# wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 04:39 pm BST

| | | |
|---|---|---|
| PDB ID | : | 7O71 / pdb_00007o71 |
| EMDB ID | : | EMD-12742 |
| Title | : | Cryo-EM structure of a respiratory complex I |
| Authors | : | Parey, K.; Vonck, J. |
| Deposited on | : | 2021-04-12 |
| Resolution | : | 2.40 Å(reported) |
| Based on initial model | : | 6RFR |

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

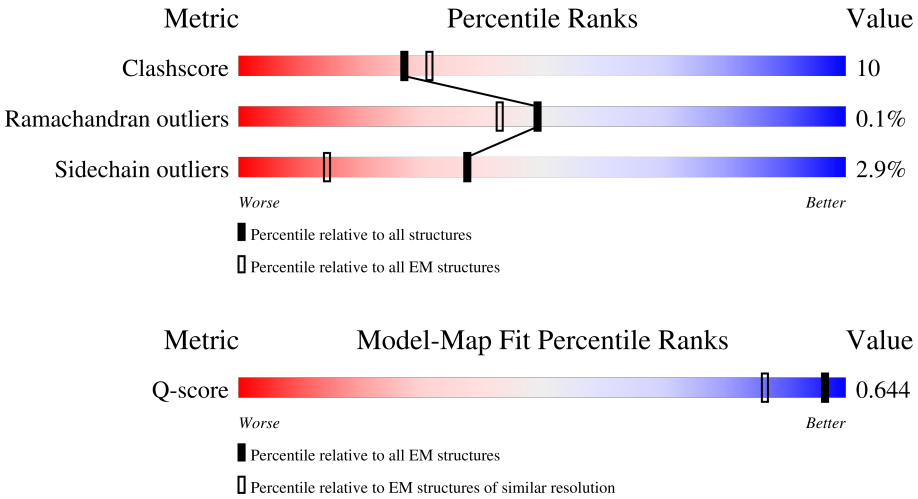
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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







| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 5628 ( 1.90 - 2.90 ) |

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 <=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 | A | 728 | 25% 74% 20% • 5% |
| 2 | B | 488 | 66% 59% 33% • 7% |
| 3 | C | 466 | 11% 73% 19% • 6% |
| 4 | G | 281 | 7% 70% 15% 15% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | H | 243 | 67% 65% 22% 11% |
| 6 | I | 229 | 7% 69% 14% 17% |
| 7 | K | 210 | 8% 65% 18% 16% |
| 8 | L | 89 | 12% 69% 29% |
| 9 | S | 249 | 55% 50% 22% 27% |
| 10 | j | 93 | 38% 83% 14% |
| 11 | 1 | 341 | 13% 77% 22% |
| 12 | 2 | 469 | 82% 17% |
| 13 | 3 | 128 | 26% 66% 32% |
| 14 | 4 | 486 | 5% 78% 21% |
| 15 | 5 | 655 | 37% 68% 30% |
| 16 | 6 | 185 | 28% 73% 25% |
| 17 | g | 78 | 36% 77% 21% |
| 18 | D | 87 | 13% 79% 20% |
| 19 | E | 375 | 25% 71% 20% 7% |
| 20 | F | 144 | 15% 67% 17% 17% |
| 21 | J | 198 | 37% 69% 20% 10% |
| 22 | M | 136 | 12% 76% 10% 14% |
| 23 | O | 109 | 61% 47% 18% 35% |
| 24 | P | 124 | 31% 73% 26% |
| 25 | Q | 132 | 63% 45% 18% 36% |
| 26 | R | 109 | 70% 64% 30% |
| 27 | U | 172 | 34% 79% 20% |
| 28 | W | 123 | 23% 77% 21% |
| 29 | X | 169 | 20% 86% 11% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 30 | Y | 161 | 13% 57% 19% 24% |
| 31 | Z | 182 | 26% 82% 15% |
| 32 | a | 149 | 54% 57% 25% 17% |
| 33 | b | 74 | 11% 70% 16% 14% |
| 34 | c | 60 | 72% 45% 28% 27% |
| 35 | d | 92 | 21% 65% 32% |
| 36 | e | 67 | 78% 61% 15% 22% |
| 37 | f | 87 | 63% 69% 24% 6% |
| 38 | h | 138 | 17% 83% 14% |
| 39 | i | 90 | 57% 70% 22% 8% |
| 40 | n | 120 | 28% 77% 18% 5% |
| 41 | 8 | 99 | 70% 52% 20% 28% |
| 42 | 9 | 89 | 47% 76% 20% |

# 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 67428 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 78 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 693 | 5269 | 3272 | 927 | 1041 | 29 | 0 | 0 |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 455 | 3517 | 2223 | 617 | 653 | 24 | 0 | 0 |

- Molecule 3 is a protein called NUCM protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 437 | 3470 | 2205 | 595 | 648 | 22 | 1 | 0 |

- Molecule 4 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | G | 239 | 1978 | 1272 | 336 | 366 | 4 | 0 | 0 |

- Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | H | 216 | 1688 | 1060 | 284 | 326 | 18 | 0 | 0 |

- Molecule 6 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | I | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1519 | 966 | 254 | 289 | 10 | | |

- Molecule 7 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | K | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1395 | 885 | 246 | 249 | 15 | | |

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | L | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 693 | 465 | 109 | 116 | 3 | | |

- Molecule 9 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | S | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1492 | 961 | 255 | 274 | 2 | | |

- Molecule 10 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 10 | j | 90 | Total | C | N | O | 0 | 0 |
| | | | 724 | 465 | 132 | 127 | | |

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | 1 | 340 | Total | C | N | O | S | 0 | 0 |
| | | | 2716 | 1850 | 393 | 466 | 7 | | |

- Molecule 12 is a protein called NADH dehydrogenase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | 2 | 469 | Total | C | N | O | S | 0 | 0 |
| | | | 3776 | 2558 | 550 | 656 | 12 | | |

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | 3 | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1027 | 701 | 151 | 172 | 3 | | |

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | 4 | 481 | Total | C | N | O | S | 0 | 0 |
| | | | 3815 | 2573 | 581 | 647 | 14 | | |

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | 5 | 654 | Total | C | N | O | S | 0 | 0 |
| | | | 5197 | 3479 | 785 | 905 | 28 | | |

- Molecule 16 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | 6 | 184 | Total | C | N | O | S | 0 | 0 |
| | | | 1453 | 985 | 208 | 251 | 9 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 6 | 1 | FME | - | insertion | UNP S5U3X7 |

- Molecule 17 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 17 | g | 76 | Total | C | N | O | 0 | 0 |
| | | | 622 | 408 | 113 | 101 | | |

- Molecule 18 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | D | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 681 | 432 | 127 | 119 | 3 | | |

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase 40 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | E | 350 | Total | C | N | O | S | 0 | 0 |
| | | | 2806 | 1782 | 490 | 524 | 10 | | |

- Molecule 20 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | F | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 981 | 624 | 164 | 191 | 2 | | |

- Molecule 21 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | J | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1319 | 838 | 238 | 238 | 5 | | |

- Molecule 22 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | M | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 912 | 568 | 163 | 176 | 5 | | |

- Molecule 23 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 23 | O | 71 | Total | C | N | O | 0 | 0 |
| | | | 543 | 344 | 83 | 116 | | |

- Molecule 24 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | P | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 1036 | 667 | 182 | 185 | 2 | | |

- Molecule 25 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Q | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 648 | 405 | 103 | 138 | 2 | | |

- Molecule 26 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | R | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 562 | 168 | 151 | 3 | | |

- Molecule 27 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | U | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1345 | 847 | 236 | 252 | 10 | | |

- Molecule 28 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | W | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 974 | 623 | 178 | 168 | 5 | | |

- Molecule 29 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | X | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1275 | 828 | 217 | 226 | 4 | | |

- Molecule 30 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | Y | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 1021 | 651 | 187 | 181 | 2 | | |

- Molecule 31 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | Z | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1389 | 893 | 240 | 255 | 1 | | |

- Molecule 32 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | a | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1030 | 669 | 165 | 194 | 2 | | |

- Molecule 33 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 33 | b | 64 | Total | C | N | O | 0 | 0 |
| | | | 490 | 326 | 83 | 81 | | |

- Molecule 34 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 34 | c | 44 | Total | C | N | O | 0 | 0 |
| | | | 353 | 229 | 67 | 57 | | |

- Molecule 35 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | d | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 751 | 467 | 136 | 145 | 3 | | |

- Molecule 36 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | e | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 436 | 293 | 75 | 65 | 3 | | |

- Molecule 37 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | f | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 642 | 403 | 121 | 117 | 1 | | |

- Molecule 38 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | h | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1130 | 727 | 193 | 208 | 2 | | |

- Molecule 39 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | i | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 646 | 413 | 117 | 115 | 1 | | |

- Molecule 40 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | n | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 913 | 587 | 154 | 171 | 1 | | |

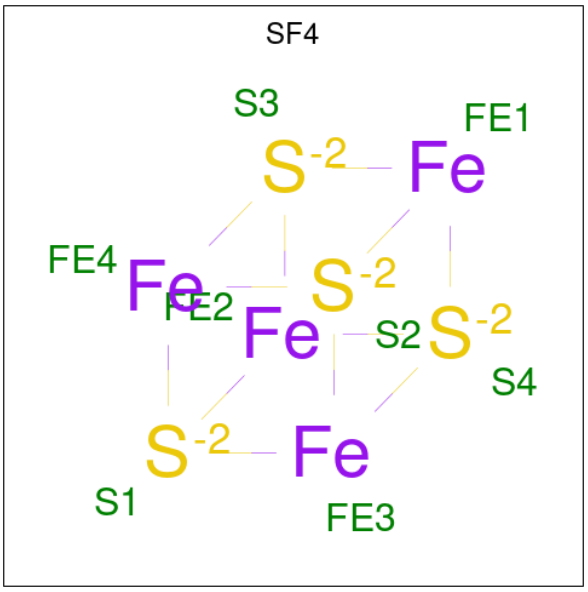
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | 8 | 71 | Total | C | N | O | S | 0 | 0 |
| | | | 594 | 375 | 109 | 102 | 8 | | |

- Molecule 42 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

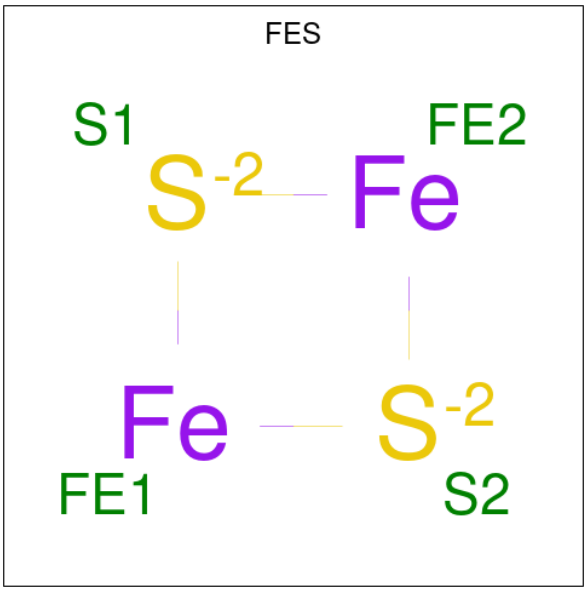
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | 9 | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 672 | 422 | 122 | 122 | 6 | | |

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: $Fe_4S_4$).



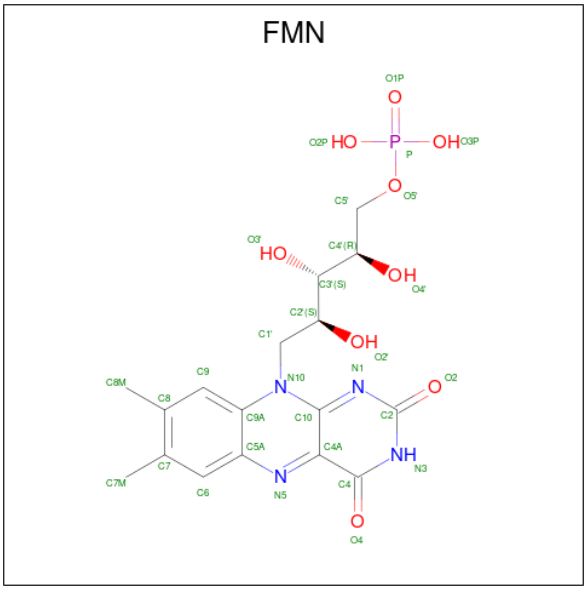

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 43 | A | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 43 | A | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 43 | B | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 43 | I | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 43 | I | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 43 | K | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: $Fe_2S_2$).



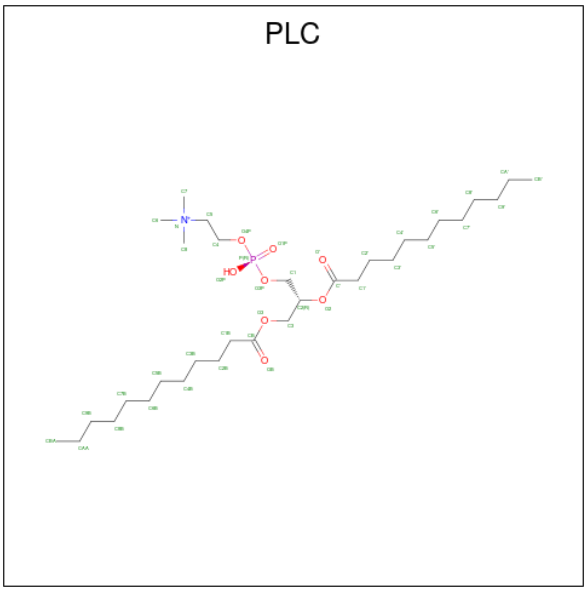

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 44 | A | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 44 | H | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



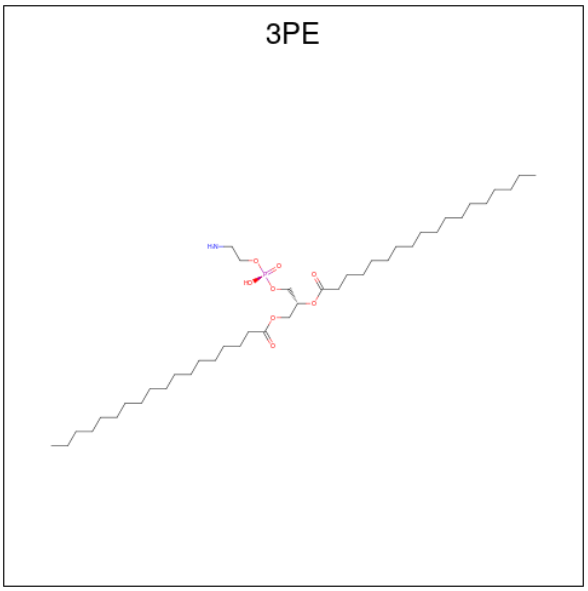

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 45 | B | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

- Molecule 46 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 46 | K | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 46 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 46 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 46 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 46 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 46 | W | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



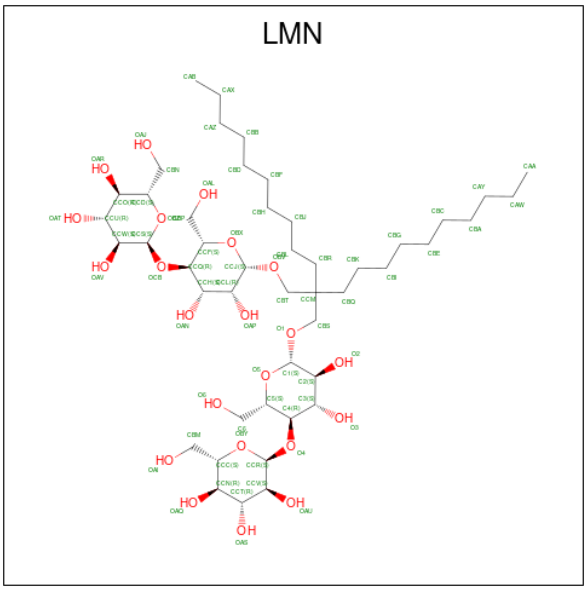

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 47 | S | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 47 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 47 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 47 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 47 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 47 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 47 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 47 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 47 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 47 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 47 | 6 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 47 | 6 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 47 | g | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 47 | E | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |

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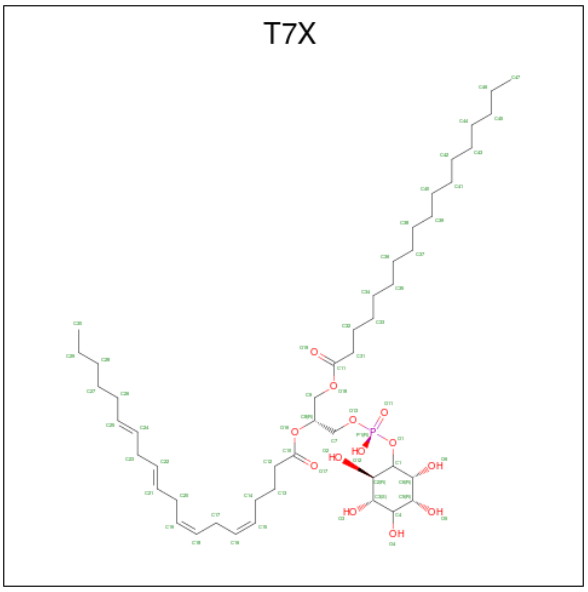
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 47 | J | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 47 | J | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 47 | J | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 47 | b | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |

- Molecule 48 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$).



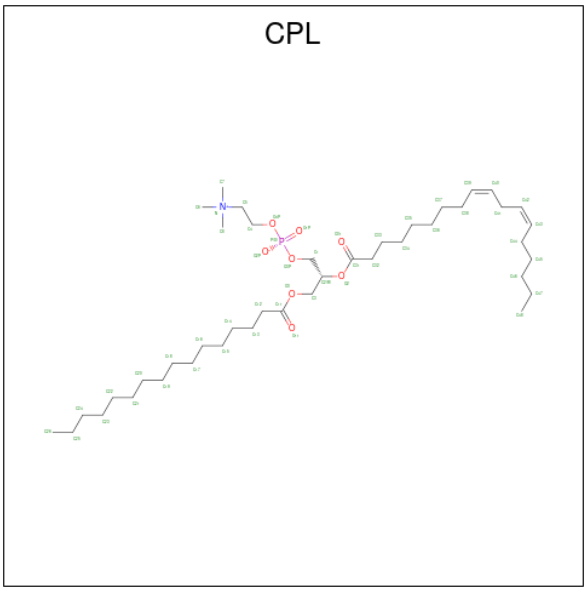

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 48 | j | 1 | Total | C | O | 0 |
| | | | 65 | 43 | 22 | |
| 48 | J | 1 | Total | C | O | 0 |
| | | | 69 | 47 | 22 | |

- Molecule 49 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



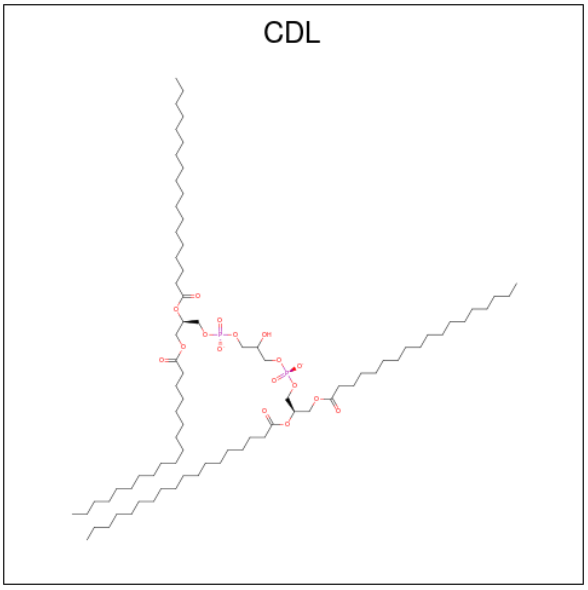

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 49 | 2 | 1 | Total | C | O | P | 0 |
| | | | 48 | 34 | 13 | 1 | |
| 49 | 2 | 1 | Total | C | O | P | 0 |
| | | | 52 | 38 | 13 | 1 | |
| 49 | 3 | 1 | Total | C | O | P | 0 |
| | | | 49 | 35 | 13 | 1 | |

- Molecule 50 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: $C_{42}H_{80}NO_8P$).



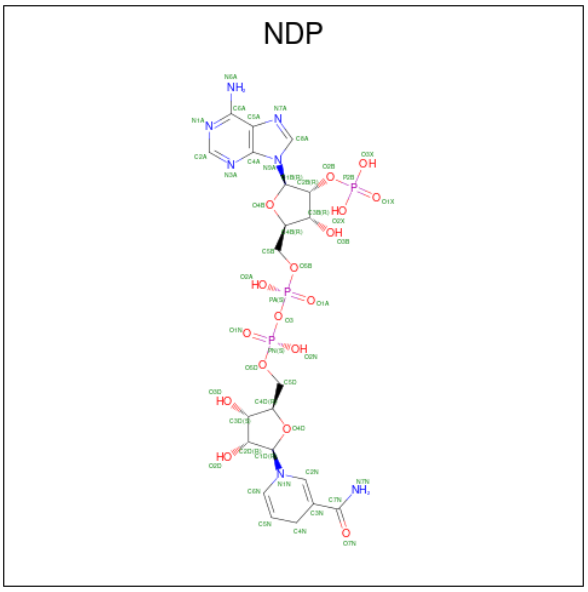
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 50 | 2 | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 51 | g | 1 | Total | C | O | P | 0 |
| | | | 83 | 64 | 17 | 2 | |
| 51 | E | 1 | Total | C | O | P | 0 |
| | | | 72 | 53 | 17 | 2 | |
| 51 | W | 1 | Total | C | O | P | 0 |
| | | | 54 | 35 | 17 | 2 | |
| 51 | X | 1 | Total | C | O | P | 0 |
| | | | 86 | 67 | 17 | 2 | |
| 51 | Z | 1 | Total | C | O | P | 0 |
| | | | 76 | 57 | 17 | 2 | |
| 51 | n | 1 | Total | C | O | P | 0 |
| | | | 92 | 73 | 17 | 2 | |

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

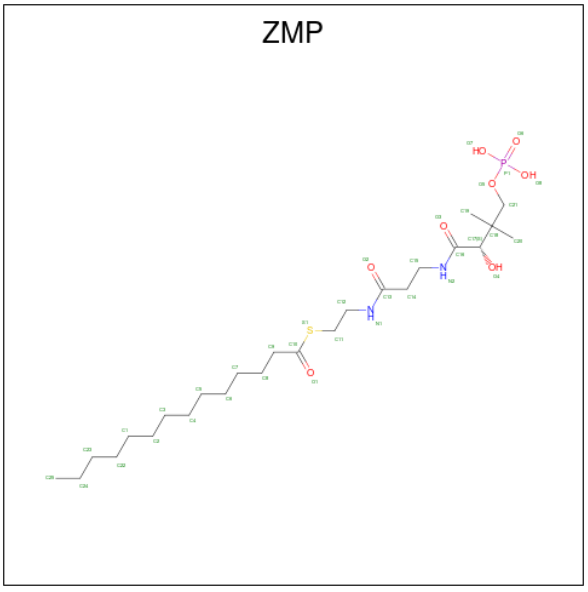



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 52 | E | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 53 | M | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 54 | O | 1 | Total | C | N | O | P | S | 0 |
| | | | 33 | 22 | 2 | 7 | 1 | 1 | |
| 54 | Q | 1 | Total | C | N | O | P | S | 0 |
| | | | 33 | 22 | 2 | 7 | 1 | 1 | |

- Molecule 55 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 55 | A | 135 | Total | O | 0 |
| | | | 135 | 135 | |
| 55 | B | 11 | Total | O | 0 |
| | | | 11 | 11 | |
| 55 | C | 168 | Total | O | 0 |
| | | | 168 | 168 | |
| 55 | G | 114 | Total | O | 0 |
| | | | 114 | 114 | |
| 55 | H | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 55 | I | 95 | Total | O | 0 |
| | | | 95 | 95 | |
| 55 | K | 78 | Total | O | 0 |
| | | | 78 | 78 | |
| 55 | L | 18 | Total | O | 0 |
| | | | 18 | 18 | |
| 55 | S | 4 | Total | O | 0 |
| | | | 4 | 4 | |
| 55 | j | 15 | Total | O | 0 |
| | | | 15 | 15 | |
| 55 | 1 | 67 | Total | O | 0 |
| | | | 67 | 67 | |
| 55 | 2 | 158 | Total | O | 0 |
| | | | 158 | 158 | |
| 55 | 3 | 10 | Total | O | 0 |
| | | | 10 | 10 | |
| 55 | 4 | 139 | Total | O | 0 |
| | | | 139 | 139 | |
| 55 | 5 | 57 | Total | O | 0 |
| | | | 57 | 57 | |
| 55 | 6 | 24 | Total | O | 0 |
| | | | 24 | 24 | |
| 55 | g | 2 | Total | O | 0 |
| | | | 2 | 2 | |
| 55 | D | 17 | Total | O | 0 |
| | | | 17 | 17 | |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 55 | E | 79 | Total O<br>79 79 | 0 |
| 55 | F | 15 | Total O<br>15 15 | 0 |
| 55 | J | 14 | Total O<br>14 14 | 0 |
| 55 | M | 45 | Total O<br>45 45 | 0 |
| 55 | P | 15 | Total O<br>15 15 | 0 |
| 55 | R | 11 | Total O<br>11 11 | 0 |
| 55 | U | 39 | Total O<br>39 39 | 0 |
| 55 | W | 23 | Total O<br>23 23 | 0 |
| 55 | X | 39 | Total O<br>39 39 | 0 |
| 55 | Y | 53 | Total O<br>53 53 | 0 |
| 55 | Z | 52 | Total O<br>52 52 | 0 |
| 55 | a | 11 | Total O<br>11 11 | 0 |
| 55 | b | 6 | Total O<br>6 6 | 0 |
| 55 | d | 8 | Total O<br>8 8 | 0 |
| 55 | h | 61 | Total O<br>61 61 | 0 |
| 55 | i | 3 | Total O<br>3 3 | 0 |
| 55 | n | 12 | Total O<br>12 12 | 0 |
| 55 | 9 | 16 | Total O<br>16 16 | 0 |

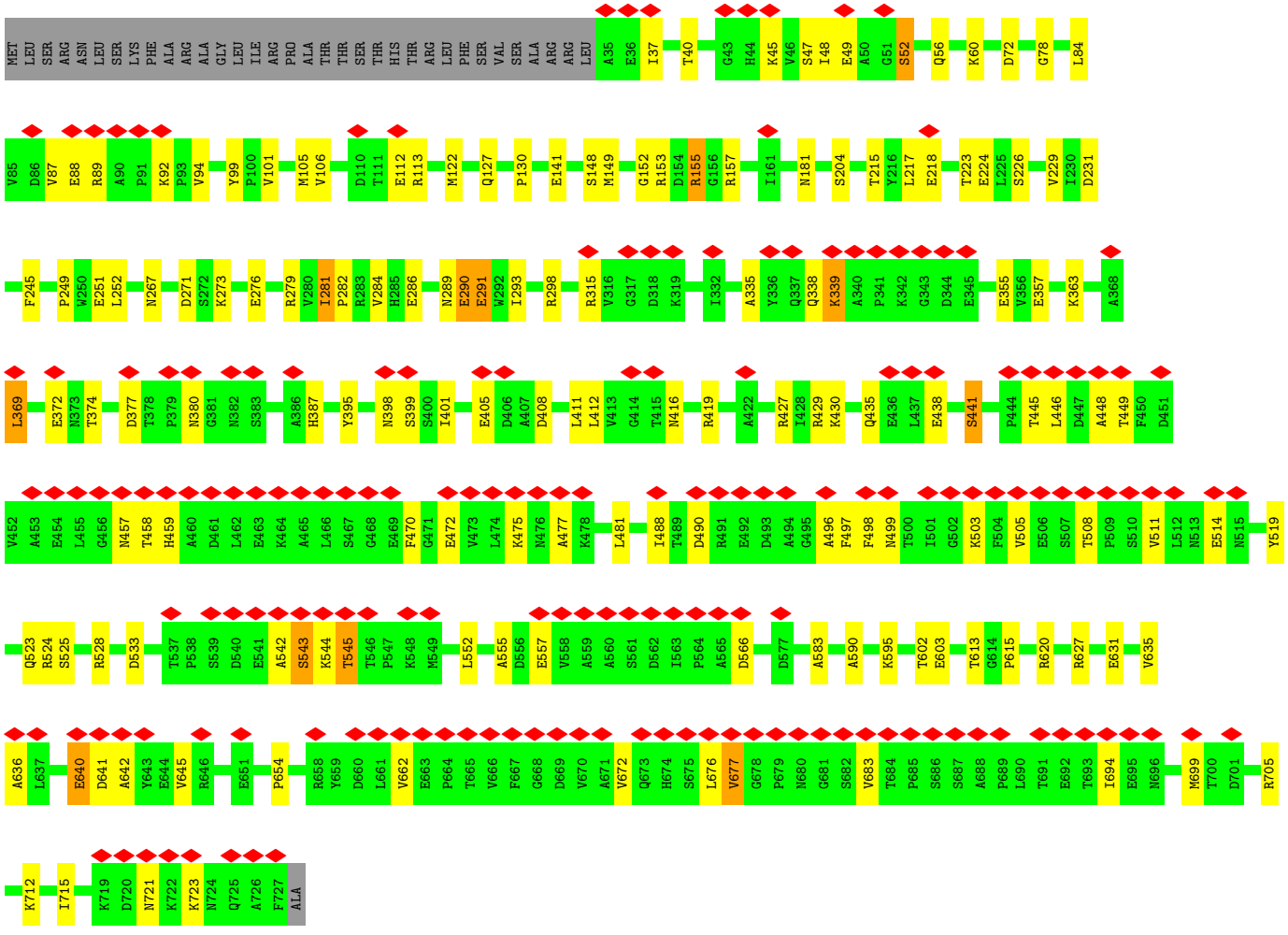
# 3 Residue-property plots (i)

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

• Molecule 1: NADH-ubiquinone oxidoreductase 78 kDa subunit

Chain A:

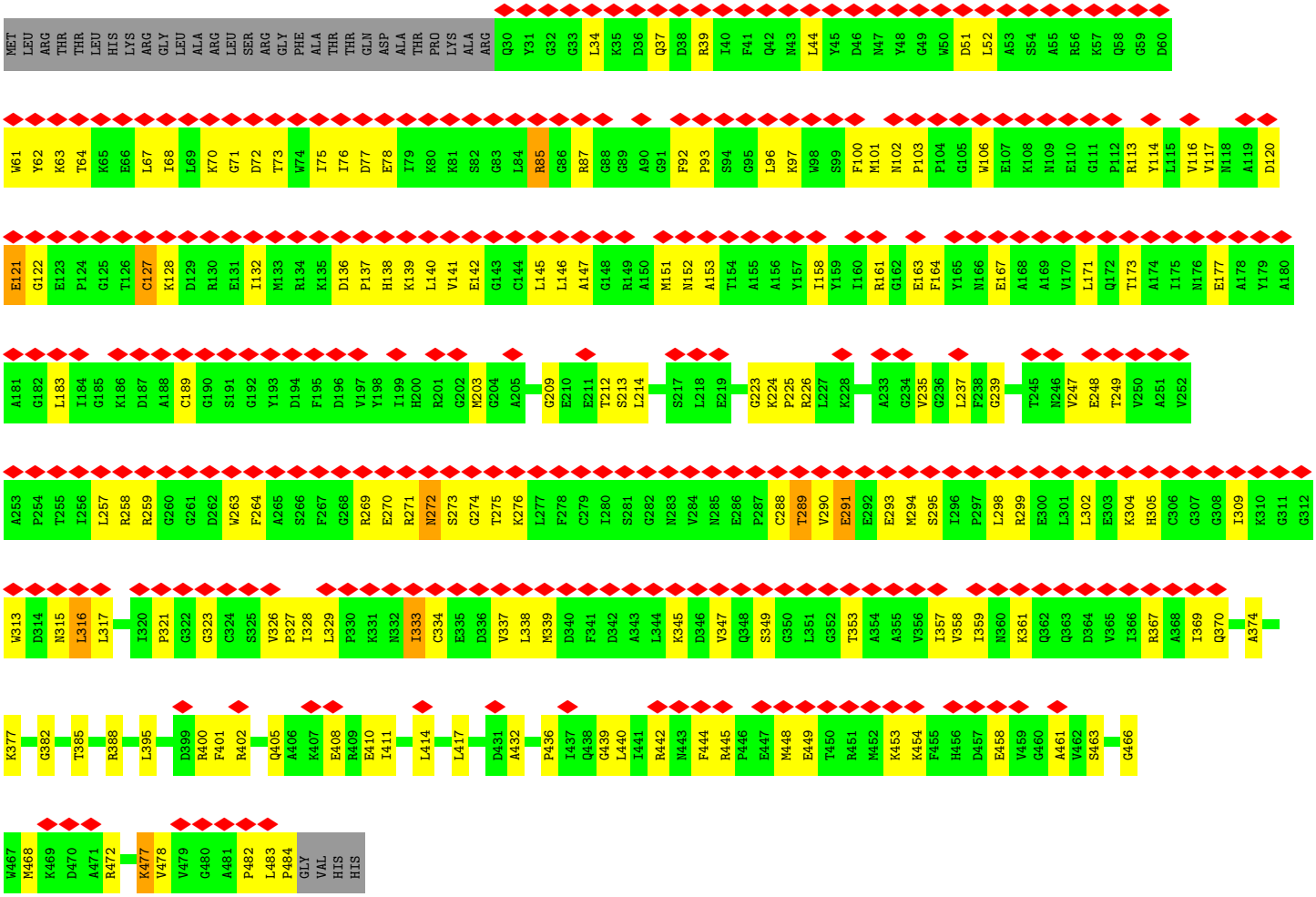



• Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:

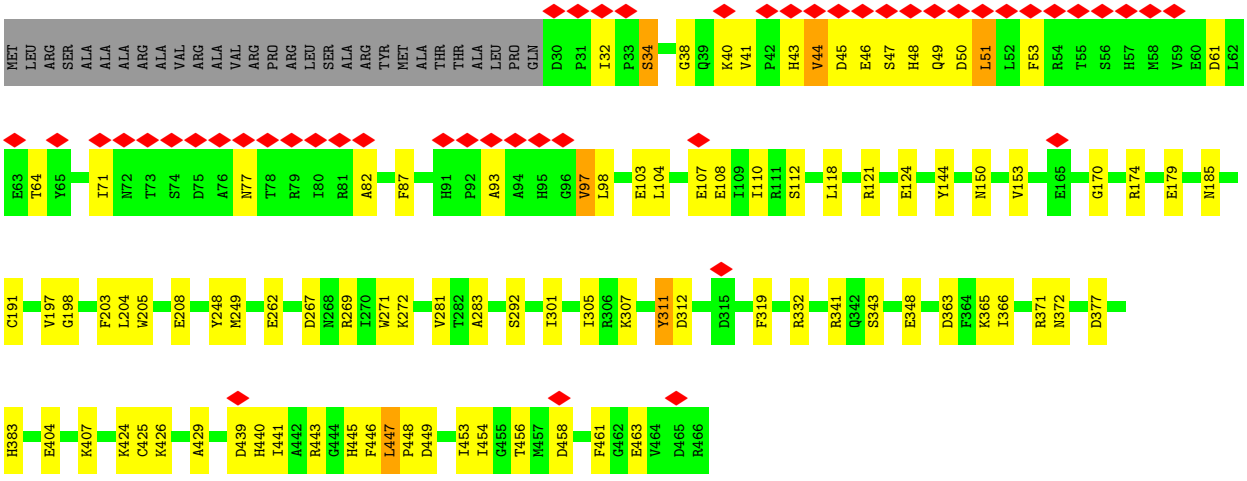




• Molecule 3: NUCM protein

Chain C:

