



wwPDB EM Validation Summary Report ⓘ

Jun 13, 2024 – 11:05 AM EDT

PDB ID : 8UEO
EMDB ID : EMD-42165
Title : In-situ complex I (Active-Apo)
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

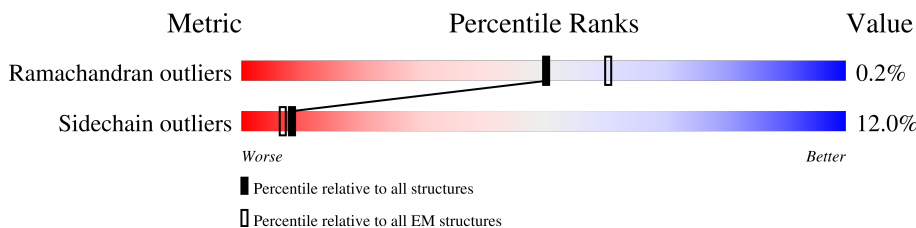
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 1A | 115 | 25% (red), 91% (green), 9% (yellow) |
| 2 | 1B | 258 | 9% (red), 50% (green), 9% (yellow), 40% (grey) |
| 3 | 1C | 264 | 14% (red), 70% (green), 8% (yellow), 21% (grey) |
| 4 | 1D | 476 | 12% (red), 80% (green), 10% (yellow), 10% (grey) |
| 5 | 1E | 249 | 57% (red), 80% (green), 6% (yellow), 14% (grey) |
| 6 | 1F | 464 | 59% (red), 84% (green), 8% (yellow), 7% (grey) |
| 7 | 1G | 727 | 35% (red), 87% (green), 9% (yellow), 1% (grey) |
| 8 | 1H | 318 | 15% (red), 89% (green), 10% (yellow) |
| 9 | 1I | 239 | 8% (red), 65% (green), 8% (yellow), 26% (grey) |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------------|
| 10 | 1J | 175 | 27% 82% 15% .. |
| 11 | 1K | 98 | 21% 82% 16% .. |
| 12 | 1L | 606 | 13% 91% 9% |
| 13 | 1M | 459 | 5% 88% 12% |
| 14 | 1N | 347 | 5% 91% 8% . |
| 15 | 1O | 357 | 46% 78% 11% 10% |
| 16 | 1P | 377 | 44% 80% 10% 9% |
| 17 | 1Q | 175 | 27% 64% 10% 26% |
| 18 | 1R | 123 | 33% 69% 9% 22% |
| 19 | 1S | 99 | 71% 69% 19% 12% |
| 20 | 1T | 156 | 41% 47% 8% 46% |
| 20 | 1U | 156 | 19% 48% 6% . 45% |
| 21 | 1V | 116 | 47% 82% 16% .. |
| 22 | 1W | 128 | 41% 76% 13% . 10% |
| 23 | 1X | 172 | 26% 91% 8% .. |
| 24 | 1Y | 141 | 14% 91% 7% .. |
| 25 | 1Z | 144 | 19% 87% 10% .. |
| 26 | 1a | 70 | 16% 90% 10% |
| 27 | 1b | 84 | 29% 90% 7% .. |
| 28 | 1c | 76 | 33% 51% 9% . 36% |
| 29 | 1d | 123 | 19% 88% 11% . |
| 30 | 1e | 106 | 17% 72% 20% . 7% |
| 31 | 1f | 135 | 22% 36% 7% 58% |
| 32 | 1g | 154 | 25% 56% 8% . 35% |
| 33 | 1h | 189 | 15% 61% 11% . 27% |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34 | 1i | 128 | |
| 35 | 1j | 105 | |
| 36 | 1k | 98 | |
| 37 | 1l | 186 | |
| 38 | 1m | 129 | |
| 39 | 1n | 179 | |
| 40 | 1o | 137 | |
| 41 | 1p | 176 | |
| 42 | 1q | 145 | |
| 43 | 1r | 113 | |
| 44 | 1s | 471 | |

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 68031 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-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | 1A | 115 | 914 | 615 | 134 | 158 | 7 | 0 | 0 |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | 1B | 155 | 1242 | 791 | 226 | 211 | 14 | 0 | 0 |

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | 1C | 209 | 1740 | 1125 | 297 | 316 | 2 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| 1C | 104 | GLN | ARG | conflict | UNP A0A286ZNN4 |
| 1C | 154 | GLY | ASP | conflict | UNP A0A286ZNN4 |

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | 1D | 429 | 3452 | 2207 | 593 | 628 | 24 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| 1D | 0 | GLY | GLU | conflict | UNP A0A8D0QM68 |

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | 1E | 214 | 1658 | 1058 | 278 | 312 | 10 | 0 | 0 |

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | 1F | 432 | 3325 | 2100 | 592 | 613 | 20 | 0 | 0 |

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | 1G | 699 | 5362 | 3360 | 933 | 1029 | 40 | 0 | 0 |

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | 1H | 317 | 2494 | 1667 | 384 | 423 | 20 | 0 | 0 |

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | 1I | 176 | 1412 | 887 | 243 | 269 | 13 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | 1J | 173 | 1322 | 888 | 188 | 234 | 12 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11 | 1K | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 488 | 112 | 127 | 13 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | 1L | 605 | Total | C | N | O | S | 0 | 0 |
| | | | 4808 | 3189 | 745 | 824 | 50 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13 | 1M | 458 | Total | C | N | O | S | 0 | 0 |
| | | | 3622 | 2405 | 571 | 608 | 38 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | 1N | 346 | Total | C | N | O | S | 0 | 0 |
| | | | 2702 | 1777 | 419 | 461 | 45 | | |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15 | 1O | 320 | Total | C | N | O | S | 0 | 0 |
| | | | 2590 | 1649 | 440 | 491 | 10 | | |

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16 | 1P | 342 | Total | C | N | O | S | 0 | 0 |
| | | | 2751 | 1783 | 481 | 478 | 9 | | |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | 1Q | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1047 | 659 | 186 | 199 | 3 | | |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | 1R | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 741 | 452 | 140 | 146 | 3 | | |

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | 1S | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 700 | 440 | 131 | 127 | 2 | | |

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | 1T | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 689 | 445 | 101 | 138 | 5 | | |
| 20 | 1U | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 694 | 448 | 102 | 139 | 5 | | |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | 1V | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 927 | 599 | 157 | 168 | 3 | | |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | 1W | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 971 | 619 | 179 | 168 | 5 | | |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23 | 1X | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1398 | 887 | 250 | 251 | 10 | | |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 24 | 1Y | 139 | 1016 | 648 | 173 | 189 | 6 | 0 | 0 |

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 25 | 1Z | 141 | 1168 | 752 | 202 | 205 | 9 | 0 | 0 |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 26 | 1a | 70 | 562 | 361 | 101 | 94 | 6 | 0 | 0 |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 27 | 1b | 83 | 643 | 417 | 110 | 115 | 1 | 0 | 0 |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 28 | 1c | 49 | 417 | 276 | 71 | 70 | 0 | 0 |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 29 | 1d | 121 | 996 | 648 | 172 | 170 | 6 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|----------------|
| 1d | -2 | ACE | - | acetylation | UNP A0A480JRW3 |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 30 | 1e | 99 | 816 | 519 | 151 | 140 | 6 | 0 | 0 |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 31 | 1f | 57 | 487 | 316 | 89 | 80 | 2 | 0 | 0 |

There are 29 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|----------------|
| 1f | -77 | MET | - | initiating methionine | UNP A0A8D1IZ33 |
| 1f | -76 | ALA | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -75 | ALA | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -74 | ALA | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -73 | ILE | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -72 | LEU | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -71 | LYS | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -70 | LEU | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -69 | GLU | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -68 | GLU | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -67 | THR | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -66 | ARG | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -65 | GLY | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -64 | GLY | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -63 | GLY | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -62 | GLU | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -61 | LYS | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -60 | CYS | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -59 | ASP | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -58 | LYS | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -57 | ASN | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -56 | GLN | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -55 | GLY | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -54 | VAL | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -53 | LYS | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -52 | GLY | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -51 | ARG | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -50 | ARG | - | expression tag | UNP A0A8D1IZ33 |
| 1f | -49 | PHE | - | expression tag | UNP A0A8D1IZ33 |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 32 | 1g | 100 | 835 | 535 | 138 | 158 | 4 | 0 | 0 |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 33 | 1h | 138 | 1151 | 754 | 195 | 199 | 3 | 0 | 0 |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 34 | 1i | 127 | 1100 | 723 | 194 | 181 | 2 | 0 | 0 |

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 35 | 1j | 71 | 601 | 394 | 99 | 107 | 1 | 0 | 0 |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 36 | 1k | 81 | 649 | 422 | 110 | 116 | 1 | 0 | 0 |

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 37 | 1l | 156 | 1310 | 847 | 213 | 242 | 8 | 0 | 0 |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 38 | 1m | 128 | 1062 | 691 | 182 | 189 | 0 | 0 |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 39 | 1n | 172 | 1495 | 956 | 273 | 258 | 8 | 0 | 0 |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 40 | 1o | 122 | 1045 | 650 | 198 | 187 | 10 | 0 | 0 |

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 41 | 1p | 173 | 1449 | 908 | 263 | 270 | 8 | 0 | 0 |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 42 | 1q | 145 | 1212 | 775 | 219 | 213 | 5 | 0 | 0 |

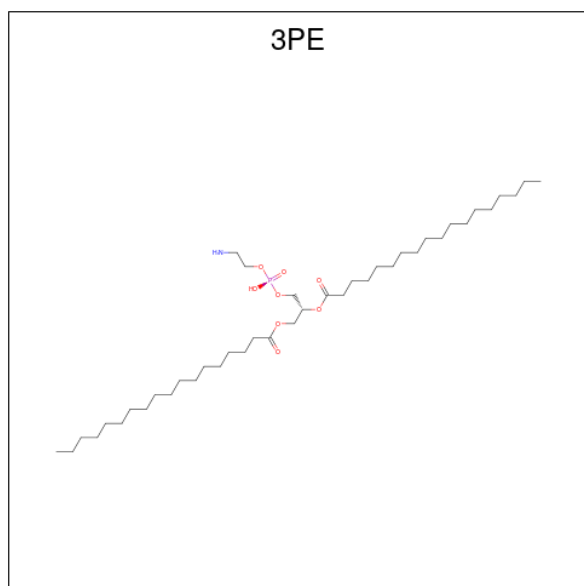
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 43 | 1r | 94 | 759 | 478 | 143 | 135 | 3 | 0 | 0 |

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

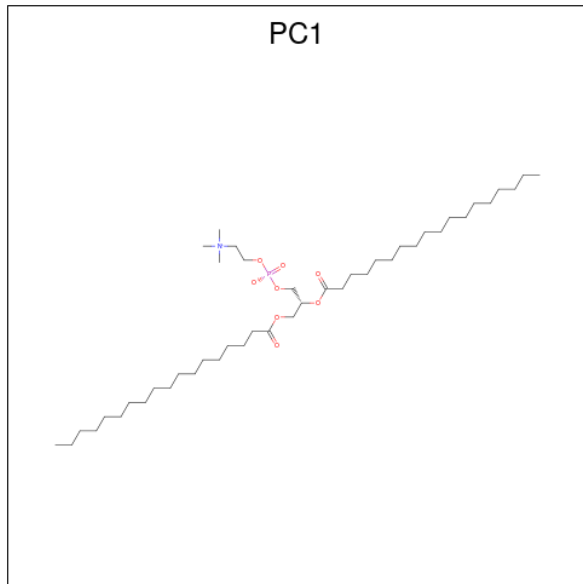
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 44 | 1s | 45 | 382 | 238 | 70 | 73 | 1 | 0 | 0 |

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| | | | Total | C | N | O | P | |
| 45 | 1A | 1 | Total 31 | C 21 | N 1 | O 8 | P 1 | 0 |
| 45 | 1D | 1 | Total 46 | C 36 | N 1 | O 8 | P 1 | 0 |
| 45 | 1L | 1 | Total 46 | C 36 | N 1 | O 8 | P 1 | 0 |
| 45 | 1L | 1 | Total 42 | C 32 | N 1 | O 8 | P 1 | 0 |
| 45 | 1M | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 45 | 1N | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 45 | 1Y | 1 | Total 31 | C 21 | N 1 | O 8 | P 1 | 0 |
| 45 | 1Y | 1 | Total 40 | C 30 | N 1 | O 8 | P 1 | 0 |
| 45 | 1Y | 1 | Total 35 | C 25 | N 1 | O 8 | P 1 | 0 |
| 45 | 1f | 1 | Total 51 | C 41 | N 1 | O 8 | P 1 | 0 |

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



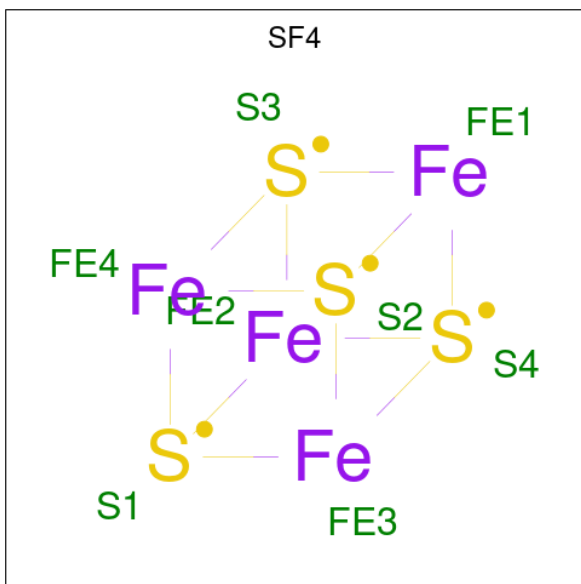
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|----|---|---|---|---------|
| | | | Total | C | N | O | P | |
| 46 | 1A | 1 | Total 27 | 17 | 1 | 8 | 1 | 0 |
| 46 | 1B | 1 | Total 34 | 24 | 1 | 8 | 1 | 0 |
| 46 | 1H | 1 | Total 54 | 44 | 1 | 8 | 1 | 0 |
| 46 | 1H | 1 | Total 34 | 24 | 1 | 8 | 1 | 0 |
| 46 | 1I | 1 | Total 44 | 34 | 1 | 8 | 1 | 0 |
| 46 | 1J | 1 | Total 32 | 22 | 1 | 8 | 1 | 0 |
| 46 | 1L | 1 | Total 38 | 28 | 1 | 8 | 1 | 0 |
| 46 | 1M | 1 | Total 35 | 25 | 1 | 8 | 1 | 0 |
| 46 | 1Y | 1 | Total 46 | 36 | 1 | 8 | 1 | 0 |
| 46 | 1d | 1 | Total 39 | 29 | 1 | 8 | 1 | 0 |
| 46 | 1f | 1 | Total 34 | 24 | 1 | 8 | 1 | 0 |
| 46 | 1h | 1 | Total 47 | 37 | 1 | 8 | 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | AltConf | |
|-----|-------|----------|-------|----|---|---|---------|---|
| | | | Total | C | N | O | | P |
| 46 | 1q | 1 | 48 | 38 | 1 | 8 | 1 | 0 |

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



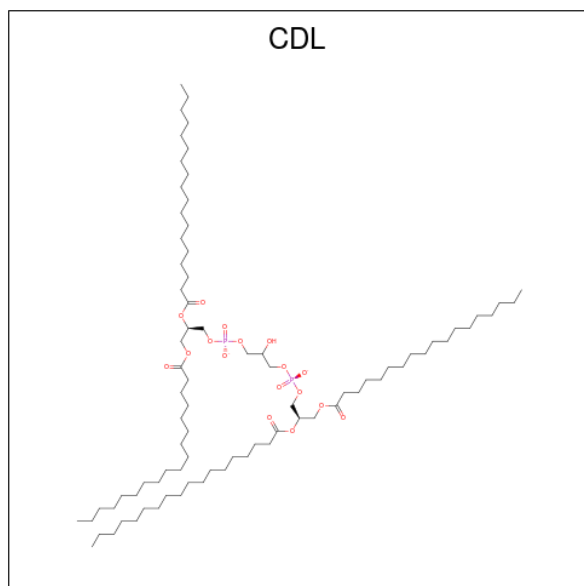
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| | | | Total | Fe | S | |
| 47 | 1B | 1 | 8 | 4 | 4 | 0 |
| 47 | 1F | 1 | 8 | 4 | 4 | 0 |
| 47 | 1G | 1 | 8 | 4 | 4 | 0 |
| 47 | 1G | 1 | 8 | 4 | 4 | 0 |
| 47 | 1I | 1 | 8 | 4 | 4 | 0 |
| 47 | 1I | 1 | 8 | 4 | 4 | 0 |

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

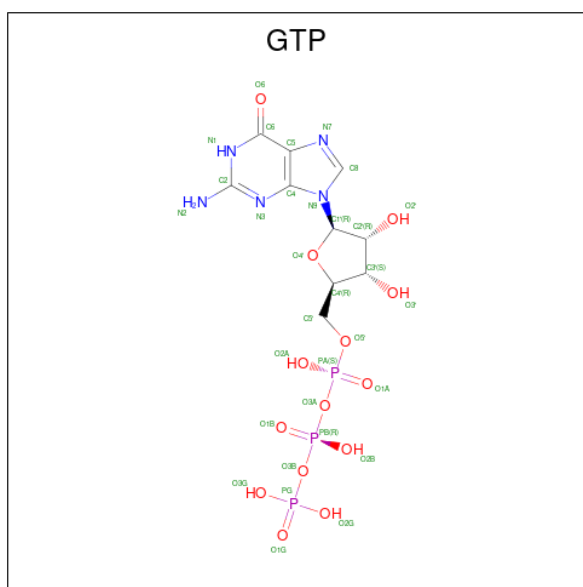
| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|----------------|---------|
| 50 | 1G | 1 | Total K 1 1 | 0 |

- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|---------------------------|---------|
| 51 | 1H | 1 | Total C O P 51 32 17 2 | 0 |
| 51 | 1L | 1 | Total C O P 76 57 17 2 | 0 |
| 51 | 1N | 1 | Total C O P 67 48 17 2 | 0 |
| 51 | 1X | 1 | Total C O P 86 67 17 2 | 0 |
| 51 | 1a | 1 | Total C O P 61 42 17 2 | 0 |
| 51 | 1d | 1 | Total C O P 65 46 17 2 | 0 |

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

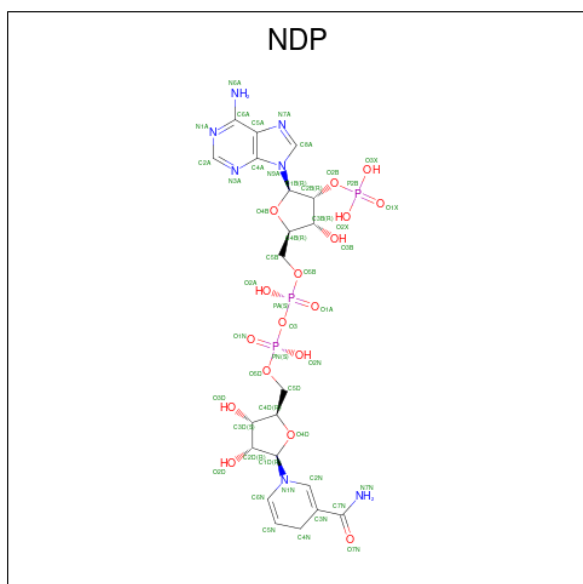


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 52 | 10 | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Mg | |
| 53 | 10 | 1 | 1 | 1 | 0 |

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

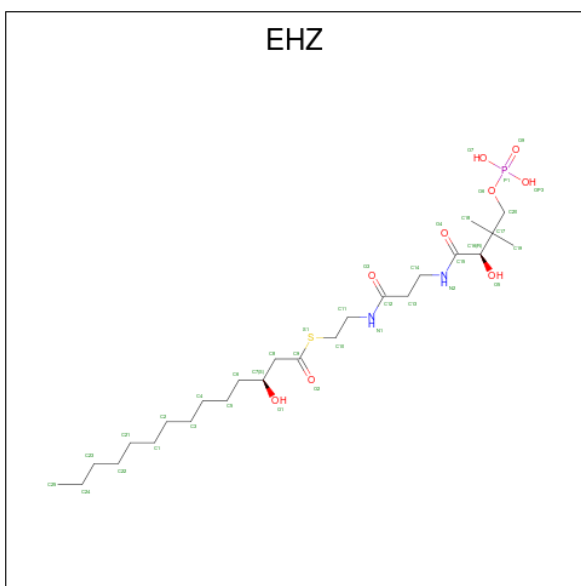


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 54 | 1P | 1 | 48 | 21 | 7 | 17 | 3 | 0 |

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

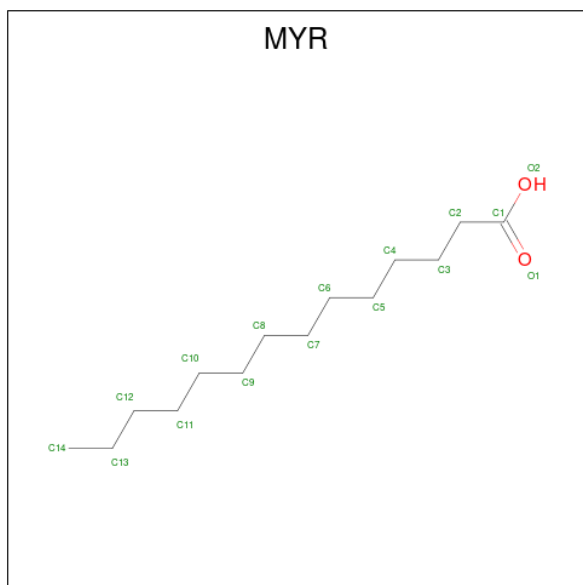
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Zn | |
| 55 | 1R | 1 | 1 | 1 | 0 |

- Molecule 56 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

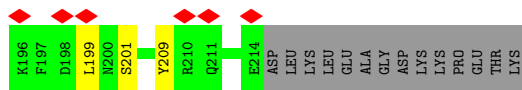


| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| | | | Total | C | N | O | P | S | |
| 56 | 1W | 1 | 37 | 25 | 2 | 8 | 1 | 1 | 0 |
| 56 | 1n | 1 | 37 | 25 | 2 | 8 | 1 | 1 | 0 |

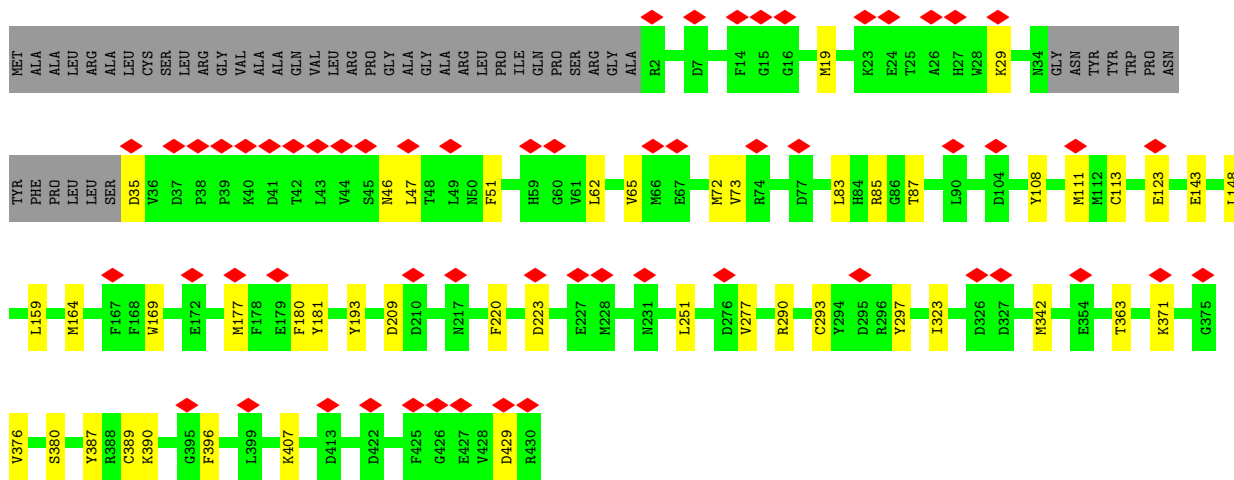
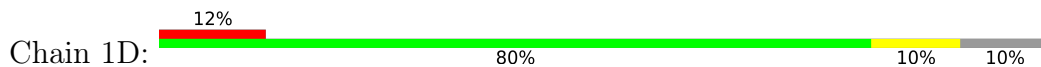
- Molecule 57 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



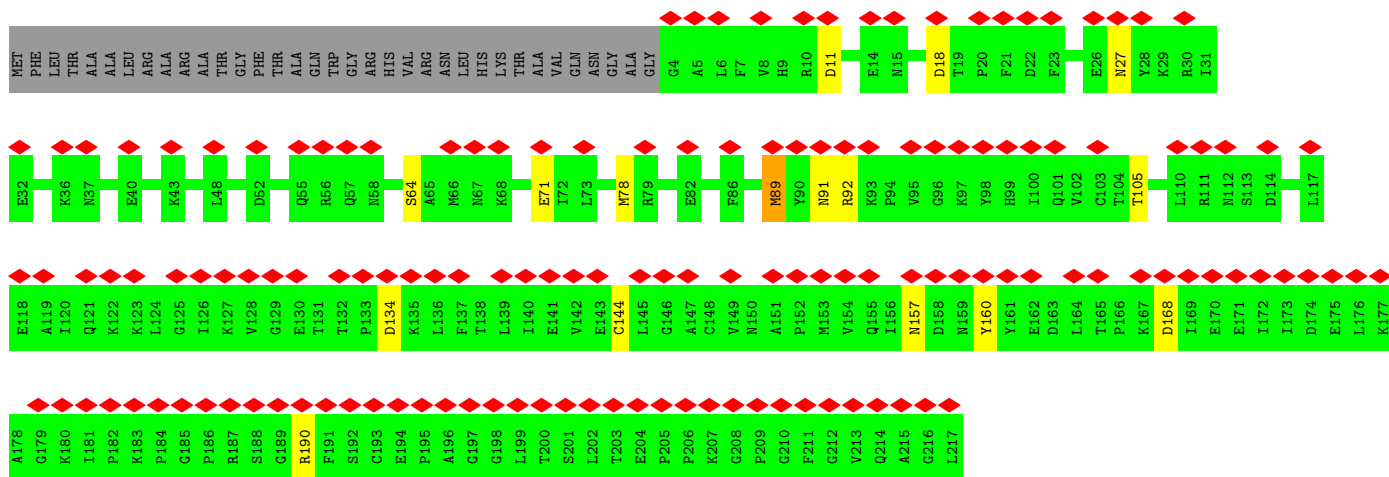
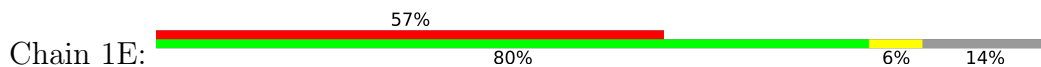
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 57 | 11 | 1 | Total | C | O | 0 |
| | | | 15 | 14 | 1 | |



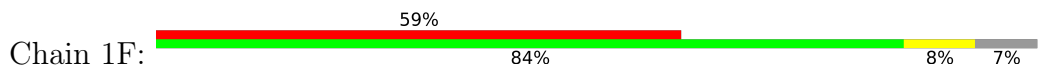
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

