



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 05:52 pm BST

PDB ID : 6ZKN / pdb_00006zkn
EMDB ID : EMD-11255
Title : Complex I inhibited by rotenone, open3
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 2.90 Å(reported)
Based on initial model : 5LNK

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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

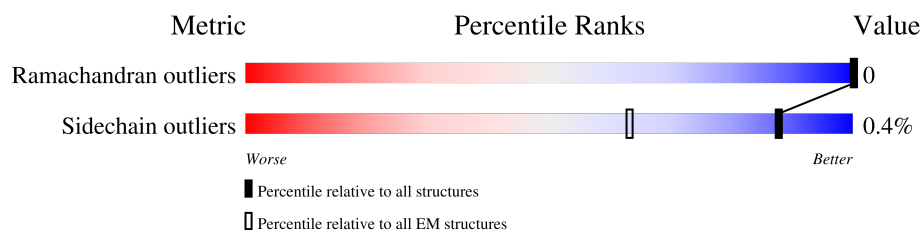
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


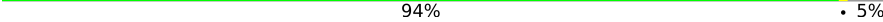




The reported resolution of this entry is 2.90 Å.

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.



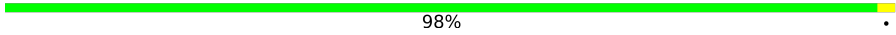

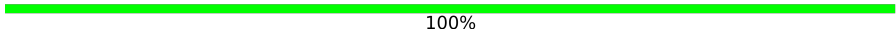
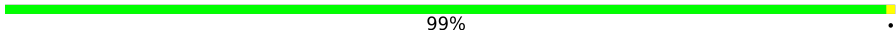




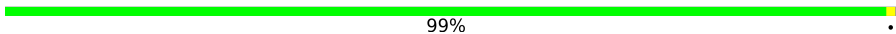
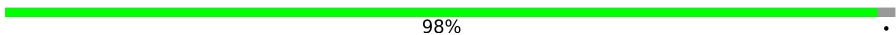





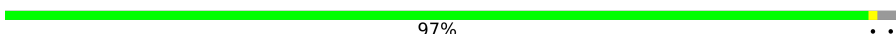


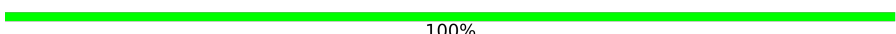

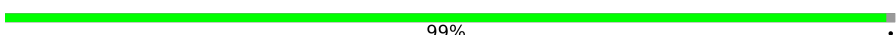
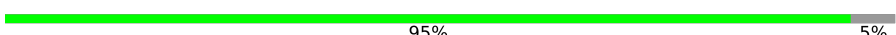

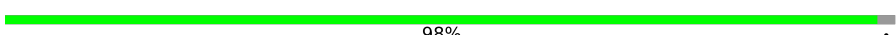
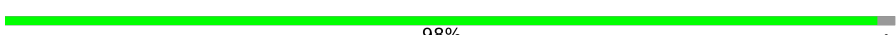
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 1 | 464 |  92% 7% |
| 2 | 2 | 246 |  86% 13% |
| 3 | 3 | 727 |  94% • 5% |
| 4 | 4 | 463 |  91% • 8% |
| 5 | 5 | 266 |  78% 22% |
| 6 | 6 | 223 |  68% • 30% |
| 7 | 9 | 217 |  81% 19% |
| 8 | A | 115 |  94% • • |
| 9 | H | 318 |  97% • • |
| 10 | J | 175 |  95% • 5% |

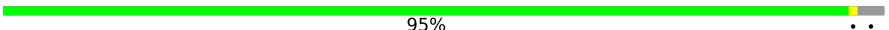


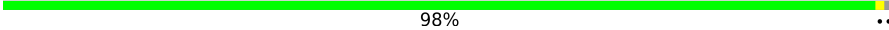




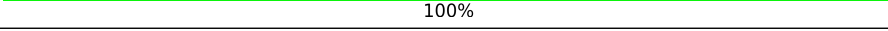
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 11 | K | 98 |  |
| 12 | L | 606 |  |
| 13 | M | 459 |  |
| 14 | N | 347 |  |
| 15 | V | 141 |  |
| 16 | W | 189 |  |
| 17 | X | 157 |  |
| 17 | j | 157 |  |
| 18 | Y | 172 |  |
| 19 | Z | 175 |  |
| 20 | a | 109 |  |
| 21 | b | 124 |  |
| 22 | c | 170 |  |
| 23 | d | 380 |  |
| 24 | e | 99 |  |
| 25 | f | 116 |  |
| 26 | g | 140 |  |
| 27 | h | 114 |  |
| 28 | i | 145 |  |
| 29 | k | 355 |  |
| 30 | l | 106 |  |
| 31 | m | 84 |  |
| 32 | n | 98 |  |
| 33 | o | 122 |  |
| 34 | p | 130 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 35 | q | 144 |  95% .. |
| 36 | r | 128 |  77% 23% |
| 37 | s | 137 |  88% . 11% |
| 38 | t | 179 |  98% .. |
| 39 | u | 108 |  60% 40% |
| 40 | v | 186 |  83% 17% |
| 41 | w | 154 |  65% . 34% |
| 42 | x | 76 |  64% 36% |
| 43 | y | 58 |  86% 14% |
| 44 | z | 70 |  100% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 50 | 970 | M | 601 | X | - | - | - |
| 53 | CDL | L | 1003 | X | - | - | - |
| 53 | CDL | o | 502 | X | - | - | - |
| 53 | CDL | y | 201 | X | - | - | - |

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 65955 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | 1 | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3312 | 2086 | 593 | 613 | 20 | | |

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | 2 | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1655 | 1058 | 278 | 309 | 10 | | |

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 3 | 3 | 688 | Total | C | N | O | S | 0 | 0 |
| | | | 5275 | 3301 | 922 | 1011 | 41 | | |

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | 4 | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3427 | 2188 | 590 | 624 | 25 | | |

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | 5 | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1726 | 1112 | 296 | 315 | 3 | | |

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6 | 6 | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1247 | 795 | 225 | 213 | 14 | | |

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7 | 9 | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1414 | 889 | 243 | 270 | 12 | | |

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | A | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 880 | 593 | 128 | 153 | 6 | | |

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | H | 314 | Total | C | N | O | S | 0 | 0 |
| | | | 2498 | 1685 | 380 | 414 | 19 | | |

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10 | J | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1273 | 856 | 182 | 222 | 13 | | |

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11 | K | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 749 | 490 | 112 | 132 | 15 | | |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | L | 558 | Total | C | N | O | S | 0 | 0 |
| | | | 4425 | 2935 | 689 | 759 | 42 | | |

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13 | M | 459 | Total | C | N | O | S | 0 | 0 |
| | | | 3647 | 2429 | 571 | 607 | 40 | | |

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | N | 347 | Total | C | N | O | S | 0 | 0 |
| | | | 2723 | 1808 | 416 | 459 | 40 | | |

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15 | V | 27 | Total | C | N | O | S | 0 | 0 |
| | | | 204 | 135 | 32 | 34 | 3 | | |

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | W | 139 | Total | C | N | O | S | 0 | 0 |
| | | | 1155 | 761 | 194 | 198 | 2 | | |

- Molecule 17 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | X | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 701 | 451 | 103 | 142 | 5 | | |
| 17 | j | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 660 | 425 | 98 | 132 | 5 | | |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18 | Y | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1403 | 889 | 253 | 251 | 10 | | |

- Molecule 19 is a protein called Mitochondrial complex I, PDSW subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | Z | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1441 | 905 | 266 | 262 | 8 | | |

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20 | a | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 371 | 233 | 66 | 71 | 1 | | |

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | b | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 737 | 451 | 139 | 144 | 3 | | |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | c | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1024 | 646 | 182 | 193 | 3 | | |

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23 | d | 297 | Total | C | N | O | S | 0 | 0 |
| | | | 2372 | 1516 | 432 | 419 | 5 | | |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | e | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 691 | 434 | 129 | 126 | 2 | | |

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | f | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 595 | 153 | 167 | 2 | | |

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | g | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 969 | 619 | 180 | 166 | 4 | | |

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | h | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 769 | 480 | 146 | 140 | 3 | | |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | i | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1209 | 778 | 216 | 210 | 5 | | |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|------|---------|-------|
| 29 | k | 320 | Total | C | N | O | P S | 0 | 0 |
| | | | 2596 | 1659 | 432 | 494 | 1 10 | | |

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | l | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 874 | 551 | 164 | 153 | 6 | | |

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | m | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 626 | 411 | 103 | 110 | 2 | | |

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | n | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 634 | 415 | 106 | 111 | 2 | | |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | o | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 1004 | 652 | 175 | 172 | 5 | | |

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | p | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1059 | 675 | 189 | 194 | 1 | | |

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | q | 139 | Total | C | N | O | S | 0 | 0 |
| | | | 1142 | 733 | 200 | 200 | 9 | | |

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | r | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 846 | 554 | 149 | 142 | 1 | | |

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | s | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 1047 | 653 | 199 | 186 | 9 | | |

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | t | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1520 | 973 | 279 | 262 | 6 | | |

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39 | u | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 563 | 372 | 93 | 97 | 1 | | |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | v | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1307 | 846 | 213 | 239 | 9 | | |

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | w | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 846 | 542 | 140 | 160 | 4 | | |

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 42 | x | 49 | Total | C | N | O | 0 | 0 |
| | | | 412 | 271 | 70 | 71 | | |

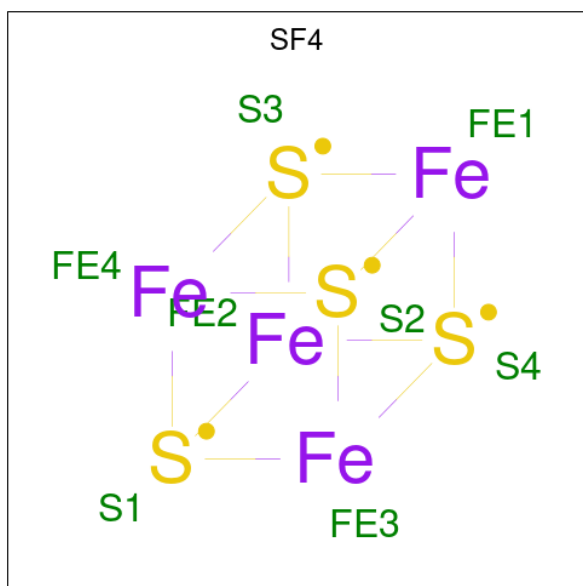
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 43 | y | 50 | Total | C | N | O | 0 | 0 |
| | | | 436 | 287 | 77 | 72 | | |

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 44 | z | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 576 | 369 | 106 | 96 | 5 | | |

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45 | 1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | 3 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | 3 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | 6 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

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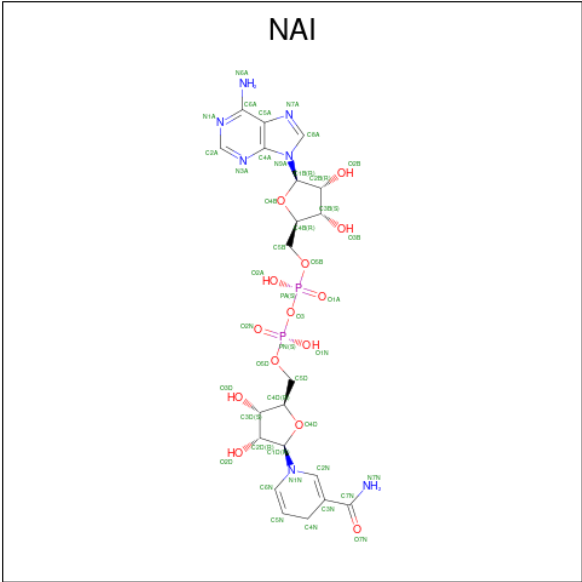
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45 | 9 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | 9 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



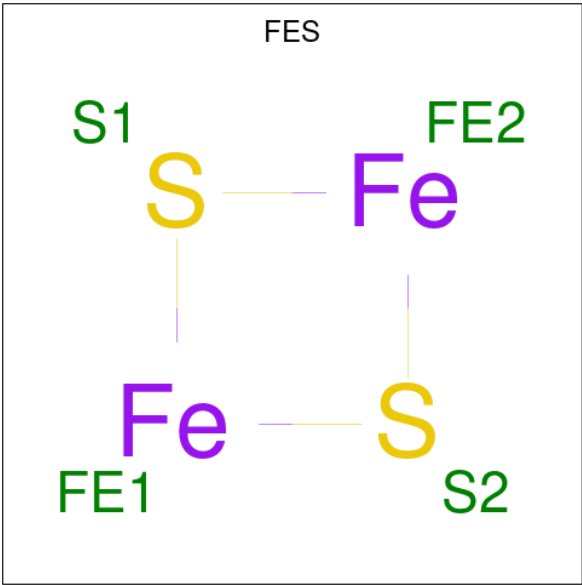
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 47 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | |

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

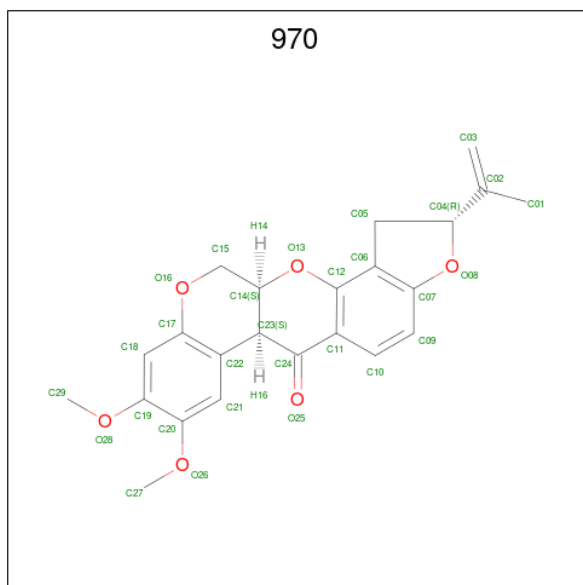


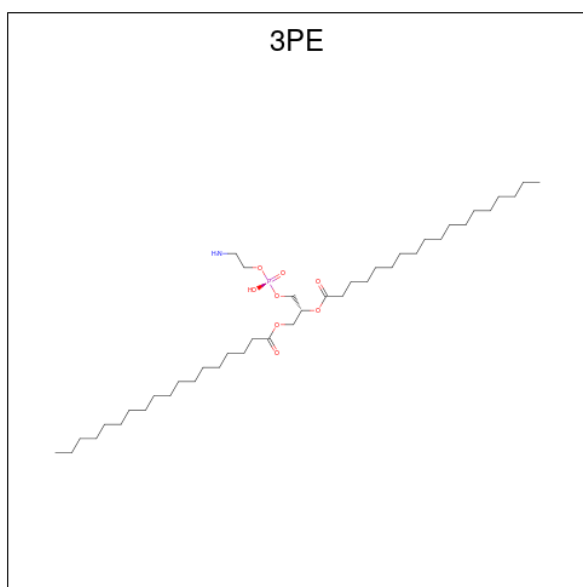
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 48 | 2 | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 48 | 3 | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|----------------|---------|
| 49 | 3 | 1 | Total K 1 1 | 0 |

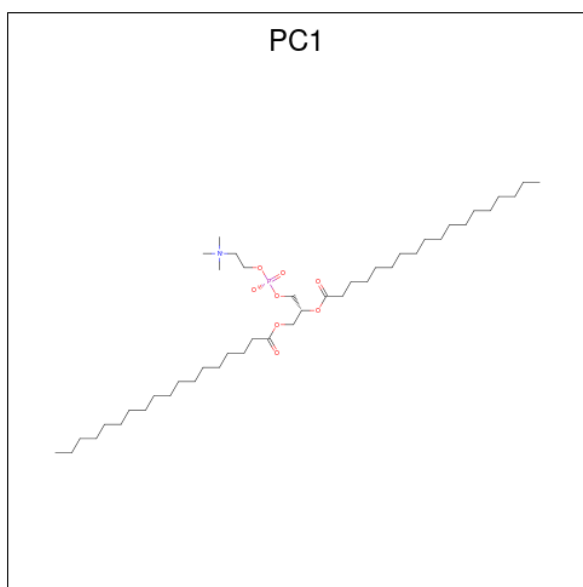
- Molecule 50 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).





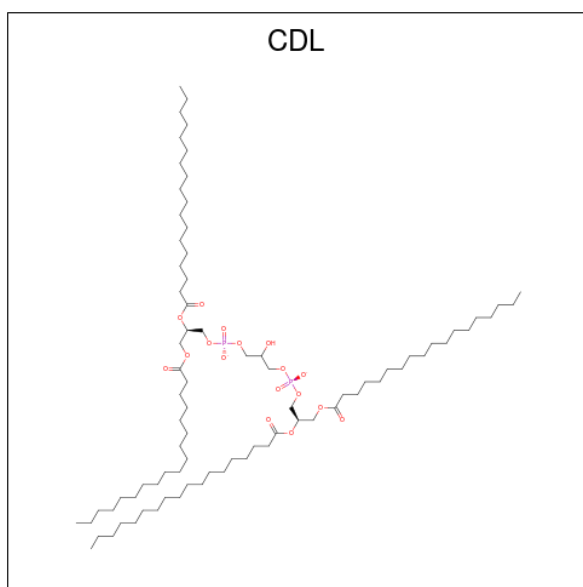
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 51 | 6 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 51 | A | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 51 | H | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 51 | L | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 51 | L | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 51 | M | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 51 | N | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 51 | i | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 51 | o | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



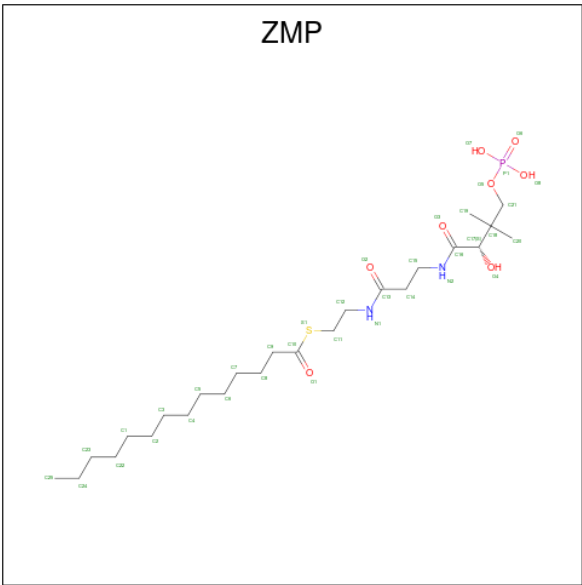
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 52 | 9 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 52 | A | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 52 | A | 1 | Total | C | N | O | P | 0 |
| | | | 37 | 27 | 1 | 8 | 1 | |
| 52 | L | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 52 | M | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 52 | w | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 53 | L | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 53 | W | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 53 | h | 1 | Total | C | O | P | 0 |
| | | | 58 | 39 | 17 | 2 | |
| 53 | o | 1 | Total | C | O | P | 0 |
| | | | 75 | 56 | 17 | 2 | |
| 53 | o | 1 | Total | C | O | P | 0 |
| | | | 90 | 71 | 17 | 2 | |
| 53 | y | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

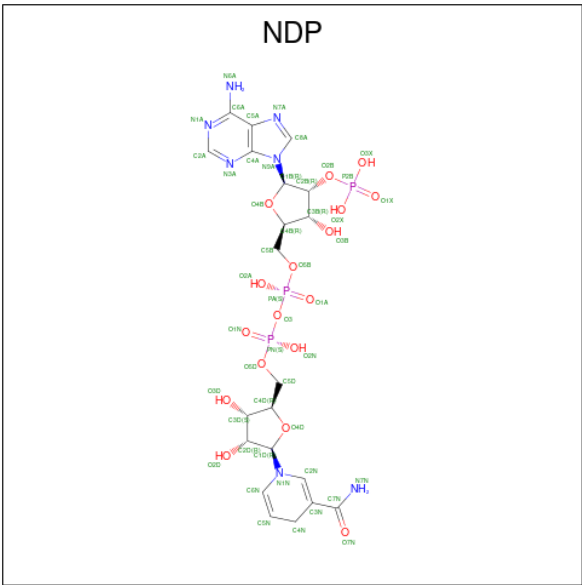


| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 54 | X | 1 | Total | C | N | O | P | S | 0 |
| | | | 31 | 20 | 2 | 7 | 1 | 1 | |
| 54 | g | 1 | Total | C | N | O | P | S | 0 |
| | | | 34 | 23 | 2 | 7 | 1 | 1 | |

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

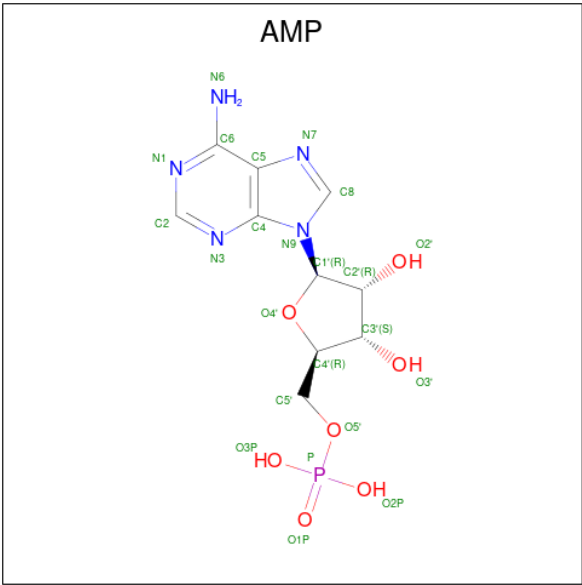
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 55 | b | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



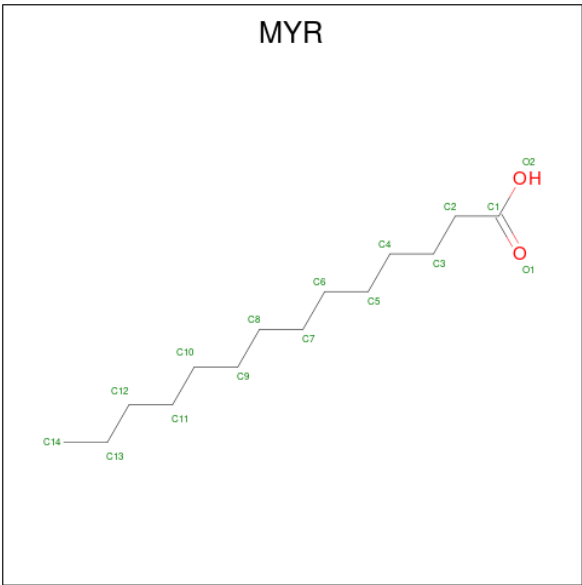
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 56 | d | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 57 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 57 | k | 1 | Total | C | N | O | P | 0 |
| | | | 23 | 10 | 5 | 7 | 1 | |

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



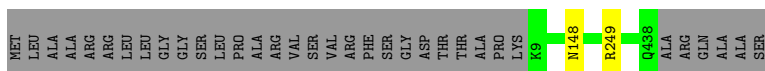
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 58 | s | 1 | Total | C | O | 0 |
| | | | 15 | 14 | 1 | |