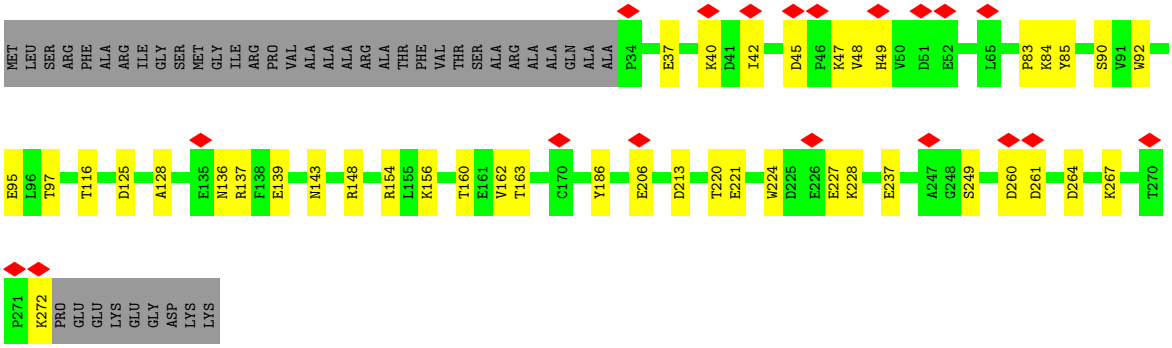


• Molecule 4: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)

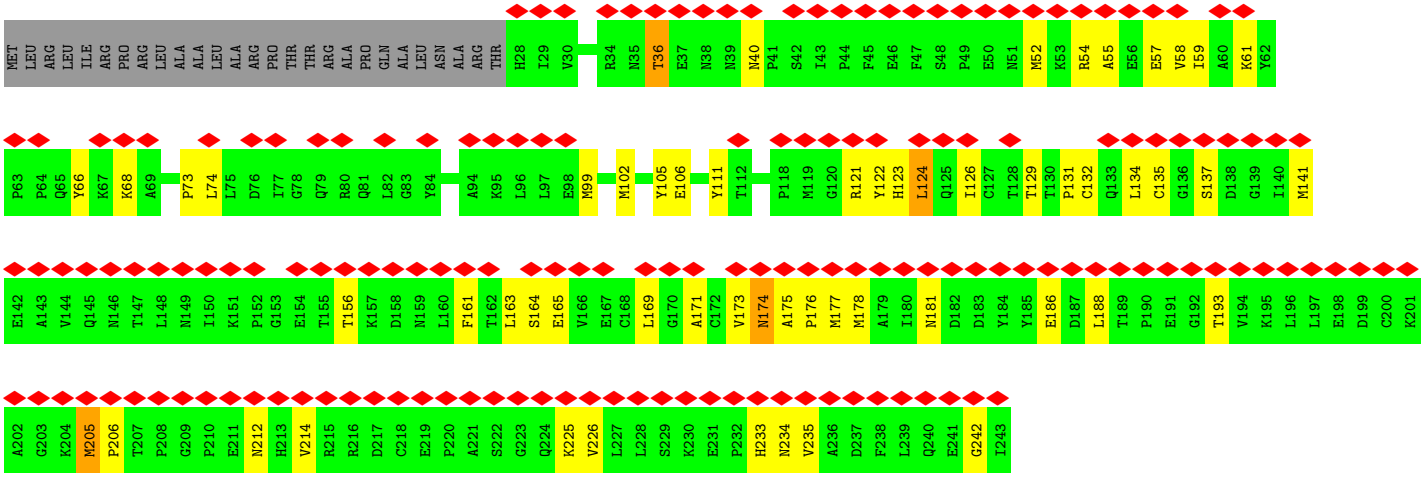
Chain G:





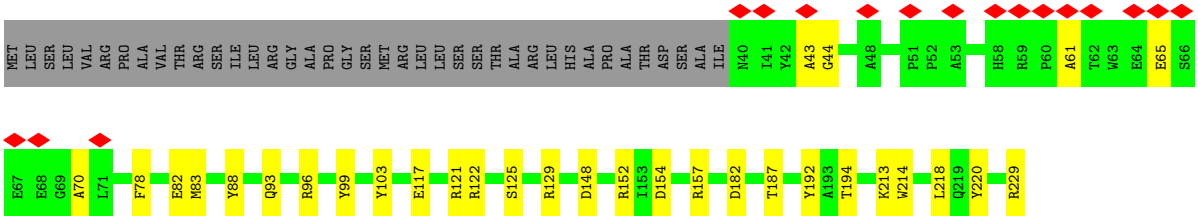

• Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)



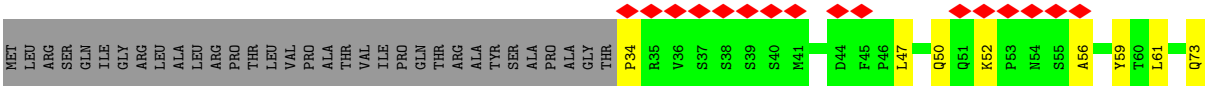

• Molecule 6: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

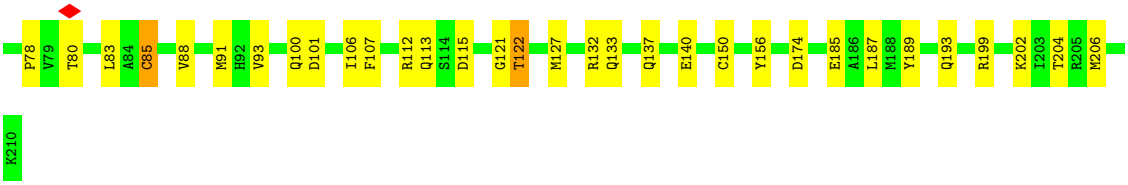



• Molecule 7: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

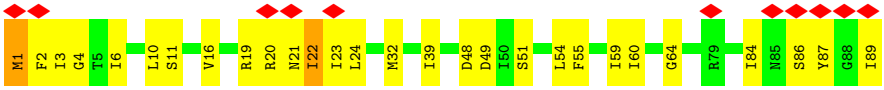




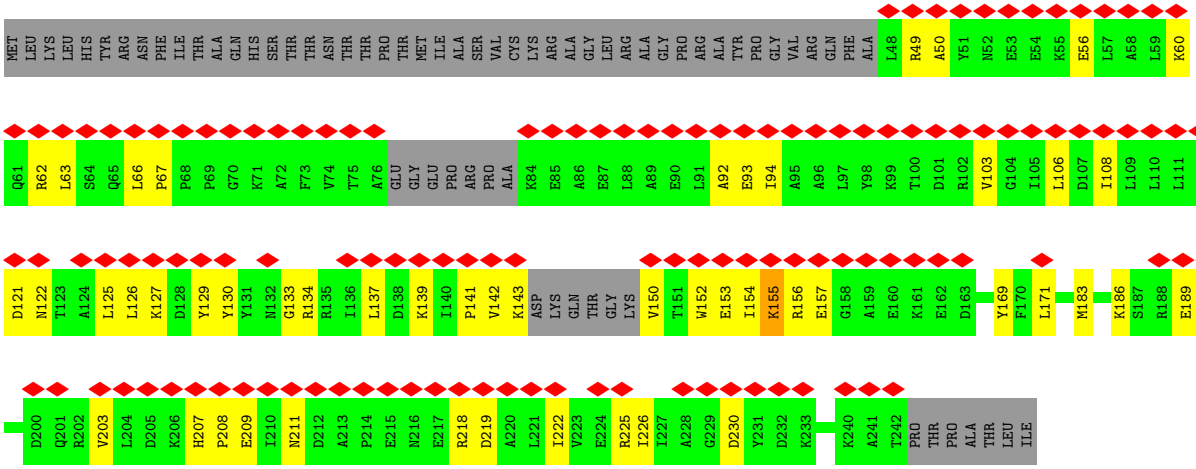

• Molecule 8: NADH-ubiquinone oxidoreductase chain 4L



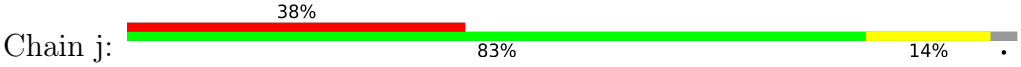



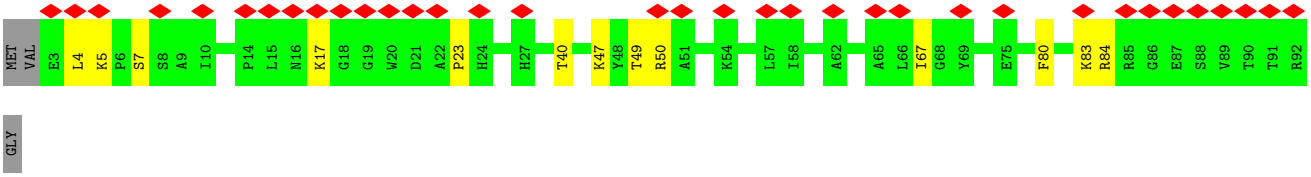

• Molecule 9: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)



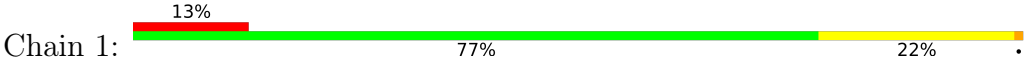



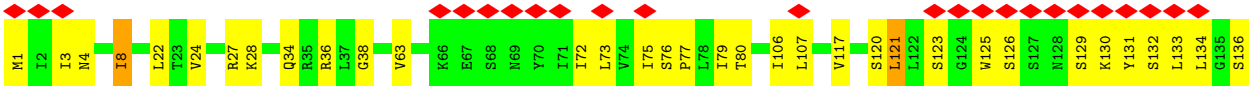

• Molecule 10: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

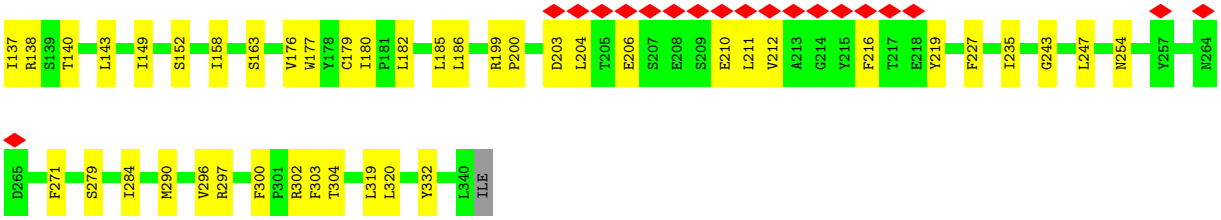


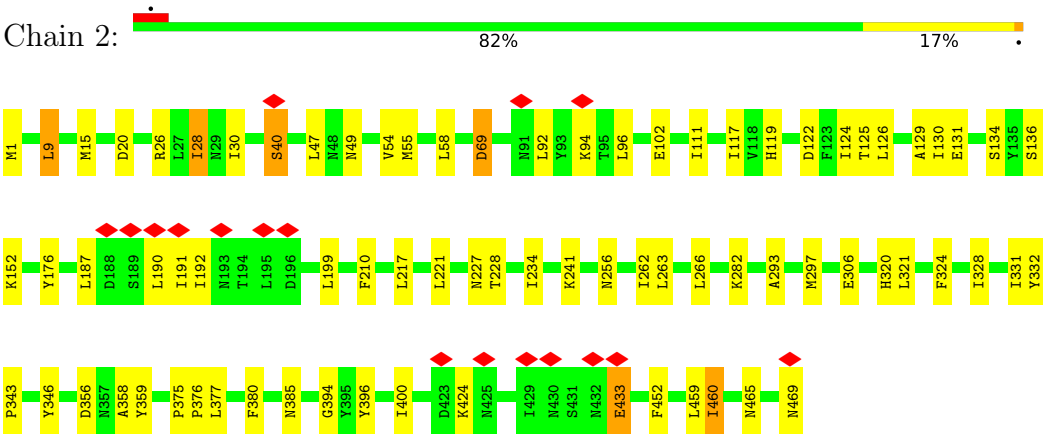

• Molecule 11: NADH-ubiquinone oxidoreductase chain 1



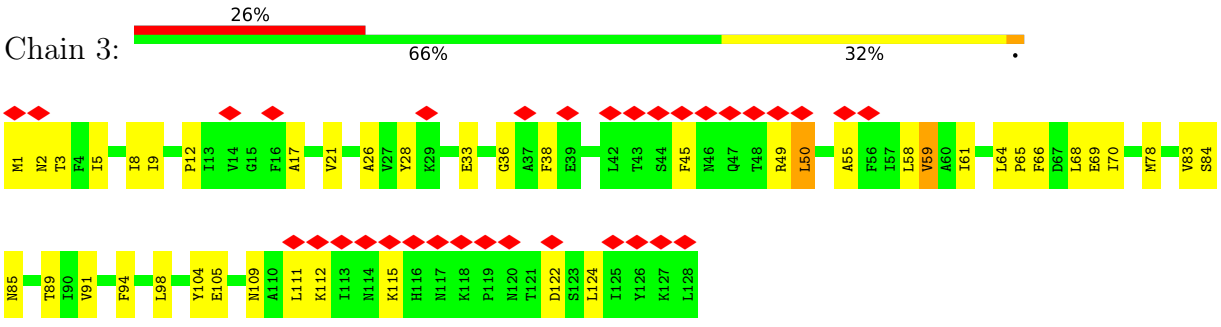





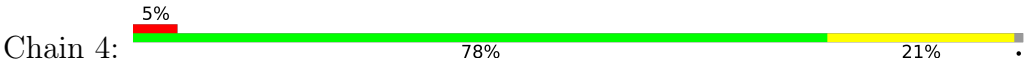

• Molecule 12: NADH dehydrogenase subunit 2

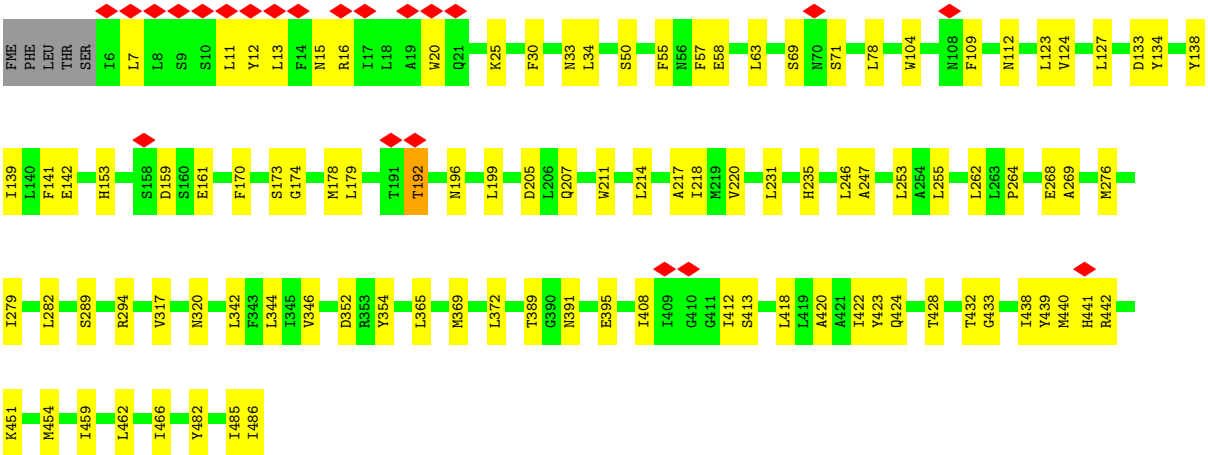



• Molecule 13: NADH-ubiquinone oxidoreductase chain 3



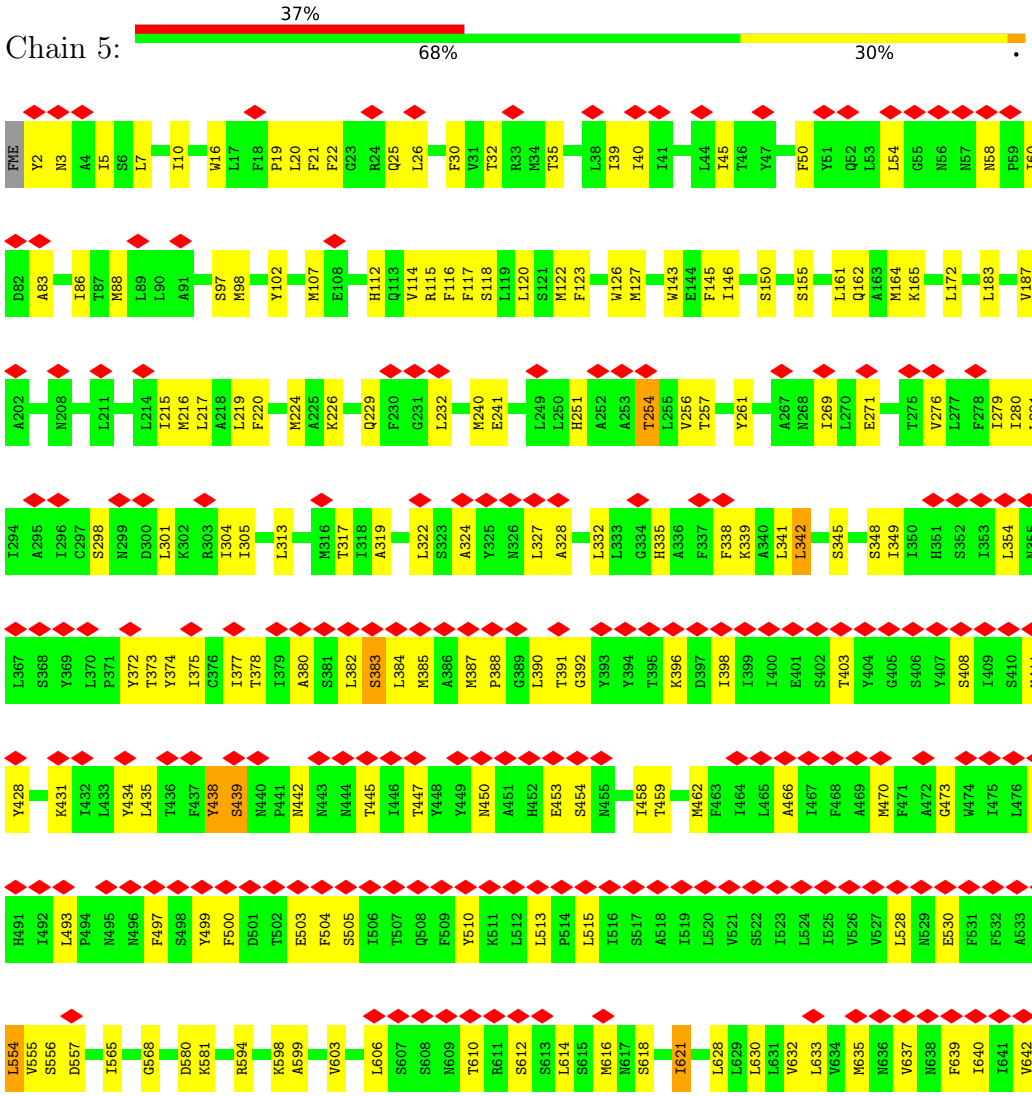

• Molecule 14: NADH-ubiquinone oxidoreductase chain 4



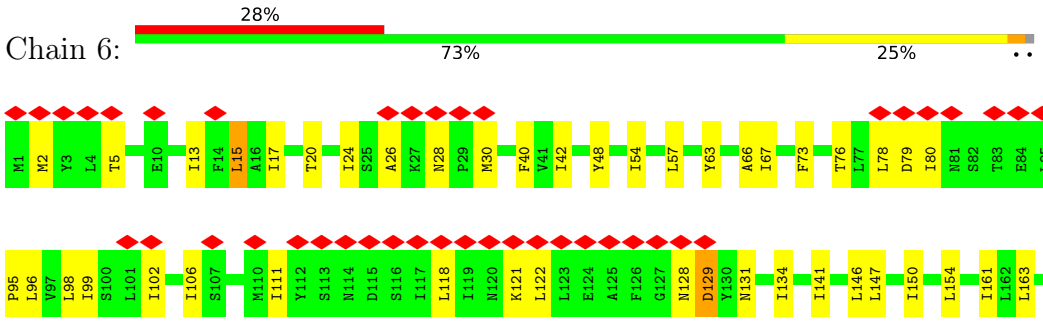
• Molecule 15: NADH-ubiquinone oxidoreductase chain 5

Chain 5:



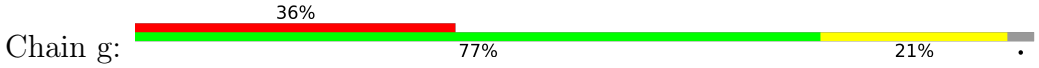

• Molecule 16: NADH-ubiquinone oxidoreductase chain 6

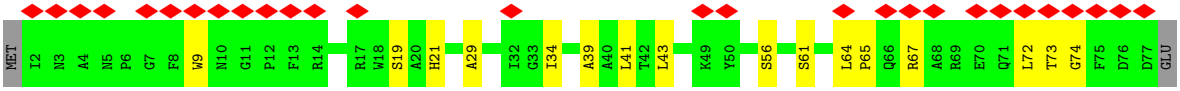
Chain 6:



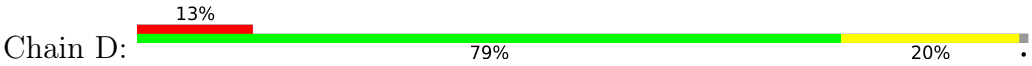

• Molecule 17: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

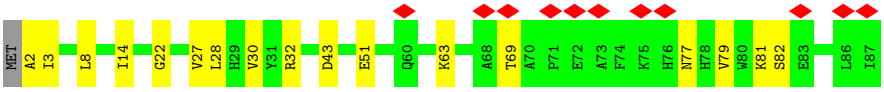
Chain g:






• Molecule 18: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)



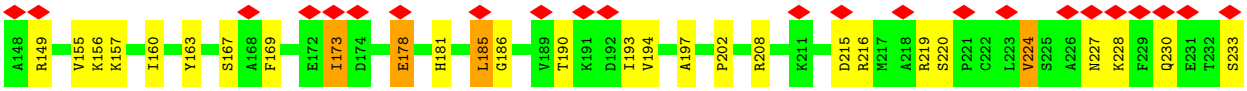



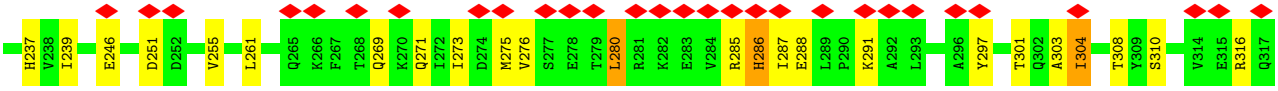

• Molecule 19: NADH-ubiquinone oxidoreductase 40 kDa subunit

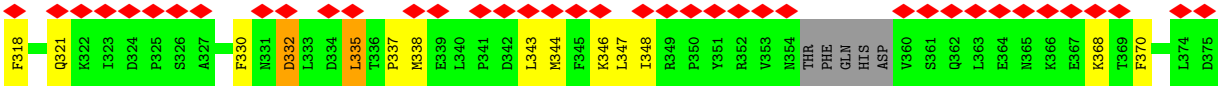






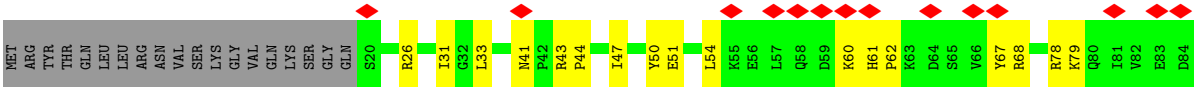



• Molecule 20: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



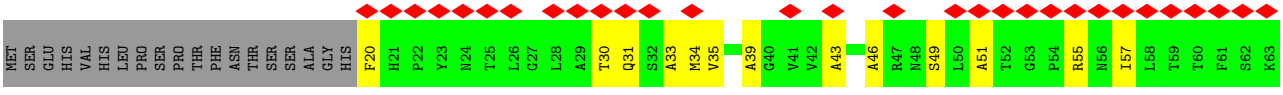



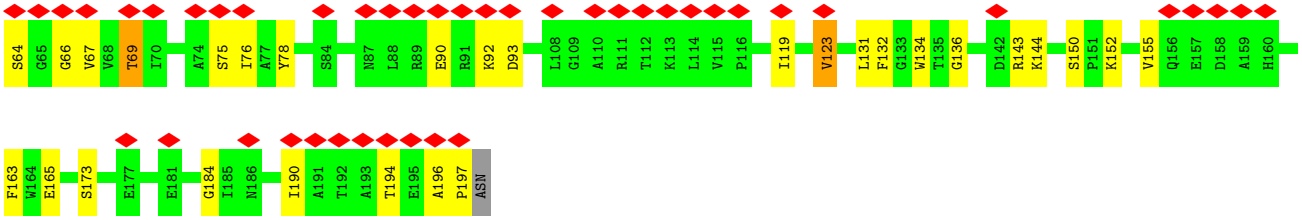




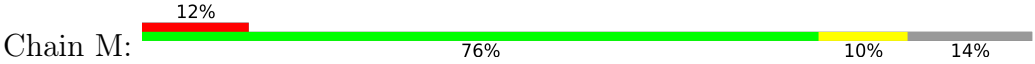
• Molecule 21: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

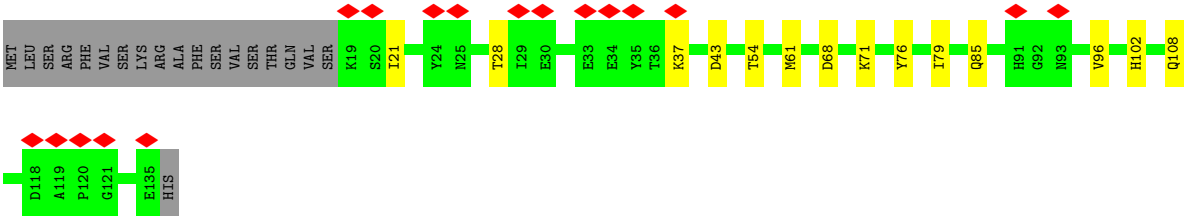




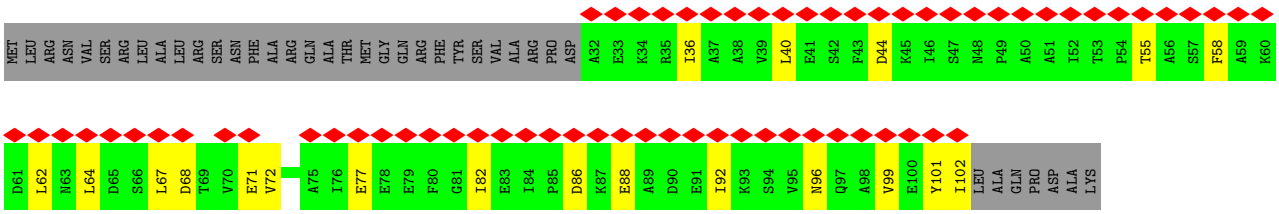

• Molecule 22: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



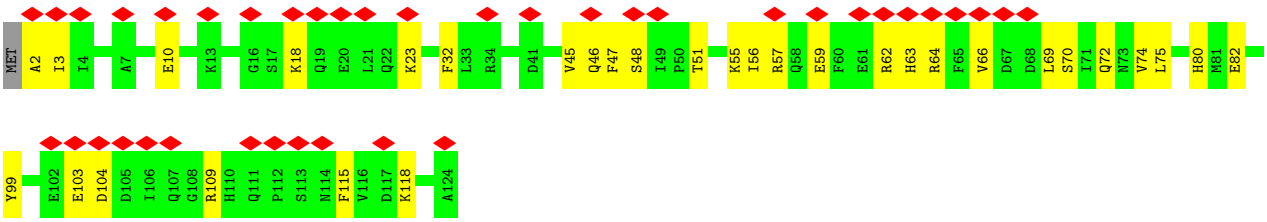

• Molecule 23: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)



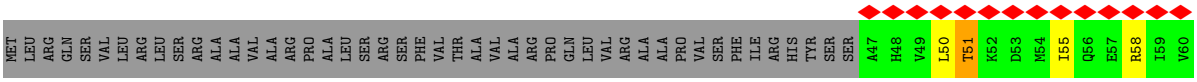

• Molecule 24: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

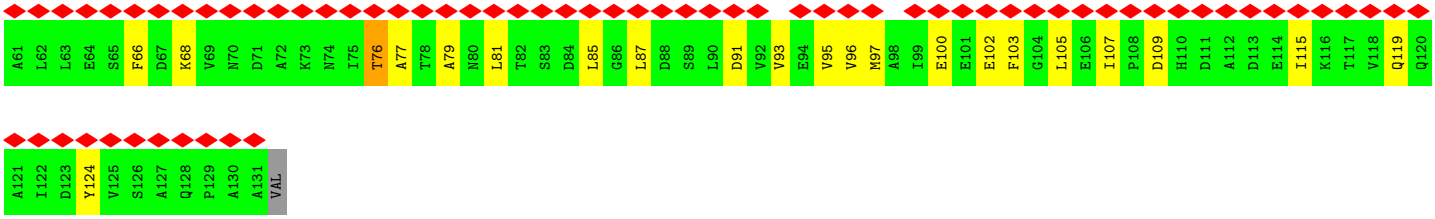



• Molecule 25: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)



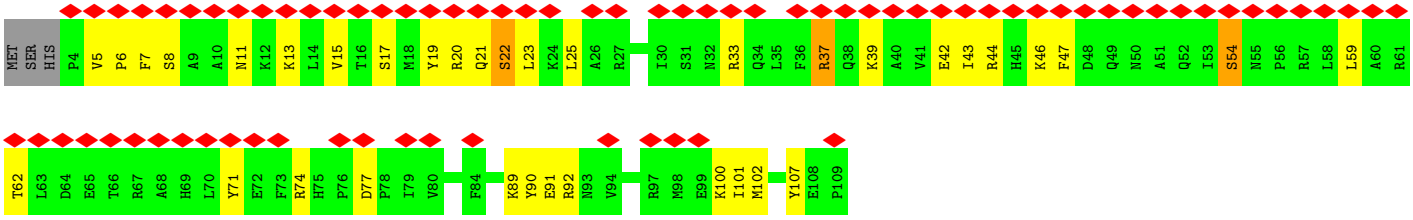






• Molecule 26: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain R:

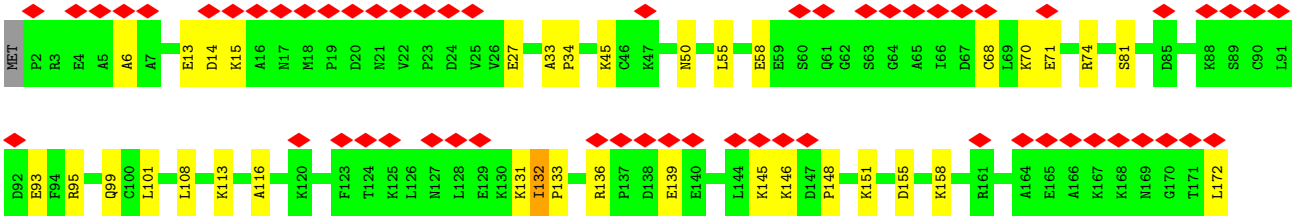



• Molecule 27: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain U:

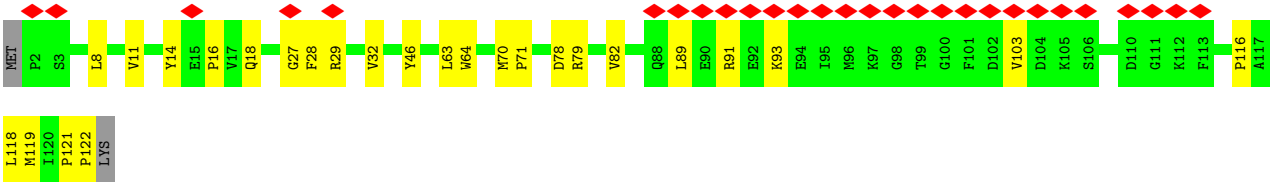



• Molecule 28: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain W:

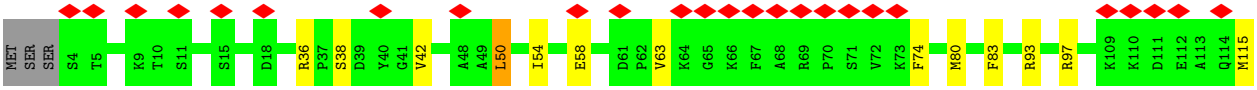



• Molecule 29: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain X:



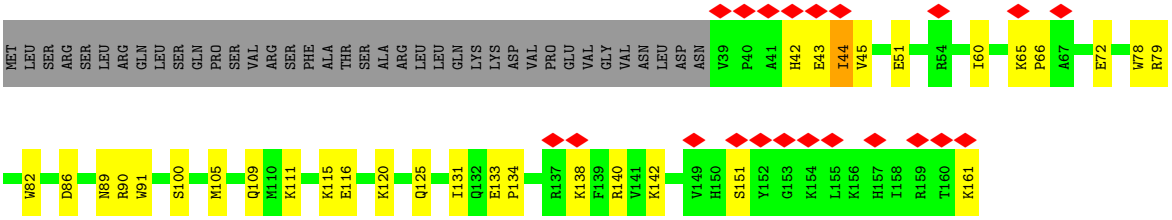






• Molecule 30: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Y:

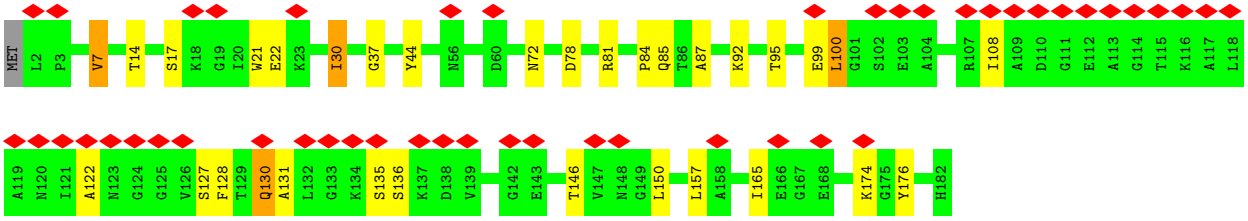



• Molecule 31: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Z:

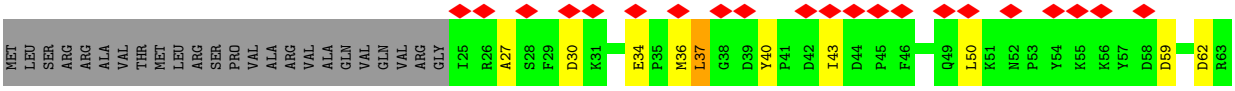


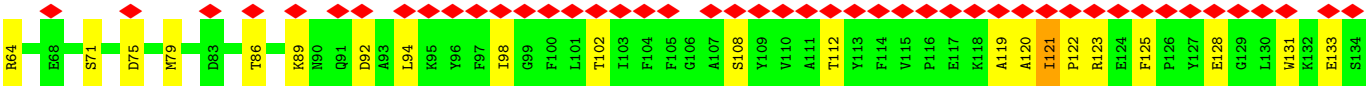



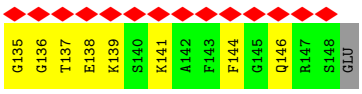

• Molecule 32: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain a:



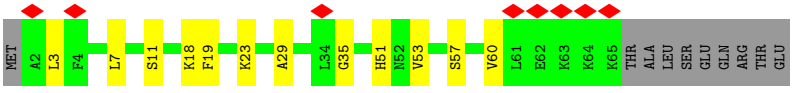




• Molecule 33: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

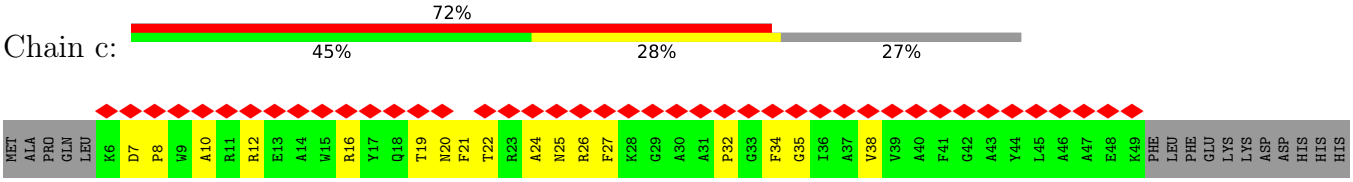
Chain b:



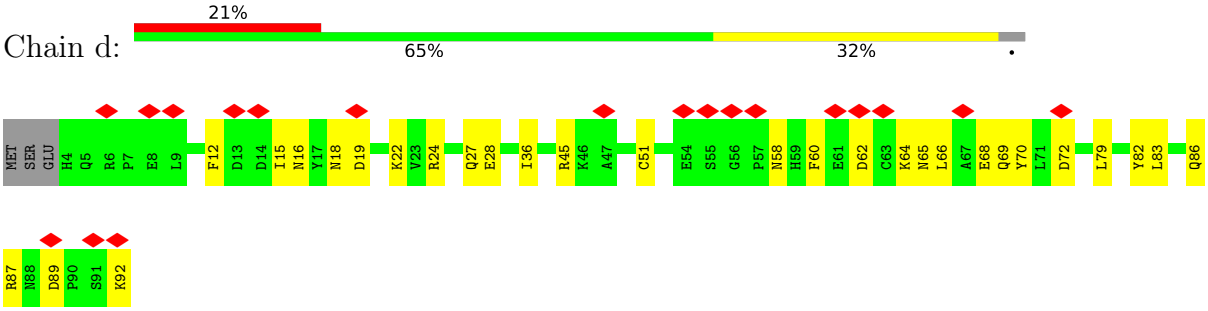

• Molecule 34: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain c:



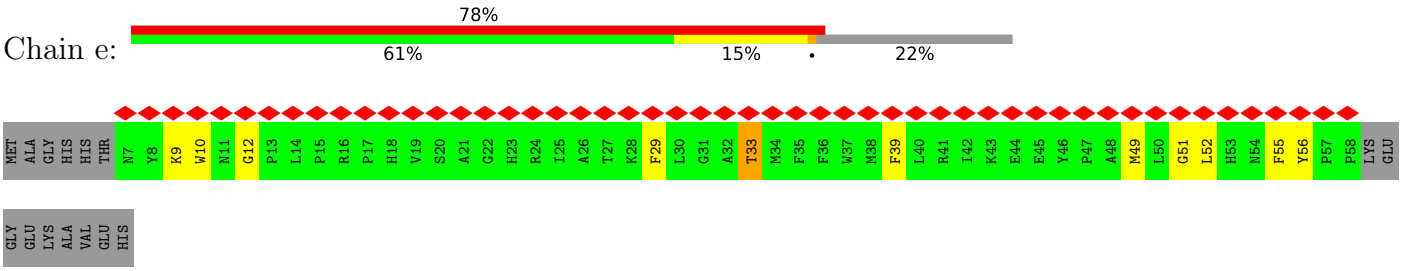

• Molecule 35: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain d:



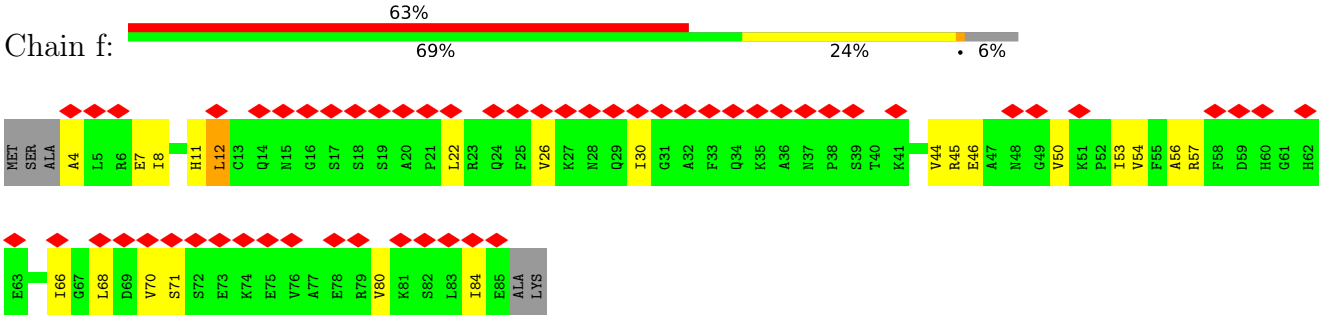

• Molecule 36: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain e:



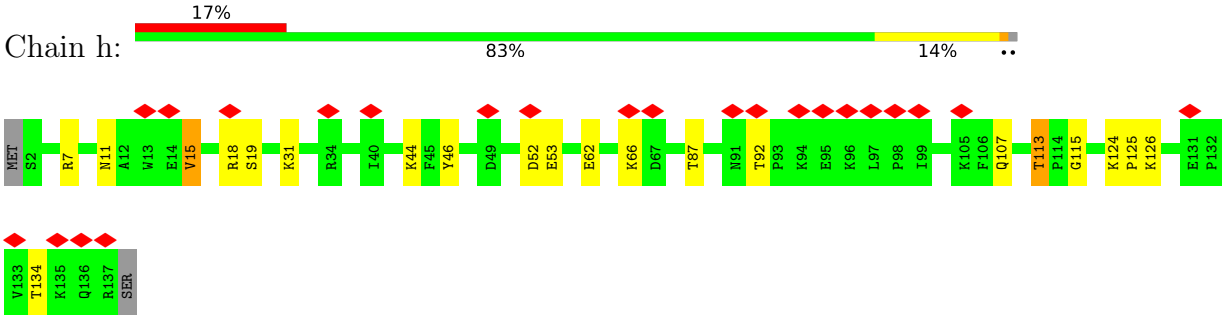

• Molecule 37: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain f:



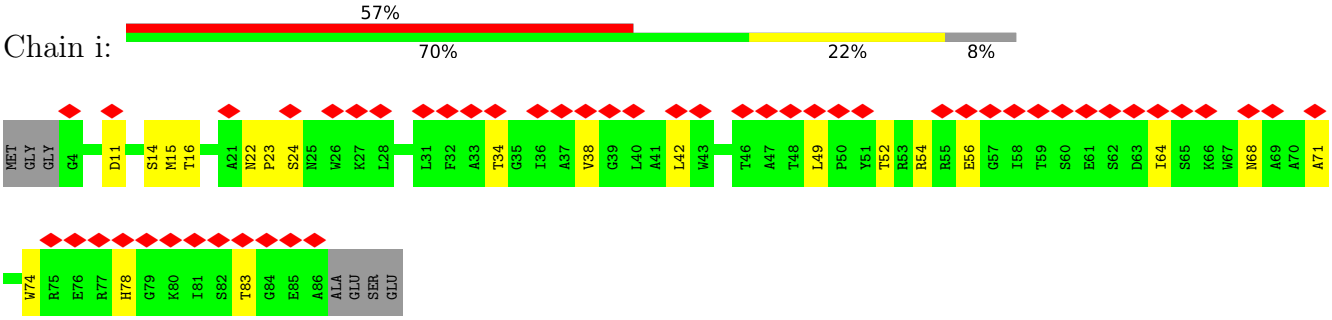

• Molecule 38: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain h:



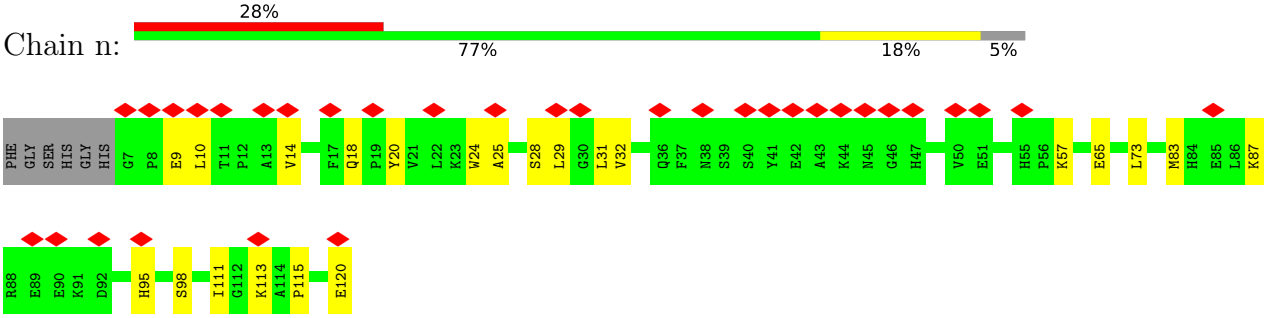

• Molecule 39: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain i:



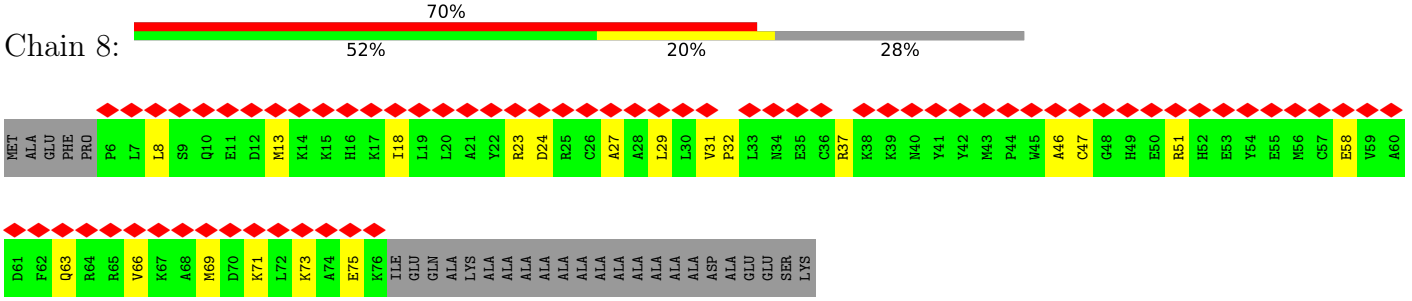

• Molecule 40: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain n:



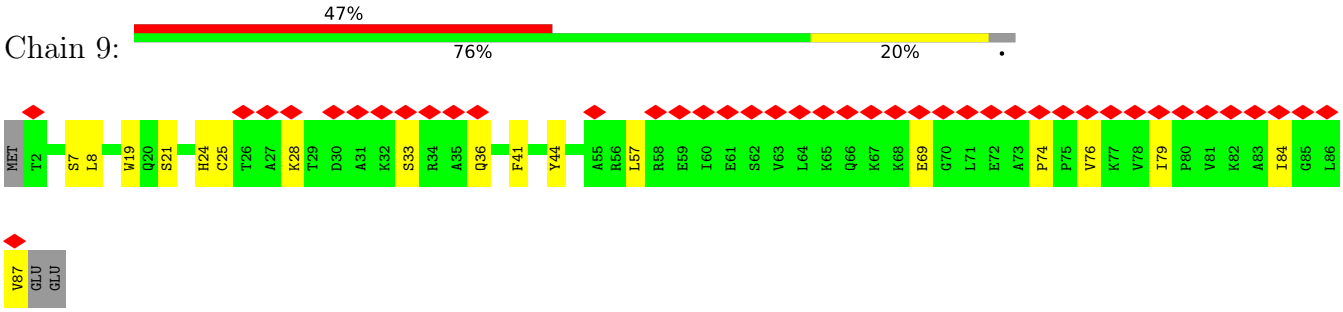

• Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 8:




• Molecule 42: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 9:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 178960 | 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 ($e^-/Å^2$) | 50.0 | Depositor |
| Minimum defocus (nm) | -800 | Depositor |
| Maximum defocus (nm) | -2200 | Depositor |
| Magnification | 96899 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.104 | Depositor |
| Minimum map value | -0.045 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.016 | Depositor |
| Map size (Å) | 309.59998, 309.59998, 309.59998 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.516, 0.516, 0.516 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PE, T7X, LMN, FMN, CPL, FME, SF4, FES, 2MR, NDP, ZMP, ZN, PLC

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 | A | 0.25 | 0/5363 | 0.49 | 2/7278 (0.0%) |
| 2 | B | 0.25 | 0/3594 | 0.48 | 0/4851 |
| 3 | C | 0.28 | 0/3541 | 0.51 | 0/4799 |
| 4 | G | 0.26 | 0/2040 | 0.52 | 2/2781 (0.1%) |
| 5 | H | 0.24 | 0/1725 | 0.57 | 1/2343 (0.0%) |
| 6 | I | 0.27 | 0/1557 | 0.44 | 0/2110 |
| 7 | K | 0.27 | 0/1434 | 0.47 | 0/1950 |
| 8 | L | 0.29 | 0/692 | 0.46 | 0/937 |
| 9 | S | 0.21 | 0/1517 | 0.48 | 0/2046 |
| 10 | j | 0.21 | 0/745 | 0.41 | 0/1006 |
| 11 | 1 | 0.27 | 0/2781 | 0.47 | 0/3798 |
| 12 | 2 | 0.26 | 0/3846 | 0.43 | 0/5242 |
| 13 | 3 | 0.25 | 0/1041 | 0.49 | 0/1420 |
| 14 | 4 | 0.25 | 0/3908 | 0.44 | 0/5337 |
| 15 | 5 | 0.25 | 0/5327 | 0.49 | 0/7273 |
| 16 | 6 | 0.25 | 0/1468 | 0.44 | 0/2003 |
| 17 | g | 0.33 | 0/648 | 0.50 | 0/887 |
| 18 | D | 0.23 | 0/697 | 0.41 | 0/940 |
| 19 | E | 0.27 | 0/2866 | 0.50 | 0/3881 |
| 20 | F | 0.24 | 0/1002 | 0.47 | 0/1359 |
| 21 | J | 0.21 | 0/1351 | 0.43 | 0/1840 |
| 22 | M | 0.24 | 0/935 | 0.42 | 0/1268 |
| 23 | O | 0.19 | 0/549 | 0.39 | 0/746 |
| 24 | P | 0.23 | 0/1061 | 0.41 | 0/1427 |
| 25 | Q | 0.18 | 0/654 | 0.38 | 0/890 |
| 26 | R | 0.23 | 0/909 | 0.46 | 0/1229 |
| 27 | U | 0.25 | 0/1374 | 0.48 | 0/1856 |
| 28 | W | 0.24 | 0/998 | 0.45 | 0/1346 |
| 29 | X | 0.24 | 0/1314 | 0.40 | 0/1783 |
| 30 | Y | 0.26 | 0/1051 | 0.44 | 0/1420 |
| 31 | Z | 0.25 | 0/1430 | 0.48 | 0/1955 |
| 32 | a | 0.23 | 0/1064 | 0.42 | 0/1439 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | b | 0.20 | 0/503 | 0.31 | 0/679 |
| 34 | c | 0.20 | 0/364 | 0.48 | 0/491 |
| 35 | d | 0.25 | 0/767 | 0.41 | 0/1031 |
| 36 | e | 0.17 | 0/456 | 0.38 | 0/619 |
| 37 | f | 0.23 | 0/652 | 0.53 | 0/874 |
| 38 | h | 0.24 | 0/1168 | 0.47 | 0/1589 |
| 39 | i | 0.21 | 0/666 | 0.39 | 0/907 |
| 40 | n | 0.28 | 0/941 | 0.41 | 0/1276 |
| 41 | 8 | 0.20 | 0/606 | 0.42 | 0/808 |
| 42 | 9 | 0.22 | 0/684 | 0.39 | 0/918 |
| All | All | 0.25 | 0/65289 | 0.47 | 5/88632 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 3 | C | 0 | 1 |
| 5 | H | 0 | 1 |
| 7 | K | 0 | 1 |
| 13 | 3 | 0 | 1 |
| 15 | 5 | 0 | 3 |
| 27 | U | 0 | 1 |
| 28 | W | 0 | 1 |
| All | All | 0 | 10 |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | G | 92 | TRP | CA-C-N | 5.80 | 132.62 | 121.54 |
| 4 | G | 92 | TRP | C-N-CA | 5.80 | 132.62 | 121.54 |
| 1 | A | 289 | ASN | CA-C-N | 5.74 | 132.50 | 121.54 |
| 1 | A | 289 | ASN | C-N-CA | 5.74 | 132.50 | 121.54 |
| 5 | H | 205 | MET | CB-CG-SD | 5.51 | 129.22 | 112.70 |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 13 | 3 | 83 | VAL | Peptide |
| 1 | A | 290 | GLU | Peptide |
| 3 | C | 311 | TYR | Peptide |
| 5 | H | 174 | ASN | Peptide |
| 7 | K | 34 | PRO | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5269 | 0 | 5168 | 95 | 0 |
| 2 | B | 3517 | 0 | 3476 | 117 | 0 |
| 3 | C | 3470 | 0 | 3403 | 76 | 0 |
| 4 | G | 1978 | 0 | 1908 | 32 | 0 |
| 5 | H | 1688 | 0 | 1660 | 38 | 0 |
| 6 | I | 1519 | 0 | 1460 | 28 | 0 |
| 7 | K | 1395 | 0 | 1375 | 30 | 0 |
| 8 | L | 693 | 0 | 753 | 27 | 0 |
| 9 | S | 1492 | 0 | 1536 | 42 | 0 |
| 10 | j | 724 | 0 | 706 | 13 | 0 |
| 11 | 1 | 2716 | 0 | 2812 | 65 | 0 |
| 12 | 2 | 3776 | 0 | 4004 | 69 | 0 |
| 13 | 3 | 1027 | 0 | 1091 | 33 | 0 |
| 14 | 4 | 3815 | 0 | 4010 | 73 | 0 |
| 15 | 5 | 5197 | 0 | 5353 | 149 | 0 |
| 16 | 6 | 1453 | 0 | 1576 | 53 | 0 |
| 17 | g | 622 | 0 | 602 | 13 | 0 |
| 18 | D | 681 | 0 | 671 | 14 | 0 |
| 19 | E | 2806 | 0 | 2792 | 65 | 0 |
| 20 | F | 981 | 0 | 969 | 22 | 0 |
| 21 | J | 1319 | 0 | 1304 | 33 | 0 |
| 22 | M | 912 | 0 | 869 | 8 | 0 |
| 23 | O | 543 | 0 | 537 | 14 | 0 |
| 24 | P | 1036 | 0 | 1018 | 27 | 0 |
| 25 | Q | 648 | 0 | 636 | 26 | 0 |
| 26 | R | 884 | 0 | 891 | 27 | 0 |
| 27 | U | 1345 | 0 | 1327 | 26 | 0 |
| 28 | W | 974 | 0 | 987 | 25 | 0 |
| 29 | X | 1275 | 0 | 1250 | 17 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 30 | Y | 1021 | 0 | 984 | 25 | 0 |
| 31 | Z | 1389 | 0 | 1395 | 21 | 0 |
| 32 | a | 1030 | 0 | 967 | 28 | 0 |
| 33 | b | 490 | 0 | 509 | 8 | 0 |
| 34 | c | 353 | 0 | 343 | 17 | 0 |
| 35 | d | 751 | 0 | 715 | 23 | 0 |
| 36 | e | 436 | 0 | 426 | 9 | 0 |
| 37 | f | 642 | 0 | 656 | 19 | 0 |
| 38 | h | 1130 | 0 | 1084 | 17 | 0 |
| 39 | i | 646 | 0 | 630 | 22 | 0 |
| 40 | n | 913 | 0 | 879 | 19 | 0 |
| 41 | 8 | 594 | 0 | 599 | 16 | 0 |
| 42 | 9 | 672 | 0 | 683 | 12 | 0 |
| 43 | A | 16 | 0 | 0 | 0 | 0 |
| 43 | B | 8 | 0 | 0 | 0 | 0 |
| 43 | I | 16 | 0 | 0 | 0 | 0 |
| 43 | K | 8 | 0 | 0 | 1 | 0 |
| 44 | A | 4 | 0 | 0 | 1 | 0 |
| 44 | H | 4 | 0 | 0 | 0 | 0 |
| 45 | B | 31 | 0 | 19 | 2 | 0 |
| 46 | 1 | 77 | 0 | 108 | 4 | 0 |
| 46 | 4 | 35 | 0 | 44 | 1 | 0 |
| 46 | 5 | 42 | 0 | 64 | 1 | 0 |
| 46 | K | 39 | 0 | 55 | 3 | 0 |
| 46 | W | 41 | 0 | 59 | 1 | 0 |
| 47 | 1 | 128 | 0 | 184 | 14 | 0 |
| 47 | 4 | 136 | 0 | 203 | 14 | 0 |
| 47 | 5 | 126 | 0 | 177 | 15 | 0 |
| 47 | 6 | 84 | 0 | 117 | 6 | 0 |
| 47 | E | 36 | 0 | 46 | 0 | 0 |
| 47 | J | 119 | 0 | 160 | 12 | 0 |
| 47 | S | 42 | 0 | 61 | 2 | 0 |
| 47 | b | 42 | 0 | 58 | 7 | 0 |
| 47 | g | 43 | 0 | 63 | 4 | 0 |
| 48 | J | 69 | 0 | 88 | 9 | 0 |
| 48 | j | 65 | 0 | 77 | 5 | 0 |
| 49 | 2 | 100 | 0 | 0 | 1 | 0 |
| 49 | 3 | 49 | 0 | 0 | 1 | 0 |
| 50 | 2 | 52 | 0 | 80 | 3 | 0 |
| 51 | E | 72 | 0 | 88 | 9 | 0 |
| 51 | W | 54 | 0 | 52 | 3 | 0 |
| 51 | X | 86 | 0 | 119 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 51 | Z | 76 | 0 | 96 | 5 | 0 |
| 51 | g | 83 | 0 | 116 | 7 | 0 |
| 51 | n | 92 | 0 | 137 | 13 | 0 |
| 52 | E | 48 | 0 | 26 | 1 | 0 |
| 53 | M | 1 | 0 | 0 | 0 | 0 |
| 54 | O | 33 | 0 | 38 | 3 | 0 |
| 54 | Q | 33 | 0 | 38 | 3 | 0 |
| 55 | 1 | 67 | 0 | 0 | 1 | 0 |
| 55 | 2 | 158 | 0 | 0 | 5 | 0 |
| 55 | 3 | 10 | 0 | 0 | 0 | 0 |
| 55 | 4 | 139 | 0 | 0 | 5 | 0 |
| 55 | 5 | 57 | 0 | 0 | 1 | 0 |
| 55 | 6 | 24 | 0 | 0 | 1 | 0 |
| 55 | 9 | 16 | 0 | 0 | 0 | 0 |
| 55 | A | 135 | 0 | 0 | 2 | 0 |
| 55 | B | 11 | 0 | 0 | 0 | 0 |
| 55 | C | 168 | 0 | 0 | 7 | 0 |
| 55 | D | 17 | 0 | 0 | 1 | 0 |
| 55 | E | 79 | 0 | 0 | 1 | 0 |
| 55 | F | 15 | 0 | 0 | 0 | 0 |
| 55 | G | 114 | 0 | 0 | 3 | 0 |
| 55 | H | 2 | 0 | 0 | 0 | 0 |
| 55 | I | 95 | 0 | 0 | 1 | 0 |
| 55 | J | 14 | 0 | 0 | 0 | 0 |
| 55 | K | 78 | 0 | 0 | 2 | 0 |
| 55 | L | 18 | 0 | 0 | 1 | 0 |
| 55 | M | 45 | 0 | 0 | 0 | 0 |
| 55 | P | 15 | 0 | 0 | 1 | 0 |
| 55 | R | 11 | 0 | 0 | 0 | 0 |
| 55 | S | 4 | 0 | 0 | 0 | 0 |
| 55 | U | 39 | 0 | 0 | 1 | 0 |
| 55 | W | 23 | 0 | 0 | 0 | 0 |
| 55 | X | 39 | 0 | 0 | 1 | 0 |
| 55 | Y | 53 | 0 | 0 | 0 | 0 |
| 55 | Z | 52 | 0 | 0 | 3 | 0 |
| 55 | a | 11 | 0 | 0 | 0 | 0 |
| 55 | b | 6 | 0 | 0 | 0 | 0 |
| 55 | d | 8 | 0 | 0 | 5 | 0 |
| 55 | g | 2 | 0 | 0 | 0 | 0 |
| 55 | h | 61 | 0 | 0 | 4 | 0 |
| 55 | i | 3 | 0 | 0 | 0 | 0 |
| 55 | j | 15 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 55 | n | 12 | 0 | 0 | 0 | 0 |
| All | All | 67428 | 0 | 66387 | 1299 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1299 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:E:173:ILE:O | 19:E:181:HIS:ND1 | 2.06 | 0.88 |
| 1:A:47:SER:O | 1:A:60:LYS:NZ | 2.07 | 0.86 |
| 15:5:354:LEU:HD21 | 15:5:450:ASN:HB2 | 1.59 | 0.83 |
| 9:S:56:GLU:HB3 | 9:S:118:LEU:HD21 | 1.61 | 0.83 |
| 2:B:64:THR:HA | 2:B:67:LEU:HD12 | 1.60 | 0.82 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 691/728 (95%) | 666 (96%) | 24 (4%) | 1 (0%) | 48 64 |
| 2 | B | 453/488 (93%) | 426 (94%) | 26 (6%) | 1 (0%) | 43 58 |
| 3 | C | 435/466 (93%) | 416 (96%) | 19 (4%) | 0 | 100 100 |
| 4 | G | 237/281 (84%) | 230 (97%) | 7 (3%) | 0 | 100 100 |
| 5 | H | 214/243 (88%) | 194 (91%) | 20 (9%) | 0 | 100 100 |
| 6 | I | 188/229 (82%) | 184 (98%) | 4 (2%) | 0 | 100 100 |
| 7 | K | 175/210 (83%) | 168 (96%) | 7 (4%) | 0 | 100 100 |
| 8 | L | 87/89 (98%) | 85 (98%) | 2 (2%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 9 | S | 176/249 (71%) | 173 (98%) | 3 (2%) | 0 | 100 | 100 |
| 10 | j | 88/93 (95%) | 85 (97%) | 3 (3%) | 0 | 100 | 100 |
| 11 | 1 | 338/341 (99%) | 328 (97%) | 10 (3%) | 0 | 100 | 100 |
| 12 | 2 | 467/469 (100%) | 462 (99%) | 5 (1%) | 0 | 100 | 100 |
| 13 | 3 | 126/128 (98%) | 124 (98%) | 1 (1%) | 1 (1%) | 16 | 25 |
| 14 | 4 | 479/486 (99%) | 466 (97%) | 13 (3%) | 0 | 100 | 100 |
| 15 | 5 | 652/655 (100%) | 624 (96%) | 26 (4%) | 2 (0%) | 36 | 50 |
| 16 | 6 | 182/185 (98%) | 179 (98%) | 3 (2%) | 0 | 100 | 100 |
| 17 | g | 74/78 (95%) | 68 (92%) | 6 (8%) | 0 | 100 | 100 |
| 18 | D | 84/87 (97%) | 83 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | E | 346/375 (92%) | 336 (97%) | 10 (3%) | 0 | 100 | 100 |
| 20 | F | 118/144 (82%) | 114 (97%) | 4 (3%) | 0 | 100 | 100 |
| 21 | J | 176/198 (89%) | 170 (97%) | 6 (3%) | 0 | 100 | 100 |
| 22 | M | 115/136 (85%) | 115 (100%) | 0 | 0 | 100 | 100 |
| 23 | O | 69/109 (63%) | 69 (100%) | 0 | 0 | 100 | 100 |
| 24 | P | 121/124 (98%) | 121 (100%) | 0 | 0 | 100 | 100 |
| 25 | Q | 83/132 (63%) | 80 (96%) | 3 (4%) | 0 | 100 | 100 |
| 26 | R | 104/109 (95%) | 102 (98%) | 2 (2%) | 0 | 100 | 100 |
| 27 | U | 169/172 (98%) | 166 (98%) | 3 (2%) | 0 | 100 | 100 |
| 28 | W | 119/123 (97%) | 118 (99%) | 1 (1%) | 0 | 100 | 100 |
| 29 | X | 162/169 (96%) | 160 (99%) | 2 (1%) | 0 | 100 | 100 |
| 30 | Y | 121/161 (75%) | 119 (98%) | 2 (2%) | 0 | 100 | 100 |
| 31 | Z | 179/182 (98%) | 174 (97%) | 5 (3%) | 0 | 100 | 100 |
| 32 | a | 122/149 (82%) | 117 (96%) | 5 (4%) | 0 | 100 | 100 |
| 33 | b | 62/74 (84%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 34 | c | 42/60 (70%) | 40 (95%) | 2 (5%) | 0 | 100 | 100 |
| 35 | d | 87/92 (95%) | 85 (98%) | 2 (2%) | 0 | 100 | 100 |
| 36 | e | 50/67 (75%) | 46 (92%) | 4 (8%) | 0 | 100 | 100 |
| 37 | f | 80/87 (92%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 38 | h | 134/138 (97%) | 130 (97%) | 4 (3%) | 0 | 100 | 100 |
| 39 | i | 81/90 (90%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 40 | n | 112/120 (93%) | 108 (96%) | 4 (4%) | 0 | 100 100 |
| 41 | 8 | 69/99 (70%) | 69 (100%) | 0 | 0 | 100 100 |
| 42 | 9 | 84/89 (94%) | 84 (100%) | 0 | 0 | 100 100 |
| All | All | 7951/8704 (91%) | 7702 (97%) | 244 (3%) | 5 (0%) | 49 64 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 5 | 555 | VAL |
| 13 | 3 | 84 | SER |
| 1 | A | 291 | GLU |
| 2 | B | 121 | GLU |
| 15 | 5 | 439 | SER |

### 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 | A | 566/595 (95%) | 542 (96%) | 24 (4%) | 26 45 |
| 2 | B | 363/389 (93%) | 341 (94%) | 22 (6%) | 17 30 |
| 3 | C | 373/393 (95%) | 366 (98%) | 7 (2%) | 50 71 |
| 4 | G | 216/245 (88%) | 213 (99%) | 3 (1%) | 59 79 |
| 5 | H | 191/212 (90%) | 186 (97%) | 5 (3%) | 40 63 |
| 6 | I | 156/187 (83%) | 154 (99%) | 2 (1%) | 61 80 |
| 7 | K | 154/180 (86%) | 148 (96%) | 6 (4%) | 28 48 |
| 8 | L | 76/76 (100%) | 74 (97%) | 2 (3%) | 40 63 |
| 9 | S | 157/211 (74%) | 152 (97%) | 5 (3%) | 34 56 |
| 10 | j | 71/73 (97%) | 70 (99%) | 1 (1%) | 59 79 |
| 11 | 1 | 300/301 (100%) | 297 (99%) | 3 (1%) | 68 84 |
| 12 | 2 | 432/432 (100%) | 422 (98%) | 10 (2%) | 44 66 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 13 | 3 | 113/113 (100%) | 107 (95%) | 6 (5%) | 20 | 36 |
| 14 | 4 | 429/433 (99%) | 419 (98%) | 10 (2%) | 44 | 66 |
| 15 | 5 | 579/579 (100%) | 561 (97%) | 18 (3%) | 35 | 57 |
| 16 | 6 | 165/166 (99%) | 160 (97%) | 5 (3%) | 36 | 58 |
| 17 | g | 63/65 (97%) | 61 (97%) | 2 (3%) | 34 | 56 |
| 18 | D | 68/69 (99%) | 65 (96%) | 3 (4%) | 25 | 43 |
| 19 | E | 306/329 (93%) | 291 (95%) | 15 (5%) | 22 | 39 |
| 20 | F | 108/129 (84%) | 107 (99%) | 1 (1%) | 70 | 85 |
| 21 | J | 129/147 (88%) | 124 (96%) | 5 (4%) | 28 | 48 |
| 22 | M | 97/115 (84%) | 94 (97%) | 3 (3%) | 35 | 57 |
| 23 | O | 60/91 (66%) | 59 (98%) | 1 (2%) | 53 | 74 |
| 24 | P | 109/110 (99%) | 108 (99%) | 1 (1%) | 70 | 85 |
| 25 | Q | 72/111 (65%) | 70 (97%) | 2 (3%) | 38 | 60 |
| 26 | R | 97/100 (97%) | 93 (96%) | 4 (4%) | 27 | 46 |
| 27 | U | 147/148 (99%) | 145 (99%) | 2 (1%) | 59 | 79 |
| 28 | W | 100/102 (98%) | 100 (100%) | 0 | 100 | 100 |
| 29 | X | 128/133 (96%) | 126 (98%) | 2 (2%) | 55 | 76 |
| 30 | Y | 105/140 (75%) | 102 (97%) | 3 (3%) | 37 | 60 |
| 31 | Z | 147/148 (99%) | 140 (95%) | 7 (5%) | 23 | 40 |
| 32 | a | 108/129 (84%) | 102 (94%) | 6 (6%) | 19 | 33 |
| 33 | b | 50/59 (85%) | 48 (96%) | 2 (4%) | 28 | 47 |
| 34 | c | 30/45 (67%) | 30 (100%) | 0 | 100 | 100 |
| 35 | d | 82/85 (96%) | 82 (100%) | 0 | 100 | 100 |
| 36 | e | 44/55 (80%) | 43 (98%) | 1 (2%) | 44 | 66 |
| 37 | f | 70/73 (96%) | 69 (99%) | 1 (1%) | 59 | 79 |
| 38 | h | 121/123 (98%) | 117 (97%) | 4 (3%) | 33 | 55 |
| 39 | i | 64/68 (94%) | 63 (98%) | 1 (2%) | 55 | 76 |
| 40 | n | 98/102 (96%) | 96 (98%) | 2 (2%) | 48 | 70 |
| 41 | 8 | 63/76 (83%) | 63 (100%) | 0 | 100 | 100 |
| 42 | 9 | 73/76 (96%) | 69 (94%) | 4 (6%) | 19 | 34 |
| All | All | 6880/7413 (93%) | 6679 (97%) | 201 (3%) | 38 | 60 |

5 of 201 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 5 | 445 | THR |
| 19 | E | 286 | HIS |
| 42 | 9 | 76 | VAL |
| 15 | 5 | 557 | ASP |
| 17 | g | 73 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | Y | 62 | GLN |
| 31 | Z | 79 | HIS |
| 38 | h | 55 | HIS |
| 14 | 4 | 15 | ASN |
| 12 | 2 | 392 | 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)

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 12 | FME | 2 | 1 | 12 | 8,9,10 | 0.92 | 0 | 7,9,11 | 1.04 | 1 (14%) |
| 3 | 2MR | C | 121 | 3 | 10,12,13 | 1.76 | 1 (10%) | 5,13,15 | 2.51 | 2 (40%) |
| 16 | FME | 6 | 1 | 16 | 8,9,10 | 0.96 | 0 | 7,9,11 | 0.95 | 0 |
| 13 | FME | 3 | 1 | 13 | 8,9,10 | 0.84 | 0 | 7,9,11 | 1.33 | 1 (14%) |
| 11 | FME | 1 | 1 | 11 | 8,9,10 | 0.95 | 0 | 7,9,11 | 1.05 | 1 (14%) |
| 8 | FME | L | 1 | 8 | 8,9,10 | 0.44 | 0 | 7,9,11 | 1.36 | 1 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 12 | FME | 2 | 1 | 12 | - | 4/7/9/11 | - |
| 3 | 2MR | C | 121 | 3 | - | 4/10/13/15 | - |
| 16 | FME | 6 | 1 | 16 | - | 4/7/9/11 | - |
| 13 | FME | 3 | 1 | 13 | - | 3/7/9/11 | - |
| 11 | FME | 1 | 1 | 11 | - | 0/7/9/11 | - |
| 8 | FME | L | 1 | 8 | - | 2/7/9/11 | - |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 121 | 2MR | CZ-NE | 4.83 | 1.44 | 1.34 |

