



Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 07:48 AM EST

PDB ID : 6WKV
EMDB ID : EMD-21810
Title : Cryo-EM structure of engineered variant of the Encapsulin from *Thermotoga maritima* (TmE)
Authors : Williams, E.; Jenkins, M.; Zhao, H.; Juneja, P.; Lutz, S.
Deposited on : 2020-04-17
Resolution : 2.99 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:

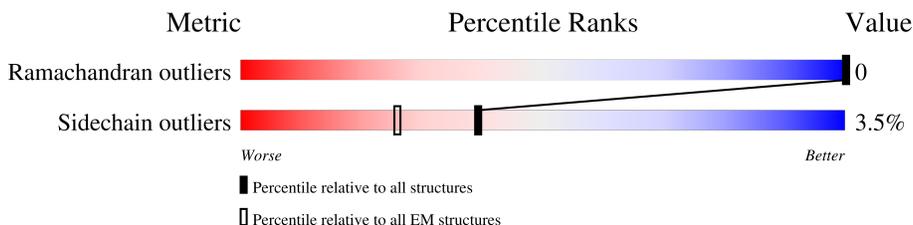
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.99 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.



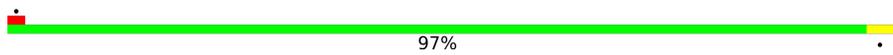
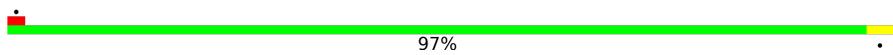
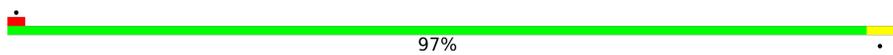
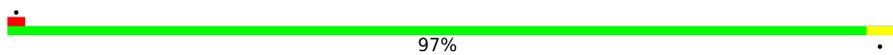
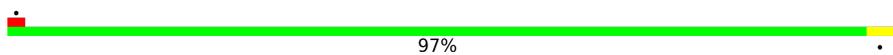
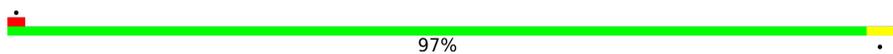
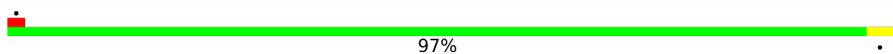
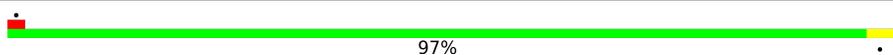
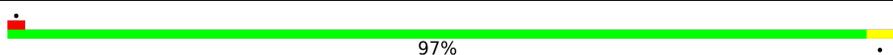
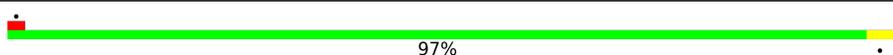
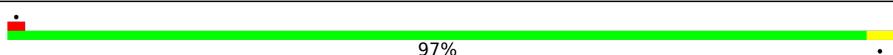
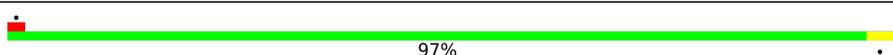
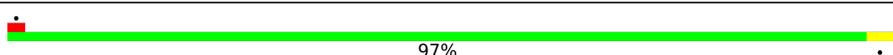
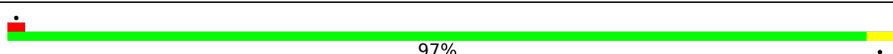
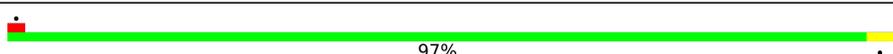
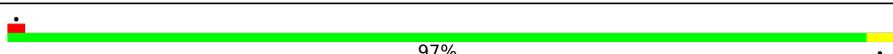
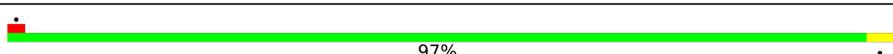
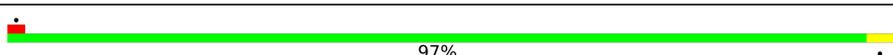
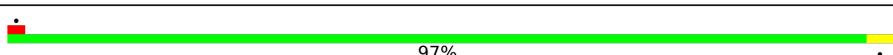
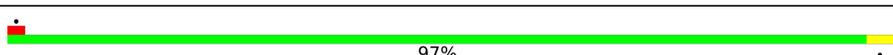
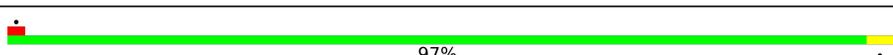
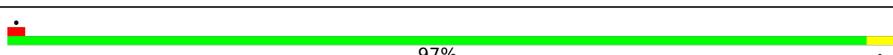
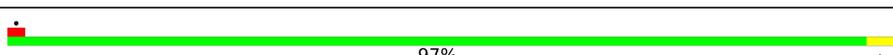
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | 0 | 258 | 97% . |
| 1 | 1 | 258 | 97% . |
| 1 | 2 | 258 | 97% . |
| 1 | 3 | 258 | 97% . |
| 1 | 4 | 258 | 97% . |
| 1 | 5 | 258 | 97% . |
| 1 | 6 | 258 | 97% . |
| 1 | 7 | 258 | 97% . |
| 1 | 8 | 258 | 97% . |

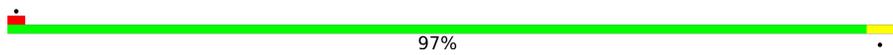
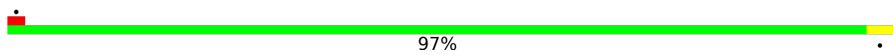
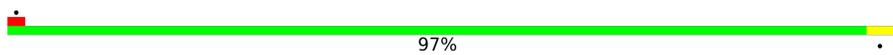
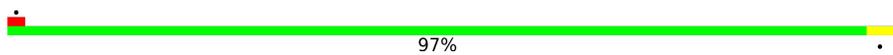
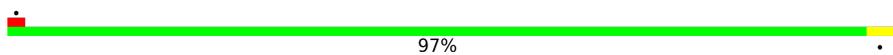
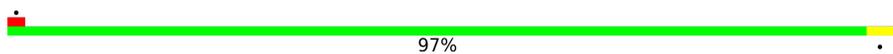
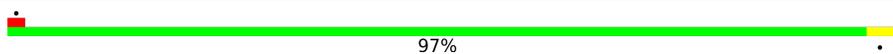
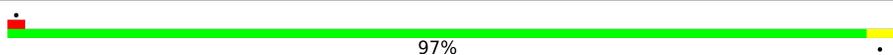
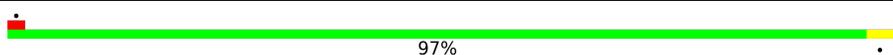
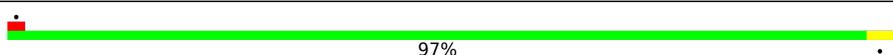
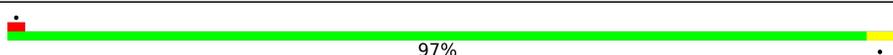
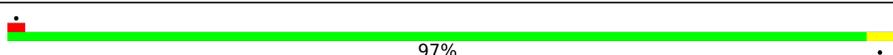
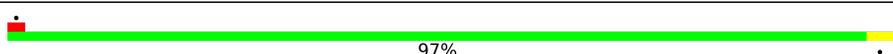
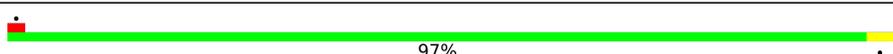
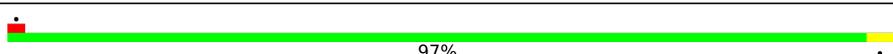
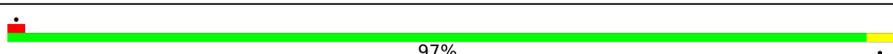
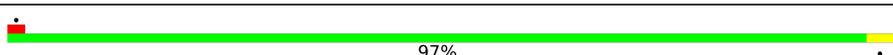
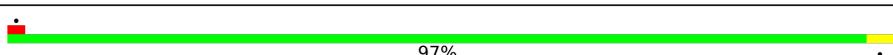
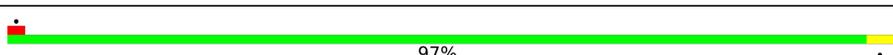
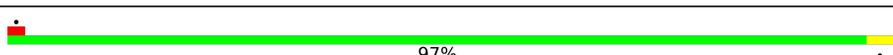
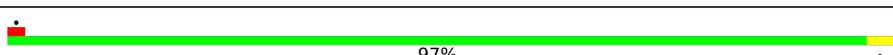
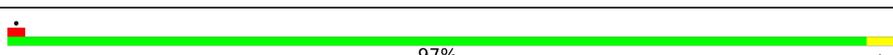
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 9 | 258 |  97% |
| 1 | A | 258 |  97% |
| 1 | B | 258 |  97% |
| 1 | C | 258 |  97% |
| 1 | D | 258 |  97% |
| 1 | E | 258 |  97% |
| 1 | F | 258 |  97% |
| 1 | G | 258 |  97% |
| 1 | H | 258 |  97% |
| 1 | I | 258 |  97% |
| 1 | J | 258 |  97% |
| 1 | K | 258 |  97% |
| 1 | L | 258 |  97% |
| 1 | M | 258 |  97% |
| 1 | N | 258 |  97% |
| 1 | O | 258 |  97% |
| 1 | P | 258 |  97% |
| 1 | Q | 258 |  97% |
| 1 | R | 258 |  97% |
| 1 | S | 258 |  97% |
| 1 | T | 258 |  97% |
| 1 | U | 258 |  97% |
| 1 | V | 258 |  97% |
| 1 | W | 258 |  97% |
| 1 | X | 258 |  97% |

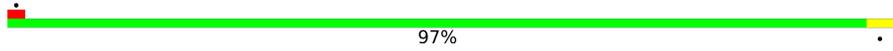
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | Y | 258 |  97% |
| 1 | Z | 258 |  97% |
| 1 | a | 258 |  97% |
| 1 | b | 258 |  97% |
| 1 | c | 258 |  97% |
| 1 | d | 258 |  97% |
| 1 | e | 258 |  97% |
| 1 | f | 258 |  97% |
| 1 | g | 258 |  97% |
| 1 | h | 258 |  97% |
| 1 | i | 258 |  97% |
| 1 | j | 258 |  97% |
| 1 | k | 258 |  97% |
| 1 | l | 258 |  97% |
| 1 | m | 258 |  97% |
| 1 | n | 258 |  97% |
| 1 | o | 258 |  97% |
| 1 | p | 258 |  97% |
| 1 | q | 258 |  97% |
| 1 | r | 258 |  97% |
| 1 | s | 258 |  97% |
| 1 | t | 258 |  97% |
| 1 | u | 258 |  97% |
| 1 | v | 258 |  97% |
| 1 | w | 258 |  97% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | x | 258 |  97% |

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 127740 atoms, of which 1140 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 Encapsulin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | B | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | C | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | D | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | E | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | F | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | G | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | H | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | I | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | J | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | K | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | L | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | M | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | N | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | O | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | P | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |
| 1 | Q | 257 | 2079 | 1333 | 348 | 395 | 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1 | R | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | S | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | T | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | U | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | V | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | W | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | X | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | Y | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | Z | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 0 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 1 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 2 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 3 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 4 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 5 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 6 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 7 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 8 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | 9 | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | a | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |
| 1 | b | 257 | Total 2079 | C 1333 | N 348 | O 395 | S 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | c | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | d | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | e | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | f | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | g | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | h | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | i | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | j | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | k | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | l | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | m | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | n | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | o | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | p | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | q | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | r | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | s | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | t | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | u | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | v | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |
| 1 | w | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | x | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1333 | 348 | 395 | 3 | | |

There are 540 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| A | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| A | ? | - | GLU | deletion | UNP Q9WZP2 |
| A | ? | - | ALA | deletion | UNP Q9WZP2 |
| A | ? | - | GLY | deletion | UNP Q9WZP2 |
| A | ? | - | HIS | deletion | UNP Q9WZP2 |
| A | ? | - | TYR | deletion | UNP Q9WZP2 |
| A | ? | - | PRO | deletion | UNP Q9WZP2 |
| A | ? | - | LEU | deletion | UNP Q9WZP2 |
| B | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| B | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| B | ? | - | GLU | deletion | UNP Q9WZP2 |
| B | ? | - | ALA | deletion | UNP Q9WZP2 |
| B | ? | - | GLY | deletion | UNP Q9WZP2 |
| B | ? | - | HIS | deletion | UNP Q9WZP2 |
| B | ? | - | TYR | deletion | UNP Q9WZP2 |
| B | ? | - | PRO | deletion | UNP Q9WZP2 |
| B | ? | - | LEU | deletion | UNP Q9WZP2 |
| C | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| C | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| C | ? | - | GLU | deletion | UNP Q9WZP2 |
| C | ? | - | ALA | deletion | UNP Q9WZP2 |
| C | ? | - | GLY | deletion | UNP Q9WZP2 |
| C | ? | - | HIS | deletion | UNP Q9WZP2 |
| C | ? | - | TYR | deletion | UNP Q9WZP2 |
| C | ? | - | PRO | deletion | UNP Q9WZP2 |
| C | ? | - | LEU | deletion | UNP Q9WZP2 |
| D | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| D | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| D | ? | - | GLU | deletion | UNP Q9WZP2 |
| D | ? | - | ALA | deletion | UNP Q9WZP2 |
| D | ? | - | GLY | deletion | UNP Q9WZP2 |
| D | ? | - | HIS | deletion | UNP Q9WZP2 |
| D | ? | - | TYR | deletion | UNP Q9WZP2 |
| D | ? | - | PRO | deletion | UNP Q9WZP2 |
| D | ? | - | LEU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| E | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| E | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| E | ? | - | GLU | deletion | UNP Q9WZP2 |
| E | ? | - | ALA | deletion | UNP Q9WZP2 |
| E | ? | - | GLY | deletion | UNP Q9WZP2 |
| E | ? | - | HIS | deletion | UNP Q9WZP2 |
| E | ? | - | TYR | deletion | UNP Q9WZP2 |
| E | ? | - | PRO | deletion | UNP Q9WZP2 |
| E | ? | - | LEU | deletion | UNP Q9WZP2 |
| F | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| F | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| F | ? | - | GLU | deletion | UNP Q9WZP2 |
| F | ? | - | ALA | deletion | UNP Q9WZP2 |
| F | ? | - | GLY | deletion | UNP Q9WZP2 |
| F | ? | - | HIS | deletion | UNP Q9WZP2 |
| F | ? | - | TYR | deletion | UNP Q9WZP2 |
| F | ? | - | PRO | deletion | UNP Q9WZP2 |
| F | ? | - | LEU | deletion | UNP Q9WZP2 |
| G | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| G | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| G | ? | - | GLU | deletion | UNP Q9WZP2 |
| G | ? | - | ALA | deletion | UNP Q9WZP2 |
| G | ? | - | GLY | deletion | UNP Q9WZP2 |
| G | ? | - | HIS | deletion | UNP Q9WZP2 |
| G | ? | - | TYR | deletion | UNP Q9WZP2 |
| G | ? | - | PRO | deletion | UNP Q9WZP2 |
| G | ? | - | LEU | deletion | UNP Q9WZP2 |
| H | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| H | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| H | ? | - | GLU | deletion | UNP Q9WZP2 |
| H | ? | - | ALA | deletion | UNP Q9WZP2 |
| H | ? | - | GLY | deletion | UNP Q9WZP2 |
| H | ? | - | HIS | deletion | UNP Q9WZP2 |
| H | ? | - | TYR | deletion | UNP Q9WZP2 |
| H | ? | - | PRO | deletion | UNP Q9WZP2 |
| H | ? | - | LEU | deletion | UNP Q9WZP2 |
| I | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| I | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| I | ? | - | GLU | deletion | UNP Q9WZP2 |
| I | ? | - | ALA | deletion | UNP Q9WZP2 |
| I | ? | - | GLY | deletion | UNP Q9WZP2 |
| I | ? | - | HIS | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| I | ? | - | TYR | deletion | UNP Q9WZP2 |
| I | ? | - | PRO | deletion | UNP Q9WZP2 |
| I | ? | - | LEU | deletion | UNP Q9WZP2 |
| J | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| J | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| J | ? | - | GLU | deletion | UNP Q9WZP2 |
| J | ? | - | ALA | deletion | UNP Q9WZP2 |
| J | ? | - | GLY | deletion | UNP Q9WZP2 |
| J | ? | - | HIS | deletion | UNP Q9WZP2 |
| J | ? | - | TYR | deletion | UNP Q9WZP2 |
| J | ? | - | PRO | deletion | UNP Q9WZP2 |
| J | ? | - | LEU | deletion | UNP Q9WZP2 |
| K | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| K | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| K | ? | - | GLU | deletion | UNP Q9WZP2 |
| K | ? | - | ALA | deletion | UNP Q9WZP2 |
| K | ? | - | GLY | deletion | UNP Q9WZP2 |
| K | ? | - | HIS | deletion | UNP Q9WZP2 |
| K | ? | - | TYR | deletion | UNP Q9WZP2 |
| K | ? | - | PRO | deletion | UNP Q9WZP2 |
| K | ? | - | LEU | deletion | UNP Q9WZP2 |
| L | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| L | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| L | ? | - | GLU | deletion | UNP Q9WZP2 |
| L | ? | - | ALA | deletion | UNP Q9WZP2 |
| L | ? | - | GLY | deletion | UNP Q9WZP2 |
| L | ? | - | HIS | deletion | UNP Q9WZP2 |
| L | ? | - | TYR | deletion | UNP Q9WZP2 |
| L | ? | - | PRO | deletion | UNP Q9WZP2 |
| L | ? | - | LEU | deletion | UNP Q9WZP2 |
| M | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| M | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| M | ? | - | GLU | deletion | UNP Q9WZP2 |
| M | ? | - | ALA | deletion | UNP Q9WZP2 |
| M | ? | - | GLY | deletion | UNP Q9WZP2 |
| M | ? | - | HIS | deletion | UNP Q9WZP2 |
| M | ? | - | TYR | deletion | UNP Q9WZP2 |
| M | ? | - | PRO | deletion | UNP Q9WZP2 |
| M | ? | - | LEU | deletion | UNP Q9WZP2 |
| N | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| N | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| N | ? | - | GLU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| N | ? | - | ALA | deletion | UNP Q9WZP2 |
| N | ? | - | GLY | deletion | UNP Q9WZP2 |
| N | ? | - | HIS | deletion | UNP Q9WZP2 |
| N | ? | - | TYR | deletion | UNP Q9WZP2 |
| N | ? | - | PRO | deletion | UNP Q9WZP2 |
| N | ? | - | LEU | deletion | UNP Q9WZP2 |
| O | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| O | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| O | ? | - | GLU | deletion | UNP Q9WZP2 |
| O | ? | - | ALA | deletion | UNP Q9WZP2 |
| O | ? | - | GLY | deletion | UNP Q9WZP2 |
| O | ? | - | HIS | deletion | UNP Q9WZP2 |
| O | ? | - | TYR | deletion | UNP Q9WZP2 |
| O | ? | - | PRO | deletion | UNP Q9WZP2 |
| O | ? | - | LEU | deletion | UNP Q9WZP2 |
| P | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| P | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| P | ? | - | GLU | deletion | UNP Q9WZP2 |
| P | ? | - | ALA | deletion | UNP Q9WZP2 |
| P | ? | - | GLY | deletion | UNP Q9WZP2 |
| P | ? | - | HIS | deletion | UNP Q9WZP2 |
| P | ? | - | TYR | deletion | UNP Q9WZP2 |
| P | ? | - | PRO | deletion | UNP Q9WZP2 |
| P | ? | - | LEU | deletion | UNP Q9WZP2 |
| Q | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| Q | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| Q | ? | - | GLU | deletion | UNP Q9WZP2 |
| Q | ? | - | ALA | deletion | UNP Q9WZP2 |
| Q | ? | - | GLY | deletion | UNP Q9WZP2 |
| Q | ? | - | HIS | deletion | UNP Q9WZP2 |
| Q | ? | - | TYR | deletion | UNP Q9WZP2 |
| Q | ? | - | PRO | deletion | UNP Q9WZP2 |
| Q | ? | - | LEU | deletion | UNP Q9WZP2 |
| R | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| R | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| R | ? | - | GLU | deletion | UNP Q9WZP2 |
| R | ? | - | ALA | deletion | UNP Q9WZP2 |
| R | ? | - | GLY | deletion | UNP Q9WZP2 |
| R | ? | - | HIS | deletion | UNP Q9WZP2 |
| R | ? | - | TYR | deletion | UNP Q9WZP2 |
| R | ? | - | PRO | deletion | UNP Q9WZP2 |
| R | ? | - | LEU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| S | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| S | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| S | ? | - | GLU | deletion | UNP Q9WZP2 |
| S | ? | - | ALA | deletion | UNP Q9WZP2 |
| S | ? | - | GLY | deletion | UNP Q9WZP2 |
| S | ? | - | HIS | deletion | UNP Q9WZP2 |
| S | ? | - | TYR | deletion | UNP Q9WZP2 |
| S | ? | - | PRO | deletion | UNP Q9WZP2 |
| S | ? | - | LEU | deletion | UNP Q9WZP2 |
| T | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| T | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| T | ? | - | GLU | deletion | UNP Q9WZP2 |
| T | ? | - | ALA | deletion | UNP Q9WZP2 |
| T | ? | - | GLY | deletion | UNP Q9WZP2 |
| T | ? | - | HIS | deletion | UNP Q9WZP2 |
| T | ? | - | TYR | deletion | UNP Q9WZP2 |
| T | ? | - | PRO | deletion | UNP Q9WZP2 |
| T | ? | - | LEU | deletion | UNP Q9WZP2 |
| U | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| U | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| U | ? | - | GLU | deletion | UNP Q9WZP2 |
| U | ? | - | ALA | deletion | UNP Q9WZP2 |
| U | ? | - | GLY | deletion | UNP Q9WZP2 |
| U | ? | - | HIS | deletion | UNP Q9WZP2 |
| U | ? | - | TYR | deletion | UNP Q9WZP2 |
| U | ? | - | PRO | deletion | UNP Q9WZP2 |
| U | ? | - | LEU | deletion | UNP Q9WZP2 |
| V | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| V | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| V | ? | - | GLU | deletion | UNP Q9WZP2 |
| V | ? | - | ALA | deletion | UNP Q9WZP2 |
| V | ? | - | GLY | deletion | UNP Q9WZP2 |
| V | ? | - | HIS | deletion | UNP Q9WZP2 |
| V | ? | - | TYR | deletion | UNP Q9WZP2 |
| V | ? | - | PRO | deletion | UNP Q9WZP2 |
| V | ? | - | LEU | deletion | UNP Q9WZP2 |
| W | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| W | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| W | ? | - | GLU | deletion | UNP Q9WZP2 |
| W | ? | - | ALA | deletion | UNP Q9WZP2 |
| W | ? | - | GLY | deletion | UNP Q9WZP2 |
| W | ? | - | HIS | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| W | ? | - | TYR | deletion | UNP Q9WZP2 |
| W | ? | - | PRO | deletion | UNP Q9WZP2 |
| W | ? | - | LEU | deletion | UNP Q9WZP2 |
| X | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| X | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| X | ? | - | GLU | deletion | UNP Q9WZP2 |
| X | ? | - | ALA | deletion | UNP Q9WZP2 |
| X | ? | - | GLY | deletion | UNP Q9WZP2 |
| X | ? | - | HIS | deletion | UNP Q9WZP2 |
| X | ? | - | TYR | deletion | UNP Q9WZP2 |
| X | ? | - | PRO | deletion | UNP Q9WZP2 |
| X | ? | - | LEU | deletion | UNP Q9WZP2 |
| Y | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| Y | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| Y | ? | - | GLU | deletion | UNP Q9WZP2 |
| Y | ? | - | ALA | deletion | UNP Q9WZP2 |
| Y | ? | - | GLY | deletion | UNP Q9WZP2 |
| Y | ? | - | HIS | deletion | UNP Q9WZP2 |
| Y | ? | - | TYR | deletion | UNP Q9WZP2 |
| Y | ? | - | PRO | deletion | UNP Q9WZP2 |
| Y | ? | - | LEU | deletion | UNP Q9WZP2 |
| Z | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| Z | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| Z | ? | - | GLU | deletion | UNP Q9WZP2 |
| Z | ? | - | ALA | deletion | UNP Q9WZP2 |
| Z | ? | - | GLY | deletion | UNP Q9WZP2 |
| Z | ? | - | HIS | deletion | UNP Q9WZP2 |
| Z | ? | - | TYR | deletion | UNP Q9WZP2 |
| Z | ? | - | PRO | deletion | UNP Q9WZP2 |
| Z | ? | - | LEU | deletion | UNP Q9WZP2 |
| 0 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 0 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 0 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 0 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 0 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 0 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 0 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 0 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 0 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 1 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 1 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 1 | ? | - | GLU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 1 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 1 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 1 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 1 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 1 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 1 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 2 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 2 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 2 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 2 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 2 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 2 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 2 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 2 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 2 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 3 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 3 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 3 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 3 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 3 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 3 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 3 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 3 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 3 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 4 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 4 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 4 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 4 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 4 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 4 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 4 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 4 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 4 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 5 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 5 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 5 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 5 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 5 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 5 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 5 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 5 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 5 | ? | - | LEU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 6 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 6 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 6 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 6 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 6 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 6 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 6 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 6 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 6 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 7 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 7 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 7 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 7 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 7 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 7 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 7 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 7 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 7 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 8 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 8 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 8 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 8 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 8 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 8 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 8 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 8 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 8 | ? | - | LEU | deletion | UNP Q9WZP2 |
| 9 | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| 9 | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| 9 | ? | - | GLU | deletion | UNP Q9WZP2 |
| 9 | ? | - | ALA | deletion | UNP Q9WZP2 |
| 9 | ? | - | GLY | deletion | UNP Q9WZP2 |
| 9 | ? | - | HIS | deletion | UNP Q9WZP2 |
| 9 | ? | - | TYR | deletion | UNP Q9WZP2 |
| 9 | ? | - | PRO | deletion | UNP Q9WZP2 |
| 9 | ? | - | LEU | deletion | UNP Q9WZP2 |
| a | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| a | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| a | ? | - | GLU | deletion | UNP Q9WZP2 |
| a | ? | - | ALA | deletion | UNP Q9WZP2 |
| a | ? | - | GLY | deletion | UNP Q9WZP2 |
| a | ? | - | HIS | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| a | ? | - | TYR | deletion | UNP Q9WZP2 |
| a | ? | - | PRO | deletion | UNP Q9WZP2 |
| a | ? | - | LEU | deletion | UNP Q9WZP2 |
| b | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| b | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| b | ? | - | GLU | deletion | UNP Q9WZP2 |
| b | ? | - | ALA | deletion | UNP Q9WZP2 |
| b | ? | - | GLY | deletion | UNP Q9WZP2 |
| b | ? | - | HIS | deletion | UNP Q9WZP2 |
| b | ? | - | TYR | deletion | UNP Q9WZP2 |
| b | ? | - | PRO | deletion | UNP Q9WZP2 |
| b | ? | - | LEU | deletion | UNP Q9WZP2 |
| c | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| c | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| c | ? | - | GLU | deletion | UNP Q9WZP2 |
| c | ? | - | ALA | deletion | UNP Q9WZP2 |
| c | ? | - | GLY | deletion | UNP Q9WZP2 |
| c | ? | - | HIS | deletion | UNP Q9WZP2 |
| c | ? | - | TYR | deletion | UNP Q9WZP2 |
| c | ? | - | PRO | deletion | UNP Q9WZP2 |
| c | ? | - | LEU | deletion | UNP Q9WZP2 |
| d | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| d | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| d | ? | - | GLU | deletion | UNP Q9WZP2 |
| d | ? | - | ALA | deletion | UNP Q9WZP2 |
| d | ? | - | GLY | deletion | UNP Q9WZP2 |
| d | ? | - | HIS | deletion | UNP Q9WZP2 |
| d | ? | - | TYR | deletion | UNP Q9WZP2 |
| d | ? | - | PRO | deletion | UNP Q9WZP2 |
| d | ? | - | LEU | deletion | UNP Q9WZP2 |
| e | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| e | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| e | ? | - | GLU | deletion | UNP Q9WZP2 |
| e | ? | - | ALA | deletion | UNP Q9WZP2 |
| e | ? | - | GLY | deletion | UNP Q9WZP2 |
| e | ? | - | HIS | deletion | UNP Q9WZP2 |
| e | ? | - | TYR | deletion | UNP Q9WZP2 |
| e | ? | - | PRO | deletion | UNP Q9WZP2 |
| e | ? | - | LEU | deletion | UNP Q9WZP2 |
| f | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| f | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| f | ? | - | GLU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| f | ? | - | ALA | deletion | UNP Q9WZP2 |
| f | ? | - | GLY | deletion | UNP Q9WZP2 |
| f | ? | - | HIS | deletion | UNP Q9WZP2 |
| f | ? | - | TYR | deletion | UNP Q9WZP2 |
| f | ? | - | PRO | deletion | UNP Q9WZP2 |
| f | ? | - | LEU | deletion | UNP Q9WZP2 |
| g | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| g | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| g | ? | - | GLU | deletion | UNP Q9WZP2 |
| g | ? | - | ALA | deletion | UNP Q9WZP2 |
| g | ? | - | GLY | deletion | UNP Q9WZP2 |
| g | ? | - | HIS | deletion | UNP Q9WZP2 |
| g | ? | - | TYR | deletion | UNP Q9WZP2 |
| g | ? | - | PRO | deletion | UNP Q9WZP2 |
| g | ? | - | LEU | deletion | UNP Q9WZP2 |
| h | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| h | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| h | ? | - | GLU | deletion | UNP Q9WZP2 |
| h | ? | - | ALA | deletion | UNP Q9WZP2 |
| h | ? | - | GLY | deletion | UNP Q9WZP2 |
| h | ? | - | HIS | deletion | UNP Q9WZP2 |
| h | ? | - | TYR | deletion | UNP Q9WZP2 |
| h | ? | - | PRO | deletion | UNP Q9WZP2 |
| h | ? | - | LEU | deletion | UNP Q9WZP2 |
| i | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| i | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| i | ? | - | GLU | deletion | UNP Q9WZP2 |
| i | ? | - | ALA | deletion | UNP Q9WZP2 |
| i | ? | - | GLY | deletion | UNP Q9WZP2 |
| i | ? | - | HIS | deletion | UNP Q9WZP2 |
| i | ? | - | TYR | deletion | UNP Q9WZP2 |
| i | ? | - | PRO | deletion | UNP Q9WZP2 |
| i | ? | - | LEU | deletion | UNP Q9WZP2 |
| j | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| j | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| j | ? | - | GLU | deletion | UNP Q9WZP2 |
| j | ? | - | ALA | deletion | UNP Q9WZP2 |
| j | ? | - | GLY | deletion | UNP Q9WZP2 |
| j | ? | - | HIS | deletion | UNP Q9WZP2 |
| j | ? | - | TYR | deletion | UNP Q9WZP2 |
| j | ? | - | PRO | deletion | UNP Q9WZP2 |
| j | ? | - | LEU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| k | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| k | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| k | ? | - | GLU | deletion | UNP Q9WZP2 |
| k | ? | - | ALA | deletion | UNP Q9WZP2 |
| k | ? | - | GLY | deletion | UNP Q9WZP2 |
| k | ? | - | HIS | deletion | UNP Q9WZP2 |
| k | ? | - | TYR | deletion | UNP Q9WZP2 |
| k | ? | - | PRO | deletion | UNP Q9WZP2 |
| k | ? | - | LEU | deletion | UNP Q9WZP2 |
| l | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| l | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| l | ? | - | GLU | deletion | UNP Q9WZP2 |
| l | ? | - | ALA | deletion | UNP Q9WZP2 |
| l | ? | - | GLY | deletion | UNP Q9WZP2 |
| l | ? | - | HIS | deletion | UNP Q9WZP2 |
| l | ? | - | TYR | deletion | UNP Q9WZP2 |
| l | ? | - | PRO | deletion | UNP Q9WZP2 |
| l | ? | - | LEU | deletion | UNP Q9WZP2 |
| m | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| m | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| m | ? | - | GLU | deletion | UNP Q9WZP2 |
| m | ? | - | ALA | deletion | UNP Q9WZP2 |
| m | ? | - | GLY | deletion | UNP Q9WZP2 |
| m | ? | - | HIS | deletion | UNP Q9WZP2 |
| m | ? | - | TYR | deletion | UNP Q9WZP2 |
| m | ? | - | PRO | deletion | UNP Q9WZP2 |
| m | ? | - | LEU | deletion | UNP Q9WZP2 |
| n | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| n | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| n | ? | - | GLU | deletion | UNP Q9WZP2 |
| n | ? | - | ALA | deletion | UNP Q9WZP2 |
| n | ? | - | GLY | deletion | UNP Q9WZP2 |
| n | ? | - | HIS | deletion | UNP Q9WZP2 |
| n | ? | - | TYR | deletion | UNP Q9WZP2 |
| n | ? | - | PRO | deletion | UNP Q9WZP2 |
| n | ? | - | LEU | deletion | UNP Q9WZP2 |
| o | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| o | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| o | ? | - | GLU | deletion | UNP Q9WZP2 |
| o | ? | - | ALA | deletion | UNP Q9WZP2 |
| o | ? | - | GLY | deletion | UNP Q9WZP2 |
| o | ? | - | HIS | deletion | UNP Q9WZP2 |

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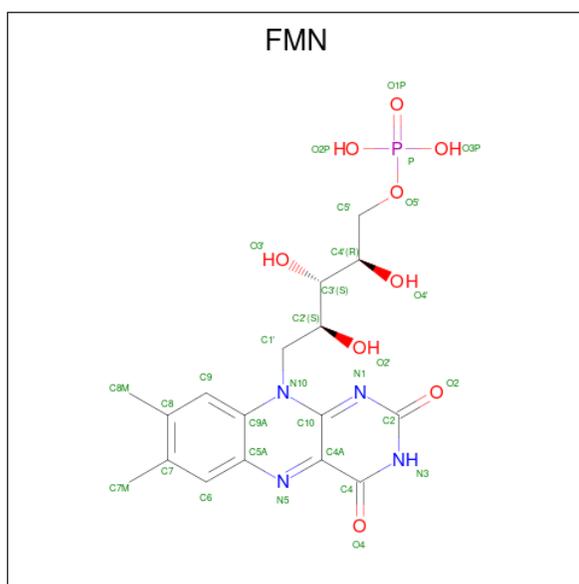
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| o | ? | - | TYR | deletion | UNP Q9WZP2 |
| o | ? | - | PRO | deletion | UNP Q9WZP2 |
| o | ? | - | LEU | deletion | UNP Q9WZP2 |
| p | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| p | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| p | ? | - | GLU | deletion | UNP Q9WZP2 |
| p | ? | - | ALA | deletion | UNP Q9WZP2 |
| p | ? | - | GLY | deletion | UNP Q9WZP2 |
| p | ? | - | HIS | deletion | UNP Q9WZP2 |
| p | ? | - | TYR | deletion | UNP Q9WZP2 |
| p | ? | - | PRO | deletion | UNP Q9WZP2 |
| p | ? | - | LEU | deletion | UNP Q9WZP2 |
| q | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| q | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| q | ? | - | GLU | deletion | UNP Q9WZP2 |
| q | ? | - | ALA | deletion | UNP Q9WZP2 |
| q | ? | - | GLY | deletion | UNP Q9WZP2 |
| q | ? | - | HIS | deletion | UNP Q9WZP2 |
| q | ? | - | TYR | deletion | UNP Q9WZP2 |
| q | ? | - | PRO | deletion | UNP Q9WZP2 |
| q | ? | - | LEU | deletion | UNP Q9WZP2 |
| r | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| r | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| r | ? | - | GLU | deletion | UNP Q9WZP2 |
| r | ? | - | ALA | deletion | UNP Q9WZP2 |
| r | ? | - | GLY | deletion | UNP Q9WZP2 |
| r | ? | - | HIS | deletion | UNP Q9WZP2 |
| r | ? | - | TYR | deletion | UNP Q9WZP2 |
| r | ? | - | PRO | deletion | UNP Q9WZP2 |
| r | ? | - | LEU | deletion | UNP Q9WZP2 |
| s | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| s | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| s | ? | - | GLU | deletion | UNP Q9WZP2 |
| s | ? | - | ALA | deletion | UNP Q9WZP2 |
| s | ? | - | GLY | deletion | UNP Q9WZP2 |
| s | ? | - | HIS | deletion | UNP Q9WZP2 |
| s | ? | - | TYR | deletion | UNP Q9WZP2 |
| s | ? | - | PRO | deletion | UNP Q9WZP2 |
| s | ? | - | LEU | deletion | UNP Q9WZP2 |
| t | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| t | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| t | ? | - | GLU | deletion | UNP Q9WZP2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| t | ? | - | ALA | deletion | UNP Q9WZP2 |
| t | ? | - | GLY | deletion | UNP Q9WZP2 |
| t | ? | - | HIS | deletion | UNP Q9WZP2 |
| t | ? | - | TYR | deletion | UNP Q9WZP2 |
| t | ? | - | PRO | deletion | UNP Q9WZP2 |
| t | ? | - | LEU | deletion | UNP Q9WZP2 |
| u | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| u | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| u | ? | - | GLU | deletion | UNP Q9WZP2 |
| u | ? | - | ALA | deletion | UNP Q9WZP2 |
| u | ? | - | GLY | deletion | UNP Q9WZP2 |
| u | ? | - | HIS | deletion | UNP Q9WZP2 |
| u | ? | - | TYR | deletion | UNP Q9WZP2 |
| u | ? | - | PRO | deletion | UNP Q9WZP2 |
| u | ? | - | LEU | deletion | UNP Q9WZP2 |
| v | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| v | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| v | ? | - | GLU | deletion | UNP Q9WZP2 |
| v | ? | - | ALA | deletion | UNP Q9WZP2 |
| v | ? | - | GLY | deletion | UNP Q9WZP2 |
| v | ? | - | HIS | deletion | UNP Q9WZP2 |
| v | ? | - | TYR | deletion | UNP Q9WZP2 |
| v | ? | - | PRO | deletion | UNP Q9WZP2 |
| v | ? | - | LEU | deletion | UNP Q9WZP2 |
| w | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| w | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| w | ? | - | GLU | deletion | UNP Q9WZP2 |
| w | ? | - | ALA | deletion | UNP Q9WZP2 |
| w | ? | - | GLY | deletion | UNP Q9WZP2 |
| w | ? | - | HIS | deletion | UNP Q9WZP2 |
| w | ? | - | TYR | deletion | UNP Q9WZP2 |
| w | ? | - | PRO | deletion | UNP Q9WZP2 |
| w | ? | - | LEU | deletion | UNP Q9WZP2 |
| x | 182 | GLY | LYS | conflict | UNP Q9WZP2 |
| x | 183 | GLY | GLU | conflict | UNP Q9WZP2 |
| x | ? | - | GLU | deletion | UNP Q9WZP2 |
| x | ? | - | ALA | deletion | UNP Q9WZP2 |
| x | ? | - | GLY | deletion | UNP Q9WZP2 |
| x | ? | - | HIS | deletion | UNP Q9WZP2 |
| x | ? | - | TYR | deletion | UNP Q9WZP2 |
| x | ? | - | PRO | deletion | UNP Q9WZP2 |
| x | ? | - | LEU | deletion | UNP Q9WZP2 |

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



| Mol | Chain | Residues | Atoms | | | | | AltConf | |
|-----|-------|----------|-------|----|----|---|---|---------|---|
| | | | Total | C | H | N | O | | P |
| 2 | A | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | B | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | C | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | D | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | D | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | E | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | F | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | G | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | G | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | I | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | J | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | M | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | M | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | |
|-----|-------|----------|-------|----|----|---|---|---------|---|
| | | | Total | C | H | N | O | | P |
| 2 | N | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | O | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | P | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | Q | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | R | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | S | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | T | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | V | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | W | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | X | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | Y | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 0 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 0 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 1 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 1 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 2 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 3 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 4 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 5 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 5 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 6 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | |
|-----|-------|----------|-------|----|----|---|---|---------|---|
| | | | Total | C | H | N | O | | P |
| 2 | 7 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | 7 | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | a | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | a | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | c | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | d | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | e | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | f | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | h | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | h | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | i | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | j | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | k | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | m | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | m | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | n | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | p | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | p | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | q | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | r | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |
| 2 | r | 1 | 50 | 17 | 19 | 4 | 9 | 1 | 0 |

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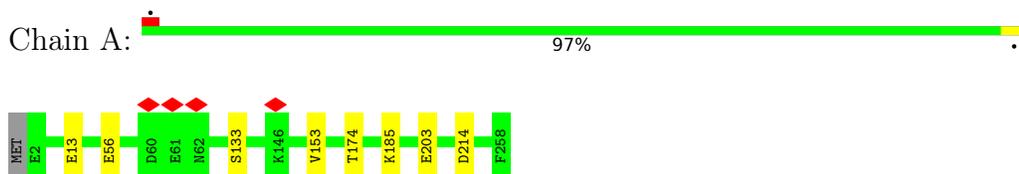
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| Mol | Chain | Residues | Atoms | | | | | AltConf | |
|-----|-------|----------|-------|----|----|---|---|---------|---|
| 2 | s | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | t | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | u | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | w | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |
| 2 | x | 1 | Total | C | H | N | O | P | 0 |
| | | | 50 | 17 | 19 | 4 | 9 | 1 | |

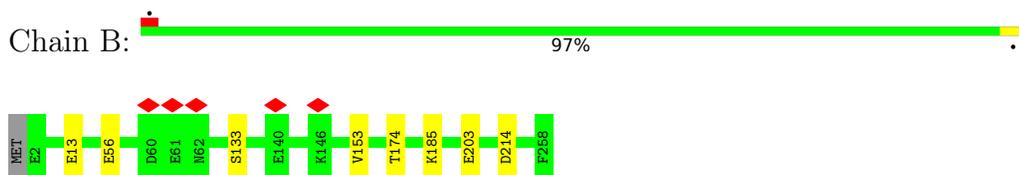
3 Residue-property plots [i](#)

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

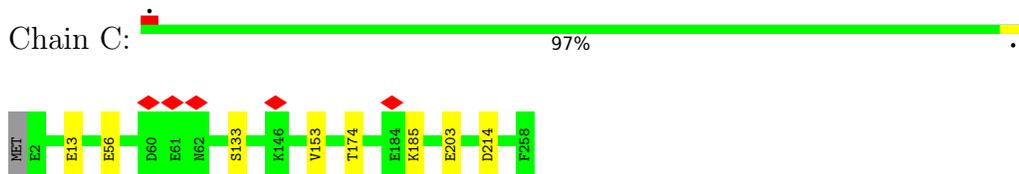
- Molecule 1: Encapsulin



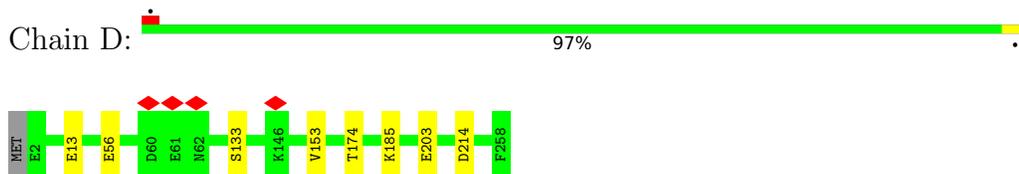
- Molecule 1: Encapsulin



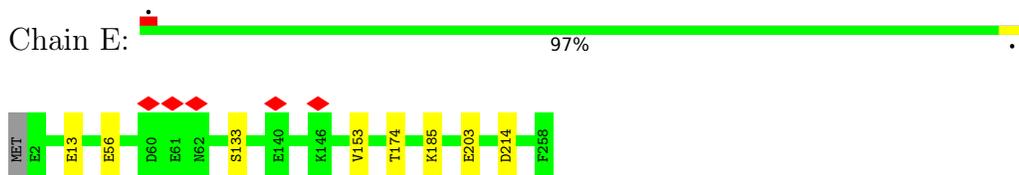
- Molecule 1: Encapsulin



- Molecule 1: Encapsulin



- Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



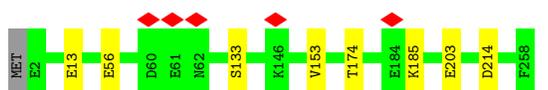
• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin





• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



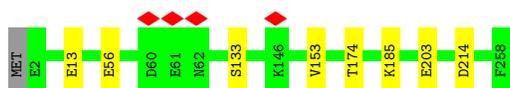
• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



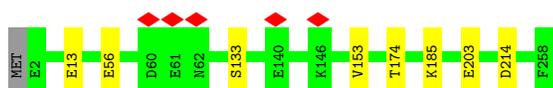
• Molecule 1: Encapsulin



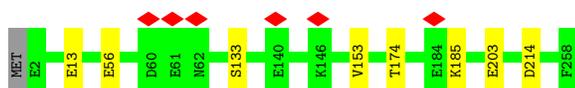
• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



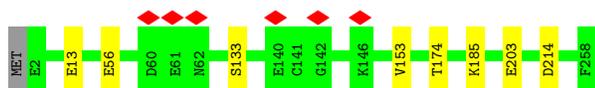
• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin





• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



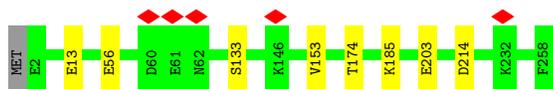
• Molecule 1: Encapsulin



• Molecule 1: Encapsulin



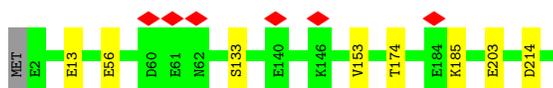
• Molecule 1: Encapsulin



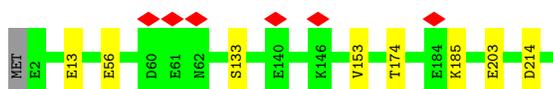
● Molecule 1: Encapsulin



● Molecule 1: Encapsulin



● Molecule 1: Encapsulin



● Molecule 1: Encapsulin



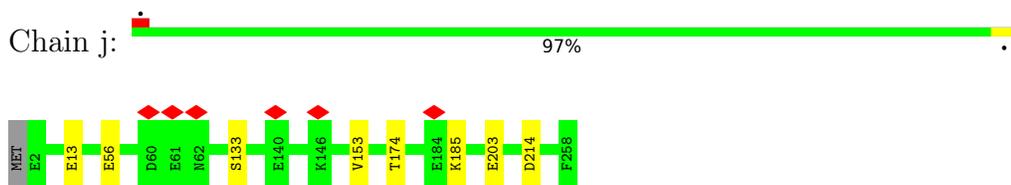
● Molecule 1: Encapsulin



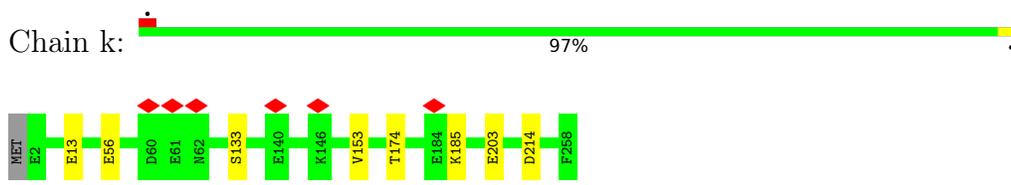
● Molecule 1: Encapsulin



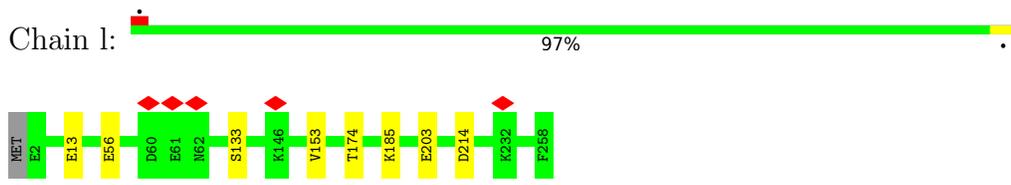
● Molecule 1: Encapsulin



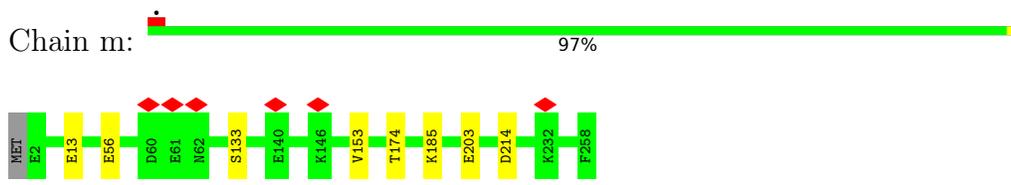
● Molecule 1: Encapsulin



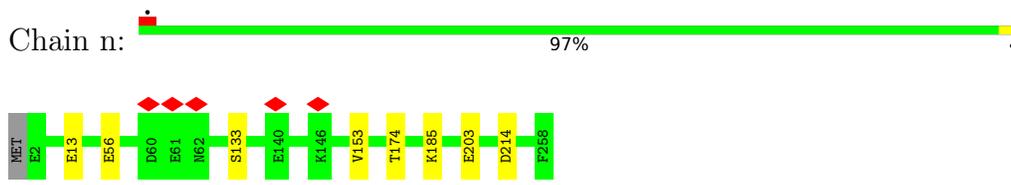
● Molecule 1: Encapsulin



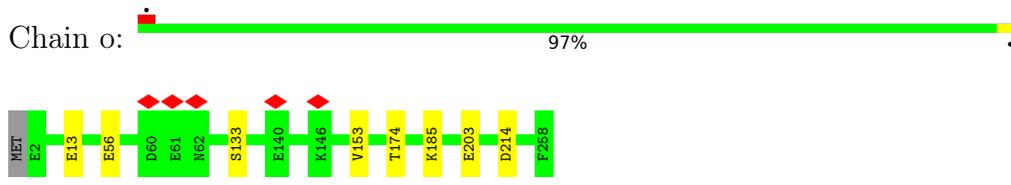
● Molecule 1: Encapsulin



● Molecule 1: Encapsulin

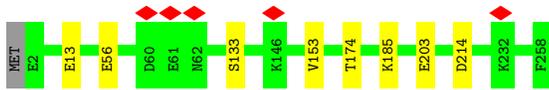


● Molecule 1: Encapsulin



● Molecule 1: Encapsulin

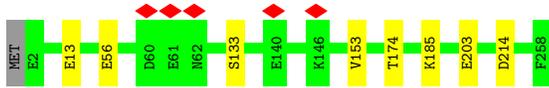




- Molecule 1: Encapsulin



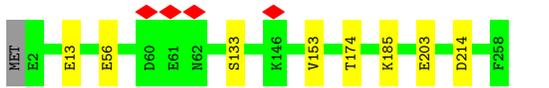
- Molecule 1: Encapsulin



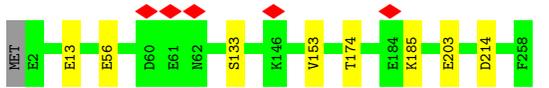
- Molecule 1: Encapsulin



- Molecule 1: Encapsulin



- Molecule 1: Encapsulin



- Molecule 1: Encapsulin



- Molecule 1: Encapsulin

Chain w:  97%



● Molecule 1: Encapsulin

Chain x:  97%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 24401 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 54 | 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 | 0.107 | Depositor |
| Minimum map value | -0.064 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.005 | Depositor |
| Recommended contour level | 0.019 | Depositor |
| Map size (Å) | 416.0, 416.0, 416.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 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: FMN

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 | 0 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 1 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 2 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 3 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 4 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 5 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 6 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 7 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 8 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | 9 | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | A | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | B | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | C | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | D | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | E | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | F | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | G | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | H | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | I | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | J | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | K | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | L | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | M | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | N | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | O | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | P | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | Q | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | R | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | S | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | T | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | U | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | V | 0.40 | 0/2118 | 0.48 | 0/2858 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|----------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | W | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | X | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | Y | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | Z | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | a | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | b | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | c | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | d | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | e | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | f | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | g | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | h | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | i | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | j | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | k | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | l | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | m | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | n | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | o | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | p | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | q | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | r | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | s | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | t | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | u | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | v | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | w | 0.40 | 0/2118 | 0.48 | 0/2858 |
| 1 | x | 0.40 | 0/2118 | 0.48 | 0/2858 |
| All | All | 0.40 | 0/127080 | 0.48 | 0/171480 |

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

5.3.1 Protein backbone

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 | 0 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 1 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 2 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 3 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 4 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 5 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 6 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 7 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 8 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | 9 | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | A | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | B | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | C | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | D | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | E | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | F | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | G | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | H | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | I | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | J | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | K | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | L | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | M | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | N | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | O | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | P | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | Q | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | R | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | S | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | T | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | U | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | V | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | W | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | X | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | Y | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | Z | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | a | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | b | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | c | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | d | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | e | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | f | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | g | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | h | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | i | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | j | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | k | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | l | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | m | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | n | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | o | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | p | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | q | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | r | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | s | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | t | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 1 | u | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | v | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | w | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| 1 | x | 255/258 (99%) | 238 (93%) | 17 (7%) | 0 | 100 | 100 |
| All | All | 15300/15480 (99%) | 14280 (93%) | 1020 (7%) | 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 | 0 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 1 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 2 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 3 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 4 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 5 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 6 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 7 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 8 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | 9 | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | A | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | B | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | C | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | D | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | E | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | F | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | G | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | H | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | I | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | J | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | K | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | L | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | M | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | N | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | O | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | P | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | Q | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | R | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | S | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | T | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | U | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | V | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | W | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | X | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | Y | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | Z | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | a | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | b | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | c | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | d | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | e | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | f | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | g | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | h | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | i | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | j | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | k | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | l | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|----------|-------------|----|
| 1 | m | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | n | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | o | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | p | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | q | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | r | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | s | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | t | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | u | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | v | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | w | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| 1 | x | 226/227 (100%) | 218 (96%) | 8 (4%) | 36 | 71 |
| All | All | 13560/13620 (100%) | 13080 (96%) | 480 (4%) | 39 | 71 |

All (480) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 13 | GLU |
| 1 | A | 56 | GLU |
| 1 | A | 133 | SER |
| 1 | A | 153 | VAL |
| 1 | A | 174 | THR |
| 1 | A | 185 | LYS |
| 1 | A | 203 | GLU |
| 1 | A | 214 | ASP |
| 1 | B | 13 | GLU |
| 1 | B | 56 | GLU |
| 1 | B | 133 | SER |
| 1 | B | 153 | VAL |
| 1 | B | 174 | THR |
| 1 | B | 185 | LYS |
| 1 | B | 203 | GLU |
| 1 | B | 214 | ASP |
| 1 | C | 13 | GLU |
| 1 | C | 56 | GLU |
| 1 | C | 133 | SER |
| 1 | C | 153 | VAL |
| 1 | C | 174 | THR |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | C | 185 | LYS |
| 1 | C | 203 | GLU |
| 1 | C | 214 | ASP |
| 1 | D | 13 | GLU |
| 1 | D | 56 | GLU |
| 1 | D | 133 | SER |
| 1 | D | 153 | VAL |
| 1 | D | 174 | THR |
| 1 | D | 185 | LYS |
| 1 | D | 203 | GLU |
| 1 | D | 214 | ASP |
| 1 | E | 13 | GLU |
| 1 | E | 56 | GLU |
| 1 | E | 133 | SER |
| 1 | E | 153 | VAL |
| 1 | E | 174 | THR |
| 1 | E | 185 | LYS |
| 1 | E | 203 | GLU |
| 1 | E | 214 | ASP |
| 1 | F | 13 | GLU |
| 1 | F | 56 | GLU |
| 1 | F | 133 | SER |
| 1 | F | 153 | VAL |
| 1 | F | 174 | THR |
| 1 | F | 185 | LYS |
| 1 | F | 203 | GLU |
| 1 | F | 214 | ASP |
| 1 | G | 13 | GLU |
| 1 | G | 56 | GLU |
| 1 | G | 133 | SER |
| 1 | G | 153 | VAL |
| 1 | G | 174 | THR |
| 1 | G | 185 | LYS |
| 1 | G | 203 | GLU |
| 1 | G | 214 | ASP |
| 1 | H | 13 | GLU |
| 1 | H | 56 | GLU |
| 1 | H | 133 | SER |
| 1 | H | 153 | VAL |
| 1 | H | 174 | THR |
| 1 | H | 185 | LYS |
| 1 | H | 203 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | H | 214 | ASP |
| 1 | I | 13 | GLU |
| 1 | I | 56 | GLU |
| 1 | I | 133 | SER |
| 1 | I | 153 | VAL |
| 1 | I | 174 | THR |
| 1 | I | 185 | LYS |
| 1 | I | 203 | GLU |
| 1 | I | 214 | ASP |
| 1 | J | 13 | GLU |
| 1 | J | 56 | GLU |
| 1 | J | 133 | SER |
| 1 | J | 153 | VAL |
| 1 | J | 174 | THR |
| 1 | J | 185 | LYS |
| 1 | J | 203 | GLU |
| 1 | J | 214 | ASP |
| 1 | K | 13 | GLU |
| 1 | K | 56 | GLU |
| 1 | K | 133 | SER |
| 1 | K | 153 | VAL |
| 1 | K | 174 | THR |
| 1 | K | 185 | LYS |
| 1 | K | 203 | GLU |
| 1 | K | 214 | ASP |
| 1 | L | 13 | GLU |
| 1 | L | 56 | GLU |
| 1 | L | 133 | SER |
| 1 | L | 153 | VAL |
| 1 | L | 174 | THR |
| 1 | L | 185 | LYS |
| 1 | L | 203 | GLU |
| 1 | L | 214 | ASP |
| 1 | M | 13 | GLU |
| 1 | M | 56 | GLU |
| 1 | M | 133 | SER |
| 1 | M | 153 | VAL |
| 1 | M | 174 | THR |
| 1 | M | 185 | LYS |
| 1 | M | 203 | GLU |
| 1 | M | 214 | ASP |
| 1 | N | 13 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | N | 56 | GLU |
| 1 | N | 133 | SER |
| 1 | N | 153 | VAL |
| 1 | N | 174 | THR |
| 1 | N | 185 | LYS |
| 1 | N | 203 | GLU |
| 1 | N | 214 | ASP |
| 1 | O | 13 | GLU |
| 1 | O | 56 | GLU |
| 1 | O | 133 | SER |
| 1 | O | 153 | VAL |
| 1 | O | 174 | THR |
| 1 | O | 185 | LYS |
| 1 | O | 203 | GLU |
| 1 | O | 214 | ASP |
| 1 | P | 13 | GLU |
| 1 | P | 56 | GLU |
| 1 | P | 133 | SER |
| 1 | P | 153 | VAL |
| 1 | P | 174 | THR |
| 1 | P | 185 | LYS |
| 1 | P | 203 | GLU |
| 1 | P | 214 | ASP |
| 1 | Q | 13 | GLU |
| 1 | Q | 56 | GLU |
| 1 | Q | 133 | SER |
| 1 | Q | 153 | VAL |
| 1 | Q | 174 | THR |
| 1 | Q | 185 | LYS |
| 1 | Q | 203 | GLU |
| 1 | Q | 214 | ASP |
| 1 | R | 13 | GLU |
| 1 | R | 56 | GLU |
| 1 | R | 133 | SER |
| 1 | R | 153 | VAL |
| 1 | R | 174 | THR |
| 1 | R | 185 | LYS |
| 1 | R | 203 | GLU |
| 1 | R | 214 | ASP |
| 1 | S | 13 | GLU |
| 1 | S | 56 | GLU |
| 1 | S | 133 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | S | 153 | VAL |
| 1 | S | 174 | THR |
| 1 | S | 185 | LYS |
| 1 | S | 203 | GLU |
| 1 | S | 214 | ASP |
| 1 | T | 13 | GLU |
| 1 | T | 56 | GLU |
| 1 | T | 133 | SER |
| 1 | T | 153 | VAL |
| 1 | T | 174 | THR |
| 1 | T | 185 | LYS |
| 1 | T | 203 | GLU |
| 1 | T | 214 | ASP |
| 1 | U | 13 | GLU |
| 1 | U | 56 | GLU |
| 1 | U | 133 | SER |
| 1 | U | 153 | VAL |
| 1 | U | 174 | THR |
| 1 | U | 185 | LYS |
| 1 | U | 203 | GLU |
| 1 | U | 214 | ASP |
| 1 | V | 13 | GLU |
| 1 | V | 56 | GLU |
| 1 | V | 133 | SER |
| 1 | V | 153 | VAL |
| 1 | V | 174 | THR |
| 1 | V | 185 | LYS |
| 1 | V | 203 | GLU |
| 1 | V | 214 | ASP |
| 1 | W | 13 | GLU |
| 1 | W | 56 | GLU |
| 1 | W | 133 | SER |
| 1 | W | 153 | VAL |
| 1 | W | 174 | THR |
| 1 | W | 185 | LYS |
| 1 | W | 203 | GLU |
| 1 | W | 214 | ASP |
| 1 | X | 13 | GLU |
| 1 | X | 56 | GLU |
| 1 | X | 133 | SER |
| 1 | X | 153 | VAL |
| 1 | X | 174 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | X | 185 | LYS |
| 1 | X | 203 | GLU |
| 1 | X | 214 | ASP |
| 1 | Y | 13 | GLU |
| 1 | Y | 56 | GLU |
| 1 | Y | 133 | SER |
| 1 | Y | 153 | VAL |
| 1 | Y | 174 | THR |
| 1 | Y | 185 | LYS |
| 1 | Y | 203 | GLU |
| 1 | Y | 214 | ASP |
| 1 | Z | 13 | GLU |
| 1 | Z | 56 | GLU |
| 1 | Z | 133 | SER |
| 1 | Z | 153 | VAL |
| 1 | Z | 174 | THR |
| 1 | Z | 185 | LYS |
| 1 | Z | 203 | GLU |
| 1 | Z | 214 | ASP |
| 1 | 0 | 13 | GLU |
| 1 | 0 | 56 | GLU |
| 1 | 0 | 133 | SER |
| 1 | 0 | 153 | VAL |
| 1 | 0 | 174 | THR |
| 1 | 0 | 185 | LYS |
| 1 | 0 | 203 | GLU |
| 1 | 0 | 214 | ASP |
| 1 | 1 | 13 | GLU |
| 1 | 1 | 56 | GLU |
| 1 | 1 | 133 | SER |
| 1 | 1 | 153 | VAL |
| 1 | 1 | 174 | THR |
| 1 | 1 | 185 | LYS |
| 1 | 1 | 203 | GLU |
| 1 | 1 | 214 | ASP |
| 1 | 2 | 13 | GLU |
| 1 | 2 | 56 | GLU |
| 1 | 2 | 133 | SER |
| 1 | 2 | 153 | VAL |
| 1 | 2 | 174 | THR |
| 1 | 2 | 185 | LYS |
| 1 | 2 | 203 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2 | 214 | ASP |
| 1 | 3 | 13 | GLU |
| 1 | 3 | 56 | GLU |
| 1 | 3 | 133 | SER |
| 1 | 3 | 153 | VAL |
| 1 | 3 | 174 | THR |
| 1 | 3 | 185 | LYS |
| 1 | 3 | 203 | GLU |
| 1 | 3 | 214 | ASP |
| 1 | 4 | 13 | GLU |
| 1 | 4 | 56 | GLU |
| 1 | 4 | 133 | SER |
| 1 | 4 | 153 | VAL |
| 1 | 4 | 174 | THR |
| 1 | 4 | 185 | LYS |
| 1 | 4 | 203 | GLU |
| 1 | 4 | 214 | ASP |
| 1 | 5 | 13 | GLU |
| 1 | 5 | 56 | GLU |
| 1 | 5 | 133 | SER |
| 1 | 5 | 153 | VAL |
| 1 | 5 | 174 | THR |
| 1 | 5 | 185 | LYS |
| 1 | 5 | 203 | GLU |
| 1 | 5 | 214 | ASP |
| 1 | 6 | 13 | GLU |
| 1 | 6 | 56 | GLU |
| 1 | 6 | 133 | SER |
| 1 | 6 | 153 | VAL |
| 1 | 6 | 174 | THR |
| 1 | 6 | 185 | LYS |
| 1 | 6 | 203 | GLU |
| 1 | 6 | 214 | ASP |
| 1 | 7 | 13 | GLU |
| 1 | 7 | 56 | GLU |
| 1 | 7 | 133 | SER |
| 1 | 7 | 153 | VAL |
| 1 | 7 | 174 | THR |
| 1 | 7 | 185 | LYS |
| 1 | 7 | 203 | GLU |
| 1 | 7 | 214 | ASP |
| 1 | 8 | 13 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 8 | 56 | GLU |
| 1 | 8 | 133 | SER |
| 1 | 8 | 153 | VAL |
| 1 | 8 | 174 | THR |
| 1 | 8 | 185 | LYS |
| 1 | 8 | 203 | GLU |
| 1 | 8 | 214 | ASP |
| 1 | 9 | 13 | GLU |
| 1 | 9 | 56 | GLU |
| 1 | 9 | 133 | SER |
| 1 | 9 | 153 | VAL |
| 1 | 9 | 174 | THR |
| 1 | 9 | 185 | LYS |
| 1 | 9 | 203 | GLU |
| 1 | 9 | 214 | ASP |
| 1 | a | 13 | GLU |
| 1 | a | 56 | GLU |
| 1 | a | 133 | SER |
| 1 | a | 153 | VAL |
| 1 | a | 174 | THR |
| 1 | a | 185 | LYS |
| 1 | a | 203 | GLU |
| 1 | a | 214 | ASP |
| 1 | b | 13 | GLU |
| 1 | b | 56 | GLU |
| 1 | b | 133 | SER |
| 1 | b | 153 | VAL |
| 1 | b | 174 | THR |
| 1 | b | 185 | LYS |
| 1 | b | 203 | GLU |
| 1 | b | 214 | ASP |
| 1 | c | 13 | GLU |
| 1 | c | 56 | GLU |
| 1 | c | 133 | SER |
| 1 | c | 153 | VAL |
| 1 | c | 174 | THR |
| 1 | c | 185 | LYS |
| 1 | c | 203 | GLU |
| 1 | c | 214 | ASP |
| 1 | d | 13 | GLU |
| 1 | d | 56 | GLU |
| 1 | d | 133 | SER |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | d | 153 | VAL |
| 1 | d | 174 | THR |
| 1 | d | 185 | LYS |
| 1 | d | 203 | GLU |
| 1 | d | 214 | ASP |
| 1 | e | 13 | GLU |
| 1 | e | 56 | GLU |
| 1 | e | 133 | SER |
| 1 | e | 153 | VAL |
| 1 | e | 174 | THR |
| 1 | e | 185 | LYS |
| 1 | e | 203 | GLU |
| 1 | e | 214 | ASP |
| 1 | f | 13 | GLU |
| 1 | f | 56 | GLU |
| 1 | f | 133 | SER |
| 1 | f | 153 | VAL |
| 1 | f | 174 | THR |
| 1 | f | 185 | LYS |
| 1 | f | 203 | GLU |
| 1 | f | 214 | ASP |
| 1 | g | 13 | GLU |
| 1 | g | 56 | GLU |
| 1 | g | 133 | SER |
| 1 | g | 153 | VAL |
| 1 | g | 174 | THR |
| 1 | g | 185 | LYS |
| 1 | g | 203 | GLU |
| 1 | g | 214 | ASP |
| 1 | h | 13 | GLU |
| 1 | h | 56 | GLU |
| 1 | h | 133 | SER |
| 1 | h | 153 | VAL |
| 1 | h | 174 | THR |
| 1 | h | 185 | LYS |
| 1 | h | 203 | GLU |
| 1 | h | 214 | ASP |
| 1 | i | 13 | GLU |
| 1 | i | 56 | GLU |
| 1 | i | 133 | SER |
| 1 | i | 153 | VAL |
| 1 | i | 174 | THR |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | i | 185 | LYS |
| 1 | i | 203 | GLU |
| 1 | i | 214 | ASP |
| 1 | j | 13 | GLU |
| 1 | j | 56 | GLU |
| 1 | j | 133 | SER |
| 1 | j | 153 | VAL |
| 1 | j | 174 | THR |
| 1 | j | 185 | LYS |
| 1 | j | 203 | GLU |
| 1 | j | 214 | ASP |
| 1 | k | 13 | GLU |
| 1 | k | 56 | GLU |
| 1 | k | 133 | SER |
| 1 | k | 153 | VAL |
| 1 | k | 174 | THR |
| 1 | k | 185 | LYS |
| 1 | k | 203 | GLU |
| 1 | k | 214 | ASP |
| 1 | l | 13 | GLU |
| 1 | l | 56 | GLU |
| 1 | l | 133 | SER |
| 1 | l | 153 | VAL |
| 1 | l | 174 | THR |
| 1 | l | 185 | LYS |
| 1 | l | 203 | GLU |
| 1 | l | 214 | ASP |
| 1 | m | 13 | GLU |
| 1 | m | 56 | GLU |
| 1 | m | 133 | SER |
| 1 | m | 153 | VAL |
| 1 | m | 174 | THR |
| 1 | m | 185 | LYS |
| 1 | m | 203 | GLU |
| 1 | m | 214 | ASP |
| 1 | n | 13 | GLU |
| 1 | n | 56 | GLU |
| 1 | n | 133 | SER |
| 1 | n | 153 | VAL |
| 1 | n | 174 | THR |
| 1 | n | 185 | LYS |
| 1 | n | 203 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | n | 214 | ASP |
| 1 | o | 13 | GLU |
| 1 | o | 56 | GLU |
| 1 | o | 133 | SER |
| 1 | o | 153 | VAL |
| 1 | o | 174 | THR |
| 1 | o | 185 | LYS |
| 1 | o | 203 | GLU |
| 1 | o | 214 | ASP |
| 1 | p | 13 | GLU |
| 1 | p | 56 | GLU |
| 1 | p | 133 | SER |
| 1 | p | 153 | VAL |
| 1 | p | 174 | THR |
| 1 | p | 185 | LYS |
| 1 | p | 203 | GLU |
| 1 | p | 214 | ASP |
| 1 | q | 13 | GLU |
| 1 | q | 56 | GLU |
| 1 | q | 133 | SER |
| 1 | q | 153 | VAL |
| 1 | q | 174 | THR |
| 1 | q | 185 | LYS |
| 1 | q | 203 | GLU |
| 1 | q | 214 | ASP |
| 1 | r | 13 | GLU |
| 1 | r | 56 | GLU |
| 1 | r | 133 | SER |
| 1 | r | 153 | VAL |
| 1 | r | 174 | THR |
| 1 | r | 185 | LYS |
| 1 | r | 203 | GLU |
| 1 | r | 214 | ASP |
| 1 | s | 13 | GLU |
| 1 | s | 56 | GLU |
| 1 | s | 133 | SER |
| 1 | s | 153 | VAL |
| 1 | s | 174 | THR |
| 1 | s | 185 | LYS |
| 1 | s | 203 | GLU |
| 1 | s | 214 | ASP |
| 1 | t | 13 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | t | 56 | GLU |
| 1 | t | 133 | SER |
| 1 | t | 153 | VAL |
| 1 | t | 174 | THR |
| 1 | t | 185 | LYS |
| 1 | t | 203 | GLU |
| 1 | t | 214 | ASP |
| 1 | u | 13 | GLU |
| 1 | u | 56 | GLU |
| 1 | u | 133 | SER |
| 1 | u | 153 | VAL |
| 1 | u | 174 | THR |
| 1 | u | 185 | LYS |
| 1 | u | 203 | GLU |
| 1 | u | 214 | ASP |
| 1 | v | 13 | GLU |
| 1 | v | 56 | GLU |
| 1 | v | 133 | SER |
| 1 | v | 153 | VAL |
| 1 | v | 174 | THR |
| 1 | v | 185 | LYS |
| 1 | v | 203 | GLU |
| 1 | v | 214 | ASP |
| 1 | w | 13 | GLU |
| 1 | w | 56 | GLU |
| 1 | w | 133 | SER |
| 1 | w | 153 | VAL |
| 1 | w | 174 | THR |
| 1 | w | 185 | LYS |
| 1 | w | 203 | GLU |
| 1 | w | 214 | ASP |
| 1 | x | 13 | GLU |
| 1 | x | 56 | GLU |
| 1 | x | 133 | SER |
| 1 | x | 153 | VAL |
| 1 | x | 174 | THR |
| 1 | x | 185 | LYS |
| 1 | x | 203 | GLU |
| 1 | x | 214 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 249 | ASN |
| 1 | B | 249 | ASN |
| 1 | C | 249 | ASN |
| 1 | D | 249 | ASN |
| 1 | E | 249 | ASN |
| 1 | F | 249 | ASN |
| 1 | G | 249 | ASN |
| 1 | H | 249 | ASN |
| 1 | I | 249 | ASN |
| 1 | J | 249 | ASN |
| 1 | K | 249 | ASN |
| 1 | L | 249 | ASN |
| 1 | M | 249 | ASN |
| 1 | N | 249 | ASN |
| 1 | O | 249 | ASN |
| 1 | P | 249 | ASN |
| 1 | Q | 249 | ASN |
| 1 | R | 249 | ASN |
| 1 | S | 249 | ASN |
| 1 | T | 249 | ASN |
| 1 | U | 249 | ASN |
| 1 | V | 249 | ASN |
| 1 | W | 249 | ASN |
| 1 | X | 249 | ASN |
| 1 | Y | 249 | ASN |
| 1 | Z | 249 | ASN |
| 1 | 0 | 249 | ASN |
| 1 | 1 | 249 | ASN |
| 1 | 2 | 249 | ASN |
| 1 | 3 | 249 | ASN |
| 1 | 4 | 249 | ASN |
| 1 | 5 | 249 | ASN |
| 1 | 6 | 249 | ASN |
| 1 | 7 | 249 | ASN |
| 1 | 8 | 249 | ASN |
| 1 | 9 | 249 | ASN |
| 1 | a | 249 | ASN |
| 1 | b | 249 | ASN |
| 1 | c | 249 | ASN |
| 1 | d | 249 | ASN |
| 1 | e | 249 | ASN |
| 1 | f | 249 | ASN |
| 1 | g | 249 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | h | 249 | ASN |
| 1 | i | 249 | ASN |
| 1 | j | 249 | ASN |
| 1 | k | 249 | ASN |
| 1 | l | 249 | ASN |
| 1 | m | 249 | ASN |
| 1 | n | 249 | ASN |
| 1 | o | 249 | ASN |
| 1 | p | 249 | ASN |
| 1 | q | 249 | ASN |
| 1 | r | 249 | ASN |
| 1 | s | 249 | ASN |
| 1 | t | 249 | ASN |
| 1 | u | 249 | ASN |
| 1 | v | 249 | ASN |
| 1 | w | 249 | ASN |
| 1 | x | 249 | 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](#)

