# wwPDB EM Validation Summary Report

Oct 21, 2024 – 02:12 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 8ESW |
| EMDB ID | : | EMD-28581 |
| Title | : | Structure of mitochondrial complex I from Drosophila melanogaster, Flexible-class 1 |
| Authors | : | Padavannil, A.; Letts, J.A. |
| Deposited on | : | 2022-10-15 |
| Resolution | : | 3.30 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

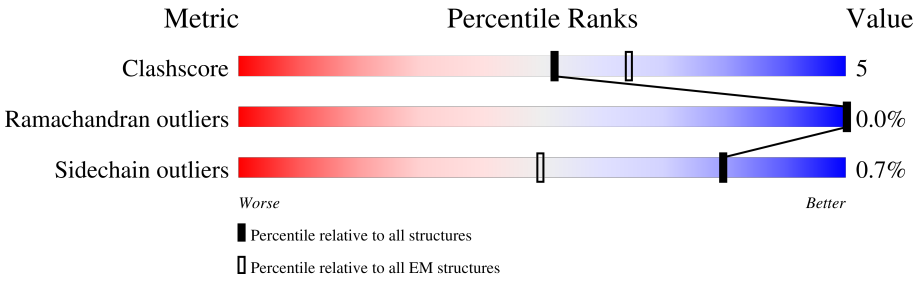
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | AN | 142 | 15% 83% 13% |
| 2 | S6 | 126 | 5% 66% 6% 29% |
| 3 | S1 | 731 | 8% 79% 14% 7% |
| 4 | S3 | 265 | 66% 12% 22% |
| 5 | V2 | 242 | 19% 75% 13% 12% |
| 6 | S7 | 221 | 64% 17% 18% |
| 7 | S8 | 217 | 67% 19% 14% |
| 8 | 3 | 117 | 68% 21% 10% |

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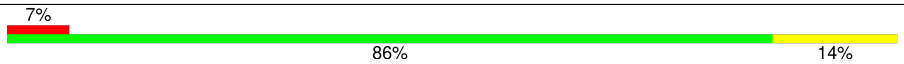
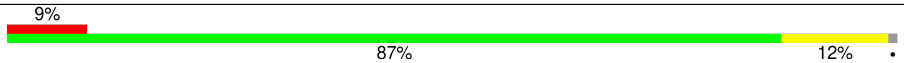
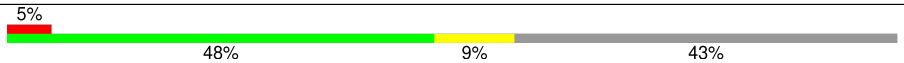
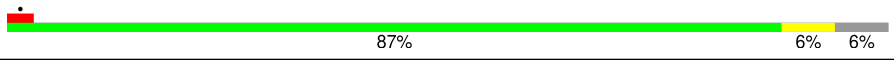
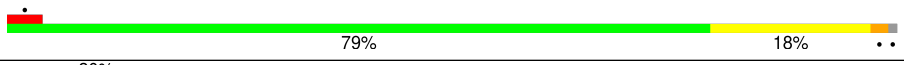
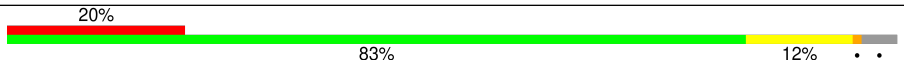
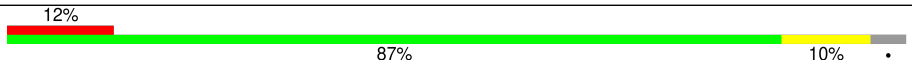
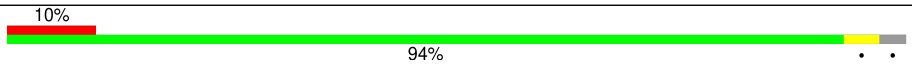
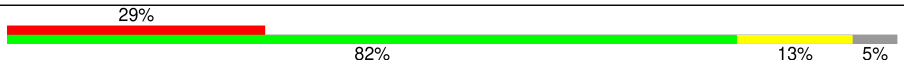
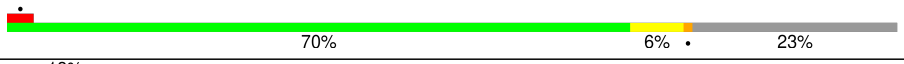
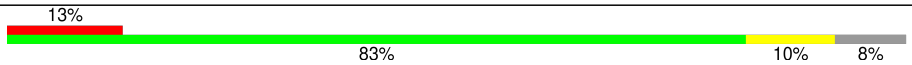
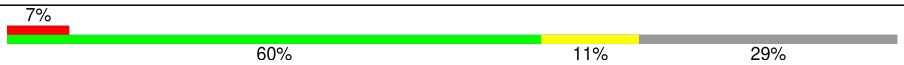
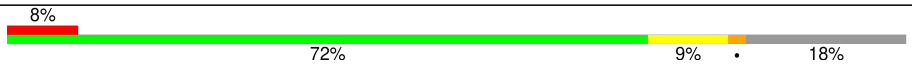
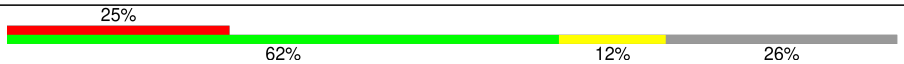
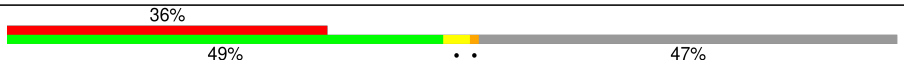
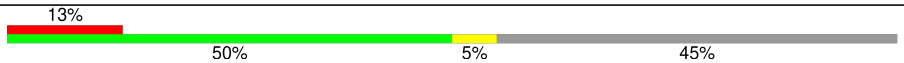
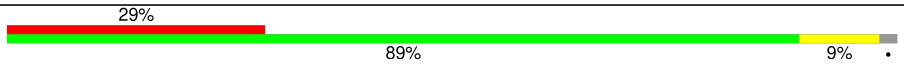
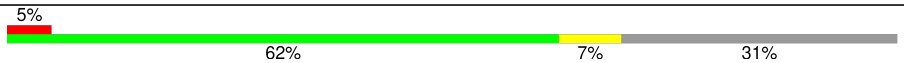
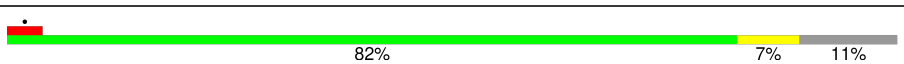
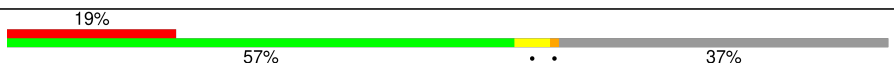
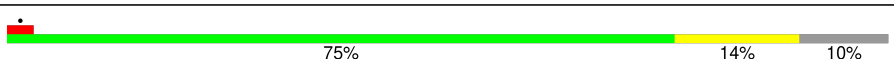
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | 1 | 315 |   |
| 10 | 4 | 446 |   |
| 11 | 5 | 577 |   |
| 12 | A8 | 175 |   |
| 13 | A1 | 123 |   |
| 14 | AO | 154 |   |
| 15 | S5 | 101 |   |
| 16 | AM | 170 |   |
| 17 | BL | 159 |   |
| 18 | B6 | 167 |   |
| 19 | B4 | 113 |   |
| 20 | B7 | 117 |   |
| 21 | B5 | 186 |   |
| 22 | B9 | 144 |   |
| 23 | BM | 150 |   |
| 24 | B8 | 175 |   |
| 25 | B3 | 110 |   |
| 26 | AB | 152 |   |
| 26 | AC | 152 |   |
| 27 | C2 | 116 |   |
| 28 | B1 | 56 |   |
| 29 | S4 | 183 |   |
| 30 | A9 | 416 |   |
| 31 | B2 | 94 |   |
| 32 | S2 | 468 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | V3 | 27 | 96% 100% |
| 34 | V1 | 474 | 11% 80% 12% 7% |
| 35 | 2 | 341 | 84% 16% |
| 36 | 4L | 96 | 6% 92% 7% |
| 37 | 6 | 174 | 81% 13% 5% |
| 38 | A7 | 103 | 12% 78% 10% 13% |
| 39 | A5 | 124 | 5% 88% 6% 6% |
| 40 | A3 | 77 | 10% 74% 13% 13% |
| 41 | A6 | 124 | 5% 81% 9% 8% |
| 42 | AL | 407 | 80% 11% 10% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 45 | SF4 | S7 | 301 | - | - | X | - |

# 2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 66555 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | AN | 137 | 1150 | 750 | 192 | 203 | 5 | 0 | 0 |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | S6 | 90 | 722 | 456 | 131 | 130 | 5 | 0 | 0 |

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | S1 | 680 | 5168 | 3239 | 915 | 985 | 29 | 0 | 0 |

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | S3 | 208 | 1719 | 1098 | 302 | 314 | 5 | 0 | 0 |

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | V2 | 214 | 1680 | 1062 | 285 | 321 | 12 | 0 | 0 |

- Molecule 6 is a protein called LD31474p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | S7 | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1435 | 920 | 251 | 250 | 14 | | |

- Molecule 7 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | S8 | 186 | Total | C | N | O | S | 0 | 0 |
| | | | 1485 | 935 | 251 | 287 | 12 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 3 | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 855 | 593 | 119 | 137 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 1 | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2571 | 1764 | 367 | 418 | 22 | | |

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | 4 | 446 | Total | C | N | O | S | 0 | 0 |
| | | | 3604 | 2448 | 533 | 581 | 42 | | |

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | 5 | 577 | Total | C | N | O | S | 0 | 0 |
| | | | 4605 | 3092 | 680 | 773 | 60 | | |

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | A8 | 174 | Total | C | N | O | S | 0 | 0 |
| | | | 1384 | 867 | 240 | 267 | 10 | | |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | A1 | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 581 | 375 | 97 | 103 | 6 | | |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | AO | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1188 | 777 | 201 | 208 | 2 | | |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | S5 | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 828 | 523 | 145 | 149 | 11 | | |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | AM | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1251 | 813 | 207 | 225 | 6 | | |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | BL | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1252 | 786 | 231 | 225 | 10 | | |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | B6 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1302 | 829 | 242 | 226 | 5 | | |

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | B4 | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 907 | 578 | 166 | 162 | 1 | | |

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | B7 | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 925 | 589 | 159 | 167 | 10 | | |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | B5 | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1221 | 787 | 209 | 222 | 3 | | |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | B9 | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1143 | 729 | 216 | 195 | 3 | | |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | BM | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 560 | 140 | 170 | 1 | | |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | B8 | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1201 | 783 | 191 | 223 | 4 | | |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | B3 | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 646 | 421 | 113 | 111 | 1 | | |

- Molecule 26 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | AC | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 677 | 437 | 102 | 136 | 2 | | |
| 26 | AB | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 652 | 421 | 99 | 130 | 2 | | |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | C2 | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 904 | 588 | 159 | 156 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | B1 | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 430 | 278 | 76 | 74 | 2 | | |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | S4 | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1023 | 640 | 192 | 187 | 4 | | |

- Molecule 30 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | A9 | 370 | Total | C | N | O | S | 0 | 0 |
| | | | 2972 | 1895 | 539 | 528 | 10 | | |

- Molecule 31 is a protein called GEO11417p1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | B2 | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 485 | 317 | 85 | 82 | 1 | | |

- Molecule 32 is a protein called Complex I-49kD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | S2 | 419 | Total | C | N | O | S | 0 | 0 |
| | | | 3349 | 2149 | 563 | 614 | 23 | | |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 33 | V3 | 27 | Total | C | N | O | 0 | 0 |
| | | | 136 | 81 | 27 | 28 | | |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | V1 | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3368 | 2126 | 600 | 616 | 26 | | |

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 2 | 341 | Total | C | N | O | S | 0 | 0 |
| | | | 2797 | 1893 | 411 | 459 | 34 | | |

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | 4L | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 785 | 535 | 112 | 126 | 12 | | |

- Molecule 37 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | 6 | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1331 | 902 | 189 | 225 | 15 | | |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | A7 | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 725 | 457 | 136 | 131 | 1 | | |

- Molecule 39 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | A5 | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 914 | 584 | 161 | 165 | 4 | | |

- Molecule 40 is a protein called RH45008p.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | A3 | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 528 | 331 | 96 | 100 | 1 | | |

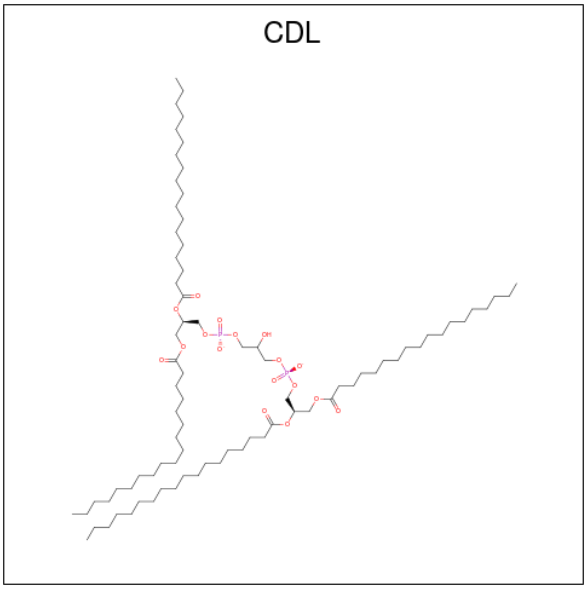
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | A6 | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 968 | 620 | 172 | 170 | 6 | | |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | AL | 368 | Total | C | N | O | S | 0 | 0 |
| | | | 3008 | 1927 | 504 | 561 | 16 | | |

- Molecule 43 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 43 | AN | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |
| 43 | S7 | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 43 | 5 | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |

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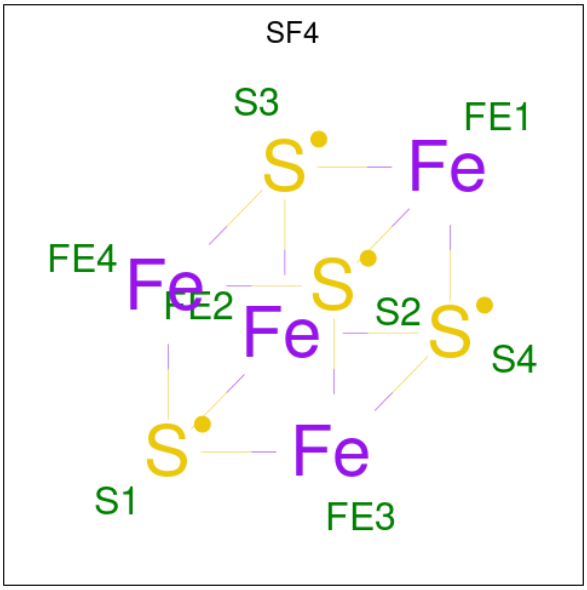
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 43 | 5 | 1 | Total | C | O | P | 0 |
| | | | 75 | 56 | 17 | 2 | |
| 43 | B6 | 1 | Total | C | O | P | 0 |
| | | | 53 | 34 | 17 | 2 | |
| 43 | B5 | 1 | Total | C | O | P | 0 |
| | | | 74 | 55 | 17 | 2 | |
| 43 | A9 | 1 | Total | C | O | P | 0 |
| | | | 54 | 35 | 17 | 2 | |
| 43 | A9 | 1 | Total | C | O | P | 0 |
| | | | 47 | 28 | 17 | 2 | |

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 44 | S6 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 45 | S1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | S1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | S7 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

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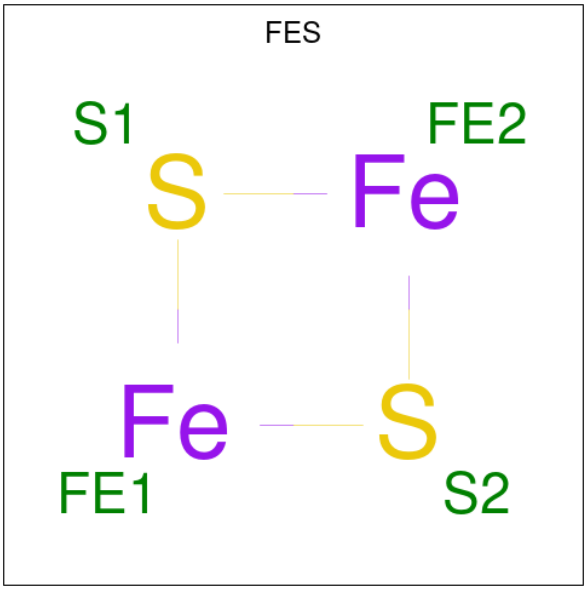
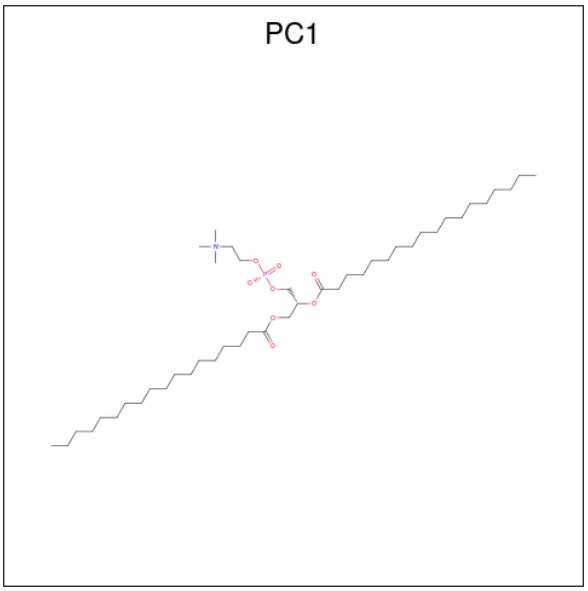
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 45 | S8 | 1 | Total Fe S<br>8 4 4 | 0 |
| 45 | S8 | 1 | Total Fe S<br>8 4 4 | 0 |
| 45 | V1 | 1 | Total Fe S<br>8 4 4 | 0 |

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: $Fe_2S_2$).



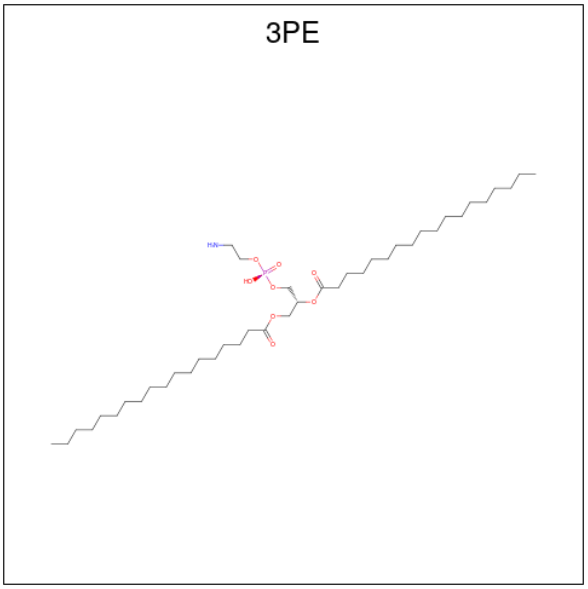

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 46 | S1 | 1 | Total Fe S<br>4 2 2 | 0 |
| 46 | V2 | 1 | Total Fe S<br>4 2 2 | 0 |

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 47 | S7 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 47 | S7 | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 47 | 1 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 47 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 47 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 47 | AM | 1 | Total | C | N | O | P | 0 |
| | | | 37 | 27 | 1 | 8 | 1 | |
| 47 | AM | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 47 | B6 | 1 | Total | C | N | O | P | 0 |
| | | | 37 | 27 | 1 | 8 | 1 | |
| 47 | B4 | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 47 | C2 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 47 | 2 | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 47 | 2 | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 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 |
| | | | 29 | 19 | 1 | 8 | 1 | |

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 48 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 48 | 4 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 48 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 48 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 48 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 48 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 48 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 48 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 48 | AM | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 48 | AM | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 48 | AM | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 48 | B6 | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |

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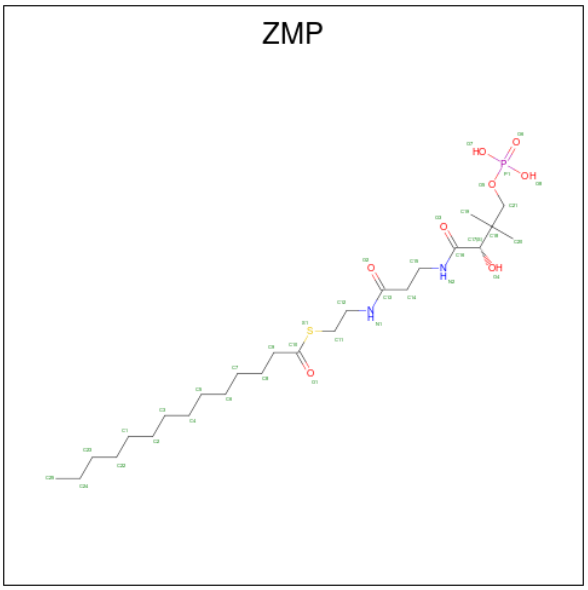
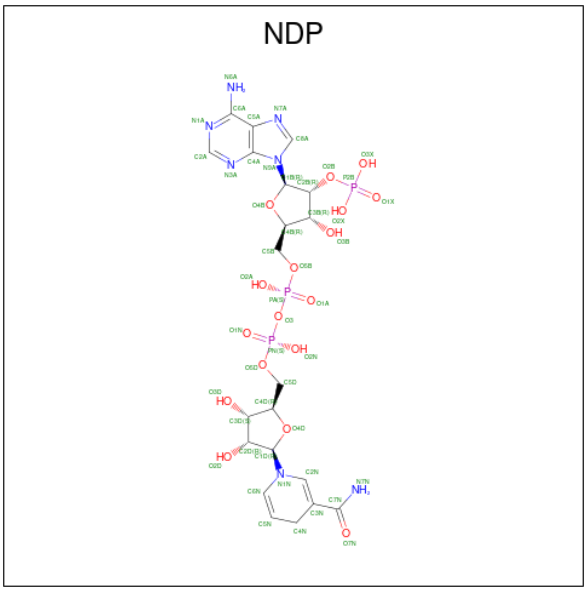
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 48 | 2 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |

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



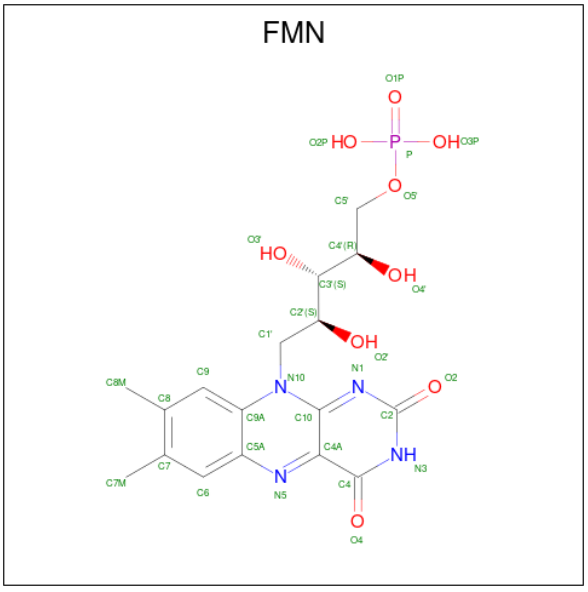

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 49 | B9 | 1 | Total | C | N | O | P | S | 0 |
| | | | 34 | 23 | 2 | 7 | 1 | 1 | |
| 49 | AB | 1 | Total | C | N | O | P | S | 0 |
| | | | 34 | 23 | 2 | 7 | 1 | 1 | |

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



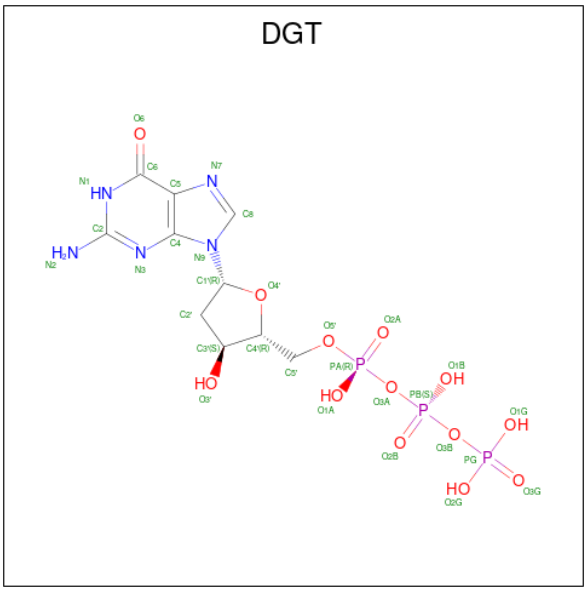

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 50 | A9 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 51 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 51 | V1 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

- Molecule 52 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



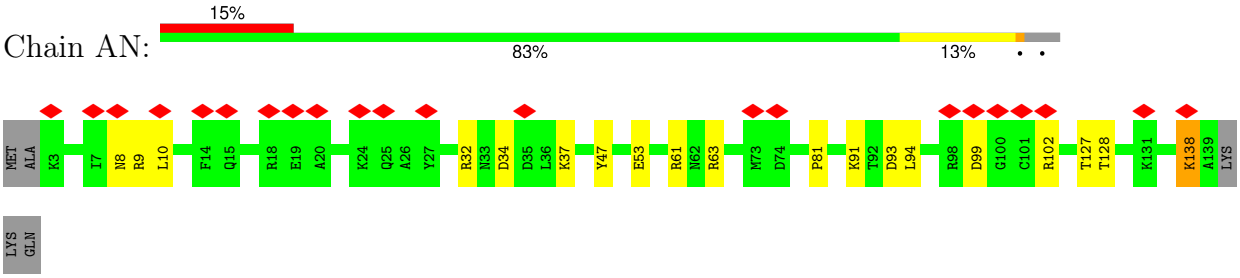

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 52 | AL | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |

# 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.

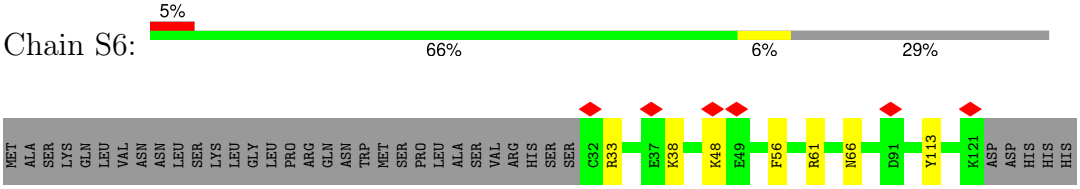
• Molecule 1: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AN:



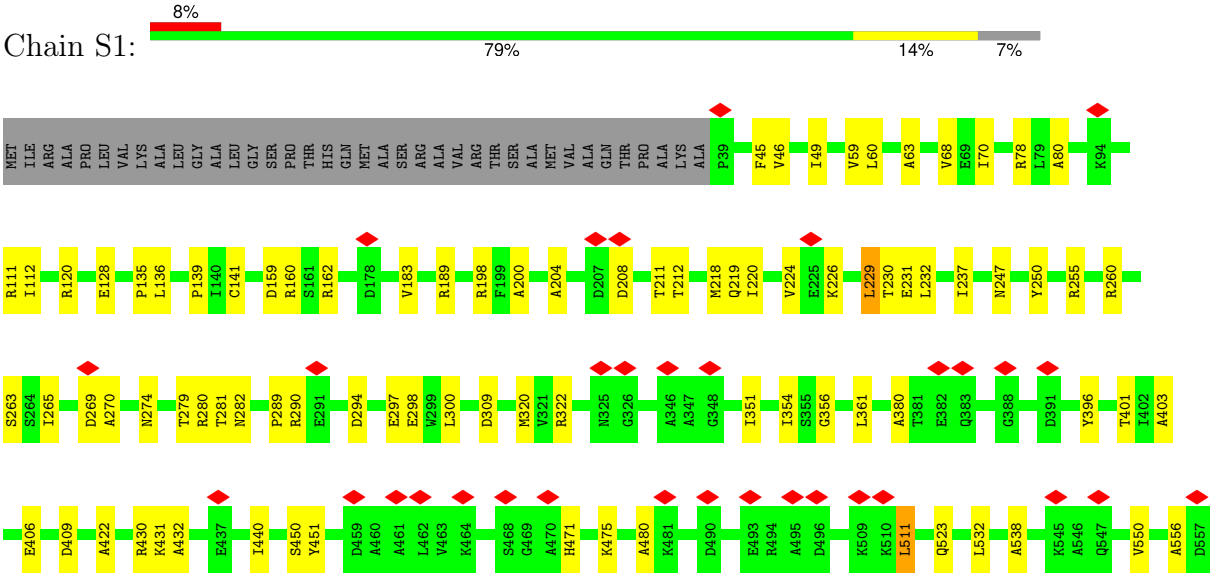

• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

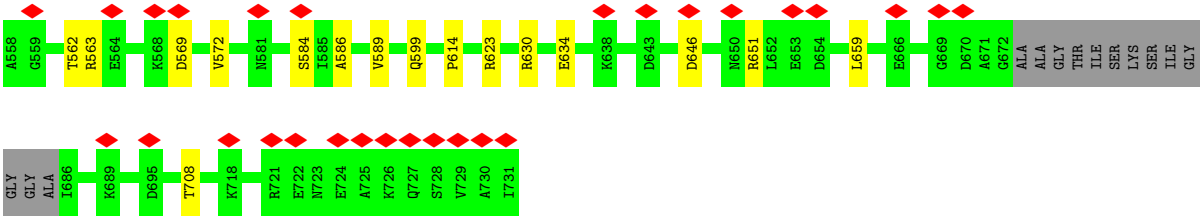
Chain S6:




• Molecule 3: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

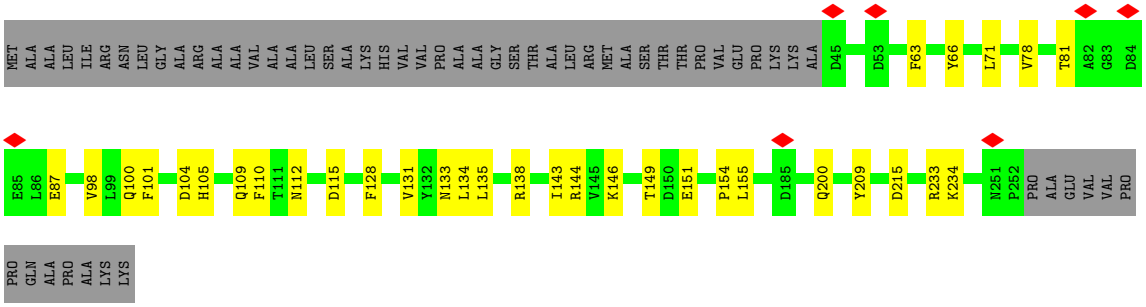
Chain S1:





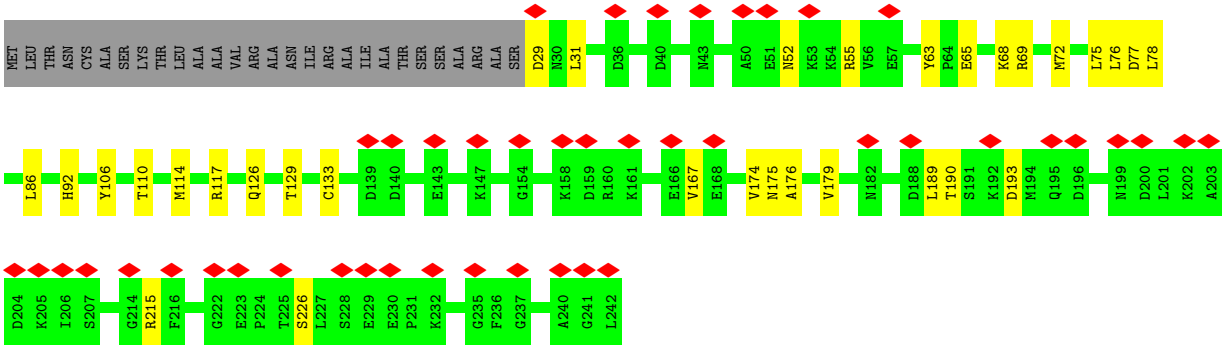

• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain S3:

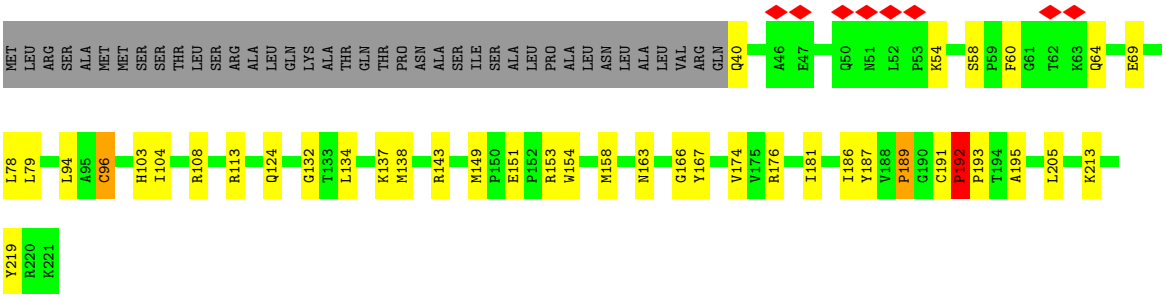

• Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A

Chain V2:

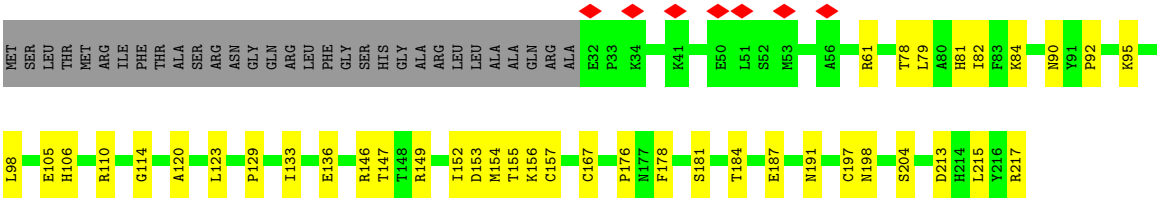

• Molecule 6: LD31474p

Chain S7:

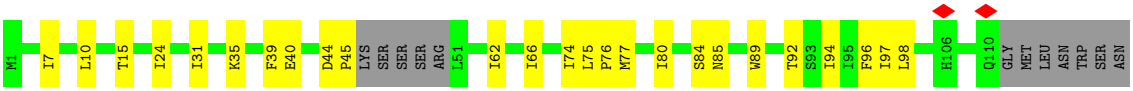

• Molecule 7: NADH dehydrogenase (ubiquinone) 23 kDa subunit

Chain S8:

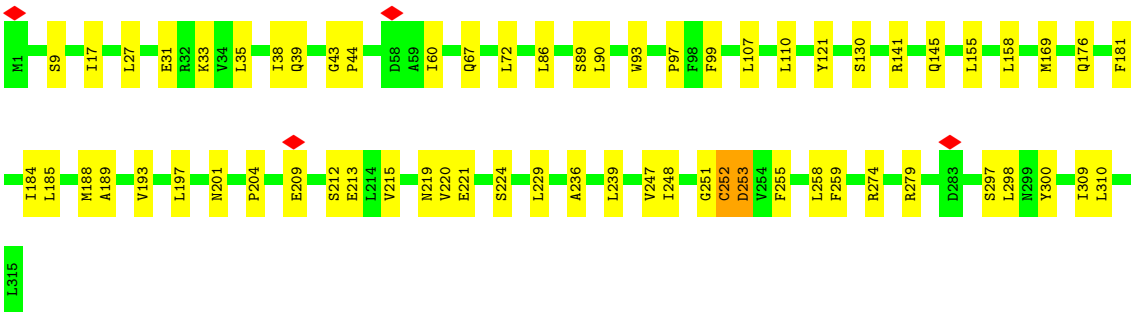

• Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain 3:

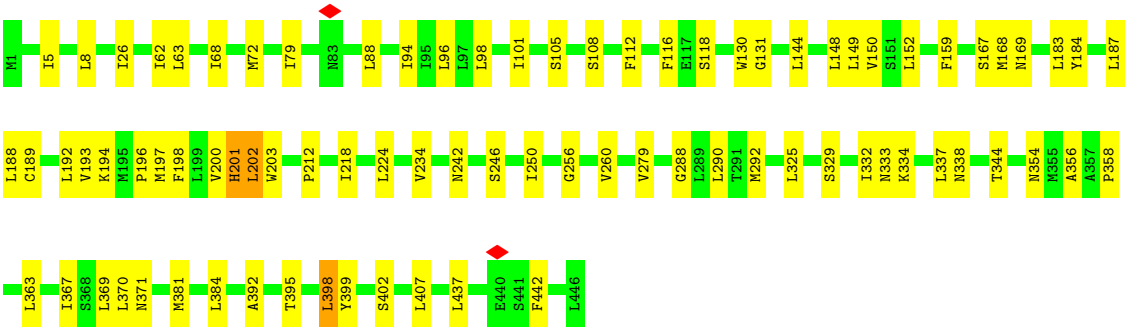

• Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain 1:

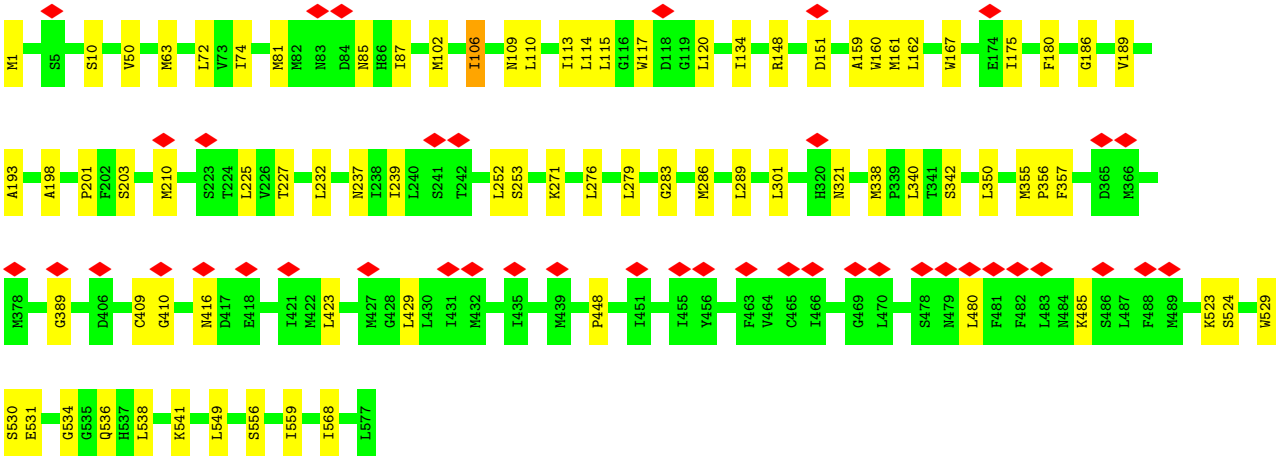

• Molecule 10: NADH-ubiquinone oxidoreductase chain 4

Chain 4:

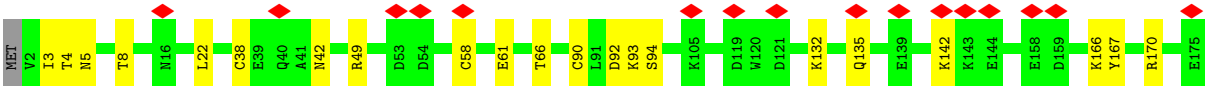

• Molecule 11: NADH-ubiquinone oxidoreductase chain 5

Chain 5:



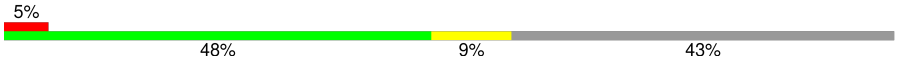

• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

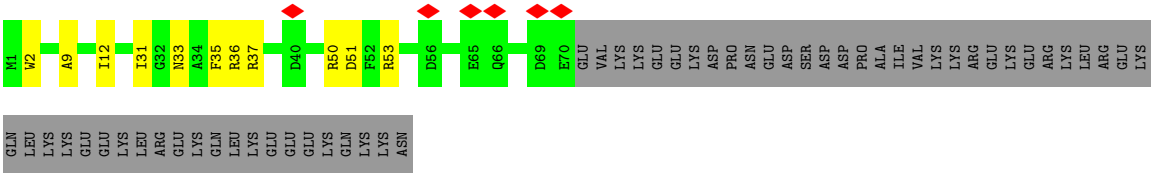
Chain A8:


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

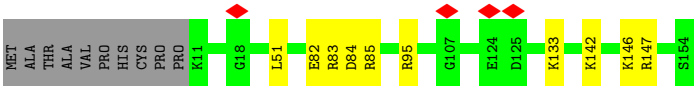
Chain A1:



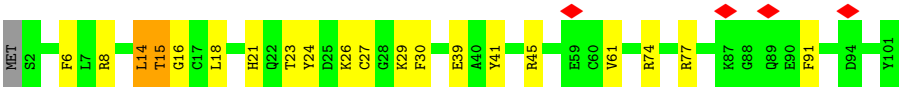

• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AO:

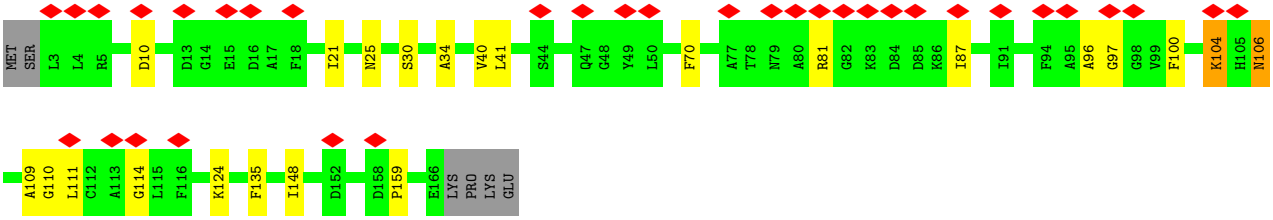

• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:

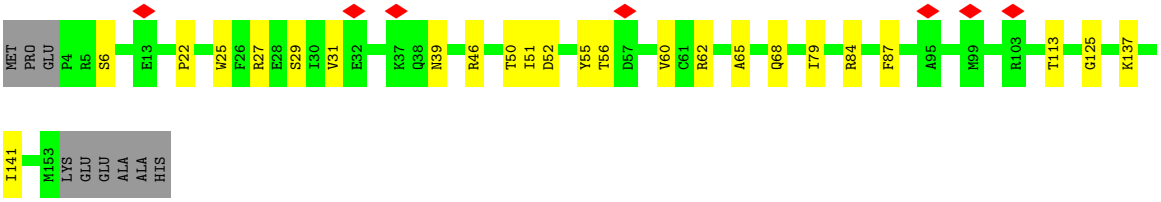

• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AM:



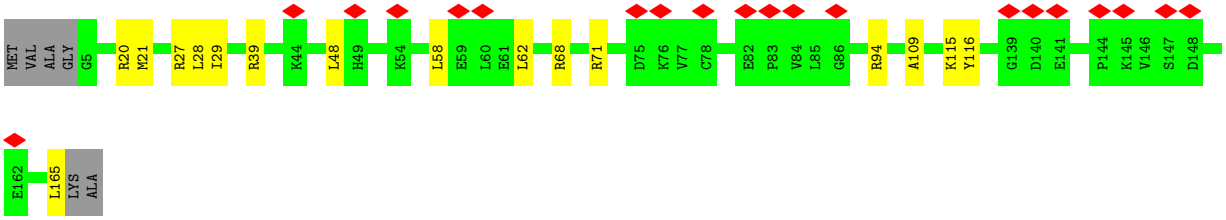

• Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BL:

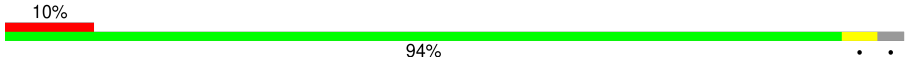

• Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

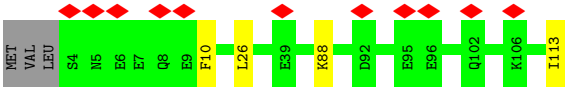
Chain B6:


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

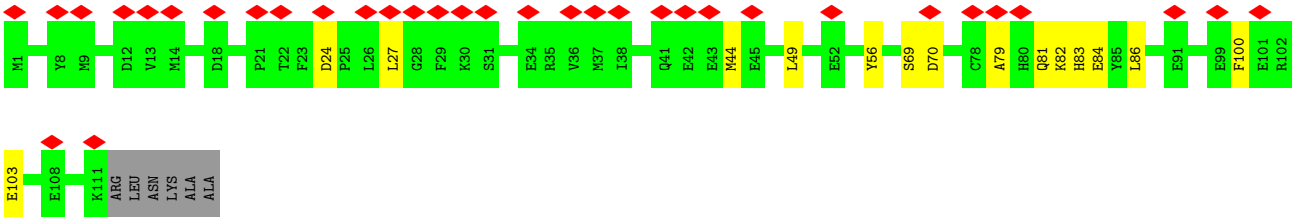
Chain B4:



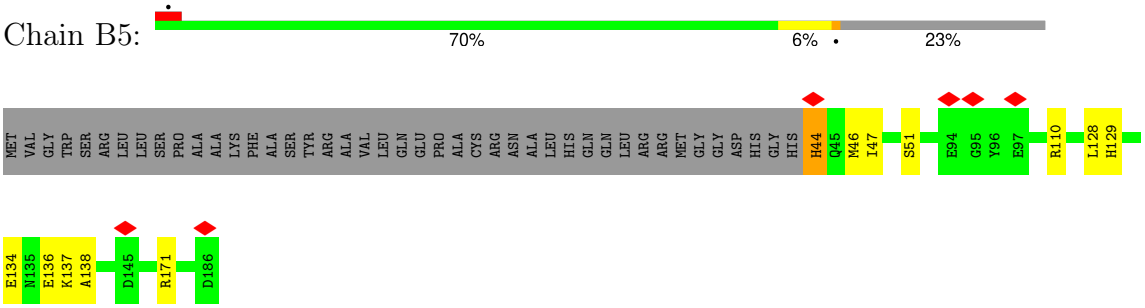

• Molecule 20: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:

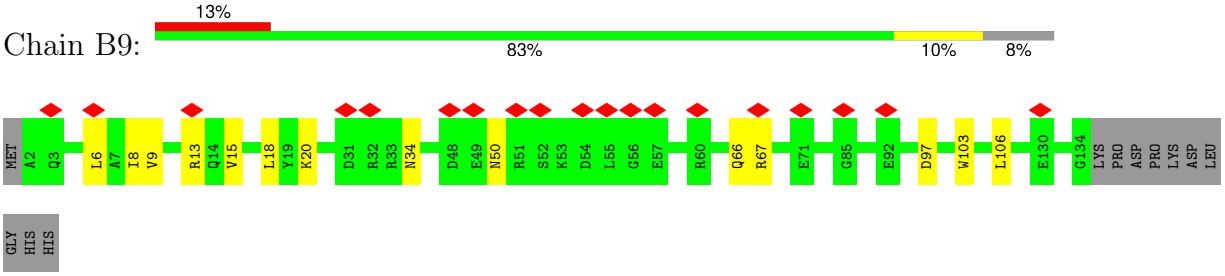

• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:



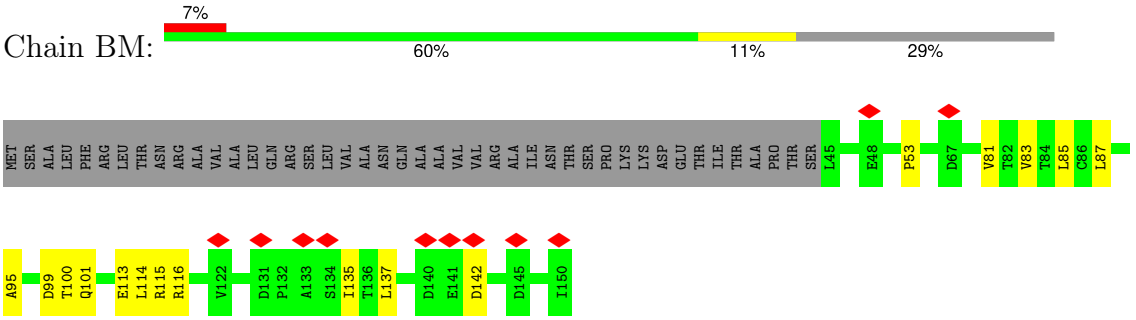

• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:



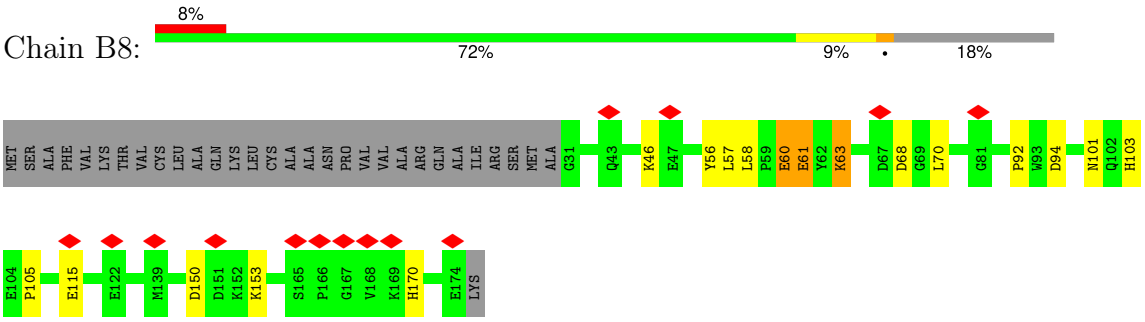

• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BM:



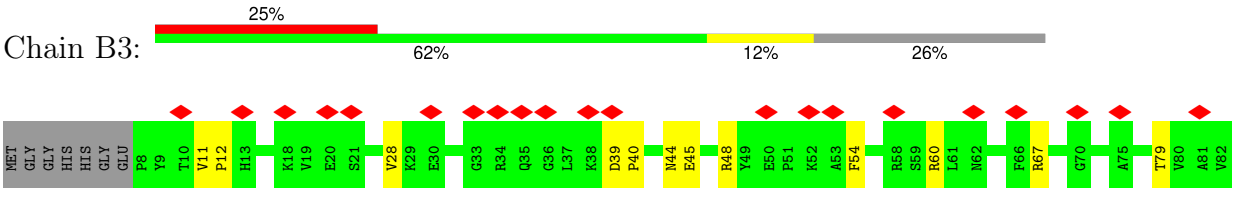

• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

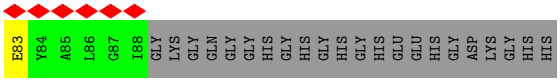
Chain B8:




• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

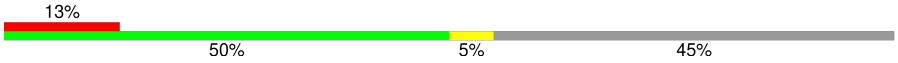
Chain B3:

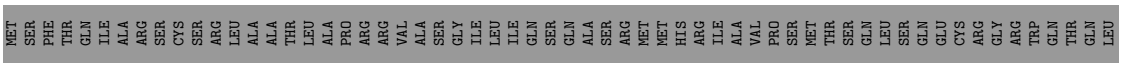


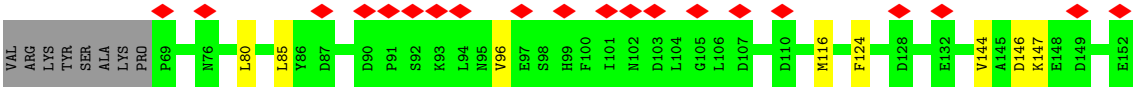



• Molecule 26: Acyl carrier protein, mitochondrial

Chain AC:



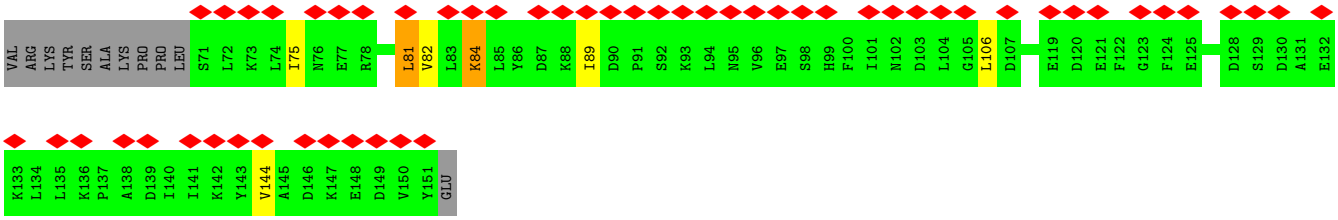




• Molecule 26: Acyl carrier protein, mitochondrial

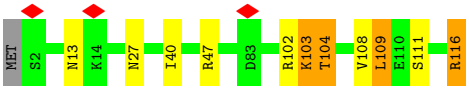
Chain AB:





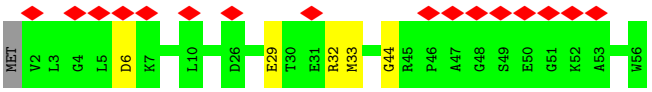

• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain C2:

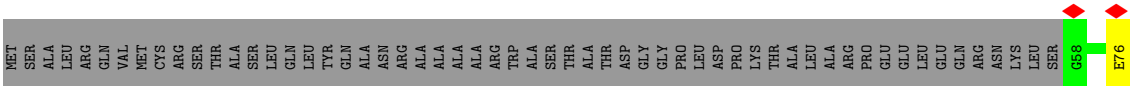

• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

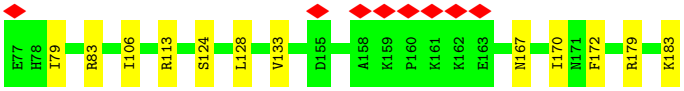
Chain B1:


• Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

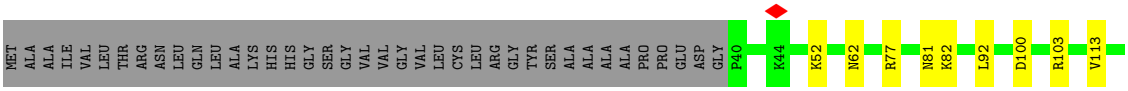
Chain S4:

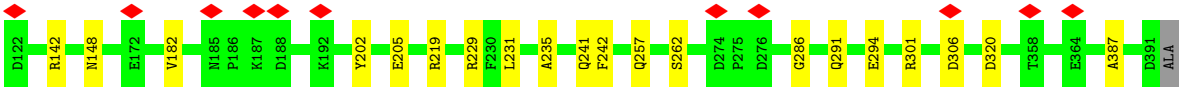



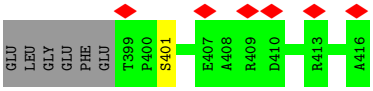



• Molecule 30: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A

Chain A9:

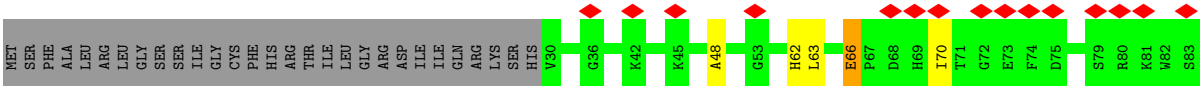



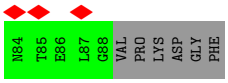




• Molecule 31: GEO11417p1

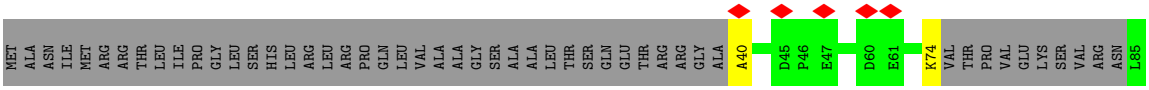
Chain B2:

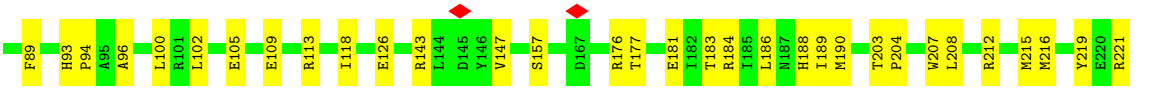



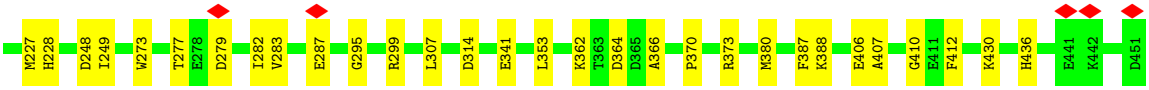



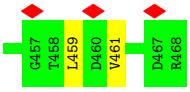

• Molecule 32: Complex I-49kD

Chain S2:

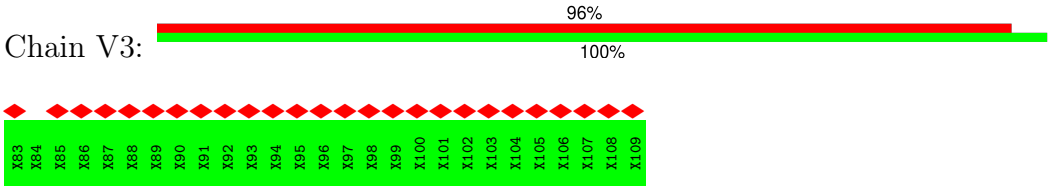



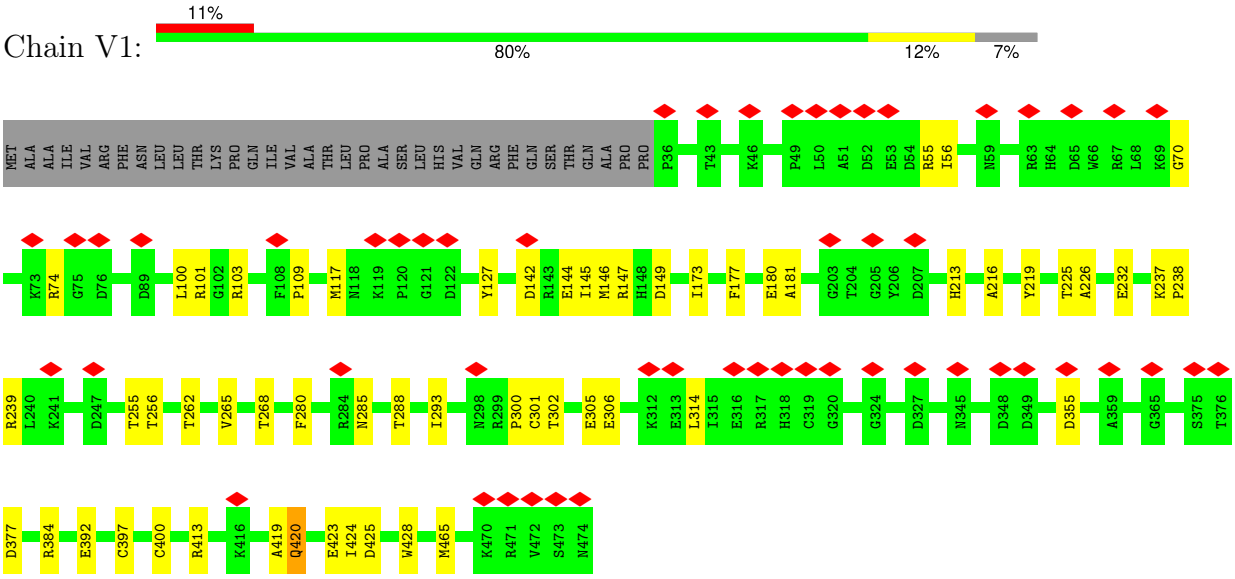

• Molecule 33: NADH dehydrogenase [ubiquinone] flavoprotein 3

Chain V3:



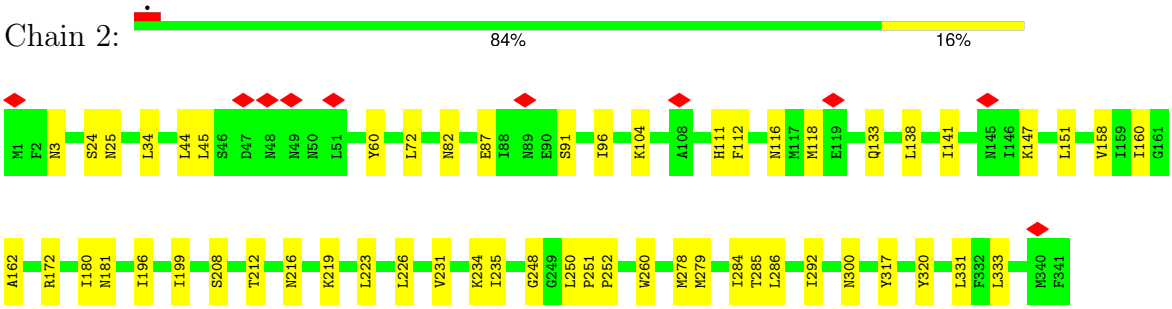

• Molecule 34: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



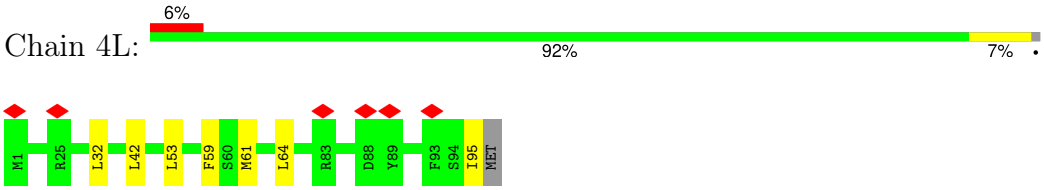

• Molecule 35: NADH-ubiquinone oxidoreductase chain 2

Chain 2:



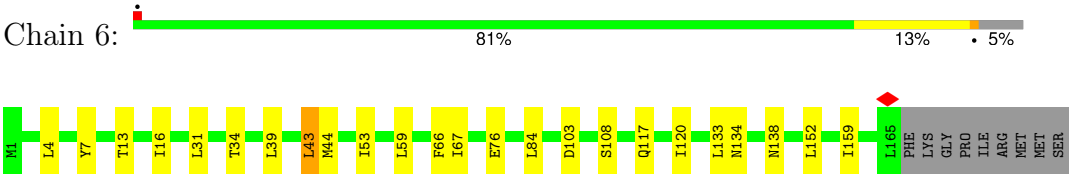

• Molecule 36: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:



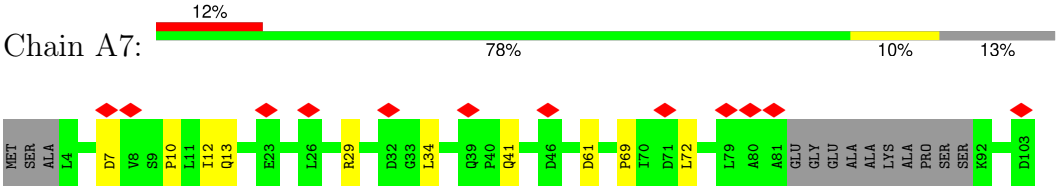

• Molecule 37: NADH-ubiquinone oxidoreductase chain 6

Chain 6:



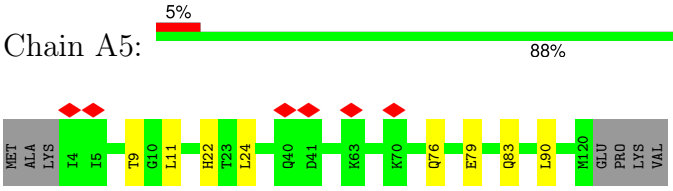
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain A7:



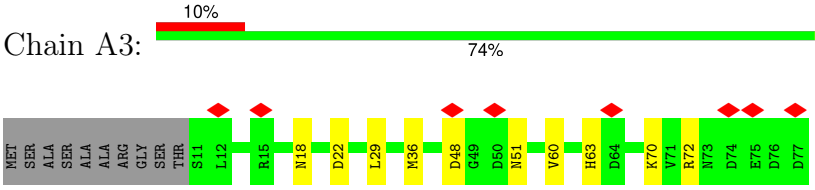

• Molecule 39: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit

Chain A5:



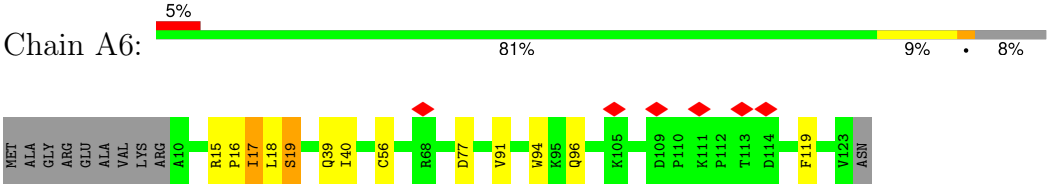

• Molecule 40: RH45008p

Chain A3:



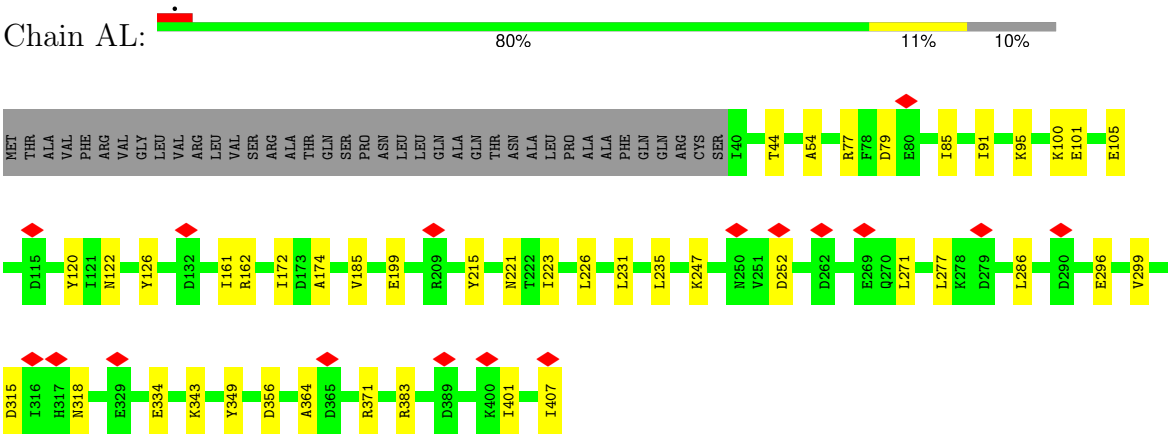

• Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AL:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 293389 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS GLACIOS | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 6.017 | Depositor |
| Minimum map value | -2.064 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.094 | Depositor |
| Recommended contour level | 0.6 | Depositor |
| Map size (Å) | 450.56, 450.56, 450.56 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.88, 0.88, 0.88 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, NDP, FES, 3PE, CDL, DGT, FMN, ZN, PC1, SF4

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 | AN | 0.31 | 0/1190 | 0.58 | 0/1612 |
| 2 | S6 | 0.29 | 0/739 | 0.55 | 0/995 |
| 3 | S1 | 0.29 | 0/5251 | 0.57 | 0/7117 |
| 4 | S3 | 0.28 | 0/1766 | 0.56 | 0/2400 |
| 5 | V2 | 0.29 | 0/1719 | 0.58 | 0/2328 |
| 6 | S7 | 0.34 | 0/1473 | 0.66 | 2/1997 (0.1%) |
| 7 | S8 | 0.33 | 0/1518 | 0.60 | 0/2050 |
| 8 | 3 | 0.32 | 0/875 | 0.61 | 0/1187 |
| 9 | 1 | 0.33 | 0/2651 | 0.60 | 0/3593 |
| 10 | 4 | 0.32 | 0/3708 | 0.61 | 1/5024 (0.0%) |
| 11 | 5 | 0.33 | 0/4725 | 0.65 | 0/6396 |
| 12 | A8 | 0.29 | 0/1417 | 0.53 | 0/1911 |
| 13 | A1 | 0.29 | 0/594 | 0.60 | 0/801 |
| 14 | AO | 0.30 | 0/1224 | 0.56 | 0/1659 |
| 15 | S5 | 0.35 | 0/846 | 0.61 | 0/1128 |
| 16 | AM | 0.31 | 0/1287 | 0.53 | 0/1749 |
| 17 | BL | 0.30 | 0/1285 | 0.57 | 0/1734 |
| 18 | B6 | 0.27 | 0/1338 | 0.57 | 0/1808 |
| 19 | B4 | 0.28 | 0/928 | 0.52 | 0/1241 |
| 20 | B7 | 0.30 | 0/948 | 0.56 | 0/1275 |
| 21 | B5 | 0.28 | 0/1255 | 0.53 | 0/1694 |
| 22 | B9 | 0.27 | 0/1176 | 0.57 | 0/1586 |
| 23 | BM | 0.27 | 0/896 | 0.52 | 0/1222 |
| 24 | B8 | 0.29 | 0/1250 | 0.57 | 0/1701 |
| 25 | B3 | 0.28 | 0/665 | 0.56 | 0/903 |
| 26 | AB | 0.30 | 0/662 | 0.64 | 0/894 |
| 26 | AC | 0.26 | 0/688 | 0.54 | 0/928 |
| 27 | C2 | 0.36 | 0/932 | 0.65 | 1/1266 (0.1%) |
| 28 | B1 | 0.27 | 0/441 | 0.56 | 0/590 |
| 29 | S4 | 0.27 | 0/1051 | 0.57 | 0/1424 |
| 30 | A9 | 0.30 | 0/3045 | 0.60 | 0/4118 |
| 31 | B2 | 0.30 | 0/508 | 0.55 | 0/698 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 32 | S2 | 0.32 | 0/3432 | 0.60 | 0/4650 |
| 34 | V1 | 0.32 | 0/3446 | 0.61 | 0/4654 |
| 35 | 2 | 0.32 | 0/2876 | 0.58 | 0/3890 |
| 36 | 4L | 0.30 | 0/806 | 0.53 | 0/1085 |
| 37 | 6 | 0.30 | 0/1356 | 0.57 | 0/1836 |
| 38 | A7 | 0.27 | 0/741 | 0.60 | 0/1006 |
| 39 | A5 | 0.27 | 0/933 | 0.56 | 0/1265 |
| 40 | A3 | 0.25 | 0/537 | 0.55 | 0/725 |
| 41 | A6 | 0.29 | 0/988 | 0.54 | 0/1329 |
| 42 | AL | 0.28 | 0/3083 | 0.56 | 0/4168 |
| All | All | 0.30 | 0/66249 | 0.59 | 4/89637 (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 |
|---|---|---|---|
| 27 | C2 | 0 | 1 |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | S7 | 192 | PRO | N-CA-C | -7.61 | 92.32 | 112.10 |
| 6 | S7 | 189 | PRO | N-CA-C | 5.92 | 127.50 | 112.10 |
| 10 | 4 | 212 | PRO | N-CA-CB | 5.83 | 110.29 | 103.30 |
| 27 | C2 | 111 | SER | N-CA-C | 5.49 | 125.82 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 27 | C2 | 116 | ARG | Sidechain |

## 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 | AN | 1150 | 0 | 1107 | 18 | 0 |
| 2 | S6 | 722 | 0 | 705 | 5 | 0 |
| 3 | S1 | 5168 | 0 | 5214 | 65 | 0 |
| 4 | S3 | 1719 | 0 | 1666 | 27 | 0 |
| 5 | V2 | 1680 | 0 | 1657 | 20 | 0 |
| 6 | S7 | 1435 | 0 | 1448 | 35 | 0 |
| 7 | S8 | 1485 | 0 | 1422 | 34 | 0 |
| 8 | 3 | 855 | 0 | 927 | 21 | 0 |
| 9 | 1 | 2571 | 0 | 2628 | 54 | 0 |
| 10 | 4 | 3604 | 0 | 3734 | 63 | 0 |
| 11 | 5 | 4605 | 0 | 4742 | 59 | 0 |
| 12 | A8 | 1384 | 0 | 1324 | 17 | 0 |
| 13 | A1 | 581 | 0 | 582 | 8 | 0 |
| 14 | AO | 1188 | 0 | 1196 | 9 | 0 |
| 15 | S5 | 828 | 0 | 805 | 13 | 0 |
| 16 | AM | 1251 | 0 | 1230 | 17 | 0 |
| 17 | BL | 1252 | 0 | 1195 | 24 | 0 |
| 18 | B6 | 1302 | 0 | 1295 | 11 | 0 |
| 19 | B4 | 907 | 0 | 896 | 8 | 0 |
| 20 | B7 | 925 | 0 | 906 | 10 | 0 |
| 21 | B5 | 1221 | 0 | 1188 | 12 | 0 |
| 22 | B9 | 1143 | 0 | 1111 | 10 | 0 |
| 23 | BM | 871 | 0 | 822 | 12 | 0 |
| 24 | B8 | 1201 | 0 | 1107 | 18 | 0 |
| 25 | B3 | 646 | 0 | 641 | 9 | 0 |
| 26 | AB | 652 | 0 | 655 | 4 | 0 |
| 26 | AC | 677 | 0 | 681 | 6 | 0 |
| 27 | C2 | 904 | 0 | 892 | 10 | 0 |
| 28 | B1 | 430 | 0 | 436 | 4 | 0 |
| 29 | S4 | 1023 | 0 | 994 | 9 | 0 |
| 30 | A9 | 2972 | 0 | 2983 | 18 | 0 |
| 31 | B2 | 485 | 0 | 450 | 5 | 0 |
| 32 | S2 | 3349 | 0 | 3314 | 44 | 0 |
| 33 | V3 | 136 | 0 | 30 | 0 | 0 |
| 34 | V1 | 3368 | 0 | 3345 | 42 | 0 |
| 35 | 2 | 2797 | 0 | 2879 | 39 | 0 |
| 36 | 4L | 785 | 0 | 809 | 8 | 0 |
| 37 | 6 | 1331 | 0 | 1439 | 19 | 0 |
| 38 | A7 | 725 | 0 | 721 | 11 | 0 |
| 39 | A5 | 914 | 0 | 944 | 8 | 0 |
| 40 | A3 | 528 | 0 | 521 | 9 | 0 |
| 41 | A6 | 968 | 0 | 991 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 42 | AL | 3008 | 0 | 2945 | 28 | 0 |
| 43 | 5 | 143 | 0 | 177 | 1 | 0 |
| 43 | A9 | 101 | 0 | 90 | 2 | 0 |
| 43 | AN | 67 | 0 | 78 | 3 | 0 |
| 43 | B5 | 74 | 0 | 95 | 4 | 0 |
| 43 | B6 | 53 | 0 | 50 | 1 | 0 |
| 43 | S7 | 71 | 0 | 86 | 2 | 0 |
| 44 | S6 | 1 | 0 | 0 | 0 | 0 |
| 45 | S1 | 16 | 0 | 0 | 0 | 0 |
| 45 | S7 | 8 | 0 | 0 | 5 | 0 |
| 45 | S8 | 16 | 0 | 0 | 1 | 0 |
| 45 | V1 | 8 | 0 | 0 | 1 | 0 |
| 46 | S1 | 4 | 0 | 0 | 0 | 0 |
| 46 | V2 | 4 | 0 | 0 | 0 | 0 |
| 47 | 1 | 54 | 0 | 88 | 1 | 0 |
| 47 | 2 | 89 | 0 | 132 | 3 | 0 |
| 47 | 4 | 83 | 0 | 114 | 7 | 0 |
| 47 | 6 | 65 | 0 | 78 | 2 | 0 |
| 47 | AM | 70 | 0 | 88 | 3 | 0 |
| 47 | B4 | 34 | 0 | 42 | 1 | 0 |
| 47 | B6 | 37 | 0 | 48 | 1 | 0 |
| 47 | C2 | 39 | 0 | 52 | 2 | 0 |
| 47 | S7 | 82 | 0 | 115 | 3 | 0 |
| 48 | 2 | 39 | 0 | 52 | 3 | 0 |
| 48 | 4 | 74 | 0 | 96 | 4 | 0 |
| 48 | 5 | 248 | 0 | 358 | 8 | 0 |
| 48 | AM | 107 | 0 | 136 | 4 | 0 |
| 48 | B6 | 44 | 0 | 65 | 2 | 0 |
| 49 | AB | 34 | 0 | 40 | 0 | 0 |
| 49 | B9 | 34 | 0 | 40 | 2 | 0 |
| 50 | A9 | 48 | 0 | 26 | 0 | 0 |
| 51 | V1 | 31 | 0 | 19 | 0 | 0 |
| 52 | AL | 31 | 0 | 12 | 3 | 0 |
| All | All | 66555 | 0 | 66754 | 690 | 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 5.

The worst 5 of 690 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) |
|---|---|---|---|
| 34:V1:397:CYS:SG | 34:V1:400:CYS:HB3 | 1.99 | 1.02 |
| 34:V1:413:ARG:NH2 | 34:V1:423:GLU:OE2 | 1.93 | 1.00 |
| 10:4:197:MET:HB2 | 10:4:200:VAL:HG22 | 1.50 | 0.91 |
| 22:B9:15:VAL:HG11 | 49:B9:201:ZMP:H19B | 1.51 | 0.90 |
| 34:V1:419:ALA:HB1 | 34:V1:423:GLU:OE1 | 1.73 | 0.87 |

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 | AN | 135/142 (95%) | 134 (99%) | 1 (1%) | 0 | 100 | 100 |
| 2 | S6 | 88/126 (70%) | 87 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | S1 | 676/731 (92%) | 653 (97%) | 23 (3%) | 0 | 100 | 100 |
| 4 | S3 | 206/265 (78%) | 202 (98%) | 4 (2%) | 0 | 100 | 100 |
| 5 | V2 | 212/242 (88%) | 206 (97%) | 6 (3%) | 0 | 100 | 100 |
| 6 | S7 | 180/221 (81%) | 173 (96%) | 6 (3%) | 1 (1%) | 22 | 53 |
| 7 | S8 | 184/217 (85%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 8 | 3 | 101/117 (86%) | 101 (100%) | 0 | 0 | 100 | 100 |
| 9 | 1 | 313/315 (99%) | 300 (96%) | 13 (4%) | 0 | 100 | 100 |
| 10 | 4 | 444/446 (100%) | 430 (97%) | 13 (3%) | 1 (0%) | 44 | 71 |
| 11 | 5 | 575/577 (100%) | 547 (95%) | 28 (5%) | 0 | 100 | 100 |
| 12 | A8 | 172/175 (98%) | 167 (97%) | 5 (3%) | 0 | 100 | 100 |
| 13 | A1 | 68/123 (55%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 14 | AO | 142/154 (92%) | 141 (99%) | 1 (1%) | 0 | 100 | 100 |
| 15 | S5 | 98/101 (97%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 16 | AM | 162/170 (95%) | 159 (98%) | 3 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 17 | BL | 148/159 (93%) | 144 (97%) | 4 (3%) | 0 | 100 | 100 |
| 18 | B6 | 159/167 (95%) | 154 (97%) | 5 (3%) | 0 | 100 | 100 |
| 19 | B4 | 108/113 (96%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | B7 | 109/117 (93%) | 108 (99%) | 1 (1%) | 0 | 100 | 100 |
| 21 | B5 | 141/186 (76%) | 139 (99%) | 2 (1%) | 0 | 100 | 100 |
| 22 | B9 | 131/144 (91%) | 130 (99%) | 1 (1%) | 0 | 100 | 100 |
| 23 | BM | 104/150 (69%) | 102 (98%) | 2 (2%) | 0 | 100 | 100 |
| 24 | B8 | 142/175 (81%) | 134 (94%) | 8 (6%) | 0 | 100 | 100 |
| 25 | B3 | 79/110 (72%) | 75 (95%) | 4 (5%) | 0 | 100 | 100 |
| 26 | AB | 79/152 (52%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | AC | 82/152 (54%) | 81 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | C2 | 113/116 (97%) | 111 (98%) | 2 (2%) | 0 | 100 | 100 |
| 28 | B1 | 53/56 (95%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |
| 29 | S4 | 124/183 (68%) | 120 (97%) | 4 (3%) | 0 | 100 | 100 |
| 30 | A9 | 366/416 (88%) | 352 (96%) | 14 (4%) | 0 | 100 | 100 |
| 31 | B2 | 57/94 (61%) | 57 (100%) | 0 | 0 | 100 | 100 |
| 32 | S2 | 415/468 (89%) | 404 (97%) | 11 (3%) | 0 | 100 | 100 |
| 34 | V1 | 437/474 (92%) | 417 (95%) | 19 (4%) | 1 (0%) | 44 | 71 |
| 35 | 2 | 339/341 (99%) | 330 (97%) | 9 (3%) | 0 | 100 | 100 |
| 36 | 4L | 93/96 (97%) | 93 (100%) | 0 | 0 | 100 | 100 |
| 37 | 6 | 163/174 (94%) | 157 (96%) | 6 (4%) | 0 | 100 | 100 |
| 38 | A7 | 86/103 (84%) | 85 (99%) | 1 (1%) | 0 | 100 | 100 |
| 39 | A5 | 115/124 (93%) | 111 (96%) | 4 (4%) | 0 | 100 | 100 |
| 40 | A3 | 65/77 (84%) | 65 (100%) | 0 | 0 | 100 | 100 |
| 41 | A6 | 112/124 (90%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 42 | AL | 366/407 (90%) | 353 (96%) | 13 (4%) | 0 | 100 | 100 |
| All | All | 7942/9000 (88%) | 7702 (97%) | 237 (3%) | 3 (0%) | 100 | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | 4 | 202 | LEU |
| 6 | S7 | 192 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | V1 | 424 | ILE |

### 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 | AN | 118/122 (97%) | 117 (99%) | 1 (1%) | 79 87 |
| 2 | S6 | 78/111 (70%) | 77 (99%) | 1 (1%) | 65 79 |
| 3 | S1 | 549/582 (94%) | 545 (99%) | 4 (1%) | 81 88 |
| 4 | S3 | 186/225 (83%) | 186 (100%) | 0 | 100 100 |
| 5 | V2 | 185/205 (90%) | 184 (100%) | 1 (0%) | 86 91 |
| 6 | S7 | 152/184 (83%) | 150 (99%) | 2 (1%) | 65 79 |
| 7 | S8 | 159/182 (87%) | 159 (100%) | 0 | 100 100 |
| 8 | 3 | 98/110 (89%) | 97 (99%) | 1 (1%) | 73 84 |
| 9 | 1 | 282/282 (100%) | 280 (99%) | 2 (1%) | 81 88 |
| 10 | 4 | 402/404 (100%) | 400 (100%) | 2 (0%) | 86 91 |
| 11 | 5 | 518/518 (100%) | 516 (100%) | 2 (0%) | 89 93 |
| 12 | A8 | 150/151 (99%) | 150 (100%) | 0 | 100 100 |
| 13 | A1 | 63/115 (55%) | 63 (100%) | 0 | 100 100 |
| 14 | AO | 126/134 (94%) | 126 (100%) | 0 | 100 100 |
| 15 | S5 | 88/89 (99%) | 81 (92%) | 7 (8%) | 10 32 |
| 16 | AM | 125/131 (95%) | 123 (98%) | 2 (2%) | 58 76 |
| 17 | BL | 133/141 (94%) | 133 (100%) | 0 | 100 100 |
| 18 | B6 | 133/136 (98%) | 132 (99%) | 1 (1%) | 79 87 |
| 19 | B4 | 91/94 (97%) | 91 (100%) | 0 | 100 100 |
| 20 | B7 | 100/104 (96%) | 99 (99%) | 1 (1%) | 73 84 |
| 21 | B5 | 129/162 (80%) | 127 (98%) | 2 (2%) | 58 76 |
| 22 | B9 | 116/126 (92%) | 115 (99%) | 1 (1%) | 75 85 |
| 23 | BM | 95/131 (72%) | 94 (99%) | 1 (1%) | 70 82 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 24 | B8 | 121/145 (83%) | 118 (98%) | 3 (2%) | 42 67 |
| 25 | B3 | 66/84 (79%) | 66 (100%) | 0 | 100 100 |
| 26 | AB | 75/136 (55%) | 73 (97%) | 2 (3%) | 40 65 |
| 26 | AC | 78/136 (57%) | 78 (100%) | 0 | 100 100 |
| 27 | C2 | 92/94 (98%) | 87 (95%) | 5 (5%) | 18 46 |
| 28 | B1 | 42/43 (98%) | 42 (100%) | 0 | 100 100 |
| 29 | S4 | 110/154 (71%) | 110 (100%) | 0 | 100 100 |
| 30 | A9 | 313/346 (90%) | 312 (100%) | 1 (0%) | 91 94 |
| 31 | B2 | 50/80 (62%) | 49 (98%) | 1 (2%) | 50 71 |
| 32 | S2 | 358/398 (90%) | 358 (100%) | 0 | 100 100 |
| 34 | V1 | 351/381 (92%) | 350 (100%) | 1 (0%) | 91 94 |
| 35 | 2 | 317/317 (100%) | 316 (100%) | 1 (0%) | 91 94 |
| 36 | 4L | 90/91 (99%) | 90 (100%) | 0 | 100 100 |
| 37 | 6 | 159/167 (95%) | 157 (99%) | 2 (1%) | 65 79 |
| 38 | A7 | 77/86 (90%) | 77 (100%) | 0 | 100 100 |
| 39 | A5 | 96/102 (94%) | 96 (100%) | 0 | 100 100 |
| 40 | A3 | 53/59 (90%) | 53 (100%) | 0 | 100 100 |
| 41 | A6 | 107/114 (94%) | 104 (97%) | 3 (3%) | 38 64 |
| 42 | AL | 324/356 (91%) | 323 (100%) | 1 (0%) | 91 94 |
| All | All | 6955/7728 (90%) | 6904 (99%) | 51 (1%) | 80 88 |