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | C | 121 | 2MR | NE-CZ-NH2 | 4.81 | 123.89 | 119.48 |
| 3 | C | 121 | 2MR | CD-NE-CZ | 2.73 | 128.53 | 123.41 |
| 13 | 3 | 1 | FME | C-CA-N | 2.69 | 114.58 | 109.73 |
| 8 | L | 1 | FME | C-CA-N | 2.58 | 114.38 | 109.73 |
| 12 | 2 | 1 | FME | C-CA-N | 2.34 | 113.95 | 109.73 |

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | C | 121 | 2MR | C-CA-CB-CG |
| 8 | L | 1 | FME | N-CA-CB-CG |
| 12 | 2 | 1 | FME | C-CA-CB-CG |
| 16 | 6 | 1 | FME | O1-CN-N-CA |
| 16 | 6 | 1 | FME | N-CA-CB-CG |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 8 | L | 1 | FME | 3 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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 | $\#\|Z\| > 2$ |
| 47 | 3PE | E | 401 | - | 35,35,50 | 1.01 | 4 (11%) | 38,40,55 | 1.18 | 2 (5%) |
| 44 | FES | H | 301 | 5 | 0,4,4 | - | - | - | | |
| 47 | 3PE | 5 | 701 | - | 41,41,50 | 0.96 | 4 (9%) | 44,46,55 | 1.17 | 2 (4%) |
| 46 | PLC | 4 | 504 | - | 34,34,41 | 1.42 | 6 (17%) | 40,42,49 | 1.23 | 2 (5%) |
| 51 | CDL | W | 402 | - | 53,53,99 | 1.18 | 7 (13%) | 59,65,111 | 1.20 | 4 (6%) |
| 47 | 3PE | 5 | 702 | - | 40,40,50 | 0.96 | 3 (7%) | 43,45,55 | 1.21 | 3 (6%) |
| 43 | SF4 | K | 301 | 7 | 0,12,12 | - | - | - | | |
| 47 | 3PE | 1 | 504 | 11 | 40,40,50 | 0.92 | 2 (5%) | 43,45,55 | 1.06 | 1 (2%) |
| 51 | CDL | E | 402 | - | 71,71,99 | 1.03 | 7 (9%) | 77,83,111 | 1.15 | 5 (6%) |
| 46 | PLC | 1 | 502 | - | 34,34,41 | 1.40 | 5 (14%) | 40,42,49 | 1.09 | 3 (7%) |
| 46 | PLC | 5 | 704 | - | 41,41,41 | 1.30 | 5 (12%) | 47,49,49 | 1.08 | 2 (4%) |
| 47 | 3PE | 5 | 703 | - | 42,42,50 | 0.99 | 3 (7%) | 45,47,55 | 1.07 | 2 (4%) |
| 47 | 3PE | 6 | 201 | - | 35,35,50 | 1.02 | 4 (11%) | 38,40,55 | 1.25 | 2 (5%) |
| 45 | FMN | B | 502 | - | 33,33,33 | 3.00 | 14 (42%) | 48,50,50 | 1.48 | 11 (22%) |
| 47 | 3PE | 4 | 501 | - | 42,42,50 | 0.94 | 4 (9%) | 45,47,55 | 1.16 | 2 (4%) |
| 48 | LMN | J | 202 | - | 72,72,72 | 1.50 | 9 (12%) | 96,98,98 | 1.48 | 11 (11%) |
| 48 | LMN | j | 101 | - | 68,68,72 | 1.58 | 10 (14%) | 92,94,98 | 1.20 | 5 (5%) |
| 47 | 3PE | g | 202 | - | 42,42,50 | 0.95 | 4 (9%) | 45,47,55 | 1.07 | 2 (4%) |
| 50 | CPL | 2 | 502 | - | 51,51,51 | 0.98 | 4 (7%) | 57,59,59 | 1.07 | 2 (3%) |
| 46 | PLC | W | 401 | - | 40,40,41 | 1.33 | 5 (12%) | 46,48,49 | 1.19 | 3 (6%) |
| 47 | 3PE | 1 | 503 | - | 35,35,50 | 1.01 | 4 (11%) | 38,40,55 | 1.13 | 2 (5%) |
| 43 | SF4 | B | 501 | 2 | 0,12,12 | - | - | - | | |
| 51 | CDL | g | 201 | - | 82,82,99 | 0.97 | 7 (8%) | 88,94,111 | 1.17 | 5 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 54 | ZMP | O | 201 | 23 | 26,32,36 | 1.81 | 5 (19%) | 31,39,45 | 1.99 | 9 (29%) |
| 47 | 3PE | 6 | 202 | - | 46,46,50 | 0.91 | 4 (8%) | 49,51,55 | 1.07 | 2 (4%) |
| 51 | CDL | X | 201 | - | 85,85,99 | 0.94 | 8 (9%) | 91,97,111 | 1.16 | 4 (4%) |
| 47 | 3PE | 4 | 502 | - | 41,41,50 | 0.95 | 4 (9%) | 44,46,55 | 1.11 | 2 (4%) |
| 44 | FES | A | 803 | 1 | 0,4,4 | - | - | - | | |
| 47 | 3PE | 4 | 503 | - | 50,50,50 | 0.85 | 3 (6%) | 53,55,55 | 1.21 | 3 (5%) |
| 43 | SF4 | A | 801 | 1 | 0,12,12 | - | - | - | | |
| 43 | SF4 | A | 802 | 1 | 0,12,12 | - | - | - | | |
| 43 | SF4 | I | 302 | 6 | 0,12,12 | - | - | - | | |
| 43 | SF4 | I | 301 | 6 | 0,12,12 | - | - | - | | |
| 47 | 3PE | J | 204 | - | 33,33,50 | 1.06 | 3 (9%) | 36,38,55 | 1.16 | 2 (5%) |
| 46 | PLC | K | 302 | - | 38,38,41 | 1.37 | 4 (10%) | 44,46,49 | 1.05 | 2 (4%) |
| 49 | T7X | 3 | 201 | - | 49,49,61 | 0.94 | 3 (6%) | 59,61,73 | 1.17 | 6 (10%) |
| 49 | T7X | 2 | 503 | - | 52,52,61 | 0.92 | 5 (9%) | 62,64,73 | 1.35 | 7 (11%) |
| 52 | NDP | E | 400 | - | 49,52,52 | 3.64 | 19 (38%) | 66,80,80 | 2.16 | 15 (22%) |
| 54 | ZMP | Q | 201 | 26,25 | 26,32,36 | 1.83 | 5 (19%) | 31,39,45 | 1.71 | 6 (19%) |
| 47 | 3PE | J | 201 | - | 40,40,50 | 0.96 | 4 (10%) | 43,45,55 | 1.14 | 2 (4%) |
| 46 | PLC | 1 | 505 | - | 41,41,41 | 1.30 | 5 (12%) | 47,49,49 | 1.11 | 2 (4%) |
| 47 | 3PE | J | 203 | 21 | 43,43,50 | 0.92 | 4 (9%) | 46,48,55 | 1.19 | 3 (6%) |
| 51 | CDL | Z | 201 | - | 75,75,99 | 1.03 | 7 (9%) | 81,87,111 | 1.16 | 6 (7%) |
| 47 | 3PE | 1 | 501 | - | 50,50,50 | 0.86 | 3 (6%) | 53,55,55 | 1.12 | 4 (7%) |
| 49 | T7X | 2 | 501 | - | 48,48,61 | 0.92 | 4 (8%) | 57,60,73 | 1.24 | 6 (10%) |
| 51 | CDL | n | 200 | - | 91,91,99 | 0.91 | 8 (8%) | 97,103,111 | 1.18 | 4 (4%) |
| 47 | 3PE | b | 201 | - | 41,41,50 | 0.96 | 4 (9%) | 44,46,55 | 1.07 | 2 (4%) |
| 47 | 3PE | S | 501 | - | 41,41,50 | 0.95 | 3 (7%) | 44,46,55 | 1.11 | 2 (4%) |

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 |
|---|---|---|---|---|---|---|---|
| 47 | 3PE | E | 401 | - | - | 14/39/39/54 | - |
| 44 | FES | H | 301 | 5 | - | - | 0/1/1/1 |
| 47 | 3PE | 5 | 701 | - | - | 15/45/45/54 | - |
| 46 | PLC | 4 | 504 | - | - | 21/38/38/45 | - |
| 51 | CDL | W | 402 | - | - | 31/64/64/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 47 | 3PE | 5 | 702 | - | - | 21/44/44/54 | - |
| 47 | 3PE | 1 | 504 | 11 | - | 15/44/44/54 | - |
| 43 | SF4 | K | 301 | 7 | - | - | 0/6/5/5 |
| 51 | CDL | E | 402 | - | - | 34/82/82/110 | - |
| 46 | PLC | 1 | 502 | - | - | 16/38/38/45 | - |
| 46 | PLC | 5 | 704 | - | - | 17/45/45/45 | - |
| 47 | 3PE | 5 | 703 | - | - | 25/46/46/54 | - |
| 47 | 3PE | 6 | 201 | - | - | 23/39/39/54 | - |
| 45 | FMN | B | 502 | - | - | 9/18/18/18 | 0/3/3/3 |
| 47 | 3PE | 4 | 501 | - | - | 19/46/46/54 | - |
| 48 | LMN | J | 202 | - | - | 34/50/130/130 | 0/4/4/4 |
| 48 | LMN | j | 101 | - | - | 21/46/126/130 | 0/4/4/4 |
| 47 | 3PE | g | 202 | - | - | 23/46/46/54 | - |
| 50 | CPL | 2 | 502 | - | - | 20/55/55/55 | - |
| 46 | PLC | W | 401 | - | - | 21/44/44/45 | - |
| 47 | 3PE | 1 | 503 | - | - | 21/39/39/54 | - |
| 43 | SF4 | B | 501 | 2 | - | - | 0/6/5/5 |
| 51 | CDL | g | 201 | - | - | 36/93/93/110 | - |
| 54 | ZMP | O | 201 | 23 | - | 17/37/39/43 | - |
| 47 | 3PE | 6 | 202 | - | - | 23/50/50/54 | - |
| 51 | CDL | X | 201 | - | - | 35/96/96/110 | - |
| 47 | 3PE | 4 | 502 | - | - | 22/45/45/54 | - |
| 44 | FES | A | 803 | 1 | - | - | 0/1/1/1 |
| 47 | 3PE | 4 | 503 | - | - | 22/54/54/54 | - |
| 43 | SF4 | A | 801 | 1 | - | - | 0/6/5/5 |
| 43 | SF4 | A | 802 | 1 | - | - | 0/6/5/5 |
| 43 | SF4 | I | 302 | 6 | - | - | 0/6/5/5 |
| 43 | SF4 | I | 301 | 6 | - | - | 0/6/5/5 |
| 47 | 3PE | J | 204 | - | - | 17/37/37/54 | - |
| 46 | PLC | K | 302 | - | - | 18/42/42/45 | - |
| 49 | T7X | 3 | 201 | - | - | 15/44/68/80 | 0/1/1/1 |
| 49 | T7X | 2 | 503 | - | - | 27/47/71/80 | 0/1/1/1 |
| 52 | NDP | E | 400 | - | - | 5/34/77/77 | 0/5/5/5 |
| 54 | ZMP | Q | 201 | 26,25 | - | 8/37/39/43 | - |
| 47 | 3PE | J | 201 | - | - | 17/44/44/54 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 46 | PLC | 1 | 505 | - | - | 28/45/45/45 | - |
| 47 | 3PE | J | 203 | 21 | - | 27/47/47/54 | - |
| 51 | CDL | Z | 201 | - | - | 40/86/86/110 | - |
| 47 | 3PE | 1 | 501 | - | - | 29/54/54/54 | - |
| 49 | T7X | 2 | 501 | - | - | 14/43/67/80 | 0/1/1/1 |
| 51 | CDL | n | 200 | - | - | 44/102/102/110 | - |
| 47 | 3PE | b | 201 | - | - | 23/45/45/54 | - |
| 47 | 3PE | S | 501 | - | - | 18/45/45/54 | - |

The worst 5 of 216 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | E | 400 | NDP | C6N-C5N | 12.27 | 1.55 | 1.33 |
| 45 | B | 502 | FMN | C4A-N5 | 7.75 | 1.45 | 1.30 |
| 52 | E | 400 | NDP | C2B-C1B | -7.58 | 1.33 | 1.53 |
| 52 | E | 400 | NDP | O4D-C1D | 7.52 | 1.59 | 1.42 |
| 52 | E | 400 | NDP | O4B-C1B | 7.40 | 1.59 | 1.42 |

The worst 5 of 160 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | J | 202 | LMN | CBR-CBL-CBJ | 6.36 | 132.13 | 113.19 |
| 52 | E | 400 | NDP | N6A-C6A-N1A | -6.15 | 104.88 | 118.35 |
| 52 | E | 400 | NDP | C4A-N9A-C1B | -6.01 | 112.28 | 126.59 |
| 54 | O | 201 | ZMP | C9-C10-S1 | 5.98 | 120.42 | 113.46 |
| 48 | j | 101 | LMN | CBR-CBL-CBJ | 5.82 | 130.53 | 113.19 |

There are no chirality outliers.

5 of 885 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 45 | B | 502 | FMN | C3'-C4'-C5'-O5' |
| 45 | B | 502 | FMN | O4'-C4'-C5'-O5' |
| 45 | B | 502 | FMN | C4'-C5'-O5'-P |
| 45 | B | 502 | FMN | C5'-O5'-P-O1P |
| 45 | B | 502 | FMN | C5'-O5'-P-O2P |

There are no ring outliers.

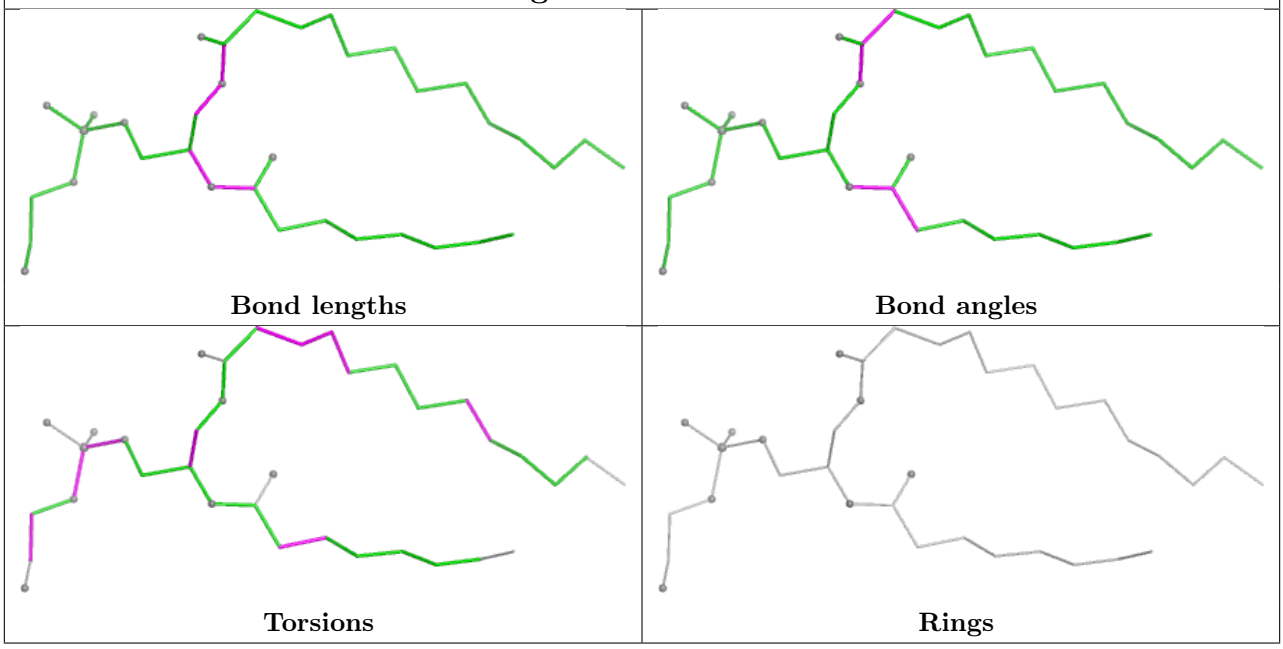
40 monomers are involved in 151 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 47 | 5 | 701 | 3PE | 5 | 0 |
| 46 | 4 | 504 | PLC | 1 | 0 |
| 51 | W | 402 | CDL | 3 | 0 |
| 47 | 5 | 702 | 3PE | 3 | 0 |
| 43 | K | 301 | SF4 | 1 | 0 |
| 47 | 1 | 504 | 3PE | 8 | 0 |
| 51 | E | 402 | CDL | 9 | 0 |
| 46 | 1 | 502 | PLC | 1 | 0 |
| 46 | 5 | 704 | PLC | 1 | 0 |
| 47 | 5 | 703 | 3PE | 7 | 0 |
| 47 | 6 | 201 | 3PE | 2 | 0 |
| 45 | B | 502 | FMN | 2 | 0 |
| 47 | 4 | 501 | 3PE | 6 | 0 |
| 48 | J | 202 | LMN | 9 | 0 |
| 48 | j | 101 | LMN | 5 | 0 |
| 47 | g | 202 | 3PE | 4 | 0 |
| 50 | 2 | 502 | CPL | 3 | 0 |
| 46 | W | 401 | PLC | 1 | 0 |
| 47 | 1 | 503 | 3PE | 2 | 0 |
| 51 | g | 201 | CDL | 7 | 0 |
| 54 | O | 201 | ZMP | 3 | 0 |
| 47 | 6 | 202 | 3PE | 4 | 0 |
| 51 | X | 201 | CDL | 10 | 0 |
| 47 | 4 | 502 | 3PE | 1 | 0 |
| 44 | A | 803 | FES | 1 | 0 |
| 47 | 4 | 503 | 3PE | 7 | 0 |
| 47 | J | 204 | 3PE | 4 | 0 |
| 46 | K | 302 | PLC | 3 | 0 |
| 49 | 3 | 201 | T7X | 1 | 0 |
| 49 | 2 | 503 | T7X | 1 | 0 |
| 52 | E | 400 | NDP | 1 | 0 |
| 54 | Q | 201 | ZMP | 3 | 0 |
| 47 | J | 201 | 3PE | 3 | 0 |
| 46 | 1 | 505 | PLC | 3 | 0 |
| 47 | J | 203 | 3PE | 5 | 0 |
| 51 | Z | 201 | CDL | 5 | 0 |
| 47 | 1 | 501 | 3PE | 4 | 0 |
| 51 | n | 200 | CDL | 13 | 0 |
| 47 | b | 201 | 3PE | 7 | 0 |
| 47 | S | 501 | 3PE | 2 | 0 |

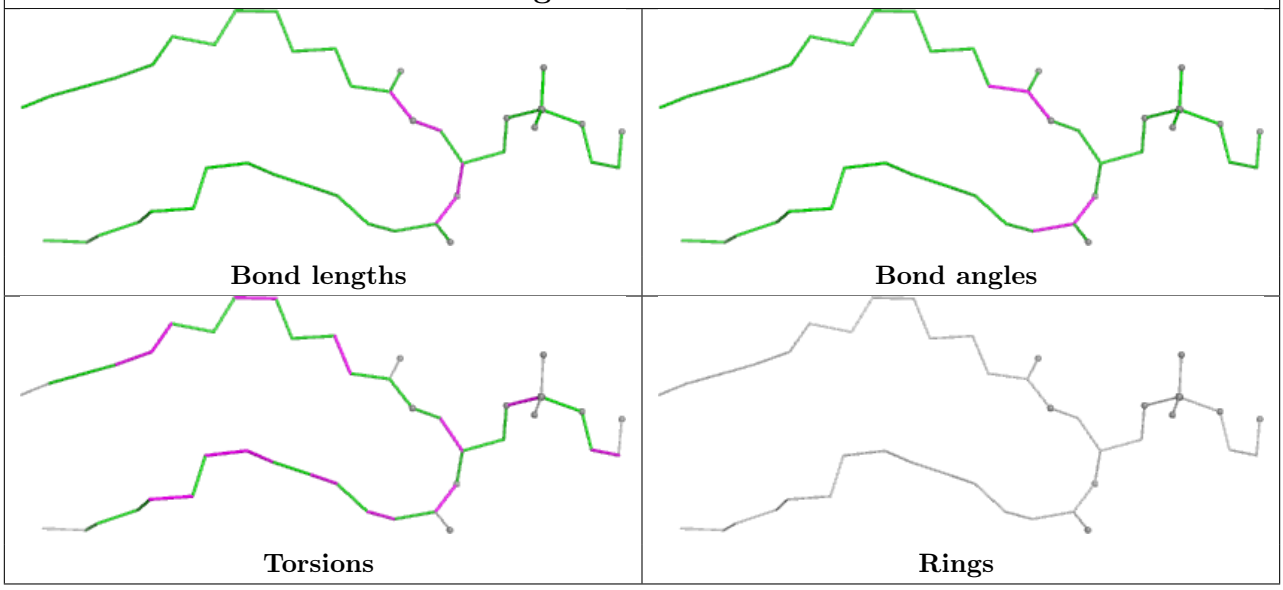
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