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

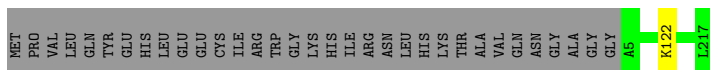
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:  92% 7%



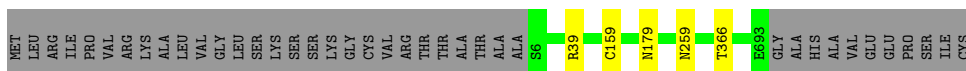
- Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2:  86% 13%




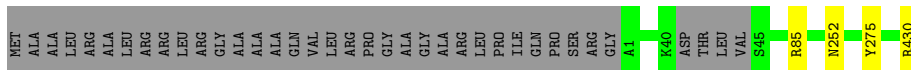
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain 3:  94% 5%



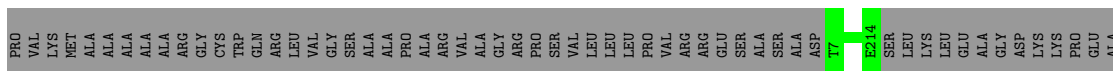
- Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:  91% 8%



- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

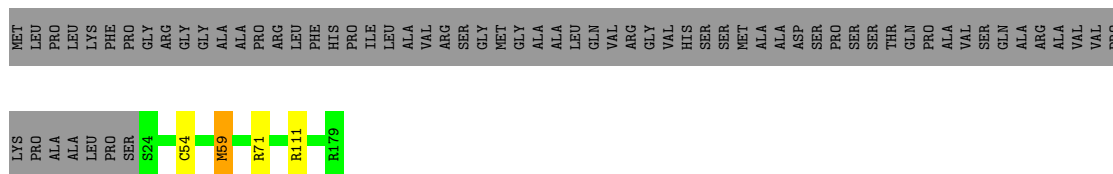
Chain 5:  78% 22%




LYS

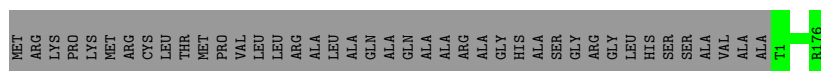
- Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6:  68% 30%



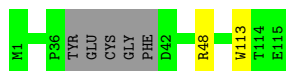
- Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:  81% 19%



- Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain A:  94%



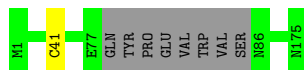
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H:  97%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  95% 5%




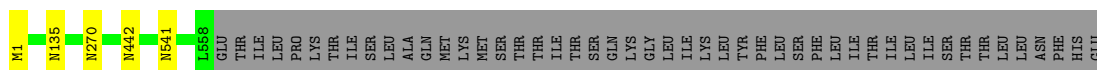
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  98%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

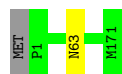
Chain L:  91% 8%



- | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|
| ARG | VAL | THR | PRO | LEU | CYS | ARG | GLN | TYR | SER | ASP | ALA | PRO | P5 | V86 | TYR | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|

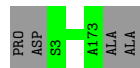
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:  99%



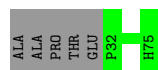
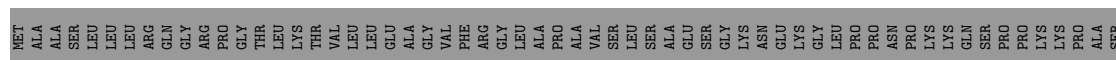
- Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:  98%



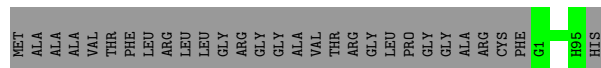
- Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:  40%



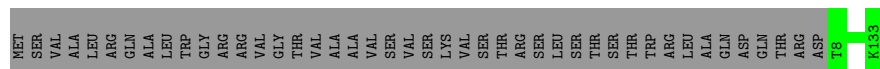
- Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:  77%




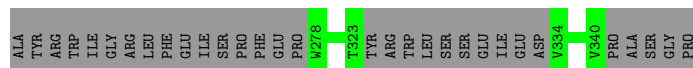
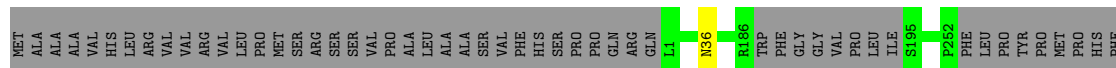
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:  74%




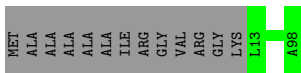
- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d:  78%



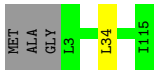
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e:  87% 13%




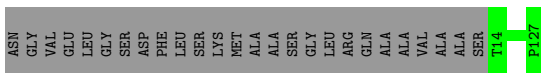
- Molecule 25: Mitochondrial complex I, B13 subunit

Chain f:  97% ..




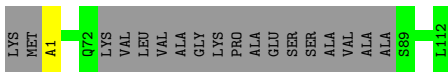
- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g:  81% 19%



- Molecule 27: Mitochondrial complex I, B14.5a subunit

Chain h:  83% 16%



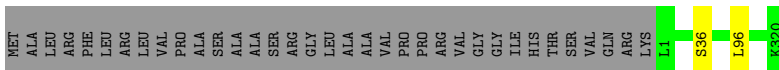
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:  90% 10%



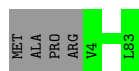
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

Chain l:  99% .



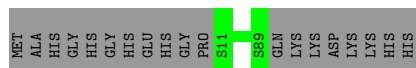
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain m:  95% 5%



- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n: 81% 19%



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o: 98% .



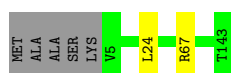
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain p: 98% .



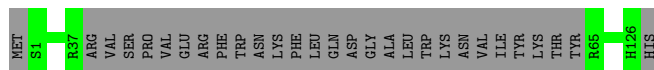
- Molecule 35: Mitochondrial complex I, B16.6 subunit

Chain q: 95% ..



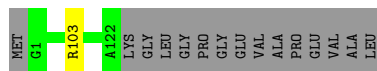
- Molecule 36: Mitochondrial complex I, B17 subunit

Chain r: 77% 23%



- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

Chain s: 88% . 11%



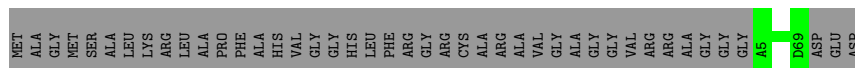
- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain t: 98% ..



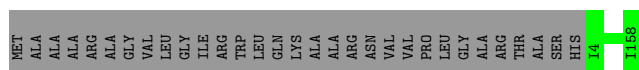
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain u: 60% 40%



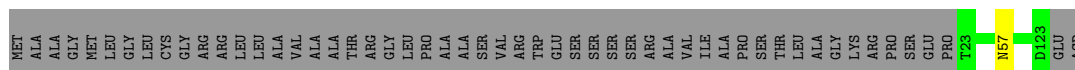
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v: 83% 17%



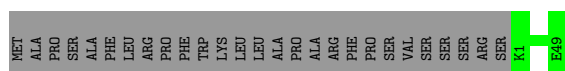
- Molecule 41: Mitochondrial complex I, ESSS subunit

Chain w: 65% . 34%



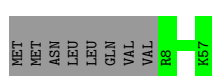
- Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x: 64% 36%



- Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y: 86% 14%



- Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 55837 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 100 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, 3PE, SEP, MYR, 2MR, K, 970, AMP, CDL, ZN, FME, ZMP, NDP, PC1, SF4, FMN, NAI, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 1 | 0.40 | 0/3386 | 0.57 | 0/4575 |
| 2 | 2 | 0.37 | 0/1695 | 0.57 | 0/2306 |
| 3 | 3 | 0.41 | 1/5362 (0.0%) | 0.57 | 0/7266 |
| 4 | 4 | 0.43 | 0/3504 | 0.58 | 0/4746 |
| 5 | 5 | 0.40 | 0/1776 | 0.56 | 0/2417 |
| 6 | 6 | 0.49 | 0/1278 | 0.60 | 1/1728 (0.1%) |
| 7 | 9 | 0.48 | 0/1445 | 0.61 | 0/1956 |
| 8 | A | 0.35 | 0/902 | 0.64 | 0/1234 |
| 9 | H | 0.42 | 0/2572 | 0.66 | 1/3517 (0.0%) |
| 10 | J | 0.40 | 1/1302 (0.1%) | 0.59 | 0/1760 |
| 11 | K | 0.37 | 0/749 | 0.66 | 0/1014 |
| 12 | L | 0.34 | 0/4537 | 0.55 | 0/6176 |
| 13 | M | 0.36 | 0/3731 | 0.61 | 0/5085 |
| 14 | N | 0.38 | 0/2787 | 0.61 | 1/3795 (0.0%) |
| 15 | V | 0.28 | 0/208 | 0.44 | 0/279 |
| 16 | W | 0.34 | 0/1188 | 0.51 | 0/1607 |
| 17 | X | 0.30 | 0/713 | 0.49 | 0/963 |
| 17 | j | 0.32 | 0/670 | 0.52 | 0/902 |
| 18 | Y | 0.37 | 0/1440 | 0.53 | 0/1942 |
| 19 | Z | 0.32 | 0/1475 | 0.48 | 0/1989 |
| 20 | a | 0.30 | 0/383 | 0.51 | 0/518 |
| 21 | b | 0.39 | 0/749 | 0.51 | 0/1009 |
| 22 | c | 0.36 | 0/1047 | 0.53 | 0/1415 |
| 23 | d | 0.35 | 0/2424 | 0.54 | 0/3276 |
| 24 | e | 0.31 | 0/702 | 0.53 | 0/945 |
| 25 | f | 0.33 | 0/937 | 0.54 | 1/1271 (0.1%) |
| 26 | g | 0.36 | 0/993 | 0.54 | 0/1336 |
| 27 | h | 0.38 | 0/779 | 0.55 | 0/1053 |
| 28 | i | 0.40 | 0/1250 | 0.52 | 0/1698 |
| 29 | k | 0.31 | 0/2646 | 0.49 | 1/3579 (0.0%) |
| 30 | l | 0.35 | 0/896 | 0.52 | 0/1200 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 31 | m | 0.32 | 0/647 | 0.53 | 0/890 |
| 32 | n | 0.29 | 0/653 | 0.45 | 0/882 |
| 33 | o | 0.36 | 0/1035 | 0.49 | 0/1398 |
| 34 | p | 0.29 | 0/1085 | 0.48 | 0/1467 |
| 35 | q | 0.35 | 0/1171 | 0.50 | 0/1579 |
| 36 | r | 0.30 | 0/874 | 0.52 | 0/1188 |
| 37 | s | 0.29 | 0/1072 | 0.47 | 0/1436 |
| 38 | t | 0.29 | 0/1573 | 0.50 | 0/2130 |
| 39 | u | 0.28 | 0/590 | 0.46 | 0/810 |
| 40 | v | 0.29 | 0/1361 | 0.49 | 0/1861 |
| 41 | w | 0.35 | 0/872 | 0.53 | 0/1185 |
| 42 | x | 0.27 | 0/425 | 0.40 | 0/576 |
| 43 | y | 0.30 | 0/449 | 0.49 | 0/605 |
| 44 | z | 0.41 | 0/591 | 0.56 | 0/795 |
| All | All | 0.37 | 2/65924 (0.0%) | 0.55 | 5/89359 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | 3 | 0 | 2 |
| 4 | 4 | 0 | 1 |
| 8 | A | 0 | 1 |
| 35 | q | 0 | 1 |
| All | All | 0 | 5 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | 3 | 159 | CYS | CB-SG | -7.18 | 1.70 | 1.82 |
| 10 | J | 41 | CYS | CB-SG | -5.20 | 1.73 | 1.81 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6 | 6 | 59 | MET | CA-CB-CG | 6.18 | 123.81 | 113.30 |
| 14 | N | 146 | LEU | CA-CB-CG | 5.69 | 128.39 | 115.30 |
| 25 | f | 34 | LEU | CA-CB-CG | 5.24 | 127.36 | 115.30 |
| 29 | k | 96 | LEU | CA-CB-CG | 5.16 | 127.17 | 115.30 |
| 9 | H | 289 | LEU | CA-CB-CG | -5.09 | 103.58 | 115.30 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 3 | 3 | 259 | ASN | Peptide |
| 3 | 3 | 366 | THR | Peptide |
| 4 | 4 | 275 | TYR | Peptide |
| 8 | A | 113 | TRP | Peptide |
| 35 | q | 24 | LEU | Peptide |

5.2 Too-close contacts

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 | 1 | 428/464 (92%) | 409 (96%) | 19 (4%) | 0 | 100 | 100 |
| 2 | 2 | 211/246 (86%) | 197 (93%) | 14 (7%) | 0 | 100 | 100 |
| 3 | 3 | 686/727 (94%) | 664 (97%) | 22 (3%) | 0 | 100 | 100 |
| 4 | 4 | 421/463 (91%) | 405 (96%) | 16 (4%) | 0 | 100 | 100 |
| 5 | 5 | 206/266 (77%) | 198 (96%) | 8 (4%) | 0 | 100 | 100 |
| 6 | 6 | 154/223 (69%) | 148 (96%) | 6 (4%) | 0 | 100 | 100 |
| 7 | 9 | 174/217 (80%) | 166 (95%) | 8 (5%) | 0 | 100 | 100 |
| 8 | A | 106/115 (92%) | 96 (91%) | 10 (9%) | 0 | 100 | 100 |
| 9 | H | 310/318 (98%) | 300 (97%) | 10 (3%) | 0 | 100 | 100 |
| 10 | J | 163/175 (93%) | 155 (95%) | 8 (5%) | 0 | 100 | 100 |
| 11 | K | 96/98 (98%) | 92 (96%) | 4 (4%) | 0 | 100 | 100 |
| 12 | L | 556/606 (92%) | 532 (96%) | 24 (4%) | 0 | 100 | 100 |
| 13 | M | 457/459 (100%) | 448 (98%) | 9 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 14 | N | 345/347 (99%) | 330 (96%) | 15 (4%) | 0 | 100 | 100 |
| 15 | V | 25/141 (18%) | 23 (92%) | 2 (8%) | 0 | 100 | 100 |
| 16 | W | 137/189 (72%) | 136 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | X | 85/157 (54%) | 83 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | j | 80/157 (51%) | 74 (92%) | 6 (8%) | 0 | 100 | 100 |
| 18 | Y | 169/172 (98%) | 163 (96%) | 6 (4%) | 0 | 100 | 100 |
| 19 | Z | 169/175 (97%) | 167 (99%) | 2 (1%) | 0 | 100 | 100 |
| 20 | a | 42/109 (38%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 21 | b | 93/124 (75%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 22 | c | 124/170 (73%) | 121 (98%) | 3 (2%) | 0 | 100 | 100 |
| 23 | d | 289/380 (76%) | 283 (98%) | 6 (2%) | 0 | 100 | 100 |
| 24 | e | 84/99 (85%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 25 | f | 111/116 (96%) | 110 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | g | 112/140 (80%) | 109 (97%) | 3 (3%) | 0 | 100 | 100 |
| 27 | h | 92/114 (81%) | 87 (95%) | 5 (5%) | 0 | 100 | 100 |
| 28 | i | 143/145 (99%) | 142 (99%) | 1 (1%) | 0 | 100 | 100 |
| 29 | k | 317/355 (89%) | 305 (96%) | 12 (4%) | 0 | 100 | 100 |
| 30 | l | 103/106 (97%) | 100 (97%) | 3 (3%) | 0 | 100 | 100 |
| 31 | m | 78/84 (93%) | 75 (96%) | 3 (4%) | 0 | 100 | 100 |
| 32 | n | 77/98 (79%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 33 | o | 118/122 (97%) | 116 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | p | 126/130 (97%) | 118 (94%) | 8 (6%) | 0 | 100 | 100 |
| 35 | q | 137/144 (95%) | 134 (98%) | 3 (2%) | 0 | 100 | 100 |
| 36 | r | 95/128 (74%) | 92 (97%) | 3 (3%) | 0 | 100 | 100 |
| 37 | s | 120/137 (88%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 38 | t | 175/179 (98%) | 171 (98%) | 4 (2%) | 0 | 100 | 100 |
| 39 | u | 63/108 (58%) | 61 (97%) | 2 (3%) | 0 | 100 | 100 |
| 40 | v | 153/186 (82%) | 144 (94%) | 9 (6%) | 0 | 100 | 100 |
| 41 | w | 99/154 (64%) | 95 (96%) | 4 (4%) | 0 | 100 | 100 |
| 42 | x | 47/76 (62%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 43 | y | 48/58 (83%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 44 | z | 68/70 (97%) | 68 (100%) | 0 | 0 | 100 | 100 |
| All | All | 7892/9247 (85%) | 7616 (96%) | 276 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | 1 | 344/368 (94%) | 342 (99%) | 2 (1%) | 84 | 95 |
| 2 | 2 | 183/210 (87%) | 182 (100%) | 1 (0%) | 86 | 96 |
| 3 | 3 | 578/608 (95%) | 576 (100%) | 2 (0%) | 91 | 97 |
| 4 | 4 | 366/391 (94%) | 364 (100%) | 2 (0%) | 86 | 96 |
| 5 | 5 | 189/230 (82%) | 189 (100%) | 0 | 100 | 100 |
| 6 | 6 | 132/181 (73%) | 128 (97%) | 4 (3%) | 36 | 71 |
| 7 | 9 | 151/179 (84%) | 151 (100%) | 0 | 100 | 100 |
| 8 | A | 99/103 (96%) | 98 (99%) | 1 (1%) | 73 | 91 |
| 9 | H | 274/278 (99%) | 270 (98%) | 4 (2%) | 60 | 85 |
| 10 | J | 136/144 (94%) | 136 (100%) | 0 | 100 | 100 |
| 11 | K | 86/86 (100%) | 84 (98%) | 2 (2%) | 45 | 77 |
| 12 | L | 492/538 (91%) | 488 (99%) | 4 (1%) | 79 | 93 |
| 13 | M | 411/411 (100%) | 410 (100%) | 1 (0%) | 92 | 98 |
| 14 | N | 315/315 (100%) | 313 (99%) | 2 (1%) | 84 | 95 |
| 15 | V | 20/102 (20%) | 20 (100%) | 0 | 100 | 100 |
| 16 | W | 122/160 (76%) | 122 (100%) | 0 | 100 | 100 |
| 17 | X | 80/141 (57%) | 80 (100%) | 0 | 100 | 100 |
| 17 | j | 76/141 (54%) | 76 (100%) | 0 | 100 | 100 |
| 18 | Y | 154/155 (99%) | 153 (99%) | 1 (1%) | 84 | 95 |
| 19 | Z | 155/157 (99%) | 155 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 20 | a | 43/93 (46%) | 43 (100%) | 0 | 100 | 100 |
| 21 | b | 79/97 (81%) | 79 (100%) | 0 | 100 | 100 |
| 22 | c | 113/150 (75%) | 113 (100%) | 0 | 100 | 100 |
| 23 | d | 255/326 (78%) | 254 (100%) | 1 (0%) | 89 | 97 |
| 24 | e | 76/82 (93%) | 76 (100%) | 0 | 100 | 100 |
| 25 | f | 101/102 (99%) | 101 (100%) | 0 | 100 | 100 |
| 26 | g | 107/124 (86%) | 107 (100%) | 0 | 100 | 100 |
| 27 | h | 84/96 (88%) | 84 (100%) | 0 | 100 | 100 |
| 28 | i | 131/131 (100%) | 131 (100%) | 0 | 100 | 100 |
| 29 | k | 283/309 (92%) | 283 (100%) | 0 | 100 | 100 |
| 30 | l | 94/95 (99%) | 94 (100%) | 0 | 100 | 100 |
| 31 | m | 69/72 (96%) | 69 (100%) | 0 | 100 | 100 |
| 32 | n | 61/76 (80%) | 61 (100%) | 0 | 100 | 100 |
| 33 | o | 107/109 (98%) | 107 (100%) | 0 | 100 | 100 |
| 34 | p | 114/116 (98%) | 114 (100%) | 0 | 100 | 100 |
| 35 | q | 119/122 (98%) | 118 (99%) | 1 (1%) | 79 | 93 |
| 36 | r | 95/122 (78%) | 95 (100%) | 0 | 100 | 100 |
| 37 | s | 110/120 (92%) | 109 (99%) | 1 (1%) | 75 | 92 |
| 38 | t | 159/161 (99%) | 158 (99%) | 1 (1%) | 84 | 95 |
| 39 | u | 59/84 (70%) | 59 (100%) | 0 | 100 | 100 |
| 40 | v | 140/160 (88%) | 140 (100%) | 0 | 100 | 100 |
| 41 | w | 92/130 (71%) | 91 (99%) | 1 (1%) | 70 | 90 |
| 42 | x | 44/67 (66%) | 44 (100%) | 0 | 100 | 100 |
| 43 | y | 46/54 (85%) | 46 (100%) | 0 | 100 | 100 |
| 44 | z | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| All | All | 7003/7955 (88%) | 6972 (100%) | 31 (0%) | 88 | 97 |