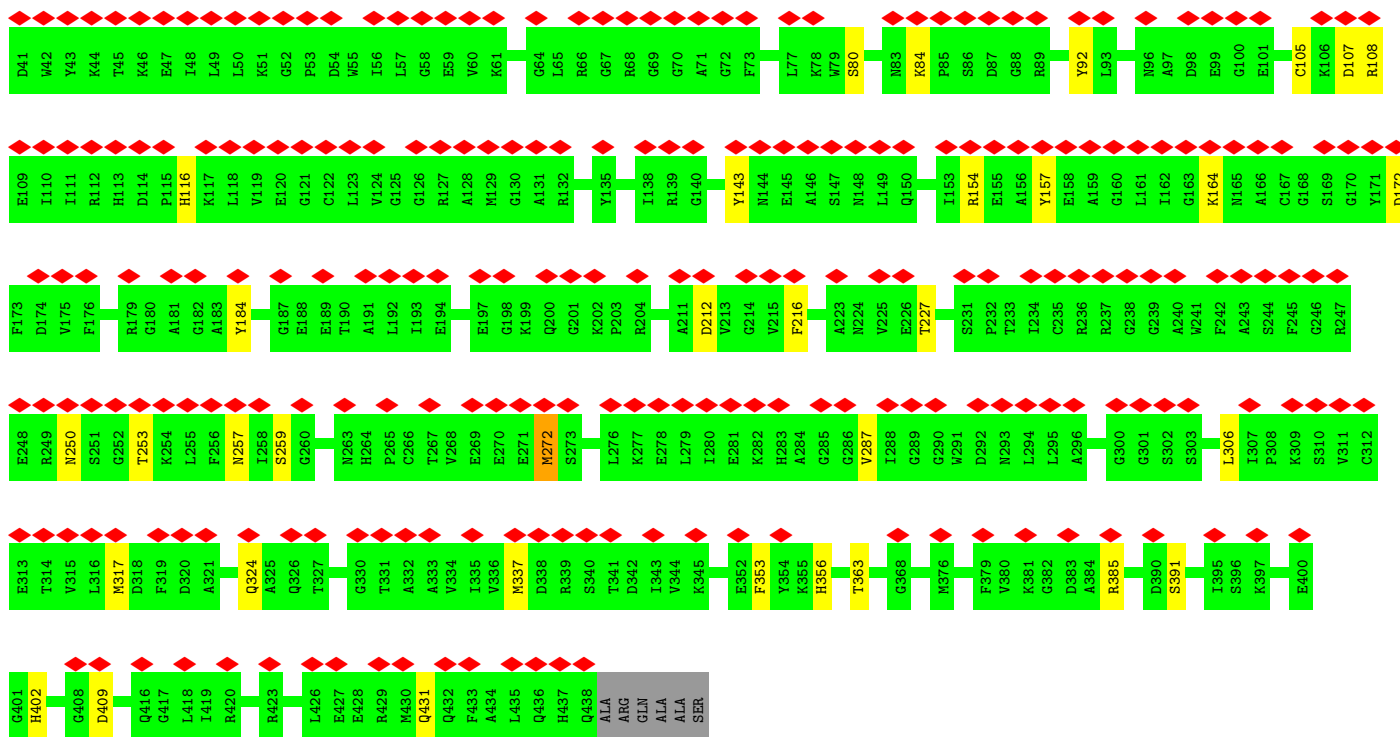


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

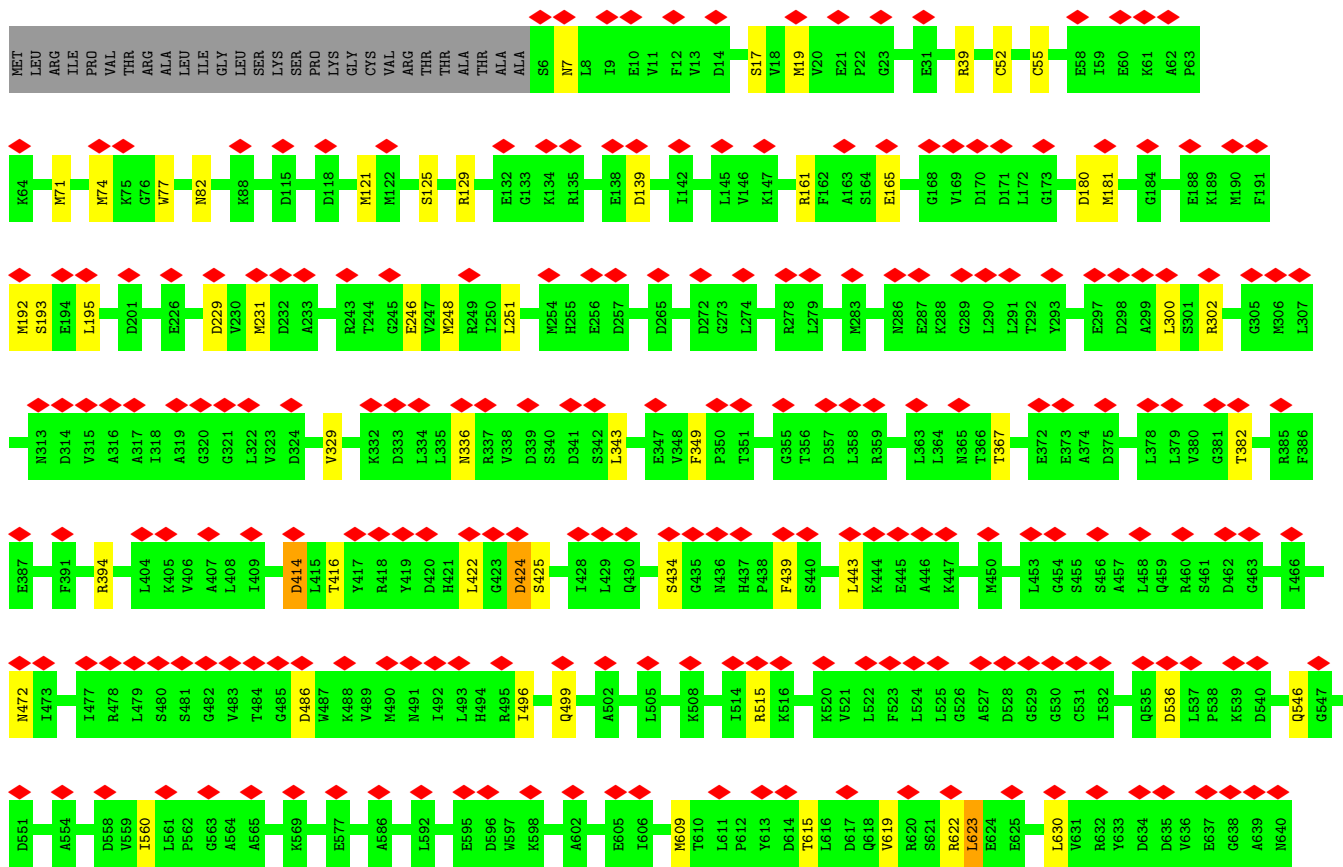
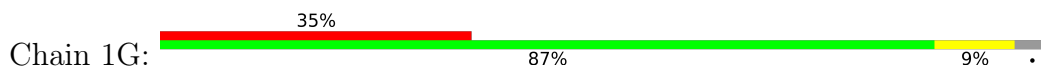


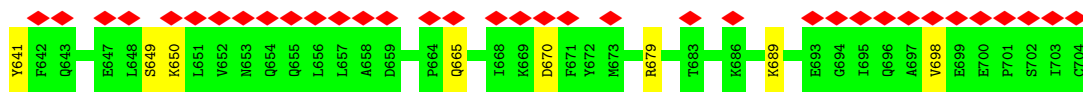
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



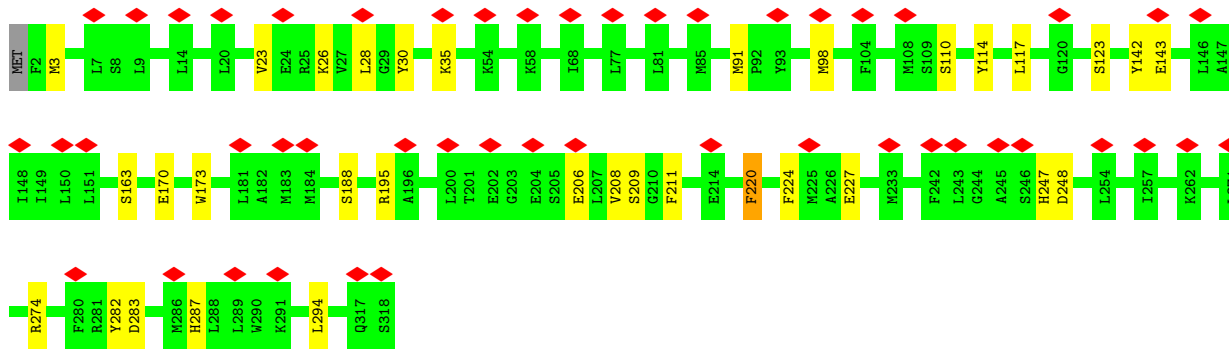
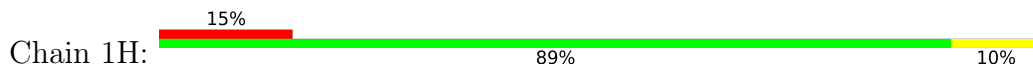


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

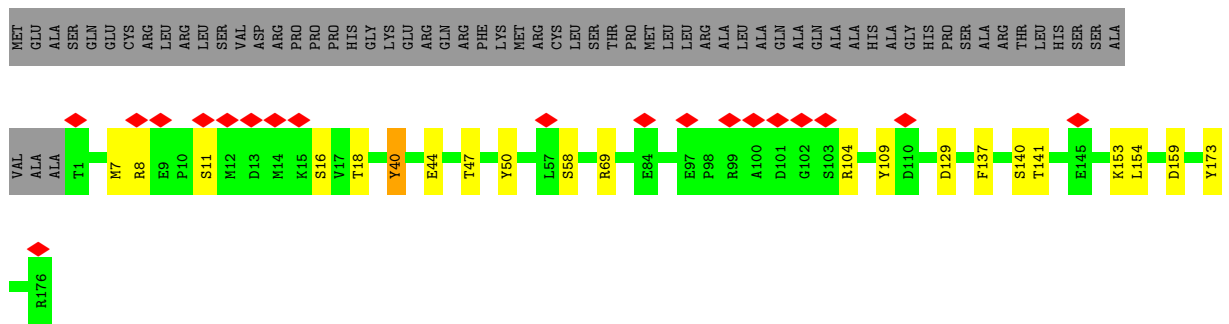




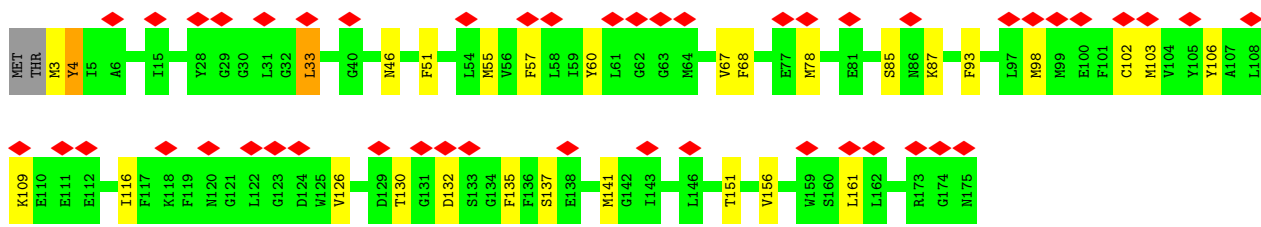
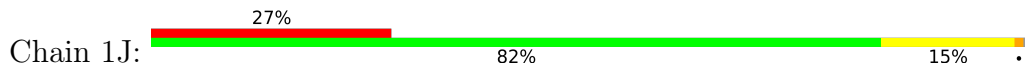
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



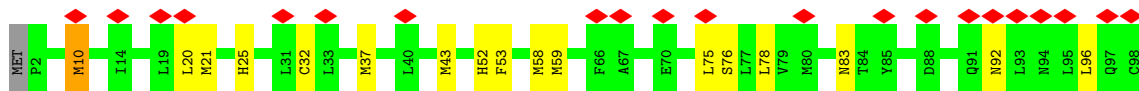
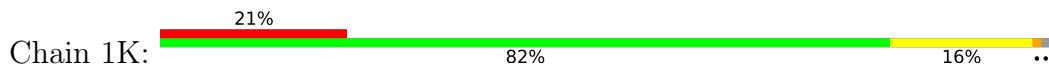
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



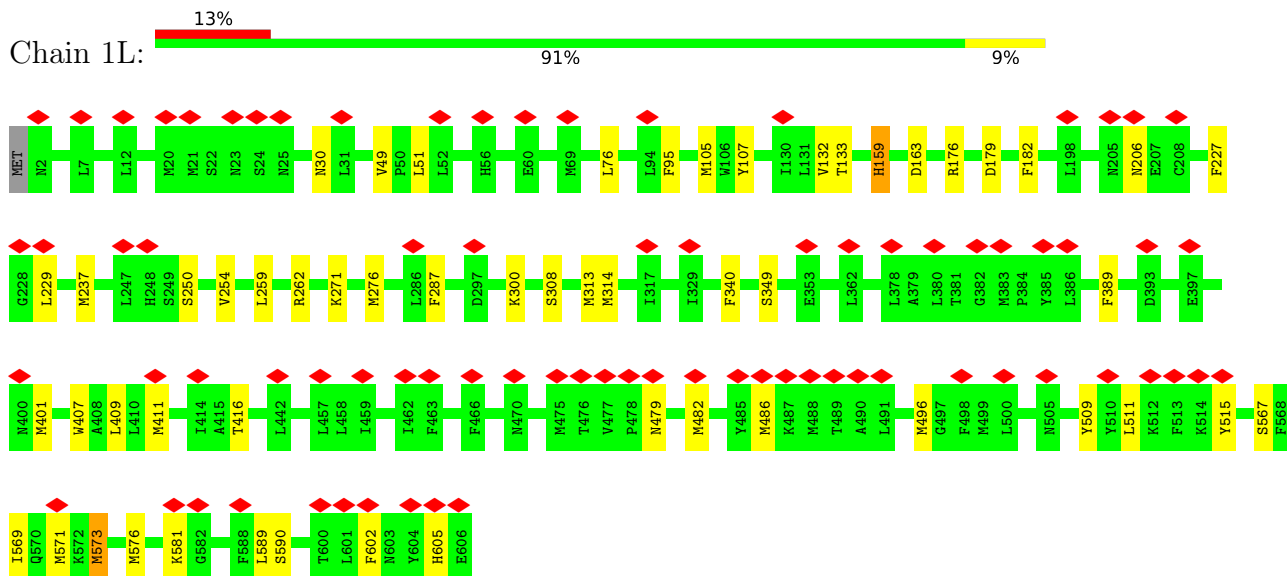
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



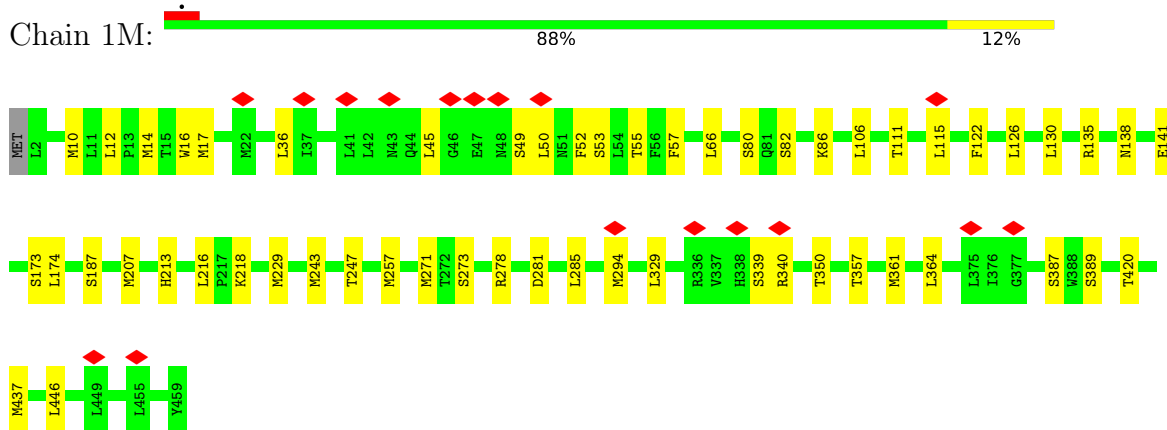
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



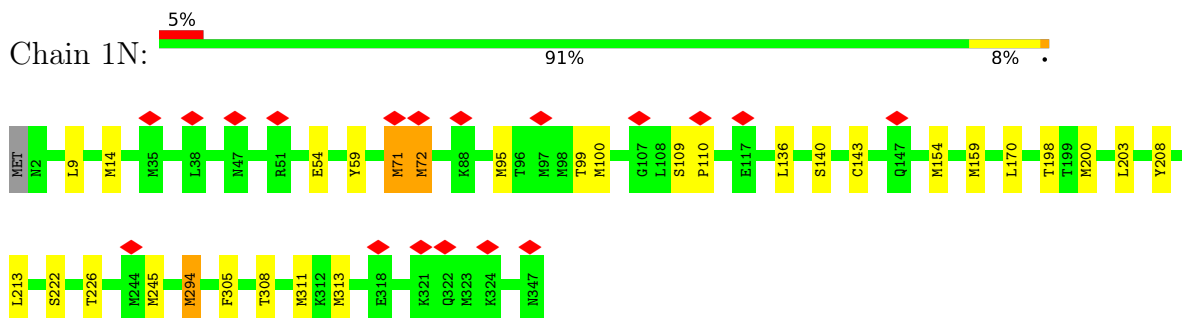
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



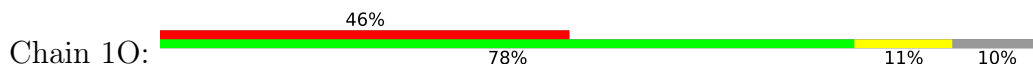
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

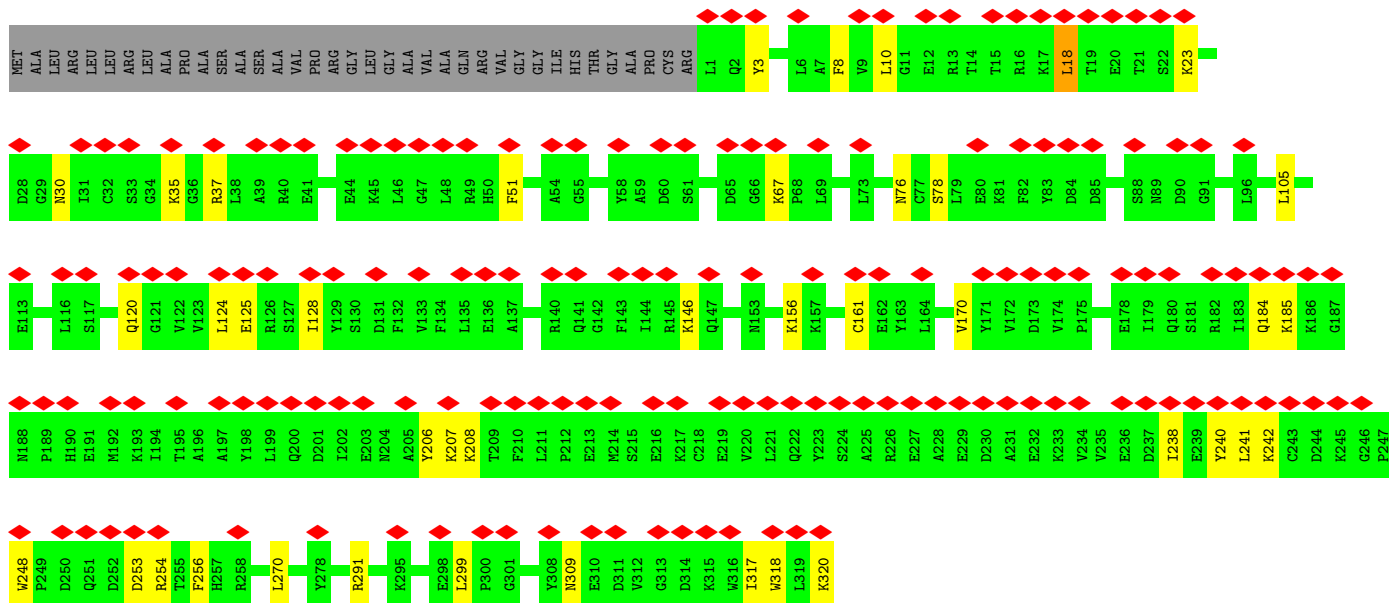


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

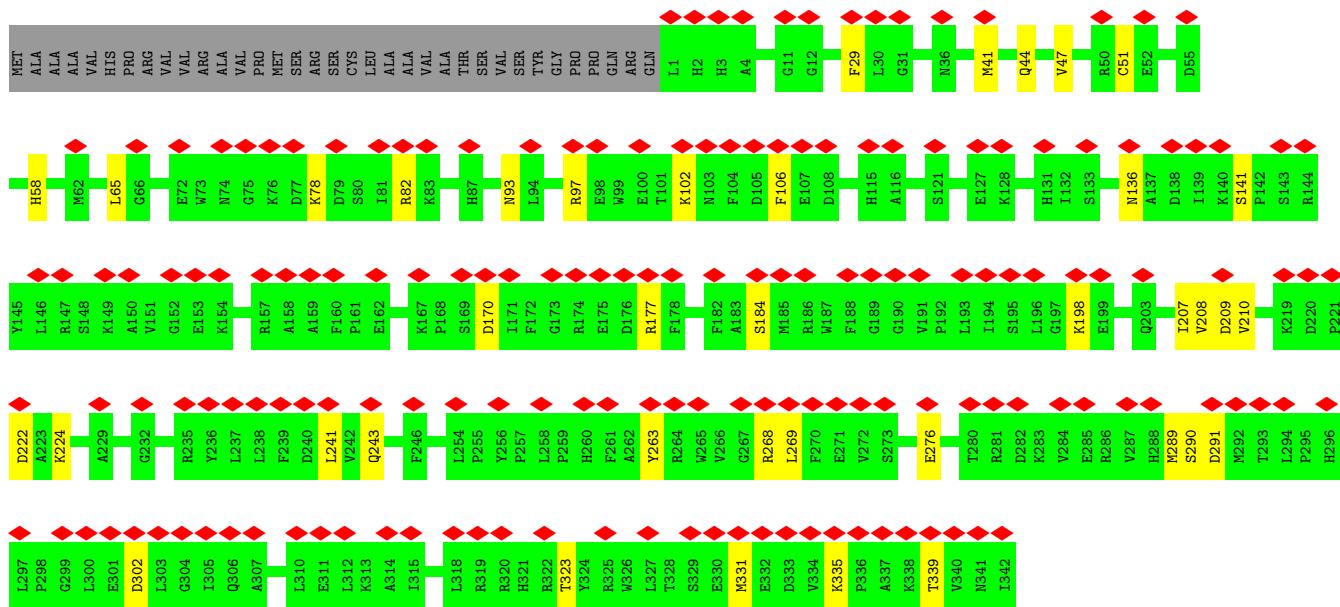
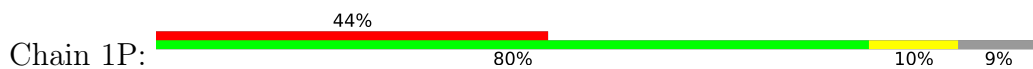


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

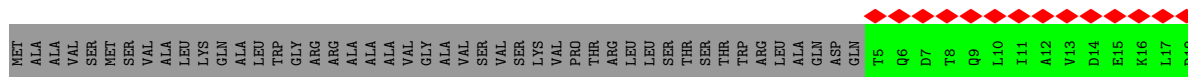


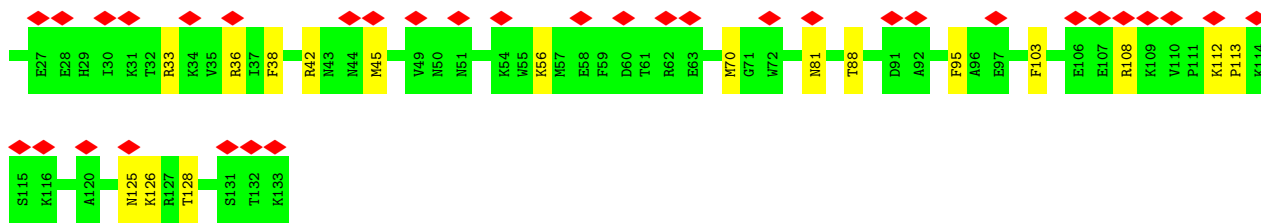


• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

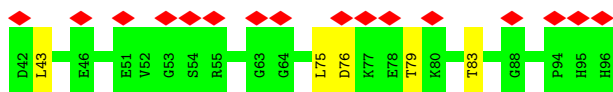
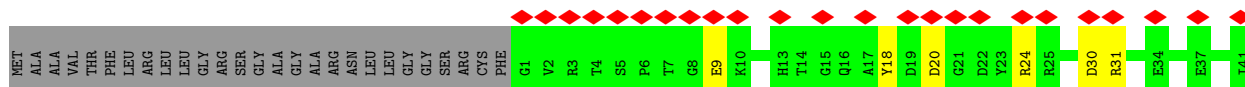


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

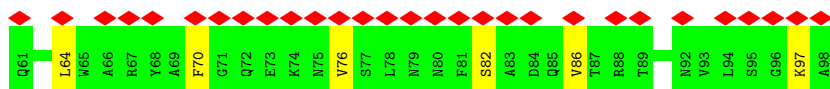
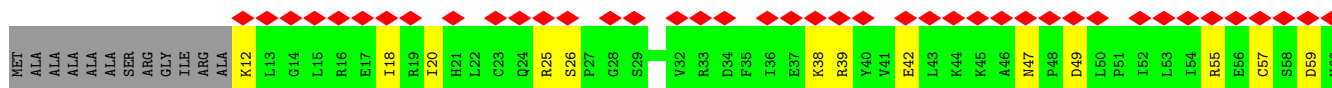




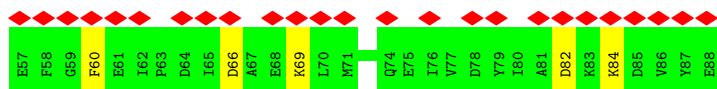
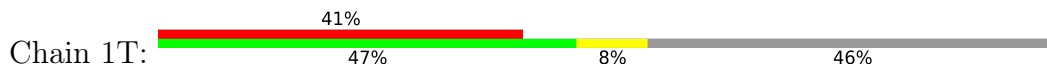
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

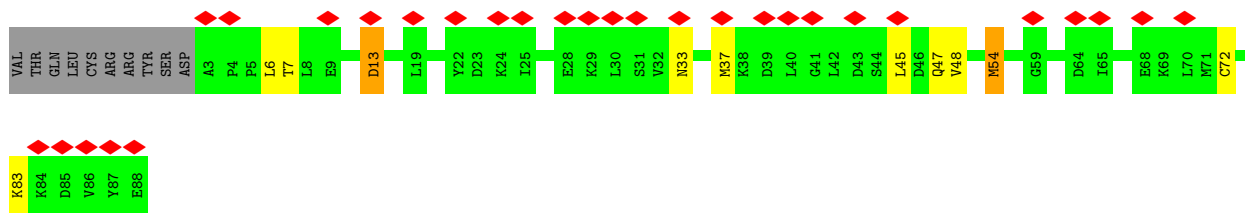


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

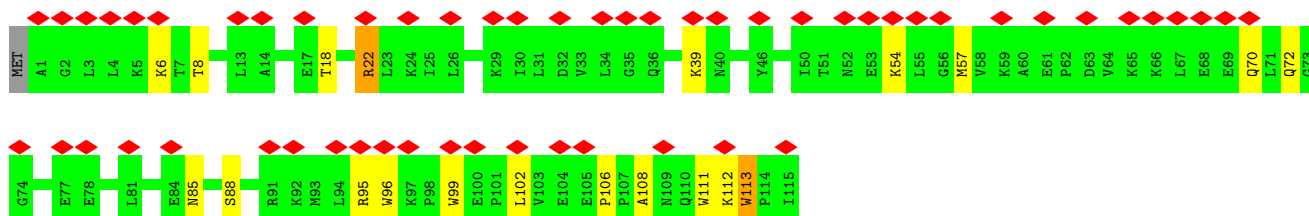
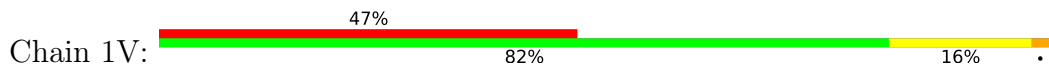