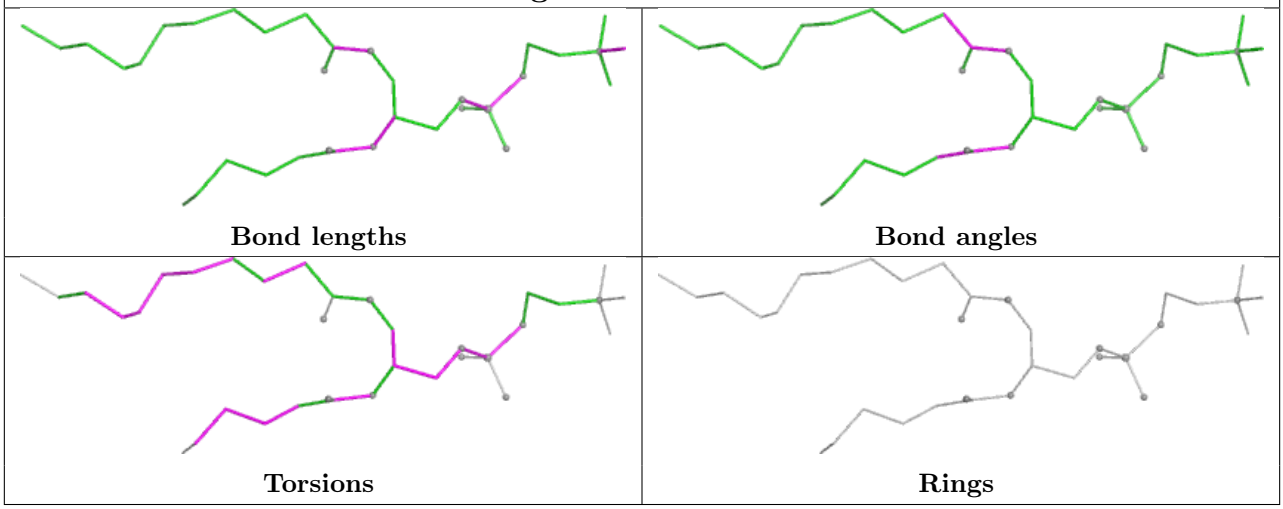
**Ligand 3PE E 401**



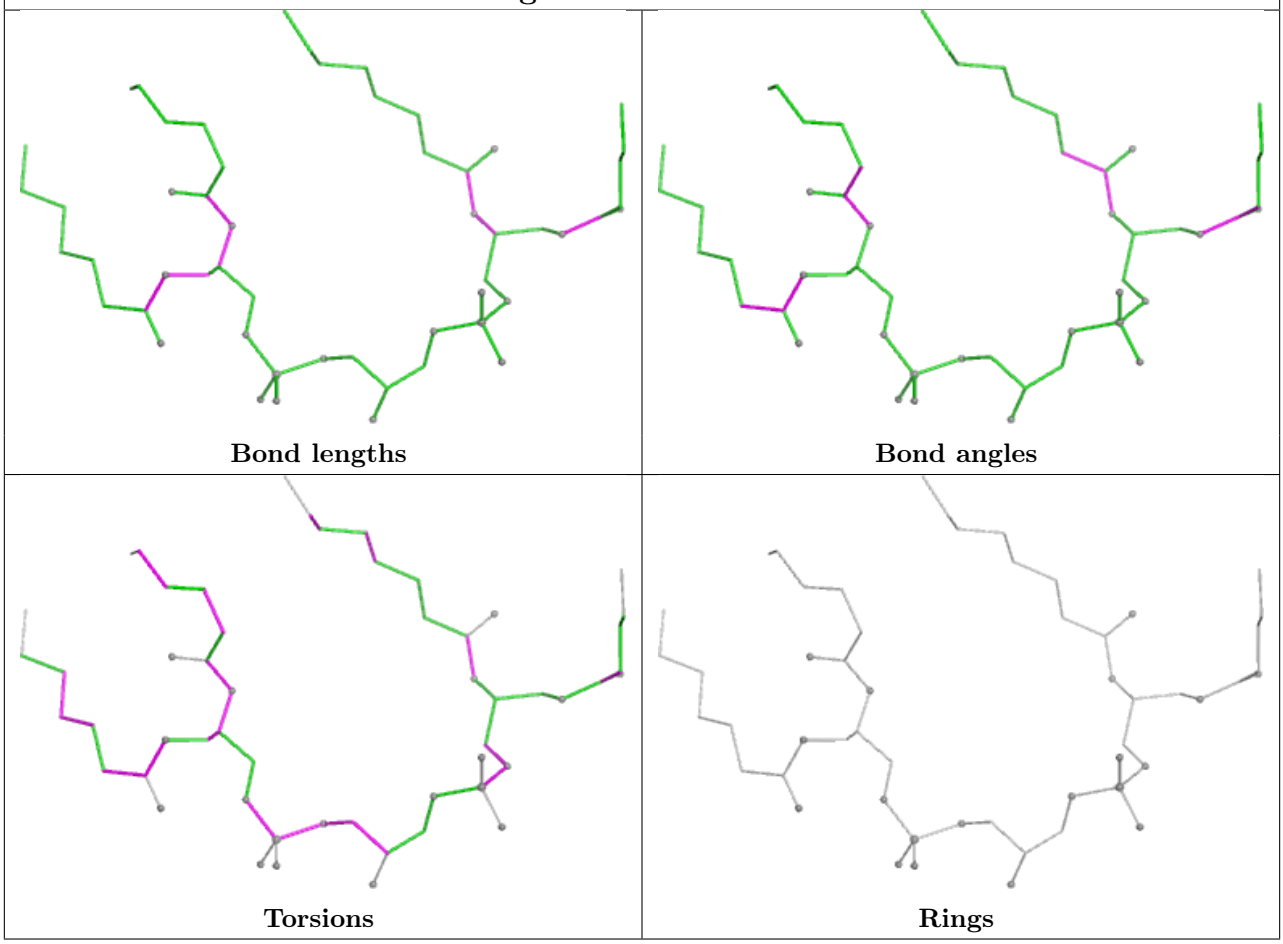

**Ligand 3PE 5 701**



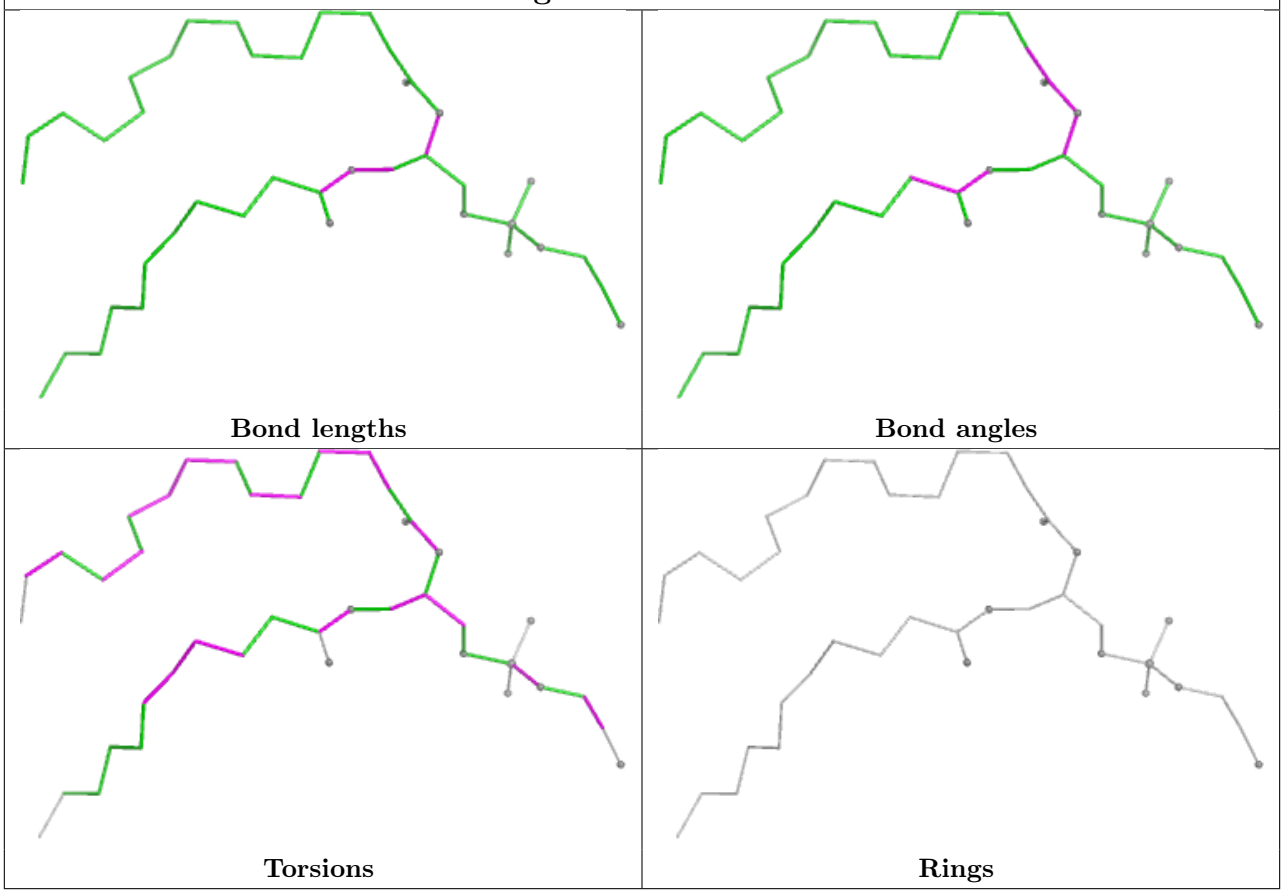
**Ligand PLC 4 504**



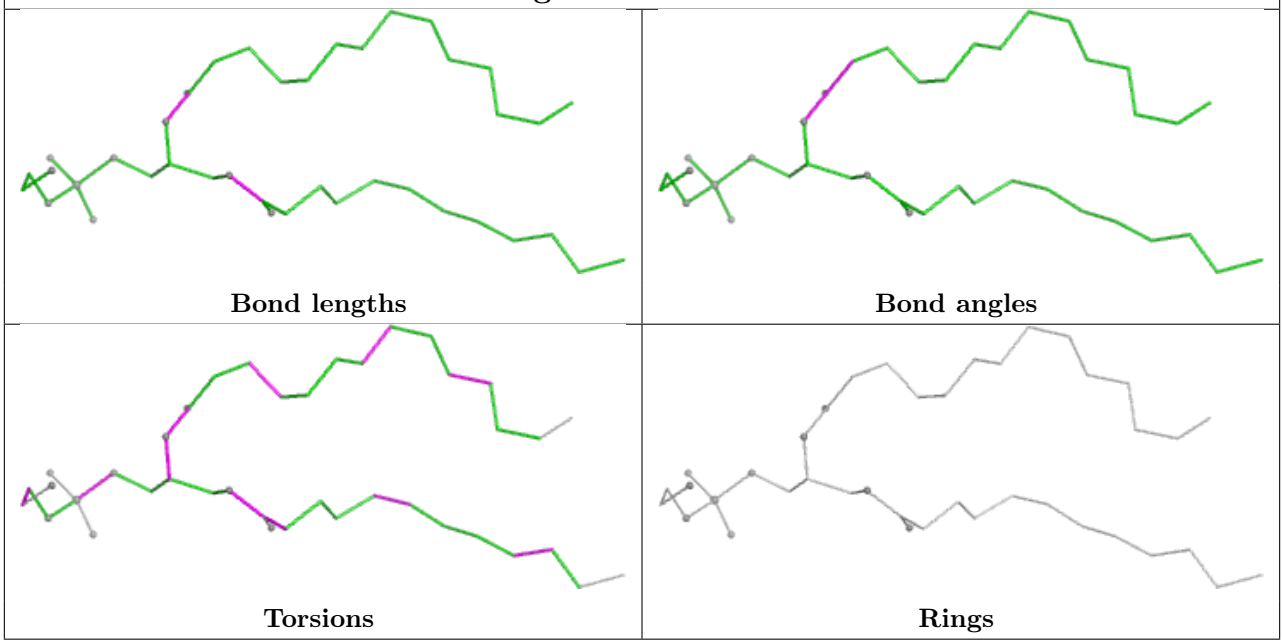

**Ligand CDL W 402**



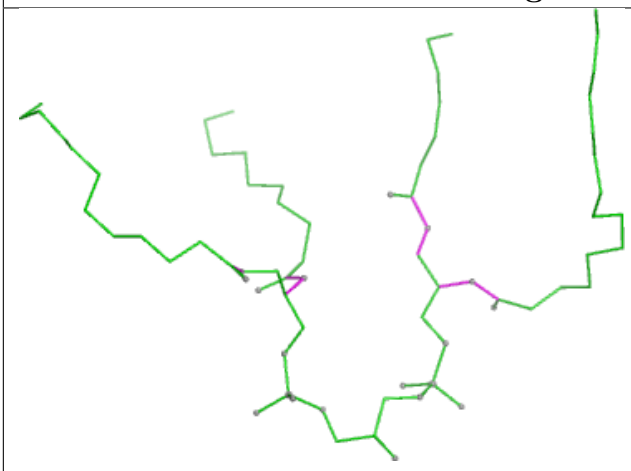
**Ligand 3PE 5 702**



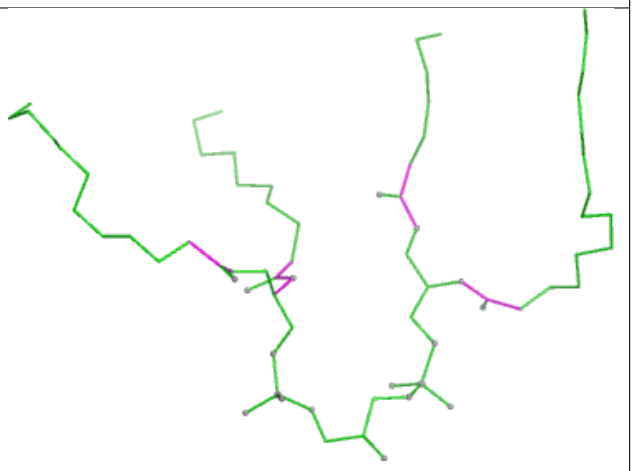

**Ligand 3PE 1 504**



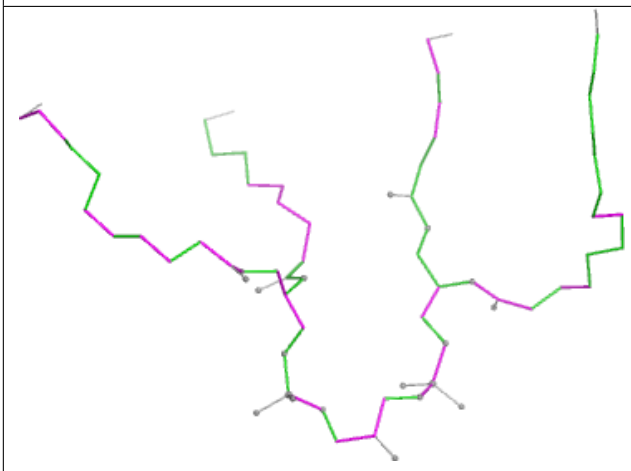
**Ligand CDL E 402**



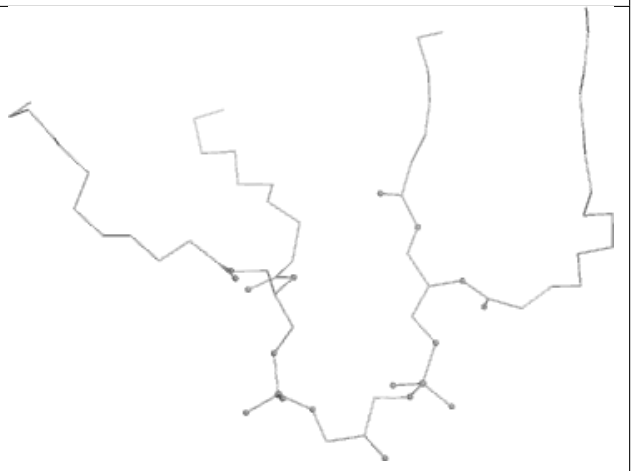
**Bond lengths**



**Bond angles**

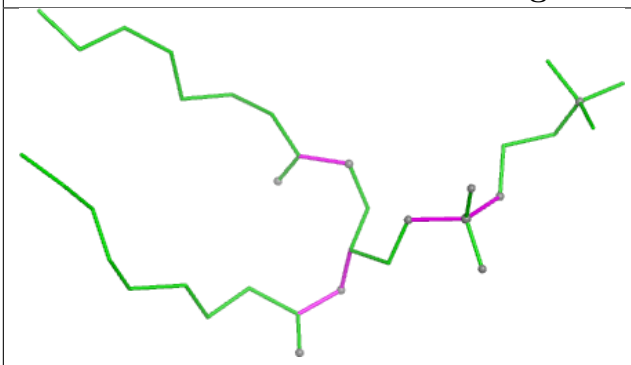


**Torsions**

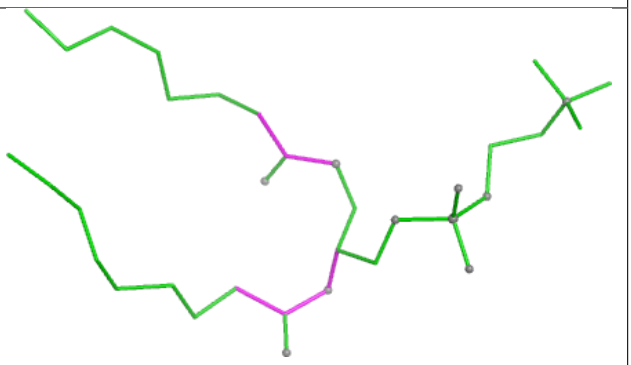


**Rings**

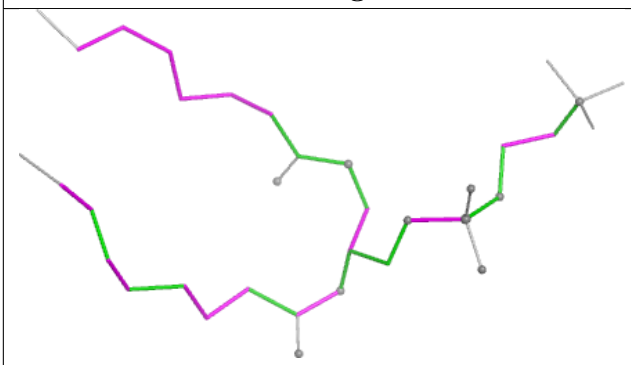
## Ligand PLC 1 502



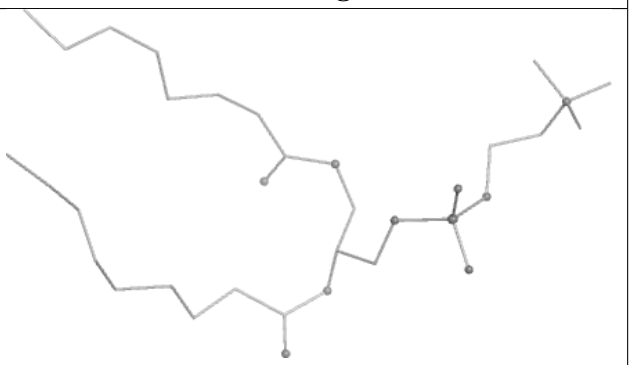
Bond lengths



Bond angles

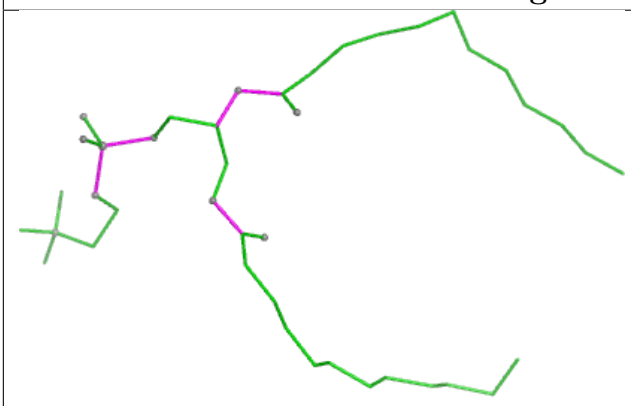


Torsions

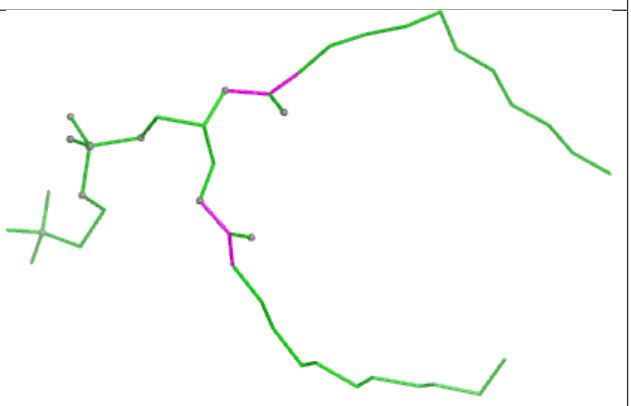


Rings

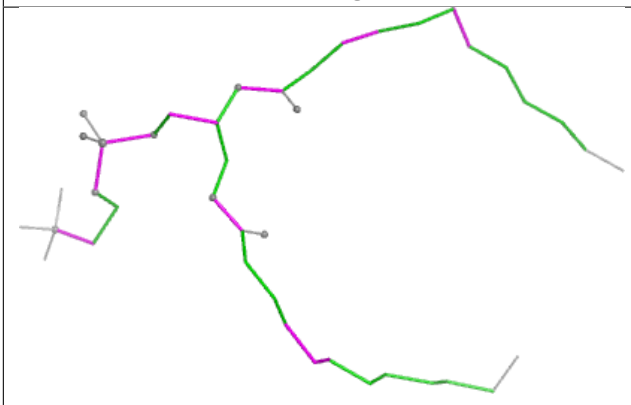
## Ligand PLC 5 704



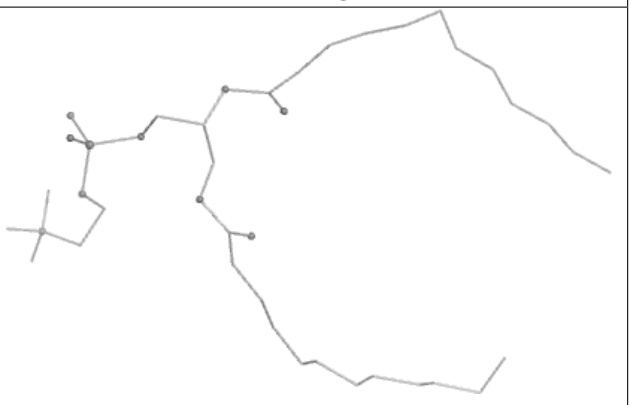
Bond lengths



Bond angles

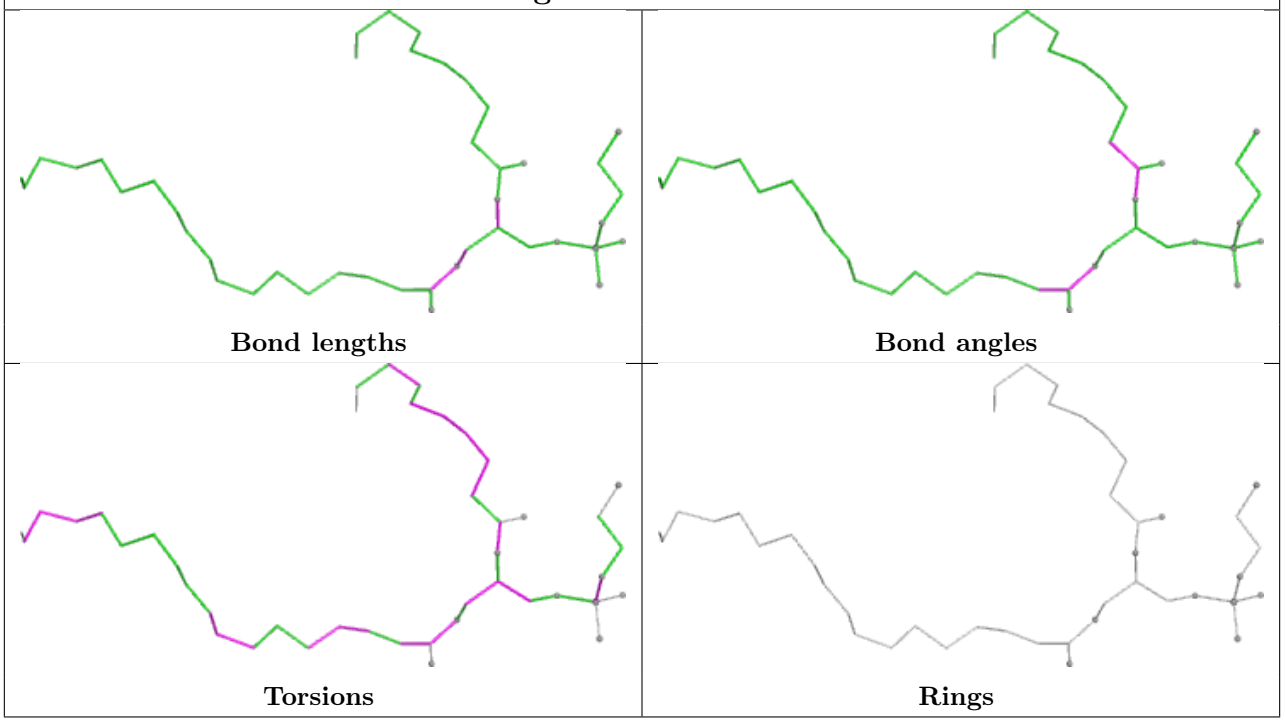


Torsions

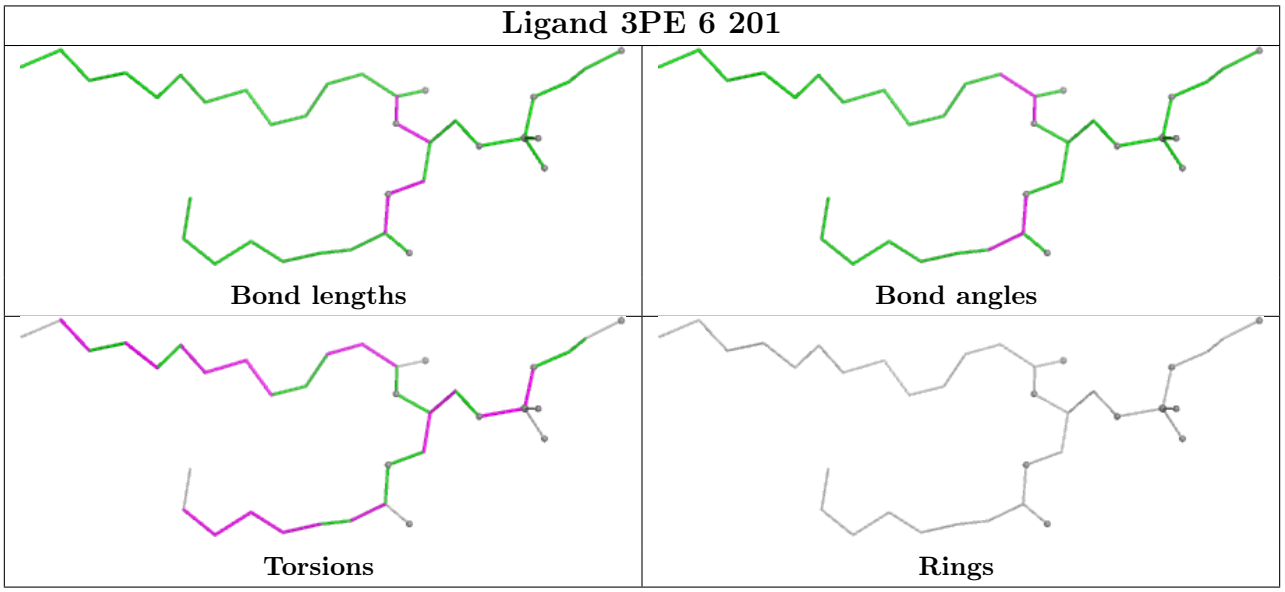


Rings

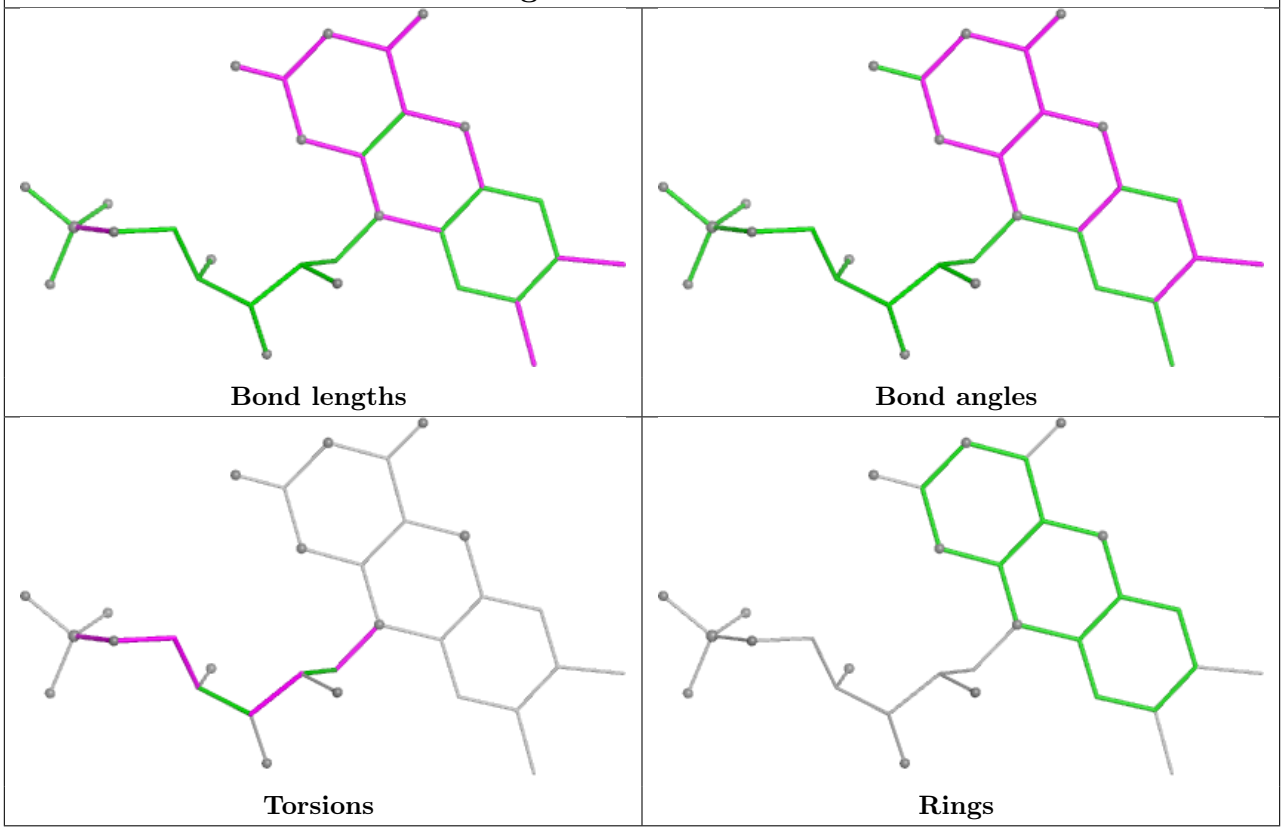
**Ligand 3PE 5 703**



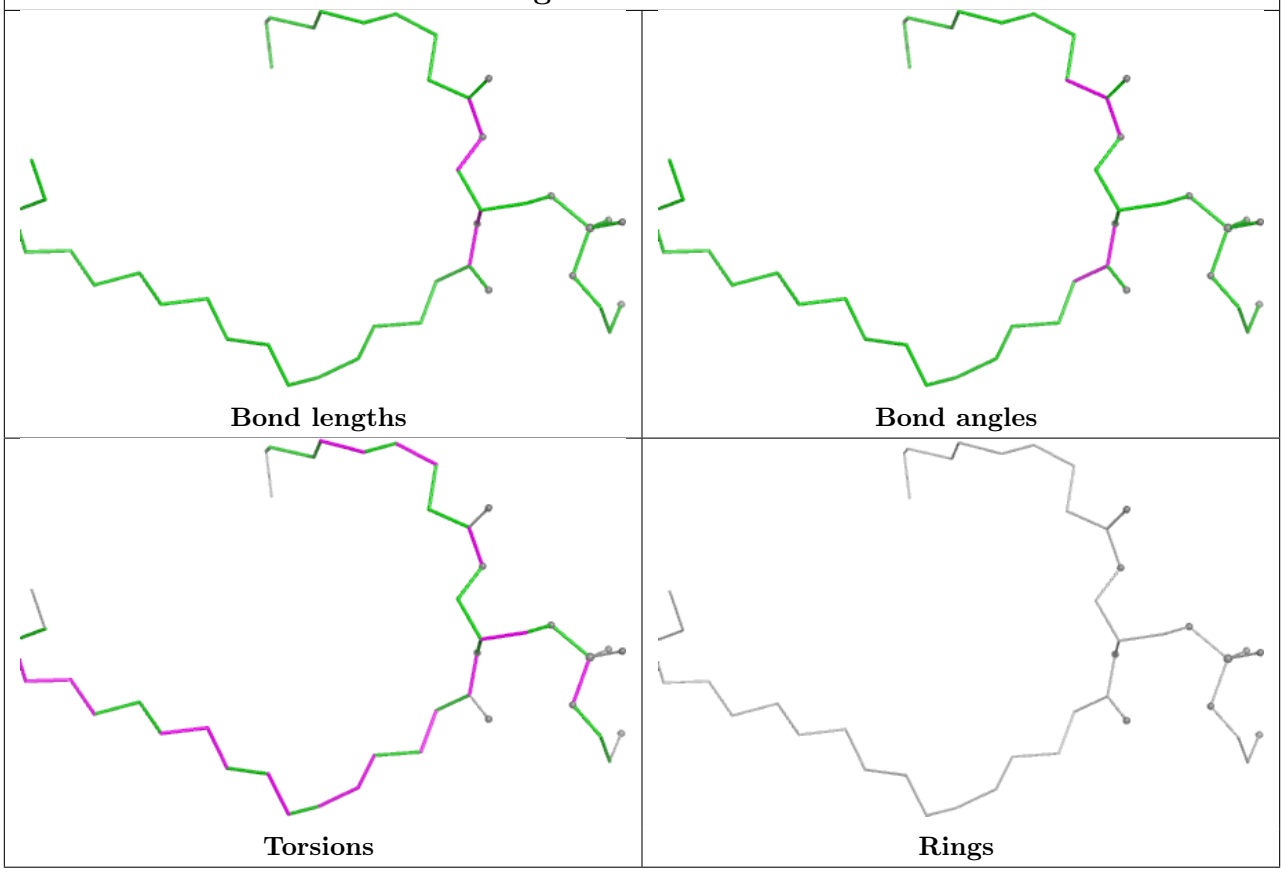

**Ligand 3PE 6 201**



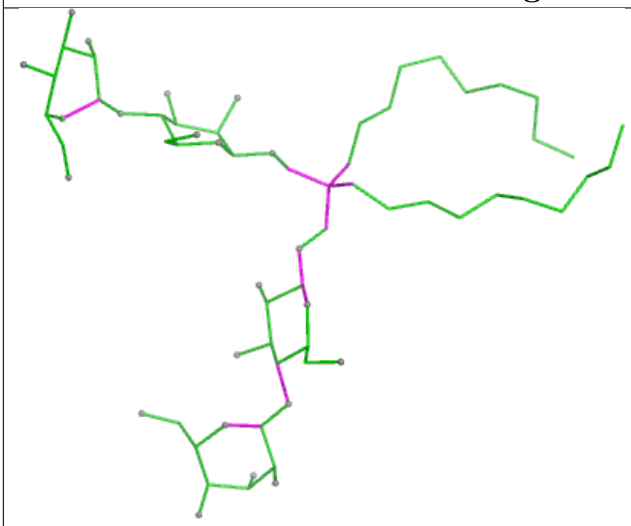
## Ligand FMN B 502



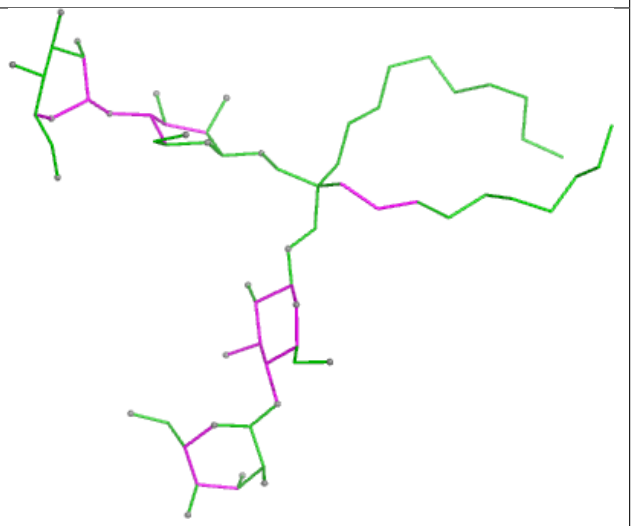

## Ligand 3PE 4 501



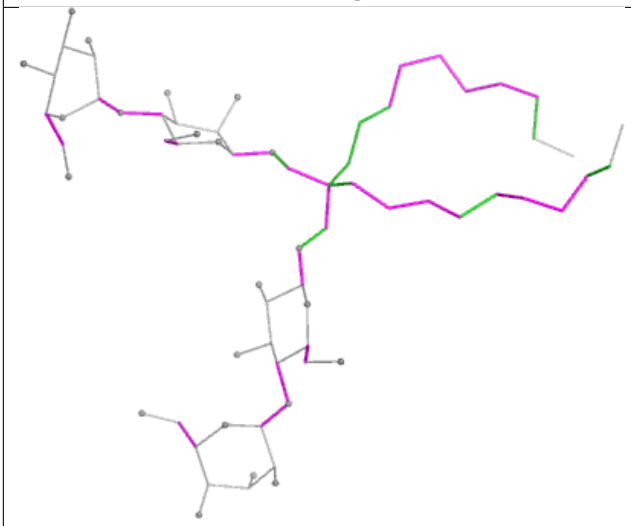
**Ligand LMN J 202**



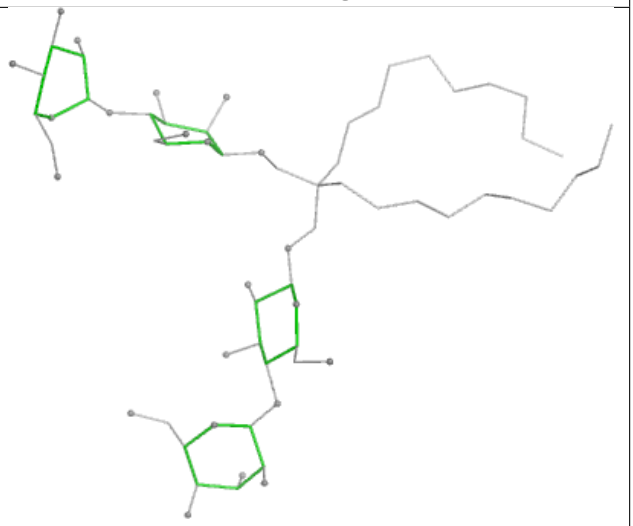
**Bond lengths**



**Bond angles**

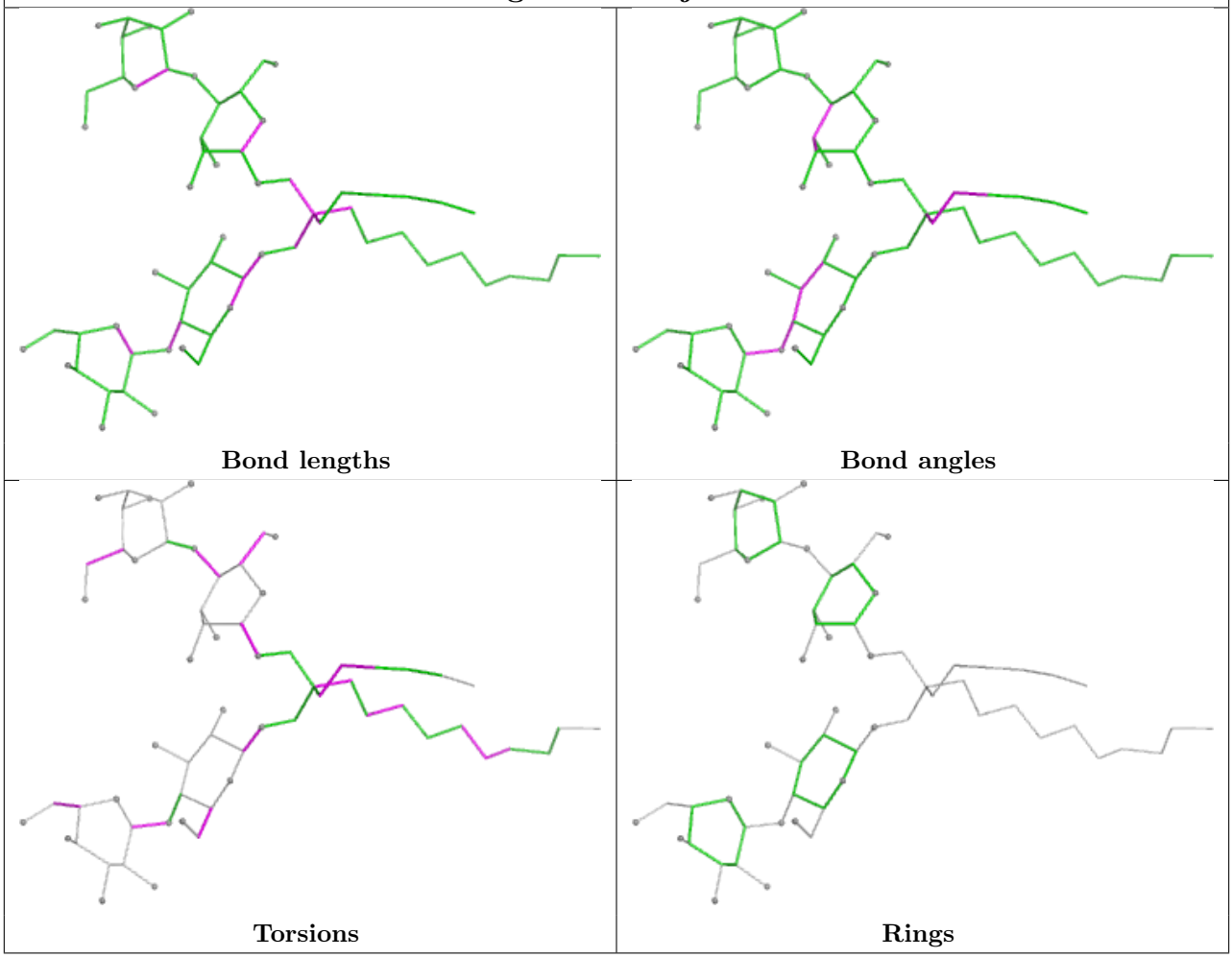


**Torsions**

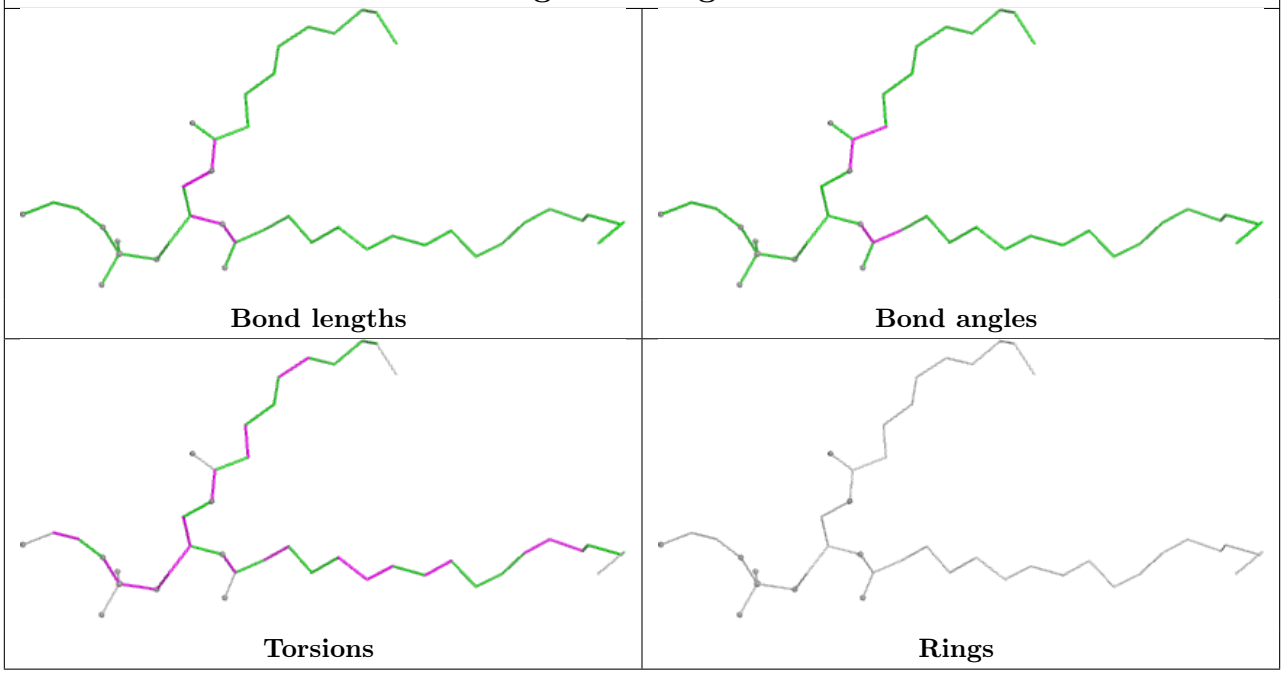


**Rings**

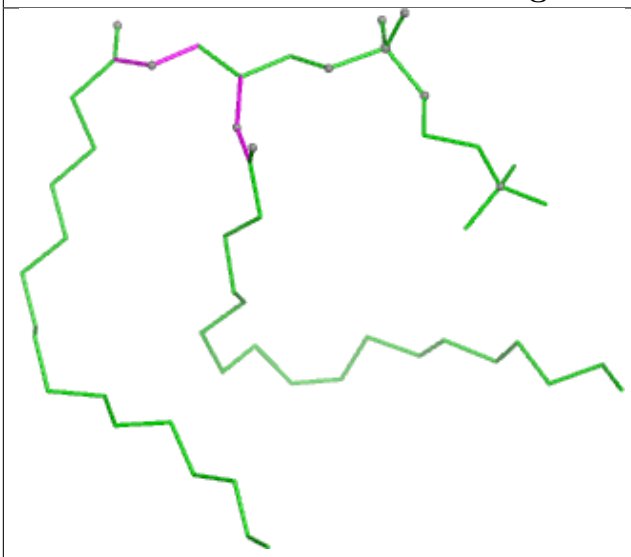
**Ligand LMN j 101**



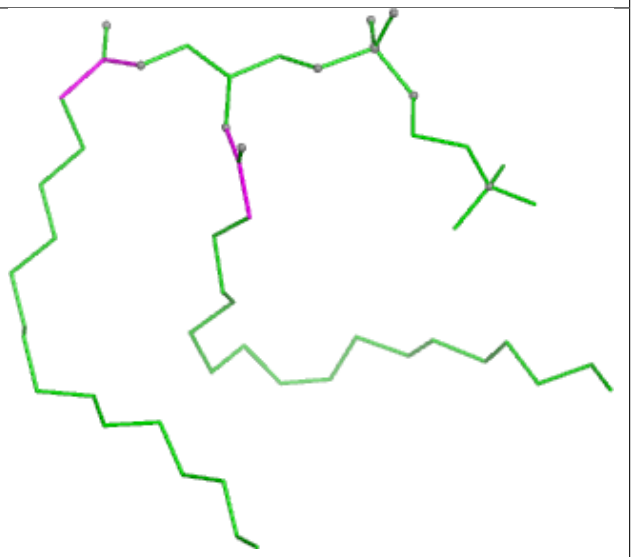

**Ligand 3PE g 202**



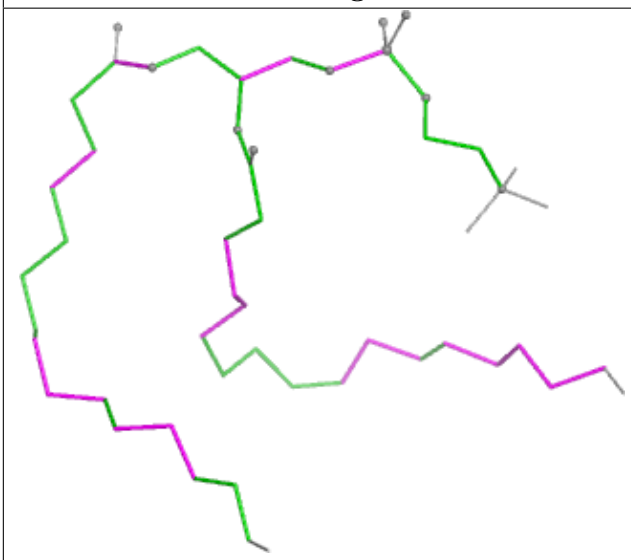
**Ligand CPL 2 502**



**Bond lengths**



**Bond angles**

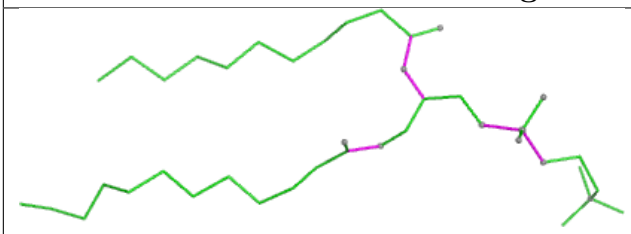


**Torsions**

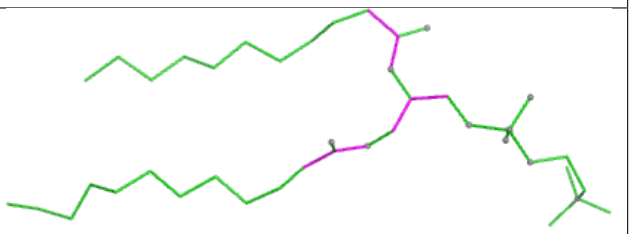


**Rings**

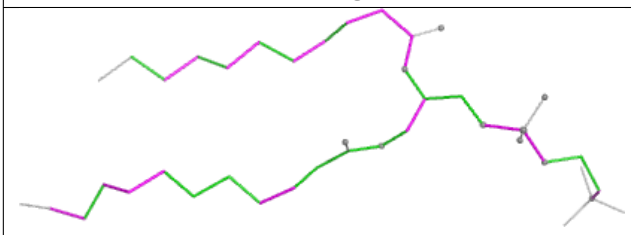
**Ligand PLC W 401**



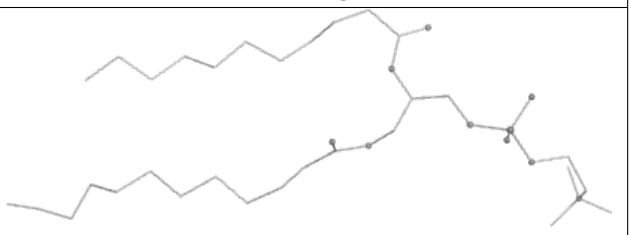
Bond lengths



Bond angles

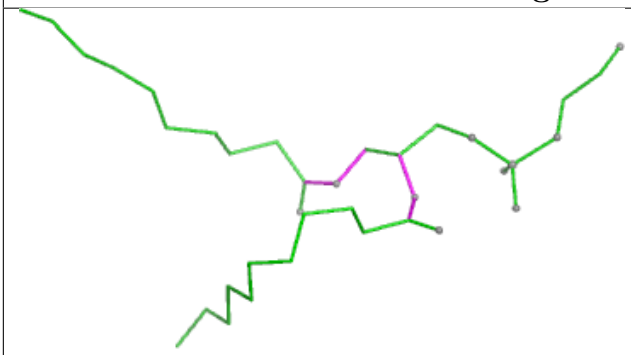


Torsions

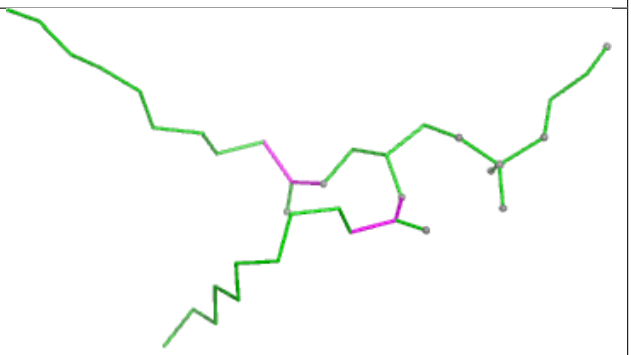


Rings

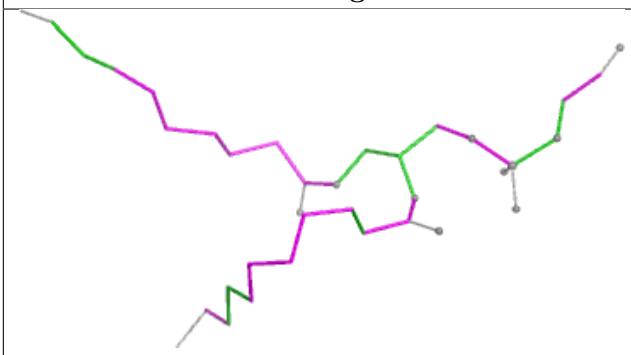