5 of 51 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | B5 | 46 | MET |
| 27 | C2 | 104 | THR |
| 26 | AB | 81 | LEU |
| 22 | B9 | 50 | ASN |
| 24 | B8 | 61 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | S1 | 134 | HIS |
| 35 | 2 | 181 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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 | PC1 | 1 | 401 | - | 53,53,53 | 0.32 | 0 | 59,61,61 | 0.54 | 1 (1%) |
| 48 | 3PE | 5 | 607 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.30 | 0 |
| 47 | PC1 | 6 | 202 | - | 28,28,53 | 0.41 | 0 | 34,36,61 | 0.40 | 0 |
| 45 | SF4 | S1 | 802 | 3 | 0,12,12 | - | - | - | | |
| 48 | 3PE | B6 | 202 | - | 43,43,50 | 0.35 | 0 | 46,48,55 | 0.73 | 3 (6%) |
| 43 | CDL | 5 | 604 | - | 67,67,99 | 0.35 | 0 | 73,79,111 | 0.32 | 0 |
| 46 | FES | S1 | 803 | 3 | 0,4,4 | - | - | - | | |
| 47 | PC1 | C2 | 201 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.35 | 0 |
| 49 | ZMP | AB | 201 | - | 28,33,36 | 0.81 | 2 (7%) | 32,40,45 | 3.16 | 9 (28%) |
| 45 | SF4 | S8 | 302 | 7 | 0,12,12 | - | - | - | | |
| 51 | FMN | V1 | 501 | - | 33,33,33 | 0.25 | 0 | 48,50,50 | 0.37 | 0 |
| 48 | 3PE | 5 | 603 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.29 | 0 |
| 43 | CDL | S7 | 302 | - | 70,70,99 | 0.34 | 0 | 76,82,111 | 0.28 | 0 |
| 45 | SF4 | S7 | 301 | 6 | 0,12,12 | - | - | - | | |
| 47 | PC1 | S7 | 303 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.43 | 0 |
| 48 | 3PE | 5 | 601 | - | 31,31,50 | 0.37 | 0 | 34,36,55 | 0.33 | 0 |
| 48 | 3PE | AM | 204 | - | 31,31,50 | 0.37 | 0 | 34,36,55 | 0.32 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 52 | DGT | AL | 501 | - | 29,33,33 | 0.97 | 3 (10%) | 37,52,52 | 0.75 | 1 (2%) |
| 43 | CDL | B6 | 203 | - | 52,52,99 | 0.41 | 0 | 58,64,111 | 0.56 | 1 (1%) |
| 47 | PC1 | AM | 205 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.37 | 0 |
| 45 | SF4 | S8 | 301 | 7 | 0,12,12 | - | - | - | | |
| 43 | CDL | A9 | 503 | - | 46,46,99 | 0.44 | 0 | 52,58,111 | 0.59 | 1 (1%) |
| 47 | PC1 | 2 | 402 | - | 43,43,53 | 0.31 | 0 | 49,51,61 | 0.33 | 0 |
| 43 | CDL | A9 | 502 | - | 53,53,99 | 0.40 | 0 | 59,65,111 | 0.36 | 0 |
| 43 | CDL | 5 | 608 | - | 74,74,99 | 0.34 | 0 | 80,86,111 | 0.30 | 0 |
| 48 | 3PE | 4 | 503 | - | 34,34,50 | 0.36 | 0 | 37,39,55 | 0.36 | 0 |
| 48 | 3PE | AM | 201 | - | 38,38,50 | 0.34 | 0 | 41,43,55 | 0.29 | 0 |
| 43 | CDL | B5 | 201 | - | 73,73,99 | 0.34 | 0 | 79,85,111 | 0.31 | 0 |
| 48 | 3PE | 2 | 401 | - | 38,38,50 | 0.37 | 0 | 41,43,55 | 0.63 | 1 (2%) |
| 47 | PC1 | 4 | 502 | - | 43,43,53 | 0.33 | 0 | 49,51,61 | 0.32 | 0 |
| 48 | 3PE | AM | 203 | - | 35,35,50 | 0.36 | 0 | 38,40,55 | 0.32 | 0 |
| 47 | PC1 | B4 | 201 | - | 33,33,53 | 0.35 | 0 | 39,41,61 | 0.36 | 0 |
| 48 | 3PE | 5 | 605 | - | 35,35,50 | 0.38 | 0 | 38,40,55 | 0.65 | 1 (2%) |
| 48 | 3PE | 5 | 602 | - | 32,32,50 | 0.37 | 0 | 35,37,55 | 0.36 | 0 |
| 45 | SF4 | S1 | 801 | 3 | 0,12,12 | - | - | - | | |
| 47 | PC1 | B6 | 201 | - | 36,36,53 | 0.36 | 0 | 42,44,61 | 0.64 | 1 (2%) |
| 47 | PC1 | 2 | 403 | - | 44,44,53 | 0.34 | 0 | 50,52,61 | 0.33 | 0 |
| 47 | PC1 | 4 | 501 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.36 | 0 |
| 48 | 3PE | 5 | 606 | - | 44,44,50 | 0.32 | 0 | 47,49,55 | 0.43 | 0 |
| 45 | SF4 | V1 | 502 | 34 | 0,12,12 | - | - | - | | |
| 47 | PC1 | AM | 202 | - | 36,36,53 | 0.34 | 0 | 42,44,61 | 0.34 | 0 |
| 46 | FES | V2 | 301 | 5 | 0,4,4 | - | - | - | | |
| 50 | NDP | A9 | 501 | - | 47,52,52 | 0.55 | 0 | 61,80,80 | 0.53 | 1 (1%) |
| 48 | 3PE | 4 | 504 | - | 38,38,50 | 0.36 | 0 | 41,43,55 | 0.64 | 1 (2%) |
| 47 | PC1 | 6 | 201 | - | 35,35,53 | 0.34 | 0 | 41,43,61 | 0.35 | 0 |
| 49 | ZMP | B9 | 201 | - | 28,33,36 | 0.23 | 0 | 32,40,45 | 0.34 | 0 |
| 43 | CDL | AN | 201 | - | 66,66,99 | 0.35 | 0 | 72,78,111 | 0.31 | 0 |
| 47 | PC1 | S7 | 304 | - | 45,45,53 | 0.33 | 0 | 51,53,61 | 0.31 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 47 | PC1 | 1 | 401 | - | - | 18/57/57/57 | - |
| 48 | 3PE | 5 | 607 | - | - | 12/54/54/54 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 47 | PC1 | 6 | 202 | - | - | 9/32/32/57 | - |
| 48 | 3PE | B6 | 202 | - | - | 12/47/47/54 | - |
| 45 | SF4 | S1 | 802 | 3 | - | - | 0/6/5/5 |
| 43 | CDL | 5 | 604 | - | - | 15/78/78/110 | - |
| 46 | FES | S1 | 803 | 3 | - | - | 0/1/1/1 |
| 47 | PC1 | C2 | 201 | - | - | 11/42/42/57 | - |
| 49 | ZMP | AB | 201 | - | - | 20/38/40/43 | - |
| 45 | SF4 | S8 | 302 | 7 | - | - | 0/6/5/5 |
| 51 | FMN | V1 | 501 | - | - | 8/18/18/18 | 0/3/3/3 |
| 48 | 3PE | 5 | 603 | - | - | 11/54/54/54 | - |
| 43 | CDL | S7 | 302 | - | - | 10/81/81/110 | - |
| 47 | PC1 | S7 | 303 | - | - | 9/39/39/57 | - |
| 48 | 3PE | 5 | 601 | - | - | 4/35/35/54 | - |
| 48 | 3PE | AM | 204 | - | - | 4/35/35/54 | - |
| 52 | DGT | AL | 501 | - | - | 4/18/34/34 | 0/3/3/3 |
| 45 | SF4 | S7 | 301 | 6 | - | - | 0/6/5/5 |
| 43 | CDL | B6 | 203 | - | - | 17/63/63/110 | - |
| 47 | PC1 | AM | 205 | - | - | 12/36/36/57 | - |
| 45 | SF4 | S8 | 301 | 7 | - | - | 0/6/5/5 |
| 43 | CDL | A9 | 503 | - | - | 18/57/57/110 | - |
| 47 | PC1 | 2 | 402 | - | - | 8/47/47/57 | - |
| 43 | CDL | A9 | 502 | - | - | 15/64/64/110 | - |
| 43 | CDL | 5 | 608 | - | - | 11/85/85/110 | - |
| 48 | 3PE | 4 | 503 | - | - | 7/38/38/54 | - |
| 48 | 3PE | AM | 201 | - | - | 7/42/42/54 | - |
| 43 | CDL | B5 | 201 | - | - | 17/84/84/110 | - |
| 48 | 3PE | 2 | 401 | - | - | 10/42/42/54 | - |
| 47 | PC1 | 4 | 502 | - | - | 9/47/47/57 | - |
| 48 | 3PE | AM | 203 | - | - | 12/39/39/54 | - |
| 47 | PC1 | B4 | 201 | - | - | 9/37/37/57 | - |
| 48 | 3PE | 5 | 605 | - | - | 3/39/39/54 | - |
| 48 | 3PE | 5 | 602 | - | - | 6/36/36/54 | - |
| 45 | SF4 | S1 | 801 | 3 | - | - | 0/6/5/5 |
| 47 | PC1 | B6 | 201 | - | - | 11/40/40/57 | - |
| 47 | PC1 | 2 | 403 | - | - | 12/48/48/57 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 47 | PC1 | 4 | 501 | - | - | 4/42/42/57 | - |
| 48 | 3PE | 5 | 606 | - | - | 15/48/48/54 | - |
| 47 | PC1 | AM | 202 | - | - | 5/40/40/57 | - |
| 45 | SF4 | V1 | 502 | 34 | - | - | 0/6/5/5 |
| 46 | FES | V2 | 301 | 5 | - | - | 0/1/1/1 |
| 50 | NDP | A9 | 501 | - | - | 5/30/77/77 | 0/5/5/5 |
| 48 | 3PE | 4 | 504 | - | - | 6/42/42/54 | - |
| 47 | PC1 | 6 | 201 | - | - | 11/39/39/57 | - |
| 49 | ZMP | B9 | 201 | - | - | 26/38/40/43 | - |
| 43 | CDL | AN | 201 | - | - | 13/77/77/110 | - |
| 47 | PC1 | S7 | 304 | - | - | 10/49/49/57 | - |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | AL | 501 | DGT | C5-C6 | -2.77 | 1.42 | 1.47 |
| 49 | AB | 201 | ZMP | C9-C10 | 2.33 | 1.53 | 1.50 |
| 49 | AB | 201 | ZMP | O4-C17 | 2.23 | 1.46 | 1.42 |
| 52 | AL | 501 | DGT | C8-N7 | -2.19 | 1.31 | 1.34 |
| 52 | AL | 501 | DGT | C5-C4 | -2.04 | 1.38 | 1.43 |

The worst 5 of 21 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 49 | AB | 201 | ZMP | C19-C18-C17 | -7.99 | 95.14 | 108.77 |
| 49 | AB | 201 | ZMP | C19-C18-C21 | 7.69 | 120.91 | 108.22 |
| 49 | AB | 201 | ZMP | C20-C18-C21 | 7.68 | 120.90 | 108.22 |
| 49 | AB | 201 | ZMP | C20-C18-C17 | -7.50 | 95.98 | 108.77 |
| 49 | AB | 201 | ZMP | C20-C18-C19 | 4.49 | 118.16 | 109.20 |

There are no chirality outliers.

5 of 426 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | AN | 201 | CDL | CA2-OA2-PA1-OA3 |
| 43 | AN | 201 | CDL | CA2-OA2-PA1-OA4 |
| 43 | AN | 201 | CDL | CA2-OA2-PA1-OA5 |
| 43 | AN | 201 | CDL | CA3-OA5-PA1-OA2 |
| 43 | AN | 201 | CDL | CB3-OB5-PB2-OB2 |

There are no ring outliers.

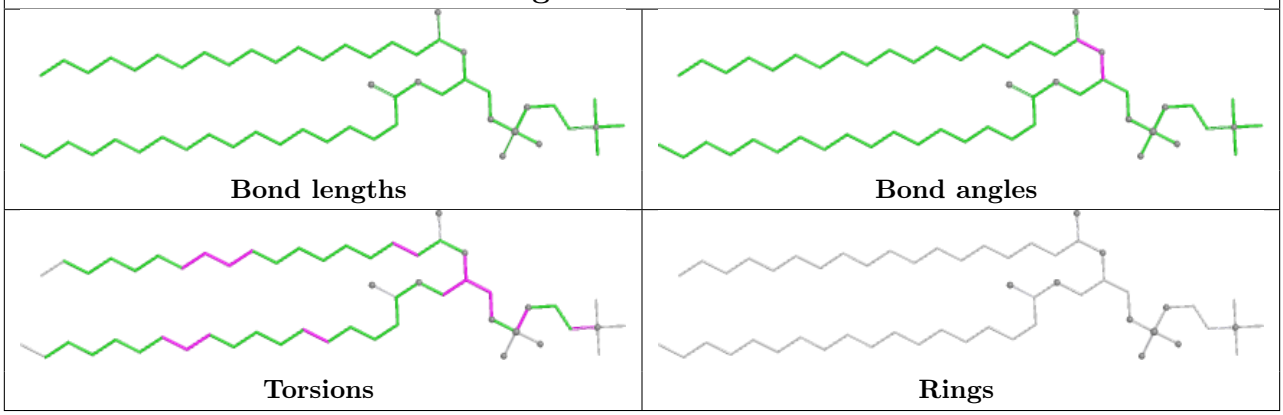
37 monomers are involved in 61 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 47 | 1 | 401 | PC1 | 1 | 0 |
| 48 | 5 | 607 | 3PE | 1 | 0 |
| 47 | 6 | 202 | PC1 | 1 | 0 |
| 48 | B6 | 202 | 3PE | 2 | 0 |
| 43 | 5 | 604 | CDL | 1 | 0 |
| 47 | C2 | 201 | PC1 | 2 | 0 |
| 48 | 5 | 603 | 3PE | 2 | 0 |
| 43 | S7 | 302 | CDL | 2 | 0 |
| 45 | S7 | 301 | SF4 | 5 | 0 |
| 47 | S7 | 303 | PC1 | 1 | 0 |
| 48 | 5 | 601 | 3PE | 2 | 0 |
| 48 | AM | 204 | 3PE | 2 | 0 |
| 52 | AL | 501 | DGT | 3 | 0 |
| 43 | B6 | 203 | CDL | 1 | 0 |
| 47 | AM | 205 | PC1 | 3 | 0 |
| 45 | S8 | 301 | SF4 | 1 | 0 |
| 43 | A9 | 503 | CDL | 1 | 0 |
| 47 | 2 | 402 | PC1 | 1 | 0 |
| 43 | A9 | 502 | CDL | 1 | 0 |
| 48 | 4 | 503 | 3PE | 2 | 0 |
| 48 | AM | 201 | 3PE | 1 | 0 |
| 43 | B5 | 201 | CDL | 4 | 0 |
| 48 | 2 | 401 | 3PE | 3 | 0 |
| 47 | 4 | 502 | PC1 | 4 | 0 |
| 48 | AM | 203 | 3PE | 1 | 0 |
| 47 | B4 | 201 | PC1 | 1 | 0 |
| 48 | 5 | 605 | 3PE | 1 | 0 |
| 48 | 5 | 602 | 3PE | 2 | 0 |
| 47 | B6 | 201 | PC1 | 1 | 0 |
| 47 | 2 | 403 | PC1 | 2 | 0 |
| 47 | 4 | 501 | PC1 | 3 | 0 |
| 45 | V1 | 502 | SF4 | 1 | 0 |
| 48 | 4 | 504 | 3PE | 2 | 0 |
| 47 | 6 | 201 | PC1 | 1 | 0 |
| 49 | B9 | 201 | ZMP | 2 | 0 |
| 43 | AN | 201 | CDL | 3 | 0 |
| 47 | S7 | 304 | PC1 | 2 | 0 |

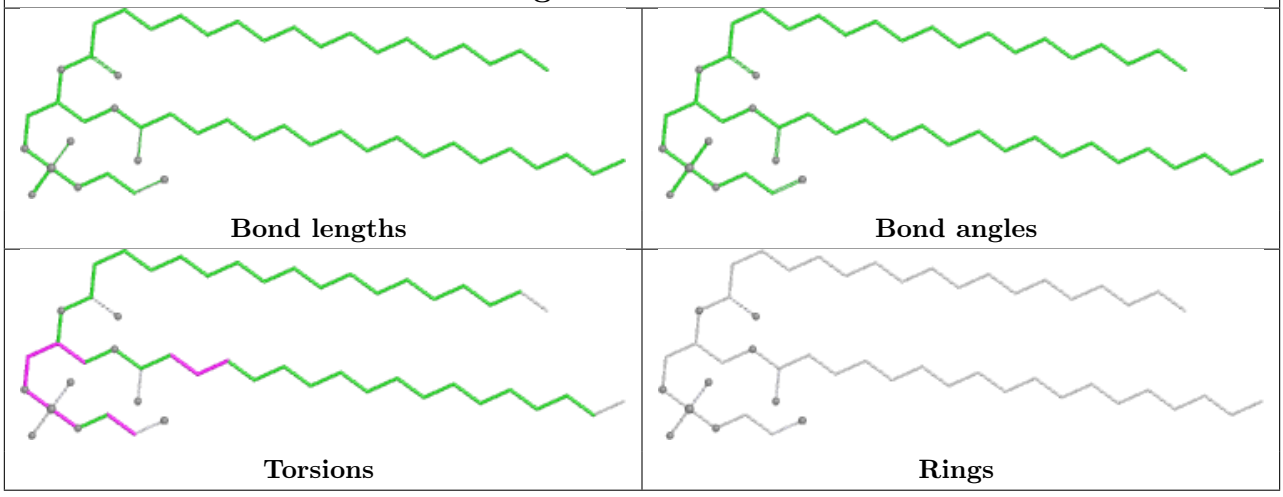
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