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

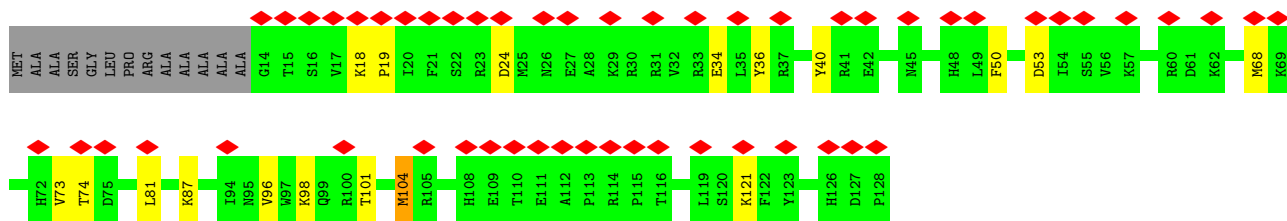
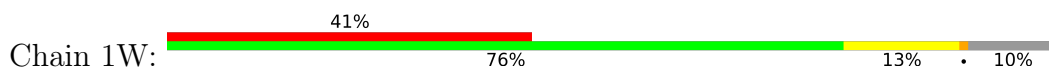




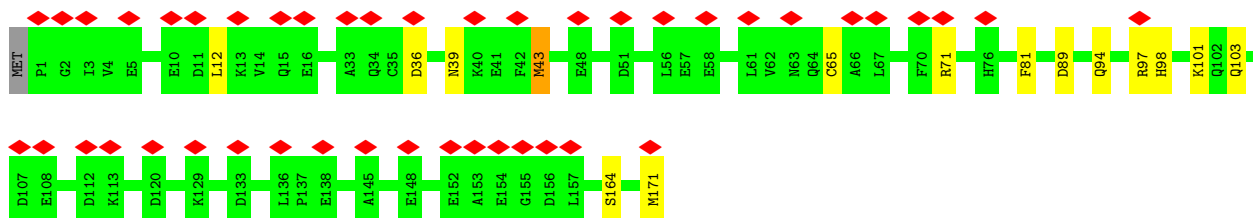
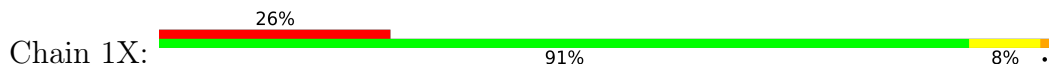
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



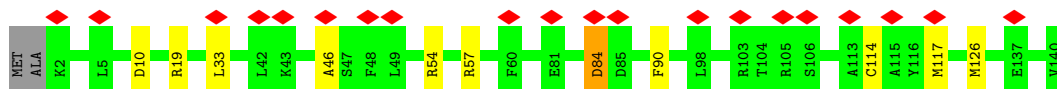
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



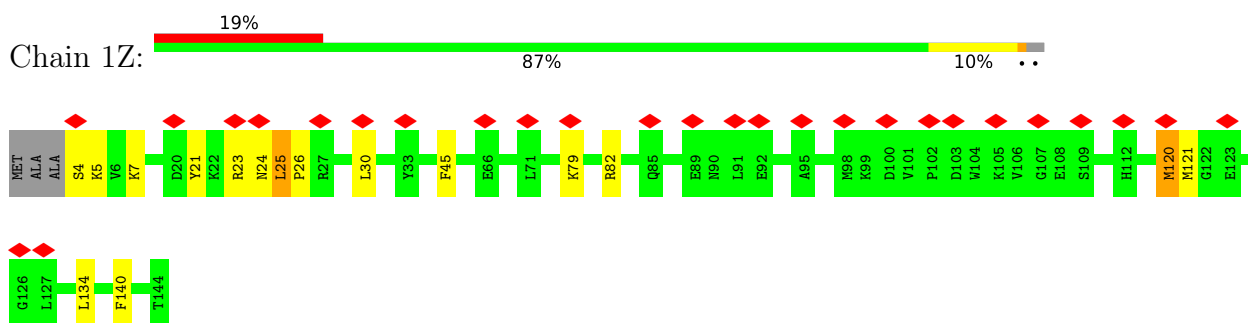
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



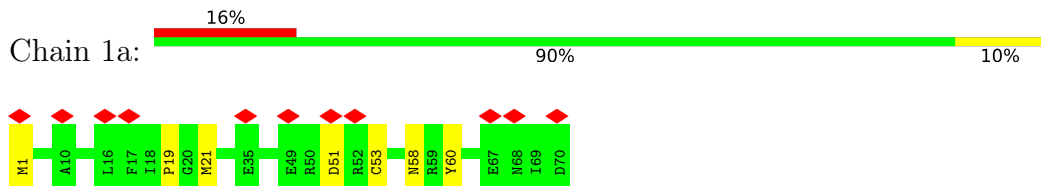
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



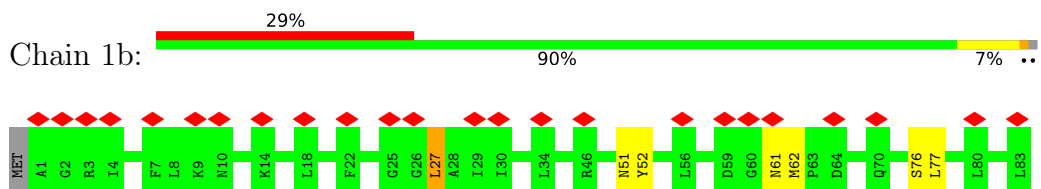
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



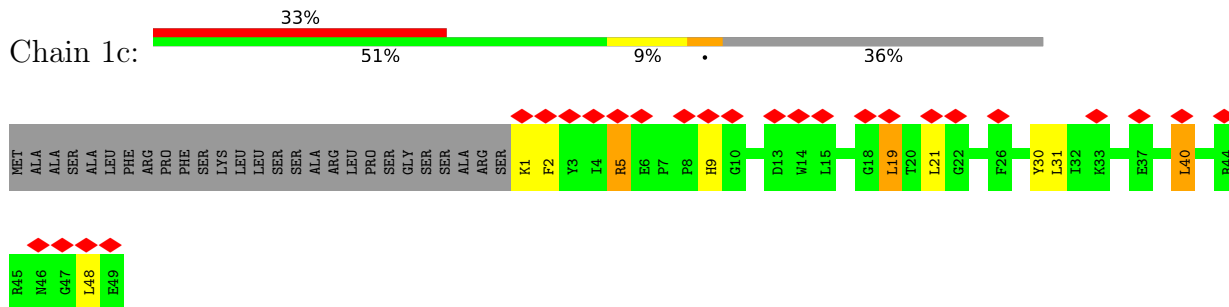
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



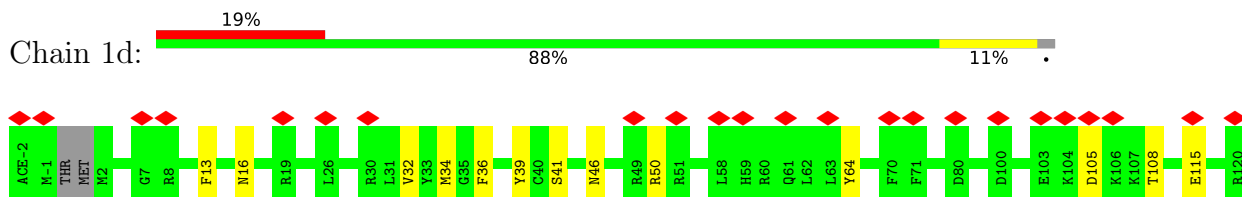
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



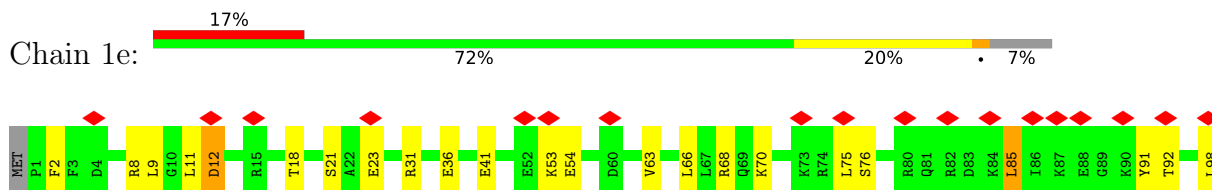
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

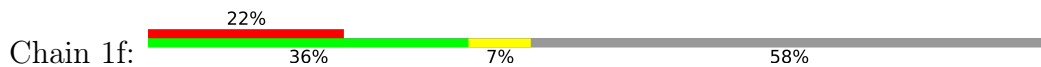


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



699
LYS
GLU
ASP
PRO
ARG
PRO

• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



MET ALA ALA ALA ILE LEU LYS LEU LEU GLU GLU THR THR ARG ARG GLY GLY GLY GLY LYS CYS ASP LYS ASN LEU LEU VAL VAL LYS GLY ARG ARG ARG PHE MET MET ILE SER ARG SER SER HIS PRO PRO LEU LEU ARG ARG GLY PRO PRO ALA ALA ASN GLY GLY ALA ASN ARG ARG ARG ARG ARG TRP TRP LEU LEU SER

PRO LEU PRO LEU VAL VAL GLY VAL VAL VAL VAL SER SER ALA ALA ALA ALA ALA MET M1 N2 V3 L4 Q5 I6 V7 R8 D9 H10 W11 I14 L15 F22 G23 C24 Y25 L26 D27 R28 R29 S30 D31 E32 K33 R38 L42 R46 E47 L48 R49 P50 M51 E52 E53 V54

K57

• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



MET ALA ALA GLY VAL LEU GLY LEU LEU CYS ALA ARG ARG ARG LEU LEU ALA ALA ALA THR ARG GLY LEU PRO PRO ALA ARG VAL ARG VAL ILE ALA PRO SER ALA LEU VAL LYS PRO PRO PRO T23 I24 R25 L26 Q27 E28 D29 F30 D31

P32 E33 D34 E35 K40 D43 D48 K49 D50 N57 M58 R59 L70 F76 V77 D82 Y83 R84 M85 R91 E94 R95 Y99 M103 G104 L105 P106 L107 M108 E109 C112 F113 D114 P115 M116 K117 I118 Q119 L120 P121 E122 ASP GLU ASP

• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

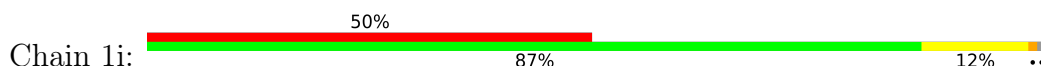


MET ALA ALA MET LEU LEU LEU ARG ALA ALA SER VAL THR ALA VAL THR LEU SER ARG ARG ARG ARG PHE PHE GLY PHE LEU THR HIS GLY PHE PRO LYS THR GLY ALA PRO THR ALA VAL ARG HIS ARG ASP HIS K6 R7 D18 R19 K23 R26

L31 I38 G39 I40 N44 V45 F46 I47 G48 E49 A50 E51 L52 A53 D54 I55 R56 E57 G58 Y59 E62 E65 K68 R73 Y80 D81 E84 K85 M91 Q95 K100 L108 R111 R112 R117 G118 D119 W122 T127 I128 K130

D142
M143

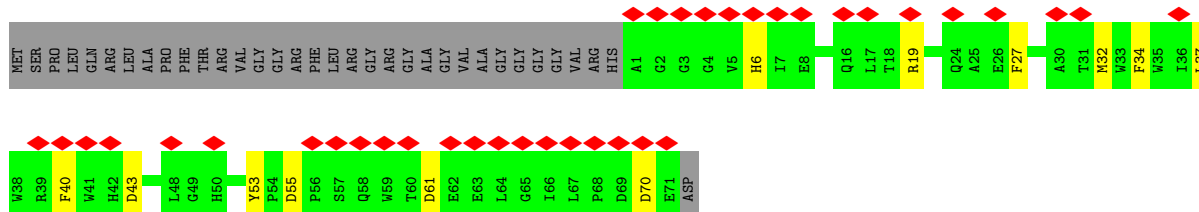
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



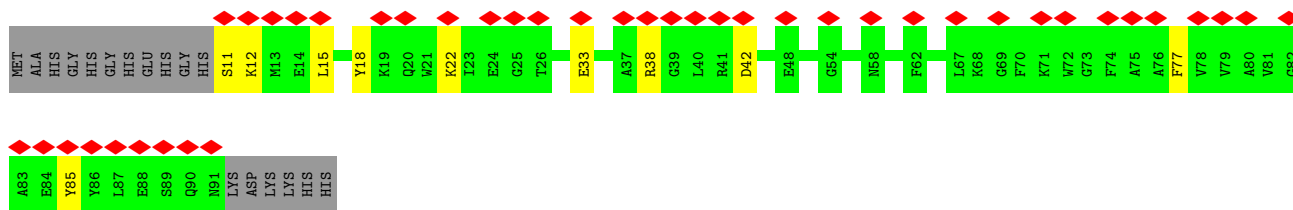
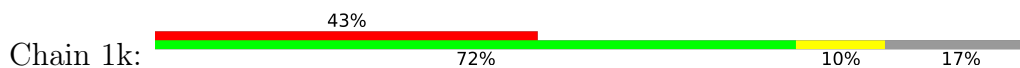
MET S1 F5 D6 L17 R18 R19 R20 W21 L22 K23 R30 L34 P35 P36 R37 R38 V39 W40 P41 M42 E43 Q44 F45 W46 N47 K48 F49 L50 Q51 D52 G53 A54 P55 W56 W57 N58 V59 I60 Y61 K62 T63 Y64 R65 H66 S67 I68 L75 I76 R82 Y83 K92



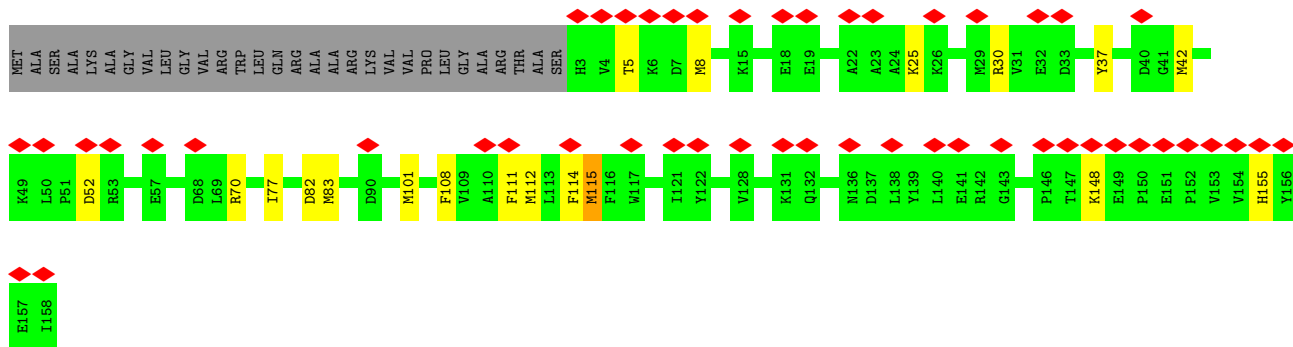
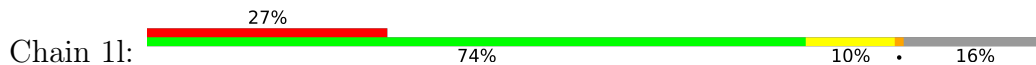
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



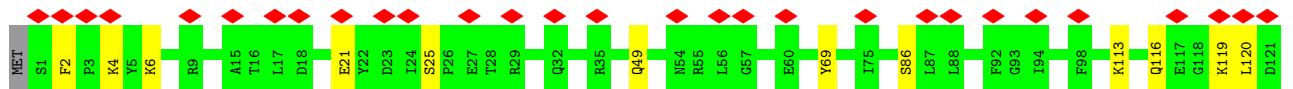
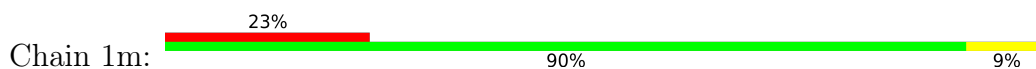
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

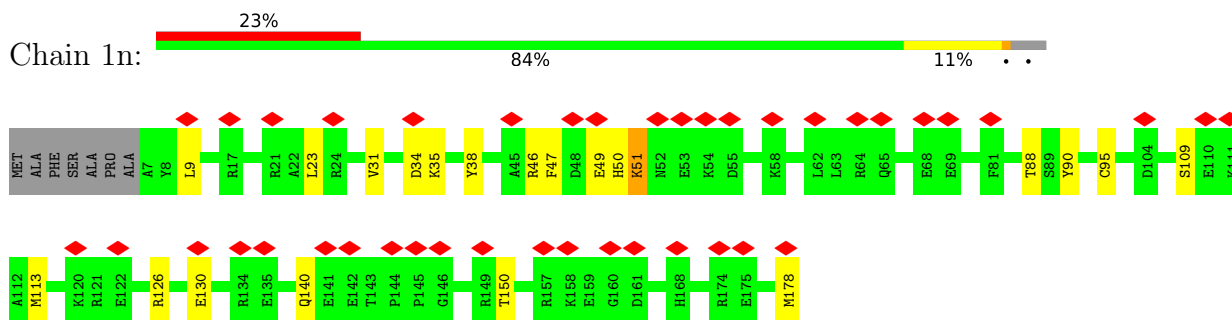


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

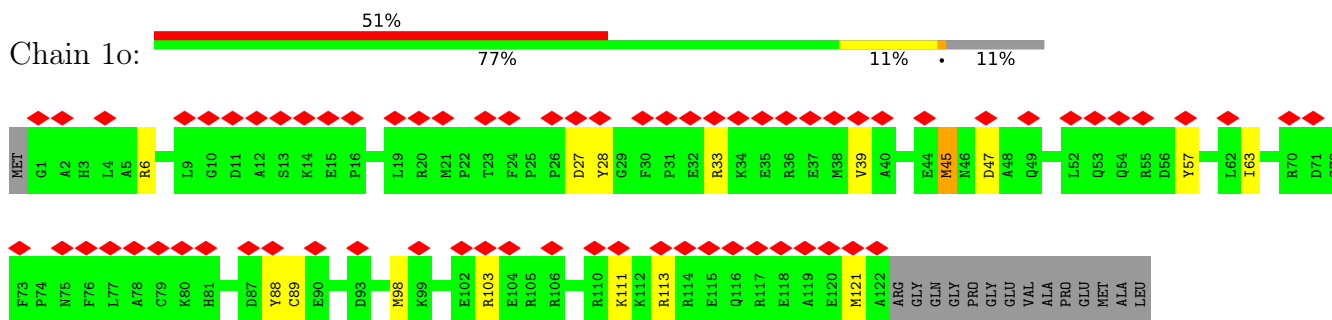




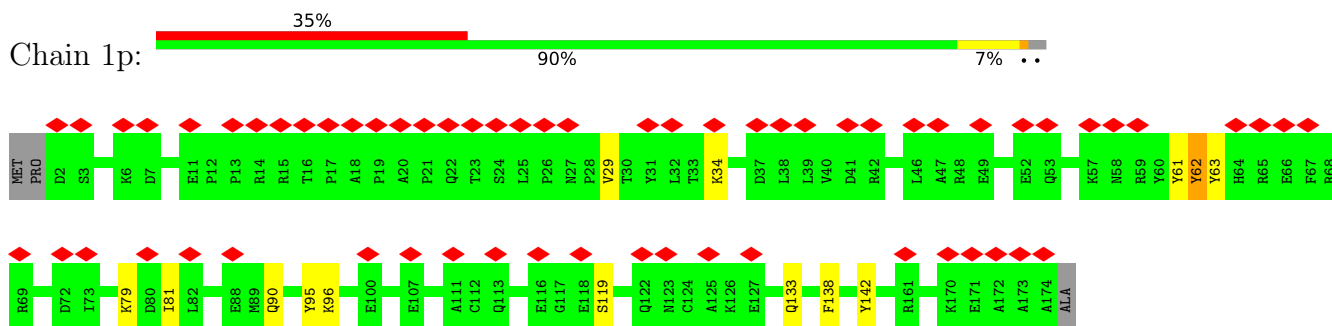
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



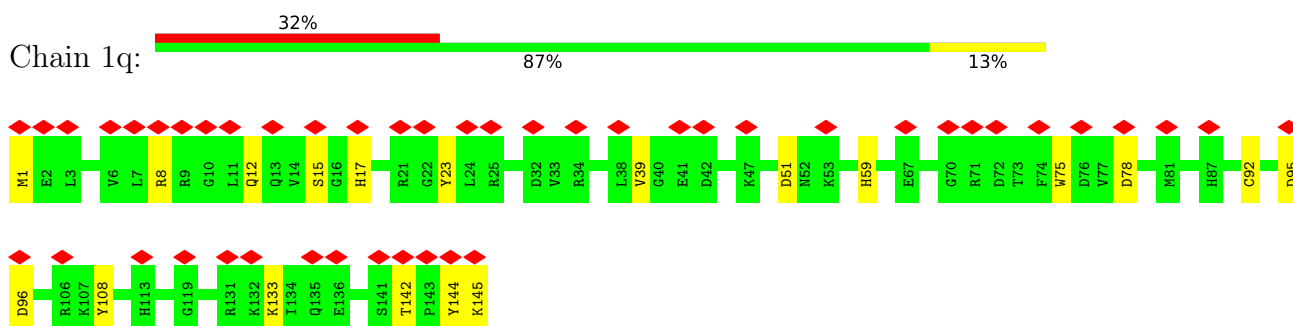
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



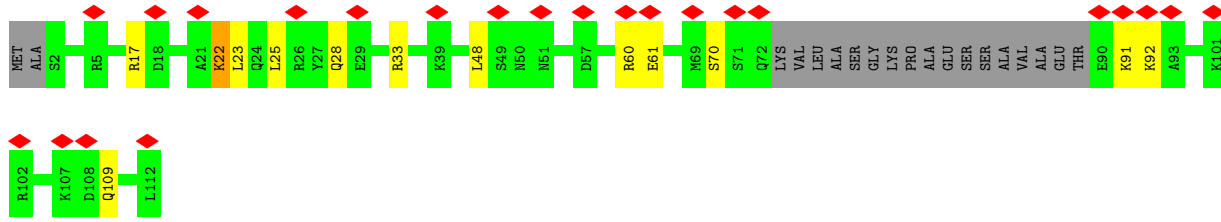
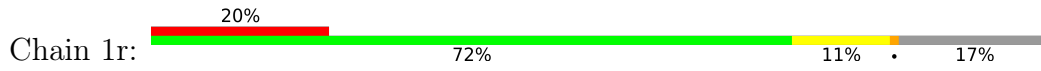
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



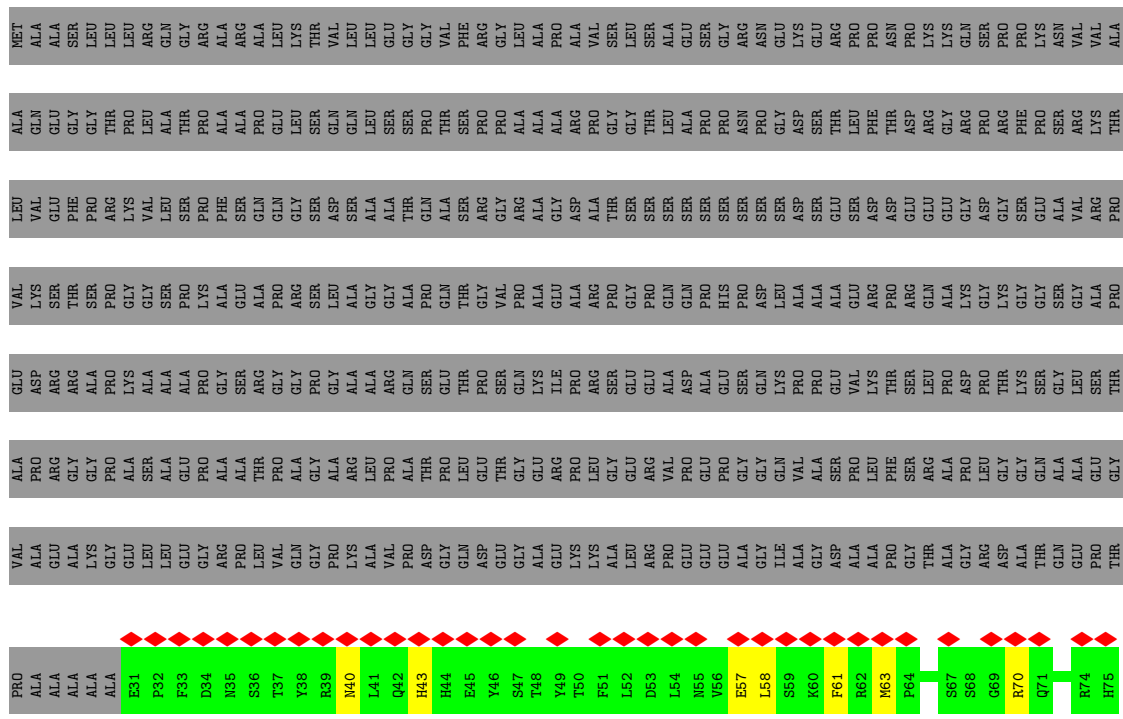
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 30000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1300 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.782 | Depositor |
| Minimum map value | -0.197 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.018 | Depositor |
| Recommended contour level | 0.12 | Depositor |
| Map size (\AA) | 426.00003, 426.00003, 426.00003 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.065, 1.065, 1.065 | Depositor |

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PE, NDP, EHZ, SF4, MYR, FMN, SAC, ACE, MG, GTP, K, ZN, PC1, 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 | 1A | 0.39 | 0/938 | 0.70 | 0/1281 |
| 2 | 1B | 0.52 | 1/1273 (0.1%) | 0.67 | 1/1722 (0.1%) |
| 3 | 1C | 0.41 | 2/1791 (0.1%) | 0.64 | 1/2439 (0.0%) |
| 4 | 1D | 0.43 | 2/3545 (0.1%) | 0.67 | 3/4806 (0.1%) |
| 5 | 1E | 0.30 | 0/1698 | 0.57 | 1/2311 (0.0%) |
| 6 | 1F | 0.32 | 0/3401 | 0.62 | 2/4595 (0.0%) |
| 7 | 1G | 0.29 | 0/5451 | 0.60 | 5/7387 (0.1%) |
| 8 | 1H | 0.46 | 2/2566 (0.1%) | 0.73 | 6/3509 (0.2%) |
| 9 | 1I | 0.47 | 1/1443 (0.1%) | 0.76 | 4/1952 (0.2%) |
| 10 | 1J | 0.43 | 1/1357 (0.1%) | 0.74 | 4/1840 (0.2%) |
| 11 | 1K | 0.53 | 0/751 | 0.99 | 4/1018 (0.4%) |
| 12 | 1L | 0.34 | 0/4939 | 0.66 | 6/6718 (0.1%) |
| 13 | 1M | 0.35 | 0/3713 | 0.71 | 7/5063 (0.1%) |
| 14 | 1N | 0.31 | 0/2765 | 0.66 | 4/3758 (0.1%) |
| 15 | 1O | 0.34 | 0/2650 | 0.58 | 2/3588 (0.1%) |
| 16 | 1P | 0.31 | 1/2828 (0.0%) | 0.57 | 1/3834 (0.0%) |
| 17 | 1Q | 0.32 | 0/1070 | 0.69 | 2/1446 (0.1%) |
| 18 | 1R | 0.32 | 0/755 | 0.63 | 0/1018 |
| 19 | 1S | 0.37 | 1/711 (0.1%) | 0.76 | 1/956 (0.1%) |
| 20 | 1T | 0.30 | 0/701 | 0.61 | 0/946 |
| 20 | 1U | 0.36 | 0/706 | 0.75 | 3/954 (0.3%) |
| 21 | 1V | 0.41 | 0/946 | 0.80 | 3/1281 (0.2%) |
| 22 | 1W | 0.69 | 2/995 (0.2%) | 1.21 | 7/1340 (0.5%) |
| 23 | 1X | 0.29 | 0/1436 | 0.64 | 3/1938 (0.2%) |
| 24 | 1Y | 0.28 | 0/1037 | 0.56 | 2/1404 (0.1%) |
| 25 | 1Z | 0.36 | 0/1199 | 0.76 | 4/1617 (0.2%) |
| 26 | 1a | 0.39 | 0/577 | 0.68 | 1/777 (0.1%) |
| 27 | 1b | 0.31 | 0/664 | 0.62 | 1/912 (0.1%) |
| 28 | 1c | 0.39 | 0/430 | 0.90 | 5/581 (0.9%) |
| 29 | 1d | 0.34 | 0/1024 | 0.64 | 1/1383 (0.1%) |
| 30 | 1e | 0.33 | 0/836 | 0.73 | 2/1118 (0.2%) |
| 31 | 1f | 0.45 | 0/499 | 0.85 | 3/673 (0.4%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | 1g | 0.47 | 1/858 (0.1%) | 0.78 | 2/1165 (0.2%) |
| 33 | 1h | 0.46 | 1/1184 (0.1%) | 0.78 | 4/1603 (0.2%) |
| 34 | 1i | 0.30 | 0/1131 | 0.71 | 1/1541 (0.1%) |
| 35 | 1j | 0.36 | 0/627 | 0.67 | 1/858 (0.1%) |
| 36 | 1k | 0.49 | 2/668 (0.3%) | 0.67 | 1/903 (0.1%) |
| 37 | 1l | 0.31 | 0/1365 | 0.66 | 5/1867 (0.3%) |
| 38 | 1m | 0.34 | 0/1092 | 0.61 | 1/1481 (0.1%) |
| 39 | 1n | 0.32 | 0/1549 | 0.63 | 1/2098 (0.0%) |
| 40 | 1o | 0.36 | 0/1069 | 0.75 | 4/1430 (0.3%) |
| 41 | 1p | 0.33 | 0/1481 | 0.62 | 1/1997 (0.1%) |
| 42 | 1q | 0.37 | 0/1253 | 0.66 | 2/1704 (0.1%) |
| 43 | 1r | 0.43 | 0/777 | 0.81 | 2/1051 (0.2%) |
| 44 | 1s | 0.41 | 0/394 | 0.75 | 1/533 (0.2%) |
| All | All | 0.37 | 17/68143 (0.0%) | 0.68 | 115/92396 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 2 | 1B | 0 | 1 |
| 7 | 1G | 0 | 1 |
| 8 | 1H | 0 | 1 |
| 12 | 1L | 0 | 1 |
| 13 | 1M | 0 | 1 |
| 14 | 1N | 0 | 2 |
| 21 | 1V | 0 | 1 |
| 34 | 1i | 0 | 1 |
| All | All | 0 | 9 |