**Ligand 3PE 1 503**



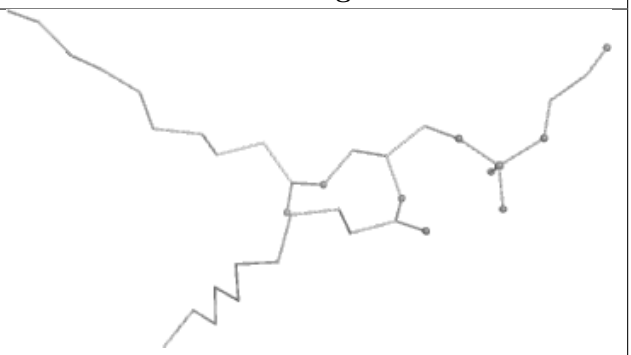
Bond lengths



Bond angles

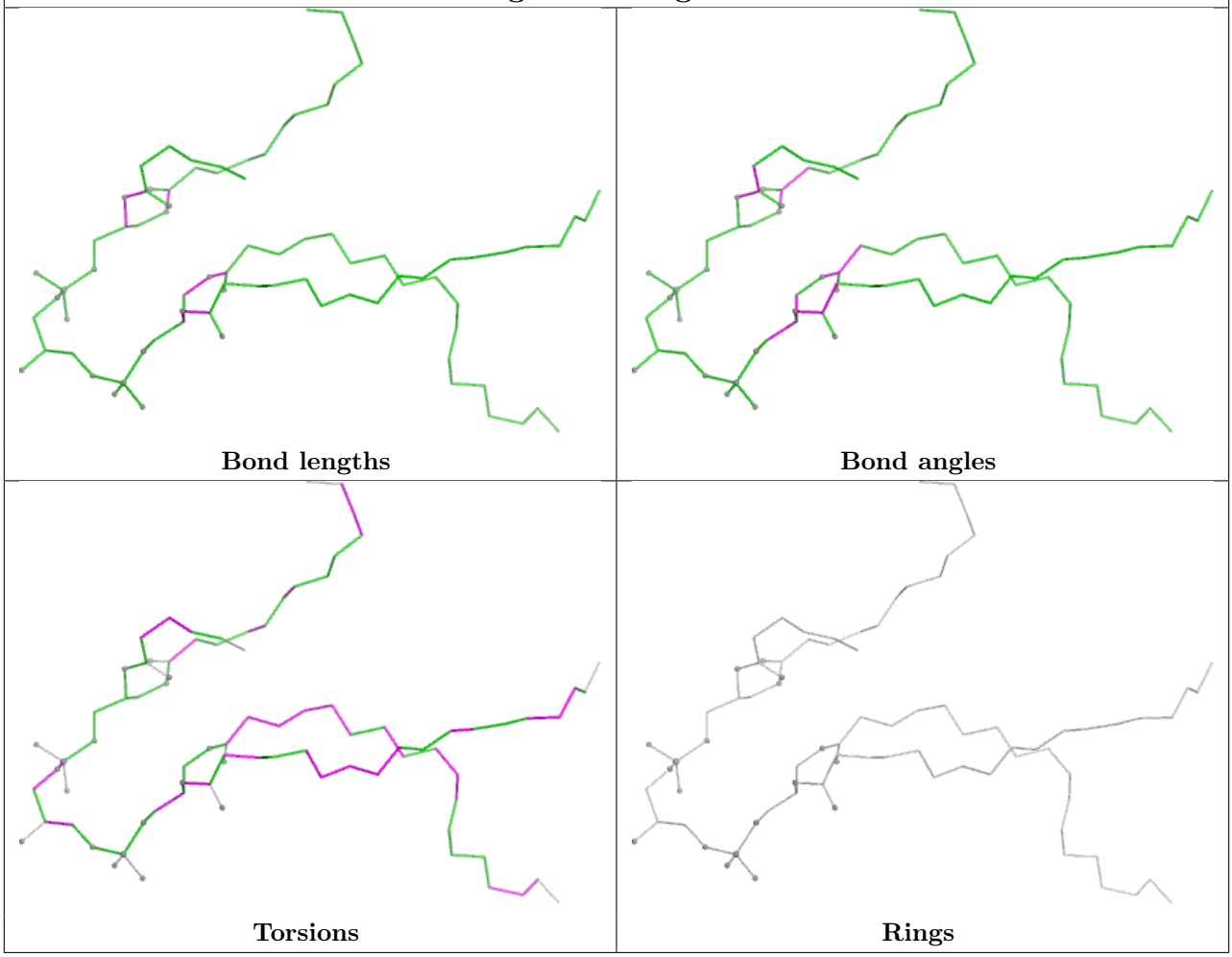


Torsions

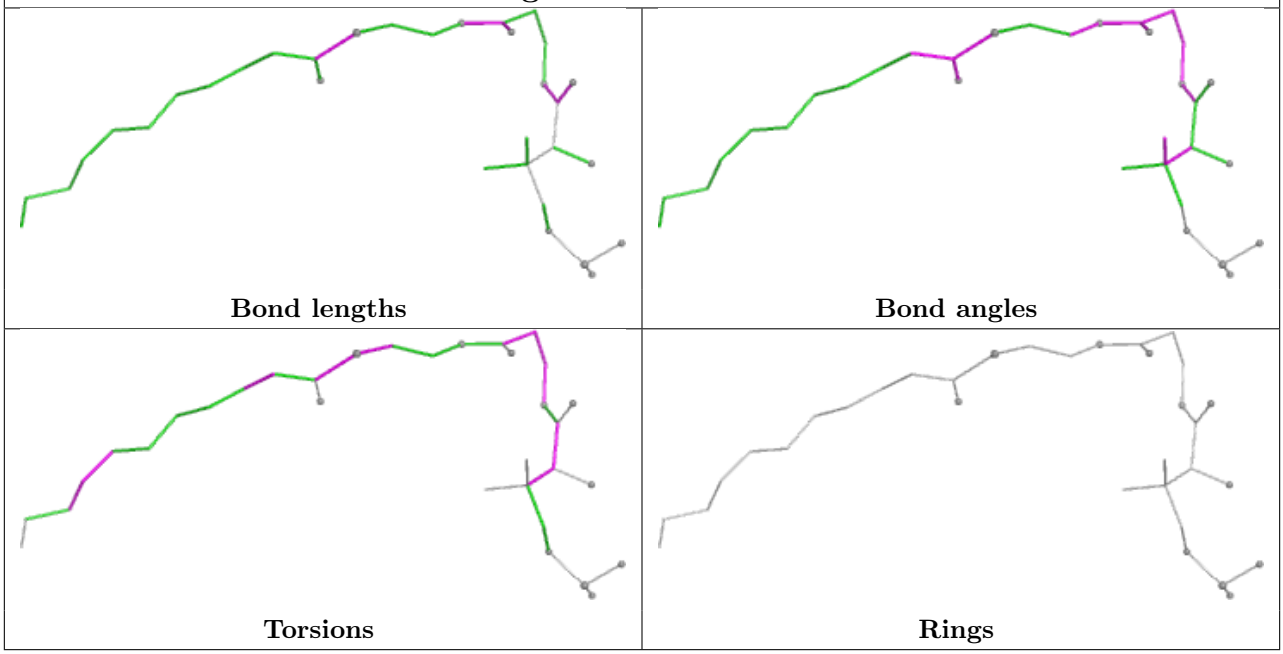


Rings

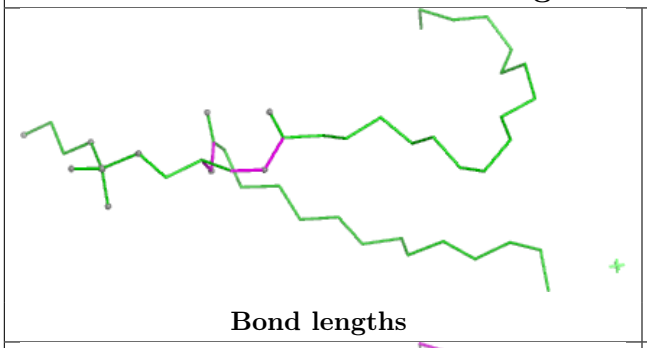
**Ligand CDL g 201**



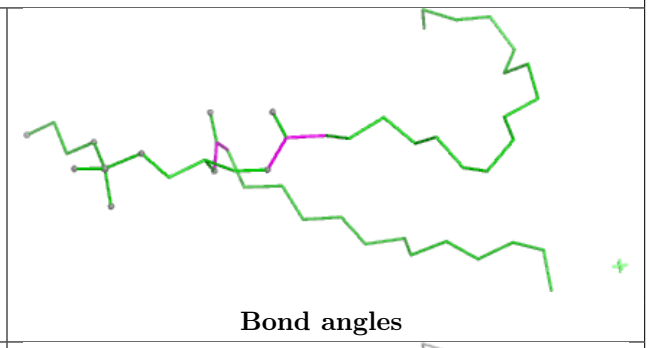

**Ligand ZMP O 201**



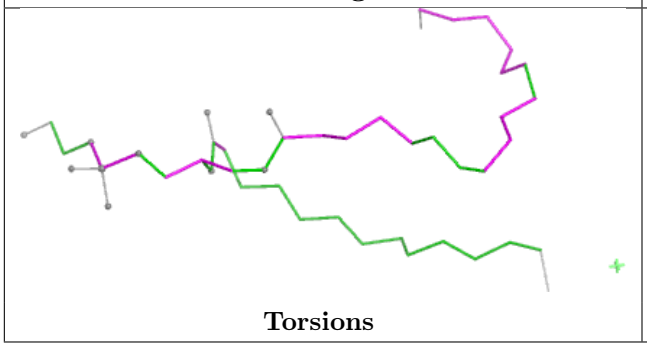
**Ligand 3PE 6 202**



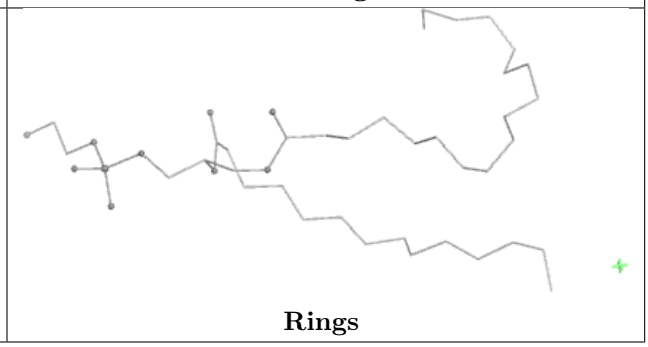
Bond lengths



Bond angles

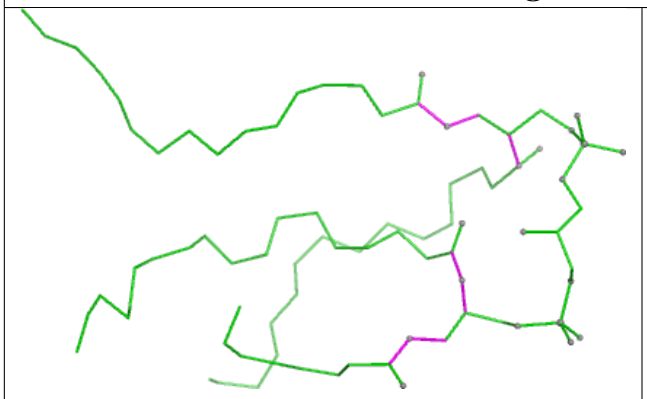


Torsions

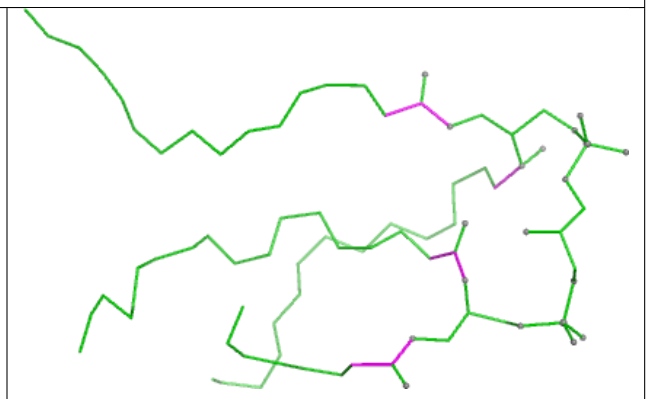


Rings

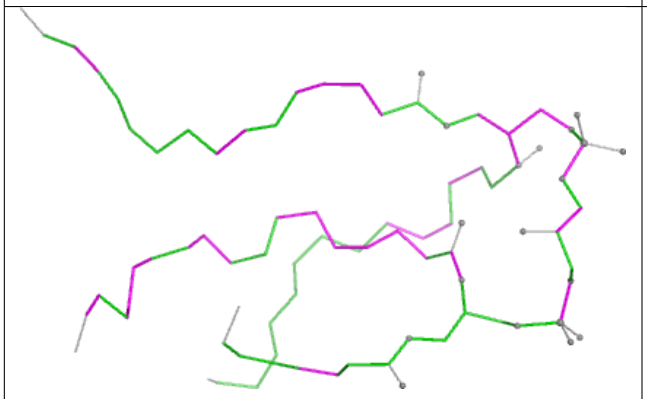
**Ligand CDL X 201**



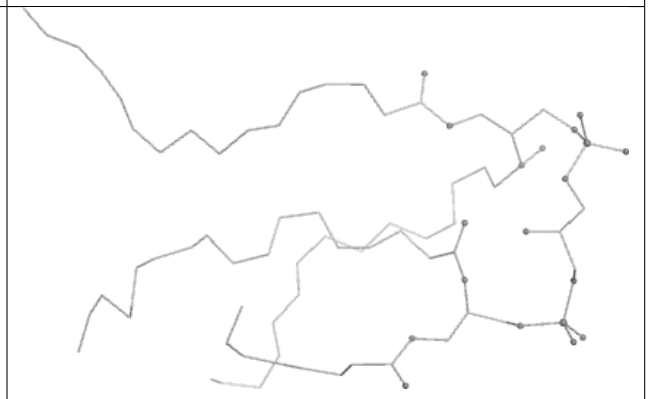
Bond lengths



Bond angles

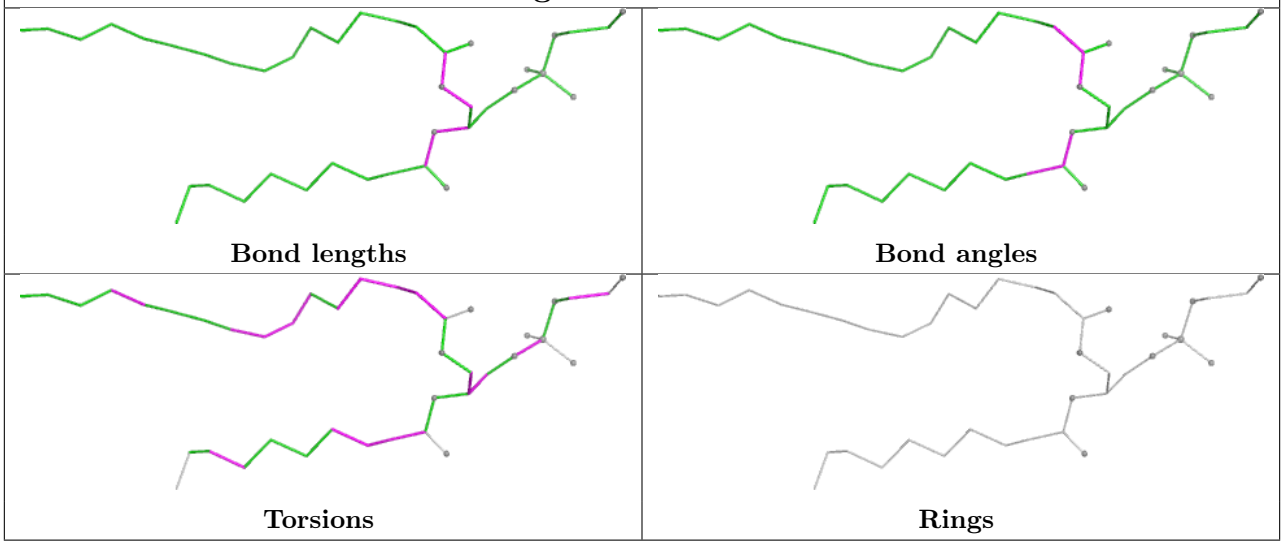


Torsions

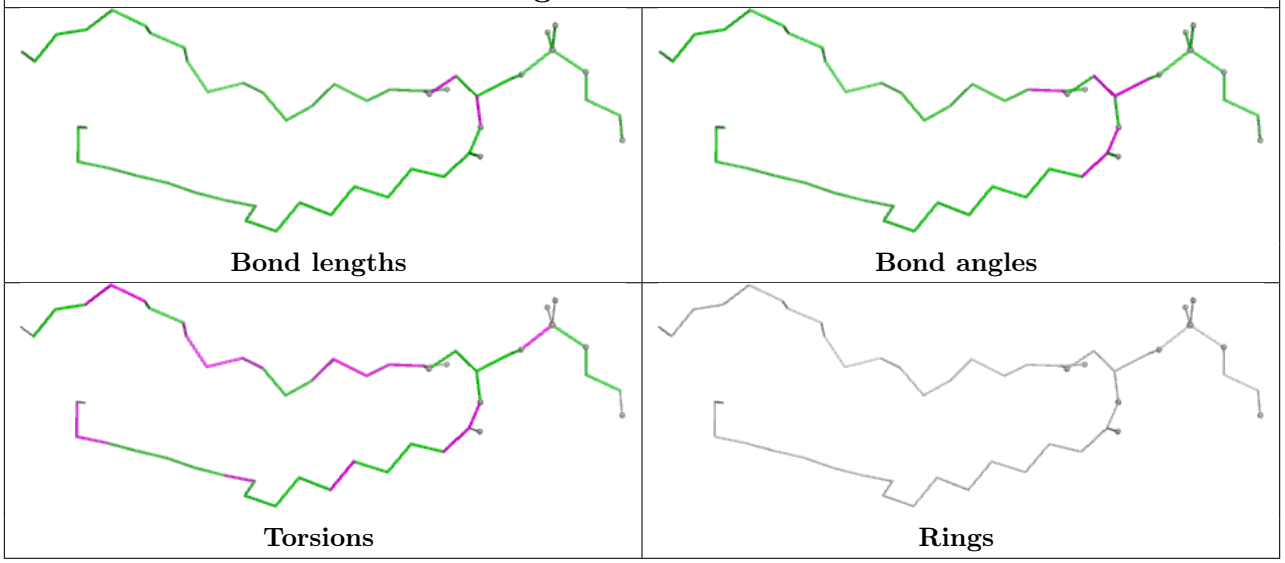


Rings

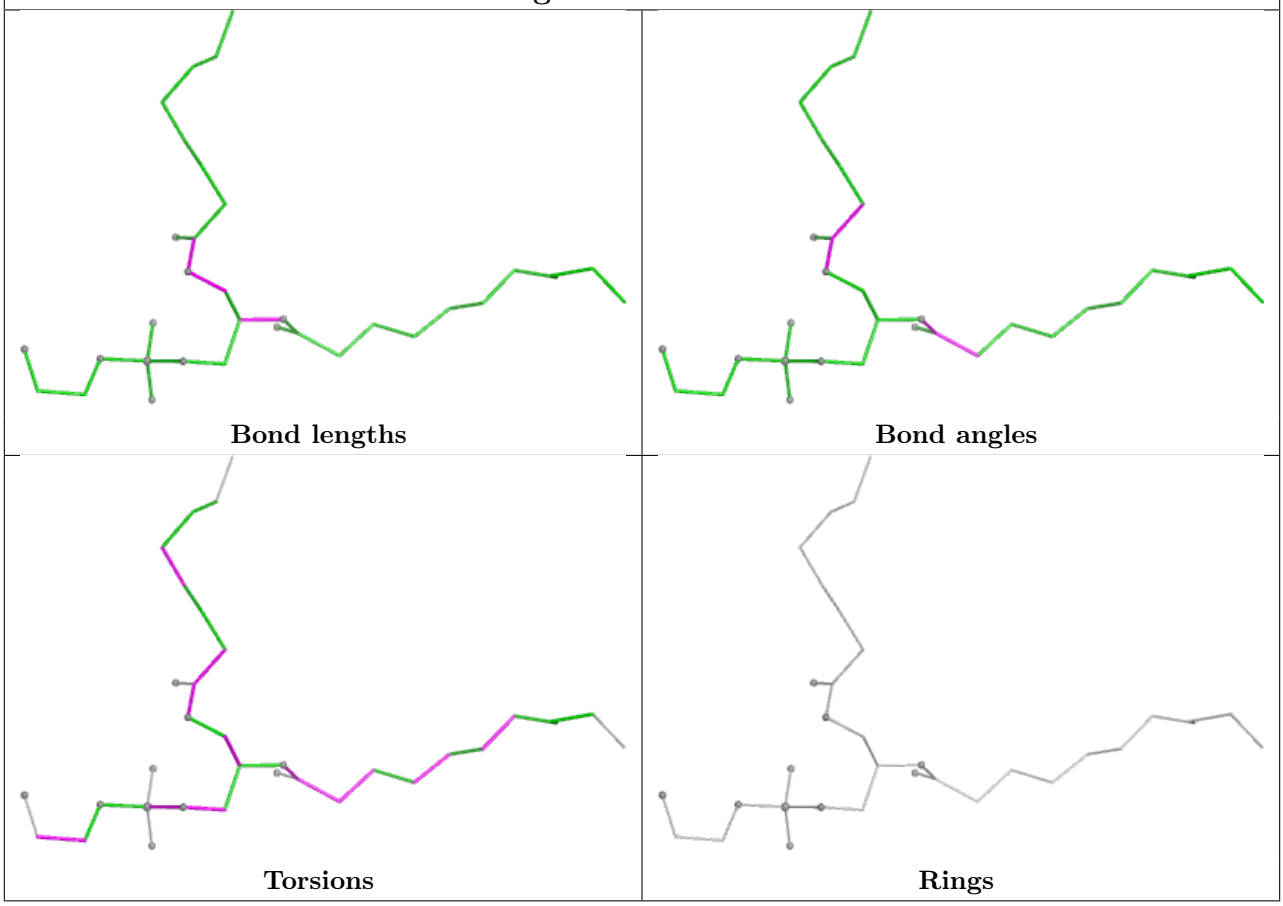
**Ligand 3PE 4 502**



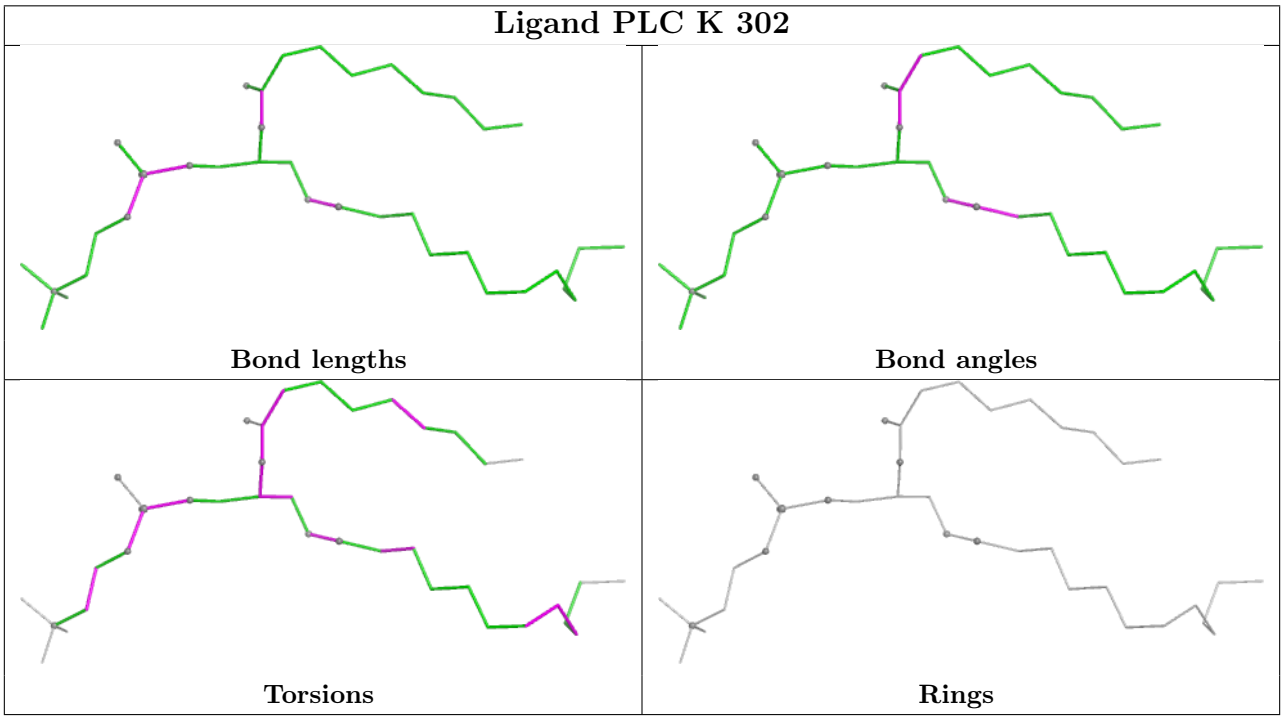

**Ligand 3PE 4 503**



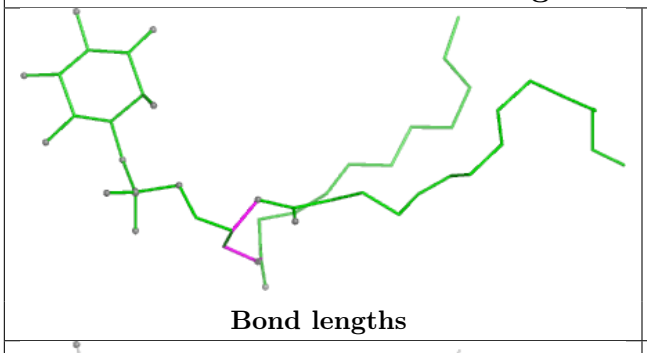
**Ligand 3PE J 204**



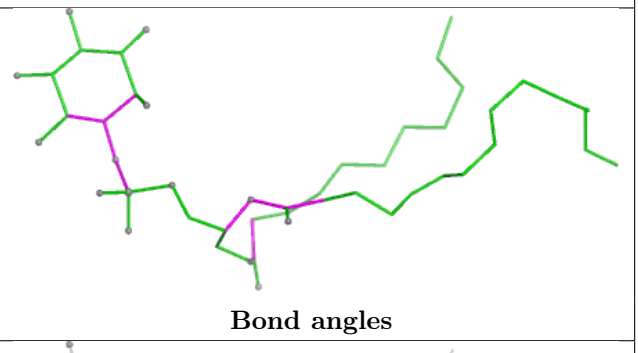

**Ligand PLC K 302**



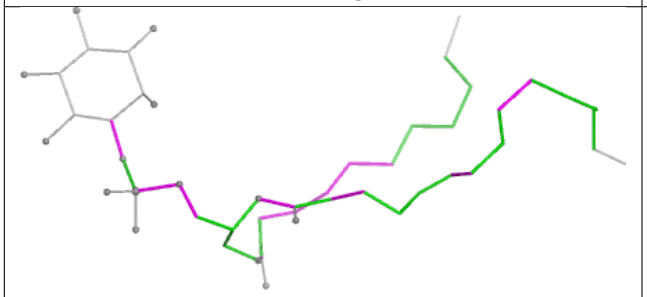
**Ligand T7X 3 201**



Bond lengths



Bond angles

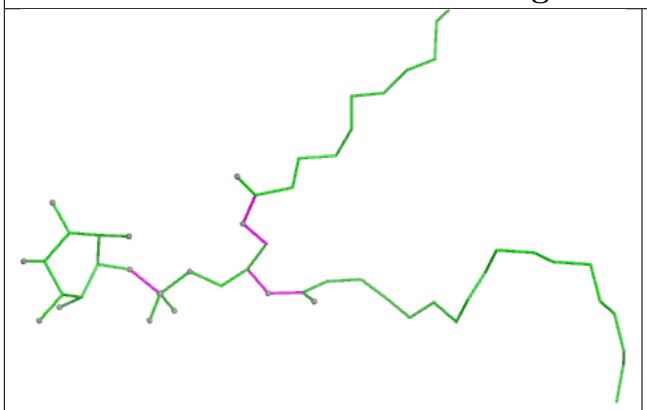


Torsions

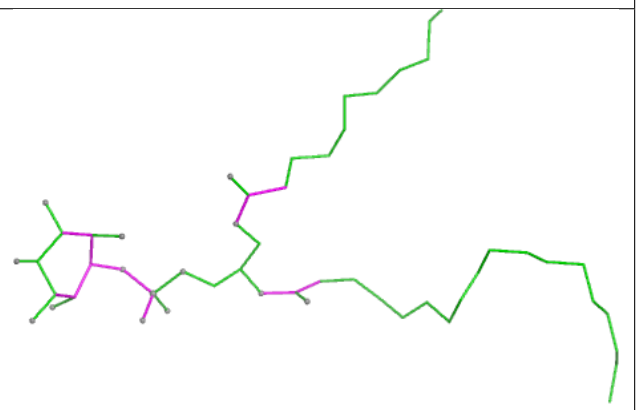


Rings

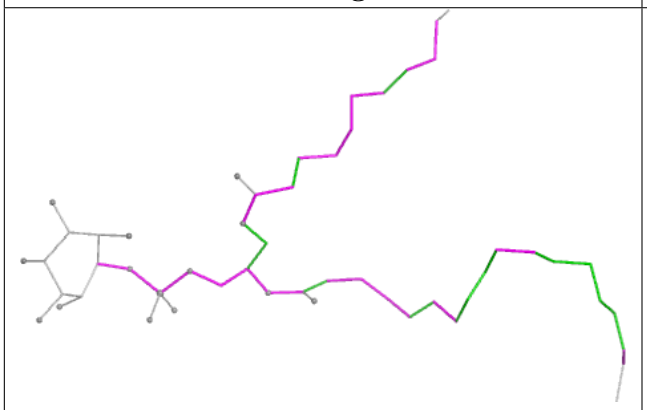
**Ligand T7X 2 503**



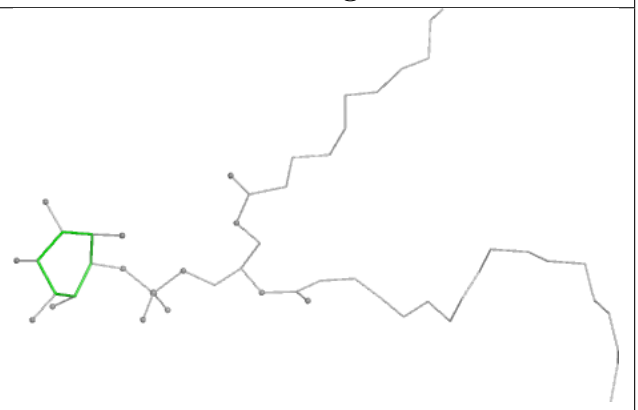
Bond lengths



Bond angles

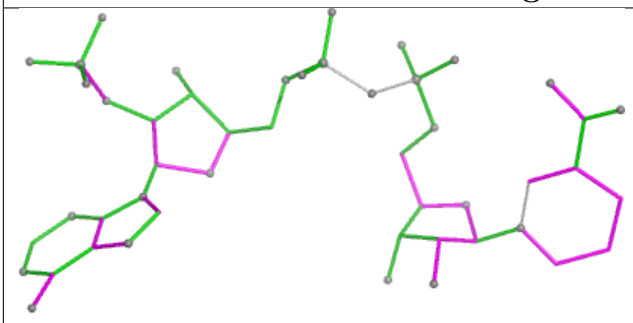


Torsions

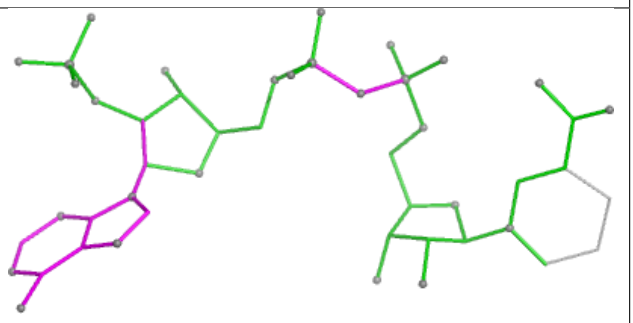


Rings

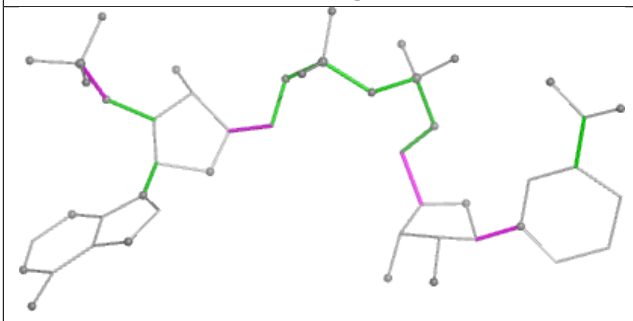
## Ligand NDP E 400



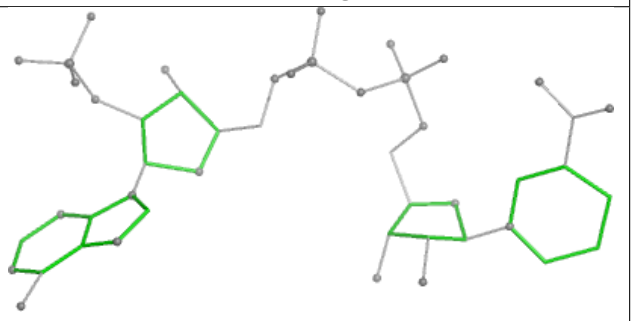
Bond lengths



Bond angles

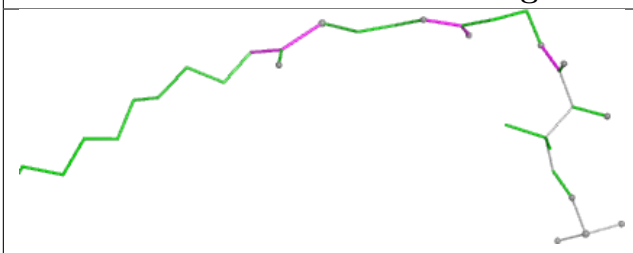


Torsions

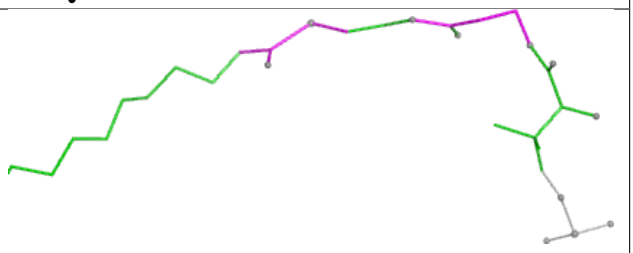


Rings

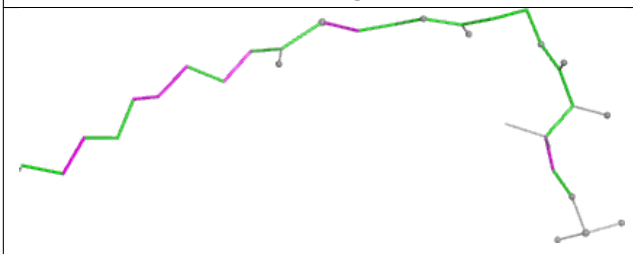
## Ligand ZMP Q 201



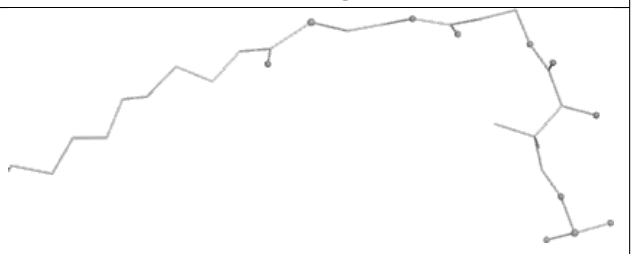
Bond lengths



Bond angles

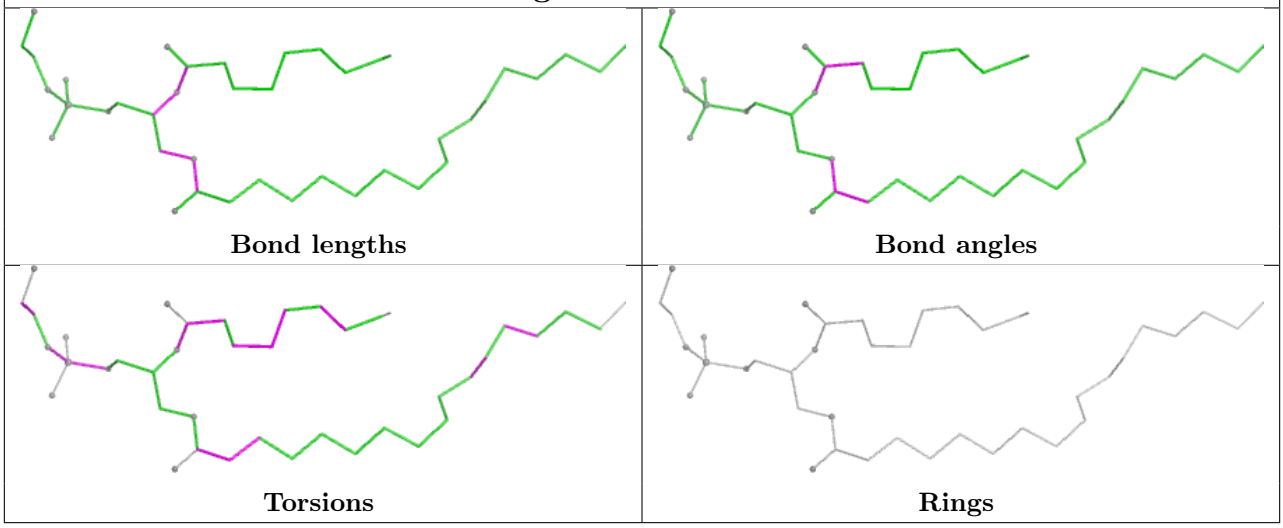


Torsions

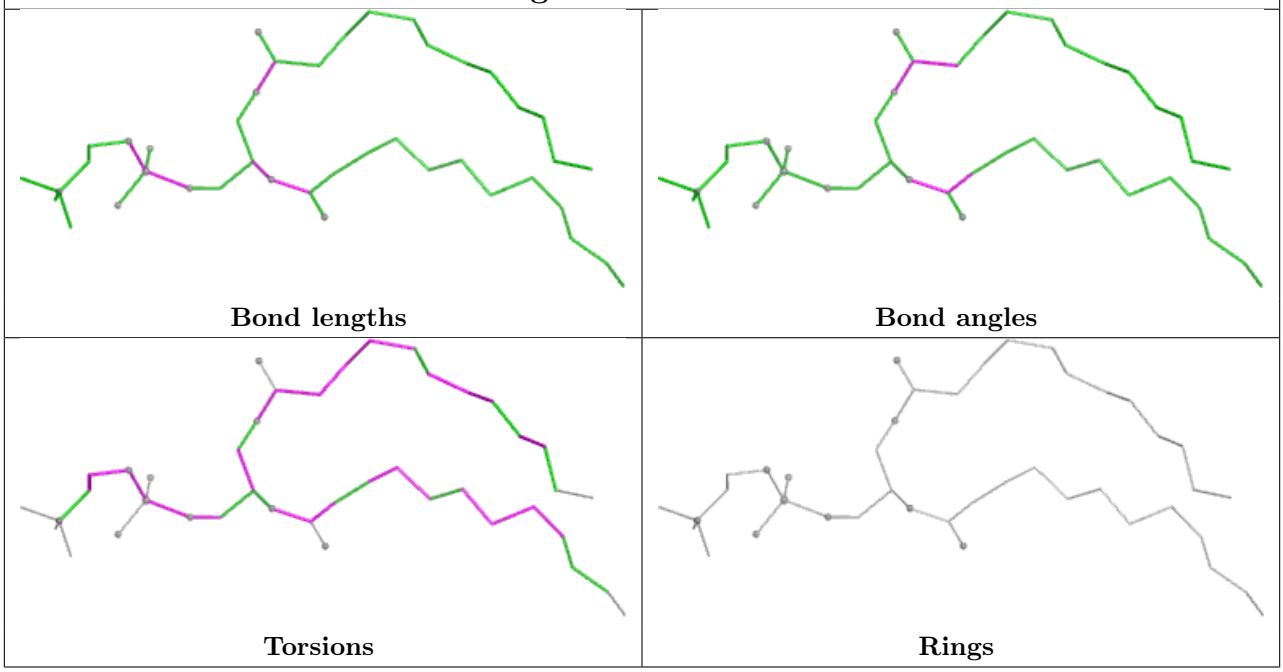


Rings

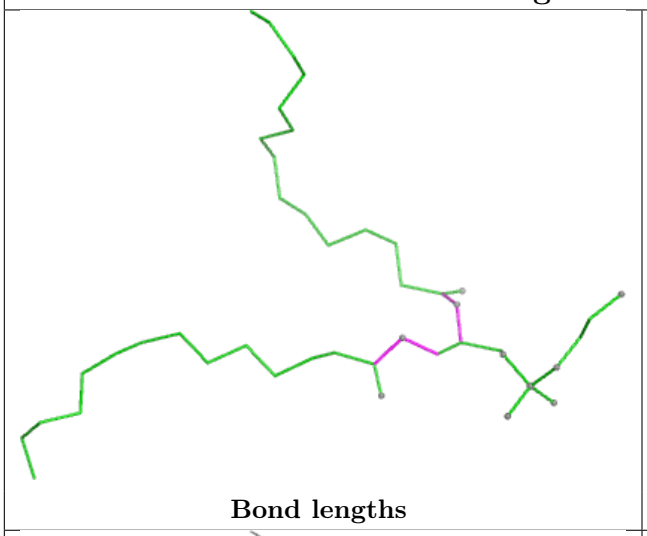
**Ligand 3PE J 201**



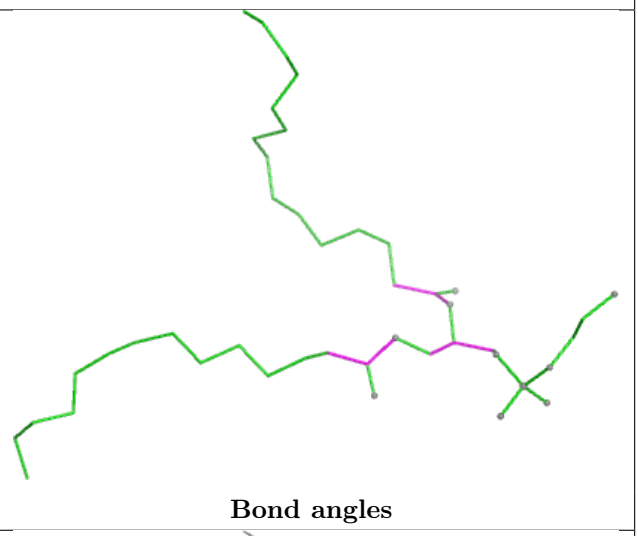

**Ligand PLC 1 505**



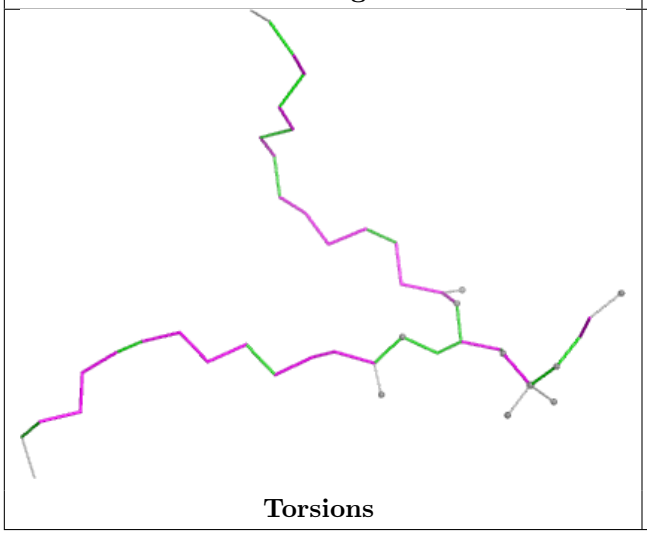
**Ligand 3PE J 203**



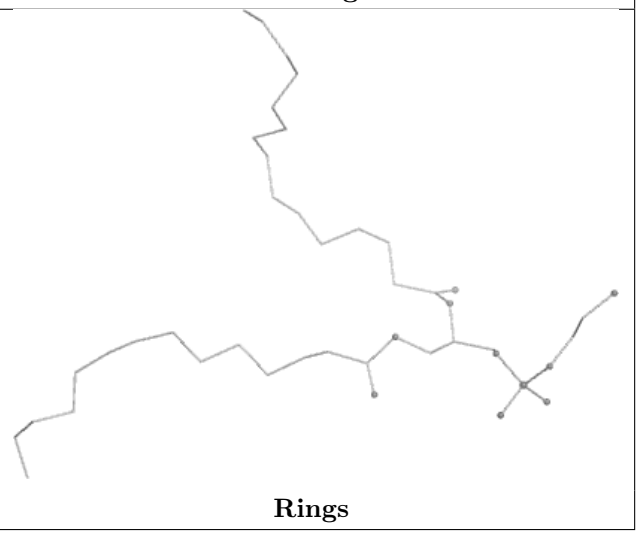
**Bond lengths**



**Bond angles**

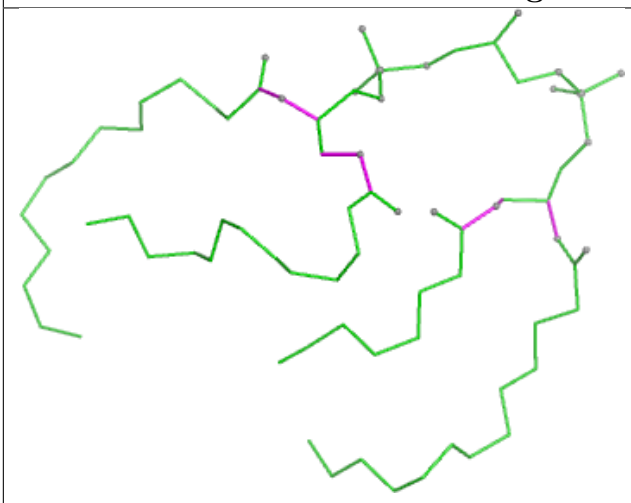