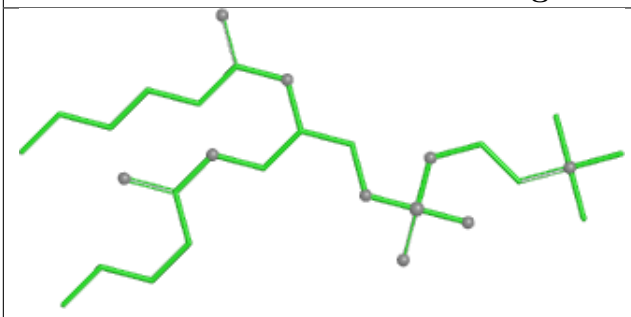
**Ligand PC1 1 401**



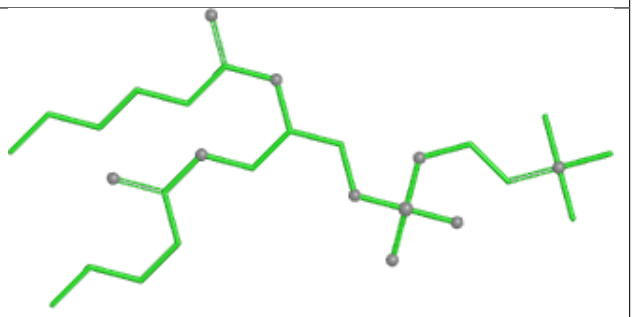

**Ligand 3PE 5 607**



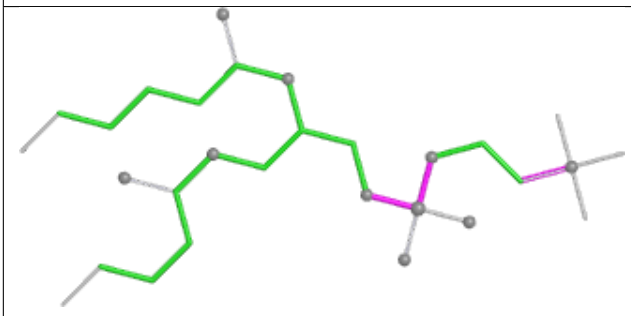
**Ligand PC1 6 202**



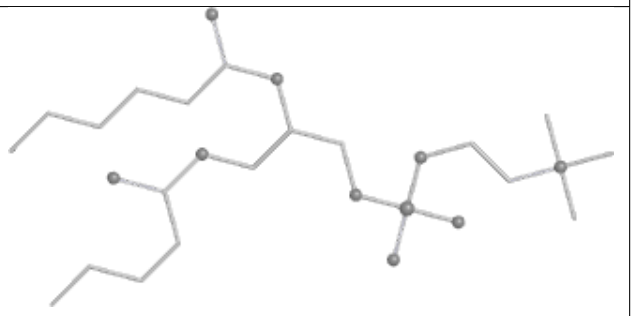
Bond lengths



Bond angles

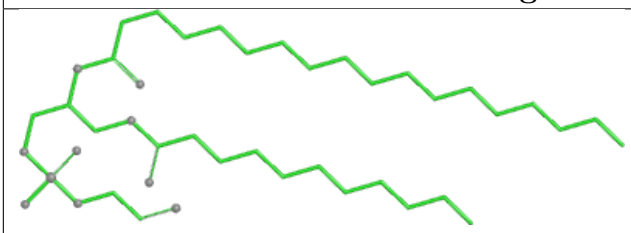


Torsions

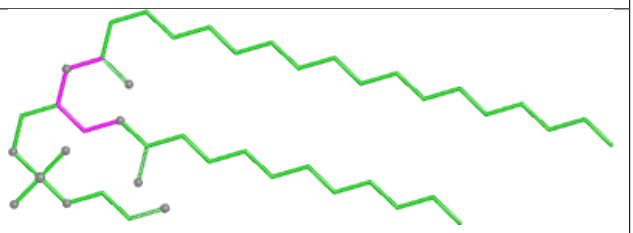


Rings

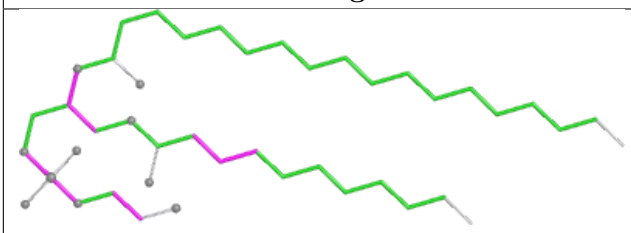
**Ligand 3PE B6 202**



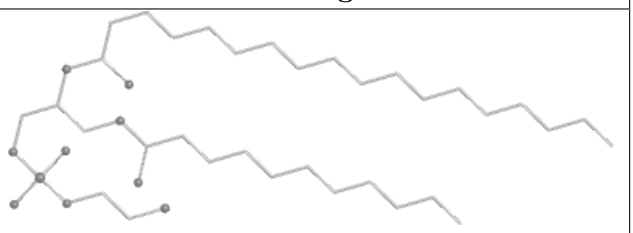
Bond lengths



Bond angles

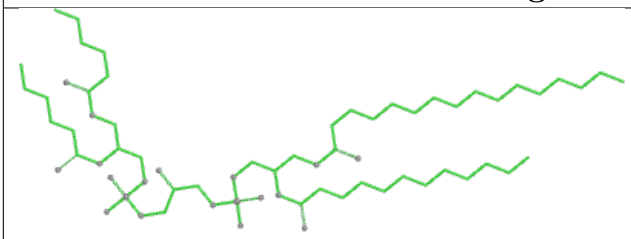


Torsions

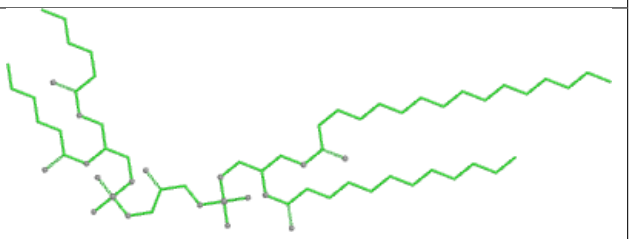


Rings

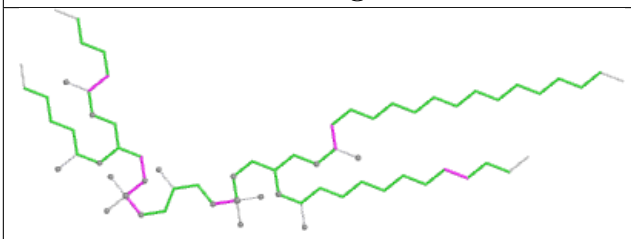
## Ligand CDL 5 604



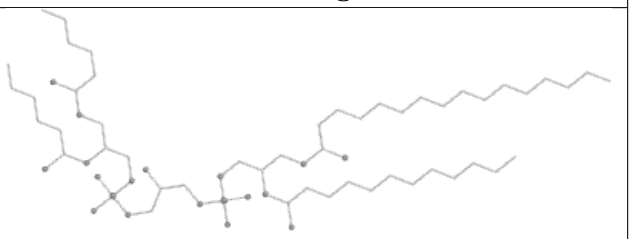
Bond lengths



Bond angles

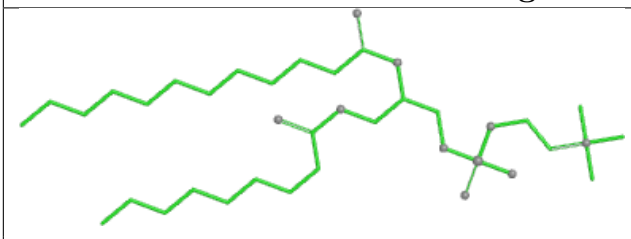


Torsions

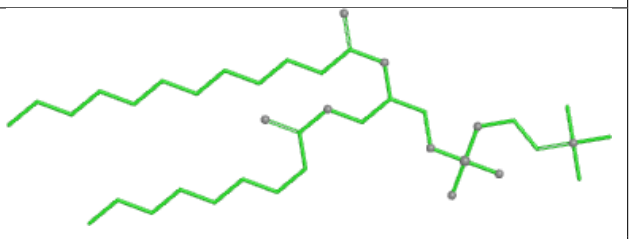


Rings

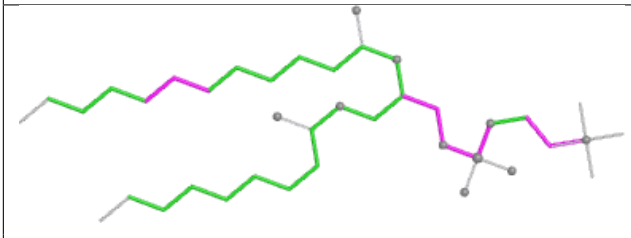
## Ligand PC1 C2 201



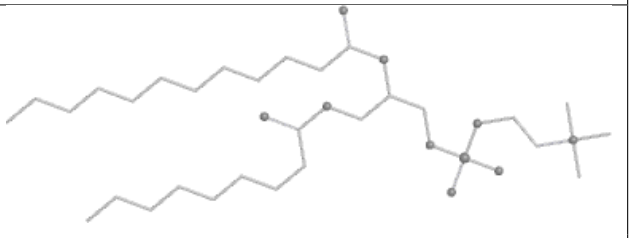
Bond lengths



Bond angles

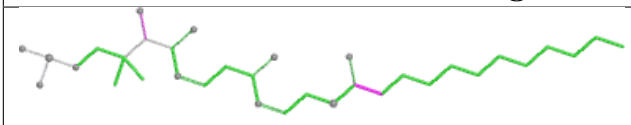


Torsions

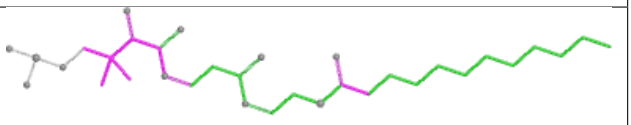


Rings

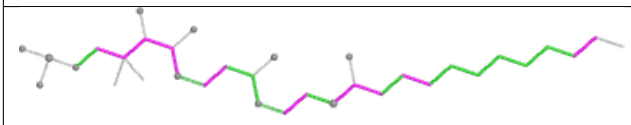
## Ligand ZMP AB 201



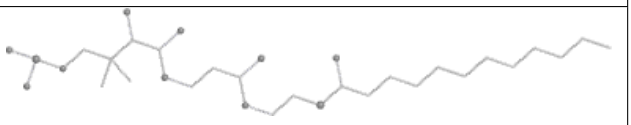
Bond lengths



Bond angles

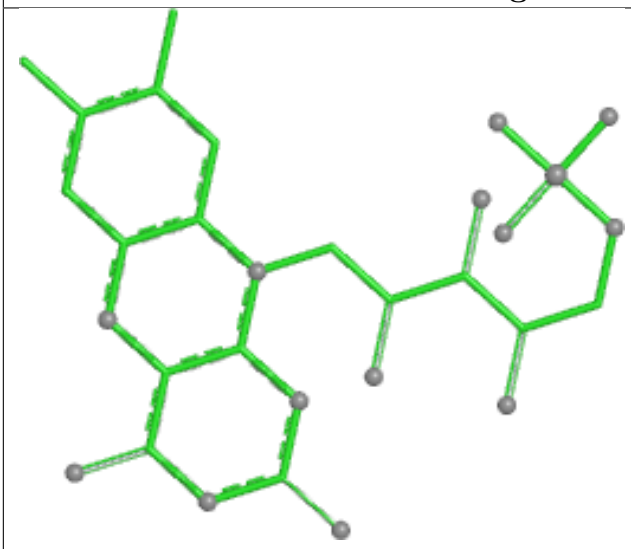


Torsions

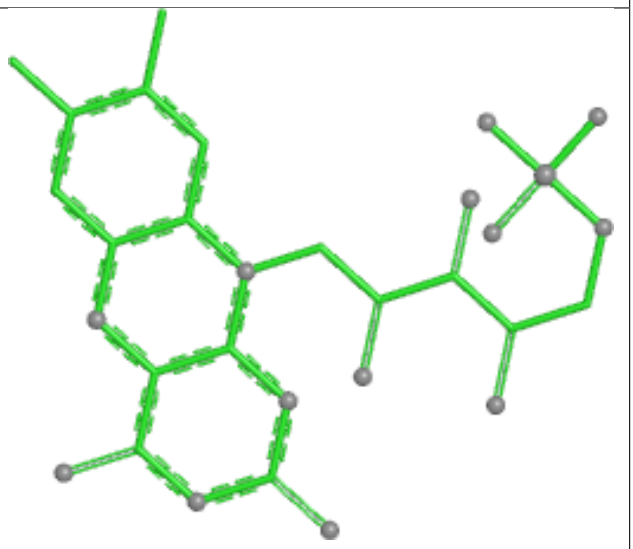


Rings

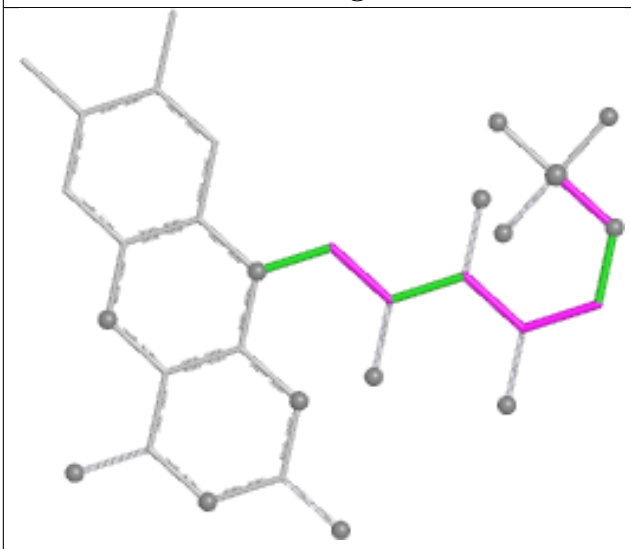
**Ligand FMN V1 501**



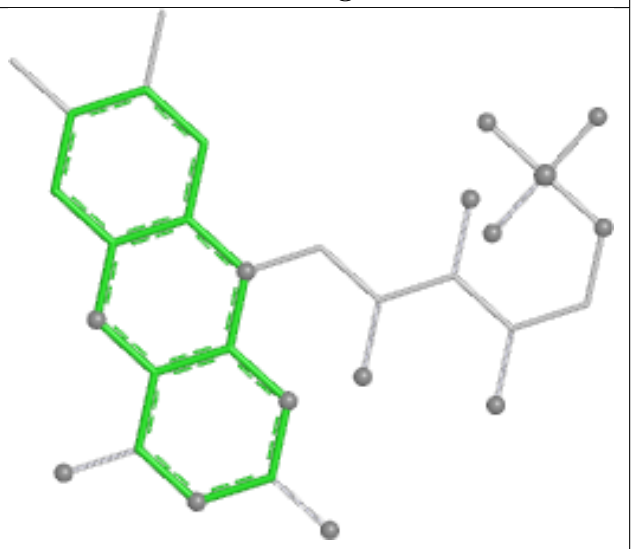
Bond lengths



Bond angles

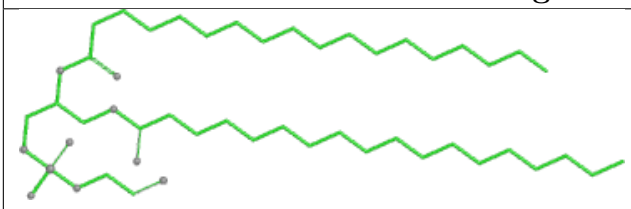


Torsions

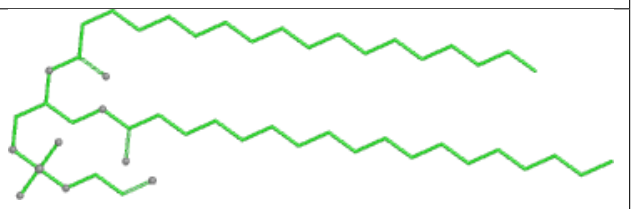


Rings

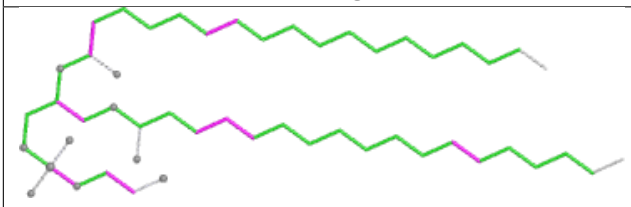
**Ligand 3PE 5 603**



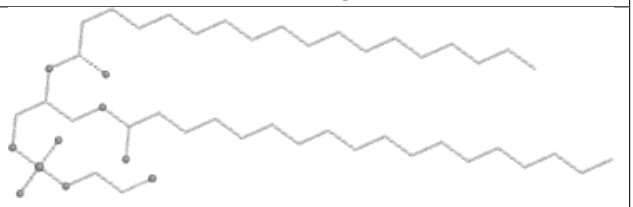
Bond lengths



Bond angles

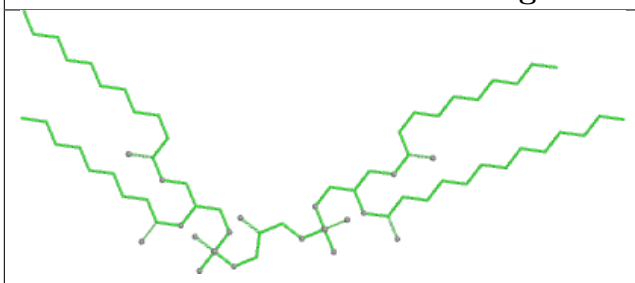


Torsions

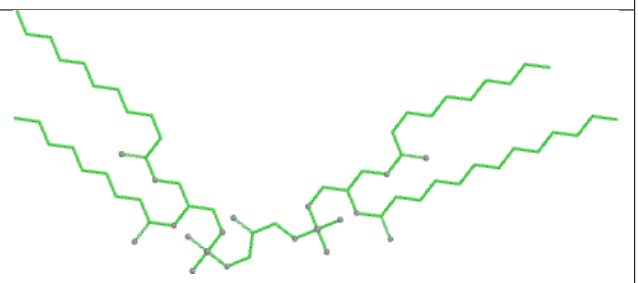


Rings

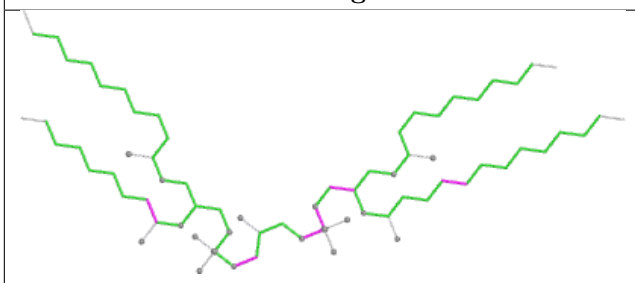
**Ligand CDL S7 302**



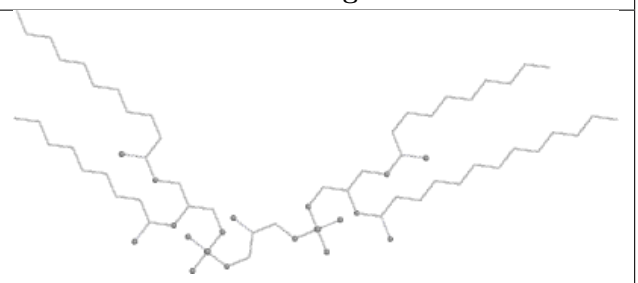
Bond lengths



Bond angles

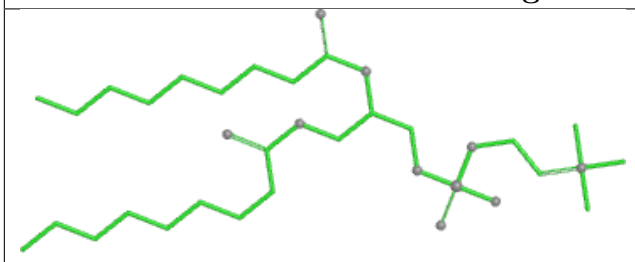


Torsions

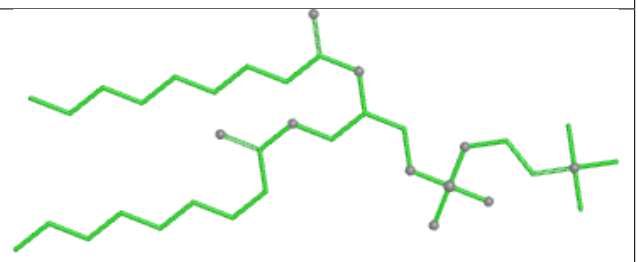


Rings

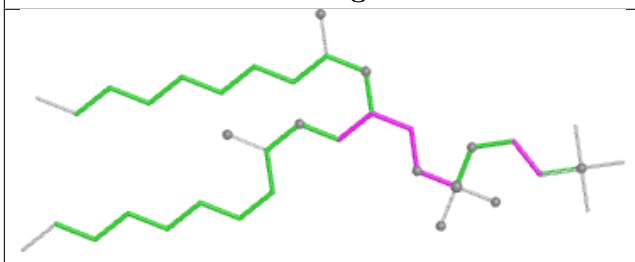
**Ligand PC1 S7 303**



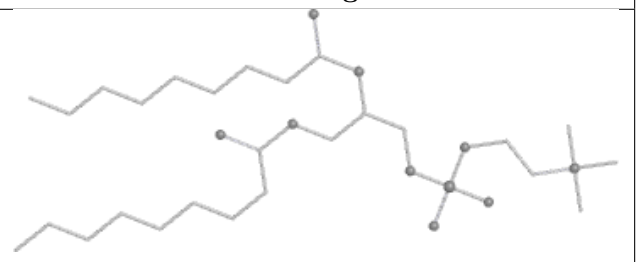
Bond lengths



Bond angles

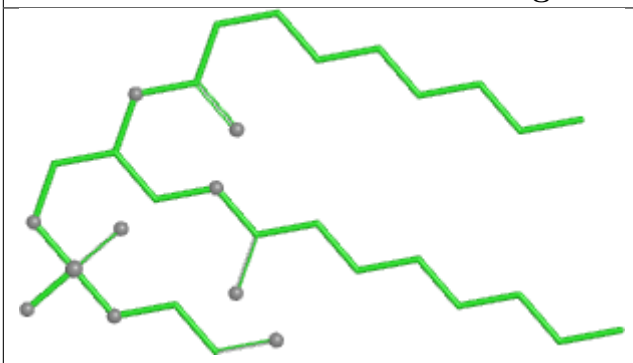


Torsions

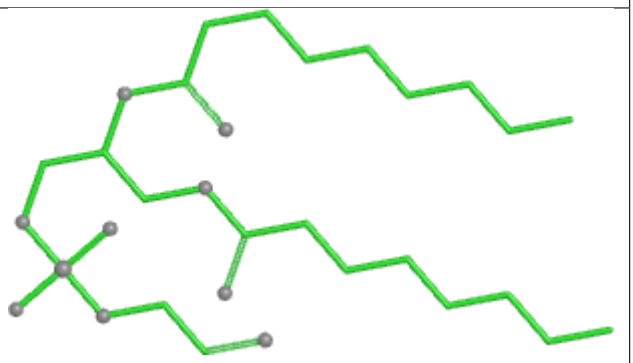


Rings

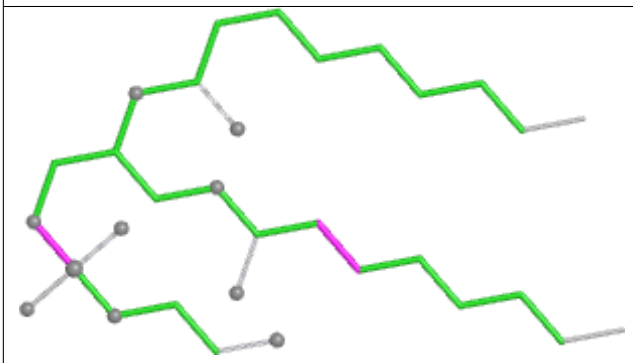
**Ligand 3PE 5 601**



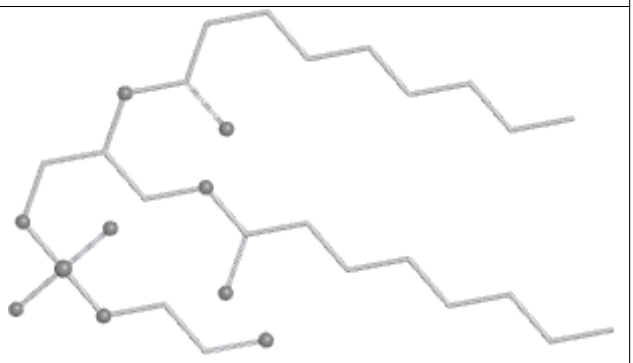
Bond lengths



Bond angles

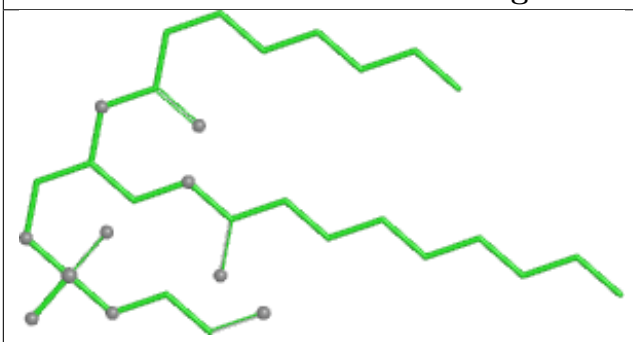


Torsions

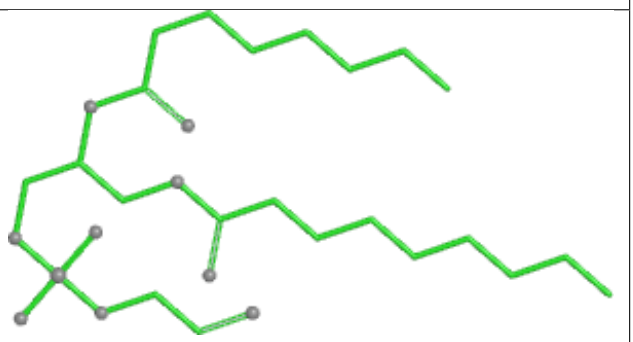


Rings

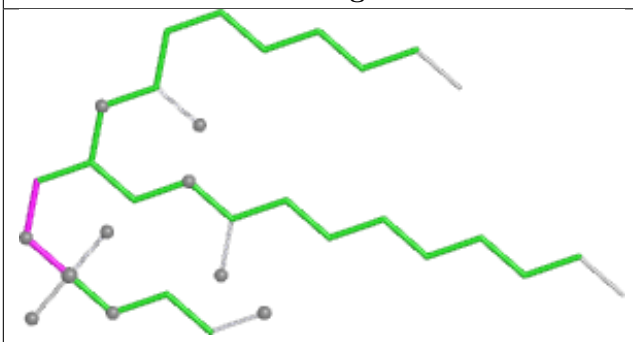
**Ligand 3PE AM 204**



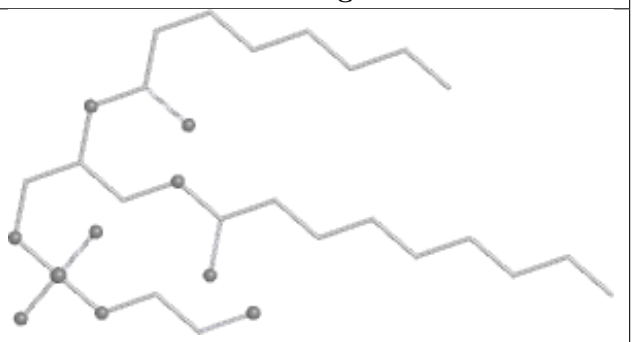
Bond lengths



Bond angles

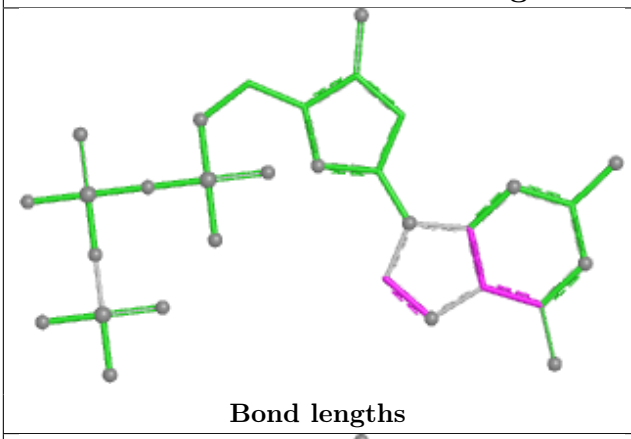


Torsions

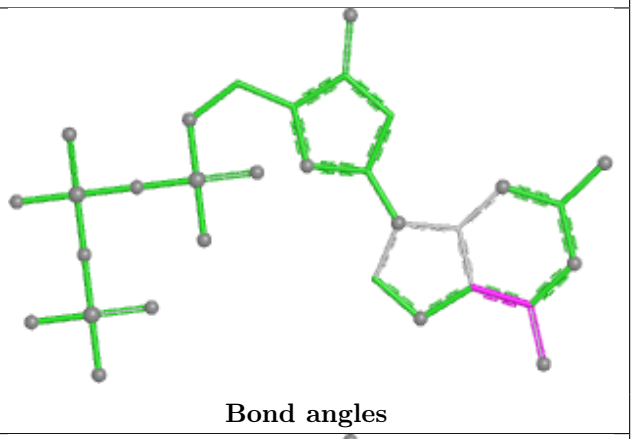


Rings

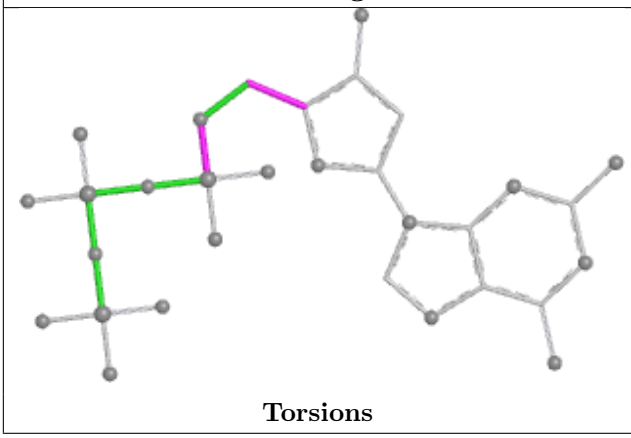
## Ligand DGT AL 501



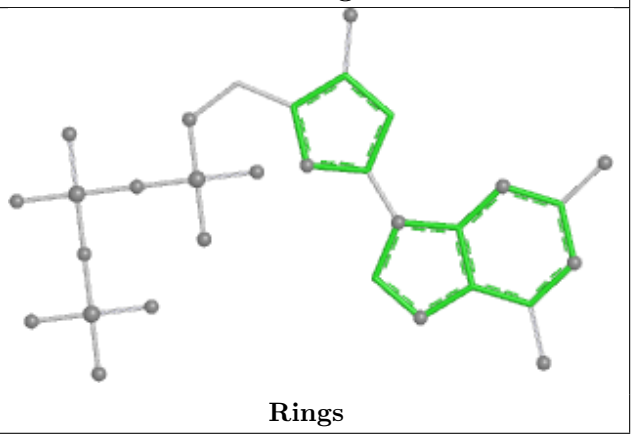
Bond lengths



Bond angles

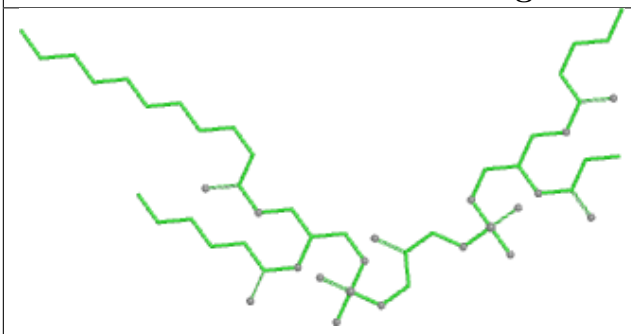


Torsions

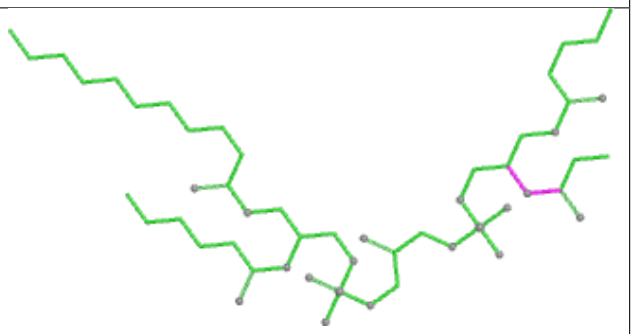


Rings

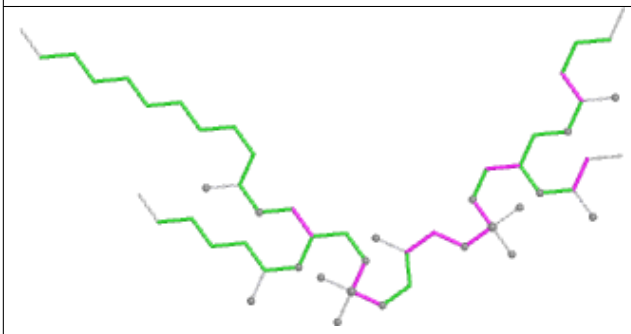
## Ligand CDL B6 203



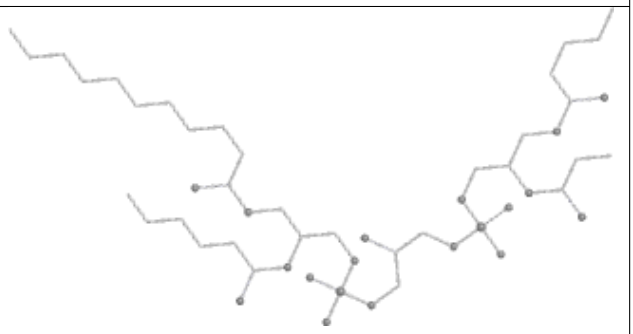
Bond lengths



Bond angles

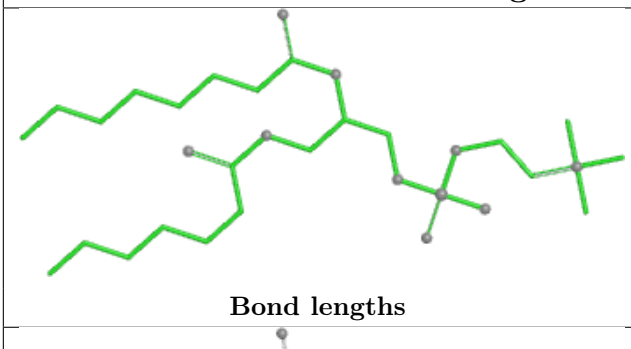


Torsions



Rings

**Ligand PC1 AM 205**



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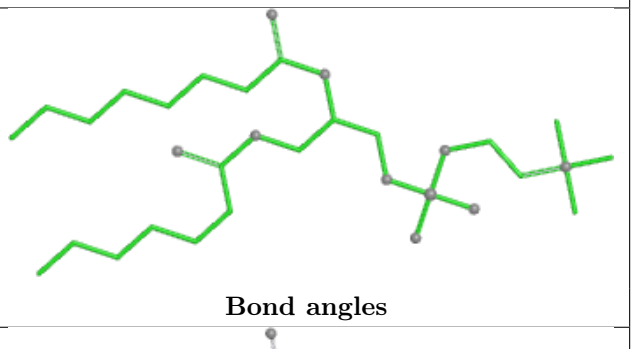
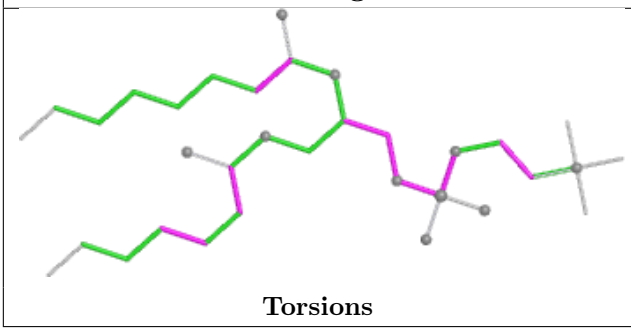
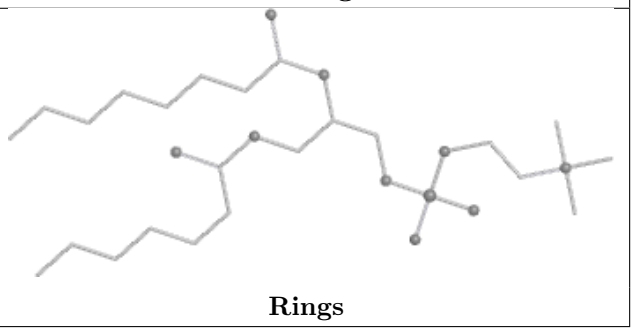


Bond angles

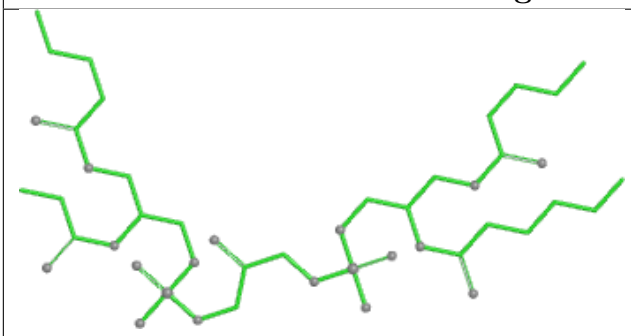


Torsions

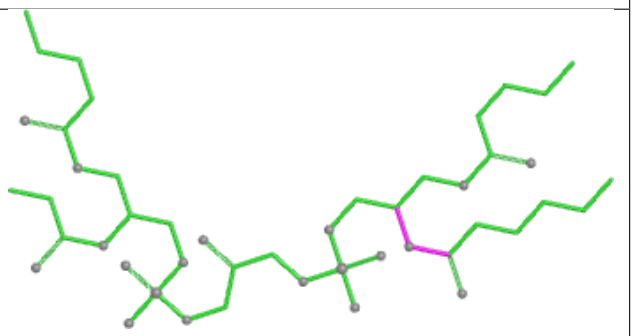


Rings

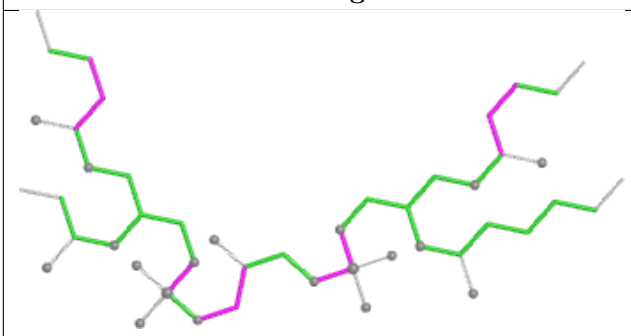
**Ligand CDL A9 503**



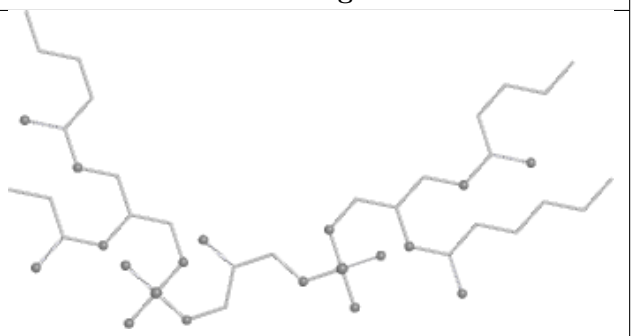
Bond lengths



Bond angles

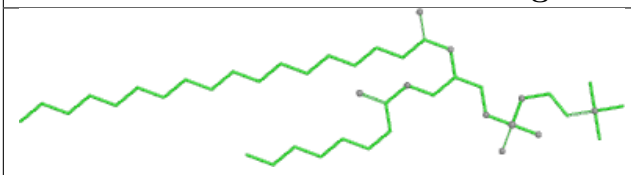


Torsions



Rings

**Ligand PC1 2 402**



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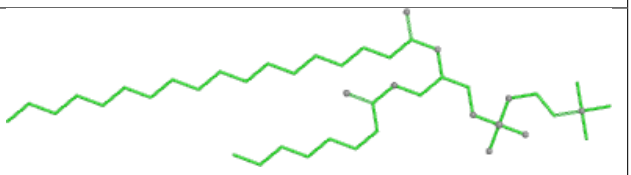
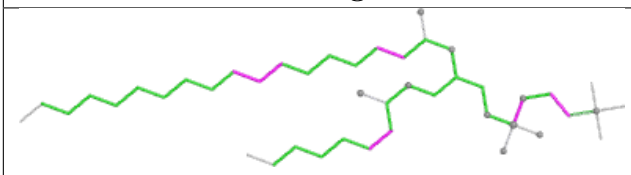
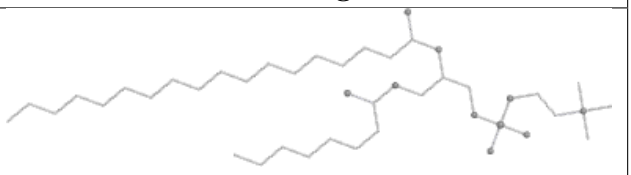


