.48 | 1.39 | 1.35 |
| 8 | w | 101 | BCL | C1B-NB | 4.48 | 1.39 | 1.35 |
| 8 | I | 101 | BCL | C1B-NB | 4.44 | 1.39 | 1.35 |
| 8 | i | 101 | BCL | C1B-NB | 4.44 | 1.39 | 1.35 |
| 8 | e | 102 | BCL | C1B-NB | 4.42 | 1.39 | 1.35 |
| 8 | P | 102 | BCL | C1B-NB | 4.42 | 1.39 | 1.35 |
| 8 | p | 102 | BCL | C1B-NB | 4.42 | 1.39 | 1.35 |
| 8 | D | 102 | BCL | MG-NA | 4.42 | 2.16 | 2.06 |
| 8 | d | 102 | BCL | MG-NA | 4.42 | 2.16 | 2.06 |
| 8 | K | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | k | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | O | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | 7 | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | o | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | 6 | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | R | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | r | 101 | BCL | C1B-NB | 4.40 | 1.39 | 1.35 |
| 8 | L | 302 | BCL | C1B-NB | 4.39 | 1.39 | 1.35 |
| 8 | l | 302 | BCL | C1B-NB | 4.39 | 1.39 | 1.35 |
| 8 | D | 102 | BCL | C1B-NB | 4.38 | 1.39 | 1.35 |
| 8 | d | 102 | BCL | C1B-NB | 4.38 | 1.39 | 1.35 |
| 8 | 7 | 102 | BCL | MG-NA | 4.37 | 2.16 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8 | 6 | 102 | BCL | MG-NA | 4.37 | 2.16 | 2.06 |
| 8 | Q | 101 | BCL | C1B-NB | 4.36 | 1.39 | 1.35 |
| 8 | q | 101 | BCL | C1B-NB | 4.36 | 1.39 | 1.35 |
| 8 | B | 101 | BCL | C1B-NB | 4.35 | 1.39 | 1.35 |
| 8 | b | 101 | BCL | C1B-NB | 4.35 | 1.39 | 1.35 |
| 8 | M | 402 | BCL | MG-NA | 4.34 | 2.16 | 2.06 |
| 8 | m | 402 | BCL | MG-NA | 4.34 | 2.16 | 2.06 |
| 8 | 9 | 101 | BCL | MG-NA | 4.30 | 2.16 | 2.06 |
| 8 | b9 | 101 | BCL | MG-NA | 4.30 | 2.16 | 2.06 |
| 8 | F | 101 | BCL | C1B-NB | 4.30 | 1.39 | 1.35 |
| 8 | f | 101 | BCL | C1B-NB | 4.30 | 1.39 | 1.35 |
| 8 | L | 301 | BCL | MG-NA | 4.29 | 2.16 | 2.06 |
| 8 | l | 301 | BCL | MG-NA | 4.28 | 2.16 | 2.06 |
| 8 | a | 101 | BCL | MG-NA | 4.27 | 2.16 | 2.06 |
| 8 | A | 101 | BCL | MG-NA | 4.27 | 2.16 | 2.06 |
| 8 | 7 | 101 | BCL | MG-NA | 4.26 | 2.16 | 2.06 |
| 8 | 6 | 101 | BCL | MG-NA | 4.26 | 2.16 | 2.06 |
| 8 | l | 302 | BCL | MG-NA | 4.25 | 2.16 | 2.06 |
| 9 | M | 404 | BPH | CBD-CGD | -4.24 | 1.46 | 1.52 |
| 9 | m | 404 | BPH | CBD-CGD | -4.24 | 1.46 | 1.52 |
| 8 | 6 | 102 | BCL | C1B-NB | 4.24 | 1.39 | 1.35 |
| 8 | L | 302 | BCL | MG-NA | 4.23 | 2.16 | 2.06 |
| 8 | 7 | 102 | BCL | C1B-NB | 4.22 | 1.39 | 1.35 |
| 8 | L | 301 | BCL | C1B-NB | 4.21 | 1.39 | 1.35 |
| 8 | M | 402 | BCL | C1B-NB | 4.21 | 1.39 | 1.35 |
| 8 | 0 | 101 | BCL | C1B-NB | 4.21 | 1.39 | 1.35 |
| 8 | l | 301 | BCL | C1B-NB | 4.21 | 1.39 | 1.35 |
| 8 | m | 402 | BCL | C1B-NB | 4.21 | 1.39 | 1.35 |
| 8 | b0 | 101 | BCL | C1B-NB | 4.21 | 1.39 | 1.35 |
| 8 | I | 101 | BCL | MG-NA | 4.21 | 2.16 | 2.06 |
| 8 | i | 101 | BCL | MG-NA | 4.21 | 2.16 | 2.06 |
| 8 | O | 101 | BCL | MG-NA | 4.20 | 2.16 | 2.06 |
| 8 | o | 101 | BCL | MG-NA | 4.20 | 2.16 | 2.06 |
| 8 | 9 | 101 | BCL | C1B-NB | 4.20 | 1.39 | 1.35 |
| 8 | b9 | 101 | BCL | C1B-NB | 4.20 | 1.39 | 1.35 |
| 8 | A | 101 | BCL | C1B-NB | 4.18 | 1.38 | 1.35 |
| 8 | a | 101 | BCL | C1B-NB | 4.18 | 1.38 | 1.35 |
| 9 | L | 303 | BPH | CBD-CGD | -4.16 | 1.46 | 1.52 |
| 9 | l | 303 | BPH | CBD-CGD | -4.13 | 1.46 | 1.52 |
| 8 | M | 403 | BCL | C1B-NB | 4.04 | 1.38 | 1.35 |
| 8 | m | 403 | BCL | C1B-NB | 4.04 | 1.38 | 1.35 |
| 8 | 5 | 101 | BCL | MG-NC | 3.59 | 2.14 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8 | 3 | 101 | BCL | MG-NC | 3.58 | 2.14 | 2.06 |
| 8 | 1 | 101 | BCL | MG-NC | 3.53 | 2.14 | 2.06 |
| 8 | b1 | 101 | BCL | MG-NC | 3.53 | 2.14 | 2.06 |
| 8 | 2 | 101 | BCL | MG-NC | 3.52 | 2.14 | 2.06 |
| 8 | 4 | 101 | BCL | MG-NC | 3.52 | 2.14 | 2.06 |
| 8 | z | 101 | BCL | MG-NC | 3.46 | 2.14 | 2.06 |
| 8 | Z | 101 | BCL | MG-NC | 3.45 | 2.14 | 2.06 |
| 10 | M | 405 | U10 | C3-C2 | -3.39 | 1.39 | 1.48 |
| 10 | m | 405 | U10 | C3-C2 | -3.39 | 1.39 | 1.48 |
| 10 | M | 405 | U10 | C4-C5 | -3.39 | 1.39 | 1.48 |
| 10 | m | 405 | U10 | C4-C5 | -3.39 | 1.39 | 1.48 |
| 10 | L | 305 | U10 | C4-C5 | -3.33 | 1.39 | 1.48 |
| 10 | l | 305 | U10 | C4-C5 | -3.33 | 1.39 | 1.48 |
| 8 | T | 101 | BCL | MG-NC | 3.30 | 2.14 | 2.06 |
| 8 | t | 101 | BCL | MG-NC | 3.30 | 2.14 | 2.06 |
| 8 | u | 101 | BCL | MG-NC | 3.30 | 2.14 | 2.06 |
| 8 | v | 101 | BCL | MG-NC | 3.30 | 2.14 | 2.06 |
| 8 | U | 101 | BCL | MG-NC | 3.29 | 2.14 | 2.06 |
| 8 | V | 101 | BCL | MG-NC | 3.29 | 2.14 | 2.06 |
| 10 | L | 304 | U10 | C4-C5 | -3.26 | 1.39 | 1.48 |
| 10 | l | 304 | U10 | C4-C5 | -3.26 | 1.39 | 1.48 |
| 8 | j | 101 | BCL | MG-NC | 3.23 | 2.14 | 2.06 |
| 8 | f | 101 | BCL | MG-NC | 3.23 | 2.13 | 2.06 |
| 8 | F | 101 | BCL | MG-NC | 3.22 | 2.13 | 2.06 |
| 8 | q | 101 | BCL | MG-NC | 3.22 | 2.13 | 2.06 |
| 8 | Q | 101 | BCL | MG-NC | 3.22 | 2.13 | 2.06 |
| 8 | J | 101 | BCL | MG-NC | 3.22 | 2.13 | 2.06 |
| 8 | G | 102 | BCL | MG-NC | 3.21 | 2.13 | 2.06 |
| 8 | R | 101 | BCL | MG-NC | 3.19 | 2.13 | 2.06 |
| 8 | r | 101 | BCL | MG-NC | 3.19 | 2.13 | 2.06 |
| 8 | C | 101 | BCL | MG-NC | 3.17 | 2.13 | 2.06 |
| 8 | g | 102 | BCL | MG-NC | 3.17 | 2.13 | 2.06 |
| 8 | c | 101 | BCL | MG-NC | 3.17 | 2.13 | 2.06 |
| 8 | w | 101 | BCL | MG-NC | 3.14 | 2.13 | 2.06 |
| 8 | N | 102 | BCL | MG-NC | 3.14 | 2.13 | 2.06 |
| 8 | W | 101 | BCL | MG-NC | 3.14 | 2.13 | 2.06 |
| 8 | P | 102 | BCL | MG-NC | 3.14 | 2.13 | 2.06 |
| 8 | p | 102 | BCL | MG-NC | 3.14 | 2.13 | 2.06 |
| 10 | L | 305 | U10 | C3-C2 | -3.13 | 1.39 | 1.48 |
| 10 | l | 305 | U10 | C3-C2 | -3.13 | 1.39 | 1.48 |
| 8 | s | 101 | BCL | MG-NC | 3.11 | 2.13 | 2.06 |
| 8 | S | 101 | BCL | MG-NC | 3.11 | 2.13 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8 | n | 102 | BCL | MG-NC | 3.10 | 2.13 | 2.06 |
| 8 | E | 102 | BCL | MG-NC | 3.09 | 2.13 | 2.06 |
| 8 | e | 102 | BCL | MG-NC | 3.09 | 2.13 | 2.06 |
| 8 | K | 101 | BCL | MG-NC | 3.03 | 2.13 | 2.06 |
| 8 | k | 101 | BCL | MG-NC | 3.03 | 2.13 | 2.06 |
| 8 | A | 101 | BCL | MG-NC | 3.01 | 2.13 | 2.06 |
| 8 | a | 101 | BCL | MG-NC | 3.01 | 2.13 | 2.06 |
| 8 | D | 102 | BCL | MG-NC | 2.95 | 2.13 | 2.06 |
| 8 | d | 102 | BCL | MG-NC | 2.95 | 2.13 | 2.06 |
| 8 | b0 | 101 | BCL | MG-NC | 2.95 | 2.13 | 2.06 |
| 8 | B | 101 | BCL | MG-NC | 2.94 | 2.13 | 2.06 |
| 8 | b | 101 | BCL | MG-NC | 2.94 | 2.13 | 2.06 |
| 8 | 0 | 101 | BCL | MG-NC | 2.94 | 2.13 | 2.06 |
| 8 | 7 | 102 | BCL | MG-NC | 2.94 | 2.13 | 2.06 |
| 8 | 6 | 102 | BCL | MG-NC | 2.94 | 2.13 | 2.06 |
| 8 | 9 | 101 | BCL | MG-NC | 2.92 | 2.13 | 2.06 |
| 8 | b9 | 101 | BCL | MG-NC | 2.92 | 2.13 | 2.06 |
| 8 | 7 | 101 | BCL | MG-NC | 2.92 | 2.13 | 2.06 |
| 8 | 6 | 101 | BCL | MG-NC | 2.92 | 2.13 | 2.06 |
| 10 | L | 304 | U10 | C3-C2 | -2.90 | 1.40 | 1.48 |
| 10 | l | 304 | U10 | C3-C2 | -2.90 | 1.40 | 1.48 |
| 8 | m | 402 | BCL | MG-NC | 2.88 | 2.13 | 2.06 |
| 8 | i | 101 | BCL | MG-NC | 2.88 | 2.13 | 2.06 |
| 8 | I | 101 | BCL | MG-NC | 2.88 | 2.13 | 2.06 |
| 8 | M | 402 | BCL | MG-NC | 2.87 | 2.13 | 2.06 |
| 10 | M | 405 | U10 | C6-C5 | -2.84 | 1.38 | 1.46 |
| 10 | m | 405 | U10 | C6-C5 | -2.84 | 1.38 | 1.46 |
| 8 | L | 301 | BCL | MG-NC | 2.77 | 2.12 | 2.06 |
| 8 | l | 301 | BCL | MG-NC | 2.77 | 2.12 | 2.06 |
| 10 | L | 305 | U10 | C6-C5 | -2.77 | 1.38 | 1.46 |
| 10 | l | 305 | U10 | C6-C5 | -2.77 | 1.38 | 1.46 |
| 8 | O | 101 | BCL | MG-NC | 2.77 | 2.12 | 2.06 |
| 8 | o | 101 | BCL | MG-NC | 2.77 | 2.12 | 2.06 |
| 8 | l | 301 | BCL | O1A-CGA | -2.76 | 1.14 | 1.22 |
| 8 | L | 301 | BCL | O1A-CGA | -2.76 | 1.14 | 1.22 |
| 10 | L | 304 | U10 | C6-C5 | -2.72 | 1.39 | 1.46 |
| 10 | l | 304 | U10 | C6-C5 | -2.72 | 1.39 | 1.46 |
| 11 | d | 101 | PC1 | O21-C2 | -2.71 | 1.39 | 1.46 |
| 11 | D | 101 | PC1 | O21-C2 | -2.67 | 1.39 | 1.46 |
| 14 | M | 407 | CDL | OA6-CA4 | -2.66 | 1.39 | 1.46 |
| 14 | m | 407 | CDL | OA6-CA4 | -2.66 | 1.39 | 1.46 |
| 8 | L | 302 | BCL | MG-NC | 2.65 | 2.12 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8 | l | 302 | BCL | MG-NC | 2.65 | 2.12 | 2.06 |
| 11 | A | 104 | PC1 | O21-C2 | -2.61 | 1.40 | 1.46 |
| 11 | a | 104 | PC1 | O21-C2 | -2.61 | 1.40 | 1.46 |
| 14 | M | 407 | CDL | OB6-CB4 | -2.61 | 1.40 | 1.46 |
| 14 | m | 407 | CDL | OB6-CB4 | -2.61 | 1.40 | 1.46 |
| 8 | M | 403 | BCL | MG-NC | 2.58 | 2.12 | 2.06 |
| 8 | m | 403 | BCL | MG-NC | 2.58 | 2.12 | 2.06 |
| 14 | F | 102 | CDL | OB6-CB4 | -2.57 | 1.40 | 1.46 |
| 14 | f | 102 | CDL | OB6-CB4 | -2.57 | 1.40 | 1.46 |
| 11 | H | 301 | PC1 | O21-C2 | -2.56 | 1.40 | 1.46 |
| 11 | h | 301 | PC1 | O21-C2 | -2.56 | 1.40 | 1.46 |
| 14 | f | 102 | CDL | OA6-CA4 | -2.56 | 1.40 | 1.46 |
| 11 | L | 307 | PC1 | O21-C2 | -2.56 | 1.40 | 1.46 |
| 11 | l | 307 | PC1 | O21-C2 | -2.56 | 1.40 | 1.46 |
| 14 | F | 102 | CDL | OA6-CA4 | -2.55 | 1.40 | 1.46 |
| 11 | A | 103 | PC1 | O21-C2 | -2.54 | 1.40 | 1.46 |
| 11 | a | 103 | PC1 | O21-C2 | -2.54 | 1.40 | 1.46 |
| 11 | L | 306 | PC1 | O21-C2 | -2.48 | 1.40 | 1.46 |
| 11 | l | 306 | PC1 | O21-C2 | -2.48 | 1.40 | 1.46 |
| 14 | F | 102 | CDL | OA8-CA7 | 2.45 | 1.40 | 1.33 |
| 14 | f | 102 | CDL | OA8-CA7 | 2.45 | 1.40 | 1.33 |
| 11 | H | 302 | PC1 | O21-C21 | 2.45 | 1.41 | 1.34 |
| 11 | h | 302 | PC1 | O21-C21 | 2.45 | 1.41 | 1.34 |
| 14 | M | 407 | CDL | OA8-CA7 | 2.44 | 1.40 | 1.33 |
| 14 | m | 407 | CDL | OA8-CA7 | 2.44 | 1.40 | 1.33 |
| 11 | A | 103 | PC1 | O31-C31 | 2.43 | 1.40 | 1.33 |
| 11 | a | 103 | PC1 | O31-C31 | 2.43 | 1.40 | 1.33 |
| 10 | M | 405 | U10 | C1-C2 | -2.43 | 1.38 | 1.47 |
| 10 | m | 405 | U10 | C1-C2 | -2.43 | 1.38 | 1.47 |
| 11 | H | 301 | PC1 | O31-C3 | -2.39 | 1.39 | 1.45 |
| 11 | h | 301 | PC1 | O31-C3 | -2.39 | 1.39 | 1.45 |
| 11 | l | 307 | PC1 | O31-C31 | 2.39 | 1.40 | 1.33 |
| 14 | F | 102 | CDL | OB8-CB7 | 2.38 | 1.40 | 1.33 |
| 14 | f | 102 | CDL | OB8-CB7 | 2.38 | 1.40 | 1.33 |
| 14 | m | 407 | CDL | OB8-CB7 | 2.37 | 1.40 | 1.33 |
| 11 | H | 302 | PC1 | O21-C2 | -2.36 | 1.40 | 1.46 |
| 11 | h | 302 | PC1 | O21-C2 | -2.36 | 1.40 | 1.46 |
| 11 | L | 306 | PC1 | O31-C31 | 2.36 | 1.40 | 1.33 |
| 11 | l | 306 | PC1 | O31-C31 | 2.36 | 1.40 | 1.33 |
| 14 | M | 407 | CDL | OB8-CB7 | 2.36 | 1.40 | 1.33 |
| 11 | L | 307 | PC1 | O31-C31 | 2.36 | 1.40 | 1.33 |
| 8 | M | 403 | BCL | CBD-CGD | -2.36 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8 | m | 403 | BCL | CBD-CGD | -2.36 | 1.45 | 1.52 |
| 11 | D | 101 | PC1 | O31-C31 | 2.33 | 1.40 | 1.33 |
| 11 | d | 101 | PC1 | O31-C31 | 2.33 | 1.40 | 1.33 |
| 8 | D | 102 | BCL | O1A-CGA | -2.31 | 1.15 | 1.22 |
| 8 | d | 102 | BCL | O1A-CGA | -2.31 | 1.15 | 1.22 |
| 8 | M | 403 | BCL | O1A-CGA | -2.30 | 1.15 | 1.22 |
| 8 | m | 403 | BCL | O1A-CGA | -2.30 | 1.15 | 1.22 |
| 11 | H | 302 | PC1 | O31-C31 | 2.30 | 1.40 | 1.33 |
| 11 | h | 302 | PC1 | O31-C31 | 2.30 | 1.40 | 1.33 |
| 11 | A | 104 | PC1 | O31-C3 | -2.27 | 1.40 | 1.45 |
| 11 | a | 104 | PC1 | O31-C3 | -2.27 | 1.40 | 1.45 |
| 11 | A | 104 | PC1 | O31-C31 | 2.26 | 1.39 | 1.33 |
| 11 | a | 104 | PC1 | O31-C31 | 2.26 | 1.39 | 1.33 |
| 8 | L | 302 | BCL | O1A-CGA | -2.24 | 1.15 | 1.22 |
| 8 | l | 302 | BCL | O1A-CGA | -2.24 | 1.15 | 1.22 |
| 11 | H | 302 | PC1 | O31-C3 | -2.23 | 1.40 | 1.45 |
| 11 | h | 302 | PC1 | O31-C3 | -2.23 | 1.40 | 1.45 |
| 8 | 9 | 101 | BCL | O1A-CGA | -2.20 | 1.16 | 1.22 |
| 8 | b9 | 101 | BCL | O1A-CGA | -2.20 | 1.16 | 1.22 |
| 10 | L | 304 | U10 | C6-C1 | 2.19 | 1.39 | 1.35 |
| 10 | l | 304 | U10 | C6-C1 | 2.19 | 1.39 | 1.35 |
| 10 | L | 305 | U10 | C6-C1 | 2.18 | 1.39 | 1.35 |
| 10 | l | 305 | U10 | C6-C1 | 2.18 | 1.39 | 1.35 |
| 11 | D | 101 | PC1 | O31-C3 | -2.17 | 1.40 | 1.45 |
| 11 | H | 301 | PC1 | O31-C31 | 2.17 | 1.39 | 1.33 |
| 11 | h | 301 | PC1 | O31-C31 | 2.17 | 1.39 | 1.33 |
| 11 | l | 307 | PC1 | O31-C3 | -2.17 | 1.40 | 1.45 |
| 10 | L | 304 | U10 | C1-C2 | -2.17 | 1.39 | 1.47 |
| 10 | l | 304 | U10 | C1-C2 | -2.17 | 1.39 | 1.47 |
| 11 | A | 103 | PC1 | O31-C3 | -2.16 | 1.40 | 1.45 |
| 11 | a | 103 | PC1 | O31-C3 | -2.16 | 1.40 | 1.45 |
| 10 | l | 305 | U10 | C1-C2 | -2.16 | 1.39 | 1.47 |
| 10 | L | 305 | U10 | C1-C2 | -2.15 | 1.39 | 1.47 |
| 11 | d | 101 | PC1 | O31-C3 | -2.15 | 1.40 | 1.45 |
| 8 | K | 101 | BCL | O1A-CGA | -2.15 | 1.16 | 1.22 |
| 8 | k | 101 | BCL | O1A-CGA | -2.15 | 1.16 | 1.22 |
| 11 | L | 307 | PC1 | O31-C3 | -2.14 | 1.40 | 1.45 |
| 14 | M | 407 | CDL | OB8-CB6 | -2.13 | 1.40 | 1.45 |
| 14 | m | 407 | CDL | OB8-CB6 | -2.13 | 1.40 | 1.45 |
| 14 | M | 407 | CDL | OA8-CA6 | -2.13 | 1.40 | 1.45 |
| 14 | m | 407 | CDL | OA8-CA6 | -2.13 | 1.40 | 1.45 |
| 11 | L | 306 | PC1 | O31-C3 | -2.12 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11 | l | 306 | PC1 | O31-C3 | -2.12 | 1.40 | 1.45 |
| 11 | A | 103 | PC1 | O21-C21 | 2.11 | 1.40 | 1.34 |
| 11 | a | 103 | PC1 | O21-C21 | 2.11 | 1.40 | 1.34 |
| 11 | H | 301 | PC1 | O21-C21 | 2.11 | 1.40 | 1.34 |
| 11 | h | 301 | PC1 | O21-C21 | 2.11 | 1.40 | 1.34 |
| 11 | L | 306 | PC1 | O21-C21 | 2.11 | 1.40 | 1.34 |
| 11 | l | 306 | PC1 | O21-C21 | 2.11 | 1.40 | 1.34 |
| 8 | I | 101 | BCL | O1A-CGA | -2.10 | 1.16 | 1.22 |
| 8 | i | 101 | BCL | O1A-CGA | -2.10 | 1.16 | 1.22 |
| 8 | 3 | 101 | BCL | OBD-CAD | 2.10 | 1.25 | 1.22 |
| 8 | 5 | 101 | BCL | OBD-CAD | 2.10 | 1.25 | 1.22 |
| 14 | F | 102 | CDL | OA6-CA5 | 2.10 | 1.40 | 1.34 |
| 14 | f | 102 | CDL | OA6-CA5 | 2.10 | 1.40 | 1.34 |
| 8 | b1 | 101 | BCL | OBD-CAD | 2.09 | 1.25 | 1.22 |
| 8 | S | 101 | BCL | O1A-CGA | -2.08 | 1.16 | 1.22 |
| 8 | s | 101 | BCL | O1A-CGA | -2.08 | 1.16 | 1.22 |
| 11 | L | 307 | PC1 | O21-C21 | 2.08 | 1.40 | 1.34 |
| 11 | d | 101 | PC1 | O21-C21 | 2.08 | 1.40 | 1.34 |
| 14 | M | 407 | CDL | OB6-CB5 | 2.08 | 1.40 | 1.34 |
| 14 | m | 407 | CDL | OB6-CB5 | 2.08 | 1.40 | 1.34 |
| 14 | M | 407 | CDL | OA6-CA5 | 2.08 | 1.40 | 1.34 |
| 14 | m | 407 | CDL | OA6-CA5 | 2.08 | 1.40 | 1.34 |
| 14 | F | 102 | CDL | OB8-CB6 | -2.08 | 1.40 | 1.45 |
| 14 | f | 102 | CDL | OB8-CB6 | -2.08 | 1.40 | 1.45 |
| 9 | M | 404 | BPH | C1C-C2C | -2.07 | 1.47 | 1.51 |
| 9 | m | 404 | BPH | C1C-C2C | -2.07 | 1.47 | 1.51 |
| 14 | f | 102 | CDL | OB6-CB5 | 2.06 | 1.40 | 1.34 |
| 11 | A | 104 | PC1 | O21-C21 | 2.06 | 1.40 | 1.34 |
| 11 | a | 104 | PC1 | O21-C21 | 2.06 | 1.40 | 1.34 |
| 11 | l | 307 | PC1 | O21-C21 | 2.05 | 1.40 | 1.34 |
| 8 | A | 101 | BCL | O1A-CGA | -2.05 | 1.16 | 1.22 |
| 8 | a | 101 | BCL | O1A-CGA | -2.05 | 1.16 | 1.22 |
| 14 | F | 102 | CDL | OB6-CB5 | 2.05 | 1.40 | 1.34 |
| 11 | D | 101 | PC1 | O21-C21 | 2.05 | 1.40 | 1.34 |
| 8 | l | 101 | BCL | OBD-CAD | 2.04 | 1.25 | 1.22 |
| 10 | M | 405 | U10 | C6-C1 | 2.03 | 1.38 | 1.35 |
| 10 | m | 405 | U10 | C6-C1 | 2.03 | 1.38 | 1.35 |
| 14 | M | 407 | CDL | PB2-OB4 | -2.02 | 1.45 | 1.55 |
| 14 | m | 407 | CDL | PB2-OB4 | -2.02 | 1.45 | 1.55 |
| 11 | H | 301 | PC1 | P-O12 | -2.02 | 1.45 | 1.55 |
| 11 | h | 301 | PC1 | P-O12 | -2.02 | 1.45 | 1.55 |
| 9 | M | 404 | BPH | O1A-CGA | -2.02 | 1.16 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9 | m | 404 | BPH | O1A-CGA | -2.02 | 1.16 | 1.22 |
| 8 | 2 | 101 | BCL | OBD-CAD | 2.02 | 1.25 | 1.22 |
| 8 | 4 | 101 | BCL | OBD-CAD | 2.02 | 1.25 | 1.22 |
| 14 | F | 102 | CDL | OA8-CA6 | -2.01 | 1.40 | 1.45 |
| 14 | f | 102 | CDL | OA8-CA6 | -2.01 | 1.40 | 1.45 |
| 8 | 3 | 101 | BCL | C4B-NB | 2.00 | 1.37 | 1.35 |
| 8 | 5 | 101 | BCL | C4B-NB | 2.00 | 1.37 | 1.35 |
| 8 | M | 403 | BCL | C3D-CAD | -2.00 | 1.41 | 1.46 |
| 8 | m | 403 | BCL | C3D-CAD | -2.00 | 1.41 | 1.46 |