60 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FMN | r | 302 | - | 33,33,33 | 3.53 | 18 (54%) | 48,50,50 | 1.22 | 7 (14%) |
| 2 | FMN | 0 | 302 | - | 33,33,33 | 3.52 | 18 (54%) | 48,50,50 | 1.19 | 8 (16%) |
| 2 | FMN | m | 302 | - | 33,33,33 | 3.56 | 18 (54%) | 48,50,50 | 1.27 | 8 (16%) |
| 2 | FMN | E | 301 | - | 33,33,33 | 3.57 | 18 (54%) | 48,50,50 | 1.33 | 8 (16%) |
| 2 | FMN | M | 301 | - | 33,33,33 | 3.55 | 18 (54%) | 48,50,50 | 1.21 | 8 (16%) |
| 2 | FMN | G | 301 | - | 33,33,33 | 3.61 | 18 (54%) | 48,50,50 | 1.26 | 9 (18%) |
| 2 | FMN | 1 | 301 | - | 33,33,33 | 3.52 | 18 (54%) | 48,50,50 | 1.22 | 6 (12%) |
| 2 | FMN | Y | 301 | - | 33,33,33 | 3.57 | 18 (54%) | 48,50,50 | 1.24 | 6 (12%) |
| 2 | FMN | D | 302 | - | 33,33,33 | 3.46 | 18 (54%) | 48,50,50 | 1.22 | 6 (12%) |
| 2 | FMN | 4 | 301 | - | 33,33,33 | 3.50 | 18 (54%) | 48,50,50 | 1.22 | 7 (14%) |
| 2 | FMN | O | 301 | - | 33,33,33 | 3.45 | 18 (54%) | 48,50,50 | 1.26 | 8 (16%) |
| 2 | FMN | p | 302 | - | 33,33,33 | 3.48 | 18 (54%) | 48,50,50 | 1.19 | 8 (16%) |
| 2 | FMN | P | 301 | - | 33,33,33 | 3.57 | 18 (54%) | 48,50,50 | 1.26 | 9 (18%) |
| 2 | FMN | q | 301 | - | 33,33,33 | 3.52 | 18 (54%) | 48,50,50 | 1.22 | 9 (18%) |
| 2 | FMN | G | 302 | - | 33,33,33 | 3.48 | 18 (54%) | 48,50,50 | 1.21 | 7 (14%) |
| 2 | FMN | x | 301 | - | 33,33,33 | 3.52 | 18 (54%) | 48,50,50 | 1.19 | 6 (12%) |
| 2 | FMN | A | 301 | - | 33,33,33 | 3.52 | 18 (54%) | 48,50,50 | 1.22 | 7 (14%) |
| 2 | FMN | 1 | 302 | - | 33,33,33 | 3.46 | 18 (54%) | 48,50,50 | 1.23 | 6 (12%) |
| 2 | FMN | T | 301 | - | 33,33,33 | 3.47 | 18 (54%) | 48,50,50 | 1.32 | 9 (18%) |
| 2 | FMN | p | 301 | - | 33,33,33 | 3.51 | 18 (54%) | 48,50,50 | 1.25 | 6 (12%) |
| 2 | FMN | t | 301 | - | 33,33,33 | 3.45 | 18 (54%) | 48,50,50 | 1.27 | 8 (16%) |
| 2 | FMN | h | 302 | - | 33,33,33 | 3.49 | 18 (54%) | 48,50,50 | 1.25 | 7 (14%) |
| 2 | FMN | s | 301 | - | 33,33,33 | 3.60 | 18 (54%) | 48,50,50 | 1.25 | 8 (16%) |
| 2 | FMN | e | 301 | - | 33,33,33 | 3.49 | 18 (54%) | 48,50,50 | 1.21 | 7 (14%) |
| 2 | FMN | j | 301 | - | 33,33,33 | 3.53 | 18 (54%) | 48,50,50 | 1.22 | 7 (14%) |
| 2 | FMN | J | 301 | - | 33,33,33 | 3.41 | 18 (54%) | 48,50,50 | 1.25 | 8 (16%) |
| 2 | FMN | 7 | 301 | - | 33,33,33 | 3.42 | 18 (54%) | 48,50,50 | 1.25 | 7 (14%) |
| 2 | FMN | c | 301 | - | 33,33,33 | 3.59 | 18 (54%) | 48,50,50 | 1.22 | 8 (16%) |
| 2 | FMN | F | 301 | - | 33,33,33 | 3.52 | 18 (54%) | 48,50,50 | 1.26 | 7 (14%) |
| 2 | FMN | f | 301 | - | 33,33,33 | 3.46 | 18 (54%) | 48,50,50 | 1.27 | 8 (16%) |
| 2 | FMN | i | 301 | - | 33,33,33 | 3.47 | 18 (54%) | 48,50,50 | 1.24 | 7 (14%) |
| 2 | FMN | 0 | 301 | - | 33,33,33 | 3.51 | 18 (54%) | 48,50,50 | 1.33 | 8 (16%) |
| 2 | FMN | a | 302 | - | 33,33,33 | 3.51 | 18 (54%) | 48,50,50 | 1.36 | 10 (20%) |
| 2 | FMN | h | 301 | - | 33,33,33 | 3.55 | 18 (54%) | 48,50,50 | 1.22 | 7 (14%) |
| 2 | FMN | d | 301 | - | 33,33,33 | 3.51 | 18 (54%) | 48,50,50 | 1.22 | 6 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FMN | D | 301 | - | 33,33,33 | 3.51 | 18 (54%) | 48,50,50 | 1.22 | 6 (12%) |
| 2 | FMN | 2 | 301 | - | 33,33,33 | 3.57 | 18 (54%) | 48,50,50 | 1.24 | 8 (16%) |
| 2 | FMN | R | 301 | - | 33,33,33 | 3.51 | 18 (54%) | 48,50,50 | 1.22 | 6 (12%) |
| 2 | FMN | Q | 301 | - | 33,33,33 | 3.49 | 18 (54%) | 48,50,50 | 1.23 | 8 (16%) |
| 2 | FMN | n | 301 | - | 33,33,33 | 3.45 | 18 (54%) | 48,50,50 | 1.23 | 7 (14%) |
| 2 | FMN | C | 301 | - | 33,33,33 | 3.53 | 18 (54%) | 48,50,50 | 1.18 | 7 (14%) |
| 2 | FMN | r | 301 | - | 33,33,33 | 3.56 | 18 (54%) | 48,50,50 | 1.23 | 8 (16%) |
| 2 | FMN | 5 | 302 | - | 33,33,33 | 3.43 | 18 (54%) | 48,50,50 | 1.21 | 6 (12%) |
| 2 | FMN | a | 301 | - | 33,33,33 | 3.51 | 18 (54%) | 48,50,50 | 1.28 | 8 (16%) |
| 2 | FMN | B | 301 | - | 33,33,33 | 3.44 | 18 (54%) | 48,50,50 | 1.27 | 10 (20%) |
| 2 | FMN | m | 301 | - | 33,33,33 | 3.46 | 18 (54%) | 48,50,50 | 1.19 | 7 (14%) |
| 2 | FMN | u | 301 | - | 33,33,33 | 3.53 | 18 (54%) | 48,50,50 | 1.27 | 7 (14%) |
| 2 | FMN | k | 301 | - | 33,33,33 | 3.53 | 18 (54%) | 48,50,50 | 1.17 | 8 (16%) |
| 2 | FMN | w | 301 | - | 33,33,33 | 3.45 | 18 (54%) | 48,50,50 | 1.25 | 8 (16%) |
| 2 | FMN | 7 | 302 | - | 33,33,33 | 3.54 | 18 (54%) | 48,50,50 | 1.21 | 6 (12%) |
| 2 | FMN | I | 301 | - | 33,33,33 | 3.52 | 18 (54%) | 48,50,50 | 1.25 | 6 (12%) |
| 2 | FMN | W | 301 | - | 33,33,33 | 3.57 | 18 (54%) | 48,50,50 | 1.25 | 7 (14%) |
| 2 | FMN | 5 | 301 | - | 33,33,33 | 3.54 | 18 (54%) | 48,50,50 | 1.23 | 8 (16%) |
| 2 | FMN | 3 | 301 | - | 33,33,33 | 3.56 | 18 (54%) | 48,50,50 | 1.21 | 7 (14%) |
| 2 | FMN | 6 | 301 | - | 33,33,33 | 3.49 | 18 (54%) | 48,50,50 | 1.39 | 8 (16%) |
| 2 | FMN | S | 301 | - | 33,33,33 | 3.55 | 18 (54%) | 48,50,50 | 1.26 | 8 (16%) |
| 2 | FMN | N | 301 | - | 33,33,33 | 3.58 | 18 (54%) | 48,50,50 | 1.26 | 8 (16%) |
| 2 | FMN | M | 302 | - | 33,33,33 | 3.48 | 18 (54%) | 48,50,50 | 1.26 | 7 (14%) |
| 2 | FMN | X | 301 | - | 33,33,33 | 3.61 | 18 (54%) | 48,50,50 | 1.27 | 8 (16%) |
| 2 | FMN | V | 301 | - | 33,33,33 | 3.57 | 18 (54%) | 48,50,50 | 1.28 | 9 (18%) |

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 |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2 | FMN | r | 302 | - | - | 5/18/18/18 | 0/3/3/3 |
| 2 | FMN | 0 | 302 | - | - | 10/18/18/18 | 0/3/3/3 |
| 2 | FMN | m | 302 | - | - | 13/18/18/18 | 0/3/3/3 |
| 2 | FMN | E | 301 | - | - | 13/18/18/18 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2 | FMN | M | 301 | - | - | 8/18/18/18 | 0/3/3/3 |
| 2 | FMN | G | 301 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | 1 | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | Y | 301 | - | - | 13/18/18/18 | 0/3/3/3 |
| 2 | FMN | D | 302 | - | - | 4/18/18/18 | 0/3/3/3 |
| 2 | FMN | 4 | 301 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | O | 301 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | p | 302 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | P | 301 | - | - | 3/18/18/18 | 0/3/3/3 |
| 2 | FMN | q | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | G | 302 | - | - | 5/18/18/18 | 0/3/3/3 |
| 2 | FMN | x | 301 | - | - | 6/18/18/18 | 0/3/3/3 |
| 2 | FMN | A | 301 | - | - | 13/18/18/18 | 0/3/3/3 |
| 2 | FMN | l | 302 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | T | 301 | - | - | 7/18/18/18 | 0/3/3/3 |
| 2 | FMN | p | 301 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | t | 301 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | h | 302 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | s | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | e | 301 | - | - | 14/18/18/18 | 0/3/3/3 |
| 2 | FMN | j | 301 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | J | 301 | - | - | 4/18/18/18 | 0/3/3/3 |
| 2 | FMN | 7 | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | c | 301 | - | - | 5/18/18/18 | 0/3/3/3 |
| 2 | FMN | F | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | f | 301 | - | - | 10/18/18/18 | 0/3/3/3 |
| 2 | FMN | i | 301 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | 0 | 301 | - | - | 14/18/18/18 | 0/3/3/3 |
| 2 | FMN | a | 302 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | h | 301 | - | - | 13/18/18/18 | 0/3/3/3 |
| 2 | FMN | d | 301 | - | - | 13/18/18/18 | 0/3/3/3 |
| 2 | FMN | D | 301 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | 2 | 301 | - | - | 7/18/18/18 | 0/3/3/3 |
| 2 | FMN | R | 301 | - | - | 13/18/18/18 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2 | FMN | Q | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | n | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | C | 301 | - | - | 2/18/18/18 | 0/3/3/3 |
| 2 | FMN | r | 301 | - | - | 8/18/18/18 | 0/3/3/3 |
| 2 | FMN | 5 | 302 | - | - | 13/18/18/18 | 0/3/3/3 |
| 2 | FMN | a | 301 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | B | 301 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | m | 301 | - | - | 10/18/18/18 | 0/3/3/3 |
| 2 | FMN | u | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | k | 301 | - | - | 11/18/18/18 | 0/3/3/3 |
| 2 | FMN | w | 301 | - | - | 8/18/18/18 | 0/3/3/3 |
| 2 | FMN | 7 | 302 | - | - | 8/18/18/18 | 0/3/3/3 |
| 2 | FMN | I | 301 | - | - | 8/18/18/18 | 0/3/3/3 |
| 2 | FMN | W | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | 5 | 301 | - | - | 10/18/18/18 | 0/3/3/3 |
| 2 | FMN | 3 | 301 | - | - | 9/18/18/18 | 0/3/3/3 |
| 2 | FMN | 6 | 301 | - | - | 15/18/18/18 | 0/3/3/3 |
| 2 | FMN | S | 301 | - | - | 12/18/18/18 | 0/3/3/3 |
| 2 | FMN | N | 301 | - | - | 15/18/18/18 | 0/3/3/3 |
| 2 | FMN | M | 302 | - | - | 8/18/18/18 | 0/3/3/3 |
| 2 | FMN | X | 301 | - | - | 10/18/18/18 | 0/3/3/3 |
| 2 | FMN | V | 301 | - | - | 4/18/18/18 | 0/3/3/3 |