All (31) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 148 | ASN |
| 1 | 1 | 249 | ARG |
| 2 | 2 | 122 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 3 | 39 | ARG |
| 3 | 3 | 179 | ASN |
| 4 | 4 | 252 | ASN |
| 4 | 4 | 430 | ARG |
| 6 | 6 | 54 | CYS |
| 6 | 6 | 59 | MET |
| 6 | 6 | 71 | ARG |
| 6 | 6 | 111 | ARG |
| 8 | A | 48 | ARG |
| 9 | H | 241 | LEU |
| 9 | H | 259 | PHE |
| 9 | H | 274 | ARG |
| 9 | H | 285 | LEU |
| 11 | K | 21 | MET |
| 11 | K | 50 | ASN |
| 12 | L | 135 | ASN |
| 12 | L | 270 | ASN |
| 12 | L | 442 | ASN |
| 12 | L | 541 | ASN |
| 13 | M | 144 | ASN |
| 14 | N | 295 | ARG |
| 14 | N | 309 | ASN |
| 18 | Y | 63 | ASN |
| 23 | d | 36 | ASN |
| 35 | q | 67 | ARG |
| 37 | s | 103 | ARG |
| 38 | t | 128 | ARG |
| 41 | w | 57 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 148 | ASN |
| 1 | 1 | 150 | GLN |
| 1 | 1 | 250 | ASN |
| 1 | 1 | 373 | ASN |
| 2 | 2 | 99 | HIS |
| 2 | 2 | 101 | GLN |
| 2 | 2 | 157 | ASN |
| 3 | 3 | 535 | GLN |
| 4 | 4 | 149 | ASN |
| 4 | 4 | 252 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 4 | 409 | HIS |
| 9 | H | 292 | ASN |
| 12 | L | 135 | ASN |
| 12 | L | 175 | ASN |
| 12 | L | 199 | GLN |
| 12 | L | 210 | ASN |
| 12 | L | 348 | HIS |
| 12 | L | 434 | GLN |
| 12 | L | 446 | ASN |
| 13 | M | 81 | GLN |
| 13 | M | 144 | ASN |
| 16 | W | 143 | ASN |
| 18 | Y | 29 | HIS |
| 19 | Z | 123 | ASN |
| 20 | a | 40 | ASN |
| 22 | c | 29 | HIS |
| 23 | d | 87 | HIS |
| 25 | f | 49 | GLN |
| 34 | p | 74 | ASN |
| 34 | p | 78 | ASN |
| 37 | s | 42 | GLN |
| 38 | t | 25 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 12 | FME | L | 1 | 12 | 8,9,10 | 0.91 | 0 | 7,9,11 | 1.77 | 2 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | 2MR | 4 | 85 | 4 | 10,12,13 | 2.26 | 3 (30%) | 5,13,15 | 2.13 | 1 (20%) |
| 27 | AYA | h | 1 | 27 | 6,7,8 | 1.26 | 1 (16%) | 5,8,10 | 1.11 | 1 (20%) |
| 29 | SEP | k | 36 | 29 | 8,9,10 | 1.54 | 1 (12%) | 8,12,14 | 1.45 | 2 (25%) |
| 11 | FME | K | 1 | 11 | 8,9,10 | 0.92 | 0 | 7,9,11 | 0.81 | 0 |
| 13 | FME | M | 1 | 13 | 8,9,10 | 0.95 | 0 | 7,9,11 | 0.80 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 12 | FME | L | 1 | 12 | - | 1/7/9/11 | - |
| 4 | 2MR | 4 | 85 | 4 | - | 1/10/13/15 | - |
| 27 | AYA | h | 1 | 27 | - | 0/4/6/8 | - |
| 29 | SEP | k | 36 | 29 | - | 3/5/8/10 | - |
| 11 | FME | K | 1 | 11 | - | 5/7/9/11 | - |
| 13 | FME | M | 1 | 13 | - | 2/7/9/11 | - |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 4 | 85 | 2MR | CZ-NH2 | 4.48 | 1.43 | 1.33 |
| 4 | 4 | 85 | 2MR | CZ-NE | 4.35 | 1.43 | 1.34 |
| 29 | k | 36 | SEP | P-O1P | 3.35 | 1.61 | 1.50 |
| 27 | h | 1 | AYA | CA-N | -2.56 | 1.43 | 1.46 |
| 4 | 4 | 85 | 2MR | CQ1-NH1 | -2.22 | 1.41 | 1.46 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4 | 4 | 85 | 2MR | NE-CZ-NH2 | -4.00 | 115.81 | 119.48 |
| 12 | L | 1 | FME | CA-N-CN | 3.36 | 127.98 | 122.82 |
| 12 | L | 1 | FME | C-CA-N | 2.87 | 114.92 | 109.73 |
| 29 | k | 36 | SEP | P-OG-CB | -2.80 | 110.58 | 118.30 |
| 29 | k | 36 | SEP | OG-CB-CA | 2.28 | 110.36 | 108.14 |
| 27 | h | 1 | AYA | CB-CA-N | 2.01 | 111.84 | 109.61 |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 11 | K | 1 | FME | O1-CN-N-CA |
| 11 | K | 1 | FME | O-C-CA-CB |
| 12 | L | 1 | FME | CA-CB-CG-SD |
| 13 | M | 1 | FME | CB-CA-N-CN |
| 13 | M | 1 | FME | C-CA-CB-CG |
| 29 | k | 36 | SEP | CB-OG-P-O1P |
| 29 | k | 36 | SEP | CB-OG-P-O2P |
| 29 | k | 36 | SEP | CB-OG-P-O3P |
| 11 | K | 1 | FME | N-CA-CB-CG |
| 11 | K | 1 | FME | CB-CA-N-CN |
| 11 | K | 1 | FME | CA-CB-CG-SD |
| 4 | 4 | 85 | 2MR | NE-CD-CG-CB |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 52 | PC1 | M | 603 | - | 41,41,53 | 0.35 | 0 | 47,49,61 | 0.48 | 0 |
| 51 | 3PE | M | 602 | - | 43,43,50 | 0.32 | 0 | 46,48,55 | 0.48 | 0 |
| 48 | FES | 3 | 803 | 3 | 0,4,4 | - | - | - | | |
| 53 | CDL | h | 201 | - | 57,57,99 | 0.37 | 0 | 63,69,111 | 0.30 | 0 |
| 52 | PC1 | 9 | 401 | - | 53,53,53 | 0.31 | 0 | 59,61,61 | 0.49 | 1 (1%) |
| 56 | NDP | d | 401 | - | 45,52,52 | 0.61 | 0 | 53,80,80 | 0.55 | 1 (1%) |
| 51 | 3PE | L | 1004 | - | 30,30,50 | 0.41 | 0 | 33,35,55 | 0.76 | 1 (3%) |
| 53 | CDL | L | 1003 | - | 99,99,99 | 0.26 | 0 | 105,111,111 | 0.30 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 51 | 3PE | o | 501 | - | 30,30,50 | 0.38 | 0 | 33,35,55 | 0.42 | 0 |
| 53 | CDL | o | 502 | - | 74,74,99 | 0.29 | 0 | 80,86,111 | 0.46 | 0 |
| 50 | 970 | M | 601 | - | 33,33,33 | 0.39 | 0 | 48,50,50 | 1.13 | 3 (6%) |
| 45 | SF4 | 6 | 502 | 6 | 0,12,12 | - | - | - | | |
| 54 | ZMP | X | 101 | 17 | 24,30,36 | 0.79 | 1 (4%) | 29,37,45 | 0.98 | 1 (3%) |
| 52 | PC1 | w | 801 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.37 | 0 |
| 51 | 3PE | i | 201 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.30 | 0 |
| 50 | 970 | 6 | 501 | - | 33,33,33 | 0.43 | 0 | 48,50,50 | 0.60 | 0 |
| 58 | MYR | s | 201 | 37 | 14,14,15 | 0.23 | 0 | 13,13,15 | 0.17 | 0 |
| 53 | CDL | o | 503 | - | 89,89,99 | 0.30 | 0 | 95,101,111 | 0.38 | 1 (1%) |
| 51 | 3PE | A | 403 | - | 50,50,50 | 0.31 | 0 | 53,55,55 | 0.42 | 0 |
| 51 | 3PE | L | 1001 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.34 | 0 |
| 52 | PC1 | A | 402 | - | 36,36,53 | 0.36 | 0 | 42,44,61 | 0.61 | 2 (4%) |
| 51 | 3PE | H | 502 | - | 50,50,50 | 0.31 | 0 | 53,55,55 | 0.52 | 1 (1%) |
| 57 | AMP | k | 501 | - | 22,25,25 | 0.87 | 1 (4%) | 25,38,38 | 1.17 | 2 (8%) |
| 46 | FMN | 1 | 502 | - | 33,33,33 | 1.09 | 2 (6%) | 48,50,50 | 1.35 | 8 (16%) |
| 45 | SF4 | 9 | 403 | 7 | 0,12,12 | - | - | - | | |
| 52 | PC1 | L | 1002 | - | 53,53,53 | 0.31 | 0 | 59,61,61 | 0.62 | 2 (3%) |
| 53 | CDL | y | 201 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.30 | 0 |
| 51 | 3PE | 6 | 503 | - | 50,50,50 | 0.31 | 0 | 53,55,55 | 0.31 | 0 |
| 54 | ZMP | g | 201 | - | 27,33,36 | 0.62 | 1 (3%) | 32,40,45 | 1.20 | 4 (12%) |
| 48 | FES | 2 | 300 | 2 | 0,4,4 | - | - | - | | |
| 53 | CDL | W | 201 | - | 99,99,99 | 0.28 | 0 | 105,111,111 | 0.30 | 0 |
| 45 | SF4 | 3 | 802 | 3 | 0,12,12 | - | - | - | | |
| 52 | PC1 | A | 401 | - | 45,45,53 | 0.32 | 0 | 51,53,61 | 0.32 | 0 |
| 45 | SF4 | 1 | 501 | 1 | 0,12,12 | - | - | - | | |
| 47 | NAI | 1 | 503 | - | 42,48,48 | 0.58 | 0 | 47,73,73 | 1.98 | 4 (8%) |
| 45 | SF4 | 3 | 801 | 3 | 0,12,12 | - | - | - | | |
| 50 | 970 | H | 501 | - | 33,33,33 | 0.35 | 0 | 48,50,50 | 0.69 | 1 (2%) |
| 45 | SF4 | 9 | 402 | 7 | 0,12,12 | - | - | - | | |
| 51 | 3PE | N | 401 | - | 50,50,50 | 0.32 | 0 | 53,55,55 | 0.52 | 1 (1%) |

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 |
|-----|------|-------|-----|------|---------|-------------|-------|
| 52 | PC1 | M | 603 | - | - | 16/45/45/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------------|---------|
| 51 | 3PE | M | 602 | - | - | 20/47/47/54 | - |
| 48 | FES | 3 | 803 | 3 | - | - | 0/1/1/1 |
| 53 | CDL | h | 201 | - | - | 19/68/68/110 | - |
| 52 | PC1 | 9 | 401 | - | - | 12/57/57/57 | - |
| 56 | NDP | d | 401 | - | - | 6/30/77/77 | 0/5/5/5 |
| 51 | 3PE | L | 1004 | - | - | 18/34/34/54 | - |
| 53 | CDL | L | 1003 | - | 1/1/9/9 | 29/110/110/110 | - |
| 51 | 3PE | o | 501 | - | - | 2/34/34/54 | - |
| 53 | CDL | o | 502 | - | 2/2/9/9 | 22/85/85/110 | - |
| 50 | 970 | M | 601 | - | 1/1/5/5 | 4/8/41/41 | 0/5/5/5 |
| 54 | ZMP | X | 101 | 17 | - | 14/35/37/43 | - |
| 45 | SF4 | 6 | 502 | 6 | - | - | 0/6/5/5 |
| 52 | PC1 | w | 801 | - | - | 8/57/57/57 | - |
| 51 | 3PE | i | 201 | - | - | 7/54/54/54 | - |
| 50 | 970 | 6 | 501 | - | - | 4/8/41/41 | 0/5/5/5 |
| 58 | MYR | s | 201 | 37 | - | 2/11/12/13 | - |
| 53 | CDL | o | 503 | - | - | 30/100/100/110 | - |
| 51 | 3PE | A | 403 | - | - | 15/54/54/54 | - |
| 51 | 3PE | L | 1001 | - | - | 9/54/54/54 | - |
| 52 | PC1 | A | 402 | - | - | 8/40/40/57 | - |
| 51 | 3PE | H | 502 | - | - | 14/54/54/54 | - |
| 57 | AMP | k | 501 | - | - | 6/6/26/26 | 0/3/3/3 |
| 46 | FMN | 1 | 502 | - | - | 9/18/18/18 | 0/3/3/3 |
| 45 | SF4 | 9 | 403 | 7 | - | - | 0/6/5/5 |
| 52 | PC1 | L | 1002 | - | - | 18/57/57/57 | - |
| 53 | CDL | y | 201 | - | 1/1/9/9 | 32/110/110/110 | - |
| 51 | 3PE | 6 | 503 | - | - | 11/54/54/54 | - |
| 54 | ZMP | g | 201 | - | - | 15/38/40/43 | - |
| 48 | FES | 2 | 300 | 2 | - | - | 0/1/1/1 |
| 53 | CDL | W | 201 | - | - | 22/110/110/110 | - |
| 45 | SF4 | 3 | 802 | 3 | - | - | 0/6/5/5 |
| 52 | PC1 | A | 401 | - | - | 14/49/49/57 | - |
| 45 | SF4 | 1 | 501 | 1 | - | - | 0/6/5/5 |
| 47 | NAI | 1 | 503 | - | - | 5/25/72/72 | 0/5/5/5 |
| 45 | SF4 | 3 | 801 | 3 | - | - | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 50 | 970 | H | 501 | - | - | 2/8/41/41 | 0/5/5/5 |
| 45 | SF4 | 9 | 402 | 7 | - | - | 0/6/5/5 |
| 51 | 3PE | N | 401 | - | - | 13/54/54/54 | - |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 46 | 1 | 502 | FMN | C4A-N5 | 3.24 | 1.37 | 1.30 |
| 57 | k | 501 | AMP | C5-C4 | 2.55 | 1.47 | 1.40 |
| 54 | X | 101 | ZMP | C9-C10 | 2.14 | 1.53 | 1.50 |
| 46 | 1 | 502 | FMN | C10-N1 | 2.03 | 1.37 | 1.33 |
| 54 | g | 201 | ZMP | C9-C10 | 2.02 | 1.52 | 1.50 |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47 | 1 | 503 | NAI | O5B-PA-O1A | -9.83 | 70.67 | 109.07 |
| 47 | 1 | 503 | NAI | O2A-PA-O1A | -8.03 | 72.55 | 112.24 |
| 50 | M | 601 | 970 | C22-C23-C14 | -4.24 | 103.63 | 109.56 |
| 46 | 1 | 502 | FMN | C4-N3-C2 | -3.44 | 119.28 | 125.64 |
| 50 | M | 601 | 970 | C12-O13-C14 | -3.25 | 110.51 | 116.06 |
| 57 | k | 501 | AMP | N3-C2-N1 | -3.08 | 123.86 | 128.68 |
| 46 | 1 | 502 | FMN | C4A-C10-N10 | 3.05 | 120.94 | 116.48 |
| 54 | g | 201 | ZMP | O1-C10-C9 | -3.04 | 120.40 | 123.99 |
| 51 | H | 502 | 3PE | O31-C3-C2 | 2.84 | 116.71 | 108.43 |
| 54 | g | 201 | ZMP | C14-C15-N2 | -2.68 | 106.48 | 111.90 |
| 46 | 1 | 502 | FMN | C4A-C4-N3 | 2.63 | 119.86 | 113.19 |
| 46 | 1 | 502 | FMN | C4A-C10-N1 | -2.61 | 118.67 | 124.73 |
| 52 | L | 1002 | PC1 | C2-O21-C21 | 2.60 | 124.19 | 117.79 |
| 54 | g | 201 | ZMP | C15-C14-C13 | -2.56 | 108.10 | 112.36 |
| 46 | 1 | 502 | FMN | O4-C4-C4A | -2.45 | 120.09 | 126.60 |
| 46 | 1 | 502 | FMN | C10-C4A-N5 | -2.43 | 119.70 | 124.86 |
| 47 | 1 | 503 | NAI | O2A-PA-O5B | 2.42 | 118.98 | 107.75 |
| 51 | L | 1004 | 3PE | C2-O21-C21 | 2.40 | 123.71 | 117.79 |
| 54 | X | 101 | ZMP | O1-C10-C9 | -2.33 | 121.23 | 123.99 |
| 46 | 1 | 502 | FMN | C4-C4A-C10 | 2.32 | 120.68 | 116.79 |
| 47 | 1 | 503 | NAI | C5A-C6A-N6A | 2.29 | 123.83 | 120.35 |
| 54 | g | 201 | ZMP | C9-C10-S1 | 2.27 | 116.10 | 113.46 |
| 50 | M | 601 | 970 | O13-C14-C15 | 2.26 | 109.61 | 106.65 |
| 52 | L | 1002 | PC1 | O21-C2-C1 | 2.25 | 116.55 | 108.40 |
| 52 | A | 402 | PC1 | O21-C2-C3 | 2.21 | 116.39 | 108.40 |
| 52 | A | 402 | PC1 | C2-O21-C21 | 2.20 | 123.21 | 117.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 57 | k | 501 | AMP | C4-C5-N7 | -2.19 | 107.12 | 109.40 |
| 51 | N | 401 | 3PE | O21-C2-C1 | 2.14 | 116.15 | 108.40 |
| 56 | d | 401 | NDP | C5A-C6A-N6A | 2.13 | 123.60 | 120.35 |
| 53 | o | 503 | CDL | CB4-OB6-CB5 | 2.06 | 122.85 | 117.79 |
| 52 | 9 | 401 | PC1 | O21-C2-C1 | 2.02 | 115.70 | 108.40 |
| 50 | H | 501 | 970 | O08-C07-C06 | 2.01 | 114.22 | 113.00 |
| 46 | 1 | 502 | FMN | C1'-C2'-C3' | 2.01 | 115.40 | 109.79 |

All (5) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 50 | M | 601 | 970 | C14 |
| 53 | L | 1003 | CDL | CB4 |
| 53 | o | 502 | CDL | CA4 |
| 53 | o | 502 | CDL | CB4 |
| 53 | y | 201 | CDL | CB4 |