All (875) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | L | 301 | BCL | CAD-C3D-C4D | -4.79 | 105.80 | 108.47 |
| 8 | l | 301 | BCL | CAD-C3D-C4D | -4.79 | 105.80 | 108.47 |
| 8 | M | 403 | BCL | CMB-C2B-C1B | -4.55 | 121.48 | 128.46 |
| 8 | m | 403 | BCL | CMB-C2B-C1B | -4.55 | 121.48 | 128.46 |
| 8 | A | 101 | BCL | CMB-C2B-C1B | -4.53 | 121.49 | 128.46 |
| 8 | a | 101 | BCL | CMB-C2B-C1B | -4.53 | 121.49 | 128.46 |
| 8 | S | 101 | BCL | CMB-C2B-C1B | -4.53 | 121.50 | 128.46 |
| 8 | s | 101 | BCL | CMB-C2B-C1B | -4.53 | 121.50 | 128.46 |
| 8 | 0 | 101 | BCL | C1-C2-C3 | 4.51 | 133.84 | 126.04 |
| 8 | b0 | 101 | BCL | C1-C2-C3 | 4.51 | 133.84 | 126.04 |
| 8 | 6 | 101 | BCL | CMB-C2B-C1B | -4.49 | 121.56 | 128.46 |
| 8 | 7 | 101 | BCL | CMB-C2B-C1B | -4.49 | 121.56 | 128.46 |
| 8 | Q | 101 | BCL | CMB-C2B-C1B | -4.47 | 121.59 | 128.46 |
| 8 | q | 101 | BCL | CMB-C2B-C1B | -4.47 | 121.59 | 128.46 |
| 8 | B | 101 | BCL | C1-C2-C3 | 4.39 | 133.63 | 126.04 |
| 8 | b | 101 | BCL | C1-C2-C3 | 4.39 | 133.63 | 126.04 |
| 8 | D | 102 | BCL | CMB-C2B-C1B | -4.35 | 121.78 | 128.46 |
| 8 | d | 102 | BCL | CMB-C2B-C1B | -4.35 | 121.78 | 128.46 |
| 8 | b9 | 101 | BCL | CMB-C2B-C1B | -4.35 | 121.78 | 128.46 |
| 8 | 9 | 101 | BCL | CMB-C2B-C1B | -4.35 | 121.78 | 128.46 |
| 10 | L | 305 | U10 | C7-C8-C9 | -4.35 | 119.56 | 126.79 |
| 10 | l | 305 | U10 | C7-C8-C9 | -4.33 | 119.59 | 126.79 |
| 11 | A | 103 | PC1 | O21-C21-C22 | 4.31 | 120.80 | 111.50 |
| 11 | a | 103 | PC1 | O21-C21-C22 | 4.31 | 120.80 | 111.50 |
| 8 | L | 301 | BCL | CMB-C2B-C1B | -4.31 | 121.84 | 128.46 |
| 8 | l | 301 | BCL | CMB-C2B-C1B | -4.31 | 121.84 | 128.46 |
| 11 | L | 306 | PC1 | O21-C21-C22 | 4.29 | 120.75 | 111.50 |
| 11 | l | 306 | PC1 | O21-C21-C22 | 4.29 | 120.75 | 111.50 |
| 8 | f | 101 | BCL | CMB-C2B-C1B | -4.23 | 121.96 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | F | 101 | BCL | CMB-C2B-C1B | -4.21 | 121.99 | 128.46 |
| 8 | 0 | 101 | BCL | CMB-C2B-C1B | -4.20 | 122.00 | 128.46 |
| 8 | b0 | 101 | BCL | CMB-C2B-C1B | -4.20 | 122.00 | 128.46 |
| 10 | L | 304 | U10 | C7-C8-C9 | -4.19 | 119.81 | 126.79 |
| 10 | l | 304 | U10 | C7-C8-C9 | -4.19 | 119.81 | 126.79 |
| 8 | 7 | 102 | BCL | CMB-C2B-C1B | -4.19 | 122.02 | 128.46 |
| 8 | 6 | 102 | BCL | CMB-C2B-C1B | -4.19 | 122.02 | 128.46 |
| 8 | L | 302 | BCL | CMB-C2B-C1B | -4.18 | 122.05 | 128.46 |
| 8 | l | 302 | BCL | CMB-C2B-C1B | -4.18 | 122.05 | 128.46 |
| 8 | L | 302 | BCL | CAD-C3D-C4D | -4.16 | 106.15 | 108.47 |
| 8 | l | 302 | BCL | CAD-C3D-C4D | -4.16 | 106.15 | 108.47 |
| 8 | K | 101 | BCL | CMB-C2B-C1B | -4.10 | 122.16 | 128.46 |
| 8 | k | 101 | BCL | CMB-C2B-C1B | -4.10 | 122.16 | 128.46 |
| 8 | m | 403 | BCL | C4A-NA-C1A | 4.08 | 108.54 | 106.71 |
| 8 | M | 403 | BCL | C4A-NA-C1A | 4.08 | 108.54 | 106.71 |
| 8 | M | 402 | BCL | CMB-C2B-C1B | -4.07 | 122.22 | 128.46 |
| 8 | m | 402 | BCL | CMB-C2B-C1B | -4.07 | 122.22 | 128.46 |
| 8 | w | 101 | BCL | CAD-C3D-C4D | -4.06 | 106.20 | 108.47 |
| 11 | A | 104 | PC1 | O21-C21-C22 | 4.05 | 120.22 | 111.50 |
| 11 | a | 104 | PC1 | O21-C21-C22 | 4.05 | 120.22 | 111.50 |
| 14 | F | 102 | CDL | OA6-CA5-C11 | 4.04 | 120.21 | 111.50 |
| 14 | f | 102 | CDL | OA6-CA5-C11 | 4.04 | 120.21 | 111.50 |
| 8 | W | 101 | BCL | CAD-C3D-C4D | -4.02 | 106.23 | 108.47 |
| 8 | U | 101 | BCL | CMB-C2B-C1B | -4.00 | 122.31 | 128.46 |
| 8 | u | 101 | BCL | CMB-C2B-C1B | -4.00 | 122.31 | 128.46 |
| 11 | H | 301 | PC1 | O21-C21-C22 | 3.98 | 120.08 | 111.50 |
| 11 | h | 301 | PC1 | O21-C21-C22 | 3.98 | 120.08 | 111.50 |
| 8 | B | 101 | BCL | CMB-C2B-C1B | -3.98 | 122.35 | 128.46 |
| 8 | b | 101 | BCL | CMB-C2B-C1B | -3.98 | 122.35 | 128.46 |
| 8 | I | 101 | BCL | CMB-C2B-C1B | -3.98 | 122.35 | 128.46 |
| 8 | i | 101 | BCL | CMB-C2B-C1B | -3.98 | 122.35 | 128.46 |
| 11 | D | 101 | PC1 | O21-C21-C22 | 3.98 | 120.07 | 111.50 |
| 11 | d | 101 | PC1 | O21-C21-C22 | 3.97 | 120.05 | 111.50 |
| 10 | L | 305 | U10 | C17-C18-C19 | -3.95 | 118.15 | 127.66 |
| 10 | l | 305 | U10 | C17-C18-C19 | -3.95 | 118.15 | 127.66 |
| 8 | G | 102 | BCL | CMB-C2B-C1B | -3.91 | 122.45 | 128.46 |
| 8 | g | 102 | BCL | CMB-C2B-C1B | -3.91 | 122.45 | 128.46 |
| 8 | J | 101 | BCL | CMB-C2B-C1B | -3.90 | 122.47 | 128.46 |
| 8 | o | 101 | BCL | C4A-NA-C1A | 3.90 | 108.46 | 106.71 |
| 14 | F | 102 | CDL | OB6-CB5-C51 | 3.90 | 119.90 | 111.50 |
| 14 | f | 102 | CDL | OB6-CB5-C51 | 3.89 | 119.89 | 111.50 |
| 8 | 7 | 102 | BCL | C11-C10-C8 | 3.88 | 128.46 | 115.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | 6 | 102 | BCL | C11-C10-C8 | 3.88 | 128.46 | 115.92 |
| 8 | j | 101 | BCL | CMB-C2B-C1B | -3.88 | 122.50 | 128.46 |
| 8 | Q | 101 | BCL | C4A-NA-C1A | 3.87 | 108.44 | 106.71 |
| 8 | q | 101 | BCL | C4A-NA-C1A | 3.87 | 108.44 | 106.71 |
| 8 | I | 101 | BCL | CAD-C3D-C4D | -3.86 | 106.32 | 108.47 |
| 8 | i | 101 | BCL | CAD-C3D-C4D | -3.86 | 106.32 | 108.47 |
| 8 | S | 101 | BCL | C4A-NA-C1A | 3.85 | 108.44 | 106.71 |
| 8 | s | 101 | BCL | C4A-NA-C1A | 3.85 | 108.44 | 106.71 |
| 8 | N | 102 | BCL | CMB-C2B-C1B | -3.84 | 122.56 | 128.46 |
| 8 | n | 102 | BCL | CMB-C2B-C1B | -3.84 | 122.56 | 128.46 |
| 8 | E | 102 | BCL | CMB-C2B-C1B | -3.84 | 122.56 | 128.46 |
| 8 | e | 102 | BCL | CMB-C2B-C1B | -3.84 | 122.56 | 128.46 |
| 14 | M | 407 | CDL | OB6-CB5-C51 | 3.83 | 119.75 | 111.50 |
| 14 | m | 407 | CDL | OB6-CB5-C51 | 3.83 | 119.75 | 111.50 |
| 14 | M | 407 | CDL | OA6-CA5-C11 | 3.83 | 119.75 | 111.50 |
| 14 | m | 407 | CDL | OA6-CA5-C11 | 3.83 | 119.75 | 111.50 |
| 8 | O | 101 | BCL | C4A-NA-C1A | 3.82 | 108.42 | 106.71 |
| 8 | O | 101 | BCL | CMB-C2B-C1B | -3.80 | 122.63 | 128.46 |
| 8 | o | 101 | BCL | CMB-C2B-C1B | -3.80 | 122.63 | 128.46 |
| 8 | 9 | 101 | BCL | C4A-NA-C1A | 3.79 | 108.41 | 106.71 |
| 8 | b9 | 101 | BCL | C4A-NA-C1A | 3.79 | 108.41 | 106.71 |
| 8 | 5 | 101 | BCL | CMB-C2B-C1B | -3.76 | 122.69 | 128.46 |
| 8 | D | 102 | BCL | C4A-NA-C1A | 3.76 | 108.40 | 106.71 |
| 8 | 3 | 101 | BCL | CMB-C2B-C1B | -3.75 | 122.70 | 128.46 |
| 8 | 1 | 101 | BCL | CMB-C2B-C1B | -3.74 | 122.72 | 128.46 |
| 8 | b1 | 101 | BCL | CMB-C2B-C1B | -3.74 | 122.72 | 128.46 |
| 8 | V | 101 | BCL | CAD-C3D-C4D | -3.72 | 106.40 | 108.47 |
| 8 | v | 101 | BCL | CAD-C3D-C4D | -3.72 | 106.40 | 108.47 |
| 8 | R | 101 | BCL | CMB-C2B-C1B | -3.71 | 122.76 | 128.46 |
| 8 | F | 101 | BCL | C4A-NA-C1A | 3.70 | 108.37 | 106.71 |
| 8 | f | 101 | BCL | C4A-NA-C1A | 3.70 | 108.37 | 106.71 |
| 11 | l | 307 | PC1 | O21-C21-C22 | 3.70 | 119.48 | 111.50 |
| 11 | L | 307 | PC1 | O21-C21-C22 | 3.70 | 119.47 | 111.50 |
| 8 | V | 101 | BCL | CMB-C2B-C1B | -3.69 | 122.79 | 128.46 |
| 8 | v | 101 | BCL | CMB-C2B-C1B | -3.69 | 122.79 | 128.46 |
| 8 | r | 101 | BCL | CMB-C2B-C1B | -3.69 | 122.79 | 128.46 |
| 8 | d | 102 | BCL | C4A-NA-C1A | 3.69 | 108.36 | 106.71 |
| 8 | M | 402 | BCL | CAD-C3D-C4D | -3.68 | 106.42 | 108.47 |
| 11 | H | 302 | PC1 | O21-C21-C22 | 3.67 | 119.42 | 111.50 |
| 11 | h | 302 | PC1 | O21-C21-C22 | 3.67 | 119.42 | 111.50 |
| 8 | K | 101 | BCL | C4A-NA-C1A | 3.67 | 108.36 | 106.71 |
| 8 | k | 101 | BCL | C4A-NA-C1A | 3.67 | 108.36 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | m | 402 | BCL | CAD-C3D-C4D | -3.65 | 106.43 | 108.47 |
| 8 | T | 101 | BCL | CMB-C2B-C1B | -3.63 | 122.88 | 128.46 |
| 8 | t | 101 | BCL | CMB-C2B-C1B | -3.63 | 122.88 | 128.46 |
| 8 | M | 403 | BCL | CAD-C3D-C4D | -3.63 | 106.44 | 108.47 |
| 8 | m | 403 | BCL | CAD-C3D-C4D | -3.63 | 106.44 | 108.47 |
| 8 | 5 | 101 | BCL | C1-C2-C3 | -3.60 | 120.93 | 126.75 |
| 8 | 3 | 101 | BCL | C1-C2-C3 | -3.59 | 120.94 | 126.75 |
| 8 | I | 101 | BCL | C4A-NA-C1A | 3.58 | 108.31 | 106.71 |
| 8 | i | 101 | BCL | C4A-NA-C1A | 3.58 | 108.31 | 106.71 |
| 8 | Q | 101 | BCL | OBD-CAD-CBD | -3.57 | 120.80 | 125.89 |
| 8 | W | 101 | BCL | CMB-C2B-C1B | -3.56 | 122.99 | 128.46 |
| 8 | w | 101 | BCL | CMB-C2B-C1B | -3.56 | 122.99 | 128.46 |
| 8 | S | 101 | BCL | OBD-CAD-CBD | -3.56 | 120.81 | 125.89 |
| 8 | g | 102 | BCL | CAD-C3D-C4D | -3.56 | 106.48 | 108.47 |
| 8 | w | 101 | BCL | C4A-NA-C1A | 3.56 | 108.31 | 106.71 |
| 8 | s | 101 | BCL | OBD-CAD-CBD | -3.55 | 120.82 | 125.89 |
| 8 | q | 101 | BCL | OBD-CAD-CBD | -3.55 | 120.82 | 125.89 |
| 8 | I | 101 | BCL | OBD-CAD-CBD | -3.54 | 120.83 | 125.89 |
| 8 | i | 101 | BCL | OBD-CAD-CBD | -3.54 | 120.83 | 125.89 |
| 8 | Z | 101 | BCL | CAD-C3D-C4D | -3.52 | 106.51 | 108.47 |
| 8 | z | 101 | BCL | CAD-C3D-C4D | -3.52 | 106.51 | 108.47 |
| 8 | 7 | 101 | BCL | OBD-CAD-CBD | -3.52 | 120.86 | 125.89 |
| 8 | 6 | 101 | BCL | OBD-CAD-CBD | -3.52 | 120.86 | 125.89 |
| 8 | A | 101 | BCL | C4A-NA-C1A | 3.51 | 108.28 | 106.71 |
| 8 | a | 101 | BCL | C4A-NA-C1A | 3.51 | 108.28 | 106.71 |
| 8 | U | 101 | BCL | C4A-NA-C1A | 3.50 | 108.28 | 106.71 |
| 8 | u | 101 | BCL | C4A-NA-C1A | 3.50 | 108.28 | 106.71 |
| 10 | L | 305 | U10 | C22-C23-C24 | -3.50 | 119.24 | 127.66 |
| 8 | G | 102 | BCL | CAD-C3D-C4D | -3.49 | 106.52 | 108.47 |
| 8 | D | 102 | BCL | OBD-CAD-CBD | -3.49 | 120.91 | 125.89 |
| 8 | d | 102 | BCL | OBD-CAD-CBD | -3.49 | 120.91 | 125.89 |
| 10 | l | 305 | U10 | C22-C23-C24 | -3.49 | 119.26 | 127.66 |
| 8 | V | 101 | BCL | OBD-CAD-CBD | -3.48 | 120.93 | 125.89 |
| 8 | v | 101 | BCL | OBD-CAD-CBD | -3.48 | 120.93 | 125.89 |
| 8 | W | 101 | BCL | C4A-NA-C1A | 3.47 | 108.27 | 106.71 |
| 8 | c | 101 | BCL | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 8 | u | 101 | BCL | OBD-CAD-CBD | -3.47 | 120.94 | 125.89 |
| 8 | C | 101 | BCL | CMB-C2B-C1B | -3.46 | 123.15 | 128.46 |
| 8 | 3 | 101 | BCL | OBD-CAD-CBD | -3.46 | 120.95 | 125.89 |
| 8 | 5 | 101 | BCL | OBD-CAD-CBD | -3.46 | 120.95 | 125.89 |
| 8 | R | 101 | BCL | OBD-CAD-CBD | -3.46 | 120.96 | 125.89 |
| 8 | r | 101 | BCL | OBD-CAD-CBD | -3.46 | 120.96 | 125.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | W | 101 | BCL | OBD-CAD-CBD | -3.46 | 120.96 | 125.89 |
| 8 | w | 101 | BCL | OBD-CAD-CBD | -3.46 | 120.96 | 125.89 |
| 8 | T | 101 | BCL | OBD-CAD-CBD | -3.45 | 120.97 | 125.89 |
| 8 | t | 101 | BCL | OBD-CAD-CBD | -3.45 | 120.97 | 125.89 |
| 8 | U | 101 | BCL | OBD-CAD-CBD | -3.44 | 120.98 | 125.89 |
| 8 | 9 | 101 | BCL | OBD-CAD-CBD | -3.44 | 120.98 | 125.89 |
| 8 | b9 | 101 | BCL | OBD-CAD-CBD | -3.44 | 120.98 | 125.89 |
| 8 | A | 101 | BCL | OBD-CAD-CBD | -3.44 | 120.98 | 125.89 |
| 8 | f | 101 | BCL | OBD-CAD-CBD | -3.43 | 120.99 | 125.89 |
| 8 | 3 | 101 | BCL | C4A-NA-C1A | 3.43 | 108.25 | 106.71 |
| 8 | 5 | 101 | BCL | C4A-NA-C1A | 3.43 | 108.25 | 106.71 |
| 8 | K | 101 | BCL | OBD-CAD-CBD | -3.43 | 120.99 | 125.89 |
| 8 | k | 101 | BCL | OBD-CAD-CBD | -3.43 | 120.99 | 125.89 |
| 8 | F | 101 | BCL | OBD-CAD-CBD | -3.43 | 121.00 | 125.89 |
| 8 | b1 | 101 | BCL | OBD-CAD-CBD | -3.43 | 121.00 | 125.89 |
| 8 | O | 101 | BCL | OBD-CAD-CBD | -3.42 | 121.01 | 125.89 |
| 8 | o | 101 | BCL | OBD-CAD-CBD | -3.42 | 121.01 | 125.89 |
| 8 | 1 | 101 | BCL | C4A-NA-C1A | 3.41 | 108.24 | 106.71 |
| 8 | b1 | 101 | BCL | C4A-NA-C1A | 3.41 | 108.24 | 106.71 |
| 8 | a | 101 | BCL | OBD-CAD-CBD | -3.41 | 121.03 | 125.89 |
| 8 | N | 102 | BCL | OBD-CAD-CBD | -3.40 | 121.04 | 125.89 |
| 8 | n | 102 | BCL | OBD-CAD-CBD | -3.40 | 121.04 | 125.89 |
| 8 | 1 | 101 | BCL | OBD-CAD-CBD | -3.40 | 121.04 | 125.89 |
| 8 | 4 | 101 | BCL | CAD-C3D-C4D | -3.40 | 106.58 | 108.47 |
| 8 | 2 | 101 | BCL | OBD-CAD-CBD | -3.39 | 121.05 | 125.89 |
| 8 | 4 | 101 | BCL | OBD-CAD-CBD | -3.39 | 121.05 | 125.89 |
| 10 | L | 304 | U10 | C17-C18-C19 | -3.39 | 119.51 | 127.66 |
| 10 | l | 304 | U10 | C17-C18-C19 | -3.39 | 119.51 | 127.66 |
| 8 | P | 102 | BCL | OBD-CAD-CBD | -3.38 | 121.06 | 125.89 |
| 8 | p | 102 | BCL | OBD-CAD-CBD | -3.38 | 121.06 | 125.89 |
| 8 | L | 301 | BCL | OBD-CAD-CBD | -3.37 | 121.08 | 125.89 |
| 8 | l | 301 | BCL | OBD-CAD-CBD | -3.37 | 121.08 | 125.89 |
| 10 | M | 405 | U10 | C27-C28-C29 | -3.37 | 119.56 | 127.66 |
| 8 | 0 | 101 | BCL | OBD-CAD-CBD | -3.36 | 121.09 | 125.89 |
| 8 | g | 102 | BCL | OBD-CAD-CBD | -3.36 | 121.09 | 125.89 |
| 8 | b0 | 101 | BCL | OBD-CAD-CBD | -3.36 | 121.09 | 125.89 |
| 8 | E | 102 | BCL | OBD-CAD-CBD | -3.36 | 121.09 | 125.89 |
| 8 | e | 102 | BCL | OBD-CAD-CBD | -3.36 | 121.09 | 125.89 |
| 8 | G | 102 | BCL | OBD-CAD-CBD | -3.36 | 121.09 | 125.89 |
| 10 | m | 405 | U10 | C27-C28-C29 | -3.36 | 119.57 | 127.66 |
| 10 | L | 305 | U10 | C15-C14-C16 | 3.36 | 120.92 | 115.27 |
| 10 | l | 305 | U10 | C15-C14-C16 | 3.36 | 120.92 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | C | 101 | BCL | OBD-CAD-CBD | -3.35 | 121.11 | 125.89 |
| 8 | c | 101 | BCL | OBD-CAD-CBD | -3.35 | 121.11 | 125.89 |
| 8 | B | 101 | BCL | OBD-CAD-CBD | -3.35 | 121.11 | 125.89 |
| 8 | b | 101 | BCL | OBD-CAD-CBD | -3.35 | 121.11 | 125.89 |
| 8 | J | 101 | BCL | OBD-CAD-CBD | -3.34 | 121.12 | 125.89 |
| 8 | j | 101 | BCL | OBD-CAD-CBD | -3.34 | 121.12 | 125.89 |
| 8 | G | 102 | BCL | C1-C2-C3 | 3.33 | 131.81 | 126.04 |
| 8 | g | 102 | BCL | C1-C2-C3 | 3.33 | 131.81 | 126.04 |
| 8 | E | 102 | BCL | CAD-C3D-C4D | -3.33 | 106.61 | 108.47 |
| 8 | e | 102 | BCL | CAD-C3D-C4D | -3.33 | 106.61 | 108.47 |
| 8 | 2 | 101 | BCL | CAD-C3D-C4D | -3.32 | 106.62 | 108.47 |
| 8 | Z | 101 | BCL | OBD-CAD-CBD | -3.32 | 121.15 | 125.89 |
| 8 | z | 101 | BCL | OBD-CAD-CBD | -3.32 | 121.15 | 125.89 |
| 8 | B | 101 | BCL | CAD-C3D-C4D | -3.32 | 106.62 | 108.47 |
| 8 | b | 101 | BCL | CAD-C3D-C4D | -3.32 | 106.62 | 108.47 |
| 8 | t | 101 | BCL | CAD-C3D-C4D | -3.32 | 106.62 | 108.47 |
| 10 | M | 405 | U10 | C25-C24-C26 | 3.31 | 120.85 | 115.27 |
| 10 | m | 405 | U10 | C25-C24-C26 | 3.31 | 120.85 | 115.27 |
| 10 | L | 304 | U10 | C15-C14-C16 | 3.31 | 120.84 | 115.27 |
| 10 | l | 304 | U10 | C15-C14-C16 | 3.31 | 120.84 | 115.27 |
| 8 | T | 101 | BCL | CAD-C3D-C4D | -3.31 | 106.62 | 108.47 |
| 8 | M | 403 | BCL | OBD-CAD-CBD | -3.30 | 121.18 | 125.89 |
| 8 | m | 403 | BCL | OBD-CAD-CBD | -3.30 | 121.18 | 125.89 |
| 8 | J | 101 | BCL | CAD-C3D-C4D | -3.30 | 106.63 | 108.47 |
| 8 | j | 101 | BCL | CAD-C3D-C4D | -3.30 | 106.63 | 108.47 |
| 8 | S | 101 | BCL | CMB-C2B-C3B | 3.30 | 130.84 | 124.68 |
| 8 | 7 | 101 | BCL | CMB-C2B-C3B | 3.30 | 130.84 | 124.68 |
| 8 | s | 101 | BCL | CMB-C2B-C3B | 3.30 | 130.84 | 124.68 |
| 8 | 6 | 101 | BCL | CMB-C2B-C3B | 3.30 | 130.84 | 124.68 |
| 8 | 7 | 102 | BCL | OBD-CAD-CBD | -3.29 | 121.19 | 125.89 |
| 8 | m | 402 | BCL | OBD-CAD-CBD | -3.29 | 121.19 | 125.89 |
| 8 | 6 | 102 | BCL | OBD-CAD-CBD | -3.29 | 121.19 | 125.89 |
| 8 | 0 | 101 | BCL | CAD-C3D-C4D | -3.29 | 106.64 | 108.47 |
| 8 | b0 | 101 | BCL | CAD-C3D-C4D | -3.29 | 106.64 | 108.47 |
| 8 | 7 | 101 | BCL | C4A-NA-C1A | 3.29 | 108.18 | 106.71 |
| 8 | 6 | 101 | BCL | C4A-NA-C1A | 3.29 | 108.18 | 106.71 |
| 8 | A | 101 | BCL | CMB-C2B-C3B | 3.28 | 130.82 | 124.68 |
| 8 | a | 101 | BCL | CMB-C2B-C3B | 3.28 | 130.82 | 124.68 |
| 8 | 2 | 101 | BCL | CMB-C2B-C1B | -3.28 | 123.42 | 128.46 |
| 8 | 4 | 101 | BCL | CMB-C2B-C1B | -3.28 | 123.42 | 128.46 |
| 10 | L | 304 | U10 | C25-C24-C26 | 3.28 | 120.78 | 115.27 |
| 8 | M | 402 | BCL | OBD-CAD-CBD | -3.27 | 121.22 | 125.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | 7 | 101 | BCL | CAD-C3D-C4D | -3.27 | 106.65 | 108.47 |
| 8 | 6 | 101 | BCL | CAD-C3D-C4D | -3.27 | 106.65 | 108.47 |
| 10 | l | 304 | U10 | C25-C24-C26 | 3.27 | 120.76 | 115.27 |
| 8 | L | 302 | BCL | OBD-CAD-CBD | -3.26 | 121.23 | 125.89 |
| 8 | l | 302 | BCL | OBD-CAD-CBD | -3.26 | 121.23 | 125.89 |
| 8 | P | 102 | BCL | CMB-C2B-C1B | -3.26 | 123.45 | 128.46 |
| 8 | p | 102 | BCL | CMB-C2B-C1B | -3.26 | 123.45 | 128.46 |
| 10 | m | 405 | U10 | C35-C34-C36 | 3.26 | 120.75 | 115.27 |
| 8 | M | 403 | BCL | CMB-C2B-C3B | 3.25 | 130.77 | 124.68 |
| 8 | m | 403 | BCL | CMB-C2B-C3B | 3.25 | 130.77 | 124.68 |
| 10 | M | 405 | U10 | C32-C33-C34 | -3.25 | 119.83 | 127.66 |
| 10 | m | 405 | U10 | C32-C33-C34 | -3.25 | 119.83 | 127.66 |
| 8 | F | 101 | BCL | C1-C2-C3 | -3.25 | 120.43 | 126.04 |
| 8 | f | 101 | BCL | C1-C2-C3 | -3.25 | 120.43 | 126.04 |
| 8 | O | 101 | BCL | CAD-C3D-C4D | -3.24 | 106.66 | 108.47 |
| 8 | o | 101 | BCL | CAD-C3D-C4D | -3.24 | 106.66 | 108.47 |
| 10 | M | 405 | U10 | C35-C34-C36 | 3.24 | 120.73 | 115.27 |
| 10 | L | 304 | U10 | C22-C23-C24 | -3.23 | 119.88 | 127.66 |
| 10 | l | 304 | U10 | C22-C23-C24 | -3.23 | 119.88 | 127.66 |
| 8 | Z | 101 | BCL | CMB-C2B-C1B | -3.21 | 123.52 | 128.46 |
| 8 | z | 101 | BCL | CMB-C2B-C1B | -3.21 | 123.52 | 128.46 |
| 8 | P | 102 | BCL | CAD-C3D-C4D | -3.21 | 106.68 | 108.47 |
| 8 | p | 102 | BCL | CAD-C3D-C4D | -3.21 | 106.68 | 108.47 |
| 8 | Q | 101 | BCL | CMB-C2B-C3B | 3.21 | 130.69 | 124.68 |
| 8 | q | 101 | BCL | CMB-C2B-C3B | 3.21 | 130.69 | 124.68 |
| 10 | M | 405 | U10 | C12-C13-C14 | -3.21 | 119.93 | 127.66 |
| 10 | m | 405 | U10 | C12-C13-C14 | -3.21 | 119.93 | 127.66 |
| 9 | M | 404 | BPH | OBD-CAD-CBD | -3.21 | 121.11 | 125.82 |
| 8 | r | 101 | BCL | CAD-C3D-C4D | -3.20 | 106.68 | 108.47 |
| 8 | Q | 101 | BCL | CAD-C3D-C4D | -3.20 | 106.69 | 108.47 |
| 8 | 1 | 101 | BCL | CAD-C3D-C4D | -3.20 | 106.69 | 108.47 |
| 8 | b1 | 101 | BCL | CAD-C3D-C4D | -3.20 | 106.69 | 108.47 |
| 9 | m | 404 | BPH | OBD-CAD-CBD | -3.19 | 121.15 | 125.82 |
| 8 | q | 101 | BCL | CAD-C3D-C4D | -3.18 | 106.69 | 108.47 |
| 8 | b0 | 101 | BCL | CHA-C1A-NA | -3.18 | 119.11 | 126.40 |
| 8 | R | 101 | BCL | CAD-C3D-C4D | -3.17 | 106.70 | 108.47 |
| 8 | 0 | 101 | BCL | CHA-C1A-NA | -3.17 | 119.14 | 126.40 |
| 8 | B | 101 | BCL | CHA-C1A-NA | -3.17 | 119.14 | 126.40 |
| 8 | b | 101 | BCL | CHA-C1A-NA | -3.17 | 119.14 | 126.40 |
| 8 | 9 | 101 | BCL | CMB-C2B-C3B | 3.16 | 130.60 | 124.68 |
| 8 | b9 | 101 | BCL | CMB-C2B-C3B | 3.16 | 130.60 | 124.68 |
| 10 | L | 305 | U10 | C27-C28-C29 | -3.16 | 120.04 | 127.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10 | l | 305 | U10 | C27-C28-C29 | -3.16 | 120.04 | 127.66 |
| 8 | F | 101 | BCL | CAD-C3D-C4D | -3.16 | 106.71 | 108.47 |
| 8 | 7 | 102 | BCL | CAD-C3D-C4D | -3.16 | 106.71 | 108.47 |
| 8 | 6 | 102 | BCL | CAD-C3D-C4D | -3.16 | 106.71 | 108.47 |
| 10 | M | 405 | U10 | C17-C18-C19 | -3.16 | 120.06 | 127.66 |
| 10 | m | 405 | U10 | C17-C18-C19 | -3.16 | 120.06 | 127.66 |
| 8 | L | 301 | BCL | CMB-C2B-C3B | 3.15 | 130.58 | 124.68 |
| 8 | l | 301 | BCL | CMB-C2B-C3B | 3.15 | 130.58 | 124.68 |
| 8 | f | 101 | BCL | CAD-C3D-C4D | -3.15 | 106.71 | 108.47 |
| 8 | m | 403 | BCL | CHA-C1A-NA | -3.15 | 119.19 | 126.40 |
| 8 | M | 403 | BCL | CHA-C1A-NA | -3.14 | 119.21 | 126.40 |
| 8 | D | 102 | BCL | CMB-C2B-C3B | 3.13 | 130.54 | 124.68 |
| 8 | d | 102 | BCL | CMB-C2B-C3B | 3.13 | 130.54 | 124.68 |
| 8 | e | 102 | BCL | CHA-C1A-NA | -3.13 | 119.24 | 126.40 |
| 10 | M | 405 | U10 | C22-C23-C24 | -3.13 | 120.14 | 127.66 |
| 10 | m | 405 | U10 | C22-C23-C24 | -3.13 | 120.14 | 127.66 |
| 8 | E | 102 | BCL | CHA-C1A-NA | -3.12 | 119.25 | 126.40 |
| 8 | g | 102 | BCL | CHA-C1A-NA | -3.12 | 119.26 | 126.40 |
| 8 | W | 101 | BCL | CHA-C1A-NA | -3.12 | 119.26 | 126.40 |
| 8 | w | 101 | BCL | CHA-C1A-NA | -3.12 | 119.26 | 126.40 |
| 8 | p | 102 | BCL | CHA-C1A-NA | -3.11 | 119.27 | 126.40 |
| 8 | G | 102 | BCL | CHA-C1A-NA | -3.11 | 119.28 | 126.40 |
| 8 | P | 102 | BCL | CHA-C1A-NA | -3.10 | 119.29 | 126.40 |
| 8 | V | 101 | BCL | CHA-C1A-NA | -3.10 | 119.30 | 126.40 |
| 8 | v | 101 | BCL | CHA-C1A-NA | -3.10 | 119.30 | 126.40 |
| 9 | L | 303 | BPH | OBD-CAD-CBD | -3.09 | 121.28 | 125.82 |
| 8 | f | 101 | BCL | CMB-C2B-C3B | 3.09 | 130.46 | 124.68 |
| 10 | l | 304 | U10 | C12-C13-C14 | -3.09 | 120.23 | 127.66 |
| 8 | 0 | 101 | BCL | CMB-C2B-C3B | 3.09 | 130.45 | 124.68 |
| 8 | b0 | 101 | BCL | CMB-C2B-C3B | 3.09 | 130.45 | 124.68 |
| 8 | T | 101 | BCL | CHA-C1A-NA | -3.09 | 119.33 | 126.40 |
| 10 | L | 304 | U10 | C12-C13-C14 | -3.08 | 120.24 | 127.66 |
| 9 | l | 303 | BPH | OBD-CAD-CBD | -3.08 | 121.31 | 125.82 |
| 8 | F | 101 | BCL | CMB-C2B-C3B | 3.08 | 130.44 | 124.68 |
| 8 | M | 402 | BCL | C2A-C1A-CHA | 3.08 | 129.24 | 123.86 |
| 8 | m | 402 | BCL | C2A-C1A-CHA | 3.08 | 129.24 | 123.86 |
| 8 | 7 | 102 | BCL | CMB-C2B-C3B | 3.07 | 130.43 | 124.68 |
| 8 | 6 | 102 | BCL | CMB-C2B-C3B | 3.07 | 130.43 | 124.68 |
| 8 | t | 101 | BCL | CHA-C1A-NA | -3.07 | 119.36 | 126.40 |
| 8 | 7 | 102 | BCL | CHA-C1A-NA | -3.07 | 119.37 | 126.40 |
| 8 | 6 | 102 | BCL | CHA-C1A-NA | -3.07 | 119.37 | 126.40 |
| 8 | s | 101 | BCL | CAD-C3D-C4D | -3.07 | 106.76 | 108.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | U | 101 | BCL | CHA-C1A-NA | -3.06 | 119.38 | 126.40 |
| 8 | u | 101 | BCL | CHA-C1A-NA | -3.06 | 119.38 | 126.40 |
| 8 | I | 101 | BCL | CHA-C1A-NA | -3.05 | 119.41 | 126.40 |
| 8 | i | 101 | BCL | CHA-C1A-NA | -3.05 | 119.41 | 126.40 |
| 8 | N | 102 | BCL | CAD-C3D-C4D | -3.05 | 106.77 | 108.47 |
| 8 | n | 102 | BCL | CAD-C3D-C4D | -3.05 | 106.77 | 108.47 |
| 8 | A | 101 | BCL | CHA-C1A-NA | -3.05 | 119.41 | 126.40 |
| 8 | a | 101 | BCL | CHA-C1A-NA | -3.05 | 119.41 | 126.40 |
| 8 | A | 101 | BCL | CAD-C3D-C4D | -3.05 | 106.77 | 108.47 |
| 8 | U | 101 | BCL | CAD-C3D-C4D | -3.05 | 106.77 | 108.47 |
| 8 | a | 101 | BCL | CAD-C3D-C4D | -3.05 | 106.77 | 108.47 |
| 8 | u | 101 | BCL | CAD-C3D-C4D | -3.05 | 106.77 | 108.47 |
| 8 | R | 101 | BCL | CHA-C1A-NA | -3.05 | 119.41 | 126.40 |
| 8 | r | 101 | BCL | CHA-C1A-NA | -3.05 | 119.41 | 126.40 |
| 8 | k | 101 | BCL | CHA-C1A-NA | -3.05 | 119.42 | 126.40 |
| 8 | 3 | 101 | BCL | CHA-C1A-NA | -3.04 | 119.43 | 126.40 |
| 8 | 5 | 101 | BCL | CHA-C1A-NA | -3.04 | 119.43 | 126.40 |
| 8 | S | 101 | BCL | CAD-C3D-C4D | -3.04 | 106.77 | 108.47 |
| 8 | Z | 101 | BCL | C4A-NA-C1A | 3.04 | 108.07 | 106.71 |
| 8 | K | 101 | BCL | CHA-C1A-NA | -3.03 | 119.45 | 126.40 |
| 8 | O | 101 | BCL | CHA-C1A-NA | -3.03 | 119.46 | 126.40 |
| 8 | Q | 101 | BCL | C16-C15-C13 | 3.03 | 125.71 | 115.92 |
| 8 | q | 101 | BCL | C16-C15-C13 | 3.03 | 125.71 | 115.92 |
| 8 | z | 101 | BCL | C4A-NA-C1A | 3.03 | 108.07 | 106.71 |
| 8 | l | 101 | BCL | CHA-C1A-NA | -3.03 | 119.47 | 126.40 |
| 8 | b1 | 101 | BCL | CHA-C1A-NA | -3.03 | 119.47 | 126.40 |
| 8 | F | 101 | BCL | CHA-C1A-NA | -3.02 | 119.47 | 126.40 |
| 8 | N | 102 | BCL | CHA-C1A-NA | -3.02 | 119.47 | 126.40 |
| 8 | f | 101 | BCL | CHA-C1A-NA | -3.02 | 119.47 | 126.40 |
| 8 | n | 102 | BCL | CHA-C1A-NA | -3.02 | 119.47 | 126.40 |
| 8 | M | 402 | BCL | CMB-C2B-C3B | 3.02 | 130.34 | 124.68 |
| 8 | m | 402 | BCL | CMB-C2B-C3B | 3.02 | 130.34 | 124.68 |
| 8 | Q | 101 | BCL | CHA-C1A-NA | -3.02 | 119.48 | 126.40 |
| 8 | q | 101 | BCL | CHA-C1A-NA | -3.02 | 119.48 | 126.40 |
| 8 | z | 101 | BCL | CHA-C1A-NA | -3.02 | 119.48 | 126.40 |
| 8 | o | 101 | BCL | CHA-C1A-NA | -3.02 | 119.49 | 126.40 |
| 8 | 9 | 101 | BCL | CHA-C1A-NA | -3.02 | 119.49 | 126.40 |
| 8 | b9 | 101 | BCL | CHA-C1A-NA | -3.02 | 119.49 | 126.40 |
| 8 | N | 102 | BCL | C4A-NA-C1A | 3.01 | 108.06 | 106.71 |
| 8 | n | 102 | BCL | C4A-NA-C1A | 3.01 | 108.06 | 106.71 |
| 8 | S | 101 | BCL | CHA-C1A-NA | -3.01 | 119.51 | 126.40 |
| 8 | s | 101 | BCL | CHA-C1A-NA | -3.01 | 119.51 | 126.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | M | 402 | BCL | C4A-NA-C1A | 3.01 | 108.06 | 106.71 |
| 8 | m | 402 | BCL | C4A-NA-C1A | 3.01 | 108.06 | 106.71 |
| 8 | Z | 101 | BCL | CHA-C1A-NA | -3.00 | 119.52 | 126.40 |
| 8 | E | 102 | BCL | C4A-NA-C1A | 3.00 | 108.06 | 106.71 |
| 8 | e | 102 | BCL | C4A-NA-C1A | 3.00 | 108.06 | 106.71 |
| 8 | J | 101 | BCL | CHA-C1A-NA | -3.00 | 119.53 | 126.40 |
| 8 | j | 101 | BCL | CHA-C1A-NA | -3.00 | 119.53 | 126.40 |
| 8 | 7 | 101 | BCL | CHA-C1A-NA | -3.00 | 119.54 | 126.40 |
| 8 | 6 | 101 | BCL | CHA-C1A-NA | -3.00 | 119.54 | 126.40 |
| 8 | K | 101 | BCL | CMB-C2B-C3B | 2.99 | 130.26 | 124.68 |
| 8 | k | 101 | BCL | CMB-C2B-C3B | 2.99 | 130.26 | 124.68 |
| 8 | W | 101 | BCL | C2A-C1A-CHA | 2.98 | 129.08 | 123.86 |
| 8 | w | 101 | BCL | C2A-C1A-CHA | 2.98 | 129.08 | 123.86 |
| 8 | 9 | 101 | BCL | CAD-C3D-C4D | -2.98 | 106.81 | 108.47 |
| 8 | b9 | 101 | BCL | CAD-C3D-C4D | -2.98 | 106.81 | 108.47 |
| 9 | L | 303 | BPH | CMB-C2B-C3B | 2.98 | 130.25 | 124.68 |
| 9 | l | 303 | BPH | CMB-C2B-C3B | 2.98 | 130.25 | 124.68 |
| 8 | J | 101 | BCL | C4A-NA-C1A | 2.97 | 108.04 | 106.71 |
| 8 | j | 101 | BCL | C4A-NA-C1A | 2.97 | 108.04 | 106.71 |
| 8 | M | 402 | BCL | CHA-C1A-NA | -2.97 | 119.59 | 126.40 |
| 8 | m | 402 | BCL | CHA-C1A-NA | -2.97 | 119.59 | 126.40 |
| 8 | L | 302 | BCL | CMB-C2B-C3B | 2.97 | 130.23 | 124.68 |
| 8 | D | 102 | BCL | CAD-C3D-C4D | -2.96 | 106.82 | 108.47 |
| 8 | d | 102 | BCL | CAD-C3D-C4D | -2.96 | 106.82 | 108.47 |
| 8 | 3 | 101 | BCL | CAD-C3D-C4D | -2.96 | 106.82 | 108.47 |
| 8 | 5 | 101 | BCL | CAD-C3D-C4D | -2.96 | 106.82 | 108.47 |
| 8 | D | 102 | BCL | CHA-C1A-NA | -2.96 | 119.62 | 126.40 |
| 8 | d | 102 | BCL | CHA-C1A-NA | -2.96 | 119.62 | 126.40 |
| 8 | P | 102 | BCL | C6-C7-C8 | -2.96 | 106.36 | 115.92 |
| 8 | p | 102 | BCL | C6-C7-C8 | -2.96 | 106.36 | 115.92 |
| 8 | l | 302 | BCL | CMB-C2B-C3B | 2.95 | 130.20 | 124.68 |
| 8 | C | 101 | BCL | CHA-C1A-NA | -2.95 | 119.65 | 126.40 |
| 8 | c | 101 | BCL | CHA-C1A-NA | -2.95 | 119.65 | 126.40 |
| 8 | U | 101 | BCL | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 8 | u | 101 | BCL | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 8 | 7 | 102 | BCL | C2A-C1A-CHA | 2.93 | 128.99 | 123.86 |
| 8 | 6 | 102 | BCL | C2A-C1A-CHA | 2.93 | 128.98 | 123.86 |
| 8 | O | 101 | BCL | C2A-C1A-CHA | 2.92 | 128.97 | 123.86 |
| 8 | o | 101 | BCL | C2A-C1A-CHA | 2.92 | 128.97 | 123.86 |
| 8 | l | 302 | BCL | CHA-C1A-NA | -2.92 | 119.71 | 126.40 |
| 8 | 2 | 101 | BCL | C2A-C1A-CHA | 2.92 | 128.96 | 123.86 |
| 8 | I | 101 | BCL | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | i | 101 | BCL | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |
| 8 | L | 302 | BCL | CHA-C1A-NA | -2.91 | 119.74 | 126.40 |
| 8 | 4 | 101 | BCL | C2A-C1A-CHA | 2.90 | 128.93 | 123.86 |
| 8 | B | 101 | BCL | CMB-C2B-C3B | 2.90 | 130.09 | 124.68 |
| 8 | b | 101 | BCL | CMB-C2B-C3B | 2.90 | 130.09 | 124.68 |
| 8 | B | 101 | BCL | C2A-C1A-CHA | 2.89 | 128.92 | 123.86 |
| 8 | b | 101 | BCL | C2A-C1A-CHA | 2.89 | 128.92 | 123.86 |
| 10 | L | 305 | U10 | C25-C24-C26 | 2.89 | 120.13 | 115.27 |
| 10 | l | 305 | U10 | C25-C24-C26 | 2.89 | 120.13 | 115.27 |
| 8 | g | 102 | BCL | C2A-C1A-CHA | 2.88 | 128.90 | 123.86 |
| 10 | L | 305 | U10 | C30-C29-C31 | 2.88 | 120.12 | 115.27 |
| 10 | l | 305 | U10 | C30-C29-C31 | 2.88 | 120.12 | 115.27 |
| 11 | A | 103 | PC1 | O31-C31-C32 | 2.88 | 120.95 | 111.91 |
| 11 | a | 103 | PC1 | O31-C31-C32 | 2.88 | 120.95 | 111.91 |
| 8 | 2 | 101 | BCL | CHA-C1A-NA | -2.88 | 119.80 | 126.40 |
| 8 | 4 | 101 | BCL | CHA-C1A-NA | -2.88 | 119.80 | 126.40 |
| 8 | b0 | 101 | BCL | C2A-C1A-CHA | 2.88 | 128.89 | 123.86 |
| 8 | C | 101 | BCL | C2A-C1A-CHA | 2.88 | 128.89 | 123.86 |
| 8 | c | 101 | BCL | C2A-C1A-CHA | 2.88 | 128.89 | 123.86 |
| 8 | V | 101 | BCL | C2A-C1A-CHA | 2.87 | 128.89 | 123.86 |
| 8 | v | 101 | BCL | C2A-C1A-CHA | 2.87 | 128.89 | 123.86 |
| 8 | 7 | 102 | BCL | C4A-NA-C1A | 2.87 | 108.00 | 106.71 |
| 8 | G | 102 | BCL | C2A-C1A-CHA | 2.87 | 128.88 | 123.86 |
| 8 | K | 101 | BCL | C1-C2-C3 | -2.87 | 121.08 | 126.04 |
| 10 | M | 405 | U10 | C15-C14-C16 | 2.87 | 120.09 | 115.27 |
| 10 | m | 405 | U10 | C15-C14-C16 | 2.87 | 120.09 | 115.27 |
| 8 | 0 | 101 | BCL | C2A-C1A-CHA | 2.87 | 128.87 | 123.86 |
| 8 | 0 | 101 | BCL | C6-C7-C8 | -2.87 | 106.66 | 115.92 |
| 8 | b0 | 101 | BCL | C6-C7-C8 | -2.87 | 106.66 | 115.92 |
| 8 | z | 101 | BCL | C2A-C1A-CHA | 2.87 | 128.87 | 123.86 |
| 8 | L | 301 | BCL | CHA-C1A-NA | -2.86 | 119.84 | 126.40 |
| 8 | l | 302 | BCL | C2A-C1A-CHA | 2.86 | 128.86 | 123.86 |
| 10 | L | 305 | U10 | C10-C9-C11 | 2.86 | 120.08 | 115.27 |
| 10 | l | 305 | U10 | C10-C9-C11 | 2.86 | 120.08 | 115.27 |
| 8 | P | 102 | BCL | C4A-NA-C1A | 2.86 | 107.99 | 106.71 |
| 8 | E | 102 | BCL | CMB-C2B-C3B | 2.86 | 130.03 | 124.68 |
| 8 | e | 102 | BCL | CMB-C2B-C3B | 2.86 | 130.03 | 124.68 |
| 8 | C | 101 | BCL | CAD-C3D-C4D | -2.86 | 106.88 | 108.47 |
| 8 | c | 101 | BCL | CAD-C3D-C4D | -2.86 | 106.88 | 108.47 |
| 8 | 6 | 102 | BCL | C4A-NA-C1A | 2.85 | 107.99 | 106.71 |
| 8 | G | 102 | BCL | CMB-C2B-C3B | 2.85 | 130.02 | 124.68 |
| 8 | g | 102 | BCL | CMB-C2B-C3B | 2.85 | 130.02 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | Z | 101 | BCL | C2A-C1A-CHA | 2.85 | 128.85 | 123.86 |
| 8 | J | 101 | BCL | CMB-C2B-C3B | 2.85 | 130.02 | 124.68 |
| 8 | k | 101 | BCL | C1-C2-C3 | -2.85 | 121.11 | 126.04 |
| 8 | l | 301 | BCL | CHA-C1A-NA | -2.85 | 119.87 | 126.40 |
| 8 | L | 302 | BCL | C2A-C1A-CHA | 2.84 | 128.83 | 123.86 |
| 8 | e | 102 | BCL | C2A-C1A-CHA | 2.84 | 128.83 | 123.86 |
| 8 | A | 101 | BCL | C2A-C1A-CHA | 2.84 | 128.83 | 123.86 |
| 8 | P | 102 | BCL | C2A-C1A-CHA | 2.84 | 128.83 | 123.86 |
| 8 | a | 101 | BCL | C2A-C1A-CHA | 2.84 | 128.83 | 123.86 |
| 8 | p | 102 | BCL | C2A-C1A-CHA | 2.84 | 128.83 | 123.86 |
| 8 | E | 102 | BCL | C2A-C1A-CHA | 2.84 | 128.82 | 123.86 |
| 8 | K | 101 | BCL | CAD-C3D-C4D | -2.84 | 106.89 | 108.47 |
| 8 | k | 101 | BCL | CAD-C3D-C4D | -2.84 | 106.89 | 108.47 |
| 8 | j | 101 | BCL | CMB-C2B-C3B | 2.83 | 129.98 | 124.68 |
| 14 | F | 102 | CDL | OB8-CB7-C71 | 2.83 | 120.79 | 111.91 |
| 14 | f | 102 | CDL | OB8-CB7-C71 | 2.83 | 120.79 | 111.91 |
| 8 | N | 102 | BCL | CMB-C2B-C3B | 2.82 | 129.96 | 124.68 |
| 8 | n | 102 | BCL | CMB-C2B-C3B | 2.82 | 129.96 | 124.68 |
| 8 | L | 301 | BCL | C2A-C1A-CHA | 2.81 | 128.78 | 123.86 |
| 8 | p | 102 | BCL | C4A-NA-C1A | 2.81 | 107.97 | 106.71 |
| 8 | N | 102 | BCL | C2A-C1A-CHA | 2.80 | 128.76 | 123.86 |
| 8 | n | 102 | BCL | C2A-C1A-CHA | 2.80 | 128.76 | 123.86 |
| 10 | M | 405 | U10 | C10-C9-C11 | 2.80 | 119.98 | 115.27 |
| 10 | m | 405 | U10 | C10-C9-C11 | 2.80 | 119.98 | 115.27 |
| 8 | 5 | 101 | BCL | CMB-C2B-C3B | 2.80 | 129.91 | 124.68 |
| 8 | l | 301 | BCL | C2A-C1A-CHA | 2.79 | 128.74 | 123.86 |
| 8 | O | 101 | BCL | CMB-C2B-C3B | 2.79 | 129.90 | 124.68 |
| 8 | o | 101 | BCL | CMB-C2B-C3B | 2.79 | 129.90 | 124.68 |
| 8 | 9 | 101 | BCL | C2A-C1A-CHA | 2.78 | 128.72 | 123.86 |
| 8 | b9 | 101 | BCL | C2A-C1A-CHA | 2.78 | 128.72 | 123.86 |
| 8 | T | 101 | BCL | C2A-C1A-CHA | 2.78 | 128.72 | 123.86 |
| 8 | 3 | 101 | BCL | CMB-C2B-C3B | 2.78 | 129.88 | 124.68 |
| 8 | m | 403 | BCL | C2A-C1A-CHA | 2.78 | 128.71 | 123.86 |
| 8 | t | 101 | BCL | C2A-C1A-CHA | 2.77 | 128.70 | 123.86 |
| 8 | M | 403 | BCL | C2A-C1A-CHA | 2.77 | 128.70 | 123.86 |
| 8 | L | 302 | BCL | C4A-NA-C1A | 2.76 | 107.95 | 106.71 |
| 8 | l | 302 | BCL | C4A-NA-C1A | 2.76 | 107.95 | 106.71 |
| 8 | F | 101 | BCL | C2A-C1A-CHA | 2.76 | 128.69 | 123.86 |
| 8 | f | 101 | BCL | C2A-C1A-CHA | 2.76 | 128.69 | 123.86 |
| 8 | l | 101 | BCL | CMB-C2B-C3B | 2.76 | 129.84 | 124.68 |
| 8 | b1 | 101 | BCL | CMB-C2B-C3B | 2.76 | 129.84 | 124.68 |
| 8 | k | 101 | BCL | C2A-C1A-CHA | 2.76 | 128.68 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | s | 101 | BCL | C1-C2-C3 | -2.76 | 121.28 | 126.04 |
| 8 | N | 102 | BCL | C1-C2-C3 | 2.75 | 130.80 | 126.04 |
| 8 | n | 102 | BCL | C1-C2-C3 | 2.75 | 130.80 | 126.04 |
| 14 | m | 407 | CDL | OB8-CB7-C71 | 2.75 | 120.54 | 111.91 |
| 8 | C | 101 | BCL | C4A-NA-C1A | 2.75 | 107.94 | 106.71 |
| 8 | c | 101 | BCL | C4A-NA-C1A | 2.75 | 107.94 | 106.71 |
| 8 | S | 101 | BCL | C1-C2-C3 | -2.75 | 121.28 | 126.04 |
| 10 | M | 405 | U10 | C30-C29-C31 | 2.75 | 119.89 | 115.27 |
| 10 | m | 405 | U10 | C30-C29-C31 | 2.75 | 119.89 | 115.27 |
| 8 | J | 101 | BCL | C2A-C1A-CHA | 2.75 | 128.66 | 123.86 |
| 8 | j | 101 | BCL | C2A-C1A-CHA | 2.75 | 128.66 | 123.86 |
| 11 | D | 101 | PC1 | O31-C31-C32 | 2.74 | 120.52 | 111.91 |
| 11 | d | 101 | PC1 | O31-C31-C32 | 2.74 | 120.52 | 111.91 |
| 14 | M | 407 | CDL | OB8-CB7-C71 | 2.74 | 120.51 | 111.91 |
| 8 | K | 101 | BCL | C2A-C1A-CHA | 2.74 | 128.65 | 123.86 |
| 11 | H | 301 | PC1 | O31-C31-C32 | 2.74 | 120.49 | 111.91 |
| 11 | h | 301 | PC1 | O31-C31-C32 | 2.74 | 120.49 | 111.91 |
| 8 | 3 | 101 | BCL | C2A-C1A-CHA | 2.73 | 128.64 | 123.86 |
| 8 | 5 | 101 | BCL | C2A-C1A-CHA | 2.73 | 128.64 | 123.86 |
| 8 | M | 403 | BCL | OBB-CAB-CBB | -2.73 | 114.02 | 120.17 |
| 8 | m | 403 | BCL | OBB-CAB-CBB | -2.73 | 114.02 | 120.17 |
| 8 | R | 101 | BCL | CMB-C2B-C3B | 2.73 | 129.79 | 124.68 |
| 8 | r | 101 | BCL | CMB-C2B-C3B | 2.73 | 129.79 | 124.68 |
| 8 | 7 | 101 | BCL | C2A-C1A-CHA | 2.73 | 128.63 | 123.86 |
| 8 | 6 | 101 | BCL | C2A-C1A-CHA | 2.73 | 128.63 | 123.86 |
| 10 | M | 405 | U10 | C20-C19-C21 | 2.72 | 119.85 | 115.27 |
| 10 | m | 405 | U10 | C20-C19-C21 | 2.72 | 119.85 | 115.27 |
| 8 | V | 101 | BCL | CMD-C2D-C3D | 2.71 | 129.75 | 124.68 |
| 8 | v | 101 | BCL | CMD-C2D-C3D | 2.71 | 129.75 | 124.68 |
| 8 | i | 101 | BCL | C1-C2-C3 | -2.71 | 121.36 | 126.04 |
| 8 | I | 101 | BCL | C2A-C1A-CHA | 2.70 | 128.59 | 123.86 |
| 8 | i | 101 | BCL | C2A-C1A-CHA | 2.70 | 128.58 | 123.86 |
| 8 | R | 101 | BCL | C2A-C1A-CHA | 2.70 | 128.57 | 123.86 |
| 8 | r | 101 | BCL | C2A-C1A-CHA | 2.70 | 128.57 | 123.86 |
| 8 | B | 101 | BCL | C4A-NA-C1A | 2.69 | 107.92 | 106.71 |
| 8 | b | 101 | BCL | C4A-NA-C1A | 2.69 | 107.92 | 106.71 |
| 8 | D | 102 | BCL | C2A-C1A-CHA | 2.69 | 128.56 | 123.86 |
| 8 | d | 102 | BCL | C2A-C1A-CHA | 2.69 | 128.56 | 123.86 |
| 8 | V | 101 | BCL | CMB-C2B-C3B | 2.69 | 129.70 | 124.68 |
| 8 | v | 101 | BCL | CMB-C2B-C3B | 2.69 | 129.70 | 124.68 |
| 8 | I | 101 | BCL | C1-C2-C3 | -2.68 | 121.40 | 126.04 |
| 8 | T | 101 | BCL | CMD-C2D-C3D | 2.68 | 129.69 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | t | 101 | BCL | CMD-C2D-C3D | 2.68 | 129.69 | 124.68 |
| 14 | M | 407 | CDL | OA8-CA7-C31 | 2.66 | 120.25 | 111.91 |
| 14 | m | 407 | CDL | OA8-CA7-C31 | 2.66 | 120.25 | 111.91 |
| 8 | U | 101 | BCL | C2A-C1A-CHA | 2.66 | 128.51 | 123.86 |
| 8 | u | 101 | BCL | C2A-C1A-CHA | 2.66 | 128.51 | 123.86 |
| 8 | E | 102 | BCL | CMD-C2D-C3D | 2.66 | 129.65 | 124.68 |
| 8 | e | 102 | BCL | CMD-C2D-C3D | 2.66 | 129.65 | 124.68 |
| 9 | M | 404 | BPH | CMB-C2B-C3B | 2.65 | 129.64 | 124.68 |
| 9 | m | 404 | BPH | CMB-C2B-C3B | 2.65 | 129.64 | 124.68 |
| 10 | L | 304 | U10 | C1M-C1-C6 | -2.65 | 120.08 | 124.40 |
| 10 | l | 304 | U10 | C1M-C1-C6 | -2.65 | 120.08 | 124.40 |
| 8 | 2 | 101 | BCL | C4A-NA-C1A | 2.64 | 107.89 | 106.71 |
| 8 | 4 | 101 | BCL | C4A-NA-C1A | 2.64 | 107.89 | 106.71 |
| 8 | T | 101 | BCL | CMB-C2B-C3B | 2.64 | 129.62 | 124.68 |
| 8 | t | 101 | BCL | CMB-C2B-C3B | 2.64 | 129.62 | 124.68 |
| 8 | 6 | 102 | BCL | C4B-C3B-CAB | -2.63 | 122.04 | 127.13 |
| 8 | p | 102 | BCL | C1-C2-C3 | 2.63 | 130.59 | 126.04 |
| 10 | L | 305 | U10 | C1M-C1-C6 | -2.63 | 120.11 | 124.40 |
| 10 | l | 305 | U10 | C1M-C1-C6 | -2.63 | 120.11 | 124.40 |
| 8 | 7 | 102 | BCL | C4B-C3B-CAB | -2.63 | 122.05 | 127.13 |
| 8 | P | 102 | BCL | C1-C2-C3 | 2.62 | 130.57 | 126.04 |
| 8 | S | 101 | BCL | C2A-C1A-CHA | 2.62 | 128.44 | 123.86 |
| 8 | s | 101 | BCL | C2A-C1A-CHA | 2.62 | 128.44 | 123.86 |
| 8 | B | 101 | BCL | C6-C7-C8 | -2.61 | 107.48 | 115.92 |
| 8 | b | 101 | BCL | C6-C7-C8 | -2.61 | 107.48 | 115.92 |
| 8 | R | 101 | BCL | CMD-C2D-C3D | 2.60 | 129.55 | 124.68 |
| 8 | r | 101 | BCL | CMD-C2D-C3D | 2.60 | 129.55 | 124.68 |
| 8 | P | 102 | BCL | CMD-C2D-C3D | 2.60 | 129.54 | 124.68 |
| 8 | p | 102 | BCL | CMD-C2D-C3D | 2.60 | 129.54 | 124.68 |
| 8 | Q | 101 | BCL | C2A-C1A-CHA | 2.60 | 128.40 | 123.86 |
| 8 | q | 101 | BCL | C2A-C1A-CHA | 2.60 | 128.40 | 123.86 |
| 8 | J | 101 | BCL | CMD-C2D-C3D | 2.59 | 129.53 | 124.68 |
| 8 | 0 | 101 | BCL | CMD-C2D-C3D | 2.59 | 129.53 | 124.68 |
| 8 | j | 101 | BCL | CMD-C2D-C3D | 2.59 | 129.53 | 124.68 |
| 8 | b0 | 101 | BCL | CMD-C2D-C3D | 2.59 | 129.53 | 124.68 |
| 8 | P | 102 | BCL | C4B-C3B-CAB | -2.59 | 122.12 | 127.13 |
| 8 | p | 102 | BCL | C4B-C3B-CAB | -2.59 | 122.12 | 127.13 |
| 8 | N | 102 | BCL | CMD-C2D-C3D | 2.59 | 129.53 | 124.68 |
| 8 | n | 102 | BCL | CMD-C2D-C3D | 2.59 | 129.53 | 124.68 |
| 8 | W | 101 | BCL | CMB-C2B-C3B | 2.59 | 129.52 | 124.68 |
| 8 | w | 101 | BCL | CMB-C2B-C3B | 2.59 | 129.52 | 124.68 |
| 8 | 7 | 102 | BCL | CMD-C2D-C3D | 2.59 | 129.52 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | 6 | 102 | BCL | CMD-C2D-C3D | 2.59 | 129.52 | 124.68 |
| 11 | L | 306 | PC1 | O31-C31-C32 | 2.57 | 119.98 | 111.91 |
| 11 | l | 306 | PC1 | O31-C31-C32 | 2.57 | 119.98 | 111.91 |
| 10 | l | 304 | U10 | C10-C9-C11 | 2.57 | 119.60 | 115.27 |
| 10 | L | 304 | U10 | C10-C9-C11 | 2.57 | 119.59 | 115.27 |
| 8 | a | 101 | BCL | CMD-C2D-C3D | 2.57 | 129.48 | 124.68 |
| 11 | A | 105 | PC1 | O12-P-O14 | 2.56 | 124.90 | 112.24 |
| 8 | B | 101 | BCL | CMD-C2D-C3D | 2.56 | 129.47 | 124.68 |
| 11 | a | 105 | PC1 | O12-P-O14 | 2.56 | 124.88 | 112.24 |
| 11 | L | 307 | PC1 | O31-C31-C32 | 2.56 | 119.93 | 111.91 |
| 11 | l | 307 | PC1 | O31-C31-C32 | 2.55 | 119.92 | 111.91 |
| 8 | c | 101 | BCL | CMD-C2D-C3D | 2.55 | 129.45 | 124.68 |
| 8 | A | 101 | BCL | CMD-C2D-C3D | 2.55 | 129.45 | 124.68 |
| 8 | R | 101 | BCL | C4A-NA-C1A | 2.55 | 107.85 | 106.71 |
| 8 | r | 101 | BCL | C4A-NA-C1A | 2.55 | 107.85 | 106.71 |
| 8 | w | 101 | BCL | C1-C2-C3 | -2.55 | 121.64 | 126.04 |
| 8 | t | 101 | BCL | C4A-NA-C1A | 2.54 | 107.85 | 106.71 |
| 8 | G | 102 | BCL | CMD-C2D-C3D | 2.54 | 129.44 | 124.68 |
| 8 | g | 102 | BCL | CMD-C2D-C3D | 2.54 | 129.44 | 124.68 |
| 8 | b | 101 | BCL | CMD-C2D-C3D | 2.54 | 129.43 | 124.68 |
| 8 | C | 101 | BCL | CMD-C2D-C3D | 2.54 | 129.43 | 124.68 |
| 8 | c | 101 | BCL | CMB-C2B-C3B | 2.54 | 129.43 | 124.68 |
| 8 | 0 | 101 | BCL | C4B-C3B-CAB | -2.53 | 122.23 | 127.13 |
| 8 | b0 | 101 | BCL | C4B-C3B-CAB | -2.53 | 122.23 | 127.13 |
| 10 | L | 305 | U10 | C20-C19-C21 | 2.53 | 119.53 | 115.27 |
| 10 | l | 305 | U10 | C20-C19-C21 | 2.53 | 119.53 | 115.27 |
| 8 | W | 101 | BCL | C1-C2-C3 | -2.53 | 121.67 | 126.04 |
| 8 | C | 101 | BCL | CMB-C2B-C3B | 2.53 | 129.41 | 124.68 |
| 8 | D | 102 | BCL | OBB-CAB-CBB | -2.52 | 114.51 | 120.17 |
| 8 | d | 102 | BCL | OBB-CAB-CBB | -2.52 | 114.51 | 120.17 |
| 8 | 0 | 101 | BCL | C4A-NA-C1A | 2.51 | 107.83 | 106.71 |
| 9 | L | 303 | BPH | CMD-C2D-C3D | 2.50 | 129.36 | 124.68 |
| 9 | l | 303 | BPH | CMD-C2D-C3D | 2.50 | 129.36 | 124.68 |
| 8 | G | 102 | BCL | C6-C7-C8 | -2.50 | 107.84 | 115.92 |
| 8 | g | 102 | BCL | C6-C7-C8 | -2.50 | 107.84 | 115.92 |
| 14 | F | 102 | CDL | OA8-CA7-C31 | 2.50 | 119.74 | 111.91 |
| 14 | f | 102 | CDL | OA8-CA7-C31 | 2.50 | 119.74 | 111.91 |
| 8 | l | 101 | BCL | C2A-C1A-CHA | 2.50 | 128.22 | 123.86 |
| 8 | b1 | 101 | BCL | C2A-C1A-CHA | 2.50 | 128.22 | 123.86 |
| 8 | E | 102 | BCL | C4B-C3B-CAB | -2.49 | 122.33 | 127.13 |
| 8 | e | 102 | BCL | C4B-C3B-CAB | -2.49 | 122.33 | 127.13 |
| 8 | T | 101 | BCL | C4A-NA-C1A | 2.48 | 107.82 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10 | l | 304 | U10 | C31-C29-C30 | 2.48 | 120.07 | 114.60 |
| 8 | 9 | 101 | BCL | CMD-C2D-C3D | 2.47 | 129.30 | 124.68 |
| 8 | b9 | 101 | BCL | CMD-C2D-C3D | 2.47 | 129.30 | 124.68 |
| 8 | Q | 101 | BCL | OBB-CAB-CBB | -2.47 | 114.62 | 120.17 |
| 8 | q | 101 | BCL | OBB-CAB-CBB | -2.47 | 114.62 | 120.17 |
| 10 | L | 304 | U10 | C31-C29-C30 | 2.46 | 120.04 | 114.60 |
| 8 | A | 101 | BCL | OBB-CAB-CBB | -2.46 | 114.63 | 120.17 |
| 8 | a | 101 | BCL | OBB-CAB-CBB | -2.46 | 114.63 | 120.17 |
| 8 | F | 101 | BCL | CMD-C2D-C3D | 2.46 | 129.28 | 124.68 |
| 8 | f | 101 | BCL | CMD-C2D-C3D | 2.46 | 129.28 | 124.68 |
| 11 | A | 104 | PC1 | O31-C31-C32 | 2.45 | 119.61 | 111.91 |
| 11 | a | 104 | PC1 | O31-C31-C32 | 2.45 | 119.61 | 111.91 |
| 8 | 7 | 101 | BCL | OBB-CAB-CBB | -2.45 | 114.65 | 120.17 |
| 8 | 6 | 101 | BCL | OBB-CAB-CBB | -2.45 | 114.65 | 120.17 |
| 8 | Q | 101 | BCL | CMD-C2D-C3D | 2.45 | 129.26 | 124.68 |
| 10 | M | 405 | U10 | C7-C8-C9 | -2.45 | 122.71 | 126.79 |
| 10 | m | 405 | U10 | C7-C8-C9 | -2.45 | 122.71 | 126.79 |
| 8 | u | 101 | BCL | CMD-C2D-C3D | 2.45 | 129.26 | 124.68 |
| 8 | K | 101 | BCL | CMD-C2D-C3D | 2.45 | 129.26 | 124.68 |
| 8 | k | 101 | BCL | CMD-C2D-C3D | 2.45 | 129.26 | 124.68 |
| 8 | R | 101 | BCL | C4B-C3B-CAB | -2.45 | 122.40 | 127.13 |
| 8 | b0 | 101 | BCL | C4A-NA-C1A | 2.45 | 107.81 | 106.71 |
| 11 | H | 302 | PC1 | O31-C31-C32 | 2.45 | 119.58 | 111.91 |
| 11 | h | 302 | PC1 | O31-C31-C32 | 2.45 | 119.58 | 111.91 |
| 8 | U | 101 | BCL | CMD-C2D-C3D | 2.44 | 129.25 | 124.68 |
| 8 | q | 101 | BCL | CMD-C2D-C3D | 2.44 | 129.25 | 124.68 |
| 8 | 3 | 101 | BCL | CMD-C2D-C3D | 2.44 | 129.25 | 124.68 |
| 8 | S | 101 | BCL | OBB-CAB-CBB | -2.44 | 114.67 | 120.17 |
| 8 | s | 101 | BCL | OBB-CAB-CBB | -2.44 | 114.67 | 120.17 |
| 8 | L | 302 | BCL | CMD-C2D-C3D | 2.44 | 129.25 | 124.68 |
| 8 | l | 302 | BCL | CMD-C2D-C3D | 2.44 | 129.25 | 124.68 |
| 8 | S | 101 | BCL | CMD-C2D-C3D | 2.44 | 129.24 | 124.68 |
| 8 | s | 101 | BCL | CMD-C2D-C3D | 2.44 | 129.24 | 124.68 |
| 8 | 5 | 101 | BCL | CMD-C2D-C3D | 2.44 | 129.24 | 124.68 |
| 8 | P | 102 | BCL | CMB-C2B-C3B | 2.44 | 129.24 | 124.68 |
| 8 | p | 102 | BCL | CMB-C2B-C3B | 2.44 | 129.24 | 124.68 |
| 8 | r | 101 | BCL | C4B-C3B-CAB | -2.43 | 122.43 | 127.13 |
| 8 | O | 101 | BCL | CMD-C2D-C3D | 2.43 | 129.22 | 124.68 |
| 8 | D | 102 | BCL | CMD-C2D-C3D | 2.43 | 129.22 | 124.68 |
| 8 | Z | 101 | BCL | CMD-C2D-C3D | 2.43 | 129.22 | 124.68 |
| 8 | d | 102 | BCL | CMD-C2D-C3D | 2.43 | 129.22 | 124.68 |
| 8 | z | 101 | BCL | CMD-C2D-C3D | 2.43 | 129.22 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | V | 101 | BCL | CBA-CAA-C2A | -2.43 | 106.70 | 113.86 |
| 8 | v | 101 | BCL | CBA-CAA-C2A | -2.43 | 106.70 | 113.86 |
| 8 | o | 101 | BCL | CMD-C2D-C3D | 2.42 | 129.21 | 124.68 |
| 9 | L | 303 | BPH | C11-C10-C8 | -2.42 | 108.09 | 115.92 |
| 9 | l | 303 | BPH | C11-C10-C8 | -2.42 | 108.09 | 115.92 |
| 8 | I | 101 | BCL | CMD-C2D-C3D | 2.42 | 129.20 | 124.68 |
| 8 | i | 101 | BCL | CMD-C2D-C3D | 2.42 | 129.20 | 124.68 |
| 8 | b1 | 101 | BCL | CMD-C2D-C3D | 2.41 | 129.19 | 124.68 |
| 8 | 1 | 101 | BCL | CMD-C2D-C3D | 2.40 | 129.17 | 124.68 |
| 10 | L | 305 | U10 | C36-C34-C35 | 2.40 | 119.90 | 114.60 |
| 10 | l | 305 | U10 | C36-C34-C35 | 2.40 | 119.90 | 114.60 |
| 11 | A | 104 | PC1 | O12-P-O14 | -2.40 | 100.39 | 112.24 |
| 8 | V | 101 | BCL | C4A-NA-C1A | 2.39 | 107.78 | 106.71 |
| 8 | v | 101 | BCL | C4A-NA-C1A | 2.39 | 107.78 | 106.71 |
| 11 | a | 104 | PC1 | O12-P-O14 | -2.39 | 100.41 | 112.24 |
| 8 | 2 | 101 | BCL | CMB-C2B-C3B | 2.39 | 129.14 | 124.68 |
| 8 | 4 | 101 | BCL | CMB-C2B-C3B | 2.39 | 129.14 | 124.68 |
| 8 | 9 | 101 | BCL | OBB-CAB-CBB | -2.38 | 114.82 | 120.17 |
| 8 | b9 | 101 | BCL | OBB-CAB-CBB | -2.38 | 114.82 | 120.17 |
| 9 | M | 404 | BPH | CMD-C2D-C3D | 2.38 | 129.12 | 124.68 |
| 9 | m | 404 | BPH | CMD-C2D-C3D | 2.38 | 129.12 | 124.68 |
| 8 | K | 101 | BCL | C1C-NC-C4C | 2.38 | 107.77 | 106.71 |
| 8 | k | 101 | BCL | C1C-NC-C4C | 2.38 | 107.77 | 106.71 |
| 8 | M | 402 | BCL | CMD-C2D-C3D | 2.37 | 129.11 | 124.68 |
| 8 | m | 402 | BCL | CMD-C2D-C3D | 2.37 | 129.11 | 124.68 |
| 8 | G | 102 | BCL | C4A-NA-C1A | 2.37 | 107.77 | 106.71 |
| 10 | M | 405 | U10 | C41-C39-C40 | 2.37 | 119.83 | 114.60 |
| 10 | m | 405 | U10 | C41-C39-C40 | 2.37 | 119.83 | 114.60 |
| 8 | 5 | 101 | BCL | C4B-C3B-CAB | -2.36 | 122.57 | 127.13 |
| 8 | 3 | 101 | BCL | C4B-C3B-CAB | -2.36 | 122.57 | 127.13 |
| 10 | L | 304 | U10 | C20-C19-C21 | 2.36 | 119.24 | 115.27 |
| 10 | l | 304 | U10 | C20-C19-C21 | 2.36 | 119.24 | 115.27 |
| 10 | L | 305 | U10 | C12-C13-C14 | -2.36 | 121.99 | 127.66 |
| 10 | l | 305 | U10 | C12-C13-C14 | -2.36 | 121.99 | 127.66 |
| 8 | m | 403 | BCL | CMD-C2D-C3D | 2.36 | 129.09 | 124.68 |
| 8 | 9 | 101 | BCL | C1C-NC-C4C | 2.36 | 107.77 | 106.71 |
| 8 | W | 101 | BCL | CMD-C2D-C3D | 2.35 | 129.07 | 124.68 |
| 8 | w | 101 | BCL | CMD-C2D-C3D | 2.35 | 129.07 | 124.68 |
| 8 | Z | 101 | BCL | CMB-C2B-C3B | 2.35 | 129.07 | 124.68 |
| 8 | z | 101 | BCL | CMB-C2B-C3B | 2.35 | 129.07 | 124.68 |
| 8 | L | 301 | BCL | OBB-CAB-CBB | -2.34 | 114.89 | 120.17 |
| 8 | O | 101 | BCL | C1-C2-C3 | -2.34 | 121.99 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | U | 101 | BCL | C4B-C3B-CAB | -2.34 | 122.61 | 127.13 |
| 8 | u | 101 | BCL | C4B-C3B-CAB | -2.34 | 122.61 | 127.13 |
| 8 | F | 101 | BCL | C4B-C3B-CAB | -2.34 | 122.61 | 127.13 |
| 14 | F | 102 | CDL | OA4-PA1-OA3 | -2.34 | 100.68 | 112.24 |
| 14 | f | 102 | CDL | OA4-PA1-OA3 | -2.34 | 100.68 | 112.24 |
| 9 | M | 404 | BPH | O2D-CGD-CBD | 2.34 | 113.96 | 111.00 |
| 9 | m | 404 | BPH | O2D-CGD-CBD | 2.34 | 113.96 | 111.00 |
| 8 | M | 403 | BCL | CMD-C2D-C3D | 2.34 | 129.05 | 124.68 |
| 8 | b9 | 101 | BCL | C1C-NC-C4C | 2.34 | 107.76 | 106.71 |
| 8 | 2 | 101 | BCL | CMD-C2D-C3D | 2.33 | 129.04 | 124.68 |
| 8 | 7 | 101 | BCL | CMD-C2D-C3D | 2.33 | 129.04 | 124.68 |
| 8 | 4 | 101 | BCL | CMD-C2D-C3D | 2.33 | 129.04 | 124.68 |
| 8 | 6 | 101 | BCL | CMD-C2D-C3D | 2.33 | 129.04 | 124.68 |
| 8 | K | 101 | BCL | C4B-C3B-CAB | -2.33 | 122.62 | 127.13 |
| 8 | k | 101 | BCL | C4B-C3B-CAB | -2.33 | 122.62 | 127.13 |
| 8 | 9 | 101 | BCL | C4B-C3B-CAB | -2.33 | 122.63 | 127.13 |
| 8 | b9 | 101 | BCL | C4B-C3B-CAB | -2.33 | 122.63 | 127.13 |
| 8 | o | 101 | BCL | C1-C2-C3 | -2.33 | 122.02 | 126.04 |
| 8 | l | 301 | BCL | OBB-CAB-CBB | -2.33 | 114.94 | 120.17 |
| 9 | l | 303 | BPH | C1-C2-C3 | -2.32 | 122.02 | 126.04 |
| 8 | l | 301 | BCL | CMD-C2D-C3D | 2.32 | 129.02 | 124.68 |
| 8 | d | 102 | BCL | C1C-NC-C4C | 2.32 | 107.75 | 106.71 |
| 9 | L | 303 | BPH | C1-C2-C3 | -2.32 | 122.03 | 126.04 |
| 8 | g | 102 | BCL | C4A-NA-C1A | 2.32 | 107.75 | 106.71 |
| 8 | f | 101 | BCL | C4B-C3B-CAB | -2.31 | 122.66 | 127.13 |
| 8 | A | 101 | BCL | C1C-NC-C4C | 2.31 | 107.75 | 106.71 |
| 8 | a | 101 | BCL | C1C-NC-C4C | 2.31 | 107.75 | 106.71 |
| 8 | 0 | 101 | BCL | OBB-CAB-CBB | -2.31 | 114.97 | 120.17 |
| 8 | b0 | 101 | BCL | OBB-CAB-CBB | -2.31 | 114.97 | 120.17 |
| 11 | H | 301 | PC1 | O12-P-O14 | -2.30 | 100.85 | 112.24 |
| 11 | h | 301 | PC1 | O12-P-O14 | -2.30 | 100.85 | 112.24 |
| 8 | L | 301 | BCL | CMD-C2D-C3D | 2.30 | 128.98 | 124.68 |
| 8 | I | 101 | BCL | C4B-C3B-CAB | -2.30 | 122.69 | 127.13 |
| 13 | q | 103 | SPO | C1-C4-C5 | -2.30 | 106.96 | 113.06 |
| 8 | 7 | 102 | BCL | OBB-CAB-CBB | -2.30 | 115.00 | 120.17 |
| 8 | U | 101 | BCL | C1-C2-C3 | -2.30 | 122.07 | 126.04 |
| 8 | u | 101 | BCL | C1-C2-C3 | -2.30 | 122.07 | 126.04 |
| 8 | M | 403 | BCL | C4B-C3B-CAB | -2.30 | 122.69 | 127.13 |
| 8 | m | 403 | BCL | C4B-C3B-CAB | -2.30 | 122.69 | 127.13 |
| 8 | C | 101 | BCL | C6-C7-C8 | -2.30 | 108.50 | 115.92 |
| 8 | c | 101 | BCL | C6-C7-C8 | -2.30 | 108.50 | 115.92 |
| 13 | Q | 103 | SPO | C1-C4-C5 | -2.30 | 106.97 | 113.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14 | F | 102 | CDL | OB4-PB2-OB3 | -2.30 | 100.89 | 112.24 |
| 14 | f | 102 | CDL | OB4-PB2-OB3 | -2.30 | 100.89 | 112.24 |
| 8 | S | 101 | BCL | C4B-C3B-CAB | -2.29 | 122.70 | 127.13 |
| 8 | s | 101 | BCL | C4B-C3B-CAB | -2.29 | 122.70 | 127.13 |
| 8 | W | 101 | BCL | C11-C10-C8 | -2.29 | 108.51 | 115.92 |
| 8 | w | 101 | BCL | C11-C10-C8 | -2.29 | 108.51 | 115.92 |
| 8 | 6 | 102 | BCL | OBB-CAB-CBB | -2.29 | 115.01 | 120.17 |
| 11 | D | 101 | PC1 | O12-P-O14 | -2.28 | 100.96 | 112.24 |
| 11 | d | 101 | PC1 | O12-P-O14 | -2.28 | 100.96 | 112.24 |
| 8 | i | 101 | BCL | C4B-C3B-CAB | -2.28 | 122.72 | 127.13 |
| 14 | M | 407 | CDL | OA4-PA1-OA3 | -2.27 | 101.03 | 112.24 |
| 14 | m | 407 | CDL | OA4-PA1-OA3 | -2.27 | 101.03 | 112.24 |
| 8 | T | 101 | BCL | C11-C10-C8 | 2.27 | 123.25 | 115.92 |
| 8 | t | 101 | BCL | C11-C10-C8 | 2.27 | 123.25 | 115.92 |
| 8 | F | 101 | BCL | OBB-CAB-CBB | -2.26 | 115.08 | 120.17 |
| 8 | f | 101 | BCL | OBB-CAB-CBB | -2.26 | 115.08 | 120.17 |
| 8 | L | 301 | BCL | C4A-NA-C1A | 2.26 | 107.72 | 106.71 |
| 8 | l | 301 | BCL | C4A-NA-C1A | 2.26 | 107.72 | 106.71 |
| 8 | B | 101 | BCL | C4B-C3B-CAB | -2.26 | 122.76 | 127.13 |
| 8 | b | 101 | BCL | C4B-C3B-CAB | -2.26 | 122.76 | 127.13 |
| 8 | 1 | 101 | BCL | C4B-C3B-CAB | -2.26 | 122.77 | 127.13 |
| 8 | b1 | 101 | BCL | C4B-C3B-CAB | -2.26 | 122.77 | 127.13 |
| 8 | D | 102 | BCL | C1C-NC-C4C | 2.25 | 107.72 | 106.71 |
| 14 | m | 407 | CDL | OB4-PB2-OB3 | -2.25 | 101.13 | 112.24 |
| 14 | M | 407 | CDL | OB4-PB2-OB3 | -2.24 | 101.15 | 112.24 |
| 8 | 7 | 101 | BCL | C1C-NC-C4C | 2.24 | 107.71 | 106.71 |
| 8 | N | 102 | BCL | C4B-C3B-CAB | -2.23 | 122.82 | 127.13 |
| 8 | n | 102 | BCL | C4B-C3B-CAB | -2.23 | 122.82 | 127.13 |
| 8 | V | 101 | BCL | C6-C7-C8 | 2.23 | 123.13 | 115.92 |
| 8 | v | 101 | BCL | C6-C7-C8 | 2.23 | 123.13 | 115.92 |
| 8 | t | 101 | BCL | C1-C2-C3 | 2.23 | 129.89 | 126.04 |
| 8 | j | 101 | BCL | C4B-C3B-CAB | -2.22 | 122.84 | 127.13 |
| 8 | 7 | 101 | BCL | C6-C7-C8 | -2.22 | 108.75 | 115.92 |
| 8 | 6 | 101 | BCL | C6-C7-C8 | -2.22 | 108.75 | 115.92 |
| 8 | T | 101 | BCL | C1-C2-C3 | 2.22 | 129.88 | 126.04 |
| 9 | L | 303 | BPH | OBB-CAB-CBB | -2.21 | 115.19 | 120.17 |
| 9 | l | 303 | BPH | OBB-CAB-CBB | -2.21 | 115.19 | 120.17 |
| 11 | A | 103 | PC1 | O12-P-O14 | -2.21 | 101.31 | 112.24 |
| 11 | a | 103 | PC1 | O12-P-O14 | -2.21 | 101.31 | 112.24 |
| 8 | L | 301 | BCL | C4B-C3B-CAB | -2.21 | 122.86 | 127.13 |
| 8 | J | 101 | BCL | C4B-C3B-CAB | -2.21 | 122.86 | 127.13 |
| 8 | Q | 101 | BCL | C1C-NC-C4C | 2.21 | 107.70 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | A | 101 | BCL | C4B-C3B-CAB | -2.21 | 122.86 | 127.13 |
| 8 | a | 101 | BCL | C4B-C3B-CAB | -2.21 | 122.86 | 127.13 |
| 8 | l | 301 | BCL | C4B-C3B-CAB | -2.20 | 122.87 | 127.13 |
| 8 | Q | 101 | BCL | C4B-C3B-CAB | -2.20 | 122.89 | 127.13 |
| 8 | q | 101 | BCL | C4B-C3B-CAB | -2.20 | 122.89 | 127.13 |
| 8 | 6 | 101 | BCL | C1C-NC-C4C | 2.20 | 107.69 | 106.71 |
| 13 | M | 406 | SPO | C2-C1-C4 | -2.20 | 107.49 | 110.86 |
| 13 | m | 406 | SPO | C2-C1-C4 | -2.20 | 107.49 | 110.86 |
| 8 | V | 101 | BCL | CAA-CBA-CGA | 2.19 | 119.65 | 113.25 |
| 8 | v | 101 | BCL | CAA-CBA-CGA | 2.19 | 119.65 | 113.25 |
| 8 | 7 | 102 | BCL | C1-C2-C3 | 2.19 | 129.82 | 126.04 |
| 8 | w | 101 | BCL | C4B-C3B-CAB | -2.18 | 122.91 | 127.13 |
| 8 | q | 101 | BCL | C1C-NC-C4C | 2.18 | 107.69 | 106.71 |
| 8 | T | 101 | BCL | C6-C7-C8 | -2.18 | 108.89 | 115.92 |
| 8 | t | 101 | BCL | C6-C7-C8 | -2.18 | 108.89 | 115.92 |
| 8 | D | 102 | BCL | C4B-C3B-CAB | -2.17 | 122.93 | 127.13 |
| 8 | O | 101 | BCL | C4B-C3B-CAB | -2.17 | 122.93 | 127.13 |
| 8 | o | 101 | BCL | C4B-C3B-CAB | -2.17 | 122.93 | 127.13 |
| 8 | S | 101 | BCL | C1C-NC-C4C | 2.17 | 107.68 | 106.71 |
| 8 | s | 101 | BCL | C1C-NC-C4C | 2.17 | 107.68 | 106.71 |
| 10 | L | 304 | U10 | C6-C1-C2 | 2.17 | 120.90 | 119.18 |
| 10 | l | 304 | U10 | C6-C1-C2 | 2.17 | 120.90 | 119.18 |
| 8 | r | 101 | BCL | C1C-NC-C4C | 2.17 | 107.68 | 106.71 |
| 8 | W | 101 | BCL | C4B-C3B-CAB | -2.17 | 122.94 | 127.13 |
| 8 | d | 102 | BCL | C4B-C3B-CAB | -2.17 | 122.95 | 127.13 |
| 8 | l | 302 | BCL | C4B-C3B-CAB | -2.16 | 122.95 | 127.13 |
| 8 | 6 | 102 | BCL | C1-C2-C3 | 2.16 | 129.78 | 126.04 |
| 8 | K | 101 | BCL | OBB-CAB-CBB | -2.16 | 115.30 | 120.17 |
| 8 | k | 101 | BCL | OBB-CAB-CBB | -2.16 | 115.30 | 120.17 |
| 8 | T | 101 | BCL | C4B-C3B-CAB | -2.16 | 122.96 | 127.13 |
| 8 | t | 101 | BCL | C4B-C3B-CAB | -2.16 | 122.96 | 127.13 |
| 8 | L | 302 | BCL | C4B-C3B-CAB | -2.15 | 122.97 | 127.13 |
| 8 | M | 402 | BCL | OBB-CAB-CBB | -2.15 | 115.33 | 120.17 |
| 8 | m | 402 | BCL | OBB-CAB-CBB | -2.14 | 115.34 | 120.17 |
| 11 | L | 306 | PC1 | O12-P-O14 | -2.13 | 101.70 | 112.24 |
| 11 | l | 306 | PC1 | O12-P-O14 | -2.13 | 101.70 | 112.24 |
| 8 | 7 | 101 | BCL | C4B-C3B-CAB | -2.12 | 123.03 | 127.13 |
| 8 | 6 | 101 | BCL | C4B-C3B-CAB | -2.12 | 123.03 | 127.13 |
| 11 | l | 307 | PC1 | O12-P-O14 | -2.12 | 101.75 | 112.24 |
| 8 | U | 101 | BCL | OBB-CAB-CBB | -2.12 | 115.40 | 120.17 |
| 8 | u | 101 | BCL | OBB-CAB-CBB | -2.12 | 115.40 | 120.17 |
| 8 | E | 102 | BCL | C1-C2-C3 | 2.12 | 129.71 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | E | 102 | BCL | C6-C7-C8 | -2.12 | 109.07 | 115.92 |
| 8 | e | 102 | BCL | C6-C7-C8 | -2.12 | 109.07 | 115.92 |
| 8 | G | 102 | BCL | C4B-C3B-CAB | -2.12 | 123.04 | 127.13 |
| 8 | g | 102 | BCL | C4B-C3B-CAB | -2.12 | 123.04 | 127.13 |
| 8 | M | 402 | BCL | C4B-C3B-CAB | -2.12 | 123.04 | 127.13 |
| 8 | e | 102 | BCL | C1-C2-C3 | 2.11 | 129.70 | 126.04 |
| 8 | Q | 101 | BCL | C17-C16-C15 | 2.11 | 122.95 | 113.24 |
| 11 | L | 307 | PC1 | O12-P-O14 | -2.11 | 101.79 | 112.24 |
| 8 | L | 302 | BCL | OBB-CAB-CBB | -2.11 | 115.42 | 120.17 |
| 8 | l | 302 | BCL | OBB-CAB-CBB | -2.11 | 115.42 | 120.17 |
| 8 | q | 101 | BCL | C17-C16-C15 | 2.11 | 122.93 | 113.24 |
| 8 | R | 101 | BCL | C1C-NC-C4C | 2.11 | 107.65 | 106.71 |
| 8 | m | 402 | BCL | C4B-C3B-CAB | -2.10 | 123.06 | 127.13 |
| 10 | M | 405 | U10 | C37-C38-C39 | -2.10 | 120.56 | 127.75 |
| 10 | m | 405 | U10 | C37-C38-C39 | -2.10 | 120.56 | 127.75 |
| 8 | E | 102 | BCL | O2A-C1-C2 | -2.10 | 103.12 | 108.64 |
| 8 | e | 102 | BCL | O2A-C1-C2 | -2.10 | 103.12 | 108.64 |
| 8 | O | 101 | BCL | OBB-CAB-CBB | -2.08 | 115.49 | 120.17 |
| 8 | o | 101 | BCL | OBB-CAB-CBB | -2.08 | 115.49 | 120.17 |
| 8 | C | 101 | BCL | C1-C2-C3 | 2.07 | 129.62 | 126.04 |
| 10 | L | 305 | U10 | C32-C33-C34 | -2.07 | 120.69 | 127.75 |
| 10 | l | 305 | U10 | C32-C33-C34 | -2.07 | 120.69 | 127.75 |
| 8 | J | 101 | BCL | C6-C7-C8 | -2.07 | 109.24 | 115.92 |
| 8 | j | 101 | BCL | C6-C7-C8 | -2.07 | 109.24 | 115.92 |
| 8 | L | 301 | BCL | C1C-NC-C4C | 2.06 | 107.63 | 106.71 |
| 8 | l | 301 | BCL | C1C-NC-C4C | 2.06 | 107.63 | 106.71 |
| 8 | E | 102 | BCL | OBB-CAB-CBB | -2.06 | 115.53 | 120.17 |
| 8 | e | 102 | BCL | OBB-CAB-CBB | -2.06 | 115.53 | 120.17 |
| 11 | H | 302 | PC1 | O12-P-O14 | -2.05 | 102.11 | 112.24 |
| 11 | h | 302 | PC1 | O12-P-O14 | -2.05 | 102.11 | 112.24 |
| 8 | N | 102 | BCL | C6-C7-C8 | -2.05 | 109.31 | 115.92 |
| 8 | n | 102 | BCL | C6-C7-C8 | -2.05 | 109.31 | 115.92 |
| 8 | c | 101 | BCL | C1-C2-C3 | 2.05 | 129.58 | 126.04 |
| 8 | 3 | 101 | BCL | OBB-CAB-CBB | -2.04 | 115.58 | 120.17 |
| 8 | 5 | 101 | BCL | OBB-CAB-CBB | -2.04 | 115.58 | 120.17 |
| 8 | B | 101 | BCL | OBB-CAB-CBB | -2.04 | 115.58 | 120.17 |
| 8 | b | 101 | BCL | OBB-CAB-CBB | -2.04 | 115.58 | 120.17 |
| 8 | 0 | 101 | BCL | C1C-NC-C4C | 2.03 | 107.62 | 106.71 |
| 8 | b0 | 101 | BCL | C1C-NC-C4C | 2.03 | 107.62 | 106.71 |
| 10 | M | 405 | U10 | O5-C5-C6 | -2.03 | 117.99 | 121.55 |
| 10 | m | 405 | U10 | O5-C5-C6 | -2.03 | 117.99 | 121.55 |
| 10 | l | 304 | U10 | C27-C28-C29 | -2.03 | 120.83 | 127.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8 | 6 | 101 | BCL | C1-C2-C3 | -2.02 | 122.54 | 126.04 |
| 8 | 7 | 101 | BCL | C1-C2-C3 | -2.02 | 122.55 | 126.04 |
| 10 | L | 304 | U10 | C27-C28-C29 | -2.02 | 120.86 | 127.75 |
| 8 | G | 102 | BCL | C1C-NC-C4C | 2.01 | 107.61 | 106.71 |
| 8 | V | 101 | BCL | C6-C5-C3 | 2.01 | 118.71 | 113.45 |
| 8 | v | 101 | BCL | C6-C5-C3 | 2.01 | 118.71 | 113.45 |

There are no chirality outliers.