All (1080) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | W | 301 | FMN | C7M-C7 | 7.88 | 1.66 | 1.51 |
| 2 | s | 301 | FMN | C7M-C7 | 7.84 | 1.66 | 1.51 |
| 2 | u | 301 | FMN | C7M-C7 | 7.84 | 1.66 | 1.51 |
| 2 | Y | 301 | FMN | C7M-C7 | 7.82 | 1.66 | 1.51 |
| 2 | r | 302 | FMN | C7M-C7 | 7.78 | 1.66 | 1.51 |
| 2 | F | 301 | FMN | C7M-C7 | 7.73 | 1.66 | 1.51 |
| 2 | h | 301 | FMN | C7M-C7 | 7.71 | 1.66 | 1.51 |
| 2 | c | 301 | FMN | C7M-C7 | 7.70 | 1.66 | 1.51 |
| 2 | N | 301 | FMN | C7M-C7 | 7.68 | 1.66 | 1.51 |
| 2 | V | 301 | FMN | C7M-C7 | 7.68 | 1.66 | 1.51 |
| 2 | m | 302 | FMN | C7M-C7 | 7.66 | 1.66 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 2 | 301 | FMN | C7M-C7 | 7.66 | 1.66 | 1.51 |
| 2 | D | 301 | FMN | C7M-C7 | 7.66 | 1.66 | 1.51 |
| 2 | 5 | 301 | FMN | C7M-C7 | 7.66 | 1.66 | 1.51 |
| 2 | r | 301 | FMN | C7M-C7 | 7.65 | 1.66 | 1.51 |
| 2 | Q | 301 | FMN | C7M-C7 | 7.65 | 1.66 | 1.51 |
| 2 | P | 301 | FMN | C7M-C7 | 7.65 | 1.66 | 1.51 |
| 2 | I | 301 | FMN | C7M-C7 | 7.63 | 1.66 | 1.51 |
| 2 | j | 301 | FMN | C7M-C7 | 7.63 | 1.66 | 1.51 |
| 2 | M | 301 | FMN | C7M-C7 | 7.62 | 1.66 | 1.51 |
| 2 | 3 | 301 | FMN | C7M-C7 | 7.61 | 1.66 | 1.51 |
| 2 | 1 | 301 | FMN | C7M-C7 | 7.61 | 1.66 | 1.51 |
| 2 | h | 302 | FMN | C7M-C7 | 7.61 | 1.66 | 1.51 |
| 2 | G | 301 | FMN | C7M-C7 | 7.61 | 1.66 | 1.51 |
| 2 | S | 301 | FMN | C7M-C7 | 7.60 | 1.66 | 1.51 |
| 2 | a | 301 | FMN | C7M-C7 | 7.59 | 1.66 | 1.51 |
| 2 | p | 301 | FMN | C7M-C7 | 7.58 | 1.66 | 1.51 |
| 2 | T | 301 | FMN | C7M-C7 | 7.56 | 1.66 | 1.51 |
| 2 | M | 302 | FMN | C7M-C7 | 7.45 | 1.66 | 1.51 |
| 2 | q | 301 | FMN | C7M-C7 | 7.45 | 1.65 | 1.51 |
| 2 | 4 | 301 | FMN | C7M-C7 | 7.45 | 1.65 | 1.51 |
| 2 | w | 301 | FMN | C7M-C7 | 7.45 | 1.65 | 1.51 |
| 2 | R | 301 | FMN | C7M-C7 | 7.44 | 1.65 | 1.51 |
| 2 | e | 301 | FMN | C7M-C7 | 7.44 | 1.65 | 1.51 |
| 2 | t | 301 | FMN | C7M-C7 | 7.43 | 1.65 | 1.51 |
| 2 | x | 301 | FMN | C7M-C7 | 7.43 | 1.65 | 1.51 |
| 2 | D | 302 | FMN | C7M-C7 | 7.42 | 1.65 | 1.51 |
| 2 | d | 301 | FMN | C7M-C7 | 7.42 | 1.65 | 1.51 |
| 2 | B | 301 | FMN | C7M-C7 | 7.41 | 1.65 | 1.51 |
| 2 | 0 | 302 | FMN | C7M-C7 | 7.41 | 1.65 | 1.51 |
| 2 | p | 302 | FMN | C7M-C7 | 7.41 | 1.65 | 1.51 |
| 2 | 0 | 301 | FMN | C7M-C7 | 7.41 | 1.65 | 1.51 |
| 2 | G | 302 | FMN | C7M-C7 | 7.41 | 1.65 | 1.51 |
| 2 | 7 | 302 | FMN | C7M-C7 | 7.41 | 1.65 | 1.51 |
| 2 | J | 301 | FMN | C7M-C7 | 7.40 | 1.65 | 1.51 |
| 2 | m | 301 | FMN | C7M-C7 | 7.40 | 1.65 | 1.51 |
| 2 | k | 301 | FMN | C7M-C7 | 7.40 | 1.65 | 1.51 |
| 2 | O | 301 | FMN | C7M-C7 | 7.40 | 1.65 | 1.51 |
| 2 | C | 301 | FMN | C7M-C7 | 7.40 | 1.65 | 1.51 |
| 2 | A | 301 | FMN | C7M-C7 | 7.39 | 1.65 | 1.51 |
| 2 | X | 301 | FMN | C7M-C7 | 7.38 | 1.65 | 1.51 |
| 2 | 1 | 302 | FMN | C7M-C7 | 7.38 | 1.65 | 1.51 |
| 2 | E | 301 | FMN | C7M-C7 | 7.37 | 1.65 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 5 | 302 | FMN | C7M-C7 | 7.36 | 1.65 | 1.51 |
| 2 | f | 301 | FMN | C7M-C7 | 7.36 | 1.65 | 1.51 |
| 2 | 7 | 301 | FMN | C7M-C7 | 7.35 | 1.65 | 1.51 |
| 2 | 6 | 301 | FMN | C7M-C7 | 7.34 | 1.65 | 1.51 |
| 2 | i | 301 | FMN | C7M-C7 | 7.31 | 1.65 | 1.51 |
| 2 | n | 301 | FMN | C7M-C7 | 7.28 | 1.65 | 1.51 |
| 2 | X | 301 | FMN | C1'-C2' | 7.12 | 1.62 | 1.52 |
| 2 | a | 302 | FMN | C1'-C2' | 6.99 | 1.62 | 1.52 |
| 2 | r | 301 | FMN | C1'-C2' | 6.82 | 1.62 | 1.52 |
| 2 | a | 302 | FMN | C7M-C7 | 6.80 | 1.64 | 1.51 |
| 2 | s | 301 | FMN | C1'-C2' | 6.72 | 1.62 | 1.52 |
| 2 | C | 301 | FMN | C1'-C2' | 6.71 | 1.62 | 1.52 |
| 2 | k | 301 | FMN | C1'-C2' | 6.66 | 1.62 | 1.52 |
| 2 | T | 301 | FMN | C1'-C2' | 6.65 | 1.62 | 1.52 |
| 2 | a | 301 | FMN | C1'-C2' | 6.64 | 1.62 | 1.52 |
| 2 | E | 301 | FMN | C1'-C2' | 6.64 | 1.62 | 1.52 |
| 2 | j | 301 | FMN | C1'-C2' | 6.62 | 1.62 | 1.52 |
| 2 | M | 301 | FMN | C1'-C2' | 6.61 | 1.62 | 1.52 |
| 2 | 7 | 302 | FMN | C1'-C2' | 6.57 | 1.61 | 1.52 |
| 2 | h | 301 | FMN | C1'-C2' | 6.56 | 1.61 | 1.52 |
| 2 | W | 301 | FMN | C1'-C2' | 6.53 | 1.61 | 1.52 |
| 2 | c | 301 | FMN | C9-C9A | 6.53 | 1.50 | 1.39 |
| 2 | F | 301 | FMN | C1'-C2' | 6.51 | 1.61 | 1.52 |
| 2 | 4 | 301 | FMN | C1'-C2' | 6.50 | 1.61 | 1.52 |
| 2 | G | 301 | FMN | C9-C9A | 6.50 | 1.50 | 1.39 |
| 2 | r | 302 | FMN | C1'-C2' | 6.49 | 1.61 | 1.52 |
| 2 | N | 301 | FMN | C9-C9A | 6.48 | 1.50 | 1.39 |
| 2 | S | 301 | FMN | C9-C9A | 6.46 | 1.50 | 1.39 |
| 2 | Y | 301 | FMN | C1'-C2' | 6.46 | 1.61 | 1.52 |
| 2 | 2 | 301 | FMN | C9-C9A | 6.45 | 1.50 | 1.39 |
| 2 | 3 | 301 | FMN | C1'-C2' | 6.45 | 1.61 | 1.52 |
| 2 | A | 301 | FMN | C1'-C2' | 6.45 | 1.61 | 1.52 |
| 2 | V | 301 | FMN | C1'-C2' | 6.44 | 1.61 | 1.52 |
| 2 | c | 301 | FMN | C1'-C2' | 6.43 | 1.61 | 1.52 |
| 2 | V | 301 | FMN | C9-C9A | 6.42 | 1.50 | 1.39 |
| 2 | p | 302 | FMN | C9-C9A | 6.41 | 1.50 | 1.39 |
| 2 | m | 302 | FMN | C9-C9A | 6.41 | 1.50 | 1.39 |
| 2 | G | 301 | FMN | C1'-C2' | 6.40 | 1.61 | 1.52 |
| 2 | P | 301 | FMN | C9-C9A | 6.40 | 1.50 | 1.39 |
| 2 | q | 301 | FMN | C1'-C2' | 6.39 | 1.61 | 1.52 |
| 2 | M | 302 | FMN | C9-C9A | 6.38 | 1.50 | 1.39 |
| 2 | x | 301 | FMN | C1'-C2' | 6.37 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 7 | 302 | FMN | C9-C9A | 6.37 | 1.50 | 1.39 |
| 2 | m | 302 | FMN | C1'-C2' | 6.37 | 1.61 | 1.52 |
| 2 | 1 | 302 | FMN | C1'-C2' | 6.36 | 1.61 | 1.52 |
| 2 | E | 301 | FMN | C9-C9A | 6.36 | 1.50 | 1.39 |
| 2 | B | 301 | FMN | C9-C9A | 6.36 | 1.50 | 1.39 |
| 2 | 5 | 301 | FMN | C1'-C2' | 6.35 | 1.61 | 1.52 |
| 2 | 1 | 302 | FMN | C9-C9A | 6.35 | 1.50 | 1.39 |
| 2 | d | 301 | FMN | C9-C9A | 6.35 | 1.50 | 1.39 |
| 2 | n | 301 | FMN | C9-C9A | 6.34 | 1.49 | 1.39 |
| 2 | x | 301 | FMN | C9-C9A | 6.33 | 1.49 | 1.39 |
| 2 | 0 | 302 | FMN | C1'-C2' | 6.33 | 1.61 | 1.52 |
| 2 | 0 | 302 | FMN | C9-C9A | 6.32 | 1.49 | 1.39 |
| 2 | I | 301 | FMN | C1'-C2' | 6.32 | 1.61 | 1.52 |
| 2 | 0 | 301 | FMN | C9-C9A | 6.32 | 1.49 | 1.39 |
| 2 | C | 301 | FMN | C9-C9A | 6.31 | 1.49 | 1.39 |
| 2 | h | 302 | FMN | C1'-C2' | 6.31 | 1.61 | 1.52 |
| 2 | 1 | 301 | FMN | C1'-C2' | 6.30 | 1.61 | 1.52 |
| 2 | 6 | 301 | FMN | C9-C9A | 6.30 | 1.49 | 1.39 |
| 2 | Q | 301 | FMN | C9-C9A | 6.29 | 1.49 | 1.39 |
| 2 | w | 301 | FMN | C9-C9A | 6.29 | 1.49 | 1.39 |
| 2 | G | 302 | FMN | C9-C9A | 6.29 | 1.49 | 1.39 |
| 2 | 0 | 301 | FMN | C1'-C2' | 6.28 | 1.61 | 1.52 |
| 2 | i | 301 | FMN | C9-C9A | 6.28 | 1.49 | 1.39 |
| 2 | a | 302 | FMN | C9-C9A | 6.28 | 1.49 | 1.39 |
| 2 | G | 302 | FMN | C1'-C2' | 6.28 | 1.61 | 1.52 |
| 2 | D | 302 | FMN | C9-C9A | 6.28 | 1.49 | 1.39 |
| 2 | f | 301 | FMN | C9-C9A | 6.27 | 1.49 | 1.39 |
| 2 | J | 301 | FMN | C1'-C2' | 6.27 | 1.61 | 1.52 |
| 2 | R | 301 | FMN | C9-C9A | 6.26 | 1.49 | 1.39 |
| 2 | k | 301 | FMN | C9-C9A | 6.26 | 1.49 | 1.39 |
| 2 | u | 301 | FMN | C9-C9A | 6.26 | 1.49 | 1.39 |
| 2 | 6 | 301 | FMN | C1'-C2' | 6.26 | 1.61 | 1.52 |
| 2 | A | 301 | FMN | C9-C9A | 6.25 | 1.49 | 1.39 |
| 2 | R | 301 | FMN | C1'-C2' | 6.25 | 1.61 | 1.52 |
| 2 | e | 301 | FMN | C1'-C2' | 6.25 | 1.61 | 1.52 |
| 2 | 5 | 301 | FMN | C9-C9A | 6.25 | 1.49 | 1.39 |
| 2 | N | 301 | FMN | C1'-C2' | 6.25 | 1.61 | 1.52 |
| 2 | u | 301 | FMN | C1'-C2' | 6.25 | 1.61 | 1.52 |
| 2 | f | 301 | FMN | C1'-C2' | 6.24 | 1.61 | 1.52 |
| 2 | 4 | 301 | FMN | C9-C9A | 6.24 | 1.49 | 1.39 |
| 2 | q | 301 | FMN | C9-C9A | 6.24 | 1.49 | 1.39 |
| 2 | W | 301 | FMN | C9-C9A | 6.24 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | O | 301 | FMN | C9-C9A | 6.24 | 1.49 | 1.39 |
| 2 | e | 301 | FMN | C9-C9A | 6.24 | 1.49 | 1.39 |
| 2 | r | 302 | FMN | C9-C9A | 6.22 | 1.49 | 1.39 |
| 2 | D | 302 | FMN | C1'-C2' | 6.22 | 1.61 | 1.52 |
| 2 | p | 301 | FMN | C9-C9A | 6.22 | 1.49 | 1.39 |
| 2 | I | 301 | FMN | C9-C9A | 6.21 | 1.49 | 1.39 |
| 2 | J | 301 | FMN | C9-C9A | 6.21 | 1.49 | 1.39 |
| 2 | D | 301 | FMN | C9-C9A | 6.21 | 1.49 | 1.39 |
| 2 | M | 301 | FMN | C9-C9A | 6.20 | 1.49 | 1.39 |
| 2 | X | 301 | FMN | C9-C9A | 6.20 | 1.49 | 1.39 |
| 2 | 7 | 301 | FMN | C9-C9A | 6.20 | 1.49 | 1.39 |
| 2 | 3 | 301 | FMN | C9-C9A | 6.18 | 1.49 | 1.39 |
| 2 | m | 301 | FMN | C9-C9A | 6.18 | 1.49 | 1.39 |
| 2 | 1 | 301 | FMN | C9-C9A | 6.18 | 1.49 | 1.39 |
| 2 | h | 301 | FMN | C9-C9A | 6.18 | 1.49 | 1.39 |
| 2 | s | 301 | FMN | C9-C9A | 6.17 | 1.49 | 1.39 |
| 2 | a | 301 | FMN | C9-C9A | 6.17 | 1.49 | 1.39 |
| 2 | F | 301 | FMN | C9-C9A | 6.17 | 1.49 | 1.39 |
| 2 | p | 301 | FMN | C1'-C2' | 6.16 | 1.61 | 1.52 |
| 2 | r | 301 | FMN | C9-C9A | 6.16 | 1.49 | 1.39 |
| 2 | j | 301 | FMN | C9-C9A | 6.15 | 1.49 | 1.39 |
| 2 | 5 | 302 | FMN | C9-C9A | 6.14 | 1.49 | 1.39 |
| 2 | P | 301 | FMN | C1'-C2' | 6.14 | 1.61 | 1.52 |
| 2 | i | 301 | FMN | C1'-C2' | 6.13 | 1.61 | 1.52 |
| 2 | d | 301 | FMN | C1'-C2' | 6.13 | 1.61 | 1.52 |
| 2 | T | 301 | FMN | C9-C9A | 6.13 | 1.49 | 1.39 |
| 2 | Q | 301 | FMN | C1'-C2' | 6.12 | 1.61 | 1.52 |
| 2 | t | 301 | FMN | C1'-C2' | 6.12 | 1.61 | 1.52 |
| 2 | 5 | 302 | FMN | C1'-C2' | 6.11 | 1.61 | 1.52 |
| 2 | X | 301 | FMN | C5'-C4' | 6.10 | 1.60 | 1.51 |
| 2 | Y | 301 | FMN | C9-C9A | 6.10 | 1.49 | 1.39 |
| 2 | 2 | 301 | FMN | C1'-C2' | 6.09 | 1.61 | 1.52 |
| 2 | t | 301 | FMN | C9-C9A | 6.09 | 1.49 | 1.39 |
| 2 | D | 301 | FMN | C1'-C2' | 6.08 | 1.61 | 1.52 |
| 2 | 7 | 302 | FMN | C5'-C4' | 6.07 | 1.60 | 1.51 |
| 2 | h | 302 | FMN | C9-C9A | 6.06 | 1.49 | 1.39 |
| 2 | O | 301 | FMN | C1'-C2' | 6.04 | 1.61 | 1.52 |
| 2 | B | 301 | FMN | C1'-C2' | 6.01 | 1.61 | 1.52 |
| 2 | Y | 301 | FMN | C5'-C4' | 5.98 | 1.60 | 1.51 |
| 2 | m | 301 | FMN | C1'-C2' | 5.97 | 1.61 | 1.52 |
| 2 | n | 301 | FMN | C1'-C2' | 5.97 | 1.61 | 1.52 |
| 2 | M | 302 | FMN | C1'-C2' | 5.95 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | w | 301 | FMN | C1'-C2' | 5.94 | 1.61 | 1.52 |
| 2 | 5 | 301 | FMN | C5'-C4' | 5.94 | 1.60 | 1.51 |
| 2 | X | 301 | FMN | C4'-C3' | 5.92 | 1.64 | 1.53 |
| 2 | 6 | 301 | FMN | C5'-C4' | 5.91 | 1.60 | 1.51 |
| 2 | d | 301 | FMN | C5'-C4' | 5.91 | 1.60 | 1.51 |
| 2 | 3 | 301 | FMN | C5'-C4' | 5.91 | 1.60 | 1.51 |
| 2 | R | 301 | FMN | C5'-C4' | 5.90 | 1.60 | 1.51 |
| 2 | p | 302 | FMN | C1'-C2' | 5.90 | 1.61 | 1.52 |
| 2 | 1 | 301 | FMN | C5'-C4' | 5.90 | 1.60 | 1.51 |
| 2 | E | 301 | FMN | C5'-C4' | 5.89 | 1.60 | 1.51 |
| 2 | r | 301 | FMN | C5'-C4' | 5.88 | 1.60 | 1.51 |
| 2 | S | 301 | FMN | C1'-C2' | 5.87 | 1.60 | 1.52 |
| 2 | t | 301 | FMN | C5'-C4' | 5.87 | 1.60 | 1.51 |
| 2 | 7 | 301 | FMN | C1'-C2' | 5.84 | 1.60 | 1.52 |
| 2 | P | 301 | FMN | C5'-C4' | 5.83 | 1.60 | 1.51 |
| 2 | q | 301 | FMN | C5'-C4' | 5.82 | 1.60 | 1.51 |
| 2 | k | 301 | FMN | C5'-C4' | 5.80 | 1.60 | 1.51 |
| 2 | p | 301 | FMN | C5'-C4' | 5.80 | 1.60 | 1.51 |
| 2 | m | 301 | FMN | C5'-C4' | 5.80 | 1.60 | 1.51 |
| 2 | j | 301 | FMN | C5'-C4' | 5.79 | 1.60 | 1.51 |
| 2 | 0 | 302 | FMN | C5'-C4' | 5.78 | 1.60 | 1.51 |
| 2 | G | 301 | FMN | C5'-C4' | 5.78 | 1.60 | 1.51 |
| 2 | I | 301 | FMN | C5'-C4' | 5.77 | 1.60 | 1.51 |
| 2 | V | 301 | FMN | C4A-N5 | 5.76 | 1.42 | 1.30 |
| 2 | C | 301 | FMN | C5'-C4' | 5.75 | 1.59 | 1.51 |
| 2 | M | 301 | FMN | C5'-C4' | 5.74 | 1.59 | 1.51 |
| 2 | S | 301 | FMN | C5'-C4' | 5.74 | 1.59 | 1.51 |
| 2 | s | 301 | FMN | C5'-C4' | 5.73 | 1.59 | 1.51 |
| 2 | i | 301 | FMN | C5'-C4' | 5.73 | 1.59 | 1.51 |
| 2 | M | 302 | FMN | C5'-C4' | 5.73 | 1.59 | 1.51 |
| 2 | e | 301 | FMN | C5'-C4' | 5.72 | 1.59 | 1.51 |
| 2 | P | 301 | FMN | C4A-N5 | 5.71 | 1.41 | 1.30 |
| 2 | 2 | 301 | FMN | C4A-N5 | 5.70 | 1.41 | 1.30 |
| 2 | m | 302 | FMN | C4A-N5 | 5.69 | 1.41 | 1.30 |
| 2 | p | 302 | FMN | C5'-C4' | 5.68 | 1.59 | 1.51 |
| 2 | G | 301 | FMN | C4A-N5 | 5.68 | 1.41 | 1.30 |
| 2 | S | 301 | FMN | C4A-N5 | 5.67 | 1.41 | 1.30 |
| 2 | N | 301 | FMN | C4A-N5 | 5.67 | 1.41 | 1.30 |
| 2 | V | 301 | FMN | C5'-C4' | 5.66 | 1.59 | 1.51 |
| 2 | h | 301 | FMN | C5'-C4' | 5.66 | 1.59 | 1.51 |
| 2 | 3 | 301 | FMN | C4'-C3' | 5.63 | 1.64 | 1.53 |
| 2 | 2 | 301 | FMN | C5'-C4' | 5.63 | 1.59 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 5 | 302 | FMN | C5'-C4' | 5.63 | 1.59 | 1.51 |
| 2 | c | 301 | FMN | C4A-N5 | 5.63 | 1.41 | 1.30 |
| 2 | E | 301 | FMN | C4'-C3' | 5.63 | 1.64 | 1.53 |
| 2 | 7 | 301 | FMN | C5'-C4' | 5.61 | 1.59 | 1.51 |
| 2 | A | 301 | FMN | C5'-C4' | 5.61 | 1.59 | 1.51 |
| 2 | O | 301 | FMN | C5'-C4' | 5.61 | 1.59 | 1.51 |
| 2 | N | 301 | FMN | C5'-C4' | 5.60 | 1.59 | 1.51 |
| 2 | D | 301 | FMN | C5'-C4' | 5.59 | 1.59 | 1.51 |
| 2 | f | 301 | FMN | C5'-C4' | 5.59 | 1.59 | 1.51 |
| 2 | B | 301 | FMN | C5'-C4' | 5.59 | 1.59 | 1.51 |
| 2 | Q | 301 | FMN | C5'-C4' | 5.59 | 1.59 | 1.51 |
| 2 | a | 301 | FMN | C4A-N5 | 5.57 | 1.41 | 1.30 |
| 2 | s | 301 | FMN | C4A-N5 | 5.57 | 1.41 | 1.30 |
| 2 | W | 301 | FMN | C5'-C4' | 5.57 | 1.59 | 1.51 |
| 2 | a | 302 | FMN | C4A-N5 | 5.56 | 1.41 | 1.30 |
| 2 | m | 302 | FMN | C5'-C4' | 5.55 | 1.59 | 1.51 |
| 2 | p | 302 | FMN | C4'-C3' | 5.55 | 1.63 | 1.53 |
| 2 | w | 301 | FMN | C5'-C4' | 5.55 | 1.59 | 1.51 |
| 2 | A | 301 | FMN | C4'-C3' | 5.55 | 1.63 | 1.53 |
| 2 | q | 301 | FMN | C4A-N5 | 5.54 | 1.41 | 1.30 |
| 2 | h | 302 | FMN | C4A-N5 | 5.53 | 1.41 | 1.30 |
| 2 | W | 301 | FMN | C4A-N5 | 5.52 | 1.41 | 1.30 |
| 2 | i | 301 | FMN | C4A-N5 | 5.52 | 1.41 | 1.30 |
| 2 | x | 301 | FMN | C5'-C4' | 5.52 | 1.59 | 1.51 |
| 2 | c | 301 | FMN | C5'-C4' | 5.51 | 1.59 | 1.51 |
| 2 | O | 301 | FMN | C4A-N5 | 5.51 | 1.41 | 1.30 |
| 2 | C | 301 | FMN | C4A-N5 | 5.50 | 1.41 | 1.30 |
| 2 | M | 301 | FMN | C4A-N5 | 5.50 | 1.41 | 1.30 |
| 2 | r | 301 | FMN | C4A-N5 | 5.50 | 1.41 | 1.30 |
| 2 | T | 301 | FMN | C4A-N5 | 5.50 | 1.41 | 1.30 |
| 2 | 5 | 301 | FMN | C4A-N5 | 5.50 | 1.41 | 1.30 |
| 2 | Q | 301 | FMN | C4A-N5 | 5.49 | 1.41 | 1.30 |
| 2 | 3 | 301 | FMN | C4A-N5 | 5.49 | 1.41 | 1.30 |
| 2 | r | 302 | FMN | C4A-N5 | 5.49 | 1.41 | 1.30 |
| 2 | x | 301 | FMN | C4'-C3' | 5.49 | 1.63 | 1.53 |
| 2 | I | 301 | FMN | C4A-N5 | 5.49 | 1.41 | 1.30 |
| 2 | r | 302 | FMN | C5'-C4' | 5.49 | 1.59 | 1.51 |
| 2 | P | 301 | FMN | C6-C5A | 5.49 | 1.48 | 1.40 |
| 2 | 7 | 302 | FMN | C4'-C3' | 5.48 | 1.63 | 1.53 |
| 2 | 0 | 301 | FMN | C5'-C4' | 5.48 | 1.59 | 1.51 |
| 2 | V | 301 | FMN | C6-C5A | 5.48 | 1.48 | 1.40 |
| 2 | Y | 301 | FMN | C4A-N5 | 5.48 | 1.41 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | w | 301 | FMN | C4A-N5 | 5.48 | 1.41 | 1.30 |
| 2 | n | 301 | FMN | C5'-C4' | 5.47 | 1.59 | 1.51 |
| 2 | l | 301 | FMN | C4A-N5 | 5.47 | 1.41 | 1.30 |
| 2 | 4 | 301 | FMN | C4A-N5 | 5.47 | 1.41 | 1.30 |
| 2 | p | 301 | FMN | C4A-N5 | 5.46 | 1.41 | 1.30 |
| 2 | F | 301 | FMN | C4A-N5 | 5.46 | 1.41 | 1.30 |
| 2 | J | 301 | FMN | C4A-N5 | 5.46 | 1.41 | 1.30 |
| 2 | A | 301 | FMN | C4A-N5 | 5.46 | 1.41 | 1.30 |
| 2 | Y | 301 | FMN | C4'-C3' | 5.46 | 1.63 | 1.53 |
| 2 | k | 301 | FMN | C4A-N5 | 5.46 | 1.41 | 1.30 |
| 2 | u | 301 | FMN | C4A-N5 | 5.46 | 1.41 | 1.30 |
| 2 | t | 301 | FMN | C4A-N5 | 5.45 | 1.41 | 1.30 |
| 2 | u | 301 | FMN | C5'-C4' | 5.45 | 1.59 | 1.51 |
| 2 | G | 302 | FMN | C5'-C4' | 5.45 | 1.59 | 1.51 |
| 2 | 0 | 301 | FMN | C4A-N5 | 5.45 | 1.41 | 1.30 |
| 2 | a | 302 | FMN | C5'-C4' | 5.44 | 1.59 | 1.51 |
| 2 | m | 301 | FMN | C4A-N5 | 5.44 | 1.41 | 1.30 |
| 2 | n | 301 | FMN | C4A-N5 | 5.44 | 1.41 | 1.30 |
| 2 | 7 | 301 | FMN | C4A-N5 | 5.44 | 1.41 | 1.30 |
| 2 | D | 301 | FMN | C4A-N5 | 5.44 | 1.41 | 1.30 |
| 2 | 2 | 301 | FMN | C6-C5A | 5.43 | 1.48 | 1.40 |
| 2 | 0 | 302 | FMN | C4A-N5 | 5.43 | 1.41 | 1.30 |
| 2 | p | 302 | FMN | C4A-N5 | 5.43 | 1.41 | 1.30 |
| 2 | G | 302 | FMN | C4A-N5 | 5.43 | 1.41 | 1.30 |
| 2 | k | 301 | FMN | C4'-C3' | 5.42 | 1.63 | 1.53 |
| 2 | B | 301 | FMN | C4A-N5 | 5.42 | 1.41 | 1.30 |
| 2 | G | 301 | FMN | C4'-C3' | 5.41 | 1.63 | 1.53 |
| 2 | a | 301 | FMN | C5'-C4' | 5.41 | 1.59 | 1.51 |
| 2 | s | 301 | FMN | C4'-C3' | 5.41 | 1.63 | 1.53 |
| 2 | x | 301 | FMN | C4A-N5 | 5.40 | 1.41 | 1.30 |
| 2 | F | 301 | FMN | C5'-C4' | 5.40 | 1.59 | 1.51 |
| 2 | M | 302 | FMN | C4A-N5 | 5.38 | 1.41 | 1.30 |
| 2 | D | 302 | FMN | C4'-C3' | 5.38 | 1.63 | 1.53 |
| 2 | h | 301 | FMN | C4A-N5 | 5.38 | 1.41 | 1.30 |
| 2 | m | 302 | FMN | C6-C5A | 5.38 | 1.48 | 1.40 |
| 2 | C | 301 | FMN | C4'-C3' | 5.37 | 1.63 | 1.53 |
| 2 | M | 301 | FMN | C4'-C3' | 5.37 | 1.63 | 1.53 |
| 2 | h | 302 | FMN | C5'-C4' | 5.37 | 1.59 | 1.51 |
| 2 | f | 301 | FMN | C4A-N5 | 5.37 | 1.41 | 1.30 |
| 2 | S | 301 | FMN | C6-C5A | 5.36 | 1.48 | 1.40 |
| 2 | 0 | 302 | FMN | C4'-C3' | 5.36 | 1.63 | 1.53 |
| 2 | 7 | 302 | FMN | C4A-N5 | 5.36 | 1.41 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | d | 301 | FMN | C4A-N5 | 5.36 | 1.41 | 1.30 |
| 2 | E | 301 | FMN | C4A-N5 | 5.36 | 1.41 | 1.30 |
| 2 | X | 301 | FMN | C4A-N5 | 5.36 | 1.41 | 1.30 |
| 2 | 4 | 301 | FMN | C4'-C3' | 5.35 | 1.63 | 1.53 |
| 2 | G | 301 | FMN | C6-C5A | 5.35 | 1.48 | 1.40 |
| 2 | D | 302 | FMN | C4A-N5 | 5.35 | 1.41 | 1.30 |
| 2 | j | 301 | FMN | C4A-N5 | 5.35 | 1.41 | 1.30 |
| 2 | R | 301 | FMN | C4A-N5 | 5.35 | 1.41 | 1.30 |
| 2 | h | 301 | FMN | C4'-C3' | 5.34 | 1.63 | 1.53 |
| 2 | e | 301 | FMN | C4A-N5 | 5.34 | 1.41 | 1.30 |
| 2 | d | 301 | FMN | C4'-C3' | 5.33 | 1.63 | 1.53 |
| 2 | 5 | 302 | FMN | C4A-N5 | 5.33 | 1.41 | 1.30 |
| 2 | e | 301 | FMN | C4'-C3' | 5.32 | 1.63 | 1.53 |
| 2 | 4 | 301 | FMN | C5'-C4' | 5.32 | 1.59 | 1.51 |
| 2 | 1 | 302 | FMN | C4A-N5 | 5.32 | 1.41 | 1.30 |
| 2 | q | 301 | FMN | C4'-C3' | 5.32 | 1.63 | 1.53 |
| 2 | M | 302 | FMN | C4'-C3' | 5.31 | 1.63 | 1.53 |
| 2 | 1 | 302 | FMN | C5'-C4' | 5.31 | 1.59 | 1.51 |
| 2 | 0 | 301 | FMN | C4'-C3' | 5.30 | 1.63 | 1.53 |
| 2 | D | 302 | FMN | C5'-C4' | 5.30 | 1.59 | 1.51 |
| 2 | R | 301 | FMN | C4'-C3' | 5.29 | 1.63 | 1.53 |
| 2 | N | 301 | FMN | C6-C5A | 5.29 | 1.48 | 1.40 |
| 2 | 5 | 301 | FMN | C4'-C3' | 5.29 | 1.63 | 1.53 |
| 2 | c | 301 | FMN | C6-C5A | 5.29 | 1.48 | 1.40 |
| 2 | 6 | 301 | FMN | C4'-C3' | 5.28 | 1.63 | 1.53 |
| 2 | 1 | 302 | FMN | C4'-C3' | 5.27 | 1.63 | 1.53 |
| 2 | r | 302 | FMN | C4'-C3' | 5.27 | 1.63 | 1.53 |
| 2 | W | 301 | FMN | C4'-C3' | 5.27 | 1.63 | 1.53 |
| 2 | c | 301 | FMN | C4'-C3' | 5.26 | 1.63 | 1.53 |
| 2 | r | 301 | FMN | C4'-C3' | 5.26 | 1.63 | 1.53 |
| 2 | 6 | 301 | FMN | C4A-N5 | 5.26 | 1.41 | 1.30 |
| 2 | Q | 301 | FMN | C4'-C3' | 5.24 | 1.63 | 1.53 |
| 2 | n | 301 | FMN | C4'-C3' | 5.23 | 1.63 | 1.53 |
| 2 | D | 301 | FMN | C4'-C3' | 5.21 | 1.63 | 1.53 |
| 2 | a | 301 | FMN | C4'-C3' | 5.21 | 1.63 | 1.53 |
| 2 | a | 302 | FMN | C4'-C3' | 5.20 | 1.63 | 1.53 |
| 2 | h | 302 | FMN | C4'-C3' | 5.20 | 1.63 | 1.53 |
| 2 | p | 301 | FMN | C4'-C3' | 5.20 | 1.63 | 1.53 |
| 2 | 1 | 301 | FMN | C4'-C3' | 5.19 | 1.63 | 1.53 |
| 2 | 2 | 301 | FMN | C4'-C3' | 5.18 | 1.63 | 1.53 |
| 2 | G | 302 | FMN | C4'-C3' | 5.18 | 1.63 | 1.53 |
| 2 | I | 301 | FMN | C4'-C3' | 5.18 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | j | 301 | FMN | C4'-C3' | 5.17 | 1.63 | 1.53 |
| 2 | 0 | 301 | FMN | C6-C5A | 5.15 | 1.48 | 1.40 |
| 2 | J | 301 | FMN | C4'-C3' | 5.15 | 1.63 | 1.53 |
| 2 | u | 301 | FMN | C4'-C3' | 5.14 | 1.63 | 1.53 |
| 2 | O | 301 | FMN | C6-C5A | 5.14 | 1.48 | 1.40 |
| 2 | m | 301 | FMN | C4'-C3' | 5.14 | 1.63 | 1.53 |
| 2 | S | 301 | FMN | C4'-C3' | 5.13 | 1.63 | 1.53 |
| 2 | 5 | 302 | FMN | C4'-C3' | 5.12 | 1.63 | 1.53 |
| 2 | F | 301 | FMN | C4'-C3' | 5.11 | 1.63 | 1.53 |
| 2 | N | 301 | FMN | C4'-C3' | 5.11 | 1.63 | 1.53 |
| 2 | i | 301 | FMN | C4'-C3' | 5.11 | 1.63 | 1.53 |
| 2 | i | 301 | FMN | C6-C5A | 5.10 | 1.48 | 1.40 |
| 2 | t | 301 | FMN | C6-C5A | 5.10 | 1.48 | 1.40 |
| 2 | h | 302 | FMN | C6-C5A | 5.09 | 1.48 | 1.40 |
| 2 | n | 301 | FMN | C6-C5A | 5.08 | 1.47 | 1.40 |
| 2 | m | 302 | FMN | C4'-C3' | 5.07 | 1.63 | 1.53 |
| 2 | M | 302 | FMN | C6-C5A | 5.07 | 1.47 | 1.40 |
| 2 | P | 301 | FMN | C4'-C3' | 5.06 | 1.63 | 1.53 |
| 2 | T | 301 | FMN | C5'-C4' | 5.06 | 1.59 | 1.51 |
| 2 | w | 301 | FMN | C4'-C3' | 5.06 | 1.63 | 1.53 |
| 2 | W | 301 | FMN | C6-C5A | 5.05 | 1.47 | 1.40 |
| 2 | t | 301 | FMN | C4'-C3' | 5.04 | 1.63 | 1.53 |
| 2 | A | 301 | FMN | C6-C5A | 5.03 | 1.47 | 1.40 |
| 2 | G | 302 | FMN | C6-C5A | 5.03 | 1.47 | 1.40 |
| 2 | 7 | 301 | FMN | C6-C5A | 5.03 | 1.47 | 1.40 |
| 2 | I | 301 | FMN | C6-C5A | 5.03 | 1.47 | 1.40 |
| 2 | f | 301 | FMN | C4'-C3' | 5.02 | 1.62 | 1.53 |
| 2 | M | 301 | FMN | C6-C5A | 5.02 | 1.47 | 1.40 |
| 2 | Y | 301 | FMN | C6-C5A | 5.02 | 1.47 | 1.40 |
| 2 | m | 301 | FMN | C6-C5A | 5.00 | 1.47 | 1.40 |
| 2 | D | 301 | FMN | C6-C5A | 5.00 | 1.47 | 1.40 |
| 2 | p | 302 | FMN | C6-C5A | 5.00 | 1.47 | 1.40 |
| 2 | w | 301 | FMN | C6-C5A | 4.99 | 1.47 | 1.40 |
| 2 | 5 | 301 | FMN | C6-C5A | 4.99 | 1.47 | 1.40 |
| 2 | s | 301 | FMN | C6-C5A | 4.98 | 1.47 | 1.40 |
| 2 | B | 301 | FMN | C4'-C3' | 4.98 | 1.62 | 1.53 |
| 2 | N | 301 | FMN | C6-C7 | 4.98 | 1.46 | 1.39 |
| 2 | F | 301 | FMN | C6-C5A | 4.98 | 1.47 | 1.40 |
| 2 | q | 301 | FMN | C6-C5A | 4.98 | 1.47 | 1.40 |
| 2 | a | 301 | FMN | C6-C5A | 4.97 | 1.47 | 1.40 |
| 2 | Q | 301 | FMN | C6-C5A | 4.97 | 1.47 | 1.40 |
| 2 | O | 301 | FMN | C4'-C3' | 4.97 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | T | 301 | FMN | C6-C7 | 4.97 | 1.46 | 1.39 |
| 2 | 3 | 301 | FMN | C6-C5A | 4.97 | 1.47 | 1.40 |
| 2 | E | 301 | FMN | C6-C5A | 4.96 | 1.47 | 1.40 |
| 2 | r | 301 | FMN | C6-C5A | 4.96 | 1.47 | 1.40 |
| 2 | C | 301 | FMN | C6-C5A | 4.96 | 1.47 | 1.40 |
| 2 | p | 301 | FMN | C6-C5A | 4.96 | 1.47 | 1.40 |
| 2 | f | 301 | FMN | C6-C5A | 4.96 | 1.47 | 1.40 |
| 2 | 7 | 301 | FMN | C4'-C3' | 4.95 | 1.62 | 1.53 |
| 2 | a | 301 | FMN | C6-C7 | 4.95 | 1.46 | 1.39 |
| 2 | r | 302 | FMN | C6-C5A | 4.94 | 1.47 | 1.40 |
| 2 | u | 301 | FMN | C6-C5A | 4.94 | 1.47 | 1.40 |
| 2 | 4 | 301 | FMN | C6-C5A | 4.93 | 1.47 | 1.40 |
| 2 | 1 | 301 | FMN | C6-C5A | 4.93 | 1.47 | 1.40 |
| 2 | W | 301 | FMN | C6-C7 | 4.92 | 1.46 | 1.39 |
| 2 | 5 | 301 | FMN | C6-C7 | 4.92 | 1.46 | 1.39 |
| 2 | 0 | 302 | FMN | C6-C5A | 4.91 | 1.47 | 1.40 |
| 2 | S | 301 | FMN | C6-C7 | 4.90 | 1.46 | 1.39 |
| 2 | J | 301 | FMN | C6-C5A | 4.90 | 1.47 | 1.40 |
| 2 | 1 | 301 | FMN | C6-C7 | 4.90 | 1.46 | 1.39 |
| 2 | s | 301 | FMN | C6-C7 | 4.90 | 1.46 | 1.39 |
| 2 | B | 301 | FMN | C6-C5A | 4.90 | 1.47 | 1.40 |
| 2 | k | 301 | FMN | C6-C5A | 4.90 | 1.47 | 1.40 |
| 2 | I | 301 | FMN | C6-C7 | 4.89 | 1.46 | 1.39 |
| 2 | T | 301 | FMN | C6-C5A | 4.89 | 1.47 | 1.40 |
| 2 | D | 302 | FMN | C6-C5A | 4.89 | 1.47 | 1.40 |
| 2 | X | 301 | FMN | C6-C5A | 4.88 | 1.47 | 1.40 |
| 2 | d | 301 | FMN | C6-C5A | 4.88 | 1.47 | 1.40 |
| 2 | h | 301 | FMN | C6-C5A | 4.88 | 1.47 | 1.40 |
| 2 | p | 301 | FMN | C6-C7 | 4.88 | 1.46 | 1.39 |
| 2 | R | 301 | FMN | C6-C5A | 4.88 | 1.47 | 1.40 |
| 2 | 5 | 302 | FMN | C6-C5A | 4.88 | 1.47 | 1.40 |
| 2 | 6 | 301 | FMN | C6-C5A | 4.88 | 1.47 | 1.40 |
| 2 | c | 301 | FMN | C6-C7 | 4.87 | 1.46 | 1.39 |
| 2 | Y | 301 | FMN | C6-C7 | 4.85 | 1.46 | 1.39 |
| 2 | e | 301 | FMN | C6-C5A | 4.84 | 1.47 | 1.40 |
| 2 | M | 301 | FMN | C6-C7 | 4.84 | 1.46 | 1.39 |
| 2 | h | 301 | FMN | C6-C7 | 4.83 | 1.46 | 1.39 |
| 2 | F | 301 | FMN | C6-C7 | 4.82 | 1.46 | 1.39 |
| 2 | h | 302 | FMN | C6-C7 | 4.82 | 1.46 | 1.39 |
| 2 | r | 302 | FMN | C6-C7 | 4.82 | 1.46 | 1.39 |
| 2 | x | 301 | FMN | C6-C5A | 4.82 | 1.47 | 1.40 |
| 2 | 3 | 301 | FMN | C6-C7 | 4.82 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | u | 301 | FMN | C6-C7 | 4.82 | 1.46 | 1.39 |
| 2 | 7 | 302 | FMN | C6-C5A | 4.80 | 1.47 | 1.40 |
| 2 | D | 301 | FMN | C6-C7 | 4.80 | 1.46 | 1.39 |
| 2 | a | 302 | FMN | C6-C7 | 4.79 | 1.46 | 1.39 |
| 2 | V | 301 | FMN | C4'-C3' | 4.79 | 1.62 | 1.53 |
| 2 | G | 301 | FMN | C6-C7 | 4.78 | 1.46 | 1.39 |
| 2 | V | 301 | FMN | C10-N1 | 4.78 | 1.43 | 1.33 |
| 2 | Q | 301 | FMN | C6-C7 | 4.77 | 1.46 | 1.39 |
| 2 | J | 301 | FMN | C5'-C4' | 4.77 | 1.58 | 1.51 |
| 2 | P | 301 | FMN | C6-C7 | 4.77 | 1.46 | 1.39 |
| 2 | j | 301 | FMN | C6-C5A | 4.77 | 1.47 | 1.40 |
| 2 | 2 | 301 | FMN | C6-C7 | 4.77 | 1.46 | 1.39 |
| 2 | 2 | 301 | FMN | C10-N1 | 4.77 | 1.43 | 1.33 |
| 2 | 1 | 302 | FMN | C6-C5A | 4.77 | 1.47 | 1.40 |
| 2 | V | 301 | FMN | C6-C7 | 4.75 | 1.46 | 1.39 |
| 2 | a | 302 | FMN | C6-C5A | 4.75 | 1.47 | 1.40 |
| 2 | a | 302 | FMN | C8M-C8 | 4.75 | 1.60 | 1.51 |
| 2 | m | 302 | FMN | C6-C7 | 4.75 | 1.46 | 1.39 |
| 2 | m | 302 | FMN | C10-N1 | 4.73 | 1.42 | 1.33 |
| 2 | r | 301 | FMN | C6-C7 | 4.73 | 1.46 | 1.39 |
| 2 | j | 301 | FMN | C6-C7 | 4.71 | 1.46 | 1.39 |
| 2 | G | 301 | FMN | C10-N1 | 4.71 | 1.42 | 1.33 |
| 2 | 4 | 301 | FMN | C6-C7 | 4.70 | 1.46 | 1.39 |
| 2 | P | 301 | FMN | C10-N1 | 4.70 | 1.42 | 1.33 |
| 2 | 0 | 301 | FMN | C10-N1 | 4.69 | 1.42 | 1.33 |
| 2 | e | 301 | FMN | P-O5' | 4.69 | 1.75 | 1.60 |
| 2 | N | 301 | FMN | C10-N1 | 4.69 | 1.42 | 1.33 |
| 2 | S | 301 | FMN | C10-N1 | 4.68 | 1.42 | 1.33 |
| 2 | c | 301 | FMN | C10-N1 | 4.66 | 1.42 | 1.33 |
| 2 | A | 301 | FMN | C6-C7 | 4.65 | 1.46 | 1.39 |
| 2 | V | 301 | FMN | P-O5' | 4.64 | 1.75 | 1.60 |
| 2 | X | 301 | FMN | C2'-C3' | 4.61 | 1.62 | 1.53 |
| 2 | p | 302 | FMN | C6-C7 | 4.61 | 1.46 | 1.39 |
| 2 | w | 301 | FMN | C10-N1 | 4.61 | 1.42 | 1.33 |
| 2 | k | 301 | FMN | C6-C7 | 4.60 | 1.46 | 1.39 |
| 2 | T | 301 | FMN | P-O5' | 4.60 | 1.75 | 1.60 |
| 2 | 7 | 302 | FMN | P-O5' | 4.60 | 1.75 | 1.60 |
| 2 | m | 301 | FMN | C6-C7 | 4.59 | 1.46 | 1.39 |
| 2 | i | 301 | FMN | C10-N1 | 4.59 | 1.42 | 1.33 |
| 2 | T | 301 | FMN | C4'-C3' | 4.59 | 1.62 | 1.53 |
| 2 | E | 301 | FMN | C6-C7 | 4.58 | 1.46 | 1.39 |
| 2 | h | 301 | FMN | P-O5' | 4.58 | 1.75 | 1.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | k | 301 | FMN | P-O5' | 4.57 | 1.74 | 1.60 |
| 2 | d | 301 | FMN | C10-N1 | 4.57 | 1.42 | 1.33 |
| 2 | n | 301 | FMN | C10-N1 | 4.57 | 1.42 | 1.33 |
| 2 | R | 301 | FMN | P-O5' | 4.57 | 1.74 | 1.60 |
| 2 | s | 301 | FMN | P-O5' | 4.57 | 1.74 | 1.60 |
| 2 | G | 302 | FMN | P-O5' | 4.57 | 1.74 | 1.60 |
| 2 | 0 | 302 | FMN | C6-C7 | 4.56 | 1.46 | 1.39 |
| 2 | e | 301 | FMN | C6-C7 | 4.56 | 1.46 | 1.39 |
| 2 | q | 301 | FMN | P-O5' | 4.56 | 1.74 | 1.60 |
| 2 | S | 301 | FMN | P-O5' | 4.56 | 1.74 | 1.60 |
| 2 | 4 | 301 | FMN | P-O5' | 4.56 | 1.74 | 1.60 |
| 2 | P | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | M | 302 | FMN | C10-N1 | 4.55 | 1.42 | 1.33 |
| 2 | A | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | G | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | x | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | 3 | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | i | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | Y | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | p | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | W | 301 | FMN | P-O5' | 4.55 | 1.74 | 1.60 |
| 2 | X | 301 | FMN | C10-N1 | 4.54 | 1.42 | 1.33 |
| 2 | O | 301 | FMN | C10-N1 | 4.54 | 1.42 | 1.33 |
| 2 | c | 301 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | 6 | 301 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | C | 301 | FMN | C6-C7 | 4.54 | 1.46 | 1.39 |
| 2 | 7 | 301 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | C | 301 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | d | 301 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | a | 302 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | n | 301 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | 2 | 301 | FMN | P-O5' | 4.54 | 1.74 | 1.60 |
| 2 | B | 301 | FMN | C6-C7 | 4.53 | 1.46 | 1.39 |
| 2 | e | 301 | FMN | C10-N1 | 4.53 | 1.42 | 1.33 |
| 2 | R | 301 | FMN | C10-N1 | 4.53 | 1.42 | 1.33 |
| 2 | x | 301 | FMN | C6-C7 | 4.53 | 1.46 | 1.39 |
| 2 | f | 301 | FMN | P-O5' | 4.53 | 1.74 | 1.60 |
| 2 | I | 301 | FMN | P-O5' | 4.52 | 1.74 | 1.60 |
| 2 | t | 301 | FMN | C6-C7 | 4.52 | 1.46 | 1.39 |
| 2 | 7 | 301 | FMN | C6-C7 | 4.52 | 1.46 | 1.39 |
| 2 | r | 301 | FMN | P-O5' | 4.52 | 1.74 | 1.60 |
| 2 | A | 301 | FMN | C10-N1 | 4.52 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | t | 301 | FMN | C10-N1 | 4.52 | 1.42 | 1.33 |
| 2 | 0 | 302 | FMN | P-O5' | 4.51 | 1.74 | 1.60 |
| 2 | D | 301 | FMN | P-O5' | 4.51 | 1.74 | 1.60 |
| 2 | j | 301 | FMN | P-O5' | 4.51 | 1.74 | 1.60 |
| 2 | 7 | 301 | FMN | C10-N1 | 4.51 | 1.42 | 1.33 |
| 2 | w | 301 | FMN | P-O5' | 4.51 | 1.74 | 1.60 |
| 2 | N | 301 | FMN | P-O5' | 4.51 | 1.74 | 1.60 |
| 2 | 5 | 302 | FMN | P-O5' | 4.51 | 1.74 | 1.60 |
| 2 | q | 301 | FMN | C6-C7 | 4.51 | 1.46 | 1.39 |
| 2 | 1 | 301 | FMN | P-O5' | 4.51 | 1.74 | 1.60 |
| 2 | D | 301 | FMN | C10-N1 | 4.51 | 1.42 | 1.33 |
| 2 | 0 | 301 | FMN | P-O5' | 4.50 | 1.74 | 1.60 |
| 2 | G | 302 | FMN | C10-N1 | 4.50 | 1.42 | 1.33 |
| 2 | E | 301 | FMN | P-O5' | 4.50 | 1.74 | 1.60 |
| 2 | D | 302 | FMN | C10-N1 | 4.50 | 1.42 | 1.33 |
| 2 | F | 301 | FMN | P-O5' | 4.50 | 1.74 | 1.60 |
| 2 | q | 301 | FMN | C10-N1 | 4.50 | 1.42 | 1.33 |
| 2 | u | 301 | FMN | C10-N1 | 4.50 | 1.42 | 1.33 |
| 2 | t | 301 | FMN | P-O5' | 4.50 | 1.74 | 1.60 |
| 2 | m | 301 | FMN | P-O5' | 4.49 | 1.74 | 1.60 |
| 2 | 0 | 302 | FMN | C10-N1 | 4.49 | 1.42 | 1.33 |
| 2 | 1 | 302 | FMN | C10-N1 | 4.49 | 1.42 | 1.33 |
| 2 | f | 301 | FMN | C6-C7 | 4.49 | 1.46 | 1.39 |
| 2 | M | 301 | FMN | C10-N1 | 4.49 | 1.42 | 1.33 |
| 2 | G | 302 | FMN | C6-C7 | 4.48 | 1.46 | 1.39 |
| 2 | 5 | 301 | FMN | P-O5' | 4.48 | 1.74 | 1.60 |
| 2 | r | 302 | FMN | C10-N1 | 4.48 | 1.42 | 1.33 |
| 2 | O | 301 | FMN | C6-C7 | 4.48 | 1.46 | 1.39 |
| 2 | Q | 301 | FMN | P-O5' | 4.48 | 1.74 | 1.60 |
| 2 | s | 301 | FMN | C10-N1 | 4.48 | 1.42 | 1.33 |
| 2 | X | 301 | FMN | P-O5' | 4.48 | 1.74 | 1.60 |
| 2 | C | 301 | FMN | C10-N1 | 4.48 | 1.42 | 1.33 |
| 2 | r | 302 | FMN | P-O5' | 4.48 | 1.74 | 1.60 |
| 2 | r | 301 | FMN | C10-N1 | 4.48 | 1.42 | 1.33 |
| 2 | M | 301 | FMN | P-O5' | 4.47 | 1.74 | 1.60 |
| 2 | E | 301 | FMN | C2'-C3' | 4.47 | 1.61 | 1.53 |
| 2 | 7 | 302 | FMN | C6-C7 | 4.47 | 1.46 | 1.39 |
| 2 | w | 301 | FMN | C6-C7 | 4.47 | 1.46 | 1.39 |
| 2 | J | 301 | FMN | C6-C7 | 4.47 | 1.46 | 1.39 |
| 2 | f | 301 | FMN | C10-N1 | 4.47 | 1.42 | 1.33 |
| 2 | B | 301 | FMN | C10-N1 | 4.47 | 1.42 | 1.33 |
| 2 | T | 301 | FMN | C10-N1 | 4.47 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | M | 302 | FMN | P-O5' | 4.47 | 1.74 | 1.60 |
| 2 | h | 301 | FMN | C10-N1 | 4.47 | 1.42 | 1.33 |
| 2 | 0 | 301 | FMN | C6-C7 | 4.46 | 1.46 | 1.39 |
| 2 | p | 301 | FMN | C10-N1 | 4.46 | 1.42 | 1.33 |
| 2 | j | 301 | FMN | C10-N1 | 4.46 | 1.42 | 1.33 |
| 2 | n | 301 | FMN | C6-C7 | 4.46 | 1.46 | 1.39 |
| 2 | J | 301 | FMN | C10-N1 | 4.46 | 1.42 | 1.33 |
| 2 | 5 | 302 | FMN | C10-N1 | 4.45 | 1.42 | 1.33 |
| 2 | 7 | 302 | FMN | C10-N1 | 4.45 | 1.42 | 1.33 |
| 2 | X | 301 | FMN | C6-C7 | 4.45 | 1.46 | 1.39 |
| 2 | a | 301 | FMN | P-O5' | 4.45 | 1.74 | 1.60 |
| 2 | a | 302 | FMN | C10-N1 | 4.45 | 1.42 | 1.33 |
| 2 | u | 301 | FMN | P-O5' | 4.45 | 1.74 | 1.60 |
| 2 | Y | 301 | FMN | C10-N1 | 4.45 | 1.42 | 1.33 |
| 2 | O | 301 | FMN | P-O5' | 4.45 | 1.74 | 1.60 |
| 2 | h | 302 | FMN | C10-N1 | 4.45 | 1.42 | 1.33 |
| 2 | 5 | 301 | FMN | C10-N1 | 4.45 | 1.42 | 1.33 |
| 2 | h | 302 | FMN | P-O5' | 4.44 | 1.74 | 1.60 |
| 2 | B | 301 | FMN | P-O5' | 4.44 | 1.74 | 1.60 |
| 2 | x | 301 | FMN | C10-N1 | 4.44 | 1.42 | 1.33 |
| 2 | i | 301 | FMN | C6-C7 | 4.44 | 1.46 | 1.39 |
| 2 | p | 302 | FMN | P-O5' | 4.44 | 1.74 | 1.60 |
| 2 | 6 | 301 | FMN | C10-N1 | 4.44 | 1.42 | 1.33 |
| 2 | 3 | 301 | FMN | C10-N1 | 4.43 | 1.42 | 1.33 |
| 2 | p | 302 | FMN | C10-N1 | 4.43 | 1.42 | 1.33 |
| 2 | m | 302 | FMN | P-O5' | 4.43 | 1.74 | 1.60 |
| 2 | W | 301 | FMN | C10-N1 | 4.43 | 1.42 | 1.33 |
| 2 | m | 301 | FMN | C10-N1 | 4.43 | 1.42 | 1.33 |
| 2 | F | 301 | FMN | C10-N1 | 4.43 | 1.42 | 1.33 |
| 2 | d | 301 | FMN | C6-C7 | 4.43 | 1.46 | 1.39 |
| 2 | I | 301 | FMN | C10-N1 | 4.43 | 1.42 | 1.33 |
| 2 | k | 301 | FMN | C10-N1 | 4.43 | 1.42 | 1.33 |
| 2 | 6 | 301 | FMN | C6-C7 | 4.42 | 1.46 | 1.39 |
| 2 | a | 301 | FMN | C10-N1 | 4.42 | 1.42 | 1.33 |
| 2 | M | 302 | FMN | C6-C7 | 4.42 | 1.46 | 1.39 |
| 2 | D | 302 | FMN | C6-C7 | 4.41 | 1.46 | 1.39 |
| 2 | D | 302 | FMN | P-O5' | 4.39 | 1.74 | 1.60 |
| 2 | 5 | 302 | FMN | C6-C7 | 4.39 | 1.46 | 1.39 |
| 2 | E | 301 | FMN | C10-N1 | 4.39 | 1.42 | 1.33 |
| 2 | 1 | 301 | FMN | C10-N1 | 4.39 | 1.42 | 1.33 |
| 2 | Q | 301 | FMN | C10-N1 | 4.38 | 1.42 | 1.33 |
| 2 | R | 301 | FMN | C6-C7 | 4.36 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 4 | 301 | FMN | C10-N1 | 4.35 | 1.42 | 1.33 |
| 2 | J | 301 | FMN | P-O5' | 4.35 | 1.74 | 1.60 |
| 2 | r | 302 | FMN | C8M-C8 | 4.32 | 1.59 | 1.51 |
| 2 | u | 301 | FMN | C8M-C8 | 4.31 | 1.59 | 1.51 |
| 2 | 2 | 301 | FMN | C8M-C8 | 4.30 | 1.59 | 1.51 |
| 2 | c | 301 | FMN | C8M-C8 | 4.30 | 1.59 | 1.51 |
| 2 | a | 301 | FMN | C8M-C8 | 4.29 | 1.59 | 1.51 |
| 2 | 1 | 302 | FMN | C6-C7 | 4.29 | 1.45 | 1.39 |
| 2 | r | 301 | FMN | C8M-C8 | 4.29 | 1.59 | 1.51 |
| 2 | W | 301 | FMN | C8M-C8 | 4.28 | 1.59 | 1.51 |
| 2 | 5 | 301 | FMN | C8M-C8 | 4.28 | 1.59 | 1.51 |
| 2 | 1 | 302 | FMN | P-O5' | 4.28 | 1.74 | 1.60 |
| 2 | S | 301 | FMN | C8M-C8 | 4.27 | 1.59 | 1.51 |
| 2 | D | 301 | FMN | C8M-C8 | 4.27 | 1.59 | 1.51 |
| 2 | T | 301 | FMN | C8M-C8 | 4.27 | 1.59 | 1.51 |
| 2 | 0 | 302 | FMN | C8M-C8 | 4.24 | 1.59 | 1.51 |
| 2 | 1 | 302 | FMN | C8M-C8 | 4.23 | 1.59 | 1.51 |
| 2 | j | 301 | FMN | C8M-C8 | 4.23 | 1.59 | 1.51 |
| 2 | Q | 301 | FMN | C8M-C8 | 4.23 | 1.59 | 1.51 |
| 2 | M | 301 | FMN | C8M-C8 | 4.23 | 1.59 | 1.51 |
| 2 | N | 301 | FMN | C8M-C8 | 4.22 | 1.59 | 1.51 |
| 2 | s | 301 | FMN | C8M-C8 | 4.22 | 1.59 | 1.51 |
| 2 | 7 | 302 | FMN | C8M-C8 | 4.21 | 1.59 | 1.51 |
| 2 | Y | 301 | FMN | C8M-C8 | 4.21 | 1.59 | 1.51 |
| 2 | 3 | 301 | FMN | C8M-C8 | 4.19 | 1.59 | 1.51 |
| 2 | h | 301 | FMN | C8M-C8 | 4.19 | 1.59 | 1.51 |
| 2 | p | 302 | FMN | C8M-C8 | 4.19 | 1.59 | 1.51 |
| 2 | p | 301 | FMN | C8M-C8 | 4.19 | 1.59 | 1.51 |
| 2 | E | 301 | FMN | C8M-C8 | 4.19 | 1.59 | 1.51 |
| 2 | F | 301 | FMN | C8M-C8 | 4.18 | 1.59 | 1.51 |
| 2 | B | 301 | FMN | C8M-C8 | 4.18 | 1.59 | 1.51 |
| 2 | P | 301 | FMN | C8M-C8 | 4.18 | 1.59 | 1.51 |
| 2 | I | 301 | FMN | C8M-C8 | 4.17 | 1.59 | 1.51 |
| 2 | q | 301 | FMN | C8M-C8 | 4.17 | 1.59 | 1.51 |
| 2 | V | 301 | FMN | C8M-C8 | 4.17 | 1.59 | 1.51 |
| 2 | d | 301 | FMN | C8M-C8 | 4.16 | 1.59 | 1.51 |
| 2 | R | 301 | FMN | C8M-C8 | 4.16 | 1.59 | 1.51 |
| 2 | 1 | 301 | FMN | C8M-C8 | 4.16 | 1.59 | 1.51 |
| 2 | x | 301 | FMN | C8M-C8 | 4.16 | 1.59 | 1.51 |
| 2 | D | 302 | FMN | C8M-C8 | 4.15 | 1.59 | 1.51 |
| 2 | G | 302 | FMN | C8M-C8 | 4.15 | 1.59 | 1.51 |
| 2 | J | 301 | FMN | C8M-C8 | 4.14 | 1.59 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | k | 301 | FMN | C8M-C8 | 4.14 | 1.59 | 1.51 |
| 2 | C | 301 | FMN | C8M-C8 | 4.14 | 1.59 | 1.51 |
| 2 | 4 | 301 | FMN | C8M-C8 | 4.14 | 1.59 | 1.51 |
| 2 | e | 301 | FMN | C8M-C8 | 4.13 | 1.59 | 1.51 |
| 2 | G | 301 | FMN | C8M-C8 | 4.13 | 1.59 | 1.51 |
| 2 | h | 302 | FMN | C8M-C8 | 4.13 | 1.59 | 1.51 |
| 2 | f | 301 | FMN | C8M-C8 | 4.09 | 1.59 | 1.51 |
| 2 | n | 301 | FMN | C8M-C8 | 4.09 | 1.59 | 1.51 |
| 2 | w | 301 | FMN | C8M-C8 | 4.08 | 1.59 | 1.51 |
| 2 | m | 301 | FMN | C8M-C8 | 4.07 | 1.59 | 1.51 |
| 2 | m | 302 | FMN | C8M-C8 | 4.07 | 1.59 | 1.51 |
| 2 | x | 301 | FMN | C2'-C3' | 4.06 | 1.61 | 1.53 |
| 2 | s | 301 | FMN | C2'-C3' | 4.06 | 1.61 | 1.53 |
| 2 | M | 302 | FMN | C8M-C8 | 4.06 | 1.59 | 1.51 |
| 2 | X | 301 | FMN | C8M-C8 | 4.05 | 1.59 | 1.51 |
| 2 | 3 | 301 | FMN | C2'-C3' | 4.04 | 1.61 | 1.53 |
| 2 | h | 301 | FMN | C2'-C3' | 4.04 | 1.61 | 1.53 |
| 2 | k | 301 | FMN | C2'-C3' | 4.03 | 1.61 | 1.53 |
| 2 | 0 | 301 | FMN | C8M-C8 | 4.03 | 1.59 | 1.51 |
| 2 | A | 301 | FMN | C8M-C8 | 4.02 | 1.59 | 1.51 |
| 2 | 7 | 301 | FMN | C8M-C8 | 4.02 | 1.59 | 1.51 |
| 2 | i | 301 | FMN | C8M-C8 | 4.02 | 1.59 | 1.51 |
| 2 | 6 | 301 | FMN | C8M-C8 | 4.02 | 1.59 | 1.51 |
| 2 | A | 301 | FMN | C2'-C3' | 4.00 | 1.61 | 1.53 |
| 2 | C | 301 | FMN | C2'-C3' | 4.00 | 1.61 | 1.53 |
| 2 | O | 301 | FMN | C8M-C8 | 3.98 | 1.59 | 1.51 |
| 2 | t | 301 | FMN | C8M-C8 | 3.97 | 1.59 | 1.51 |
| 2 | G | 301 | FMN | C2'-C3' | 3.96 | 1.60 | 1.53 |
| 2 | Y | 301 | FMN | C2'-C3' | 3.95 | 1.60 | 1.53 |
| 2 | R | 301 | FMN | C2'-C3' | 3.94 | 1.60 | 1.53 |
| 2 | F | 301 | FMN | C2'-C3' | 3.94 | 1.60 | 1.53 |
| 2 | 1 | 301 | FMN | C2'-C3' | 3.93 | 1.60 | 1.53 |
| 2 | W | 301 | FMN | C2'-C3' | 3.93 | 1.60 | 1.53 |
| 2 | c | 301 | FMN | C2'-C3' | 3.93 | 1.60 | 1.53 |
| 2 | 7 | 302 | FMN | C2'-C3' | 3.92 | 1.60 | 1.53 |
| 2 | 6 | 301 | FMN | C1'-N10 | 3.92 | 1.58 | 1.48 |
| 2 | d | 301 | FMN | C2'-C3' | 3.90 | 1.60 | 1.53 |
| 2 | 5 | 302 | FMN | C8M-C8 | 3.90 | 1.58 | 1.51 |
| 2 | 6 | 301 | FMN | C2'-C3' | 3.90 | 1.60 | 1.53 |
| 2 | j | 301 | FMN | C2'-C3' | 3.89 | 1.60 | 1.53 |
| 2 | I | 301 | FMN | C2'-C3' | 3.89 | 1.60 | 1.53 |
| 2 | M | 301 | FMN | C2'-C3' | 3.88 | 1.60 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | p | 301 | FMN | C2'-C3' | 3.87 | 1.60 | 1.53 |
| 2 | 4 | 301 | FMN | C2'-C3' | 3.85 | 1.60 | 1.53 |
| 2 | 5 | 302 | FMN | C2'-C3' | 3.84 | 1.60 | 1.53 |
| 2 | 1 | 302 | FMN | C2'-C3' | 3.84 | 1.60 | 1.53 |
| 2 | 0 | 302 | FMN | C2'-C3' | 3.84 | 1.60 | 1.53 |
| 2 | E | 301 | FMN | C1'-N10 | 3.83 | 1.57 | 1.48 |
| 2 | 0 | 301 | FMN | C1'-N10 | 3.82 | 1.57 | 1.48 |
| 2 | G | 302 | FMN | C2'-C3' | 3.79 | 1.60 | 1.53 |
| 2 | e | 301 | FMN | C2'-C3' | 3.78 | 1.60 | 1.53 |
| 2 | u | 301 | FMN | C2'-C3' | 3.78 | 1.60 | 1.53 |
| 2 | q | 301 | FMN | C2'-C3' | 3.77 | 1.60 | 1.53 |
| 2 | D | 302 | FMN | C2'-C3' | 3.76 | 1.60 | 1.53 |
| 2 | D | 301 | FMN | C2'-C3' | 3.74 | 1.60 | 1.53 |
| 2 | m | 301 | FMN | C2'-C3' | 3.73 | 1.60 | 1.53 |
| 2 | m | 302 | FMN | C2'-C3' | 3.73 | 1.60 | 1.53 |
| 2 | r | 301 | FMN | C2'-C3' | 3.72 | 1.60 | 1.53 |
| 2 | 2 | 301 | FMN | C2'-C3' | 3.72 | 1.60 | 1.53 |
| 2 | a | 302 | FMN | C2'-C3' | 3.72 | 1.60 | 1.53 |
| 2 | 5 | 301 | FMN | C2'-C3' | 3.71 | 1.60 | 1.53 |
| 2 | a | 302 | FMN | C1'-N10 | 3.71 | 1.57 | 1.48 |
| 2 | 0 | 301 | FMN | C2'-C3' | 3.71 | 1.60 | 1.53 |
| 2 | e | 301 | FMN | C1'-N10 | 3.68 | 1.57 | 1.48 |
| 2 | r | 302 | FMN | C2'-C3' | 3.68 | 1.60 | 1.53 |
| 2 | h | 302 | FMN | C2'-C3' | 3.68 | 1.60 | 1.53 |
| 2 | X | 301 | FMN | C1'-N10 | 3.67 | 1.57 | 1.48 |
| 2 | s | 301 | FMN | C1'-N10 | 3.66 | 1.57 | 1.48 |
| 2 | N | 301 | FMN | C1'-N10 | 3.66 | 1.57 | 1.48 |
| 2 | J | 301 | FMN | C2'-C3' | 3.65 | 1.60 | 1.53 |
| 2 | n | 301 | FMN | C2'-C3' | 3.65 | 1.60 | 1.53 |
| 2 | m | 302 | FMN | C1'-N10 | 3.65 | 1.57 | 1.48 |
| 2 | G | 301 | FMN | C1'-N10 | 3.64 | 1.57 | 1.48 |
| 2 | V | 301 | FMN | C2'-C3' | 3.64 | 1.60 | 1.53 |
| 2 | M | 302 | FMN | C1'-N10 | 3.64 | 1.57 | 1.48 |
| 2 | P | 301 | FMN | C2'-C3' | 3.63 | 1.60 | 1.53 |
| 2 | N | 301 | FMN | C2'-C3' | 3.63 | 1.60 | 1.53 |
| 2 | f | 301 | FMN | C2'-C3' | 3.62 | 1.60 | 1.53 |
| 2 | R | 301 | FMN | C1'-N10 | 3.62 | 1.57 | 1.48 |
| 2 | d | 301 | FMN | C1'-N10 | 3.62 | 1.57 | 1.48 |
| 2 | u | 301 | FMN | C1'-N10 | 3.61 | 1.57 | 1.48 |
| 2 | S | 301 | FMN | C2'-C3' | 3.60 | 1.60 | 1.53 |
| 2 | 2 | 301 | FMN | C1'-N10 | 3.60 | 1.57 | 1.48 |
| 2 | F | 301 | FMN | C1'-N10 | 3.60 | 1.57 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | h | 301 | FMN | C1'-N10 | 3.59 | 1.57 | 1.48 |
| 2 | i | 301 | FMN | C2'-C3' | 3.59 | 1.60 | 1.53 |
| 2 | W | 301 | FMN | C1'-N10 | 3.59 | 1.57 | 1.48 |
| 2 | j | 301 | FMN | C1'-N10 | 3.55 | 1.57 | 1.48 |
| 2 | O | 301 | FMN | C1'-N10 | 3.55 | 1.57 | 1.48 |
| 2 | S | 301 | FMN | C1'-N10 | 3.55 | 1.57 | 1.48 |
| 2 | Y | 301 | FMN | C1'-N10 | 3.55 | 1.57 | 1.48 |
| 2 | P | 301 | FMN | C1'-N10 | 3.54 | 1.57 | 1.48 |
| 2 | f | 301 | FMN | C1'-N10 | 3.53 | 1.57 | 1.48 |
| 2 | l | 302 | FMN | C1'-N10 | 3.53 | 1.57 | 1.48 |
| 2 | p | 302 | FMN | C2'-C3' | 3.52 | 1.60 | 1.53 |
| 2 | a | 301 | FMN | C2'-C3' | 3.52 | 1.60 | 1.53 |
| 2 | n | 301 | FMN | C1'-N10 | 3.52 | 1.57 | 1.48 |
| 2 | 4 | 301 | FMN | C1'-N10 | 3.51 | 1.57 | 1.48 |
| 2 | V | 301 | FMN | C1'-N10 | 3.51 | 1.57 | 1.48 |
| 2 | D | 301 | FMN | C1'-N10 | 3.51 | 1.57 | 1.48 |
| 2 | x | 301 | FMN | C1'-N10 | 3.51 | 1.57 | 1.48 |
| 2 | Q | 301 | FMN | C2'-C3' | 3.51 | 1.60 | 1.53 |
| 2 | 3 | 301 | FMN | C1'-N10 | 3.50 | 1.57 | 1.48 |
| 2 | 7 | 302 | FMN | C9-C8 | 3.50 | 1.44 | 1.39 |
| 2 | t | 301 | FMN | C1'-N10 | 3.49 | 1.57 | 1.48 |
| 2 | 5 | 302 | FMN | C1'-N10 | 3.49 | 1.57 | 1.48 |
| 2 | i | 301 | FMN | C1'-N10 | 3.49 | 1.57 | 1.48 |
| 2 | q | 301 | FMN | C1'-N10 | 3.48 | 1.57 | 1.48 |
| 2 | r | 301 | FMN | C1'-N10 | 3.47 | 1.57 | 1.48 |
| 2 | l | 302 | FMN | C9-C8 | 3.47 | 1.44 | 1.39 |
| 2 | 0 | 302 | FMN | C1'-N10 | 3.47 | 1.56 | 1.48 |
| 2 | w | 301 | FMN | C2'-C3' | 3.47 | 1.60 | 1.53 |
| 2 | I | 301 | FMN | C1'-N10 | 3.46 | 1.56 | 1.48 |
| 2 | r | 302 | FMN | C9-C8 | 3.45 | 1.44 | 1.39 |
| 2 | x | 301 | FMN | C9-C8 | 3.45 | 1.44 | 1.39 |
| 2 | p | 301 | FMN | C1'-N10 | 3.45 | 1.56 | 1.48 |
| 2 | k | 301 | FMN | C1'-N10 | 3.45 | 1.56 | 1.48 |
| 2 | r | 301 | FMN | C9-C8 | 3.45 | 1.44 | 1.39 |
| 2 | D | 301 | FMN | C9-C8 | 3.45 | 1.44 | 1.39 |
| 2 | u | 301 | FMN | C9-C8 | 3.45 | 1.44 | 1.39 |
| 2 | O | 301 | FMN | C2'-C3' | 3.45 | 1.60 | 1.53 |
| 2 | 7 | 302 | FMN | C1'-N10 | 3.45 | 1.56 | 1.48 |
| 2 | l | 301 | FMN | C1'-N10 | 3.44 | 1.56 | 1.48 |
| 2 | 0 | 302 | FMN | C9-C8 | 3.44 | 1.44 | 1.39 |
| 2 | A | 301 | FMN | C1'-N10 | 3.44 | 1.56 | 1.48 |
| 2 | j | 301 | FMN | C9-C8 | 3.44 | 1.44 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | c | 301 | FMN | C1'-N10 | 3.44 | 1.56 | 1.48 |
| 2 | 7 | 301 | FMN | C1'-N10 | 3.43 | 1.56 | 1.48 |
| 2 | t | 301 | FMN | C2'-C3' | 3.43 | 1.59 | 1.53 |
| 2 | w | 301 | FMN | C1'-N10 | 3.43 | 1.56 | 1.48 |
| 2 | M | 302 | FMN | C2'-C3' | 3.43 | 1.59 | 1.53 |
| 2 | q | 301 | FMN | C9-C8 | 3.43 | 1.44 | 1.39 |
| 2 | h | 301 | FMN | C9-C8 | 3.43 | 1.44 | 1.39 |
| 2 | T | 301 | FMN | C1'-N10 | 3.42 | 1.56 | 1.48 |
| 2 | p | 302 | FMN | C1'-N10 | 3.42 | 1.56 | 1.48 |
| 2 | c | 301 | FMN | C9-C8 | 3.42 | 1.44 | 1.39 |
| 2 | W | 301 | FMN | C9-C8 | 3.42 | 1.44 | 1.39 |
| 2 | m | 301 | FMN | C1'-N10 | 3.42 | 1.56 | 1.48 |
| 2 | h | 302 | FMN | C1'-N10 | 3.41 | 1.56 | 1.48 |
| 2 | Q | 301 | FMN | C9-C8 | 3.41 | 1.44 | 1.39 |
| 2 | 5 | 301 | FMN | C1'-N10 | 3.41 | 1.56 | 1.48 |
| 2 | N | 301 | FMN | C9-C8 | 3.41 | 1.44 | 1.39 |
| 2 | M | 301 | FMN | C1'-N10 | 3.41 | 1.56 | 1.48 |
| 2 | G | 302 | FMN | C1'-N10 | 3.40 | 1.56 | 1.48 |
| 2 | F | 301 | FMN | C9-C8 | 3.40 | 1.44 | 1.39 |
| 2 | D | 302 | FMN | C1'-N10 | 3.39 | 1.56 | 1.48 |
| 2 | B | 301 | FMN | C1'-N10 | 3.39 | 1.56 | 1.48 |
| 2 | D | 302 | FMN | C9-C8 | 3.39 | 1.44 | 1.39 |
| 2 | 7 | 301 | FMN | C2'-C3' | 3.38 | 1.59 | 1.53 |
| 2 | M | 301 | FMN | C9-C8 | 3.38 | 1.44 | 1.39 |
| 2 | V | 301 | FMN | C9-C8 | 3.38 | 1.44 | 1.39 |
| 2 | X | 301 | FMN | C9-C8 | 3.38 | 1.44 | 1.39 |
| 2 | J | 301 | FMN | C1'-N10 | 3.37 | 1.56 | 1.48 |
| 2 | R | 301 | FMN | C9-C8 | 3.37 | 1.44 | 1.39 |
| 2 | B | 301 | FMN | C2'-C3' | 3.37 | 1.59 | 1.53 |
| 2 | d | 301 | FMN | C9-C8 | 3.36 | 1.44 | 1.39 |
| 2 | P | 301 | FMN | C9-C8 | 3.35 | 1.44 | 1.39 |
| 2 | G | 302 | FMN | C9-C8 | 3.35 | 1.44 | 1.39 |
| 2 | Q | 301 | FMN | C1'-N10 | 3.35 | 1.56 | 1.48 |
| 2 | p | 302 | FMN | C9-C8 | 3.34 | 1.44 | 1.39 |
| 2 | s | 301 | FMN | C9-C8 | 3.34 | 1.44 | 1.39 |
| 2 | 5 | 301 | FMN | C9-C8 | 3.34 | 1.44 | 1.39 |
| 2 | 0 | 301 | FMN | C9-C8 | 3.33 | 1.44 | 1.39 |
| 2 | 2 | 301 | FMN | C9-C8 | 3.33 | 1.44 | 1.39 |
| 2 | Y | 301 | FMN | C9-C8 | 3.32 | 1.44 | 1.39 |
| 2 | k | 301 | FMN | C9-C8 | 3.32 | 1.44 | 1.39 |
| 2 | T | 301 | FMN | C9-C8 | 3.31 | 1.44 | 1.39 |
| 2 | h | 302 | FMN | C9-C8 | 3.30 | 1.44 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | r | 302 | FMN | C1'-N10 | 3.30 | 1.56 | 1.48 |
| 2 | C | 301 | FMN | C1'-N10 | 3.29 | 1.56 | 1.48 |
| 2 | w | 301 | FMN | C9-C8 | 3.29 | 1.44 | 1.39 |
| 2 | T | 301 | FMN | C2'-C3' | 3.29 | 1.59 | 1.53 |
| 2 | M | 302 | FMN | C9-C8 | 3.28 | 1.44 | 1.39 |
| 2 | J | 301 | FMN | C9-C8 | 3.27 | 1.44 | 1.39 |
| 2 | a | 301 | FMN | C1'-N10 | 3.27 | 1.56 | 1.48 |
| 2 | 4 | 301 | FMN | C9-C8 | 3.25 | 1.44 | 1.39 |
| 2 | 3 | 301 | FMN | C9-C8 | 3.24 | 1.44 | 1.39 |
| 2 | E | 301 | FMN | C9-C8 | 3.24 | 1.44 | 1.39 |
| 2 | G | 301 | FMN | C9-C8 | 3.23 | 1.44 | 1.39 |
| 2 | B | 301 | FMN | C9-C8 | 3.23 | 1.44 | 1.39 |
| 2 | p | 301 | FMN | C9-C8 | 3.23 | 1.44 | 1.39 |
| 2 | C | 301 | FMN | C9-C8 | 3.22 | 1.44 | 1.39 |
| 2 | a | 301 | FMN | C9-C8 | 3.20 | 1.44 | 1.39 |
| 2 | 1 | 301 | FMN | C9-C8 | 3.19 | 1.44 | 1.39 |
| 2 | I | 301 | FMN | C9-C8 | 3.19 | 1.44 | 1.39 |
| 2 | S | 301 | FMN | C9-C8 | 3.18 | 1.44 | 1.39 |
| 2 | i | 301 | FMN | C9-C8 | 3.18 | 1.44 | 1.39 |
| 2 | n | 301 | FMN | C9-C8 | 3.18 | 1.44 | 1.39 |
| 2 | m | 302 | FMN | C9-C8 | 3.17 | 1.44 | 1.39 |
| 2 | f | 301 | FMN | C9-C8 | 3.17 | 1.44 | 1.39 |
| 2 | a | 302 | FMN | C9-C8 | 3.17 | 1.44 | 1.39 |
| 2 | e | 301 | FMN | C9-C8 | 3.13 | 1.44 | 1.39 |
| 2 | O | 301 | FMN | C9-C8 | 3.13 | 1.44 | 1.39 |
| 2 | 5 | 302 | FMN | C9-C8 | 3.12 | 1.44 | 1.39 |
| 2 | m | 301 | FMN | C9-C8 | 3.11 | 1.44 | 1.39 |
| 2 | 6 | 301 | FMN | C9-C8 | 3.11 | 1.44 | 1.39 |
| 2 | A | 301 | FMN | C9-C8 | 3.08 | 1.44 | 1.39 |
| 2 | 7 | 301 | FMN | C9-C8 | 3.05 | 1.44 | 1.39 |
| 2 | t | 301 | FMN | C9-C8 | 3.05 | 1.44 | 1.39 |
| 2 | 0 | 301 | FMN | C10-N10 | 2.75 | 1.43 | 1.37 |
| 2 | r | 302 | FMN | C8-C7 | 2.74 | 1.47 | 1.40 |
| 2 | R | 301 | FMN | C8-C7 | 2.73 | 1.47 | 1.40 |
| 2 | 6 | 301 | FMN | C10-N10 | 2.70 | 1.43 | 1.37 |
| 2 | a | 301 | FMN | C8-C7 | 2.67 | 1.47 | 1.40 |
| 2 | u | 301 | FMN | C8-C7 | 2.67 | 1.47 | 1.40 |
| 2 | 1 | 302 | FMN | P-O1P | 2.67 | 1.59 | 1.50 |
| 2 | D | 302 | FMN | C8-C7 | 2.67 | 1.47 | 1.40 |
| 2 | T | 301 | FMN | C8-C7 | 2.67 | 1.47 | 1.40 |
| 2 | u | 301 | FMN | P-O1P | 2.66 | 1.59 | 1.50 |
| 2 | f | 301 | FMN | P-O1P | 2.66 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | i | 301 | FMN | P-O1P | 2.65 | 1.59 | 1.50 |
| 2 | J | 301 | FMN | C8-C7 | 2.65 | 1.47 | 1.40 |
| 2 | 0 | 302 | FMN | C8-C7 | 2.64 | 1.47 | 1.40 |
| 2 | M | 301 | FMN | P-O1P | 2.64 | 1.59 | 1.50 |
| 2 | F | 301 | FMN | P-O1P | 2.64 | 1.59 | 1.50 |
| 2 | x | 301 | FMN | P-O1P | 2.63 | 1.59 | 1.50 |
| 2 | m | 302 | FMN | P-O1P | 2.63 | 1.59 | 1.50 |
| 2 | 3 | 301 | FMN | P-O1P | 2.63 | 1.59 | 1.50 |
| 2 | X | 301 | FMN | C8-C7 | 2.63 | 1.47 | 1.40 |
| 2 | j | 301 | FMN | P-O1P | 2.63 | 1.59 | 1.50 |
| 2 | T | 301 | FMN | P-O1P | 2.63 | 1.59 | 1.50 |
| 2 | d | 301 | FMN | C8-C7 | 2.62 | 1.47 | 1.40 |
| 2 | q | 301 | FMN | C8-C7 | 2.62 | 1.47 | 1.40 |
| 2 | 4 | 301 | FMN | P-O1P | 2.62 | 1.59 | 1.50 |
| 2 | s | 301 | FMN | C8-C7 | 2.62 | 1.47 | 1.40 |
| 2 | P | 301 | FMN | C8-C7 | 2.62 | 1.47 | 1.40 |
| 2 | w | 301 | FMN | C8-C7 | 2.62 | 1.47 | 1.40 |
| 2 | k | 301 | FMN | P-O1P | 2.62 | 1.59 | 1.50 |
| 2 | s | 301 | FMN | P-O1P | 2.62 | 1.59 | 1.50 |
| 2 | A | 301 | FMN | C8-C7 | 2.62 | 1.47 | 1.40 |
| 2 | 7 | 302 | FMN | C8-C7 | 2.62 | 1.47 | 1.40 |
| 2 | R | 301 | FMN | P-O1P | 2.61 | 1.59 | 1.50 |
| 2 | 6 | 301 | FMN | P-O1P | 2.61 | 1.59 | 1.50 |
| 2 | Y | 301 | FMN | P-O1P | 2.61 | 1.59 | 1.50 |
| 2 | Q | 301 | FMN | C8-C7 | 2.61 | 1.47 | 1.40 |
| 2 | W | 301 | FMN | C8-C7 | 2.61 | 1.47 | 1.40 |
| 2 | O | 301 | FMN | P-O1P | 2.61 | 1.59 | 1.50 |
| 2 | B | 301 | FMN | P-O1P | 2.61 | 1.58 | 1.50 |
| 2 | S | 301 | FMN | P-O1P | 2.61 | 1.58 | 1.50 |
| 2 | 6 | 301 | FMN | C8-C7 | 2.61 | 1.47 | 1.40 |
| 2 | W | 301 | FMN | P-O1P | 2.61 | 1.58 | 1.50 |
| 2 | Q | 301 | FMN | P-O1P | 2.61 | 1.58 | 1.50 |
| 2 | 0 | 301 | FMN | P-O1P | 2.60 | 1.58 | 1.50 |
| 2 | C | 301 | FMN | C8-C7 | 2.60 | 1.47 | 1.40 |
| 2 | N | 301 | FMN | C8-C7 | 2.60 | 1.47 | 1.40 |
| 2 | j | 301 | FMN | C8-C7 | 2.60 | 1.47 | 1.40 |
| 2 | G | 302 | FMN | P-O1P | 2.60 | 1.58 | 1.50 |
| 2 | w | 301 | FMN | P-O1P | 2.60 | 1.58 | 1.50 |
| 2 | X | 301 | FMN | P-O1P | 2.60 | 1.58 | 1.50 |
| 2 | V | 301 | FMN | P-O1P | 2.60 | 1.58 | 1.50 |
| 2 | c | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | h | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | F | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | E | 301 | FMN | C10-N10 | 2.59 | 1.43 | 1.37 |
| 2 | D | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | m | 302 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | h | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | m | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | C | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | G | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | B | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | A | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | I | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | D | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | N | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | a | 302 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | n | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | E | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | 4 | 301 | FMN | C8-C7 | 2.59 | 1.47 | 1.40 |
| 2 | 5 | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | P | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | 2 | 301 | FMN | P-O1P | 2.59 | 1.58 | 1.50 |
| 2 | r | 301 | FMN | P-O1P | 2.58 | 1.58 | 1.50 |
| 2 | p | 301 | FMN | P-O1P | 2.58 | 1.58 | 1.50 |
| 2 | a | 301 | FMN | P-O1P | 2.58 | 1.58 | 1.50 |
| 2 | 1 | 302 | FMN | C8-C7 | 2.58 | 1.47 | 1.40 |
| 2 | m | 301 | FMN | P-O1P | 2.58 | 1.58 | 1.50 |
| 2 | 5 | 301 | FMN | C8-C7 | 2.58 | 1.47 | 1.40 |
| 2 | M | 301 | FMN | C8-C7 | 2.58 | 1.47 | 1.40 |
| 2 | p | 302 | FMN | P-O1P | 2.58 | 1.58 | 1.50 |
| 2 | E | 301 | FMN | P-O1P | 2.58 | 1.58 | 1.50 |
| 2 | 0 | 301 | FMN | C8-C7 | 2.58 | 1.47 | 1.40 |
| 2 | 7 | 301 | FMN | P-O1P | 2.57 | 1.58 | 1.50 |
| 2 | r | 302 | FMN | P-O1P | 2.57 | 1.58 | 1.50 |
| 2 | h | 302 | FMN | P-O1P | 2.57 | 1.58 | 1.50 |
| 2 | 0 | 302 | FMN | P-O1P | 2.57 | 1.58 | 1.50 |
| 2 | 5 | 302 | FMN | P-O1P | 2.57 | 1.58 | 1.50 |
| 2 | q | 301 | FMN | P-O1P | 2.57 | 1.58 | 1.50 |
| 2 | G | 302 | FMN | C8-C7 | 2.57 | 1.47 | 1.40 |
| 2 | S | 301 | FMN | C8-C7 | 2.57 | 1.47 | 1.40 |
| 2 | 1 | 301 | FMN | P-O1P | 2.56 | 1.58 | 1.50 |
| 2 | k | 301 | FMN | C8-C7 | 2.56 | 1.47 | 1.40 |
| 2 | c | 301 | FMN | P-O1P | 2.56 | 1.58 | 1.50 |
| 2 | e | 301 | FMN | C8-C7 | 2.56 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | x | 301 | FMN | C8-C7 | 2.56 | 1.47 | 1.40 |
| 2 | r | 301 | FMN | C8-C7 | 2.56 | 1.47 | 1.40 |
| 2 | 2 | 301 | FMN | C8-C7 | 2.56 | 1.47 | 1.40 |
| 2 | t | 301 | FMN | P-O1P | 2.56 | 1.58 | 1.50 |
| 2 | m | 302 | FMN | C10-N10 | 2.56 | 1.42 | 1.37 |
| 2 | f | 301 | FMN | C8-C7 | 2.56 | 1.47 | 1.40 |
| 2 | t | 301 | FMN | C8-C7 | 2.55 | 1.47 | 1.40 |
| 2 | i | 301 | FMN | C8-C7 | 2.55 | 1.47 | 1.40 |
| 2 | 1 | 301 | FMN | C8-C7 | 2.55 | 1.47 | 1.40 |
| 2 | G | 301 | FMN | C8-C7 | 2.55 | 1.47 | 1.40 |
| 2 | d | 301 | FMN | P-O1P | 2.55 | 1.58 | 1.50 |
| 2 | M | 302 | FMN | P-O1P | 2.55 | 1.58 | 1.50 |
| 2 | N | 301 | FMN | C10-N10 | 2.54 | 1.42 | 1.37 |
| 2 | 5 | 302 | FMN | C8-C7 | 2.54 | 1.47 | 1.40 |
| 2 | n | 301 | FMN | C8-C7 | 2.54 | 1.47 | 1.40 |
| 2 | e | 301 | FMN | P-O1P | 2.54 | 1.58 | 1.50 |
| 2 | 7 | 301 | FMN | C8-C7 | 2.53 | 1.47 | 1.40 |
| 2 | M | 302 | FMN | C8-C7 | 2.53 | 1.47 | 1.40 |
| 2 | h | 302 | FMN | C8-C7 | 2.52 | 1.47 | 1.40 |
| 2 | p | 301 | FMN | C8-C7 | 2.52 | 1.47 | 1.40 |
| 2 | V | 301 | FMN | C8-C7 | 2.52 | 1.47 | 1.40 |
| 2 | Y | 301 | FMN | C8-C7 | 2.51 | 1.47 | 1.40 |
| 2 | p | 302 | FMN | C8-C7 | 2.51 | 1.47 | 1.40 |
| 2 | 7 | 302 | FMN | P-O1P | 2.50 | 1.58 | 1.50 |
| 2 | 2 | 301 | FMN | C10-N10 | 2.49 | 1.42 | 1.37 |
| 2 | 3 | 301 | FMN | C8-C7 | 2.48 | 1.47 | 1.40 |
| 2 | G | 301 | FMN | C10-N10 | 2.47 | 1.42 | 1.37 |
| 2 | J | 301 | FMN | P-O1P | 2.46 | 1.58 | 1.50 |
| 2 | O | 301 | FMN | C8-C7 | 2.46 | 1.47 | 1.40 |
| 2 | S | 301 | FMN | C10-N10 | 2.46 | 1.42 | 1.37 |
| 2 | P | 301 | FMN | C10-N10 | 2.44 | 1.42 | 1.37 |
| 2 | I | 301 | FMN | C8-C7 | 2.43 | 1.47 | 1.40 |
| 2 | D | 302 | FMN | P-O1P | 2.42 | 1.58 | 1.50 |
| 2 | M | 302 | FMN | C10-N10 | 2.41 | 1.42 | 1.37 |
| 2 | c | 301 | FMN | C10-N10 | 2.41 | 1.42 | 1.37 |
| 2 | s | 301 | FMN | C9A-C5A | 2.38 | 1.45 | 1.41 |
| 2 | j | 301 | FMN | C10-N10 | 2.37 | 1.42 | 1.37 |
| 2 | X | 301 | FMN | C10-N10 | 2.36 | 1.42 | 1.37 |
| 2 | x | 301 | FMN | C9A-C5A | 2.36 | 1.45 | 1.41 |
| 2 | R | 301 | FMN | C10-N10 | 2.35 | 1.42 | 1.37 |
| 2 | a | 302 | FMN | C8-C7 | 2.35 | 1.46 | 1.40 |
| 2 | h | 301 | FMN | C10-N10 | 2.35 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | V | 301 | FMN | C10-N10 | 2.34 | 1.42 | 1.37 |
| 2 | e | 301 | FMN | C10-N10 | 2.34 | 1.42 | 1.37 |
| 2 | d | 301 | FMN | C10-N10 | 2.34 | 1.42 | 1.37 |
| 2 | F | 301 | FMN | C10-N10 | 2.33 | 1.42 | 1.37 |
| 2 | f | 301 | FMN | C9A-C5A | 2.31 | 1.45 | 1.41 |
| 2 | a | 302 | FMN | C9A-C5A | 2.30 | 1.45 | 1.41 |
| 2 | W | 301 | FMN | C9A-C5A | 2.30 | 1.45 | 1.41 |
| 2 | a | 302 | FMN | C10-N10 | 2.30 | 1.42 | 1.37 |
| 2 | 1 | 302 | FMN | C10-N10 | 2.29 | 1.42 | 1.37 |
| 2 | 4 | 301 | FMN | C9A-C5A | 2.29 | 1.45 | 1.41 |
| 2 | s | 301 | FMN | C10-N10 | 2.29 | 1.42 | 1.37 |
| 2 | n | 301 | FMN | C10-N10 | 2.29 | 1.42 | 1.37 |
| 2 | D | 301 | FMN | C10-N10 | 2.28 | 1.42 | 1.37 |
| 2 | 3 | 301 | FMN | C10-N10 | 2.28 | 1.42 | 1.37 |
| 2 | M | 302 | FMN | C9A-C5A | 2.28 | 1.45 | 1.41 |
| 2 | m | 302 | FMN | C9A-C5A | 2.27 | 1.45 | 1.41 |
| 2 | h | 301 | FMN | C9A-C5A | 2.27 | 1.45 | 1.41 |
| 2 | i | 301 | FMN | C9A-C5A | 2.27 | 1.45 | 1.41 |
| 2 | u | 301 | FMN | C10-N10 | 2.27 | 1.42 | 1.37 |
| 2 | 1 | 302 | FMN | C9A-C5A | 2.27 | 1.45 | 1.41 |
| 2 | 7 | 302 | FMN | C9A-C5A | 2.26 | 1.45 | 1.41 |
| 2 | p | 301 | FMN | C9A-C5A | 2.26 | 1.45 | 1.41 |
| 2 | O | 301 | FMN | C9A-C5A | 2.26 | 1.45 | 1.41 |
| 2 | W | 301 | FMN | C10-N10 | 2.26 | 1.42 | 1.37 |
| 2 | G | 301 | FMN | C9A-C5A | 2.26 | 1.45 | 1.41 |
| 2 | 3 | 301 | FMN | C9A-C5A | 2.26 | 1.45 | 1.41 |
| 2 | O | 301 | FMN | C10-N10 | 2.26 | 1.42 | 1.37 |
| 2 | 5 | 302 | FMN | C9A-C5A | 2.25 | 1.45 | 1.41 |
| 2 | T | 301 | FMN | C10-N10 | 2.25 | 1.42 | 1.37 |
| 2 | N | 301 | FMN | C9A-C5A | 2.25 | 1.45 | 1.41 |
| 2 | 5 | 301 | FMN | C9A-C5A | 2.25 | 1.45 | 1.41 |
| 2 | A | 301 | FMN | C9A-C5A | 2.25 | 1.45 | 1.41 |
| 2 | d | 301 | FMN | C9A-C5A | 2.25 | 1.45 | 1.41 |
| 2 | G | 302 | FMN | C9A-C5A | 2.25 | 1.44 | 1.41 |
| 2 | I | 301 | FMN | C9A-C5A | 2.25 | 1.44 | 1.41 |
| 2 | x | 301 | FMN | C10-N10 | 2.24 | 1.42 | 1.37 |
| 2 | D | 301 | FMN | C9A-C5A | 2.24 | 1.44 | 1.41 |
| 2 | F | 301 | FMN | C9A-C5A | 2.24 | 1.44 | 1.41 |
| 2 | u | 301 | FMN | C9A-C5A | 2.24 | 1.44 | 1.41 |
| 2 | R | 301 | FMN | C9A-C5A | 2.23 | 1.44 | 1.41 |
| 2 | w | 301 | FMN | C9A-C5A | 2.23 | 1.44 | 1.41 |
| 2 | r | 301 | FMN | C9A-C5A | 2.23 | 1.44 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | E | 301 | FMN | C9A-C5A | 2.23 | 1.44 | 1.41 |
| 2 | h | 302 | FMN | C9A-C5A | 2.22 | 1.44 | 1.41 |
| 2 | n | 301 | FMN | C9A-C5A | 2.22 | 1.44 | 1.41 |
| 2 | w | 301 | FMN | C10-N10 | 2.22 | 1.42 | 1.37 |
| 2 | X | 301 | FMN | C9A-C5A | 2.22 | 1.44 | 1.41 |
| 2 | 1 | 301 | FMN | C9A-C5A | 2.22 | 1.44 | 1.41 |
| 2 | 7 | 302 | FMN | C10-N10 | 2.22 | 1.42 | 1.37 |
| 2 | Y | 301 | FMN | C10-N10 | 2.22 | 1.42 | 1.37 |
| 2 | D | 302 | FMN | C10-N10 | 2.21 | 1.42 | 1.37 |
| 2 | 0 | 301 | FMN | C9A-C5A | 2.21 | 1.44 | 1.41 |
| 2 | B | 301 | FMN | C9A-C5A | 2.21 | 1.44 | 1.41 |
| 2 | m | 301 | FMN | C9A-C5A | 2.21 | 1.44 | 1.41 |
| 2 | 0 | 302 | FMN | C10-N10 | 2.21 | 1.42 | 1.37 |
| 2 | r | 301 | FMN | C10-N10 | 2.21 | 1.42 | 1.37 |
| 2 | Y | 301 | FMN | C9A-C5A | 2.20 | 1.44 | 1.41 |
| 2 | 7 | 301 | FMN | C9A-C5A | 2.20 | 1.44 | 1.41 |
| 2 | M | 301 | FMN | C10-N10 | 2.20 | 1.42 | 1.37 |
| 2 | q | 301 | FMN | C9A-C5A | 2.20 | 1.44 | 1.41 |
| 2 | f | 301 | FMN | C10-N10 | 2.20 | 1.42 | 1.37 |
| 2 | 0 | 302 | FMN | C9A-C5A | 2.20 | 1.44 | 1.41 |
| 2 | t | 301 | FMN | C9A-C5A | 2.20 | 1.44 | 1.41 |
| 2 | q | 301 | FMN | C10-N10 | 2.19 | 1.42 | 1.37 |
| 2 | 2 | 301 | FMN | C9A-C5A | 2.19 | 1.44 | 1.41 |
| 2 | D | 302 | FMN | C9A-C5A | 2.19 | 1.44 | 1.41 |
| 2 | 5 | 302 | FMN | C10-N10 | 2.19 | 1.42 | 1.37 |
| 2 | C | 301 | FMN | C9A-C5A | 2.19 | 1.44 | 1.41 |
| 2 | p | 302 | FMN | C10-N10 | 2.19 | 1.42 | 1.37 |
| 2 | k | 301 | FMN | C10-N10 | 2.18 | 1.42 | 1.37 |
| 2 | t | 301 | FMN | C10-N10 | 2.18 | 1.42 | 1.37 |
| 2 | p | 302 | FMN | C9A-C5A | 2.17 | 1.44 | 1.41 |
| 2 | B | 301 | FMN | C10-N10 | 2.17 | 1.42 | 1.37 |
| 2 | i | 301 | FMN | C10-N10 | 2.17 | 1.42 | 1.37 |
| 2 | T | 301 | FMN | C9A-C5A | 2.17 | 1.44 | 1.41 |
| 2 | P | 301 | FMN | C9A-C5A | 2.17 | 1.44 | 1.41 |
| 2 | c | 301 | FMN | C9A-C5A | 2.17 | 1.44 | 1.41 |
| 2 | k | 301 | FMN | C9A-C5A | 2.17 | 1.44 | 1.41 |
| 2 | Q | 301 | FMN | C9A-C5A | 2.16 | 1.44 | 1.41 |
| 2 | J | 301 | FMN | C9A-C5A | 2.16 | 1.44 | 1.41 |
| 2 | e | 301 | FMN | C9A-C5A | 2.16 | 1.44 | 1.41 |
| 2 | a | 301 | FMN | C9A-C5A | 2.16 | 1.44 | 1.41 |
| 2 | j | 301 | FMN | C9A-C5A | 2.15 | 1.44 | 1.41 |
| 2 | 7 | 301 | FMN | C10-N10 | 2.15 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | h | 302 | FMN | C10-N10 | 2.15 | 1.42 | 1.37 |
| 2 | 6 | 301 | FMN | C9A-C5A | 2.14 | 1.44 | 1.41 |
| 2 | l | 301 | FMN | C10-N10 | 2.14 | 1.42 | 1.37 |
| 2 | S | 301 | FMN | C9A-C5A | 2.13 | 1.44 | 1.41 |
| 2 | M | 301 | FMN | C9A-C5A | 2.13 | 1.44 | 1.41 |
| 2 | J | 301 | FMN | C10-N10 | 2.12 | 1.42 | 1.37 |
| 2 | V | 301 | FMN | C9A-C5A | 2.12 | 1.44 | 1.41 |
| 2 | p | 301 | FMN | C10-N10 | 2.12 | 1.42 | 1.37 |
| 2 | G | 302 | FMN | C10-N10 | 2.11 | 1.41 | 1.37 |
| 2 | r | 302 | FMN | C10-N10 | 2.10 | 1.41 | 1.37 |
| 2 | C | 301 | FMN | C10-N10 | 2.09 | 1.41 | 1.37 |
| 2 | m | 301 | FMN | C10-N10 | 2.09 | 1.41 | 1.37 |
| 2 | 4 | 301 | FMN | C10-N10 | 2.08 | 1.41 | 1.37 |
| 2 | r | 302 | FMN | C9A-C5A | 2.08 | 1.44 | 1.41 |
| 2 | 5 | 301 | FMN | C10-N10 | 2.08 | 1.41 | 1.37 |
| 2 | A | 301 | FMN | C10-N10 | 2.05 | 1.41 | 1.37 |
| 2 | I | 301 | FMN | C10-N10 | 2.05 | 1.41 | 1.37 |
| 2 | Q | 301 | FMN | C10-N10 | 2.04 | 1.41 | 1.37 |
| 2 | a | 301 | FMN | C10-N10 | 2.01 | 1.41 | 1.37 |