All (406) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 46 | 1 | 502 | FMN | N10-C1'-C2'-O2' |
| 46 | 1 | 502 | FMN | N10-C1'-C2'-C3' |
| 46 | 1 | 502 | FMN | C5'-O5'-P-O2P |
| 46 | 1 | 502 | FMN | C5'-O5'-P-O3P |
| 50 | 6 | 501 | 970 | C01-C02-C04-C05 |
| 50 | 6 | 501 | 970 | C01-C02-C04-O08 |
| 50 | 6 | 501 | 970 | C03-C02-C04-C05 |
| 50 | 6 | 501 | 970 | C03-C02-C04-O08 |
| 50 | M | 601 | 970 | C03-C02-C04-C05 |
| 50 | M | 601 | 970 | C03-C02-C04-O08 |
| 51 | 6 | 503 | 3PE | C1-O11-P-O12 |
| 51 | 6 | 503 | 3PE | O13-C11-C12-N |
| 51 | A | 403 | 3PE | C1-O11-P-O12 |
| 51 | A | 403 | 3PE | C11-O13-P-O12 |
| 51 | A | 403 | 3PE | O13-C11-C12-N |
| 51 | H | 502 | 3PE | C11-O13-P-O12 |
| 51 | H | 502 | 3PE | O13-C11-C12-N |
| 51 | L | 1001 | 3PE | C1-O11-P-O14 |
| 51 | L | 1001 | 3PE | O13-C11-C12-N |
| 51 | L | 1004 | 3PE | C1-O11-P-O12 |
| 51 | L | 1004 | 3PE | C1-O11-P-O14 |
| 51 | L | 1004 | 3PE | C11-O13-P-O12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 51 | L | 1004 | 3PE | O13-C11-C12-N |
| 51 | M | 602 | 3PE | C1-O11-P-O12 |
| 51 | M | 602 | 3PE | C1-O11-P-O13 |
| 51 | M | 602 | 3PE | C1-O11-P-O14 |
| 51 | N | 401 | 3PE | C11-O13-P-O14 |
| 51 | N | 401 | 3PE | O13-C11-C12-N |
| 51 | i | 201 | 3PE | C1-O11-P-O12 |
| 52 | 9 | 401 | PC1 | C1-O11-P-O13 |
| 52 | A | 401 | PC1 | C11-O13-P-O12 |
| 52 | A | 401 | PC1 | C11-O13-P-O14 |
| 52 | A | 401 | PC1 | C1-O11-P-O14 |
| 52 | A | 402 | PC1 | C11-O13-P-O12 |
| 52 | A | 402 | PC1 | C1-O11-P-O14 |
| 52 | L | 1002 | PC1 | C1-O11-P-O12 |
| 52 | L | 1002 | PC1 | C1-O11-P-O14 |
| 52 | M | 603 | PC1 | C11-O13-P-O14 |
| 52 | M | 603 | PC1 | C11-O13-P-O11 |
| 52 | M | 603 | PC1 | C1-O11-P-O12 |
| 53 | L | 1003 | CDL | CA2-OA2-PA1-OA3 |
| 53 | L | 1003 | CDL | CA3-OA5-PA1-OA3 |
| 53 | L | 1003 | CDL | CA3-OA5-PA1-OA4 |
| 53 | L | 1003 | CDL | CB2-OB2-PB2-OB3 |
| 53 | W | 201 | CDL | CB3-OB5-PB2-OB3 |
| 53 | W | 201 | CDL | CB3-OB5-PB2-OB4 |
| 53 | h | 201 | CDL | CA2-OA2-PA1-OA3 |
| 53 | h | 201 | CDL | CA2-OA2-PA1-OA4 |
| 53 | h | 201 | CDL | CB2-OB2-PB2-OB4 |
| 53 | o | 502 | CDL | CA2-OA2-PA1-OA3 |
| 53 | o | 502 | CDL | CA2-OA2-PA1-OA4 |
| 53 | o | 502 | CDL | CA3-OA5-PA1-OA2 |
| 53 | o | 502 | CDL | CA3-OA5-PA1-OA3 |
| 53 | o | 502 | CDL | CA3-OA5-PA1-OA4 |
| 53 | o | 503 | CDL | CA2-OA2-PA1-OA4 |
| 53 | o | 503 | CDL | CA3-OA5-PA1-OA2 |
| 53 | o | 503 | CDL | CA3-OA5-PA1-OA3 |
| 53 | o | 503 | CDL | CB2-OB2-PB2-OB3 |
| 53 | o | 503 | CDL | CB2-OB2-PB2-OB4 |
| 53 | y | 201 | CDL | CA2-C1-CB2-OB2 |
| 53 | y | 201 | CDL | CB3-OB5-PB2-OB2 |
| 53 | y | 201 | CDL | CB3-OB5-PB2-OB4 |
| 54 | X | 101 | ZMP | C17-C18-C21-O5 |
| 54 | X | 101 | ZMP | C16-C17-C18-C21 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 54 | X | 101 | ZMP | O3-C16-C17-O4 |
| 54 | X | 101 | ZMP | C17-C16-N2-C15 |
| 54 | g | 201 | ZMP | S1-C11-C12-N1 |
| 54 | g | 201 | ZMP | C12-C11-S1-C10 |
| 57 | k | 501 | AMP | C5'-O5'-P-O1P |
| 57 | k | 501 | AMP | C5'-O5'-P-O2P |
| 57 | k | 501 | AMP | C5'-O5'-P-O3P |
| 57 | k | 501 | AMP | C3'-C4'-C5'-O5' |
| 58 | s | 201 | MYR | C1-C2-C3-C4 |
| 53 | h | 201 | CDL | O1-C1-CB2-OB2 |
| 53 | y | 201 | CDL | O1-C1-CB2-OB2 |
| 54 | X | 101 | ZMP | O3-C16-N2-C15 |
| 53 | W | 201 | CDL | CA2-C1-CB2-OB2 |
| 53 | W | 201 | CDL | OB5-CB3-CB4-OB6 |
| 53 | W | 201 | CDL | O1-C1-CB2-OB2 |
| 53 | L | 1003 | CDL | CB7-C71-C72-C73 |
| 52 | M | 603 | PC1 | C11-C12-N-C14 |
| 52 | A | 402 | PC1 | C22-C23-C24-C25 |
| 53 | o | 502 | CDL | O1-C1-CB2-OB2 |
| 51 | A | 403 | 3PE | C1-O11-P-O13 |
| 51 | H | 502 | 3PE | C11-O13-P-O11 |
| 51 | L | 1001 | 3PE | C11-O13-P-O11 |
| 51 | L | 1004 | 3PE | C1-O11-P-O13 |
| 51 | M | 602 | 3PE | C11-O13-P-O11 |
| 51 | i | 201 | 3PE | C1-O11-P-O13 |
| 52 | A | 401 | PC1 | C11-O13-P-O11 |
| 52 | A | 402 | PC1 | C11-O13-P-O11 |
| 52 | A | 402 | PC1 | C1-O11-P-O13 |
| 52 | L | 1002 | PC1 | C1-O11-P-O13 |
| 52 | w | 801 | PC1 | C11-O13-P-O11 |
| 53 | L | 1003 | CDL | CA3-OA5-PA1-OA2 |
| 53 | W | 201 | CDL | CB3-OB5-PB2-OB2 |
| 53 | h | 201 | CDL | CA2-OA2-PA1-OA5 |
| 53 | o | 502 | CDL | CA2-OA2-PA1-OA5 |
| 53 | o | 503 | CDL | CA2-OA2-PA1-OA5 |
| 53 | o | 503 | CDL | CB2-OB2-PB2-OB5 |
| 53 | h | 201 | CDL | CA2-C1-CB2-OB2 |
| 52 | M | 603 | PC1 | C11-C12-N-C15 |
| 53 | o | 503 | CDL | CB5-C51-C52-C53 |
| 53 | L | 1003 | CDL | C56-C57-C58-C59 |
| 51 | 6 | 503 | 3PE | C3C-C3D-C3E-C3F |
| 51 | A | 403 | 3PE | C2C-C2D-C2E-C2F |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 51 | N | 401 | 3PE | C32-C33-C34-C35 |
| 53 | L | 1003 | CDL | C82-C83-C84-C85 |
| 51 | A | 403 | 3PE | C2E-C2F-C2G-C2H |
| 51 | i | 201 | 3PE | C29-C2A-C2B-C2C |
| 53 | o | 503 | CDL | C78-C79-C80-C81 |
| 53 | y | 201 | CDL | C12-C13-C14-C15 |
| 53 | L | 1003 | CDL | C21-C22-C23-C24 |
| 53 | W | 201 | CDL | C72-C73-C74-C75 |
| 52 | 9 | 401 | PC1 | C3B-C3C-C3D-C3E |
| 52 | 9 | 401 | PC1 | C3C-C3D-C3E-C3F |
| 53 | W | 201 | CDL | C35-C36-C37-C38 |
| 53 | W | 201 | CDL | C78-C79-C80-C81 |
| 54 | X | 101 | ZMP | C3-C4-C5-C6 |
| 52 | A | 401 | PC1 | C3B-C3C-C3D-C3E |
| 53 | W | 201 | CDL | C31-C32-C33-C34 |
| 53 | y | 201 | CDL | C13-C14-C15-C16 |
| 52 | L | 1002 | PC1 | C3A-C3B-C3C-C3D |
| 53 | L | 1003 | CDL | C77-C78-C79-C80 |
| 52 | 9 | 401 | PC1 | C2B-C2C-C2D-C2E |
| 53 | y | 201 | CDL | C59-C60-C61-C62 |
| 54 | g | 201 | ZMP | C3-C4-C5-C6 |
| 51 | N | 401 | 3PE | C21-C22-C23-C24 |
| 53 | W | 201 | CDL | CB5-C51-C52-C53 |
| 53 | L | 1003 | CDL | C17-C18-C19-C20 |
| 53 | L | 1003 | CDL | C41-C42-C43-C44 |
| 52 | 9 | 401 | PC1 | C27-C28-C29-C2A |
| 51 | H | 502 | 3PE | C28-C29-C2A-C2B |
| 53 | o | 503 | CDL | C19-C20-C21-C22 |
| 53 | W | 201 | CDL | C82-C83-C84-C85 |
| 53 | y | 201 | CDL | C81-C82-C83-C84 |
| 52 | M | 603 | PC1 | C11-C12-N-C13 |
| 52 | 9 | 401 | PC1 | C22-C21-O21-C2 |
| 53 | L | 1003 | CDL | C22-C23-C24-C25 |
| 53 | o | 503 | CDL | C56-C57-C58-C59 |
| 54 | g | 201 | ZMP | C1-C2-C3-C4 |
| 53 | L | 1003 | CDL | CB5-C51-C52-C53 |
| 53 | o | 503 | CDL | C76-C77-C78-C79 |
| 54 | X | 101 | ZMP | C5-C6-C7-C8 |
| 57 | k | 501 | AMP | O4'-C4'-C5'-O5' |
| 52 | 9 | 401 | PC1 | O22-C21-O21-C2 |
| 51 | A | 403 | 3PE | C11-O13-P-O11 |
| 51 | L | 1001 | 3PE | C1-O11-P-O13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 51 | L | 1004 | 3PE | C11-O13-P-O11 |
| 52 | A | 401 | PC1 | C1-O11-P-O13 |
| 53 | h | 201 | CDL | CB2-OB2-PB2-OB5 |
| 51 | H | 502 | 3PE | O11-C1-C2-C3 |
| 53 | L | 1003 | CDL | OB5-CB3-CB4-CB6 |
| 53 | W | 201 | CDL | OA5-CA3-CA4-CA6 |
| 53 | o | 503 | CDL | C81-C82-C83-C84 |
| 51 | N | 401 | 3PE | C1-C2-C3-O31 |
| 53 | h | 201 | CDL | CA3-CA4-CA6-OA8 |
| 53 | y | 201 | CDL | CA3-CA4-CA6-OA8 |
| 53 | o | 503 | CDL | C84-C85-C86-C87 |
| 53 | y | 201 | CDL | C15-C16-C17-C18 |
| 53 | h | 201 | CDL | CB7-C71-C72-C73 |
| 52 | L | 1002 | PC1 | C38-C39-C3A-C3B |
| 46 | 1 | 502 | FMN | C5'-O5'-P-O1P |
| 52 | M | 603 | PC1 | C23-C24-C25-C26 |
| 54 | g | 201 | ZMP | O4-C17-C18-C20 |
| 51 | 6 | 503 | 3PE | C33-C34-C35-C36 |
| 52 | 9 | 401 | PC1 | C22-C23-C24-C25 |
| 52 | L | 1002 | PC1 | O11-C1-C2-C3 |
| 52 | M | 603 | PC1 | O11-C1-C2-C3 |
| 51 | N | 401 | 3PE | C2C-C2D-C2E-C2F |
| 53 | h | 201 | CDL | C52-C53-C54-C55 |
| 53 | y | 201 | CDL | CB7-C71-C72-C73 |
| 51 | M | 602 | 3PE | C23-C24-C25-C26 |
| 52 | w | 801 | PC1 | C26-C27-C28-C29 |
| 53 | L | 1003 | CDL | C32-C33-C34-C35 |
| 51 | L | 1004 | 3PE | C2-C1-O11-P |
| 52 | 9 | 401 | PC1 | C2-C1-O11-P |
| 53 | L | 1003 | CDL | C1-CA2-OA2-PA1 |
| 51 | N | 401 | 3PE | C31-C32-C33-C34 |
| 54 | g | 201 | ZMP | C22-C1-C2-C3 |
| 53 | L | 1003 | CDL | OB5-CB3-CB4-OB6 |
| 53 | W | 201 | CDL | OA5-CA3-CA4-OA6 |
| 53 | o | 502 | CDL | OB5-CB3-CB4-OB6 |
| 53 | L | 1003 | CDL | C37-C38-C39-C40 |
| 53 | o | 503 | CDL | C64-C65-C66-C67 |
| 53 | y | 201 | CDL | C37-C38-C39-C40 |
| 53 | y | 201 | CDL | C57-C58-C59-C60 |
| 53 | W | 201 | CDL | OB6-CB4-CB6-OB8 |
| 53 | y | 201 | CDL | OA6-CA4-CA6-OA8 |
| 51 | 6 | 503 | 3PE | C36-C37-C38-C39 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 51 | H | 502 | 3PE | C2-C1-O11-P |
| 52 | M | 603 | PC1 | C2-C1-O11-P |
| 53 | o | 502 | CDL | CA4-CA3-OA5-PA1 |
| 53 | o | 503 | CDL | CB4-CB3-OB5-PB2 |
| 52 | w | 801 | PC1 | C39-C3A-C3B-C3C |
| 53 | o | 503 | CDL | C71-C72-C73-C74 |
| 52 | L | 1002 | PC1 | C21-C22-C23-C24 |
| 53 | y | 201 | CDL | C11-C12-C13-C14 |
| 53 | W | 201 | CDL | OB5-CB3-CB4-CB6 |
| 53 | o | 503 | CDL | OB5-CB3-CB4-CB6 |
| 52 | L | 1002 | PC1 | C3F-C3G-C3H-C3I |
| 52 | L | 1002 | PC1 | C23-C24-C25-C26 |
| 54 | g | 201 | ZMP | N2-C16-C17-O4 |
| 51 | M | 602 | 3PE | C36-C37-C38-C39 |
| 51 | N | 401 | 3PE | C3C-C3D-C3E-C3F |
| 51 | A | 403 | 3PE | C35-C36-C37-C38 |
| 52 | L | 1002 | PC1 | C2-C1-O11-P |
| 53 | L | 1003 | CDL | CA3-CA4-CA6-OA8 |
| 53 | W | 201 | CDL | C1-CA2-OA2-PA1 |
| 53 | h | 201 | CDL | C1-CB2-OB2-PB2 |
| 53 | h | 201 | CDL | CB3-CB4-CB6-OB8 |
| 53 | o | 503 | CDL | CA3-CA4-CA6-OA8 |
| 51 | L | 1004 | 3PE | O11-C1-C2-O21 |
| 52 | A | 402 | PC1 | O11-C1-C2-O21 |
| 52 | L | 1002 | PC1 | O11-C1-C2-O21 |
| 52 | M | 603 | PC1 | O11-C1-C2-O21 |
| 54 | X | 101 | ZMP | C16-C17-C18-C19 |
| 54 | X | 101 | ZMP | C16-C17-C18-C20 |
| 54 | g | 201 | ZMP | C16-C17-C18-C20 |
| 51 | N | 401 | 3PE | O21-C2-C3-O31 |
| 53 | L | 1003 | CDL | OA6-CA4-CA6-OA8 |
| 53 | h | 201 | CDL | OA6-CA4-CA6-OA8 |
| 53 | o | 503 | CDL | OA6-CA4-CA6-OA8 |
| 51 | M | 602 | 3PE | C3D-C3E-C3F-C3G |
| 52 | L | 1002 | PC1 | C3E-C3F-C3G-C3H |
| 53 | o | 502 | CDL | CA7-C31-C32-C33 |
| 53 | L | 1003 | CDL | CB2-OB2-PB2-OB5 |
| 46 | 1 | 502 | FMN | C4'-C5'-O5'-P |
| 51 | M | 602 | 3PE | C2-C1-O11-P |
| 53 | L | 1003 | CDL | CA4-CA3-OA5-PA1 |
| 53 | h | 201 | CDL | CB4-CB3-OB5-PB2 |
| 53 | y | 201 | CDL | C1-CB2-OB2-PB2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 47 | 1 | 503 | NAI | C5B-O5B-PA-O1A |
| 51 | 6 | 503 | 3PE | C1-O11-P-O14 |
| 51 | A | 403 | 3PE | C11-O13-P-O14 |
| 51 | L | 1001 | 3PE | C11-O13-P-O14 |
| 51 | L | 1004 | 3PE | C11-O13-P-O14 |
| 51 | M | 602 | 3PE | C11-O13-P-O14 |
| 51 | i | 201 | 3PE | C1-O11-P-O14 |
| 52 | 9 | 401 | PC1 | C1-O11-P-O12 |
| 52 | A | 401 | PC1 | C1-O11-P-O12 |
| 52 | A | 401 | PC1 | C11-C12-N-C14 |
| 52 | A | 402 | PC1 | C1-O11-P-O12 |
| 52 | M | 603 | PC1 | C1-O11-P-O14 |
| 52 | w | 801 | PC1 | C11-O13-P-O14 |
| 53 | h | 201 | CDL | CB2-OB2-PB2-OB3 |
| 53 | o | 503 | CDL | CA2-OA2-PA1-OA3 |
| 53 | y | 201 | CDL | CB3-OB5-PB2-OB3 |
| 51 | H | 502 | 3PE | C32-C31-O31-C3 |
| 53 | o | 502 | CDL | OB5-CB3-CB4-CB6 |
| 53 | y | 201 | CDL | OB5-CB3-CB4-CB6 |
| 52 | w | 801 | PC1 | C3E-C3F-C3G-C3H |
| 50 | H | 501 | 970 | C01-C02-C04-O08 |
| 51 | A | 403 | 3PE | C12-C11-O13-P |
| 51 | H | 502 | 3PE | C12-C11-O13-P |
| 53 | o | 503 | CDL | C31-C32-C33-C34 |
| 51 | H | 502 | 3PE | O11-C1-C2-O21 |
| 53 | y | 201 | CDL | OB5-CB3-CB4-OB6 |
| 51 | A | 403 | 3PE | C38-C39-C3A-C3B |
| 53 | L | 1003 | CDL | C58-C59-C60-C61 |
| 58 | s | 201 | MYR | C11-C10-C9-C8 |
| 52 | w | 801 | PC1 | O13-C11-C12-N |
| 54 | g | 201 | ZMP | O4-C17-C18-C21 |
| 53 | o | 502 | CDL | C12-C13-C14-C15 |
| 53 | y | 201 | CDL | C56-C57-C58-C59 |
| 52 | A | 401 | PC1 | C11-C12-N-C13 |
| 52 | A | 402 | PC1 | O21-C21-C22-C23 |
| 54 | X | 101 | ZMP | C19-C18-C21-O5 |
| 54 | X | 101 | ZMP | C20-C18-C21-O5 |
| 53 | y | 201 | CDL | OA5-CA3-CA4-CA6 |
| 53 | y | 201 | CDL | C32-C33-C34-C35 |
| 46 | 1 | 502 | FMN | C2'-C3'-C4'-O4' |
| 51 | A | 403 | 3PE | C2-C1-O11-P |
| 51 | M | 602 | 3PE | O11-C1-C2-O21 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 47 | 1 | 503 | NAI | O4D-C1D-N1N-C2N |
| 51 | H | 502 | 3PE | C33-C34-C35-C36 |
| 51 | 6 | 503 | 3PE | C11-O13-P-O11 |
| 51 | H | 502 | 3PE | C1-O11-P-O13 |
| 51 | N | 401 | 3PE | C11-O13-P-O11 |
| 51 | i | 201 | 3PE | C11-O13-P-O11 |
| 51 | o | 501 | 3PE | C11-O13-P-O11 |
| 53 | L | 1003 | CDL | CA2-OA2-PA1-OA5 |
| 53 | W | 201 | CDL | CA2-OA2-PA1-OA5 |
| 53 | o | 502 | CDL | CB2-OB2-PB2-OB5 |
| 54 | g | 201 | ZMP | O4-C17-C18-C19 |
| 51 | A | 403 | 3PE | C24-C25-C26-C27 |
| 56 | d | 401 | NDP | PN-O3-PA-O1A |
| 53 | o | 502 | CDL | C71-C72-C73-C74 |
| 53 | o | 502 | CDL | CA2-C1-CB2-OB2 |
| 53 | y | 201 | CDL | C58-C59-C60-C61 |
| 53 | y | 201 | CDL | CA5-C11-C12-C13 |
| 51 | N | 401 | 3PE | C2B-C2C-C2D-C2E |
| 52 | L | 1002 | PC1 | C29-C2A-C2B-C2C |
| 51 | H | 502 | 3PE | O32-C31-O31-C3 |
| 56 | d | 401 | NDP | O4D-C1D-N1N-C6N |
| 52 | L | 1002 | PC1 | C2A-C2B-C2C-C2D |
| 53 | L | 1003 | CDL | C60-C61-C62-C63 |
| 53 | o | 502 | CDL | C14-C15-C16-C17 |
| 51 | M | 602 | 3PE | C32-C33-C34-C35 |
| 53 | L | 1003 | CDL | C1-CB2-OB2-PB2 |
| 57 | k | 501 | AMP | C4'-C5'-O5'-P |
| 52 | A | 401 | PC1 | C11-C12-N-C15 |
| 51 | 6 | 503 | 3PE | C25-C26-C27-C28 |
| 53 | o | 502 | CDL | CA3-CA4-CA6-OA8 |
| 51 | L | 1001 | 3PE | C24-C25-C26-C27 |
| 52 | 9 | 401 | PC1 | C3-C2-O21-C21 |
| 52 | L | 1002 | PC1 | C1-C2-O21-C21 |
| 52 | M | 603 | PC1 | C1-O11-P-O13 |
| 53 | h | 201 | CDL | CB3-OB5-PB2-OB2 |
| 52 | A | 401 | PC1 | C26-C27-C28-C29 |
| 51 | H | 502 | 3PE | C2F-C2G-C2H-C2I |
| 51 | M | 602 | 3PE | O11-C1-C2-C3 |
| 51 | M | 602 | 3PE | C34-C35-C36-C37 |
| 53 | o | 502 | CDL | OA6-CA4-CA6-OA8 |
| 51 | M | 602 | 3PE | C37-C38-C39-C3A |
| 51 | A | 403 | 3PE | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 53 | L | 1003 | CDL | C39-C40-C41-C42 |
| 51 | M | 602 | 3PE | C26-C27-C28-C29 |
| 47 | 1 | 503 | NAI | C2D-C1D-N1N-C2N |
| 52 | M | 603 | PC1 | O21-C21-C22-C23 |
| 53 | o | 502 | CDL | C52-C51-CB5-OB6 |
| 51 | L | 1001 | 3PE | C35-C36-C37-C38 |
| 53 | W | 201 | CDL | CA5-C11-C12-C13 |
| 56 | d | 401 | NDP | PN-O3-PA-O2A |
| 53 | o | 503 | CDL | C34-C35-C36-C37 |
| 51 | 6 | 503 | 3PE | C23-C24-C25-C26 |
| 54 | g | 201 | ZMP | O1-C10-S1-C11 |
| 53 | L | 1003 | CDL | C79-C80-C81-C82 |
| 51 | L | 1004 | 3PE | C33-C34-C35-C36 |
| 47 | 1 | 503 | NAI | PN-O3-PA-O5B |
| 51 | L | 1004 | 3PE | O11-C1-C2-C3 |
| 54 | X | 101 | ZMP | C7-C8-C9-C10 |
| 51 | A | 403 | 3PE | O21-C2-C3-O31 |
| 51 | o | 501 | 3PE | C25-C26-C27-C28 |
| 51 | 6 | 503 | 3PE | O21-C21-C22-C23 |
| 54 | X | 101 | ZMP | N2-C16-C17-O4 |
| 56 | d | 401 | NDP | C2B-O2B-P2B-O1X |
| 52 | L | 1002 | PC1 | C31-C32-C33-C34 |
| 51 | L | 1004 | 3PE | O21-C21-C22-C23 |
| 51 | i | 201 | 3PE | O21-C21-C22-C23 |
| 51 | M | 602 | 3PE | C33-C34-C35-C36 |
| 53 | y | 201 | CDL | C36-C37-C38-C39 |
| 51 | M | 602 | 3PE | C27-C28-C29-C2A |
| 53 | o | 503 | CDL | CA5-C11-C12-C13 |
| 51 | N | 401 | 3PE | C3-C2-O21-C21 |
| 53 | o | 503 | CDL | CB3-CB4-OB6-CB5 |
| 46 | 1 | 502 | FMN | O3'-C3'-C4'-C5' |
| 51 | M | 602 | 3PE | O21-C21-C22-C23 |
| 53 | y | 201 | CDL | C12-C11-CA5-OA6 |
| 51 | 6 | 503 | 3PE | C37-C38-C39-C3A |
| 53 | W | 201 | CDL | CB3-CB4-CB6-OB8 |
| 54 | g | 201 | ZMP | C16-C17-C18-C19 |
| 54 | g | 201 | ZMP | C6-C7-C8-C9 |
| 53 | o | 503 | CDL | C72-C71-CB7-OB8 |
| 56 | d | 401 | NDP | C2B-O2B-P2B-O2X |
| 53 | o | 503 | CDL | CA4-CA3-OA5-PA1 |
| 52 | M | 603 | PC1 | O31-C31-C32-C33 |
| 51 | i | 201 | 3PE | O22-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 53 | W | 201 | CDL | C19-C20-C21-C22 |
| 51 | L | 1004 | 3PE | C23-C24-C25-C26 |
| 53 | y | 201 | CDL | C63-C64-C65-C66 |
| 46 | 1 | 502 | FMN | C2'-C3'-C4'-C5' |
| 51 | L | 1004 | 3PE | O22-C21-C22-C23 |
| 52 | L | 1002 | PC1 | C33-C34-C35-C36 |
| 53 | y | 201 | CDL | C12-C11-CA5-OA7 |
| 53 | y | 201 | CDL | C72-C73-C74-C75 |
| 51 | M | 602 | 3PE | O22-C21-C22-C23 |
| 53 | o | 502 | CDL | C72-C71-CB7-OB8 |
| 53 | y | 201 | CDL | C52-C51-CB5-OB6 |
| 54 | X | 101 | ZMP | C6-C7-C8-C9 |
| 47 | 1 | 503 | NAI | C2N-C3N-C7N-N7N |
| 51 | L | 1001 | 3PE | C1-O11-P-O12 |
| 52 | w | 801 | PC1 | C1-O11-P-O14 |
| 53 | h | 201 | CDL | CB3-OB5-PB2-OB4 |
| 53 | o | 503 | CDL | CB3-OB5-PB2-OB3 |
| 56 | d | 401 | NDP | O4B-C4B-C5B-O5B |
| 51 | H | 502 | 3PE | C29-C2A-C2B-C2C |
| 51 | N | 401 | 3PE | O31-C31-C32-C33 |
| 50 | H | 501 | 970 | C01-C02-C04-C05 |
| 50 | M | 601 | 970 | C01-C02-C04-C05 |
| 50 | M | 601 | 970 | C01-C02-C04-O08 |
| 51 | L | 1004 | 3PE | C12-C11-O13-P |
| 51 | L | 1004 | 3PE | C1-C2-O21-C21 |
| 51 | M | 602 | 3PE | C12-C11-O13-P |
| 53 | o | 502 | CDL | CB6-CB4-OB6-CB5 |
| 54 | g | 201 | ZMP | O3-C16-C17-C18 |
| 53 | h | 201 | CDL | C52-C51-CB5-OB6 |
| 53 | o | 503 | CDL | C72-C71-CB7-OB9 |
| 51 | L | 1001 | 3PE | C3B-C3C-C3D-C3E |
| 53 | W | 201 | CDL | CA7-C31-C32-C33 |
| 52 | A | 401 | PC1 | O31-C31-C32-C33 |
| 52 | A | 401 | PC1 | C35-C36-C37-C38 |
| 53 | h | 201 | CDL | C52-C51-CB5-OB7 |
| 54 | g | 201 | ZMP | C16-C17-C18-C21 |
| 53 | y | 201 | CDL | C52-C51-CB5-OB7 |
| 51 | L | 1004 | 3PE | O31-C31-C32-C33 |
| 52 | 9 | 401 | PC1 | O31-C31-C32-C33 |
| 52 | M | 603 | PC1 | C28-C29-C2A-C2B |
| 52 | A | 401 | PC1 | C22-C23-C24-C25 |
| 53 | o | 503 | CDL | C72-C73-C74-C75 |