All (1239) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 8 | J | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | 7 | 101 | BCL | C2-C3-C5-C6 |
| 8 | 7 | 101 | BCL | C4-C3-C5-C6 |
| 8 | 7 | 102 | BCL | C4-C3-C5-C6 |
| 8 | 0 | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | j | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | 6 | 101 | BCL | C4-C3-C5-C6 |
| 8 | 6 | 102 | BCL | C4-C3-C5-C6 |
| 8 | b0 | 101 | BCL | C2A-CAA-CBA-CGA |
| 9 | M | 404 | BPH | C2-C3-C5-C6 |
| 9 | M | 404 | BPH | C4-C3-C5-C6 |
| 9 | m | 404 | BPH | C2-C3-C5-C6 |
| 9 | m | 404 | BPH | C4-C3-C5-C6 |
| 10 | L | 305 | U10 | C24-C26-C27-C28 |
| 10 | l | 305 | U10 | C24-C26-C27-C28 |
| 11 | L | 306 | PC1 | C11-O13-P-O12 |
| 11 | L | 306 | PC1 | C11-O13-P-O14 |
| 11 | L | 306 | PC1 | C1-O11-P-O12 |
| 11 | L | 306 | PC1 | C1-O11-P-O14 |
| 11 | L | 306 | PC1 | C1-O11-P-O13 |
| 11 | L | 306 | PC1 | O21-C2-C3-O31 |
| 11 | L | 307 | PC1 | C11-O13-P-O12 |
| 11 | L | 307 | PC1 | C11-O13-P-O14 |
| 11 | L | 307 | PC1 | C11-O13-P-O11 |
| 11 | L | 307 | PC1 | C1-O11-P-O12 |
| 11 | L | 307 | PC1 | O11-C1-C2-O21 |
| 11 | H | 301 | PC1 | O13-C11-C12-N |
| 11 | H | 302 | PC1 | C1-O11-P-O14 |
| 11 | H | 302 | PC1 | O13-C11-C12-N |
| 11 | H | 302 | PC1 | O21-C2-C3-O31 |
| 11 | A | 103 | PC1 | C11-O13-P-O14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | A | 103 | PC1 | C1-O11-P-O12 |
| 11 | A | 103 | PC1 | C1-O11-P-O14 |
| 11 | A | 103 | PC1 | C1-O11-P-O13 |
| 11 | A | 104 | PC1 | C1-O11-P-O14 |
| 11 | A | 104 | PC1 | C12-C11-O13-P |
| 11 | A | 104 | PC1 | O11-C1-C2-O21 |
| 11 | A | 105 | PC1 | C11-O13-P-O14 |
| 11 | A | 105 | PC1 | C11-O13-P-O11 |
| 11 | A | 105 | PC1 | C1-O11-P-O12 |
| 11 | D | 101 | PC1 | C1-O11-P-O12 |
| 11 | D | 101 | PC1 | C1-O11-P-O14 |
| 11 | D | 101 | PC1 | O13-C11-C12-N |
| 11 | l | 306 | PC1 | C11-O13-P-O12 |
| 11 | l | 306 | PC1 | C11-O13-P-O14 |
| 11 | l | 306 | PC1 | C1-O11-P-O12 |
| 11 | l | 306 | PC1 | C1-O11-P-O14 |
| 11 | l | 306 | PC1 | C1-O11-P-O13 |
| 11 | l | 306 | PC1 | O21-C2-C3-O31 |
| 11 | l | 307 | PC1 | C11-O13-P-O12 |
| 11 | l | 307 | PC1 | C11-O13-P-O14 |
| 11 | l | 307 | PC1 | C11-O13-P-O11 |
| 11 | l | 307 | PC1 | C1-O11-P-O12 |
| 11 | l | 307 | PC1 | O11-C1-C2-O21 |
| 11 | h | 301 | PC1 | O13-C11-C12-N |
| 11 | h | 302 | PC1 | C1-O11-P-O14 |
| 11 | h | 302 | PC1 | O13-C11-C12-N |
| 11 | h | 302 | PC1 | O21-C2-C3-O31 |
| 11 | a | 103 | PC1 | C11-O13-P-O14 |
| 11 | a | 103 | PC1 | C1-O11-P-O12 |
| 11 | a | 103 | PC1 | C1-O11-P-O14 |
| 11 | a | 103 | PC1 | C1-O11-P-O13 |
| 11 | a | 104 | PC1 | C1-O11-P-O14 |
| 11 | a | 104 | PC1 | C12-C11-O13-P |
| 11 | a | 104 | PC1 | O11-C1-C2-O21 |
| 11 | a | 105 | PC1 | C11-O13-P-O14 |
| 11 | a | 105 | PC1 | C11-O13-P-O11 |
| 11 | a | 105 | PC1 | C1-O11-P-O12 |
| 11 | d | 101 | PC1 | C1-O11-P-O12 |
| 11 | d | 101 | PC1 | C1-O11-P-O14 |
| 11 | d | 101 | PC1 | O13-C11-C12-N |
| 13 | M | 406 | SPO | C4-C1-O1-CM1 |
| 13 | A | 102 | SPO | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | A | 102 | SPO | C15-C16-C17-C18 |
| 13 | B | 102 | SPO | C2-C1-C4-C5 |
| 13 | B | 102 | SPO | C3-C1-C4-C5 |
| 13 | B | 102 | SPO | C5-C6-C7-C8 |
| 13 | B | 102 | SPO | C5-C6-C7-C9 |
| 13 | B | 102 | SPO | C10-C11-C12-C13 |
| 13 | B | 102 | SPO | C10-C11-C12-C14 |
| 13 | D | 103 | SPO | O1-C1-C4-C5 |
| 13 | D | 103 | SPO | C2-C1-C4-C5 |
| 13 | D | 103 | SPO | C3-C1-C4-C5 |
| 13 | D | 103 | SPO | C5-C6-C7-C8 |
| 13 | D | 103 | SPO | C5-C6-C7-C9 |
| 13 | D | 103 | SPO | C10-C11-C12-C13 |
| 13 | D | 103 | SPO | C10-C11-C12-C14 |
| 13 | E | 101 | SPO | C10-C11-C12-C13 |
| 13 | E | 101 | SPO | C10-C11-C12-C14 |
| 13 | E | 101 | SPO | C15-C16-C17-C18 |
| 13 | E | 101 | SPO | C33-C35-C36-C37 |
| 13 | E | 103 | SPO | C5-C6-C7-C8 |
| 13 | E | 103 | SPO | C5-C6-C7-C9 |
| 13 | E | 103 | SPO | C10-C11-C12-C13 |
| 13 | E | 103 | SPO | C10-C11-C12-C14 |
| 13 | E | 103 | SPO | C28-C30-C31-C32 |
| 13 | G | 101 | SPO | C10-C11-C12-C13 |
| 13 | G | 101 | SPO | C10-C11-C12-C14 |
| 13 | G | 101 | SPO | C33-C35-C36-C37 |
| 13 | G | 103 | SPO | C10-C11-C12-C13 |
| 13 | G | 103 | SPO | C10-C11-C12-C14 |
| 13 | G | 103 | SPO | C27-C28-C30-C31 |
| 13 | G | 103 | SPO | C29-C28-C30-C31 |
| 13 | G | 103 | SPO | C32-C33-C35-C36 |
| 13 | G | 103 | SPO | C34-C33-C35-C36 |
| 13 | I | 102 | SPO | C10-C11-C12-C13 |
| 13 | I | 102 | SPO | C15-C16-C17-C18 |
| 13 | I | 102 | SPO | C15-C16-C17-C19 |
| 13 | I | 102 | SPO | C33-C35-C36-C37 |
| 13 | J | 102 | SPO | C2-C1-C4-C5 |
| 13 | J | 102 | SPO | C3-C1-C4-C5 |
| 13 | J | 102 | SPO | C10-C11-C12-C13 |
| 13 | J | 102 | SPO | C10-C11-C12-C14 |
| 13 | J | 102 | SPO | C32-C33-C35-C36 |
| 13 | J | 102 | SPO | C34-C33-C35-C36 |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|-----------------|
| 13 | N | 101 | SPO | C10-C11-C12-C13 |
| 13 | N | 101 | SPO | C10-C11-C12-C14 |
| 13 | N | 101 | SPO | C15-C16-C17-C18 |
| 13 | N | 101 | SPO | C15-C16-C17-C19 |
| 13 | N | 101 | SPO | C33-C35-C36-C37 |
| 13 | O | 102 | SPO | O1-C1-C4-C5 |
| 13 | O | 102 | SPO | C2-C1-C4-C5 |
| 13 | O | 102 | SPO | C3-C1-C4-C5 |
| 13 | O | 102 | SPO | C15-C16-C17-C18 |
| 13 | O | 102 | SPO | C15-C16-C17-C19 |
| 13 | O | 102 | SPO | C22-C23-C25-C26 |
| 13 | O | 102 | SPO | C24-C23-C25-C26 |
| 13 | P | 101 | SPO | C10-C11-C12-C13 |
| 13 | P | 101 | SPO | C10-C11-C12-C14 |
| 13 | P | 101 | SPO | C32-C33-C35-C36 |
| 13 | P | 101 | SPO | C34-C33-C35-C36 |
| 13 | Q | 102 | SPO | C10-C11-C12-C13 |
| 13 | Q | 102 | SPO | C10-C11-C12-C14 |
| 13 | Q | 102 | SPO | C33-C35-C36-C37 |
| 13 | Q | 103 | SPO | C5-C6-C7-C8 |
| 13 | Q | 103 | SPO | C5-C6-C7-C9 |
| 13 | Q | 103 | SPO | C10-C11-C12-C13 |
| 13 | Q | 103 | SPO | C10-C11-C12-C14 |
| 13 | Q | 103 | SPO | C27-C28-C30-C31 |
| 13 | Q | 103 | SPO | C29-C28-C30-C31 |
| 13 | Q | 104 | SPO | C10-C11-C12-C13 |
| 13 | Q | 104 | SPO | C10-C11-C12-C14 |
| 13 | Q | 104 | SPO | C32-C33-C35-C36 |
| 13 | Q | 104 | SPO | C34-C33-C35-C36 |
| 13 | S | 102 | SPO | C3-C1-C4-C5 |
| 13 | S | 102 | SPO | C5-C6-C7-C8 |
| 13 | S | 102 | SPO | C5-C6-C7-C9 |
| 13 | S | 102 | SPO | C10-C11-C12-C13 |
| 13 | S | 102 | SPO | C10-C11-C12-C14 |
| 13 | S | 102 | SPO | C27-C28-C30-C31 |
| 13 | S | 102 | SPO | C29-C28-C30-C31 |
| 13 | S | 103 | SPO | C5-C6-C7-C8 |
| 13 | S | 103 | SPO | C5-C6-C7-C9 |
| 13 | S | 103 | SPO | C10-C11-C12-C13 |
| 13 | S | 103 | SPO | C10-C11-C12-C14 |
| 13 | U | 102 | SPO | C10-C11-C12-C13 |
| 13 | U | 102 | SPO | C10-C11-C12-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | U | 102 | SPO | C32-C33-C35-C36 |
| 13 | U | 102 | SPO | C34-C33-C35-C36 |
| 13 | U | 103 | SPO | C33-C35-C36-C37 |
| 13 | C | 102 | SPO | C11-C10-C9-C7 |
| 13 | C | 102 | SPO | C10-C11-C12-C13 |
| 13 | C | 102 | SPO | C10-C11-C12-C14 |
| 13 | C | 102 | SPO | C15-C16-C17-C18 |
| 13 | C | 102 | SPO | C15-C16-C17-C19 |
| 13 | C | 102 | SPO | C27-C28-C30-C31 |
| 13 | C | 102 | SPO | C29-C28-C30-C31 |
| 13 | 3 | 102 | SPO | C10-C11-C12-C13 |
| 13 | 3 | 102 | SPO | C10-C11-C12-C14 |
| 13 | 3 | 102 | SPO | C15-C16-C17-C18 |
| 13 | 3 | 102 | SPO | C15-C16-C17-C19 |
| 13 | 3 | 102 | SPO | C32-C33-C35-C36 |
| 13 | 3 | 102 | SPO | C34-C33-C35-C36 |
| 13 | 3 | 103 | SPO | C5-C6-C7-C8 |
| 13 | 3 | 103 | SPO | C11-C10-C9-C7 |
| 13 | 3 | 103 | SPO | C10-C11-C12-C13 |
| 13 | 3 | 103 | SPO | C10-C11-C12-C14 |
| 13 | 3 | 103 | SPO | C27-C28-C30-C31 |
| 13 | 3 | 103 | SPO | C29-C28-C30-C31 |
| 13 | 3 | 103 | SPO | C32-C33-C35-C36 |
| 13 | 3 | 103 | SPO | C34-C33-C35-C36 |
| 13 | 9 | 102 | SPO | C15-C16-C17-C18 |
| 13 | 9 | 102 | SPO | C15-C16-C17-C19 |
| 13 | 9 | 102 | SPO | C32-C33-C35-C36 |
| 13 | 9 | 102 | SPO | C34-C33-C35-C36 |
| 13 | 0 | 102 | SPO | C2-C1-C4-C5 |
| 13 | 0 | 102 | SPO | C3-C1-C4-C5 |
| 13 | 0 | 102 | SPO | C1-C4-C5-C6 |
| 13 | 0 | 102 | SPO | C10-C11-C12-C13 |
| 13 | 0 | 102 | SPO | C10-C11-C12-C14 |
| 13 | X | 101 | SPO | C10-C11-C12-C13 |
| 13 | X | 101 | SPO | C10-C11-C12-C14 |
| 13 | X | 101 | SPO | C15-C16-C17-C18 |
| 13 | X | 101 | SPO | C15-C16-C17-C19 |
| 13 | X | 101 | SPO | C32-C33-C35-C36 |
| 13 | X | 101 | SPO | C34-C33-C35-C36 |
| 13 | m | 406 | SPO | C4-C1-O1-CM1 |
| 13 | a | 102 | SPO | C10-C11-C12-C13 |
| 13 | a | 102 | SPO | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | b | 102 | SPO | C2-C1-C4-C5 |
| 13 | b | 102 | SPO | C3-C1-C4-C5 |
| 13 | b | 102 | SPO | C5-C6-C7-C8 |
| 13 | b | 102 | SPO | C5-C6-C7-C9 |
| 13 | b | 102 | SPO | C10-C11-C12-C13 |
| 13 | b | 102 | SPO | C10-C11-C12-C14 |
| 13 | d | 103 | SPO | O1-C1-C4-C5 |
| 13 | d | 103 | SPO | C2-C1-C4-C5 |
| 13 | d | 103 | SPO | C3-C1-C4-C5 |
| 13 | d | 103 | SPO | C5-C6-C7-C8 |
| 13 | d | 103 | SPO | C5-C6-C7-C9 |
| 13 | d | 103 | SPO | C10-C11-C12-C13 |
| 13 | d | 103 | SPO | C10-C11-C12-C14 |
| 13 | e | 101 | SPO | C10-C11-C12-C13 |
| 13 | e | 101 | SPO | C10-C11-C12-C14 |
| 13 | e | 101 | SPO | C15-C16-C17-C18 |
| 13 | e | 101 | SPO | C33-C35-C36-C37 |
| 13 | e | 103 | SPO | C5-C6-C7-C8 |
| 13 | e | 103 | SPO | C5-C6-C7-C9 |
| 13 | e | 103 | SPO | C10-C11-C12-C13 |
| 13 | e | 103 | SPO | C10-C11-C12-C14 |
| 13 | e | 103 | SPO | C28-C30-C31-C32 |
| 13 | g | 101 | SPO | C10-C11-C12-C13 |
| 13 | g | 101 | SPO | C10-C11-C12-C14 |
| 13 | g | 101 | SPO | C33-C35-C36-C37 |
| 13 | g | 103 | SPO | C10-C11-C12-C13 |
| 13 | g | 103 | SPO | C10-C11-C12-C14 |
| 13 | g | 103 | SPO | C27-C28-C30-C31 |
| 13 | g | 103 | SPO | C29-C28-C30-C31 |
| 13 | g | 103 | SPO | C32-C33-C35-C36 |
| 13 | g | 103 | SPO | C34-C33-C35-C36 |
| 13 | i | 102 | SPO | C10-C11-C12-C13 |
| 13 | i | 102 | SPO | C15-C16-C17-C18 |
| 13 | i | 102 | SPO | C15-C16-C17-C19 |
| 13 | i | 102 | SPO | C33-C35-C36-C37 |
| 13 | j | 102 | SPO | C2-C1-C4-C5 |
| 13 | j | 102 | SPO | C3-C1-C4-C5 |
| 13 | j | 102 | SPO | C10-C11-C12-C13 |
| 13 | j | 102 | SPO | C10-C11-C12-C14 |
| 13 | j | 102 | SPO | C32-C33-C35-C36 |
| 13 | j | 102 | SPO | C34-C33-C35-C36 |
| 13 | n | 101 | SPO | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | n | 101 | SPO | C10-C11-C12-C14 |
| 13 | n | 101 | SPO | C15-C16-C17-C18 |
| 13 | n | 101 | SPO | C15-C16-C17-C19 |
| 13 | n | 101 | SPO | C33-C35-C36-C37 |
| 13 | o | 102 | SPO | O1-C1-C4-C5 |
| 13 | o | 102 | SPO | C2-C1-C4-C5 |
| 13 | o | 102 | SPO | C3-C1-C4-C5 |
| 13 | o | 102 | SPO | C15-C16-C17-C18 |
| 13 | o | 102 | SPO | C15-C16-C17-C19 |
| 13 | o | 102 | SPO | C22-C23-C25-C26 |
| 13 | o | 102 | SPO | C24-C23-C25-C26 |
| 13 | p | 101 | SPO | C10-C11-C12-C13 |
| 13 | p | 101 | SPO | C10-C11-C12-C14 |
| 13 | p | 101 | SPO | C32-C33-C35-C36 |
| 13 | p | 101 | SPO | C34-C33-C35-C36 |
| 13 | q | 102 | SPO | C10-C11-C12-C13 |
| 13 | q | 102 | SPO | C10-C11-C12-C14 |
| 13 | q | 102 | SPO | C33-C35-C36-C37 |
| 13 | q | 103 | SPO | C5-C6-C7-C8 |
| 13 | q | 103 | SPO | C5-C6-C7-C9 |
| 13 | q | 103 | SPO | C10-C11-C12-C13 |
| 13 | q | 103 | SPO | C10-C11-C12-C14 |
| 13 | q | 103 | SPO | C27-C28-C30-C31 |
| 13 | q | 103 | SPO | C29-C28-C30-C31 |
| 13 | q | 104 | SPO | C10-C11-C12-C13 |
| 13 | q | 104 | SPO | C10-C11-C12-C14 |
| 13 | q | 104 | SPO | C32-C33-C35-C36 |
| 13 | q | 104 | SPO | C34-C33-C35-C36 |
| 13 | s | 102 | SPO | C3-C1-C4-C5 |
| 13 | s | 102 | SPO | C5-C6-C7-C8 |
| 13 | s | 102 | SPO | C5-C6-C7-C9 |
| 13 | s | 102 | SPO | C10-C11-C12-C13 |
| 13 | s | 102 | SPO | C10-C11-C12-C14 |
| 13 | s | 102 | SPO | C27-C28-C30-C31 |
| 13 | s | 102 | SPO | C29-C28-C30-C31 |
| 13 | s | 103 | SPO | C5-C6-C7-C8 |
| 13 | s | 103 | SPO | C5-C6-C7-C9 |
| 13 | s | 103 | SPO | C10-C11-C12-C13 |
| 13 | s | 103 | SPO | C10-C11-C12-C14 |
| 13 | u | 102 | SPO | C10-C11-C12-C13 |
| 13 | u | 102 | SPO | C10-C11-C12-C14 |
| 13 | u | 102 | SPO | C32-C33-C35-C36 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | u | 102 | SPO | C34-C33-C35-C36 |
| 13 | u | 103 | SPO | C33-C35-C36-C37 |
| 13 | c | 102 | SPO | C11-C10-C9-C7 |
| 13 | c | 102 | SPO | C10-C11-C12-C13 |
| 13 | c | 102 | SPO | C10-C11-C12-C14 |
| 13 | c | 102 | SPO | C15-C16-C17-C18 |
| 13 | c | 102 | SPO | C15-C16-C17-C19 |
| 13 | c | 102 | SPO | C27-C28-C30-C31 |
| 13 | c | 102 | SPO | C29-C28-C30-C31 |
| 13 | 5 | 102 | SPO | C10-C11-C12-C13 |
| 13 | 5 | 102 | SPO | C10-C11-C12-C14 |
| 13 | 5 | 102 | SPO | C15-C16-C17-C18 |
| 13 | 5 | 102 | SPO | C15-C16-C17-C19 |
| 13 | 5 | 102 | SPO | C32-C33-C35-C36 |
| 13 | 5 | 102 | SPO | C34-C33-C35-C36 |
| 13 | 5 | 103 | SPO | C5-C6-C7-C8 |
| 13 | 5 | 103 | SPO | C11-C10-C9-C7 |
| 13 | 5 | 103 | SPO | C10-C11-C12-C13 |
| 13 | 5 | 103 | SPO | C10-C11-C12-C14 |
| 13 | 5 | 103 | SPO | C27-C28-C30-C31 |
| 13 | 5 | 103 | SPO | C29-C28-C30-C31 |
| 13 | 5 | 103 | SPO | C32-C33-C35-C36 |
| 13 | 5 | 103 | SPO | C34-C33-C35-C36 |
| 13 | b9 | 102 | SPO | C15-C16-C17-C18 |
| 13 | b9 | 102 | SPO | C15-C16-C17-C19 |
| 13 | b9 | 102 | SPO | C32-C33-C35-C36 |
| 13 | b9 | 102 | SPO | C34-C33-C35-C36 |
| 13 | b0 | 102 | SPO | C2-C1-C4-C5 |
| 13 | b0 | 102 | SPO | C3-C1-C4-C5 |
| 13 | b0 | 102 | SPO | C1-C4-C5-C6 |
| 13 | b0 | 102 | SPO | C10-C11-C12-C13 |
| 13 | b0 | 102 | SPO | C10-C11-C12-C14 |
| 13 | x | 101 | SPO | C10-C11-C12-C13 |
| 13 | x | 101 | SPO | C10-C11-C12-C14 |
| 13 | x | 101 | SPO | C15-C16-C17-C18 |
| 13 | x | 101 | SPO | C15-C16-C17-C19 |
| 13 | x | 101 | SPO | C32-C33-C35-C36 |
| 13 | x | 101 | SPO | C34-C33-C35-C36 |
| 14 | M | 407 | CDL | CA3-OA5-PA1-OA2 |
| 14 | M | 407 | CDL | CA3-OA5-PA1-OA3 |
| 14 | M | 407 | CDL | C51-CB5-OB6-CB4 |
| 14 | F | 102 | CDL | CA2-OA2-PA1-OA3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 14 | F | 102 | CDL | CA2-OA2-PA1-OA4 |
| 14 | F | 102 | CDL | C11-CA5-OA6-CA4 |
| 14 | F | 102 | CDL | CB2-OB2-PB2-OB3 |
| 14 | F | 102 | CDL | CB2-OB2-PB2-OB4 |
| 14 | F | 102 | CDL | CB2-OB2-PB2-OB5 |
| 14 | m | 407 | CDL | CA3-OA5-PA1-OA2 |
| 14 | m | 407 | CDL | CA3-OA5-PA1-OA3 |
| 14 | m | 407 | CDL | C51-CB5-OB6-CB4 |
| 14 | f | 102 | CDL | CA2-OA2-PA1-OA3 |
| 14 | f | 102 | CDL | CA2-OA2-PA1-OA4 |
| 14 | f | 102 | CDL | C11-CA5-OA6-CA4 |
| 14 | f | 102 | CDL | CB2-OB2-PB2-OB3 |
| 14 | f | 102 | CDL | CB2-OB2-PB2-OB4 |
| 14 | f | 102 | CDL | CB2-OB2-PB2-OB5 |
| 11 | A | 105 | PC1 | O32-C31-O31-C3 |
| 11 | a | 105 | PC1 | O32-C31-O31-C3 |
| 14 | F | 102 | CDL | OA9-CA7-OA8-CA6 |
| 14 | f | 102 | CDL | OA9-CA7-OA8-CA6 |
| 11 | L | 307 | PC1 | O22-C21-O21-C2 |
| 11 | l | 307 | PC1 | O22-C21-O21-C2 |
| 14 | M | 407 | CDL | OB7-CB5-OB6-CB4 |
| 14 | F | 102 | CDL | OA7-CA5-OA6-CA4 |
| 14 | m | 407 | CDL | OB7-CB5-OB6-CB4 |
| 14 | f | 102 | CDL | OA7-CA5-OA6-CA4 |
| 11 | A | 105 | PC1 | C32-C31-O31-C3 |
| 11 | a | 105 | PC1 | C32-C31-O31-C3 |
| 14 | F | 102 | CDL | C31-CA7-OA8-CA6 |
| 14 | f | 102 | CDL | C31-CA7-OA8-CA6 |
| 11 | L | 307 | PC1 | C22-C21-O21-C2 |
| 11 | l | 307 | PC1 | C22-C21-O21-C2 |
| 10 | M | 405 | U10 | C37-C38-C39-C40 |
| 10 | m | 405 | U10 | C37-C38-C39-C40 |
| 13 | A | 102 | SPO | C34-C33-C35-C36 |
| 13 | 0 | 102 | SPO | C29-C28-C30-C31 |
| 13 | a | 102 | SPO | C34-C33-C35-C36 |
| 13 | b0 | 102 | SPO | C29-C28-C30-C31 |
| 8 | 6 | 101 | BCL | C2-C3-C5-C6 |
| 8 | B | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | N | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | R | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | T | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | b | 101 | BCL | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 8 | n | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | r | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | t | 101 | BCL | C2A-CAA-CBA-CGA |
| 11 | A | 105 | PC1 | C11-C12-N-C13 |
| 11 | a | 105 | PC1 | C11-C12-N-C13 |
| 10 | M | 405 | U10 | C37-C38-C39-C41 |
| 10 | m | 405 | U10 | C37-C38-C39-C41 |
| 10 | L | 305 | U10 | C25-C24-C26-C27 |
| 10 | l | 305 | U10 | C25-C24-C26-C27 |
| 13 | M | 406 | SPO | C34-C33-C35-C36 |
| 13 | B | 102 | SPO | C34-C33-C35-C36 |
| 13 | D | 103 | SPO | C34-C33-C35-C36 |
| 13 | Q | 103 | SPO | C34-C33-C35-C36 |
| 13 | S | 102 | SPO | C34-C33-C35-C36 |
| 13 | 0 | 102 | SPO | C34-C33-C35-C36 |
| 13 | m | 406 | SPO | C34-C33-C35-C36 |
| 13 | b | 102 | SPO | C34-C33-C35-C36 |
| 13 | d | 103 | SPO | C34-C33-C35-C36 |
| 13 | q | 103 | SPO | C34-C33-C35-C36 |
| 13 | s | 102 | SPO | C34-C33-C35-C36 |
| 13 | b0 | 102 | SPO | C34-C33-C35-C36 |
| 8 | 7 | 102 | BCL | C2-C3-C5-C6 |
| 8 | 6 | 102 | BCL | C2-C3-C5-C6 |
| 10 | L | 305 | U10 | C23-C24-C26-C27 |
| 10 | l | 305 | U10 | C23-C24-C26-C27 |
| 13 | M | 406 | SPO | C32-C33-C35-C36 |
| 13 | A | 102 | SPO | C32-C33-C35-C36 |
| 13 | B | 102 | SPO | C32-C33-C35-C36 |
| 13 | D | 103 | SPO | C32-C33-C35-C36 |
| 13 | Q | 103 | SPO | C32-C33-C35-C36 |
| 13 | S | 102 | SPO | C32-C33-C35-C36 |
| 13 | 0 | 102 | SPO | C32-C33-C35-C36 |
| 13 | m | 406 | SPO | C32-C33-C35-C36 |
| 13 | a | 102 | SPO | C32-C33-C35-C36 |
| 13 | b | 102 | SPO | C32-C33-C35-C36 |
| 13 | d | 103 | SPO | C32-C33-C35-C36 |
| 13 | q | 103 | SPO | C32-C33-C35-C36 |
| 13 | s | 102 | SPO | C32-C33-C35-C36 |
| 13 | b0 | 102 | SPO | C32-C33-C35-C36 |
| 10 | L | 304 | U10 | C14-C16-C17-C18 |
| 10 | L | 304 | U10 | C19-C21-C22-C23 |
| 10 | l | 304 | U10 | C14-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 10 | l | 304 | U10 | C19-C21-C22-C23 |
| 13 | A | 102 | SPO | C33-C35-C36-C37 |
| 13 | B | 102 | SPO | C33-C35-C36-C37 |
| 13 | D | 103 | SPO | C33-C35-C36-C37 |
| 13 | E | 103 | SPO | C33-C35-C36-C37 |
| 13 | P | 101 | SPO | C33-C35-C36-C37 |
| 13 | S | 103 | SPO | C33-C35-C36-C37 |
| 13 | 3 | 102 | SPO | C33-C35-C36-C37 |
| 13 | a | 102 | SPO | C33-C35-C36-C37 |
| 13 | b | 102 | SPO | C33-C35-C36-C37 |
| 13 | d | 103 | SPO | C33-C35-C36-C37 |
| 13 | e | 103 | SPO | C33-C35-C36-C37 |
| 13 | p | 101 | SPO | C33-C35-C36-C37 |
| 13 | s | 103 | SPO | C33-C35-C36-C37 |
| 13 | 5 | 102 | SPO | C33-C35-C36-C37 |
| 13 | E | 103 | SPO | C11-C10-C9-C7 |
| 13 | G | 103 | SPO | C12-C14-C15-C16 |
| 13 | O | 102 | SPO | C11-C10-C9-C7 |
| 13 | e | 103 | SPO | C11-C10-C9-C7 |
| 13 | g | 103 | SPO | C12-C14-C15-C16 |
| 13 | o | 102 | SPO | C11-C10-C9-C7 |
| 14 | M | 407 | CDL | OB6-CB4-CB6-OB8 |
| 14 | m | 407 | CDL | OB6-CB4-CB6-OB8 |
| 10 | L | 305 | U10 | C12-C11-C9-C10 |
| 10 | l | 305 | U10 | C12-C11-C9-C10 |
| 13 | 0 | 102 | SPO | C27-C28-C30-C31 |
| 13 | b0 | 102 | SPO | C27-C28-C30-C31 |
| 8 | G | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | g | 102 | BCL | C2A-CAA-CBA-CGA |
| 13 | E | 103 | SPO | C15-C16-C17-C18 |
| 13 | G | 101 | SPO | C15-C16-C17-C18 |
| 13 | J | 102 | SPO | C5-C6-C7-C8 |
| 13 | O | 102 | SPO | C5-C6-C7-C8 |
| 13 | Q | 102 | SPO | C15-C16-C17-C18 |
| 13 | S | 103 | SPO | C15-C16-C17-C18 |
| 13 | U | 103 | SPO | C10-C11-C12-C13 |
| 13 | C | 102 | SPO | C5-C6-C7-C8 |
| 13 | 9 | 102 | SPO | C10-C11-C12-C13 |
| 13 | e | 103 | SPO | C15-C16-C17-C18 |
| 13 | g | 101 | SPO | C15-C16-C17-C18 |
| 13 | j | 102 | SPO | C5-C6-C7-C8 |
| 13 | o | 102 | SPO | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | q | 102 | SPO | C15-C16-C17-C18 |
| 13 | s | 103 | SPO | C15-C16-C17-C18 |
| 13 | u | 103 | SPO | C10-C11-C12-C13 |
| 13 | c | 102 | SPO | C5-C6-C7-C8 |
| 13 | b9 | 102 | SPO | C10-C11-C12-C13 |
| 13 | A | 102 | SPO | C10-C11-C12-C14 |
| 13 | I | 102 | SPO | C10-C11-C12-C14 |
| 13 | J | 102 | SPO | C5-C6-C7-C9 |
| 13 | C | 102 | SPO | C5-C6-C7-C9 |
| 13 | 3 | 103 | SPO | C5-C6-C7-C9 |
| 13 | 9 | 102 | SPO | C10-C11-C12-C14 |
| 13 | a | 102 | SPO | C10-C11-C12-C14 |
| 13 | i | 102 | SPO | C10-C11-C12-C14 |
| 13 | j | 102 | SPO | C5-C6-C7-C9 |
| 13 | c | 102 | SPO | C5-C6-C7-C9 |
| 13 | 5 | 103 | SPO | C5-C6-C7-C9 |
| 13 | b9 | 102 | SPO | C10-C11-C12-C14 |
| 11 | A | 104 | PC1 | C22-C21-O21-C2 |
| 11 | a | 104 | PC1 | C22-C21-O21-C2 |
| 11 | A | 103 | PC1 | C31-C32-C33-C34 |
| 11 | a | 103 | PC1 | C31-C32-C33-C34 |
| 13 | 0 | 102 | SPO | C11-C10-C9-C7 |
| 13 | b0 | 102 | SPO | C11-C10-C9-C7 |
| 8 | E | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | P | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | 7 | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | e | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | p | 102 | BCL | C2A-CAA-CBA-CGA |
| 8 | 6 | 102 | BCL | C2A-CAA-CBA-CGA |
| 10 | L | 304 | U10 | C9-C11-C12-C13 |
| 10 | L | 304 | U10 | C24-C26-C27-C28 |
| 10 | L | 305 | U10 | C29-C31-C32-C33 |
| 10 | l | 304 | U10 | C9-C11-C12-C13 |
| 10 | l | 304 | U10 | C24-C26-C27-C28 |
| 10 | l | 305 | U10 | C29-C31-C32-C33 |
| 13 | Q | 104 | SPO | C33-C35-C36-C37 |
| 13 | q | 104 | SPO | C33-C35-C36-C37 |
| 11 | L | 306 | PC1 | C11-O13-P-O11 |
| 11 | L | 307 | PC1 | C1-O11-P-O13 |
| 11 | A | 103 | PC1 | C11-O13-P-O11 |
| 11 | A | 105 | PC1 | C1-O11-P-O13 |
| 11 | D | 101 | PC1 | C1-O11-P-O13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | l | 306 | PC1 | C11-O13-P-O11 |
| 11 | l | 307 | PC1 | C1-O11-P-O13 |
| 11 | a | 103 | PC1 | C11-O13-P-O11 |
| 11 | a | 105 | PC1 | C1-O11-P-O13 |
| 11 | d | 101 | PC1 | C1-O11-P-O13 |
| 11 | A | 104 | PC1 | O22-C21-O21-C2 |
| 11 | A | 105 | PC1 | O22-C21-O21-C2 |
| 11 | a | 104 | PC1 | O22-C21-O21-C2 |
| 11 | a | 105 | PC1 | O22-C21-O21-C2 |
| 13 | E | 103 | SPO | C29-C28-C30-C31 |
| 13 | e | 103 | SPO | C29-C28-C30-C31 |
| 11 | A | 105 | PC1 | C11-C12-N-C15 |
| 11 | a | 105 | PC1 | C11-C12-N-C15 |
| 13 | I | 102 | SPO | C11-C10-C9-C7 |
| 13 | O | 102 | SPO | C12-C14-C15-C16 |
| 13 | X | 101 | SPO | C11-C10-C9-C7 |
| 13 | i | 102 | SPO | C11-C10-C9-C7 |
| 13 | o | 102 | SPO | C12-C14-C15-C16 |
| 13 | x | 101 | SPO | C11-C10-C9-C7 |
| 11 | A | 105 | PC1 | C22-C21-O21-C2 |
| 11 | a | 105 | PC1 | C22-C21-O21-C2 |
| 14 | F | 102 | CDL | O1-C1-CA2-OA2 |
| 14 | f | 102 | CDL | O1-C1-CA2-OA2 |
| 14 | M | 407 | CDL | C71-CB7-OB8-CB6 |
| 14 | m | 407 | CDL | C71-CB7-OB8-CB6 |
| 8 | R | 101 | BCL | C4-C3-C5-C6 |
| 8 | r | 101 | BCL | C4-C3-C5-C6 |
| 8 | P | 102 | BCL | C2-C3-C5-C6 |
| 8 | p | 102 | BCL | C2-C3-C5-C6 |
| 8 | F | 101 | BCL | C11-C10-C8-C9 |
| 8 | I | 101 | BCL | C11-C10-C8-C9 |
| 8 | f | 101 | BCL | C11-C10-C8-C9 |
| 8 | i | 101 | BCL | C11-C10-C8-C9 |
| 14 | F | 102 | CDL | C71-C72-C73-C74 |
| 14 | f | 102 | CDL | C71-C72-C73-C74 |
| 13 | G | 103 | SPO | C15-C16-C17-C18 |
| 13 | g | 103 | SPO | C15-C16-C17-C18 |
| 13 | G | 103 | SPO | C15-C16-C17-C19 |
| 13 | O | 102 | SPO | C5-C6-C7-C9 |
| 13 | g | 103 | SPO | C15-C16-C17-C19 |
| 13 | o | 102 | SPO | C5-C6-C7-C9 |
| 11 | L | 307 | PC1 | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | l | 307 | PC1 | C22-C23-C24-C25 |
| 11 | L | 307 | PC1 | C23-C24-C25-C26 |
| 11 | A | 103 | PC1 | C32-C33-C34-C35 |
| 11 | l | 307 | PC1 | C23-C24-C25-C26 |
| 11 | a | 103 | PC1 | C32-C33-C34-C35 |
| 11 | A | 105 | PC1 | C11-C12-N-C14 |
| 11 | a | 105 | PC1 | C11-C12-N-C14 |
| 13 | S | 102 | SPO | C33-C35-C36-C37 |
| 13 | s | 102 | SPO | C33-C35-C36-C37 |
| 11 | H | 301 | PC1 | C37-C38-C39-C3A |
| 11 | h | 301 | PC1 | C37-C38-C39-C3A |
| 11 | L | 307 | PC1 | C1-C2-C3-O31 |
| 11 | l | 307 | PC1 | C1-C2-C3-O31 |
| 8 | 7 | 102 | BCL | O2A-C1-C2-C3 |
| 8 | 6 | 102 | BCL | O2A-C1-C2-C3 |
| 8 | E | 102 | BCL | C4-C3-C5-C6 |
| 8 | P | 102 | BCL | C4-C3-C5-C6 |
| 8 | C | 101 | BCL | C4-C3-C5-C6 |
| 8 | e | 102 | BCL | C4-C3-C5-C6 |
| 8 | p | 102 | BCL | C4-C3-C5-C6 |
| 8 | c | 101 | BCL | C4-C3-C5-C6 |
| 10 | L | 304 | U10 | C20-C19-C21-C22 |
| 10 | l | 304 | U10 | C20-C19-C21-C22 |
| 8 | E | 102 | BCL | C2-C3-C5-C6 |
| 8 | R | 101 | BCL | C2-C3-C5-C6 |
| 8 | C | 101 | BCL | C2-C3-C5-C6 |
| 8 | e | 102 | BCL | C2-C3-C5-C6 |
| 8 | r | 101 | BCL | C2-C3-C5-C6 |
| 8 | c | 101 | BCL | C2-C3-C5-C6 |
| 14 | M | 407 | CDL | OB9-CB7-OB8-CB6 |
| 14 | m | 407 | CDL | OB9-CB7-OB8-CB6 |
| 11 | A | 103 | PC1 | C23-C24-C25-C26 |
| 11 | a | 103 | PC1 | C23-C24-C25-C26 |
| 10 | L | 304 | U10 | C27-C28-C29-C30 |
| 10 | l | 304 | U10 | C27-C28-C29-C30 |
| 8 | J | 101 | BCL | C4-C3-C5-C6 |
| 8 | N | 102 | BCL | C4-C3-C5-C6 |
| 8 | j | 101 | BCL | C4-C3-C5-C6 |
| 8 | n | 102 | BCL | C4-C3-C5-C6 |
| 13 | G | 101 | SPO | C34-C33-C35-C36 |
| 13 | g | 101 | SPO | C34-C33-C35-C36 |
| 8 | A | 101 | BCL | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 8 | F | 101 | BCL | C11-C10-C8-C7 |
| 8 | I | 101 | BCL | C11-C10-C8-C7 |
| 8 | N | 102 | BCL | C2-C3-C5-C6 |
| 8 | Z | 101 | BCL | C2-C3-C5-C6 |
| 8 | a | 101 | BCL | C11-C10-C8-C7 |
| 8 | f | 101 | BCL | C11-C10-C8-C7 |
| 8 | i | 101 | BCL | C11-C10-C8-C7 |
| 8 | n | 102 | BCL | C2-C3-C5-C6 |
| 8 | z | 101 | BCL | C2-C3-C5-C6 |
| 10 | L | 304 | U10 | C18-C19-C21-C22 |
| 10 | l | 304 | U10 | C18-C19-C21-C22 |
| 11 | L | 306 | PC1 | C21-C22-C23-C24 |
| 11 | l | 306 | PC1 | C21-C22-C23-C24 |
| 11 | H | 301 | PC1 | C36-C37-C38-C39 |
| 11 | h | 301 | PC1 | C36-C37-C38-C39 |
| 10 | M | 405 | U10 | C34-C36-C37-C38 |
| 10 | m | 405 | U10 | C34-C36-C37-C38 |
| 11 | A | 104 | PC1 | C21-C22-C23-C24 |
| 11 | a | 104 | PC1 | C21-C22-C23-C24 |
| 11 | D | 101 | PC1 | O21-C2-C3-O31 |
| 11 | d | 101 | PC1 | O21-C2-C3-O31 |
| 8 | Z | 101 | BCL | C4-C3-C5-C6 |
| 8 | z | 101 | BCL | C4-C3-C5-C6 |
| 8 | J | 101 | BCL | C2-C3-C5-C6 |
| 8 | j | 101 | BCL | C2-C3-C5-C6 |
| 10 | L | 305 | U10 | C12-C11-C9-C8 |
| 10 | l | 305 | U10 | C12-C11-C9-C8 |
| 13 | E | 103 | SPO | C27-C28-C30-C31 |
| 13 | e | 103 | SPO | C27-C28-C30-C31 |
| 8 | A | 101 | BCL | C11-C10-C8-C9 |
| 8 | a | 101 | BCL | C11-C10-C8-C9 |
| 13 | M | 406 | SPO | C15-C16-C17-C18 |
| 13 | E | 101 | SPO | C5-C6-C7-C8 |
| 13 | Q | 102 | SPO | C5-C6-C7-C8 |
| 13 | 9 | 102 | SPO | C5-C6-C7-C8 |
| 13 | m | 406 | SPO | C15-C16-C17-C18 |
| 13 | q | 102 | SPO | C5-C6-C7-C8 |
| 13 | b9 | 102 | SPO | C5-C6-C7-C8 |
| 13 | E | 101 | SPO | C5-C6-C7-C9 |
| 13 | E | 101 | SPO | C15-C16-C17-C19 |
| 13 | Q | 102 | SPO | C5-C6-C7-C9 |
| 13 | 9 | 102 | SPO | C5-C6-C7-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | e | 101 | SPO | C5-C6-C7-C9 |
| 13 | e | 101 | SPO | C15-C16-C17-C19 |
| 13 | q | 102 | SPO | C5-C6-C7-C9 |
| 13 | b9 | 102 | SPO | C5-C6-C7-C9 |
| 11 | H | 302 | PC1 | C1-O11-P-O13 |
| 11 | A | 104 | PC1 | C1-O11-P-O13 |
| 11 | h | 302 | PC1 | C1-O11-P-O13 |
| 11 | a | 104 | PC1 | C1-O11-P-O13 |
| 14 | F | 102 | CDL | CA2-OA2-PA1-OA5 |
| 14 | F | 102 | CDL | CA3-OA5-PA1-OA2 |
| 14 | f | 102 | CDL | CA2-OA2-PA1-OA5 |
| 14 | f | 102 | CDL | CA3-OA5-PA1-OA2 |
| 11 | L | 306 | PC1 | O11-C1-C2-C3 |
| 11 | A | 104 | PC1 | O11-C1-C2-C3 |
| 11 | A | 105 | PC1 | O11-C1-C2-C3 |
| 11 | l | 306 | PC1 | O11-C1-C2-C3 |
| 11 | a | 104 | PC1 | O11-C1-C2-C3 |
| 11 | a | 105 | PC1 | O11-C1-C2-C3 |
| 13 | E | 103 | SPO | C1-C4-C5-C6 |
| 13 | G | 103 | SPO | C1-C4-C5-C6 |
| 13 | e | 103 | SPO | C1-C4-C5-C6 |
| 13 | g | 103 | SPO | C1-C4-C5-C6 |
| 13 | G | 101 | SPO | C32-C33-C35-C36 |
| 13 | g | 101 | SPO | C32-C33-C35-C36 |
| 14 | F | 102 | CDL | C73-C74-C75-C76 |
| 14 | f | 102 | CDL | C73-C74-C75-C76 |
| 14 | M | 407 | CDL | C11-CA5-OA6-CA4 |
| 14 | F | 102 | CDL | C51-CB5-OB6-CB4 |
| 14 | m | 407 | CDL | C11-CA5-OA6-CA4 |
| 14 | f | 102 | CDL | C51-CB5-OB6-CB4 |
| 11 | A | 104 | PC1 | C1-C2-C3-O31 |
| 11 | D | 101 | PC1 | C1-C2-C3-O31 |
| 11 | a | 104 | PC1 | C1-C2-C3-O31 |
| 11 | d | 101 | PC1 | C1-C2-C3-O31 |
| 14 | M | 407 | CDL | C55-C56-C57-C58 |
| 14 | m | 407 | CDL | C55-C56-C57-C58 |
| 10 | M | 405 | U10 | C35-C34-C36-C37 |
| 10 | m | 405 | U10 | C35-C34-C36-C37 |
| 11 | D | 101 | PC1 | O11-C1-C2-O21 |
| 11 | d | 101 | PC1 | O11-C1-C2-O21 |
| 14 | M | 407 | CDL | OA5-CA3-CA4-OA6 |
| 14 | m | 407 | CDL | OA5-CA3-CA4-OA6 |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|-----------------|
| 11 | D | 101 | PC1 | C22-C23-C24-C25 |
| 11 | d | 101 | PC1 | C22-C23-C24-C25 |
| 13 | M | 406 | SPO | C2-C1-O1-CM1 |
| 13 | m | 406 | SPO | C2-C1-O1-CM1 |
| 11 | L | 307 | PC1 | O21-C2-C3-O31 |
| 11 | l | 307 | PC1 | O21-C2-C3-O31 |
| 14 | F | 102 | CDL | OA6-CA4-CA6-OA8 |
| 14 | F | 102 | CDL | OB6-CB4-CB6-OB8 |
| 14 | f | 102 | CDL | OA6-CA4-CA6-OA8 |
| 14 | f | 102 | CDL | OB6-CB4-CB6-OB8 |
| 13 | S | 102 | SPO | C2-C1-C4-C5 |
| 13 | 9 | 102 | SPO | C2-C1-C4-C5 |
| 13 | 9 | 102 | SPO | C3-C1-C4-C5 |
| 13 | s | 102 | SPO | C2-C1-C4-C5 |
| 13 | b9 | 102 | SPO | C2-C1-C4-C5 |
| 13 | b9 | 102 | SPO | C3-C1-C4-C5 |
| 9 | L | 303 | BPH | C11-C10-C8-C7 |
| 9 | l | 303 | BPH | C11-C10-C8-C7 |
| 10 | M | 405 | U10 | C33-C34-C36-C37 |
| 10 | m | 405 | U10 | C33-C34-C36-C37 |
| 9 | L | 303 | BPH | C11-C10-C8-C9 |
| 9 | l | 303 | BPH | C11-C10-C8-C9 |
| 13 | A | 102 | SPO | C11-C10-C9-C7 |
| 13 | a | 102 | SPO | C11-C10-C9-C7 |
| 11 | H | 301 | PC1 | C32-C31-O31-C3 |
| 11 | h | 301 | PC1 | C32-C31-O31-C3 |
| 11 | H | 301 | PC1 | C29-C2A-C2B-C2C |
| 11 | h | 301 | PC1 | C29-C2A-C2B-C2C |
| 13 | B | 102 | SPO | O1-C1-C4-C5 |
| 13 | J | 102 | SPO | O1-C1-C4-C5 |
| 13 | 0 | 102 | SPO | O1-C1-C4-C5 |
| 13 | b | 102 | SPO | O1-C1-C4-C5 |
| 13 | j | 102 | SPO | O1-C1-C4-C5 |
| 13 | b0 | 102 | SPO | O1-C1-C4-C5 |
| 13 | G | 101 | SPO | C5-C6-C7-C8 |
| 13 | I | 102 | SPO | C5-C6-C7-C8 |
| 13 | N | 101 | SPO | C5-C6-C7-C8 |
| 13 | P | 101 | SPO | C5-C6-C7-C8 |
| 13 | Q | 104 | SPO | C5-C6-C7-C8 |
| 13 | U | 103 | SPO | C5-C6-C7-C8 |
| 13 | 3 | 102 | SPO | C5-C6-C7-C8 |
| 13 | X | 101 | SPO | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | e | 101 | SPO | C5-C6-C7-C8 |
| 13 | g | 101 | SPO | C5-C6-C7-C8 |
| 13 | i | 102 | SPO | C5-C6-C7-C8 |
| 13 | n | 101 | SPO | C5-C6-C7-C8 |
| 13 | p | 101 | SPO | C5-C6-C7-C8 |
| 13 | q | 104 | SPO | C5-C6-C7-C8 |
| 13 | u | 103 | SPO | C5-C6-C7-C8 |
| 13 | 5 | 102 | SPO | C5-C6-C7-C8 |
| 13 | x | 101 | SPO | C5-C6-C7-C8 |
| 13 | A | 102 | SPO | C15-C16-C17-C19 |
| 13 | G | 101 | SPO | C5-C6-C7-C9 |
| 13 | G | 101 | SPO | C15-C16-C17-C19 |
| 13 | I | 102 | SPO | C5-C6-C7-C9 |
| 13 | N | 101 | SPO | C5-C6-C7-C9 |
| 13 | Q | 102 | SPO | C15-C16-C17-C19 |
| 13 | Q | 104 | SPO | C5-C6-C7-C9 |
| 13 | S | 103 | SPO | C15-C16-C17-C19 |
| 13 | X | 101 | SPO | C5-C6-C7-C9 |
| 13 | a | 102 | SPO | C15-C16-C17-C19 |
| 13 | g | 101 | SPO | C5-C6-C7-C9 |
| 13 | g | 101 | SPO | C15-C16-C17-C19 |
| 13 | i | 102 | SPO | C5-C6-C7-C9 |
| 13 | n | 101 | SPO | C5-C6-C7-C9 |
| 13 | q | 102 | SPO | C15-C16-C17-C19 |
| 13 | q | 104 | SPO | C5-C6-C7-C9 |
| 13 | s | 103 | SPO | C15-C16-C17-C19 |
| 13 | x | 101 | SPO | C5-C6-C7-C9 |
| 14 | m | 407 | CDL | C61-C62-C63-C64 |
| 14 | M | 407 | CDL | C61-C62-C63-C64 |
| 14 | M | 407 | CDL | OA5-CA3-CA4-CA6 |
| 14 | m | 407 | CDL | OA5-CA3-CA4-CA6 |
| 10 | M | 405 | U10 | C30-C29-C31-C32 |
| 10 | m | 405 | U10 | C30-C29-C31-C32 |
| 10 | M | 405 | U10 | C28-C29-C31-C32 |
| 10 | m | 405 | U10 | C28-C29-C31-C32 |
| 10 | L | 304 | U10 | C27-C28-C29-C31 |
| 10 | l | 304 | U10 | C27-C28-C29-C31 |
| 13 | 3 | 102 | SPO | C11-C10-C9-C7 |
| 13 | 5 | 102 | SPO | C11-C10-C9-C7 |
| 14 | M | 407 | CDL | C56-C57-C58-C59 |
| 14 | m | 407 | CDL | C56-C57-C58-C59 |
| 11 | L | 306 | PC1 | C1-C2-C3-O31 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | H | 302 | PC1 | C1-C2-C3-O31 |
| 11 | A | 103 | PC1 | C1-C2-C3-O31 |
| 11 | A | 105 | PC1 | C1-C2-C3-O31 |
| 11 | l | 306 | PC1 | C1-C2-C3-O31 |
| 11 | h | 302 | PC1 | C1-C2-C3-O31 |
| 11 | a | 103 | PC1 | C1-C2-C3-O31 |
| 11 | a | 105 | PC1 | C1-C2-C3-O31 |
| 14 | M | 407 | CDL | CA3-CA4-CA6-OA8 |
| 14 | M | 407 | CDL | CB3-CB4-CB6-OB8 |
| 14 | m | 407 | CDL | CA3-CA4-CA6-OA8 |
| 14 | m | 407 | CDL | CB3-CB4-CB6-OB8 |
| 11 | H | 301 | PC1 | C34-C35-C36-C37 |
| 11 | h | 301 | PC1 | C34-C35-C36-C37 |
| 8 | C | 101 | BCL | C2A-CAA-CBA-CGA |
| 8 | c | 101 | BCL | C2A-CAA-CBA-CGA |
| 11 | L | 306 | PC1 | O11-C1-C2-O21 |
| 11 | A | 103 | PC1 | O11-C1-C2-O21 |
| 11 | A | 105 | PC1 | O11-C1-C2-O21 |
| 11 | l | 306 | PC1 | O11-C1-C2-O21 |
| 11 | a | 103 | PC1 | O11-C1-C2-O21 |
| 11 | a | 105 | PC1 | O11-C1-C2-O21 |
| 11 | H | 301 | PC1 | O32-C31-O31-C3 |
| 11 | h | 301 | PC1 | O32-C31-O31-C3 |
| 11 | A | 103 | PC1 | O21-C2-C3-O31 |
| 11 | A | 105 | PC1 | O21-C2-C3-O31 |
| 11 | a | 103 | PC1 | O21-C2-C3-O31 |
| 11 | a | 105 | PC1 | O21-C2-C3-O31 |
| 14 | M | 407 | CDL | OA6-CA4-CA6-OA8 |
| 14 | m | 407 | CDL | OA6-CA4-CA6-OA8 |
| 11 | A | 103 | PC1 | C27-C28-C29-C2A |
| 11 | a | 103 | PC1 | C27-C28-C29-C2A |
| 10 | L | 305 | U10 | C19-C21-C22-C23 |
| 10 | l | 305 | U10 | C19-C21-C22-C23 |
| 13 | C | 102 | SPO | C33-C35-C36-C37 |
| 13 | 3 | 103 | SPO | C33-C35-C36-C37 |
| 13 | c | 102 | SPO | C33-C35-C36-C37 |
| 13 | 5 | 103 | SPO | C33-C35-C36-C37 |
| 14 | M | 407 | CDL | OA7-CA5-OA6-CA4 |
| 14 | F | 102 | CDL | OB7-CB5-OB6-CB4 |
| 14 | m | 407 | CDL | OA7-CA5-OA6-CA4 |
| 14 | f | 102 | CDL | OB7-CB5-OB6-CB4 |
| 11 | H | 301 | PC1 | C2-C1-O11-P |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | h | 301 | PC1 | C2-C1-O11-P |
| 13 | Q | 104 | SPO | C15-C16-C17-C18 |
| 13 | q | 104 | SPO | C15-C16-C17-C18 |
| 13 | U | 103 | SPO | C5-C6-C7-C9 |
| 13 | U | 103 | SPO | C10-C11-C12-C14 |
| 13 | u | 103 | SPO | C5-C6-C7-C9 |
| 13 | u | 103 | SPO | C10-C11-C12-C14 |
| 11 | H | 302 | PC1 | O11-C1-C2-C3 |
| 11 | h | 302 | PC1 | O11-C1-C2-C3 |
| 8 | B | 101 | BCL | C4-C3-C5-C6 |
| 8 | b | 101 | BCL | C4-C3-C5-C6 |
| 13 | D | 103 | SPO | C11-C10-C9-C7 |
| 13 | Q | 103 | SPO | C25-C26-C27-C28 |
| 13 | C | 102 | SPO | C25-C26-C27-C28 |
| 13 | 9 | 102 | SPO | C11-C10-C9-C7 |
| 13 | d | 103 | SPO | C11-C10-C9-C7 |
| 13 | q | 103 | SPO | C25-C26-C27-C28 |
| 13 | c | 102 | SPO | C25-C26-C27-C28 |
| 13 | b9 | 102 | SPO | C11-C10-C9-C7 |
| 8 | M | 403 | BCL | CAD-CBD-CGD-O2D |
| 8 | m | 403 | BCL | CAD-CBD-CGD-O2D |
| 14 | M | 407 | CDL | C62-C63-C64-C65 |
| 14 | m | 407 | CDL | C62-C63-C64-C65 |
| 10 | L | 304 | U10 | C5-C4-O4-C4M |
| 10 | L | 305 | U10 | C5-C4-O4-C4M |
| 10 | l | 304 | U10 | C5-C4-O4-C4M |
| 10 | l | 305 | U10 | C5-C4-O4-C4M |
| 11 | H | 302 | PC1 | O11-C1-C2-O21 |
| 11 | h | 302 | PC1 | O11-C1-C2-O21 |
| 11 | A | 104 | PC1 | O21-C2-C3-O31 |
| 11 | a | 104 | PC1 | O21-C2-C3-O31 |
| 10 | L | 304 | U10 | C25-C24-C26-C27 |
| 10 | l | 304 | U10 | C25-C24-C26-C27 |
| 8 | D | 102 | BCL | C11-C10-C8-C9 |
| 8 | d | 102 | BCL | C11-C10-C8-C9 |
| 14 | F | 102 | CDL | C72-C73-C74-C75 |
| 14 | f | 102 | CDL | C72-C73-C74-C75 |
| 13 | A | 102 | SPO | C5-C6-C7-C8 |
| 13 | O | 102 | SPO | C10-C11-C12-C13 |
| 13 | U | 102 | SPO | C5-C6-C7-C8 |
| 13 | 0 | 102 | SPO | C5-C6-C7-C8 |
| 13 | a | 102 | SPO | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | o | 102 | SPO | C10-C11-C12-C13 |
| 13 | u | 102 | SPO | C5-C6-C7-C8 |
| 13 | b0 | 102 | SPO | C5-C6-C7-C8 |
| 13 | A | 102 | SPO | C5-C6-C7-C9 |
| 13 | E | 103 | SPO | C15-C16-C17-C19 |
| 13 | O | 102 | SPO | C10-C11-C12-C14 |
| 13 | P | 101 | SPO | C5-C6-C7-C9 |
| 13 | U | 102 | SPO | C5-C6-C7-C9 |
| 13 | 3 | 102 | SPO | C5-C6-C7-C9 |
| 13 | 0 | 102 | SPO | C5-C6-C7-C9 |
| 13 | a | 102 | SPO | C5-C6-C7-C9 |
| 13 | e | 103 | SPO | C15-C16-C17-C19 |
| 13 | o | 102 | SPO | C10-C11-C12-C14 |
| 13 | p | 101 | SPO | C5-C6-C7-C9 |
| 13 | u | 102 | SPO | C5-C6-C7-C9 |
| 13 | 5 | 102 | SPO | C5-C6-C7-C9 |
| 13 | b0 | 102 | SPO | C5-C6-C7-C9 |
| 11 | h | 302 | PC1 | C33-C34-C35-C36 |
| 9 | M | 404 | BPH | C2-C1-O2A-CGA |
| 9 | m | 404 | BPH | C2-C1-O2A-CGA |
| 11 | H | 302 | PC1 | C33-C34-C35-C36 |
| 13 | B | 102 | SPO | C11-C10-C9-C7 |
| 13 | b | 102 | SPO | C11-C10-C9-C7 |
| 13 | U | 103 | SPO | C29-C28-C30-C31 |
| 13 | u | 103 | SPO | C29-C28-C30-C31 |
| 11 | A | 104 | PC1 | C2-C1-O11-P |
| 11 | a | 104 | PC1 | C2-C1-O11-P |
| 11 | L | 307 | PC1 | C1-O11-P-O14 |
| 11 | H | 301 | PC1 | C11-O13-P-O14 |
| 11 | A | 103 | PC1 | C11-O13-P-O12 |
| 11 | A | 104 | PC1 | C11-O13-P-O14 |
| 11 | A | 105 | PC1 | C11-O13-P-O12 |
| 11 | D | 101 | PC1 | C11-O13-P-O12 |
| 11 | l | 307 | PC1 | C1-O11-P-O14 |
| 11 | h | 301 | PC1 | C11-O13-P-O14 |
| 11 | a | 103 | PC1 | C11-O13-P-O12 |
| 11 | a | 104 | PC1 | C11-O13-P-O14 |
| 11 | a | 105 | PC1 | C11-O13-P-O12 |
| 11 | d | 101 | PC1 | C11-O13-P-O12 |
| 14 | M | 407 | CDL | CA3-OA5-PA1-OA4 |
| 14 | F | 102 | CDL | CA3-OA5-PA1-OA4 |
| 14 | F | 102 | CDL | CB3-OB5-PB2-OB3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 14 | m | 407 | CDL | CA3-OA5-PA1-OA4 |
| 14 | f | 102 | CDL | CA3-OA5-PA1-OA4 |
| 14 | f | 102 | CDL | CB3-OB5-PB2-OB3 |
| 11 | L | 307 | PC1 | O11-C1-C2-C3 |
| 11 | D | 101 | PC1 | O11-C1-C2-C3 |
| 11 | l | 307 | PC1 | O11-C1-C2-C3 |
| 11 | d | 101 | PC1 | O11-C1-C2-C3 |
| 14 | F | 102 | CDL | OB5-CB3-CB4-CB6 |
| 14 | f | 102 | CDL | OB5-CB3-CB4-CB6 |
| 10 | L | 305 | U10 | C27-C28-C29-C30 |
| 10 | l | 305 | U10 | C27-C28-C29-C30 |
| 13 | C | 102 | SPO | C28-C30-C31-C32 |
| 13 | 3 | 103 | SPO | C28-C30-C31-C32 |
| 13 | c | 102 | SPO | C28-C30-C31-C32 |
| 13 | 5 | 103 | SPO | C28-C30-C31-C32 |
| 11 | H | 302 | PC1 | C12-C11-O13-P |
| 11 | h | 302 | PC1 | C12-C11-O13-P |
| 13 | B | 102 | SPO | C1-C4-C5-C6 |
| 13 | b | 102 | SPO | C1-C4-C5-C6 |
| 11 | D | 101 | PC1 | C21-C22-C23-C24 |
| 11 | d | 101 | PC1 | C21-C22-C23-C24 |
| 14 | M | 407 | CDL | C12-C13-C14-C15 |
| 14 | m | 407 | CDL | C12-C13-C14-C15 |
| 8 | B | 101 | BCL | C2-C3-C5-C6 |
| 8 | b | 101 | BCL | C2-C3-C5-C6 |
| 14 | F | 102 | CDL | OB5-CB3-CB4-OB6 |
| 14 | f | 102 | CDL | OB5-CB3-CB4-OB6 |
| 13 | N | 101 | SPO | C11-C10-C9-C7 |
| 13 | n | 101 | SPO | C11-C10-C9-C7 |
| 11 | A | 104 | PC1 | C11-C12-N-C13 |
| 11 | a | 104 | PC1 | C11-C12-N-C13 |
| 11 | L | 307 | PC1 | O13-C11-C12-N |
| 11 | l | 307 | PC1 | O13-C11-C12-N |
| 11 | H | 302 | PC1 | C34-C35-C36-C37 |
| 11 | h | 302 | PC1 | C34-C35-C36-C37 |
| 8 | 7 | 102 | BCL | C6-C7-C8-C9 |
| 8 | 6 | 102 | BCL | C6-C7-C8-C9 |
| 10 | M | 405 | U10 | C24-C26-C27-C28 |
| 10 | m | 405 | U10 | C24-C26-C27-C28 |
| 13 | B | 102 | SPO | C9-C10-C11-C12 |
| 13 | D | 103 | SPO | C9-C10-C11-C12 |
| 13 | E | 103 | SPO | C9-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|-----------------|
| 13 | G | 103 | SPO | C9-C10-C11-C12 |
| 13 | J | 102 | SPO | C9-C10-C11-C12 |
| 13 | S | 102 | SPO | C9-C10-C11-C12 |
| 13 | C | 102 | SPO | C14-C15-C16-C17 |
| 13 | 0 | 102 | SPO | C9-C10-C11-C12 |
| 13 | b | 102 | SPO | C9-C10-C11-C12 |
| 13 | d | 103 | SPO | C9-C10-C11-C12 |
| 13 | e | 103 | SPO | C9-C10-C11-C12 |
| 13 | g | 103 | SPO | C9-C10-C11-C12 |
| 13 | j | 102 | SPO | C9-C10-C11-C12 |
| 13 | s | 102 | SPO | C9-C10-C11-C12 |
| 13 | c | 102 | SPO | C14-C15-C16-C17 |
| 13 | b0 | 102 | SPO | C9-C10-C11-C12 |
| 13 | 3 | 102 | SPO | C12-C14-C15-C16 |
| 13 | 5 | 102 | SPO | C12-C14-C15-C16 |
| 14 | M | 407 | CDL | C33-C34-C35-C36 |
| 14 | m | 407 | CDL | C33-C34-C35-C36 |
| 13 | Q | 104 | SPO | C15-C16-C17-C19 |
| 13 | q | 104 | SPO | C15-C16-C17-C19 |
| 14 | m | 407 | CDL | C59-C60-C61-C62 |
| 14 | M | 407 | CDL | C59-C60-C61-C62 |
| 10 | L | 304 | U10 | C23-C24-C26-C27 |
| 10 | l | 304 | U10 | C23-C24-C26-C27 |
| 13 | U | 103 | SPO | C27-C28-C30-C31 |
| 13 | u | 103 | SPO | C27-C28-C30-C31 |
| 13 | M | 406 | SPO | C3-C1-O1-CM1 |
| 13 | 9 | 102 | SPO | C33-C35-C36-C37 |
| 13 | m | 406 | SPO | C3-C1-O1-CM1 |
| 13 | b9 | 102 | SPO | C33-C35-C36-C37 |
| 11 | D | 101 | PC1 | C11-O13-P-O11 |
| 11 | d | 101 | PC1 | C11-O13-P-O11 |
| 14 | M | 407 | CDL | CA2-OA2-PA1-OA5 |
| 14 | M | 407 | CDL | CB2-OB2-PB2-OB5 |
| 14 | m | 407 | CDL | CA2-OA2-PA1-OA5 |
| 14 | m | 407 | CDL | CB2-OB2-PB2-OB5 |
| 13 | U | 103 | SPO | C2-C1-C4-C5 |
| 13 | u | 103 | SPO | C2-C1-C4-C5 |
| 14 | F | 102 | CDL | CA3-CA4-CA6-OA8 |
| 14 | F | 102 | CDL | CB3-CB4-CB6-OB8 |
| 14 | f | 102 | CDL | CA3-CA4-CA6-OA8 |
| 14 | f | 102 | CDL | CB3-CB4-CB6-OB8 |
| 11 | H | 302 | PC1 | C36-C37-C38-C39 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | h | 302 | PC1 | C36-C37-C38-C39 |
| 8 | D | 102 | BCL | C11-C10-C8-C7 |
| 8 | d | 102 | BCL | C11-C10-C8-C7 |
| 13 | D | 103 | SPO | C12-C14-C15-C16 |
| 13 | Q | 103 | SPO | C12-C14-C15-C16 |
| 13 | Q | 104 | SPO | C11-C10-C9-C7 |
| 13 | d | 103 | SPO | C12-C14-C15-C16 |
| 13 | q | 103 | SPO | C12-C14-C15-C16 |
| 13 | q | 104 | SPO | C11-C10-C9-C7 |
| 11 | H | 302 | PC1 | C32-C31-O31-C3 |
| 11 | h | 302 | PC1 | C32-C31-O31-C3 |
| 13 | M | 406 | SPO | C15-C16-C17-C19 |
| 13 | m | 406 | SPO | C15-C16-C17-C19 |
| 13 | J | 102 | SPO | C29-C28-C30-C31 |
| 13 | j | 102 | SPO | C29-C28-C30-C31 |
| 11 | A | 103 | PC1 | C32-C31-O31-C3 |
| 11 | a | 103 | PC1 | C32-C31-O31-C3 |
| 11 | L | 307 | PC1 | O21-C21-C22-C23 |
| 11 | l | 307 | PC1 | O21-C21-C22-C23 |
| 13 | J | 102 | SPO | C12-C14-C15-C16 |
| 13 | S | 102 | SPO | C11-C10-C9-C7 |
| 13 | 3 | 102 | SPO | C17-C19-C20-C21 |
| 13 | j | 102 | SPO | C12-C14-C15-C16 |
| 13 | s | 102 | SPO | C11-C10-C9-C7 |
| 13 | 5 | 102 | SPO | C17-C19-C20-C21 |
| 8 | T | 101 | BCL | C4-C3-C5-C6 |
| 8 | t | 101 | BCL | C4-C3-C5-C6 |
| 8 | T | 101 | BCL | C2-C3-C5-C6 |
| 8 | t | 101 | BCL | C2-C3-C5-C6 |
| 11 | A | 104 | PC1 | C11-C12-N-C14 |
| 11 | a | 104 | PC1 | C11-C12-N-C14 |
| 8 | 0 | 101 | BCL | C4-C3-C5-C6 |
| 8 | b0 | 101 | BCL | C4-C3-C5-C6 |
| 13 | E | 103 | SPO | C8-C7-C9-C10 |
| 13 | C | 102 | SPO | C13-C12-C14-C15 |
| 13 | e | 103 | SPO | C8-C7-C9-C10 |
| 13 | c | 102 | SPO | C13-C12-C14-C15 |
| 11 | H | 302 | PC1 | O32-C31-O31-C3 |
| 11 | h | 302 | PC1 | O32-C31-O31-C3 |
| 11 | a | 105 | PC1 | C24-C25-C26-C27 |
| 13 | 3 | 103 | SPO | C15-C16-C17-C18 |
| 13 | 5 | 103 | SPO | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | A | 105 | PC1 | C24-C25-C26-C27 |
| 11 | A | 104 | PC1 | C11-C12-N-C15 |
| 11 | a | 104 | PC1 | C11-C12-N-C15 |
| 8 | M | 402 | BCL | C11-C10-C8-C7 |
| 8 | 0 | 101 | BCL | C2-C3-C5-C6 |
| 8 | m | 402 | BCL | C11-C10-C8-C7 |
| 8 | b0 | 101 | BCL | C2-C3-C5-C6 |
| 11 | A | 103 | PC1 | O32-C31-O31-C3 |
| 11 | a | 103 | PC1 | O32-C31-O31-C3 |
| 10 | L | 304 | U10 | C3-C4-O4-C4M |
| 10 | l | 304 | U10 | C3-C4-O4-C4M |
| 14 | F | 102 | CDL | CB3-OB5-PB2-OB2 |
| 14 | f | 102 | CDL | CB3-OB5-PB2-OB2 |
| 8 | Q | 101 | BCL | C8-C10-C11-C12 |
| 8 | q | 101 | BCL | C8-C10-C11-C12 |
| 8 | B | 101 | BCL | C10-C11-C12-C13 |
| 8 | b | 101 | BCL | C10-C11-C12-C13 |
| 10 | L | 304 | U10 | C12-C11-C9-C10 |
| 10 | l | 304 | U10 | C12-C11-C9-C10 |
| 13 | N | 101 | SPO | C29-C28-C30-C31 |
| 13 | P | 101 | SPO | C29-C28-C30-C31 |
| 13 | Q | 104 | SPO | C29-C28-C30-C31 |
| 13 | n | 101 | SPO | C29-C28-C30-C31 |
| 13 | p | 101 | SPO | C29-C28-C30-C31 |
| 13 | q | 104 | SPO | C29-C28-C30-C31 |
| 10 | M | 405 | U10 | C5-C4-O4-C4M |
| 10 | m | 405 | U10 | C5-C4-O4-C4M |
| 13 | E | 103 | SPO | C6-C7-C9-C10 |
| 13 | C | 102 | SPO | C11-C12-C14-C15 |
| 13 | e | 103 | SPO | C6-C7-C9-C10 |
| 13 | c | 102 | SPO | C11-C12-C14-C15 |
| 13 | P | 101 | SPO | C11-C10-C9-C7 |
| 13 | p | 101 | SPO | C11-C10-C9-C7 |
| 13 | I | 102 | SPO | C34-C33-C35-C36 |
| 13 | i | 102 | SPO | C34-C33-C35-C36 |
| 8 | D | 102 | BCL | C8-C10-C11-C12 |
| 8 | d | 102 | BCL | C8-C10-C11-C12 |
| 8 | M | 402 | BCL | C4-C3-C5-C6 |
| 8 | m | 402 | BCL | C4-C3-C5-C6 |
| 13 | D | 103 | SPO | C29-C28-C30-C31 |
| 13 | G | 101 | SPO | C29-C28-C30-C31 |
| 13 | O | 102 | SPO | C29-C28-C30-C31 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | 9 | 102 | SPO | C29-C28-C30-C31 |
| 13 | d | 103 | SPO | C29-C28-C30-C31 |
| 13 | g | 101 | SPO | C29-C28-C30-C31 |
| 13 | o | 102 | SPO | C29-C28-C30-C31 |
| 13 | b9 | 102 | SPO | C29-C28-C30-C31 |
| 11 | L | 307 | PC1 | C36-C37-C38-C39 |
| 11 | l | 307 | PC1 | C36-C37-C38-C39 |
| 11 | A | 103 | PC1 | C28-C29-C2A-C2B |
| 11 | a | 103 | PC1 | C28-C29-C2A-C2B |
| 8 | b9 | 101 | BCL | C4-C3-C5-C6 |
| 13 | A | 102 | SPO | C29-C28-C30-C31 |
| 13 | I | 102 | SPO | C29-C28-C30-C31 |
| 13 | U | 102 | SPO | C29-C28-C30-C31 |
| 13 | a | 102 | SPO | C29-C28-C30-C31 |
| 13 | i | 102 | SPO | C29-C28-C30-C31 |
| 13 | u | 102 | SPO | C29-C28-C30-C31 |
| 13 | Q | 104 | SPO | C27-C28-C30-C31 |
| 13 | q | 104 | SPO | C27-C28-C30-C31 |
| 13 | D | 103 | SPO | C25-C26-C27-C28 |
| 13 | U | 103 | SPO | C11-C10-C9-C7 |
| 13 | d | 103 | SPO | C25-C26-C27-C28 |
| 13 | u | 103 | SPO | C11-C10-C9-C7 |
| 8 | Z | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | z | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | K | 101 | BCL | C4-C3-C5-C6 |
| 8 | 9 | 101 | BCL | C4-C3-C5-C6 |
| 8 | k | 101 | BCL | C4-C3-C5-C6 |
| 13 | E | 101 | SPO | C29-C28-C30-C31 |
| 13 | S | 103 | SPO | C34-C33-C35-C36 |
| 13 | e | 101 | SPO | C29-C28-C30-C31 |
| 13 | s | 103 | SPO | C34-C33-C35-C36 |
| 8 | E | 102 | BCL | C10-C11-C12-C13 |
| 8 | e | 102 | BCL | C10-C11-C12-C13 |
| 8 | M | 402 | BCL | C2-C3-C5-C6 |
| 8 | m | 402 | BCL | C2-C3-C5-C6 |
| 10 | L | 304 | U10 | C12-C11-C9-C8 |
| 10 | l | 304 | U10 | C12-C11-C9-C8 |
| 14 | m | 407 | CDL | C31-C32-C33-C34 |
| 8 | M | 402 | BCL | C11-C10-C8-C9 |
| 8 | V | 101 | BCL | C6-C7-C8-C9 |
| 8 | m | 402 | BCL | C11-C10-C8-C9 |
| 8 | v | 101 | BCL | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 14 | M | 407 | CDL | C31-C32-C33-C34 |
| 8 | E | 102 | BCL | CAA-CBA-CGA-O2A |
| 8 | e | 102 | BCL | CAA-CBA-CGA-O2A |
| 11 | H | 301 | PC1 | O21-C21-C22-C23 |
| 11 | h | 301 | PC1 | O21-C21-C22-C23 |
| 9 | M | 404 | BPH | CAD-CBD-CGD-O2D |
| 9 | m | 404 | BPH | CAD-CBD-CGD-O2D |
| 8 | 7 | 102 | BCL | C8-C10-C11-C12 |
| 8 | 6 | 102 | BCL | C8-C10-C11-C12 |
| 8 | V | 101 | BCL | C4-C3-C5-C6 |
| 8 | v | 101 | BCL | C4-C3-C5-C6 |
| 13 | B | 102 | SPO | C29-C28-C30-C31 |
| 13 | E | 101 | SPO | C34-C33-C35-C36 |
| 13 | S | 103 | SPO | C29-C28-C30-C31 |
| 13 | b | 102 | SPO | C29-C28-C30-C31 |
| 13 | e | 101 | SPO | C34-C33-C35-C36 |
| 13 | s | 103 | SPO | C29-C28-C30-C31 |
| 8 | 2 | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | 4 | 101 | BCL | CAA-CBA-CGA-O2A |
| 13 | I | 102 | SPO | C27-C28-C30-C31 |
| 13 | N | 101 | SPO | C27-C28-C30-C31 |
| 13 | P | 101 | SPO | C27-C28-C30-C31 |
| 13 | 9 | 102 | SPO | C27-C28-C30-C31 |
| 13 | i | 102 | SPO | C27-C28-C30-C31 |
| 13 | n | 101 | SPO | C27-C28-C30-C31 |
| 13 | p | 101 | SPO | C27-C28-C30-C31 |
| 13 | b9 | 102 | SPO | C27-C28-C30-C31 |
| 11 | D | 101 | PC1 | C24-C25-C26-C27 |
| 11 | d | 101 | PC1 | C24-C25-C26-C27 |
| 13 | M | 406 | SPO | C33-C35-C36-C37 |
| 13 | m | 406 | SPO | C33-C35-C36-C37 |
| 8 | 2 | 101 | BCL | CAA-CBA-CGA-O1A |
| 8 | 4 | 101 | BCL | CAA-CBA-CGA-O1A |
| 8 | V | 101 | BCL | O2A-C1-C2-C3 |
| 8 | 7 | 101 | BCL | O2A-C1-C2-C3 |
| 8 | v | 101 | BCL | O2A-C1-C2-C3 |
| 8 | 6 | 101 | BCL | O2A-C1-C2-C3 |
| 8 | J | 101 | BCL | CHA-CBD-CGD-O2D |
| 8 | C | 101 | BCL | CHA-CBD-CGD-O2D |
| 8 | 1 | 101 | BCL | CHA-CBD-CGD-O1D |
| 8 | 1 | 101 | BCL | CHA-CBD-CGD-O2D |
| 8 | j | 101 | BCL | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 8 | c | 101 | BCL | CHA-CBD-CGD-O2D |
| 8 | b1 | 101 | BCL | CHA-CBD-CGD-O1D |
| 8 | b1 | 101 | BCL | CHA-CBD-CGD-O2D |
| 11 | L | 306 | PC1 | O21-C21-C22-C23 |
| 11 | l | 306 | PC1 | O21-C21-C22-C23 |
| 11 | A | 103 | PC1 | O11-C1-C2-C3 |
| 11 | a | 103 | PC1 | O11-C1-C2-C3 |
| 13 | Q | 103 | SPO | C2-C1-C4-C5 |
| 13 | q | 103 | SPO | C2-C1-C4-C5 |
| 8 | A | 101 | BCL | C8-C10-C11-C12 |
| 8 | a | 101 | BCL | C8-C10-C11-C12 |
| 8 | V | 101 | BCL | C6-C7-C8-C10 |
| 8 | v | 101 | BCL | C6-C7-C8-C10 |
| 13 | A | 102 | SPO | C27-C28-C30-C31 |
| 13 | E | 101 | SPO | C27-C28-C30-C31 |
| 13 | J | 102 | SPO | C27-C28-C30-C31 |
| 13 | a | 102 | SPO | C27-C28-C30-C31 |
| 13 | e | 101 | SPO | C27-C28-C30-C31 |
| 13 | j | 102 | SPO | C27-C28-C30-C31 |
| 8 | n | 102 | BCL | C10-C11-C12-C13 |
| 8 | Q | 101 | BCL | C6-C7-C8-C9 |
| 8 | q | 101 | BCL | C6-C7-C8-C9 |
| 8 | N | 102 | BCL | C10-C11-C12-C13 |
| 11 | A | 105 | PC1 | C36-C37-C38-C39 |
| 11 | a | 105 | PC1 | C36-C37-C38-C39 |
| 13 | S | 102 | SPO | O1-C1-C4-C5 |
| 13 | s | 102 | SPO | O1-C1-C4-C5 |
| 10 | L | 305 | U10 | C15-C14-C16-C17 |
| 10 | l | 305 | U10 | C15-C14-C16-C17 |
| 13 | 3 | 102 | SPO | C29-C28-C30-C31 |
| 13 | 5 | 102 | SPO | C29-C28-C30-C31 |
| 8 | E | 102 | BCL | CAA-CBA-CGA-O1A |
| 11 | l | 307 | PC1 | C32-C33-C34-C35 |
| 14 | F | 102 | CDL | C71-CB7-OB8-CB6 |
| 14 | f | 102 | CDL | C71-CB7-OB8-CB6 |
| 11 | L | 307 | PC1 | C32-C33-C34-C35 |
| 14 | F | 102 | CDL | C52-C53-C54-C55 |
| 8 | Z | 101 | BCL | CAA-CBA-CGA-O1A |
| 8 | e | 102 | BCL | CAA-CBA-CGA-O1A |
| 8 | z | 101 | BCL | CAA-CBA-CGA-O1A |
| 11 | H | 301 | PC1 | O22-C21-C22-C23 |
| 11 | h | 301 | PC1 | O22-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 14 | f | 102 | CDL | C52-C53-C54-C55 |
| 13 | Q | 102 | SPO | C34-C33-C35-C36 |
| 11 | A | 104 | PC1 | O21-C21-C22-C23 |
| 11 | a | 104 | PC1 | O21-C21-C22-C23 |
| 14 | M | 407 | CDL | CB3-OB5-PB2-OB3 |
| 14 | m | 407 | CDL | CB3-OB5-PB2-OB3 |
| 14 | F | 102 | CDL | OB9-CB7-OB8-CB6 |
| 14 | f | 102 | CDL | OB9-CB7-OB8-CB6 |
| 13 | q | 102 | SPO | C34-C33-C35-C36 |
| 8 | N | 102 | BCL | CAD-CBD-CGD-O1D |
| 8 | n | 102 | BCL | CAD-CBD-CGD-O1D |
| 11 | H | 301 | PC1 | C12-C11-O13-P |
| 11 | h | 301 | PC1 | C12-C11-O13-P |
| 11 | L | 307 | PC1 | O31-C31-C32-C33 |
| 11 | l | 307 | PC1 | O31-C31-C32-C33 |
| 8 | Q | 101 | BCL | C11-C10-C8-C9 |
| 8 | 7 | 101 | BCL | C11-C10-C8-C9 |
| 8 | 9 | 101 | BCL | C11-C10-C8-C9 |
| 8 | q | 101 | BCL | C11-C10-C8-C9 |
| 8 | 6 | 101 | BCL | C11-C10-C8-C9 |
| 8 | b9 | 101 | BCL | C11-C10-C8-C9 |
| 14 | M | 407 | CDL | C72-C71-CB7-OB8 |
| 14 | m | 407 | CDL | C72-C71-CB7-OB8 |
| 13 | M | 406 | SPO | C1-C4-C5-C6 |
| 13 | Q | 103 | SPO | C1-C4-C5-C6 |
| 13 | m | 406 | SPO | C1-C4-C5-C6 |
| 13 | q | 103 | SPO | C1-C4-C5-C6 |
| 8 | T | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | 7 | 102 | BCL | CAA-CBA-CGA-O2A |
| 8 | t | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | 6 | 102 | BCL | CAA-CBA-CGA-O2A |
| 10 | M | 405 | U10 | C25-C24-C26-C27 |
| 10 | m | 405 | U10 | C25-C24-C26-C27 |
| 8 | Q | 101 | BCL | C6-C7-C8-C10 |
| 8 | 7 | 101 | BCL | C11-C10-C8-C7 |
| 8 | 9 | 101 | BCL | C11-C10-C8-C7 |
| 8 | q | 101 | BCL | C6-C7-C8-C10 |
| 8 | 6 | 101 | BCL | C11-C10-C8-C7 |
| 8 | b9 | 101 | BCL | C11-C10-C8-C7 |
| 13 | G | 101 | SPO | C27-C28-C30-C31 |
| 13 | I | 102 | SPO | C32-C33-C35-C36 |
| 13 | O | 102 | SPO | C27-C28-C30-C31 |