All (447) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 6 | 301 | FMN | C4A-C10-N1 | -3.32 | 117.03 | 124.73 |
| 2 | 0 | 301 | FMN | C4A-C10-N1 | -3.20 | 117.31 | 124.73 |
| 2 | E | 301 | FMN | C4A-C10-N1 | -3.19 | 117.33 | 124.73 |
| 2 | a | 301 | FMN | C4'-C3'-C2' | -3.19 | 106.73 | 113.36 |
| 2 | 4 | 301 | FMN | C4A-C10-N10 | 3.07 | 120.97 | 116.48 |
| 2 | f | 301 | FMN | C4A-C10-N10 | 2.98 | 120.84 | 116.48 |
| 2 | V | 301 | FMN | C4'-C3'-C2' | -2.97 | 107.19 | 113.36 |
| 2 | 5 | 301 | FMN | C4A-C10-N10 | 2.96 | 120.81 | 116.48 |
| 2 | 7 | 302 | FMN | C4A-C10-N10 | 2.95 | 120.80 | 116.48 |
| 2 | 6 | 301 | FMN | C4-N3-C2 | -2.94 | 120.21 | 125.64 |
| 2 | a | 302 | FMN | C4A-C10-N10 | 2.93 | 120.77 | 116.48 |
| 2 | A | 301 | FMN | C4A-C10-N10 | 2.92 | 120.76 | 116.48 |
| 2 | E | 301 | FMN | C4A-C10-N10 | 2.91 | 120.74 | 116.48 |
| 2 | a | 302 | FMN | C4-N3-C2 | -2.91 | 120.27 | 125.64 |
| 2 | Y | 301 | FMN | O4-C4-C4A | -2.91 | 118.89 | 126.60 |
| 2 | B | 301 | FMN | C4A-C10-N10 | 2.90 | 120.71 | 116.48 |
| 2 | m | 301 | FMN | C4A-C10-N10 | 2.89 | 120.71 | 116.48 |
| 2 | E | 301 | FMN | C4-N3-C2 | -2.89 | 120.30 | 125.64 |
| 2 | I | 301 | FMN | O4-C4-C4A | -2.89 | 118.94 | 126.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 1 | 302 | FMN | C4A-C10-N10 | 2.88 | 120.69 | 116.48 |
| 2 | T | 301 | FMN | C5'-C4'-C3' | -2.87 | 106.66 | 112.20 |
| 2 | s | 301 | FMN | C4-N3-C2 | -2.87 | 120.35 | 125.64 |
| 2 | x | 301 | FMN | C4A-C10-N10 | 2.86 | 120.66 | 116.48 |
| 2 | k | 301 | FMN | C4A-C10-N10 | 2.84 | 120.64 | 116.48 |
| 2 | s | 301 | FMN | O4-C4-C4A | -2.84 | 119.06 | 126.60 |
| 2 | W | 301 | FMN | O4-C4-C4A | -2.84 | 119.07 | 126.60 |
| 2 | d | 301 | FMN | C4A-C10-N10 | 2.83 | 120.62 | 116.48 |
| 2 | M | 302 | FMN | C4A-C10-N1 | -2.83 | 118.17 | 124.73 |
| 2 | u | 301 | FMN | O4-C4-C4A | -2.83 | 119.10 | 126.60 |
| 2 | m | 302 | FMN | C4A-C10-N1 | -2.83 | 118.17 | 124.73 |
| 2 | 5 | 302 | FMN | C4A-C10-N10 | 2.82 | 120.60 | 116.48 |
| 2 | h | 301 | FMN | C4A-C10-N10 | 2.82 | 120.60 | 116.48 |
| 2 | N | 301 | FMN | C4A-C10-N1 | -2.81 | 118.20 | 124.73 |
| 2 | W | 301 | FMN | C4-N3-C2 | -2.81 | 120.45 | 125.64 |
| 2 | M | 302 | FMN | C4A-C10-N10 | 2.81 | 120.59 | 116.48 |
| 2 | p | 301 | FMN | C4A-C10-N10 | 2.81 | 120.59 | 116.48 |
| 2 | R | 301 | FMN | C4A-C10-N10 | 2.80 | 120.57 | 116.48 |
| 2 | F | 301 | FMN | C4-N3-C2 | -2.80 | 120.47 | 125.64 |
| 2 | 0 | 301 | FMN | C4-N3-C2 | -2.80 | 120.47 | 125.64 |
| 2 | s | 301 | FMN | C4A-C10-N10 | 2.80 | 120.57 | 116.48 |
| 2 | e | 301 | FMN | C4A-C10-N1 | -2.79 | 118.25 | 124.73 |
| 2 | S | 301 | FMN | C4-N3-C2 | -2.79 | 120.48 | 125.64 |
| 2 | e | 301 | FMN | C4A-C10-N10 | 2.79 | 120.56 | 116.48 |
| 2 | h | 301 | FMN | C4-N3-C2 | -2.79 | 120.49 | 125.64 |
| 2 | h | 301 | FMN | C4A-C10-N1 | -2.79 | 118.26 | 124.73 |
| 2 | c | 301 | FMN | C4-N3-C2 | -2.79 | 120.49 | 125.64 |
| 2 | Y | 301 | FMN | C4-N3-C2 | -2.79 | 120.49 | 125.64 |
| 2 | q | 301 | FMN | C4A-C10-N10 | 2.78 | 120.55 | 116.48 |
| 2 | 6 | 301 | FMN | C4'-C3'-C2' | -2.78 | 107.57 | 113.36 |
| 2 | J | 301 | FMN | C4A-C10-N10 | 2.78 | 120.55 | 116.48 |
| 2 | 2 | 301 | FMN | C4-N3-C2 | -2.78 | 120.50 | 125.64 |
| 2 | 0 | 302 | FMN | C4A-C10-N10 | 2.78 | 120.55 | 116.48 |
| 2 | 1 | 301 | FMN | C4A-C10-N10 | 2.78 | 120.54 | 116.48 |
| 2 | G | 302 | FMN | C4A-C10-N10 | 2.78 | 120.54 | 116.48 |
| 2 | u | 301 | FMN | C4-N3-C2 | -2.78 | 120.51 | 125.64 |
| 2 | 6 | 301 | FMN | C4A-C10-N10 | 2.78 | 120.54 | 116.48 |
| 2 | Q | 301 | FMN | C4A-C10-N10 | 2.77 | 120.53 | 116.48 |
| 2 | W | 301 | FMN | C4A-C10-N10 | 2.77 | 120.53 | 116.48 |
| 2 | M | 301 | FMN | C4A-C10-N10 | 2.77 | 120.53 | 116.48 |
| 2 | T | 301 | FMN | C4A-C10-N10 | 2.77 | 120.53 | 116.48 |
| 2 | i | 301 | FMN | C4A-C10-N10 | 2.77 | 120.53 | 116.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | w | 301 | FMN | C4A-C10-N10 | 2.77 | 120.53 | 116.48 |
| 2 | 3 | 301 | FMN | C4A-C10-N10 | 2.77 | 120.53 | 116.48 |
| 2 | I | 301 | FMN | C4A-C10-N10 | 2.76 | 120.52 | 116.48 |
| 2 | n | 301 | FMN | C4A-C10-N10 | 2.76 | 120.52 | 116.48 |
| 2 | 3 | 301 | FMN | C4-N3-C2 | -2.76 | 120.54 | 125.64 |
| 2 | r | 301 | FMN | C4-N3-C2 | -2.76 | 120.54 | 125.64 |
| 2 | m | 302 | FMN | C4-N3-C2 | -2.76 | 120.54 | 125.64 |
| 2 | p | 302 | FMN | C4A-C10-N10 | 2.76 | 120.52 | 116.48 |
| 2 | 7 | 301 | FMN | C4A-C10-N10 | 2.76 | 120.51 | 116.48 |
| 2 | N | 301 | FMN | C4A-C10-N10 | 2.76 | 120.51 | 116.48 |
| 2 | j | 301 | FMN | C4-N3-C2 | -2.75 | 120.56 | 125.64 |
| 2 | p | 301 | FMN | O4-C4-C4A | -2.75 | 119.30 | 126.60 |
| 2 | a | 301 | FMN | C4A-C10-N10 | 2.75 | 120.50 | 116.48 |
| 2 | X | 301 | FMN | C4A-C10-N1 | -2.75 | 118.35 | 124.73 |
| 2 | F | 301 | FMN | C4A-C10-N10 | 2.75 | 120.50 | 116.48 |
| 2 | F | 301 | FMN | C4A-C10-N1 | -2.75 | 118.36 | 124.73 |
| 2 | G | 301 | FMN | C4-N3-C2 | -2.74 | 120.58 | 125.64 |
| 2 | D | 302 | FMN | C4A-C10-N10 | 2.74 | 120.48 | 116.48 |
| 2 | P | 301 | FMN | C4A-C10-N1 | -2.73 | 118.39 | 124.73 |
| 2 | f | 301 | FMN | C4-N3-C2 | -2.73 | 120.60 | 125.64 |
| 2 | u | 301 | FMN | C4A-C10-N10 | 2.73 | 120.47 | 116.48 |
| 2 | I | 301 | FMN | C4-N3-C2 | -2.73 | 120.61 | 125.64 |
| 2 | C | 301 | FMN | C4A-C10-N10 | 2.73 | 120.47 | 116.48 |
| 2 | s | 301 | FMN | C4A-C10-N1 | -2.73 | 118.41 | 124.73 |
| 2 | r | 301 | FMN | C4A-C10-N10 | 2.72 | 120.46 | 116.48 |
| 2 | j | 301 | FMN | C4A-C10-N1 | -2.72 | 118.41 | 124.73 |
| 2 | 0 | 302 | FMN | C4-N3-C2 | -2.72 | 120.61 | 125.64 |
| 2 | G | 301 | FMN | C4A-C10-N1 | -2.72 | 118.42 | 124.73 |
| 2 | 1 | 302 | FMN | C4-N3-C2 | -2.72 | 120.62 | 125.64 |
| 2 | r | 302 | FMN | C4'-C3'-C2' | -2.72 | 107.71 | 113.36 |
| 2 | P | 301 | FMN | C4-N3-C2 | -2.72 | 120.62 | 125.64 |
| 2 | d | 301 | FMN | C4-N3-C2 | -2.72 | 120.62 | 125.64 |
| 2 | O | 301 | FMN | C4A-C10-N10 | 2.72 | 120.45 | 116.48 |
| 2 | F | 301 | FMN | O4-C4-C4A | -2.72 | 119.40 | 126.60 |
| 2 | S | 301 | FMN | C4A-C10-N1 | -2.71 | 118.44 | 124.73 |
| 2 | R | 301 | FMN | C4-N3-C2 | -2.71 | 120.63 | 125.64 |
| 2 | h | 301 | FMN | O4-C4-C4A | -2.71 | 119.41 | 126.60 |
| 2 | M | 302 | FMN | C4-N3-C2 | -2.71 | 120.64 | 125.64 |
| 2 | B | 301 | FMN | C4-N3-C2 | -2.71 | 120.64 | 125.64 |
| 2 | R | 301 | FMN | C4A-C10-N1 | -2.71 | 118.45 | 124.73 |
| 2 | 7 | 302 | FMN | C4-N3-C2 | -2.70 | 120.64 | 125.64 |
| 2 | M | 301 | FMN | C4-N3-C2 | -2.70 | 120.65 | 125.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 2 | 301 | FMN | C4A-C10-N1 | -2.70 | 118.46 | 124.73 |
| 2 | D | 302 | FMN | C4-N3-C2 | -2.70 | 120.65 | 125.64 |
| 2 | V | 301 | FMN | C4-N3-C2 | -2.70 | 120.65 | 125.64 |
| 2 | N | 301 | FMN | C4-N3-C2 | -2.70 | 120.66 | 125.64 |
| 2 | d | 301 | FMN | C4A-C10-N1 | -2.70 | 118.47 | 124.73 |
| 2 | a | 302 | FMN | C4A-C10-N1 | -2.70 | 118.47 | 124.73 |
| 2 | c | 301 | FMN | C4A-C10-N1 | -2.69 | 118.48 | 124.73 |
| 2 | p | 301 | FMN | C4-N3-C2 | -2.69 | 120.67 | 125.64 |
| 2 | Q | 301 | FMN | C4-N3-C2 | -2.69 | 120.68 | 125.64 |
| 2 | D | 301 | FMN | C4-N3-C2 | -2.69 | 120.68 | 125.64 |
| 2 | Q | 301 | FMN | O4-C4-C4A | -2.68 | 119.49 | 126.60 |
| 2 | Y | 301 | FMN | C4A-C10-N10 | 2.68 | 120.40 | 116.48 |
| 2 | 5 | 301 | FMN | C4-N3-C2 | -2.68 | 120.69 | 125.64 |
| 2 | n | 301 | FMN | C4-N3-C2 | -2.68 | 120.69 | 125.64 |
| 2 | e | 301 | FMN | C4-N3-C2 | -2.67 | 120.70 | 125.64 |
| 2 | f | 301 | FMN | C4A-C10-N1 | -2.67 | 118.53 | 124.73 |
| 2 | m | 302 | FMN | C4A-C10-N10 | 2.67 | 120.38 | 116.48 |
| 2 | X | 301 | FMN | C4-N3-C2 | -2.67 | 120.71 | 125.64 |
| 2 | E | 301 | FMN | C10-N1-C2 | 2.67 | 122.24 | 116.90 |
| 2 | 1 | 302 | FMN | C4A-C10-N1 | -2.67 | 118.54 | 124.73 |
| 2 | X | 301 | FMN | C4A-C10-N10 | 2.67 | 120.38 | 116.48 |
| 2 | p | 302 | FMN | C4-N3-C2 | -2.67 | 120.72 | 125.64 |
| 2 | 3 | 301 | FMN | O4-C4-C4A | -2.66 | 119.53 | 126.60 |
| 2 | u | 301 | FMN | C4A-C10-N1 | -2.66 | 118.56 | 124.73 |
| 2 | t | 301 | FMN | C4A-C10-N10 | 2.66 | 120.37 | 116.48 |
| 2 | 0 | 301 | FMN | C10-N1-C2 | 2.66 | 122.21 | 116.90 |
| 2 | O | 301 | FMN | C4A-C10-N1 | -2.65 | 118.57 | 124.73 |
| 2 | T | 301 | FMN | C4-N3-C2 | -2.65 | 120.74 | 125.64 |
| 2 | 1 | 301 | FMN | C4-N3-C2 | -2.65 | 120.74 | 125.64 |
| 2 | O | 301 | FMN | C4-N3-C2 | -2.65 | 120.75 | 125.64 |
| 2 | 5 | 301 | FMN | O4-C4-C4A | -2.65 | 119.57 | 126.60 |
| 2 | i | 301 | FMN | C4-N3-C2 | -2.65 | 120.75 | 125.64 |
| 2 | q | 301 | FMN | C4-N3-C2 | -2.64 | 120.76 | 125.64 |
| 2 | W | 301 | FMN | C4A-C10-N1 | -2.64 | 118.60 | 124.73 |
| 2 | 7 | 301 | FMN | C4-N3-C2 | -2.64 | 120.76 | 125.64 |
| 2 | j | 301 | FMN | C4A-C10-N10 | 2.64 | 120.34 | 116.48 |
| 2 | 3 | 301 | FMN | C4A-C10-N1 | -2.64 | 118.61 | 124.73 |
| 2 | h | 302 | FMN | C4-N3-C2 | -2.64 | 120.77 | 125.64 |
| 2 | t | 301 | FMN | C4-N3-C2 | -2.64 | 120.77 | 125.64 |
| 2 | G | 301 | FMN | C4A-C10-N10 | 2.64 | 120.34 | 116.48 |
| 2 | 7 | 302 | FMN | C4A-C10-N1 | -2.64 | 118.61 | 124.73 |
| 2 | A | 301 | FMN | C4-N3-C2 | -2.63 | 120.77 | 125.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 6 | 301 | FMN | C10-N1-C2 | 2.63 | 122.17 | 116.90 |
| 2 | G | 302 | FMN | C4-N3-C2 | -2.63 | 120.78 | 125.64 |
| 2 | r | 301 | FMN | O4-C4-C4A | -2.63 | 119.62 | 126.60 |
| 2 | 0 | 301 | FMN | C4A-C10-N10 | 2.63 | 120.32 | 116.48 |
| 2 | B | 301 | FMN | C4A-C10-N1 | -2.62 | 118.64 | 124.73 |
| 2 | k | 301 | FMN | C4-N3-C2 | -2.62 | 120.80 | 125.64 |
| 2 | Y | 301 | FMN | C4A-C10-N1 | -2.62 | 118.64 | 124.73 |
| 2 | T | 301 | FMN | C4A-C10-N1 | -2.62 | 118.65 | 124.73 |
| 2 | x | 301 | FMN | C4-N3-C2 | -2.62 | 120.80 | 125.64 |
| 2 | D | 301 | FMN | C4A-C10-N10 | 2.62 | 120.31 | 116.48 |
| 2 | M | 301 | FMN | C4A-C10-N1 | -2.61 | 118.67 | 124.73 |
| 2 | h | 302 | FMN | C4A-C10-N10 | 2.61 | 120.30 | 116.48 |
| 2 | J | 301 | FMN | C4-N3-C2 | -2.61 | 120.82 | 125.64 |
| 2 | r | 302 | FMN | C4A-C10-N10 | 2.61 | 120.30 | 116.48 |
| 2 | w | 301 | FMN | C4-N3-C2 | -2.61 | 120.82 | 125.64 |
| 2 | 0 | 302 | FMN | C4A-C10-N1 | -2.61 | 118.68 | 124.73 |
| 2 | x | 301 | FMN | C4A-C10-N1 | -2.61 | 118.68 | 124.73 |
| 2 | D | 301 | FMN | C4A-C10-N1 | -2.60 | 118.69 | 124.73 |
| 2 | C | 301 | FMN | C4-N3-C2 | -2.60 | 120.83 | 125.64 |
| 2 | 1 | 301 | FMN | O4-C4-C4A | -2.60 | 119.70 | 126.60 |
| 2 | 4 | 301 | FMN | C4-N3-C2 | -2.60 | 120.84 | 125.64 |
| 2 | m | 301 | FMN | C4-N3-C2 | -2.59 | 120.85 | 125.64 |
| 2 | r | 302 | FMN | O4-C4-C4A | -2.59 | 119.73 | 126.60 |
| 2 | n | 301 | FMN | C4A-C10-N1 | -2.59 | 118.73 | 124.73 |
| 2 | k | 301 | FMN | C4A-C10-N1 | -2.58 | 118.74 | 124.73 |
| 2 | q | 301 | FMN | C4A-C10-N1 | -2.58 | 118.74 | 124.73 |
| 2 | 5 | 302 | FMN | C4-N3-C2 | -2.58 | 120.88 | 125.64 |
| 2 | D | 301 | FMN | O4-C4-C4A | -2.57 | 119.77 | 126.60 |
| 2 | j | 301 | FMN | O4-C4-C4A | -2.57 | 119.78 | 126.60 |
| 2 | r | 302 | FMN | C4-N3-C2 | -2.57 | 120.89 | 125.64 |
| 2 | V | 301 | FMN | C4A-C10-N1 | -2.57 | 118.77 | 124.73 |
| 2 | P | 301 | FMN | C4A-C10-N10 | 2.57 | 120.23 | 116.48 |
| 2 | S | 301 | FMN | C4A-C10-N10 | 2.56 | 120.23 | 116.48 |
| 2 | D | 302 | FMN | C4A-C10-N1 | -2.56 | 118.79 | 124.73 |
| 2 | r | 301 | FMN | C4A-C10-N1 | -2.55 | 118.80 | 124.73 |
| 2 | w | 301 | FMN | C4A-C10-N1 | -2.55 | 118.82 | 124.73 |
| 2 | a | 301 | FMN | C4-N3-C2 | -2.54 | 120.94 | 125.64 |
| 2 | 7 | 301 | FMN | C4A-C10-N1 | -2.54 | 118.83 | 124.73 |
| 2 | 5 | 302 | FMN | C4A-C10-N1 | -2.54 | 118.83 | 124.73 |
| 2 | t | 301 | FMN | C4A-C10-N1 | -2.54 | 118.84 | 124.73 |
| 2 | p | 302 | FMN | C4A-C10-N1 | -2.53 | 118.85 | 124.73 |
| 2 | T | 301 | FMN | O4-C4-C4A | -2.53 | 119.89 | 126.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | p | 301 | FMN | C4A-C10-N1 | -2.52 | 118.87 | 124.73 |
| 2 | h | 302 | FMN | O4-C4-C4A | -2.52 | 119.91 | 126.60 |
| 2 | J | 301 | FMN | C4A-C10-N1 | -2.51 | 118.90 | 124.73 |
| 2 | 5 | 301 | FMN | C4A-C10-N1 | -2.51 | 118.91 | 124.73 |
| 2 | c | 301 | FMN | C4A-C10-N10 | 2.51 | 120.15 | 116.48 |
| 2 | 1 | 301 | FMN | C4A-C10-N1 | -2.51 | 118.92 | 124.73 |
| 2 | M | 301 | FMN | O4-C4-C4A | -2.50 | 119.98 | 126.60 |
| 2 | i | 301 | FMN | C4A-C10-N1 | -2.50 | 118.94 | 124.73 |
| 2 | 2 | 301 | FMN | C4A-C10-N10 | 2.49 | 120.13 | 116.48 |
| 2 | 4 | 301 | FMN | C4A-C10-N1 | -2.49 | 118.94 | 124.73 |
| 2 | 7 | 301 | FMN | O4-C4-C4A | -2.49 | 119.99 | 126.60 |
| 2 | 6 | 301 | FMN | O4-C4-C4A | -2.48 | 120.01 | 126.60 |
| 2 | a | 301 | FMN | O4-C4-C4A | -2.48 | 120.02 | 126.60 |
| 2 | e | 301 | FMN | O4-C4-C4A | -2.48 | 120.02 | 126.60 |
| 2 | A | 301 | FMN | C4A-C10-N1 | -2.48 | 118.98 | 124.73 |
| 2 | G | 302 | FMN | C4A-C10-N1 | -2.48 | 118.98 | 124.73 |
| 2 | h | 302 | FMN | C4A-C10-N1 | -2.48 | 118.98 | 124.73 |
| 2 | m | 302 | FMN | C4A-C4-N3 | 2.48 | 119.48 | 113.19 |
| 2 | 6 | 301 | FMN | C5A-C9A-N10 | 2.47 | 120.51 | 117.95 |
| 2 | O | 301 | FMN | O4-C4-C4A | -2.47 | 120.04 | 126.60 |
| 2 | 0 | 301 | FMN | O4-C4-C4A | -2.46 | 120.07 | 126.60 |
| 2 | Q | 301 | FMN | C4A-C10-N1 | -2.46 | 119.03 | 124.73 |
| 2 | N | 301 | FMN | C10-C4A-N5 | -2.46 | 119.64 | 124.86 |
| 2 | I | 301 | FMN | C4A-C10-N1 | -2.46 | 119.03 | 124.73 |
| 2 | t | 301 | FMN | O4-C4-C4A | -2.45 | 120.09 | 126.60 |
| 2 | s | 301 | FMN | C4A-C4-N3 | 2.45 | 119.42 | 113.19 |
| 2 | X | 301 | FMN | O4-C4-C4A | -2.45 | 120.10 | 126.60 |
| 2 | 5 | 302 | FMN | O4-C4-C4A | -2.45 | 120.11 | 126.60 |
| 2 | P | 301 | FMN | C10-C4A-N5 | -2.45 | 119.66 | 124.86 |
| 2 | 0 | 302 | FMN | O4-C4-C4A | -2.44 | 120.12 | 126.60 |
| 2 | 1 | 302 | FMN | O4-C4-C4A | -2.44 | 120.13 | 126.60 |
| 2 | m | 301 | FMN | C4A-C10-N1 | -2.44 | 119.08 | 124.73 |
| 2 | V | 301 | FMN | C4A-C4-N3 | 2.44 | 119.38 | 113.19 |
| 2 | N | 301 | FMN | C4-C4A-N5 | 2.43 | 121.69 | 118.23 |
| 2 | 0 | 301 | FMN | C4A-C4-N3 | 2.43 | 119.37 | 113.19 |
| 2 | f | 301 | FMN | O4-C4-C4A | -2.43 | 120.15 | 126.60 |
| 2 | J | 301 | FMN | O4-C4-C4A | -2.43 | 120.16 | 126.60 |
| 2 | D | 302 | FMN | O4-C4-C4A | -2.43 | 120.16 | 126.60 |
| 2 | G | 301 | FMN | C4A-C4-N3 | 2.42 | 119.35 | 113.19 |
| 2 | V | 301 | FMN | C4A-C10-N10 | 2.42 | 120.02 | 116.48 |
| 2 | 2 | 301 | FMN | C4A-C4-N3 | 2.42 | 119.34 | 113.19 |
| 2 | r | 302 | FMN | C4A-C10-N1 | -2.42 | 119.12 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | N | 301 | FMN | C4A-C4-N3 | 2.41 | 119.32 | 113.19 |
| 2 | Y | 301 | FMN | C4A-C4-N3 | 2.41 | 119.31 | 113.19 |
| 2 | 7 | 302 | FMN | O4-C4-C4A | -2.41 | 120.21 | 126.60 |
| 2 | N | 301 | FMN | C10-N1-C2 | 2.41 | 121.71 | 116.90 |
| 2 | c | 301 | FMN | C4A-C4-N3 | 2.41 | 119.30 | 113.19 |
| 2 | k | 301 | FMN | O4-C4-C4A | -2.40 | 120.22 | 126.60 |
| 2 | a | 301 | FMN | C4-C4A-N5 | 2.40 | 121.65 | 118.23 |
| 2 | E | 301 | FMN | O4-C4-C4A | -2.40 | 120.22 | 126.60 |
| 2 | P | 301 | FMN | C4A-C4-N3 | 2.40 | 119.29 | 113.19 |
| 2 | A | 301 | FMN | O4-C4-C4A | -2.40 | 120.23 | 126.60 |
| 2 | I | 301 | FMN | C4A-C4-N3 | 2.40 | 119.29 | 113.19 |
| 2 | S | 301 | FMN | C10-C4A-N5 | -2.40 | 119.76 | 124.86 |
| 2 | G | 302 | FMN | O4-C4-C4A | -2.40 | 120.23 | 126.60 |
| 2 | p | 302 | FMN | O4-C4-C4A | -2.40 | 120.23 | 126.60 |
| 2 | m | 302 | FMN | C10-N1-C2 | 2.40 | 121.70 | 116.90 |
| 2 | C | 301 | FMN | C4A-C10-N1 | -2.40 | 119.17 | 124.73 |
| 2 | i | 301 | FMN | O4-C4-C4A | -2.40 | 120.25 | 126.60 |
| 2 | c | 301 | FMN | C10-C4A-N5 | -2.39 | 119.78 | 124.86 |
| 2 | m | 301 | FMN | O4-C4-C4A | -2.39 | 120.26 | 126.60 |
| 2 | B | 301 | FMN | O4-C4-C4A | -2.39 | 120.26 | 126.60 |
| 2 | S | 301 | FMN | C4A-C4-N3 | 2.39 | 119.26 | 113.19 |
| 2 | 4 | 301 | FMN | O4-C4-C4A | -2.39 | 120.26 | 126.60 |
| 2 | C | 301 | FMN | O4-C4-C4A | -2.39 | 120.27 | 126.60 |
| 2 | N | 301 | FMN | O4-C4-C4A | -2.39 | 120.27 | 126.60 |
| 2 | B | 301 | FMN | C10-C4A-N5 | -2.39 | 119.79 | 124.86 |
| 2 | G | 301 | FMN | C10-C4A-N5 | -2.39 | 119.79 | 124.86 |
| 2 | x | 301 | FMN | O4-C4-C4A | -2.39 | 120.27 | 126.60 |
| 2 | V | 301 | FMN | C4-C4A-N5 | 2.39 | 121.63 | 118.23 |
| 2 | P | 301 | FMN | C4-C4A-N5 | 2.38 | 121.62 | 118.23 |
| 2 | P | 301 | FMN | O4-C4-C4A | -2.38 | 120.28 | 126.60 |
| 2 | q | 301 | FMN | O4-C4-C4A | -2.38 | 120.28 | 126.60 |
| 2 | n | 301 | FMN | O4-C4-C4A | -2.38 | 120.28 | 126.60 |
| 2 | R | 301 | FMN | O4-C4-C4A | -2.38 | 120.29 | 126.60 |
| 2 | M | 302 | FMN | O4-C4-C4A | -2.38 | 120.29 | 126.60 |
| 2 | d | 301 | FMN | O4-C4-C4A | -2.38 | 120.29 | 126.60 |
| 2 | V | 301 | FMN | C10-C4A-N5 | -2.38 | 119.81 | 124.86 |
| 2 | m | 302 | FMN | C10-C4A-N5 | -2.37 | 119.82 | 124.86 |
| 2 | c | 301 | FMN | O4-C4-C4A | -2.37 | 120.30 | 126.60 |
| 2 | G | 301 | FMN | O4-C4-C4A | -2.37 | 120.31 | 126.60 |
| 2 | S | 301 | FMN | O4-C4-C4A | -2.37 | 120.31 | 126.60 |
| 2 | X | 301 | FMN | C1'-C2'-C3' | 2.37 | 116.40 | 109.79 |
| 2 | 2 | 301 | FMN | C10-C4A-N5 | -2.37 | 119.83 | 124.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | W | 301 | FMN | C4A-C4-N3 | 2.37 | 119.20 | 113.19 |
| 2 | w | 301 | FMN | O4-C4-C4A | -2.36 | 120.33 | 126.60 |
| 2 | 0 | 301 | FMN | C5A-C9A-N10 | 2.36 | 120.39 | 117.95 |
| 2 | p | 302 | FMN | C10-C4A-N5 | -2.36 | 119.84 | 124.86 |
| 2 | u | 301 | FMN | C4A-C4-N3 | 2.36 | 119.19 | 113.19 |
| 2 | E | 301 | FMN | C4A-C4-N3 | 2.36 | 119.19 | 113.19 |
| 2 | r | 301 | FMN | C4A-C4-N3 | 2.36 | 119.18 | 113.19 |
| 2 | 6 | 301 | FMN | C4A-C4-N3 | 2.36 | 119.18 | 113.19 |
| 2 | O | 301 | FMN | C4A-C4-N3 | 2.35 | 119.17 | 113.19 |
| 2 | 2 | 301 | FMN | O4-C4-C4A | -2.35 | 120.37 | 126.60 |
| 2 | M | 302 | FMN | C4A-C4-N3 | 2.35 | 119.15 | 113.19 |
| 2 | a | 301 | FMN | C4A-C10-N1 | -2.35 | 119.29 | 124.73 |
| 2 | f | 301 | FMN | C4A-C4-N3 | 2.34 | 119.13 | 113.19 |
| 2 | m | 302 | FMN | O4-C4-C4A | -2.34 | 120.40 | 126.60 |
| 2 | 4 | 301 | FMN | C10-C4A-N5 | -2.34 | 119.90 | 124.86 |
| 2 | i | 301 | FMN | C4A-C4-N3 | 2.33 | 119.12 | 113.19 |
| 2 | a | 302 | FMN | O2-C2-N1 | -2.33 | 117.96 | 121.83 |
| 2 | t | 301 | FMN | C4A-C4-N3 | 2.33 | 119.12 | 113.19 |
| 2 | a | 301 | FMN | C10-C4A-N5 | -2.33 | 119.91 | 124.86 |
| 2 | Q | 301 | FMN | C4A-C4-N3 | 2.33 | 119.10 | 113.19 |
| 2 | A | 301 | FMN | C10-C4A-N5 | -2.32 | 119.94 | 124.86 |
| 2 | V | 301 | FMN | O4-C4-C4A | -2.32 | 120.45 | 126.60 |
| 2 | 0 | 302 | FMN | C4A-C4-N3 | 2.31 | 119.07 | 113.19 |
| 2 | M | 301 | FMN | C4A-C4-N3 | 2.31 | 119.06 | 113.19 |
| 2 | q | 301 | FMN | C4A-C4-N3 | 2.31 | 119.05 | 113.19 |
| 2 | w | 301 | FMN | C10-C4A-N5 | -2.31 | 119.96 | 124.86 |
| 2 | p | 301 | FMN | C4A-C4-N3 | 2.31 | 119.05 | 113.19 |
| 2 | 3 | 301 | FMN | C4A-C4-N3 | 2.31 | 119.05 | 113.19 |
| 2 | a | 302 | FMN | C4A-C4-N3 | 2.31 | 119.05 | 113.19 |
| 2 | n | 301 | FMN | C4A-C4-N3 | 2.31 | 119.04 | 113.19 |
| 2 | m | 302 | FMN | C4-C4A-N5 | 2.30 | 121.50 | 118.23 |
| 2 | G | 302 | FMN | C4A-C4-N3 | 2.29 | 119.01 | 113.19 |
| 2 | C | 301 | FMN | C10-C4A-N5 | -2.29 | 119.99 | 124.86 |
| 2 | w | 301 | FMN | C4A-C4-N3 | 2.29 | 119.01 | 113.19 |
| 2 | e | 301 | FMN | C4A-C4-N3 | 2.29 | 119.01 | 113.19 |
| 2 | j | 301 | FMN | C4A-C4-N3 | 2.29 | 119.01 | 113.19 |
| 2 | 5 | 301 | FMN | C4A-C4-N3 | 2.29 | 119.00 | 113.19 |
| 2 | f | 301 | FMN | C10-C4A-N5 | -2.29 | 120.00 | 124.86 |
| 2 | B | 301 | FMN | C4A-C4-N3 | 2.29 | 119.00 | 113.19 |
| 2 | G | 301 | FMN | C4-C4A-N5 | 2.28 | 121.48 | 118.23 |
| 2 | 5 | 301 | FMN | C10-C4A-N5 | -2.28 | 120.02 | 124.86 |
| 2 | A | 301 | FMN | C4A-C4-N3 | 2.28 | 118.98 | 113.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 7 | 302 | FMN | C10-C4A-N5 | -2.28 | 120.02 | 124.86 |
| 2 | h | 301 | FMN | C4A-C4-N3 | 2.28 | 118.97 | 113.19 |
| 2 | a | 302 | FMN | C10-C4A-N5 | -2.28 | 120.03 | 124.86 |
| 2 | h | 302 | FMN | C4A-C4-N3 | 2.28 | 118.97 | 113.19 |
| 2 | p | 302 | FMN | C4A-C4-N3 | 2.27 | 118.97 | 113.19 |
| 2 | 7 | 301 | FMN | C4A-C4-N3 | 2.27 | 118.96 | 113.19 |
| 2 | 0 | 302 | FMN | C10-C4A-N5 | -2.27 | 120.03 | 124.86 |
| 2 | G | 302 | FMN | C10-C4A-N5 | -2.27 | 120.03 | 124.86 |
| 2 | F | 301 | FMN | C4A-C4-N3 | 2.27 | 118.96 | 113.19 |
| 2 | J | 301 | FMN | C10-C4A-N5 | -2.27 | 120.04 | 124.86 |
| 2 | 1 | 302 | FMN | C4A-C4-N3 | 2.27 | 118.96 | 113.19 |
| 2 | D | 301 | FMN | C4A-C4-N3 | 2.27 | 118.96 | 113.19 |
| 2 | C | 301 | FMN | C4A-C4-N3 | 2.27 | 118.95 | 113.19 |
| 2 | M | 302 | FMN | C10-N1-C2 | 2.27 | 121.44 | 116.90 |
| 2 | D | 302 | FMN | C4A-C4-N3 | 2.27 | 118.94 | 113.19 |
| 2 | 7 | 301 | FMN | C4'-C3'-C2' | -2.27 | 108.65 | 113.36 |
| 2 | J | 301 | FMN | C4A-C4-N3 | 2.26 | 118.94 | 113.19 |
| 2 | k | 301 | FMN | C4A-C4-N3 | 2.26 | 118.93 | 113.19 |
| 2 | C | 301 | FMN | C4-C4A-N5 | 2.26 | 121.45 | 118.23 |
| 2 | m | 301 | FMN | C10-C4A-N5 | -2.26 | 120.06 | 124.86 |
| 2 | a | 301 | FMN | C4A-C4-N3 | 2.26 | 118.93 | 113.19 |
| 2 | k | 301 | FMN | C10-C4A-N5 | -2.26 | 120.06 | 124.86 |
| 2 | 7 | 302 | FMN | C4A-C4-N3 | 2.26 | 118.92 | 113.19 |
| 2 | r | 302 | FMN | C4A-C4-N3 | 2.25 | 118.92 | 113.19 |
| 2 | P | 301 | FMN | C10-N1-C2 | 2.25 | 121.41 | 116.90 |
| 2 | i | 301 | FMN | C10-C4A-N5 | -2.25 | 120.08 | 124.86 |
| 2 | 1 | 301 | FMN | C4A-C4-N3 | 2.25 | 118.91 | 113.19 |
| 2 | q | 301 | FMN | C10-C4A-N5 | -2.25 | 120.09 | 124.86 |
| 2 | T | 301 | FMN | C4A-C4-N3 | 2.24 | 118.89 | 113.19 |
| 2 | M | 301 | FMN | C10-C4A-N5 | -2.24 | 120.10 | 124.86 |
| 2 | X | 301 | FMN | C4A-C4-N3 | 2.24 | 118.88 | 113.19 |
| 2 | c | 301 | FMN | C4-C4A-N5 | 2.24 | 121.42 | 118.23 |
| 2 | M | 302 | FMN | C10-C4A-N5 | -2.23 | 120.12 | 124.86 |
| 2 | O | 301 | FMN | C10-N1-C2 | 2.23 | 121.37 | 116.90 |
| 2 | m | 301 | FMN | C4A-C4-N3 | 2.23 | 118.85 | 113.19 |
| 2 | O | 301 | FMN | C10-C4A-N5 | -2.23 | 120.13 | 124.86 |
| 2 | n | 301 | FMN | C10-C4A-N5 | -2.22 | 120.14 | 124.86 |
| 2 | a | 302 | FMN | C4'-C3'-C2' | -2.22 | 108.74 | 113.36 |
| 2 | p | 302 | FMN | C4-C4A-N5 | 2.22 | 121.39 | 118.23 |
| 2 | d | 301 | FMN | C4A-C4-N3 | 2.22 | 118.82 | 113.19 |
| 2 | S | 301 | FMN | C4-C4A-N5 | 2.21 | 121.38 | 118.23 |
| 2 | R | 301 | FMN | C4A-C4-N3 | 2.21 | 118.81 | 113.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 7 | 301 | FMN | C10-C4A-N5 | -2.21 | 120.17 | 124.86 |
| 2 | d | 301 | FMN | C10-C4A-N5 | -2.21 | 120.17 | 124.86 |
| 2 | 2 | 301 | FMN | C4-C4A-N5 | 2.21 | 121.37 | 118.23 |
| 2 | 5 | 302 | FMN | C4A-C4-N3 | 2.21 | 118.79 | 113.19 |
| 2 | Q | 301 | FMN | C10-C4A-N5 | -2.20 | 120.18 | 124.86 |
| 2 | 4 | 301 | FMN | C4A-C4-N3 | 2.20 | 118.78 | 113.19 |
| 2 | T | 301 | FMN | C4'-C3'-C2' | -2.20 | 108.79 | 113.36 |
| 2 | A | 301 | FMN | C4-C4A-N5 | 2.20 | 121.36 | 118.23 |
| 2 | t | 301 | FMN | C10-C4A-N5 | -2.19 | 120.20 | 124.86 |
| 2 | x | 301 | FMN | C10-C4A-N5 | -2.19 | 120.20 | 124.86 |
| 2 | D | 302 | FMN | C10-C4A-N5 | -2.19 | 120.21 | 124.86 |
| 2 | T | 301 | FMN | C10-C4A-N5 | -2.19 | 120.21 | 124.86 |
| 2 | B | 301 | FMN | C4'-C3'-C2' | -2.19 | 108.81 | 113.36 |
| 2 | i | 301 | FMN | C4-C4A-N5 | 2.19 | 121.34 | 118.23 |
| 2 | R | 301 | FMN | C10-C4A-N5 | -2.18 | 120.23 | 124.86 |
| 2 | 4 | 301 | FMN | C4-C4A-N5 | 2.18 | 121.33 | 118.23 |
| 2 | 5 | 302 | FMN | C10-C4A-N5 | -2.17 | 120.24 | 124.86 |
| 2 | x | 301 | FMN | C4A-C4-N3 | 2.17 | 118.71 | 113.19 |
| 2 | 1 | 302 | FMN | C10-C4A-N5 | -2.17 | 120.25 | 124.86 |
| 2 | E | 301 | FMN | C10-C4A-N5 | -2.17 | 120.25 | 124.86 |
| 2 | p | 301 | FMN | C10-C4A-N5 | -2.16 | 120.27 | 124.86 |
| 2 | l | 301 | FMN | C10-C4A-N5 | -2.16 | 120.27 | 124.86 |
| 2 | f | 301 | FMN | C10-N1-C2 | 2.16 | 121.23 | 116.90 |
| 2 | r | 302 | FMN | C10-C4A-N5 | -2.16 | 120.27 | 124.86 |
| 2 | G | 302 | FMN | C4-C4A-N5 | 2.16 | 121.31 | 118.23 |
| 2 | s | 301 | FMN | C10-N1-C2 | 2.15 | 121.20 | 116.90 |
| 2 | h | 302 | FMN | C4'-C3'-C2' | -2.15 | 108.89 | 113.36 |
| 2 | B | 301 | FMN | C4-C4A-N5 | 2.15 | 121.29 | 118.23 |
| 2 | G | 301 | FMN | C10-N1-C2 | 2.14 | 121.19 | 116.90 |
| 2 | w | 301 | FMN | C4-C4A-N5 | 2.13 | 121.27 | 118.23 |
| 2 | e | 301 | FMN | C10-C4A-N5 | -2.13 | 120.33 | 124.86 |
| 2 | h | 302 | FMN | C10-C4A-N5 | -2.13 | 120.34 | 124.86 |
| 2 | e | 301 | FMN | C10-N1-C2 | 2.13 | 121.15 | 116.90 |
| 2 | 2 | 301 | FMN | C10-N1-C2 | 2.12 | 121.15 | 116.90 |
| 2 | 3 | 301 | FMN | C10-C4A-N5 | -2.12 | 120.35 | 124.86 |
| 2 | S | 301 | FMN | C10-N1-C2 | 2.12 | 121.14 | 116.90 |
| 2 | r | 301 | FMN | C10-C4A-N5 | -2.12 | 120.36 | 124.86 |
| 2 | 5 | 301 | FMN | C4-C4A-N5 | 2.12 | 121.24 | 118.23 |
| 2 | u | 301 | FMN | C5'-C4'-C3' | -2.11 | 108.13 | 112.20 |
| 2 | a | 302 | FMN | C9-C9A-N10 | -2.10 | 118.99 | 121.84 |
| 2 | r | 301 | FMN | C5'-C4'-C3' | -2.10 | 108.15 | 112.20 |
| 2 | h | 301 | FMN | C10-N1-C2 | 2.09 | 121.09 | 116.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 301 | FMN | C10-C4A-N5 | -2.09 | 120.42 | 124.86 |
| 2 | m | 301 | FMN | C4-C4A-N5 | 2.09 | 121.21 | 118.23 |
| 2 | V | 301 | FMN | C10-N1-C2 | 2.09 | 121.08 | 116.90 |
| 2 | t | 301 | FMN | C10-N1-C2 | 2.09 | 121.08 | 116.90 |
| 2 | f | 301 | FMN | C4-C4A-N5 | 2.09 | 121.21 | 118.23 |
| 2 | F | 301 | FMN | C10-C4A-N5 | -2.09 | 120.42 | 124.86 |
| 2 | c | 301 | FMN | C10-N1-C2 | 2.09 | 121.08 | 116.90 |
| 2 | O | 301 | FMN | C4-C4A-N5 | 2.09 | 121.20 | 118.23 |
| 2 | J | 301 | FMN | C4-C4A-N5 | 2.08 | 121.19 | 118.23 |
| 2 | Y | 301 | FMN | C10-N1-C2 | 2.08 | 121.06 | 116.90 |
| 2 | q | 301 | FMN | C4-C4A-N5 | 2.07 | 121.18 | 118.23 |
| 2 | W | 301 | FMN | C10-N1-C2 | 2.07 | 121.04 | 116.90 |
| 2 | P | 301 | FMN | C4'-C3'-C2' | -2.07 | 109.06 | 113.36 |
| 2 | t | 301 | FMN | C4-C4A-N5 | 2.07 | 121.18 | 118.23 |
| 2 | W | 301 | FMN | C10-C4A-N5 | -2.07 | 120.47 | 124.86 |
| 2 | M | 301 | FMN | C10-N1-C2 | 2.07 | 121.03 | 116.90 |
| 2 | J | 301 | FMN | C4'-C3'-C2' | -2.06 | 109.07 | 113.36 |
| 2 | B | 301 | FMN | C10-N1-C2 | 2.06 | 121.03 | 116.90 |
| 2 | I | 301 | FMN | C10-C4A-N5 | -2.06 | 120.48 | 124.86 |
| 2 | Q | 301 | FMN | C4-C4A-N5 | 2.06 | 121.17 | 118.23 |
| 2 | q | 301 | FMN | C10-N1-C2 | 2.06 | 121.02 | 116.90 |
| 2 | Q | 301 | FMN | C5'-C4'-C3' | -2.06 | 108.23 | 112.20 |
| 2 | u | 301 | FMN | C10-N1-C2 | 2.05 | 121.00 | 116.90 |
| 2 | h | 301 | FMN | C10-C4A-N5 | -2.05 | 120.51 | 124.86 |
| 2 | 0 | 301 | FMN | C10-C4A-N5 | -2.04 | 120.52 | 124.86 |
| 2 | j | 301 | FMN | C10-C4A-N5 | -2.04 | 120.52 | 124.86 |
| 2 | X | 301 | FMN | C10-C4A-N5 | -2.04 | 120.53 | 124.86 |
| 2 | G | 301 | FMN | C4'-C3'-C2' | -2.04 | 109.12 | 113.36 |
| 2 | s | 301 | FMN | C5A-C9A-N10 | 2.04 | 120.06 | 117.95 |
| 2 | F | 301 | FMN | C10-N1-C2 | 2.03 | 120.97 | 116.90 |
| 2 | j | 301 | FMN | C10-N1-C2 | 2.03 | 120.96 | 116.90 |
| 2 | k | 301 | FMN | C4-C4A-N5 | 2.03 | 121.12 | 118.23 |
| 2 | X | 301 | FMN | C5A-C9A-N10 | 2.03 | 120.05 | 117.95 |
| 2 | k | 301 | FMN | C10-N1-C2 | 2.03 | 120.96 | 116.90 |
| 2 | B | 301 | FMN | C5'-C4'-C3' | -2.03 | 108.28 | 112.20 |
| 2 | 0 | 302 | FMN | C4-C4A-N5 | 2.03 | 121.12 | 118.23 |
| 2 | T | 301 | FMN | C10-N1-C2 | 2.02 | 120.95 | 116.90 |
| 2 | E | 301 | FMN | C5A-C9A-N10 | 2.02 | 120.04 | 117.95 |
| 2 | M | 301 | FMN | C4-C4A-N5 | 2.02 | 121.11 | 118.23 |
| 2 | s | 301 | FMN | C10-C4A-N5 | -2.02 | 120.58 | 124.86 |
| 2 | p | 302 | FMN | C10-N1-C2 | 2.01 | 120.93 | 116.90 |
| 2 | n | 301 | FMN | C10-N1-C2 | 2.01 | 120.92 | 116.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 0 | 302 | FMN | C10-N1-C2 | 2.01 | 120.92 | 116.90 |
| 2 | 3 | 301 | FMN | C10-N1-C2 | 2.01 | 120.92 | 116.90 |
| 2 | 5 | 301 | FMN | C10-N1-C2 | 2.01 | 120.92 | 116.90 |
| 2 | w | 301 | FMN | C5'-C4'-C3' | -2.00 | 108.33 | 112.20 |
| 2 | a | 302 | FMN | C6-C7-C8 | 2.00 | 122.54 | 119.67 |
| 2 | q | 301 | FMN | C5'-C4'-C3' | -2.00 | 108.33 | 112.20 |
| 2 | a | 302 | FMN | O4-C4-C4A | -2.00 | 121.29 | 126.60 |
| 2 | r | 301 | FMN | C10-N1-C2 | 2.00 | 120.91 | 116.90 |

There are no chirality outliers.

All (586) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | A | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | A | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | A | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | A | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | A | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | A | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | A | 301 | FMN | C5'-O5'-P-O2P |
| 2 | A | 301 | FMN | C5'-O5'-P-O3P |
| 2 | B | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | B | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | B | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | B | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | B | 301 | FMN | C5'-O5'-P-O2P |
| 2 | B | 301 | FMN | C5'-O5'-P-O3P |
| 2 | C | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | C | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | D | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | D | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | D | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | D | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | D | 301 | FMN | C5'-O5'-P-O2P |
| 2 | D | 301 | FMN | C5'-O5'-P-O3P |
| 2 | D | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | D | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | D | 302 | FMN | O4'-C4'-C5'-O5' |
| 2 | E | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | E | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | E | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | E | 301 | FMN | C1'-C2'-C3'-O3' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | E | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | E | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | E | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | F | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | F | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | F | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | F | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | F | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | F | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | F | 301 | FMN | C5'-O5'-P-O2P |
| 2 | F | 301 | FMN | C5'-O5'-P-O3P |
| 2 | G | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | G | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | G | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | G | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | G | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | G | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | G | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | G | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | G | 301 | FMN | C5'-O5'-P-O1P |
| 2 | G | 301 | FMN | C5'-O5'-P-O2P |
| 2 | G | 301 | FMN | C5'-O5'-P-O3P |
| 2 | G | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | G | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | G | 302 | FMN | C5'-O5'-P-O1P |
| 2 | G | 302 | FMN | C5'-O5'-P-O2P |
| 2 | G | 302 | FMN | C5'-O5'-P-O3P |
| 2 | I | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | I | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | I | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | I | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | I | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | I | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | I | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | I | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | J | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | J | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | J | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | J | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | M | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | M | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | M | 302 | FMN | C2'-C1'-N10-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | M | 302 | FMN | C1'-C2'-C3'-O3' |
| 2 | M | 302 | FMN | C1'-C2'-C3'-C4' |
| 2 | M | 302 | FMN | O2'-C2'-C3'-C4' |
| 2 | M | 302 | FMN | C5'-O5'-P-O1P |
| 2 | N | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | N | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | N | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | N | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | N | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | N | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | N | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | N | 301 | FMN | C5'-O5'-P-O1P |
| 2 | N | 301 | FMN | C5'-O5'-P-O2P |
| 2 | N | 301 | FMN | C5'-O5'-P-O3P |
| 2 | O | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | O | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | O | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | O | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | O | 301 | FMN | C5'-O5'-P-O2P |
| 2 | O | 301 | FMN | C5'-O5'-P-O3P |
| 2 | P | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | P | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | Q | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | Q | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | Q | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | Q | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | Q | 301 | FMN | C5'-O5'-P-O2P |
| 2 | Q | 301 | FMN | C5'-O5'-P-O3P |
| 2 | R | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | R | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | R | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | R | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | R | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | R | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | R | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | S | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | S | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | S | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | S | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | S | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | S | 301 | FMN | C5'-O5'-P-O2P |
| 2 | S | 301 | FMN | C5'-O5'-P-O3P |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | T | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | T | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | T | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | V | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | V | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | V | 301 | FMN | C4'-C5'-O5'-P |
| 2 | W | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | W | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | W | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | W | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | W | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | W | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | W | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | W | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | X | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | X | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | X | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | X | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | X | 301 | FMN | C5'-O5'-P-O1P |
| 2 | X | 301 | FMN | C5'-O5'-P-O2P |
| 2 | X | 301 | FMN | C5'-O5'-P-O3P |
| 2 | Y | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | Y | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | Y | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | Y | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | Y | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | Y | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | Y | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | Y | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 0 | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | 0 | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | 0 | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | 0 | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | 0 | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | 0 | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | 0 | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | 0 | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 0 | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 0 | 301 | FMN | C5'-O5'-P-O1P |
| 2 | 0 | 301 | FMN | C5'-O5'-P-O2P |
| 2 | 0 | 301 | FMN | C5'-O5'-P-O3P |
| 2 | 0 | 302 | FMN | N10-C1'-C2'-O2' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 0 | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | 0 | 302 | FMN | C1'-C2'-C3'-O3' |
| 2 | 0 | 302 | FMN | C1'-C2'-C3'-C4' |
| 2 | 0 | 302 | FMN | C5'-O5'-P-O1P |
| 2 | 0 | 302 | FMN | C5'-O5'-P-O2P |
| 2 | 0 | 302 | FMN | C5'-O5'-P-O3P |
| 2 | 1 | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | 1 | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | 1 | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | 1 | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | 1 | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | 1 | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | 1 | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 1 | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 1 | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | 1 | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | 1 | 302 | FMN | C5'-O5'-P-O1P |
| 2 | 1 | 302 | FMN | C5'-O5'-P-O2P |
| 2 | 1 | 302 | FMN | C5'-O5'-P-O3P |
| 2 | 2 | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | 2 | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | 3 | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | 3 | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | 3 | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | 3 | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | 3 | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 3 | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 4 | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | 4 | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | 4 | 301 | FMN | C5'-O5'-P-O2P |
| 2 | 4 | 301 | FMN | C5'-O5'-P-O3P |
| 2 | 5 | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | 5 | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | 5 | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | 5 | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | 5 | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | 5 | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 5 | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | 5 | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 5 | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 5 | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | 5 | 302 | FMN | N10-C1'-C2'-C3' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 5 | 302 | FMN | C1'-C2'-C3'-O3' |
| 2 | 5 | 302 | FMN | C1'-C2'-C3'-C4' |
| 2 | 5 | 302 | FMN | O2'-C2'-C3'-O3' |
| 2 | 5 | 302 | FMN | O2'-C2'-C3'-C4' |
| 2 | 5 | 302 | FMN | O4'-C4'-C5'-O5' |
| 2 | 6 | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | 6 | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | 6 | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | 6 | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | 6 | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | 6 | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | 6 | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | 6 | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 6 | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 6 | 301 | FMN | C5'-O5'-P-O1P |
| 2 | 6 | 301 | FMN | C5'-O5'-P-O2P |
| 2 | 6 | 301 | FMN | C5'-O5'-P-O3P |
| 2 | 7 | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 7 | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 7 | 301 | FMN | C5'-O5'-P-O1P |
| 2 | 7 | 301 | FMN | C5'-O5'-P-O2P |
| 2 | 7 | 301 | FMN | C5'-O5'-P-O3P |
| 2 | 7 | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | 7 | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | 7 | 302 | FMN | C2'-C3'-C4'-O4' |
| 2 | 7 | 302 | FMN | O3'-C3'-C4'-O4' |
| 2 | 7 | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | 7 | 302 | FMN | O4'-C4'-C5'-O5' |
| 2 | a | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | a | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | a | 301 | FMN | C5'-O5'-P-O3P |
| 2 | a | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | a | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | a | 302 | FMN | C1'-C2'-C3'-O3' |
| 2 | a | 302 | FMN | C1'-C2'-C3'-C4' |
| 2 | a | 302 | FMN | C5'-O5'-P-O1P |
| 2 | a | 302 | FMN | C5'-O5'-P-O2P |
| 2 | a | 302 | FMN | C5'-O5'-P-O3P |
| 2 | c | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | c | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | c | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | c | 301 | FMN | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | c | 301 | FMN | C4'-C5'-O5'-P |
| 2 | d | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | d | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | d | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | d | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | d | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | d | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | d | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | e | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | e | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | e | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | e | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | e | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | e | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | e | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | e | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | e | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | f | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | f | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | f | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | f | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | f | 301 | FMN | C4'-C5'-O5'-P |
| 2 | h | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | h | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | h | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | h | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | h | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | h | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | h | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | h | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | h | 301 | FMN | C4'-C5'-O5'-P |
| 2 | h | 301 | FMN | C5'-O5'-P-O1P |
| 2 | h | 301 | FMN | C5'-O5'-P-O2P |
| 2 | h | 301 | FMN | C5'-O5'-P-O3P |
| 2 | h | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | h | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | h | 302 | FMN | C2'-C3'-C4'-O4' |
| 2 | h | 302 | FMN | O3'-C3'-C4'-O4' |
| 2 | h | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | h | 302 | FMN | O4'-C4'-C5'-O5' |
| 2 | h | 302 | FMN | C5'-O5'-P-O2P |
| 2 | i | 301 | FMN | C1'-C2'-C3'-O3' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | i | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | i | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | i | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | i | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | i | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | j | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | j | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | j | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | j | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | j | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | j | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | j | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | j | 301 | FMN | C4'-C5'-O5'-P |
| 2 | j | 301 | FMN | C5'-O5'-P-O1P |
| 2 | j | 301 | FMN | C5'-O5'-P-O2P |
| 2 | j | 301 | FMN | C5'-O5'-P-O3P |
| 2 | k | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | k | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | k | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | k | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | k | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | k | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | k | 301 | FMN | C5'-O5'-P-O2P |
| 2 | k | 301 | FMN | C5'-O5'-P-O3P |
| 2 | m | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | m | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | m | 302 | FMN | C2'-C1'-N10-C10 |
| 2 | m | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | m | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | m | 302 | FMN | C1'-C2'-C3'-O3' |
| 2 | m | 302 | FMN | C1'-C2'-C3'-C4' |
| 2 | m | 302 | FMN | O2'-C2'-C3'-O3' |
| 2 | m | 302 | FMN | O2'-C2'-C3'-C4' |
| 2 | m | 302 | FMN | C5'-O5'-P-O2P |
| 2 | m | 302 | FMN | C5'-O5'-P-O3P |
| 2 | n | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | n | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | n | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | n | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | p | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | p | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | p | 301 | FMN | C1'-C2'-C3'-O3' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | p | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | p | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | p | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | p | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | p | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | p | 301 | FMN | C5'-O5'-P-O2P |
| 2 | p | 301 | FMN | C5'-O5'-P-O3P |
| 2 | p | 302 | FMN | N10-C1'-C2'-O2' |
| 2 | p | 302 | FMN | C2'-C3'-C4'-O4' |
| 2 | p | 302 | FMN | C2'-C3'-C4'-C5' |
| 2 | p | 302 | FMN | O3'-C3'-C4'-O4' |
| 2 | p | 302 | FMN | O3'-C3'-C4'-C5' |
| 2 | p | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | p | 302 | FMN | O4'-C4'-C5'-O5' |
| 2 | p | 302 | FMN | C5'-O5'-P-O1P |
| 2 | p | 302 | FMN | C5'-O5'-P-O2P |
| 2 | p | 302 | FMN | C5'-O5'-P-O3P |
| 2 | q | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | q | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | q | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | q | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | q | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | r | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | r | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | r | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | r | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | r | 302 | FMN | C1'-C2'-C3'-C4' |
| 2 | r | 302 | FMN | C5'-O5'-P-O2P |
| 2 | s | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | s | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | s | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | s | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | s | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | s | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | t | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | t | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | t | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | t | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | t | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | t | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | t | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | t | 301 | FMN | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | t | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | u | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | u | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | u | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | w | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | w | 301 | FMN | C1'-C2'-C3'-C4' |
| 2 | w | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | w | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | w | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | w | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | x | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | x | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | x | 301 | FMN | C4'-C5'-O5'-P |
| 2 | x | 301 | FMN | C5'-O5'-P-O3P |
| 2 | M | 302 | FMN | O2'-C2'-C3'-O3' |
| 2 | S | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | e | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | e | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | m | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | D | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | S | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | Y | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | 3 | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | e | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | m | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | t | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | a | 302 | FMN | C4'-C5'-O5'-P |
| 2 | A | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | D | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | Y | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | 2 | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | 5 | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | 7 | 302 | FMN | O3'-C3'-C4'-C5' |
| 2 | d | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | h | 302 | FMN | O3'-C3'-C4'-C5' |
| 2 | q | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | r | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | D | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | Y | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 7 | 302 | FMN | C2'-C3'-C4'-C5' |
| 2 | d | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | e | 301 | FMN | C2'-C3'-C4'-C5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | h | 302 | FMN | C2'-C3'-C4'-C5' |
| 2 | q | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | r | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 0 | 302 | FMN | O2'-C2'-C3'-C4' |
| 2 | d | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | k | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | W | 301 | FMN | C4'-C5'-O5'-P |
| 2 | 0 | 301 | FMN | C4'-C5'-O5'-P |
| 2 | B | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | R | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | S | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | 4 | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | a | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | B | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | R | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | S | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 2 | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 4 | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | a | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | D | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | E | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | M | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | R | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | T | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | X | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | Y | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | 0 | 302 | FMN | O2'-C2'-C3'-O3' |
| 2 | 2 | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | 3 | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | a | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | a | 302 | FMN | O2'-C2'-C3'-O3' |
| 2 | d | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | k | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | n | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | B | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | M | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | R | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | T | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | 2 | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | 4 | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | a | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | n | 301 | FMN | O2'-C2'-C3'-C4' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | A | 301 | FMN | C4'-C5'-O5'-P |
| 2 | Q | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | 4 | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | a | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | s | 301 | FMN | O4'-C4'-C5'-O5' |
| 2 | M | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | B | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | 4 | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | r | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | X | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | a | 302 | FMN | O2'-C2'-C3'-C4' |
| 2 | E | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | M | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | O | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | u | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | E | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | r | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | u | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | M | 301 | FMN | C4'-C5'-O5'-P |
| 2 | Q | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | R | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 4 | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | d | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | j | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | m | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | s | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 6 | 301 | FMN | C2'-C1'-N10-C9A |
| 2 | N | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | E | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | O | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | A | 301 | FMN | C5'-O5'-P-O1P |
| 2 | D | 301 | FMN | C5'-O5'-P-O1P |
| 2 | O | 301 | FMN | C5'-O5'-P-O1P |
| 2 | S | 301 | FMN | C5'-O5'-P-O1P |
| 2 | 4 | 301 | FMN | C5'-O5'-P-O1P |
| 2 | k | 301 | FMN | C5'-O5'-P-O1P |
| 2 | m | 302 | FMN | C5'-O5'-P-O1P |
| 2 | x | 301 | FMN | C5'-O5'-P-O1P |
| 2 | Y | 301 | FMN | C4'-C5'-O5'-P |
| 2 | s | 301 | FMN | C4'-C5'-O5'-P |
| 2 | B | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | G | 301 | FMN | C2'-C1'-N10-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | O | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | P | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | 2 | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | 7 | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | f | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | i | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | n | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | p | 302 | FMN | C2'-C1'-N10-C10 |
| 2 | t | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | w | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | f | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | E | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | N | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 1 | 302 | FMN | C2'-C3'-C4'-C5' |
| 2 | f | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | N | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | 1 | 302 | FMN | O3'-C3'-C4'-C5' |
| 2 | 5 | 302 | FMN | O3'-C3'-C4'-C5' |
| 2 | 1 | 302 | FMN | O3'-C3'-C4'-O4' |
| 2 | f | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | u | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | M | 302 | FMN | C5'-O5'-P-O3P |
| 2 | a | 301 | FMN | C5'-O5'-P-O2P |
| 2 | h | 302 | FMN | C5'-O5'-P-O3P |
| 2 | r | 302 | FMN | C5'-O5'-P-O3P |
| 2 | x | 301 | FMN | C5'-O5'-P-O2P |
| 2 | p | 301 | FMN | C4'-C5'-O5'-P |
| 2 | O | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 3 | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 5 | 302 | FMN | C2'-C3'-C4'-C5' |
| 2 | 1 | 302 | FMN | C4'-C5'-O5'-P |
| 2 | q | 301 | FMN | C4'-C5'-O5'-P |
| 2 | w | 301 | FMN | C4'-C5'-O5'-P |
| 2 | M | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | M | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | m | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | T | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | u | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | D | 302 | FMN | N10-C1'-C2'-C3' |
| 2 | m | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | n | 301 | FMN | N10-C1'-C2'-O2' |
| 2 | r | 302 | FMN | N10-C1'-C2'-O2' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | m | 302 | FMN | O4'-C4'-C5'-O5' |
| 2 | N | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | 1 | 302 | FMN | C2'-C3'-C4'-O4' |
| 2 | 7 | 301 | FMN | O2'-C2'-C3'-C4' |
| 2 | i | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | d | 301 | FMN | C4'-C5'-O5'-P |
| 2 | E | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | N | 301 | FMN | C4'-C5'-O5'-P |
| 2 | R | 301 | FMN | C4'-C5'-O5'-P |
| 2 | T | 301 | FMN | C5'-O5'-P-O1P |
| 2 | a | 301 | FMN | C5'-O5'-P-O1P |
| 2 | h | 302 | FMN | C5'-O5'-P-O1P |
| 2 | m | 301 | FMN | C5'-O5'-P-O1P |
| 2 | r | 302 | FMN | C5'-O5'-P-O1P |
| 2 | O | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | u | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | m | 302 | FMN | C4'-C5'-O5'-P |
| 2 | 5 | 302 | FMN | O3'-C3'-C4'-O4' |
| 2 | 6 | 301 | FMN | C4'-C5'-O5'-P |
| 2 | u | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | A | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | V | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | 5 | 302 | FMN | C2'-C1'-N10-C10 |
| 2 | m | 301 | FMN | C2'-C1'-N10-C10 |
| 2 | i | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | 0 | 301 | FMN | C2'-C1'-N10-C9A |
| 2 | f | 301 | FMN | C2'-C3'-C4'-O4' |
| 2 | i | 301 | FMN | O3'-C3'-C4'-O4' |
| 2 | 1 | 301 | FMN | C5'-O5'-P-O3P |
| 2 | e | 301 | FMN | C5'-O5'-P-O2P |
| 2 | m | 301 | FMN | C5'-O5'-P-O3P |
| 2 | n | 301 | FMN | C5'-O5'-P-O2P |
| 2 | q | 301 | FMN | C5'-O5'-P-O2P |
| 2 | t | 301 | FMN | C5'-O5'-P-O3P |
| 2 | 0 | 302 | FMN | O4'-C4'-C5'-O5' |
| 2 | p | 302 | FMN | O2'-C2'-C3'-O3' |
| 2 | B | 301 | FMN | C5'-O5'-P-O1P |
| 2 | F | 301 | FMN | C5'-O5'-P-O1P |
| 2 | Q | 301 | FMN | C5'-O5'-P-O1P |
| 2 | p | 301 | FMN | C5'-O5'-P-O1P |
| 2 | i | 301 | FMN | C2'-C3'-C4'-C5' |
| 2 | 6 | 301 | FMN | O3'-C3'-C4'-O4' |