Bond angles

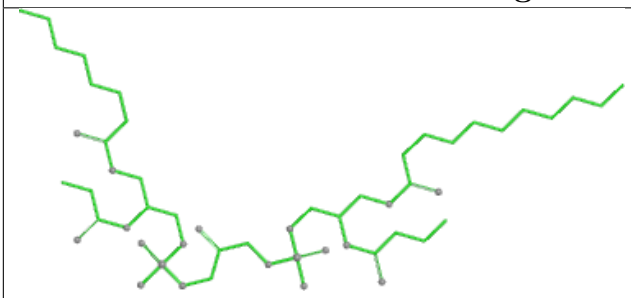


Torsions

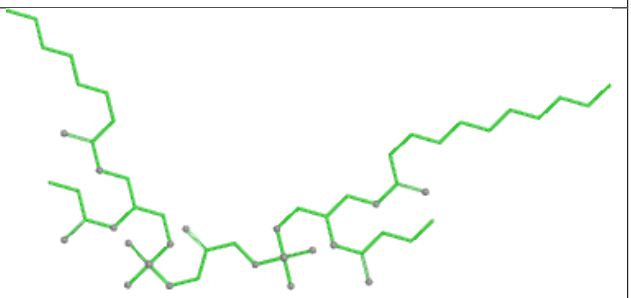


Rings

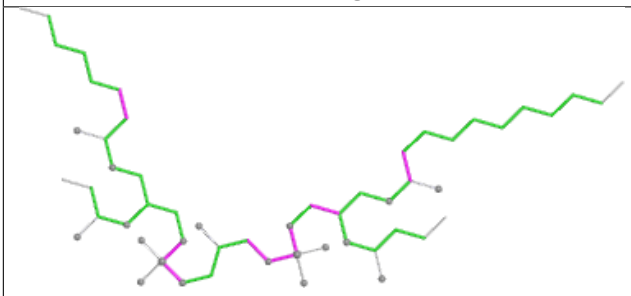
**Ligand CDL A9 502**



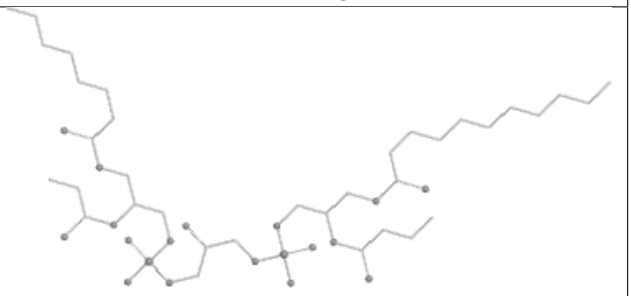
Bond lengths



Bond angles

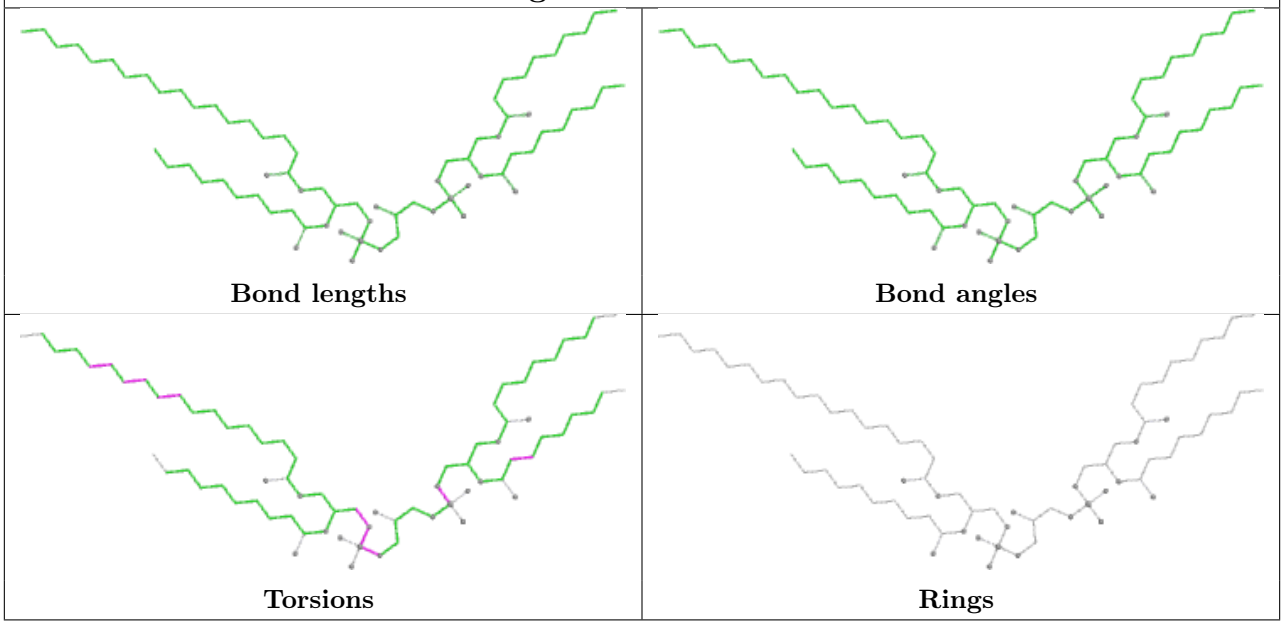


Torsions

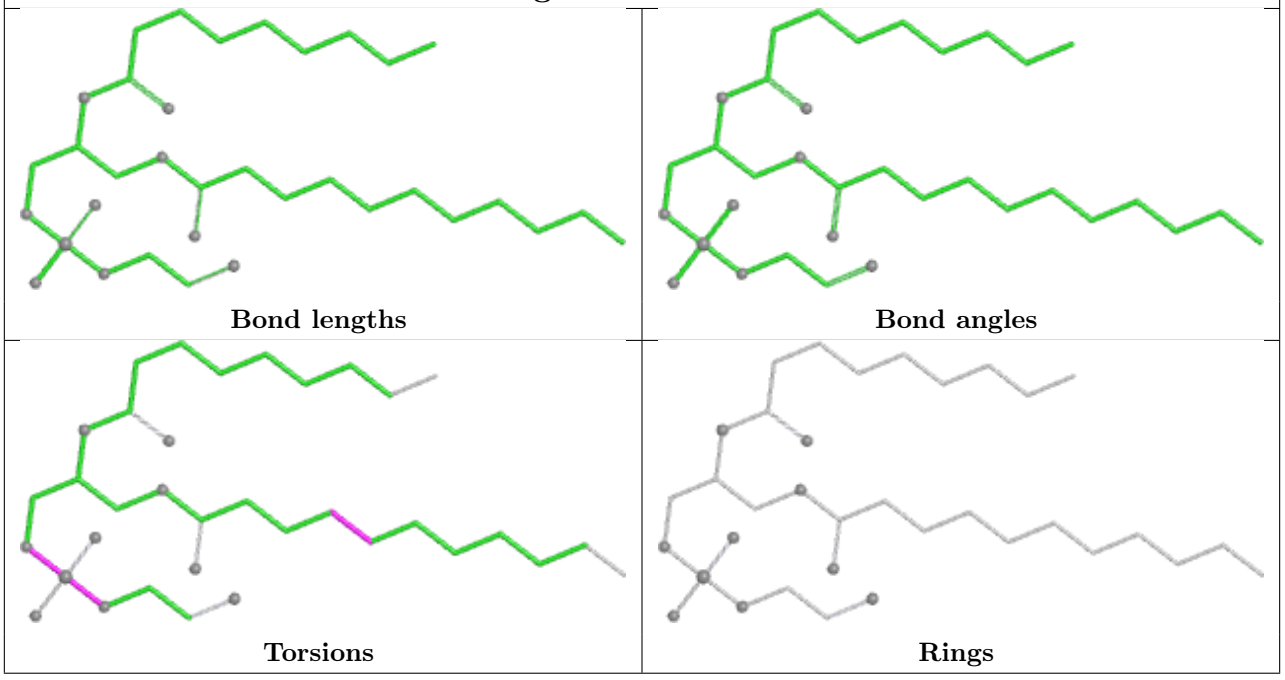


Rings

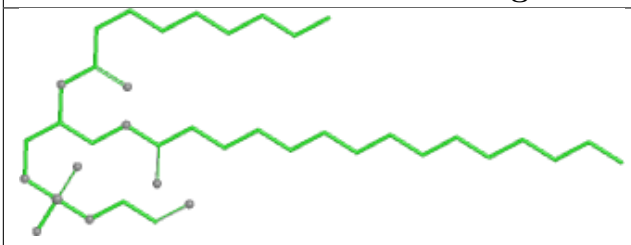
**Ligand CDL 5 608**



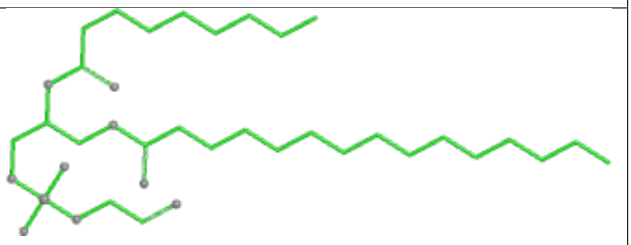

**Ligand 3PE 4 503**



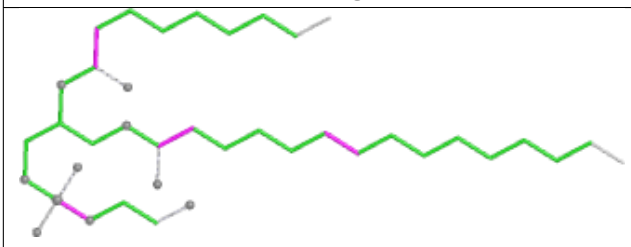
## Ligand 3PE AM 201



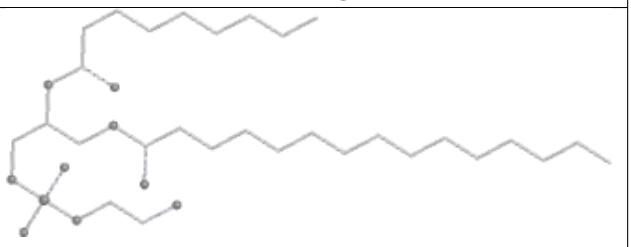
Bond lengths



Bond angles

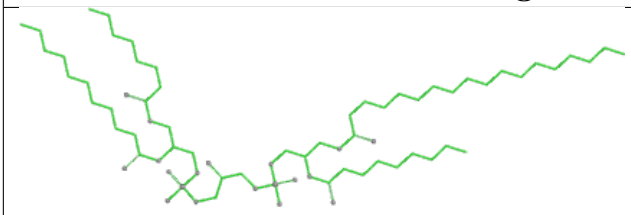


Torsions

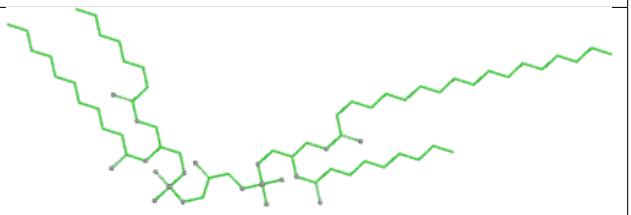


Rings

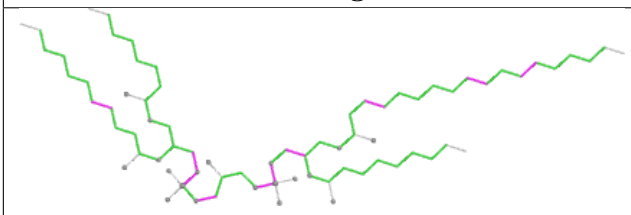
## Ligand CDL B5 201



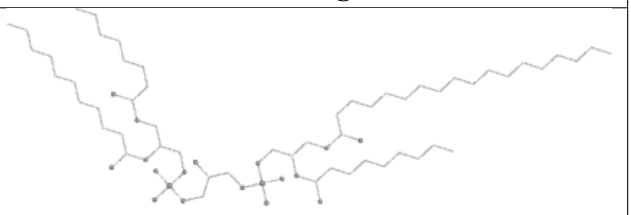
Bond lengths



Bond angles

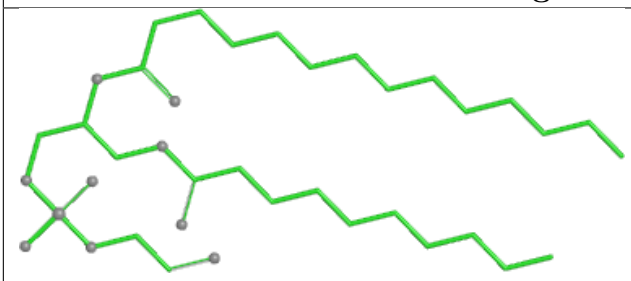


Torsions

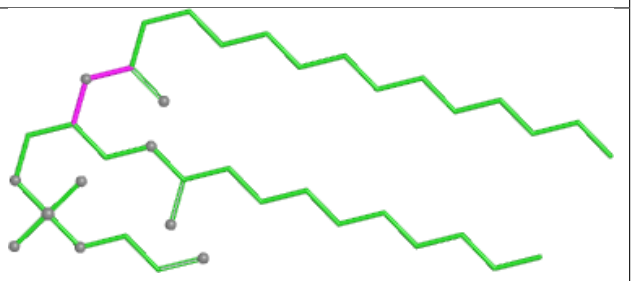


Rings

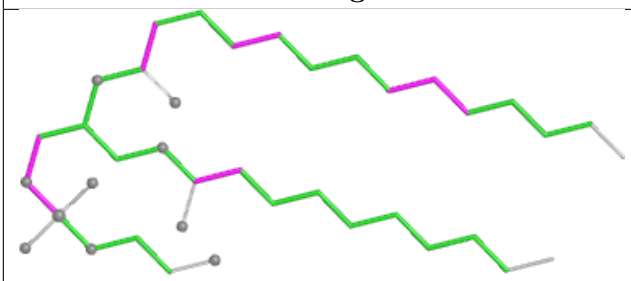
**Ligand 3PE 2 401**



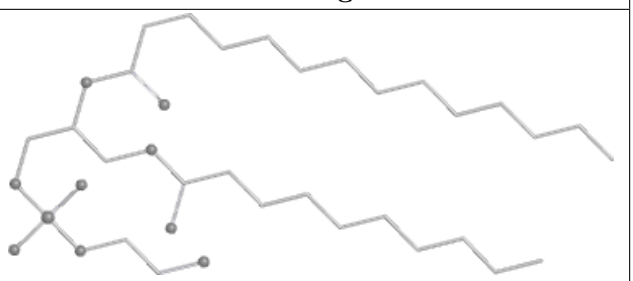
Bond lengths



Bond angles

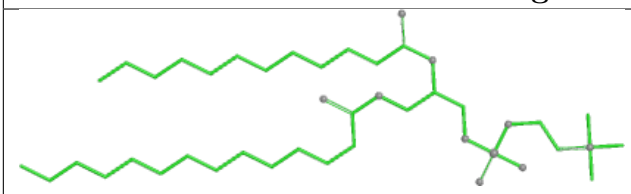


Torsions

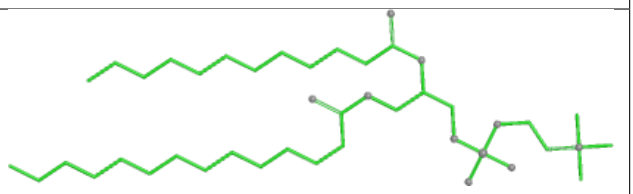


Rings

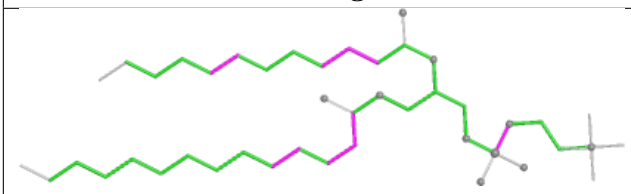
**Ligand PC1 4 502**



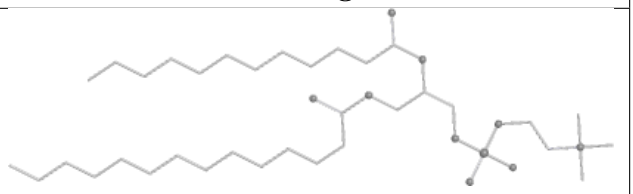
Bond lengths



Bond angles

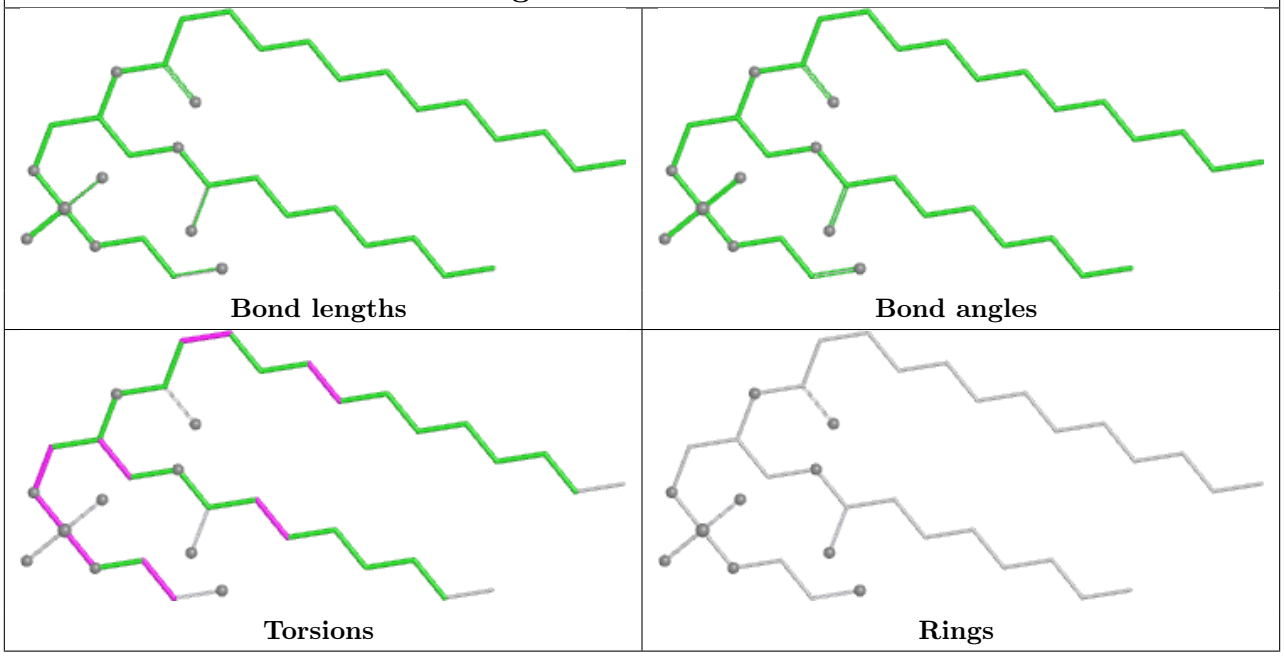


Torsions

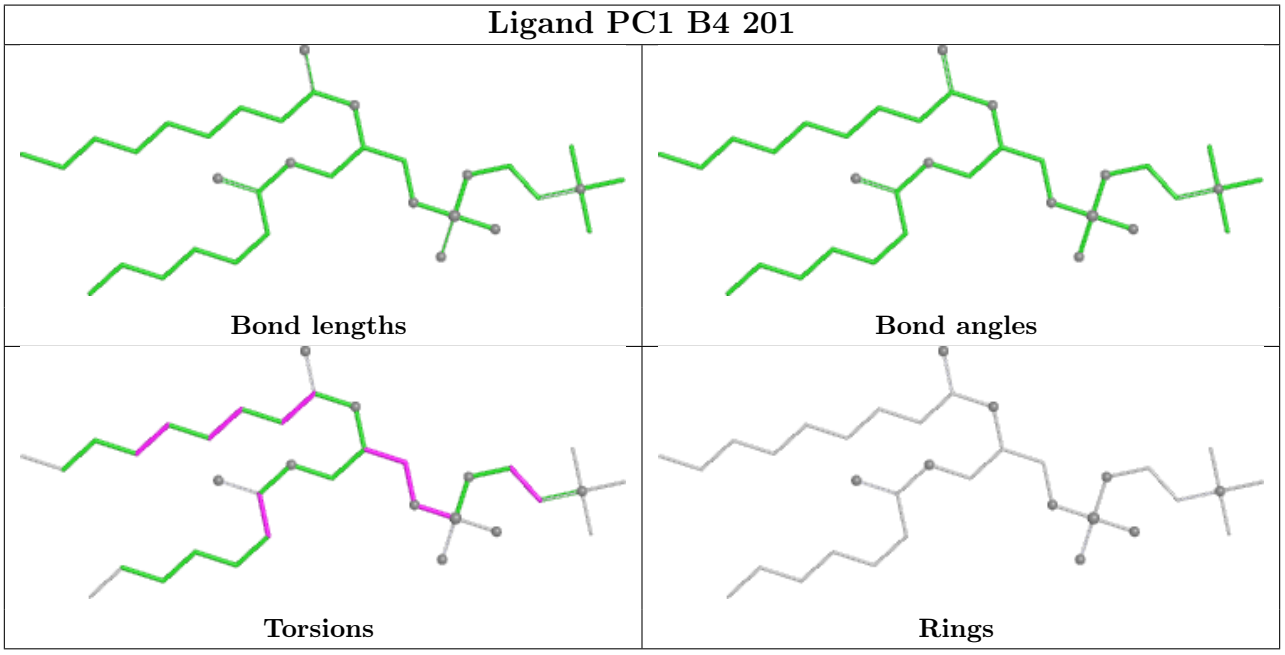


Rings

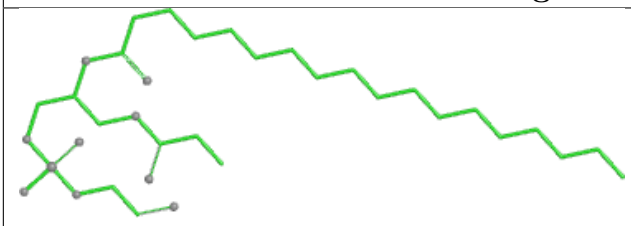
**Ligand 3PE AM 203**



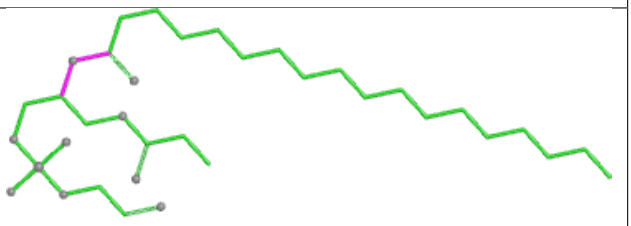

**Ligand PC1 B4 201**



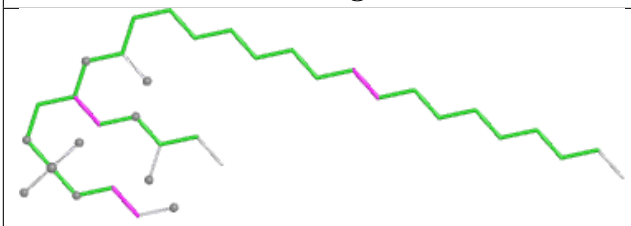
**Ligand 3PE 5 605**



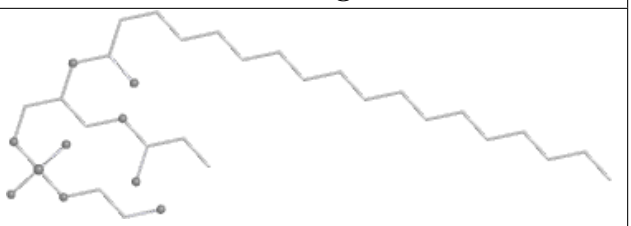
Bond lengths



Bond angles

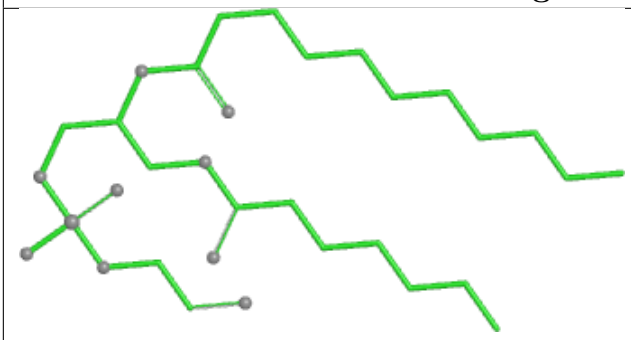


Torsions

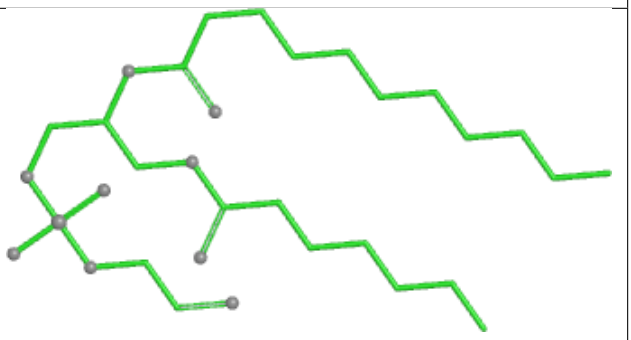


Rings

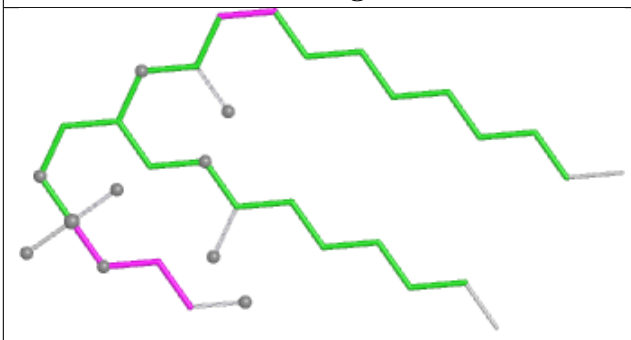
**Ligand 3PE 5 602**



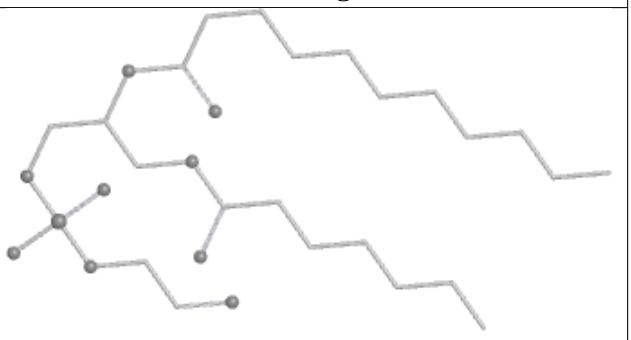
Bond lengths



Bond angles

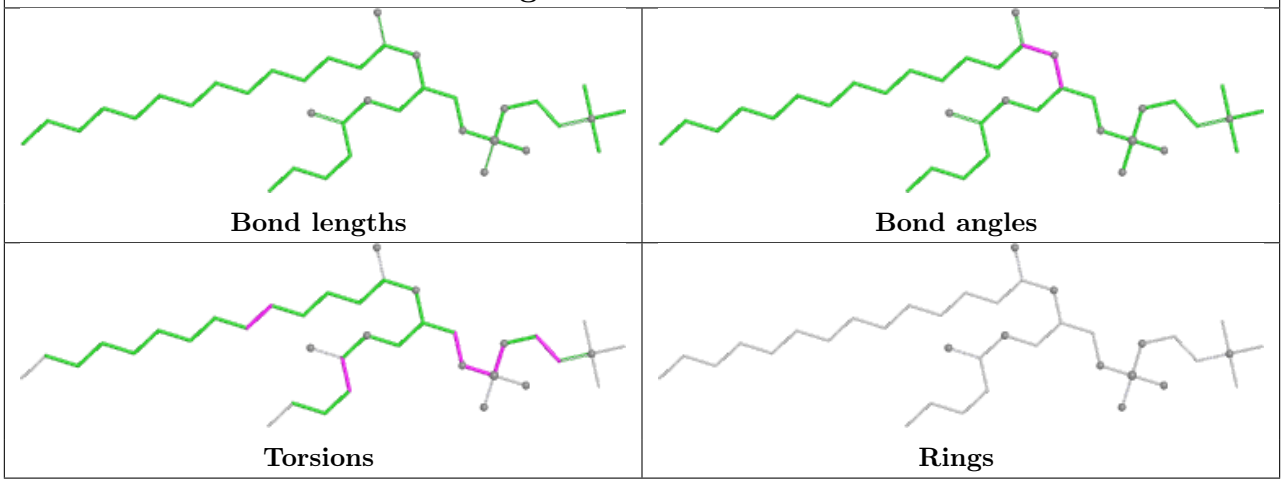


Torsions

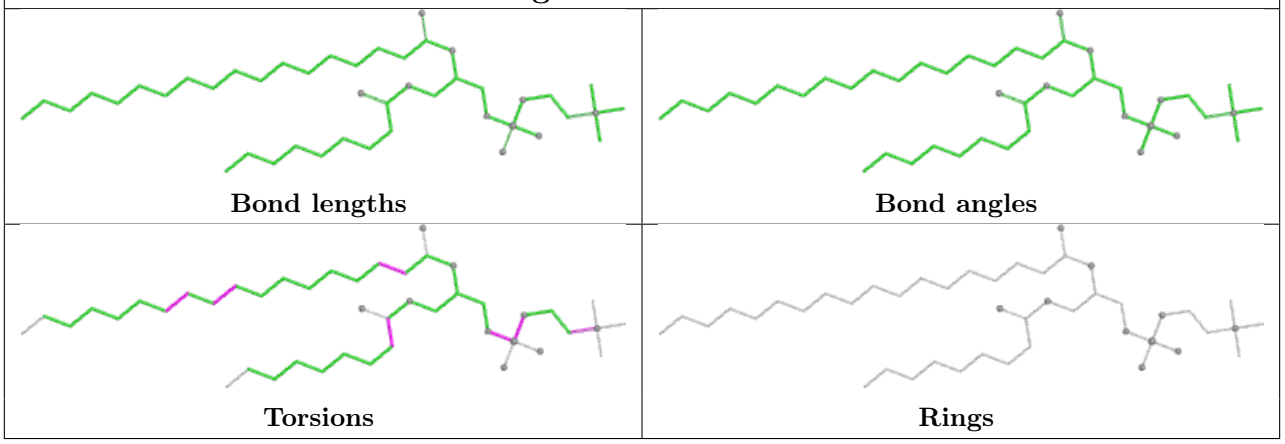


Rings

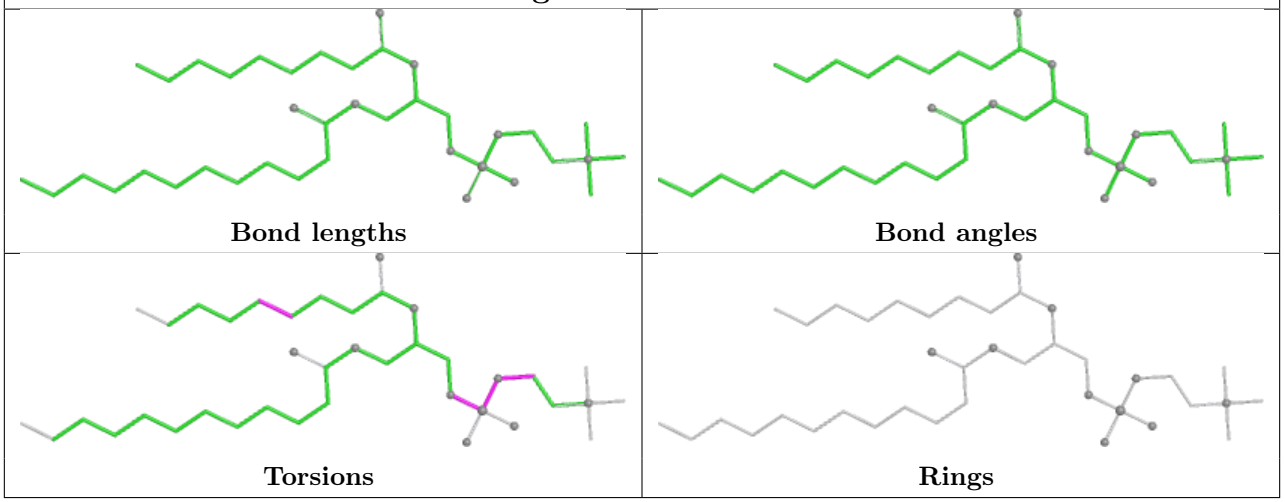
**Ligand PC1 B6 201**



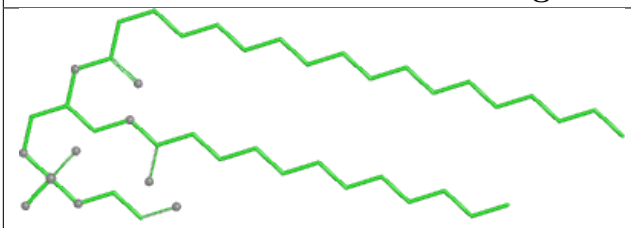

**Ligand PC1 2 403**



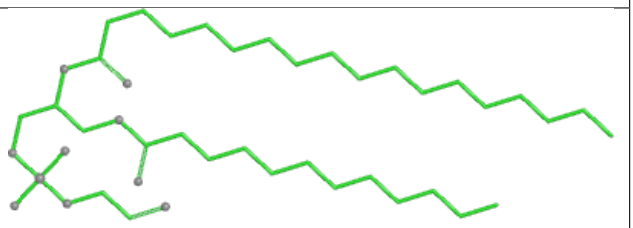

**Ligand PC1 4 501**



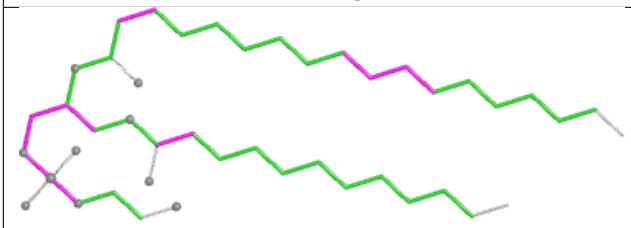
**Ligand 3PE 5 606**



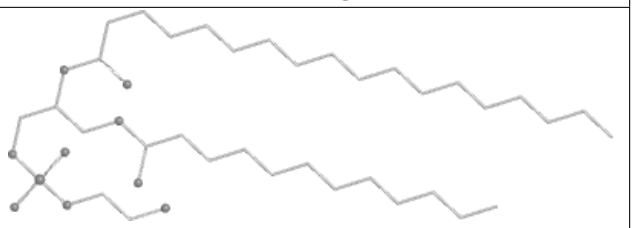
Bond lengths



Bond angles

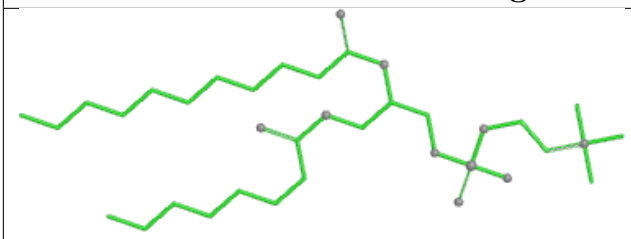


Torsions

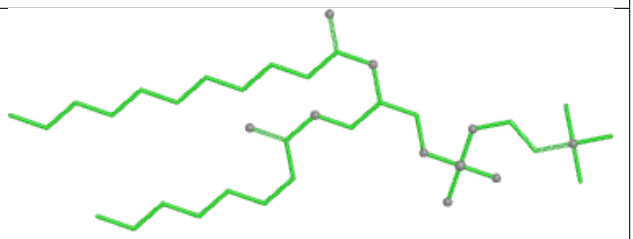


Rings

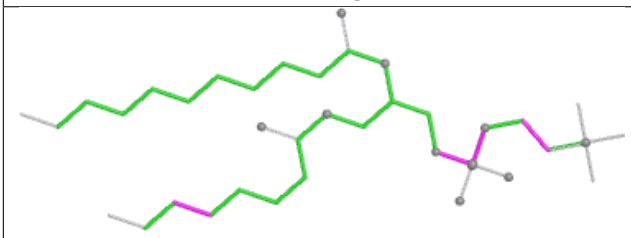
**Ligand PC1 AM 202**



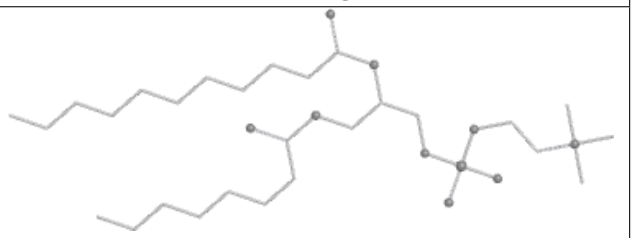
Bond lengths



Bond angles

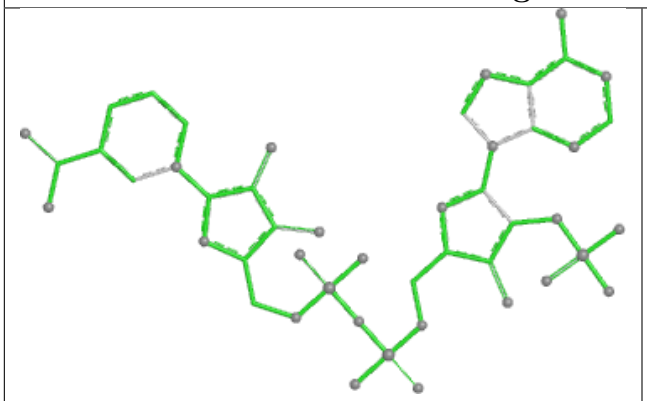


Torsions

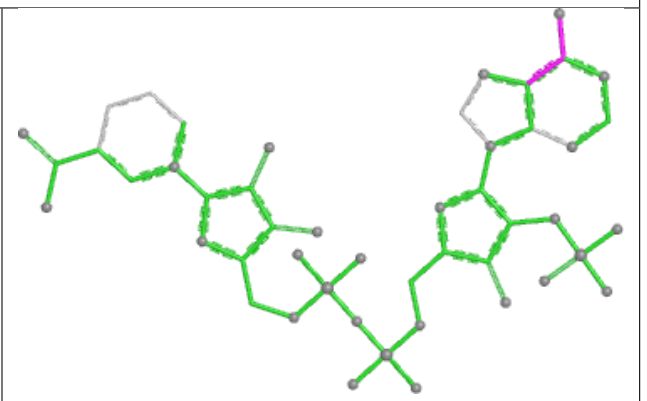


Rings

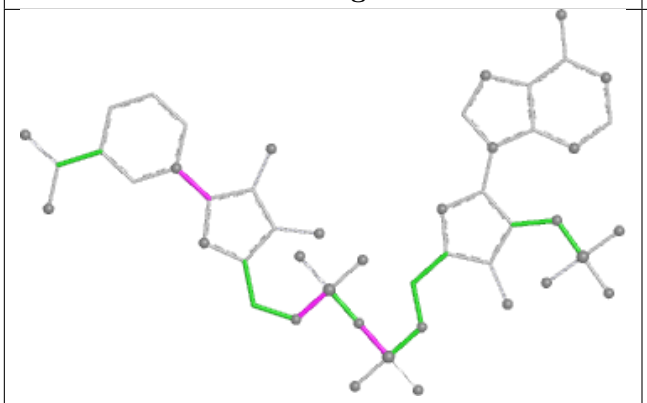