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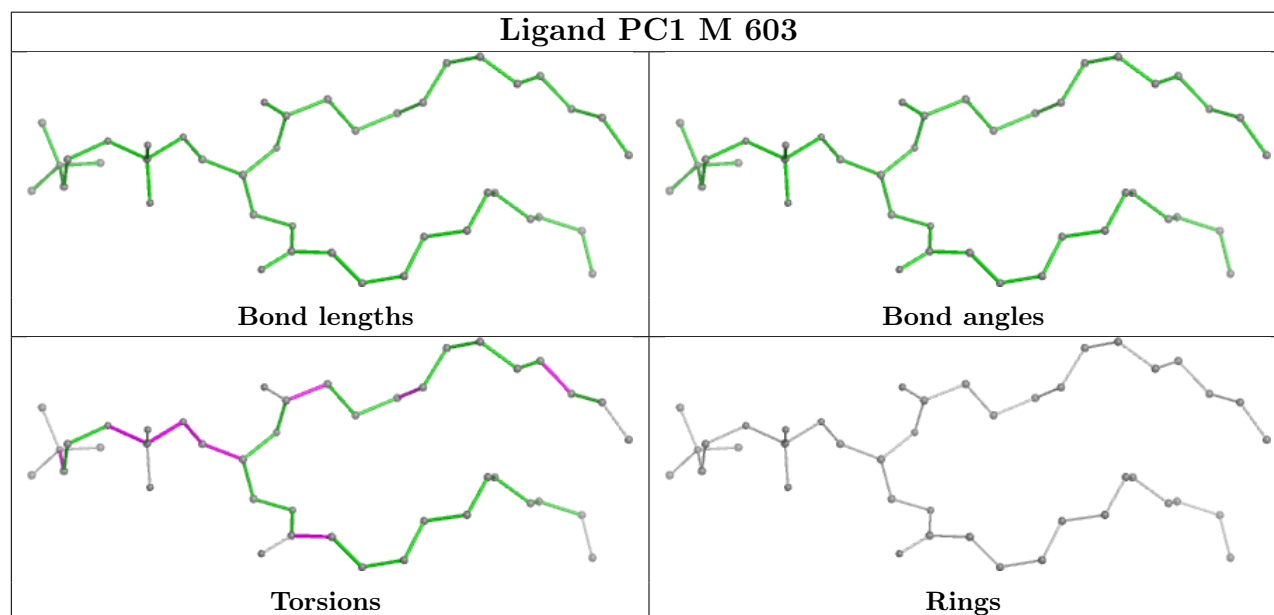
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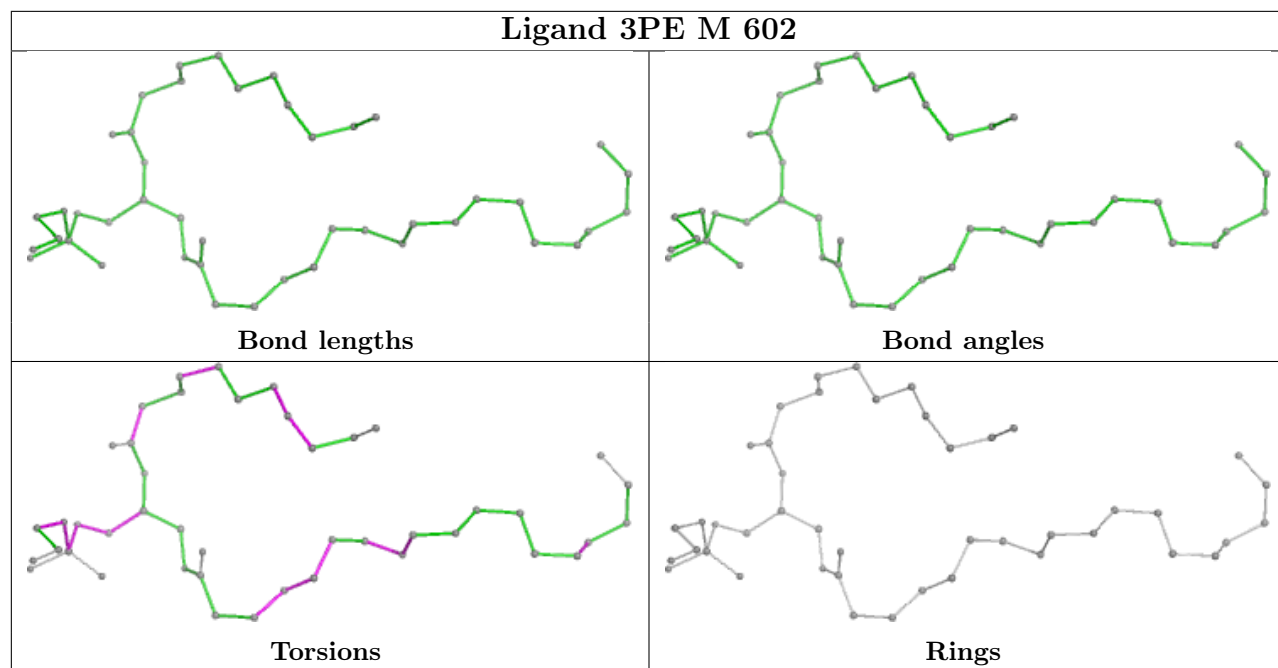
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 53 | y | 201 | CDL | C60-C61-C62-C63 |
| 51 | L | 1004 | 3PE | O32-C31-C32-C33 |
| 53 | o | 502 | CDL | C72-C71-CB7-OB9 |
| 52 | L | 1002 | PC1 | C2F-C2G-C2H-C2I |
| 52 | M | 603 | PC1 | O32-C31-C32-C33 |
| 52 | w | 801 | PC1 | C34-C35-C36-C37 |

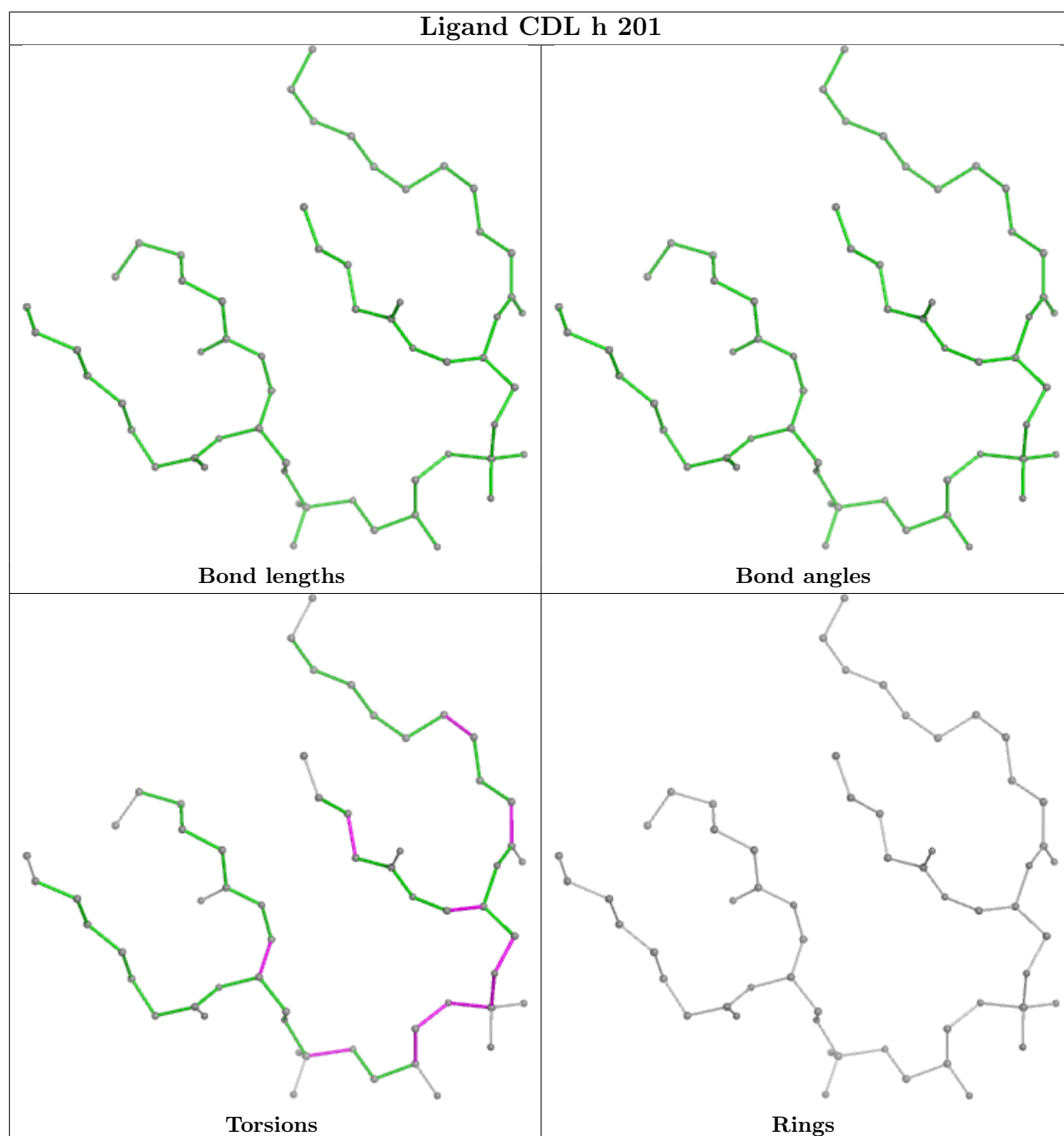
There are no ring outliers.

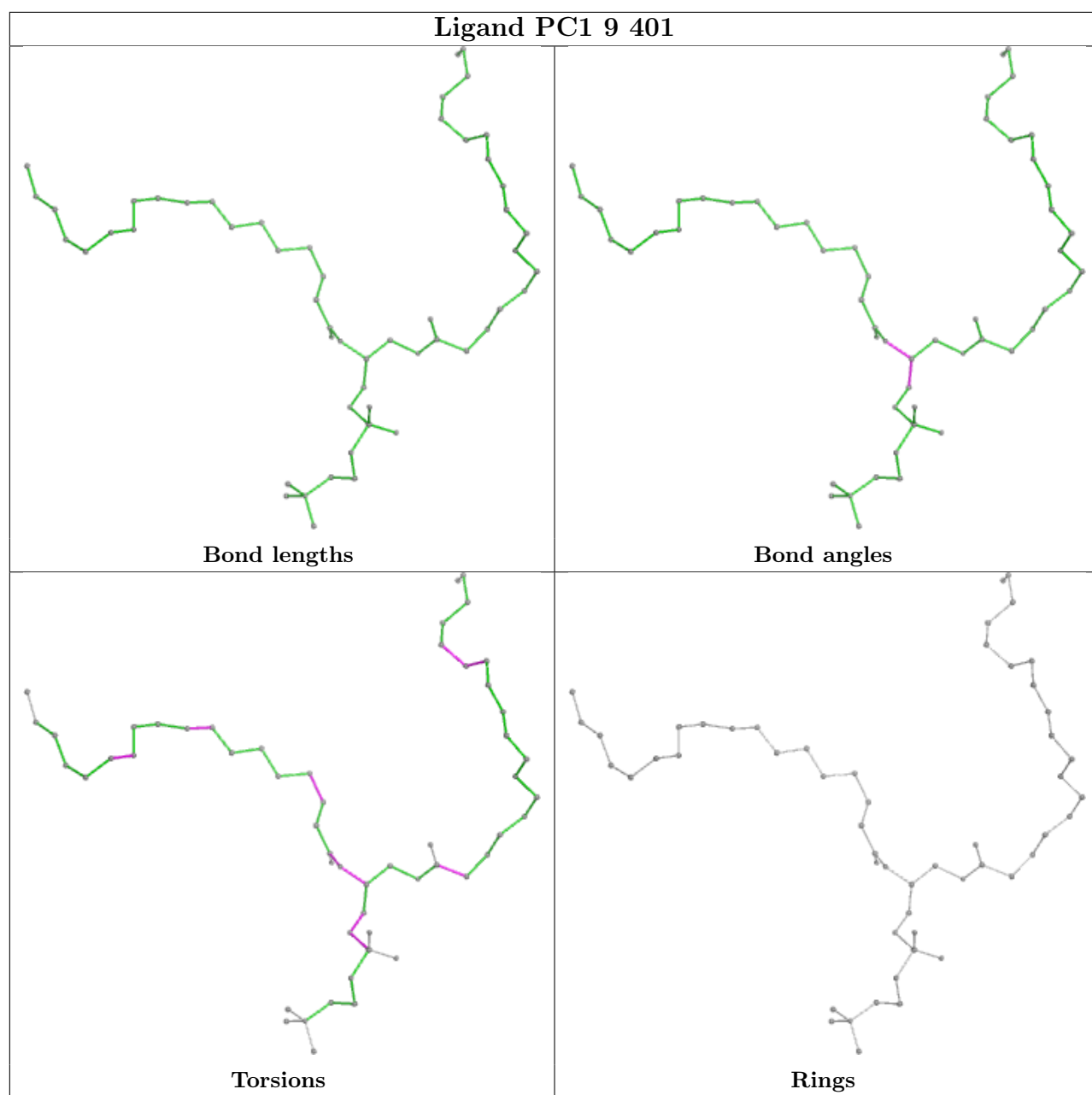
No monomer is involved in short contacts.

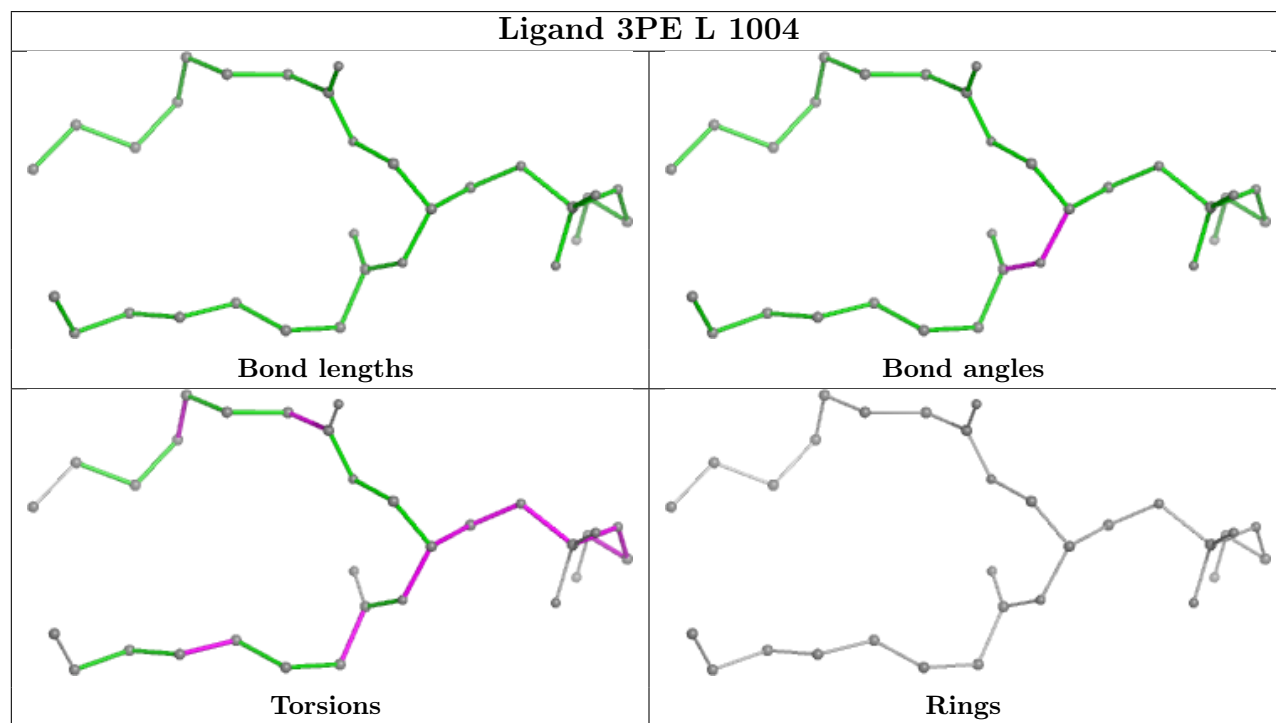
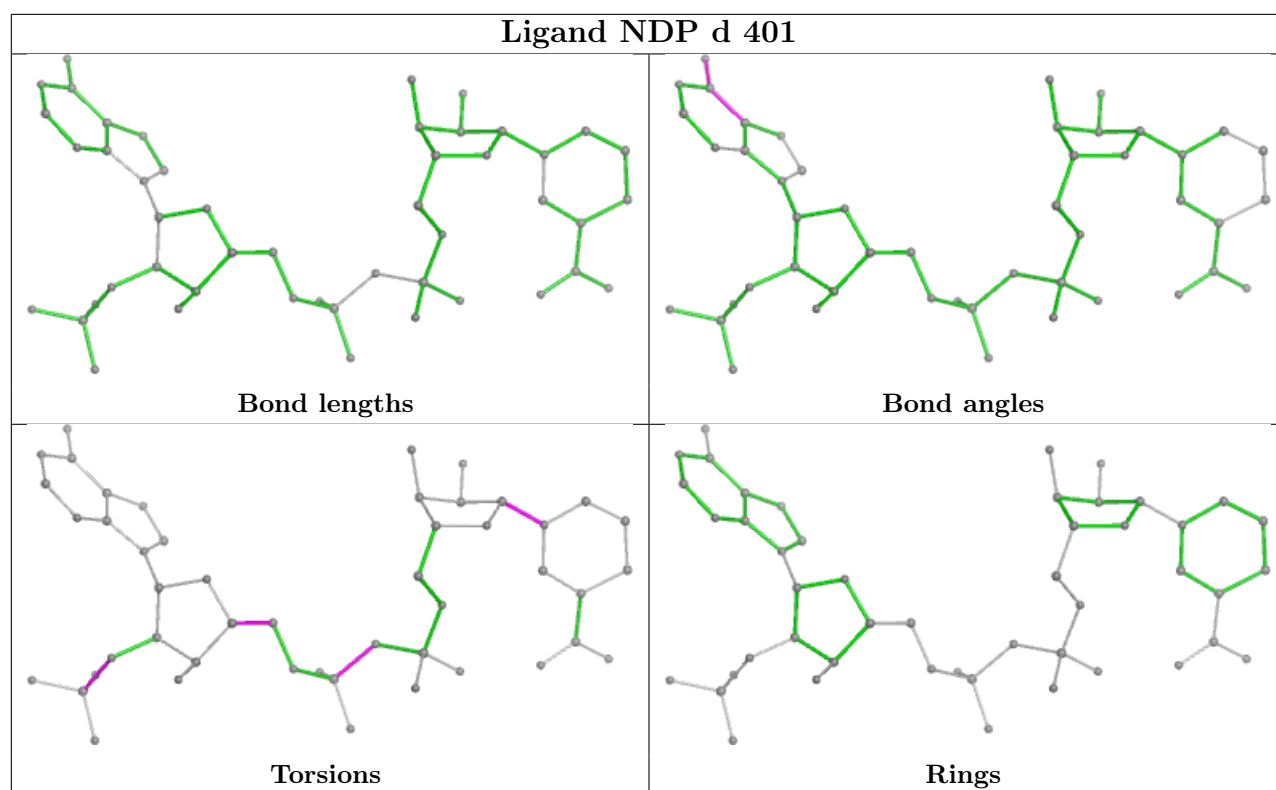
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