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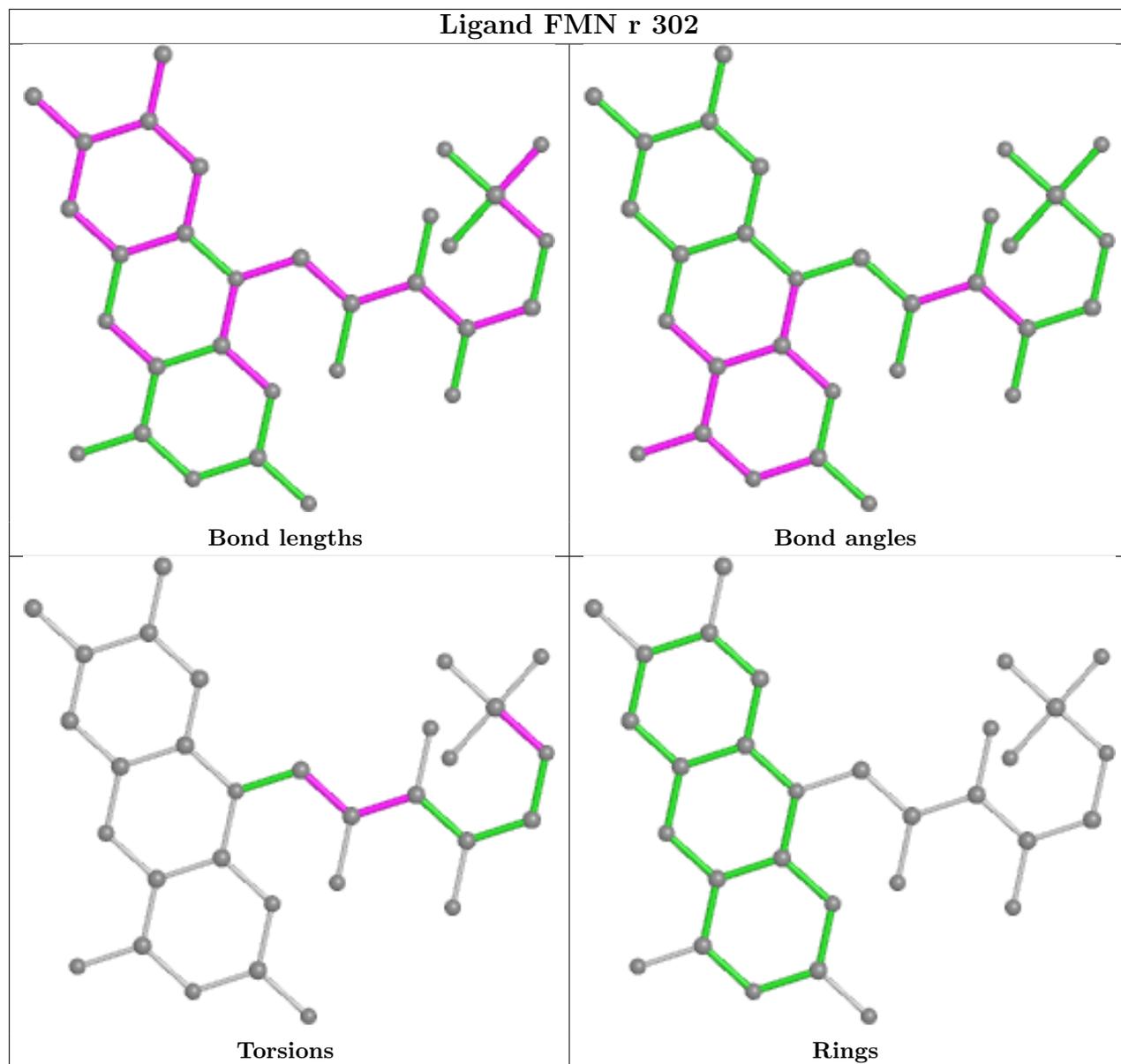
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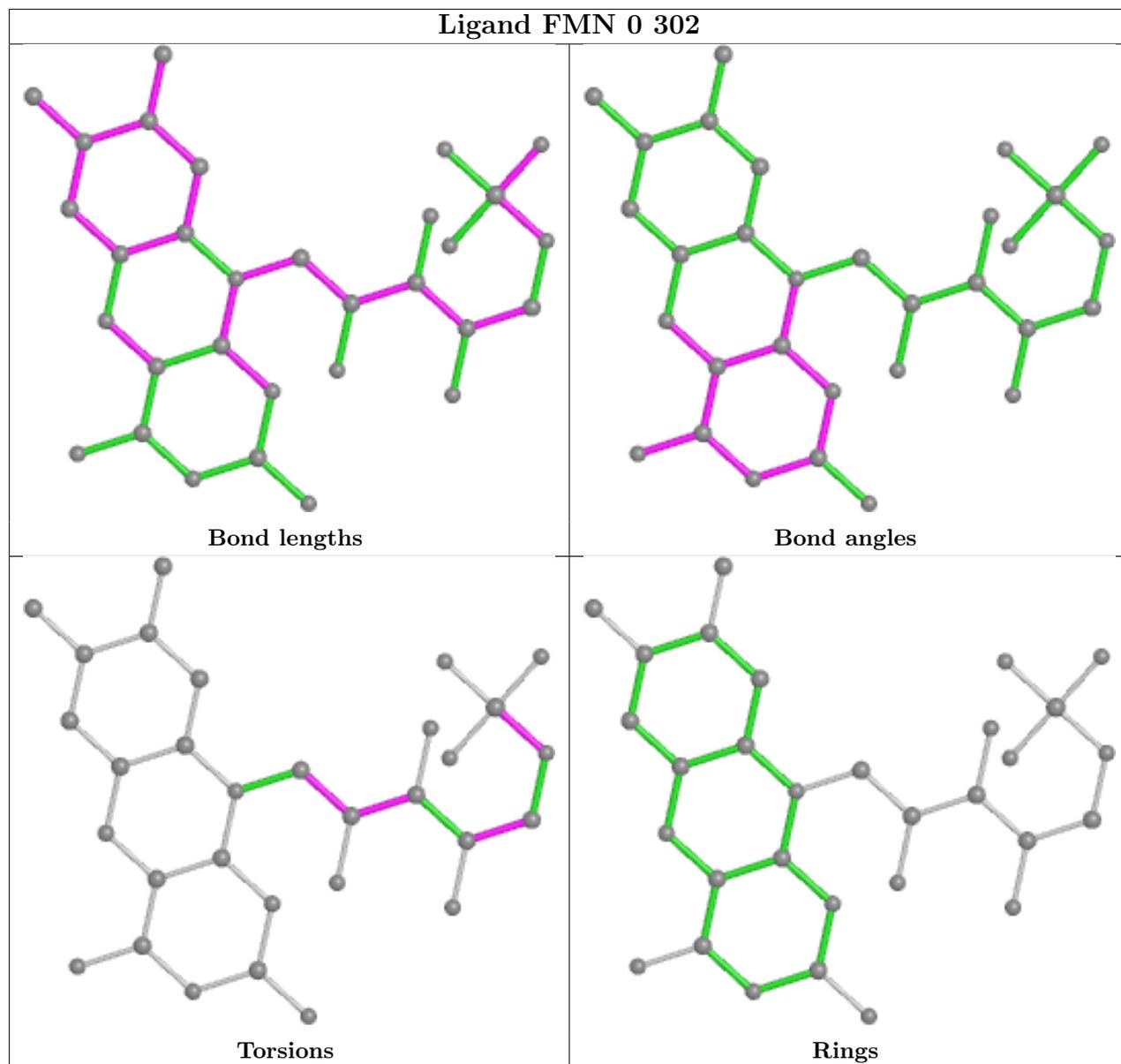
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | h | 301 | FMN | O3'-C3'-C4'-C5' |
| 2 | 7 | 301 | FMN | O2'-C2'-C3'-O3' |
| 2 | X | 301 | FMN | C4'-C5'-O5'-P |
| 2 | 5 | 302 | FMN | C4'-C5'-O5'-P |
| 2 | A | 301 | FMN | C3'-C4'-C5'-O5' |
| 2 | 1 | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | 5 | 302 | FMN | C3'-C4'-C5'-O5' |
| 2 | 7 | 301 | FMN | C1'-C2'-C3'-O3' |
| 2 | a | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | m | 301 | FMN | N10-C1'-C2'-C3' |
| 2 | a | 302 | FMN | C2'-C1'-N10-C10 |

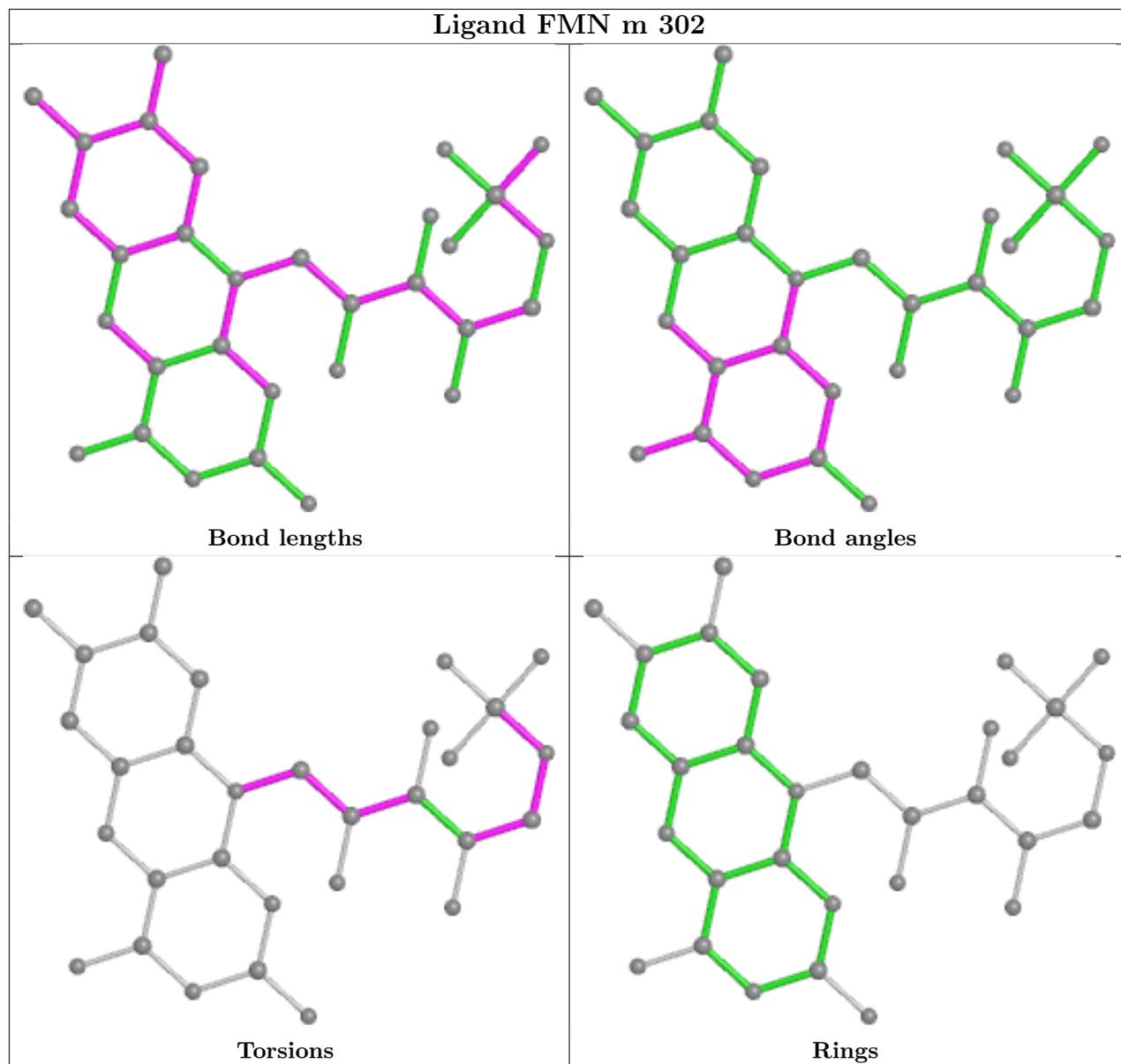
There are no ring outliers.

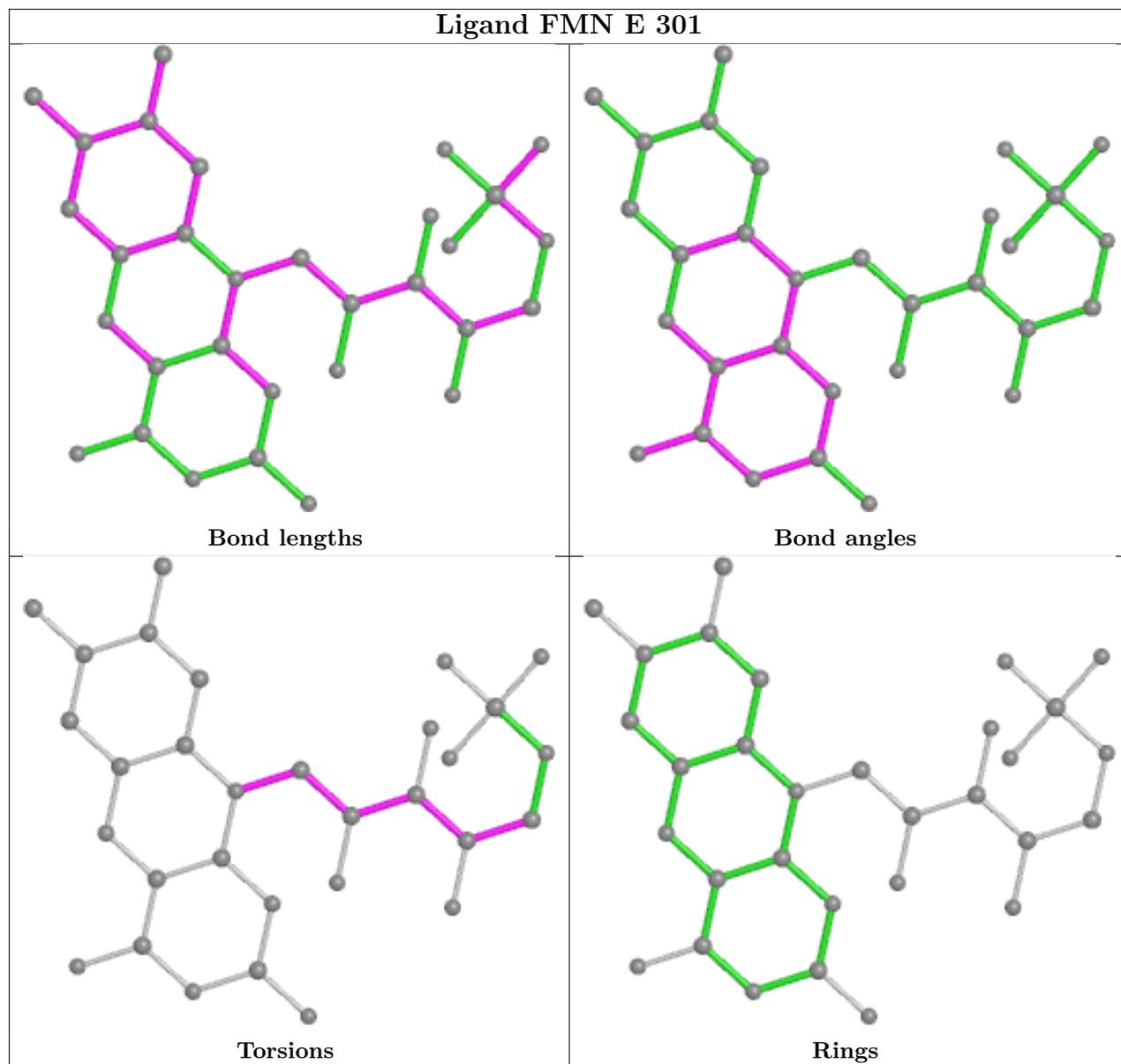
No monomer is involved in short contacts.

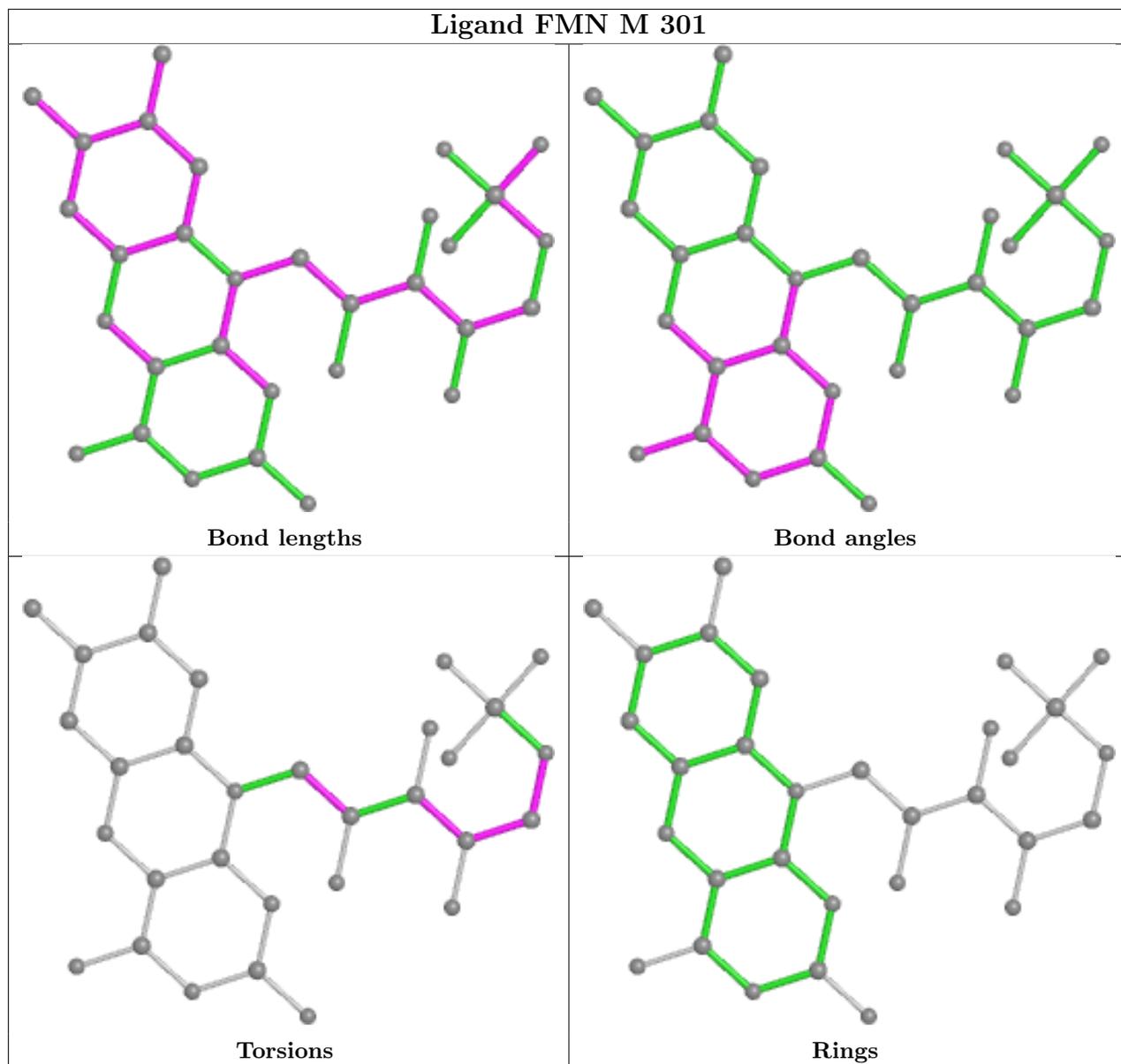
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