## Ligand NDP A9 501



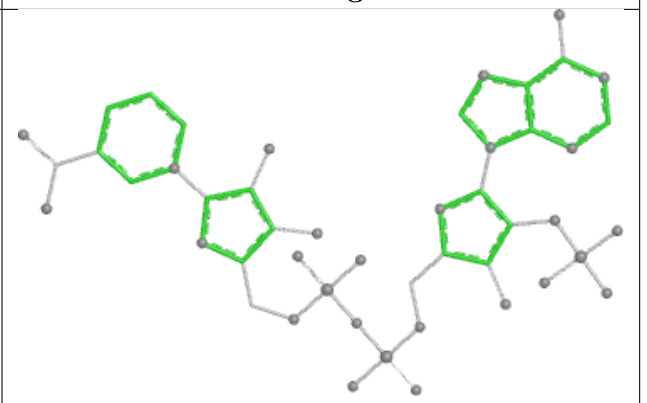
Bond lengths



Bond angles

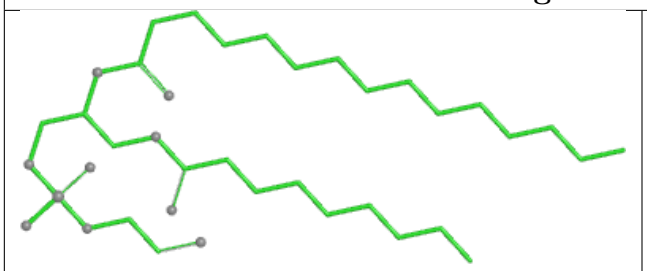


Torsions

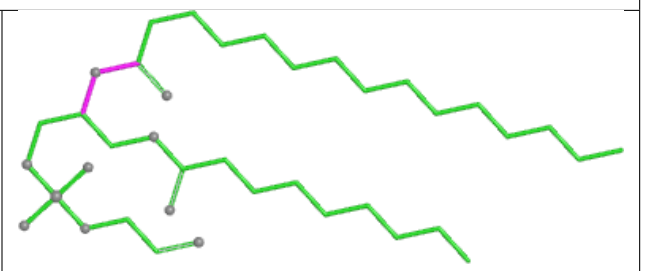


Rings

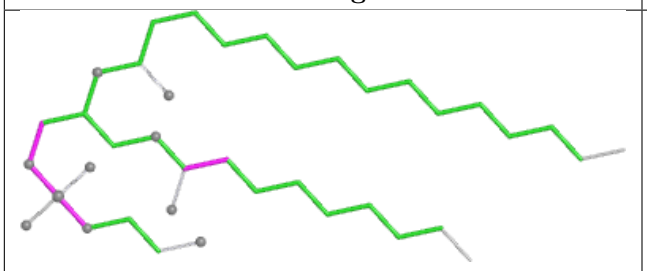
## Ligand 3PE 4 504



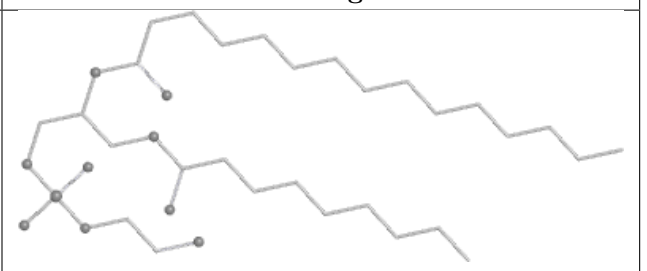
Bond lengths



Bond angles

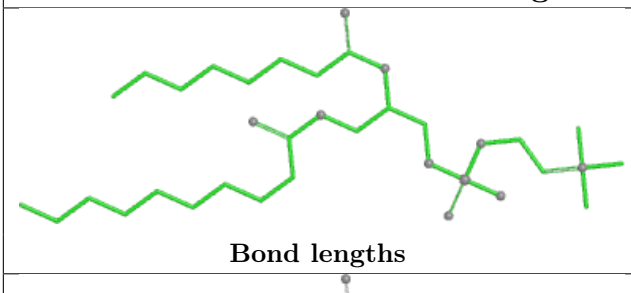


Torsions

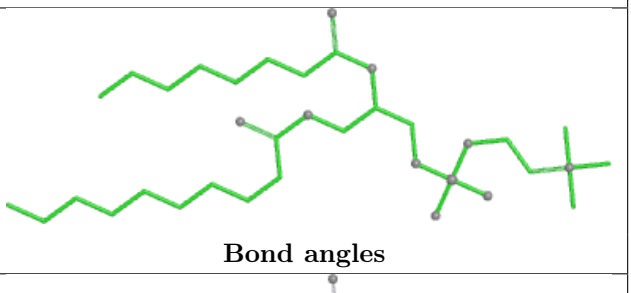


Rings

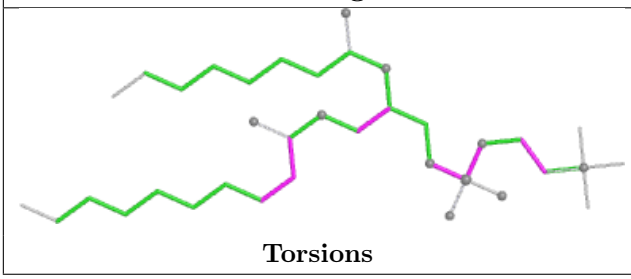
## Ligand PC1 6 201



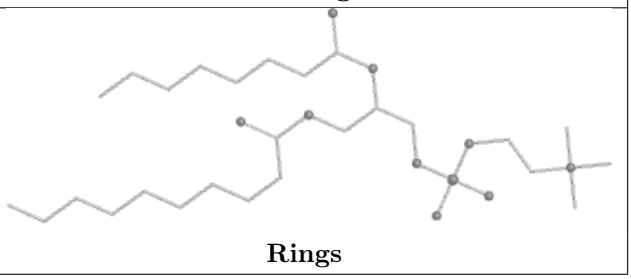
Bond lengths



Bond angles

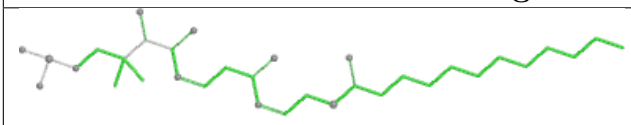


Torsions

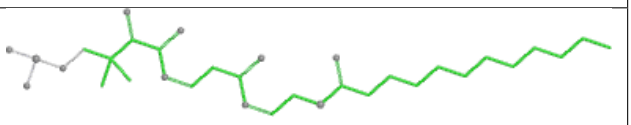


Rings

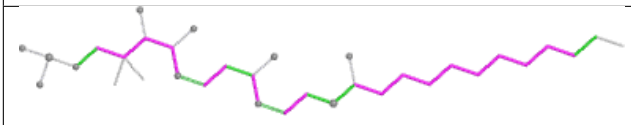
## Ligand ZMP B9 201



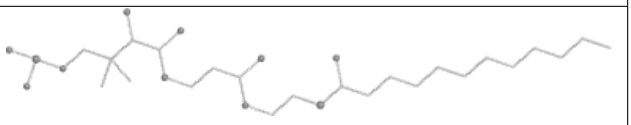
Bond lengths



Bond angles

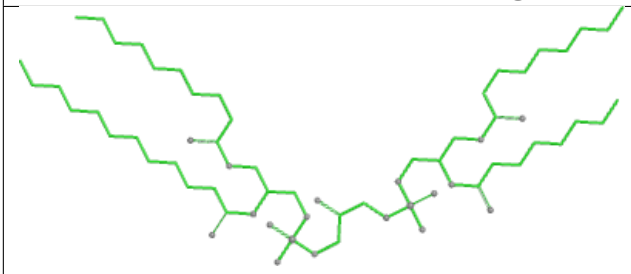


Torsions

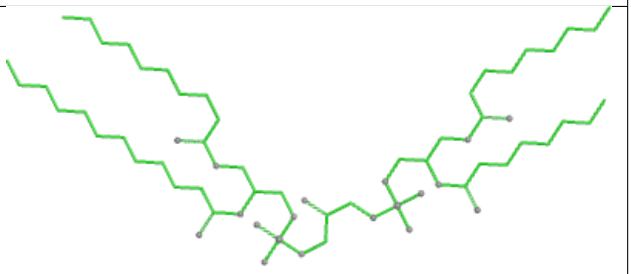


Rings

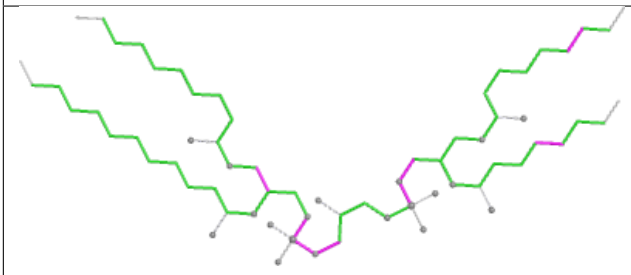
## Ligand CDL AN 201



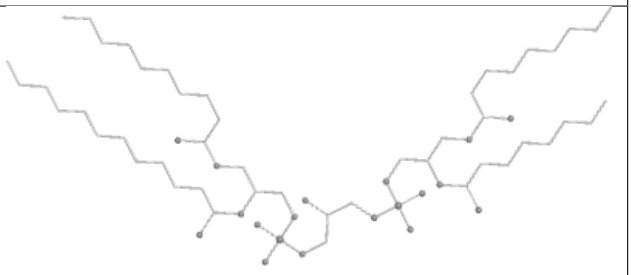
Bond lengths



Bond angles

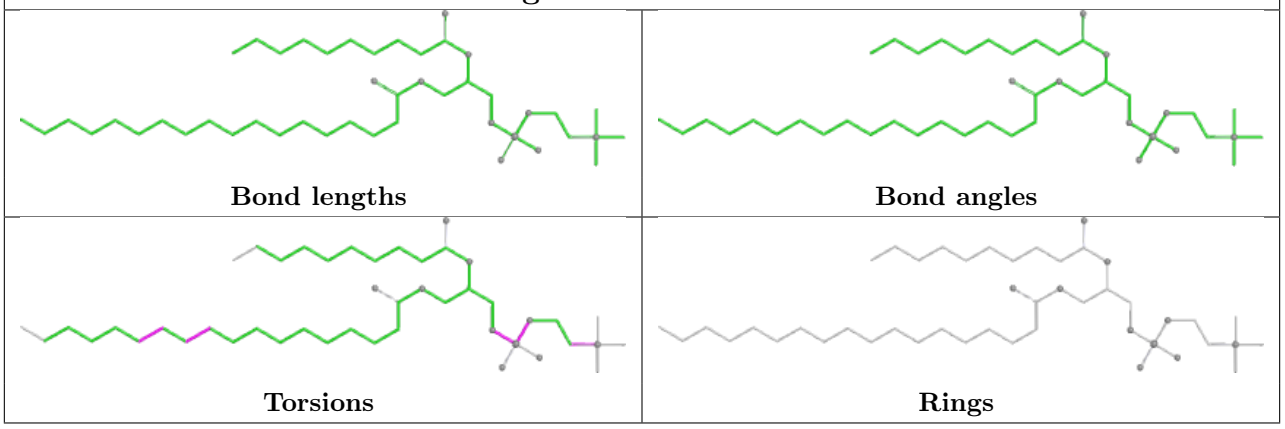


Torsions



Rings

**Ligand PC1 S7 304**




## 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.

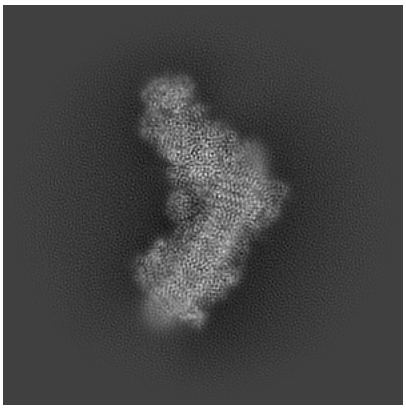
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28581. These allow visual inspection of the internal detail of the map and identification of artifacts.

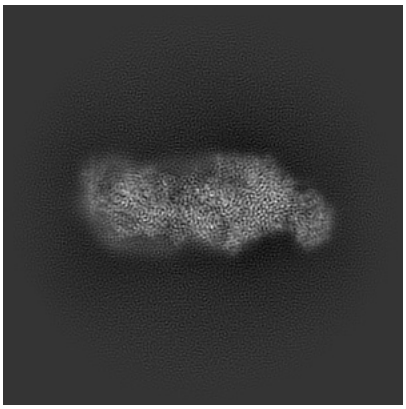
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

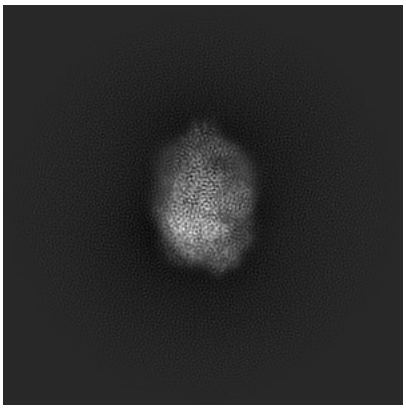
### 6.1.1 Primary map



X

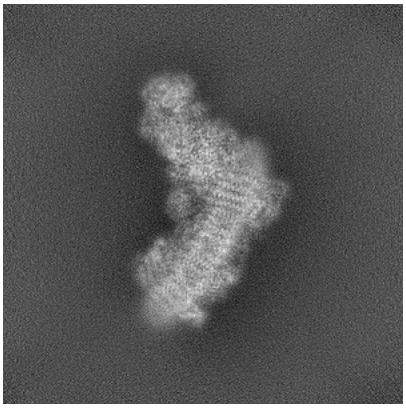


Y

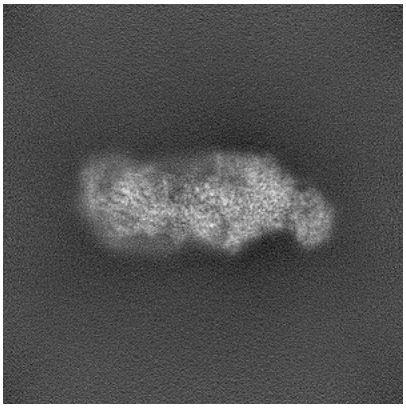


Z

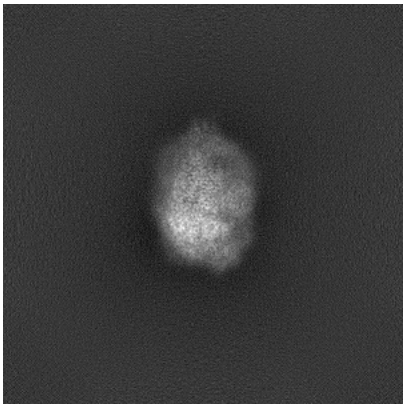
### 6.1.2 Raw map



X



Y

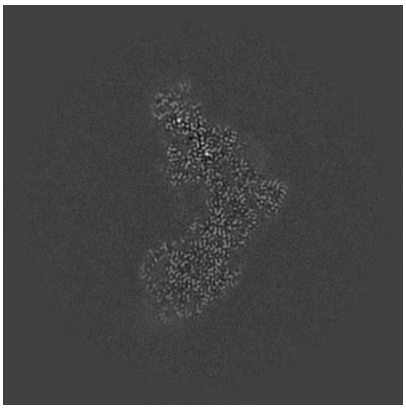


Z

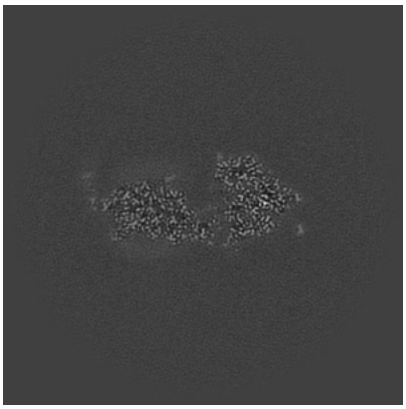
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

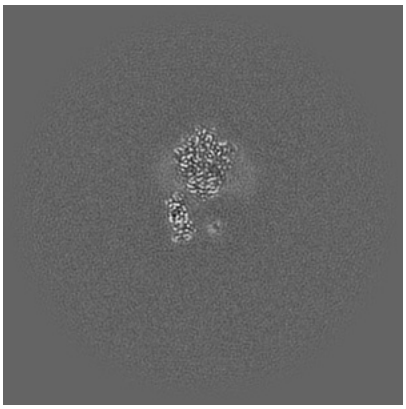
### 6.2.1 Primary map



X Index: 256

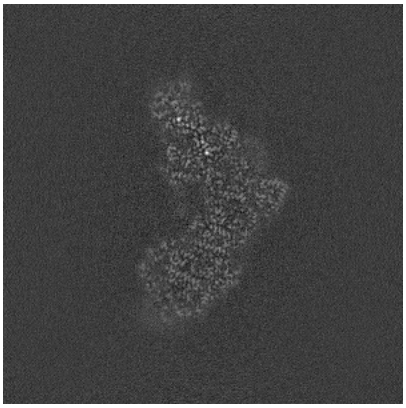


Y Index: 256

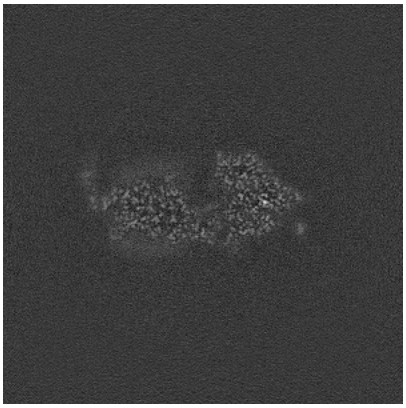


Z Index: 256

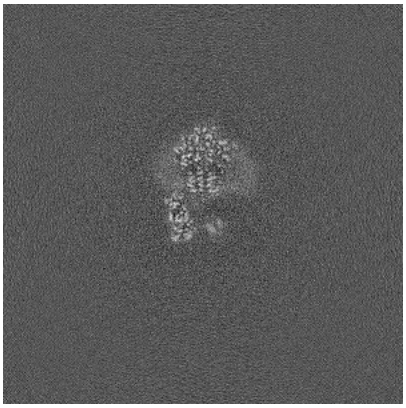
### 6.2.2 Raw map



X Index: 256



Y Index: 256

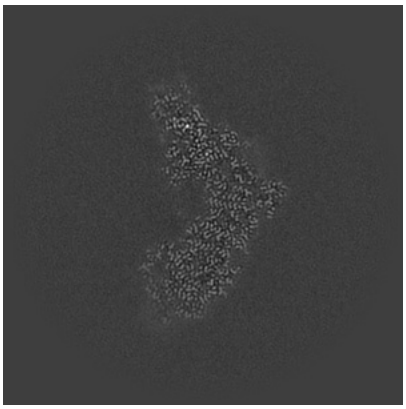


Z Index: 256

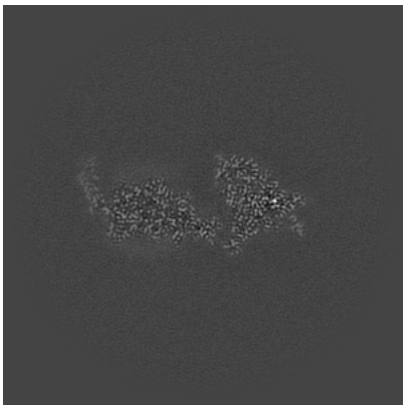
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

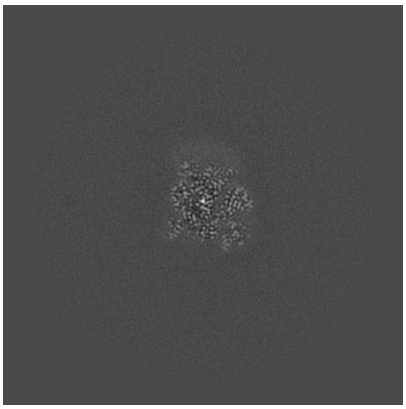
### 6.3.1 Primary map



X Index: 254

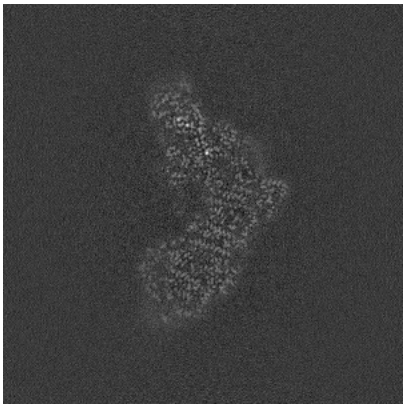


Y Index: 251

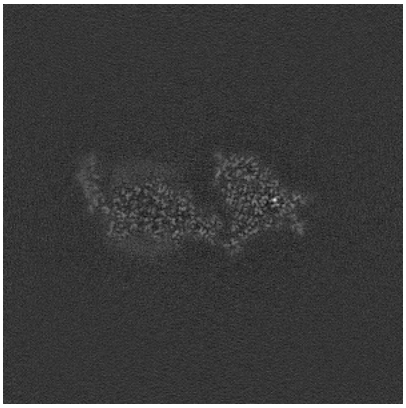


Z Index: 320

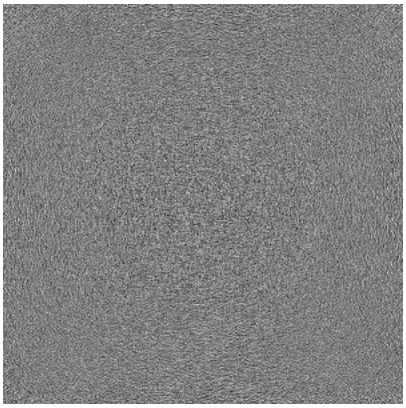
### 6.3.2 Raw map



X Index: 255



Y Index: 251

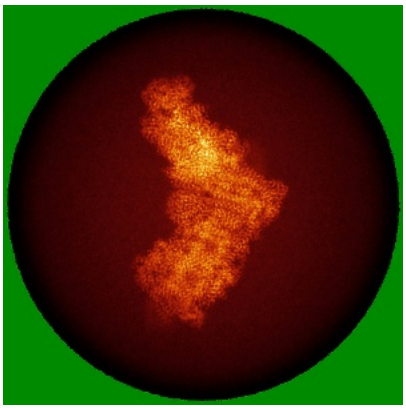


Z Index: 0

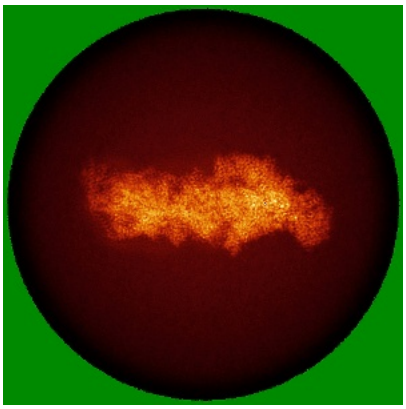
The images above show the largest variance slices of the map in three orthogonal directions.