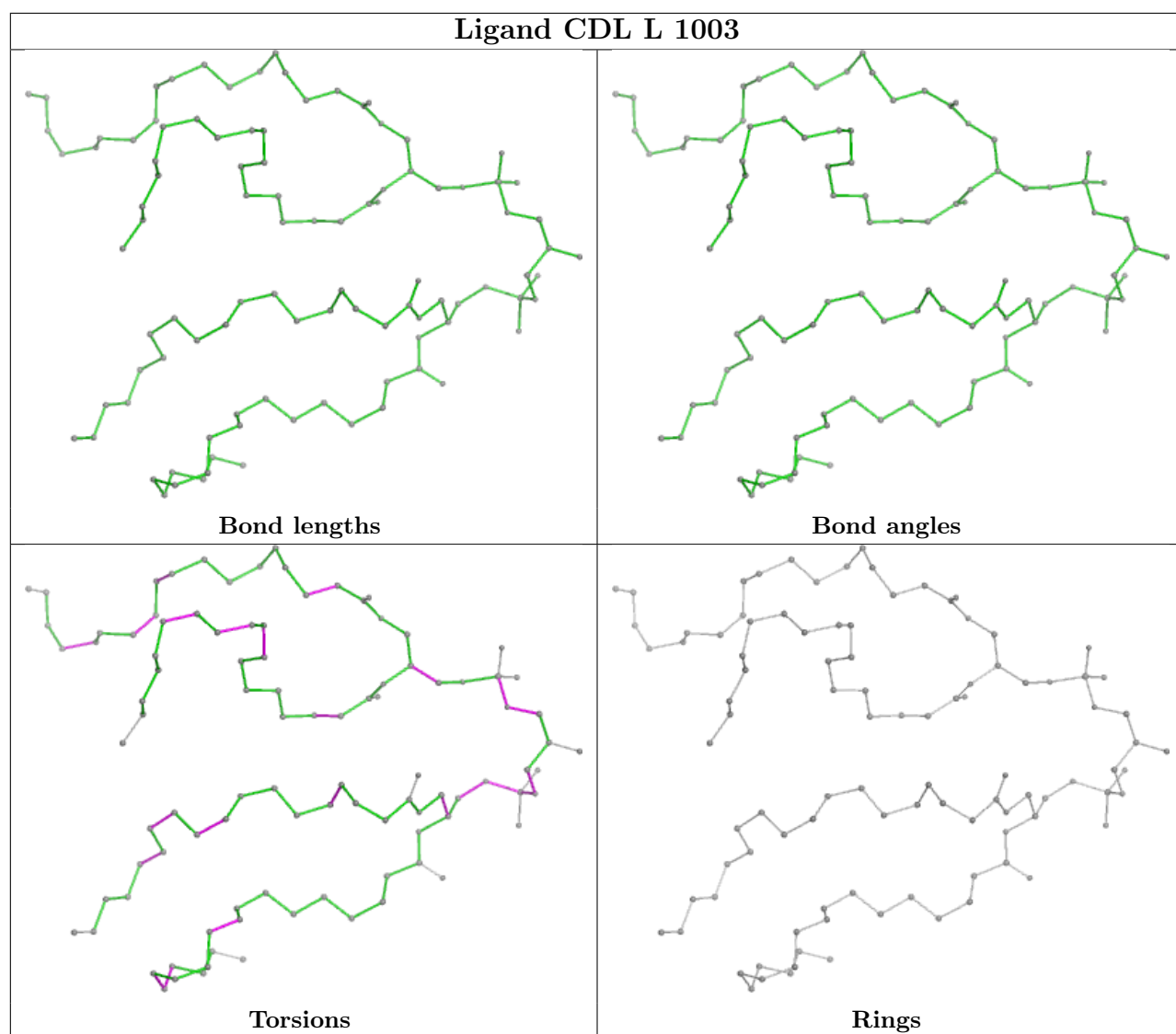


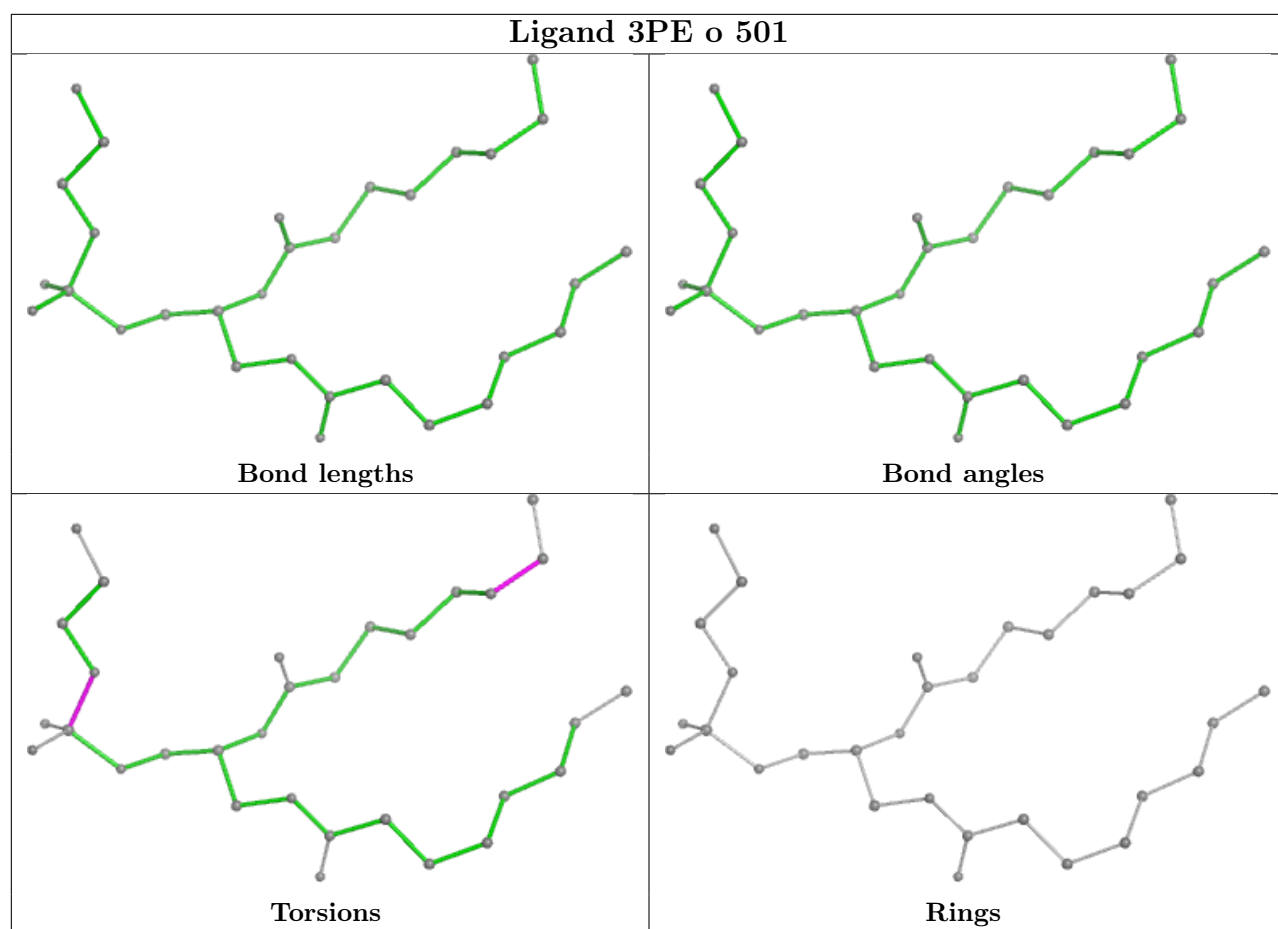


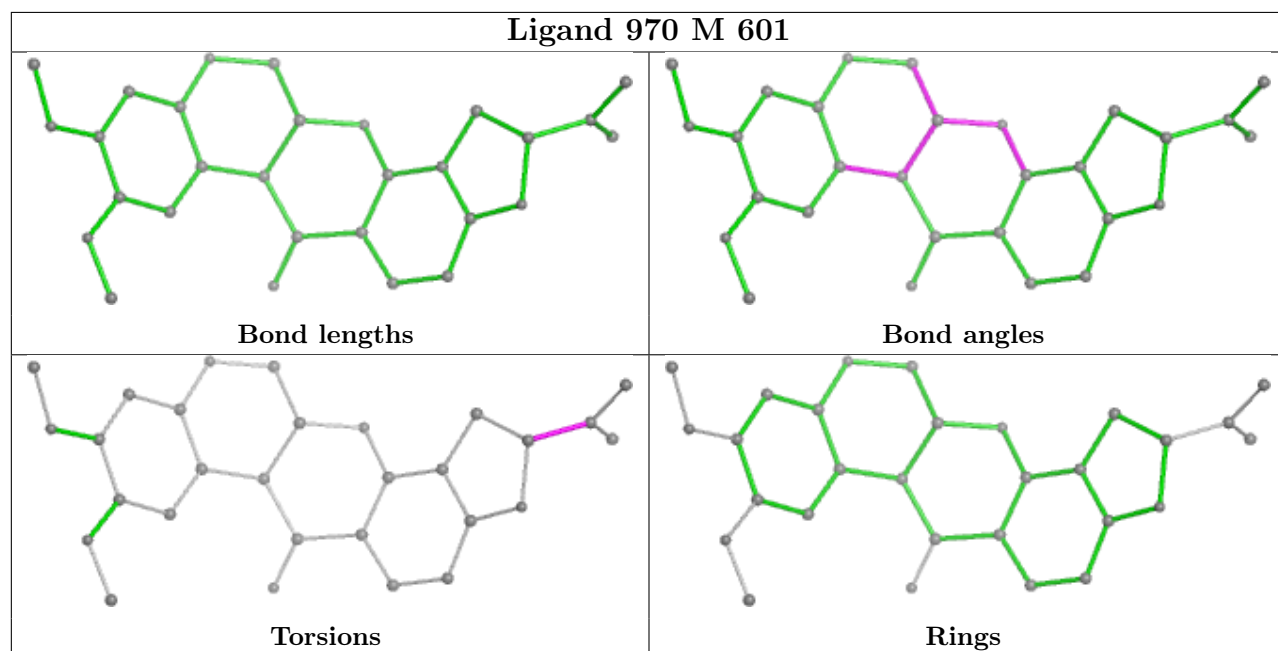
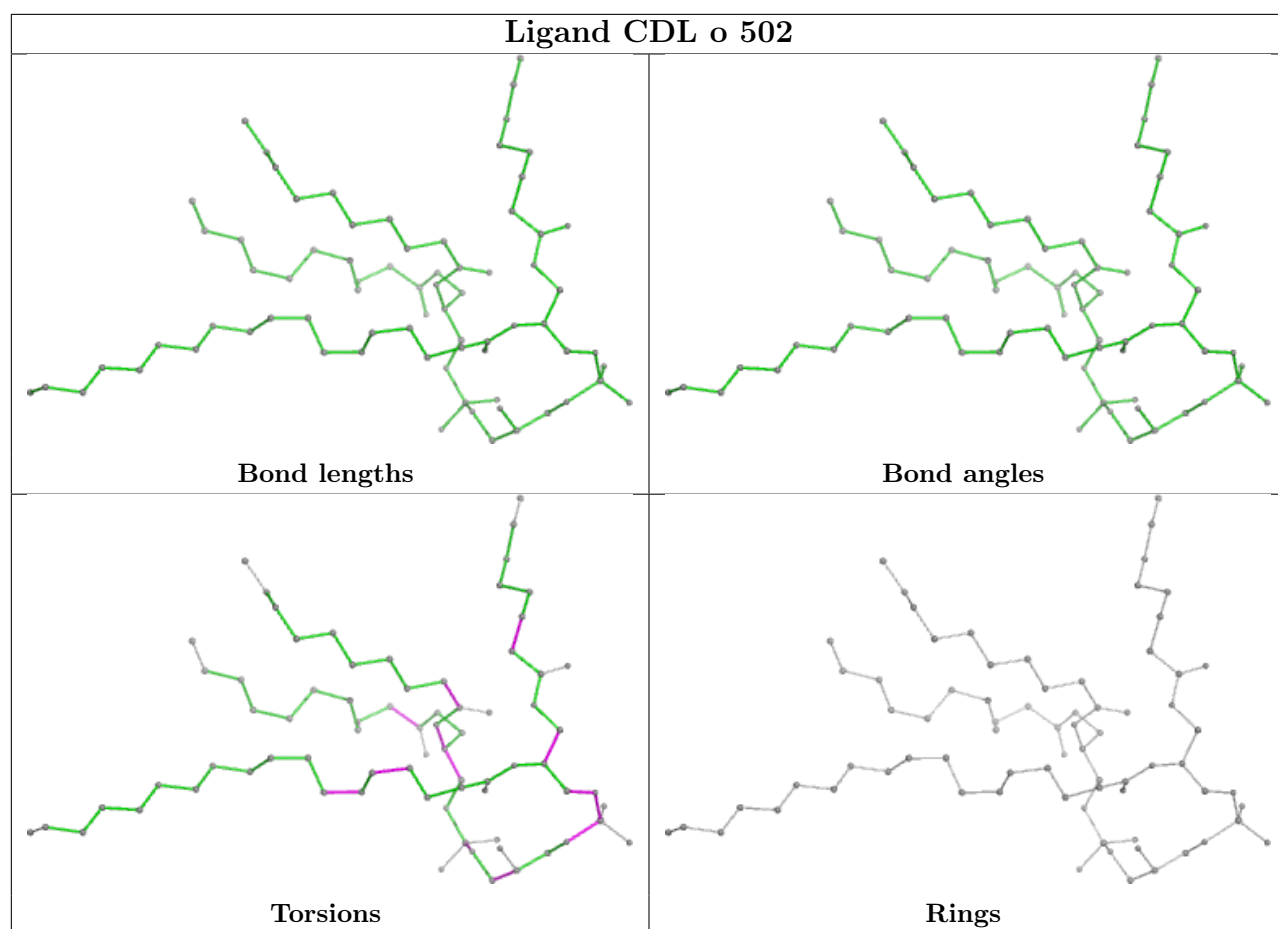


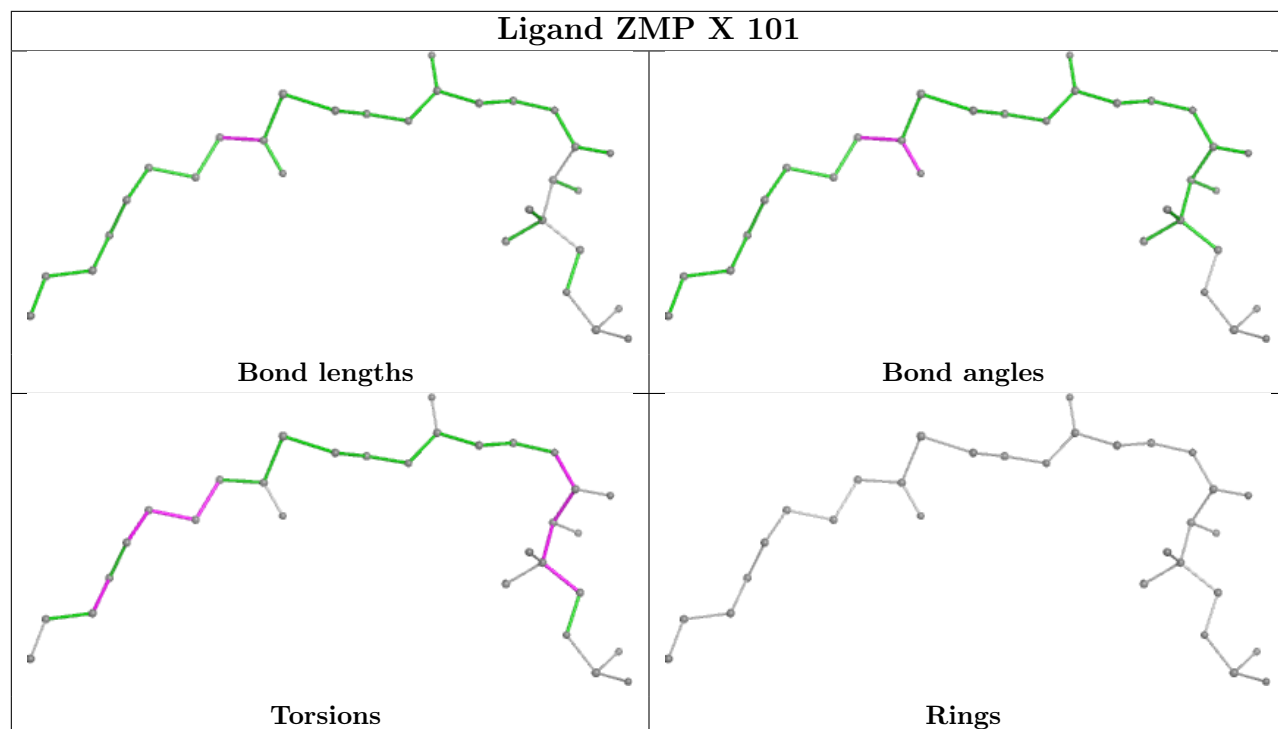


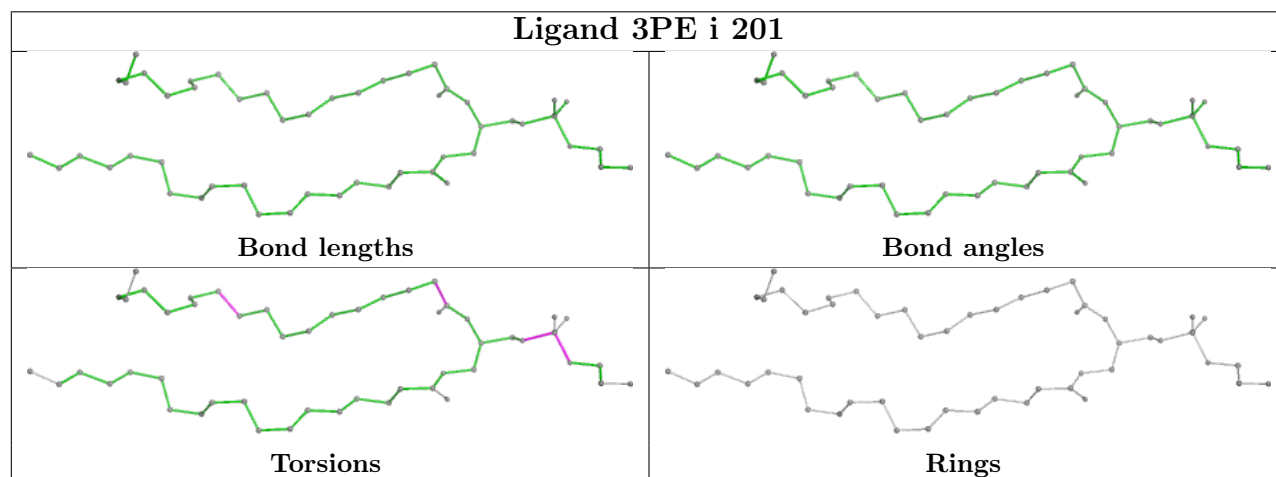
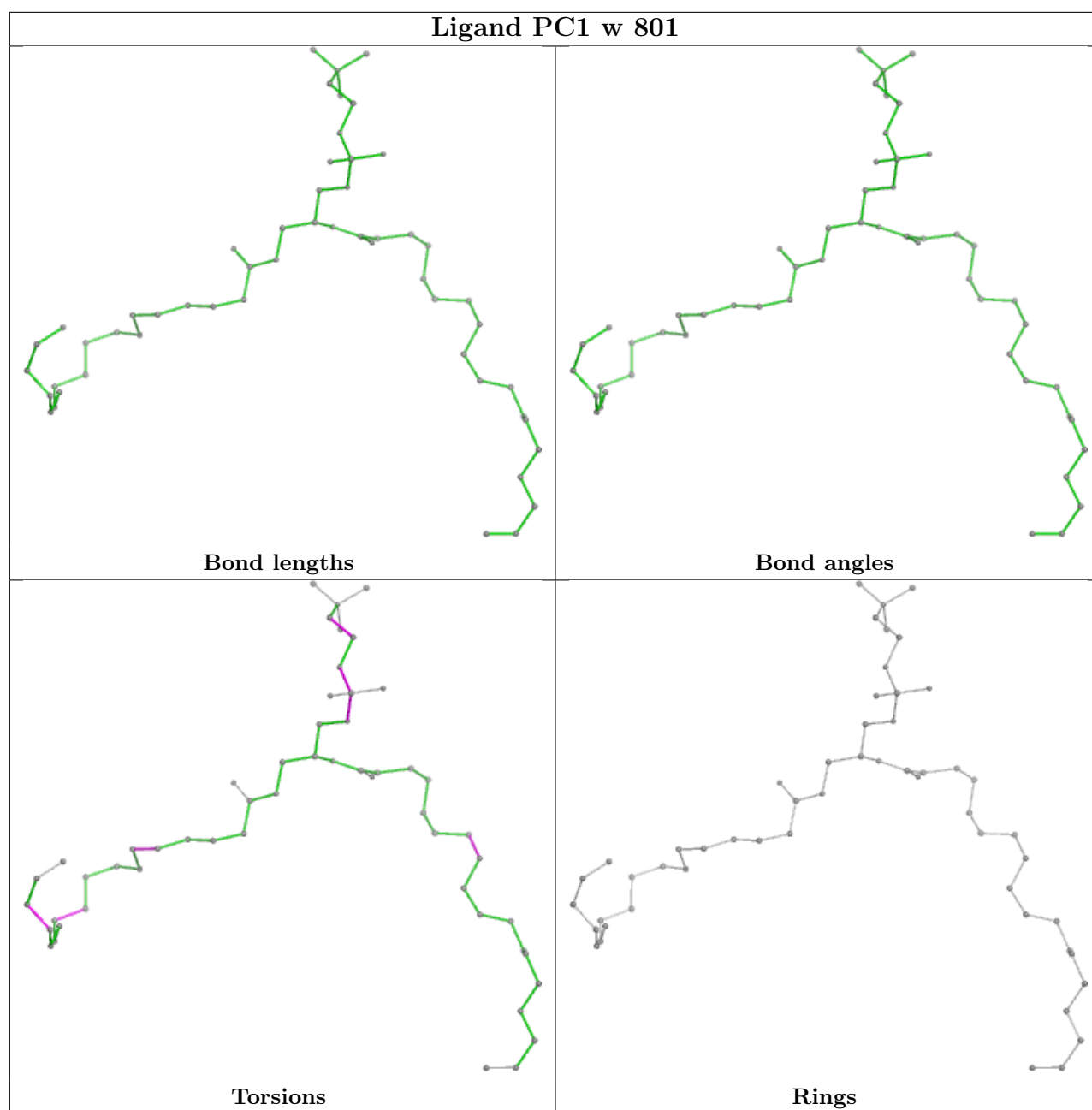


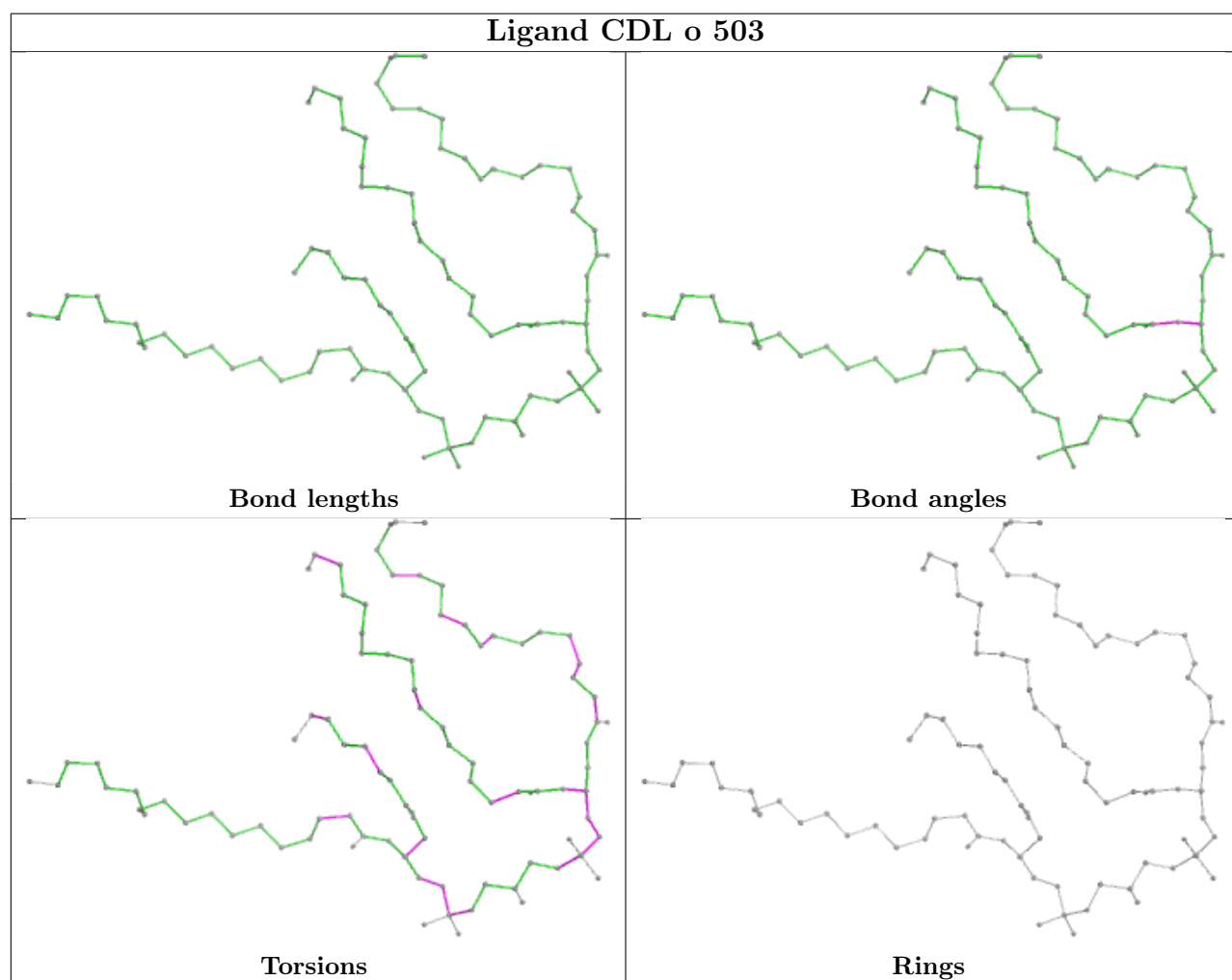
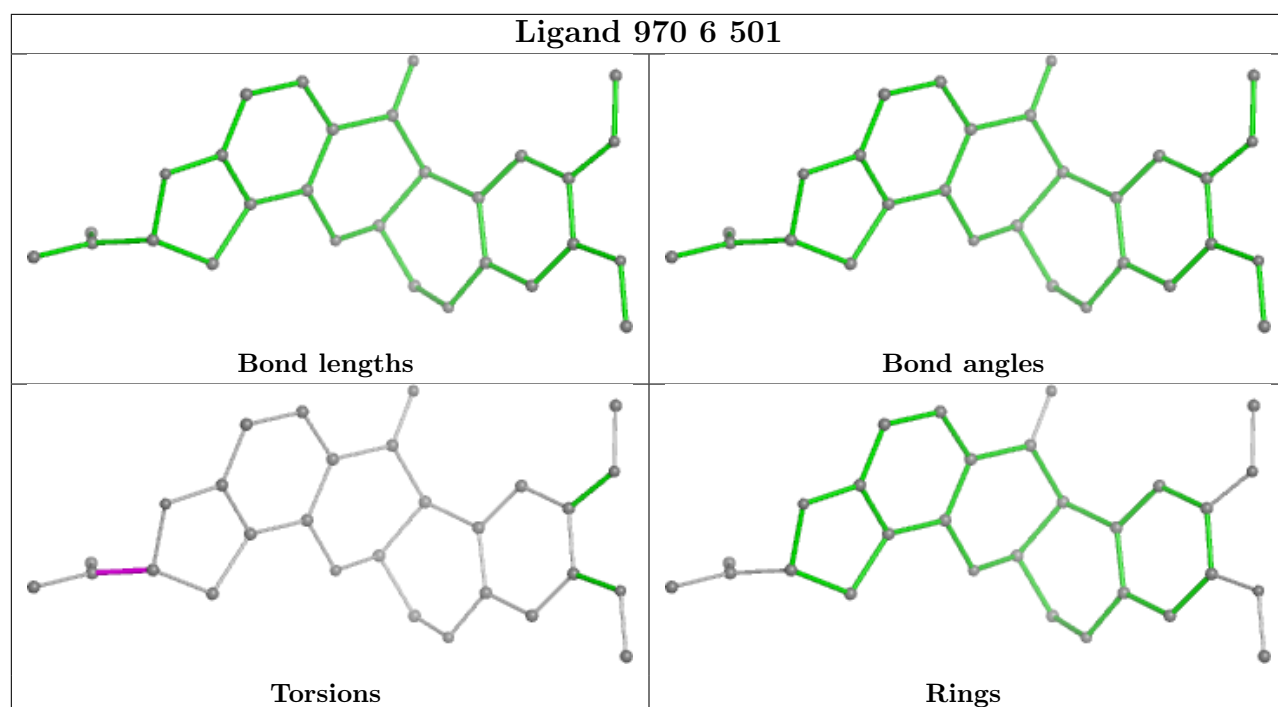