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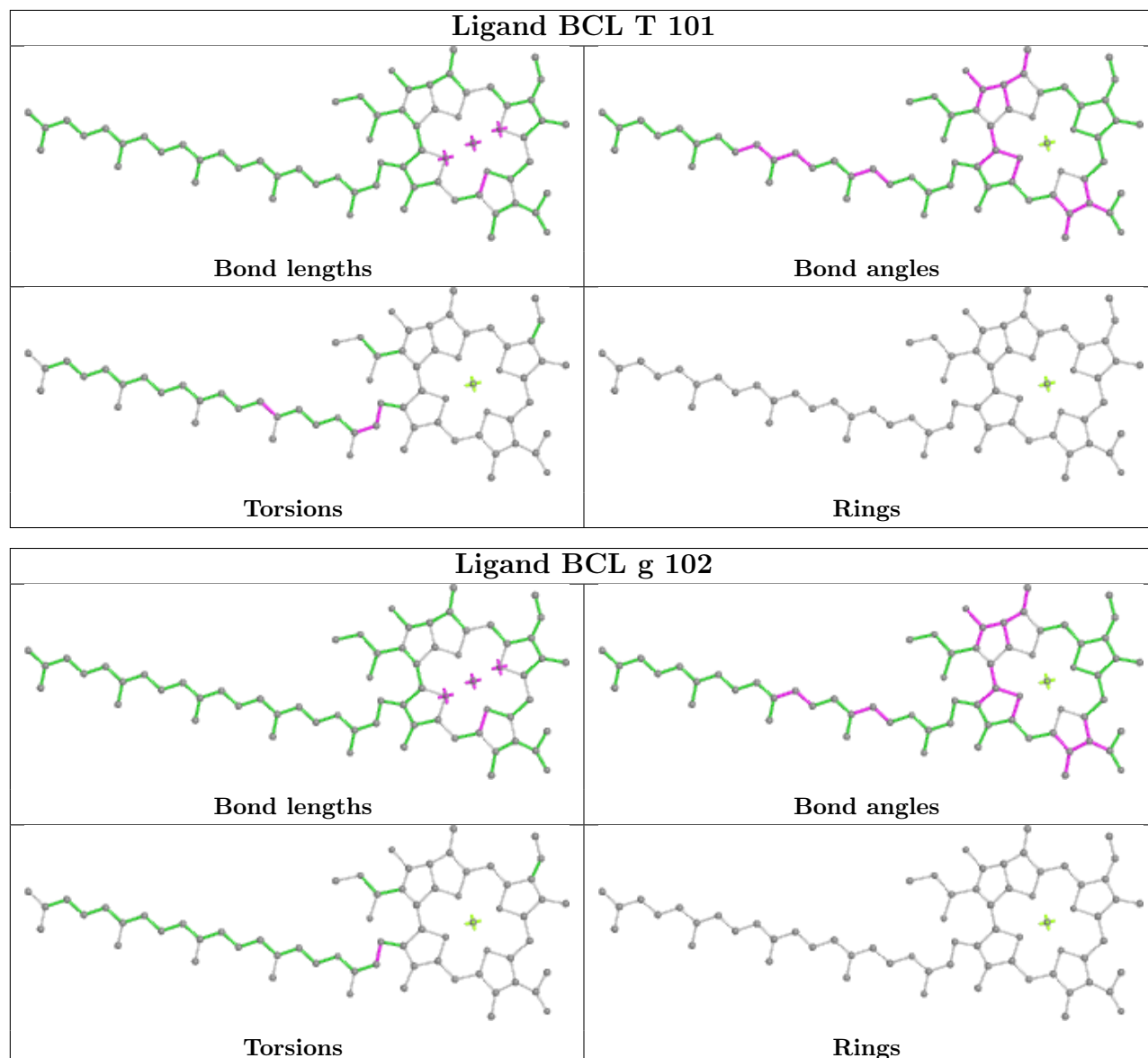
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 13 | g | 101 | SPO | C27-C28-C30-C31 |
| 13 | i | 102 | SPO | C32-C33-C35-C36 |
| 13 | o | 102 | SPO | C27-C28-C30-C31 |
| 8 | R | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | r | 101 | BCL | CAA-CBA-CGA-O2A |
| 13 | P | 101 | SPO | C15-C16-C17-C19 |
| 13 | 3 | 103 | SPO | C15-C16-C17-C19 |
| 13 | p | 101 | SPO | C15-C16-C17-C19 |
| 13 | 5 | 103 | SPO | C15-C16-C17-C19 |
| 13 | E | 101 | SPO | C11-C10-C9-C7 |
| 13 | E | 103 | SPO | C17-C19-C20-C21 |
| 13 | C | 102 | SPO | C17-C19-C20-C21 |
| 13 | e | 101 | SPO | C11-C10-C9-C7 |
| 13 | e | 103 | SPO | C17-C19-C20-C21 |
| 13 | c | 102 | SPO | C17-C19-C20-C21 |
| 11 | A | 104 | PC1 | O22-C21-C22-C23 |
| 11 | a | 104 | PC1 | O22-C21-C22-C23 |
| 13 | G | 101 | SPO | C28-C30-C31-C32 |
| 13 | I | 102 | SPO | C28-C30-C31-C32 |
| 13 | P | 101 | SPO | C28-C30-C31-C32 |
| 13 | g | 101 | SPO | C28-C30-C31-C32 |
| 13 | i | 102 | SPO | C28-C30-C31-C32 |
| 13 | p | 101 | SPO | C28-C30-C31-C32 |
| 8 | J | 101 | BCL | C10-C11-C12-C13 |
| 8 | j | 101 | BCL | C10-C11-C12-C13 |
| 8 | r | 101 | BCL | CAA-CBA-CGA-O1A |
| 8 | B | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | P | 102 | BCL | CAA-CBA-CGA-O2A |
| 8 | b | 101 | BCL | CAA-CBA-CGA-O2A |
| 8 | p | 102 | BCL | CAA-CBA-CGA-O2A |
| 8 | 7 | 101 | BCL | C8-C10-C11-C12 |
| 8 | 6 | 101 | BCL | C8-C10-C11-C12 |

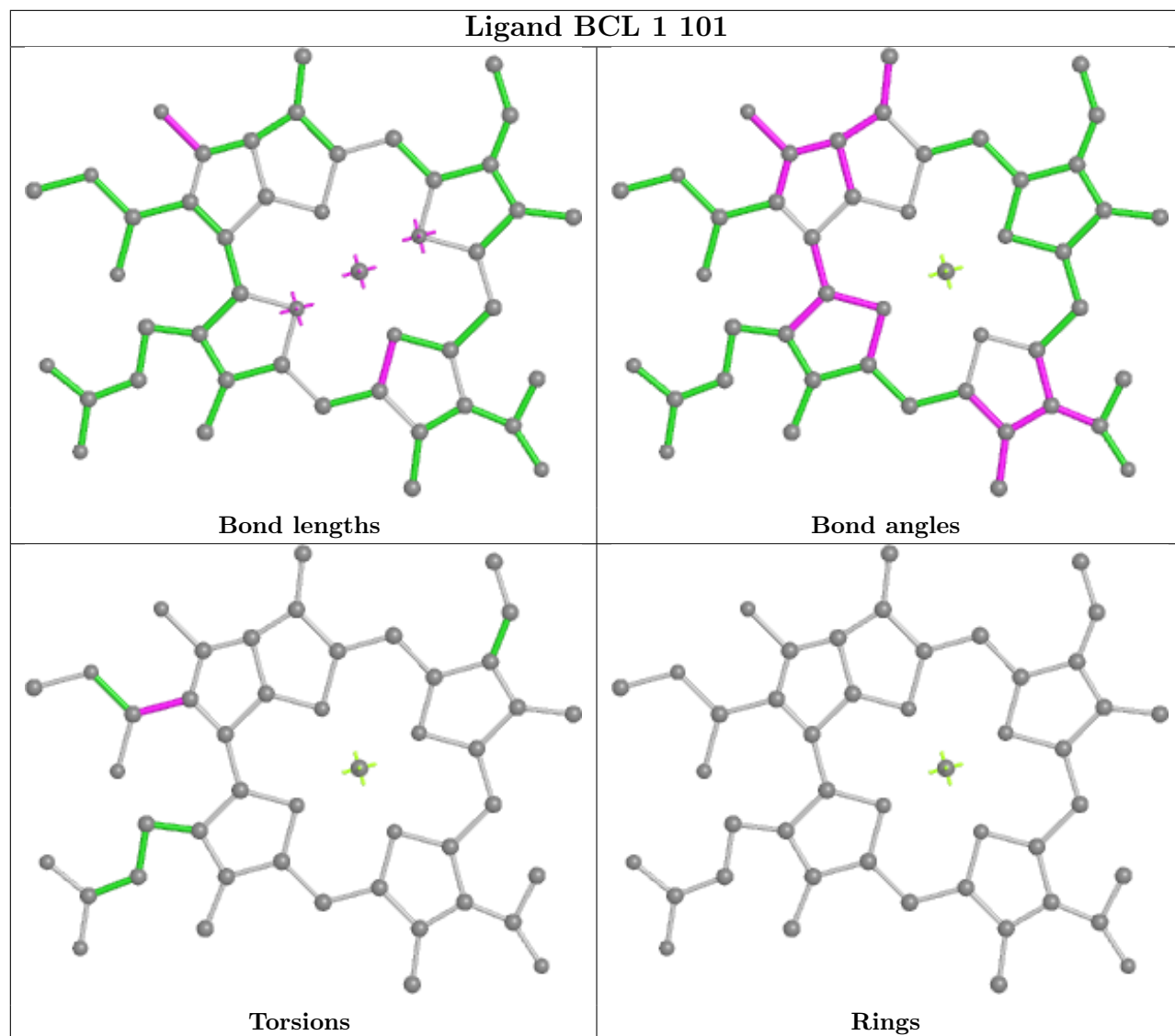
There are no ring outliers.

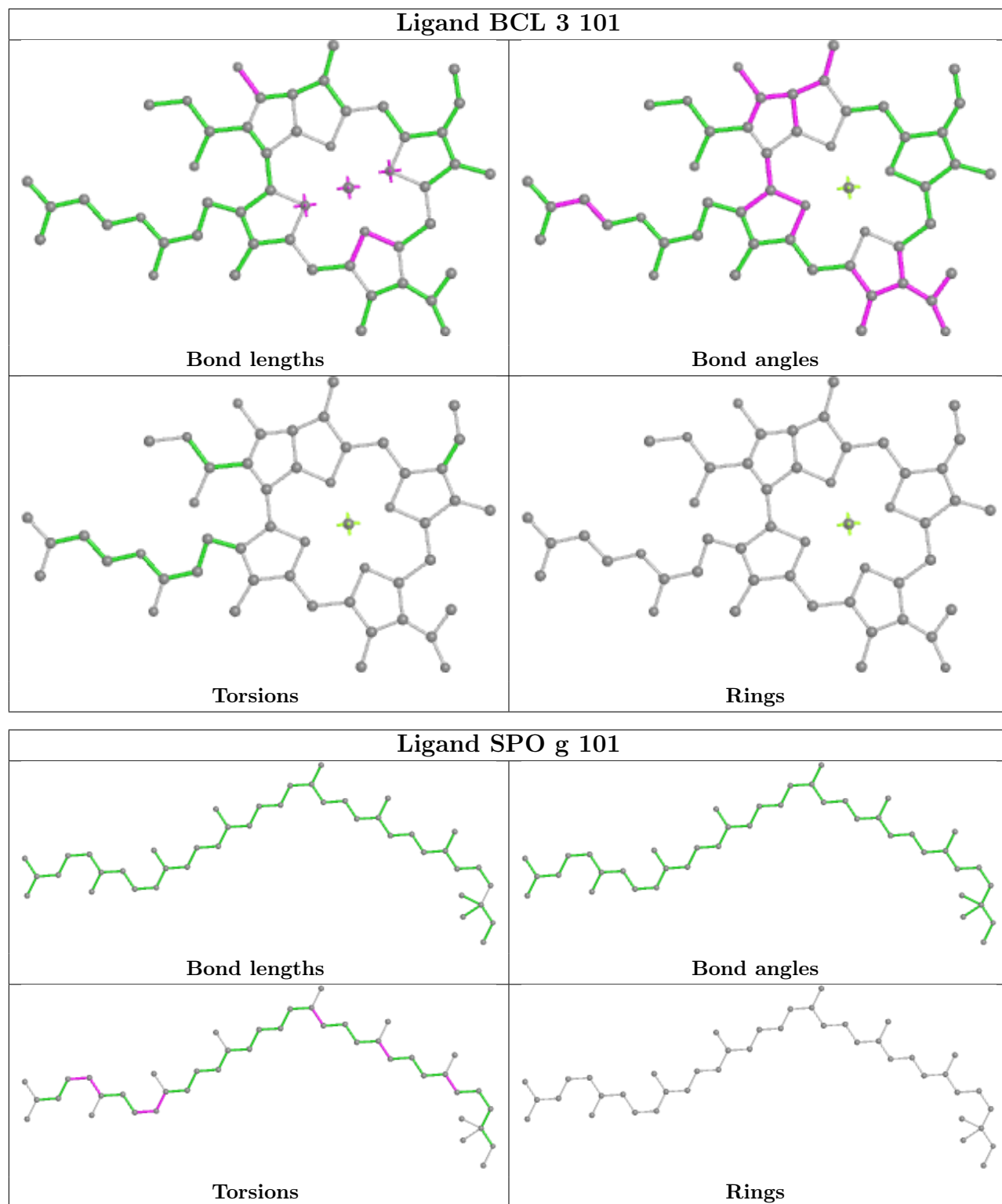
No monomer is involved in short contacts.

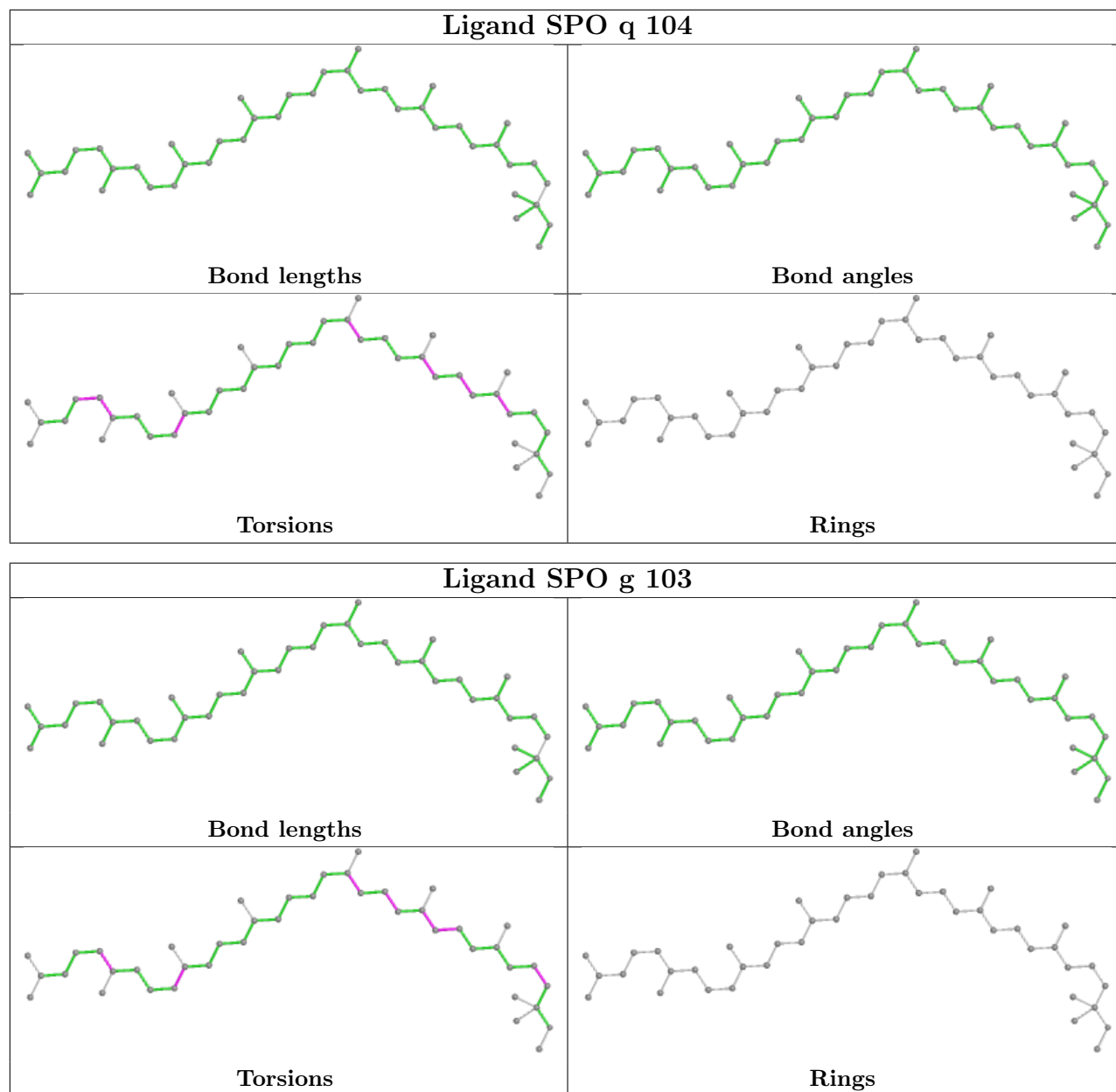
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

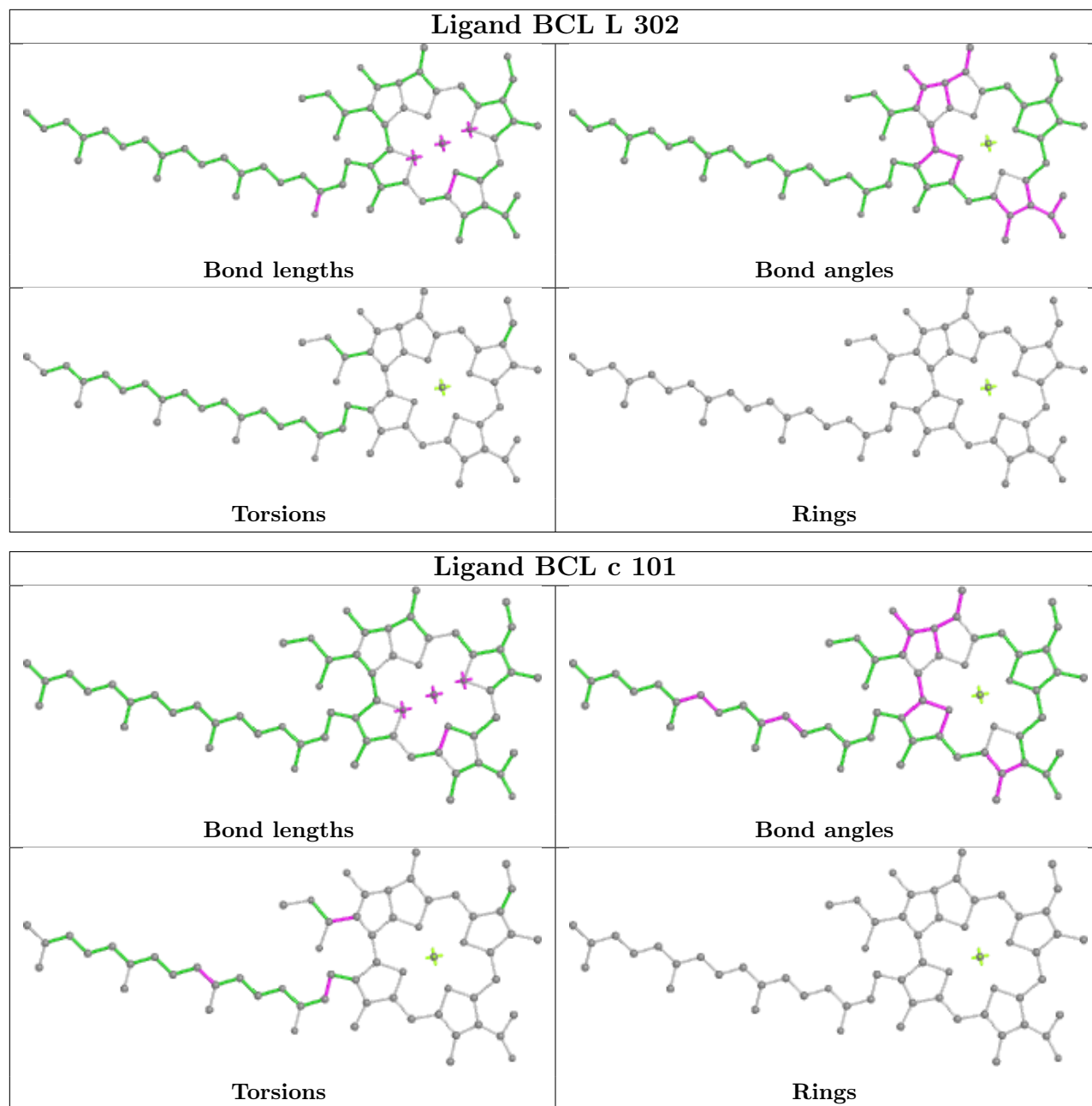
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

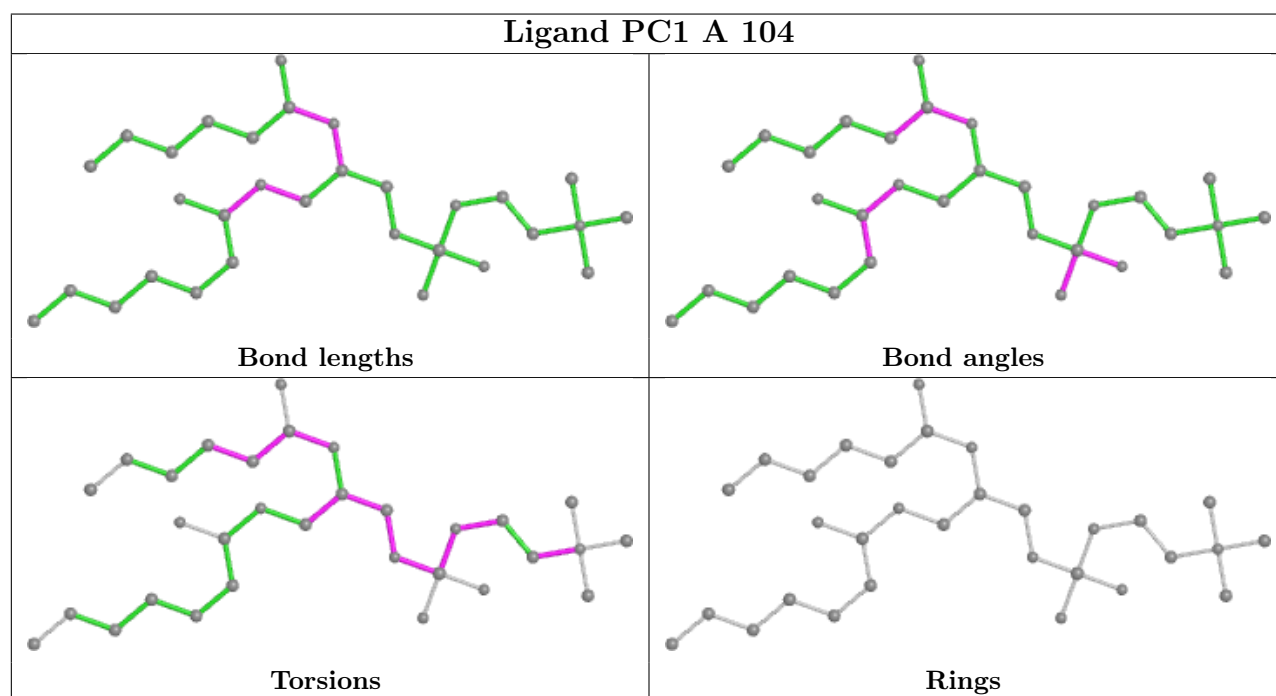
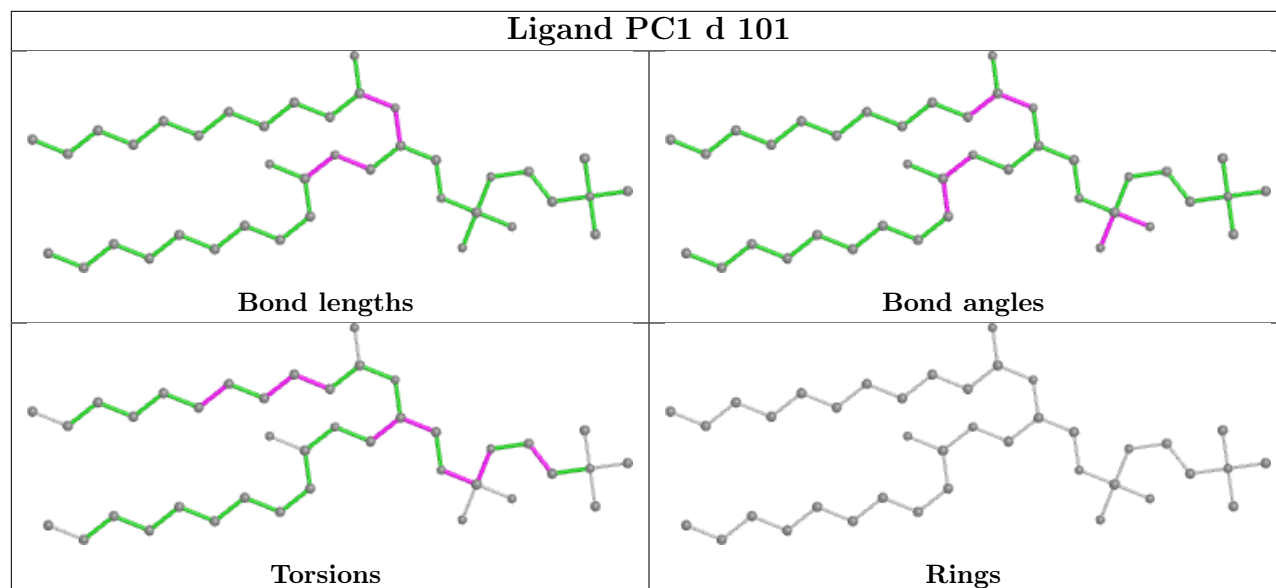


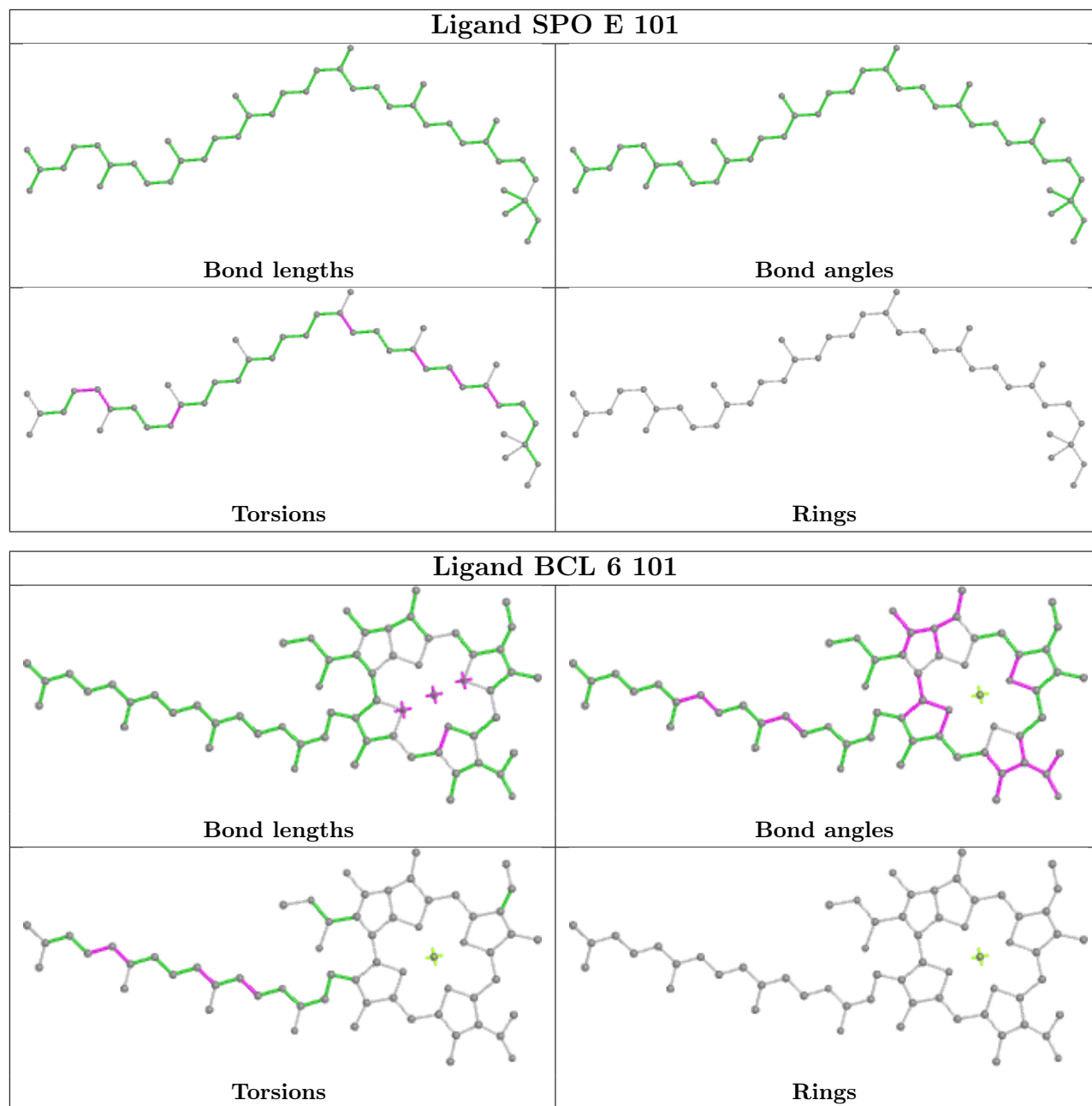


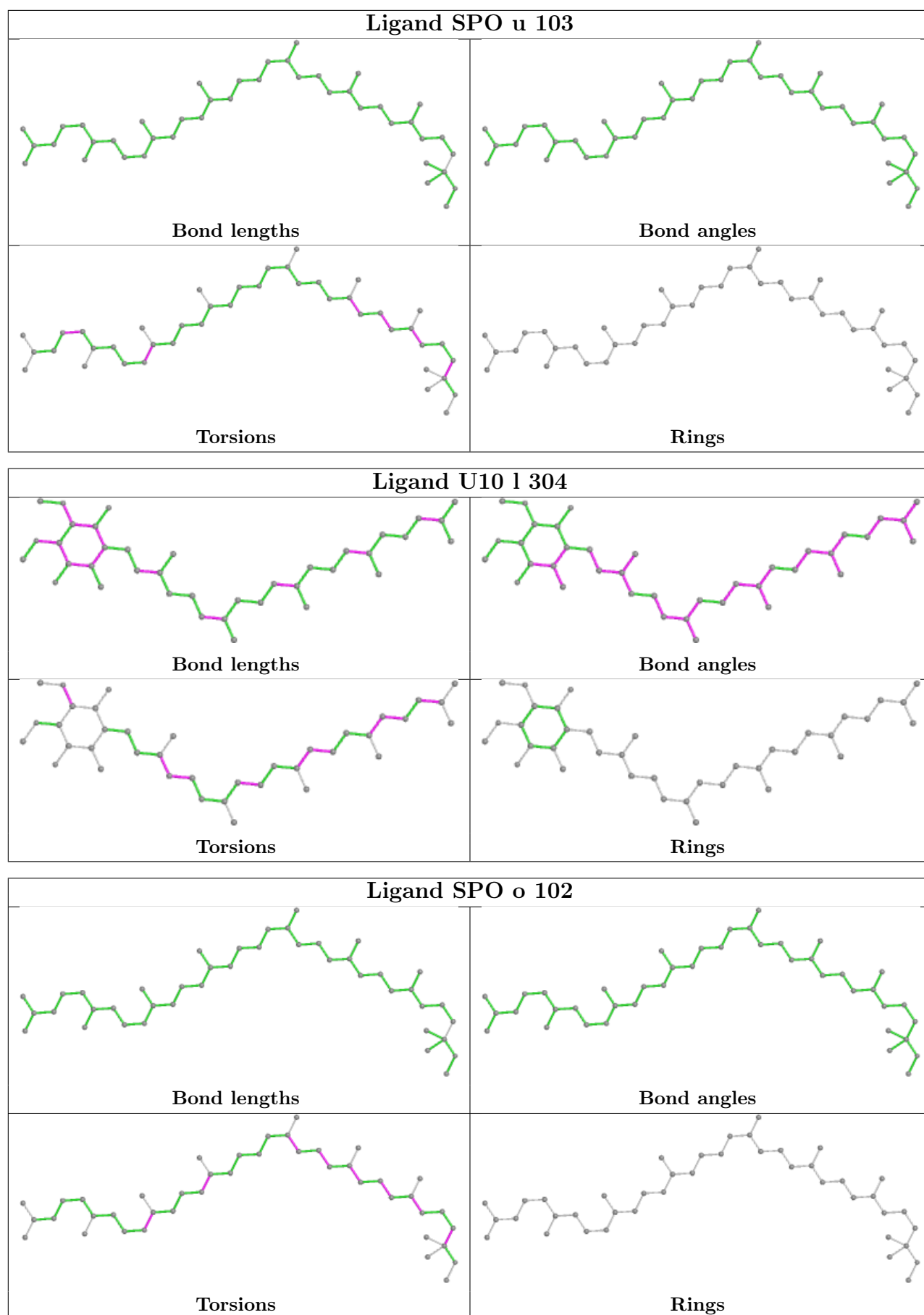


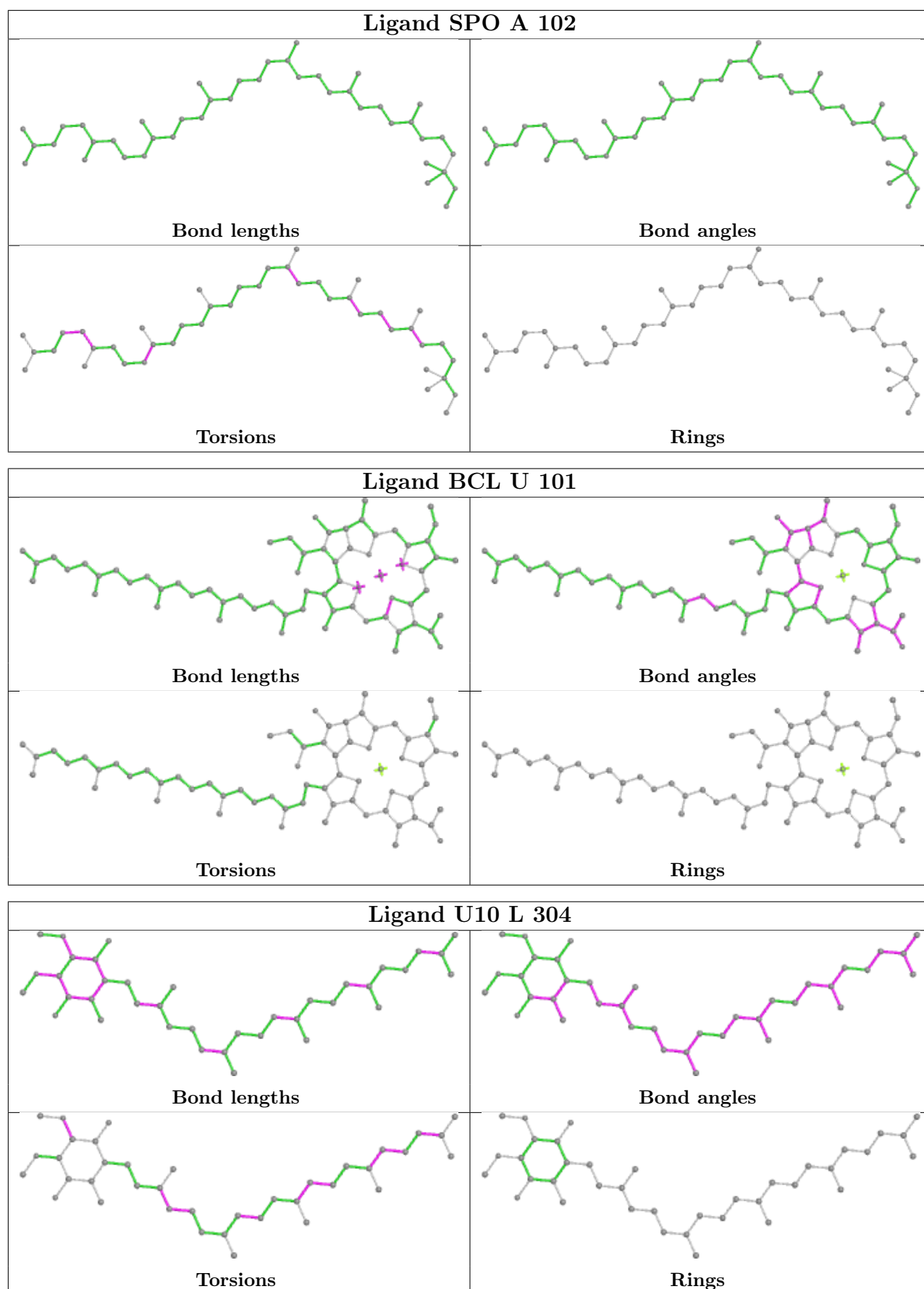


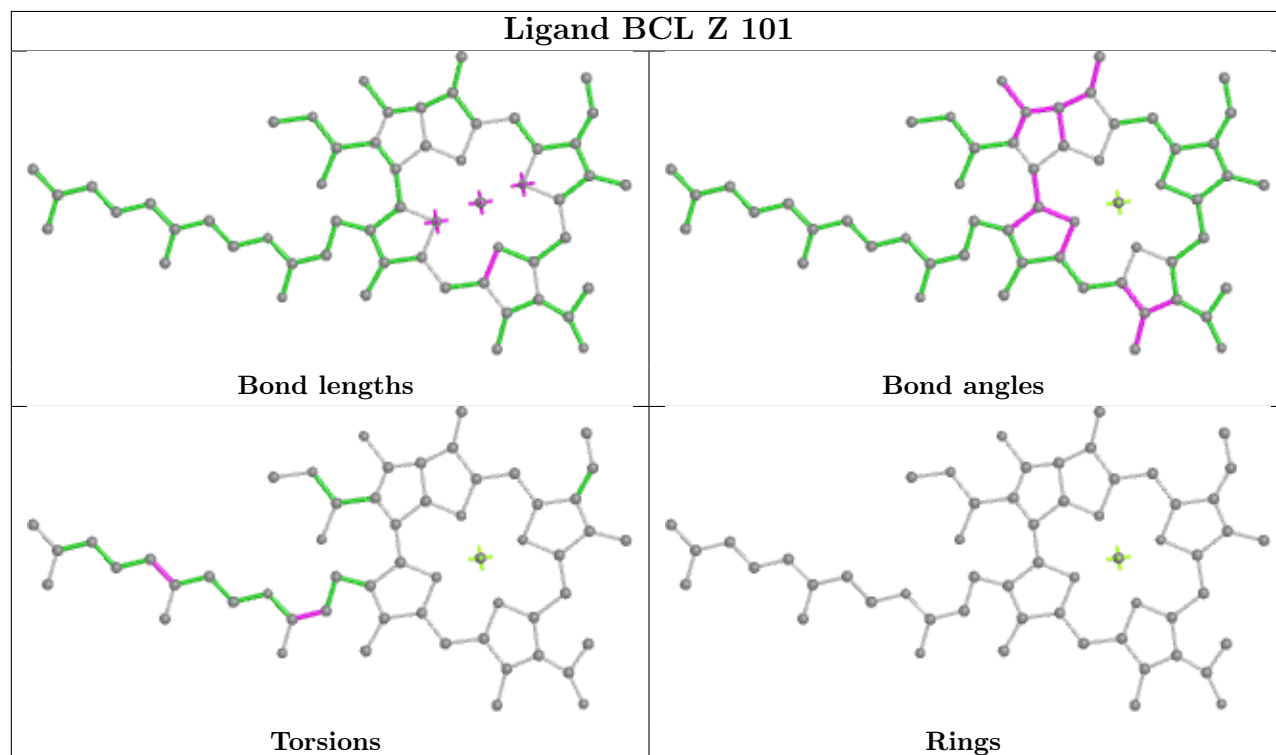
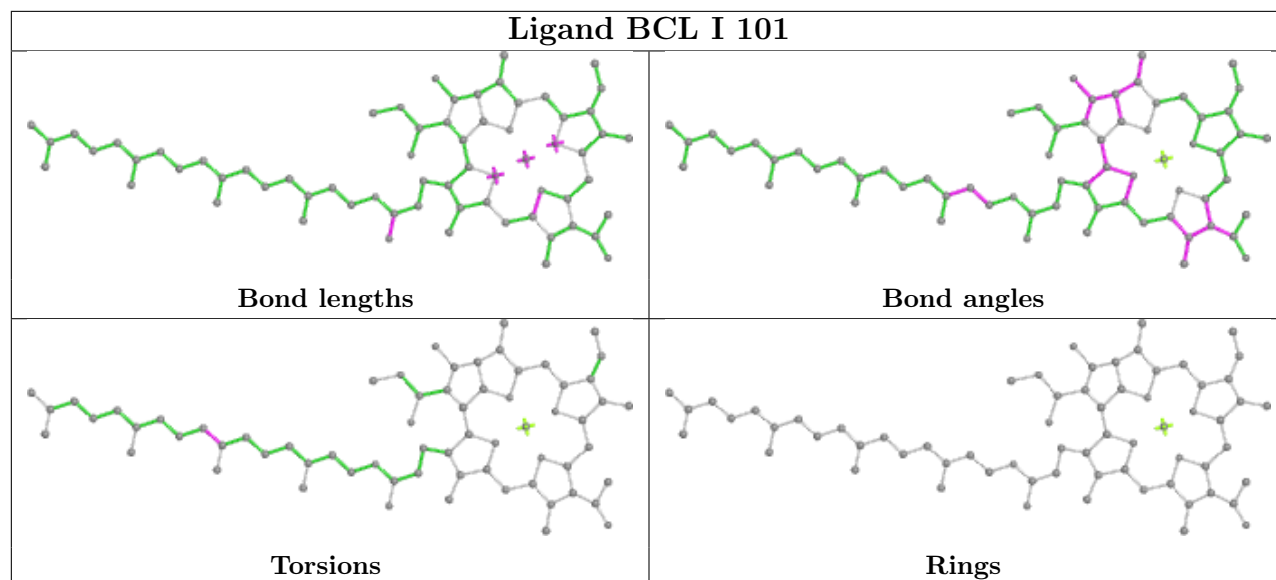