The worst 5 of 17 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 22 | 1W | 19 | PRO | CB-CG | -12.27 | 0.88 | 1.50 |
| 22 | 1W | 19 | PRO | CG-CD | -8.29 | 1.23 | 1.50 |
| 9 | 1I | 40 | TYR | CD1-CE1 | -7.36 | 1.28 | 1.39 |
| 8 | 1H | 220 | PHE | CD1-CE1 | -7.02 | 1.25 | 1.39 |
| 33 | 1h | 84 | GLU | CG-CD | -6.99 | 1.41 | 1.51 |

The worst 5 of 115 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 22 | 1W | 19 | PRO | CB-CG-CD | 18.84 | 179.97 | 106.50 |
| 22 | 1W | 19 | PRO | N-CD-CG | -18.78 | 75.03 | 103.20 |
| 13 | 1M | 271 | MET | CG-SD-CE | -18.27 | 70.97 | 100.20 |
| 8 | 1H | 26 | LYS | CD-CE-NZ | -16.36 | 74.06 | 111.70 |
| 22 | 1W | 19 | PRO | CA-CB-CG | -15.32 | 74.90 | 104.00 |

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | 1B | 81 | ARG | Peptide |
| 7 | 1G | 649 | SER | Peptide |
| 8 | 1H | 91 | MET | Peptide |
| 12 | 1L | 159 | HIS | Peptide |
| 13 | 1M | 278 | ARG | Sidechain |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | 1A | 113/115 (98%) | 105 (93%) | 7 (6%) | 1 (1%) | 17 | 54 |
| 2 | 1B | 153/258 (59%) | 142 (93%) | 11 (7%) | 0 | 100 | 100 |
| 3 | 1C | 207/264 (78%) | 189 (91%) | 17 (8%) | 1 (0%) | 29 | 66 |
| 4 | 1D | 427/476 (90%) | 398 (93%) | 29 (7%) | 0 | 100 | 100 |
| 5 | 1E | 212/249 (85%) | 185 (87%) | 26 (12%) | 1 (0%) | 29 | 66 |
| 6 | 1F | 430/464 (93%) | 398 (93%) | 31 (7%) | 1 (0%) | 47 | 79 |
| 7 | 1G | 697/727 (96%) | 648 (93%) | 45 (6%) | 4 (1%) | 25 | 62 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 8 | 1H | 315/318 (99%) | 294 (93%) | 20 (6%) | 1 (0%) | 41 | 74 |
| 9 | 1I | 174/239 (73%) | 160 (92%) | 14 (8%) | 0 | 100 | 100 |
| 10 | 1J | 171/175 (98%) | 155 (91%) | 14 (8%) | 2 (1%) | 13 | 50 |
| 11 | 1K | 95/98 (97%) | 85 (90%) | 10 (10%) | 0 | 100 | 100 |
| 12 | 1L | 603/606 (100%) | 558 (92%) | 44 (7%) | 1 (0%) | 47 | 79 |
| 13 | 1M | 456/459 (99%) | 427 (94%) | 28 (6%) | 1 (0%) | 47 | 79 |
| 14 | 1N | 344/347 (99%) | 318 (92%) | 25 (7%) | 1 (0%) | 41 | 74 |
| 15 | 1O | 318/357 (89%) | 299 (94%) | 19 (6%) | 0 | 100 | 100 |
| 16 | 1P | 340/377 (90%) | 324 (95%) | 16 (5%) | 0 | 100 | 100 |
| 17 | 1Q | 127/175 (73%) | 118 (93%) | 9 (7%) | 0 | 100 | 100 |
| 18 | 1R | 94/123 (76%) | 86 (92%) | 8 (8%) | 0 | 100 | 100 |
| 19 | 1S | 85/99 (86%) | 81 (95%) | 4 (5%) | 0 | 100 | 100 |
| 20 | 1T | 83/156 (53%) | 78 (94%) | 5 (6%) | 0 | 100 | 100 |
| 20 | 1U | 84/156 (54%) | 79 (94%) | 5 (6%) | 0 | 100 | 100 |
| 21 | 1V | 113/116 (97%) | 99 (88%) | 13 (12%) | 1 (1%) | 17 | 54 |
| 22 | 1W | 113/128 (88%) | 103 (91%) | 9 (8%) | 1 (1%) | 17 | 54 |
| 23 | 1X | 169/172 (98%) | 154 (91%) | 15 (9%) | 0 | 100 | 100 |
| 24 | 1Y | 137/141 (97%) | 133 (97%) | 3 (2%) | 1 (1%) | 22 | 60 |
| 25 | 1Z | 139/144 (96%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 26 | 1a | 68/70 (97%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 27 | 1b | 81/84 (96%) | 73 (90%) | 8 (10%) | 0 | 100 | 100 |
| 28 | 1c | 47/76 (62%) | 43 (92%) | 4 (8%) | 0 | 100 | 100 |
| 29 | 1d | 117/123 (95%) | 105 (90%) | 12 (10%) | 0 | 100 | 100 |
| 30 | 1e | 97/106 (92%) | 88 (91%) | 8 (8%) | 1 (1%) | 15 | 52 |
| 31 | 1f | 55/135 (41%) | 47 (86%) | 8 (14%) | 0 | 100 | 100 |
| 32 | 1g | 98/154 (64%) | 84 (86%) | 14 (14%) | 0 | 100 | 100 |
| 33 | 1h | 136/189 (72%) | 126 (93%) | 10 (7%) | 0 | 100 | 100 |
| 34 | 1i | 124/128 (97%) | 113 (91%) | 11 (9%) | 0 | 100 | 100 |
| 35 | 1j | 69/105 (66%) | 62 (90%) | 7 (10%) | 0 | 100 | 100 |
| 36 | 1k | 79/98 (81%) | 72 (91%) | 7 (9%) | 0 | 100 | 100 |
| 37 | 1l | 154/186 (83%) | 141 (92%) | 13 (8%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 38 | 1m | 126/129 (98%) | 119 (94%) | 7 (6%) | 0 | 100 | 100 |
| 39 | 1n | 170/179 (95%) | 161 (95%) | 8 (5%) | 1 (1%) | 25 | 62 |
| 40 | 1o | 120/137 (88%) | 115 (96%) | 5 (4%) | 0 | 100 | 100 |
| 41 | 1p | 171/176 (97%) | 161 (94%) | 10 (6%) | 0 | 100 | 100 |
| 42 | 1q | 143/145 (99%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 43 | 1r | 90/113 (80%) | 85 (94%) | 5 (6%) | 0 | 100 | 100 |
| 44 | 1s | 43/471 (9%) | 40 (93%) | 3 (7%) | 0 | 100 | 100 |
| All | All | 8187/9743 (84%) | 7582 (93%) | 586 (7%) | 19 (0%) | 50 | 79 |

5 of 19 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 46 | SER |
| 3 | 1C | 89 | ARG |
| 7 | 1G | 499 | GLN |
| 8 | 1H | 208 | VAL |
| 10 | 1J | 4 | TYR |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | 1A | 100/100 (100%) | 91 (91%) | 9 (9%) | 9 | 37 |
| 2 | 1B | 131/212 (62%) | 107 (82%) | 24 (18%) | 1 | 11 |
| 3 | 1C | 190/227 (84%) | 169 (89%) | 21 (11%) | 6 | 29 |
| 4 | 1D | 371/405 (92%) | 329 (89%) | 42 (11%) | 6 | 28 |
| 5 | 1E | 183/207 (88%) | 168 (92%) | 15 (8%) | 11 | 40 |
| 6 | 1F | 346/368 (94%) | 307 (89%) | 39 (11%) | 6 | 28 |
| 7 | 1G | 588/610 (96%) | 530 (90%) | 58 (10%) | 8 | 32 |
| 8 | 1H | 274/275 (100%) | 247 (90%) | 27 (10%) | 8 | 32 |
| 9 | 1I | 151/201 (75%) | 131 (87%) | 20 (13%) | 4 | 22 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 10 | 1J | 139/141 (99%) | 115 (83%) | 24 (17%) | 2 | 13 |
| 11 | 1K | 84/85 (99%) | 70 (83%) | 14 (17%) | 2 | 15 |
| 12 | 1L | 539/540 (100%) | 489 (91%) | 50 (9%) | 9 | 35 |
| 13 | 1M | 408/409 (100%) | 362 (89%) | 46 (11%) | 6 | 28 |
| 14 | 1N | 310/311 (100%) | 283 (91%) | 27 (9%) | 10 | 38 |
| 15 | 1O | 283/307 (92%) | 243 (86%) | 40 (14%) | 3 | 21 |
| 16 | 1P | 296/323 (92%) | 259 (88%) | 37 (12%) | 4 | 24 |
| 17 | 1Q | 117/152 (77%) | 102 (87%) | 15 (13%) | 4 | 23 |
| 18 | 1R | 79/97 (81%) | 68 (86%) | 11 (14%) | 3 | 21 |
| 19 | 1S | 77/82 (94%) | 60 (78%) | 17 (22%) | 1 | 6 |
| 20 | 1T | 79/133 (59%) | 67 (85%) | 12 (15%) | 3 | 18 |
| 20 | 1U | 79/133 (59%) | 69 (87%) | 10 (13%) | 4 | 23 |
| 21 | 1V | 100/101 (99%) | 82 (82%) | 18 (18%) | 1 | 12 |
| 22 | 1W | 107/112 (96%) | 91 (85%) | 16 (15%) | 3 | 18 |
| 23 | 1X | 153/154 (99%) | 140 (92%) | 13 (8%) | 10 | 40 |
| 24 | 1Y | 101/102 (99%) | 92 (91%) | 9 (9%) | 9 | 38 |
| 25 | 1Z | 123/124 (99%) | 109 (89%) | 14 (11%) | 5 | 28 |
| 26 | 1a | 58/58 (100%) | 52 (90%) | 6 (10%) | 7 | 31 |
| 27 | 1b | 69/70 (99%) | 62 (90%) | 7 (10%) | 7 | 32 |
| 28 | 1c | 45/66 (68%) | 37 (82%) | 8 (18%) | 2 | 12 |
| 29 | 1d | 107/109 (98%) | 95 (89%) | 12 (11%) | 6 | 28 |
| 30 | 1e | 87/94 (93%) | 65 (75%) | 22 (25%) | 0 | 4 |
| 31 | 1f | 54/113 (48%) | 47 (87%) | 7 (13%) | 4 | 23 |
| 32 | 1g | 92/129 (71%) | 80 (87%) | 12 (13%) | 4 | 23 |
| 33 | 1h | 121/158 (77%) | 102 (84%) | 19 (16%) | 2 | 17 |
| 34 | 1i | 119/120 (99%) | 105 (88%) | 14 (12%) | 5 | 26 |
| 35 | 1j | 62/84 (74%) | 51 (82%) | 11 (18%) | 2 | 13 |
| 36 | 1k | 63/76 (83%) | 55 (87%) | 8 (13%) | 4 | 23 |
| 37 | 1l | 141/161 (88%) | 125 (89%) | 16 (11%) | 6 | 28 |
| 38 | 1m | 113/114 (99%) | 102 (90%) | 11 (10%) | 8 | 33 |
| 39 | 1n | 156/160 (98%) | 136 (87%) | 20 (13%) | 4 | 23 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 40 | 1o | 110/120 (92%) | 96 (87%) | 14 (13%) | 4 | 23 |
| 41 | 1p | 154/156 (99%) | 140 (91%) | 14 (9%) | 9 | 36 |
| 42 | 1q | 131/131 (100%) | 114 (87%) | 17 (13%) | 4 | 23 |
| 43 | 1r | 85/98 (87%) | 73 (86%) | 12 (14%) | 3 | 21 |
| 44 | 1s | 44/351 (12%) | 38 (86%) | 6 (14%) | 3 | 22 |
| All | All | 7219/8279 (87%) | 6355 (88%) | 864 (12%) | 8 | 25 |

5 of 864 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | 1P | 78 | LYS |
| 21 | 1V | 111 | TRP |
| 39 | 1n | 150 | THR |
| 16 | 1P | 209 | ASP |
| 16 | 1P | 65 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | 1O | 153 | ASN |
| 44 | 1s | 55 | ASN |
| 22 | 1W | 72 | HIS |
| 42 | 1q | 31 | ASN |
| 38 | 1m | 125 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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 |
| 34 | SAC | 1i | 1 | - | 7,8,9 | 0.54 | 0 | 8,9,11 | 1.06 | 1 (12%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 34 | SAC | 1i | 1 | - | - | 2/7/8/10 | - |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 34 | 1i | 1 | SAC | O-C-CA | -2.91 | 117.15 | 124.78 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 34 | 1i | 1 | SAC | C2A-C1A-N-CA |
| 34 | 1i | 1 | SAC | OAC-C1A-N-CA |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 3 are monoatomic - leaving 43 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 |
| 51 | CDL | 1N | 402 | - | 66,66,99 | 0.30 | 0 | 72,78,111 | 0.46 | 0 |
| 48 | FES | 1E | 301 | 5 | 0,4,4 | - | - | - | | |
| 46 | PC1 | 1I | 203 | - | 43,43,53 | 0.30 | 0 | 49,51,61 | 0.43 | 0 |
| 45 | 3PE | 1L | 701 | - | 45,45,50 | 0.28 | 0 | 48,50,55 | 0.37 | 0 |
| 51 | CDL | 1a | 101 | - | 60,60,99 | 0.33 | 0 | 66,72,111 | 0.42 | 0 |
| 46 | PC1 | 1B | 202 | - | 33,33,53 | 0.32 | 0 | 39,41,61 | 0.33 | 0 |
| 45 | 3PE | 1A | 201 | - | 30,30,50 | 0.33 | 0 | 33,35,55 | 0.40 | 0 |
| 56 | EHZ | 1n | 201 | - | 29,36,37 | 0.18 | 0 | 35,44,47 | 1.16 | 1 (2%) |
| 52 | GTP | 1O | 401 | 53 | 26,34,34 | 0.97 | 2 (7%) | 32,54,54 | 0.80 | 0 |
| 45 | 3PE | 1M | 502 | - | 37,37,50 | 0.30 | 0 | 40,42,55 | 0.40 | 0 |
| 49 | FMN | 1F | 501 | - | 33,33,33 | 0.58 | 0 | 48,50,50 | 0.66 | 1 (2%) |
| 46 | PC1 | 1f | 101 | - | 33,33,53 | 0.68 | 1 (3%) | 39,41,61 | 0.96 | 3 (7%) |
| 46 | PC1 | 1M | 501 | - | 34,34,53 | 0.32 | 0 | 40,42,61 | 0.36 | 0 |
| 46 | PC1 | 1H | 401 | - | 53,53,53 | 0.27 | 0 | 59,61,61 | 0.36 | 0 |
| 47 | SF4 | 1F | 502 | 6 | 0,12,12 | - | - | - | | |
| 45 | 3PE | 1Y | 802 | - | 39,39,50 | 0.29 | 0 | 42,44,55 | 0.40 | 0 |
| 51 | CDL | 1L | 702 | - | 75,75,99 | 0.31 | 0 | 81,87,111 | 0.36 | 0 |
| 45 | 3PE | 1Y | 804 | - | 34,34,50 | 0.31 | 0 | 37,39,55 | 0.57 | 1 (2%) |
| 46 | PC1 | 1H | 402 | - | 33,33,53 | 0.33 | 0 | 39,41,61 | 0.40 | 0 |
| 46 | PC1 | 1q | 201 | - | 47,47,53 | 0.27 | 0 | 53,55,61 | 0.41 | 0 |
| 47 | SF4 | 1G | 802 | 7 | 0,12,12 | - | - | - | | |
| 46 | PC1 | 1d | 202 | - | 38,38,53 | 0.32 | 0 | 44,46,61 | 0.42 | 0 |
| 47 | SF4 | 1B | 201 | 2 | 0,12,12 | - | - | - | | |
| 45 | 3PE | 1D | 901 | - | 45,45,50 | 0.28 | 0 | 48,50,55 | 0.33 | 0 |
| 47 | SF4 | 1I | 202 | 9 | 0,12,12 | - | - | - | | |
| 45 | 3PE | 1f | 102 | - | 50,50,50 | 0.28 | 0 | 53,55,55 | 0.99 | 4 (7%) |
| 46 | PC1 | 1A | 202 | - | 25,25,53 | 0.38 | 0 | 29,32,61 | 0.51 | 0 |
| 46 | PC1 | 1Y | 803 | - | 45,45,53 | 0.29 | 0 | 51,53,61 | 0.34 | 0 |
| 45 | 3PE | 1N | 401 | - | 37,37,50 | 0.31 | 0 | 40,42,55 | 0.43 | 0 |
| 45 | 3PE | 1Y | 801 | - | 30,30,50 | 0.35 | 0 | 33,35,55 | 1.30 | 4 (12%) |
| 46 | PC1 | 1J | 201 | - | 31,31,53 | 0.34 | 0 | 37,39,61 | 0.35 | 0 |
| 47 | SF4 | 1G | 801 | 7 | 0,12,12 | - | - | - | | |
| 51 | CDL | 1X | 201 | - | 85,85,99 | 0.28 | 0 | 91,97,111 | 0.33 | 0 |
| 57 | MYR | 1l | 201 | - | 14,14,15 | 0.34 | 0 | 13,13,15 | 0.40 | 0 |
| 51 | CDL | 1H | 403 | - | 50,50,99 | 0.36 | 0 | 56,62,111 | 0.54 | 1 (1%) |
| 51 | CDL | 1d | 201 | - | 64,64,99 | 0.32 | 0 | 70,76,111 | 0.37 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 45 | 3PE | 1L | 704 | - | 41,41,50 | 0.29 | 0 | 44,46,55 | 0.38 | 0 |
| 46 | PC1 | 1L | 703 | - | 37,37,53 | 0.29 | 0 | 43,45,61 | 0.34 | 0 |
| 48 | FES | 1G | 803 | 7 | 0,4,4 | - | - | - | - | - |
| 56 | EHZ | 1W | 201 | - | 29,36,37 | 0.20 | 0 | 35,44,47 | 1.49 | 1 (2%) |
| 46 | PC1 | 1h | 201 | - | 46,46,53 | 0.26 | 0 | 52,54,61 | 0.43 | 0 |
| 47 | SF4 | 1I | 201 | 9 | 0,12,12 | - | - | - | - | - |
| 54 | NDP | 1P | 501 | - | 45,52,52 | 0.60 | 0 | 53,80,80 | 0.71 | 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 |
|-----|------|-------|-----|------|---------|--------------|---------|
| 51 | CDL | 1N | 402 | - | - | 10/76/76/110 | - |
| 48 | FES | 1E | 301 | 5 | - | - | 0/1/1/1 |
| 46 | PC1 | 1I | 203 | - | - | 11/47/47/57 | - |
| 45 | 3PE | 1L | 701 | - | - | 4/49/49/54 | - |
| 51 | CDL | 1a | 101 | - | - | 9/71/71/110 | - |
| 46 | PC1 | 1B | 202 | - | - | 14/37/37/57 | - |
| 45 | 3PE | 1A | 201 | - | - | 5/34/34/54 | - |
| 56 | EHZ | 1n | 201 | - | - | 8/42/44/45 | - |
| 52 | GTP | 1O | 401 | 53 | - | 0/18/38/38 | 0/3/3/3 |
| 45 | 3PE | 1M | 502 | - | - | 10/41/41/54 | - |
| 49 | FMN | 1F | 501 | - | - | 2/18/18/18 | 0/3/3/3 |
| 46 | PC1 | 1f | 101 | - | - | 10/36/36/57 | - |
| 46 | PC1 | 1M | 501 | - | - | 4/38/38/57 | - |
| 46 | PC1 | 1H | 401 | - | - | 3/57/57/57 | - |
| 51 | CDL | 1L | 702 | - | - | 13/86/86/110 | - |
| 45 | 3PE | 1Y | 802 | - | - | 11/43/43/54 | - |
| 47 | SF4 | 1F | 502 | 6 | - | - | 0/6/5/5 |
| 45 | 3PE | 1Y | 804 | - | - | 10/38/38/54 | - |
| 46 | PC1 | 1H | 402 | - | - | 4/37/37/57 | - |
| 46 | PC1 | 1q | 201 | - | - | 11/51/51/57 | - |
| 47 | SF4 | 1G | 802 | 7 | - | - | 0/6/5/5 |
| 46 | PC1 | 1d | 202 | - | - | 15/42/42/57 | - |
| 47 | SF4 | 1B | 201 | 2 | - | - | 0/6/5/5 |
| 45 | 3PE | 1D | 901 | - | - | 2/49/49/54 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|---------|
| 47 | SF4 | 1I | 202 | 9 | - | - | 0/6/5/5 |
| 45 | 3PE | 1f | 102 | - | - | 14/54/54/54 | - |
| 46 | PC1 | 1A | 202 | - | - | 4/28/28/57 | - |
| 46 | PC1 | 1Y | 803 | - | - | 8/49/49/57 | - |
| 45 | 3PE | 1N | 401 | - | - | 7/41/41/54 | - |
| 45 | 3PE | 1Y | 801 | - | - | 7/34/34/54 | - |
| 46 | PC1 | 1J | 201 | - | - | 6/35/35/57 | - |
| 51 | CDL | 1X | 201 | - | - | 22/96/96/110 | - |
| 47 | SF4 | 1G | 801 | 7 | - | - | 0/6/5/5 |
| 57 | MYR | 1l | 201 | - | - | 2/11/12/13 | - |
| 51 | CDL | 1H | 403 | - | - | 8/61/61/110 | - |
| 51 | CDL | 1d | 201 | - | - | 13/75/75/110 | - |
| 45 | 3PE | 1L | 704 | - | - | 2/45/45/54 | - |
| 46 | PC1 | 1L | 703 | - | - | 3/40/40/57 | - |
| 48 | FES | 1G | 803 | 7 | - | - | 0/1/1/1 |
| 56 | EHZ | 1W | 201 | - | - | 18/42/44/45 | - |
| 46 | PC1 | 1h | 201 | - | - | 16/50/50/57 | - |
| 47 | SF4 | 1I | 201 | 9 | - | - | 0/6/5/5 |
| 54 | NDP | 1P | 501 | - | - | 9/30/77/77 | 0/5/5/5 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 52 | 1O | 401 | GTP | C5-C6 | -2.67 | 1.42 | 1.47 |
| 52 | 1O | 401 | GTP | C8-N7 | -2.13 | 1.31 | 1.35 |
| 46 | 1f | 101 | PC1 | O11-C1 | 2.05 | 1.52 | 1.44 |

The worst 5 of 17 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 56 | 1W | 201 | EHZ | C10-S1-C9 | 8.02 | 126.85 | 101.87 |
| 56 | 1n | 201 | EHZ | C10-S1-C9 | 5.92 | 120.30 | 101.87 |
| 45 | 1Y | 801 | 3PE | O21-C21-C22 | 5.60 | 123.58 | 111.50 |
| 45 | 1f | 102 | 3PE | O21-C21-C22 | 5.01 | 122.29 | 111.50 |
| 46 | 1f | 101 | PC1 | C3-C2-C1 | 3.39 | 119.80 | 111.79 |

There are no chirality outliers.