**Torsions**

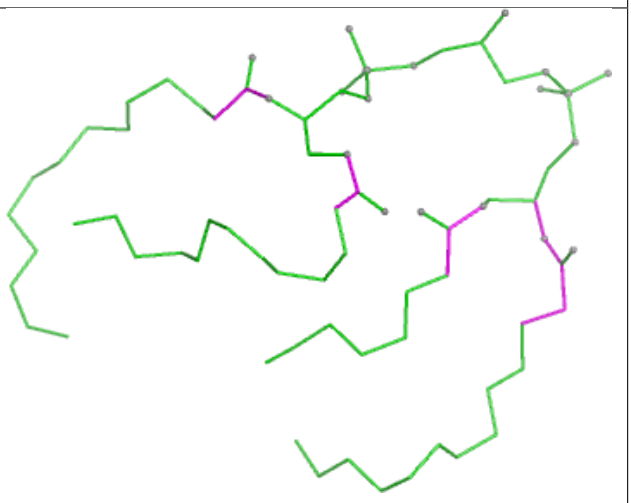


**Rings**

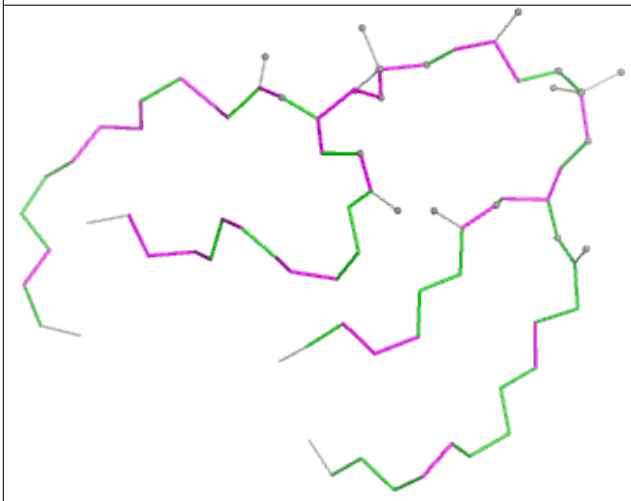
**Ligand CDL Z 201**



**Bond lengths**



**Bond angles**

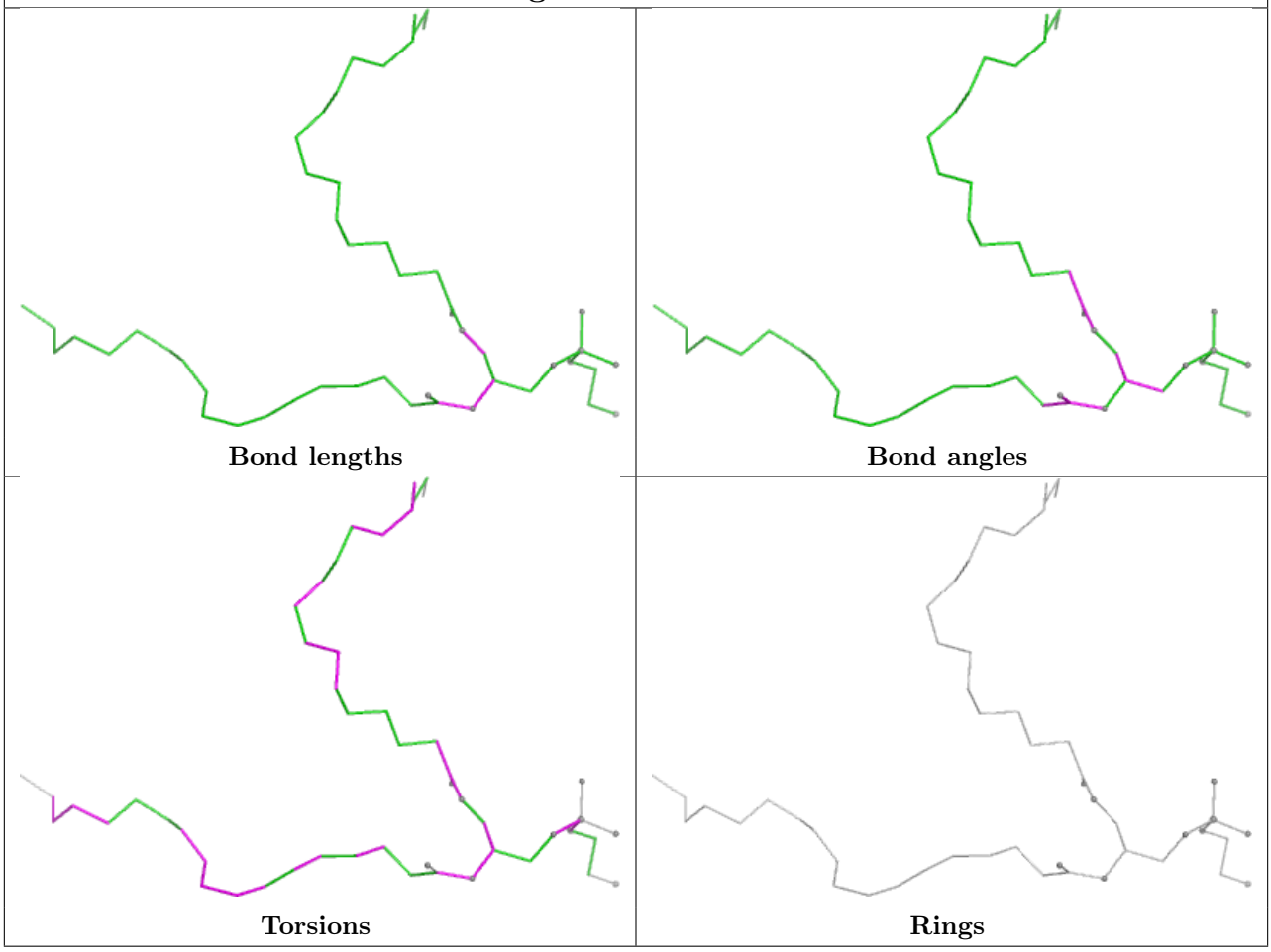


**Torsions**

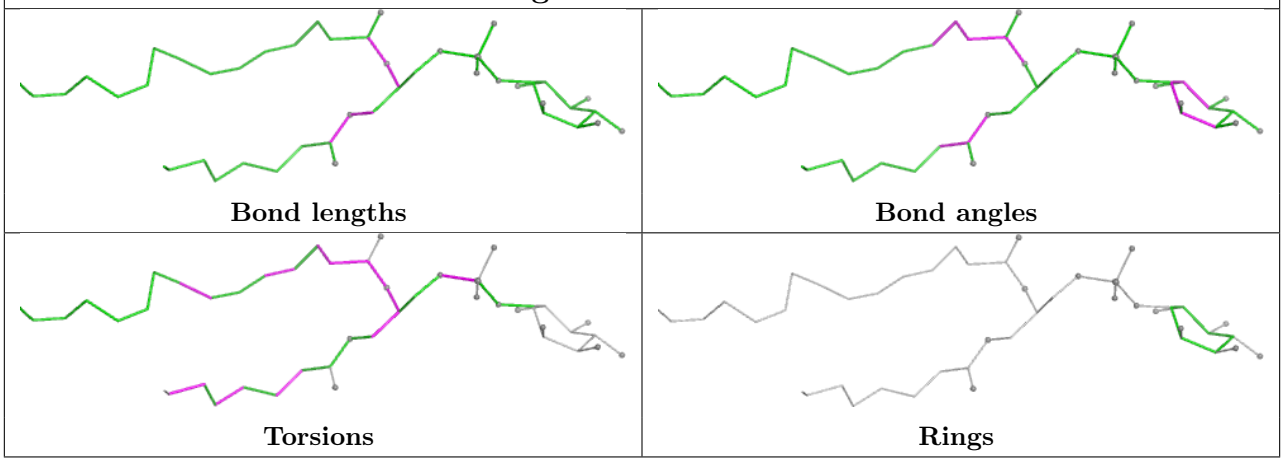


**Rings**

**Ligand 3PE 1 501**




**Ligand T7X 2 501**



**Ligand CDL n 200**



**Bond lengths**



**Bond angles**

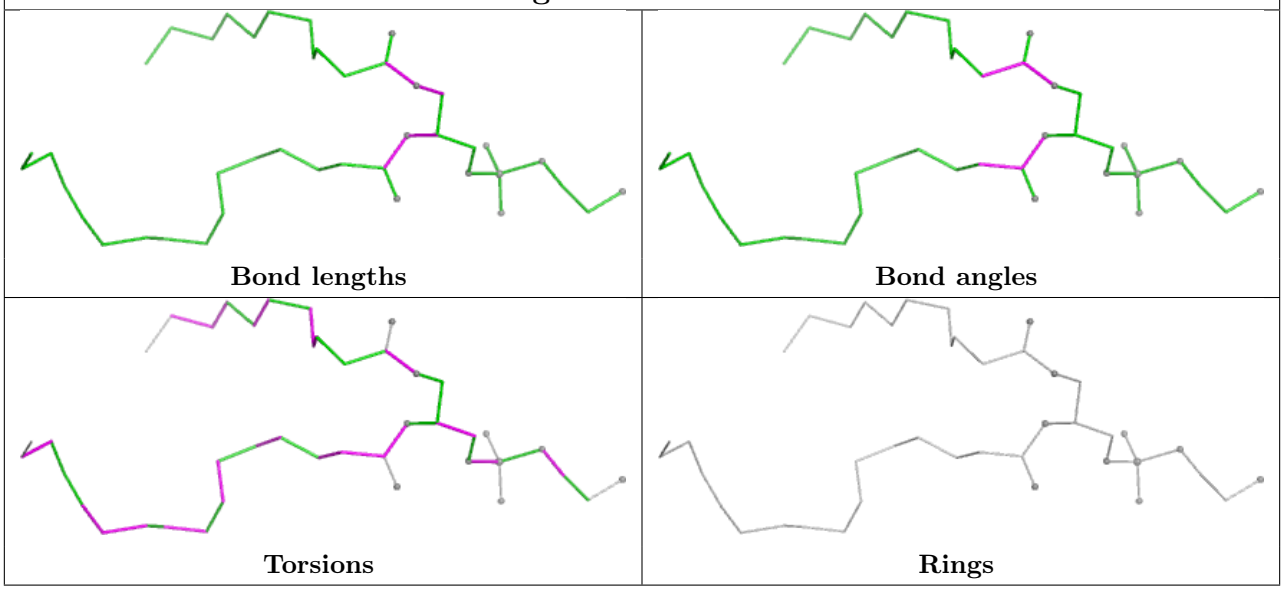


**Torsions**

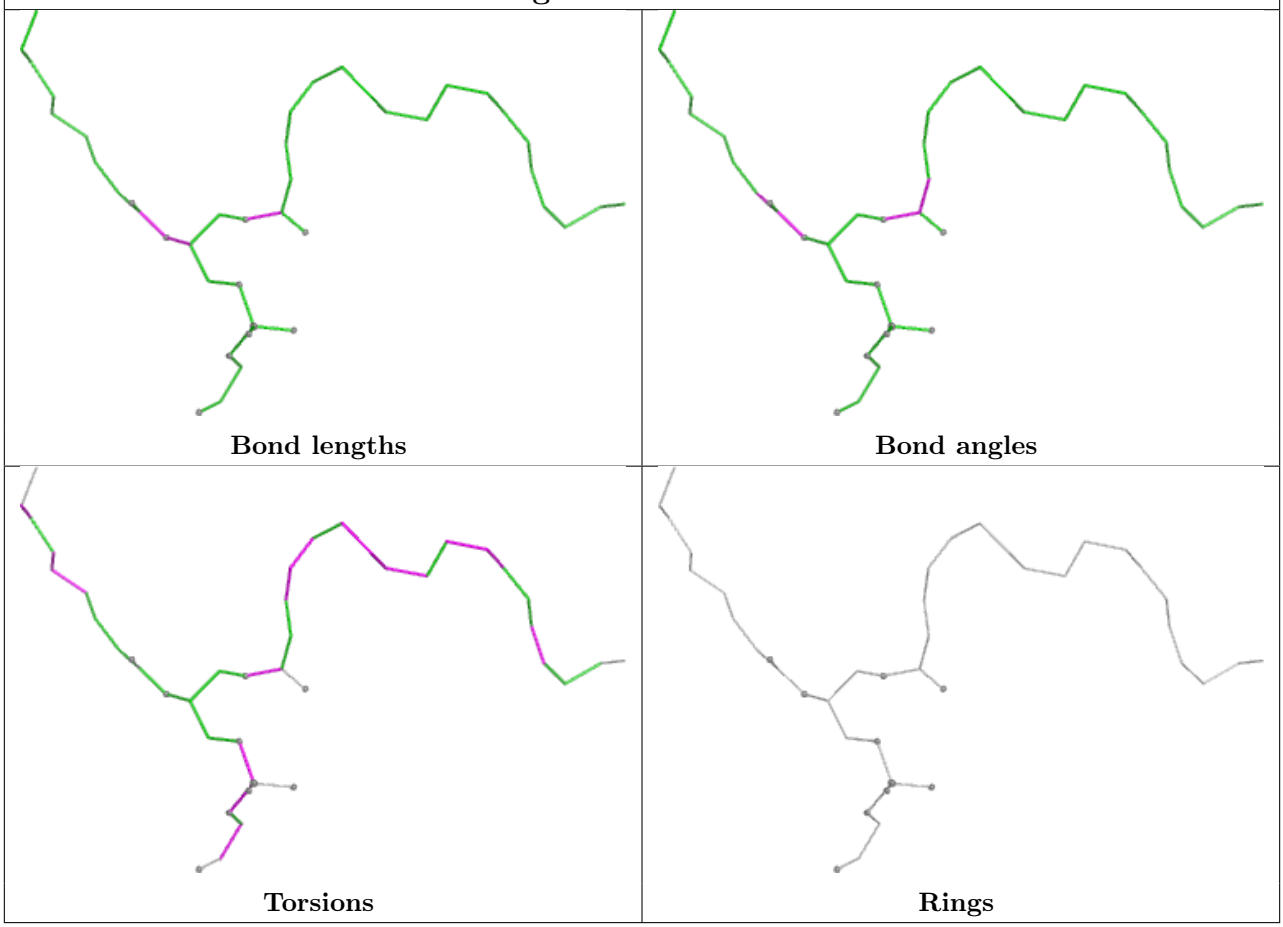


**Rings**

**Ligand 3PE b 201**




**Ligand 3PE S 501**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

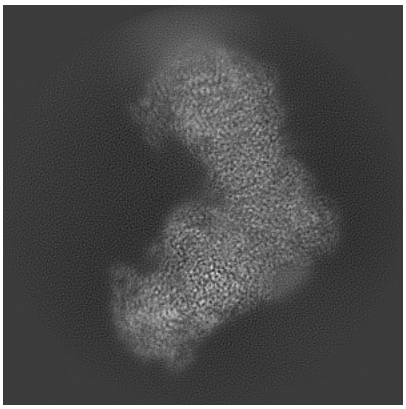
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12742. These allow visual inspection of the internal detail of the map and identification of artifacts.

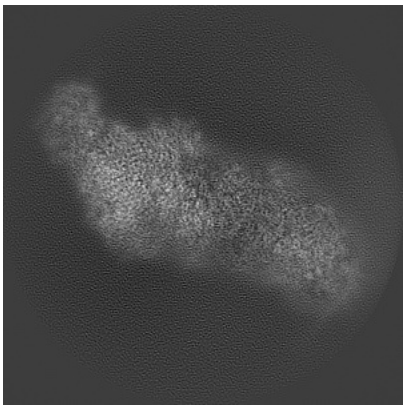
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

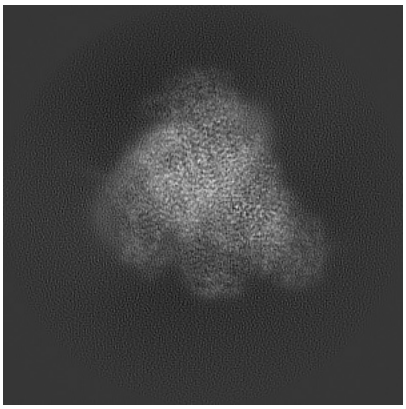
### 6.1.1 Primary map



X

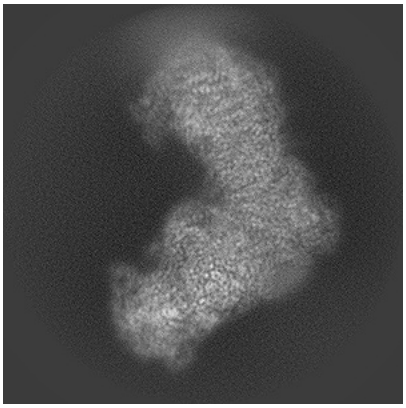


Y

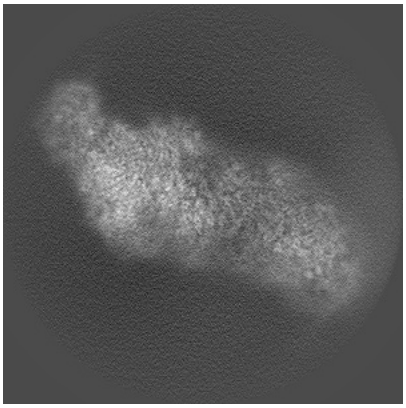


Z

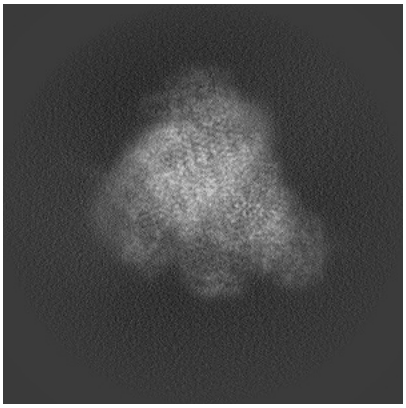
### 6.1.2 Raw map



X



Y

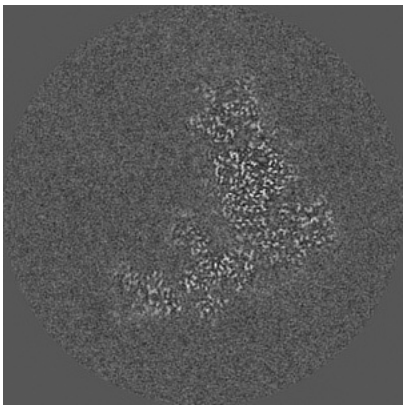


Z

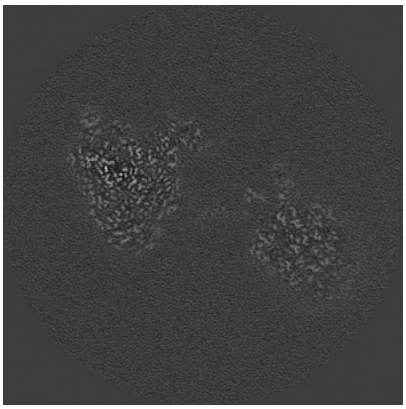
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

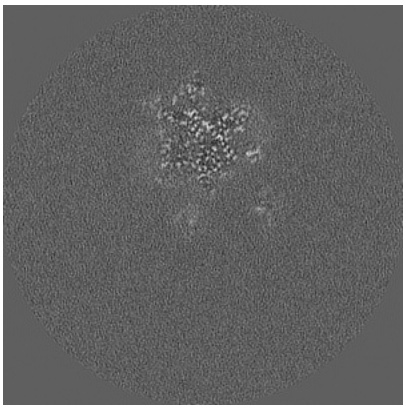
### 6.2.1 Primary map



X Index: 300

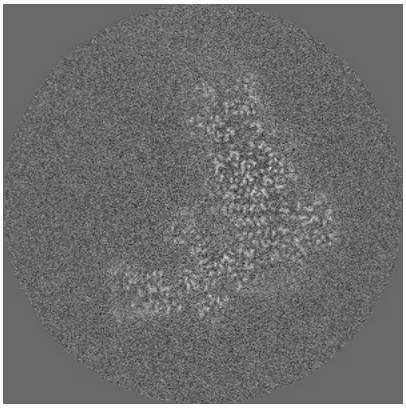


Y Index: 300

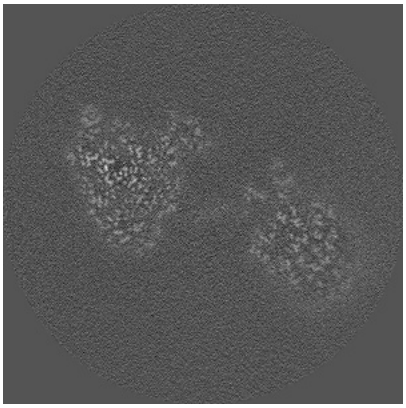


Z Index: 300

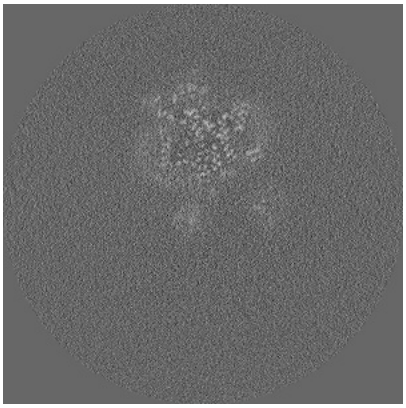
### 6.2.2 Raw map



X Index: 300



Y Index: 300

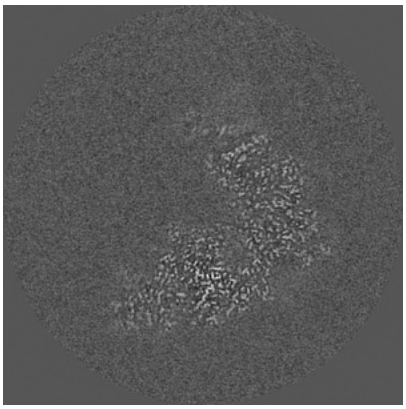


Z Index: 300

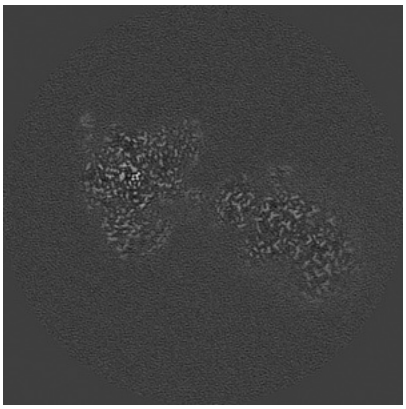
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

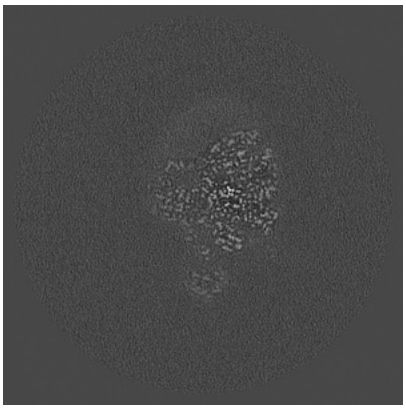
### 6.3.1 Primary map



X Index: 332

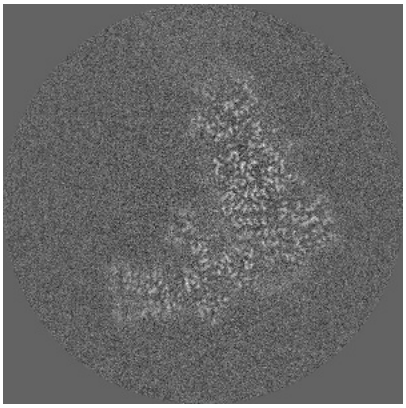


Y Index: 319

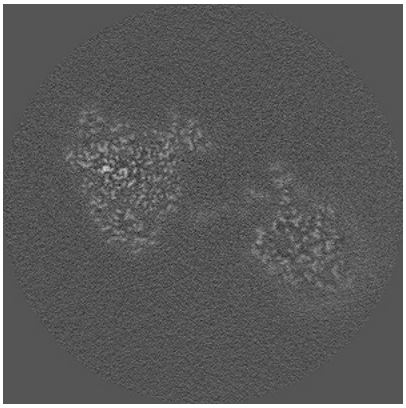


Z Index: 197

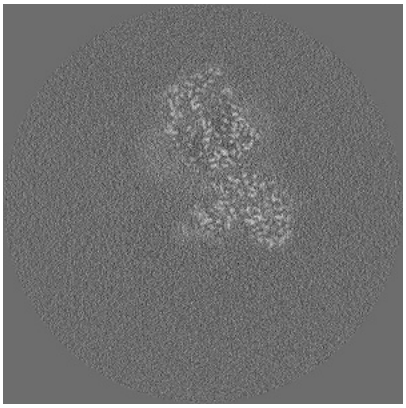
### 6.3.2 Raw map



X Index: 301



Y Index: 298

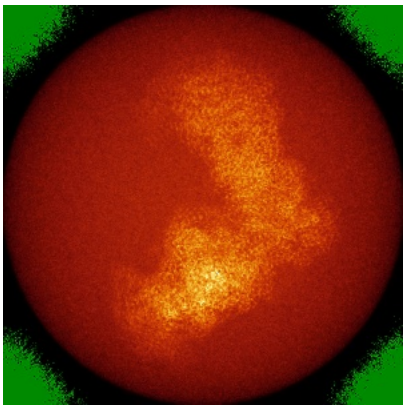


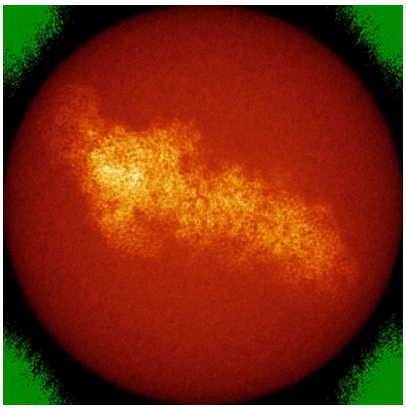
Z Index: 261

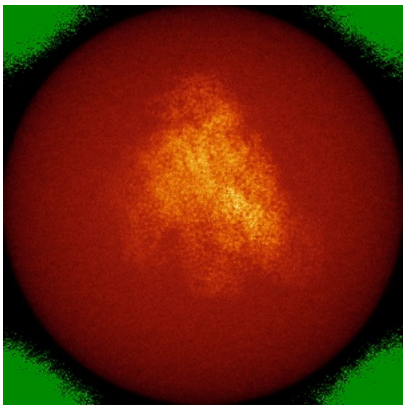
The images above show the largest variance slices of the map in three orthogonal directions.