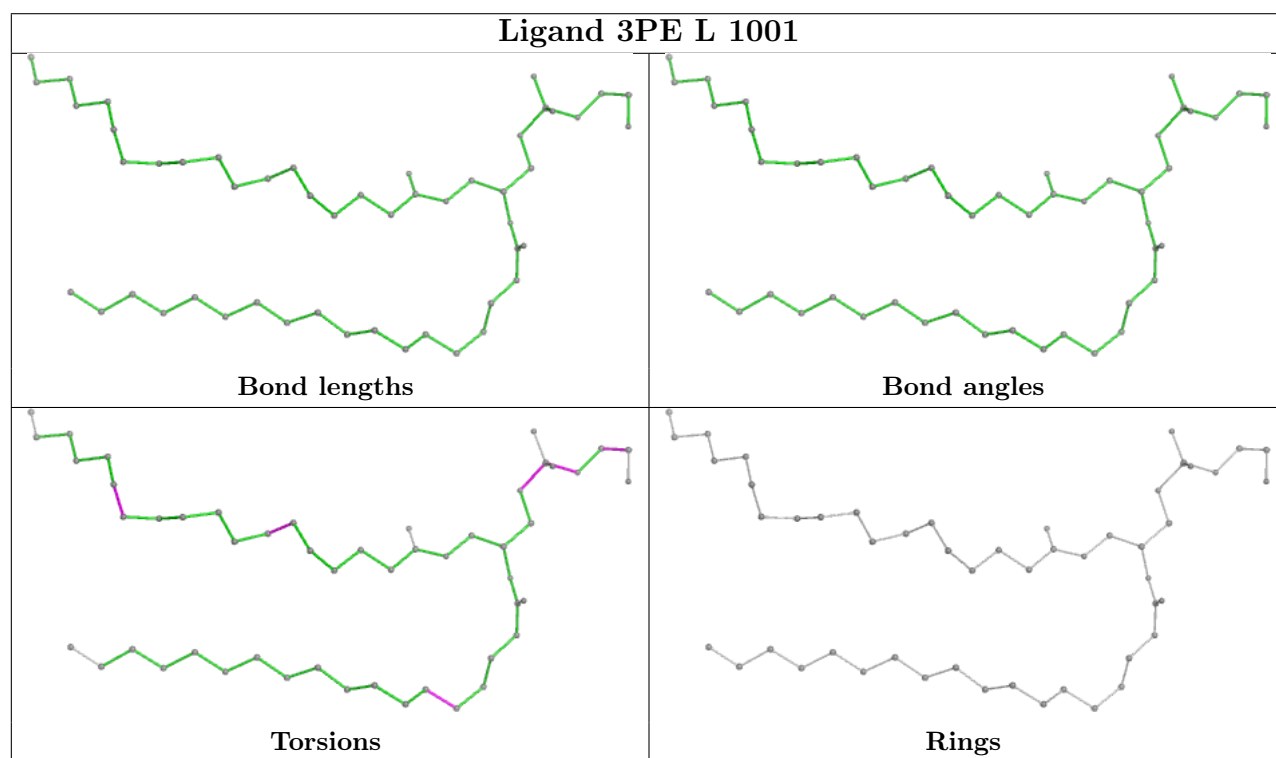
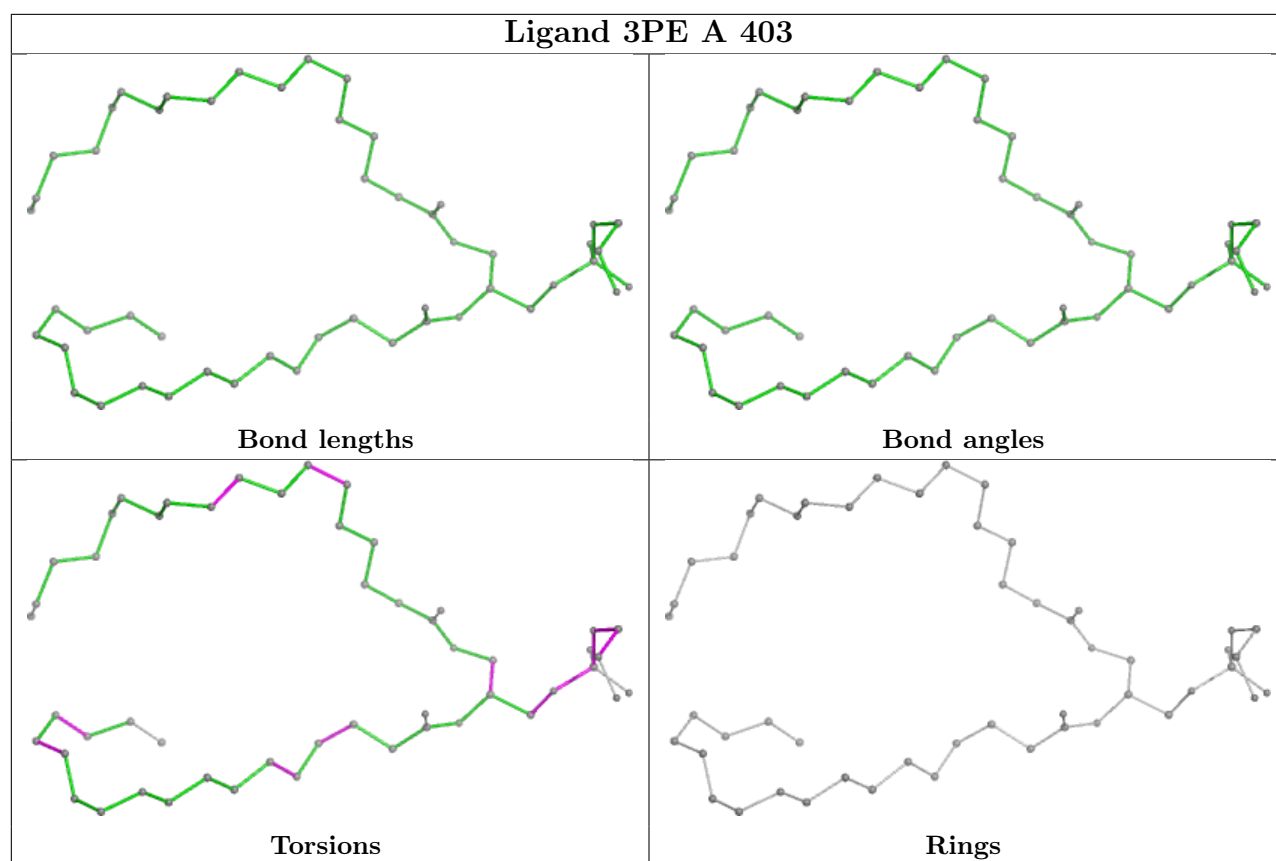


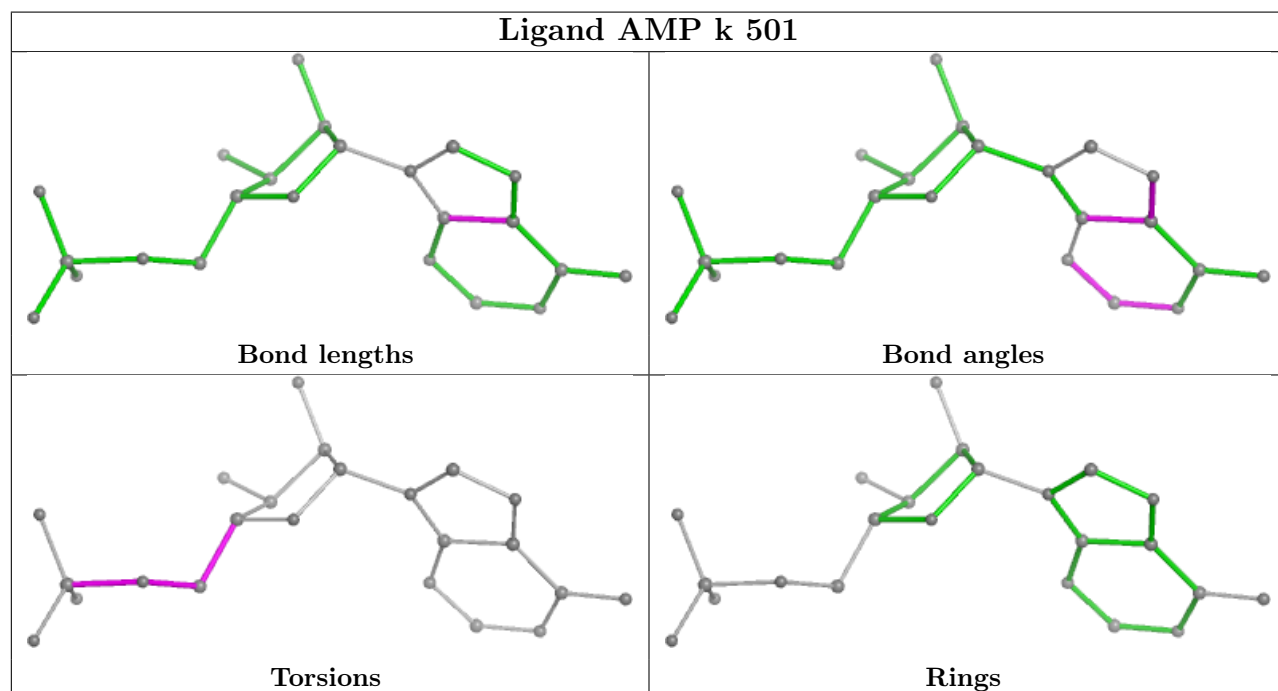
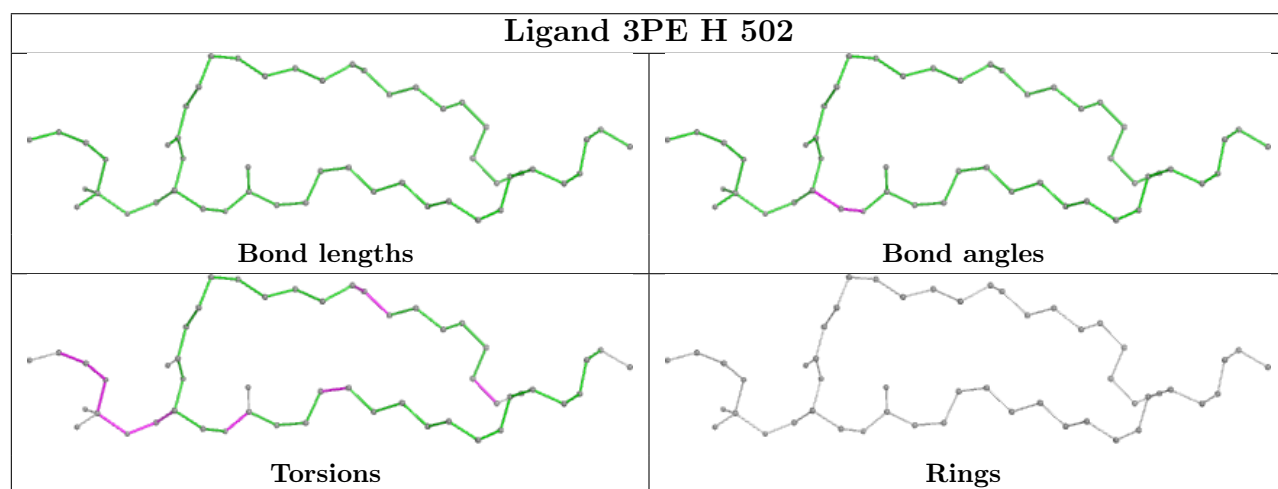
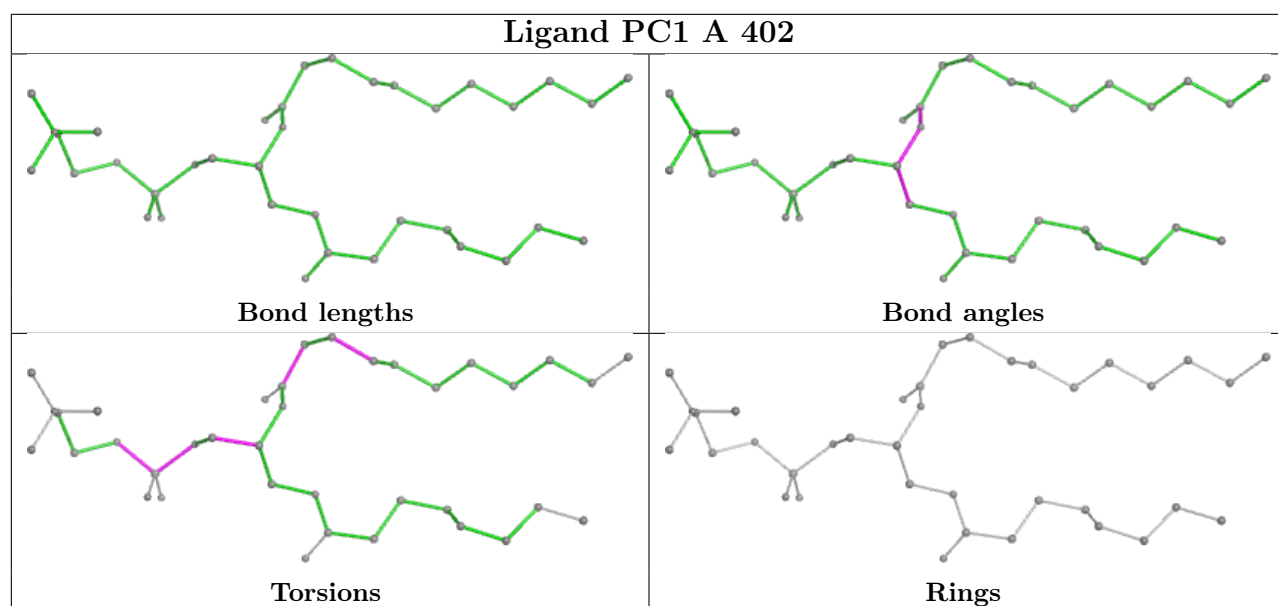


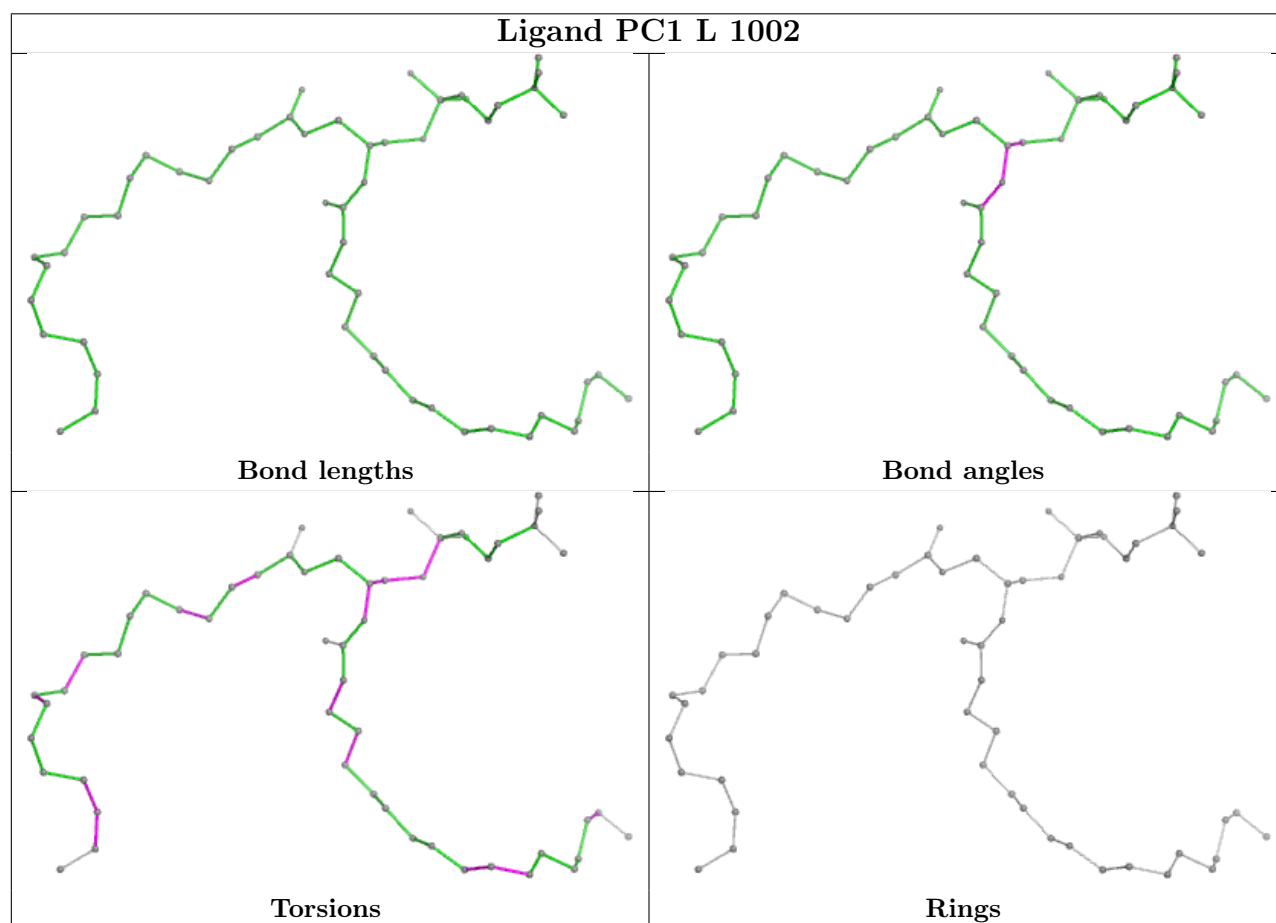
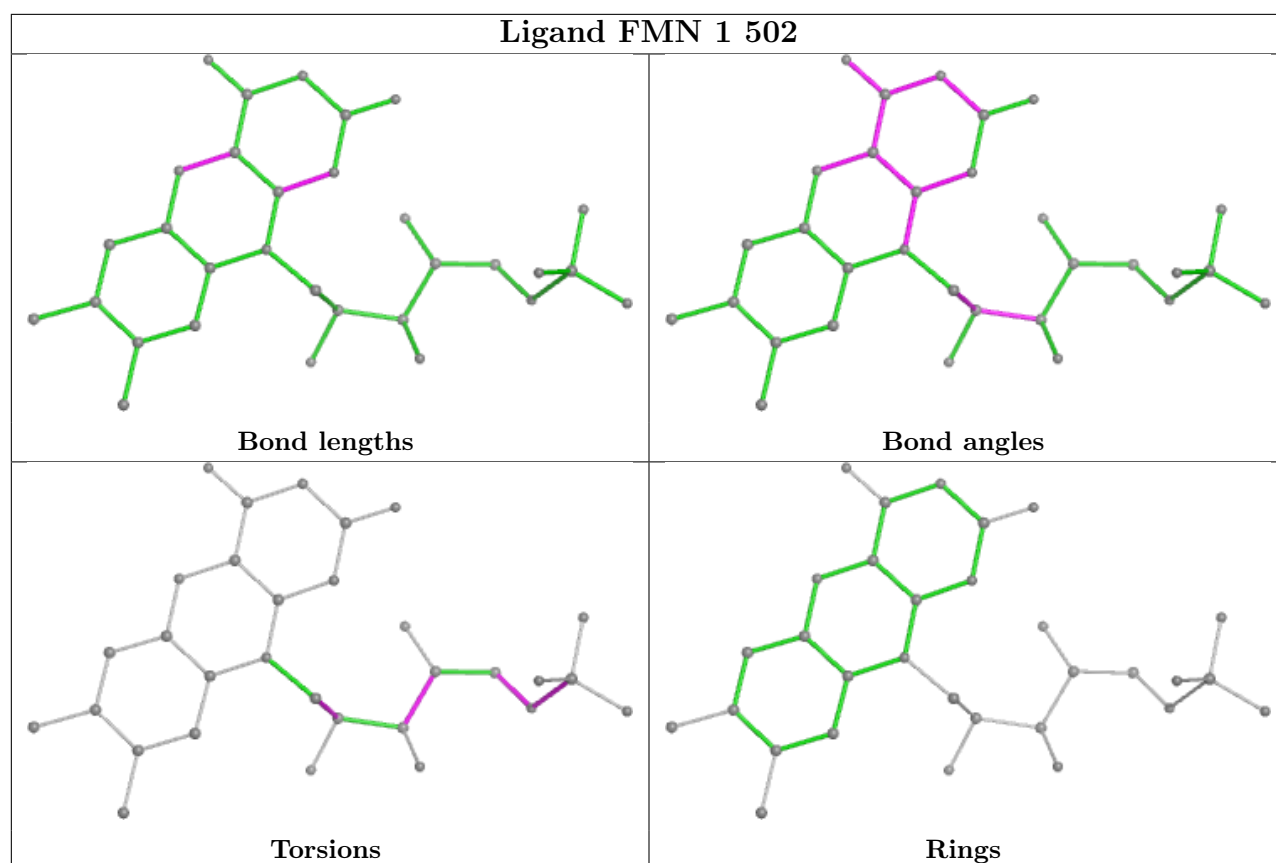