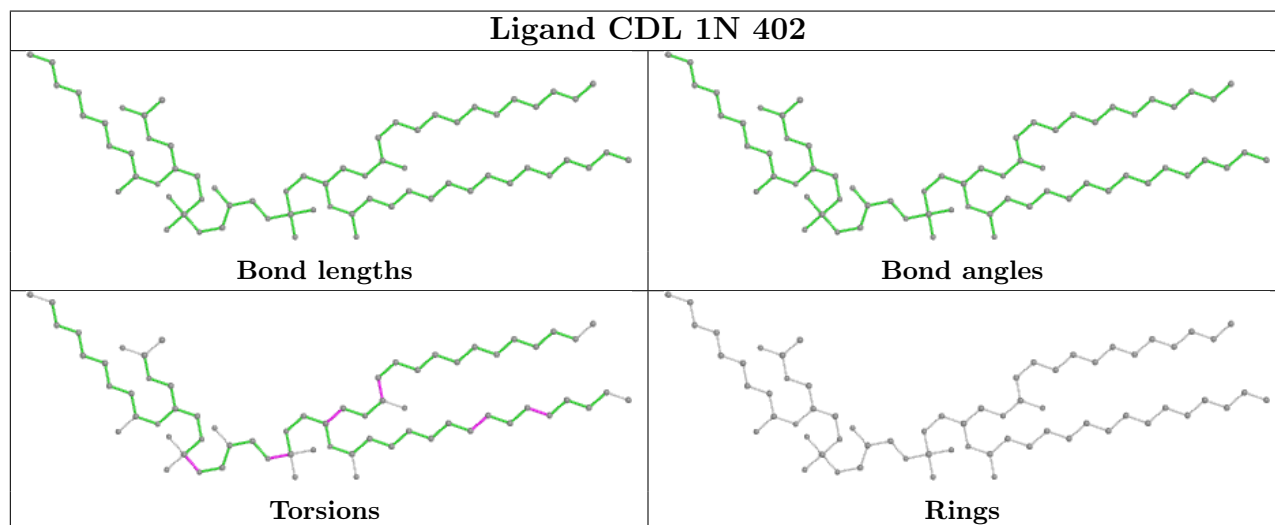
5 of 295 torsion outliers are listed below:

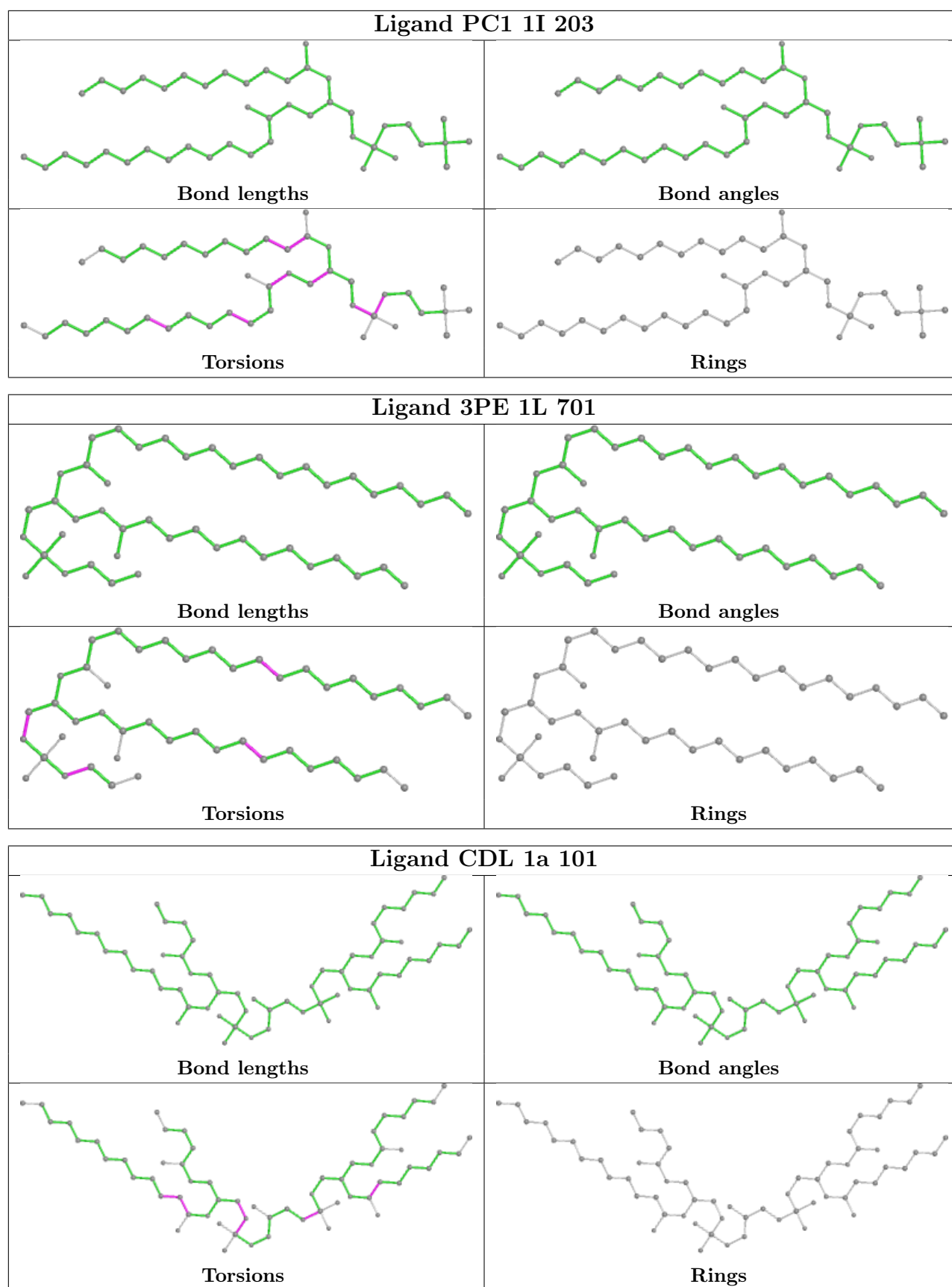
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 45 | 1N | 401 | 3PE | C1-O11-P-O14 |
| 45 | 1N | 401 | 3PE | C12-C11-O13-P |
| 45 | 1Y | 801 | 3PE | C1-O11-P-O13 |
| 45 | 1Y | 801 | 3PE | C2-C1-O11-P |
| 45 | 1Y | 801 | 3PE | O32-C31-O31-C3 |

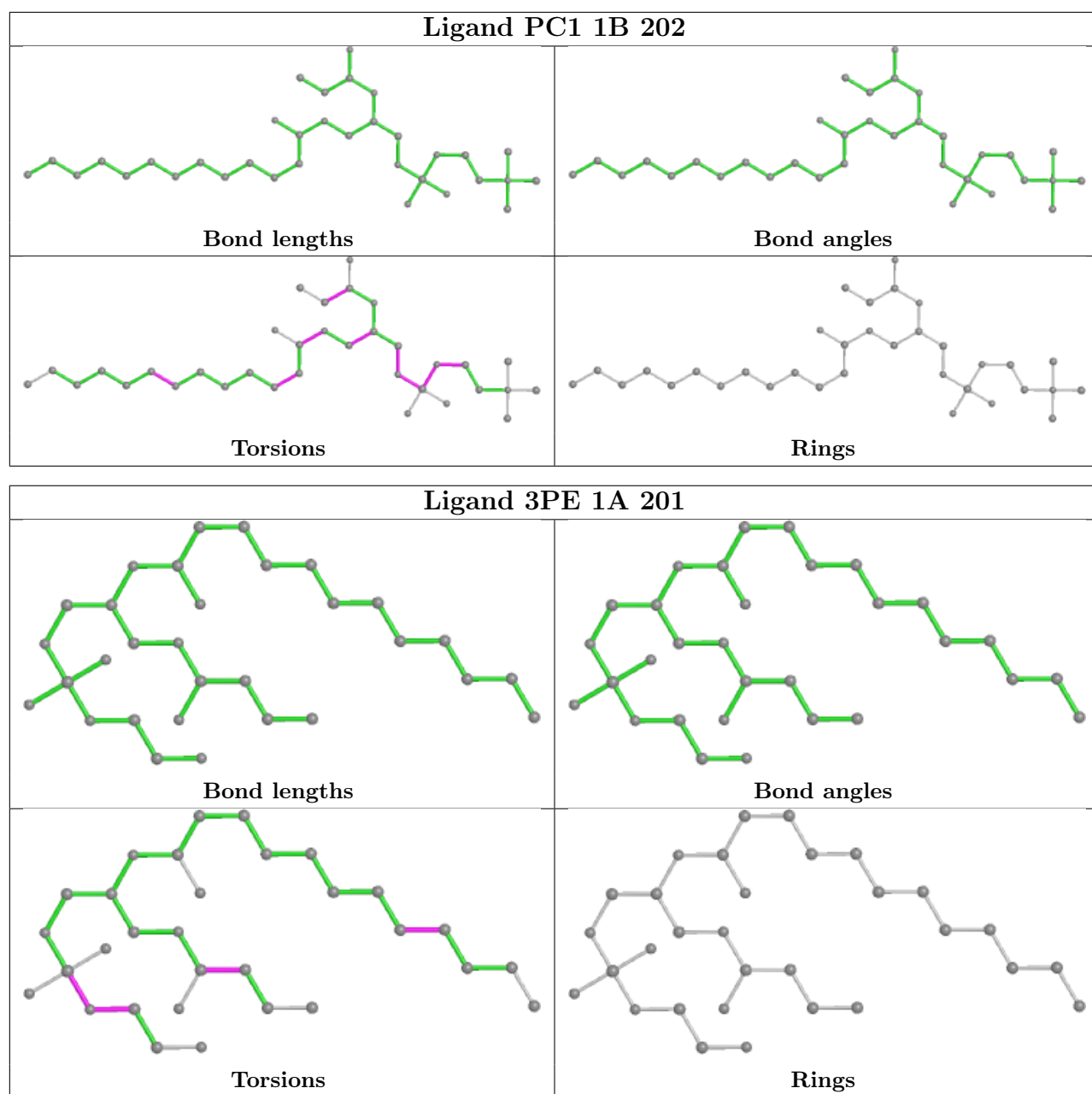
There are no ring outliers.

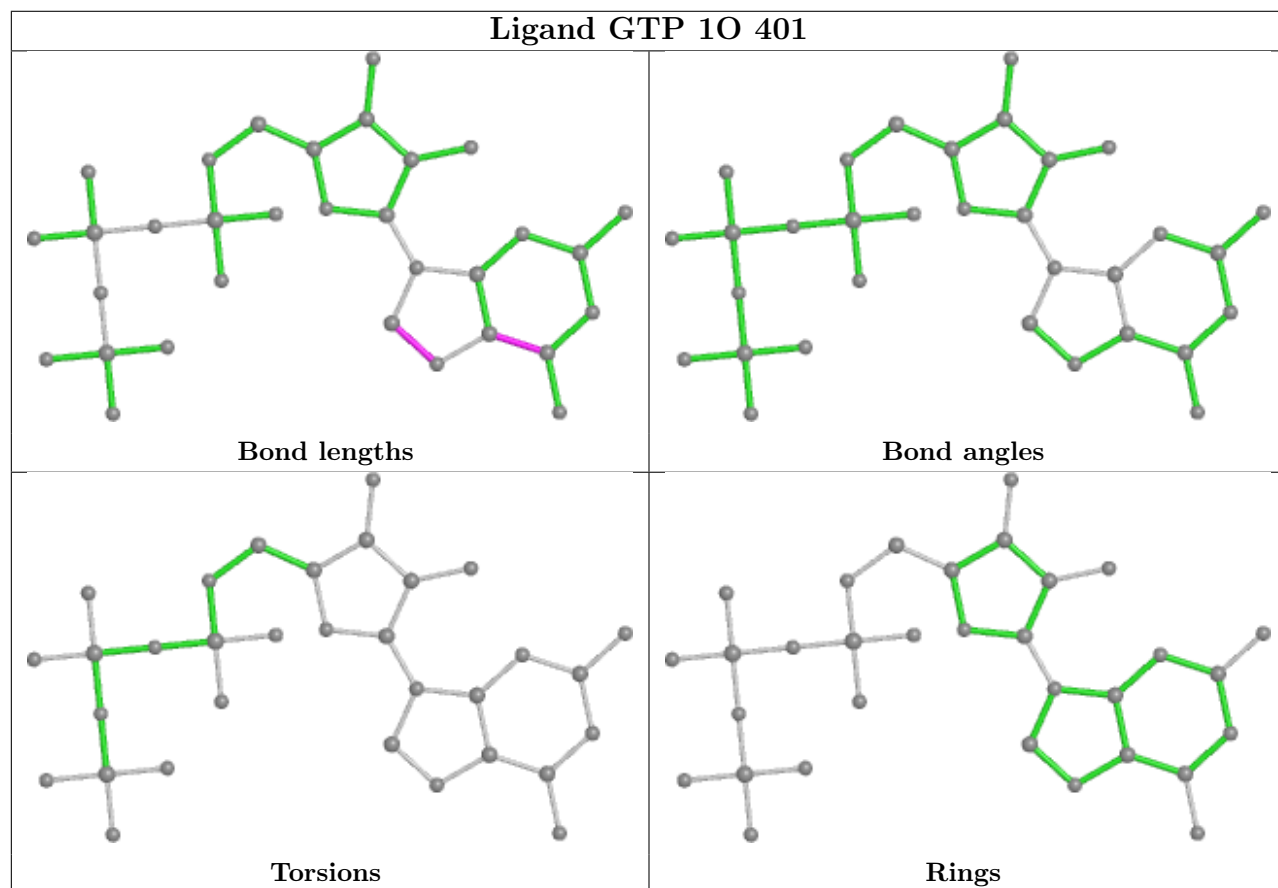
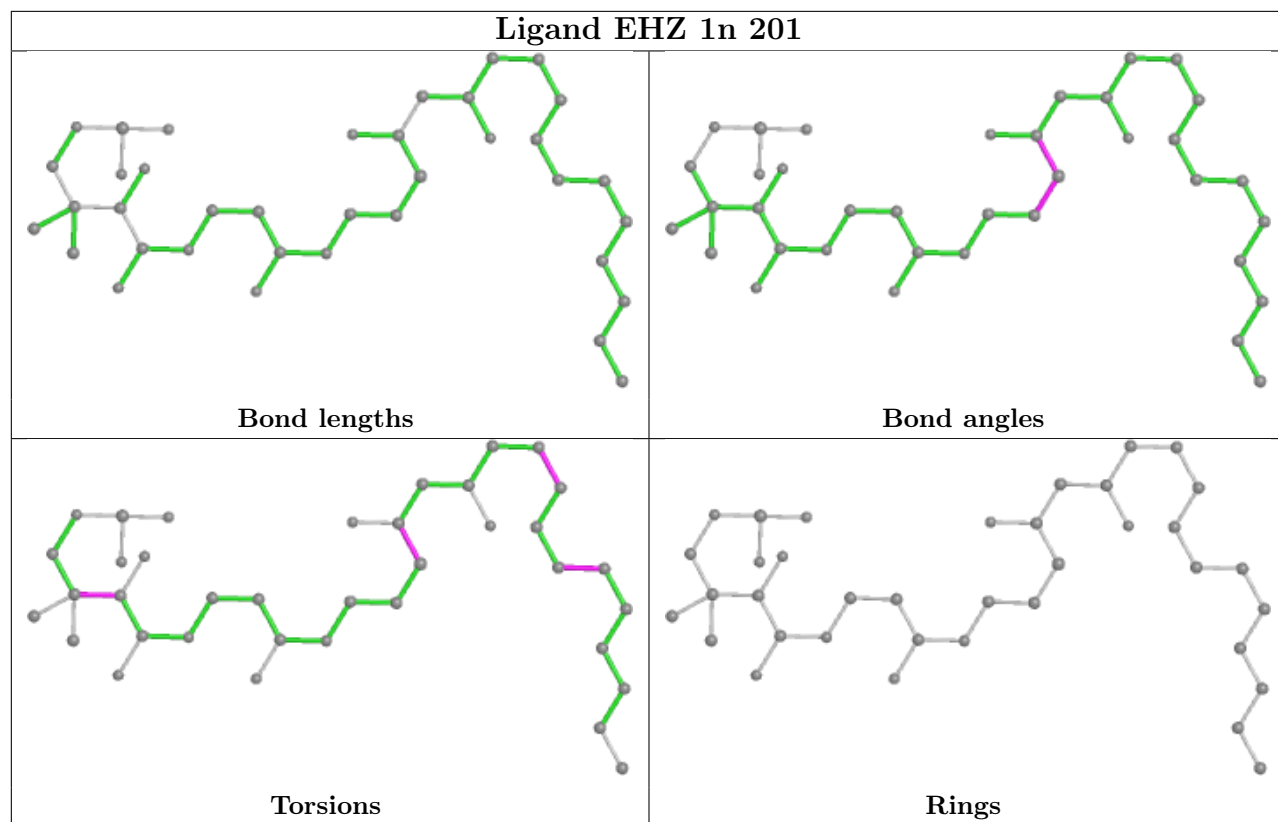
No monomer is involved in short contacts.

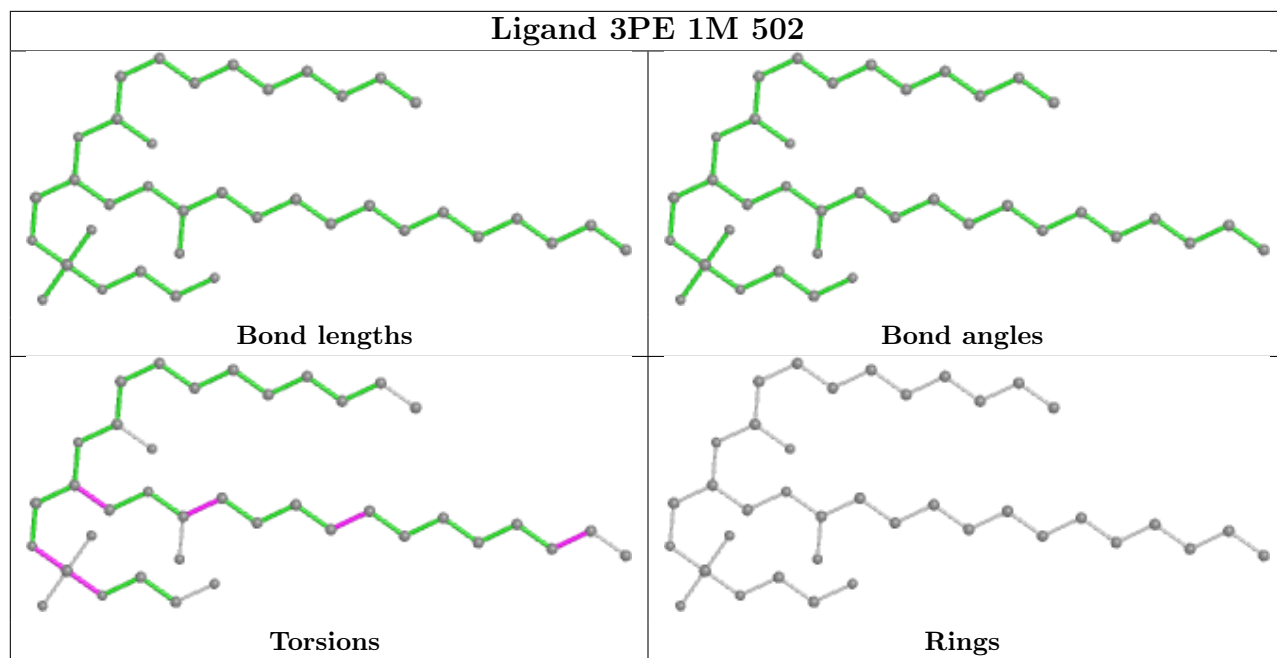
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

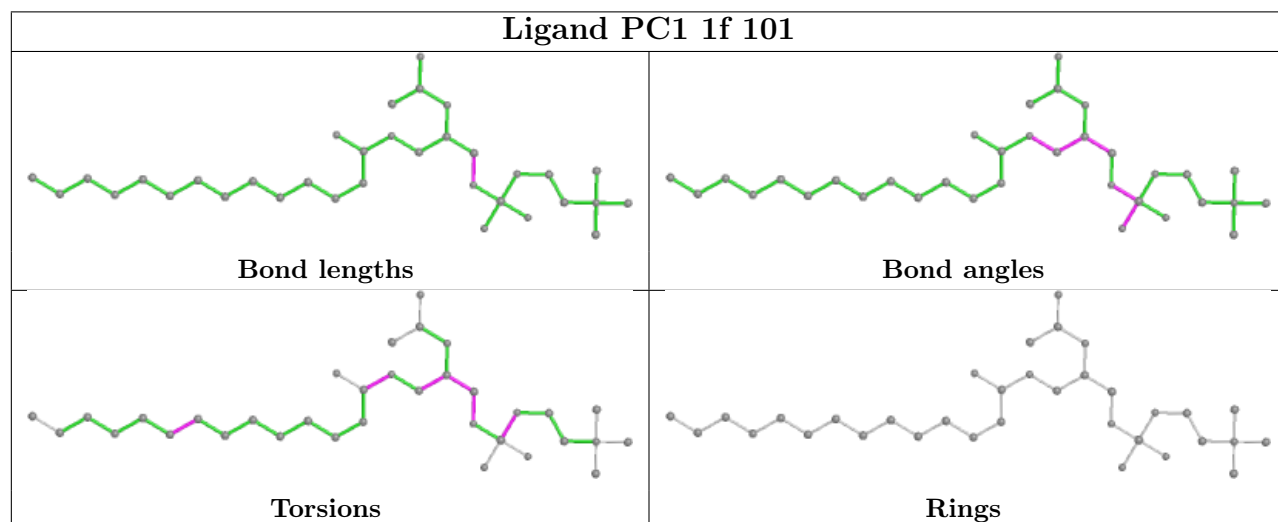
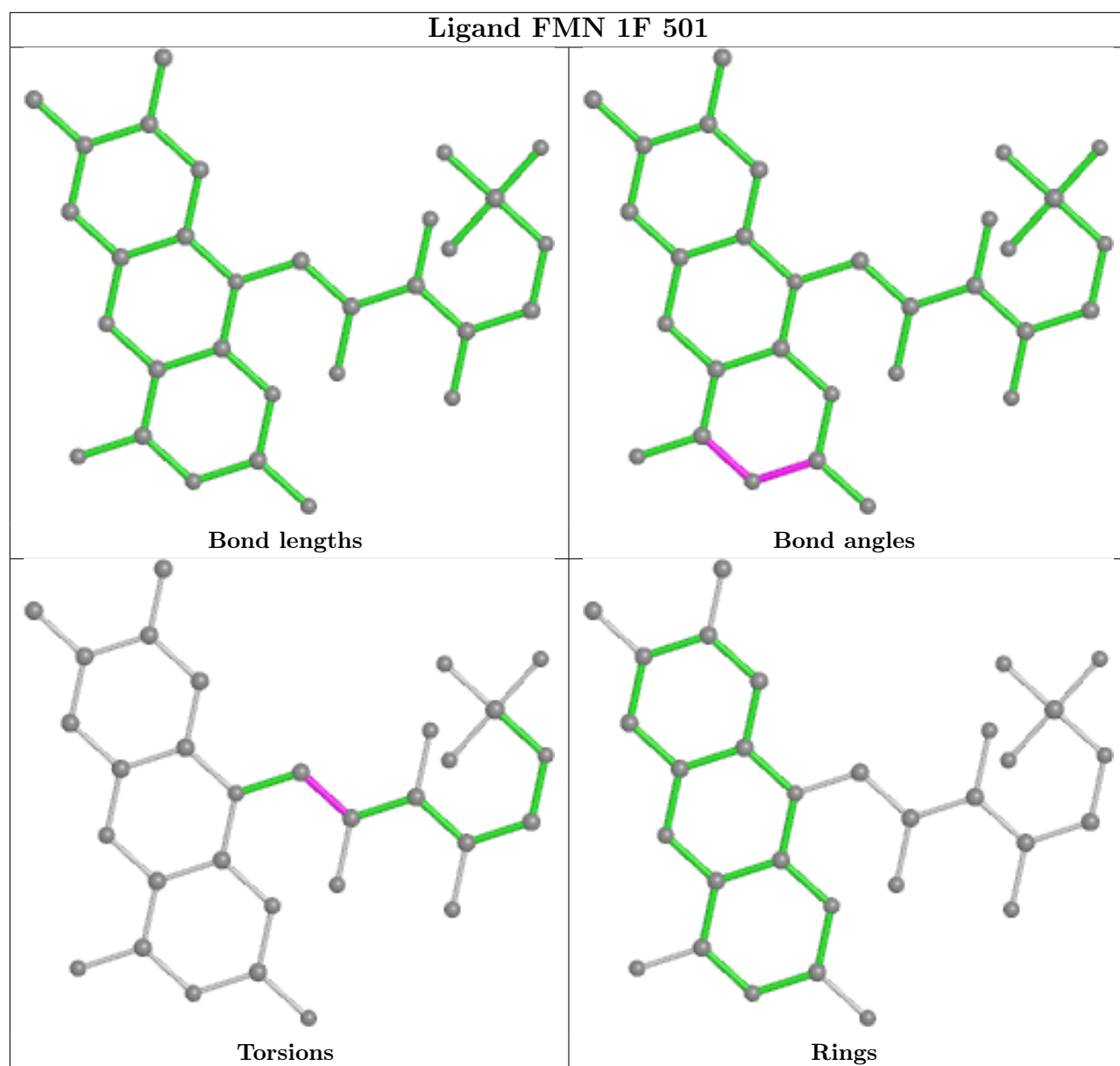


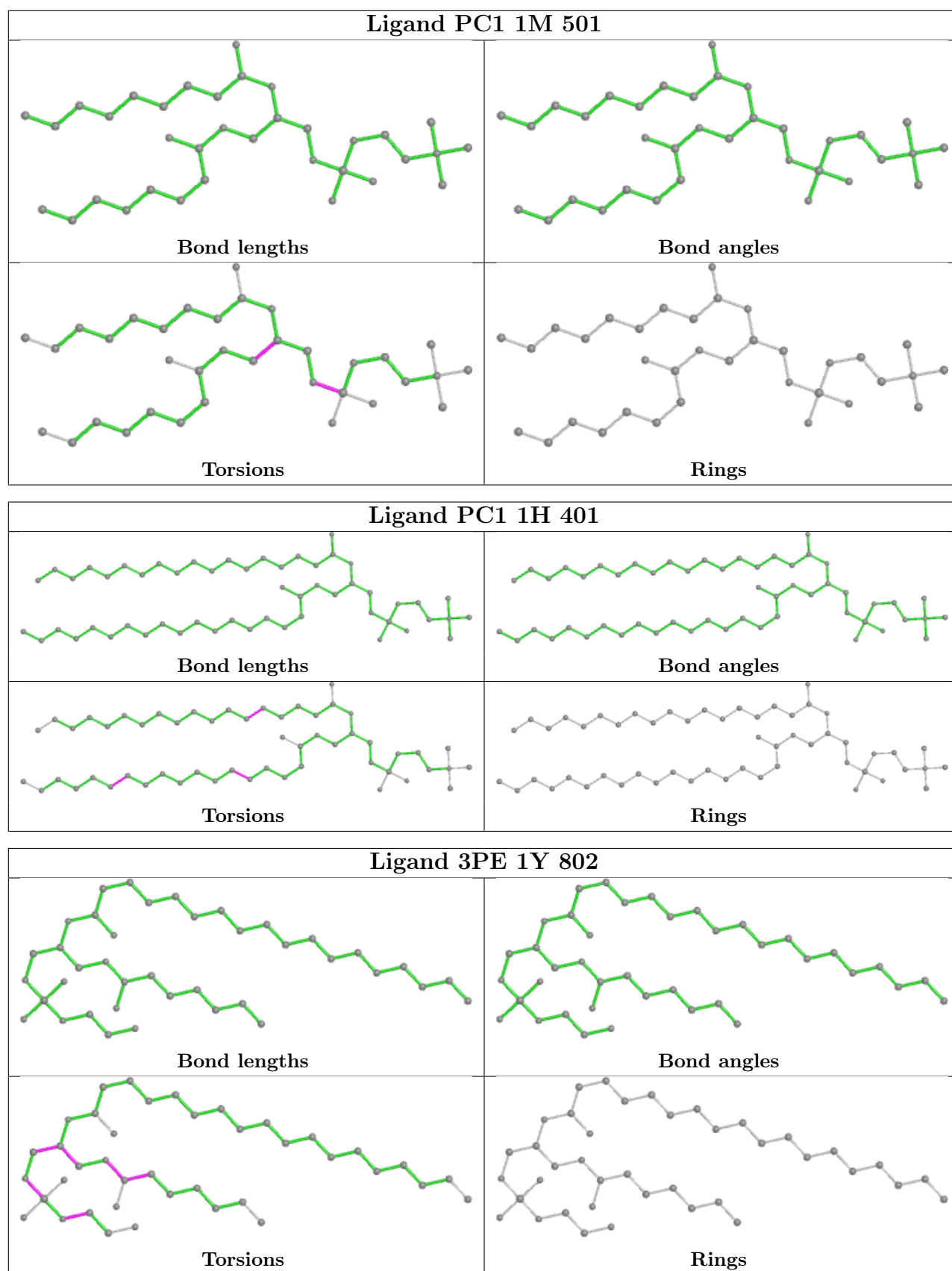


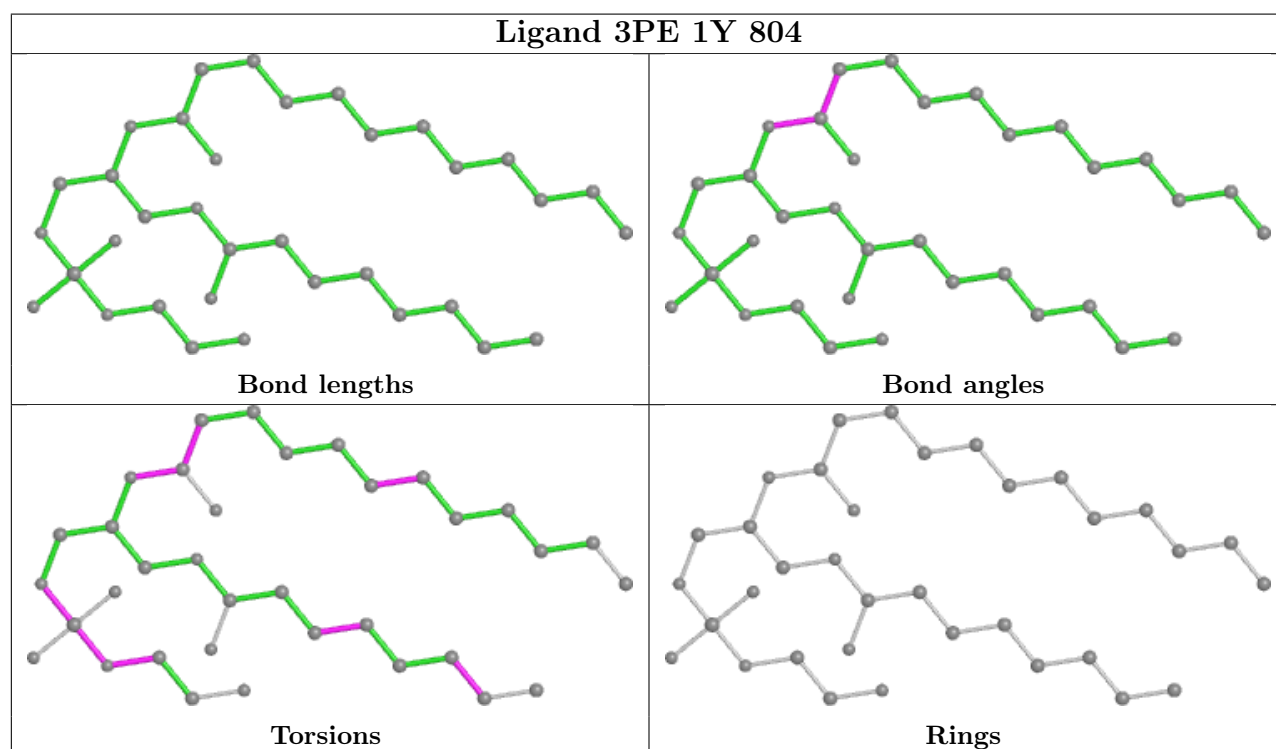
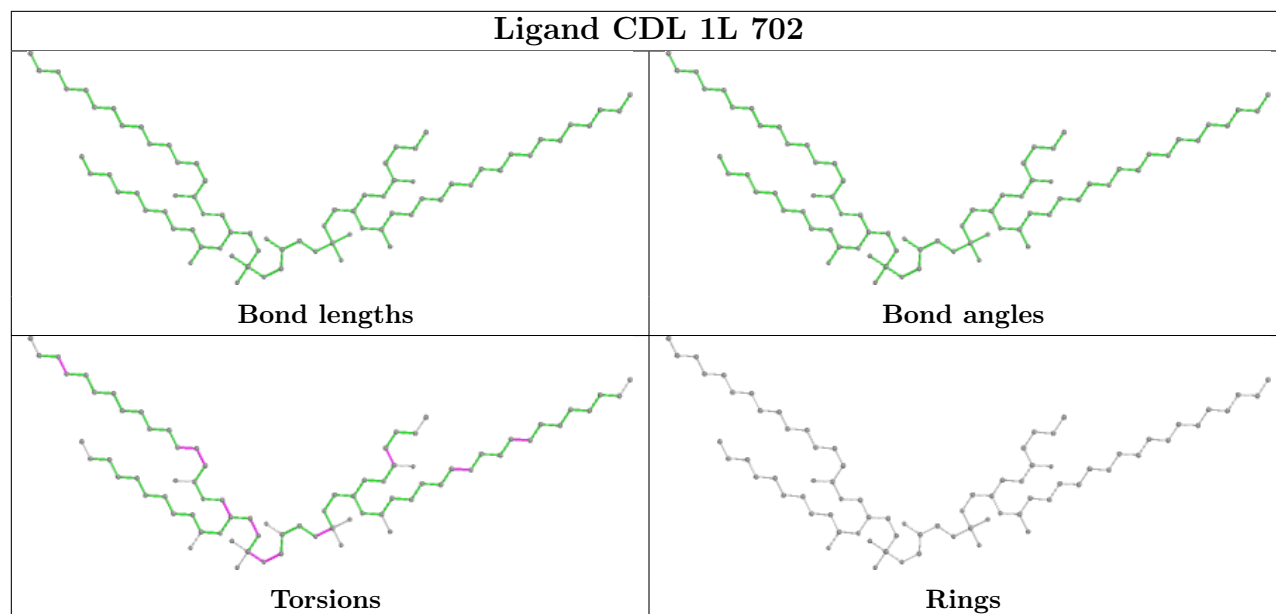