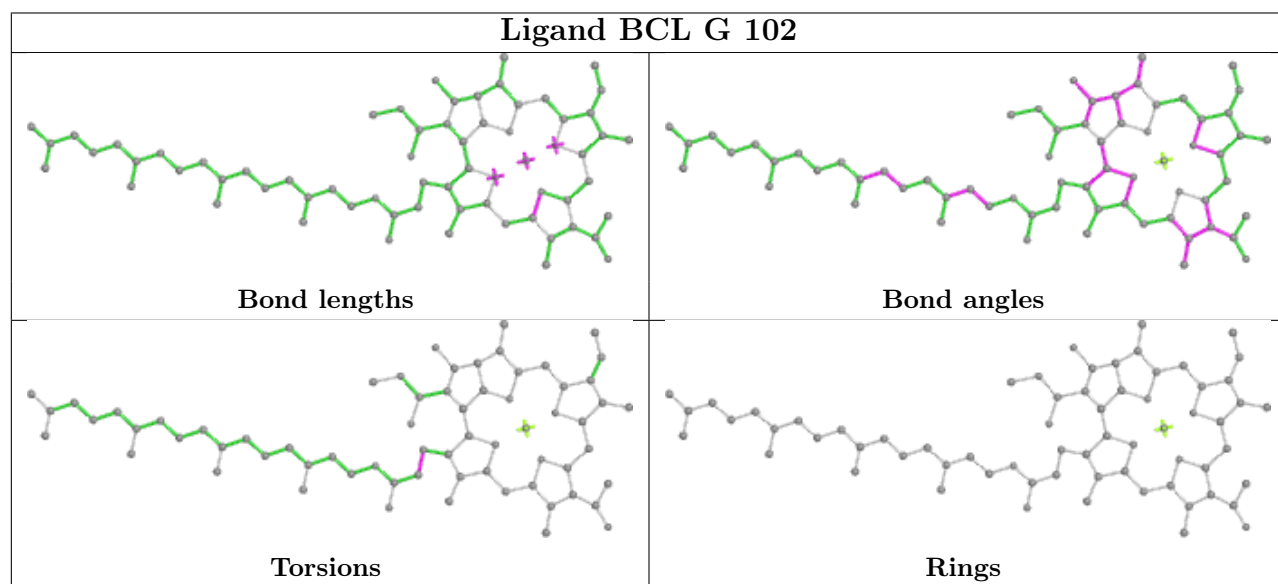
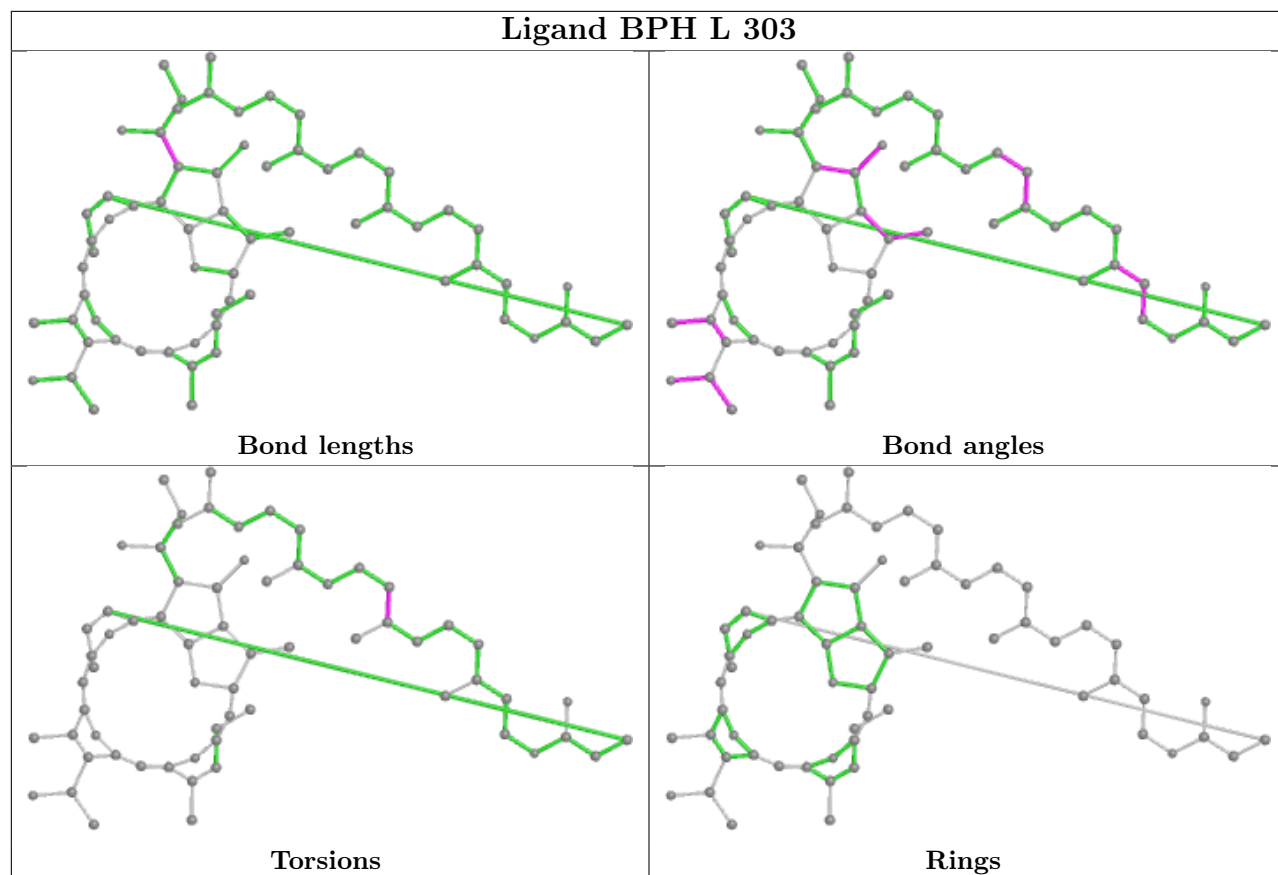


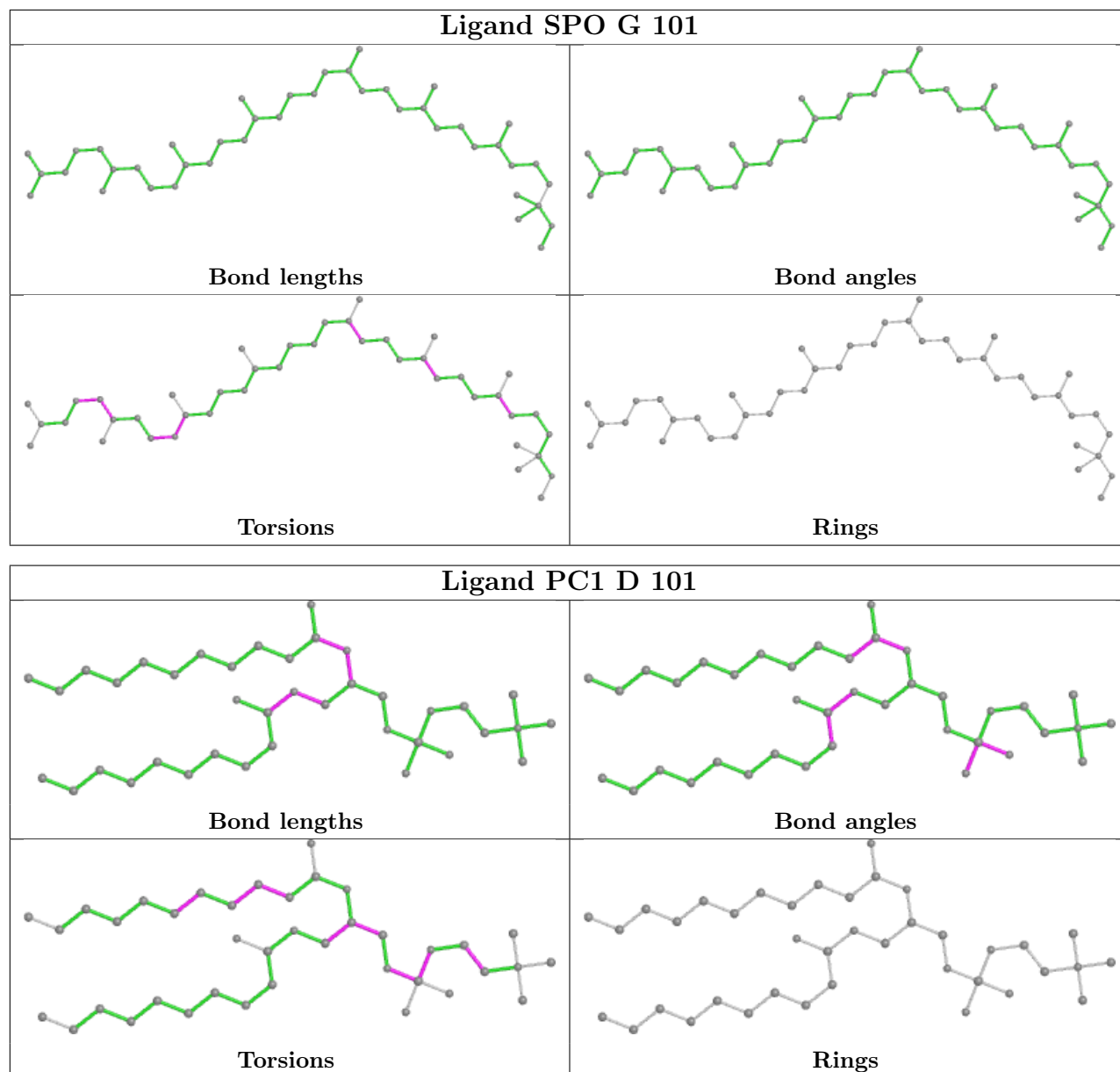


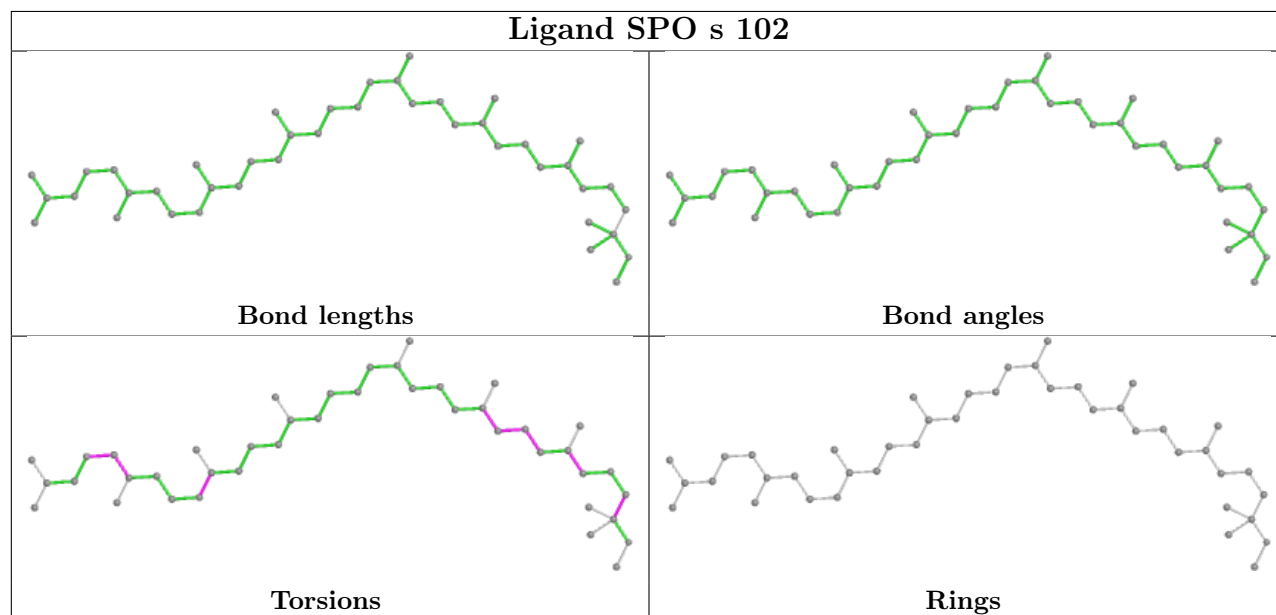
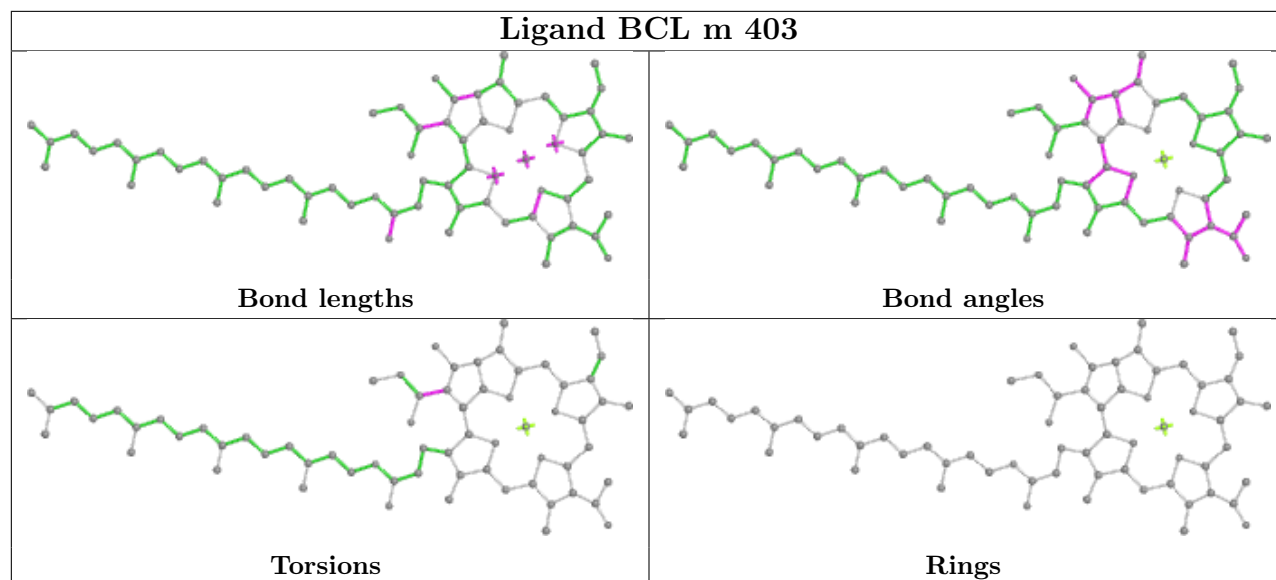


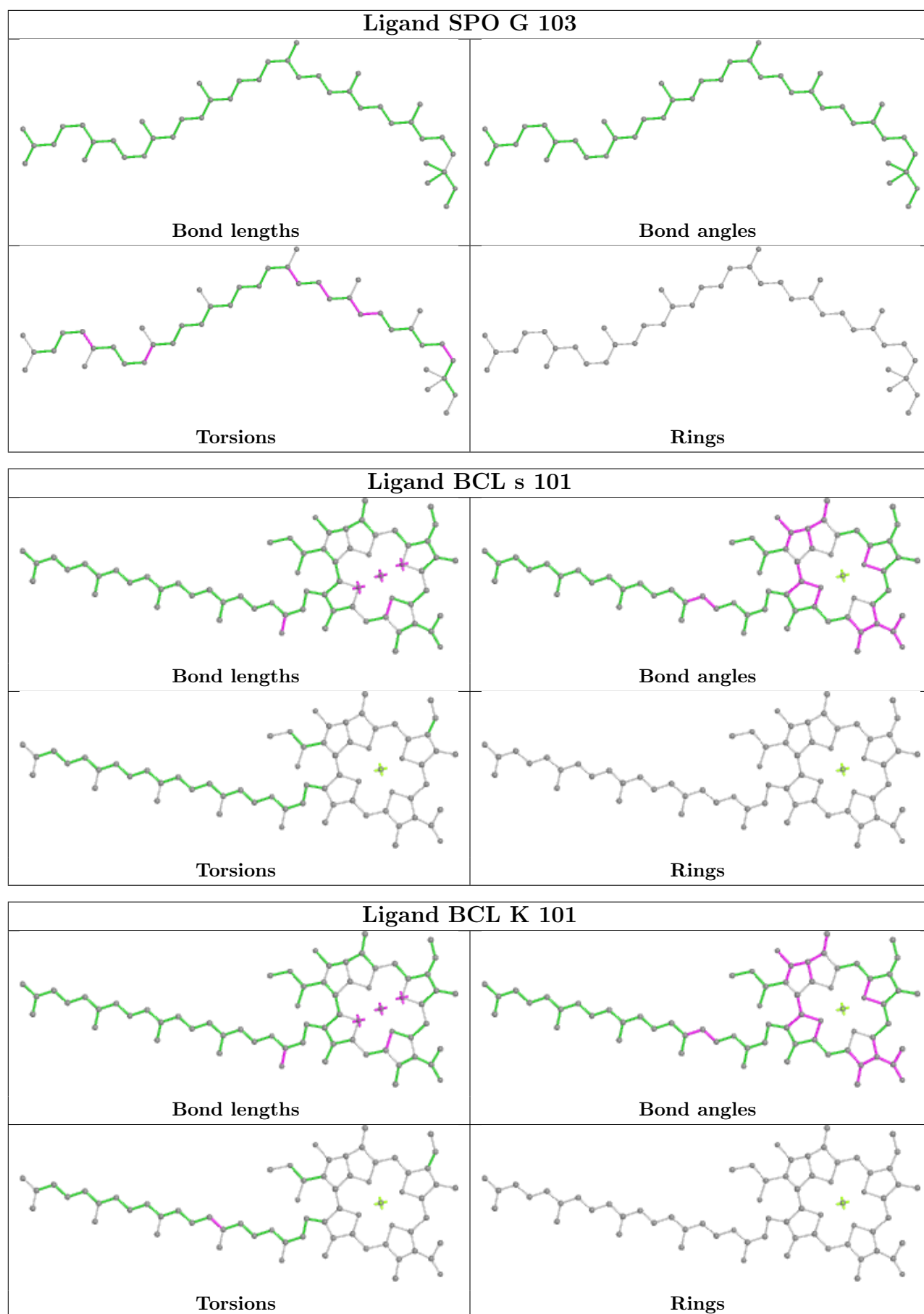


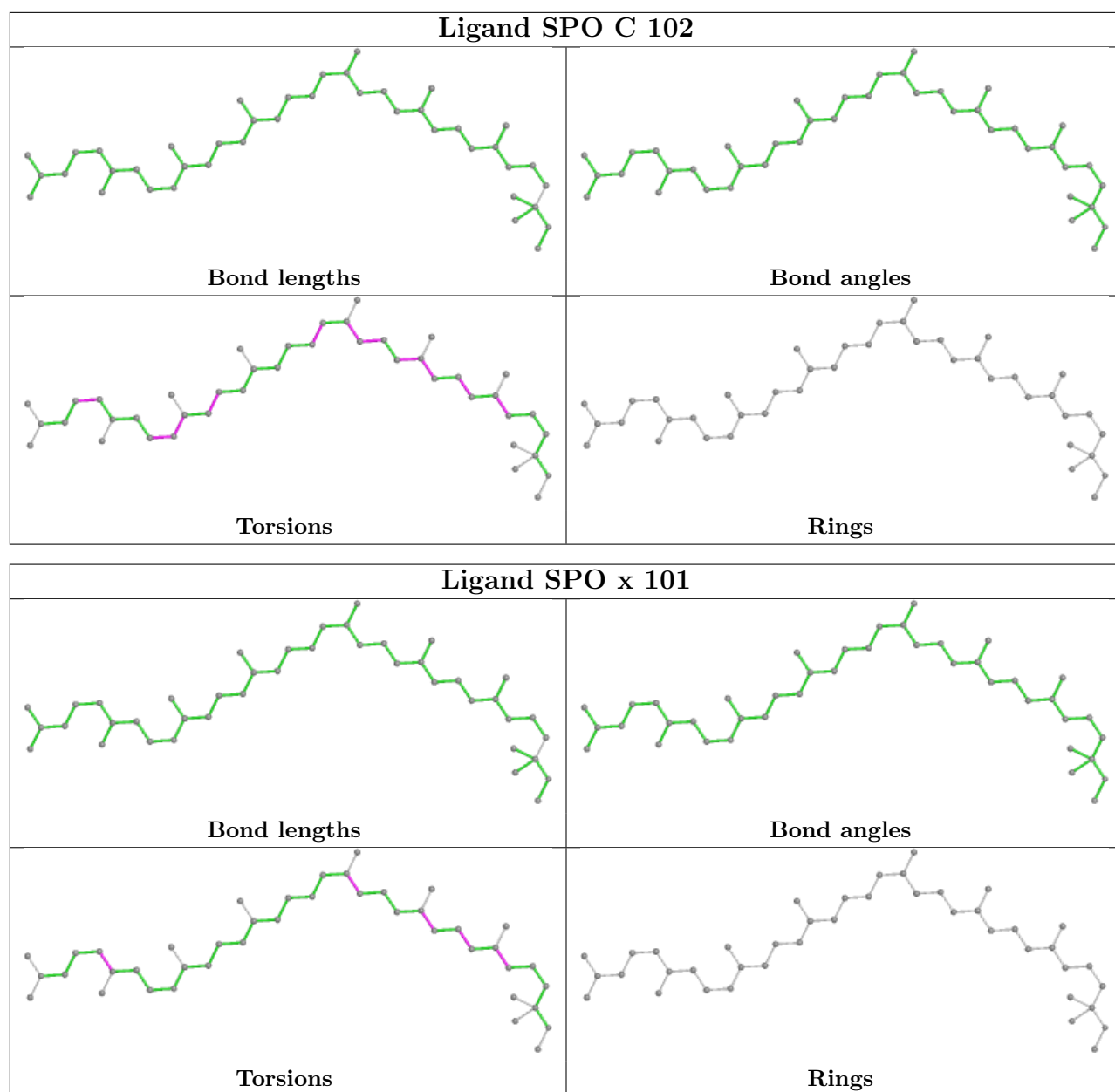


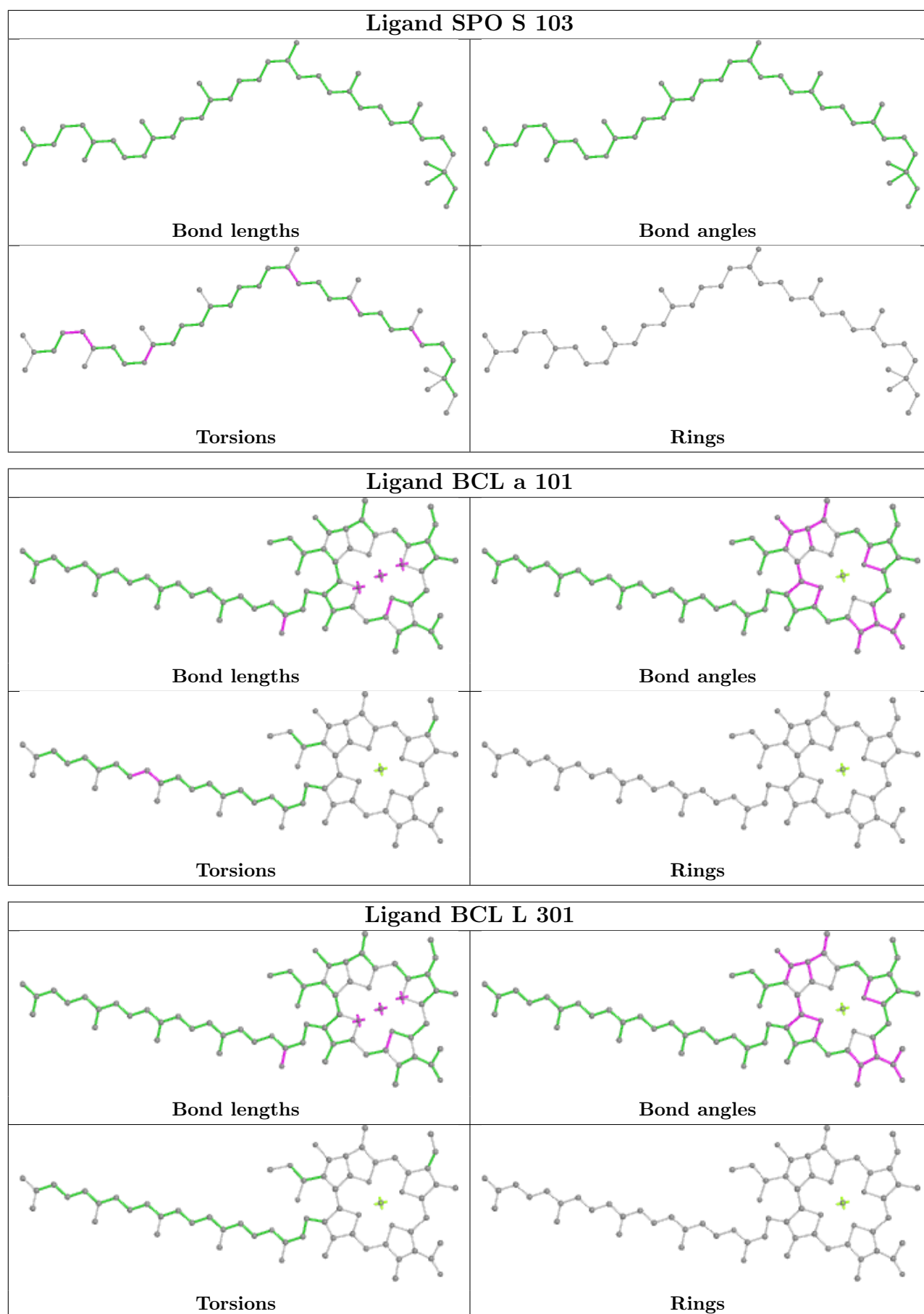


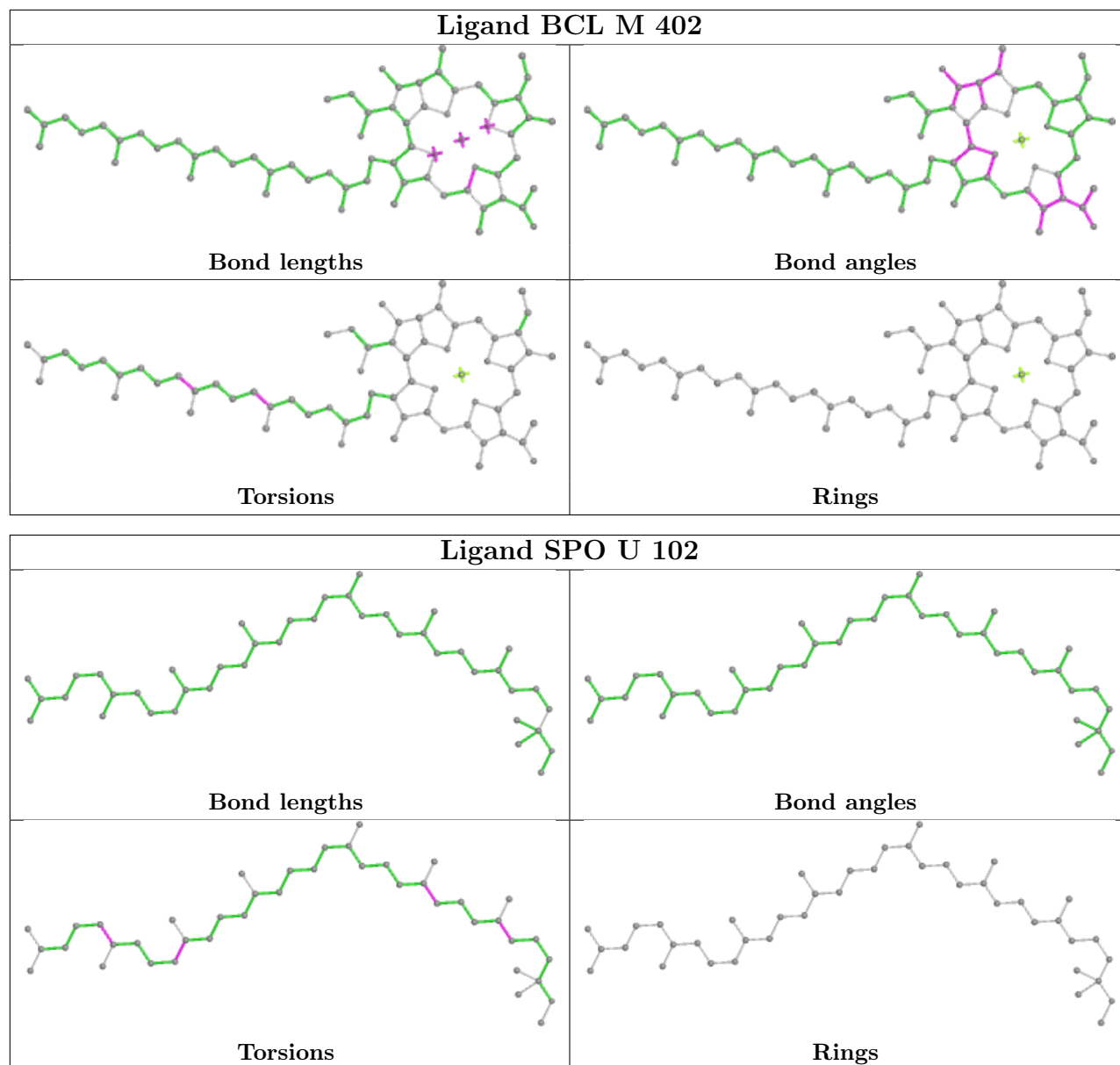


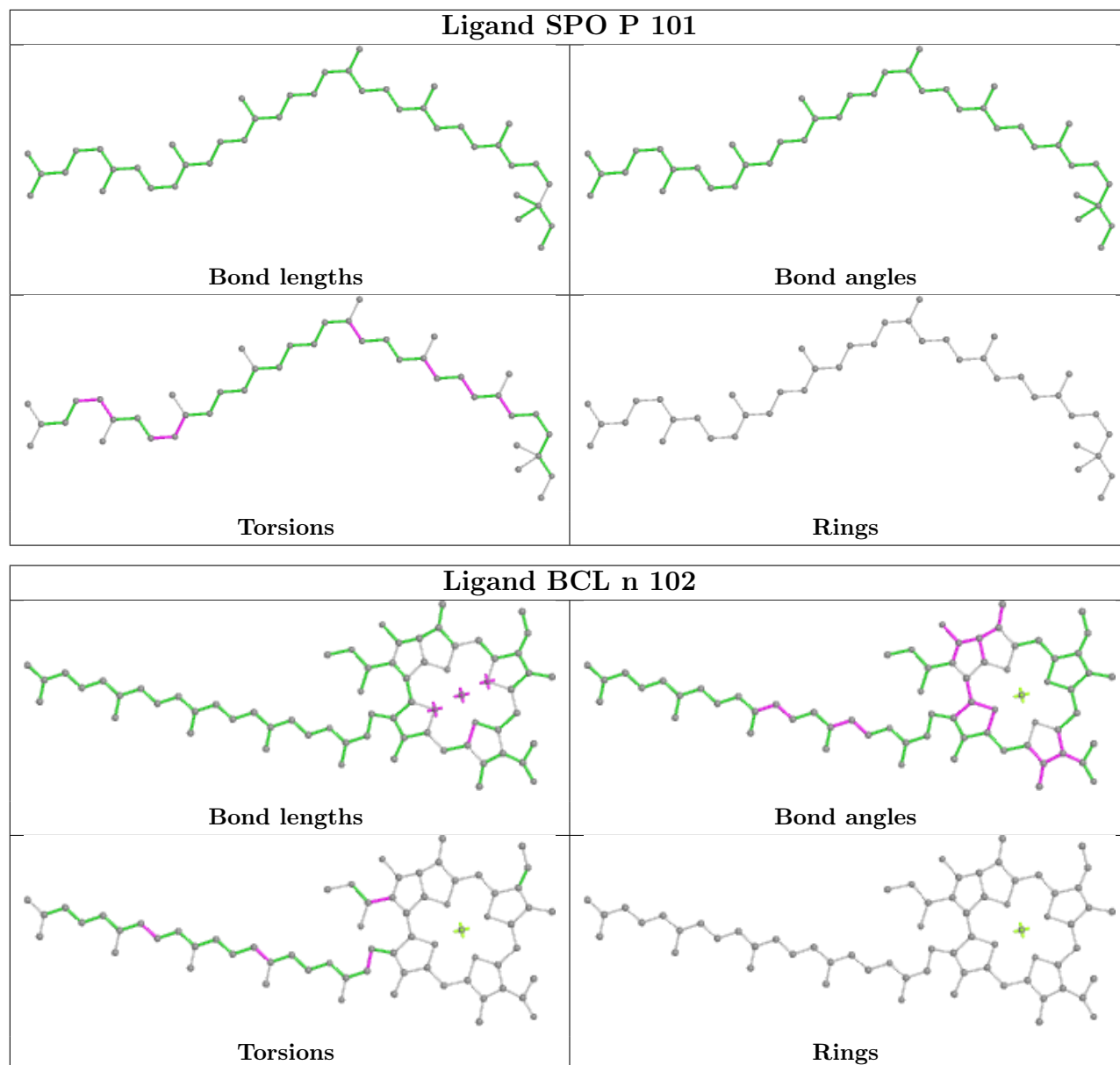


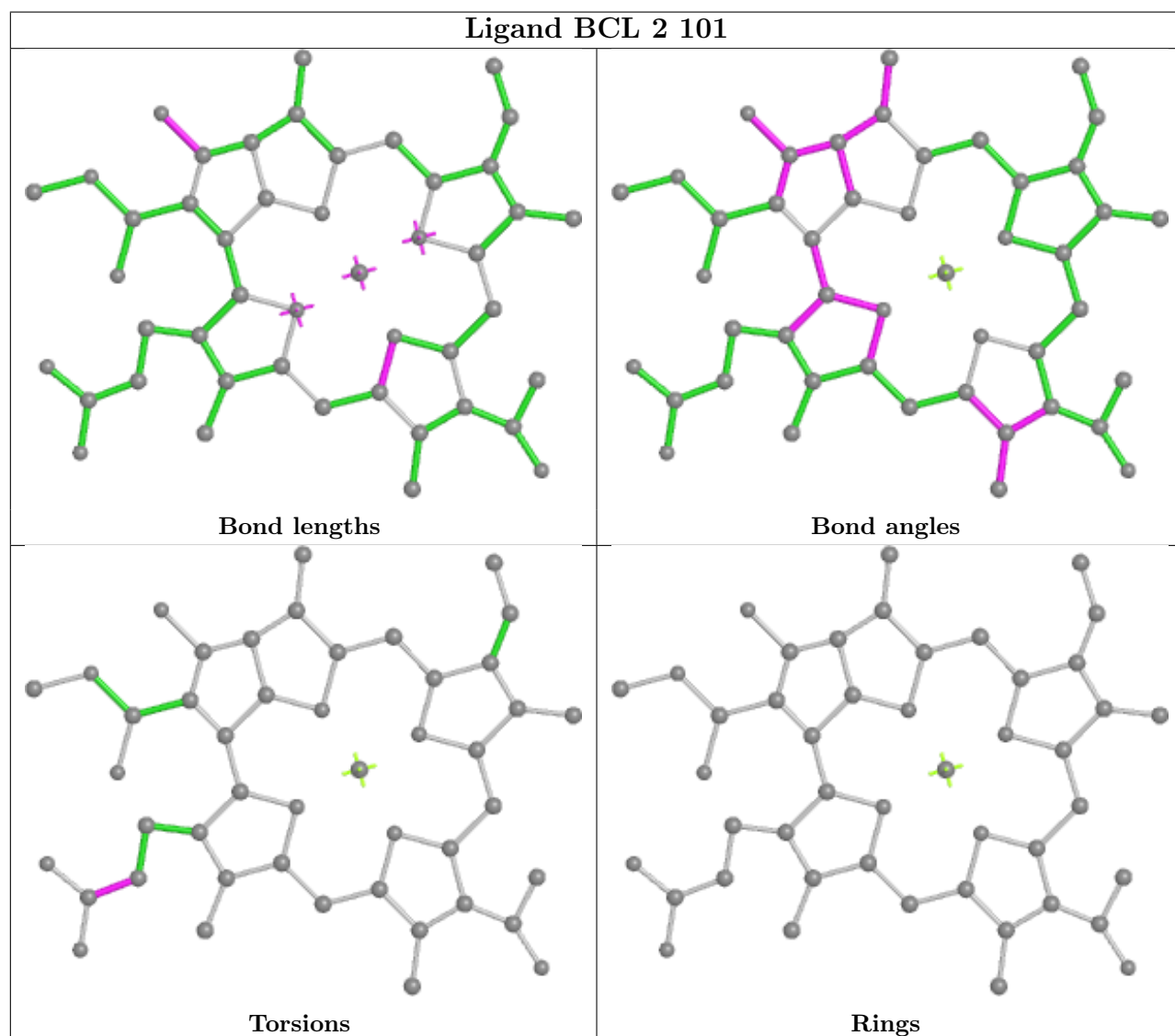
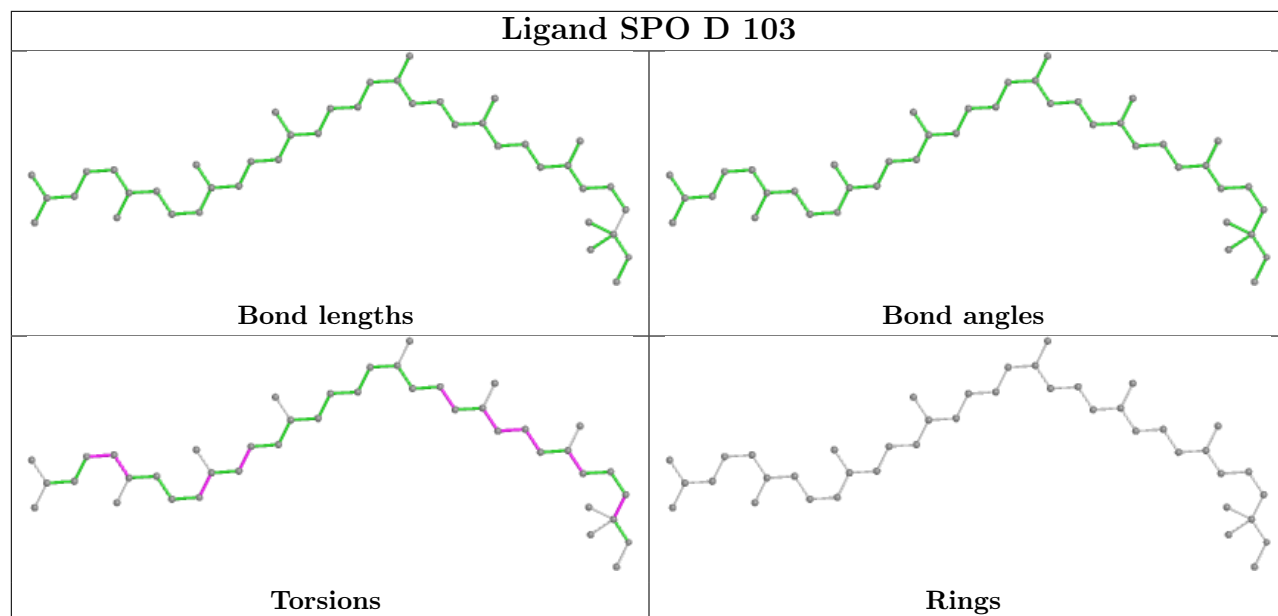


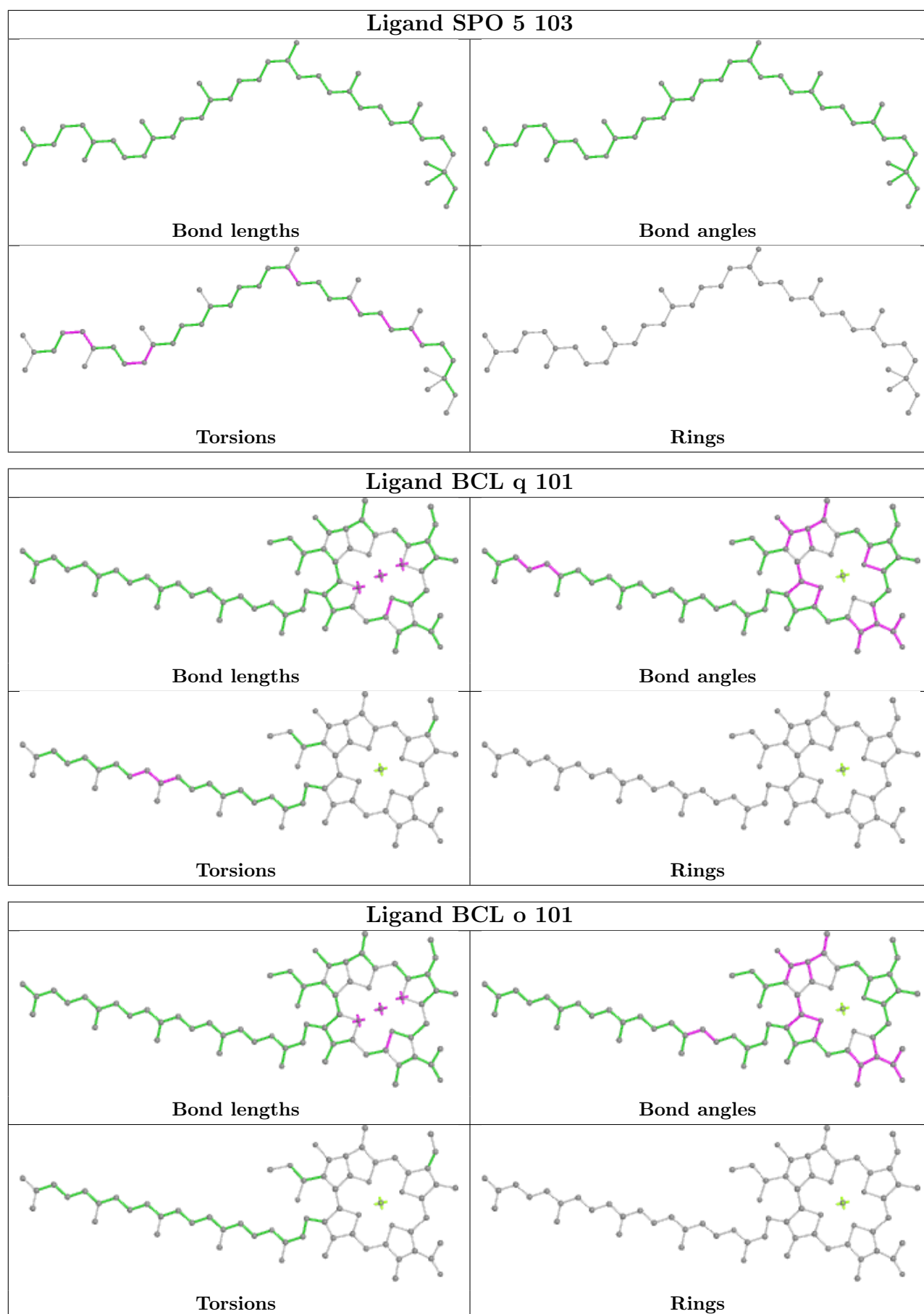


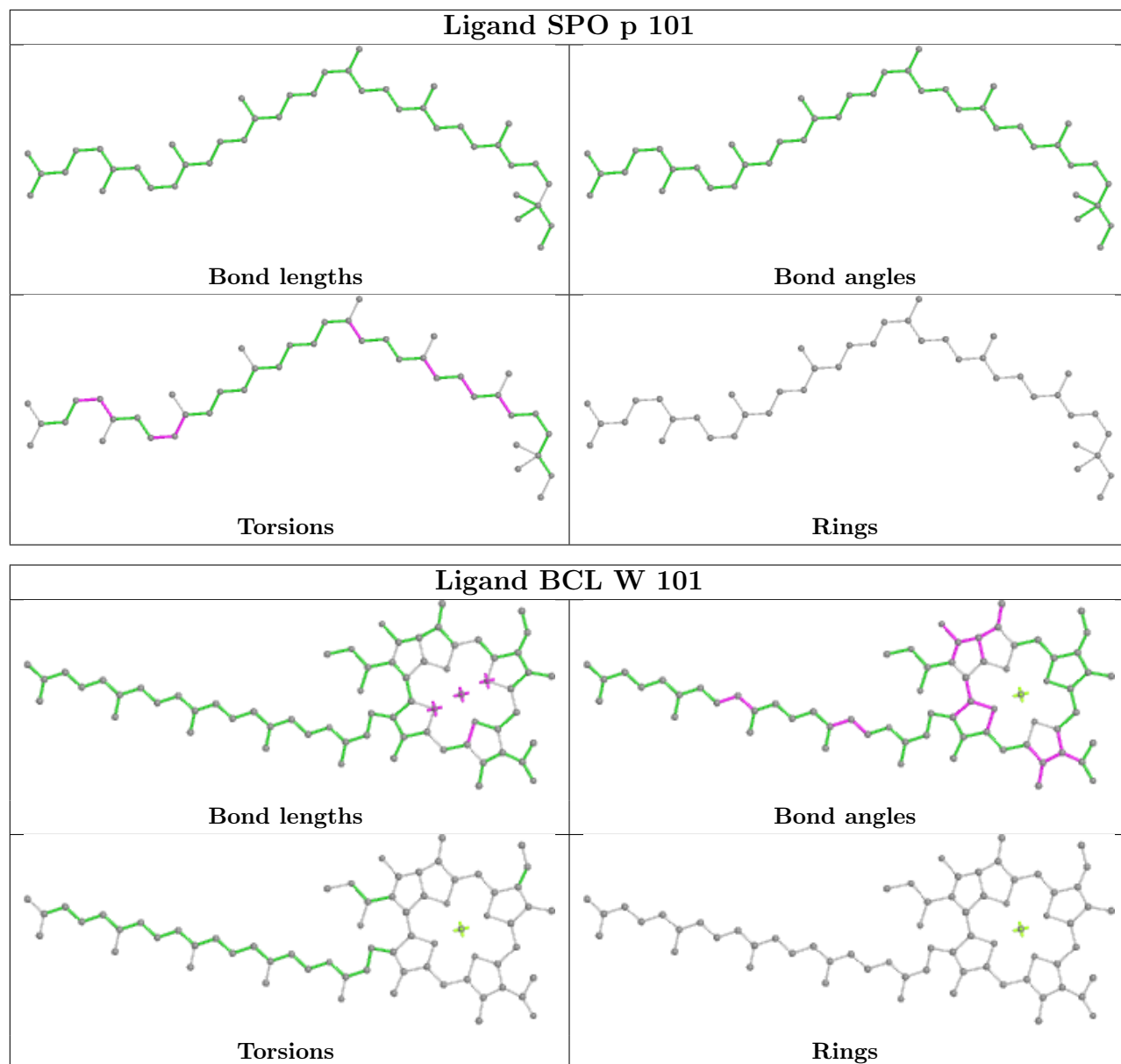


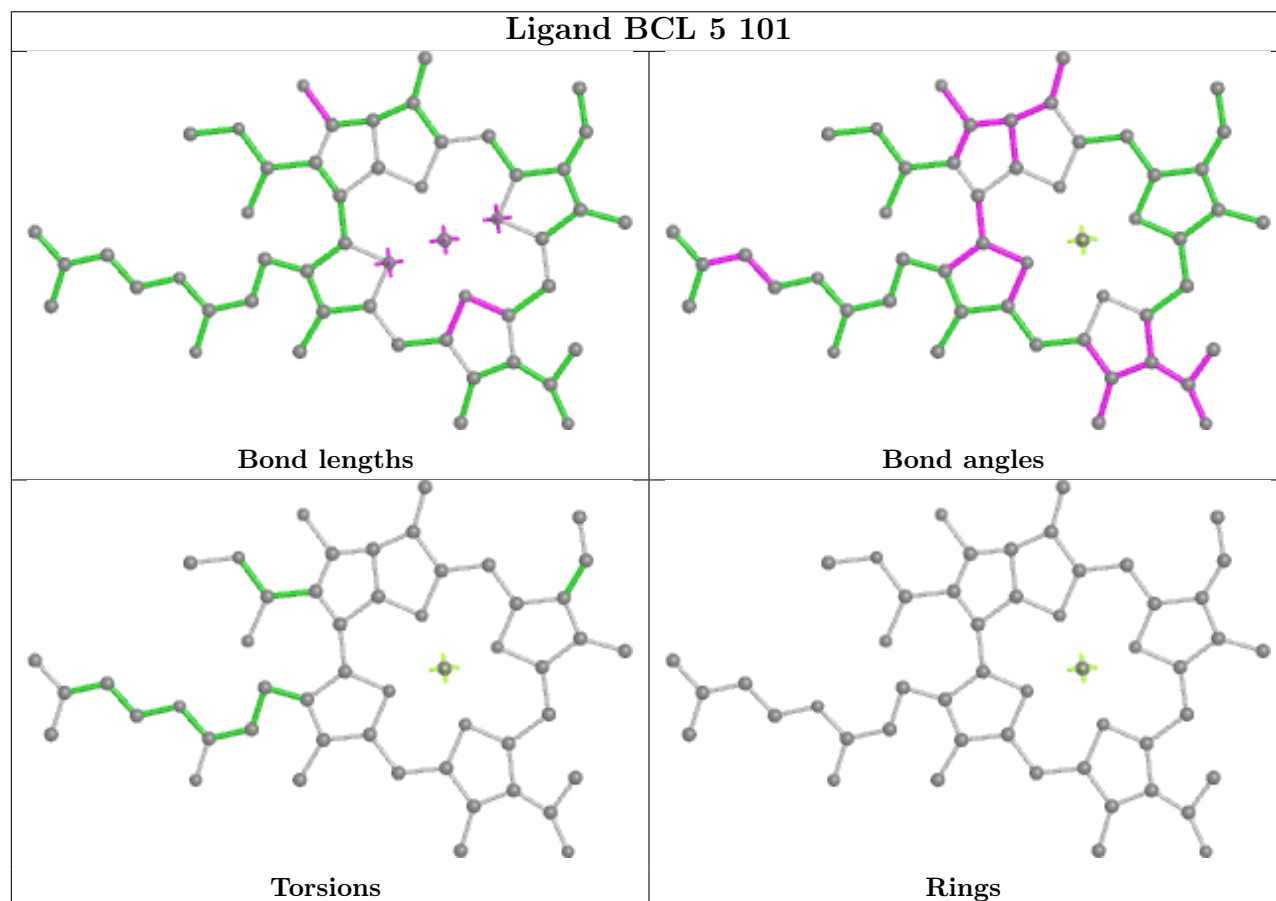
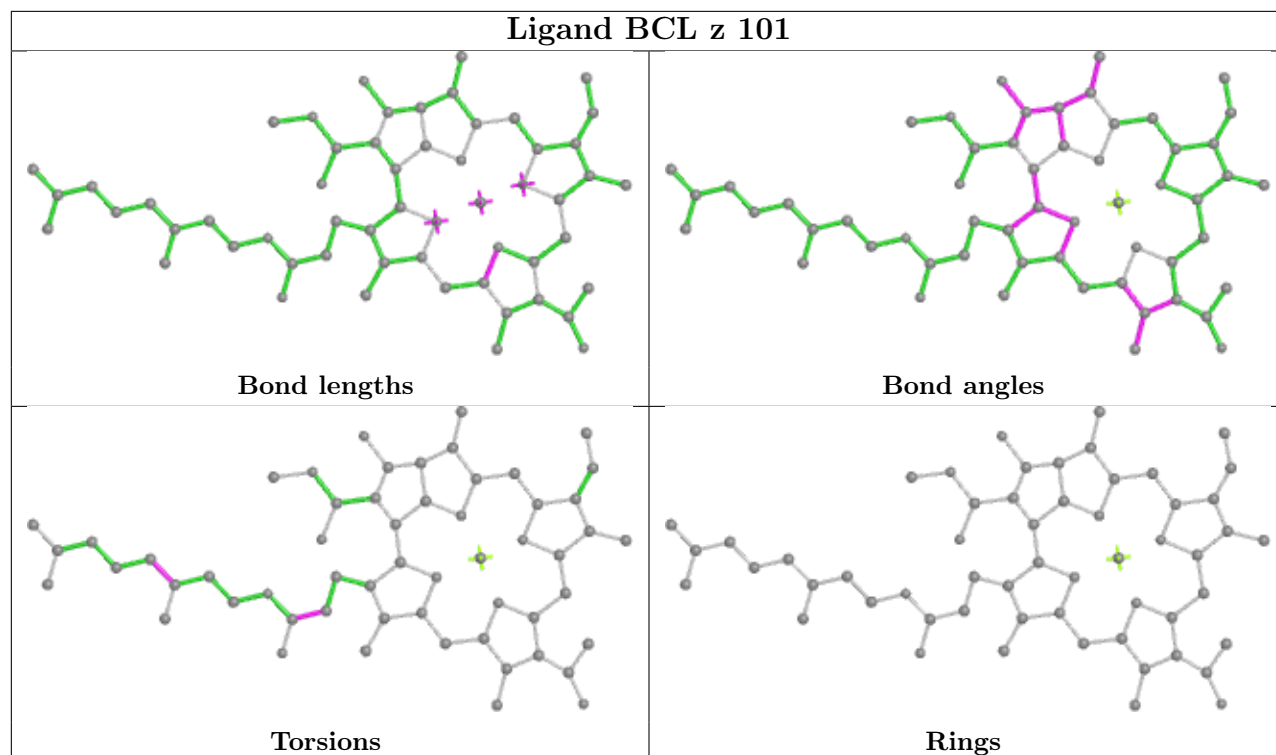