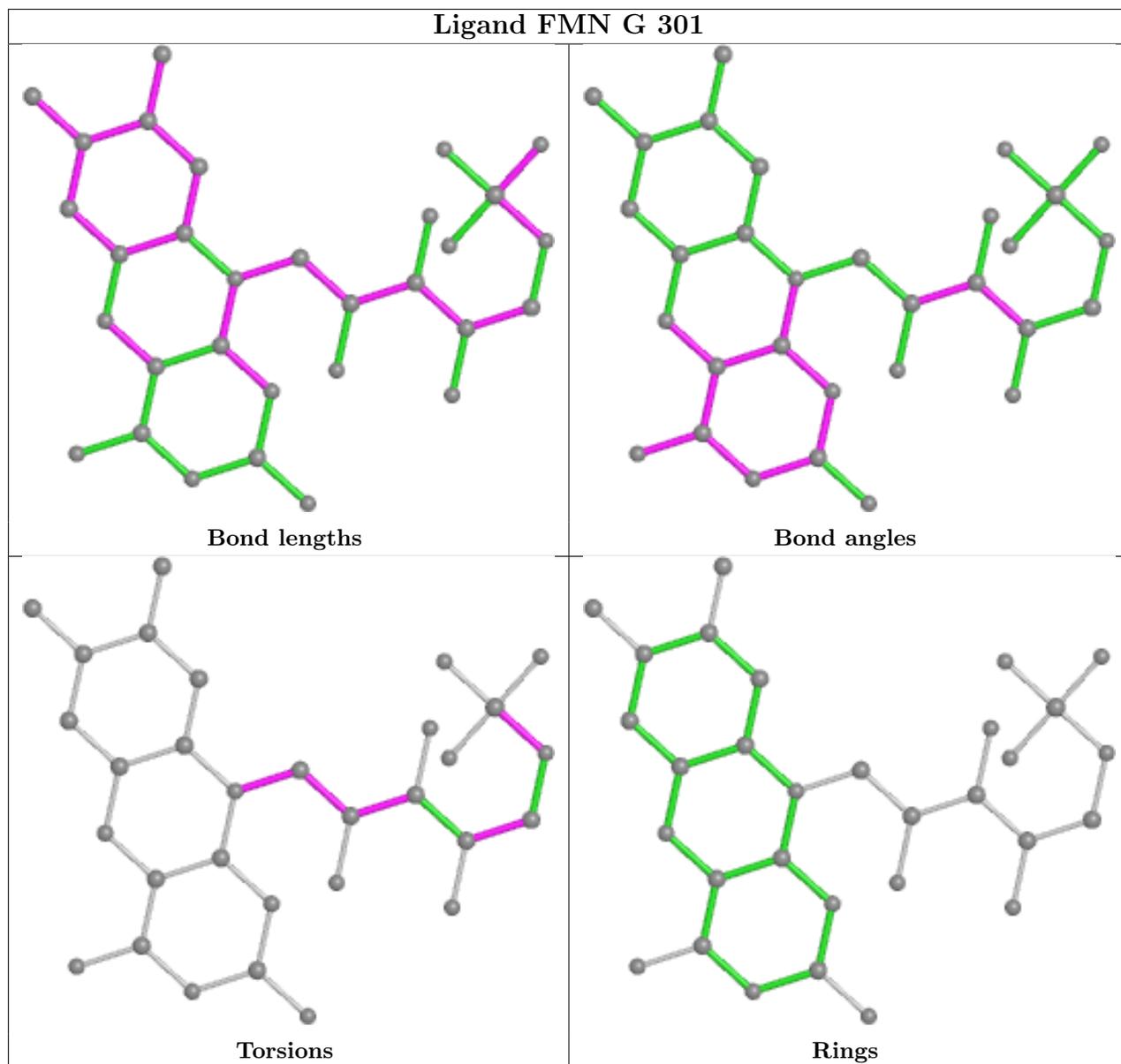


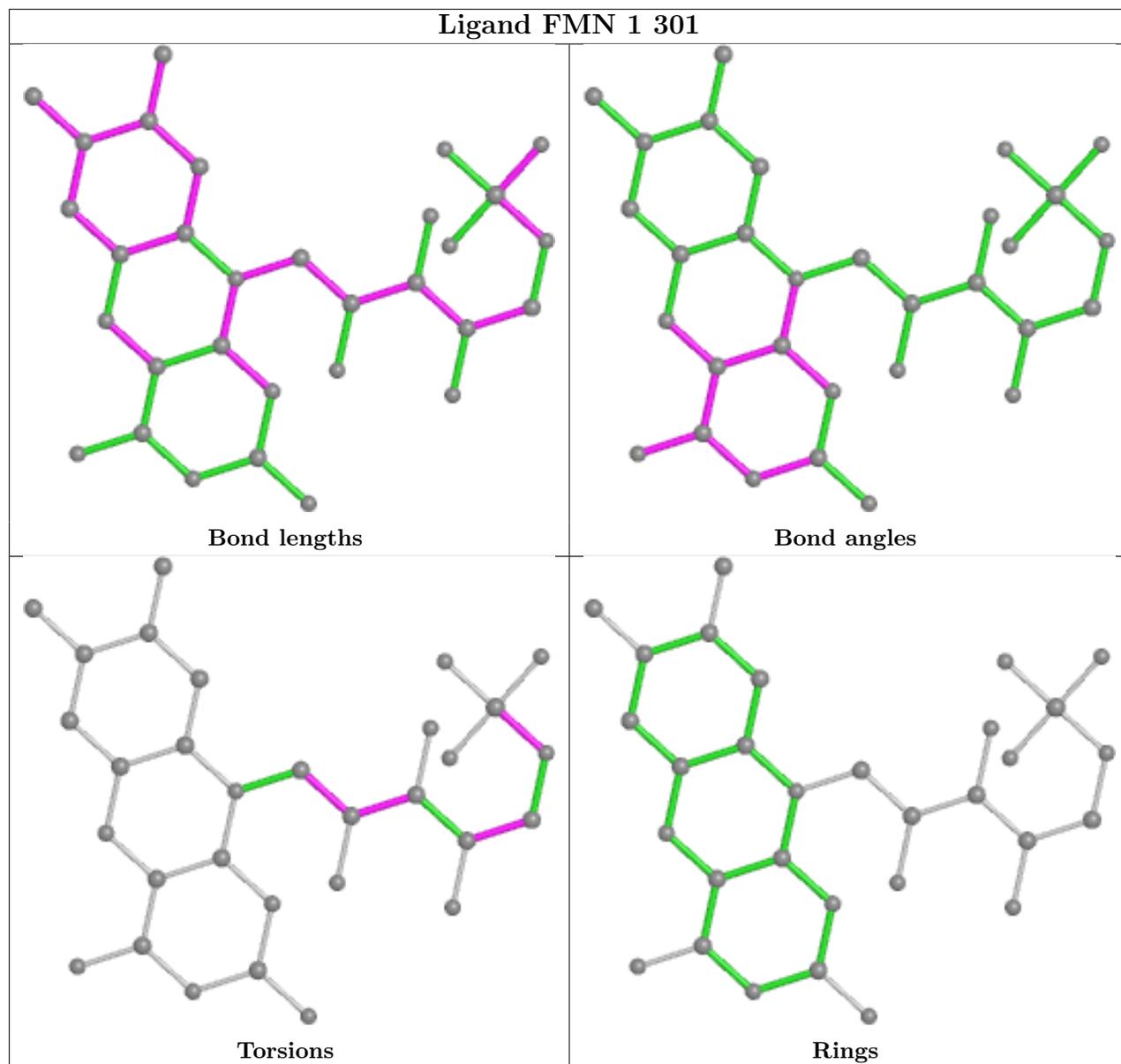


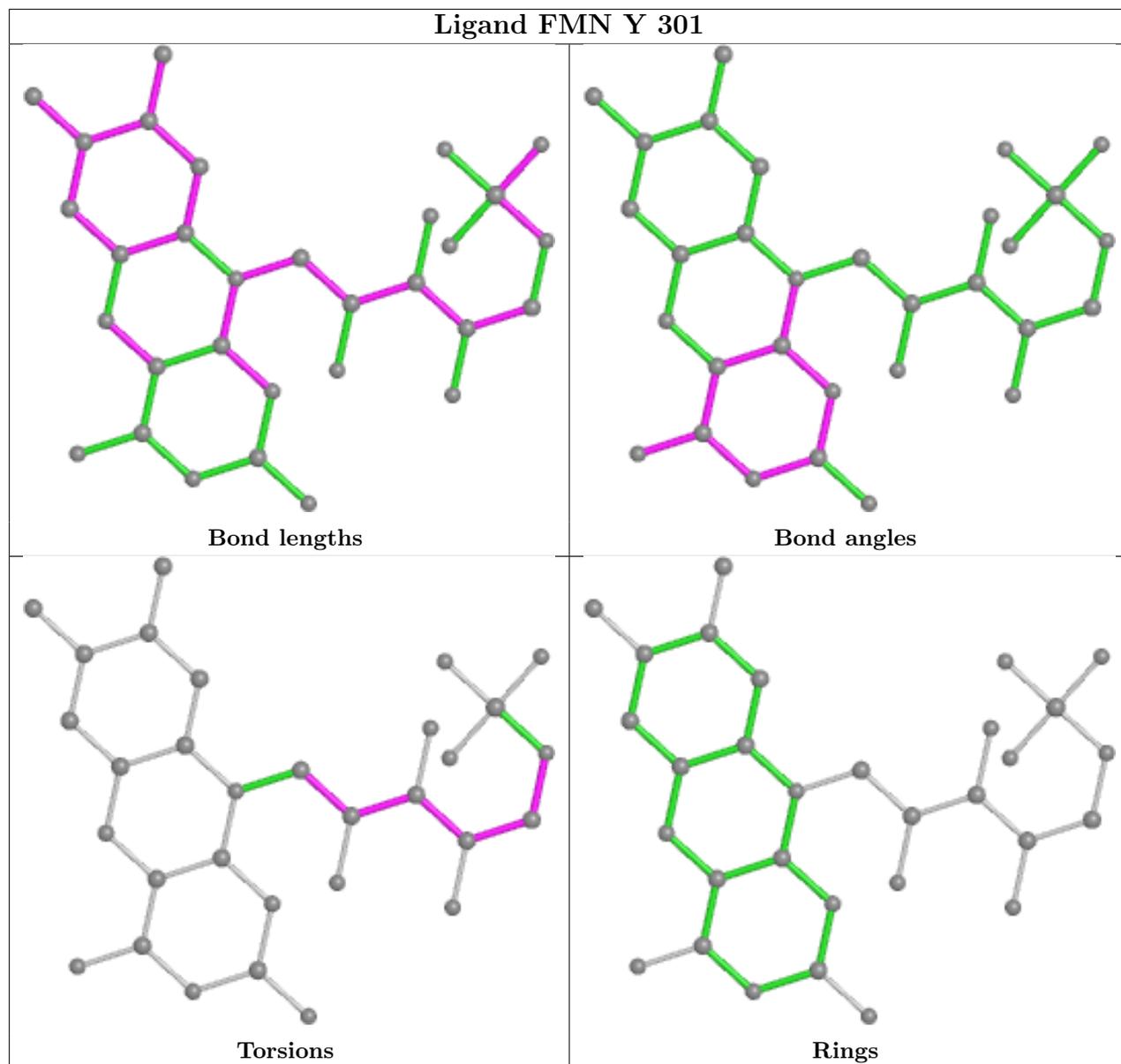


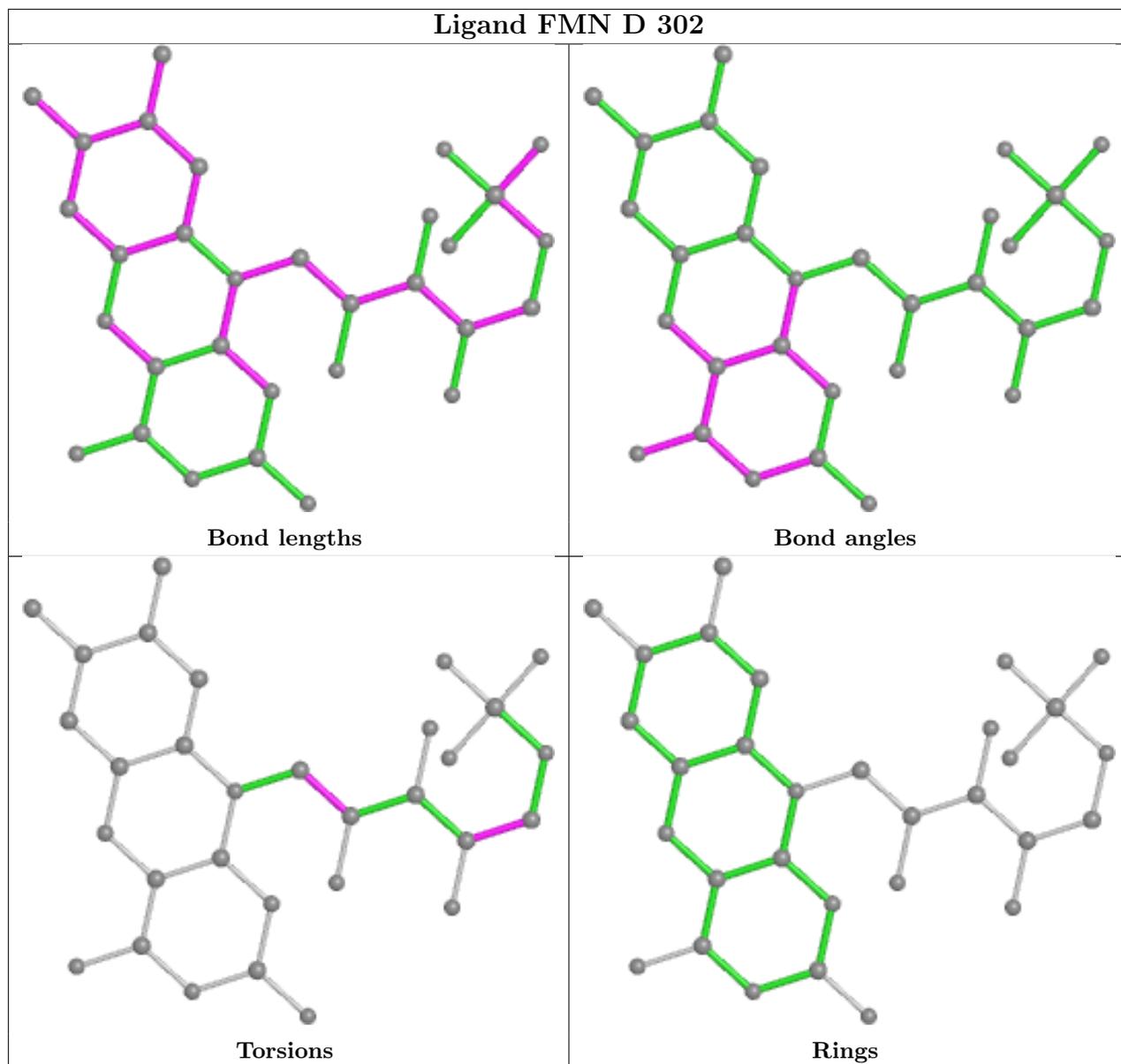


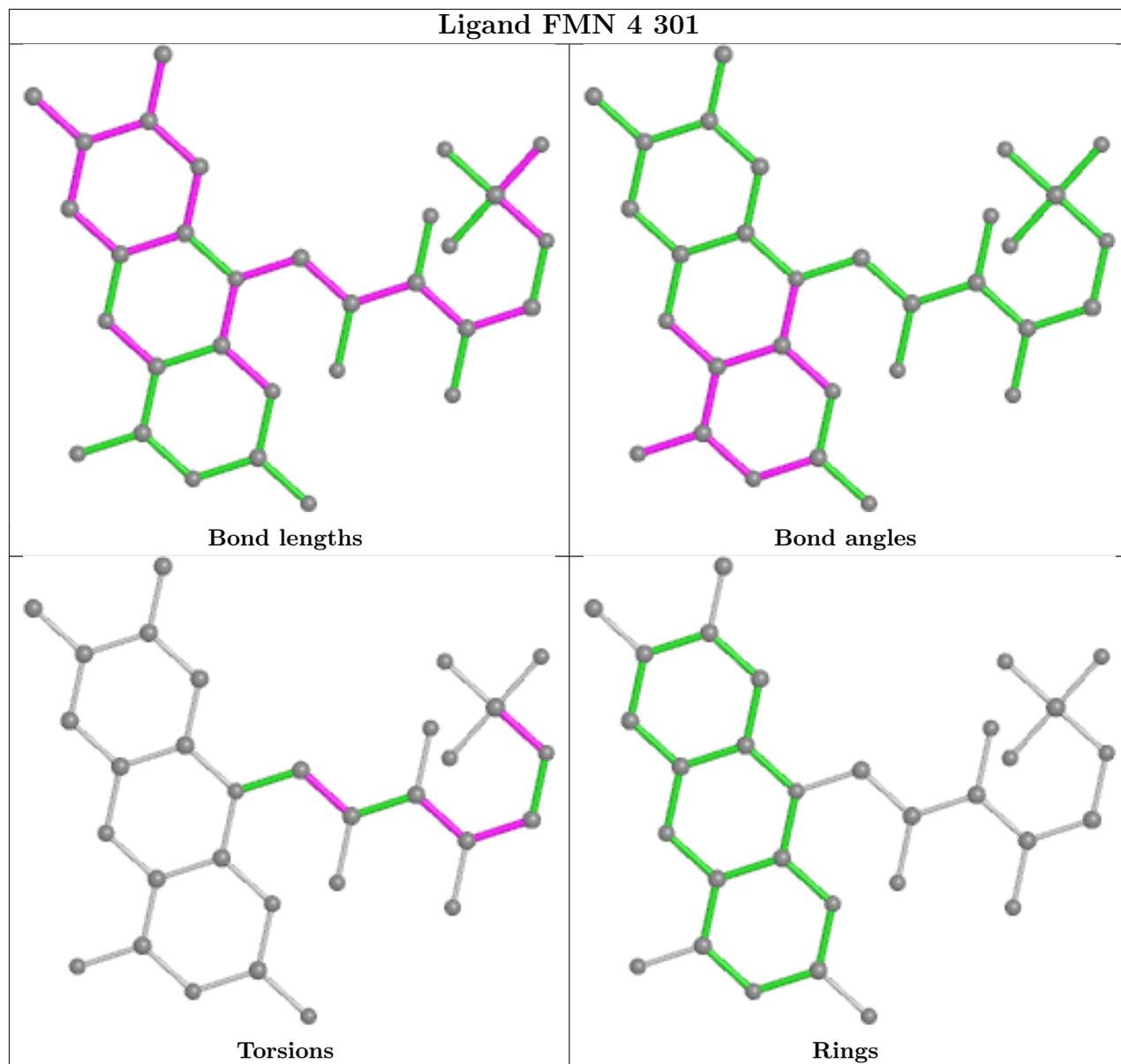


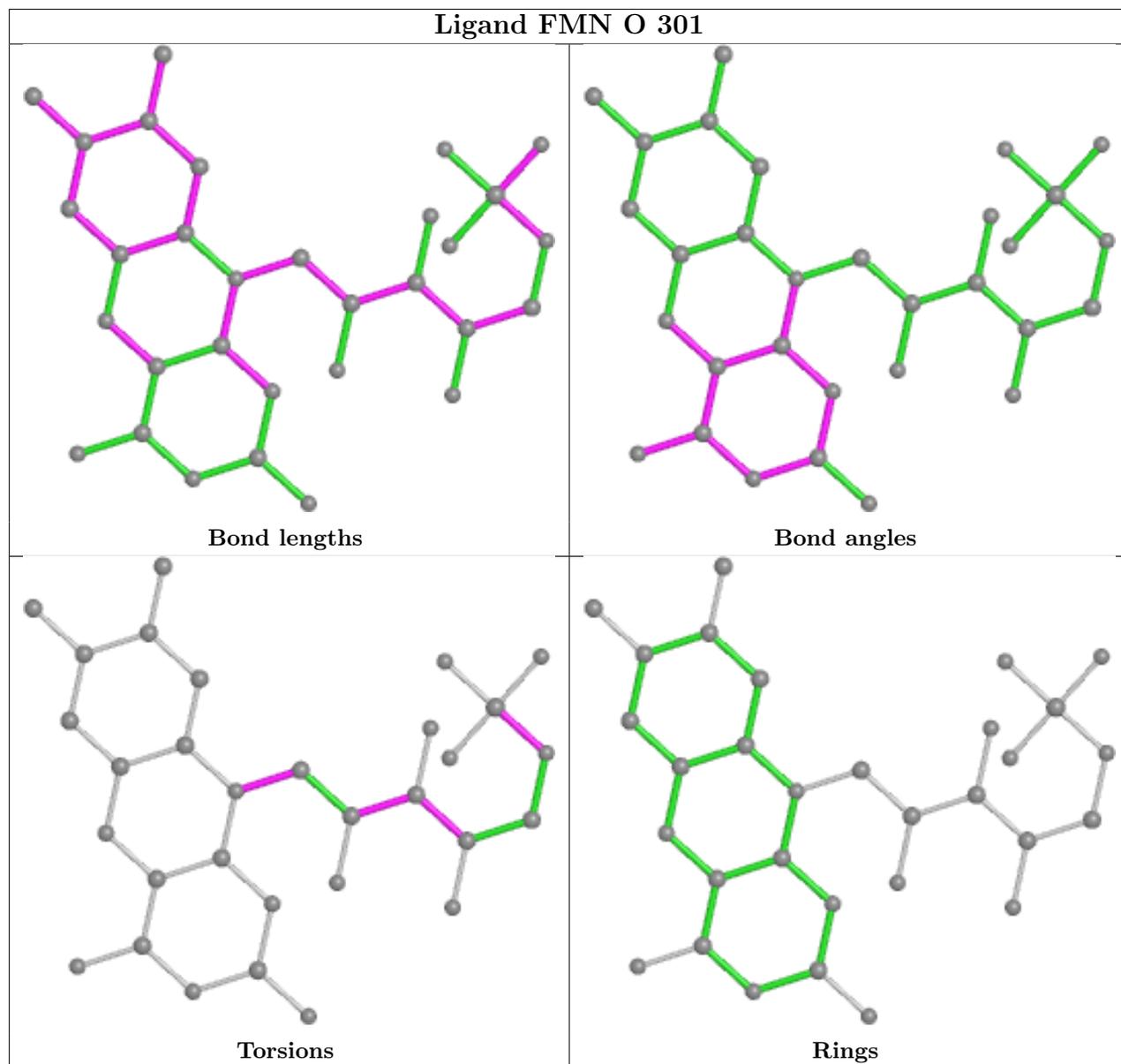


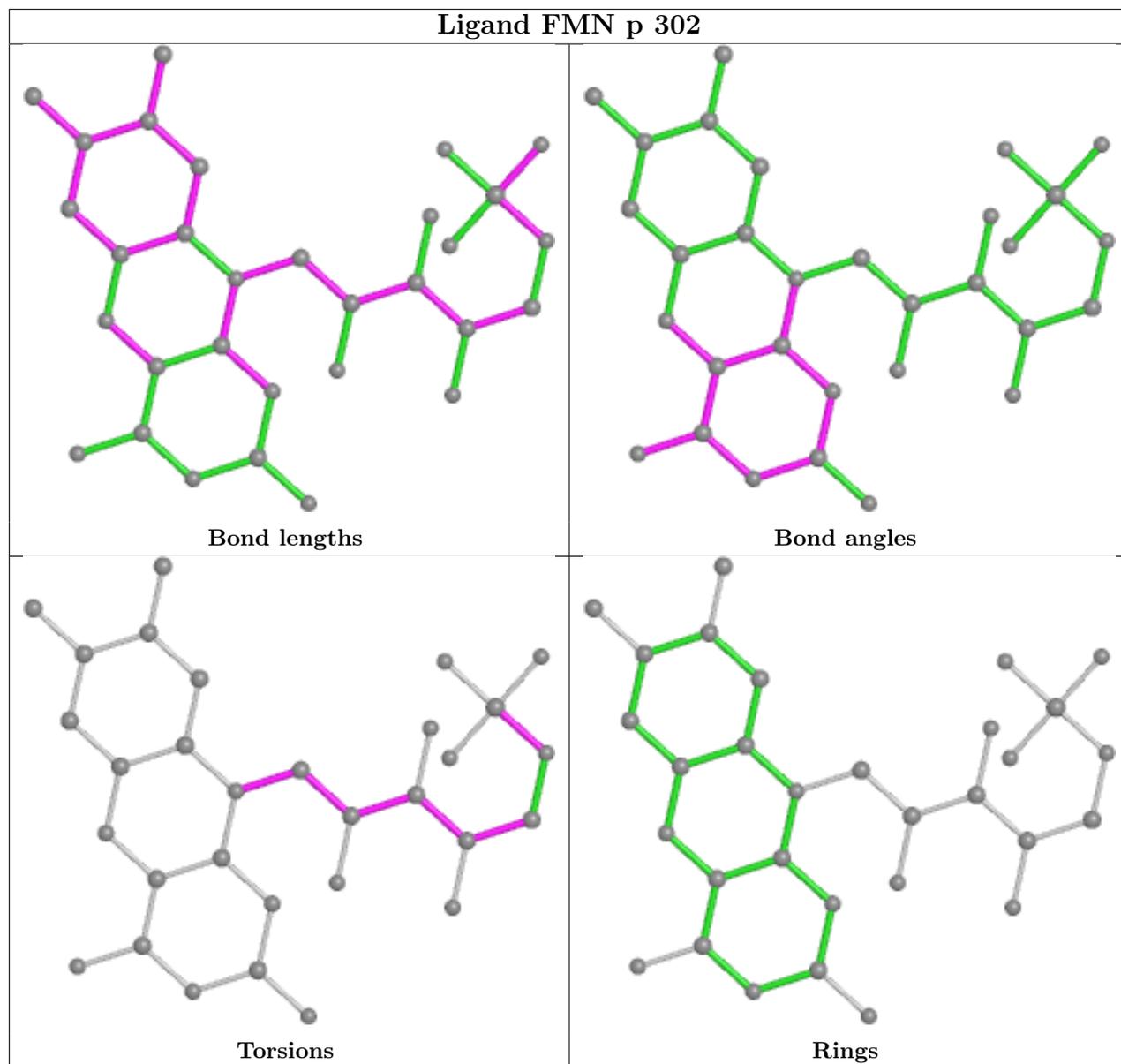


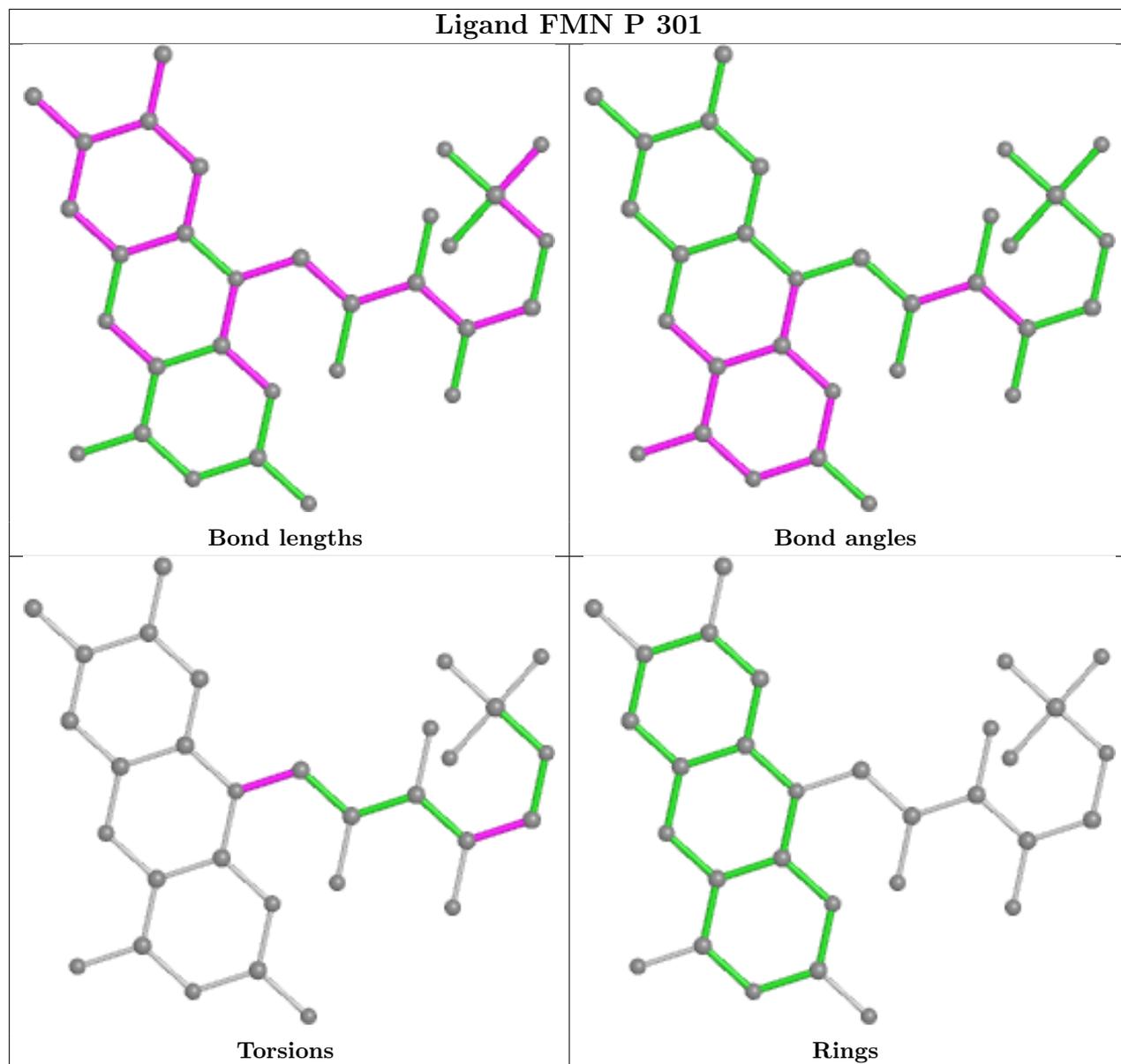


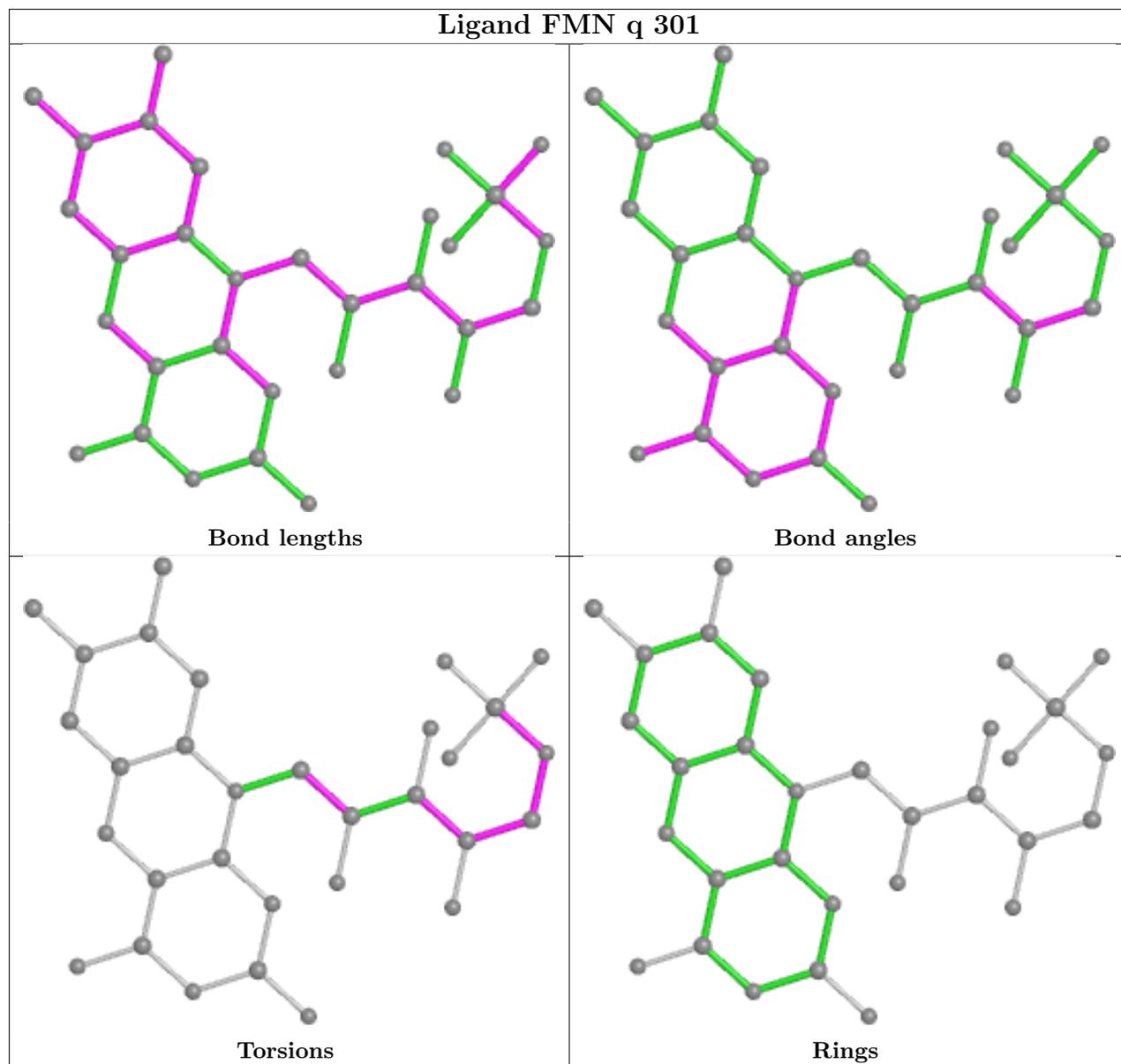


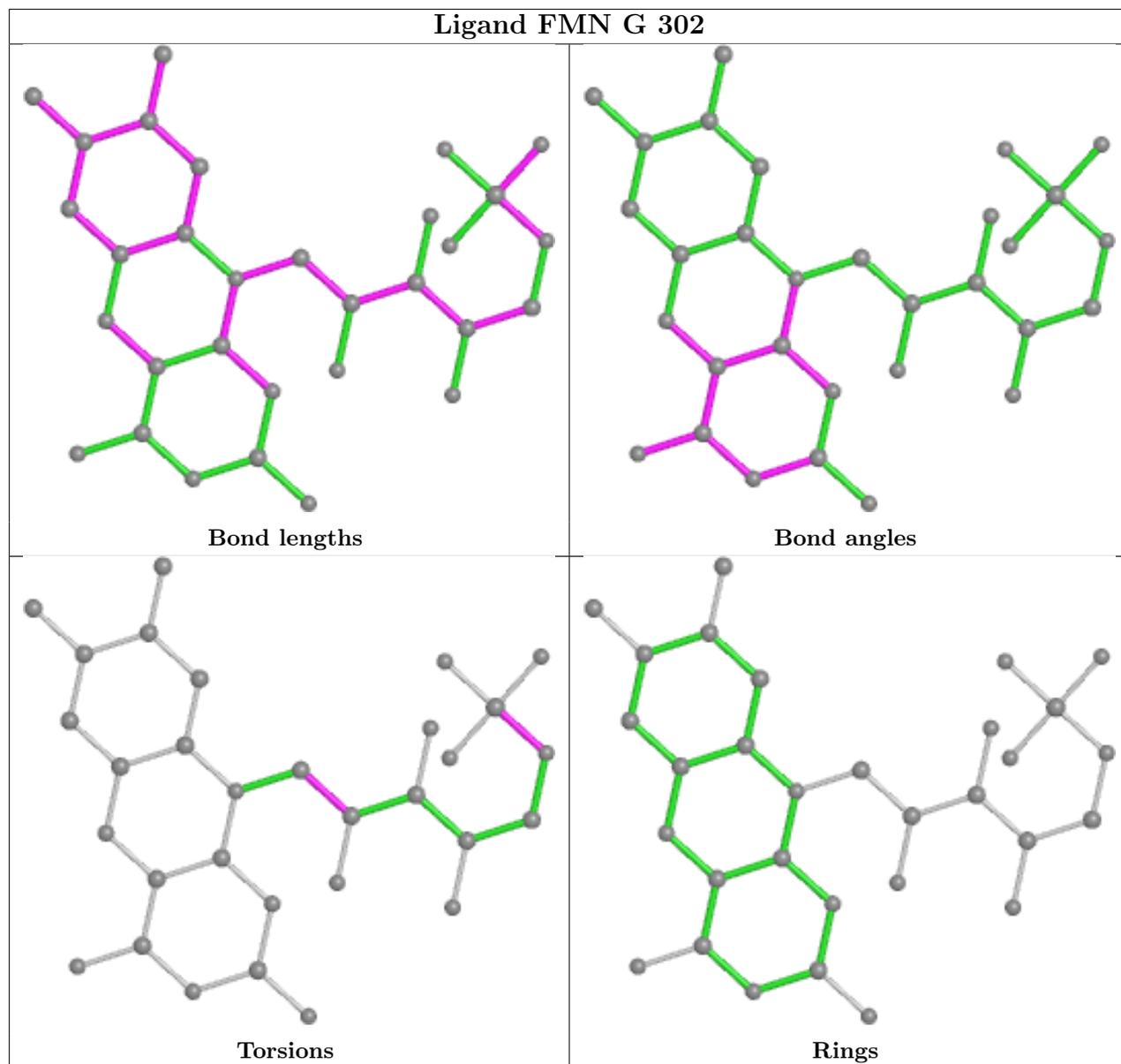


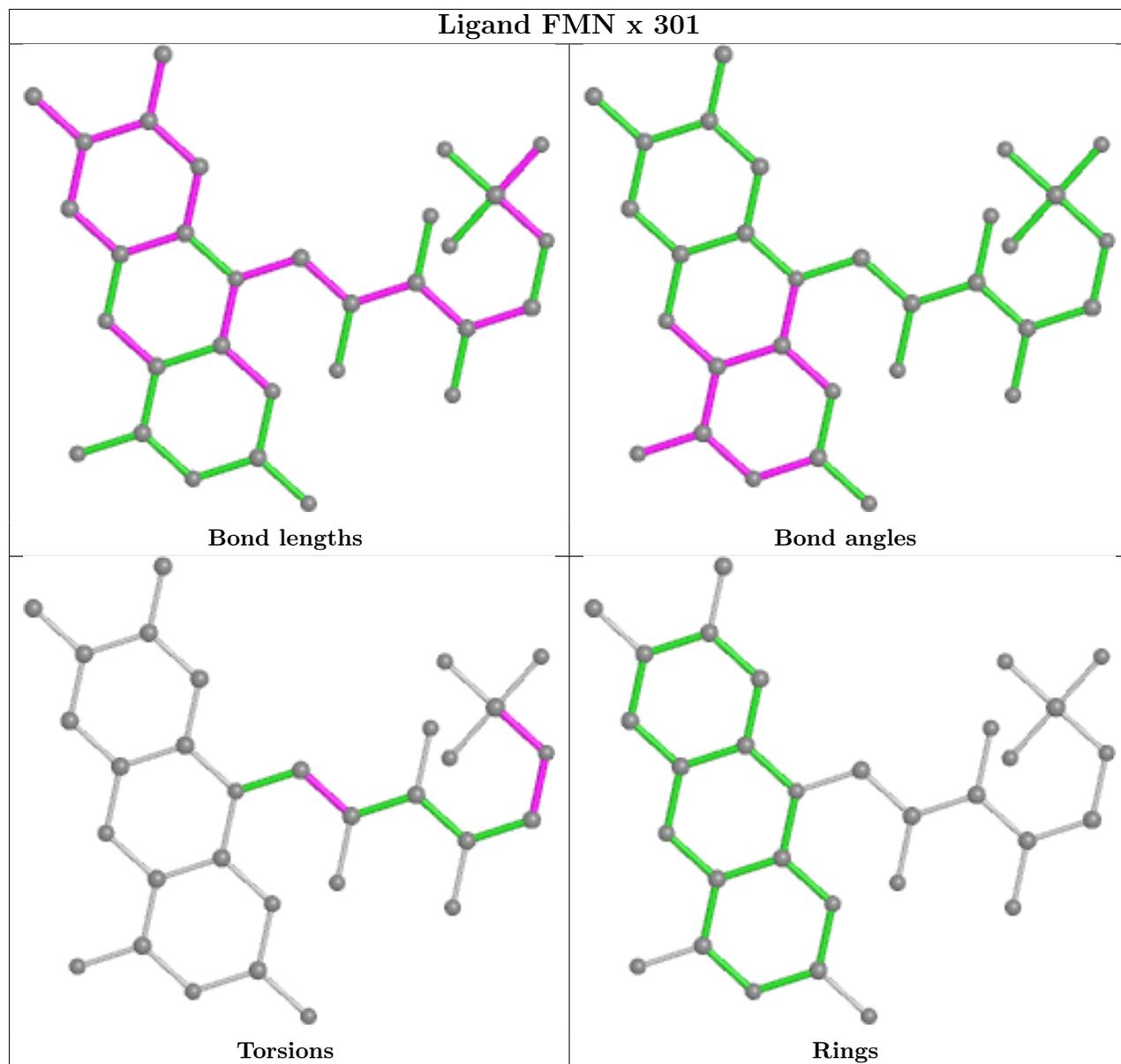


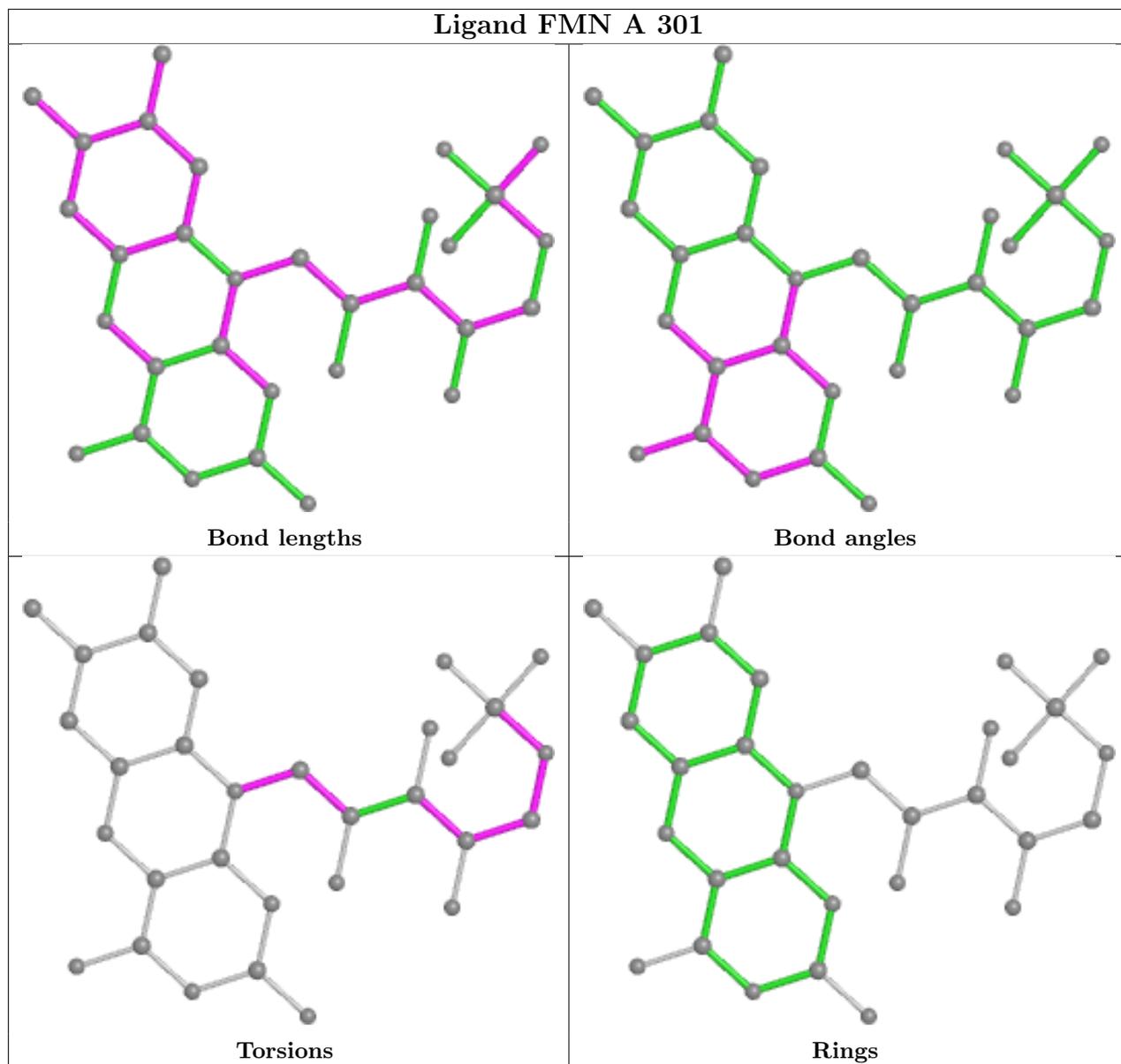


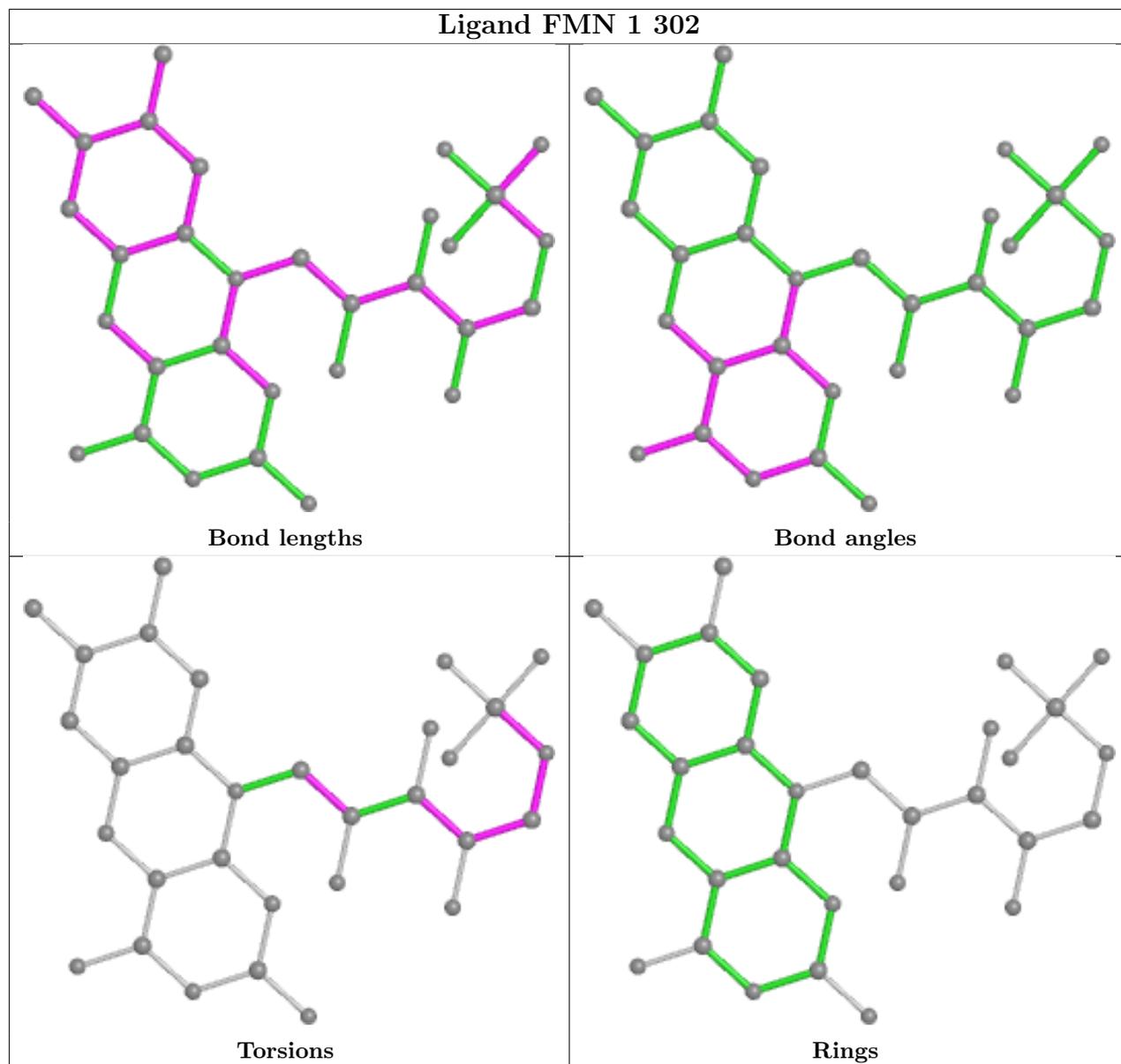


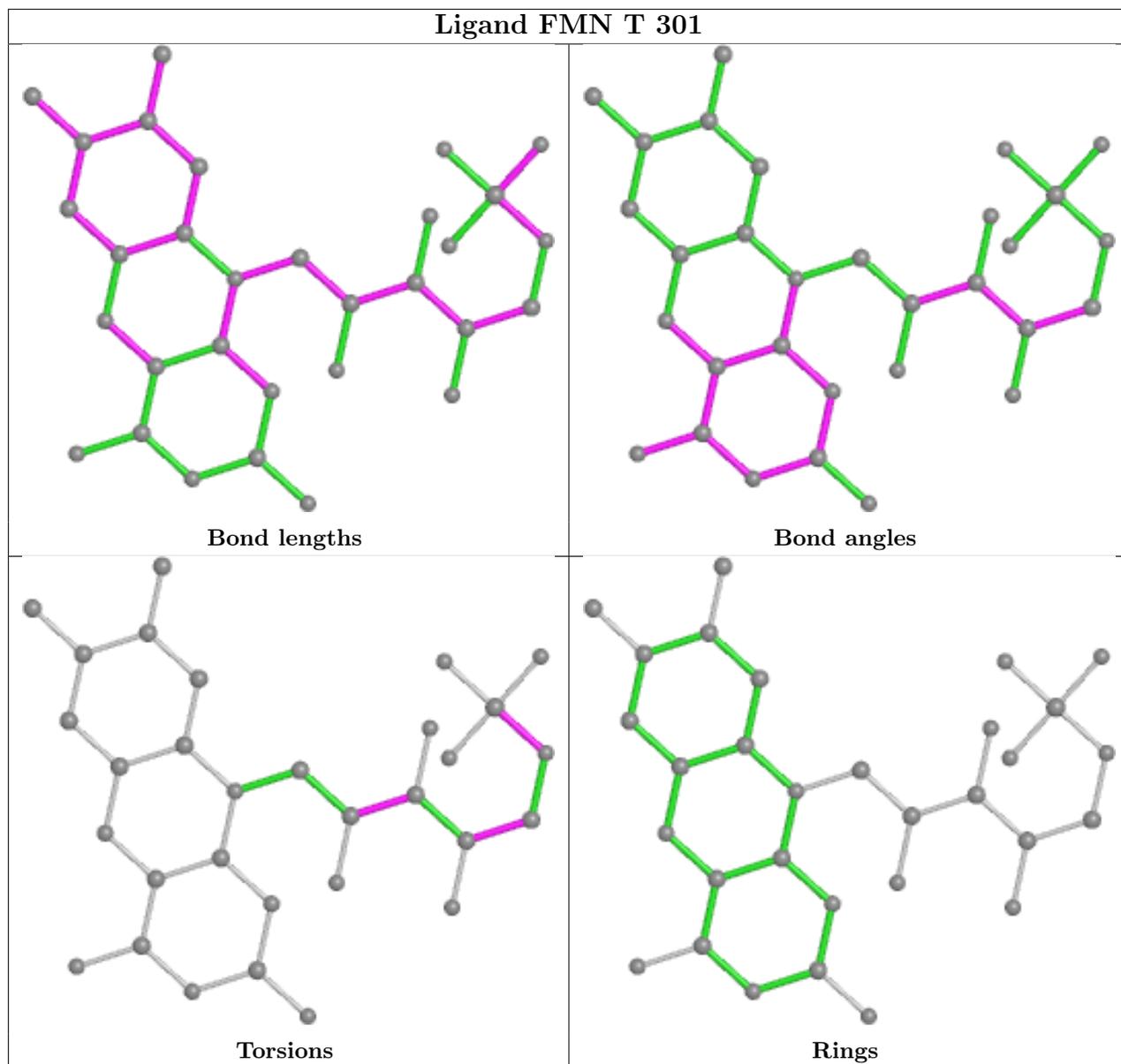


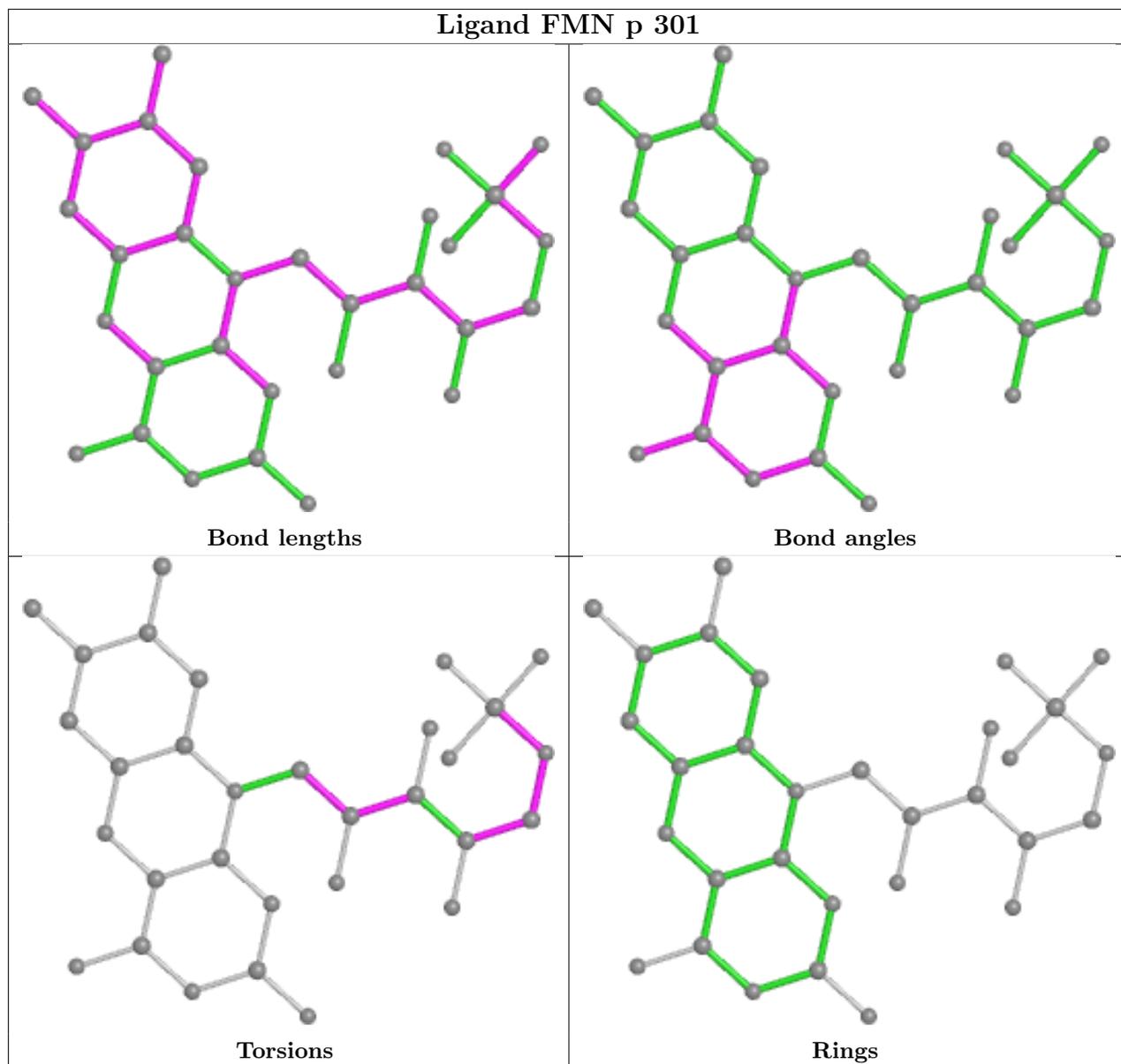


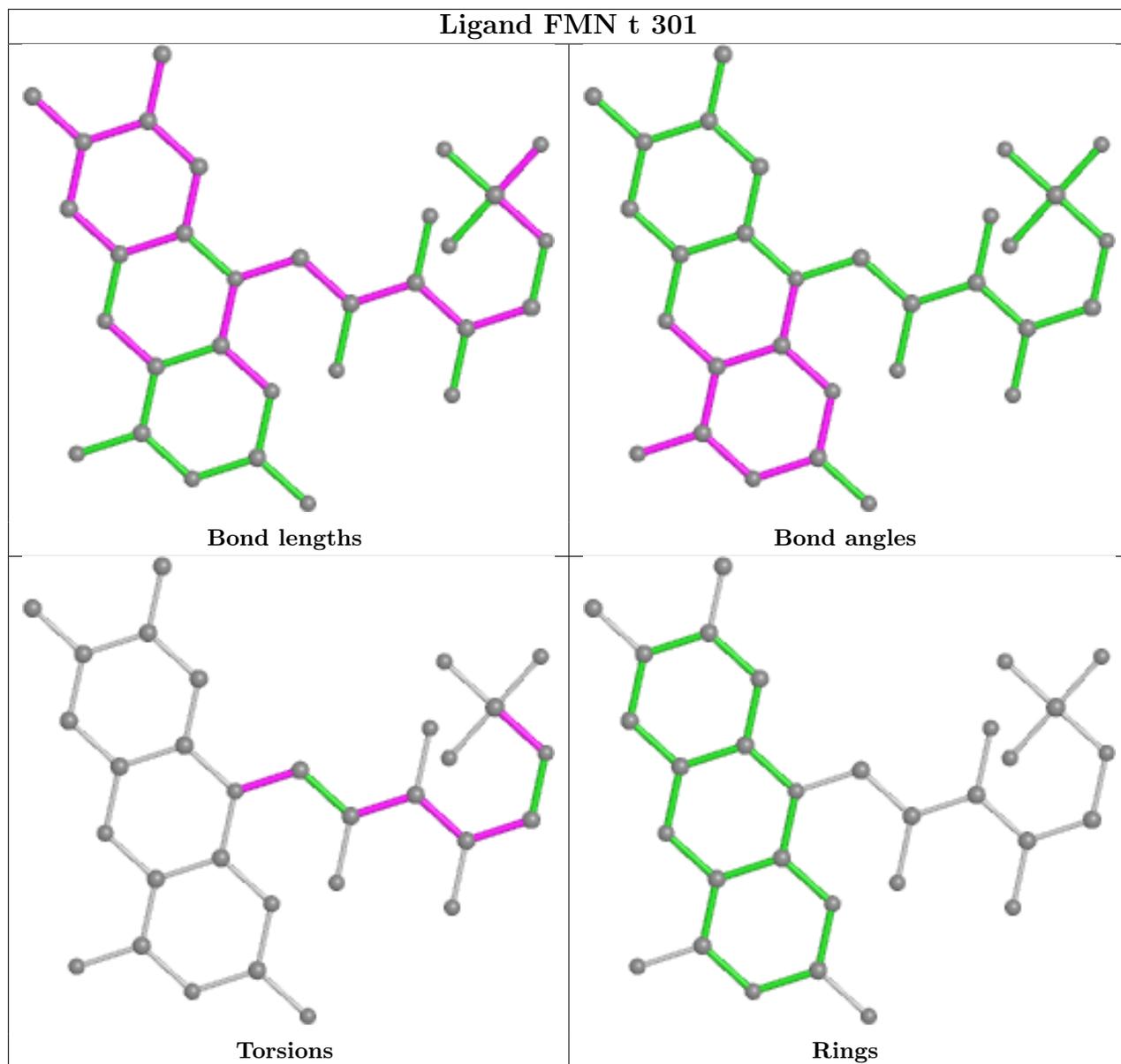


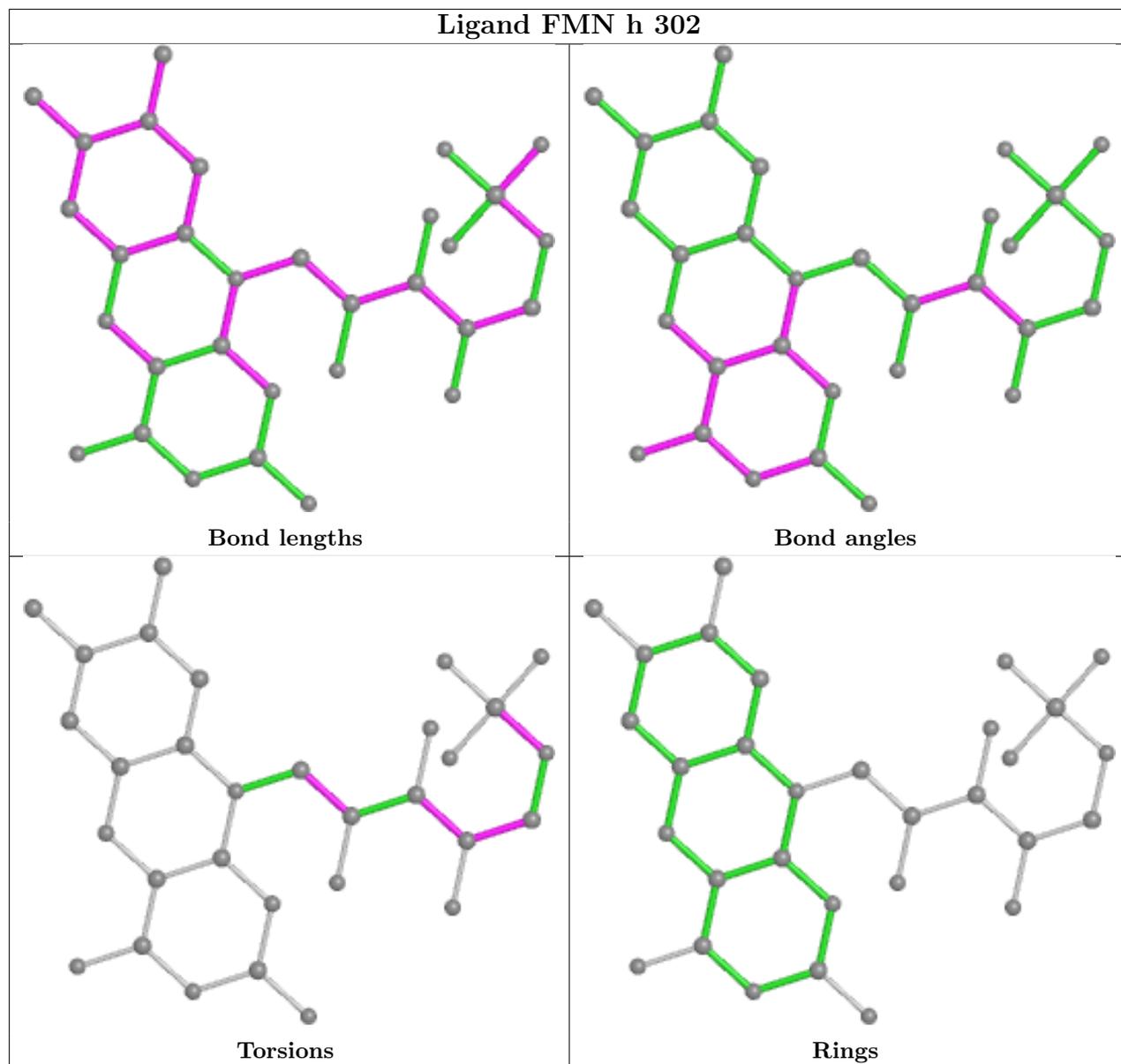


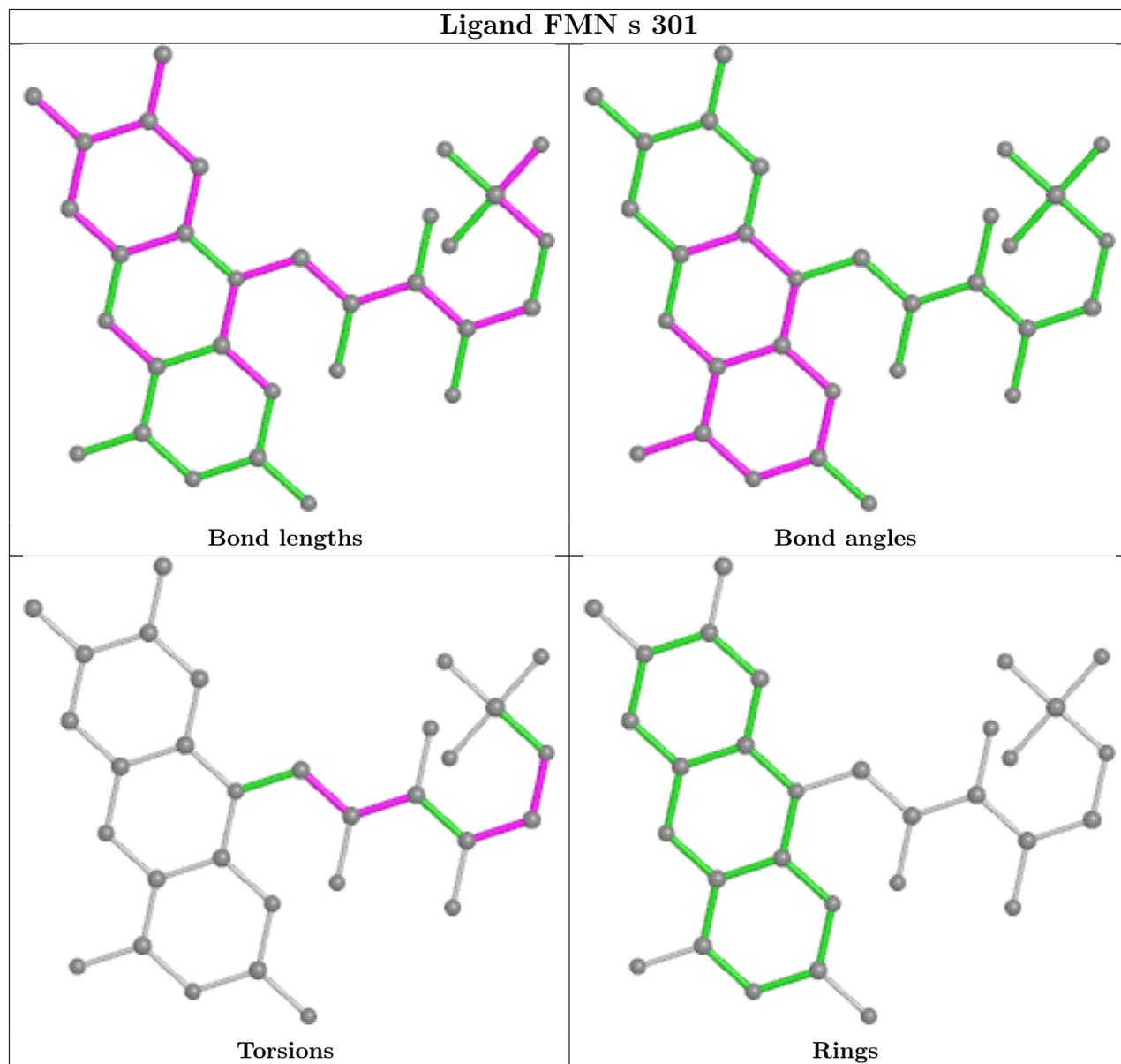


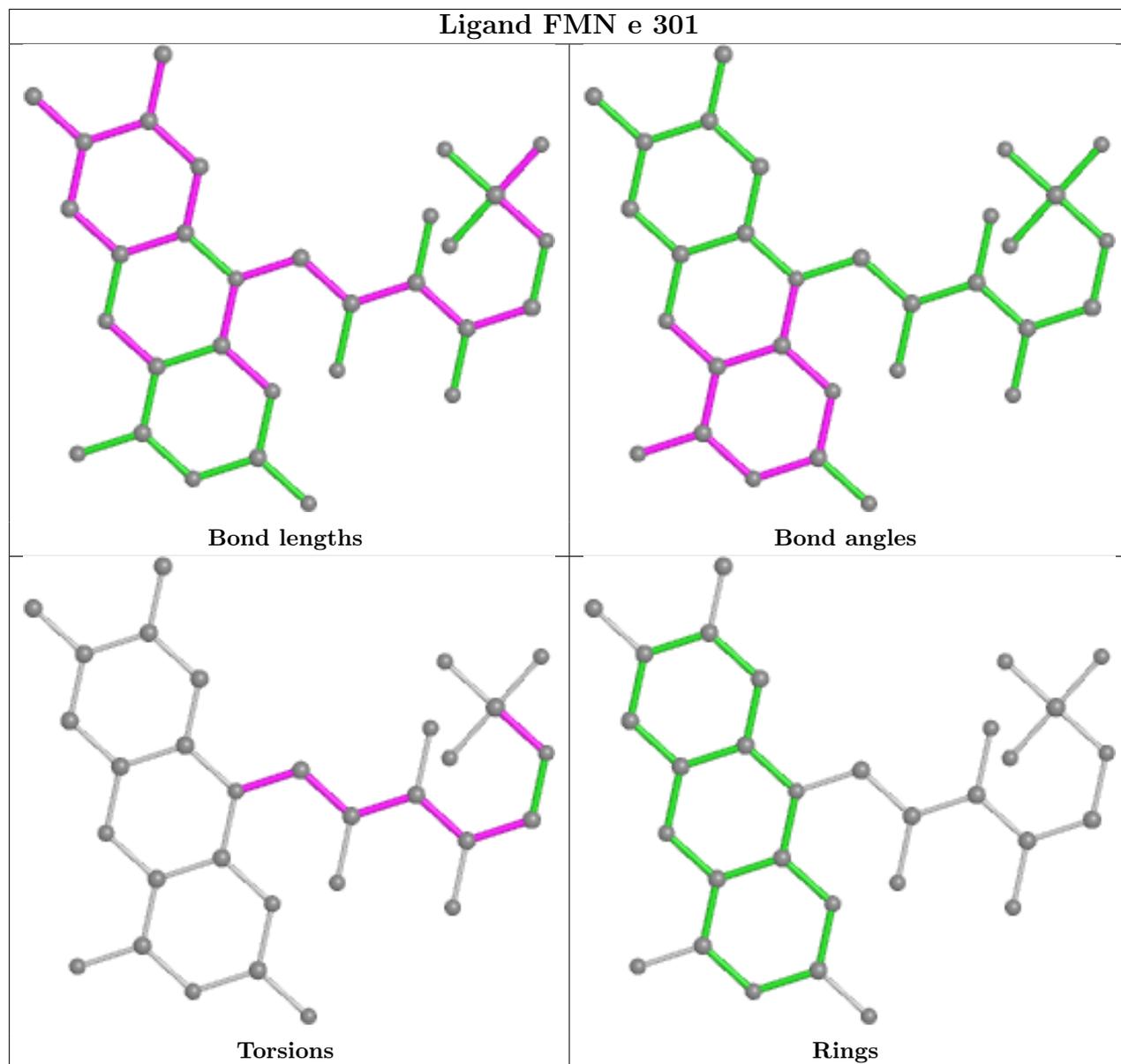


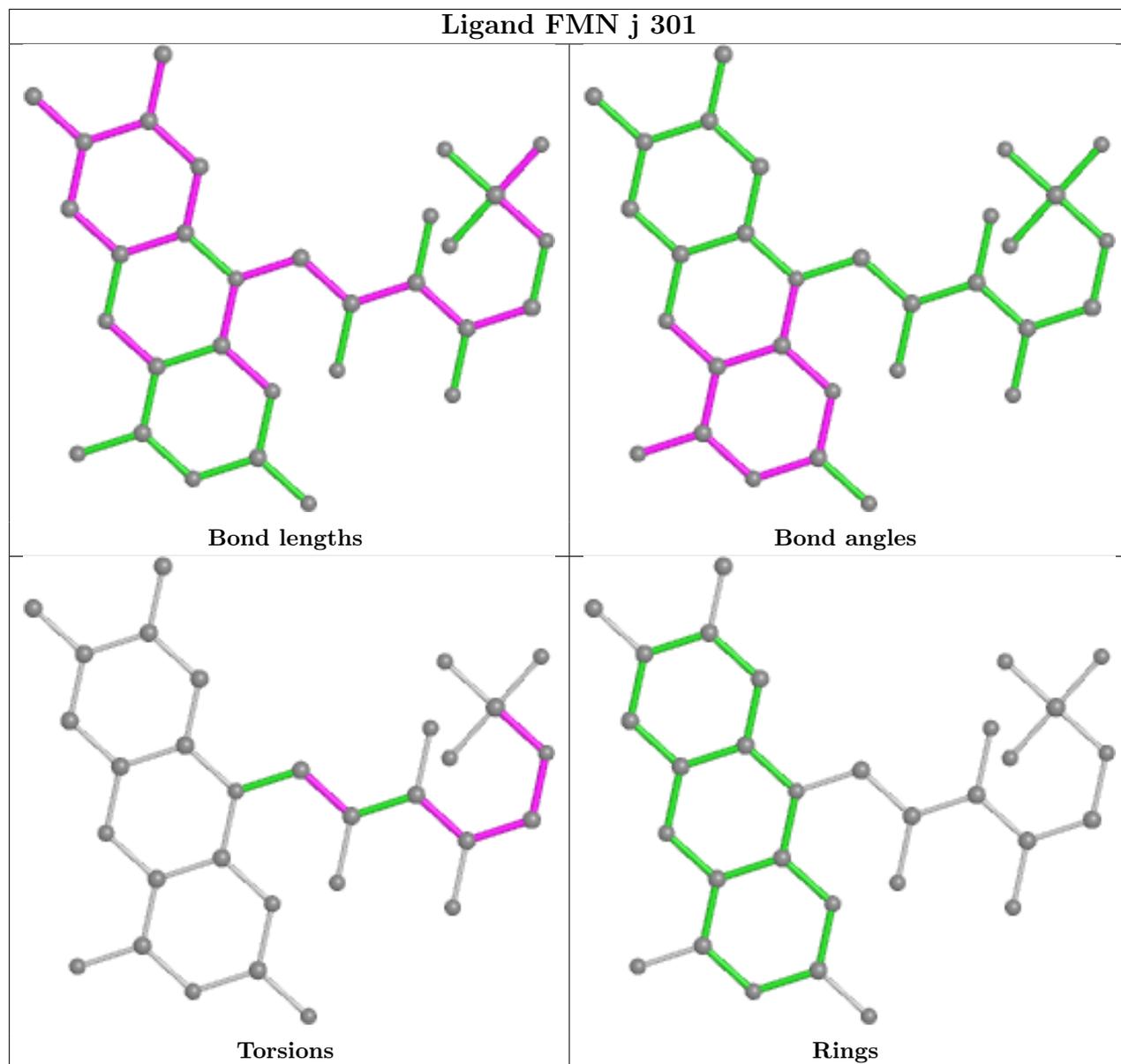


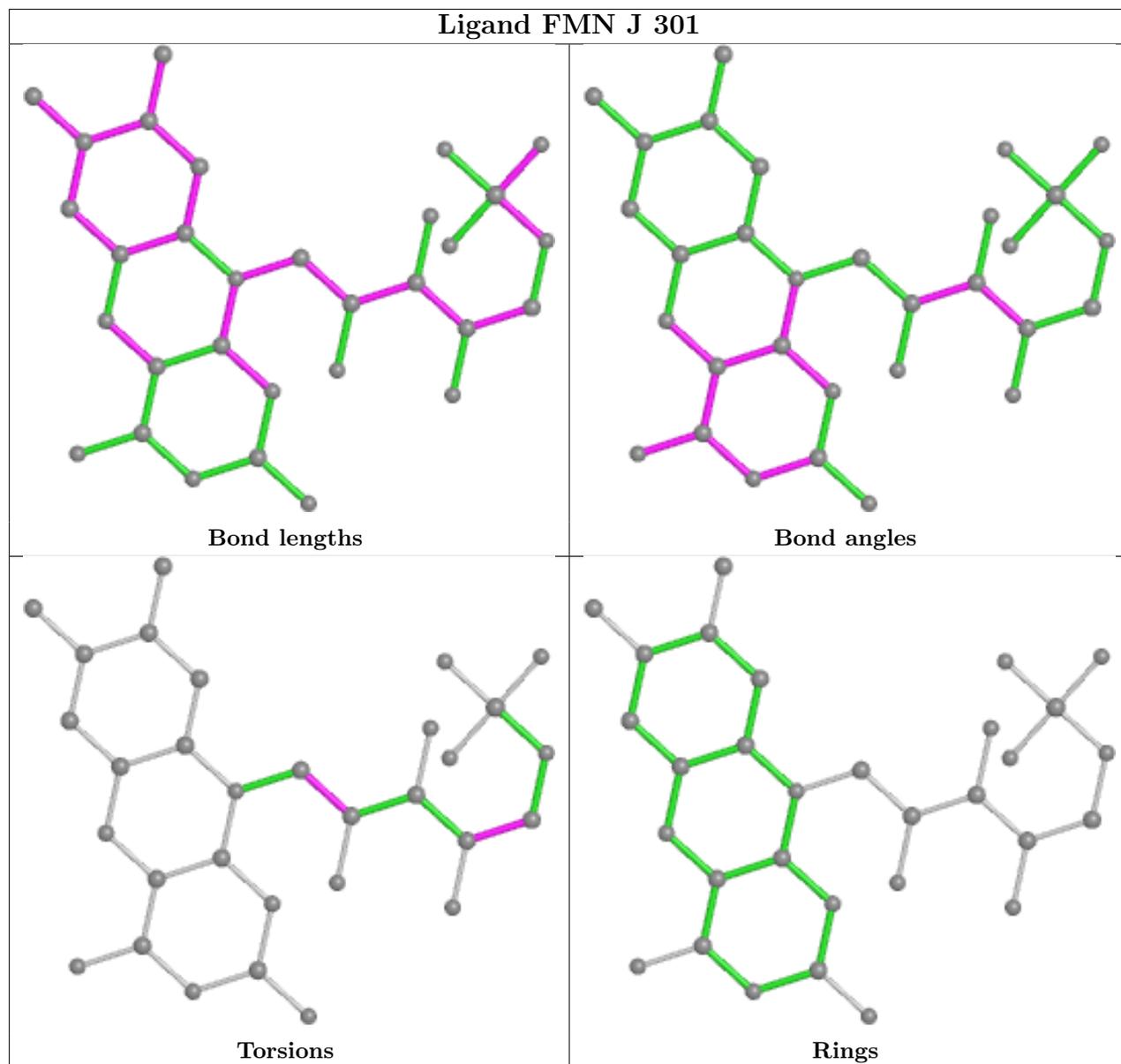


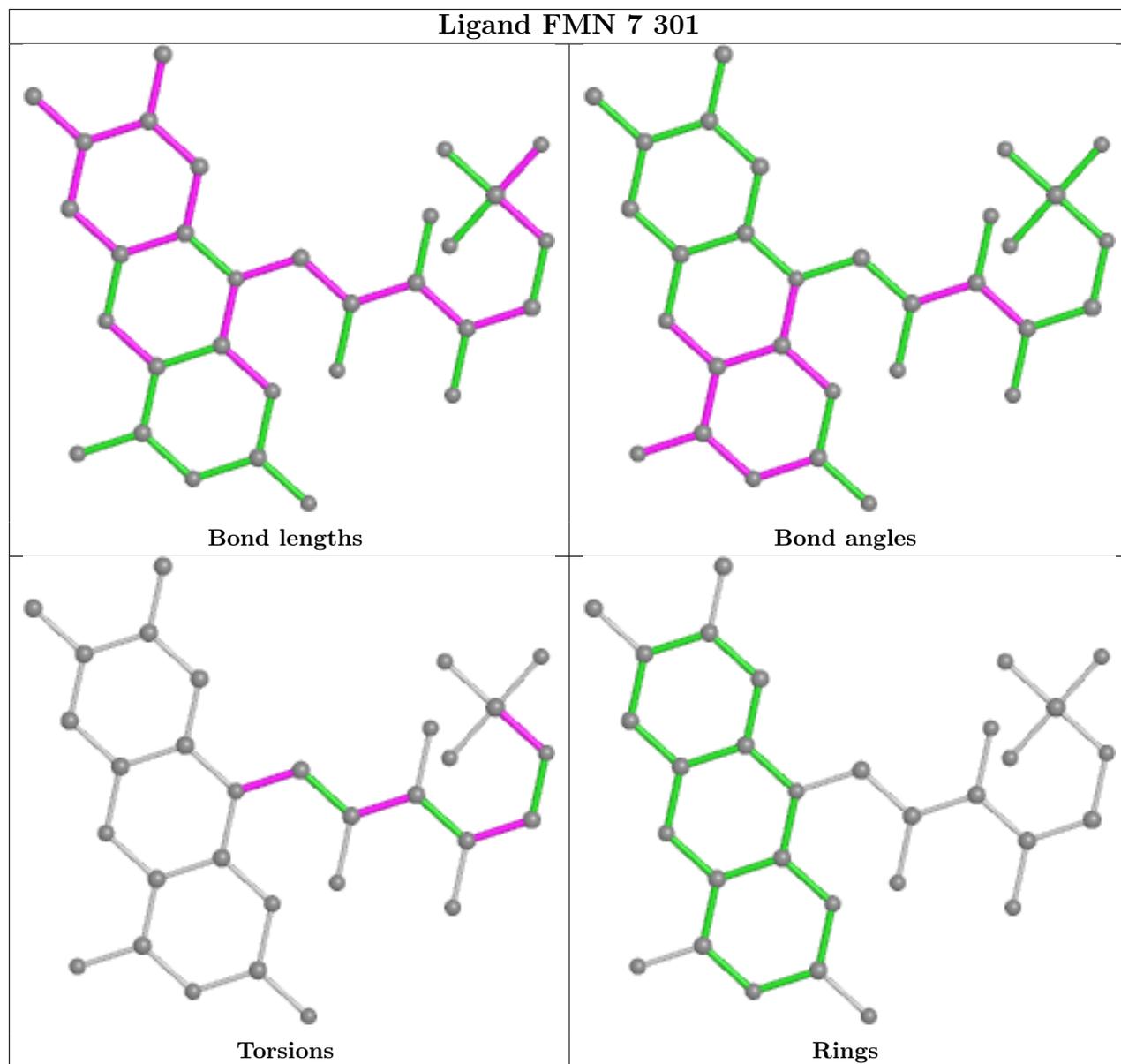


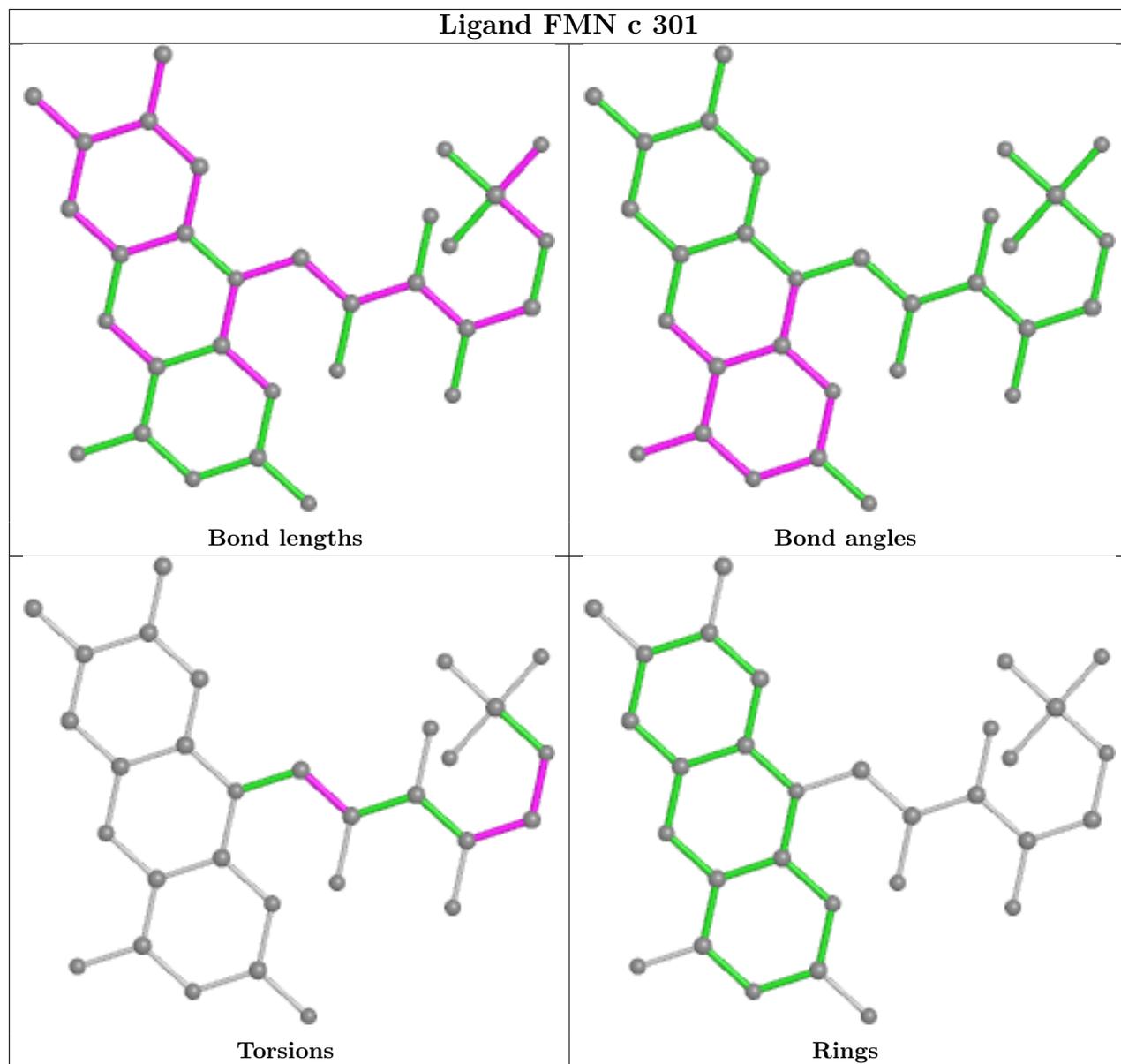


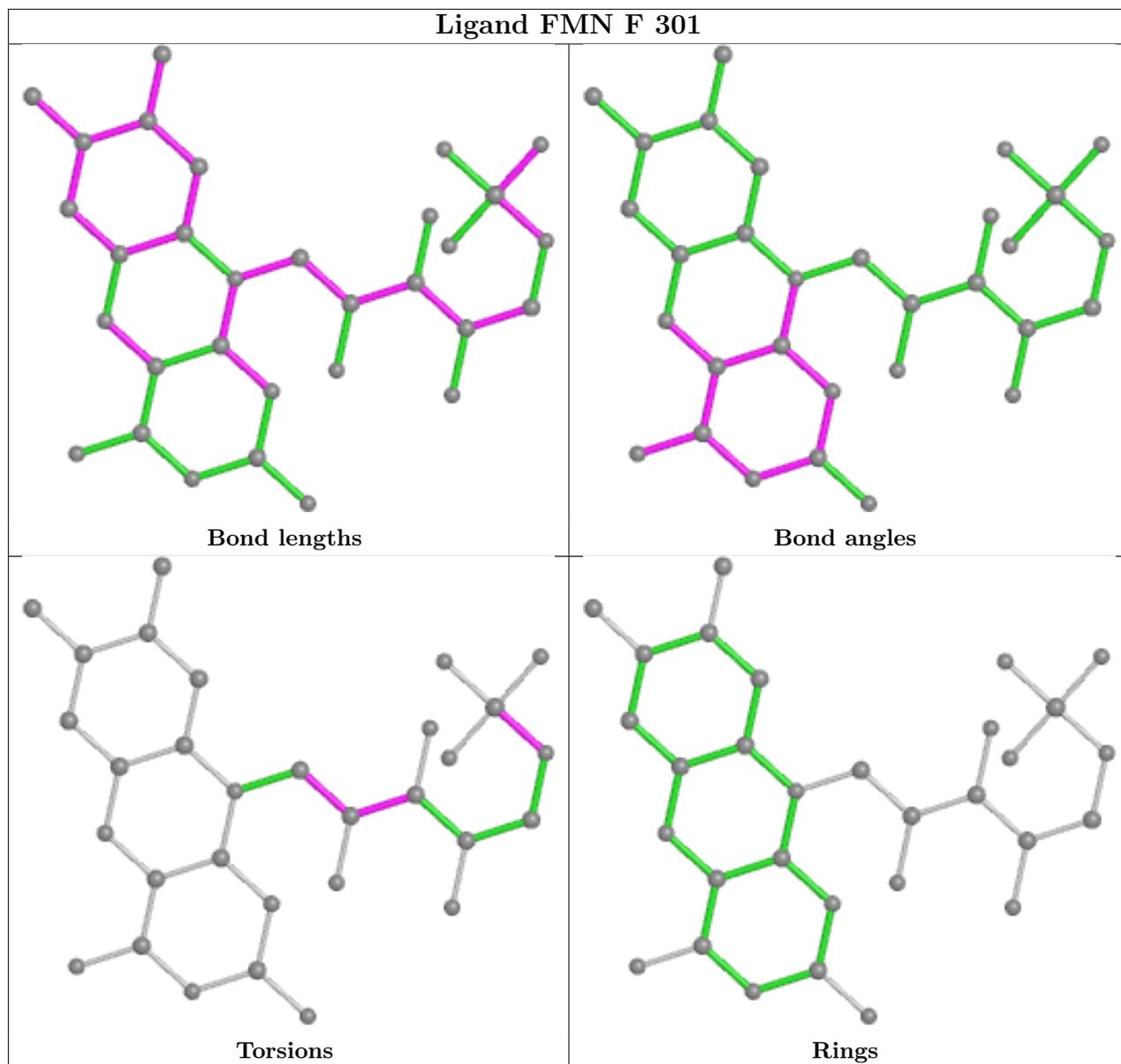


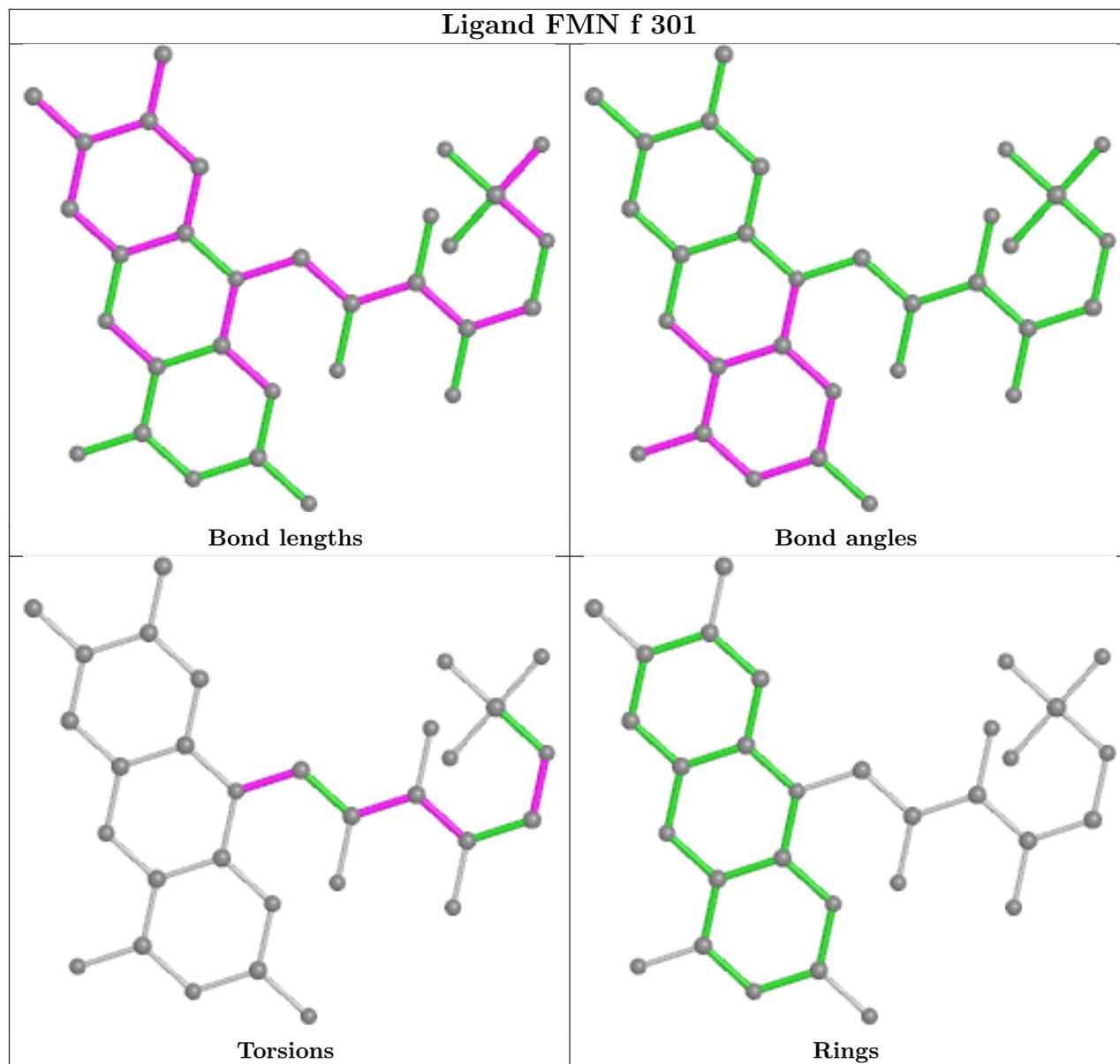


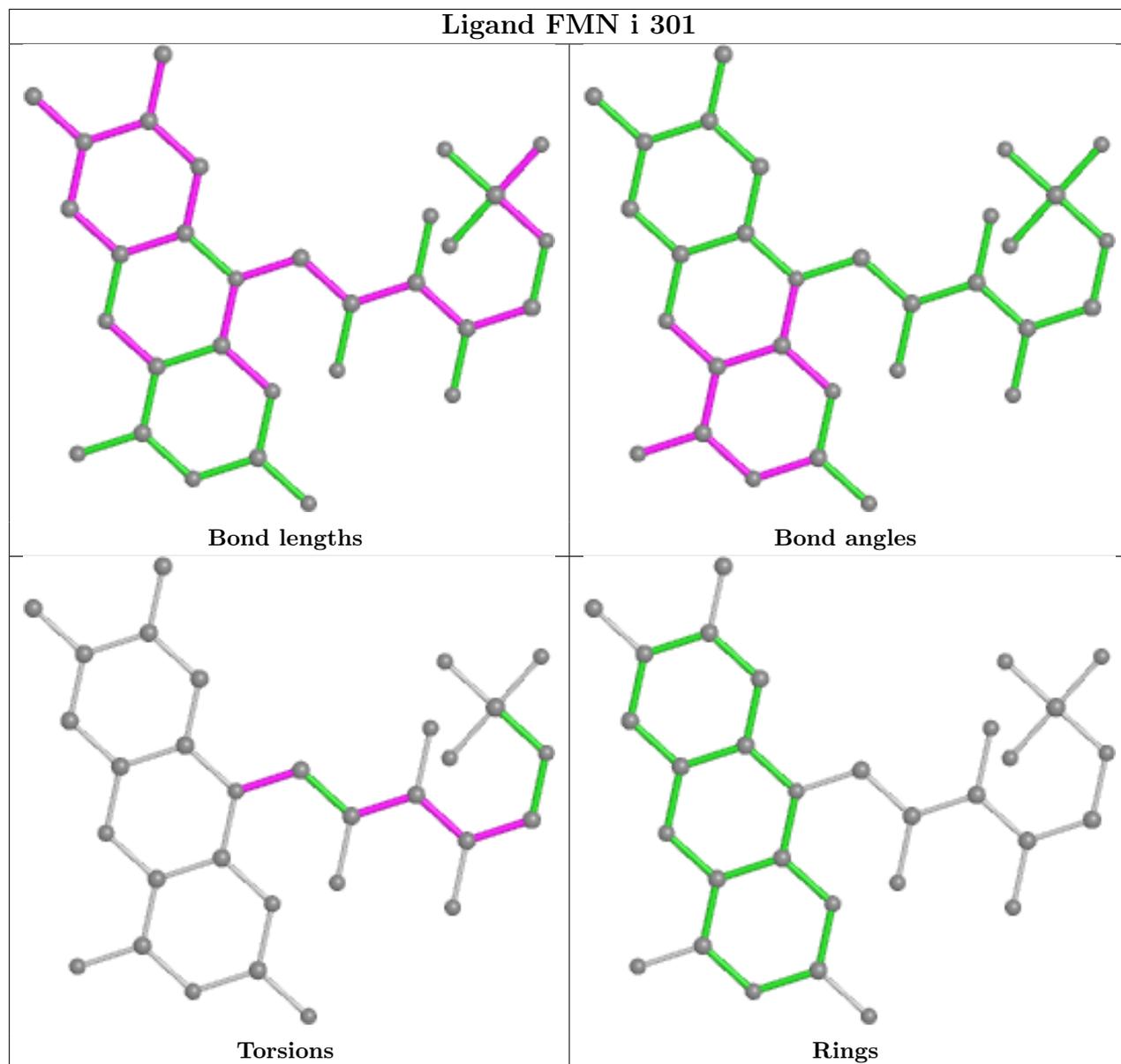


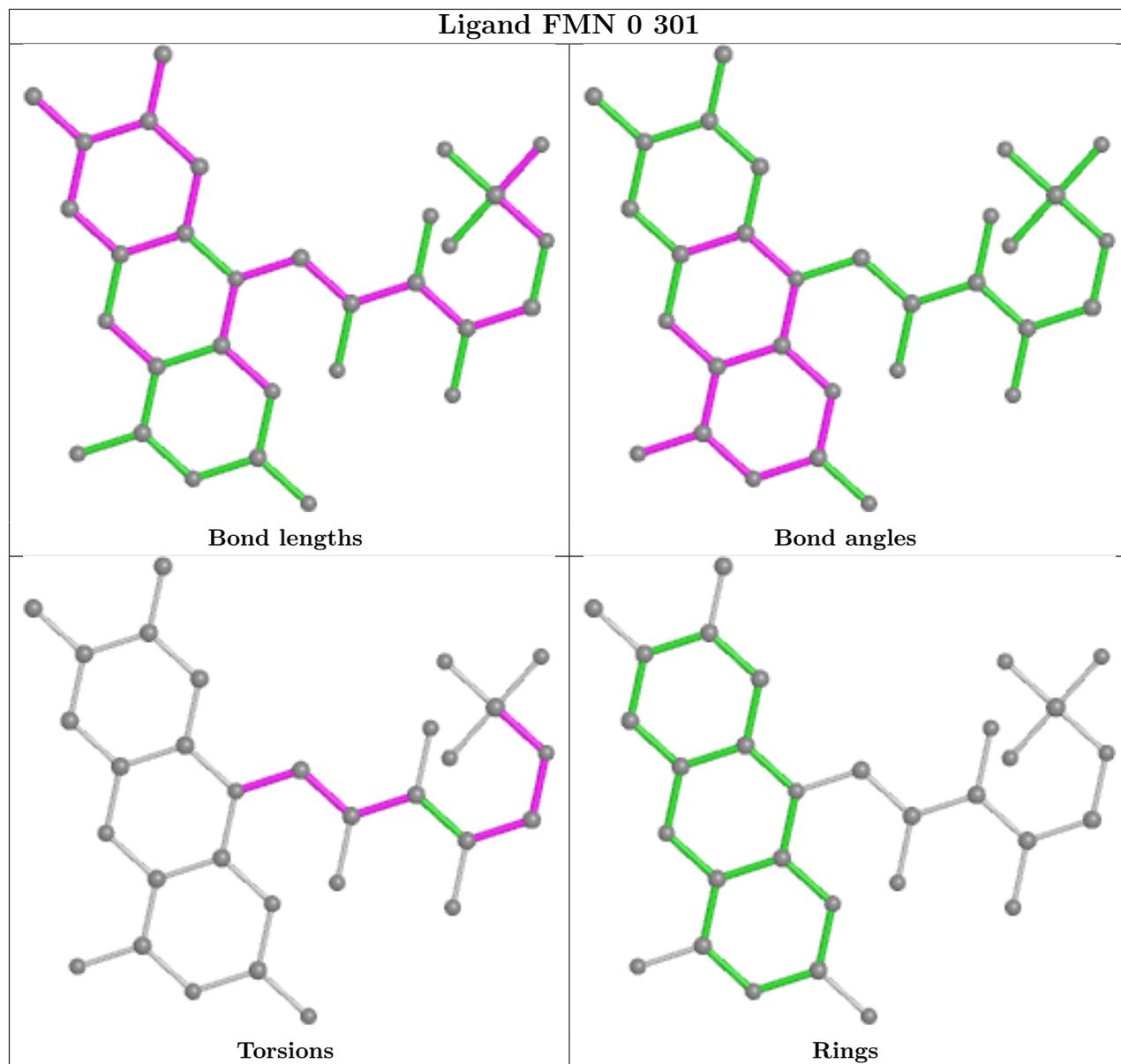


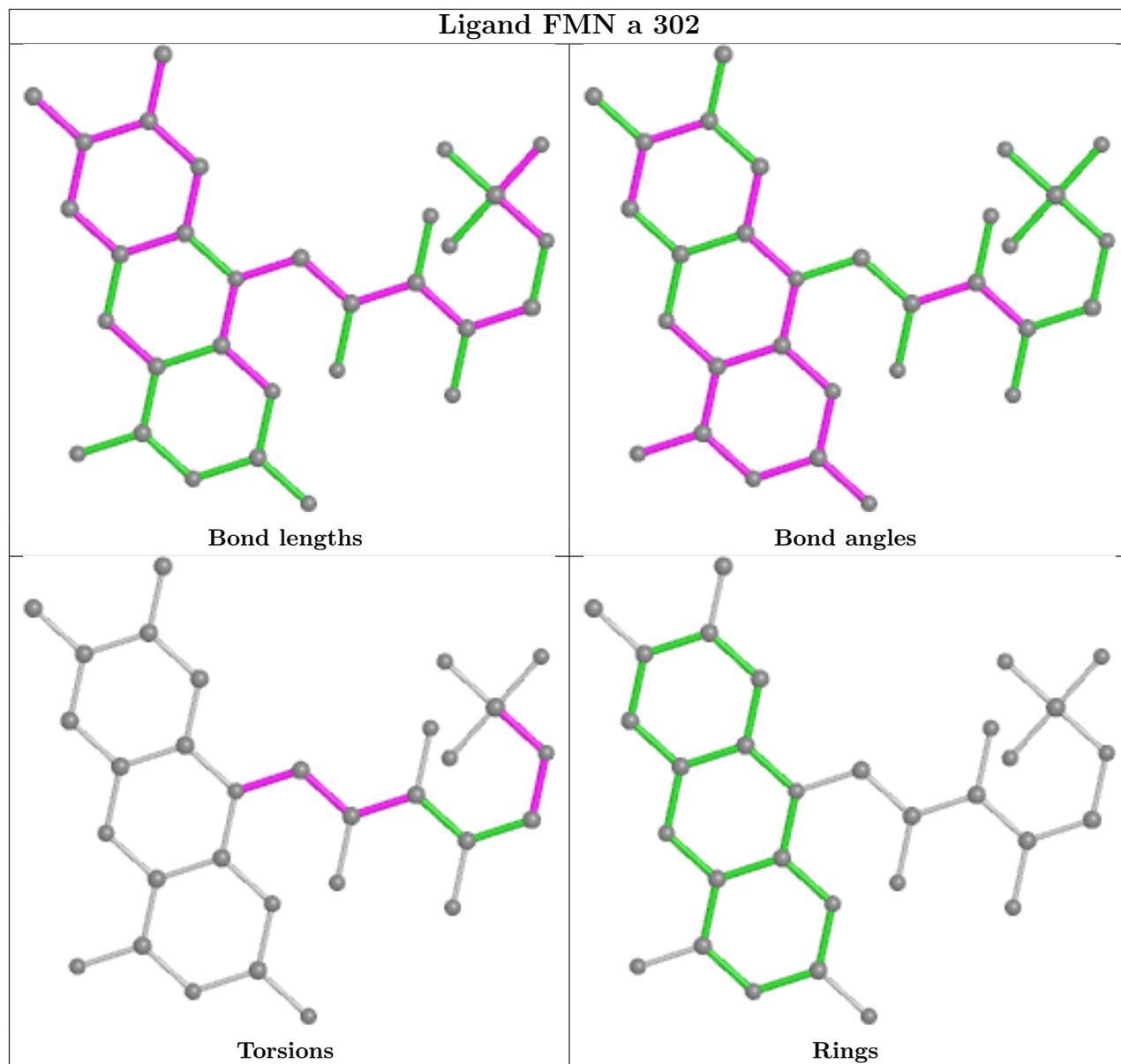


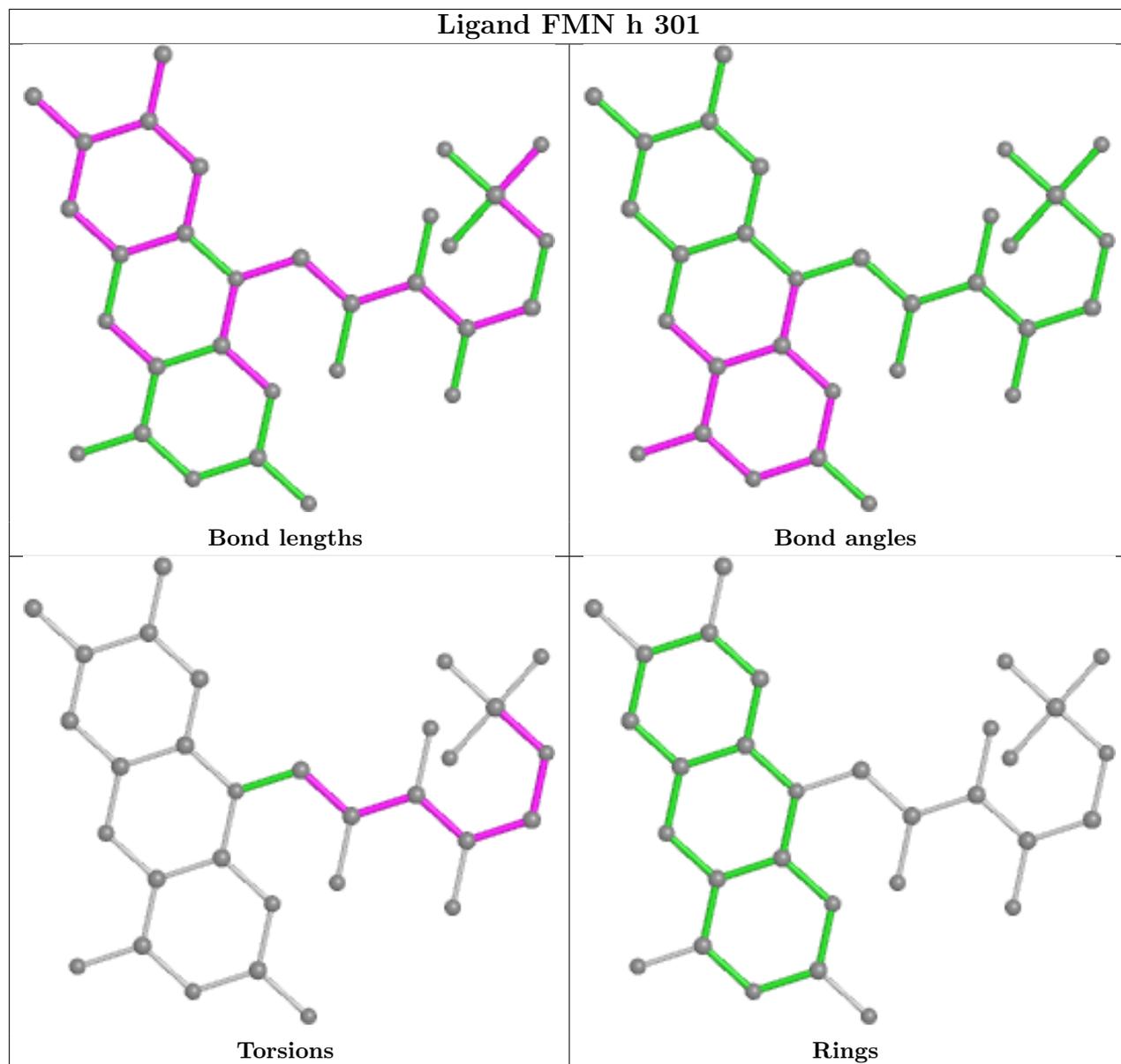


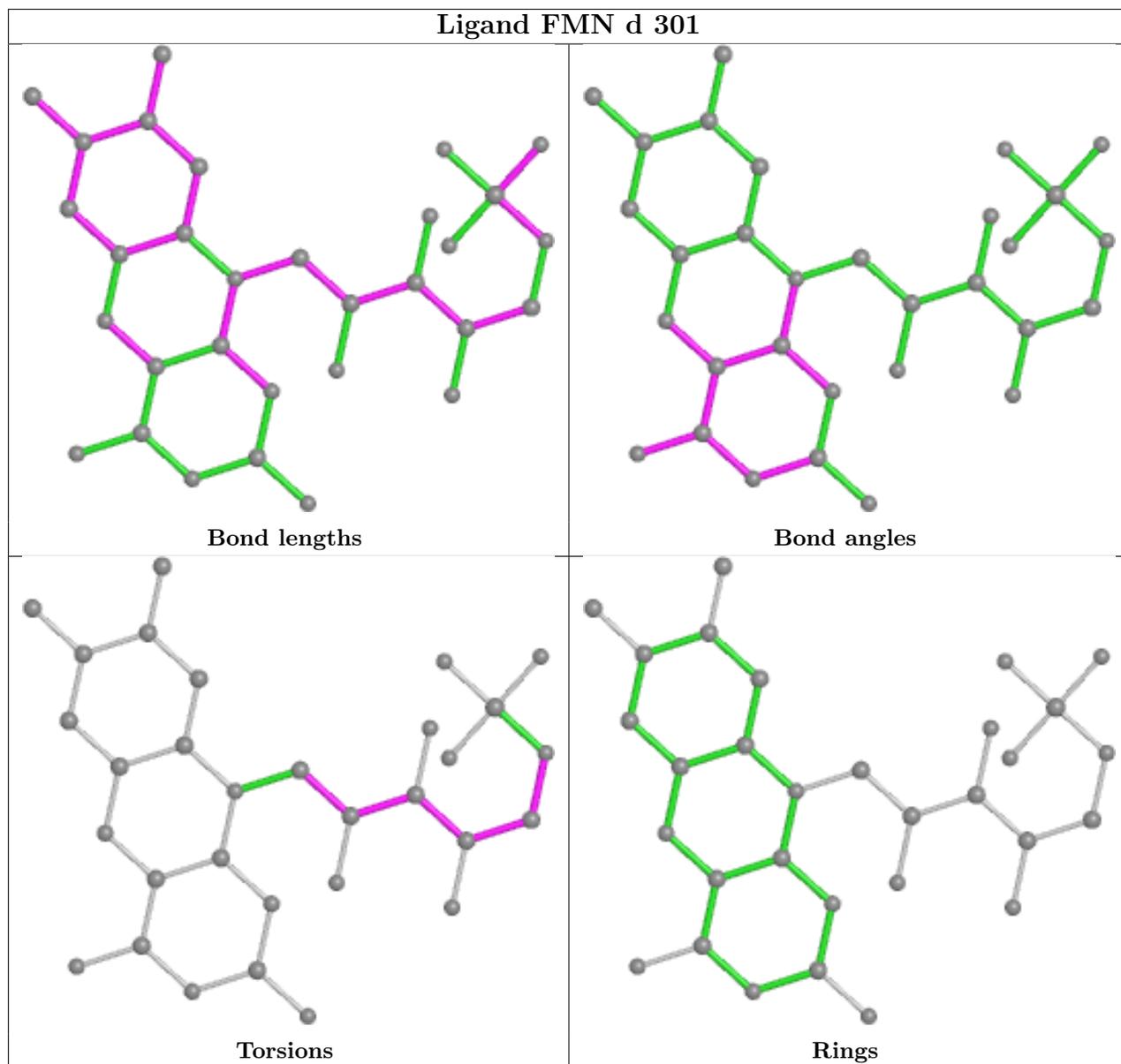


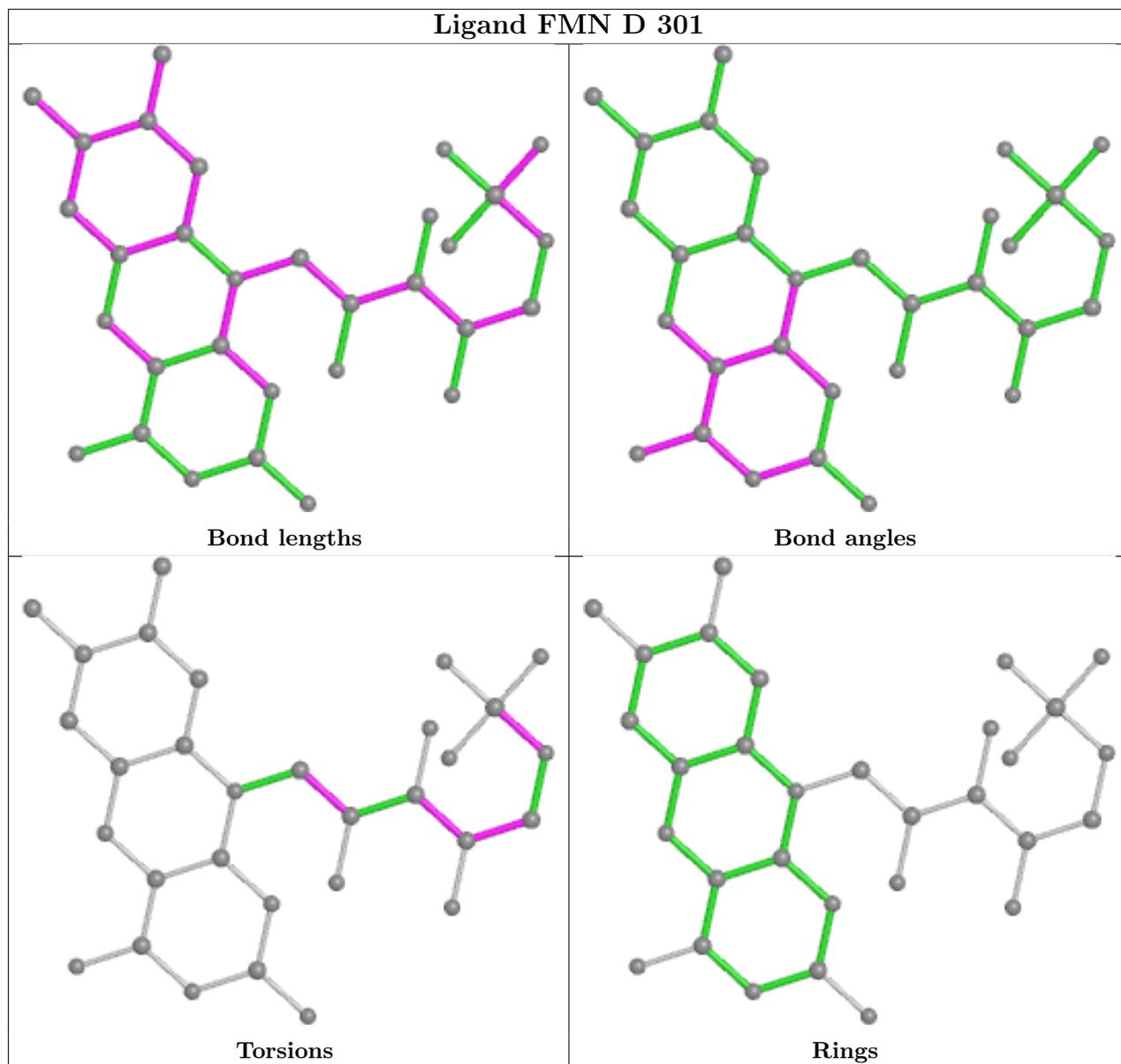


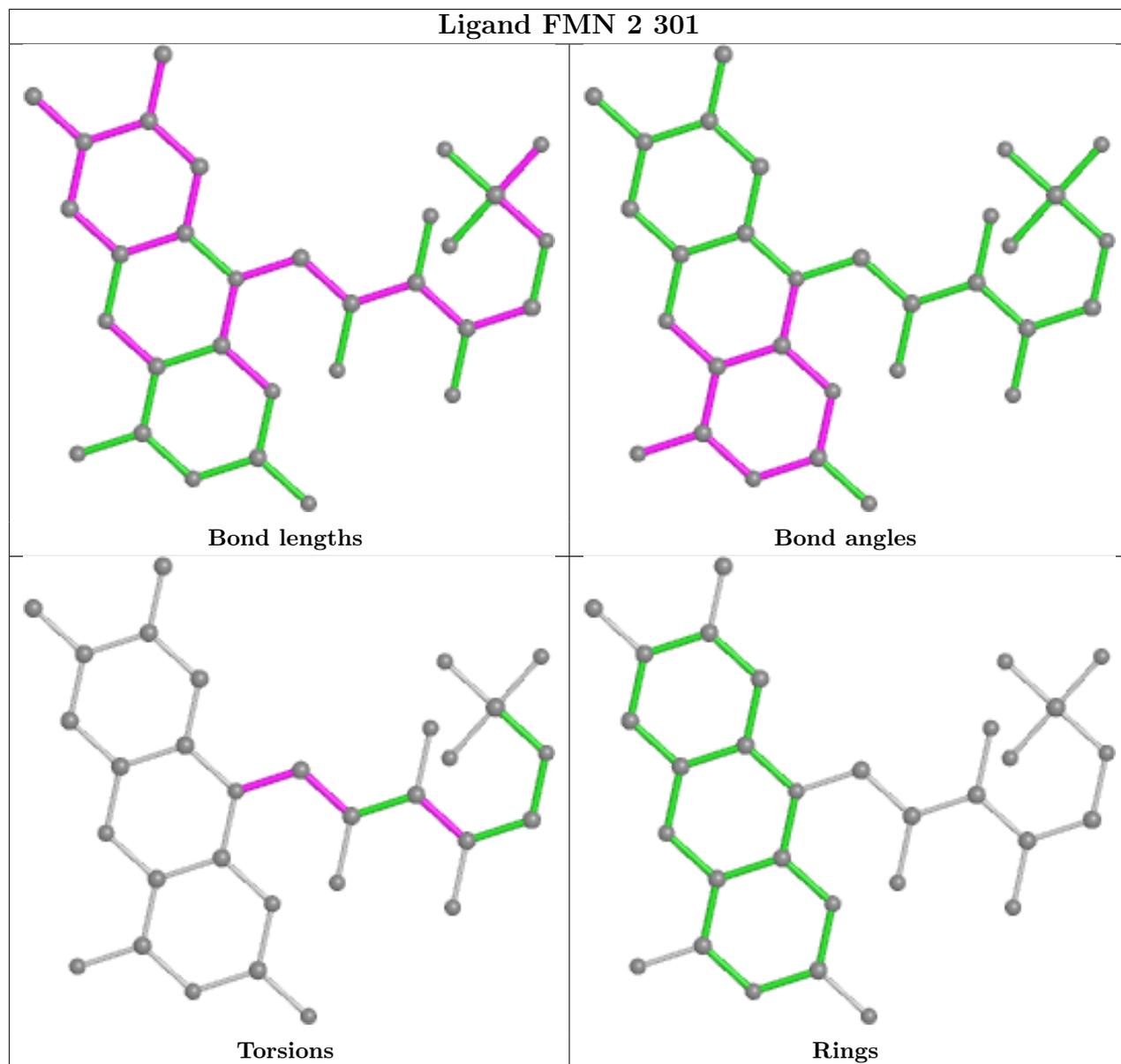


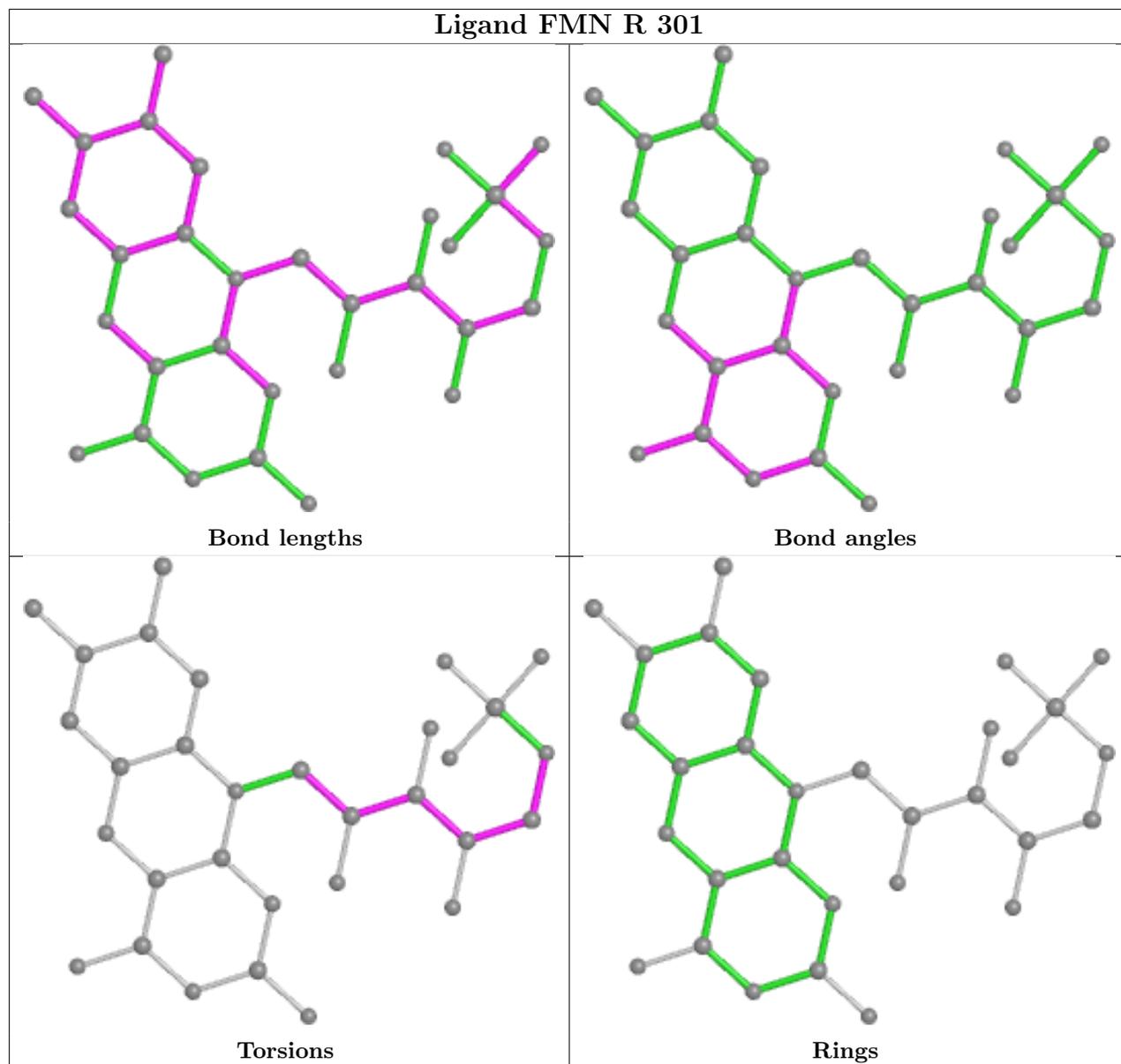


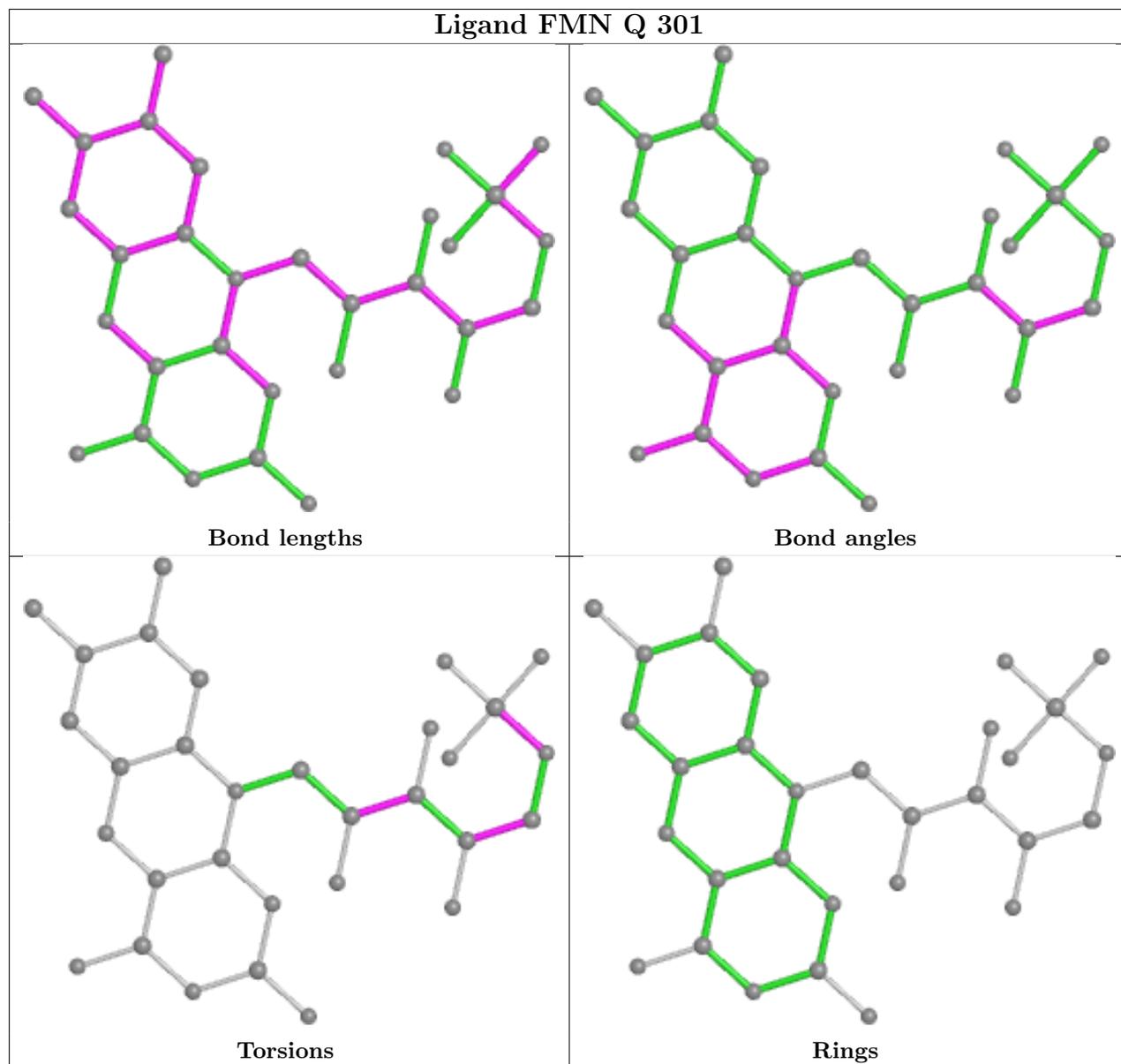


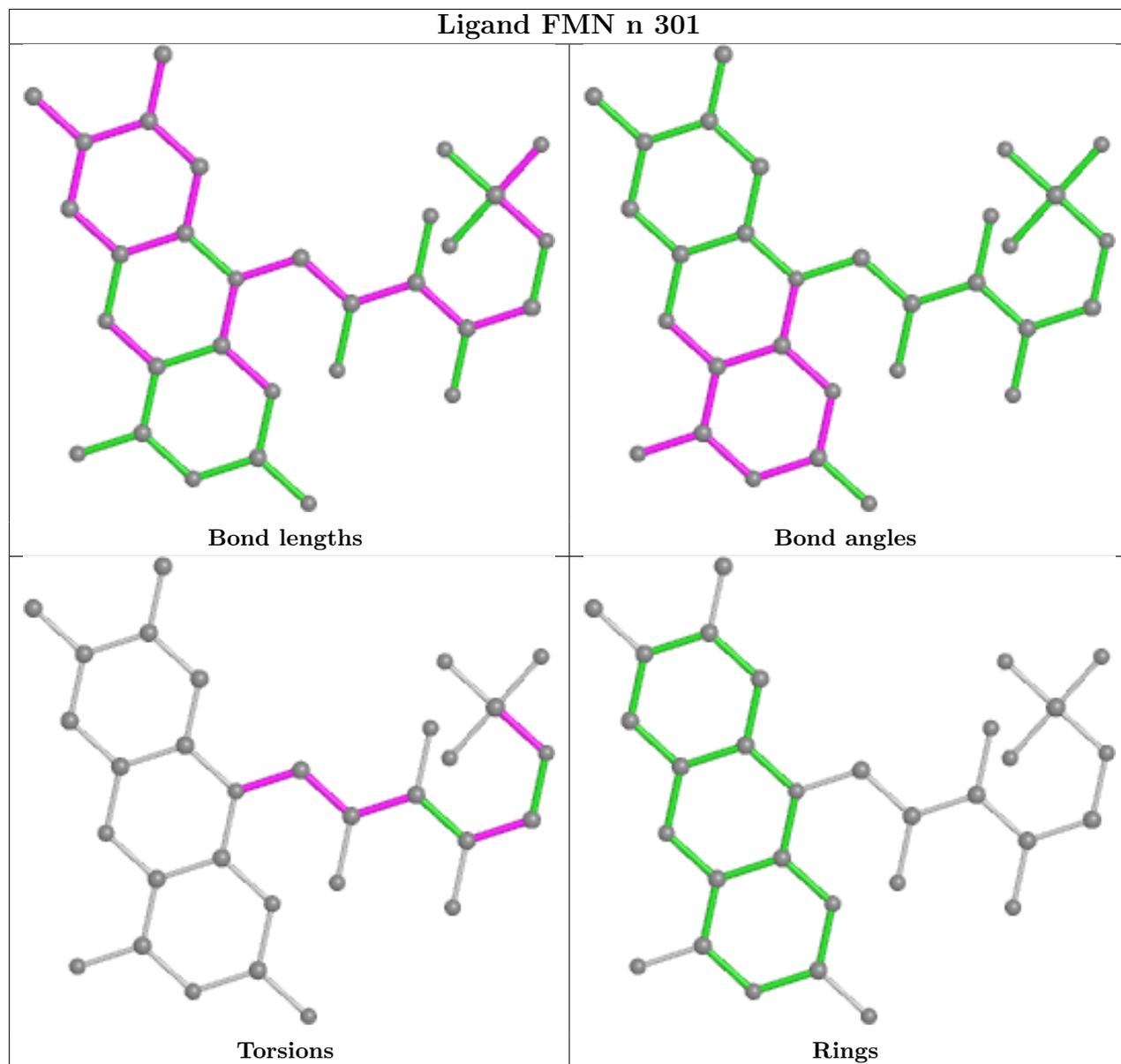


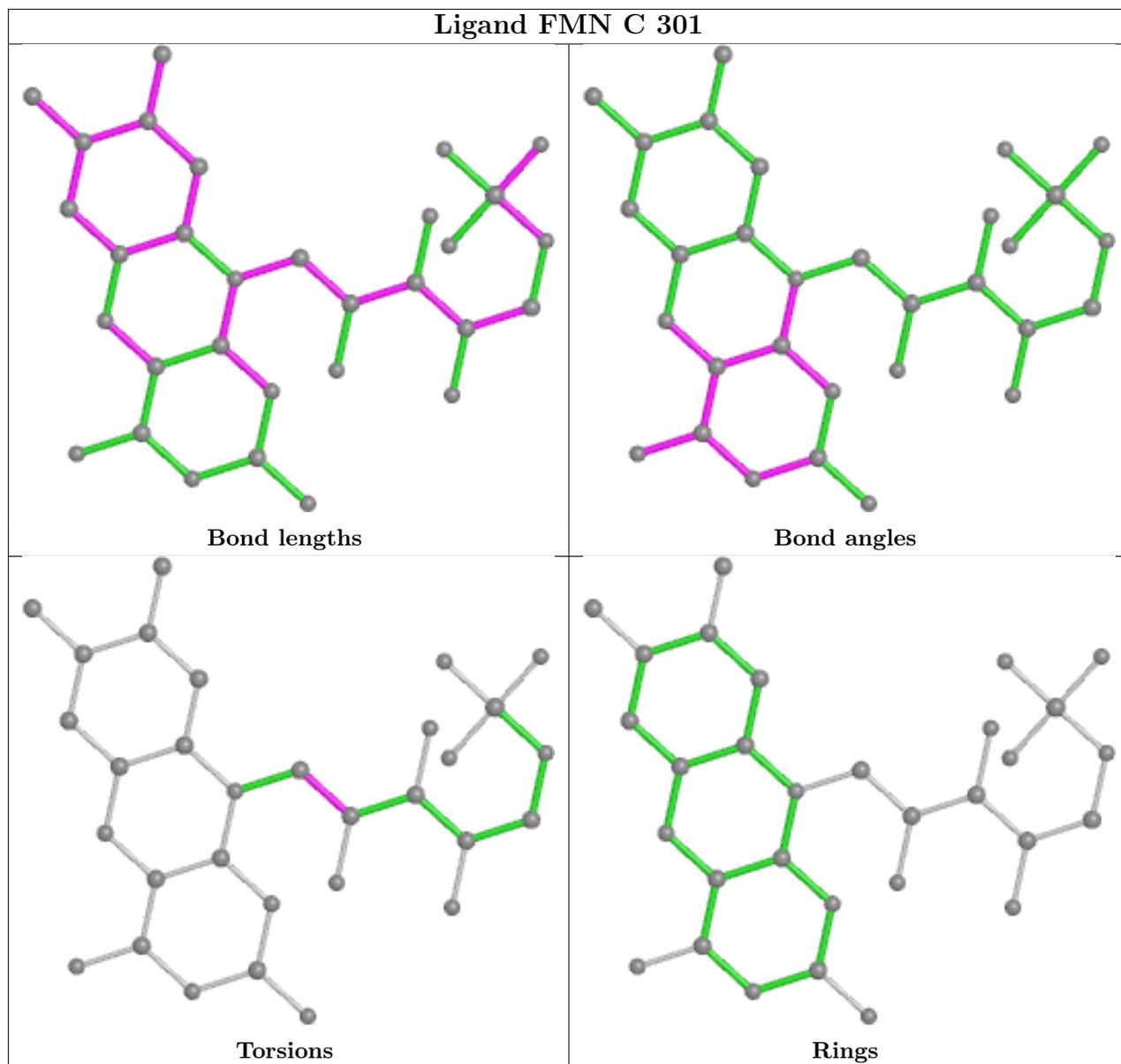


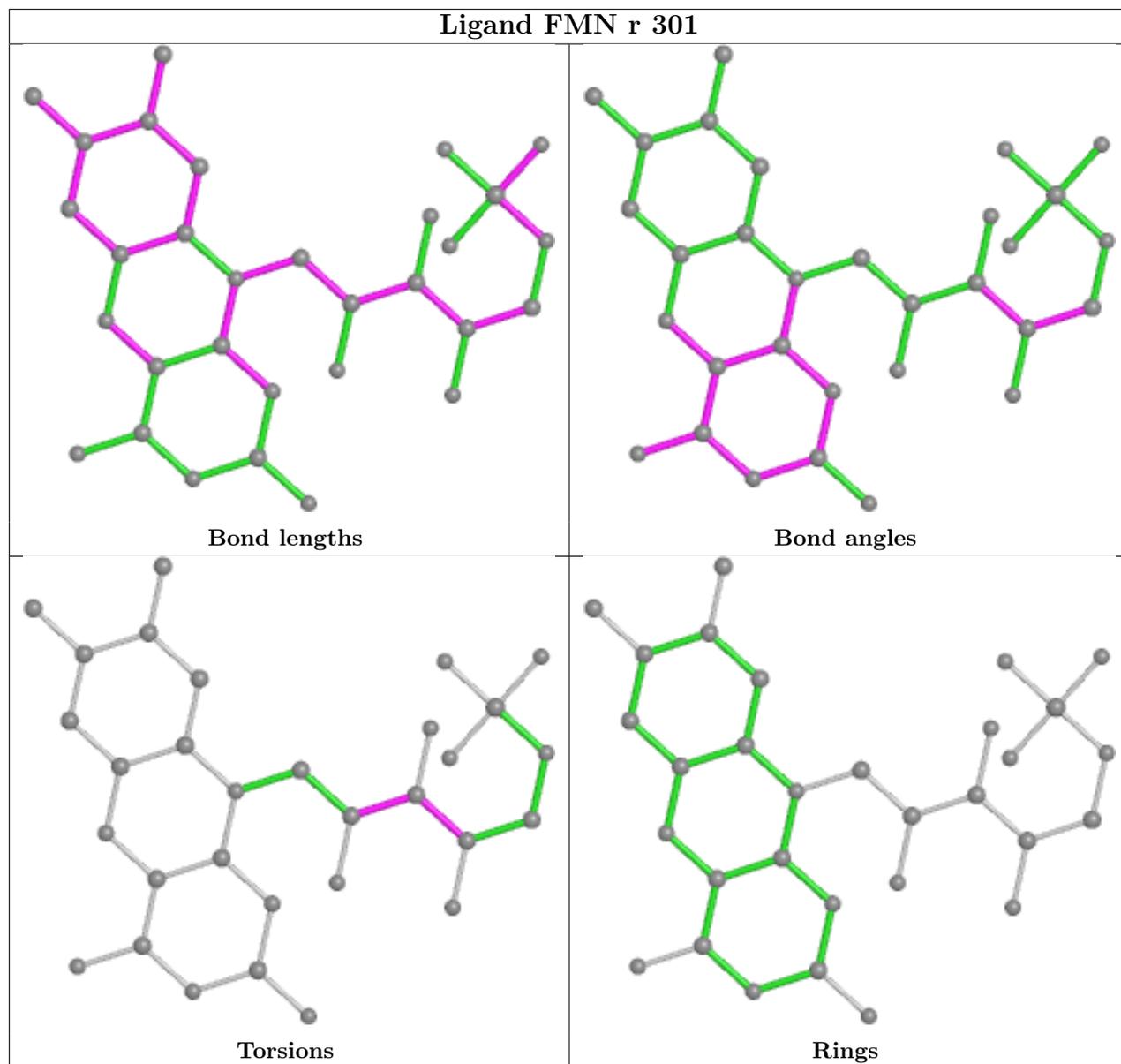


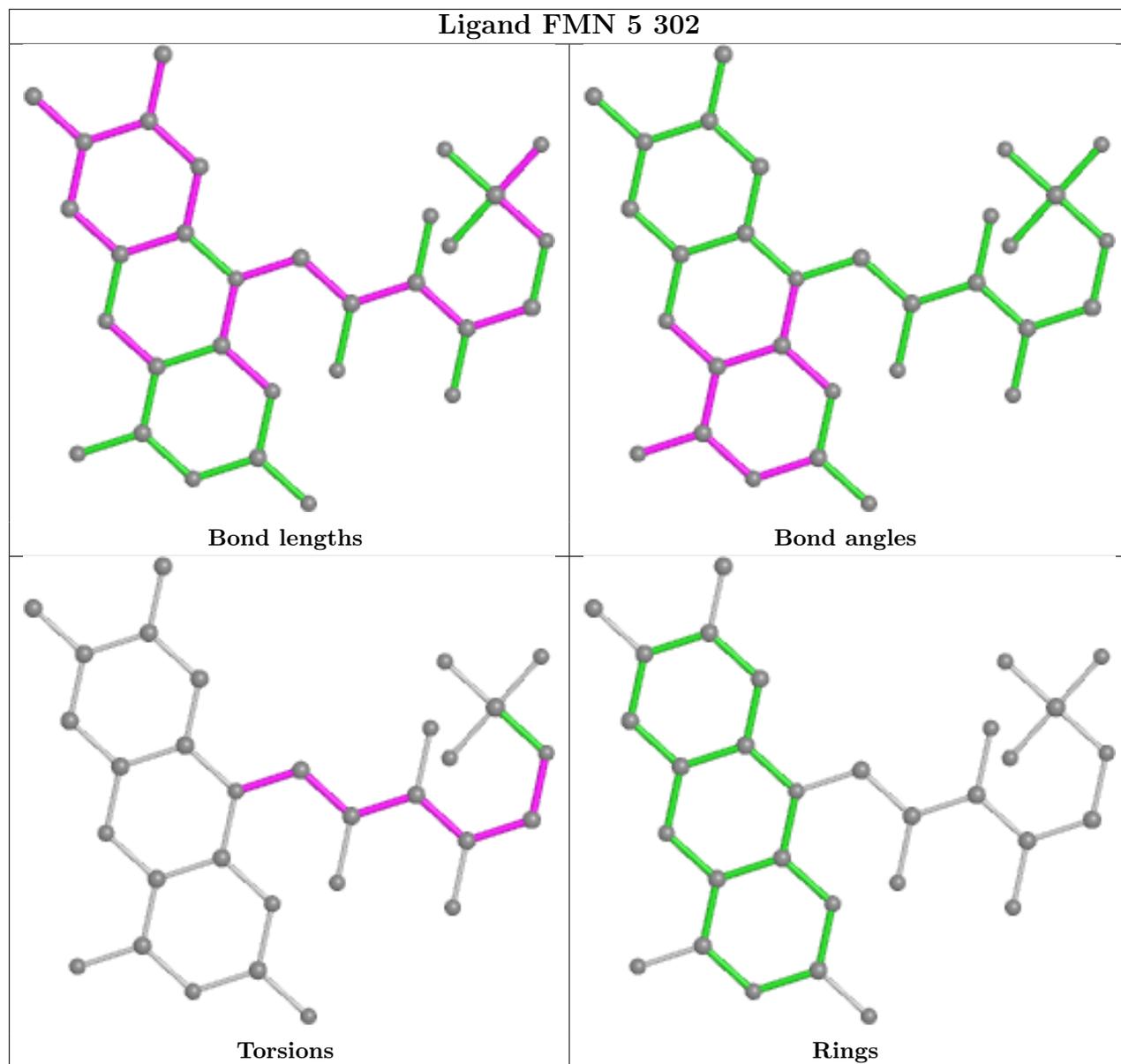


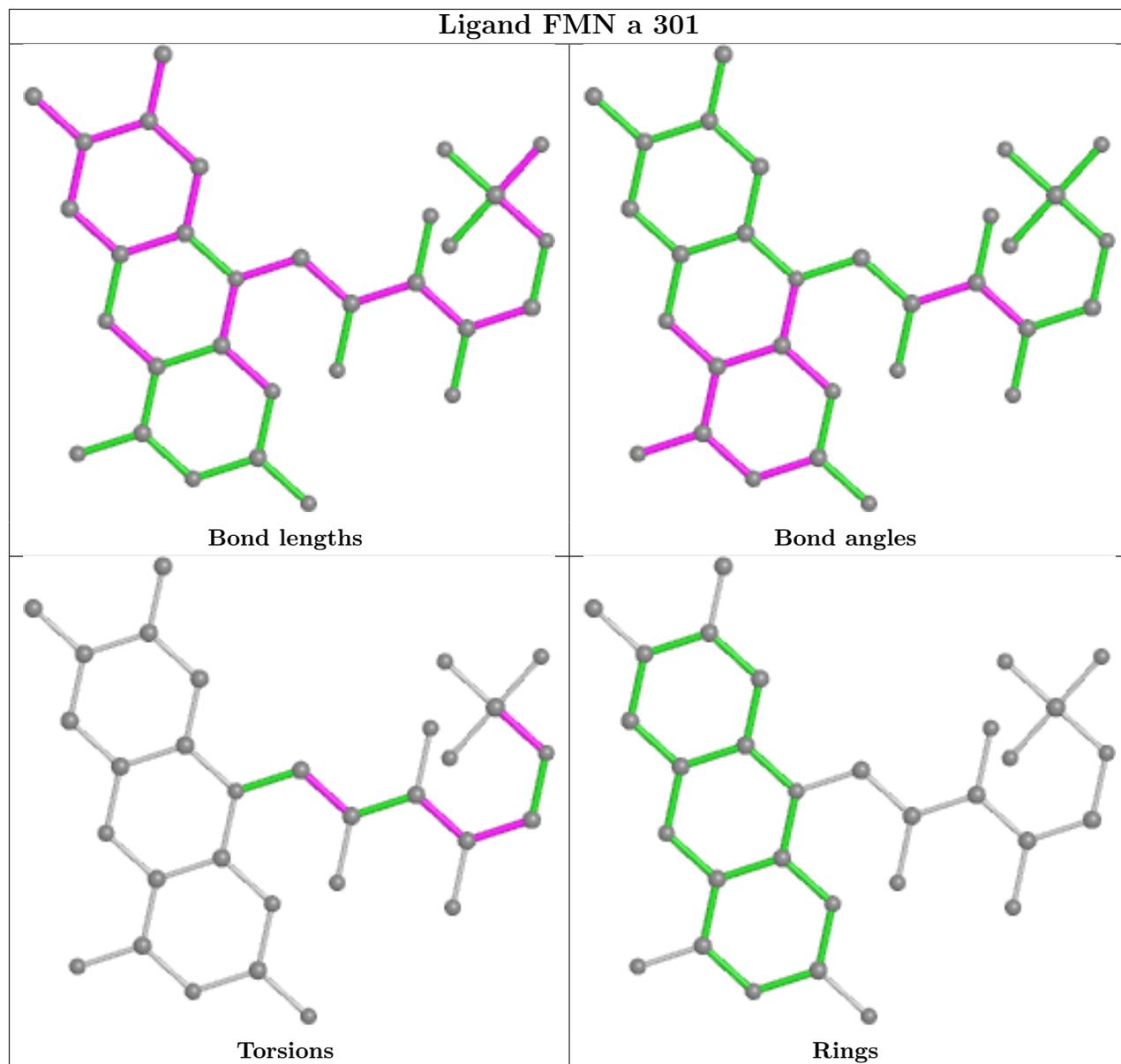


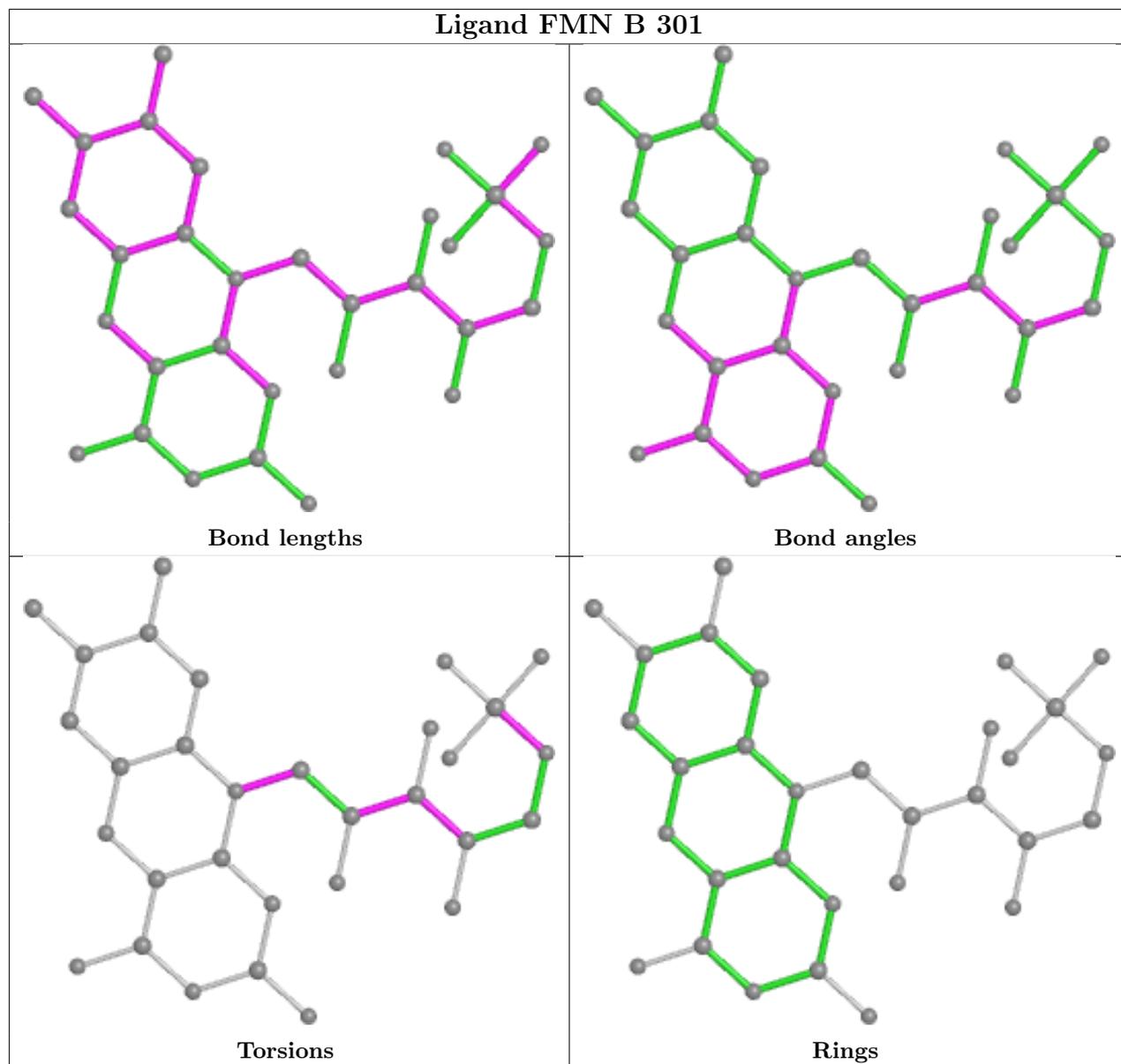


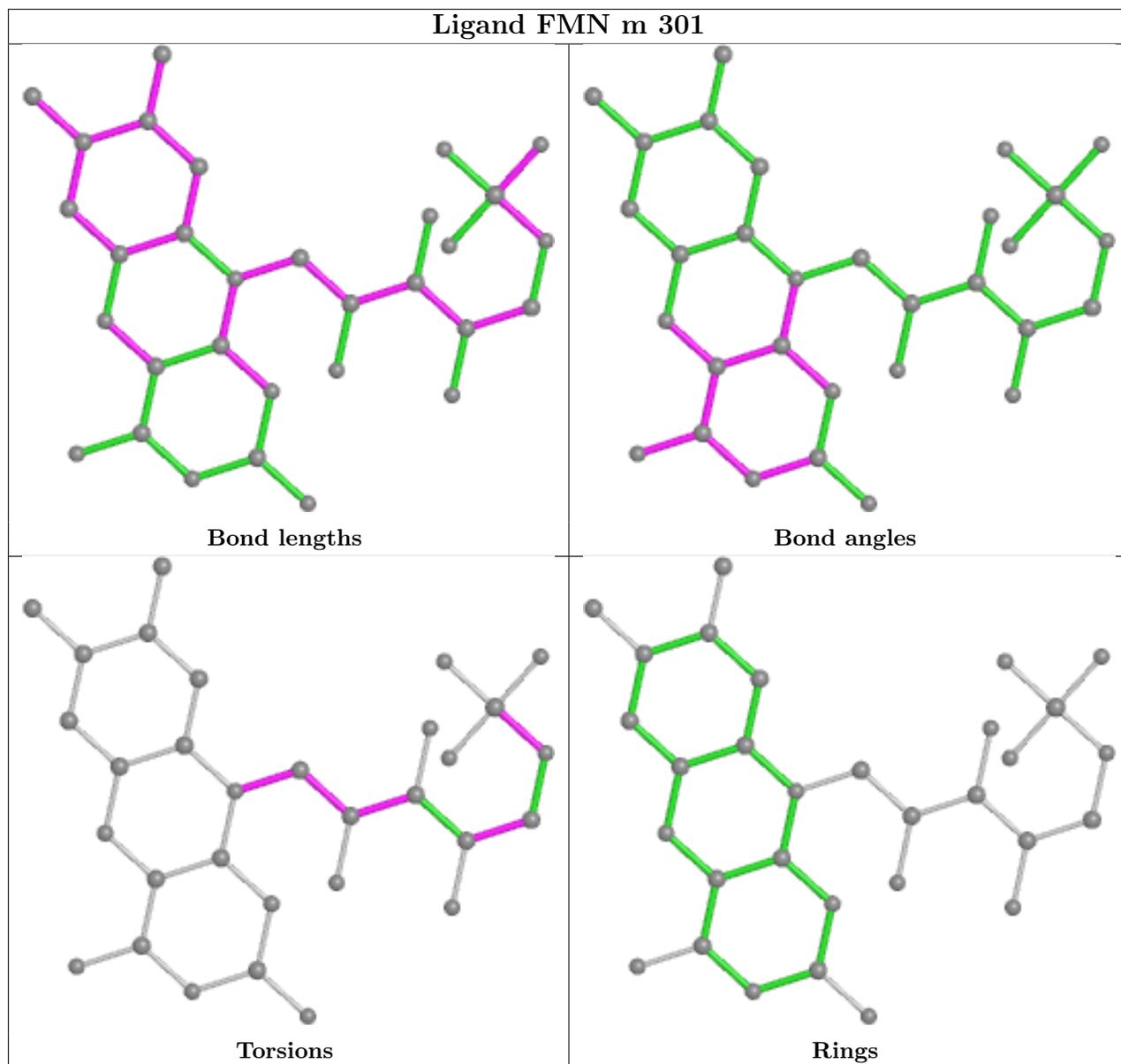


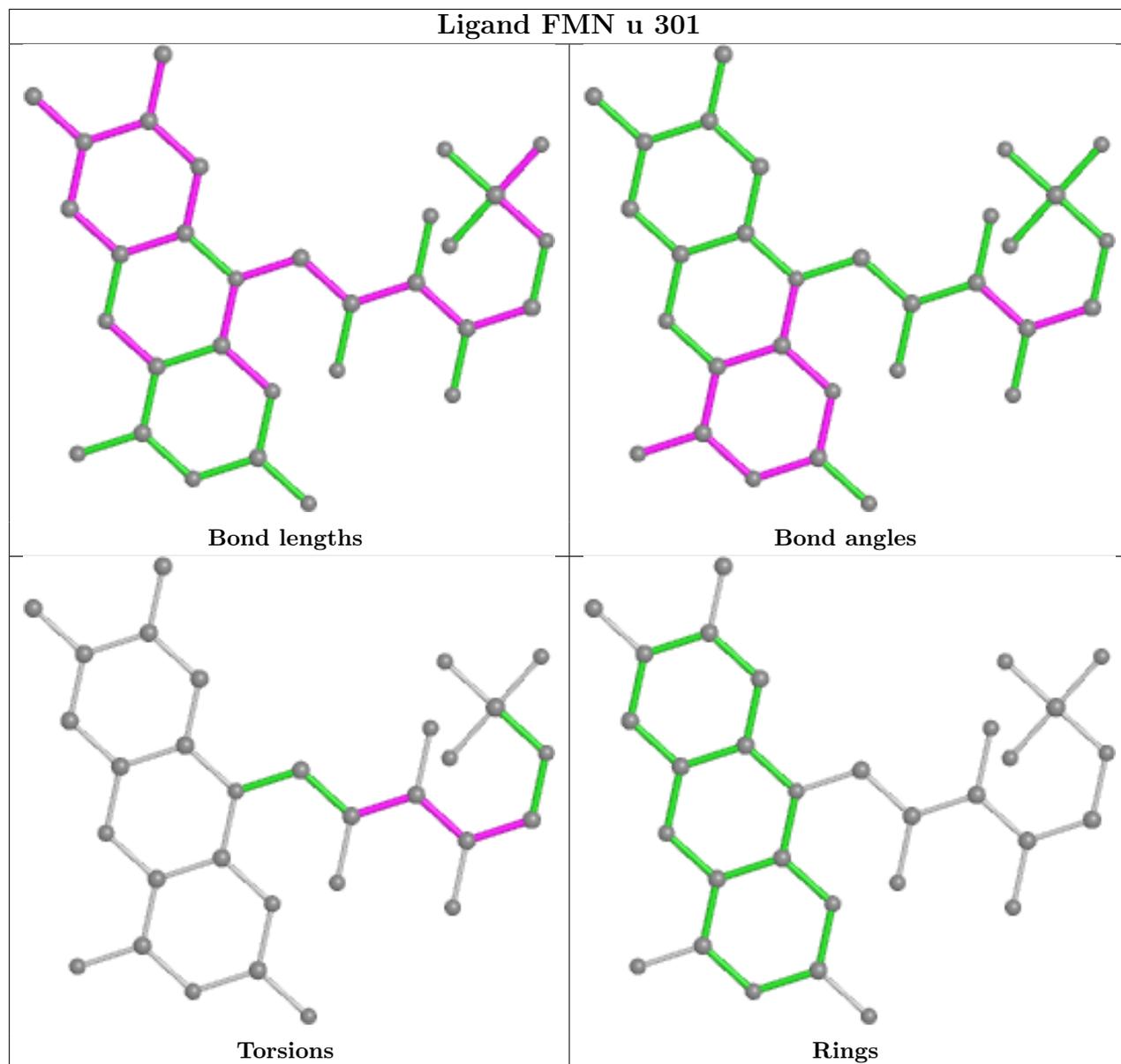


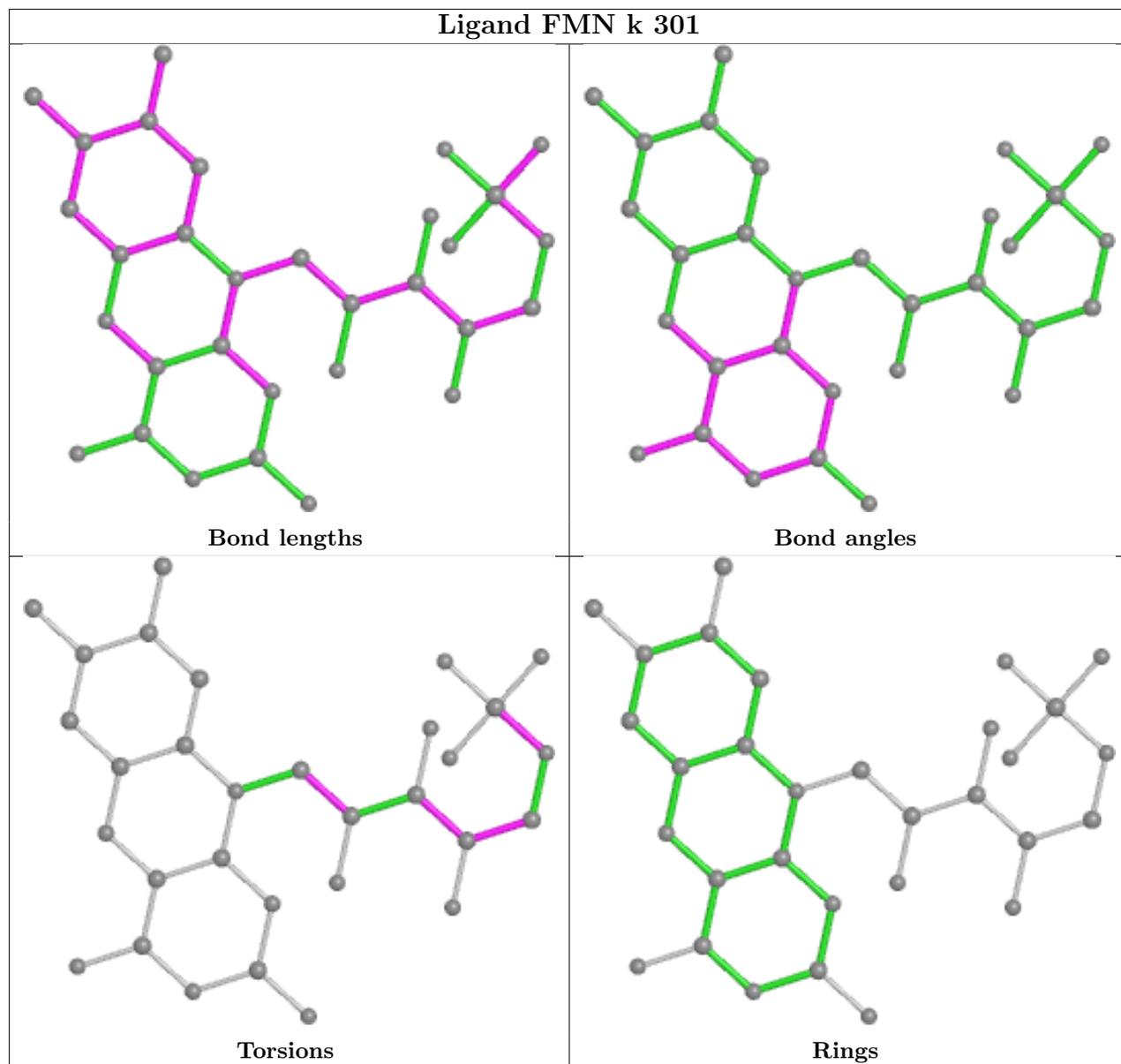


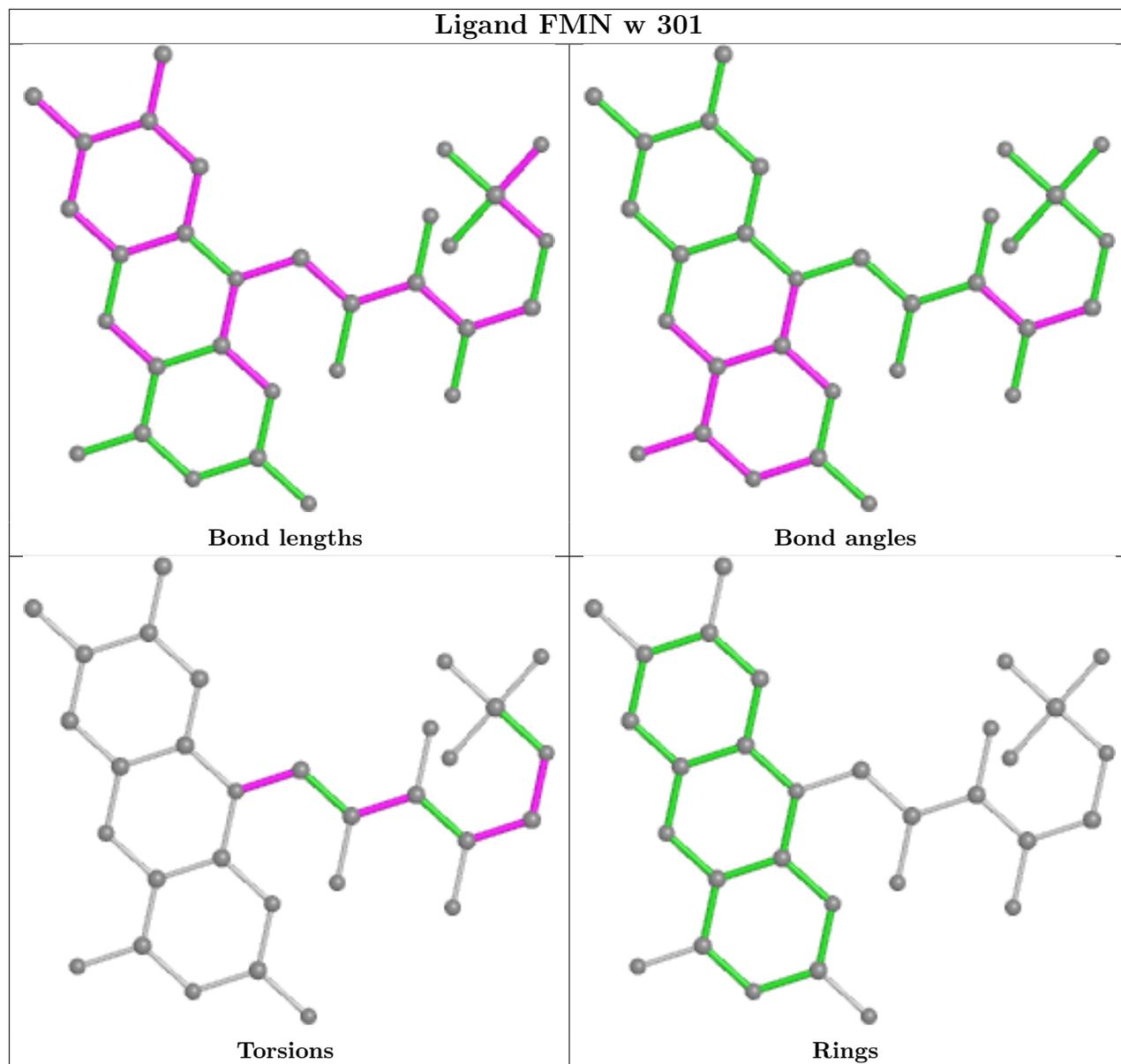


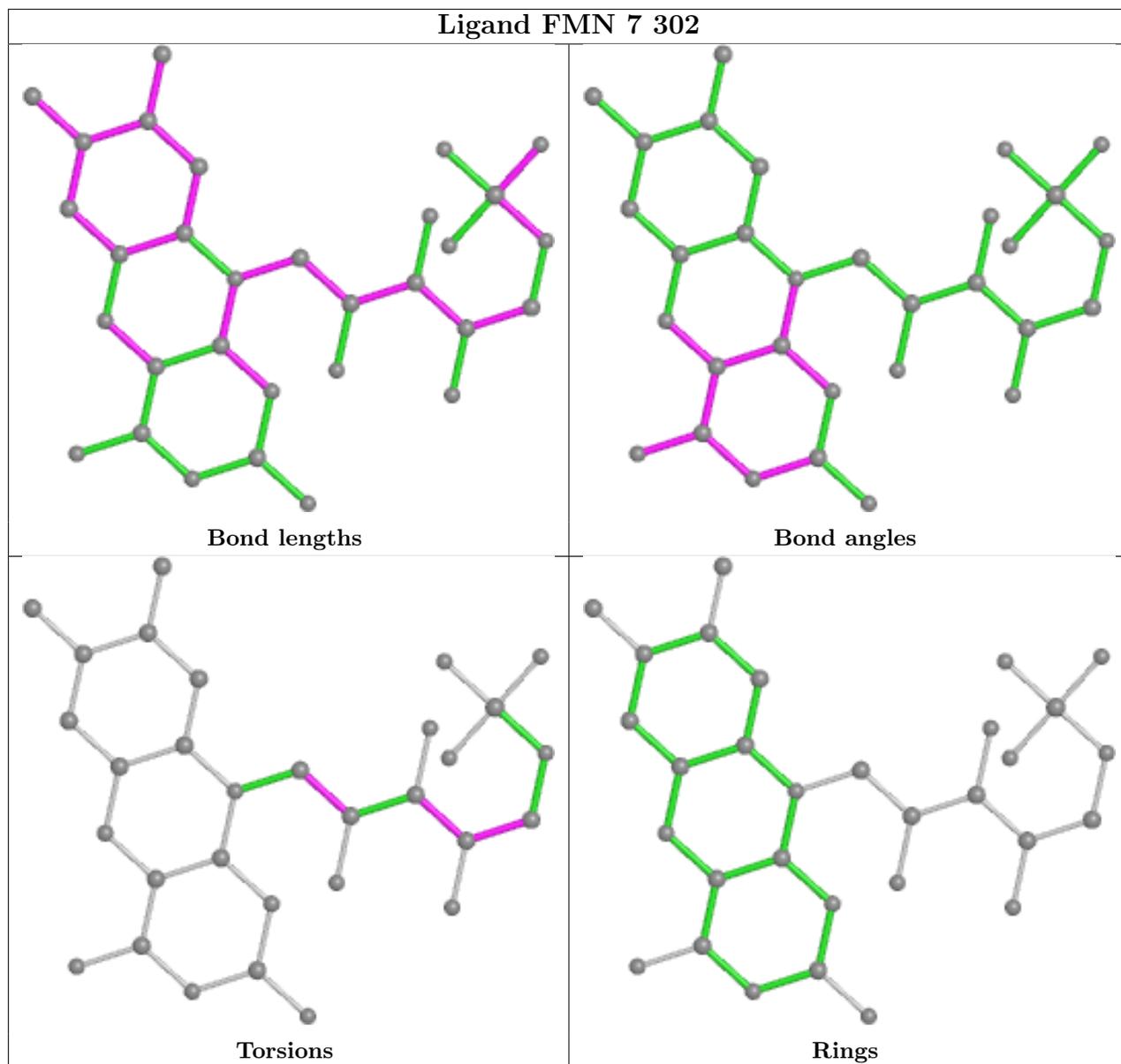


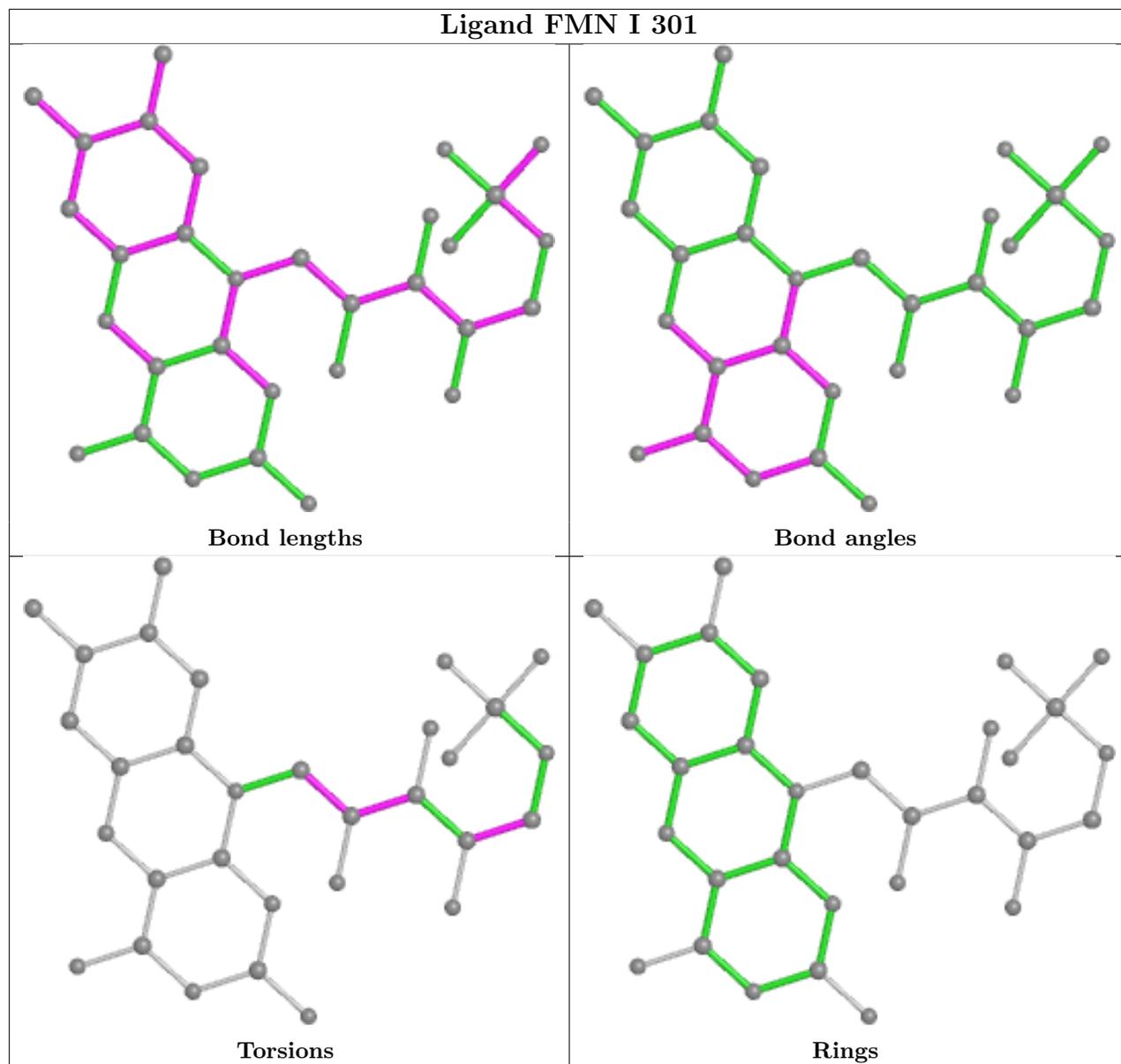


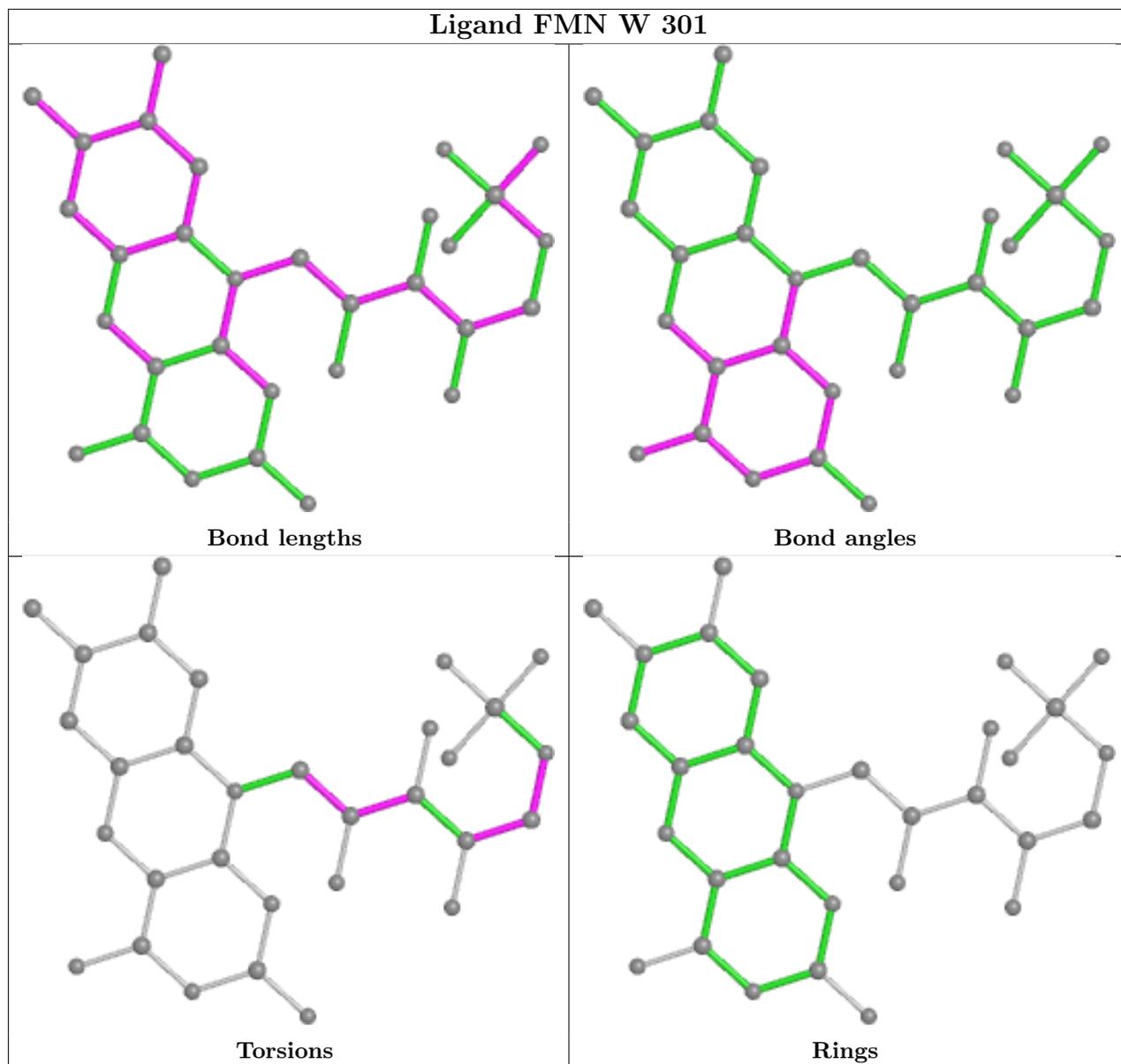


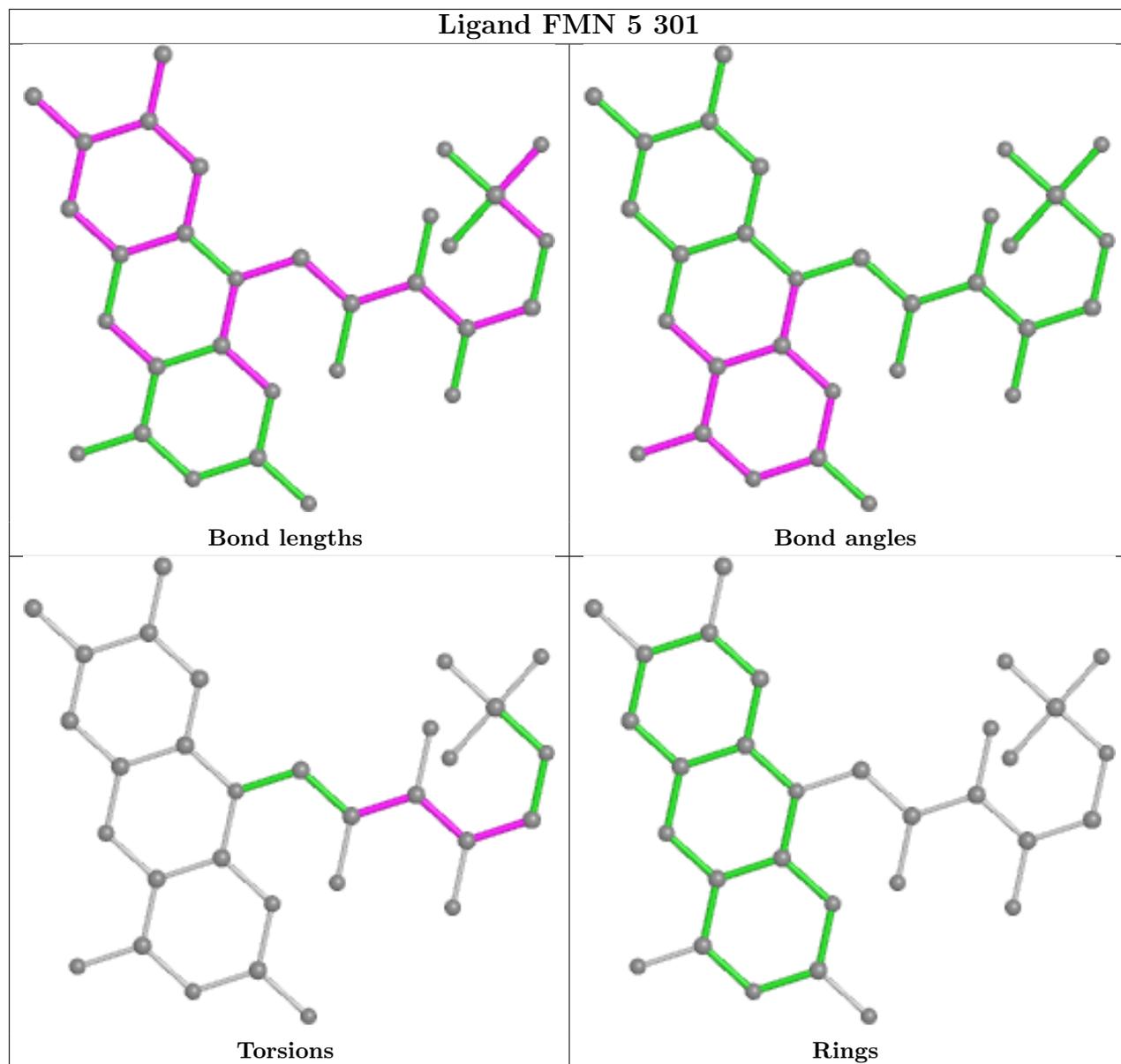


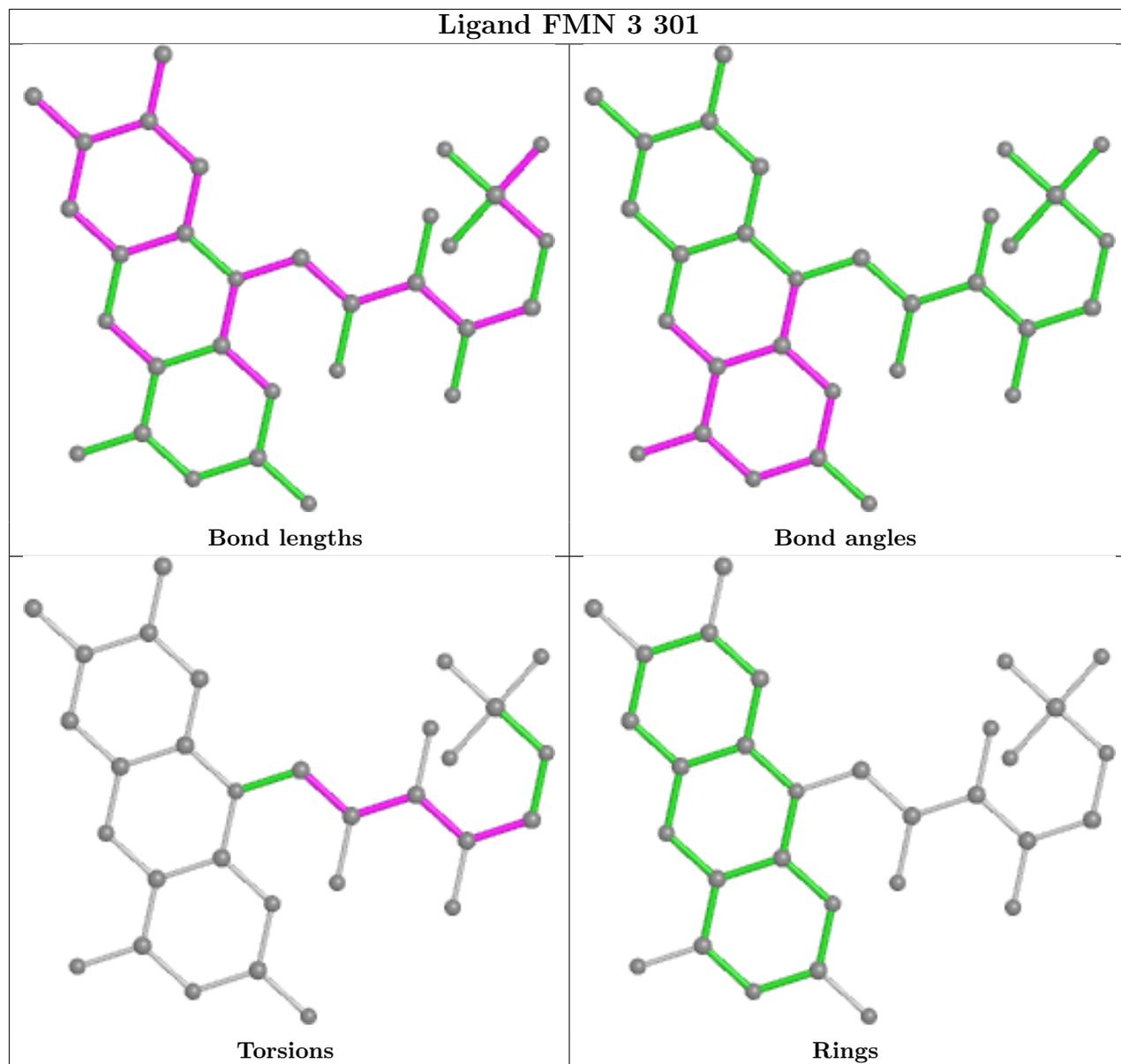


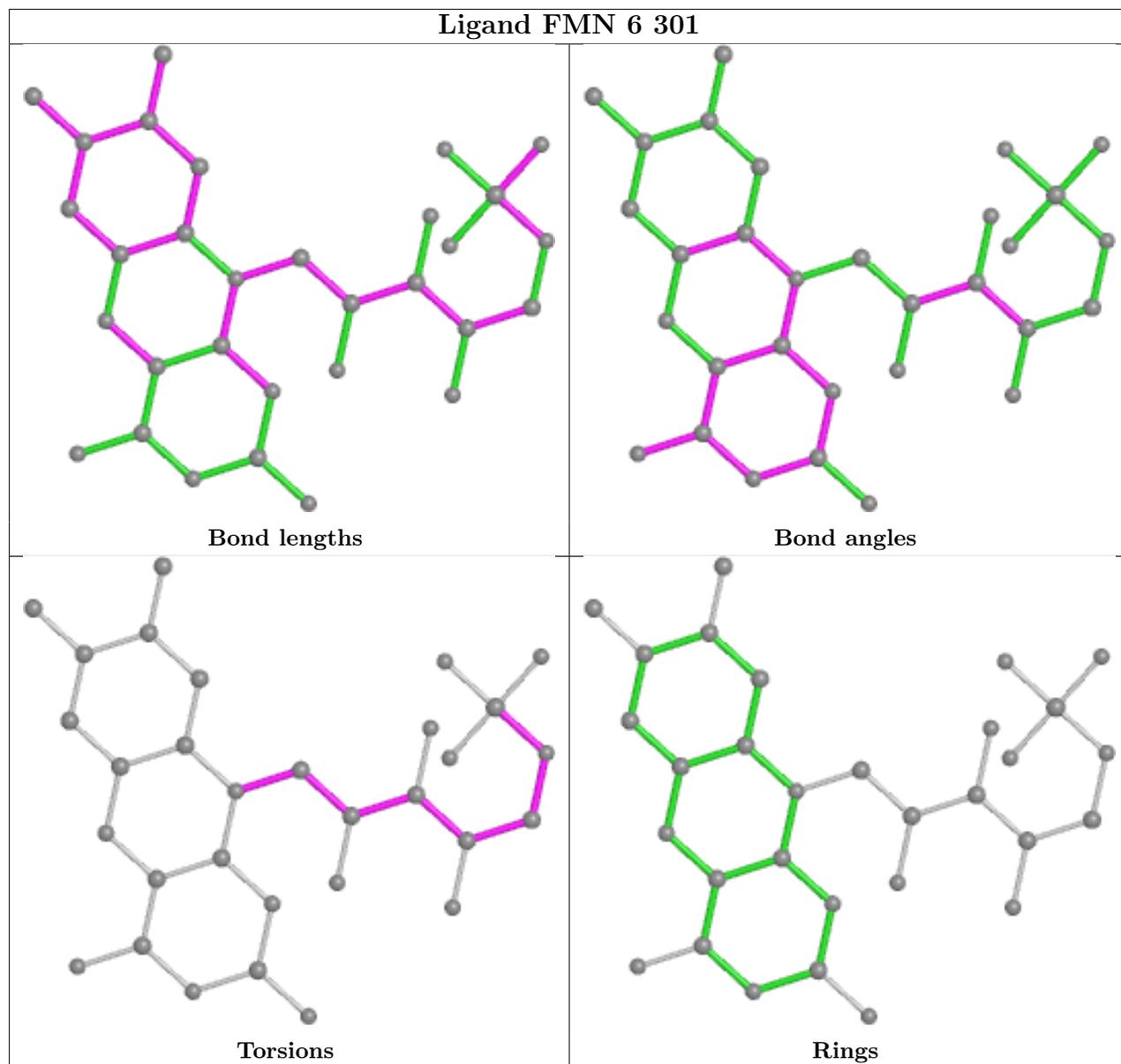