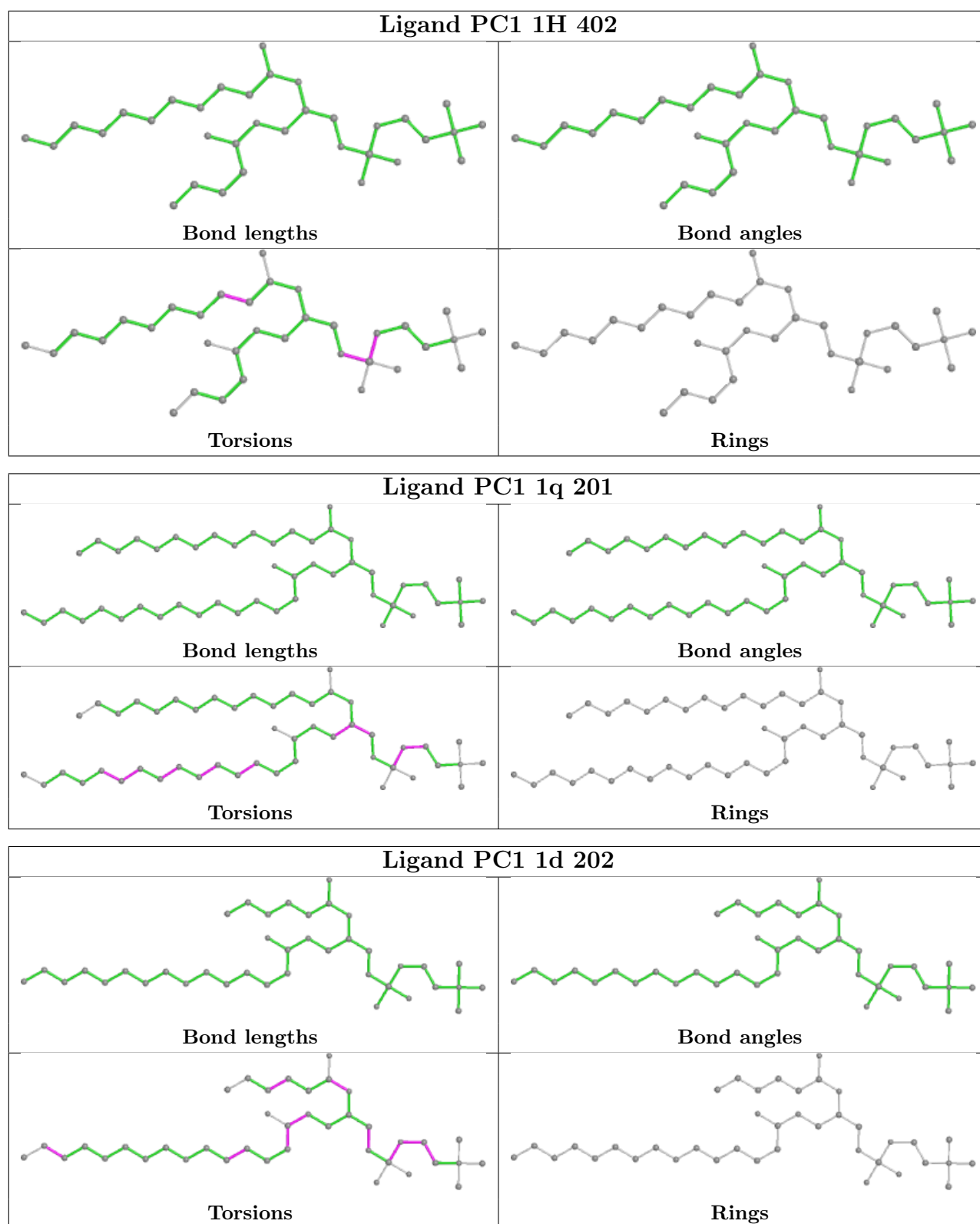


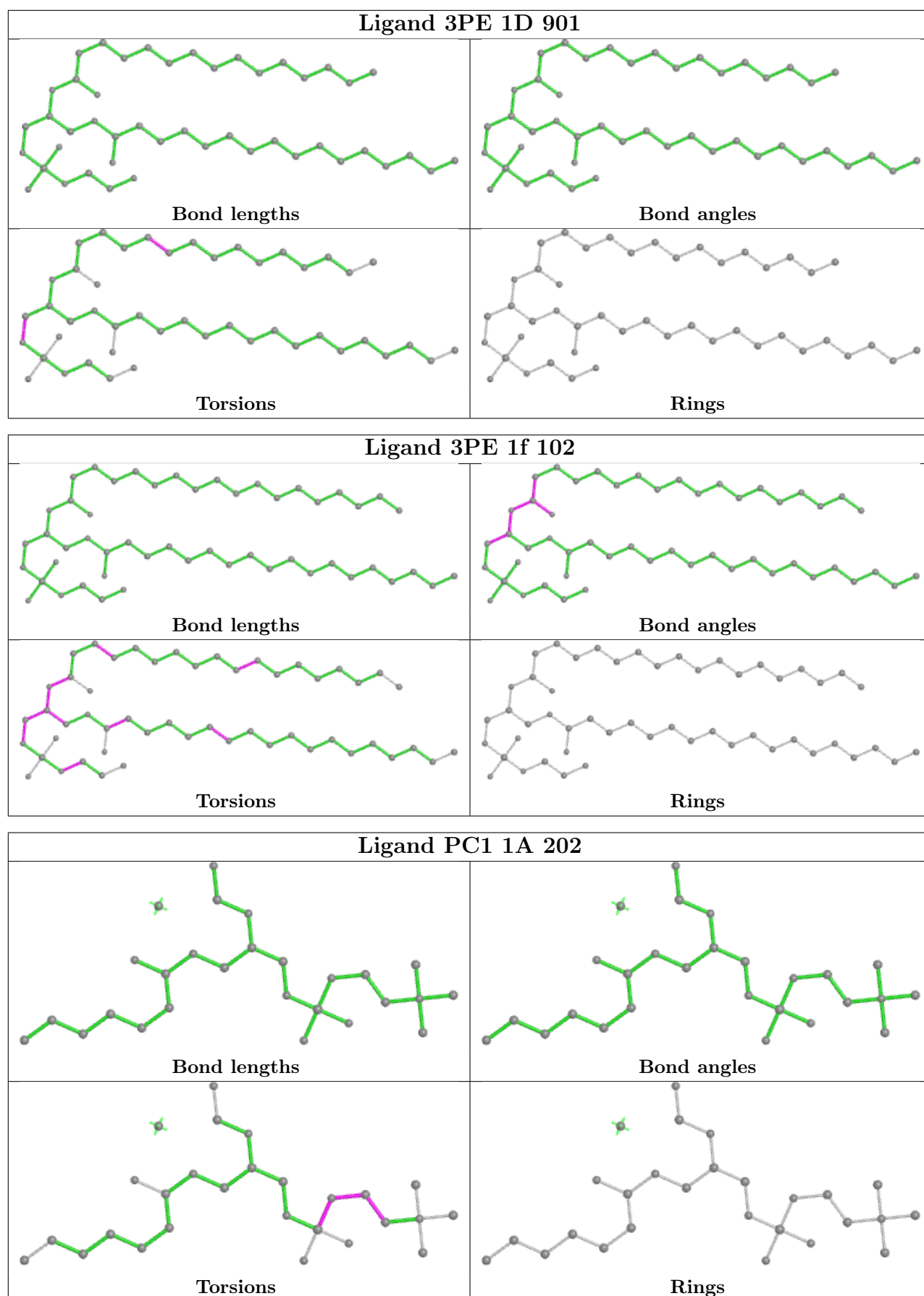


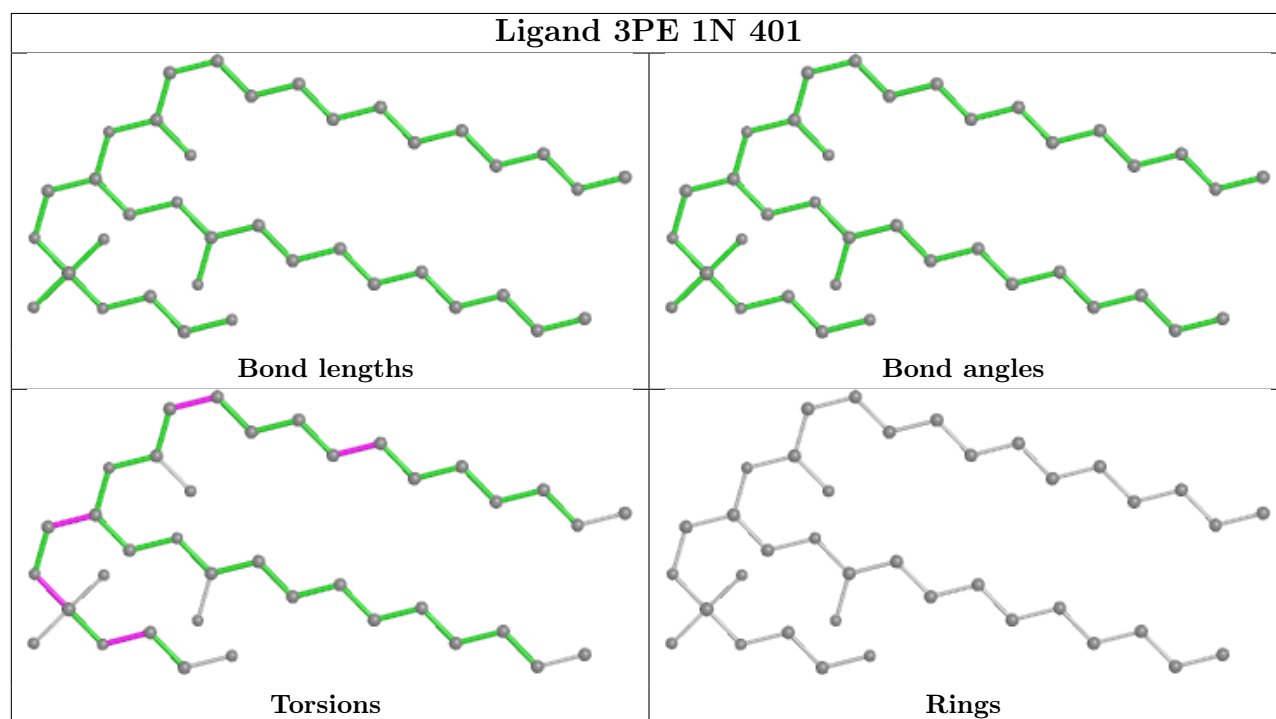
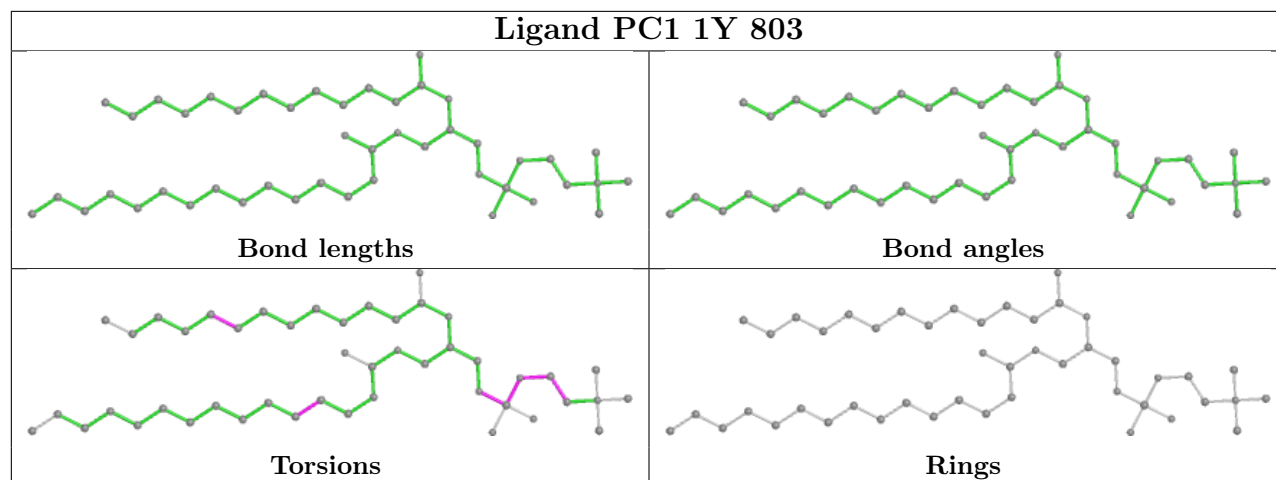


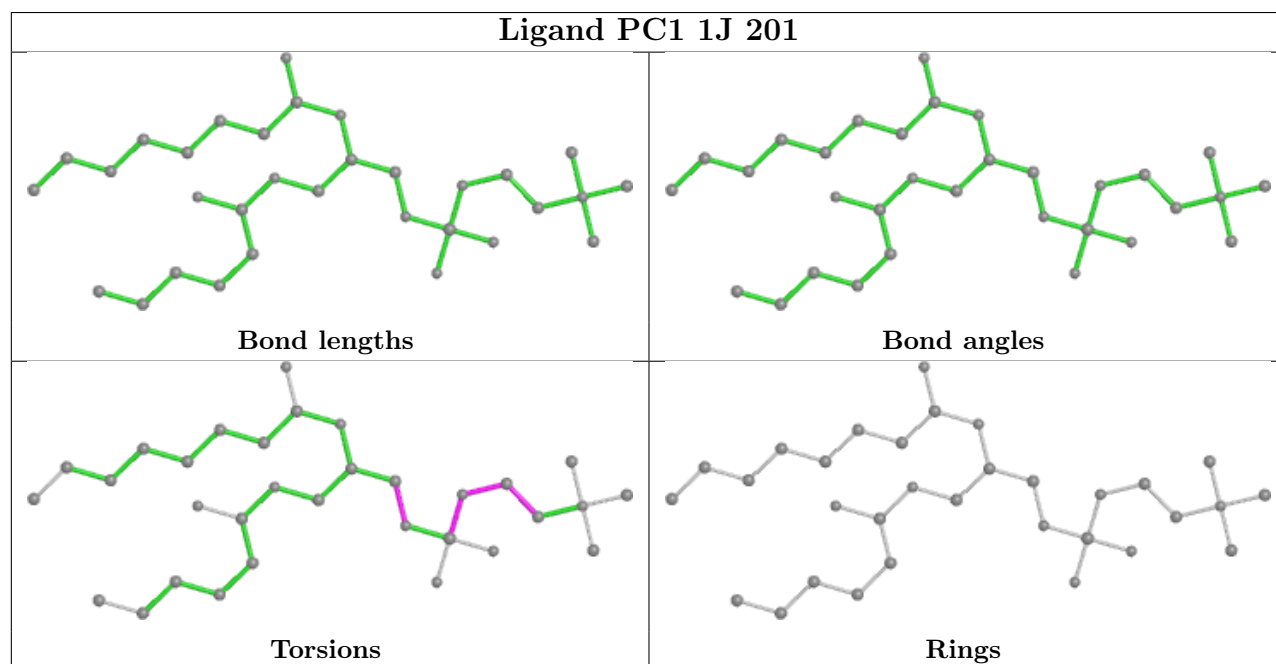
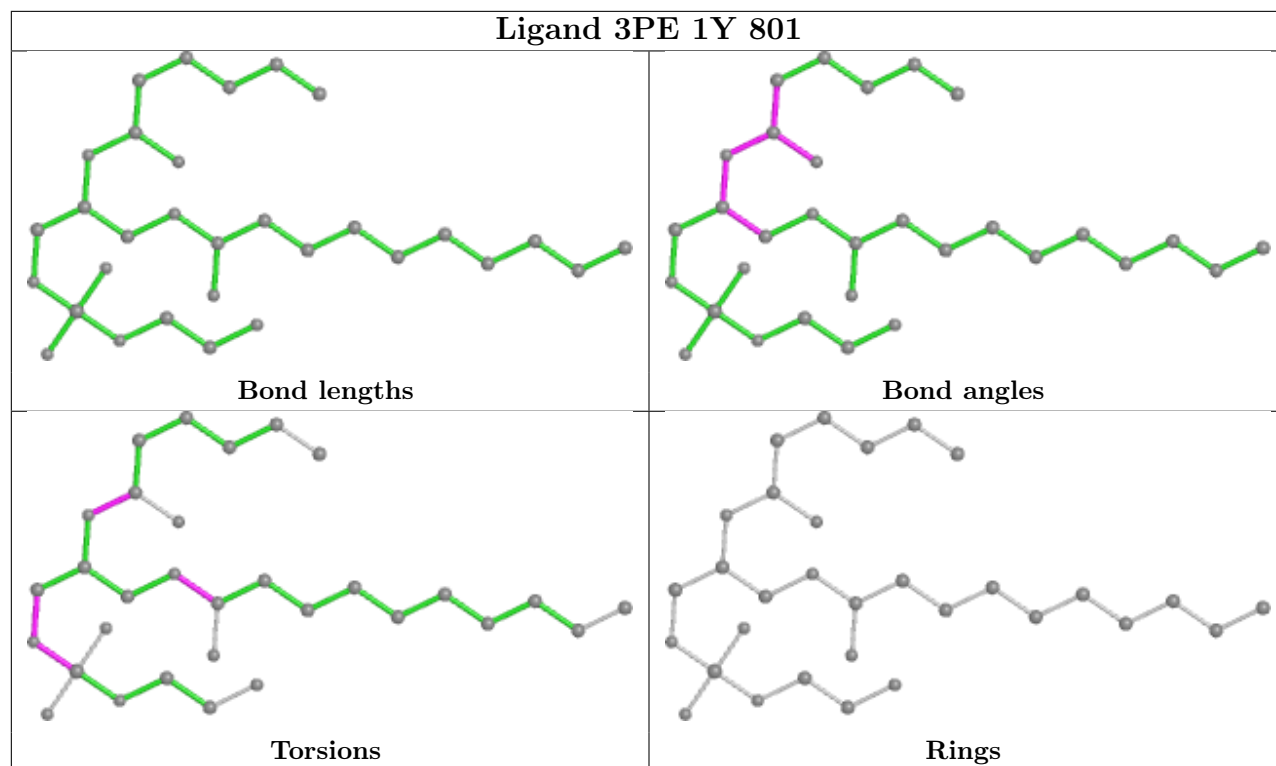


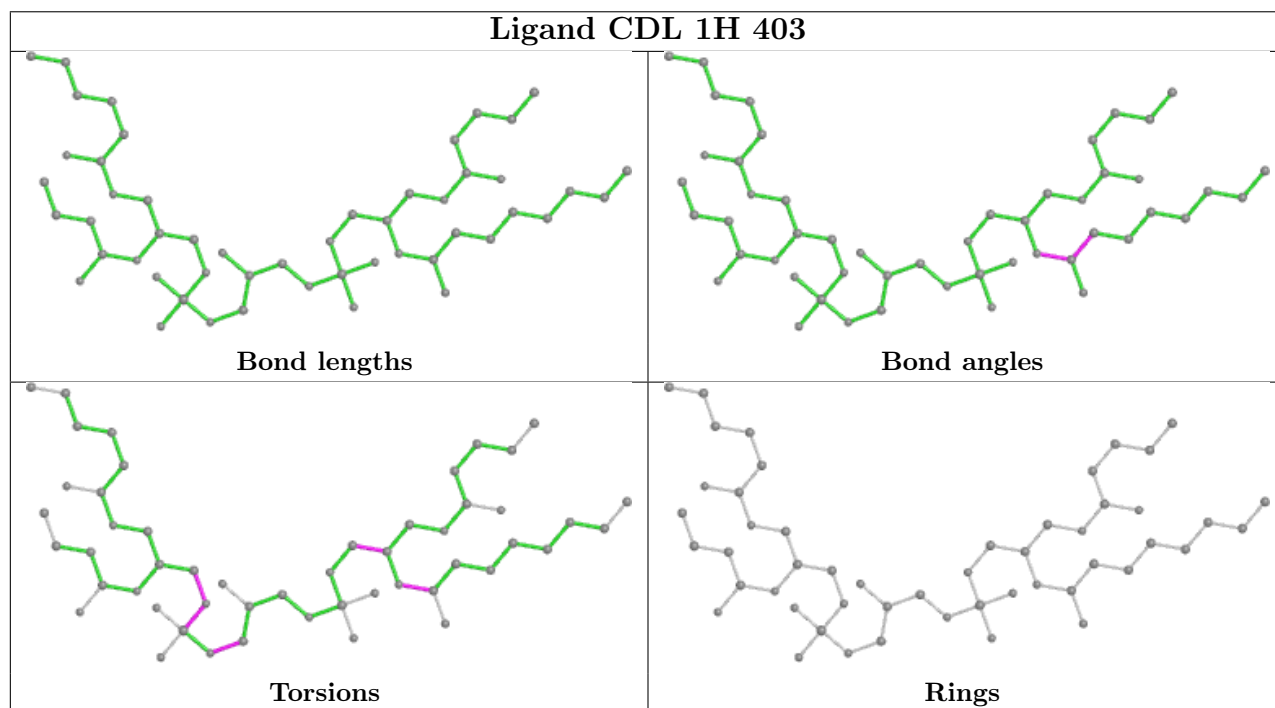
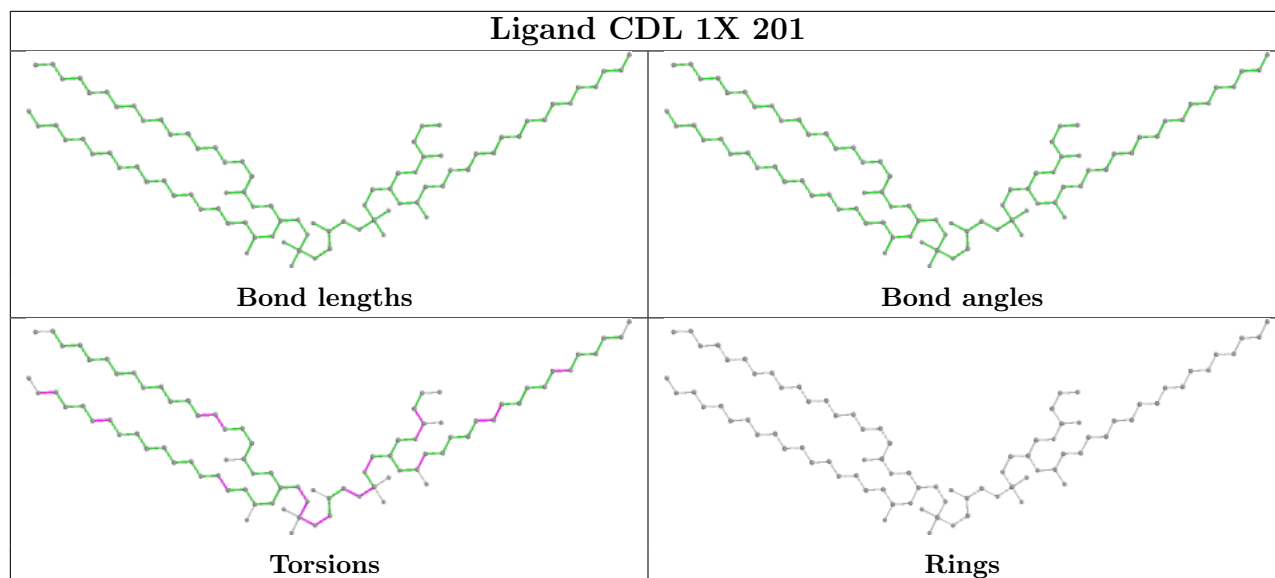