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

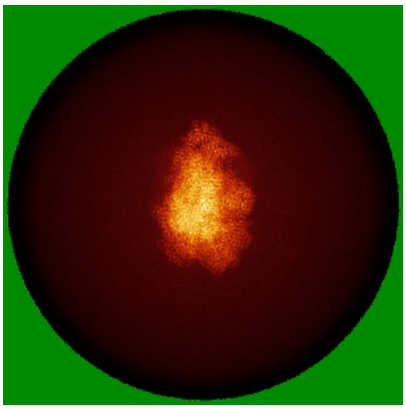
### 6.4.1 Primary map



X

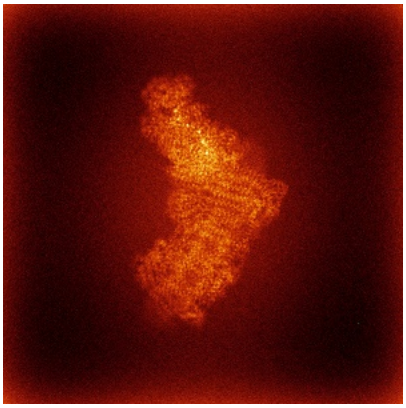


Y

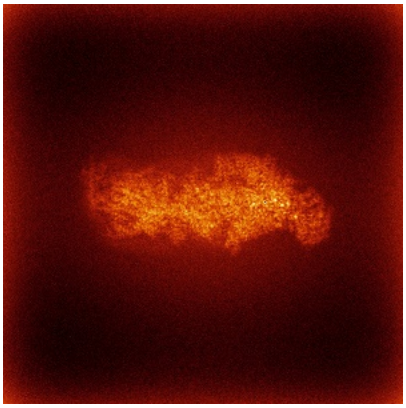


Z

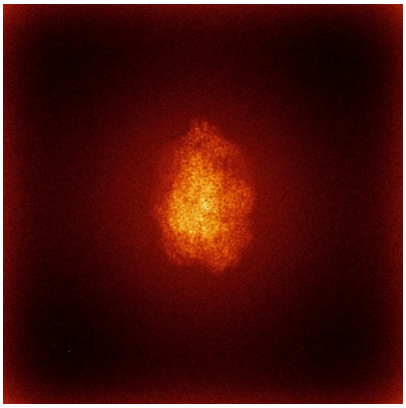
### 6.4.2 Raw map



X



Y

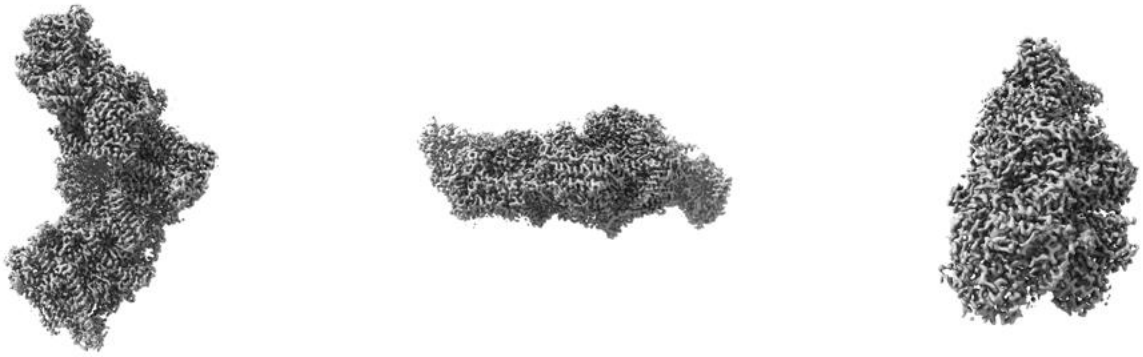


Z

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 0.6. 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.

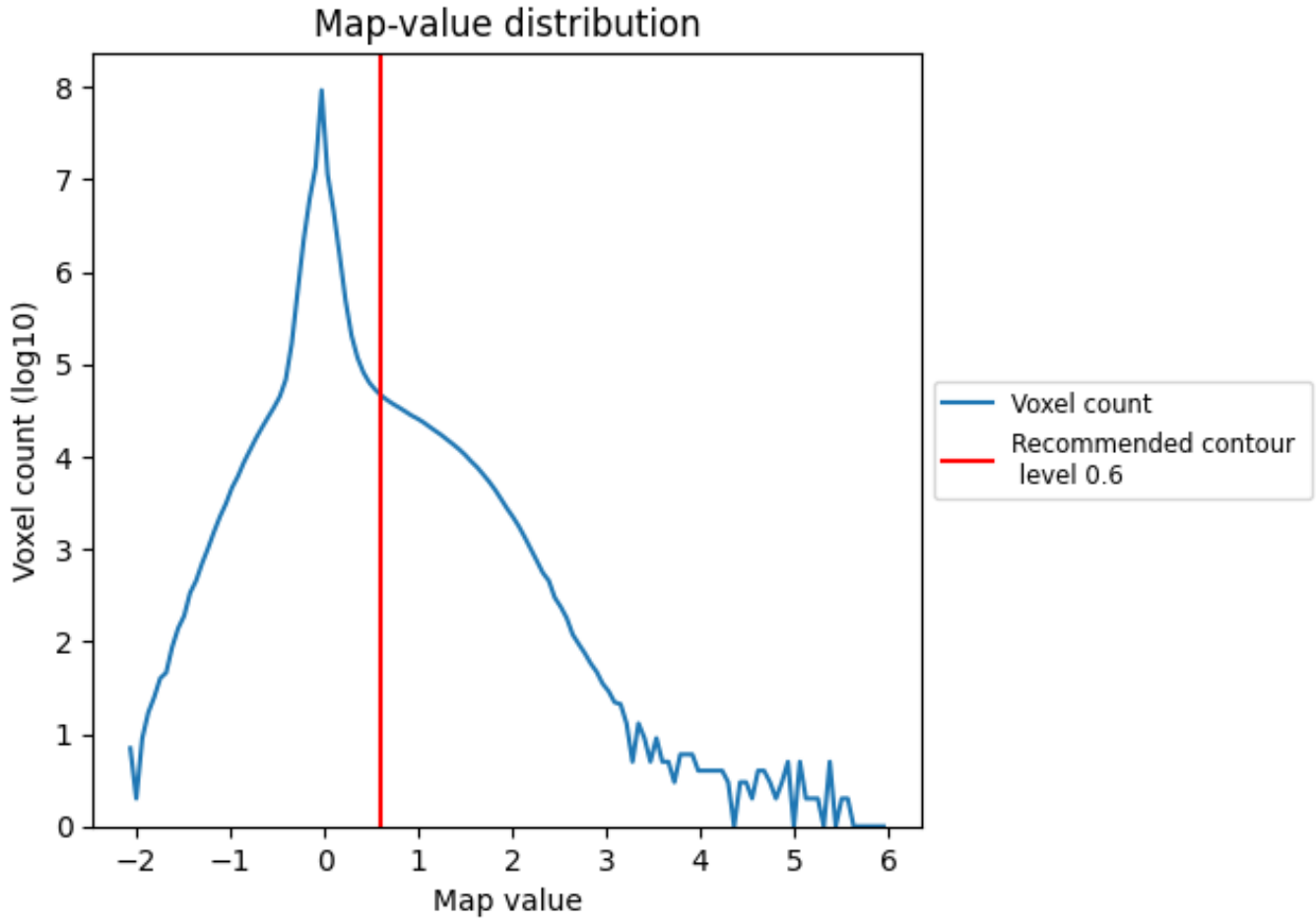
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

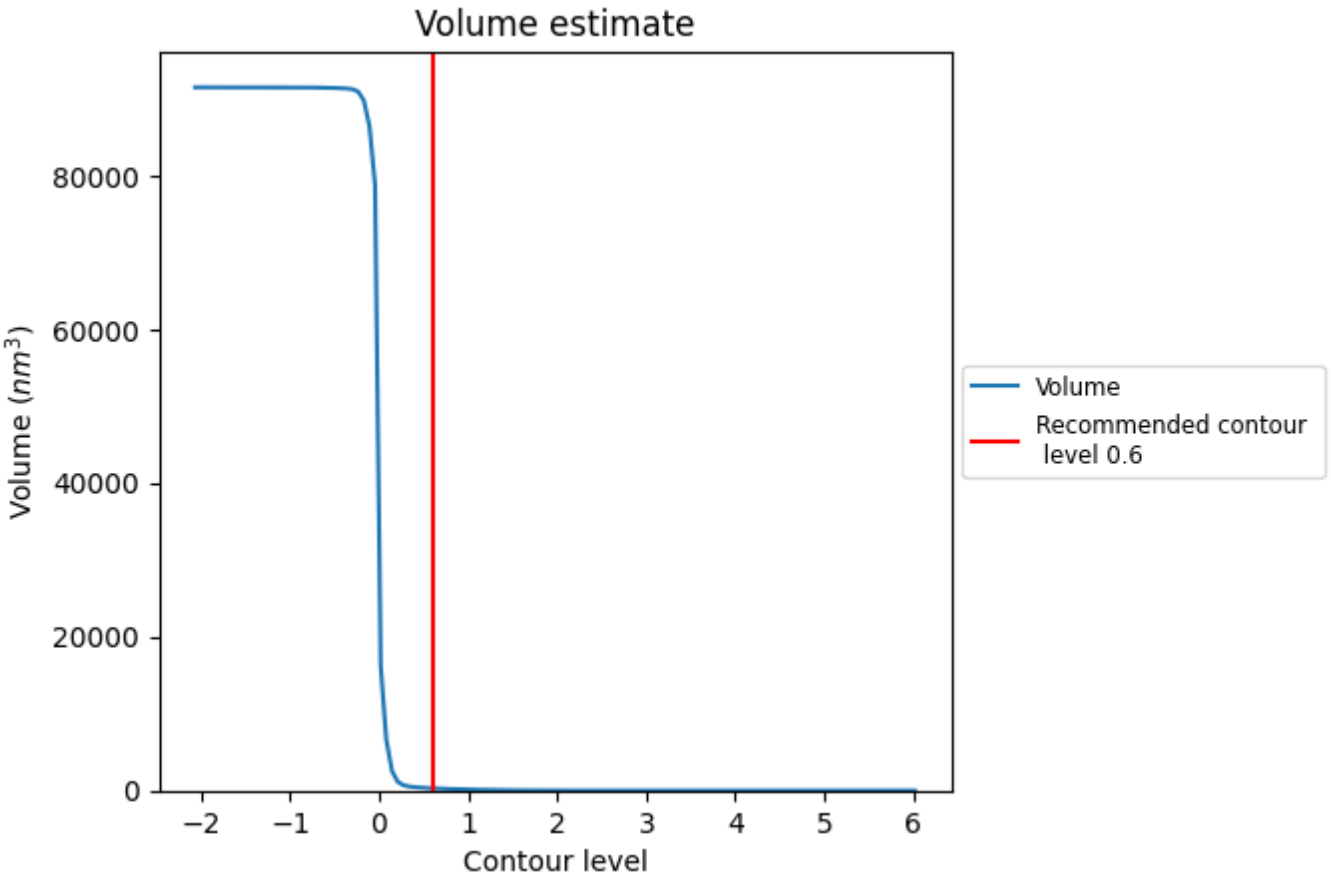
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

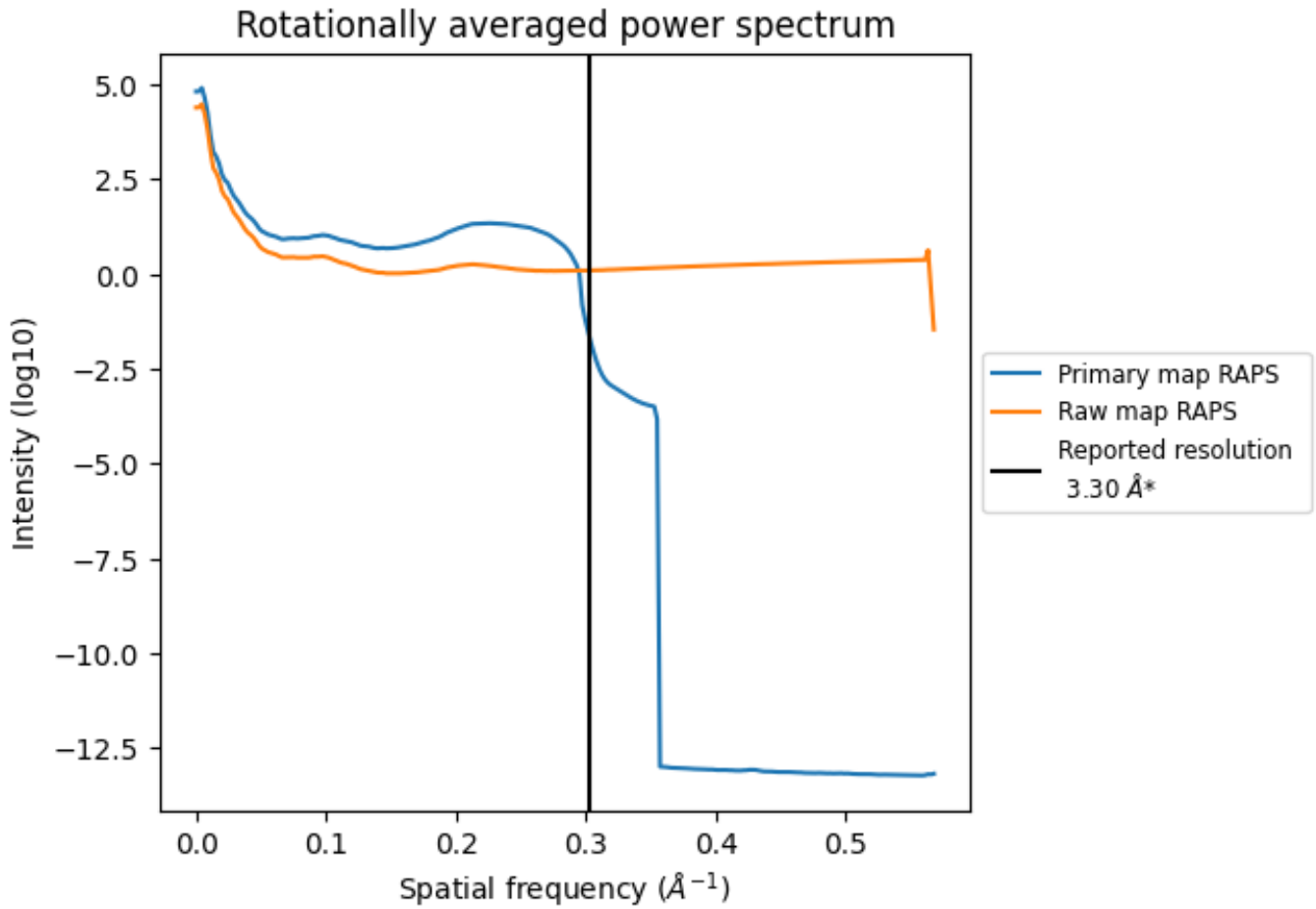
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 293 $nm^3$; this corresponds to an approximate mass of 265 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)

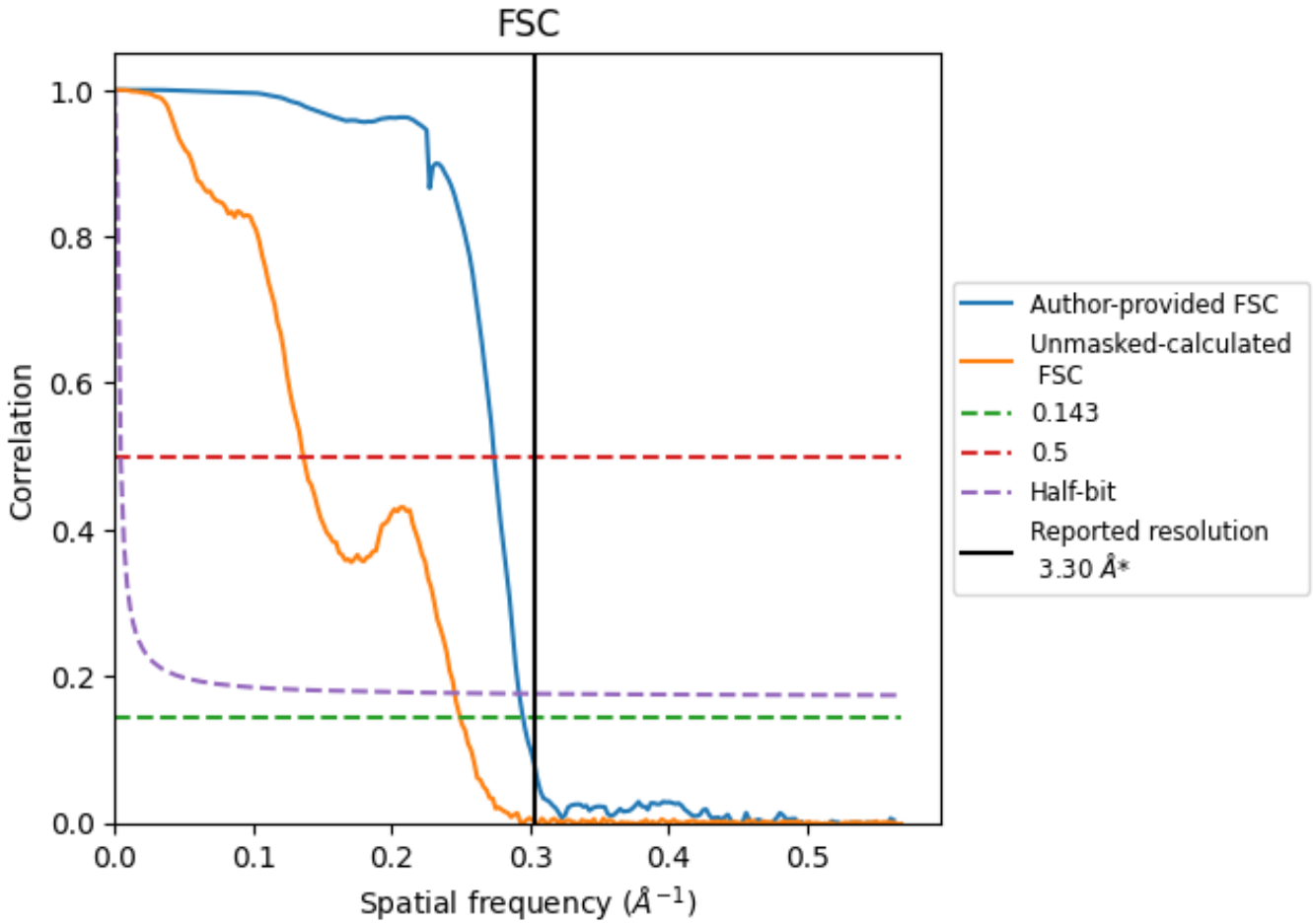



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

# 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 0.303 Å$^{-1}$

## 8.2 Resolution estimates (i)

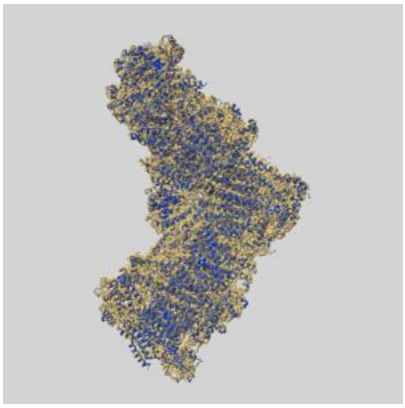
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.30 | - | - |
| Author-provided FSC curve | 3.39 | 3.65 | 3.42 |
| Unmasked-calculated* | 4.01 | 7.34 | 4.07 |

*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 4.01 differs from the reported value 3.3 by more than 10 %

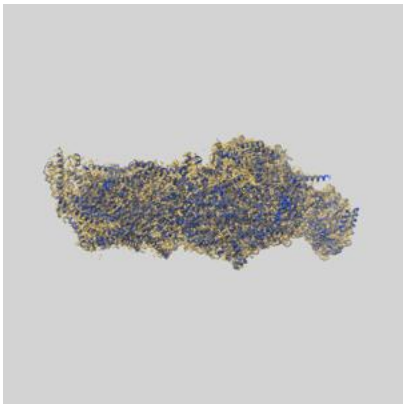
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28581 and PDB model 8ESW. Per-residue inclusion information can be found in section 3 on page 19.

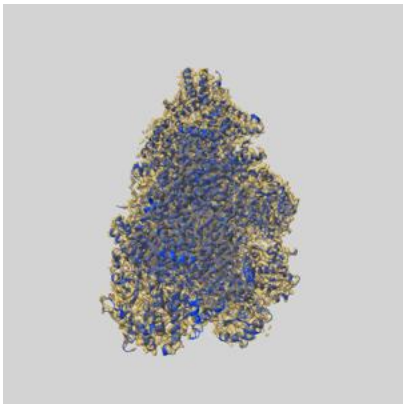
## 9.1 Map-model overlay



X



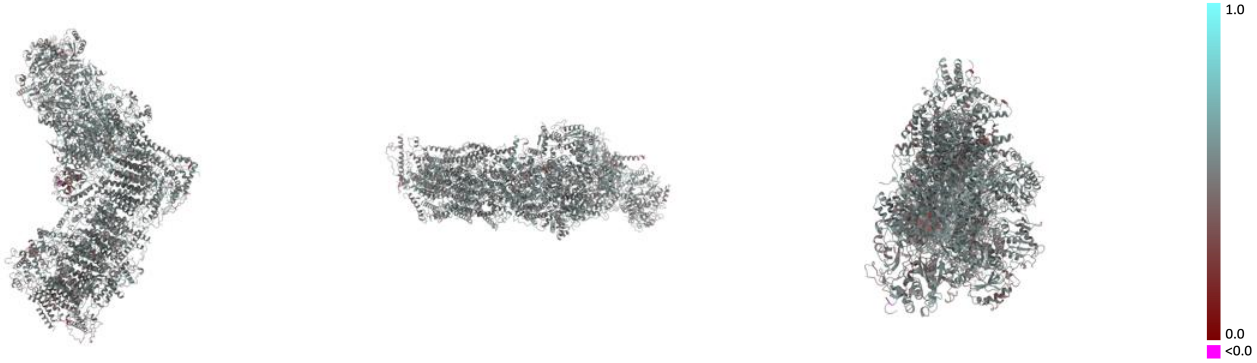
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

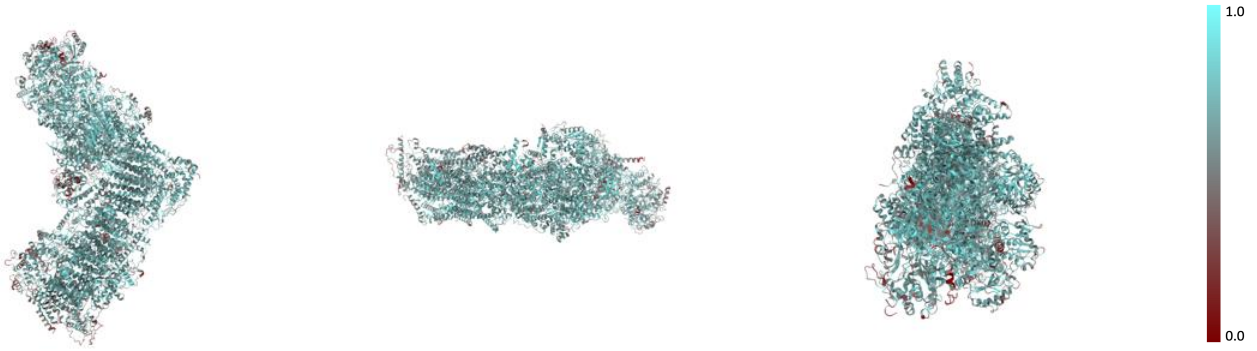
## 9.2 Q-score mapped to coordinate model




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.

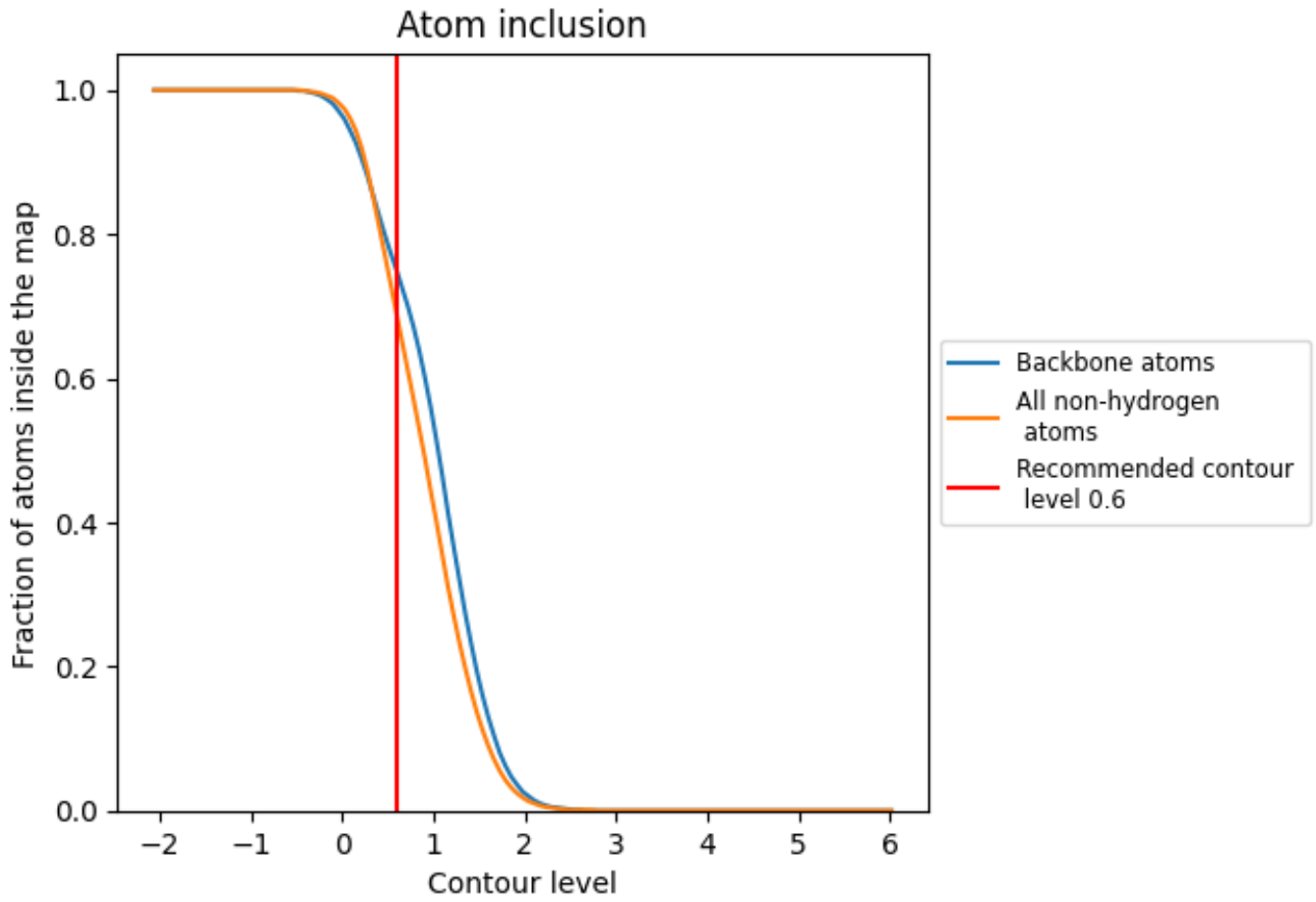
## 9.3 Atom inclusion mapped to coordinate model




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 (0.6).

## 9.4 Atom inclusion (i)




At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6850 | 0.5040 |
| 1 | 0.7340 | 0.5070 |
| 2 | 0.7330 | 0.5160 |
| 3 | 0.7000 | 0.4960 |
| 4 | 0.7420 | 0.5190 |
| 4L | 0.7080 | 0.5130 |
| 5 | 0.6510 | 0.4910 |
| 6 | 0.7120 | 0.5080 |
| A1 | 0.6860 | 0.4920 |
| A3 | 0.6610 | 0.5080 |
| A5 | 0.6960 | 0.5100 |
| A6 | 0.7050 | 0.5120 |
| A7 | 0.6720 | 0.5060 |
| A8 | 0.6840 | 0.5100 |
| A9 | 0.7290 | 0.5210 |
| AB | 0.3290 | 0.3620 |
| AC | 0.5520 | 0.4780 |
| AL | 0.7180 | 0.5200 |
| AM | 0.5900 | 0.4920 |
| AN | 0.6380 | 0.5060 |
| AO | 0.7290 | 0.5150 |
| B1 | 0.5940 | 0.4890 |
| B2 | 0.5180 | 0.4460 |
| B3 | 0.5110 | 0.4670 |
| B4 | 0.6600 | 0.4990 |
| B5 | 0.7120 | 0.5190 |
| B6 | 0.6140 | 0.4920 |
| B7 | 0.5370 | 0.4510 |
| B8 | 0.6670 | 0.5000 |
| B9 | 0.6420 | 0.4990 |
| BL | 0.7300 | 0.5030 |
| BM | 0.6820 | 0.5080 |
| C2 | 0.7130 | 0.5170 |
| S1 | 0.6920 | 0.5050 |
| S2 | 0.7450 | 0.5180 |


*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| S3 | 0.7600 | 0.5360 |
| S4 | 0.7060 | 0.5140 |
| S5 | 0.7290 | 0.5160 |
| S6 | 0.7080 | 0.5360 |
| S7 | 0.7110 | 0.5080 |
| S8 | 0.7560 | 0.5240 |
| V1 | 0.6560 | 0.4890 |
| V2 | 0.6140 | 0.4810 |
| V3 | 0.1470 | 0.4370 |