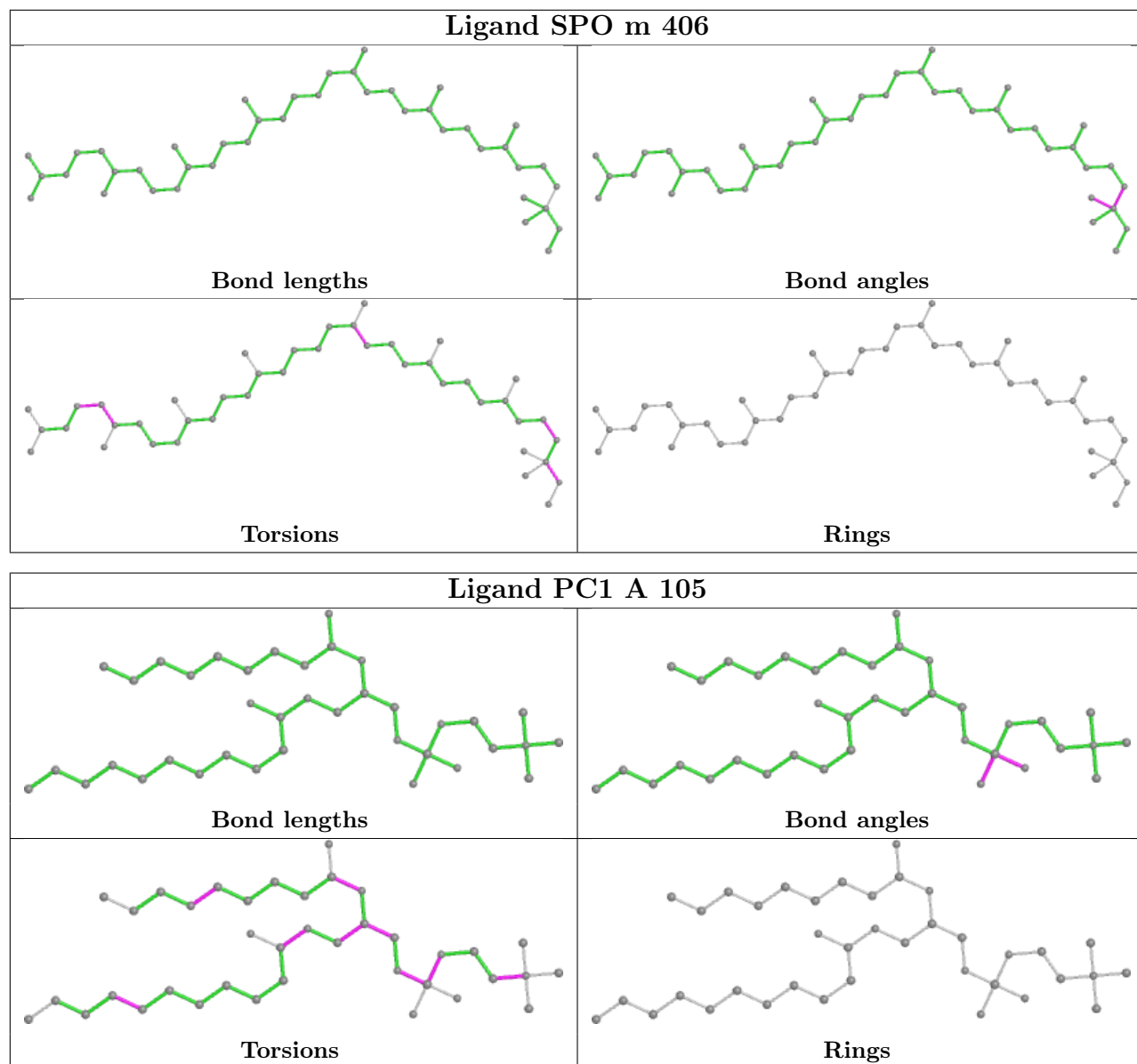


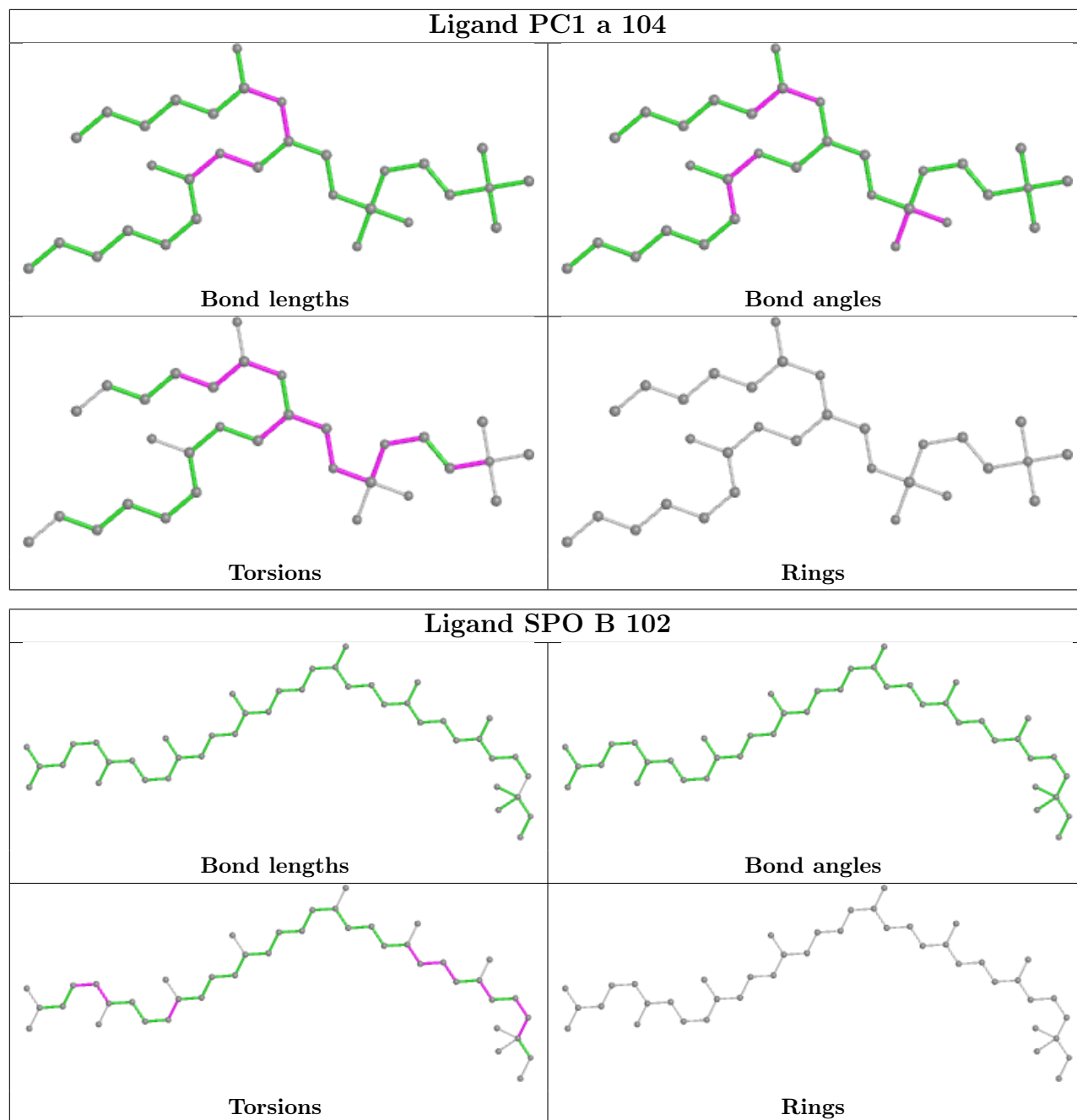


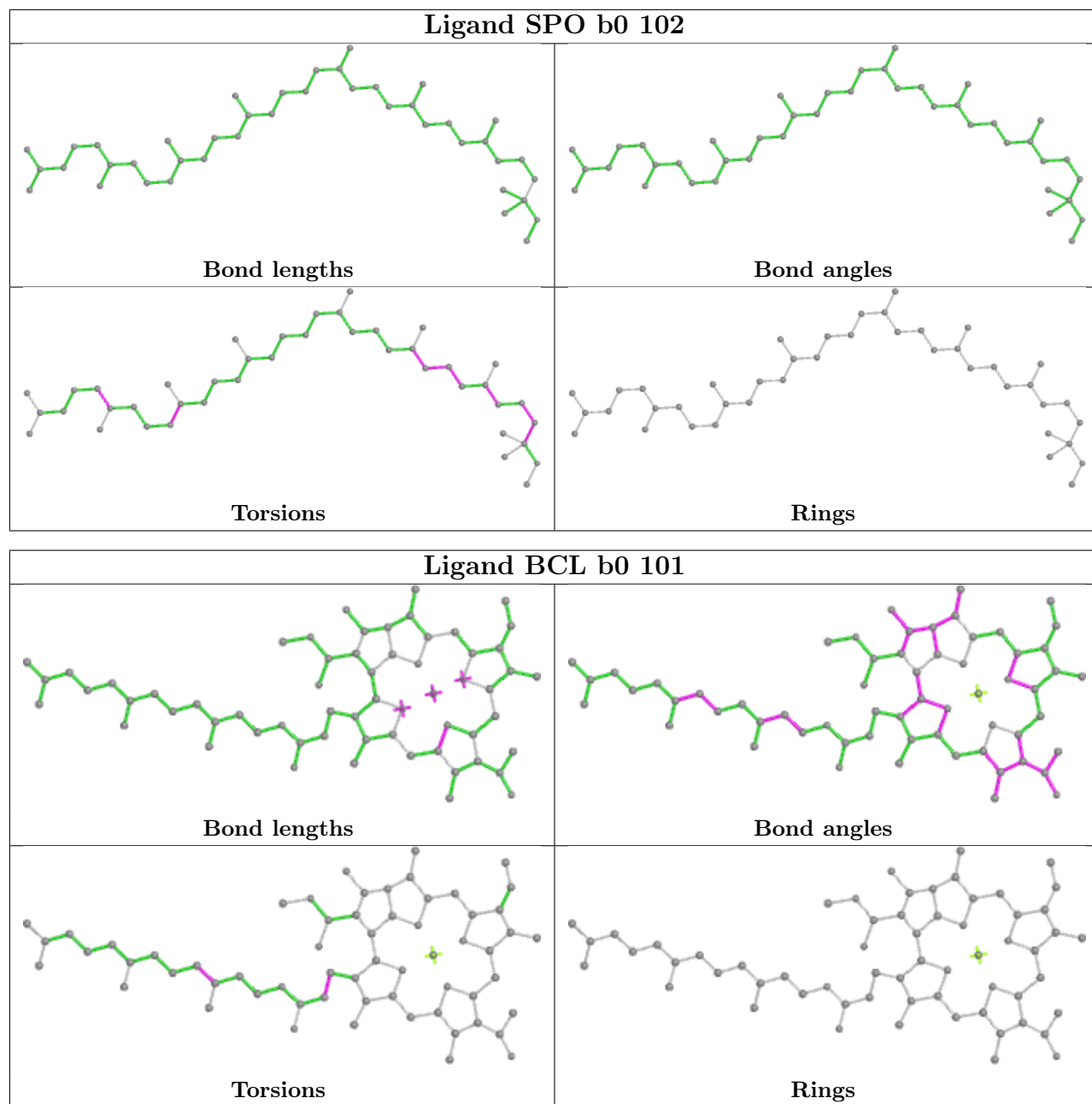


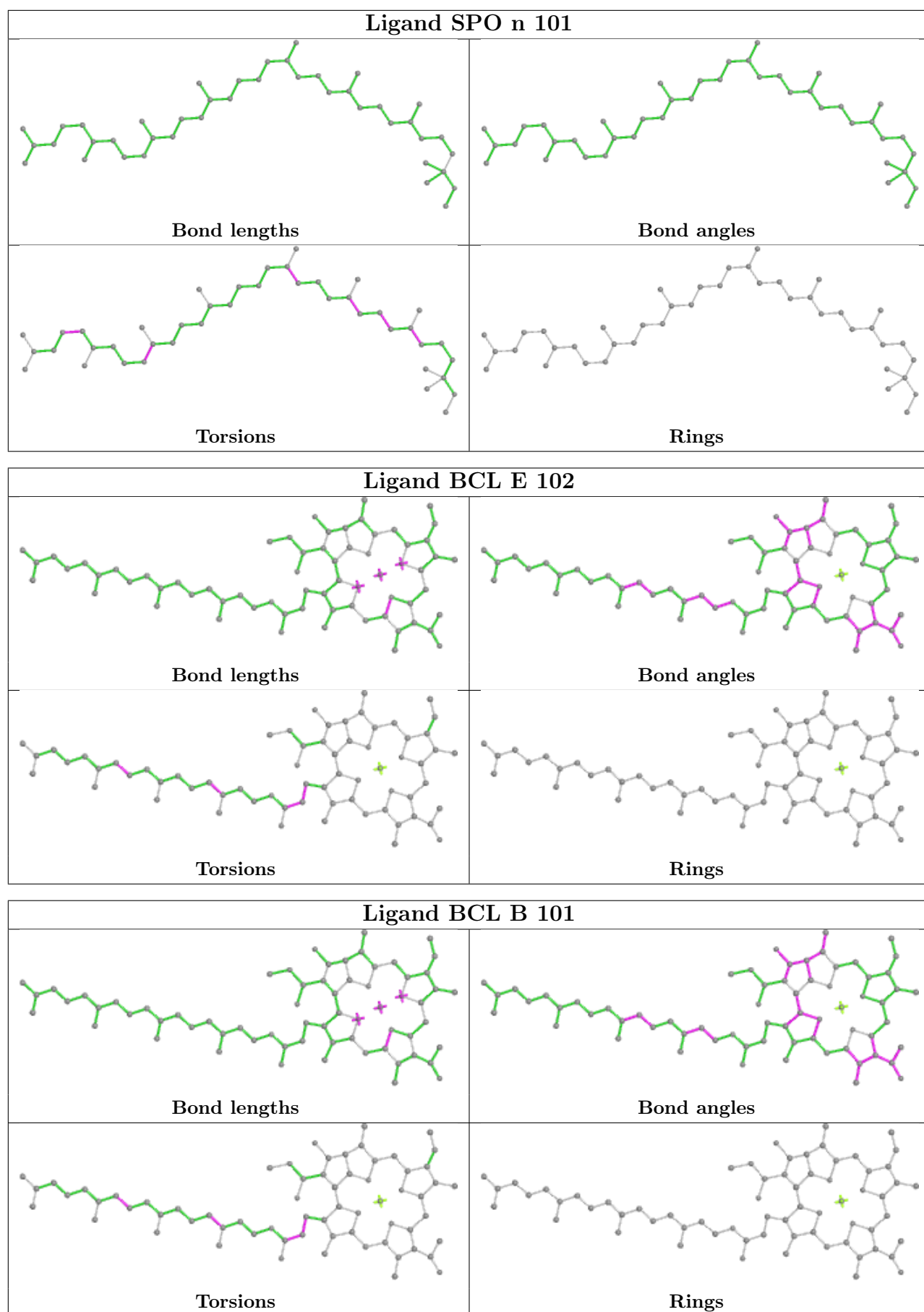


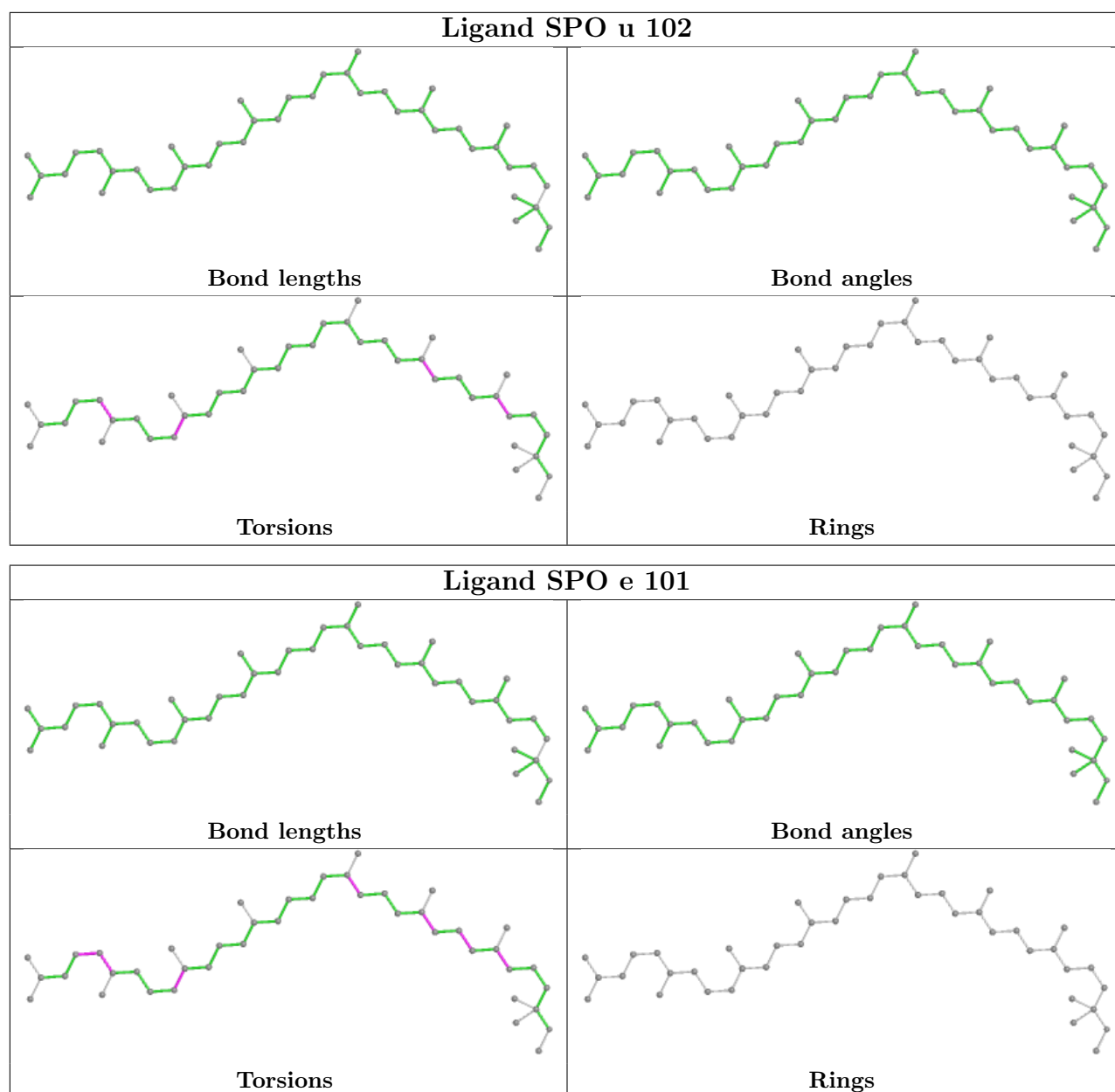


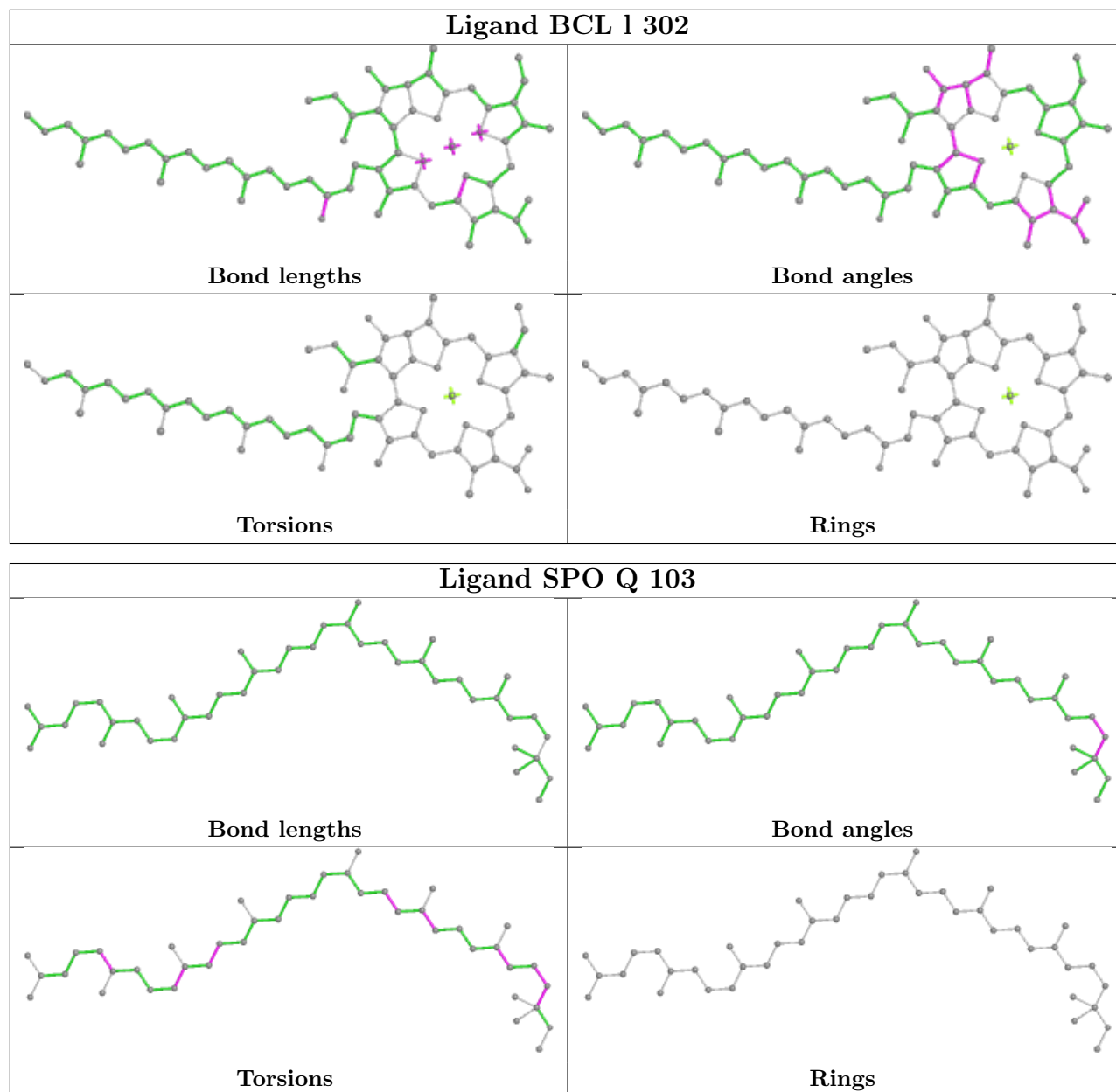


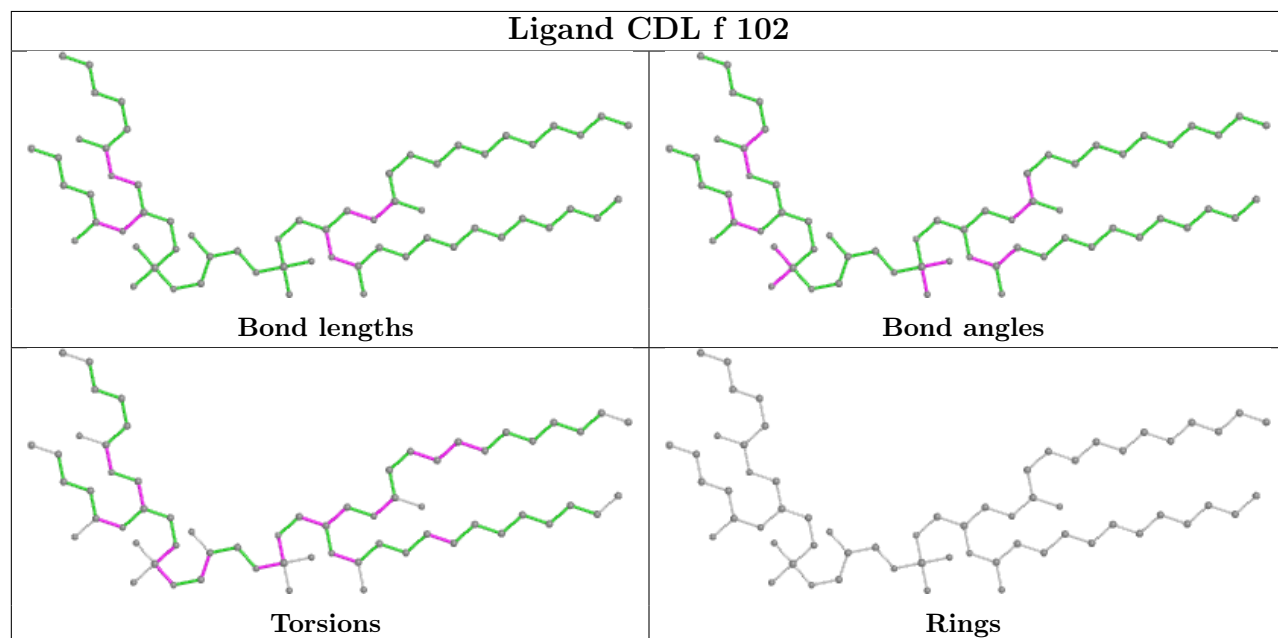
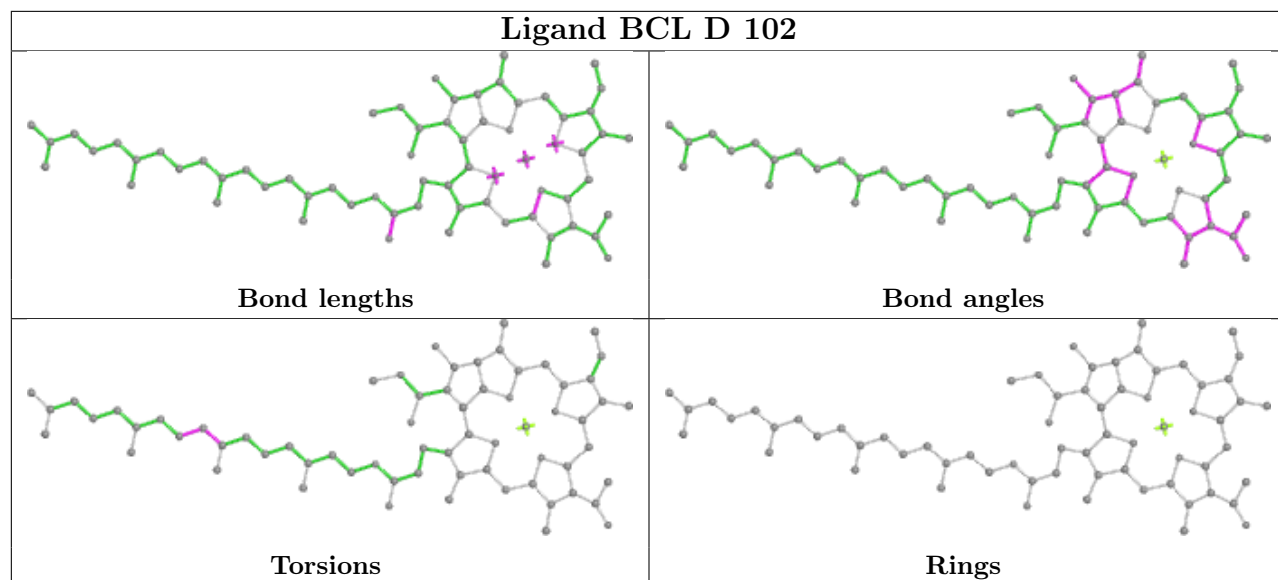


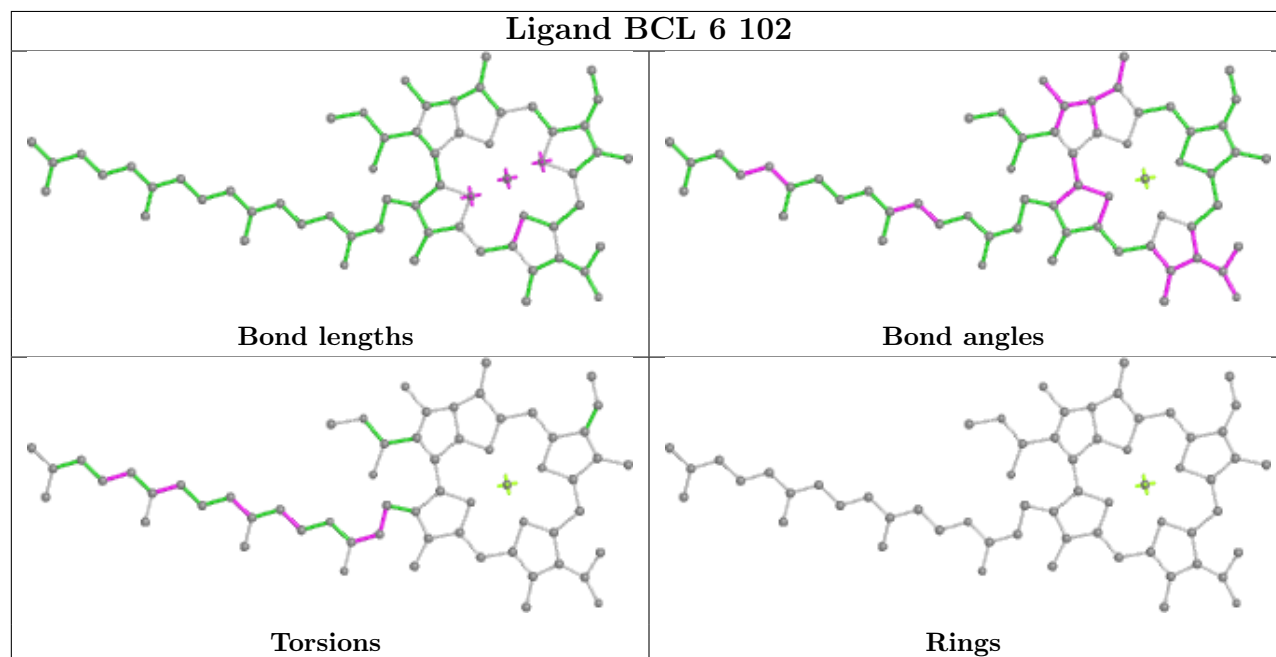
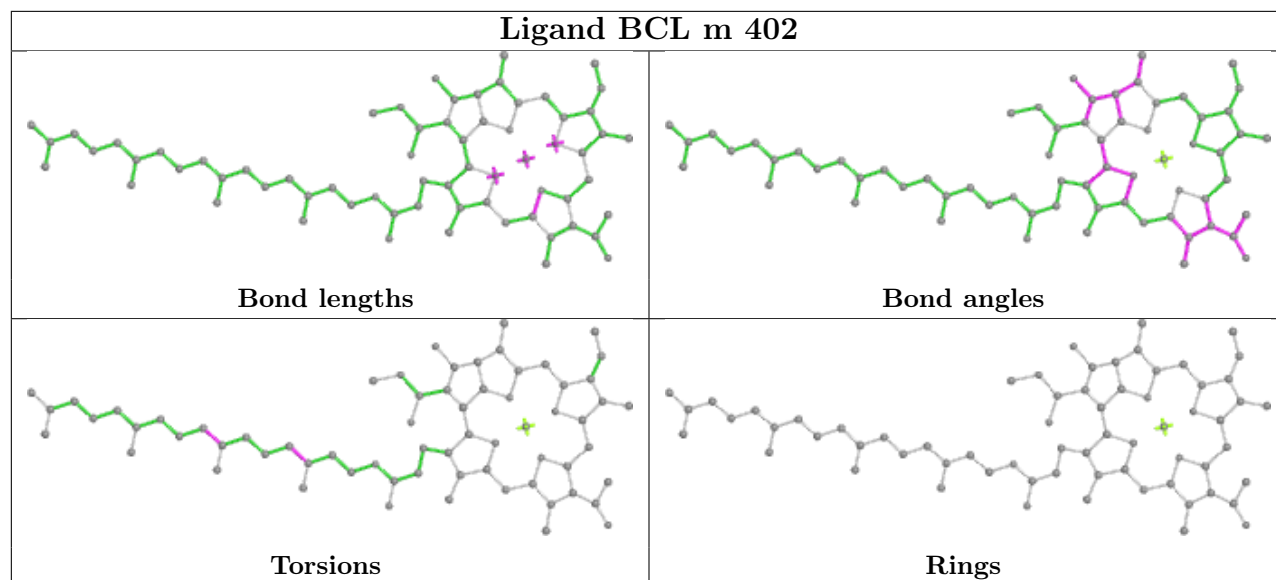


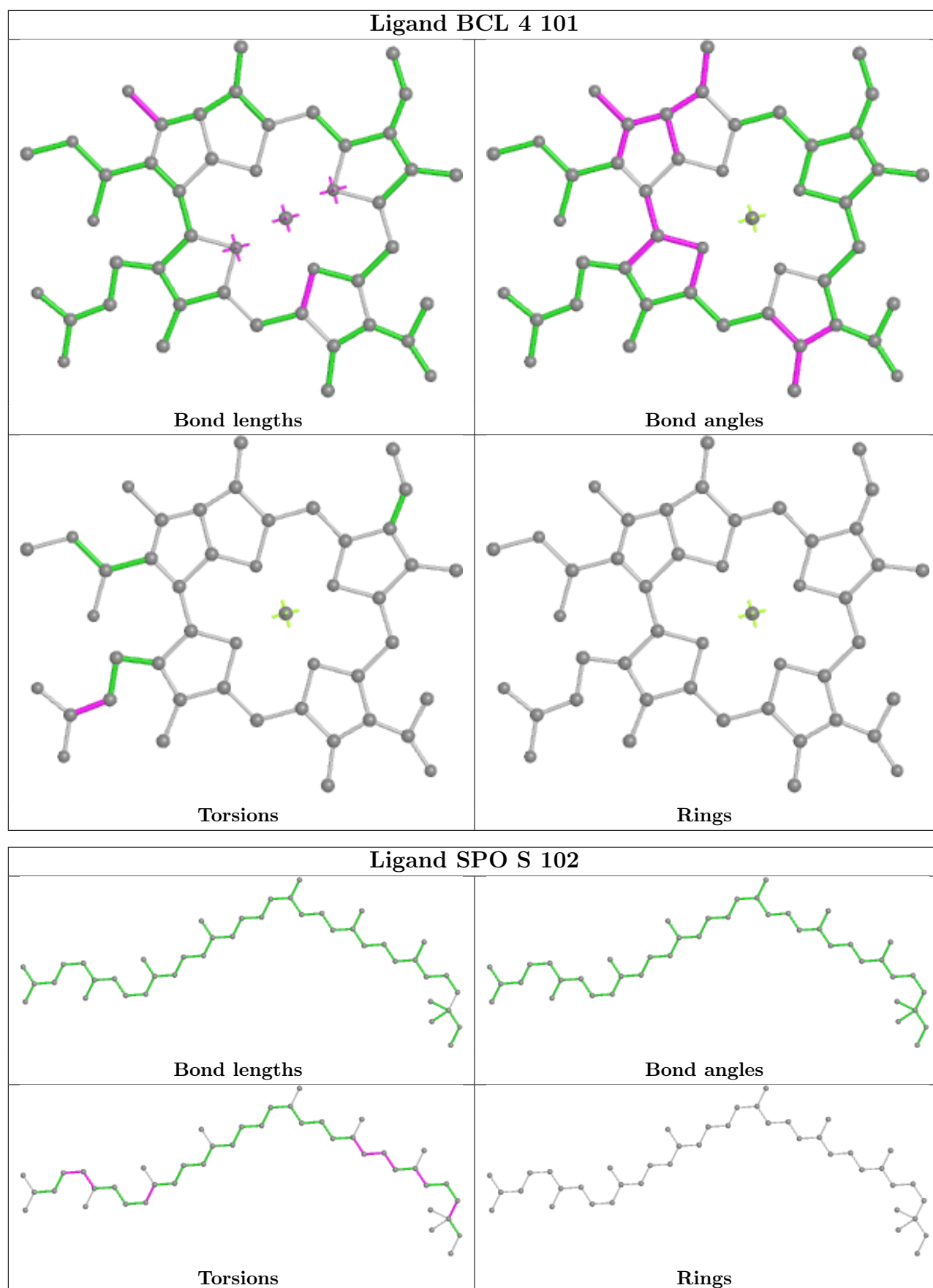


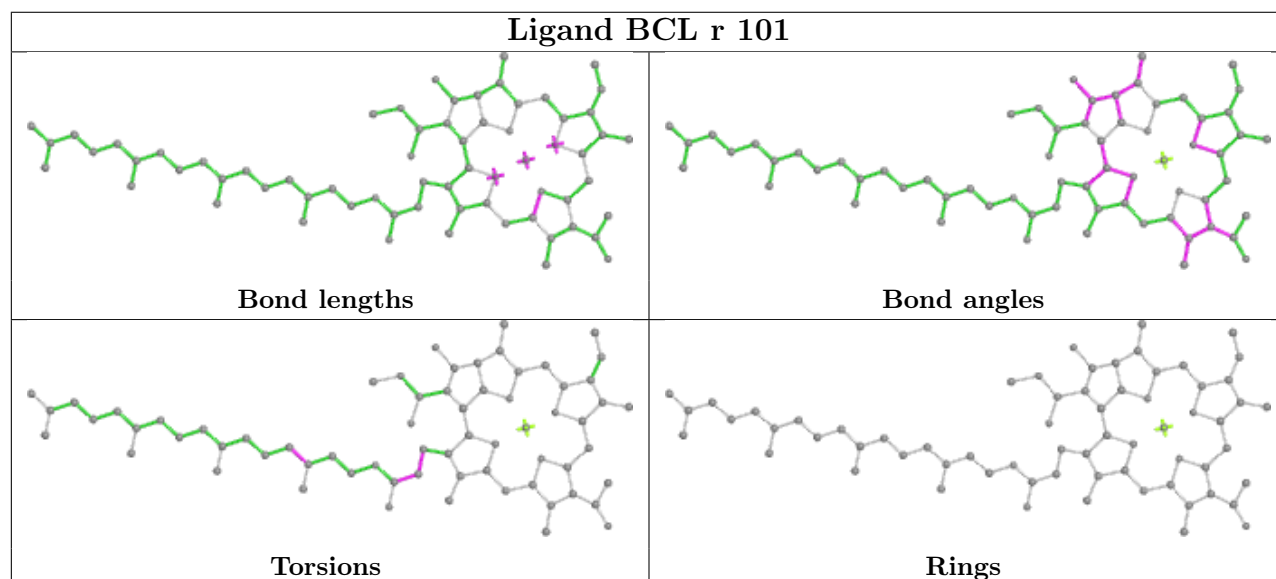
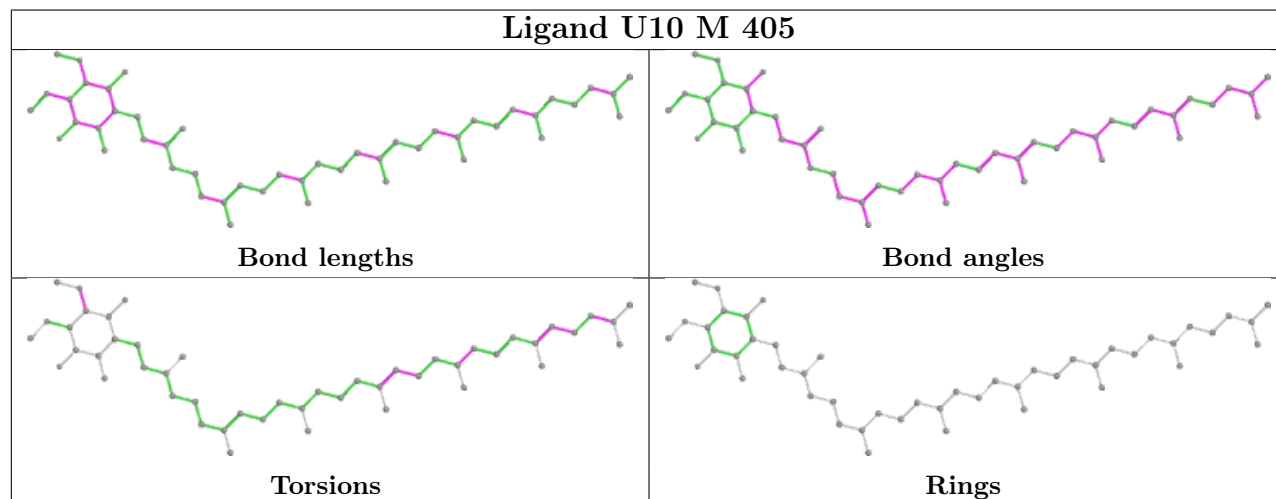
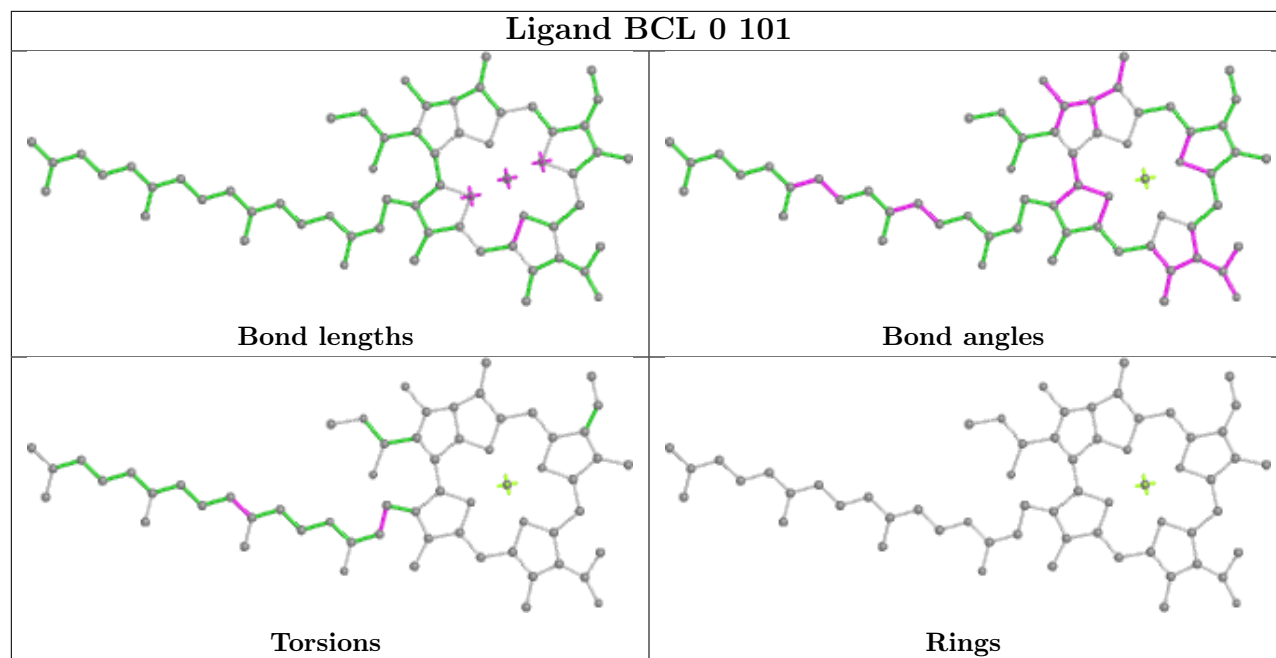


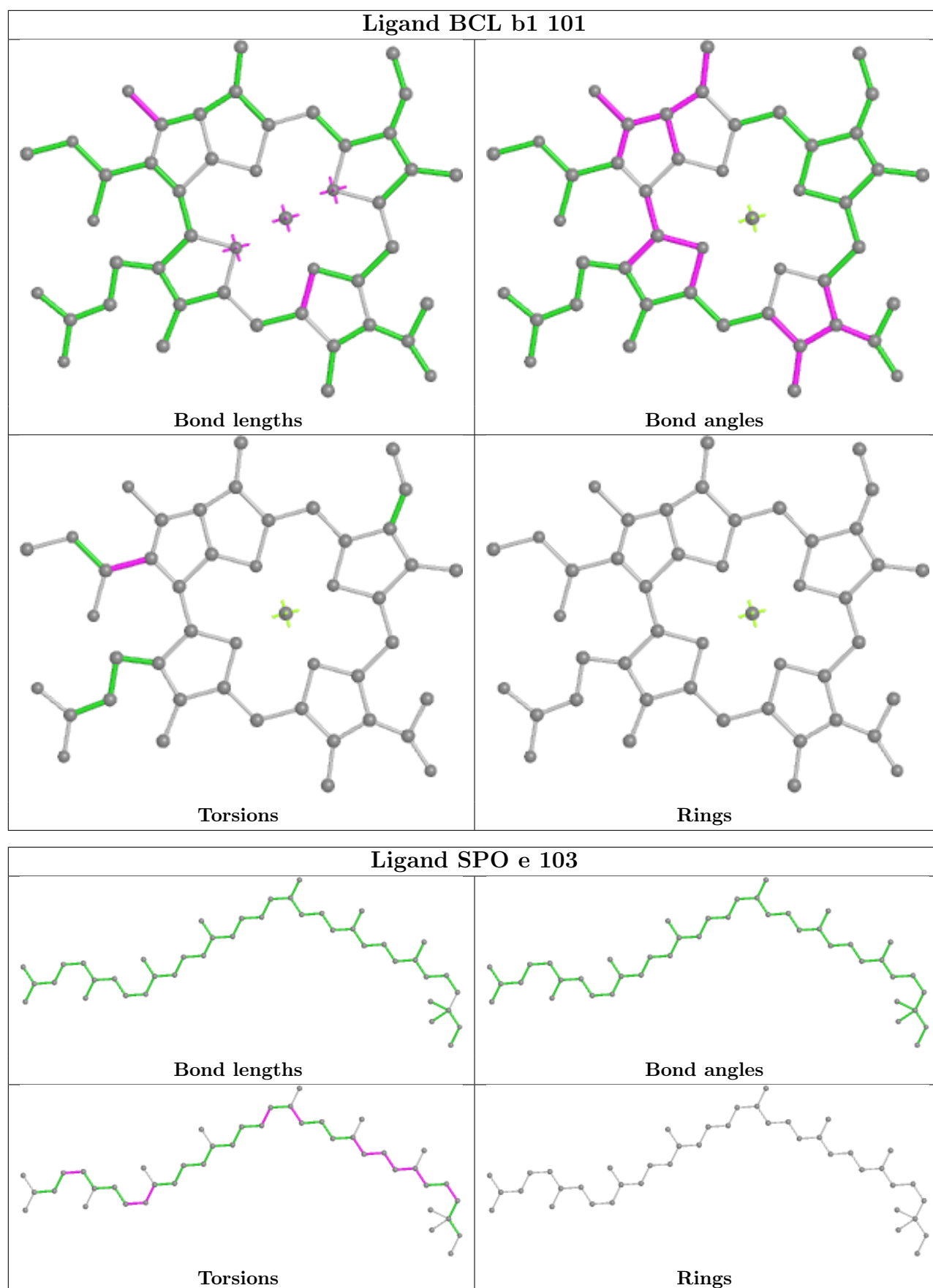


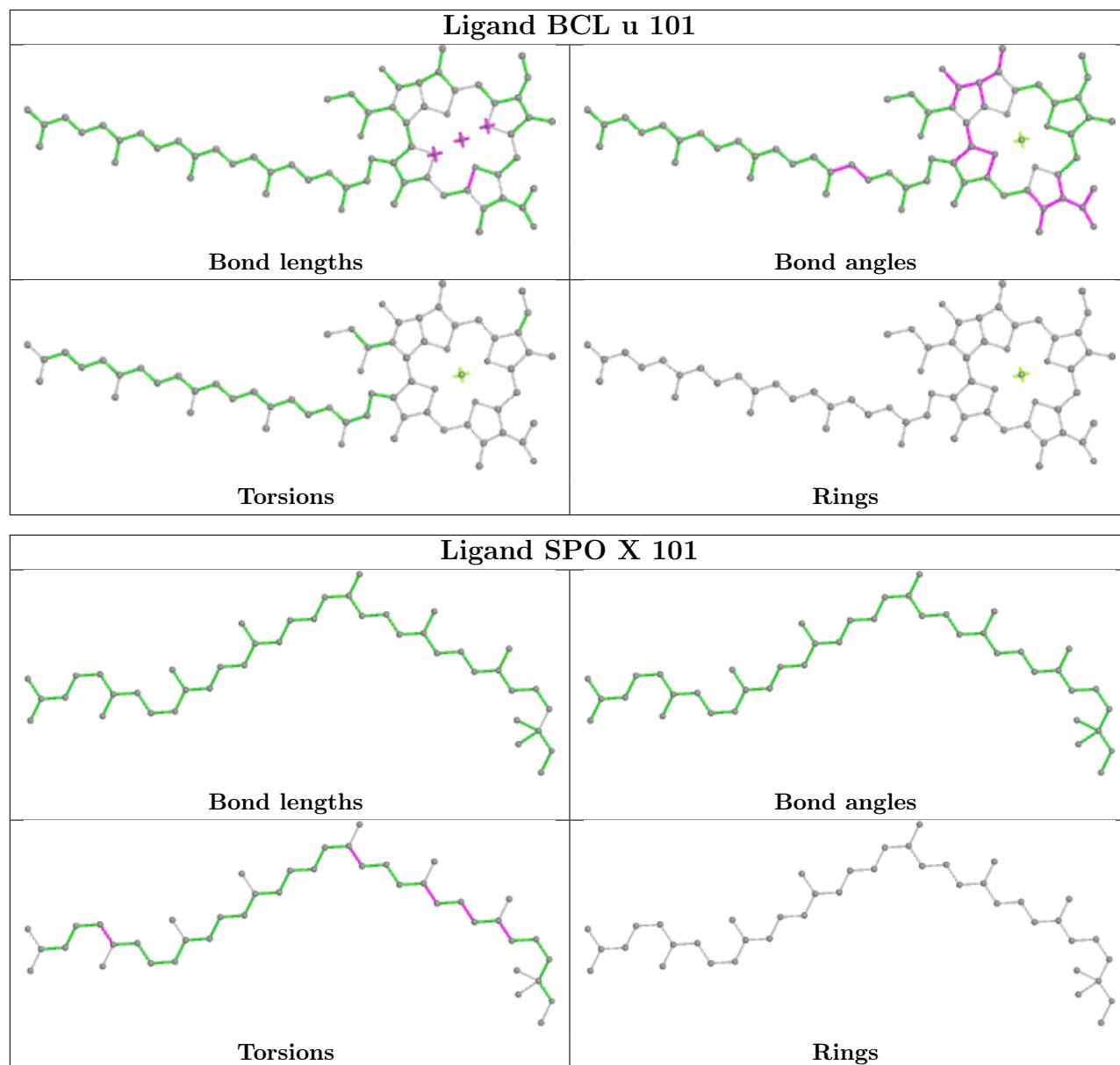


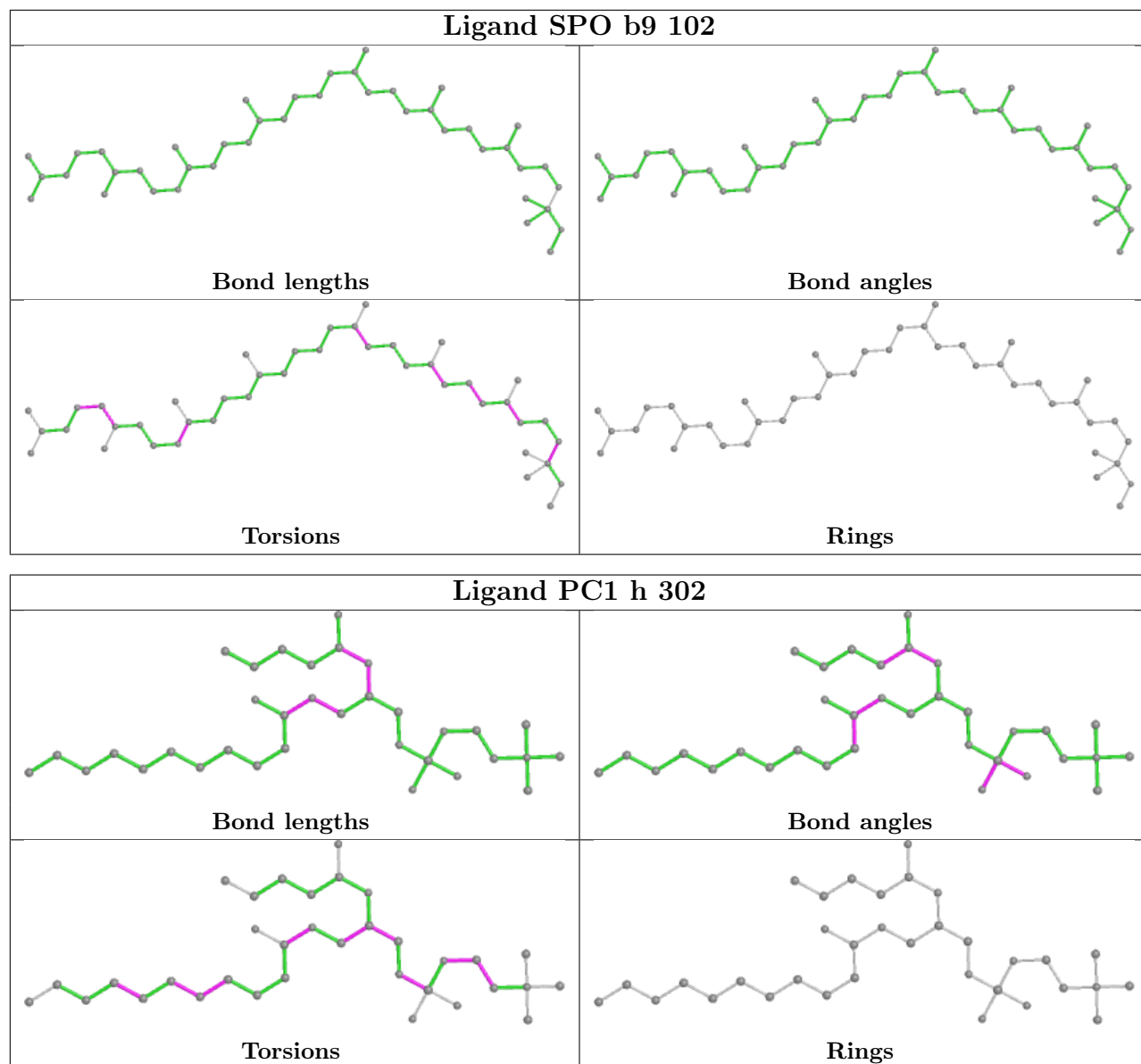


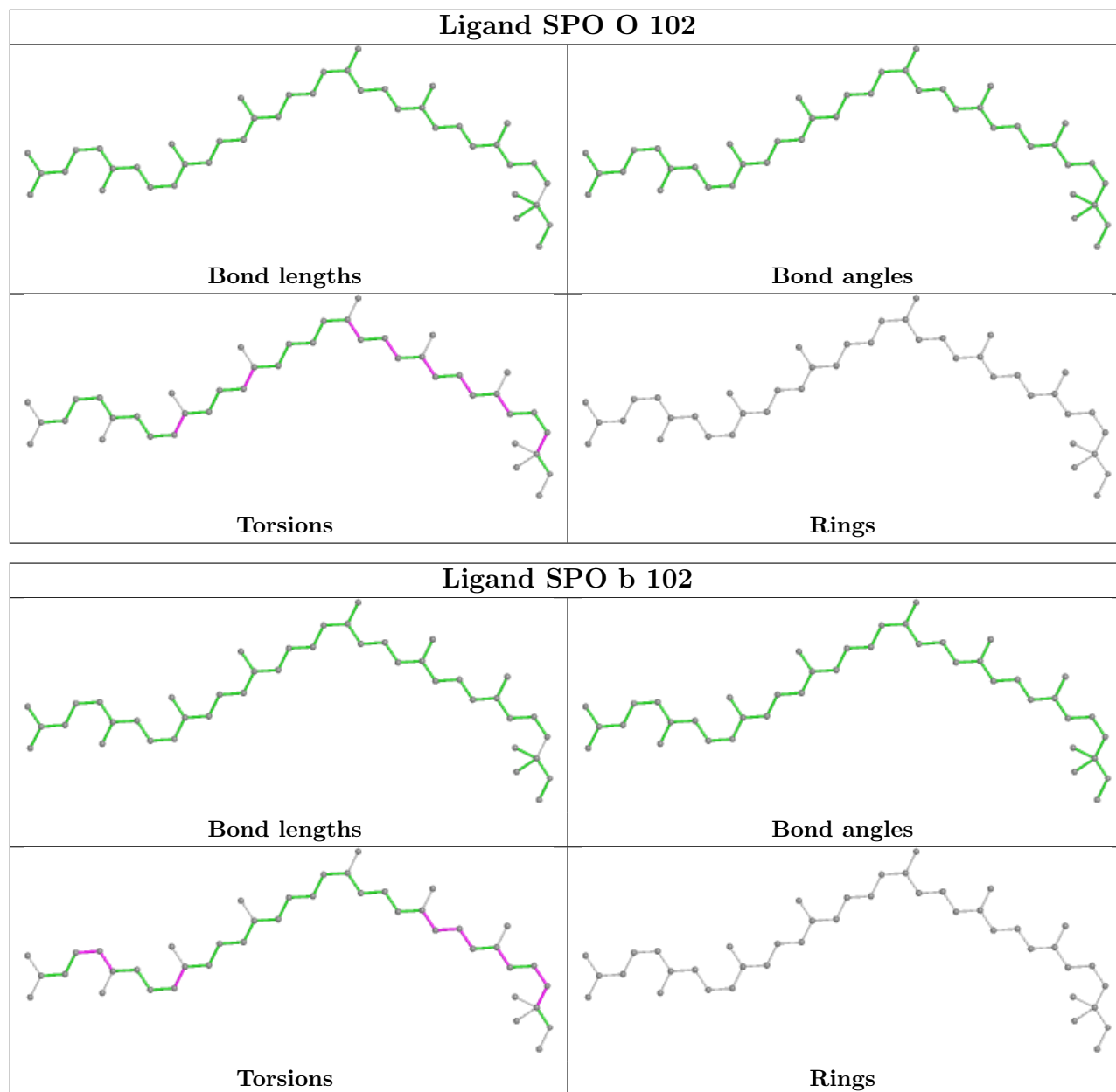


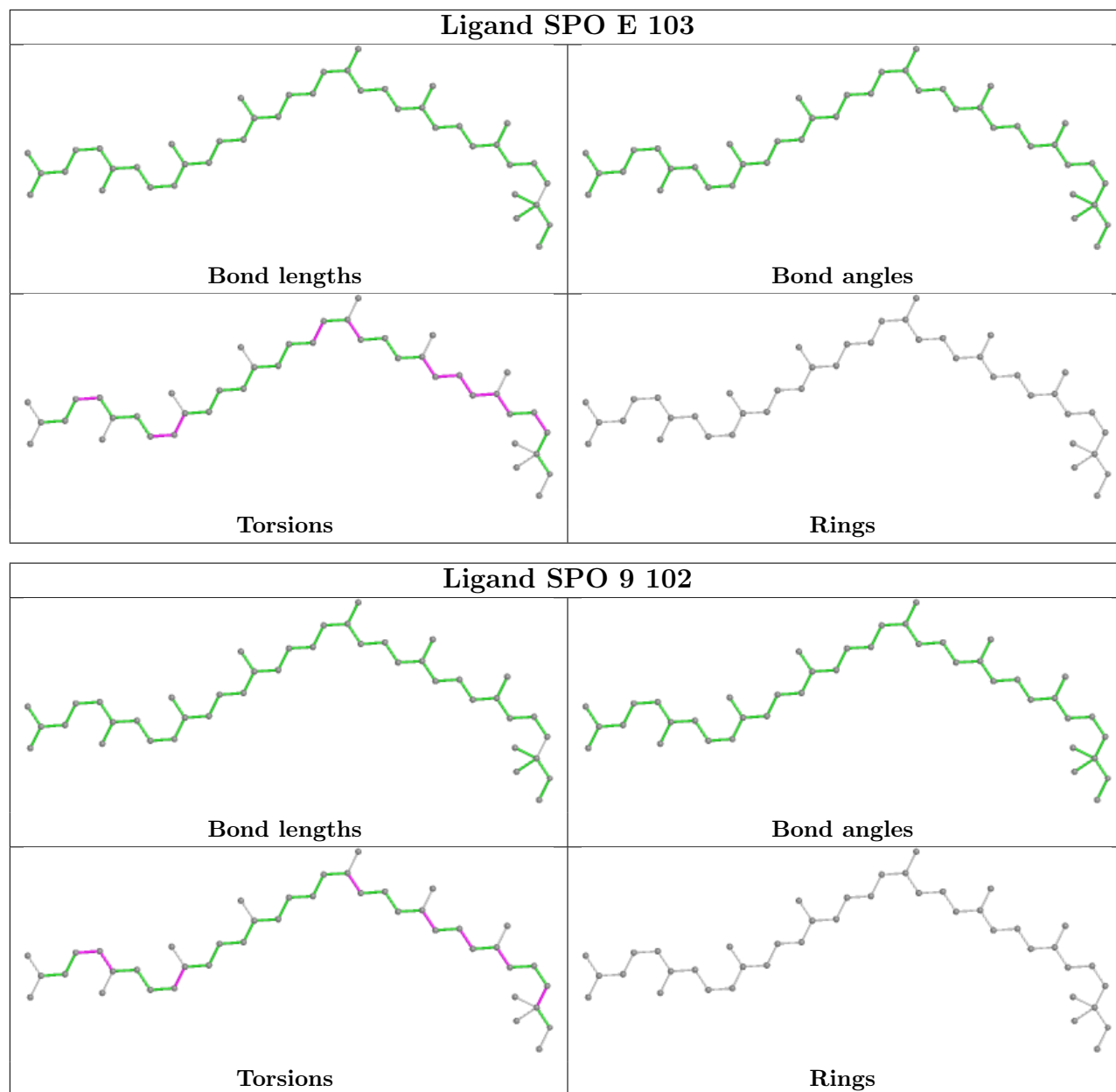


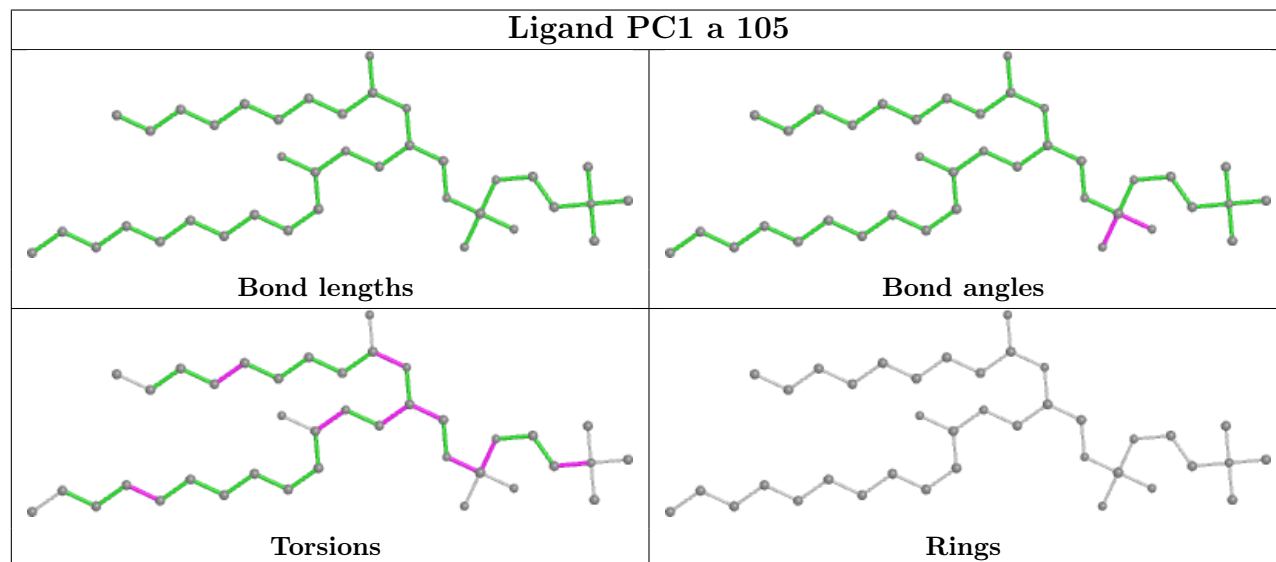
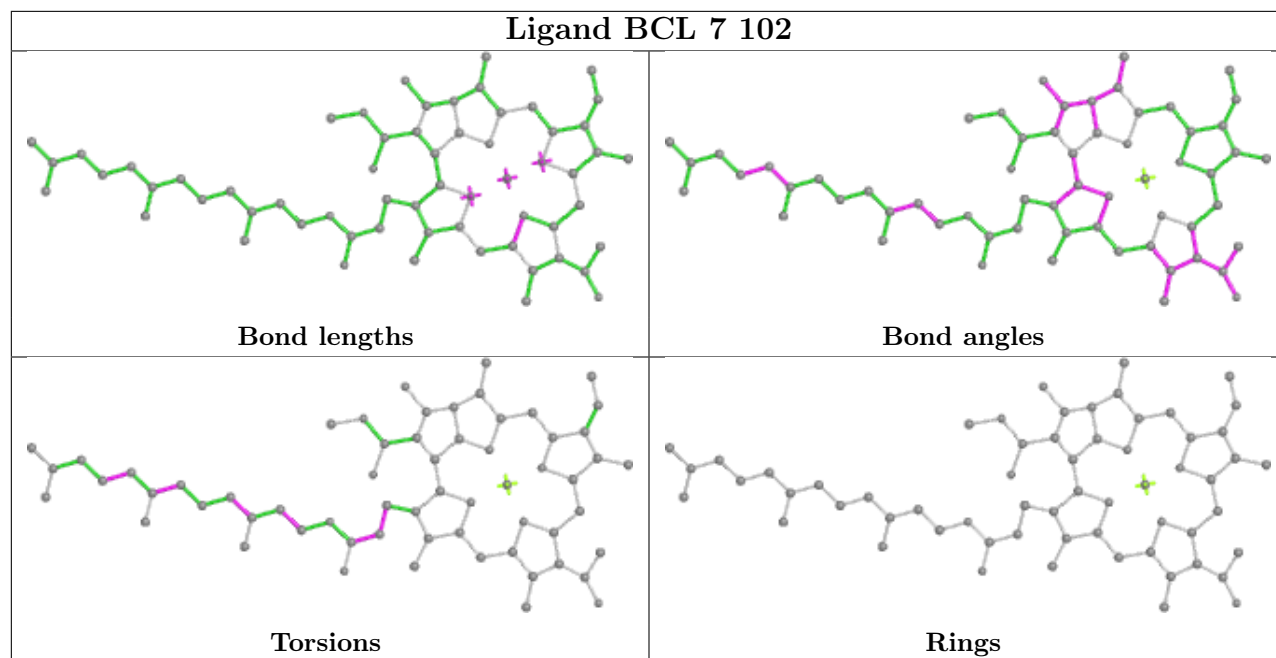