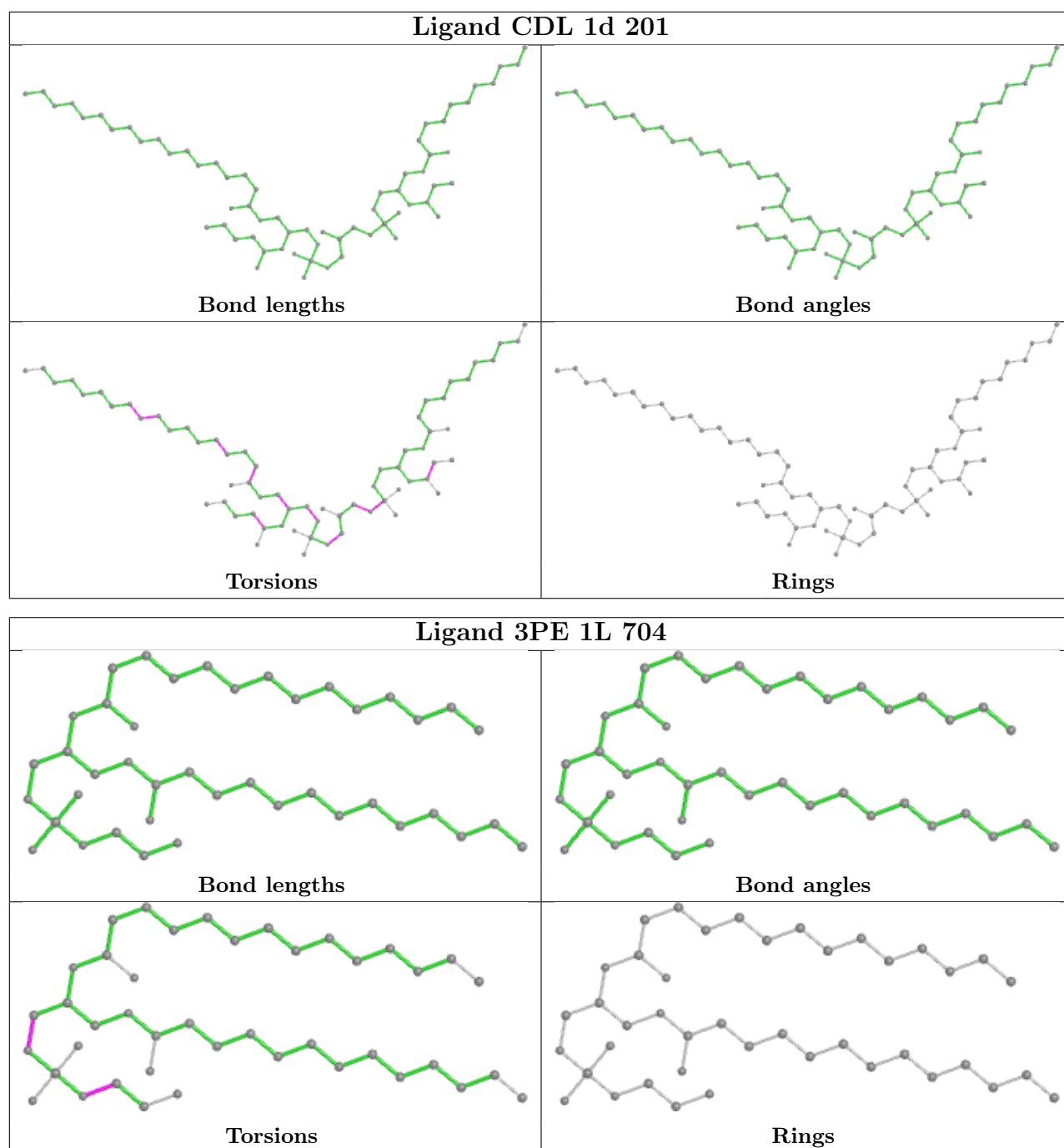


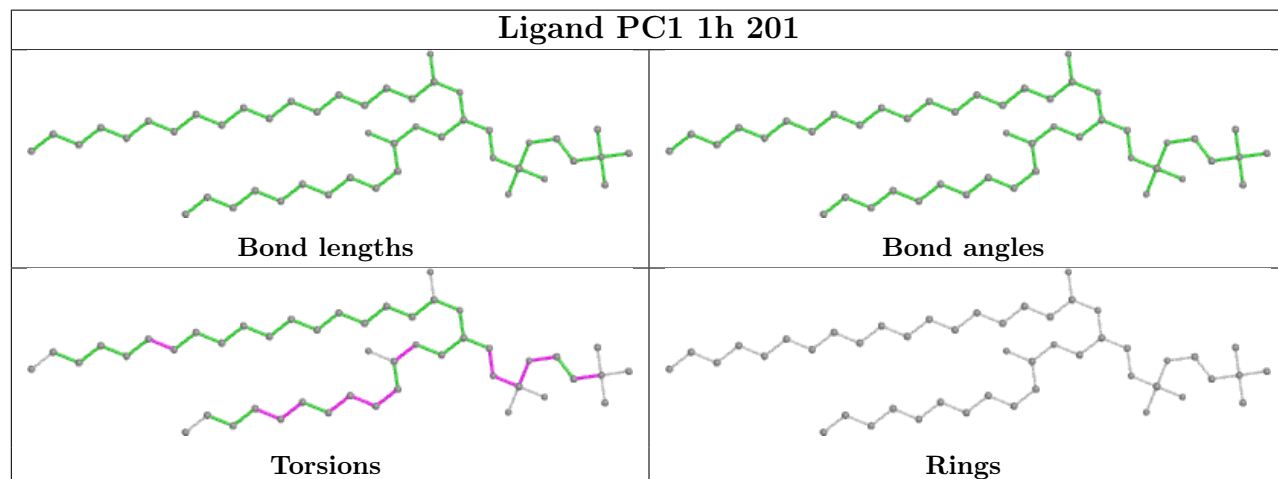
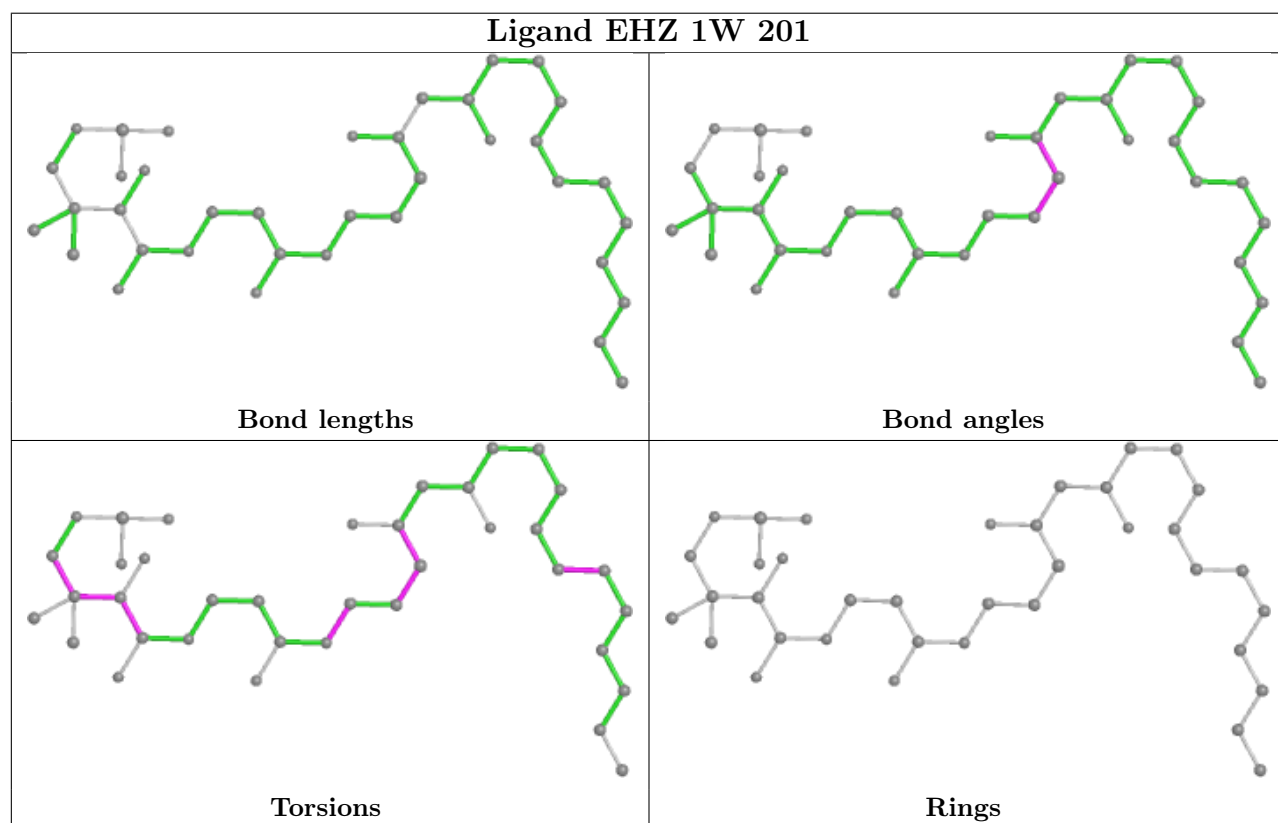
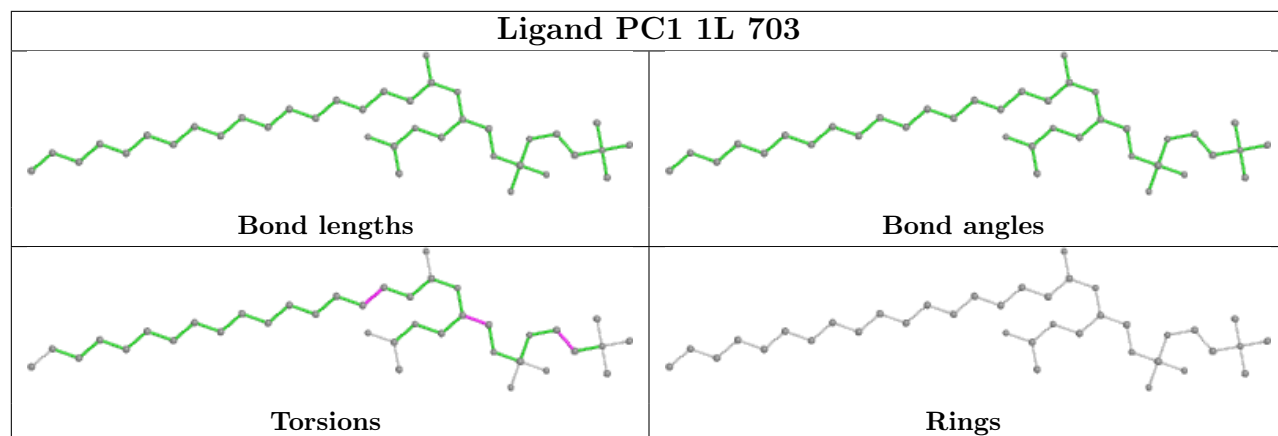


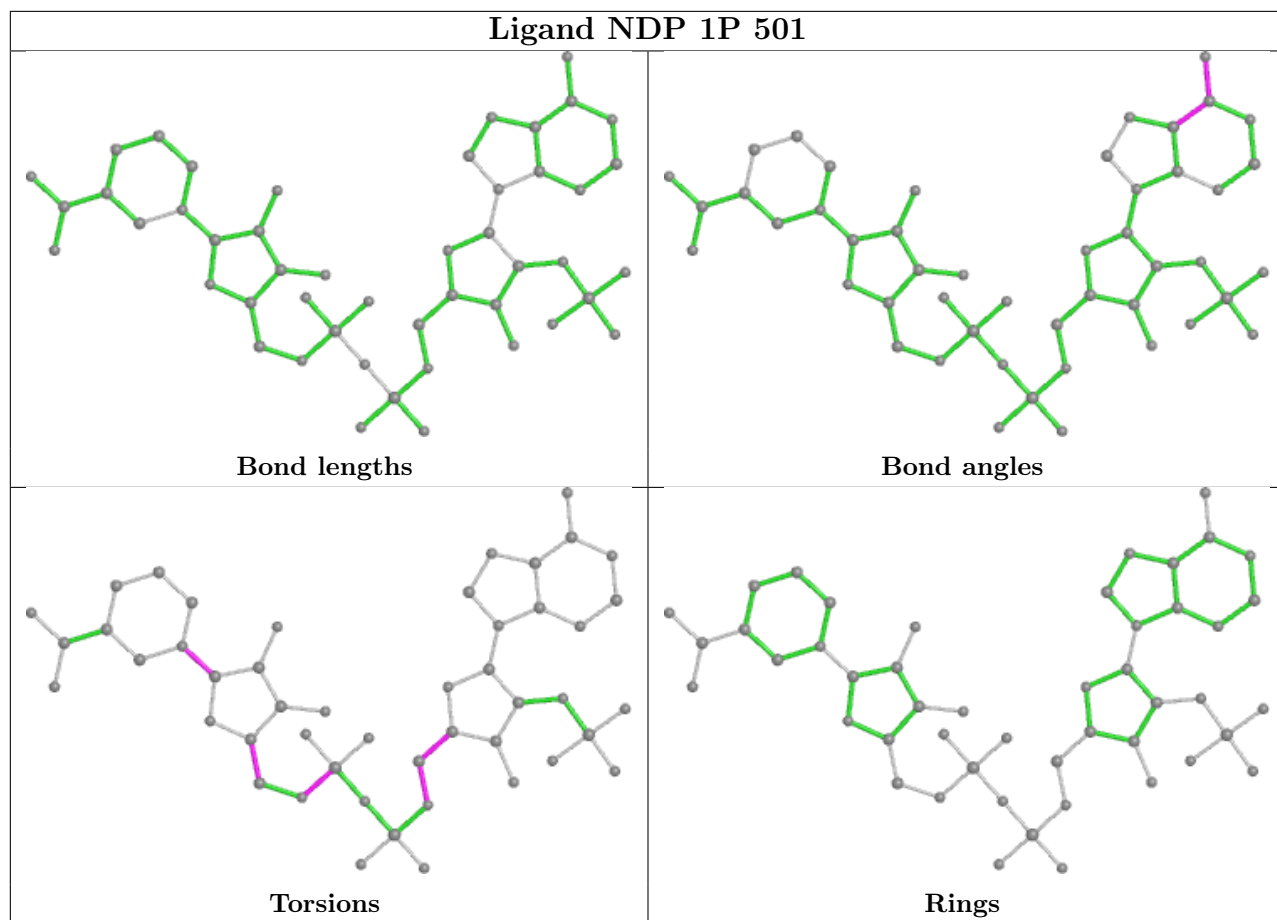












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 34 | 1i | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 1i | 1:SAC | C | 2:GLY | N | 5.29 |

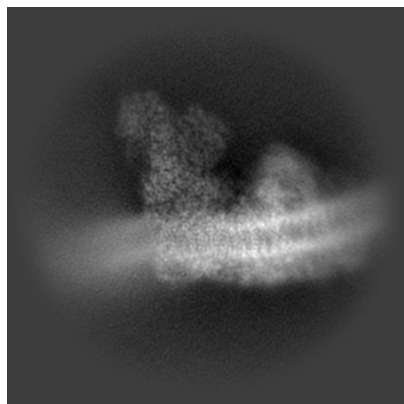
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42165. These allow visual inspection of the internal detail of the map and identification of artifacts.

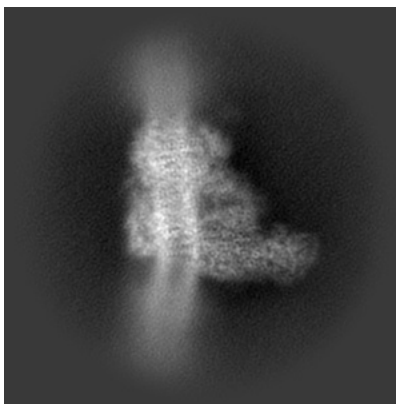
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

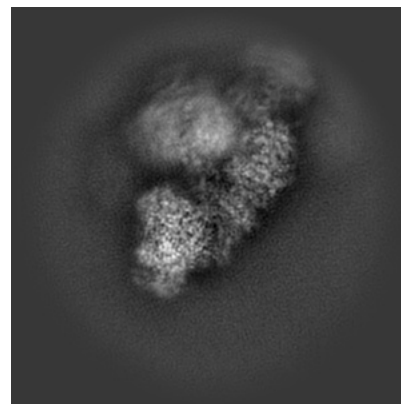
6.1.1 Primary map



X

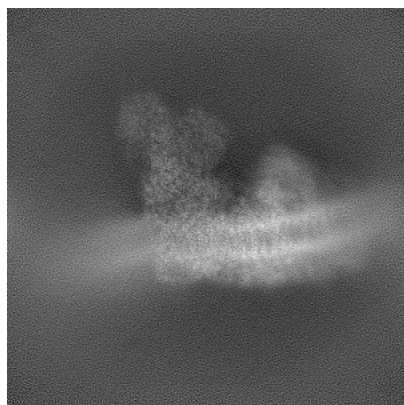


Y

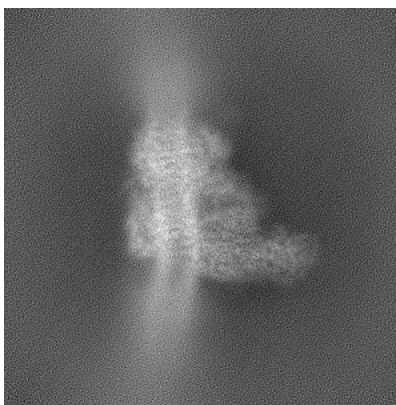


Z

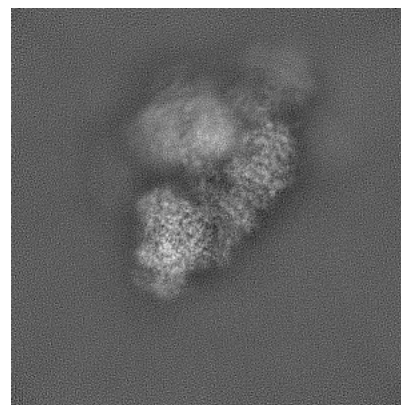
6.1.2 Raw map



X



Y

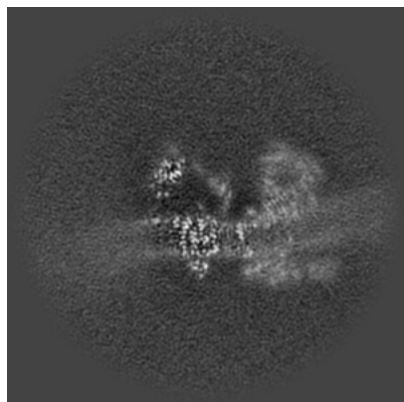


Z

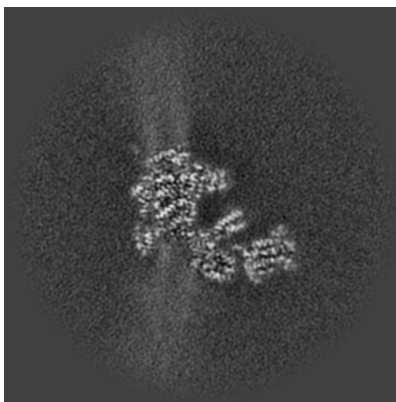
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

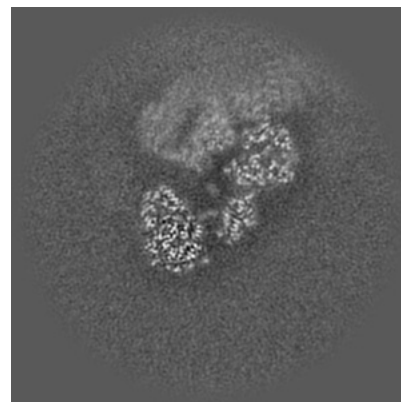
6.2.1 Primary map



X Index: 200

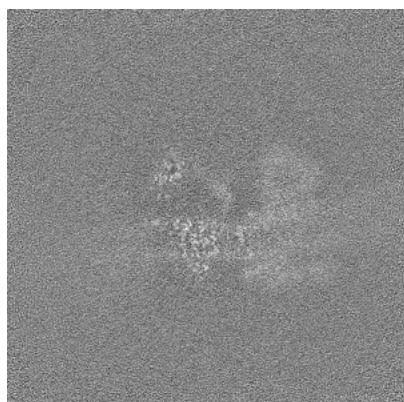


Y Index: 200

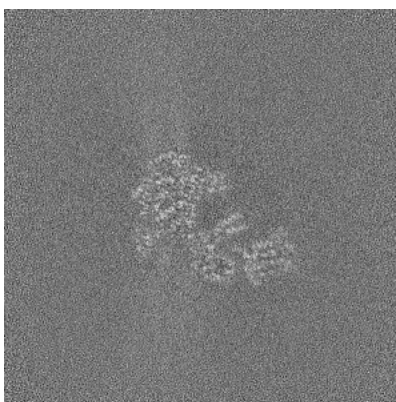


Z Index: 200

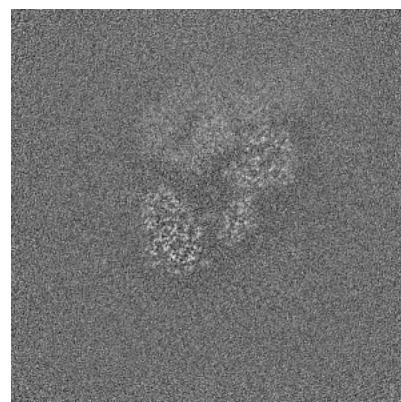
6.2.2 Raw map



X Index: 200



Y Index: 200

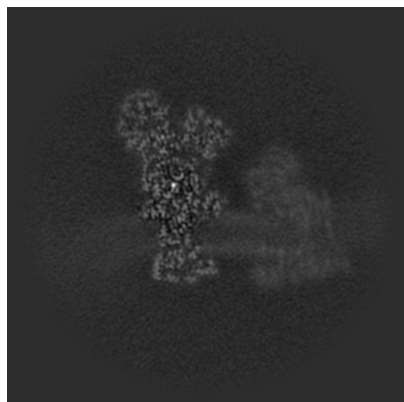


Z Index: 200

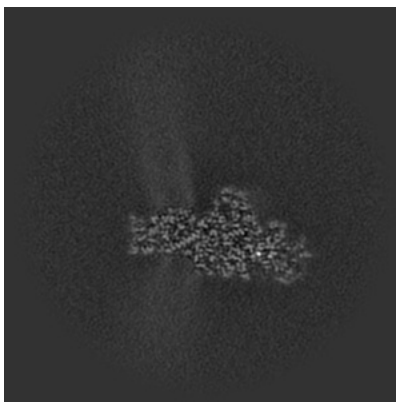
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

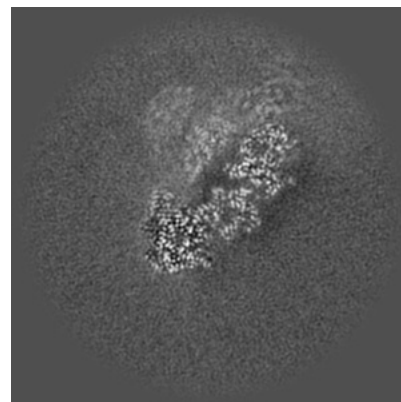
6.3.1 Primary map



X Index: 162

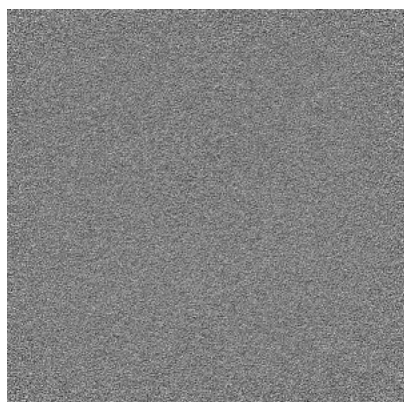


Y Index: 157

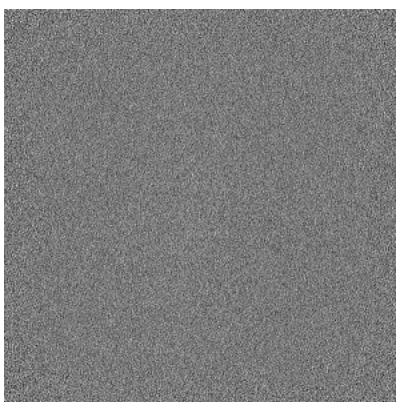


Z Index: 190

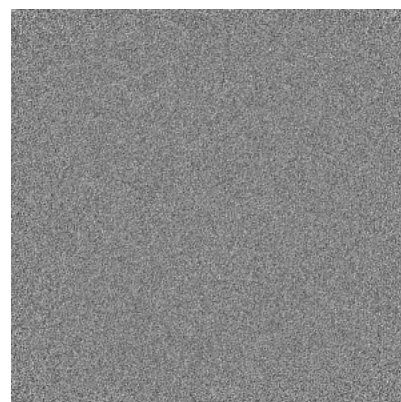
6.3.2 Raw map



X Index: 0



Y Index: 0

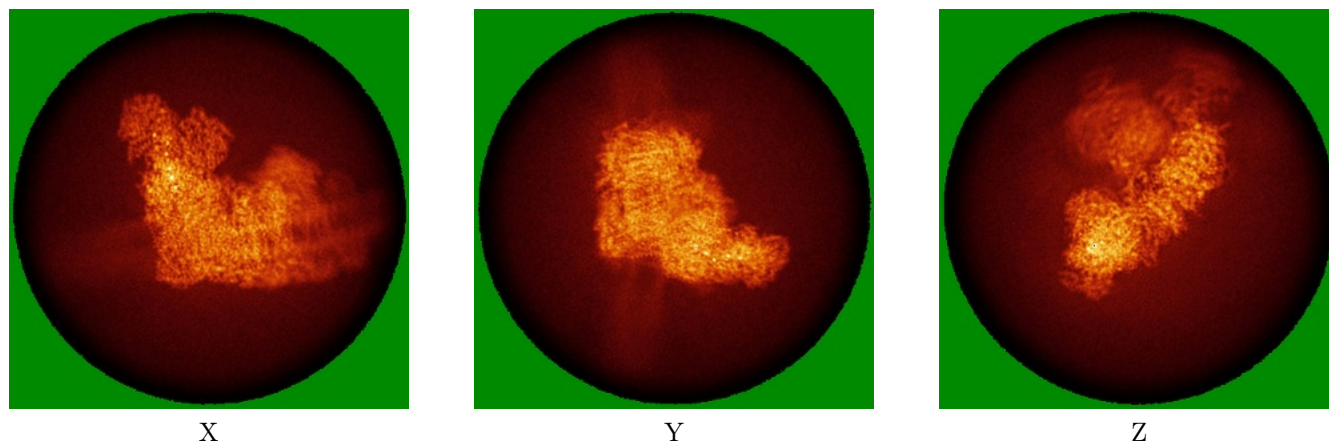


Z Index: 0

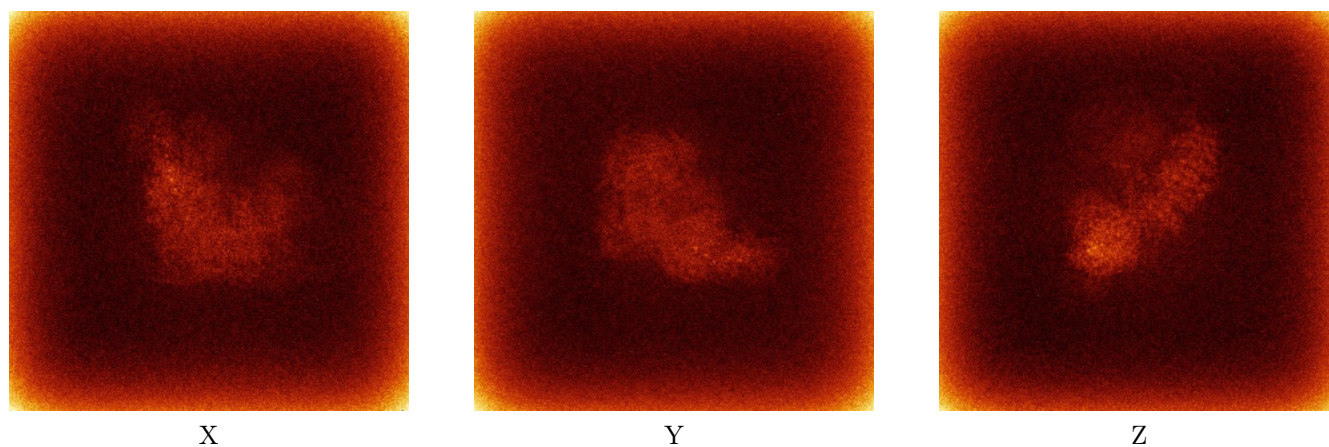
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