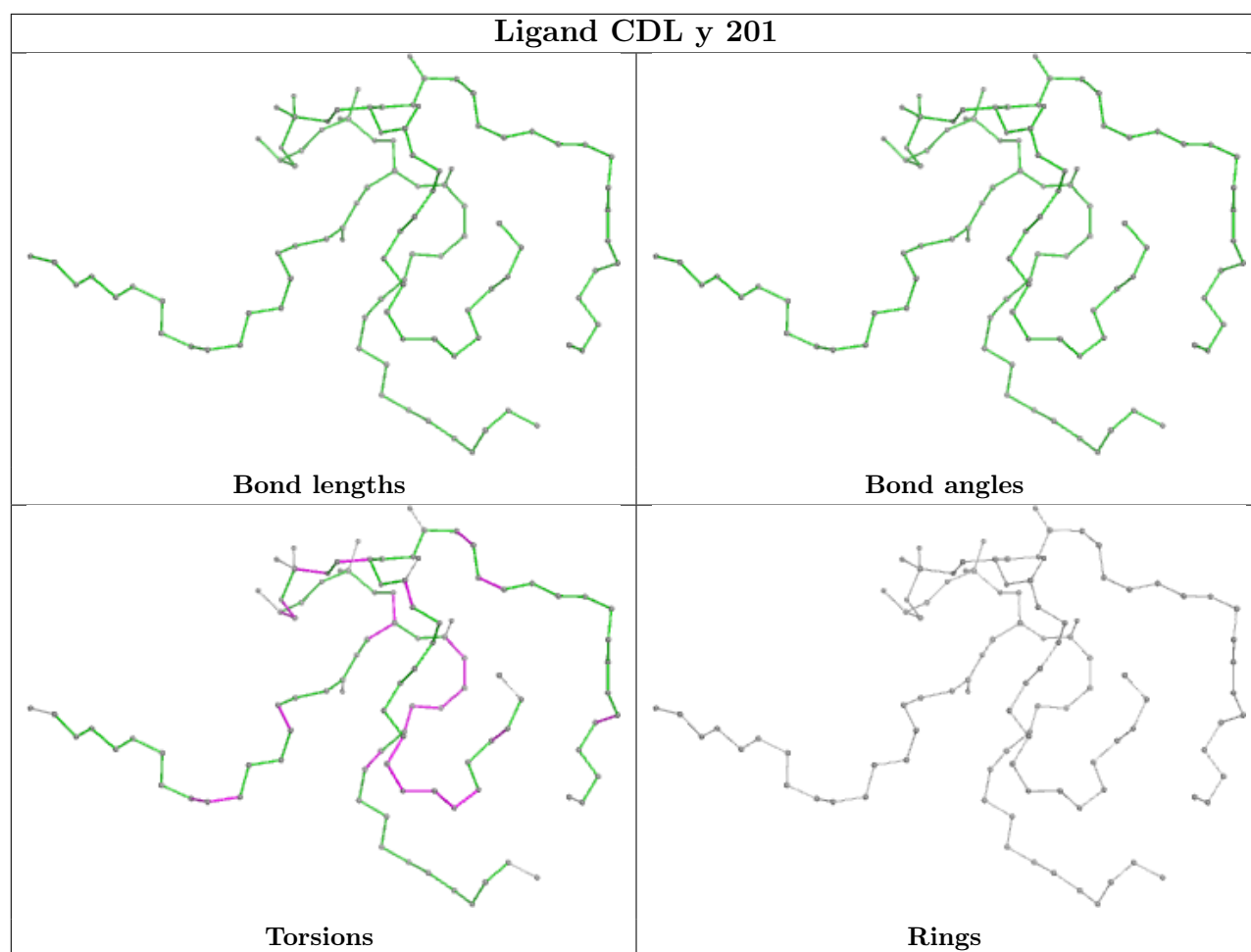




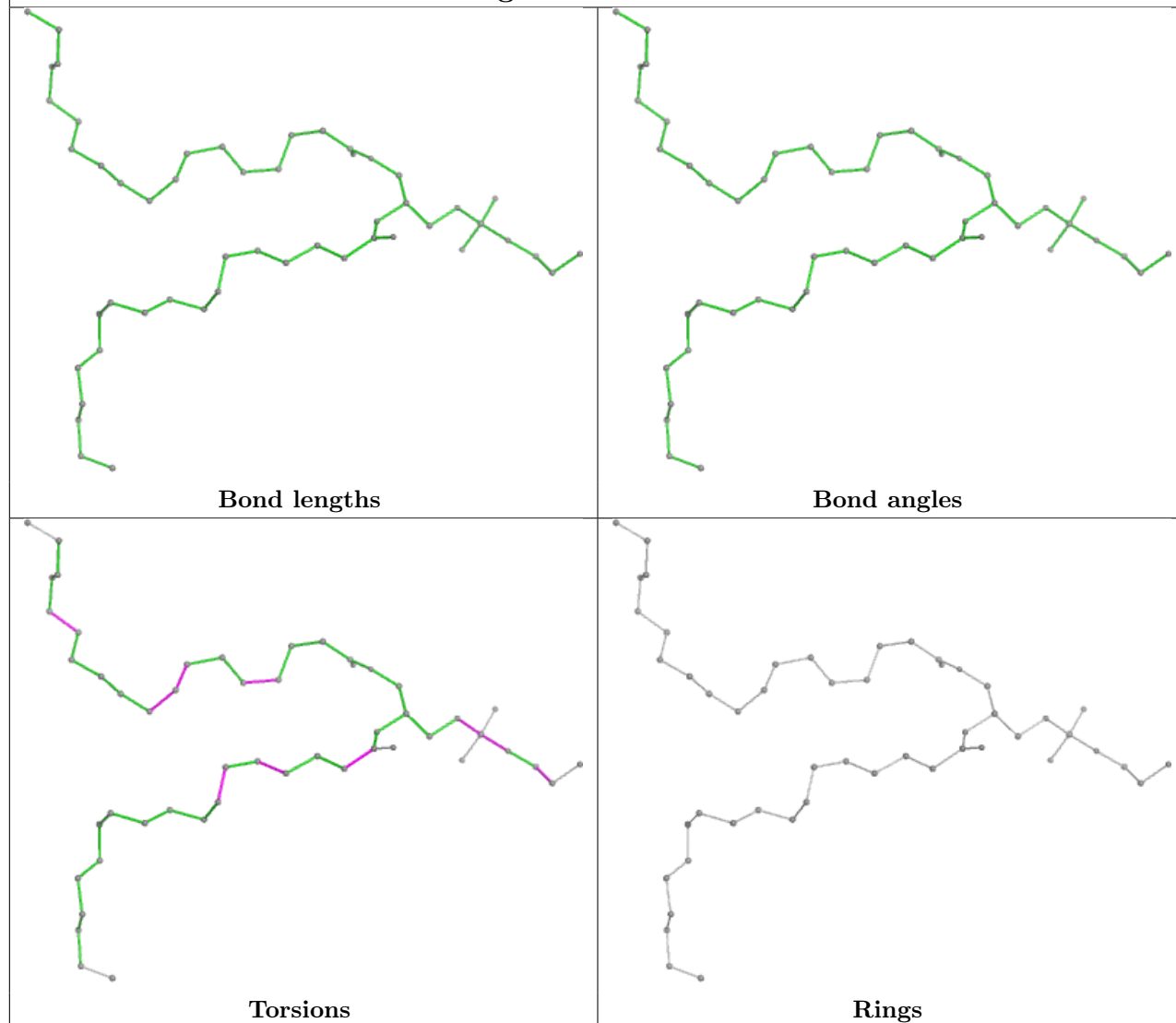




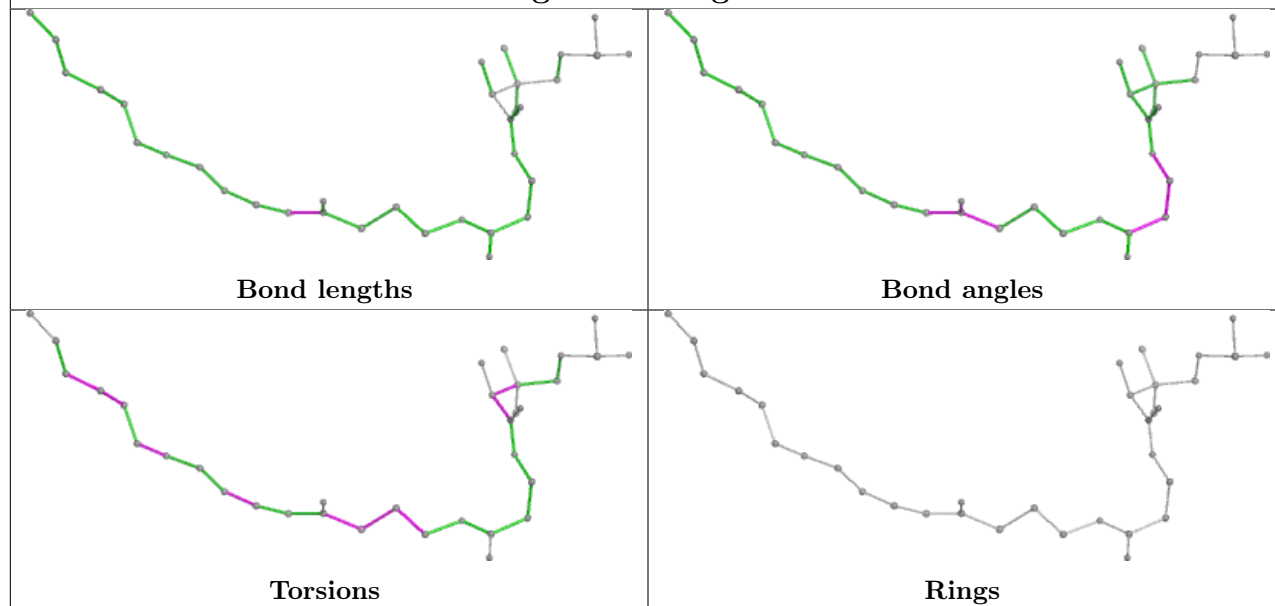


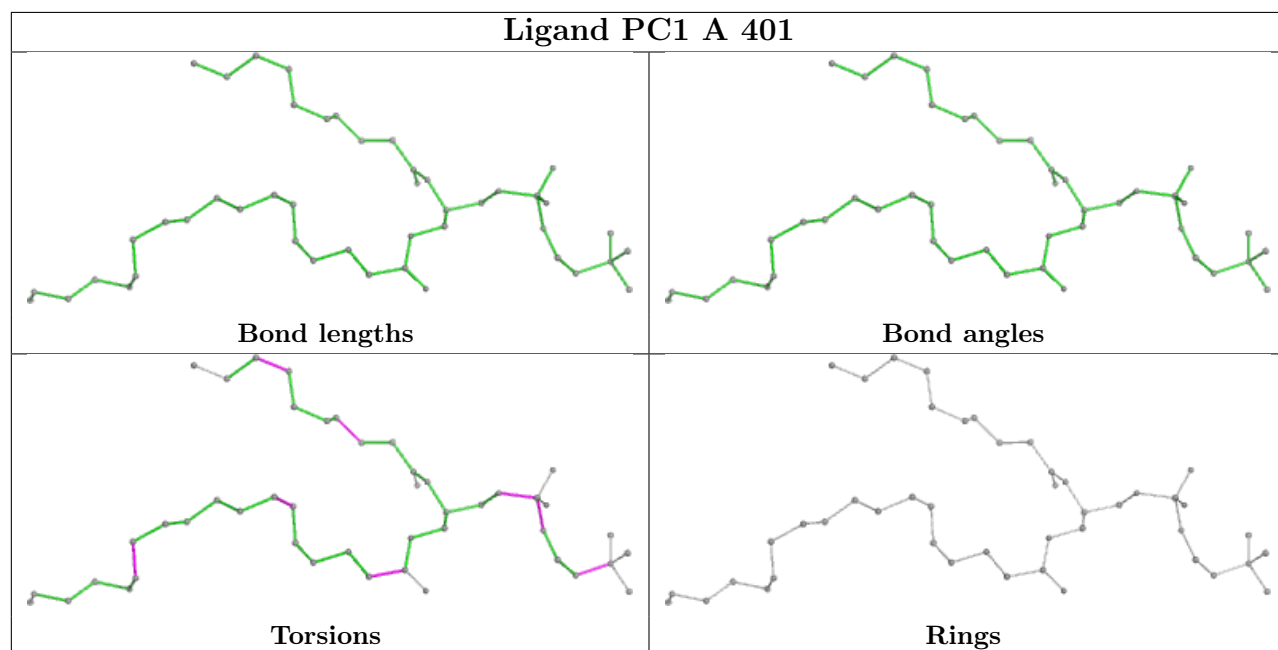
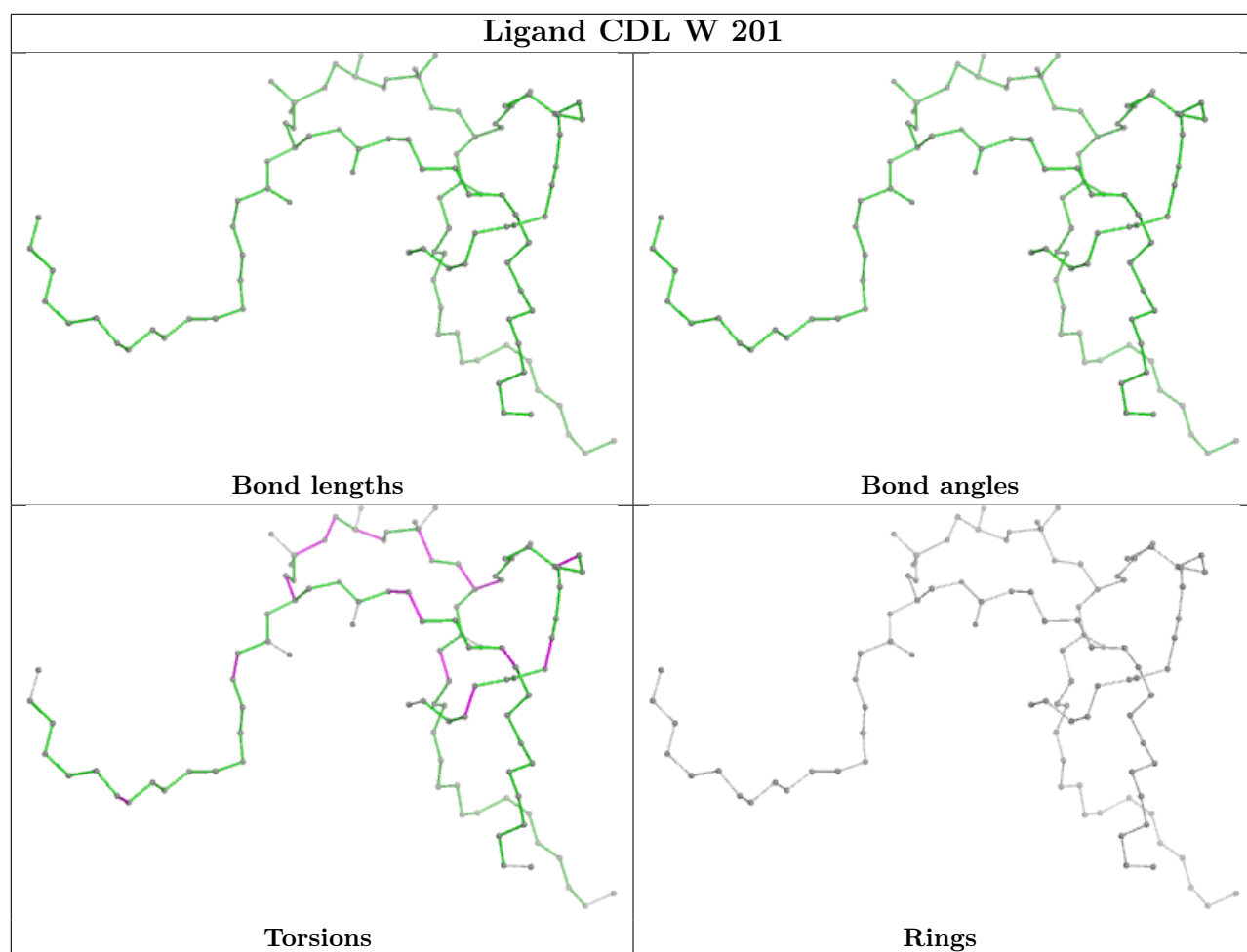


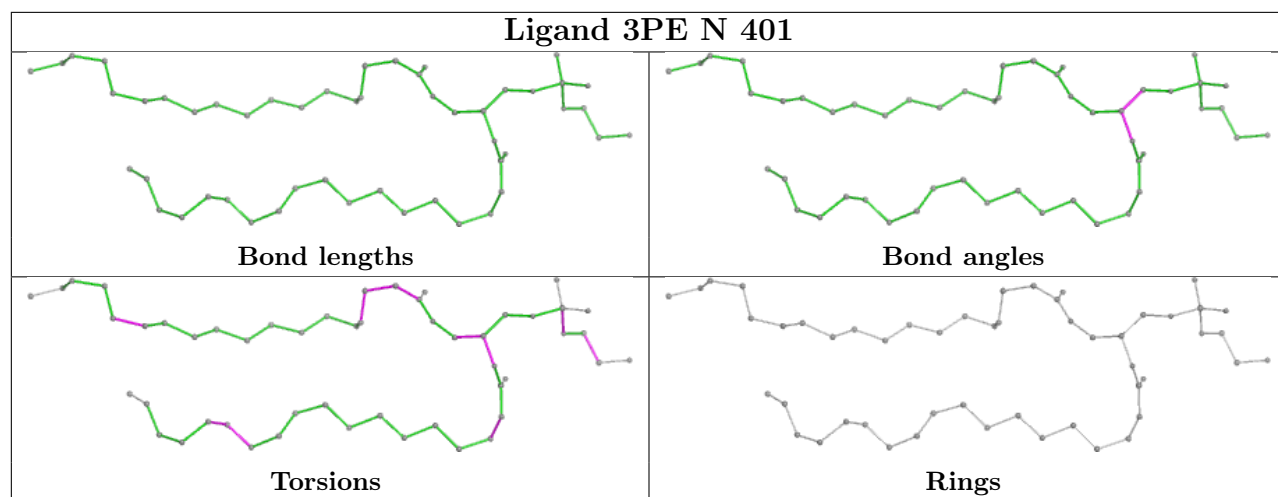
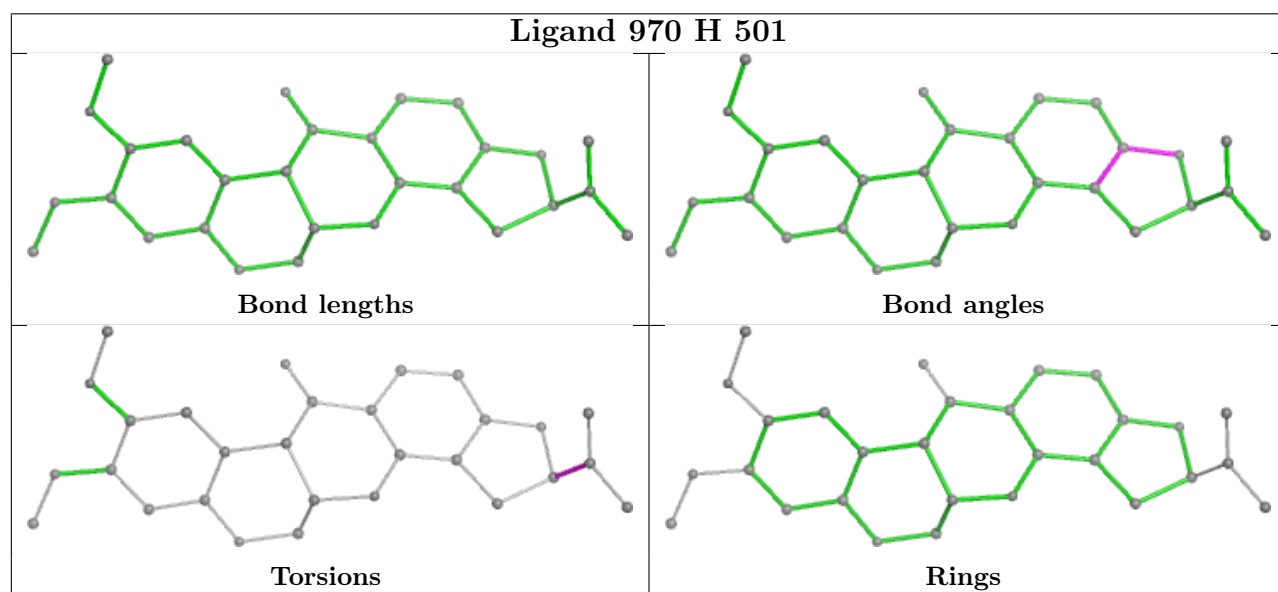
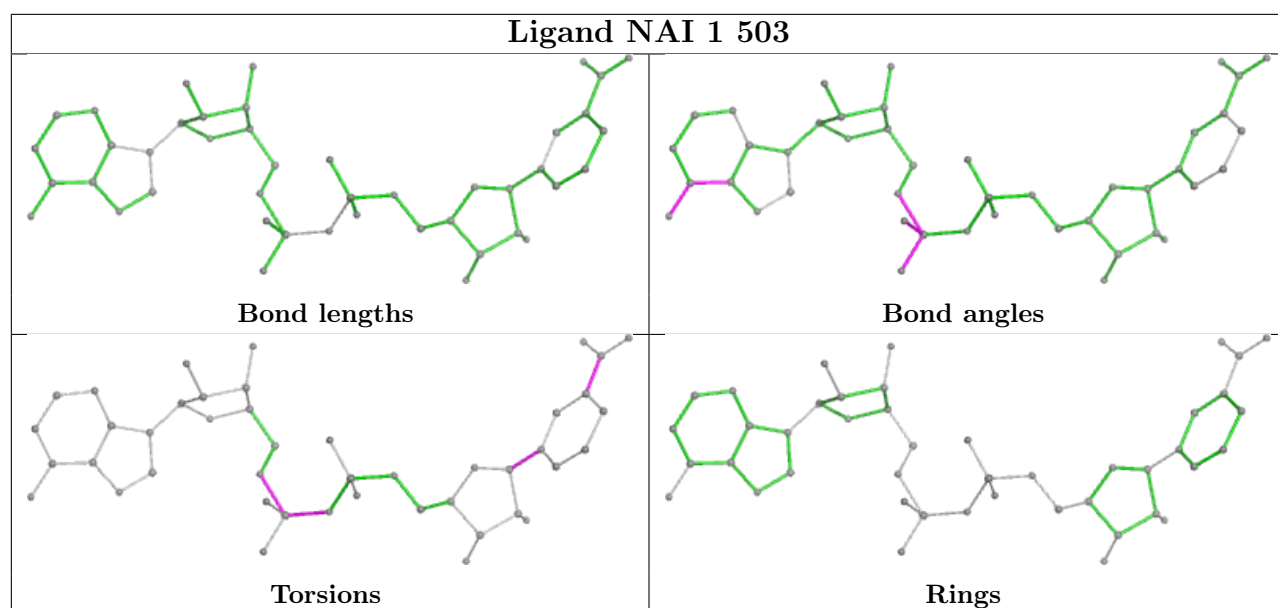
Ligand 3PE 6 503



Ligand ZMP g 201







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-11255. 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](#)

This section was not generated.

6.2 Central slices [i](#)

This section was not generated.

6.3 Largest variance slices [i](#)

This section was not generated.

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

This section was not generated.

6.5 Orthogonal surface views [i](#)

This section was not generated.

6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.