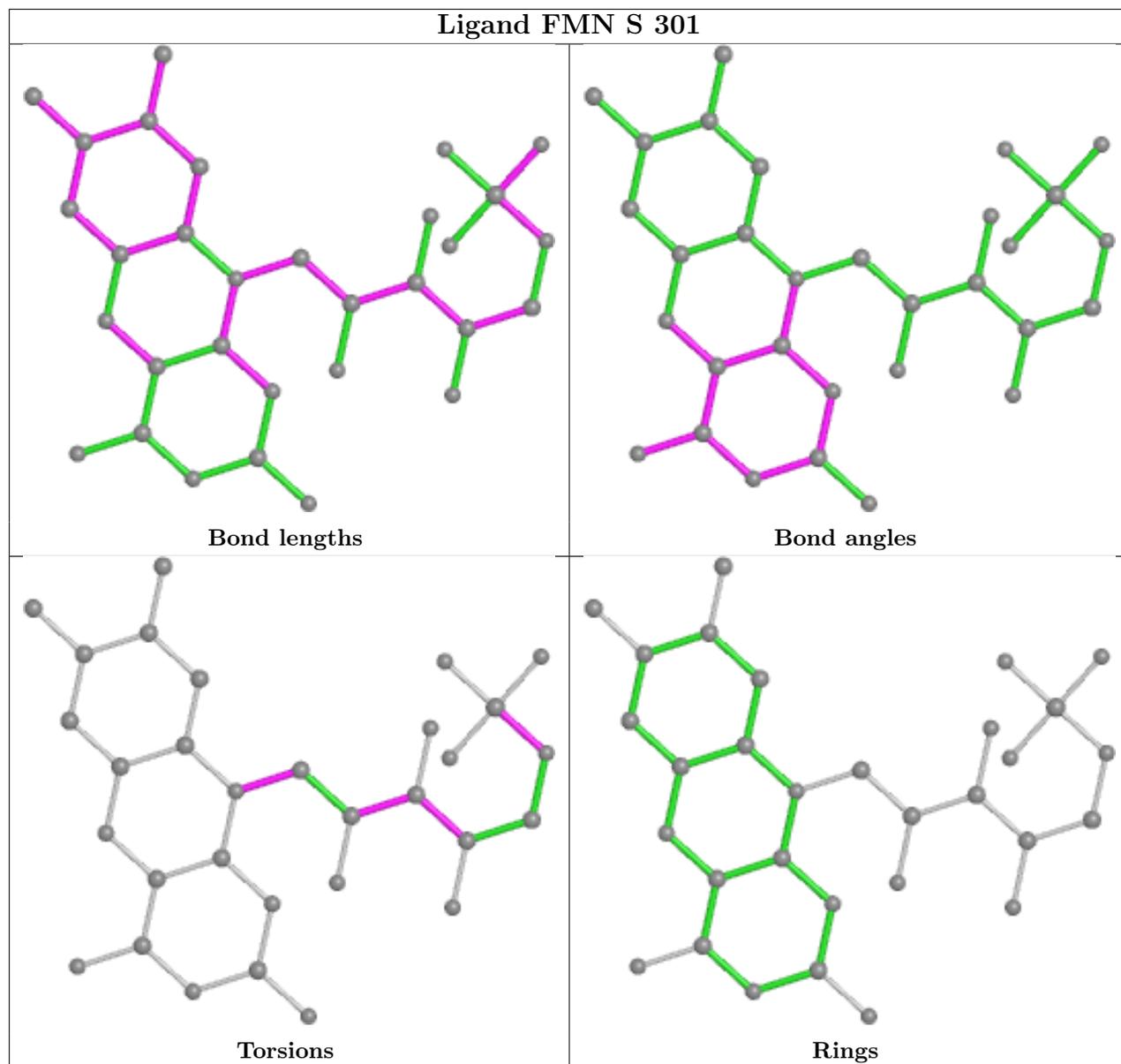


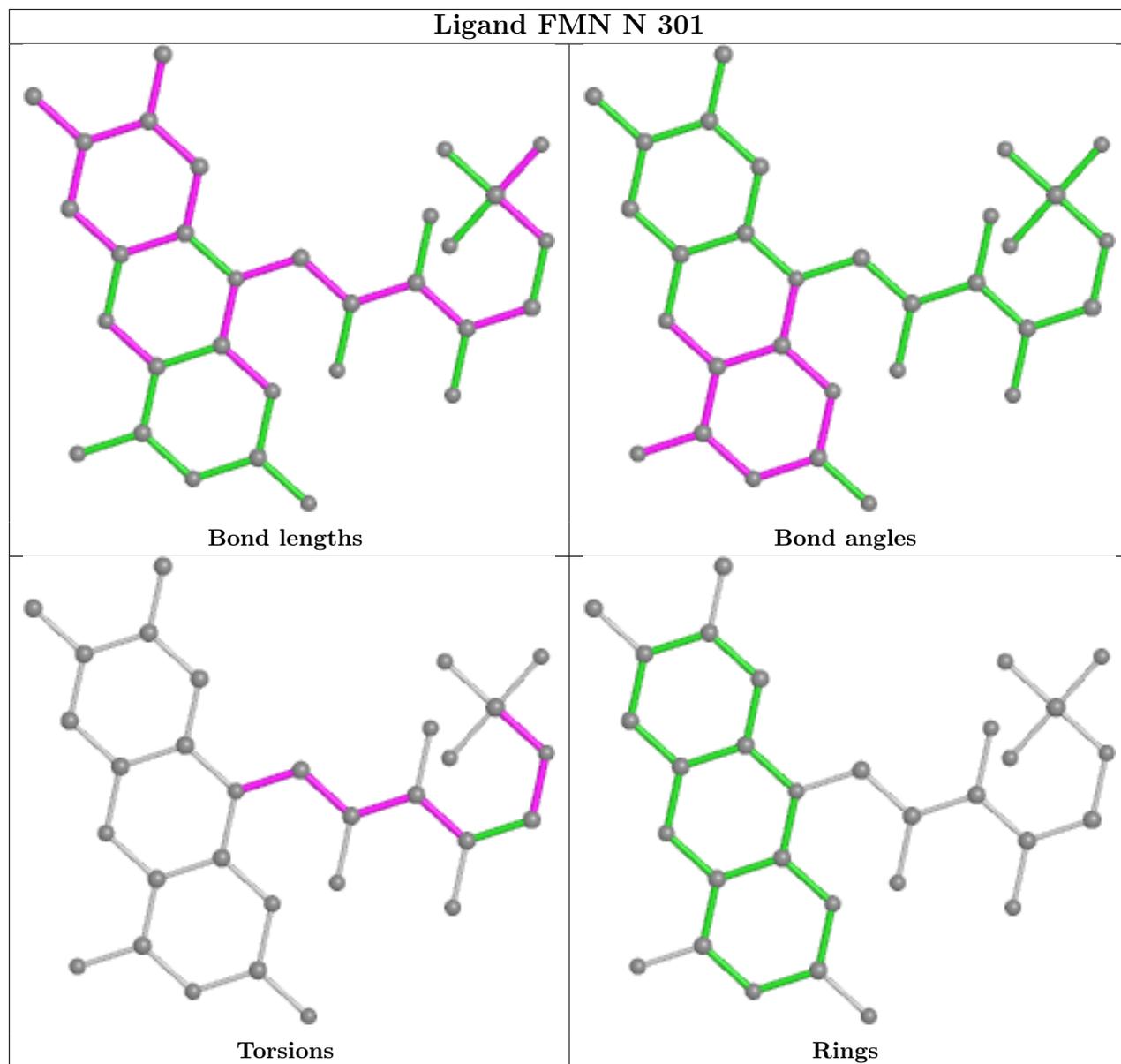


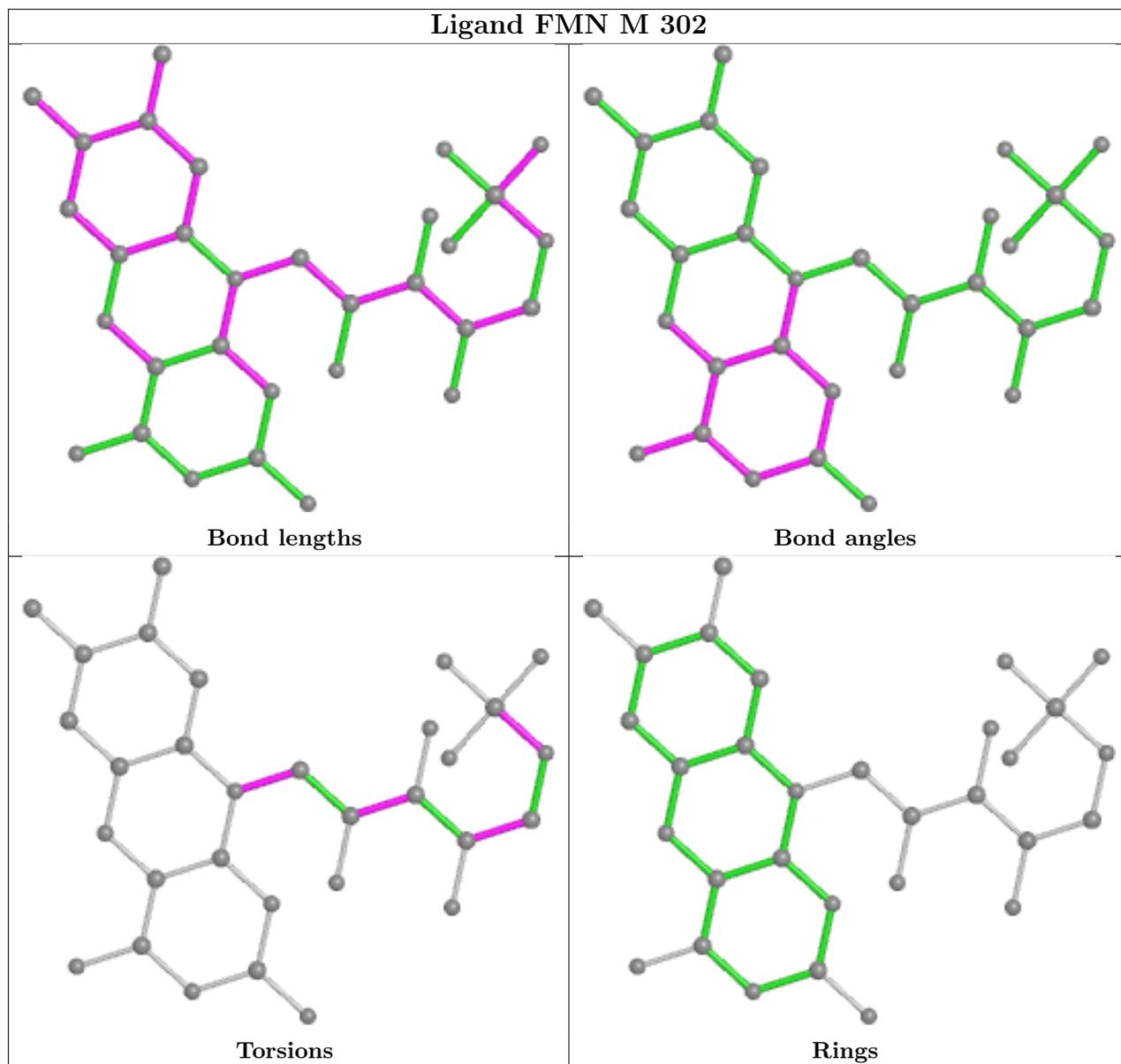


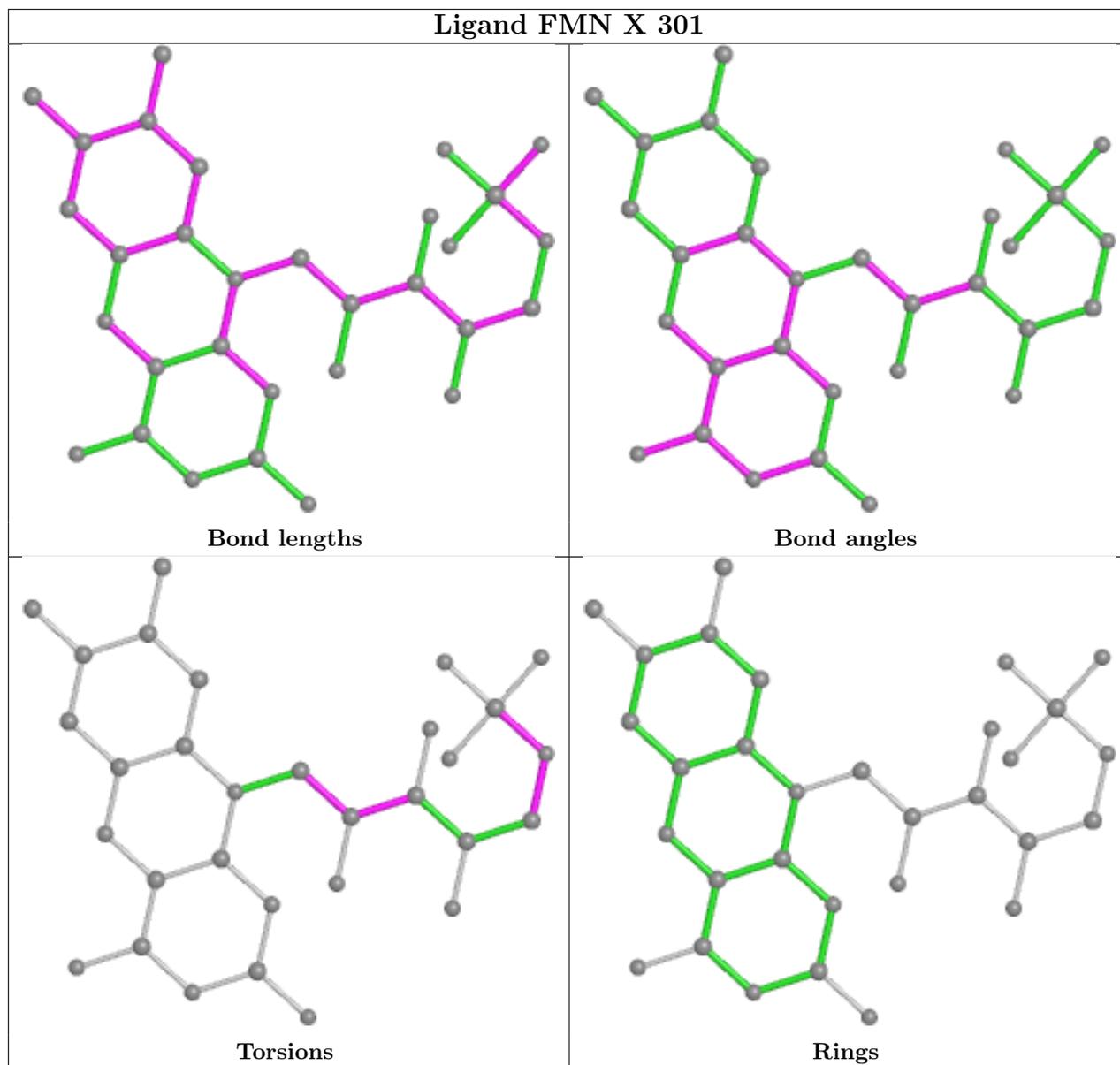


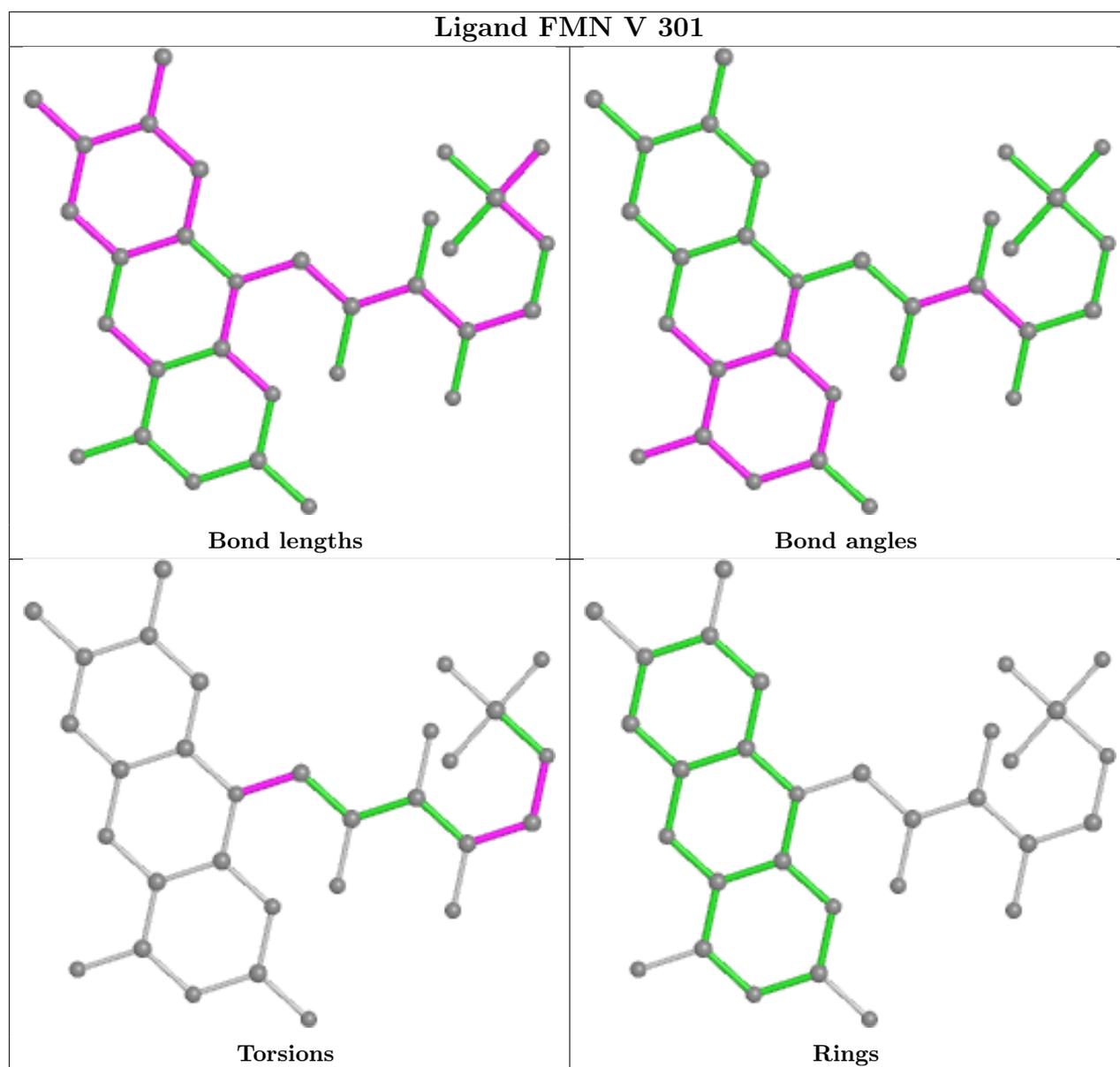












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

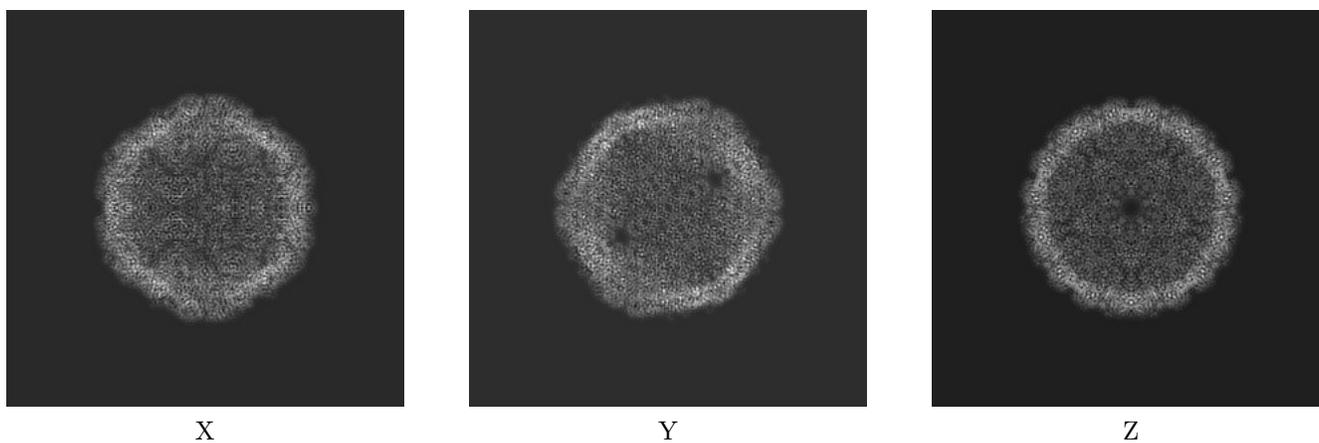
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21810. 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](#)

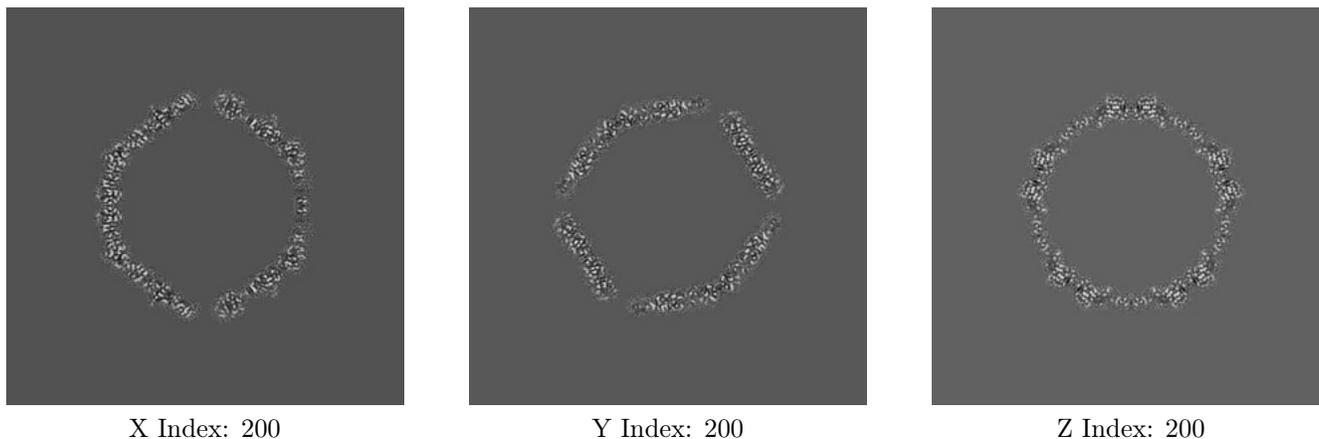
6.1.1 Primary map



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

6.2 Central slices [i](#)

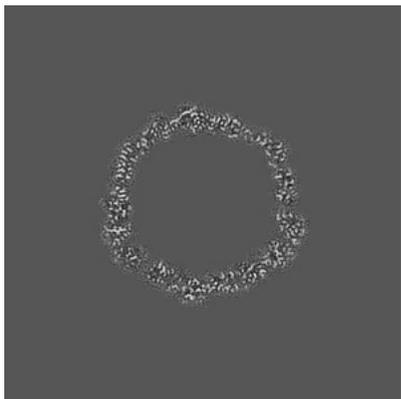
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

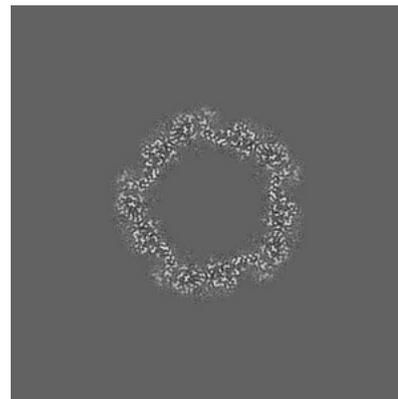
6.3.1 Primary map



X Index: 153



Y Index: 222

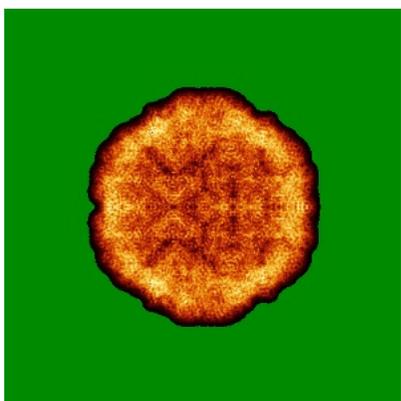


Z Index: 136

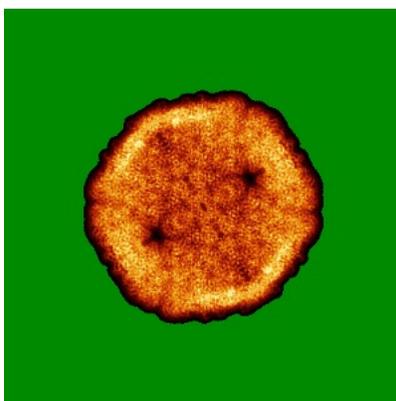
The images above show the largest variance slices of the map in three orthogonal directions.

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

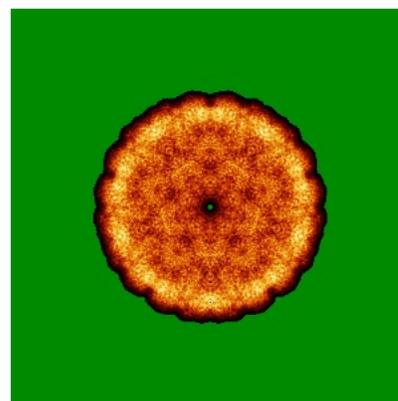
6.4.1 Primary map



X



Y

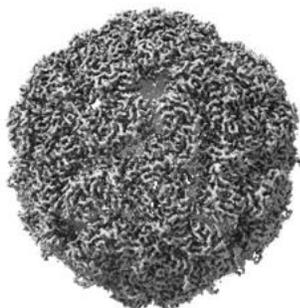


Z

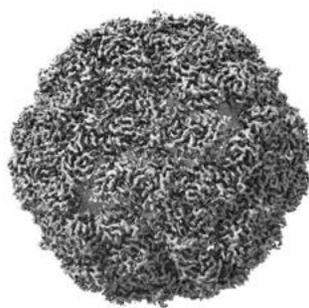
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

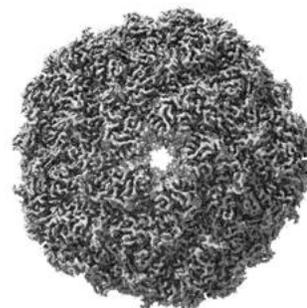
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

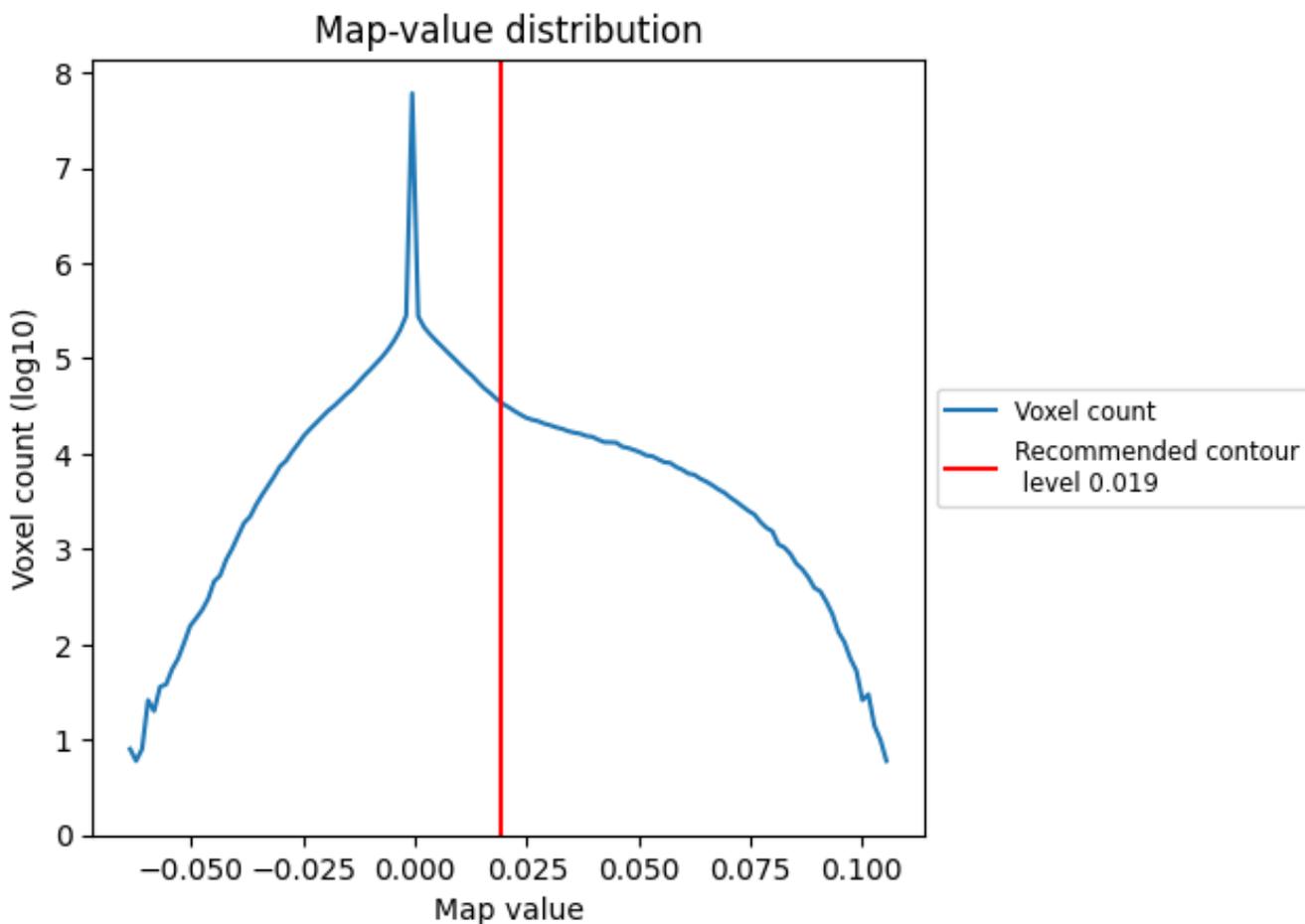
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

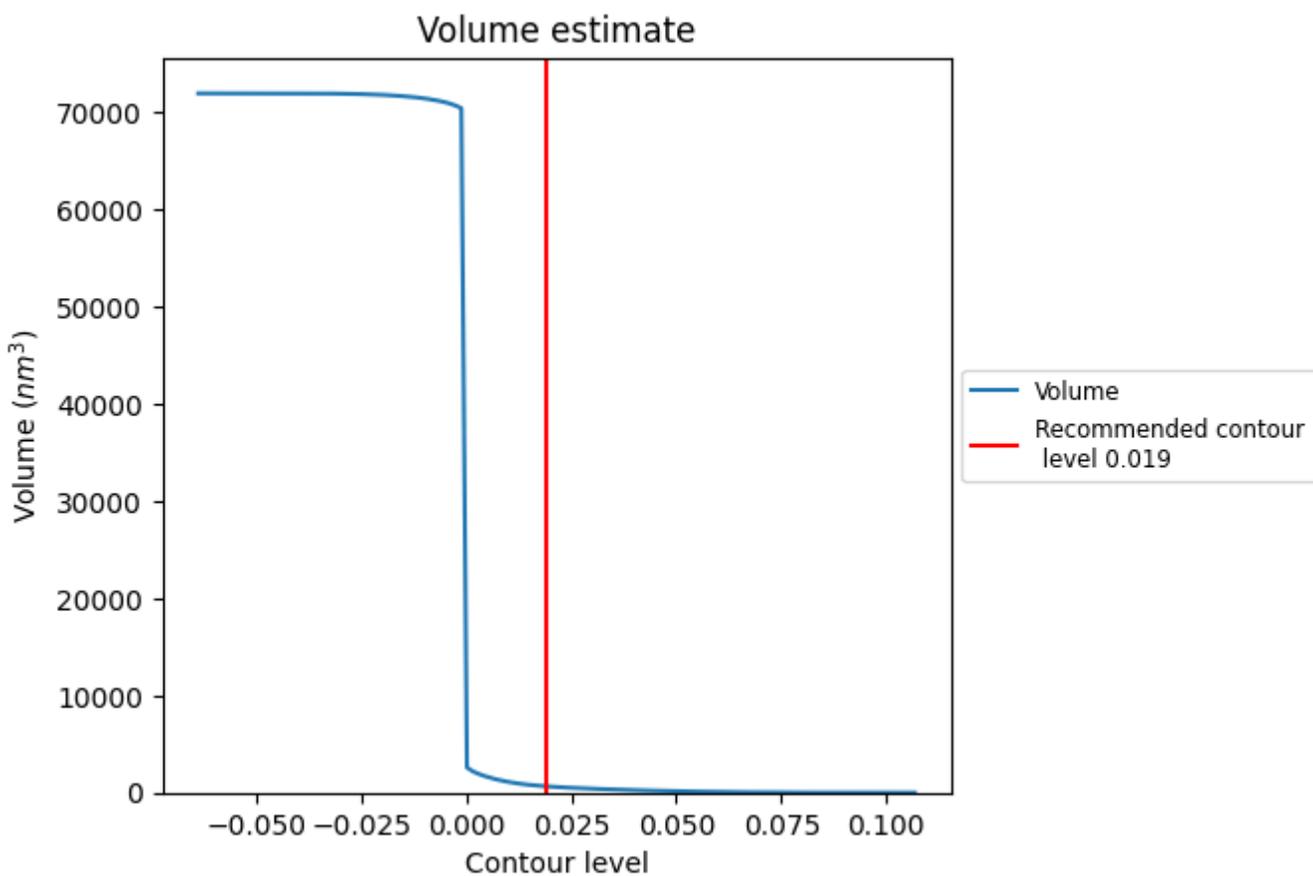
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

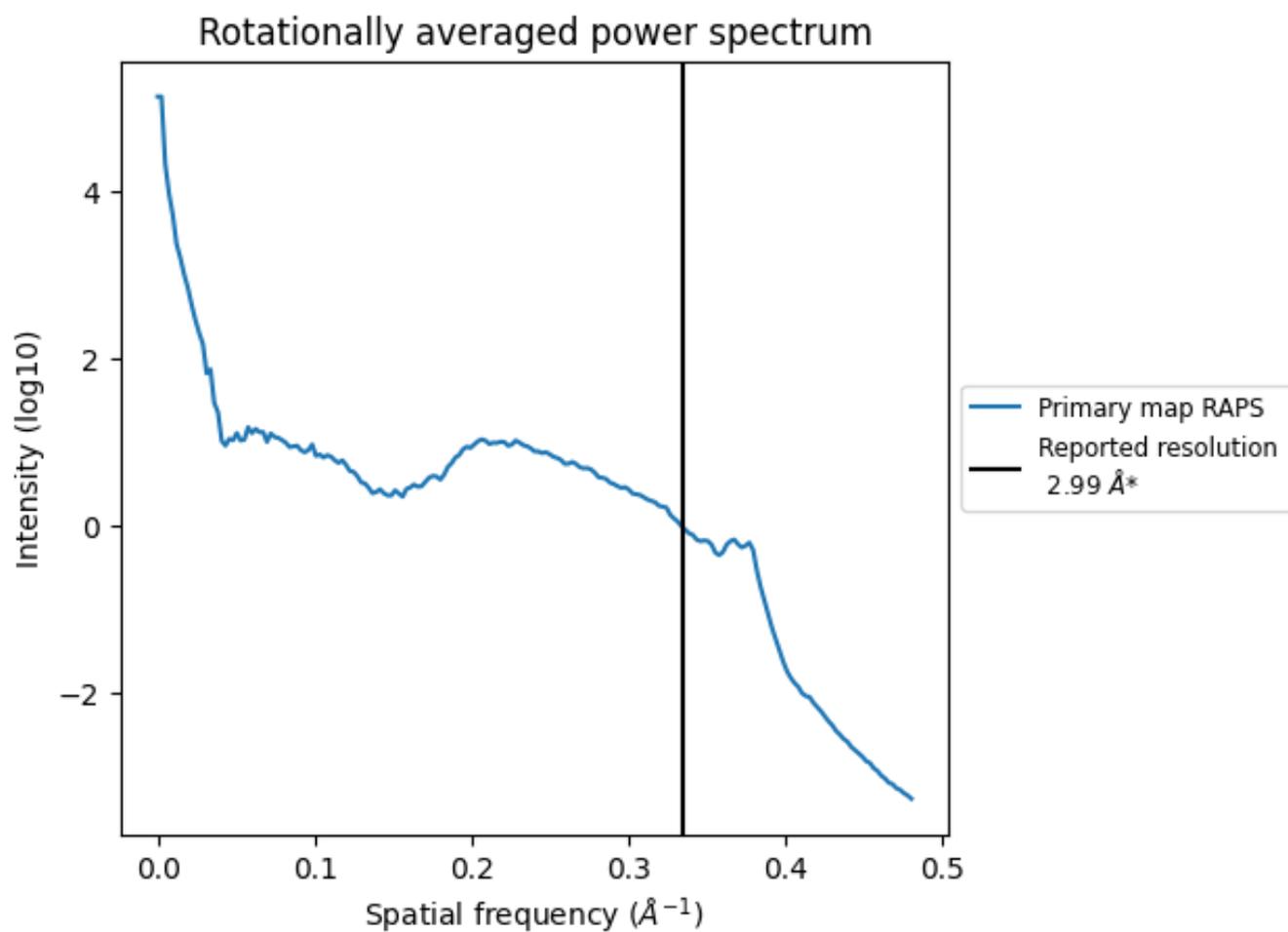
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 649 nm³; this corresponds to an approximate mass of 586 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

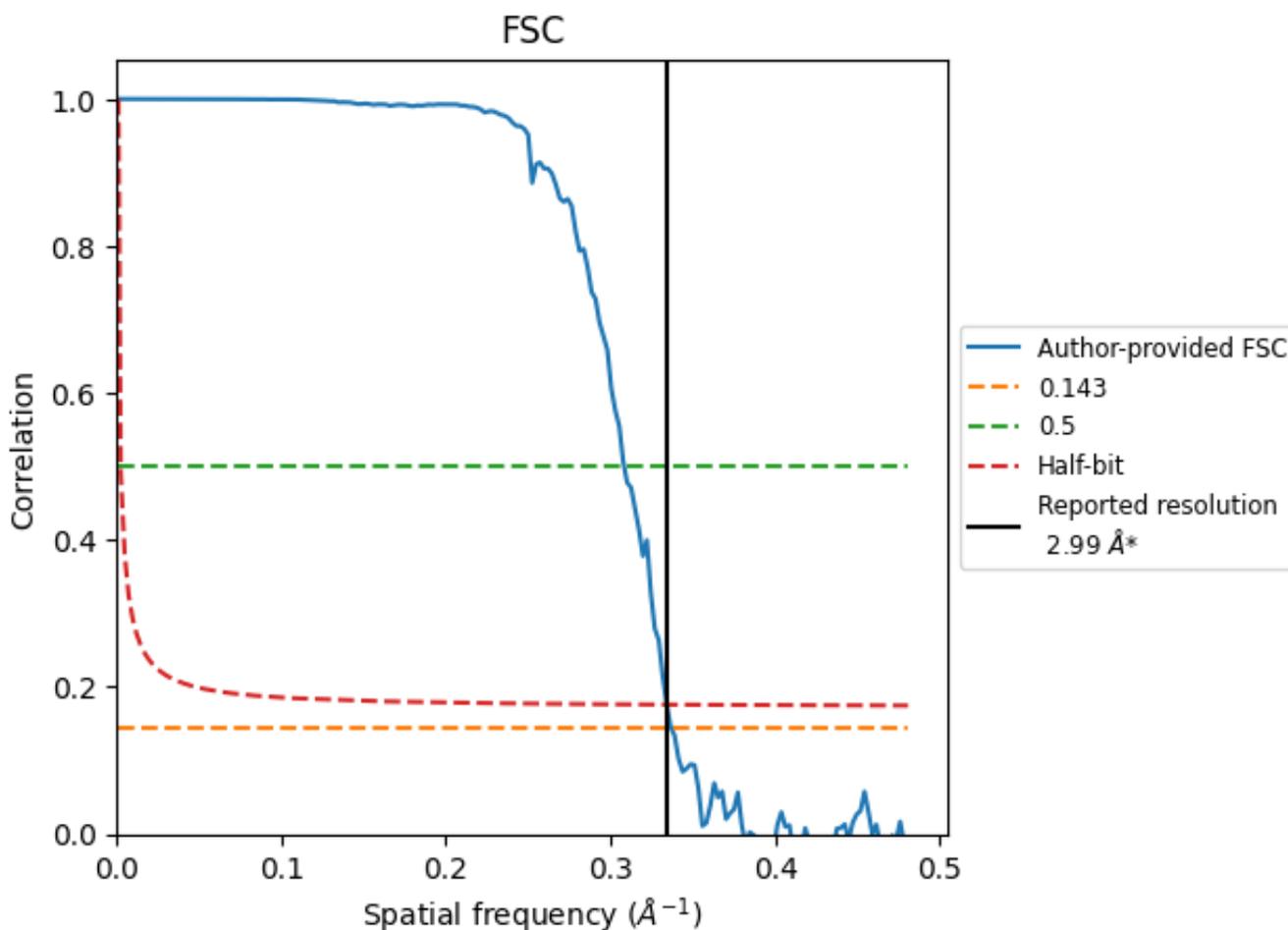


*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

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

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

8.2 Resolution estimates [i](#)

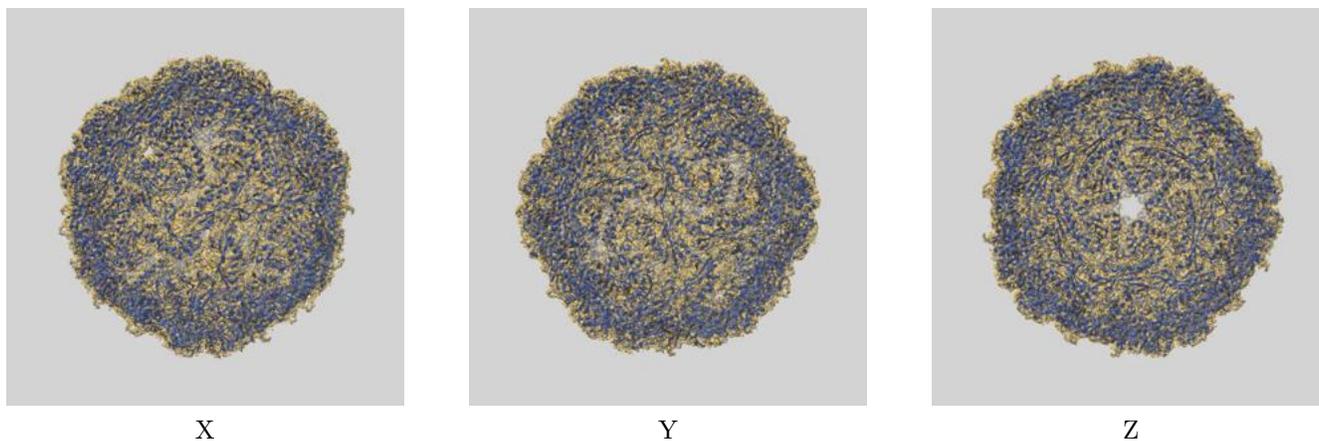
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.99 | - | - |
| Author-provided FSC curve | 2.97 | 3.24 | 2.99 |
| Unmasked-calculated* | - | - | - |