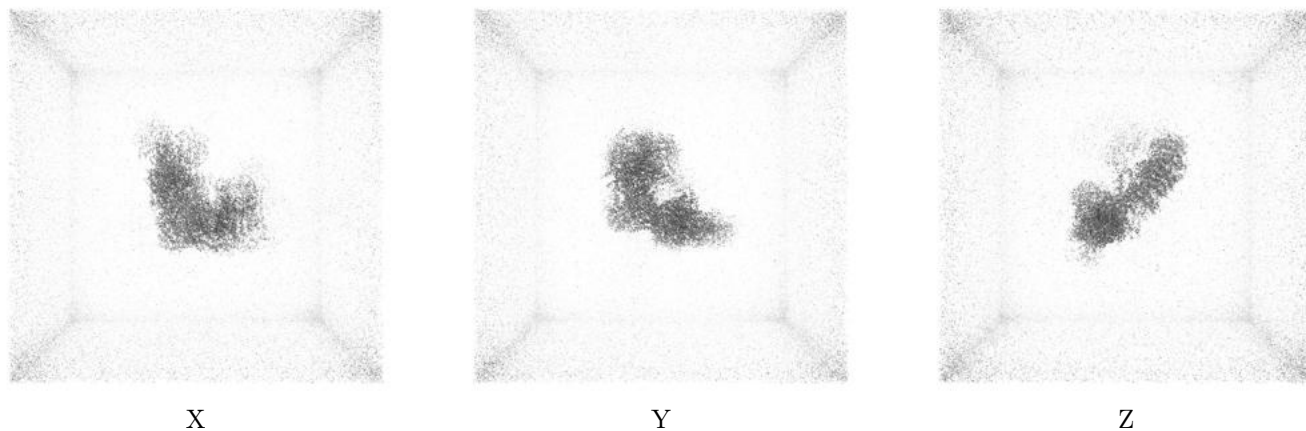
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

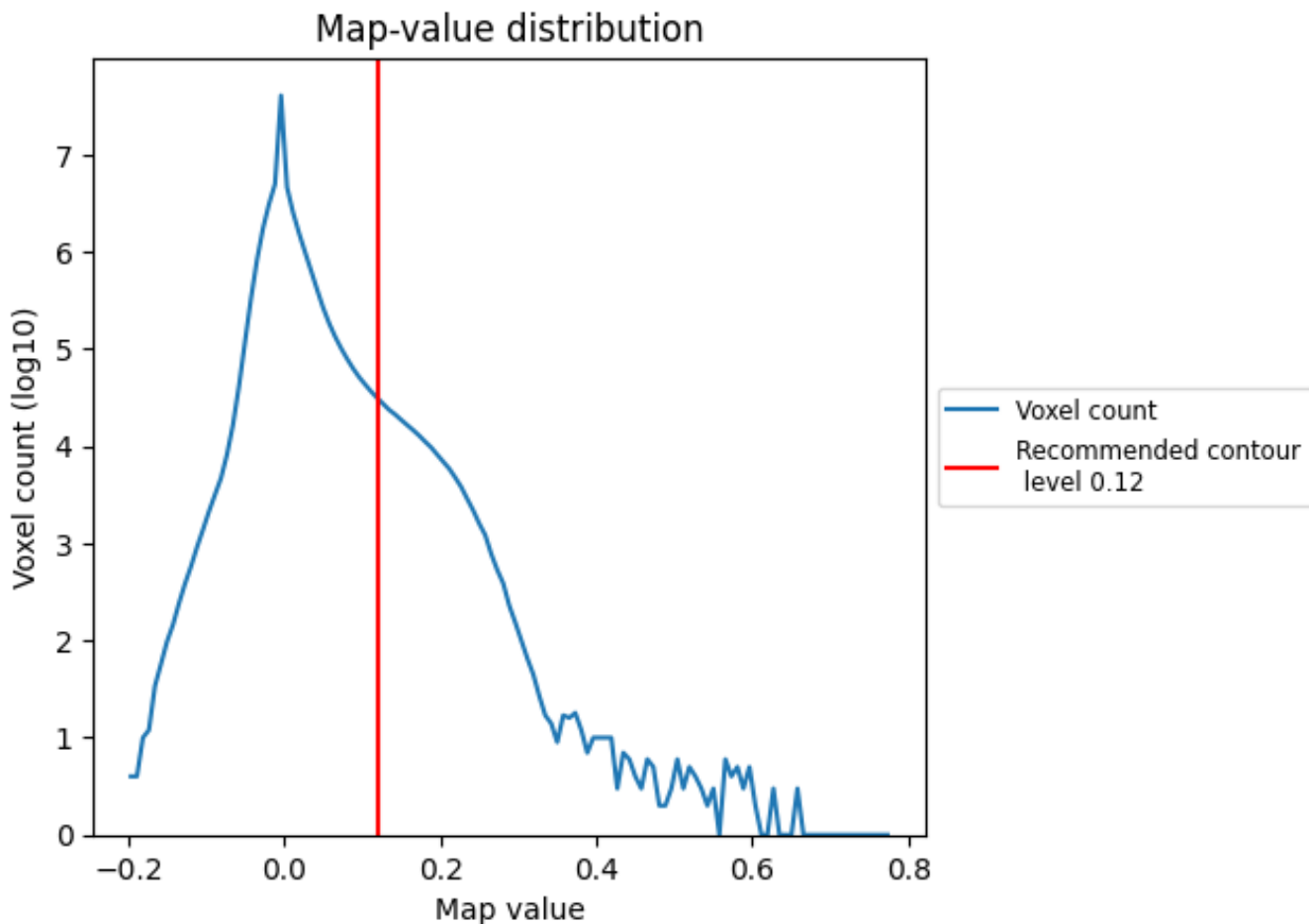
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

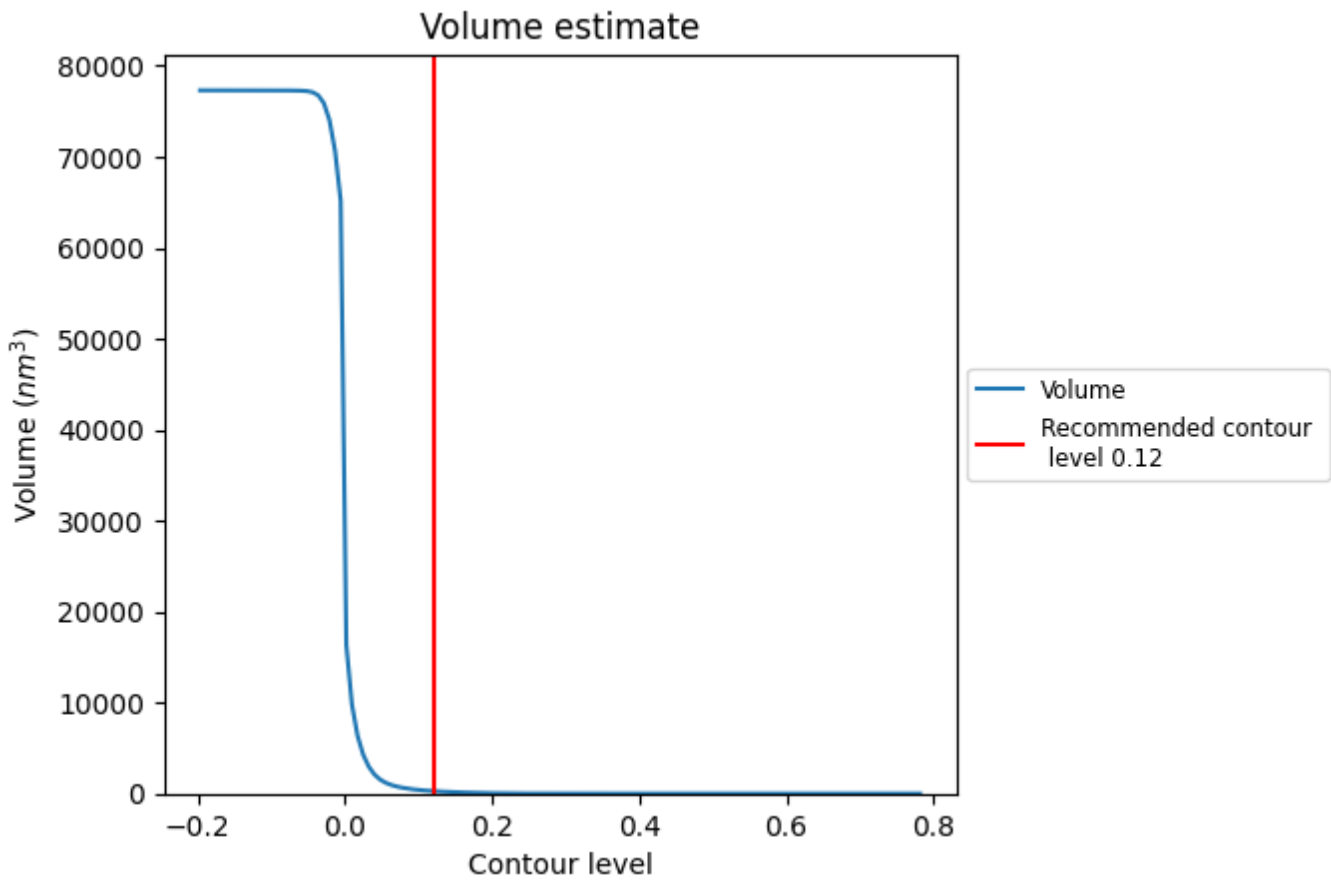
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

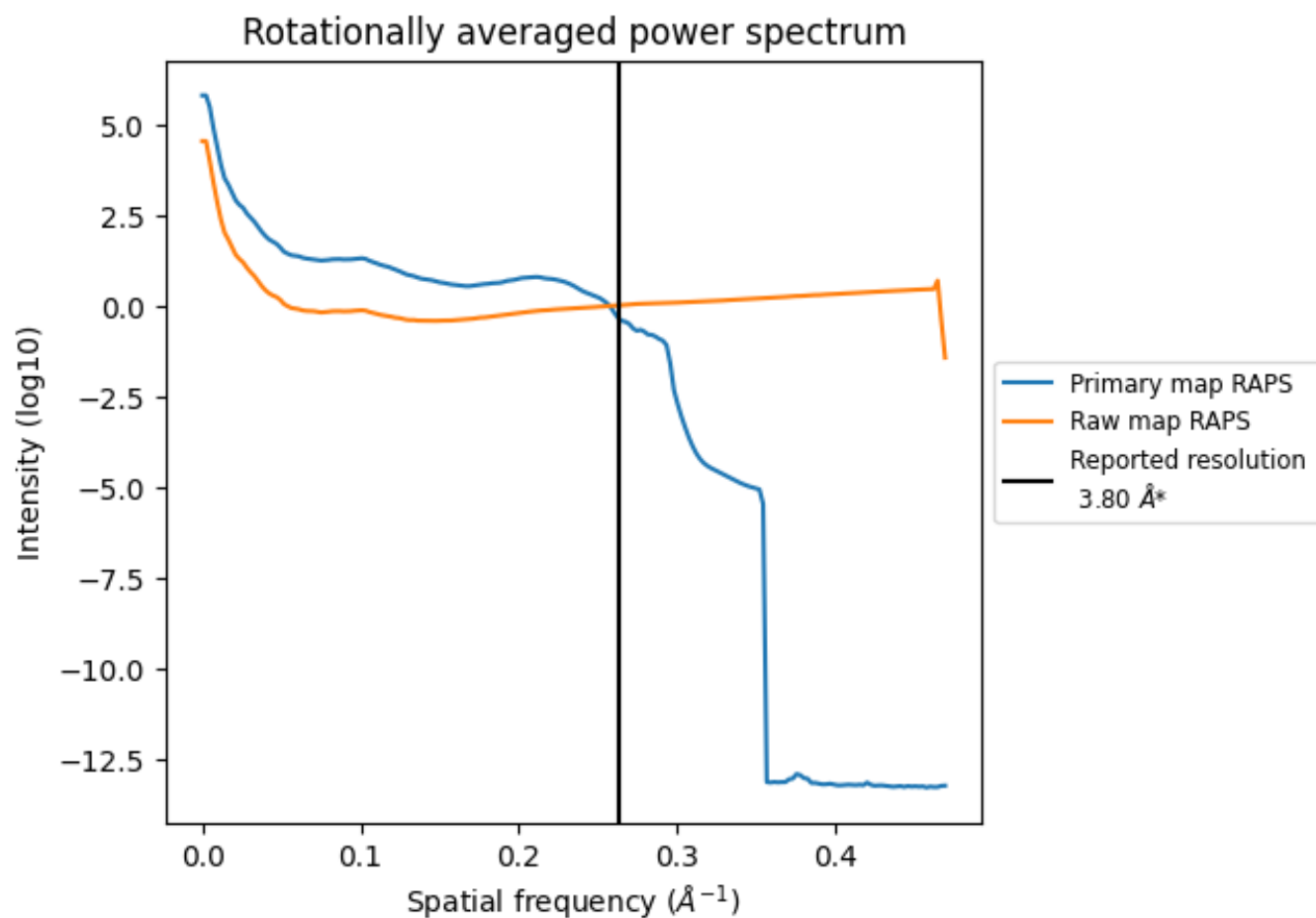
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

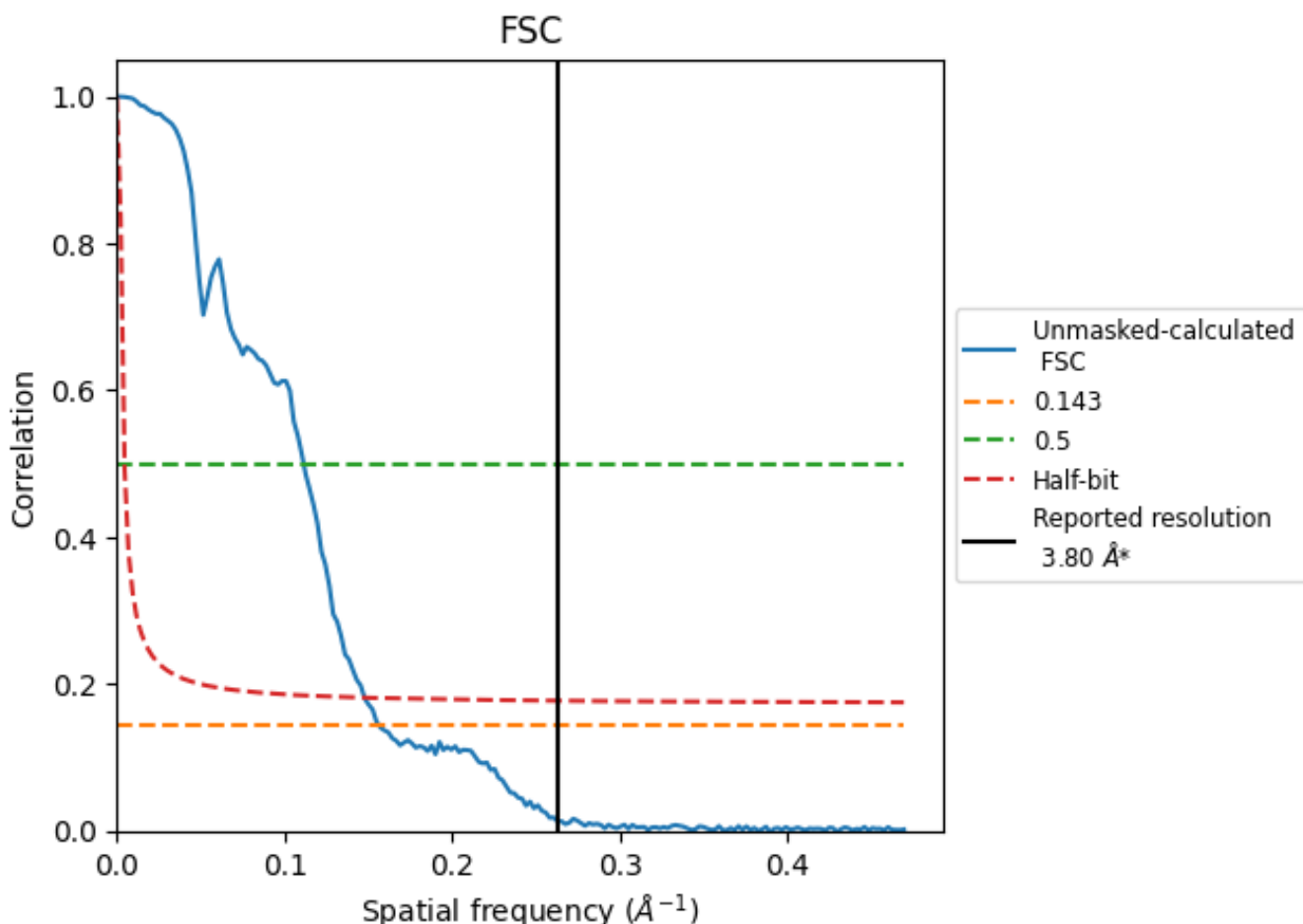


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

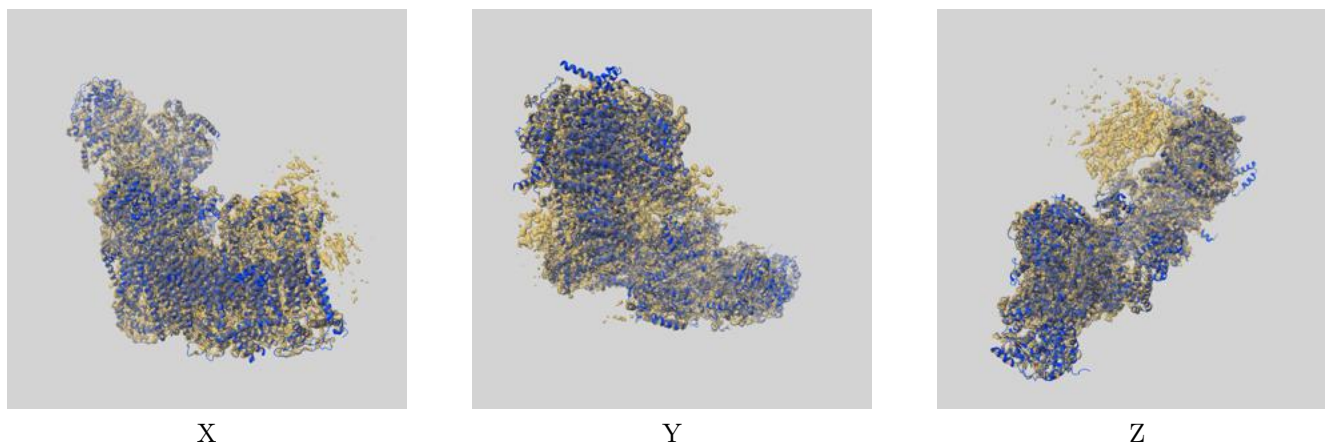
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.80 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 6.39 | 8.98 | 6.77 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.39 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

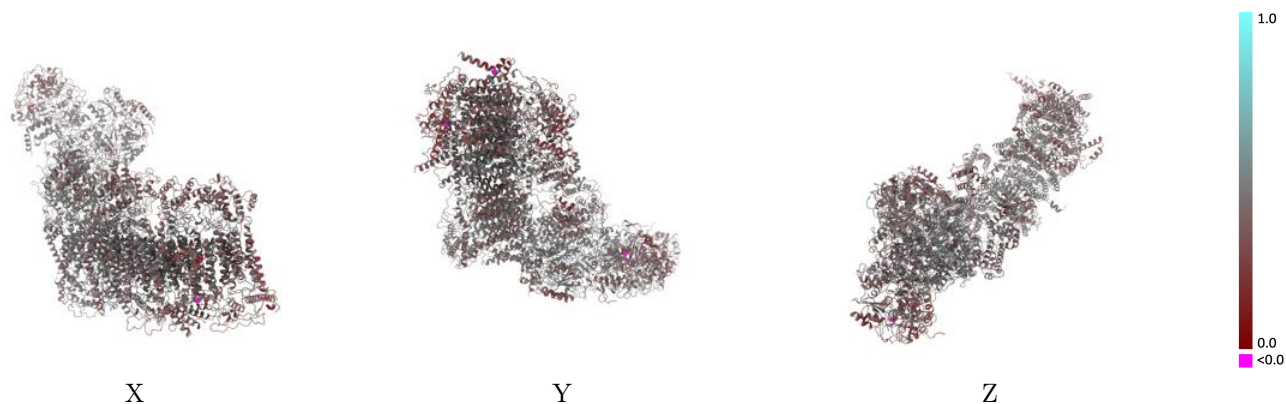
This section contains information regarding the fit between EMDB map EMD-42165 and PDB model 8UEO. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



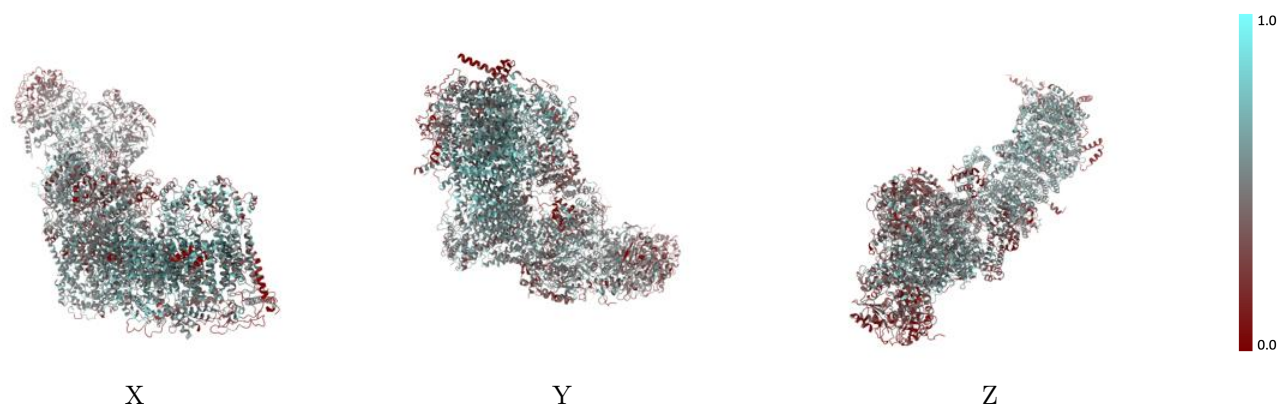
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



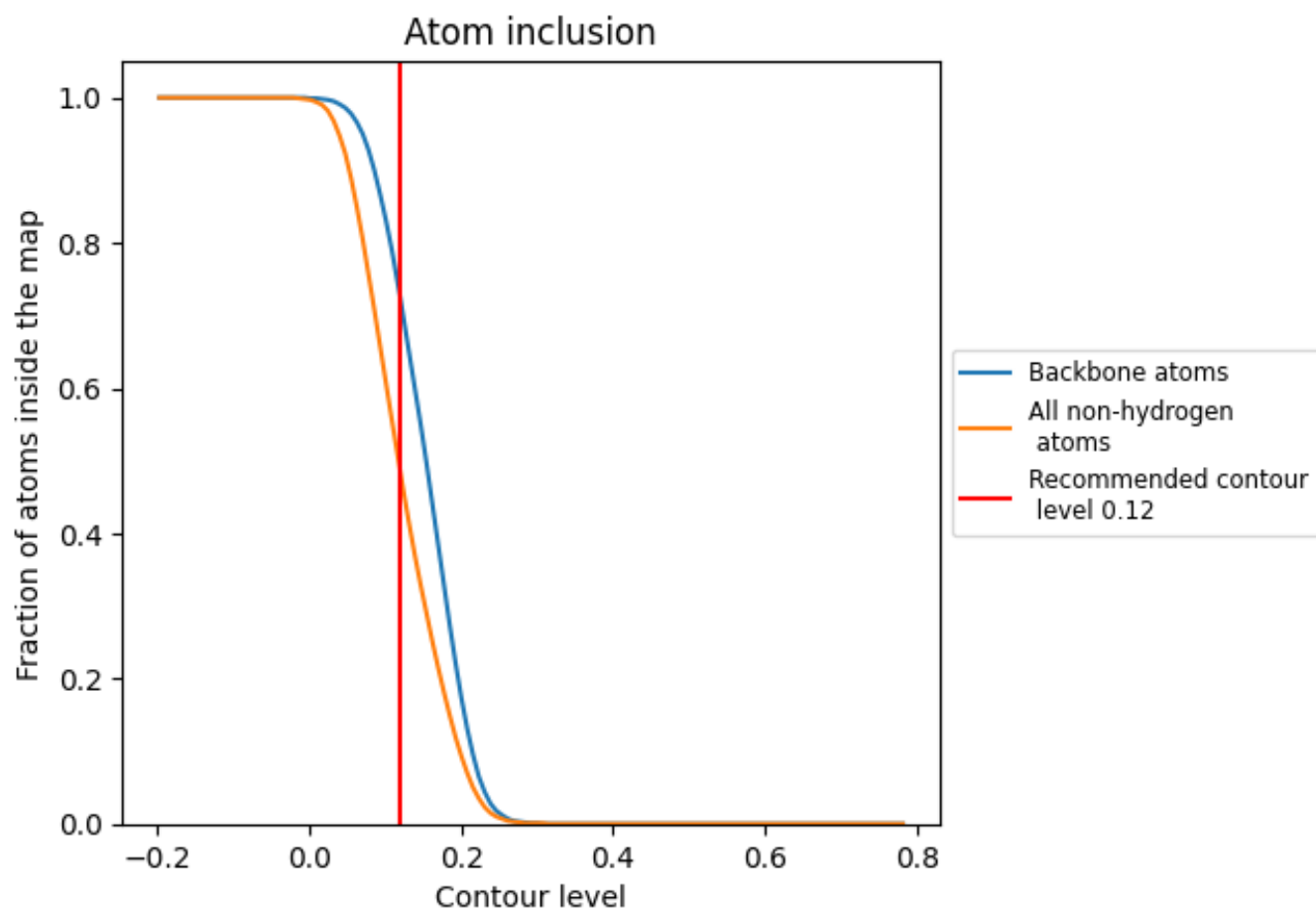
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.4840 |  0.4170 |
| 1A |  0.4750 |  0.4300 |
| 1B |  0.5830 |  0.4660 |
| 1C |  0.5470 |  0.4570 |
| 1D |  0.5740 |  0.4590 |
| 1E |  0.3180 |  0.3810 |
| 1F |  0.3400 |  0.3850 |
| 1G |  0.4550 |  0.4240 |
| 1H |  0.5360 |  0.4520 |
| 1I |  0.5830 |  0.4450 |
| 1J |  0.5040 |  0.4230 |
| 1K |  0.5290 |  0.4270 |
| 1L |  0.5600 |  0.4110 |
| 1M |  0.6320 |  0.4510 |
| 1N |  0.5900 |  0.4470 |
| 1O |  0.3810 |  0.3990 |
| 1P |  0.4110 |  0.4260 |
| 1Q |  0.4210 |  0.4320 |
| 1R |  0.4470 |  0.4490 |
| 1S |  0.2950 |  0.3410 |
| 1T |  0.2030 |  0.3280 |
| 1U |  0.4880 |  0.3610 |
| 1V |  0.3990 |  0.4050 |
| 1W |  0.3970 |  0.4100 |
| 1X |  0.5010 |  0.4220 |
| 1Y |  0.5050 |  0.4110 |
| 1Z |  0.5490 |  0.4340 |
| 1a |  0.5380 |  0.4380 |
| 1b |  0.4850 |  0.4200 |
| 1c |  0.3890 |  0.3930 |
| 1d |  0.5170 |  0.4270 |
| 1e |  0.5440 |  0.4390 |
| 1f |  0.3150 |  0.4040 |
| 1g |  0.4770 |  0.3930 |
| 1h |  0.5450 |  0.4130 |



Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 1i |  0.3270 |  0.3500 |
| 1j |  0.3750 |  0.3500 |
| 1k |  0.3710 |  0.3710 |
| 1l |  0.5130 |  0.4060 |
| 1m |  0.5690 |  0.4060 |
| 1n |  0.5380 |  0.3800 |
| 1o |  0.3510 |  0.3070 |
| 1p |  0.4850 |  0.3880 |
| 1q |  0.4860 |  0.4520 |
| 1r |  0.5250 |  0.4600 |
| 1s |  0.2020 |  0.3390 |