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

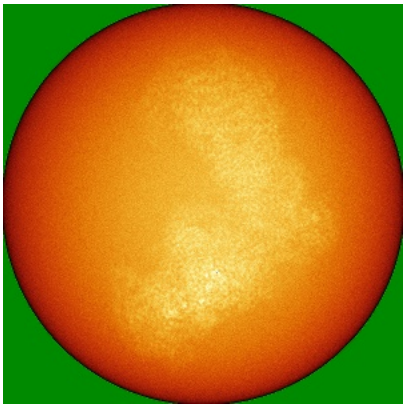
### 6.4.1 Primary map

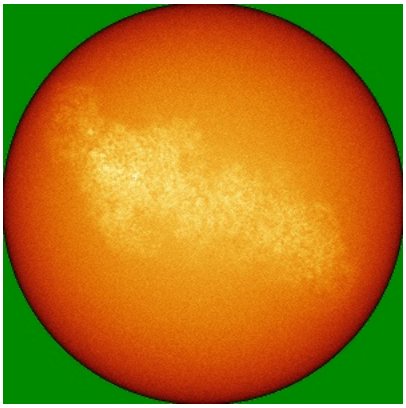

X

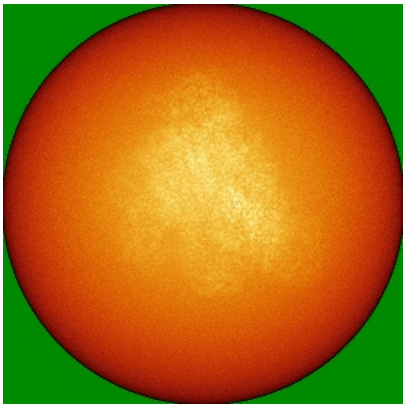

Y


Z

### 6.4.2 Raw map


X


Y


Z

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

## 6.5 Orthogonal surface views (i)

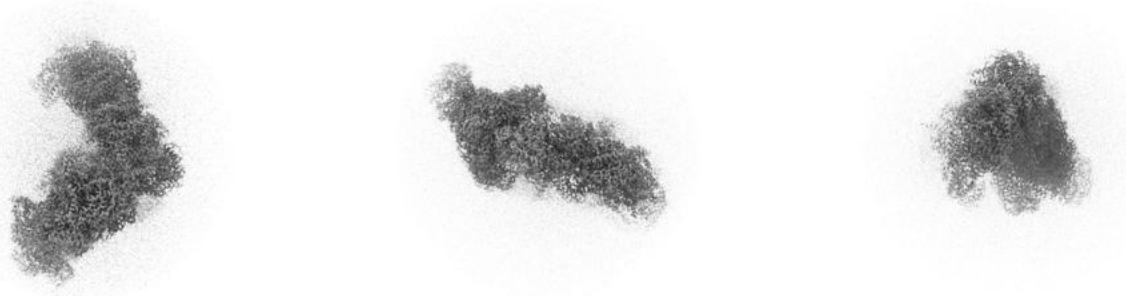
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. 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



X Y Z

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.

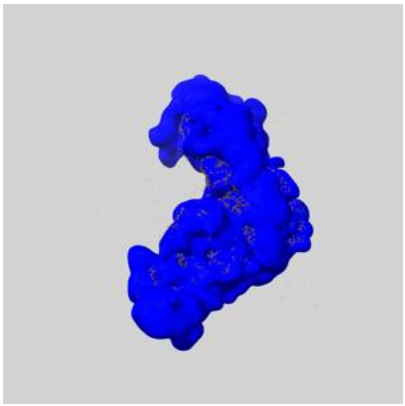
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

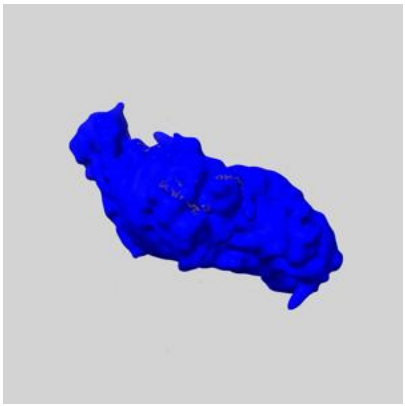
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

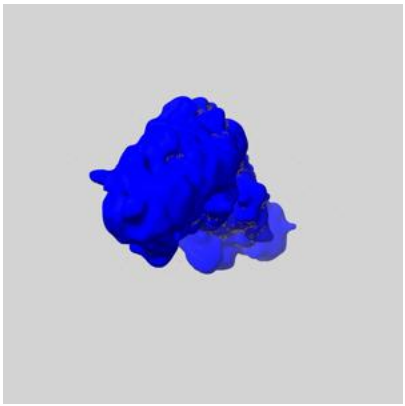
### 6.6.1 emd_12742_msk_1.map (i)



X



Y

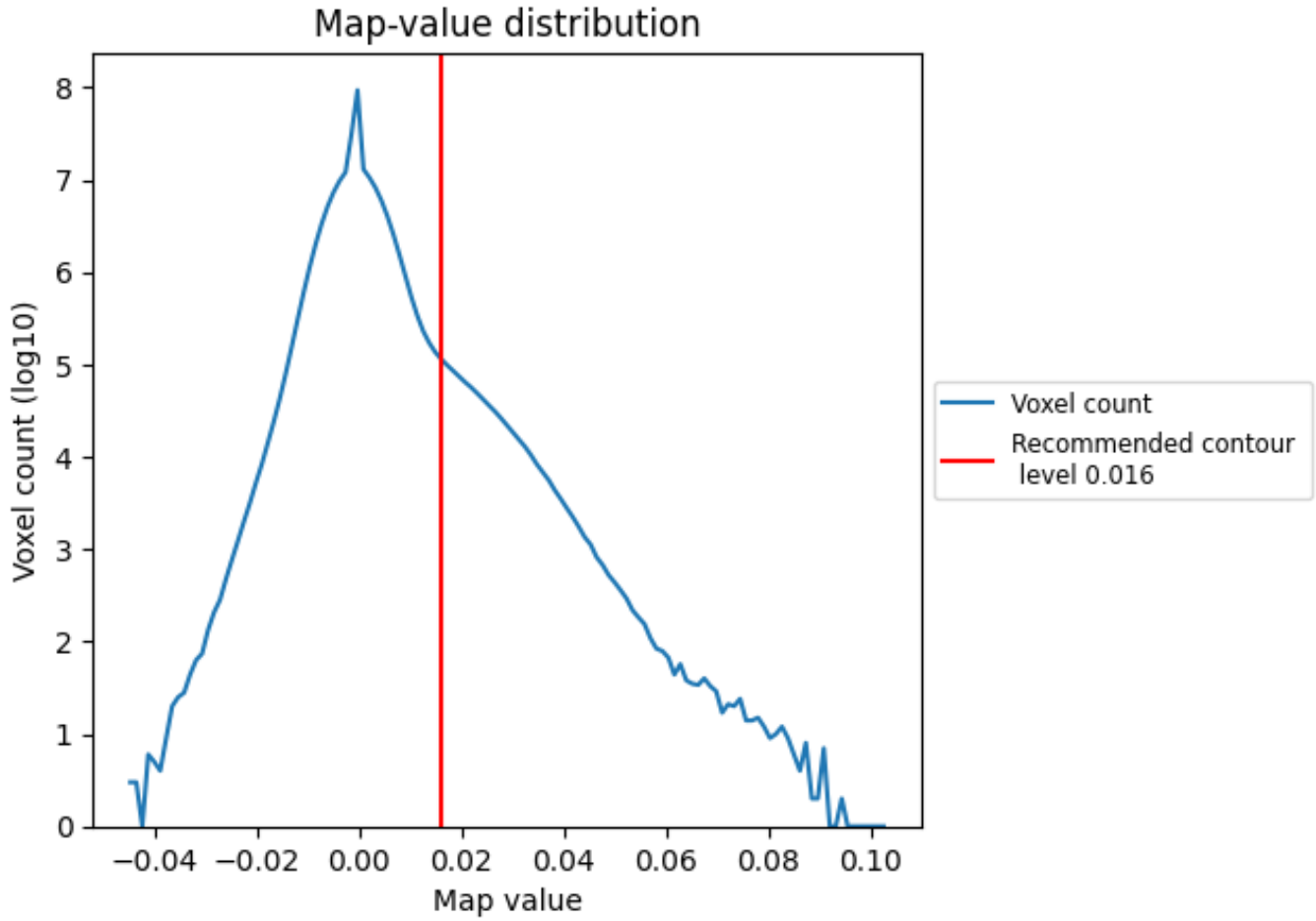


Z

# 7 Map analysis

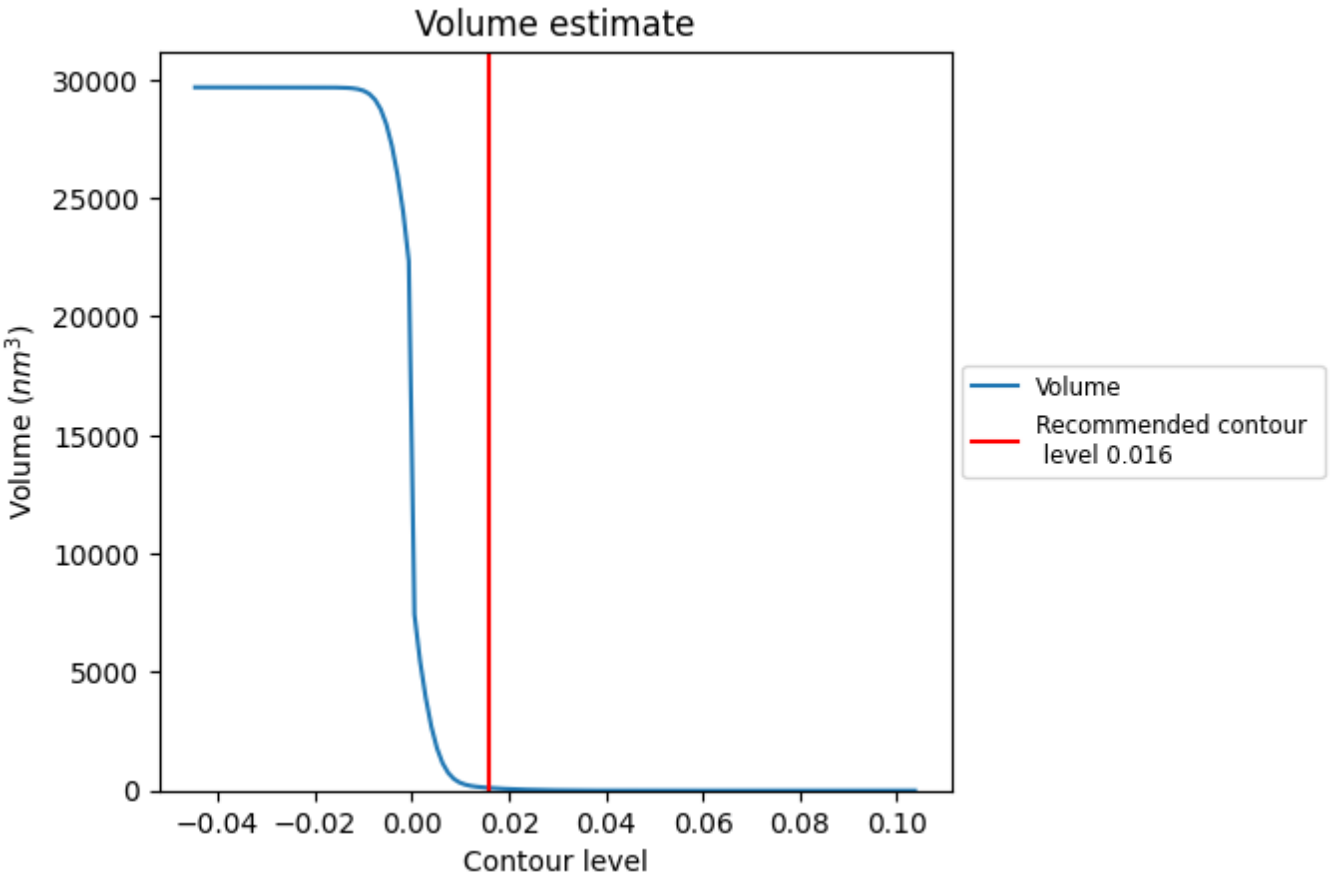
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

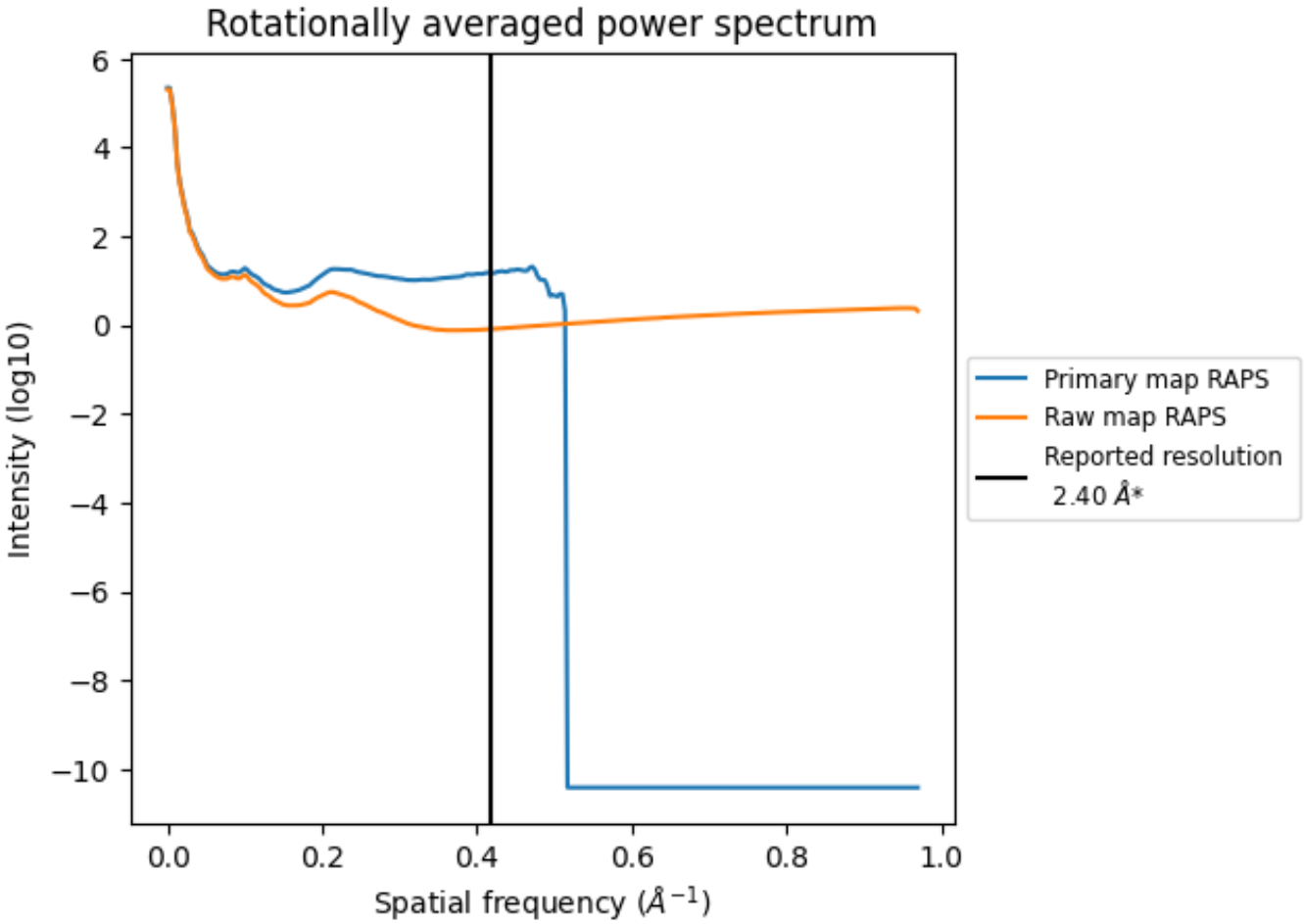
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 112 $nm^3$; this corresponds to an approximate mass of 101 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)

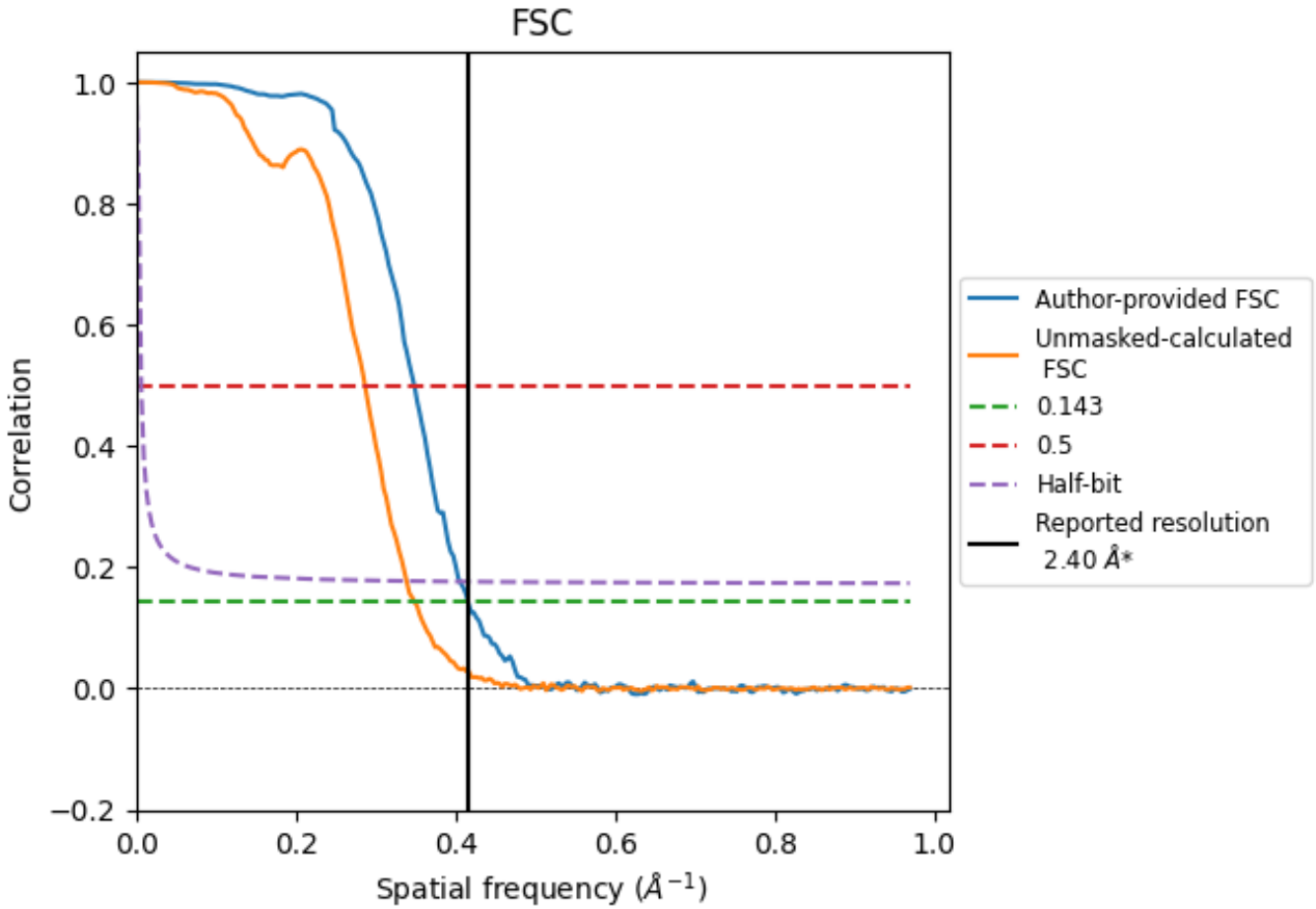



*Reported resolution corresponds to spatial frequency of 0.417 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.417 Å$^{-1}$

## 8.2 Resolution estimates (i)

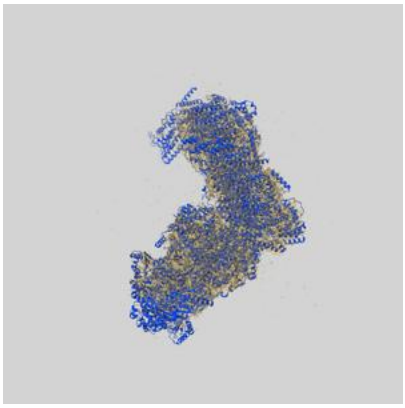
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.40 | - | - |
| Author-provided FSC curve | 2.41 | 2.87 | 2.46 |
| Unmasked-calculated* | 2.87 | 3.49 | 2.95 |

*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 2.87 differs from the reported value 2.4 by more than 10 %

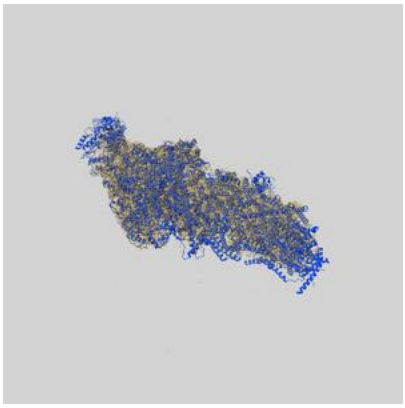
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12742 and PDB model 7O71. Per-residue inclusion information can be found in section 3 on page 22.

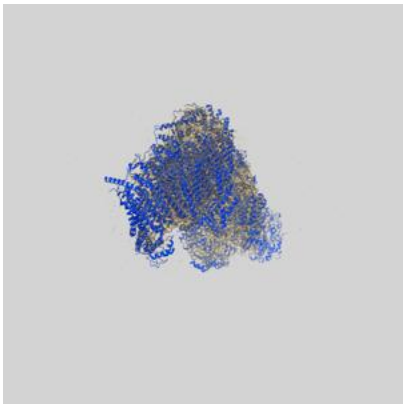
## 9.1 Map-model overlay



X



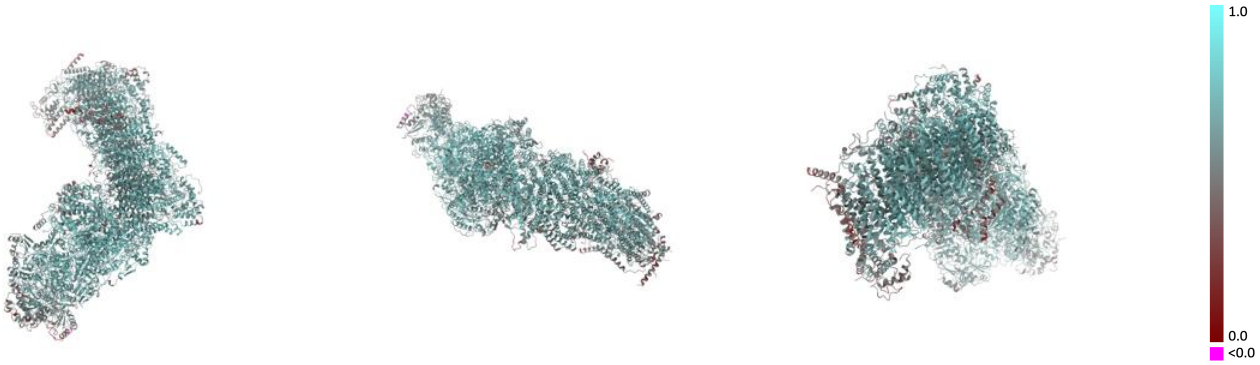
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

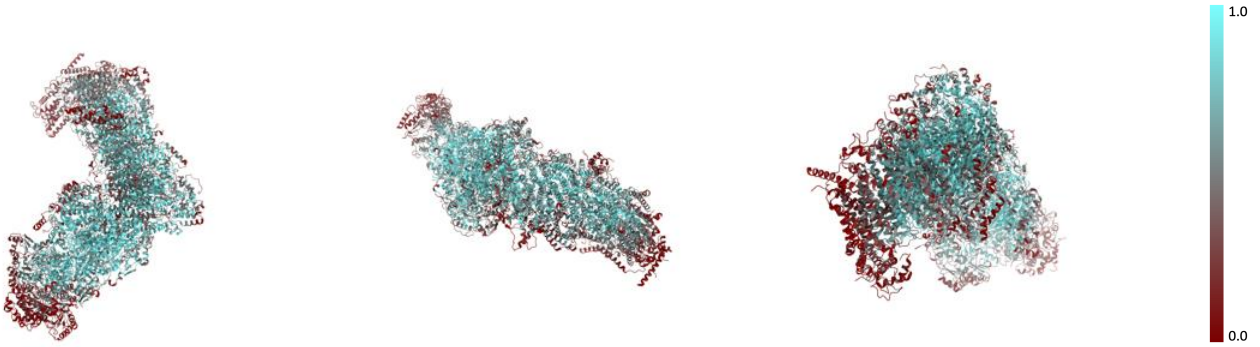
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

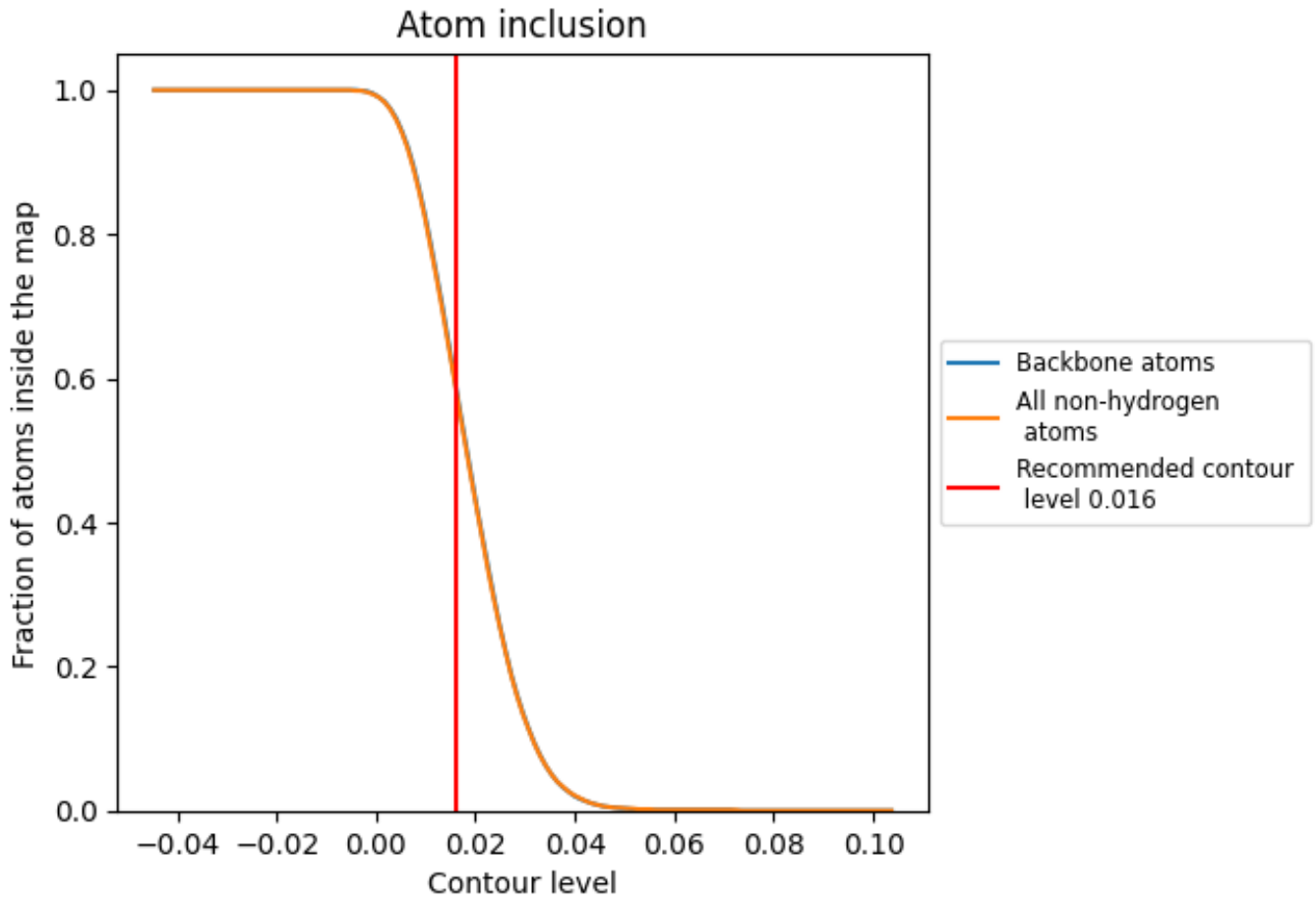
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (0.016).

## 9.4 Atom inclusion (i)




At the recommended contour level, 59% of all backbone atoms, 59% 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 (0.016) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5880 | 0.6440 |
| 1 | 0.7260 | 0.6880 |
| 2 | 0.8590 | 0.7290 |
| 3 | 0.5810 | 0.6340 |
| 4 | 0.7920 | 0.7060 |
| 5 | 0.5100 | 0.6360 |
| 6 | 0.5600 | 0.6440 |
| 8 | 0.1180 | 0.4910 |
| 9 | 0.4610 | 0.5950 |
| A | 0.6350 | 0.6650 |
| B | 0.3000 | 0.5630 |
| C | 0.8160 | 0.7170 |
| D | 0.7120 | 0.6900 |
| E | 0.5920 | 0.6440 |
| F | 0.6100 | 0.6600 |
| G | 0.8290 | 0.7160 |
| H | 0.2400 | 0.5030 |
| I | 0.8610 | 0.7310 |
| J | 0.4410 | 0.5980 |
| K | 0.8220 | 0.7180 |
| L | 0.7590 | 0.7020 |
| M | 0.7430 | 0.6940 |
| O | 0.0860 | 0.3970 |
| P | 0.5850 | 0.6400 |
| Q | 0.0900 | 0.4420 |
| R | 0.2720 | 0.5240 |
| S | 0.2550 | 0.4720 |
| U | 0.5590 | 0.6450 |
| W | 0.6160 | 0.6560 |
| X | 0.6650 | 0.6740 |
| Y | 0.7270 | 0.6820 |
| Z | 0.6250 | 0.6560 |
| a | 0.3340 | 0.5810 |
| b | 0.6560 | 0.6750 |
| c | 0.1180 | 0.4570 |




*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| d | 0.6180 | 0.6570 |
| e | 0.1010 | 0.4670 |
| f | 0.3030 | 0.5590 |
| g | 0.4910 | 0.6220 |
| h | 0.7380 | 0.6880 |
| i | 0.3720 | 0.5910 |
| j | 0.4910 | 0.6040 |
| n | 0.5060 | 0.6310 |