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

9 Map-model fit [i](#)

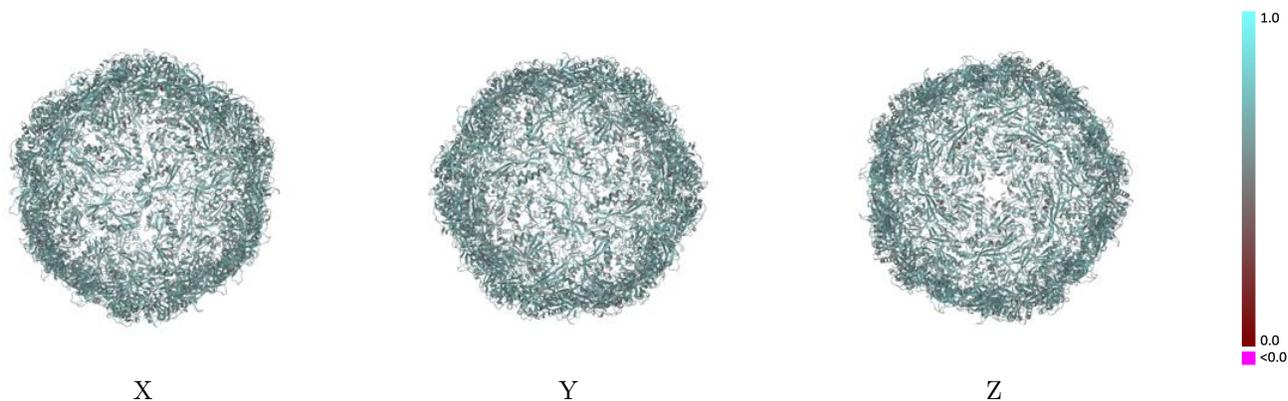
This section contains information regarding the fit between EMDB map EMD-21810 and PDB model 6WKV. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



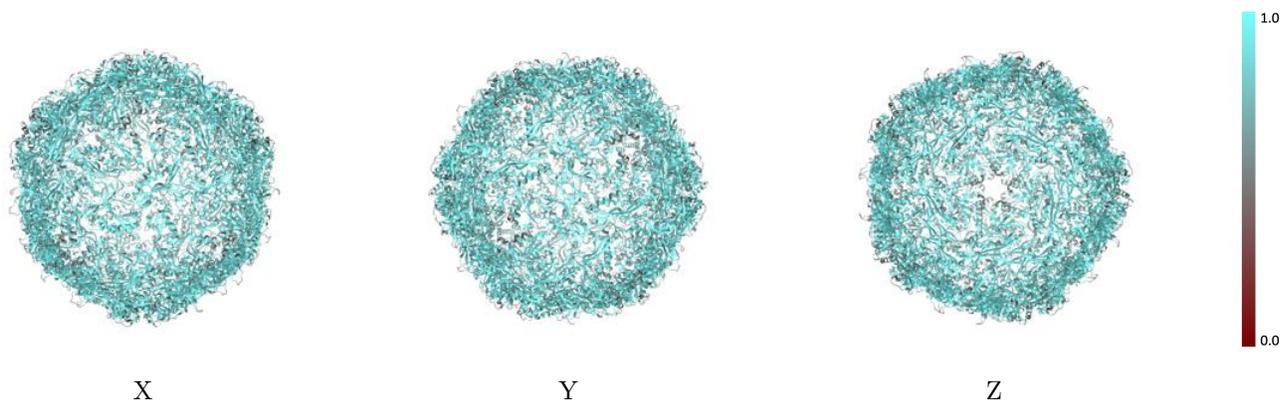
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



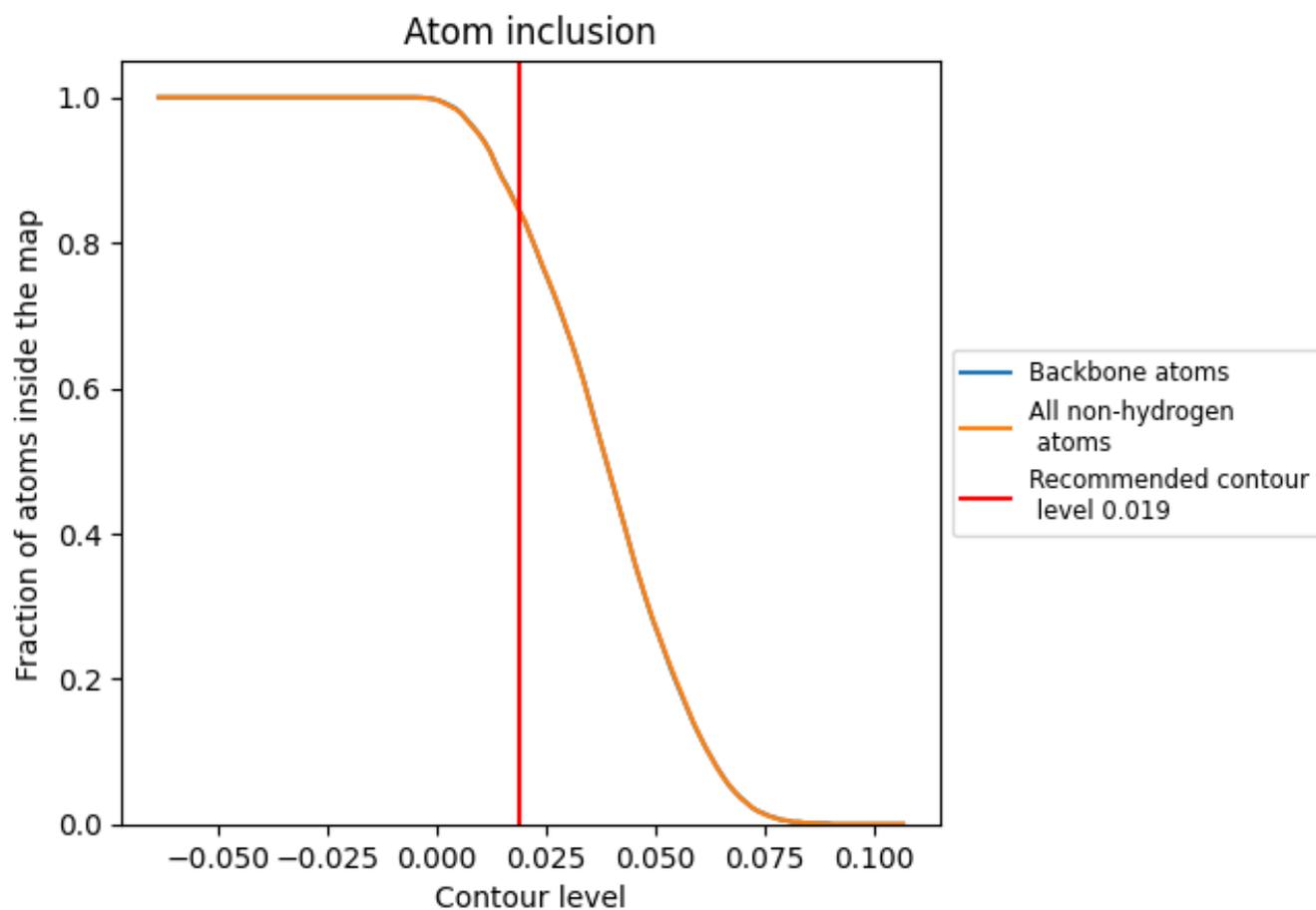
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.019) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8420 |  0.6110 |
| 0 |  0.8450 |  0.6080 |
| 1 |  0.8420 |  0.6100 |
| 2 |  0.8430 |  0.6110 |
| 3 |  0.8430 |  0.6100 |
| 4 |  0.8410 |  0.6120 |
| 5 |  0.8420 |  0.6100 |
| 6 |  0.8440 |  0.6100 |
| 7 |  0.8430 |  0.6100 |
| 8 |  0.8490 |  0.6110 |
| 9 |  0.8490 |  0.6130 |
| A |  0.8450 |  0.6100 |
| B |  0.8450 |  0.6100 |
| C |  0.8450 |  0.6110 |
| D |  0.8410 |  0.6090 |
| E |  0.8430 |  0.6090 |
| F |  0.8420 |  0.6090 |
| G |  0.8430 |  0.6120 |
| H |  0.8530 |  0.6130 |
| I |  0.8450 |  0.6100 |
| J |  0.8420 |  0.6110 |
| K |  0.8510 |  0.6120 |
| L |  0.8460 |  0.6120 |
| M |  0.8420 |  0.6090 |
| N |  0.8440 |  0.6120 |
| O |  0.8480 |  0.6120 |
| P |  0.8510 |  0.6110 |
| Q |  0.8450 |  0.6110 |
| R |  0.8450 |  0.6130 |
| S |  0.8450 |  0.6120 |
| T |  0.8430 |  0.6110 |
| U |  0.8470 |  0.6120 |
| V |  0.8410 |  0.6100 |
| W |  0.8470 |  0.6110 |
| X |  0.8490 |  0.6110 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Y |  0.8440 |  0.6110 |
| Z |  0.8470 |  0.6140 |
| a |  0.8380 |  0.6090 |
| b |  0.8540 |  0.6120 |
| c |  0.8450 |  0.6110 |
| d |  0.8440 |  0.6100 |
| e |  0.8450 |  0.6110 |
| f |  0.8420 |  0.6110 |
| g |  0.8480 |  0.6110 |
| h |  0.8430 |  0.6080 |
| i |  0.8450 |  0.6110 |
| j |  0.8430 |  0.6100 |
| k |  0.8420 |  0.6100 |
| l |  0.8480 |  0.6100 |
| m |  0.8420 |  0.6090 |
| n |  0.8460 |  0.6120 |
| o |  0.8480 |  0.6120 |
| p |  0.8400 |  0.6090 |
| q |  0.8450 |  0.6110 |
| r |  0.8440 |  0.6080 |
| s |  0.8450 |  0.6100 |
| t |  0.8470 |  0.6110 |
| u |  0.8470 |  0.6100 |
| v |  0.8460 |  0.6140 |
| w |  0.8430 |  0.6090 |
| x |  0.8430 |  0.6120 |