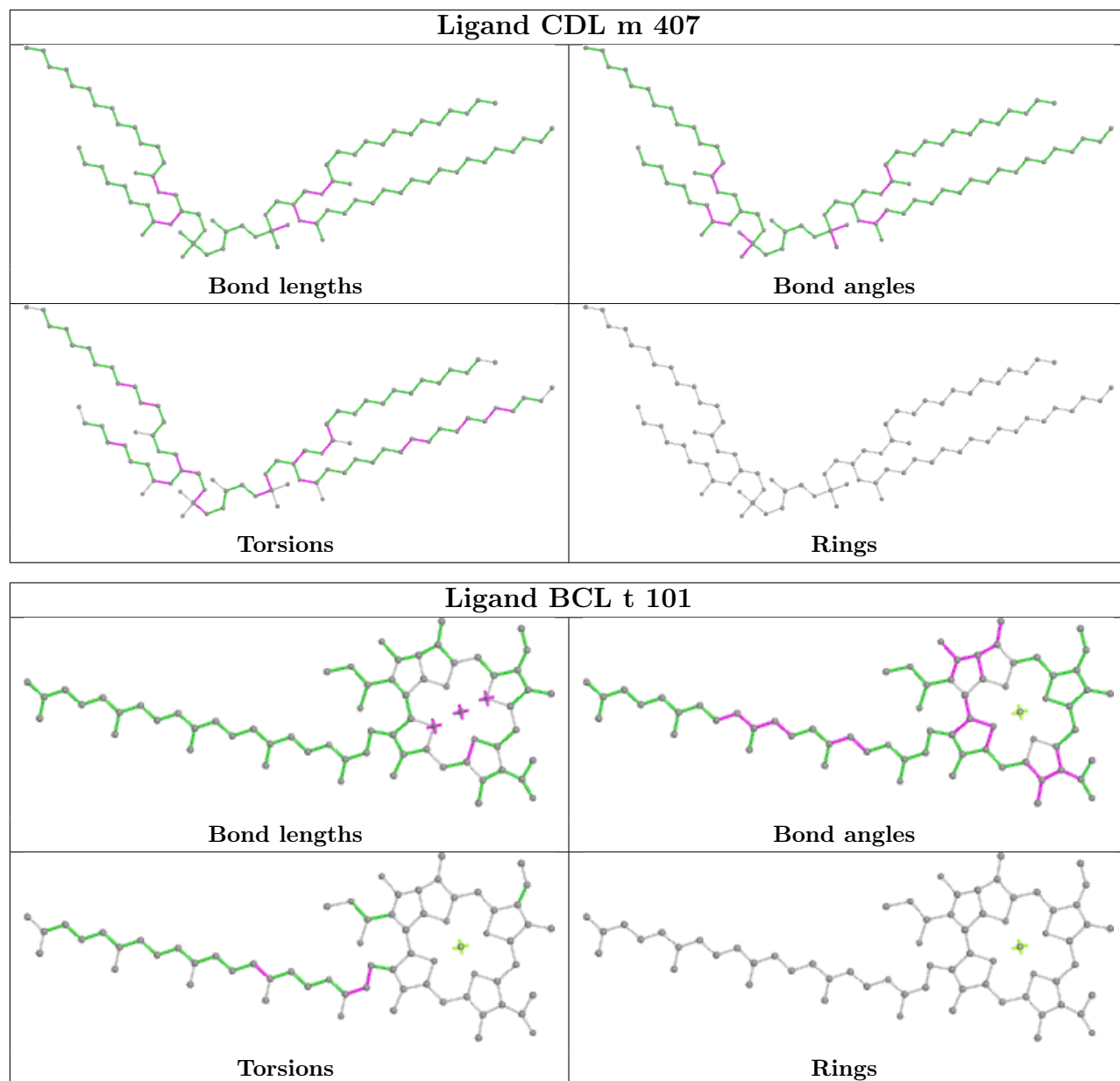


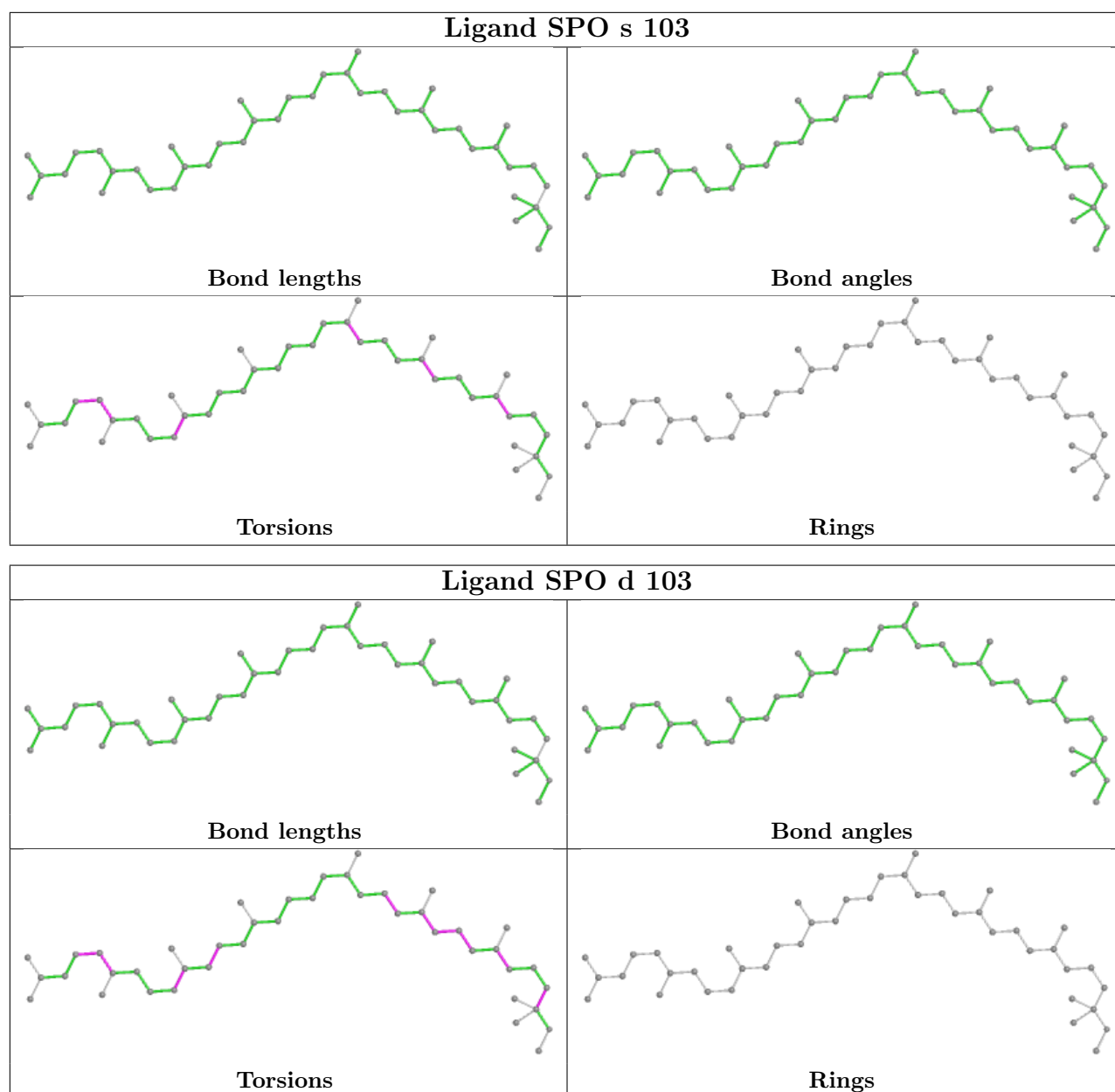


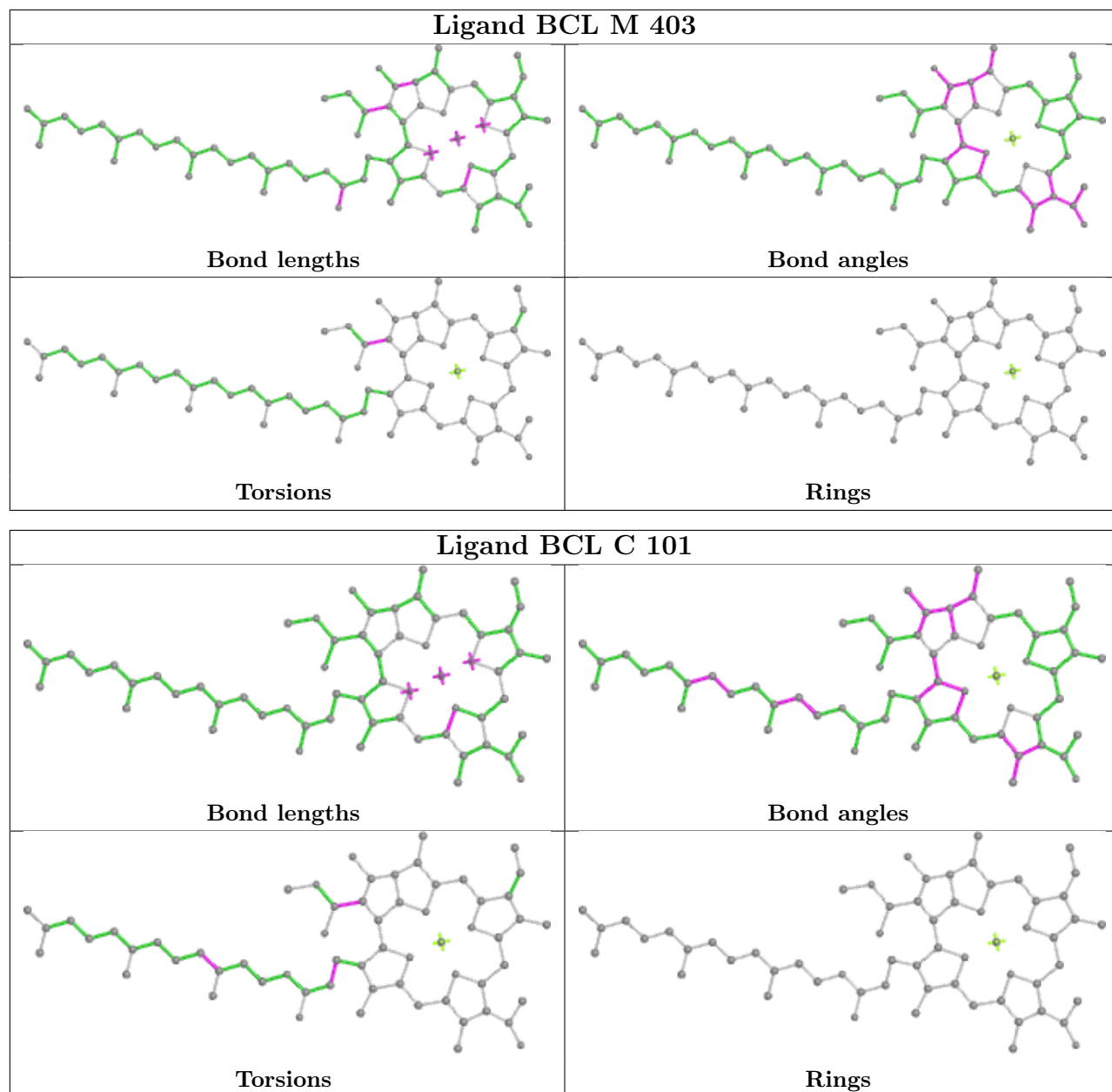


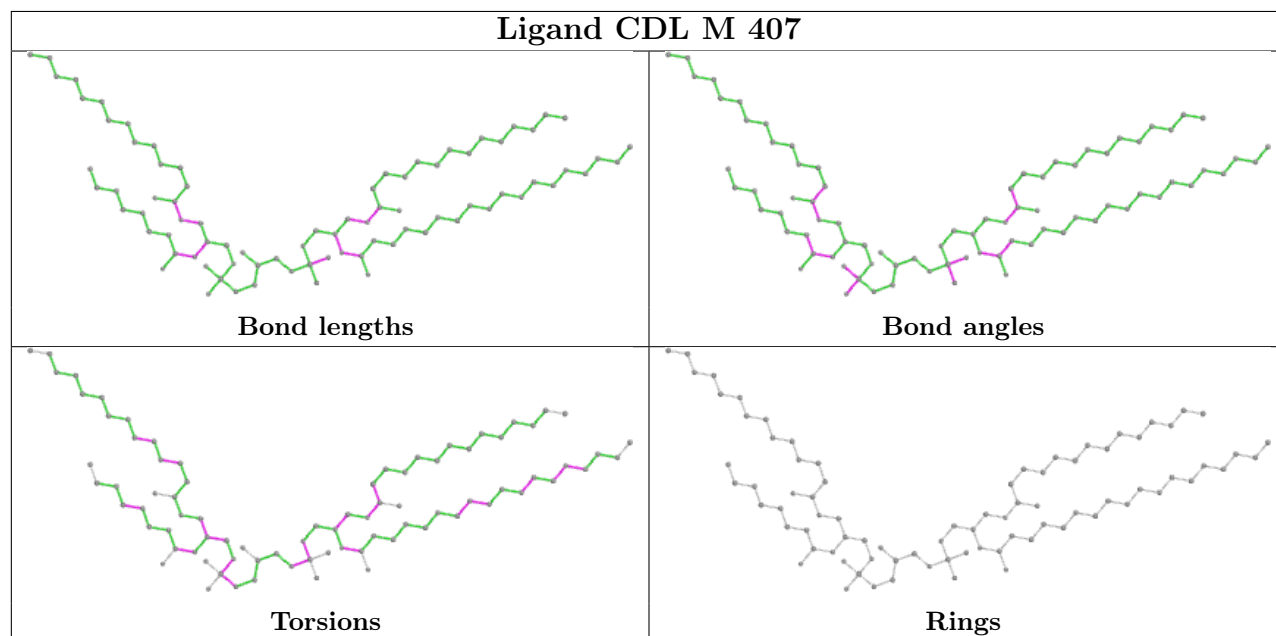
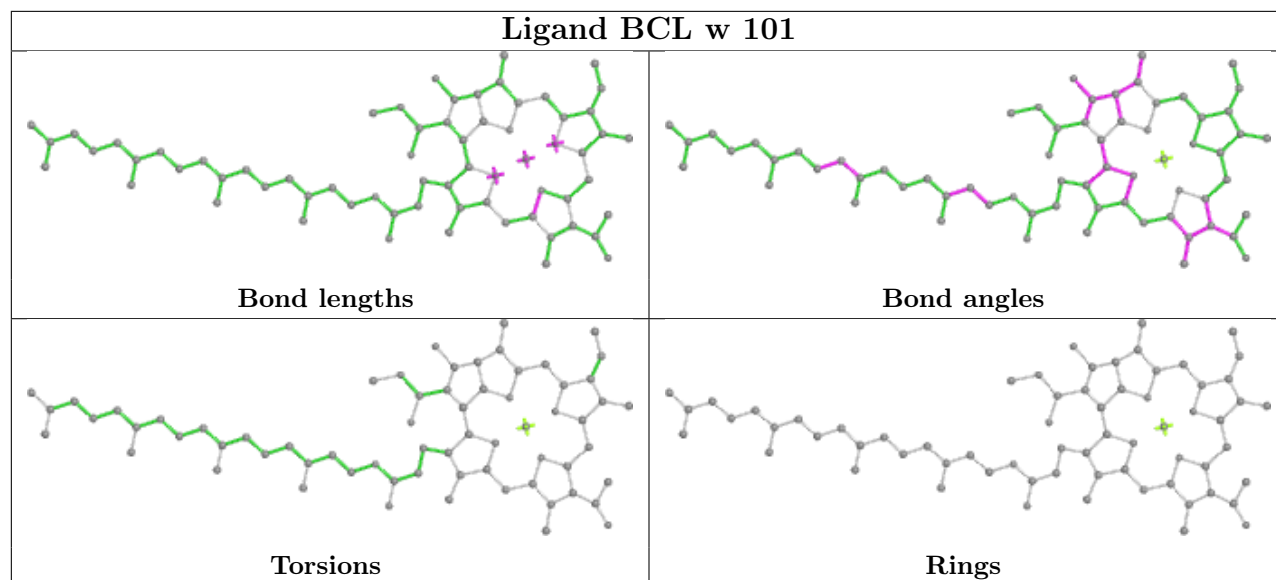


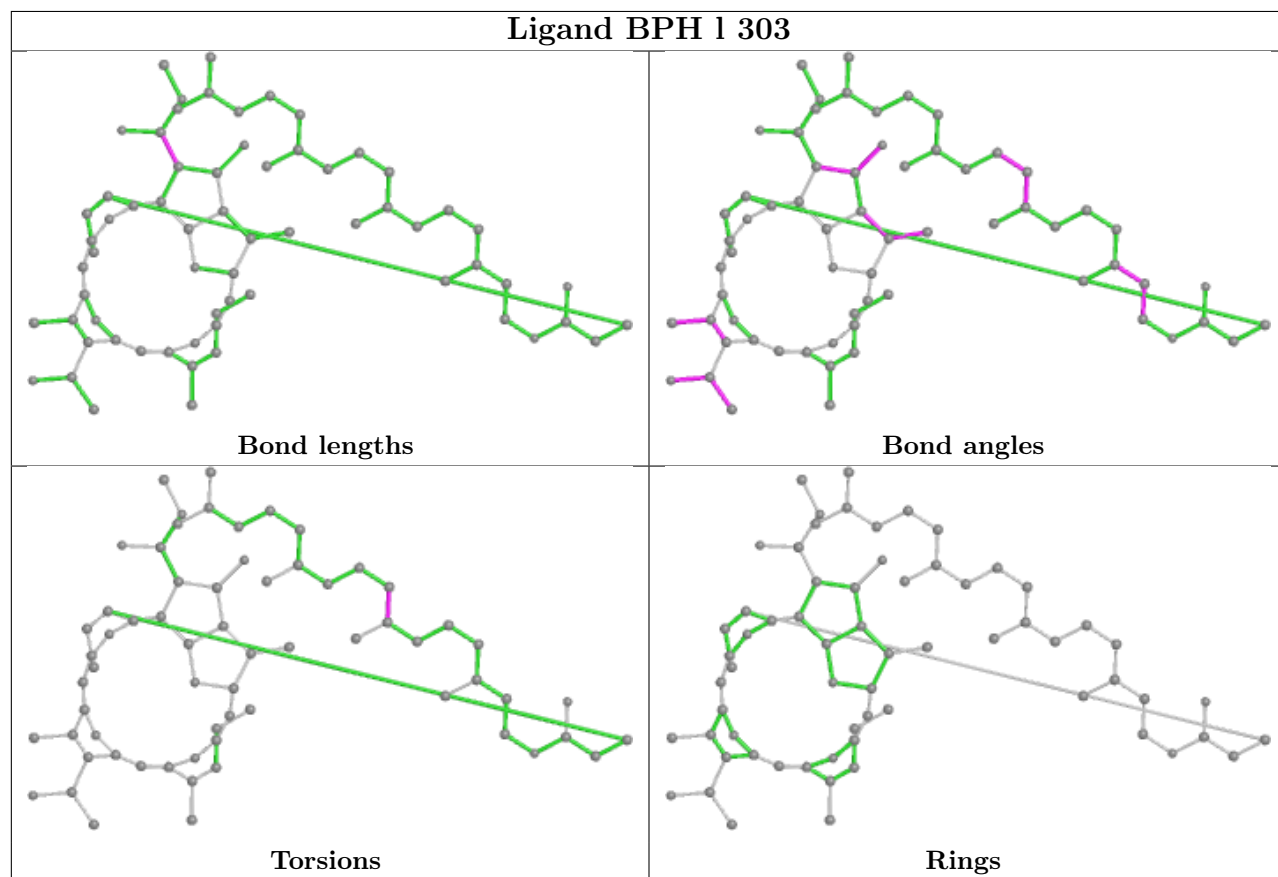
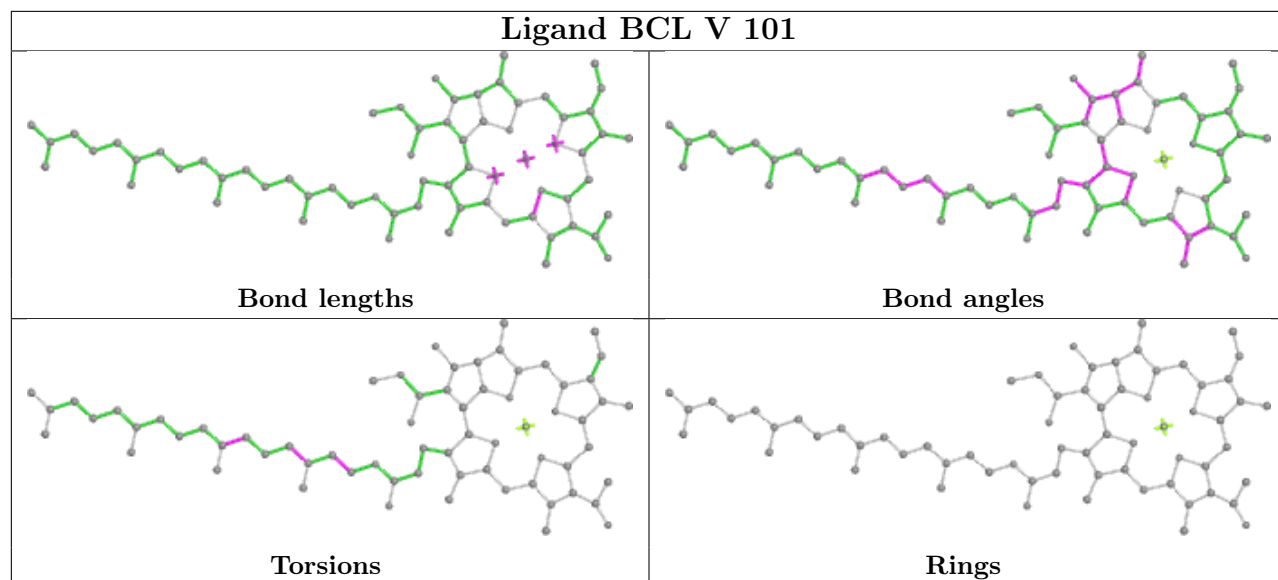


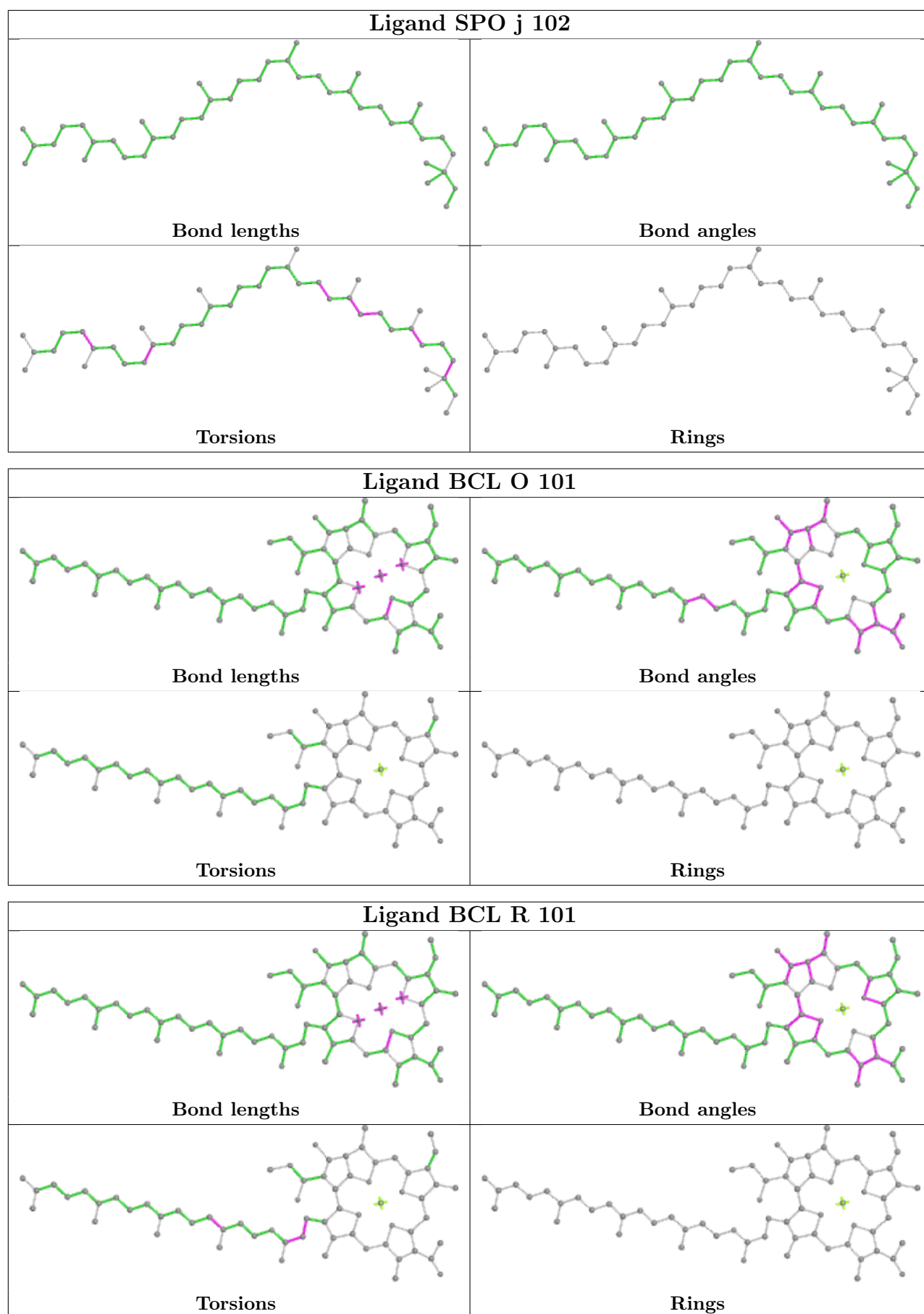


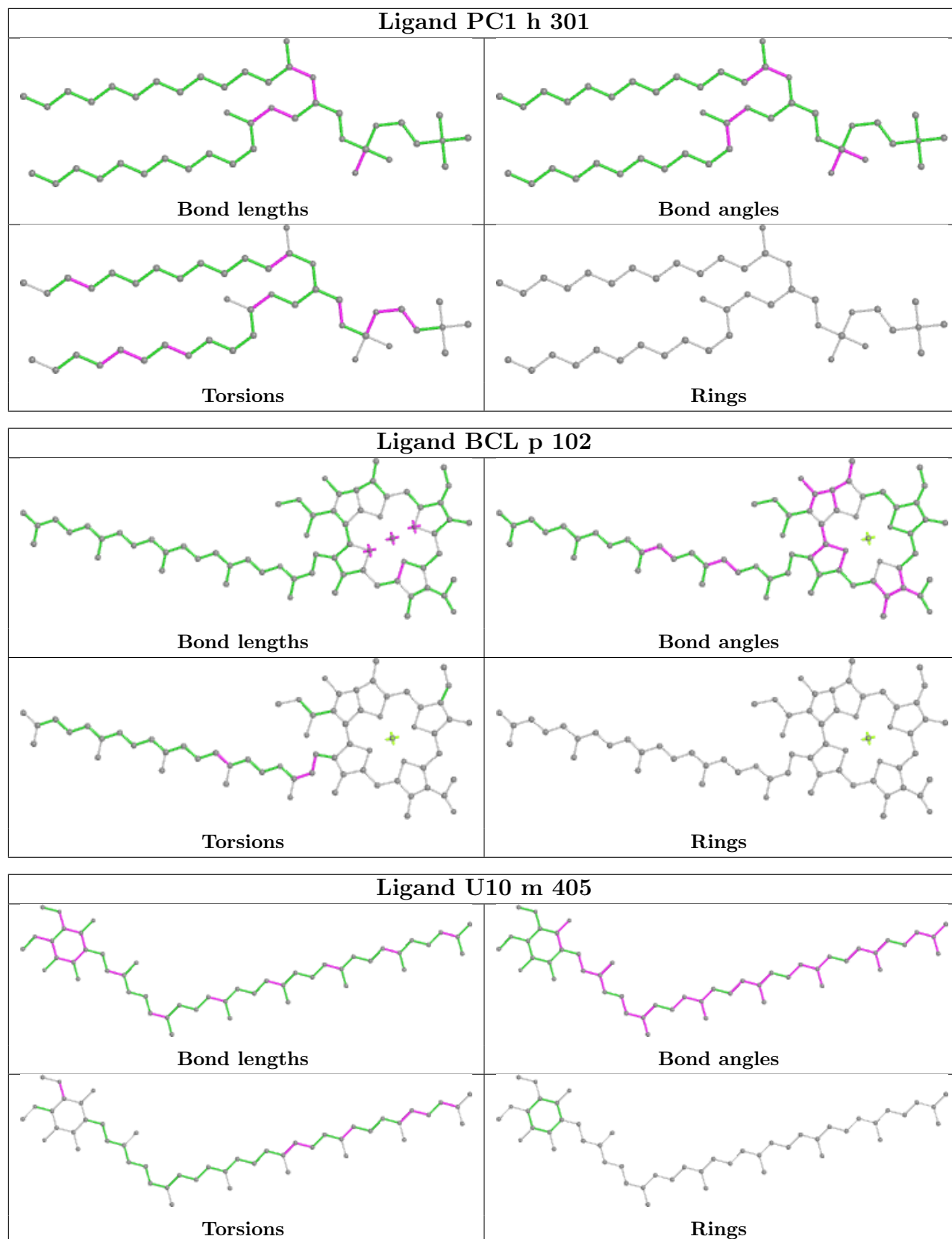


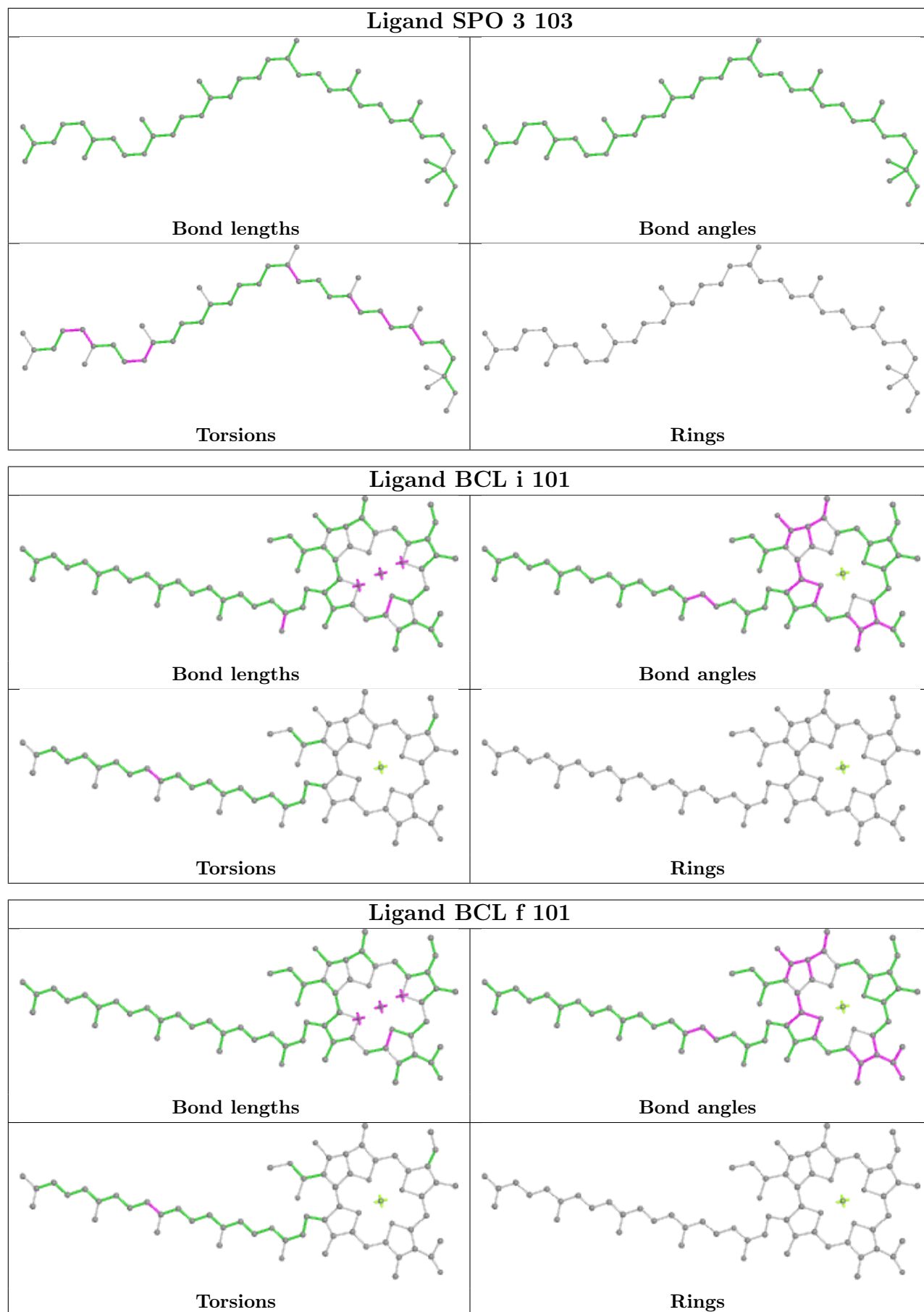


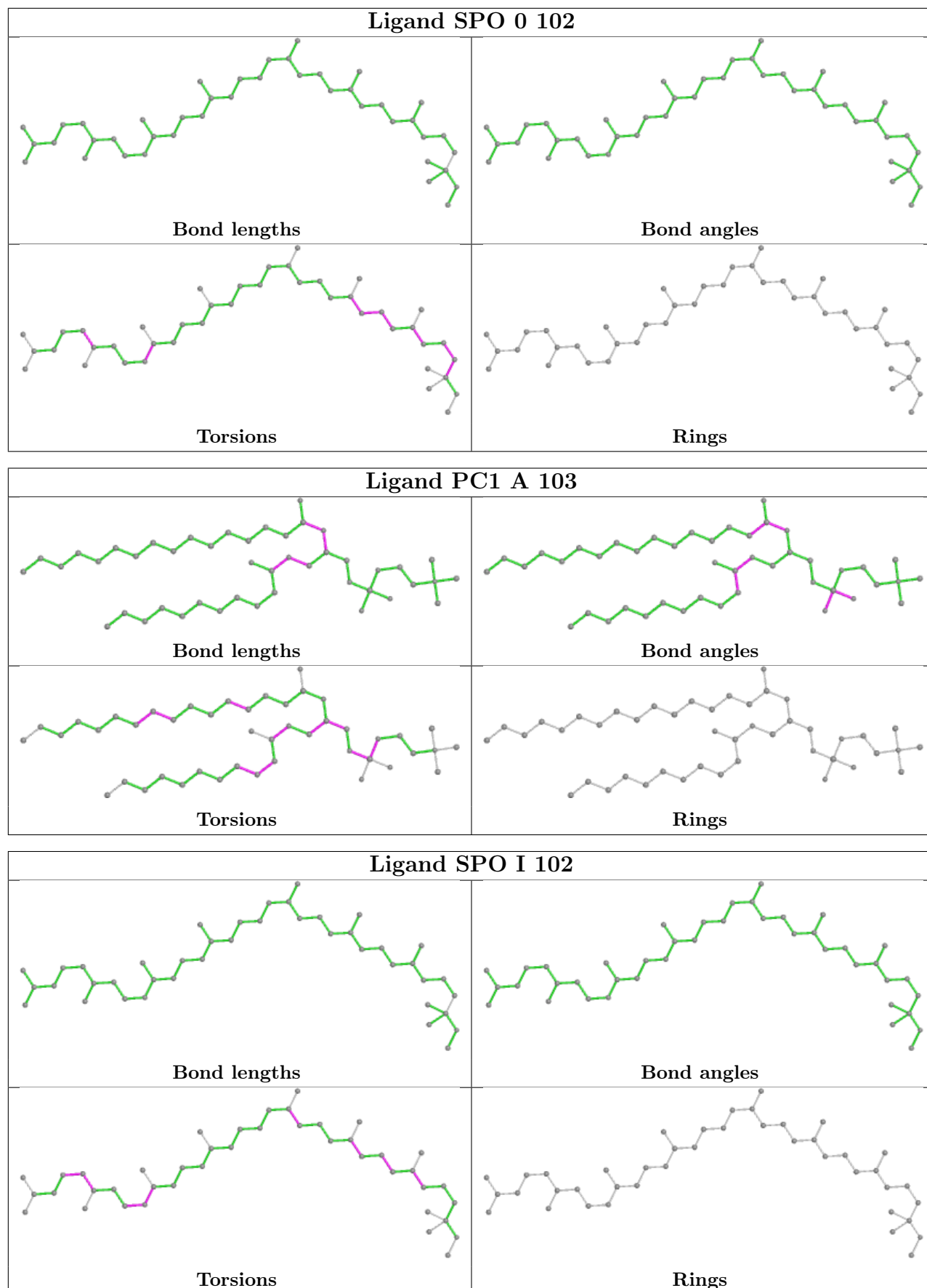


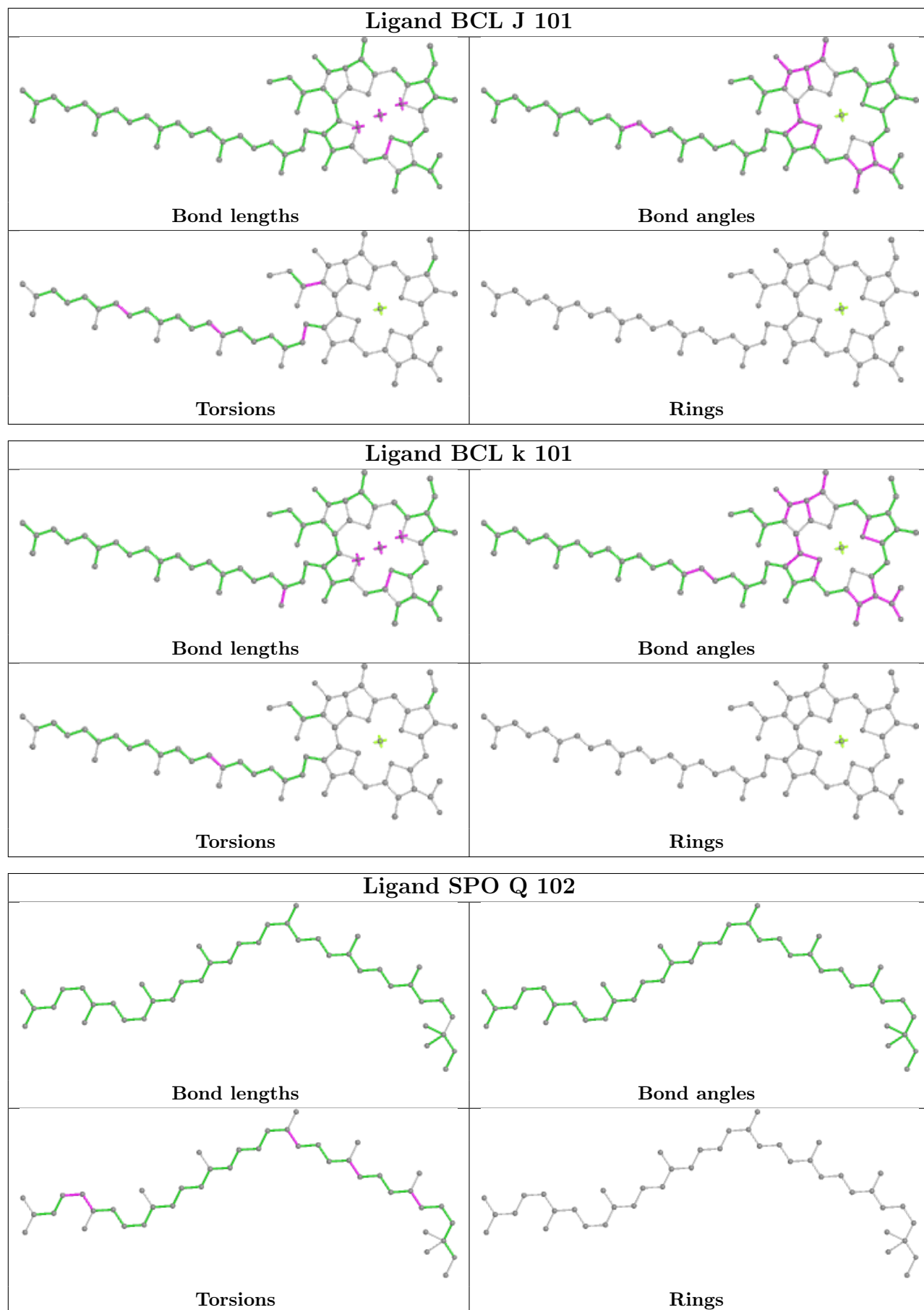


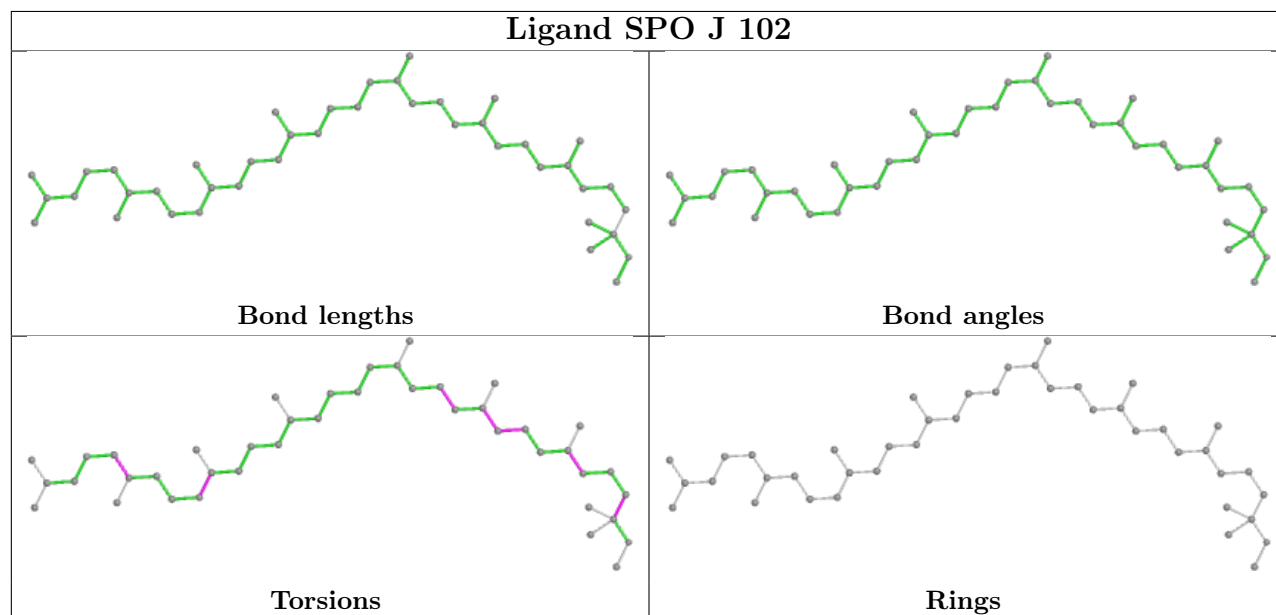
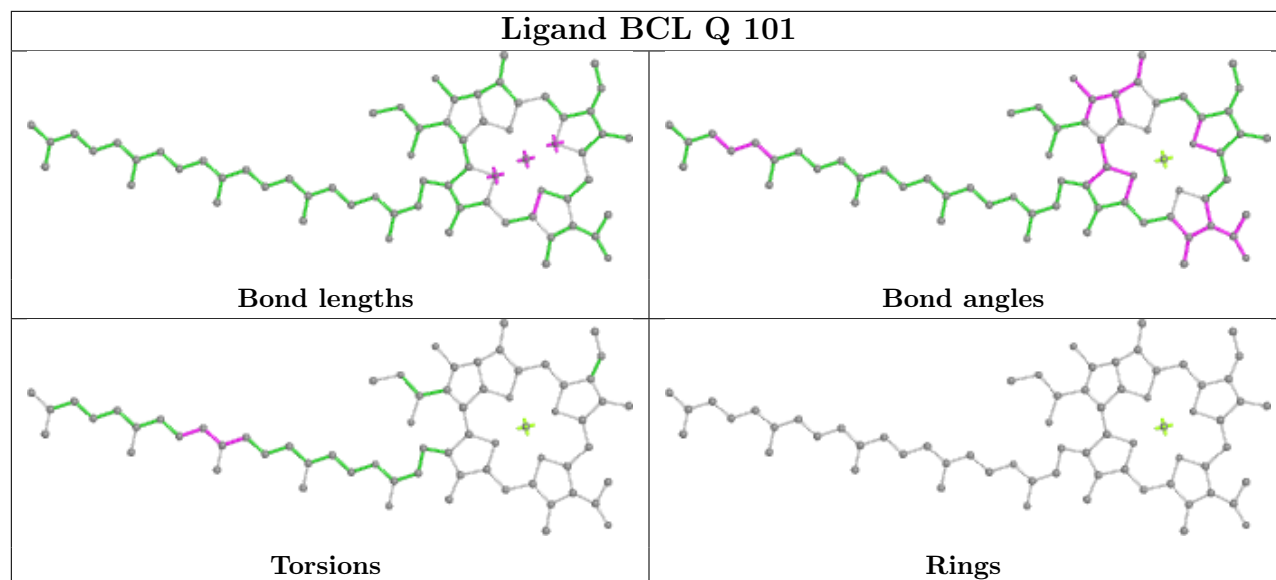


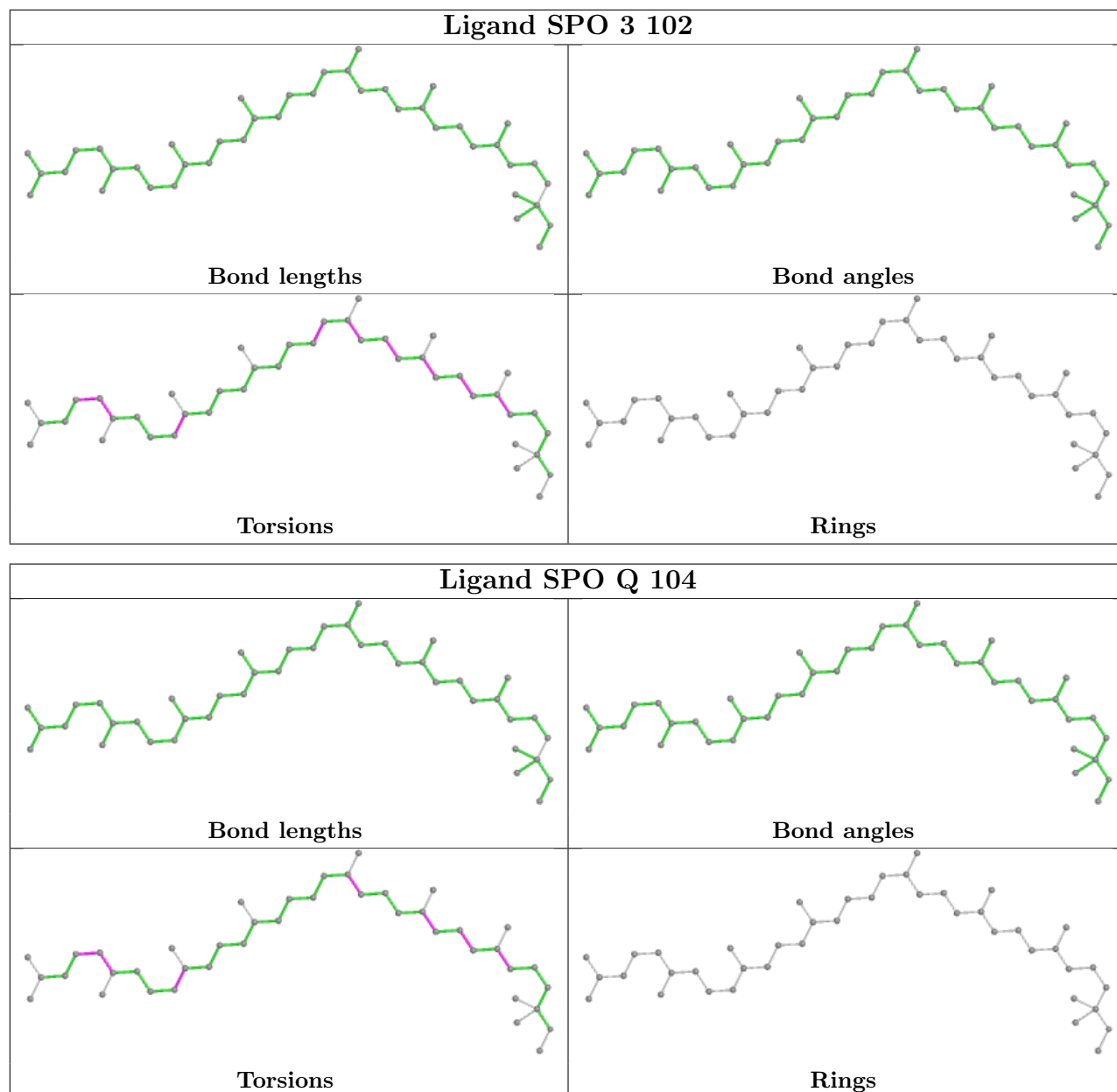


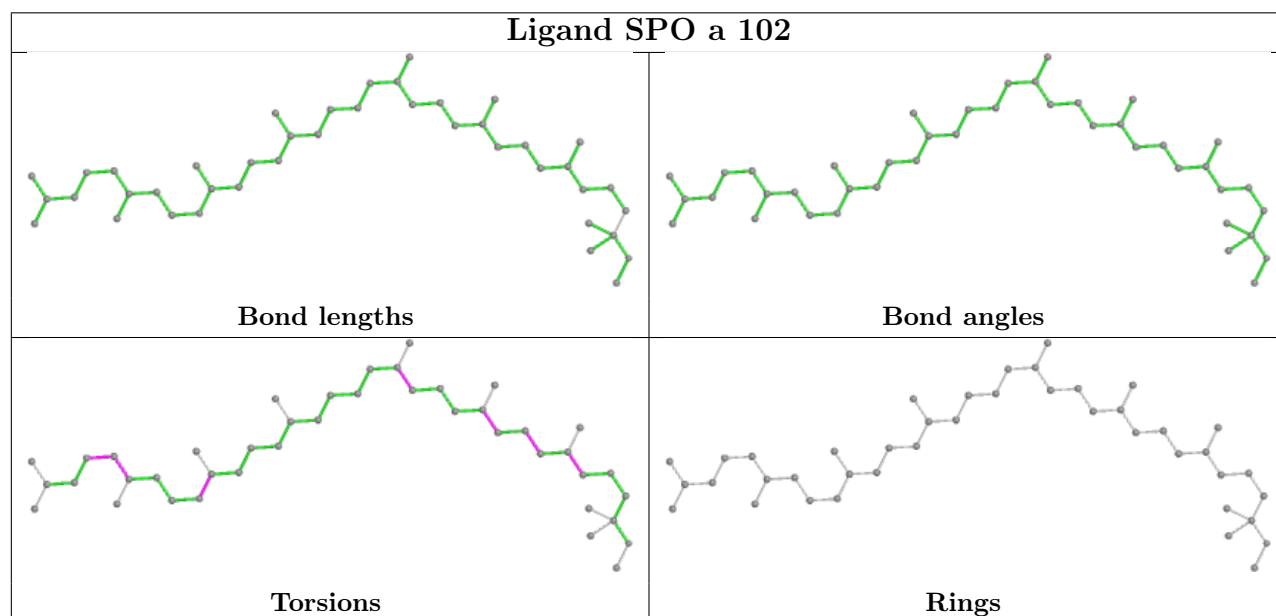
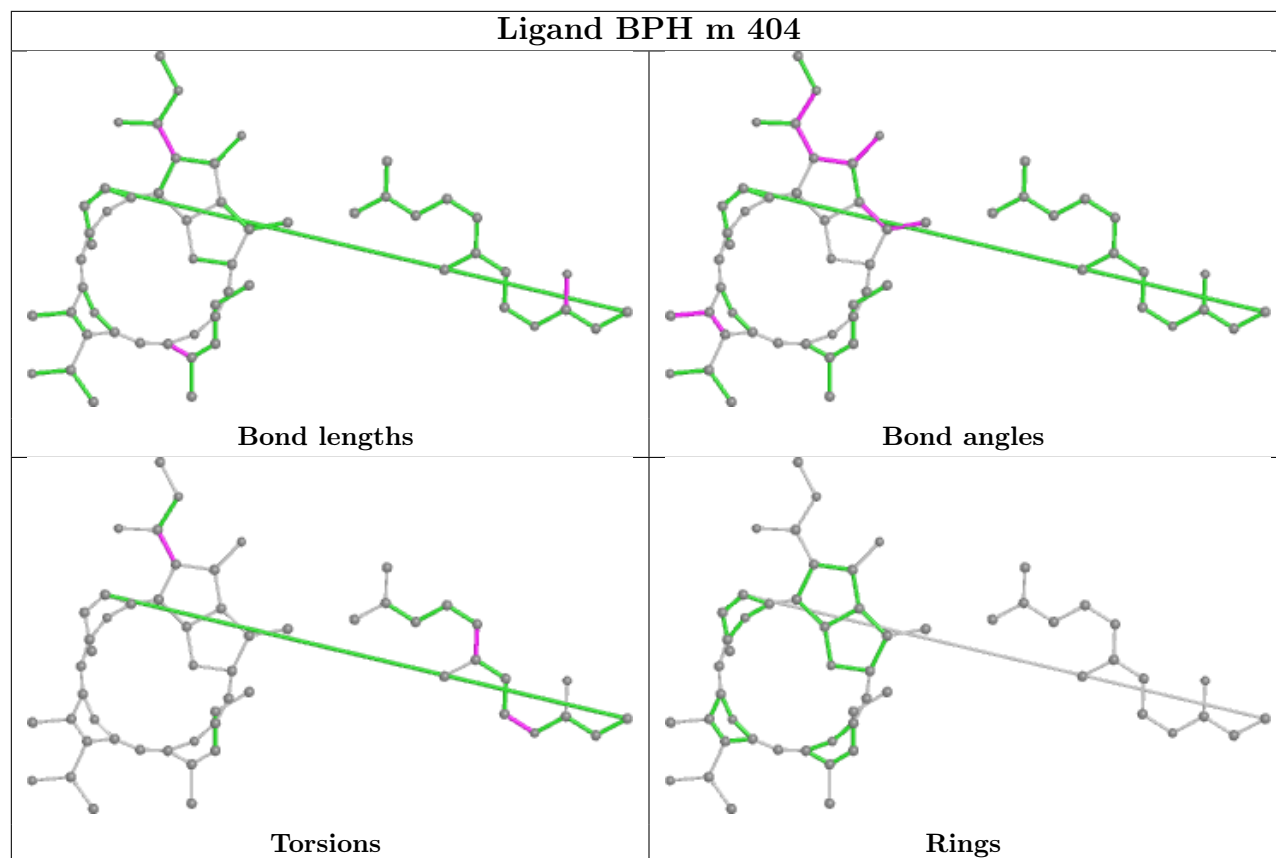


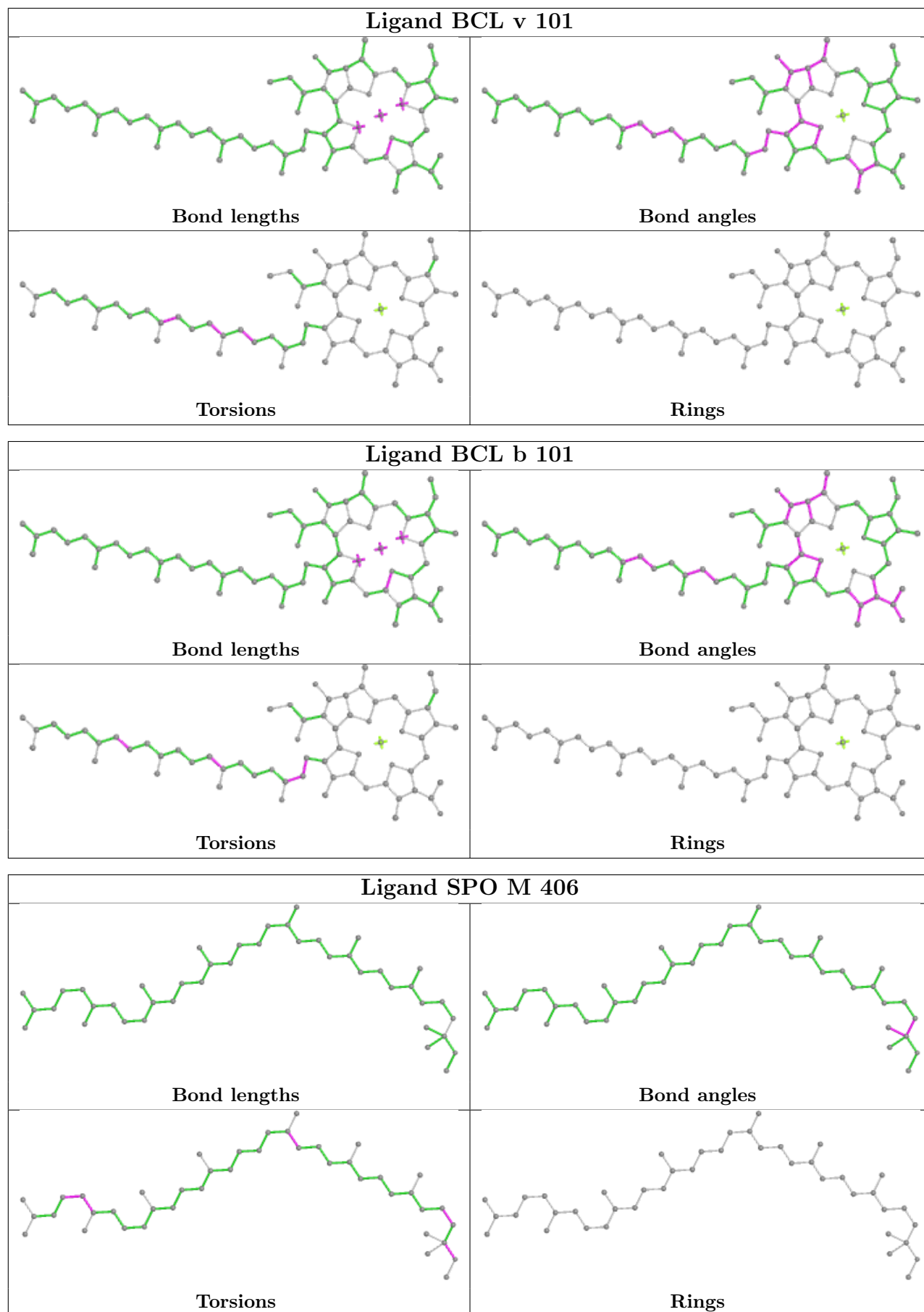


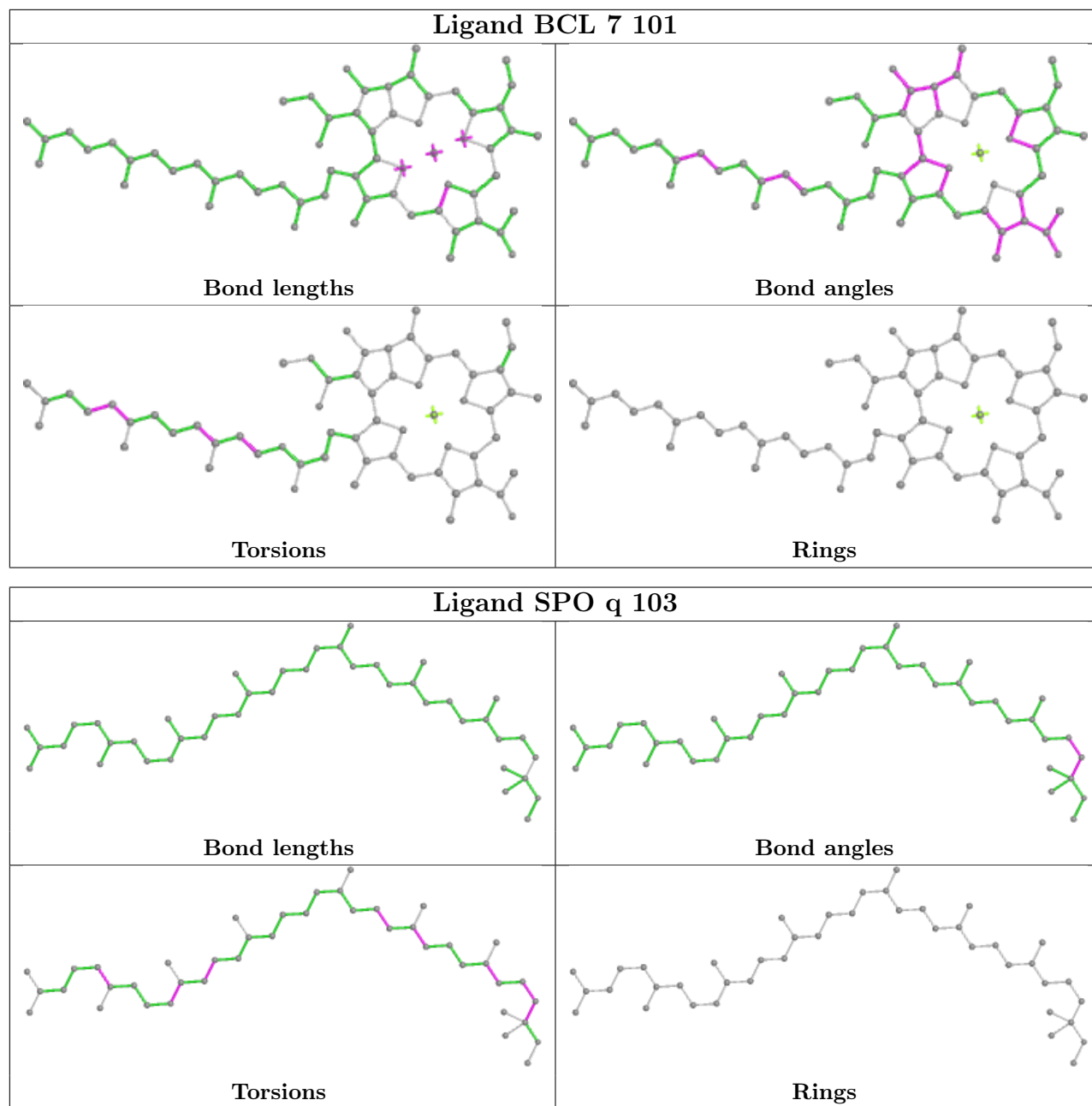


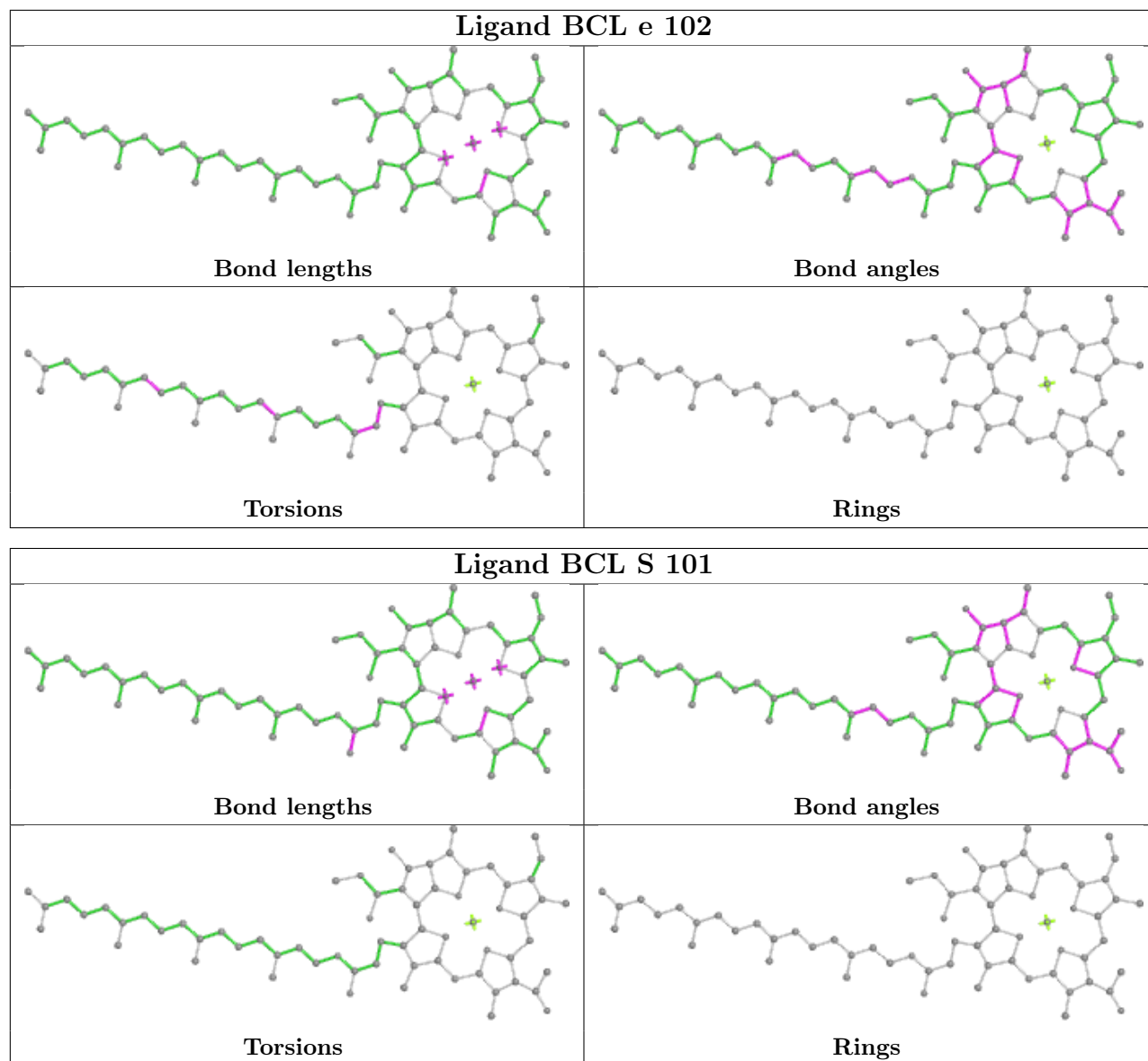


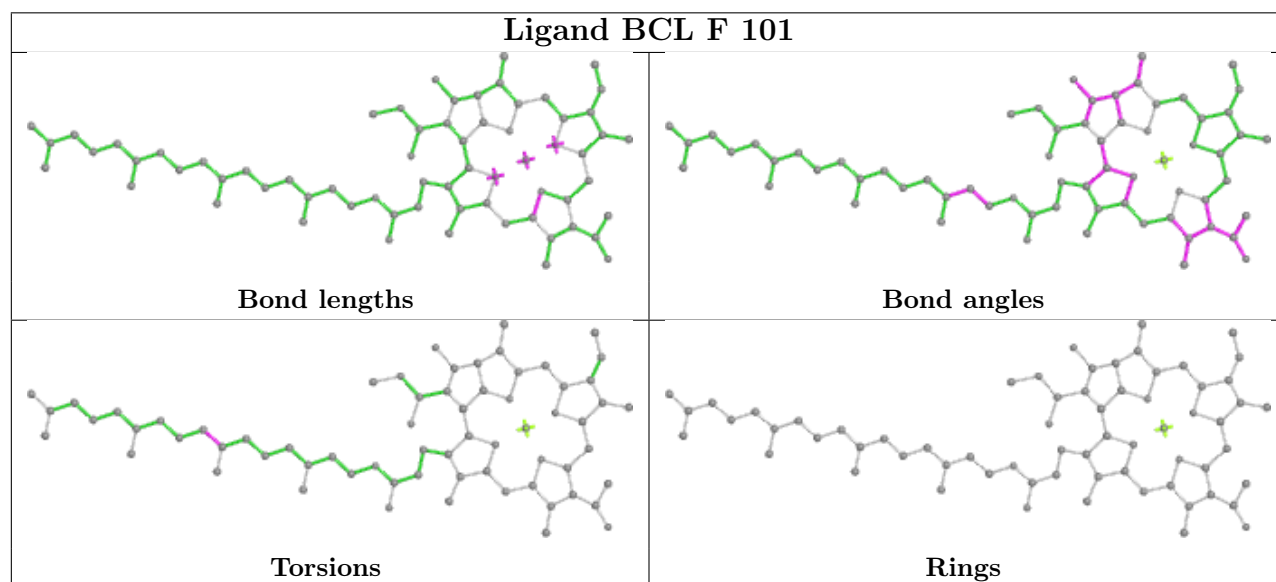
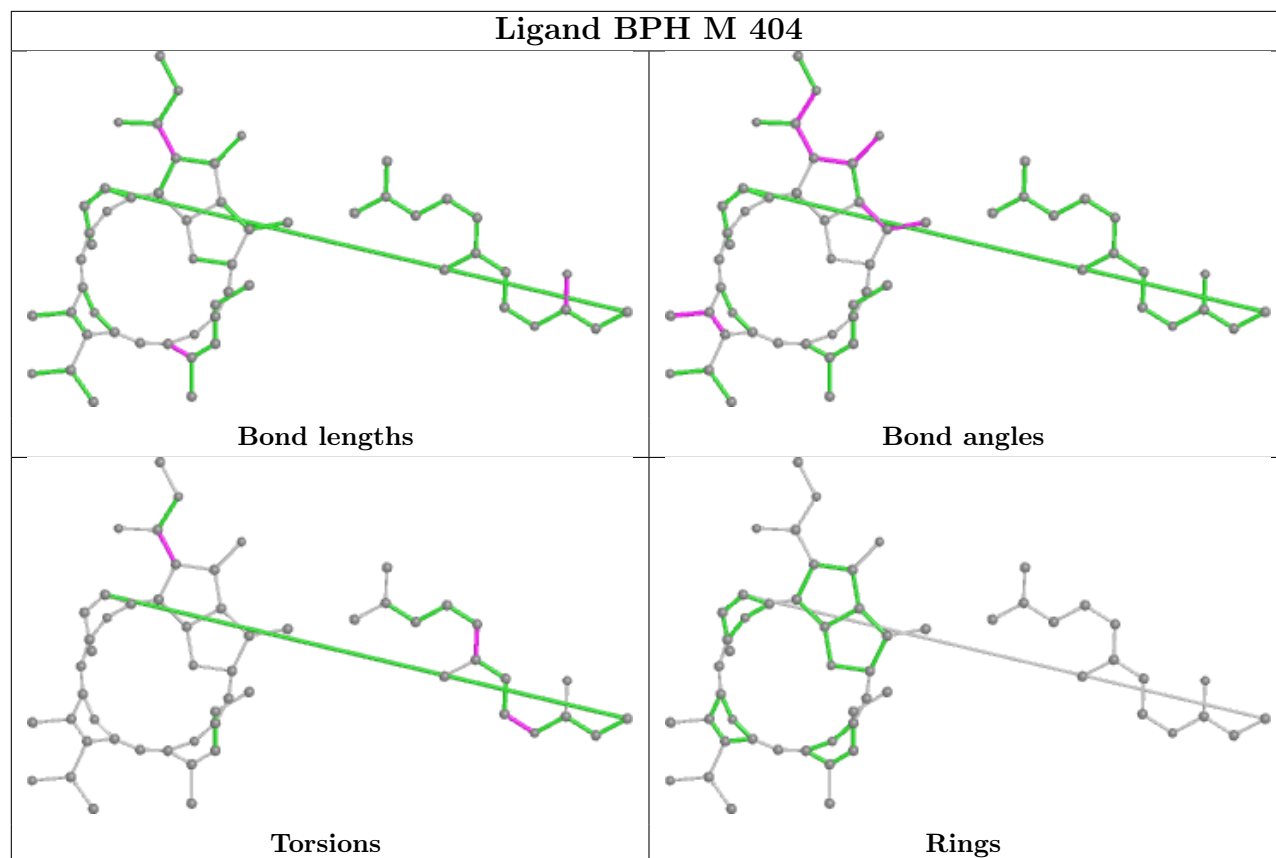


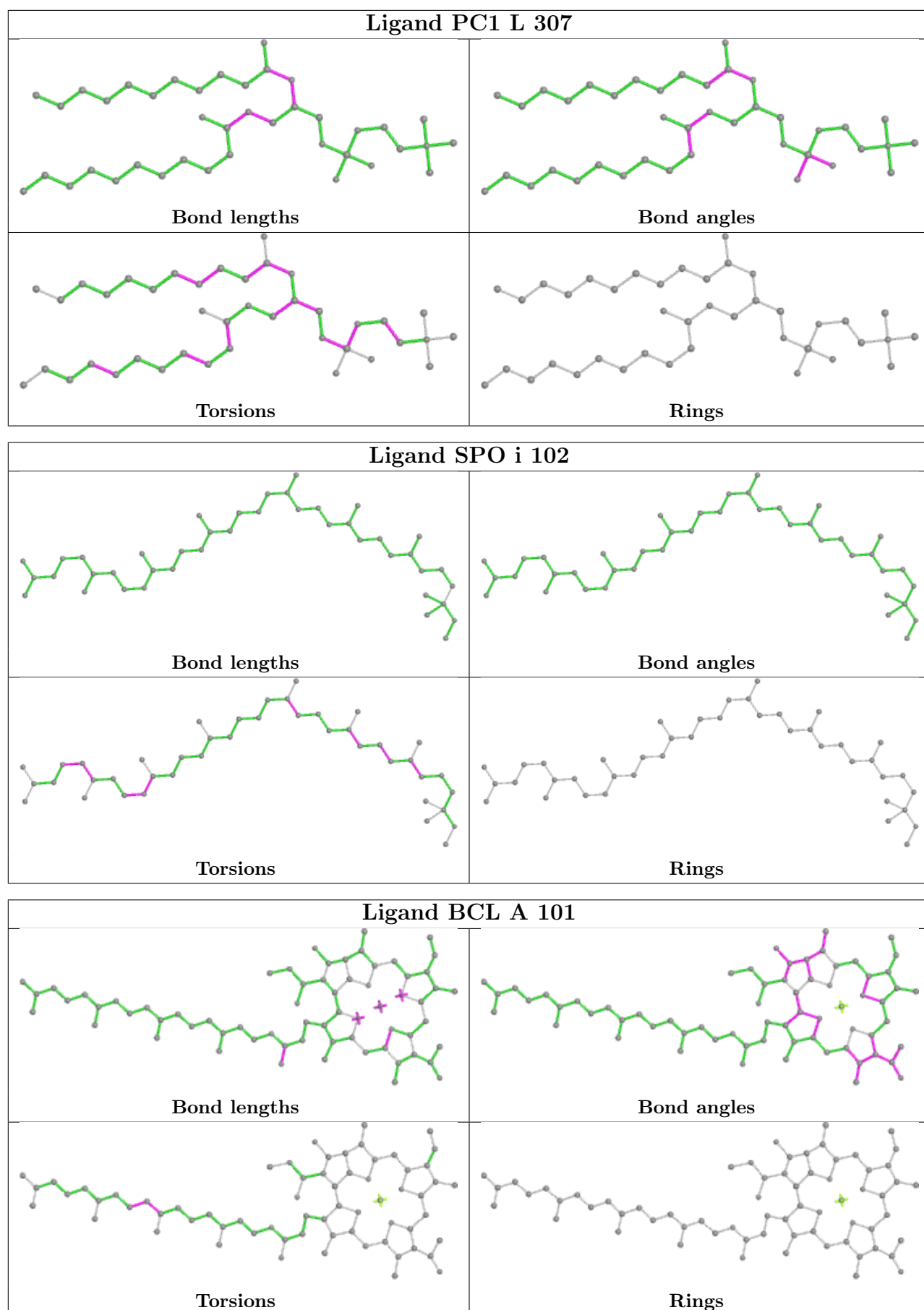


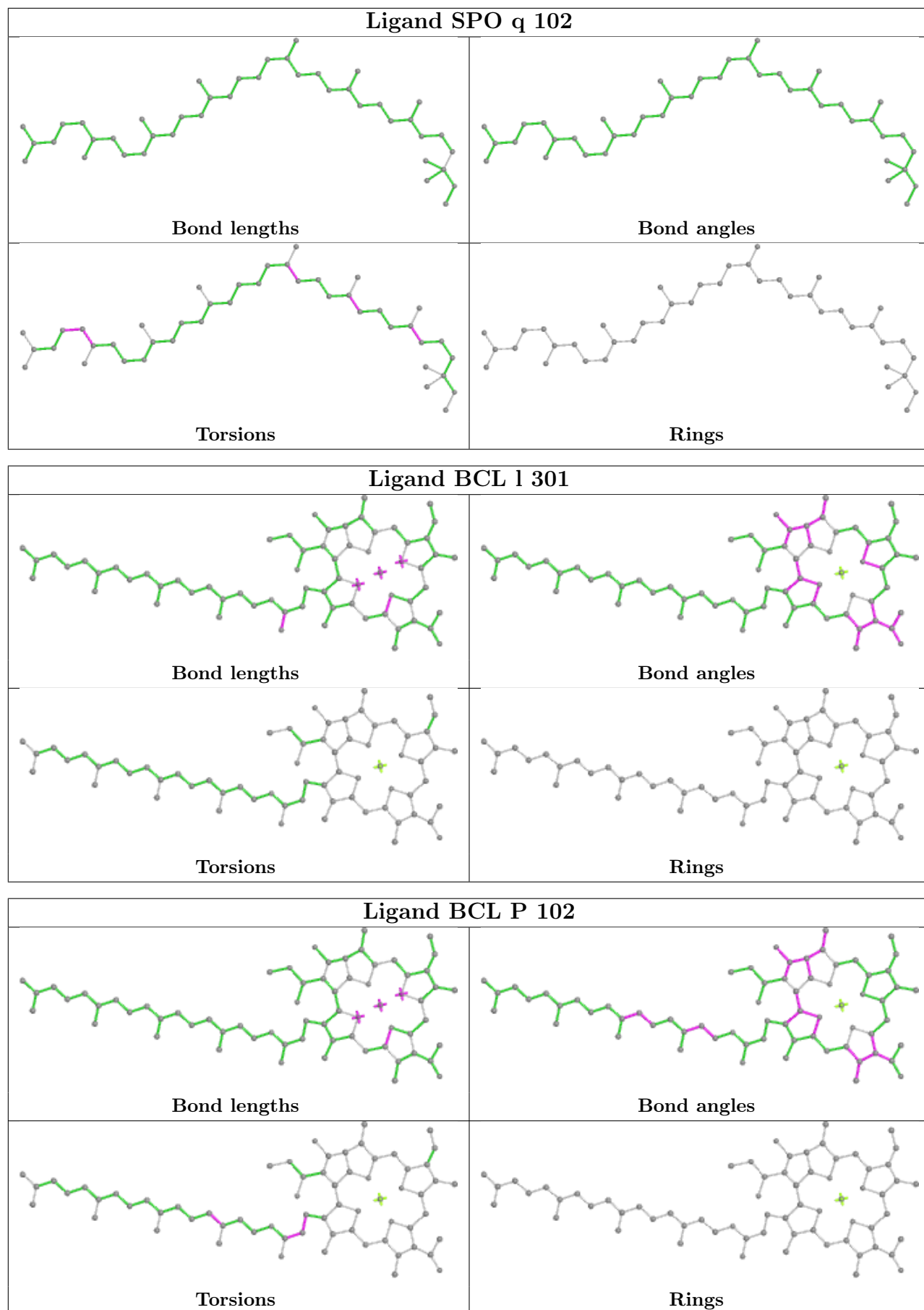


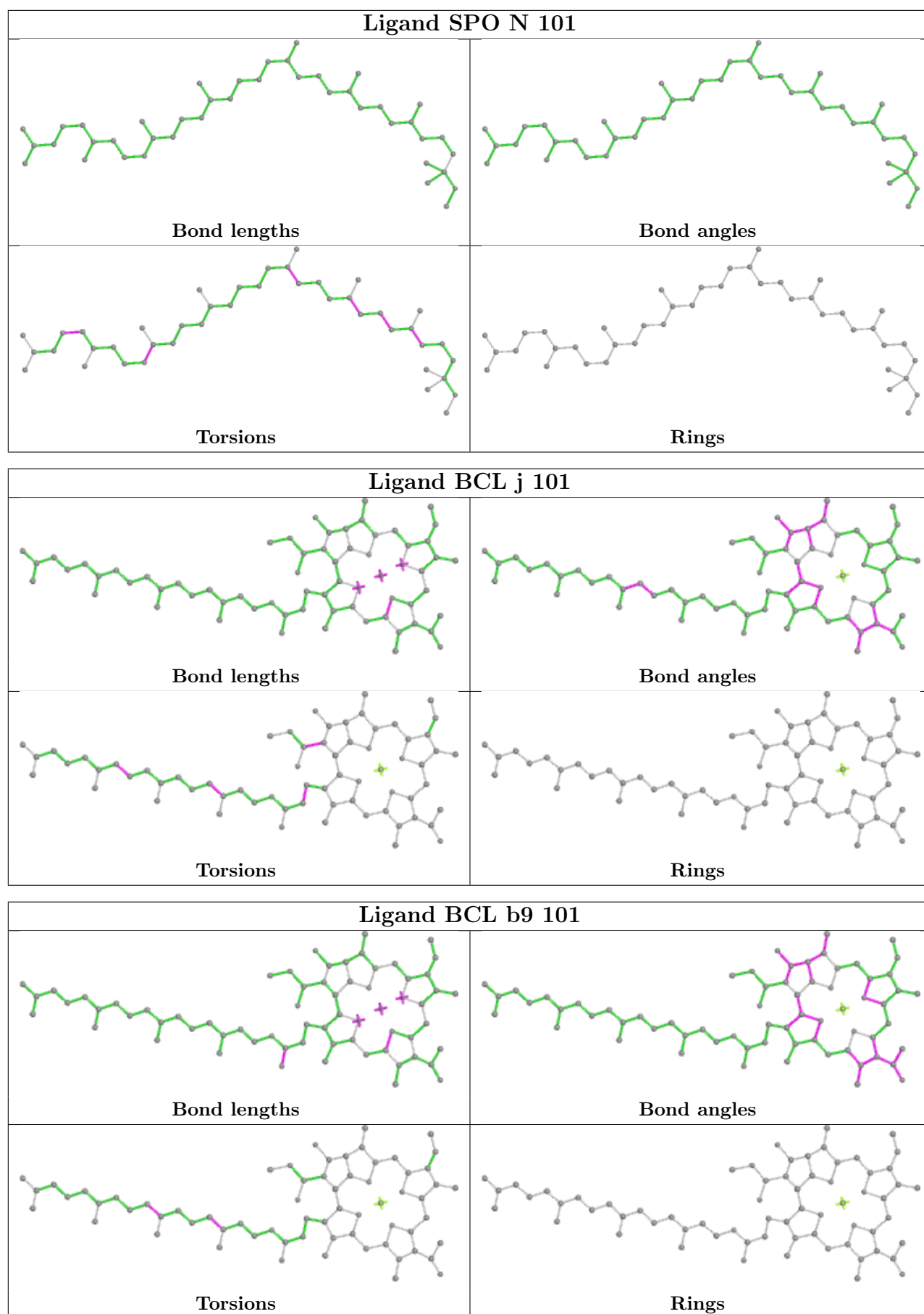


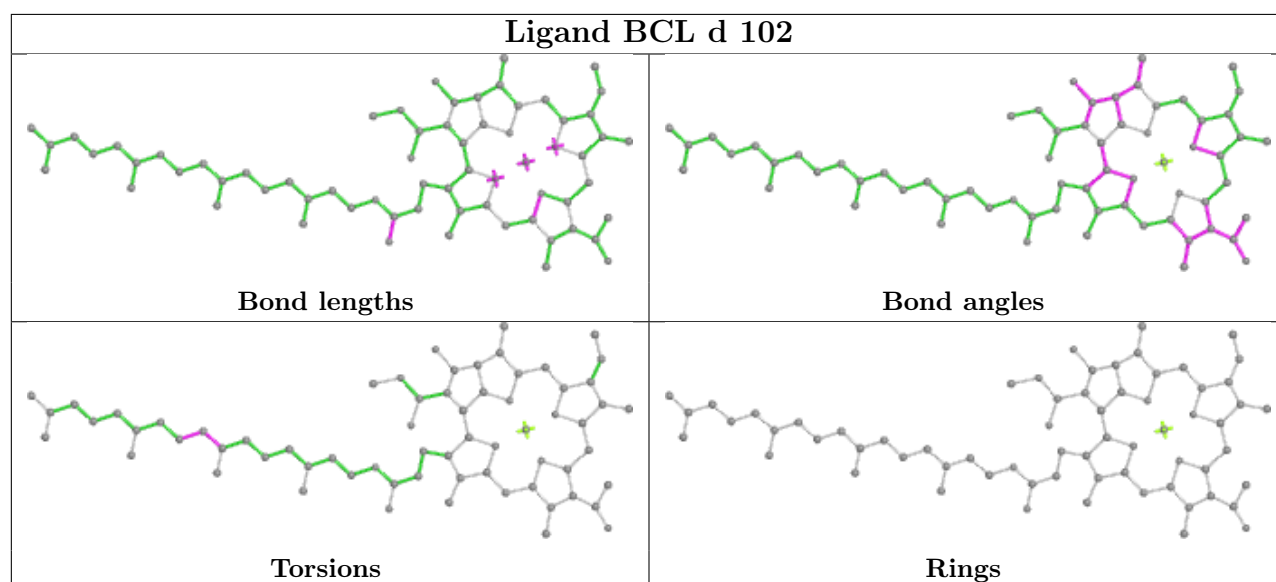
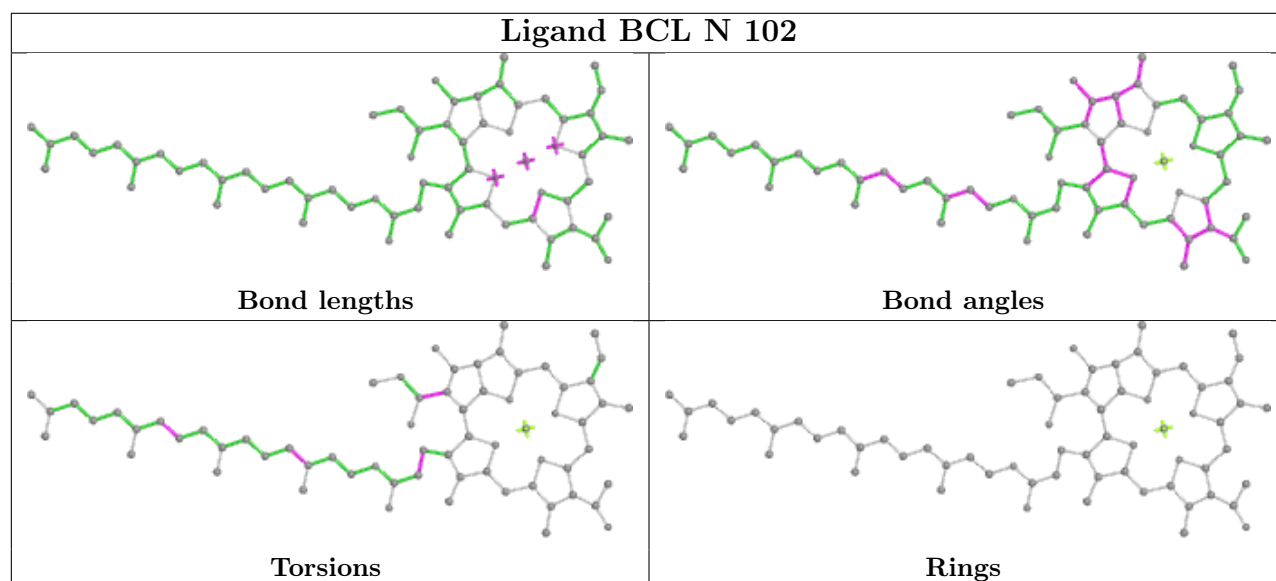
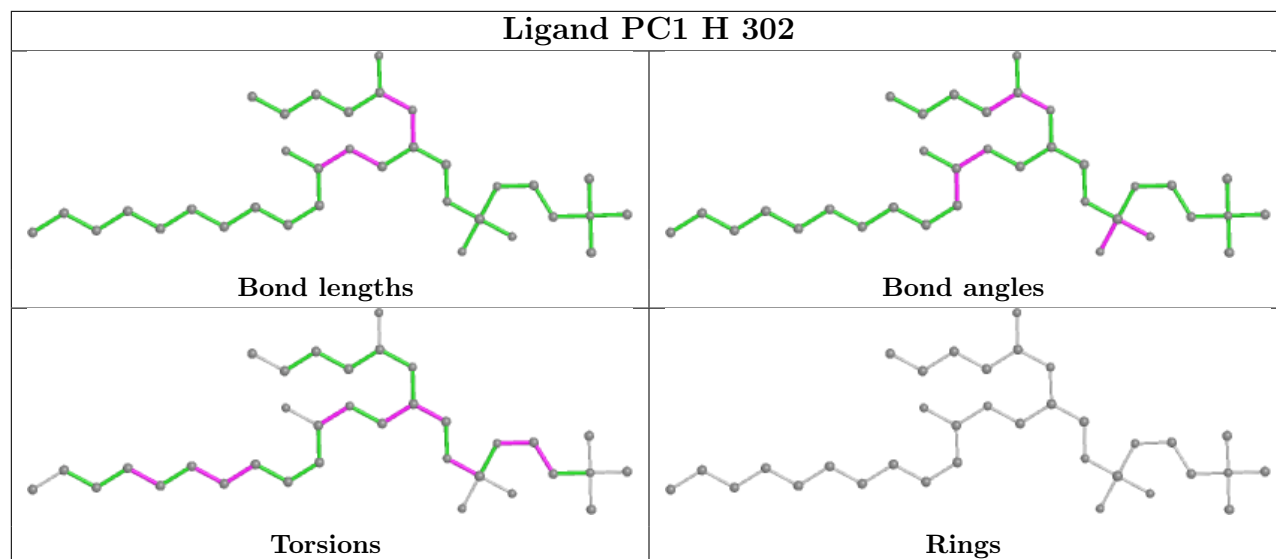


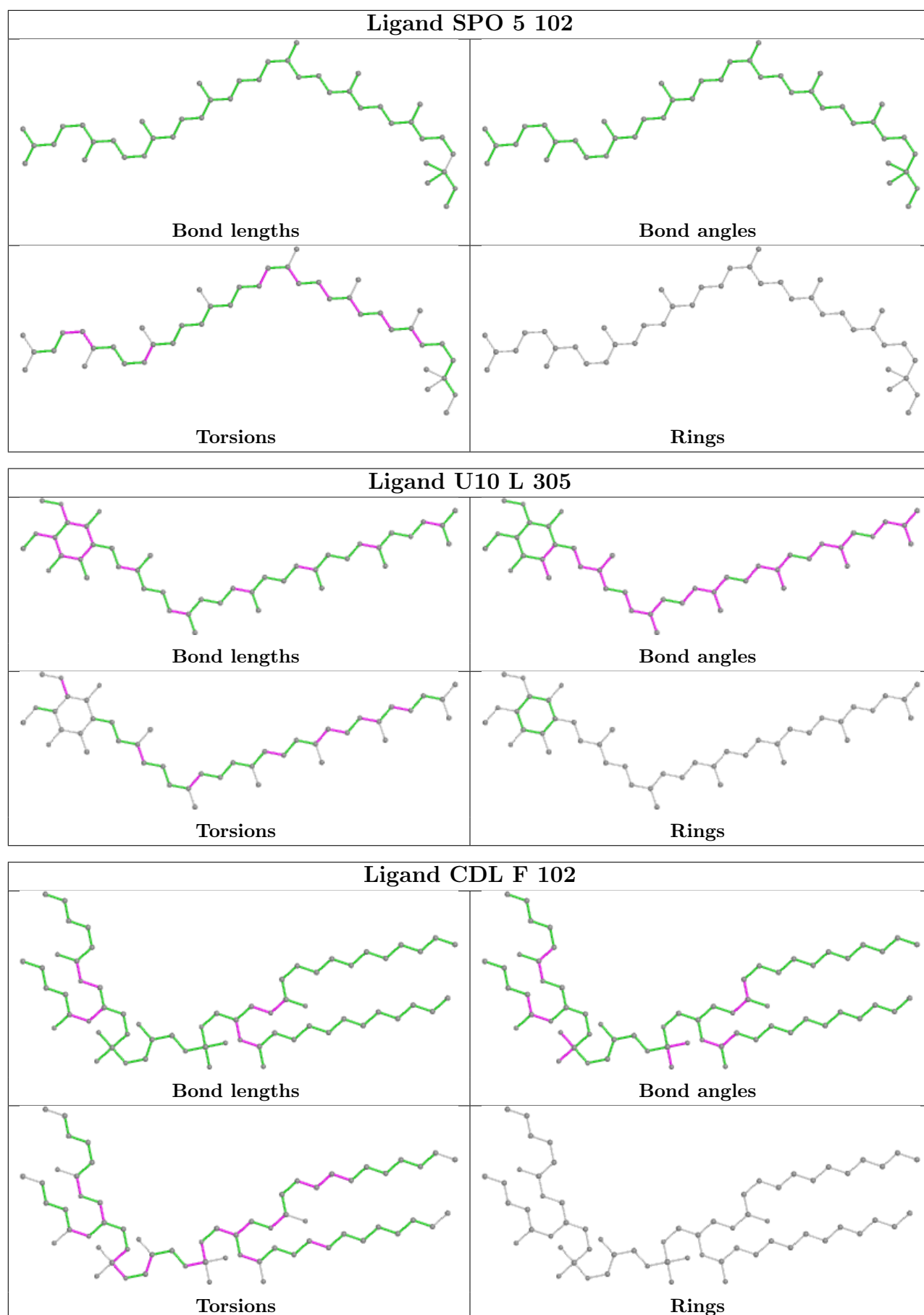


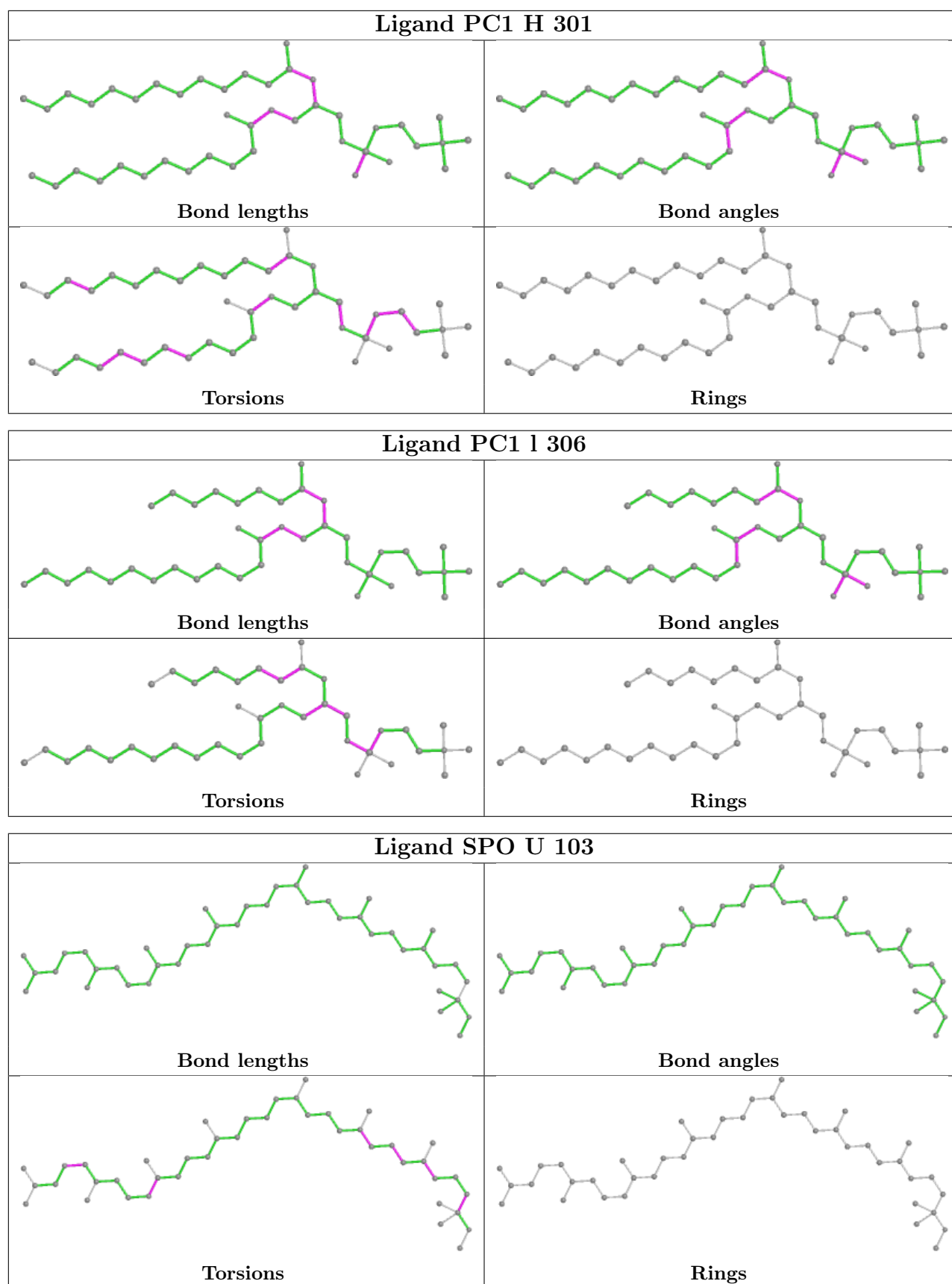


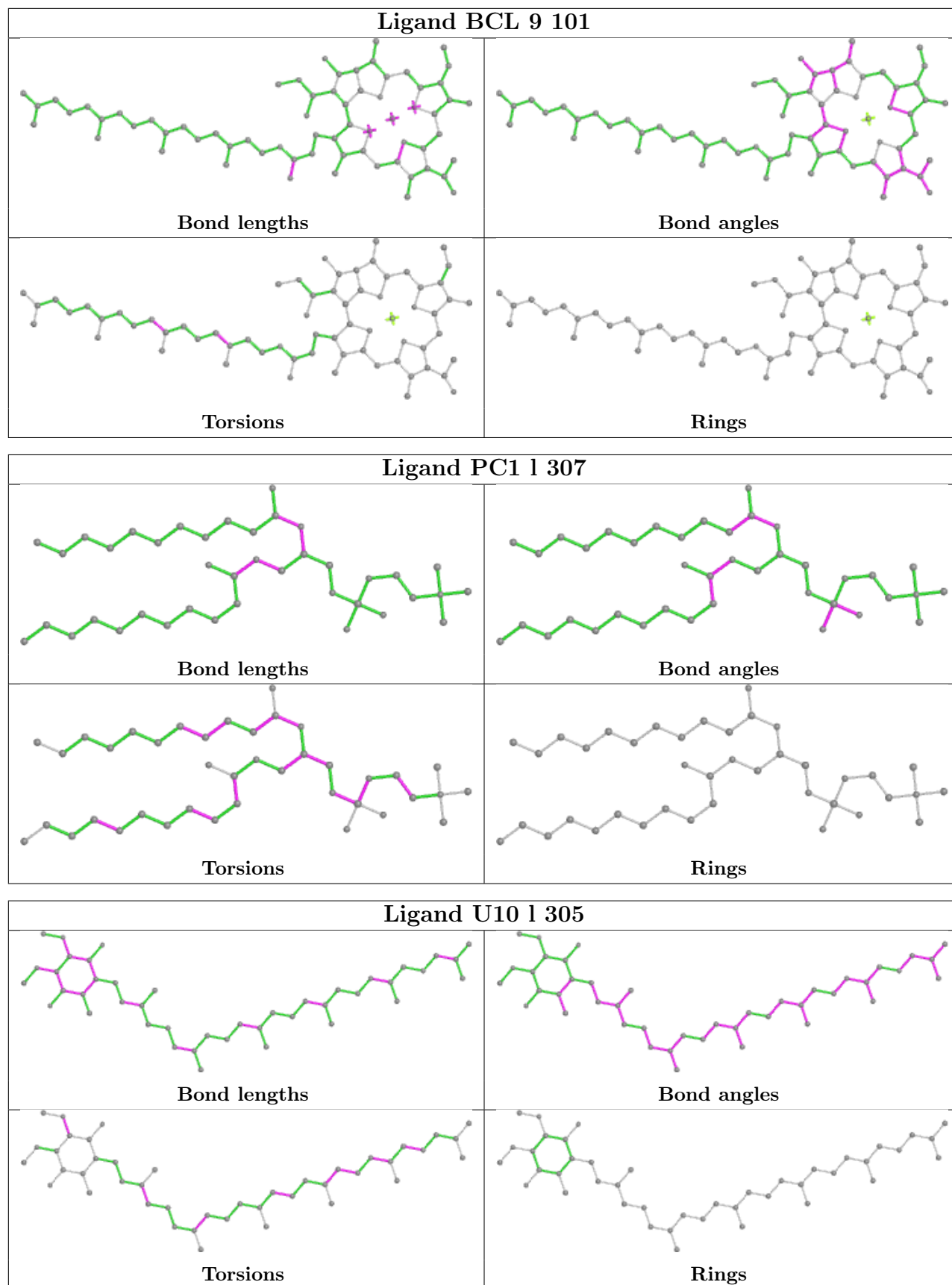


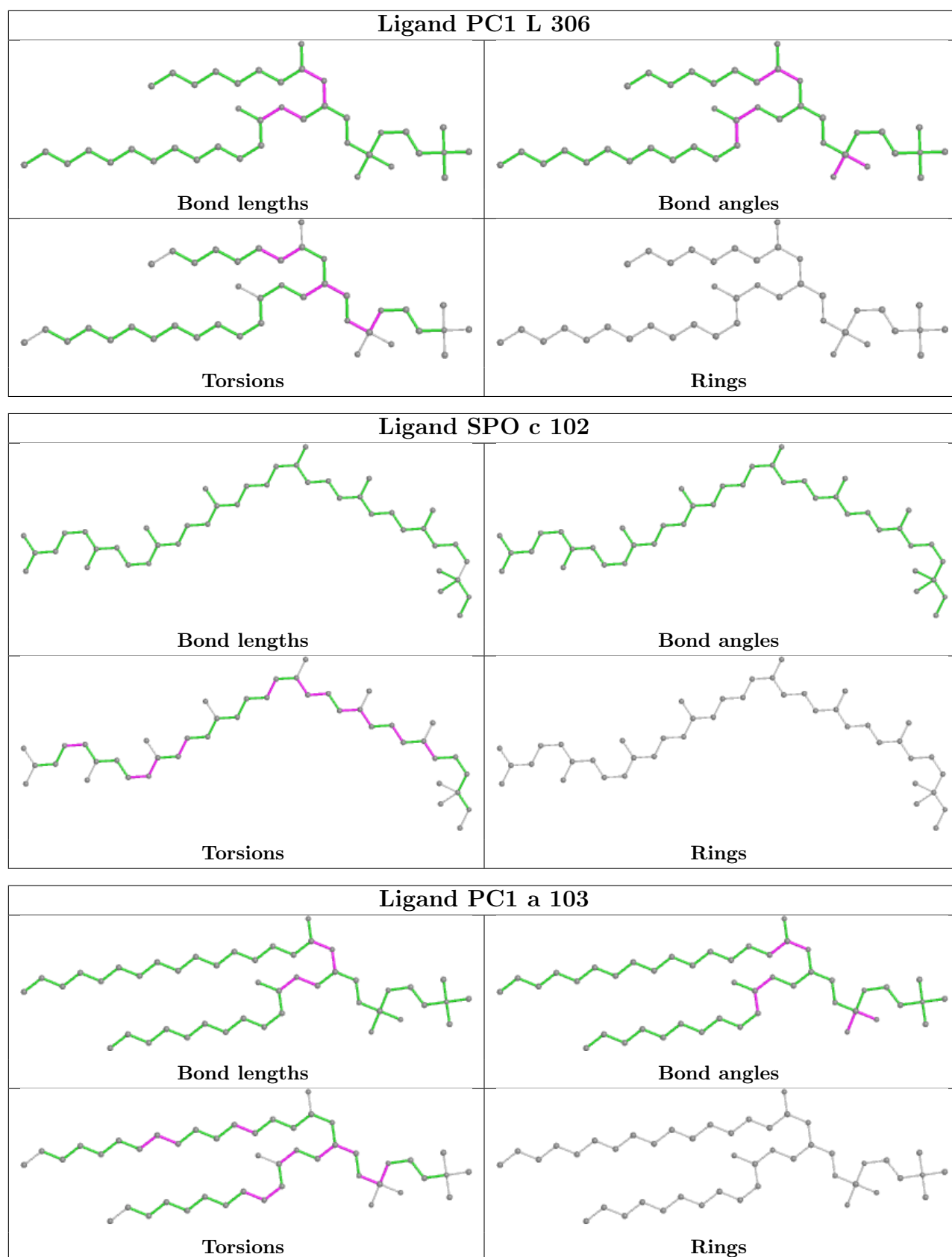












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

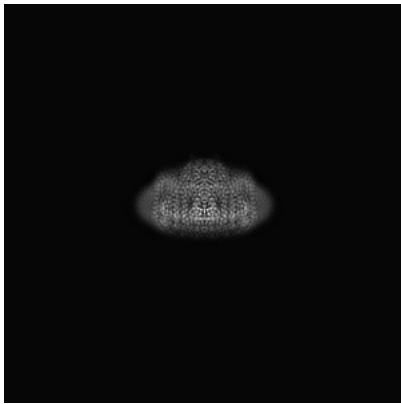
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32058. These allow visual inspection of the internal detail of the map and identification of artifacts.

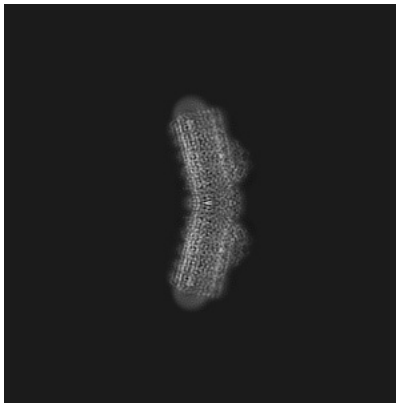
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

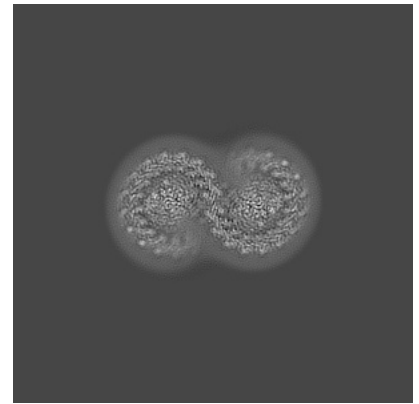
6.1.1 Primary map



X



Y

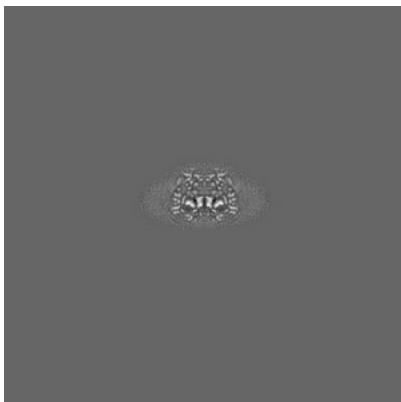


Z

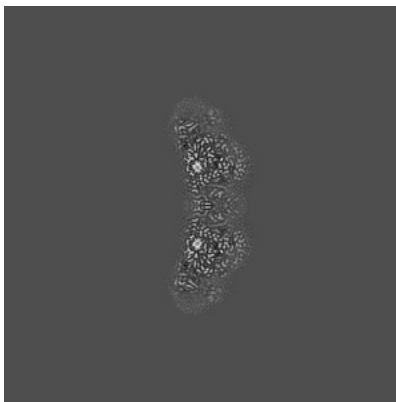
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

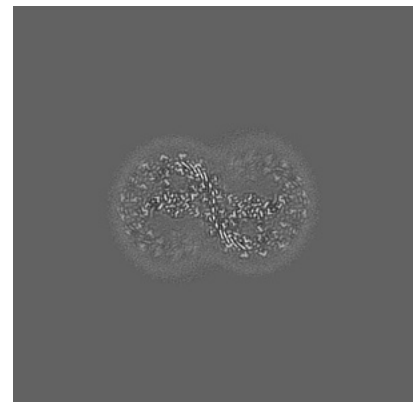
6.2.1 Primary map



X Index: 208



Y Index: 208

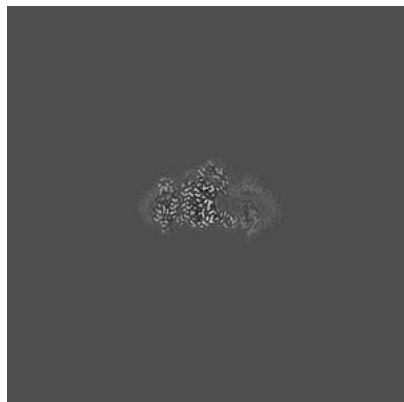


Z Index: 208

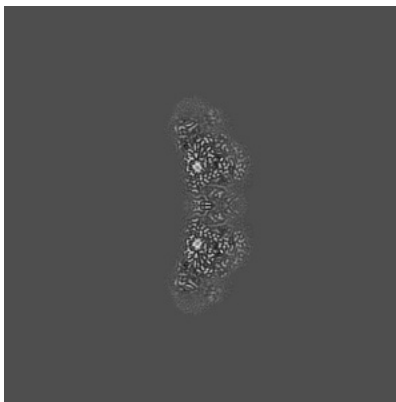
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

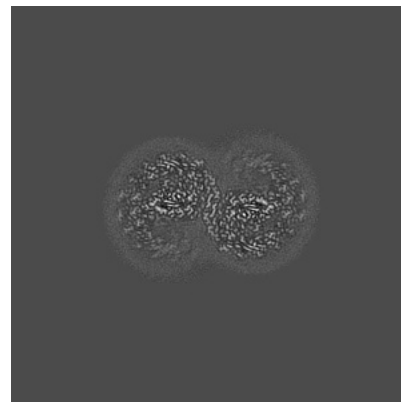
6.3.1 Primary map



X Index: 257



Y Index: 208

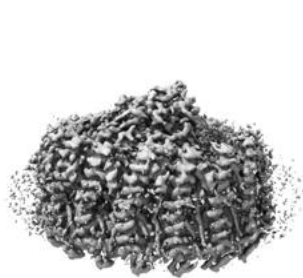


Z Index: 202

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

6.4 Orthogonal surface views [i](#)

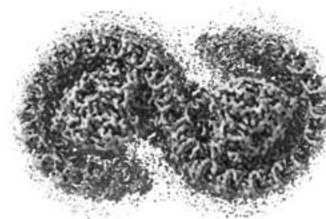
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

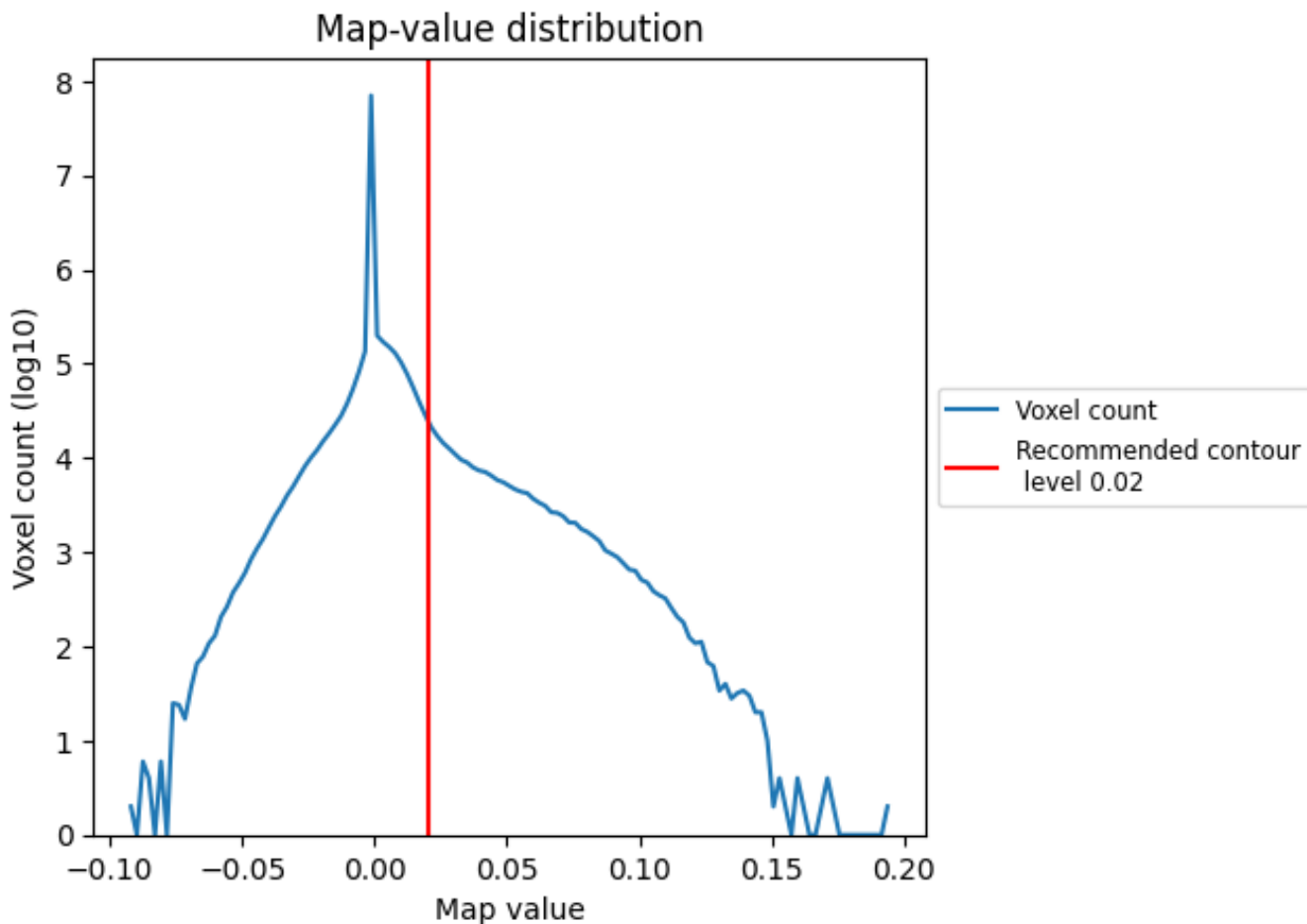
6.5 Mask visualisation

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

7 Map analysis [i](#)

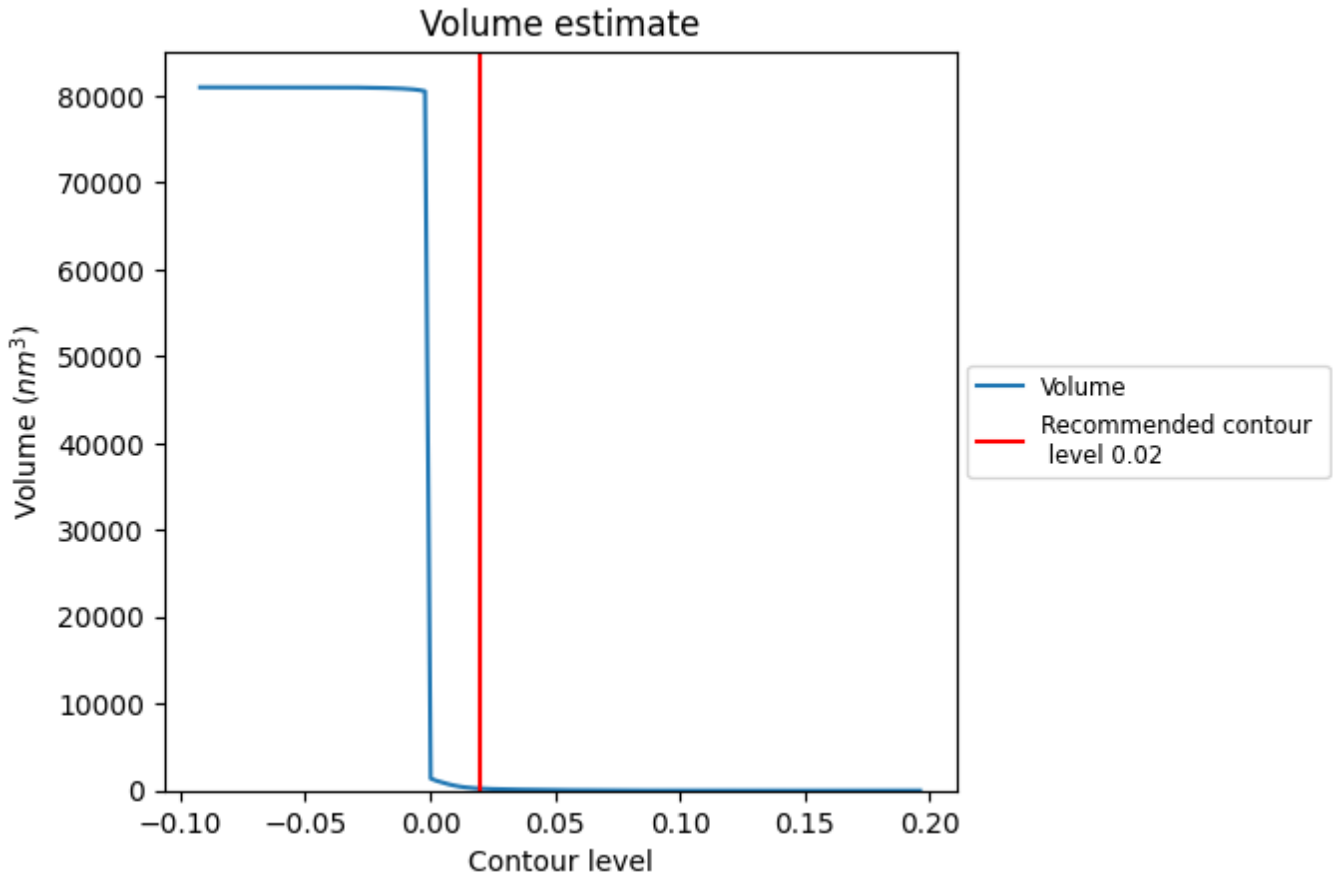
This section contains the results of statistical analysis of the map.

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.

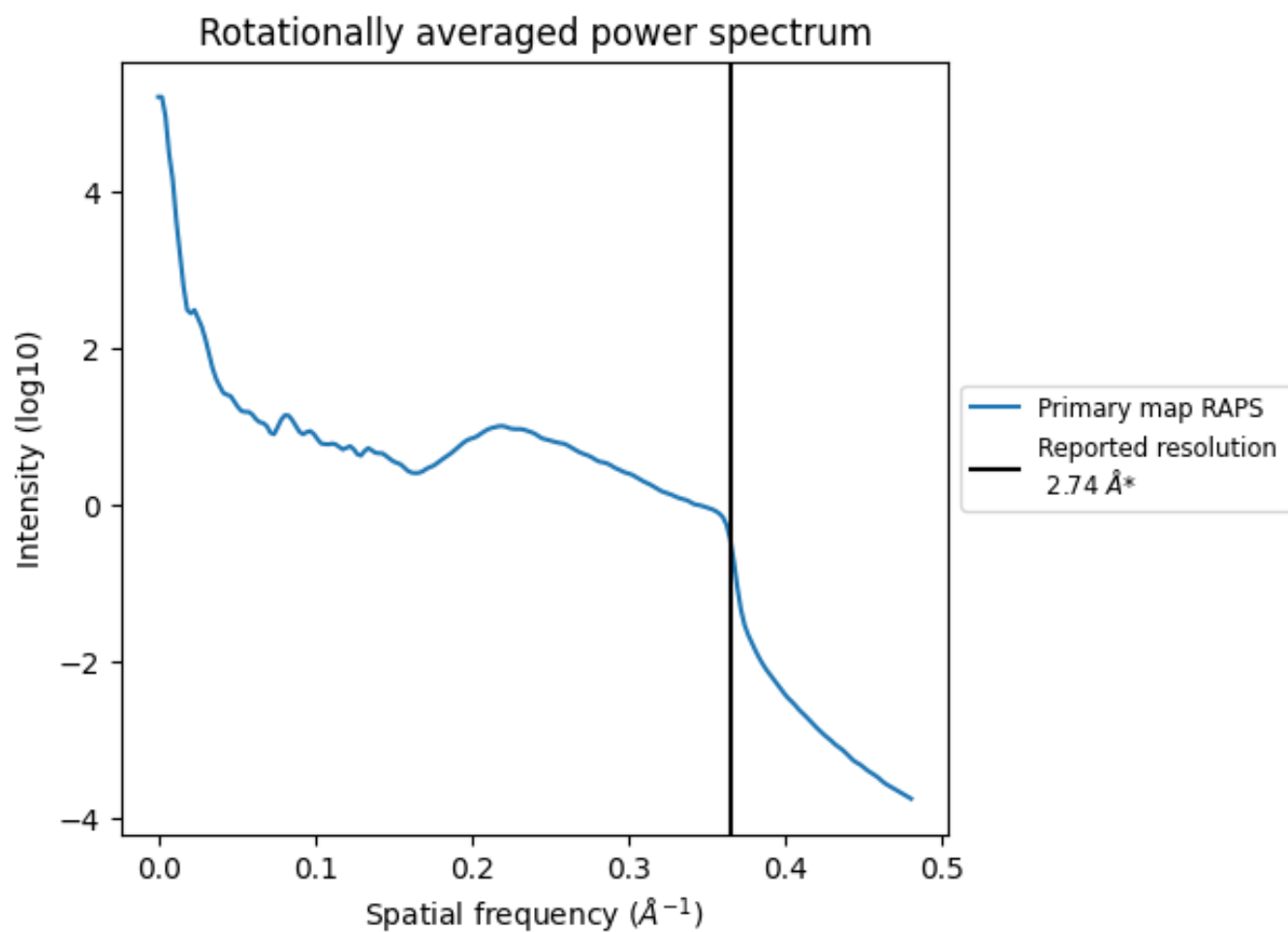
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm³; this corresponds to an approximate mass of 211 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.365\AA^{-1}

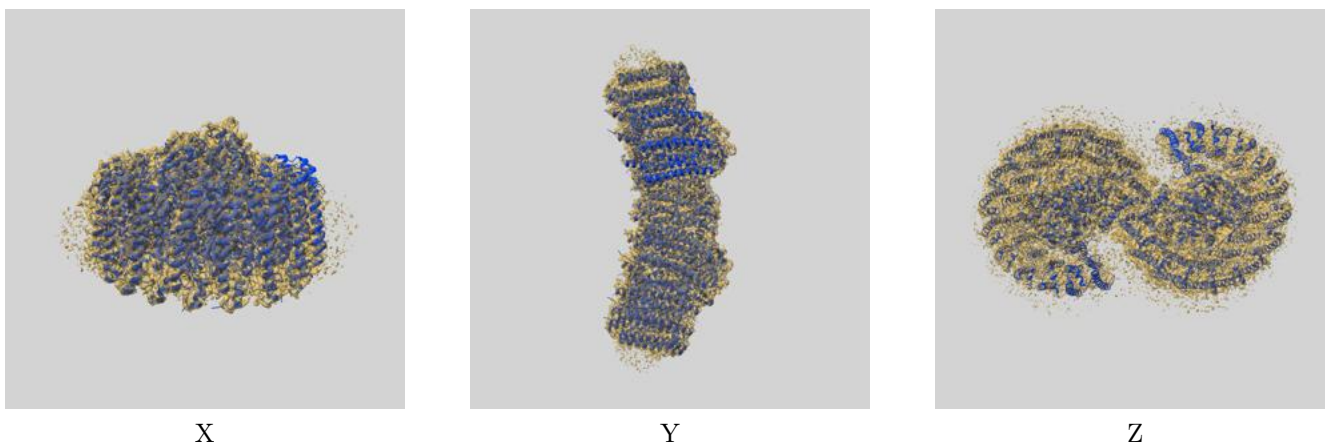
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32058 and PDB model 7VOR. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

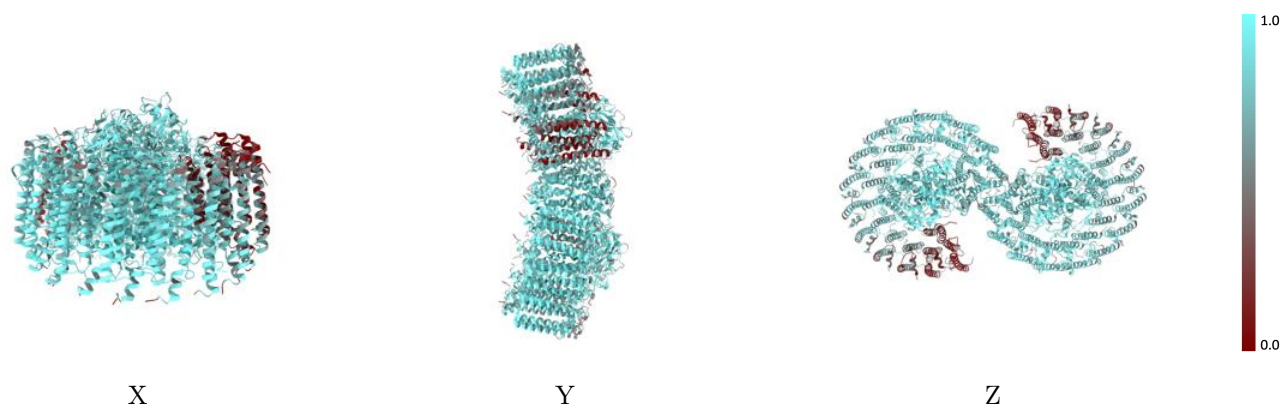


The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

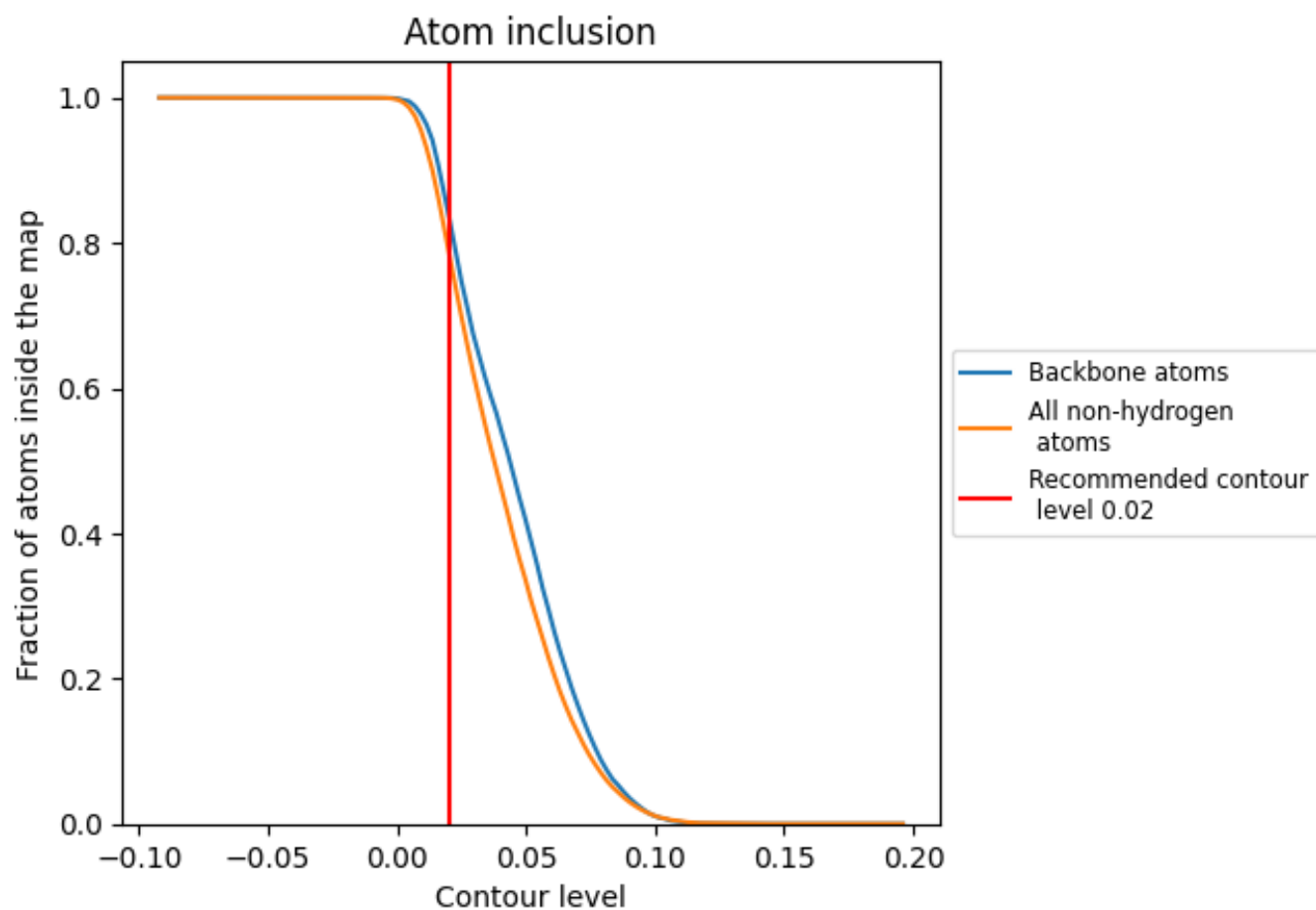
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).




































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion |
|-------|--|
| All |  0.7893 |
| 0 |  0.8736 |
| 1 |  0.2547 |
| 2 |  0.1715 |
| 3 |  0.3645 |
| 4 |  0.1715 |
| 5 |  0.3662 |
| 6 |  0.9057 |
| 7 |  0.9057 |
| 8 |  0.8949 |
| 9 |  0.9295 |
| A |  0.8981 |
| B |  0.8684 |
| C |  0.4598 |
| D |  0.8868 |
| E |  0.8653 |
| F |  0.8467 |
| G |  0.8052 |
| H |  0.8449 |
| I |  0.8631 |
| J |  0.8080 |
| K |  0.8250 |
| L |  0.9387 |
| M |  0.9358 |
| N |  0.7932 |
| O |  0.8139 |
| P |  0.7857 |
| Q |  0.8132 |
| R |  0.7857 |
| S |  0.7798 |
| T |  0.7688 |
| U |  0.7096 |
| V |  0.6583 |
| W |  0.5606 |
| X |  0.8082 |



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| Chain | Atom inclusion |
|-------|--|
| Y |  0.2151 |
| Z |  0.2861 |
| a |  0.8981 |
| b |  0.8662 |
| b0 |  0.8714 |
| b1 |  0.2571 |
| b8 |  0.8949 |
| b9 |  0.9259 |
| c |  0.4575 |
| d |  0.8834 |
| e |  0.8612 |
| f |  0.8484 |
| g |  0.8072 |
| h |  0.8424 |
| i |  0.8650 |
| j |  0.8080 |
| k |  0.8250 |
| l |  0.9383 |
| m |  0.9354 |
| n |  0.7955 |
| o |  0.8139 |
| p |  0.7857 |
| q |  0.8163 |
| r |  0.7833 |
| s |  0.7815 |
| t |  0.7714 |
| u |  0.7079 |
| v |  0.6608 |
| w |  0.5586 |
| x |  0.8082 |
| y |  0.2151 |
| z |  0.2835 |