# wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 01:00 am GMT

| | | |
|---|---|---|
| PDB ID | : | 6G2J |
| EMDB ID | : | EMD-4345 |
| Title | : | Mouse mitochondrial complex I in the active state |
| Authors | : | Agip, A.N.A.; Blaza, J.N.; Bridges, H.R.; Viscomi, C.; Rawson, S.; Muench, S.P.; Hirst, J. |
| Deposited on | : | 2018-03-23 |
| 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

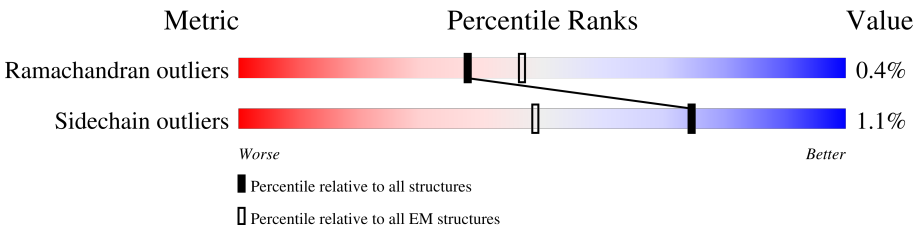
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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) |
|---|---|---|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 115 | 17%, 97%, • |
| 2 | B | 224 | 7%, 67%, •, 31% |
| 3 | C | 263 | 13%, 75%, •, 22% |
| 4 | D | 463 | 11%, 91%, •, 7% |
| 5 | E | 248 | 37%, 84%, •, 15% |
| 6 | F | 428 | 33%, 99%, • |
| 7 | G | 727 | 24%, 93%, •, 5% |
| 8 | H | 318 | 11%, 98%, • |
| 9 | I | 212 | 8%, 83%, •, 16% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | J | 172 | 30% 98% |
| 11 | K | 98 | 11% 98% |
| 12 | L | 607 | 26% 98% |
| 13 | M | 459 | 11% 98% |
| 14 | N | 345 | 9% 97% |
| 15 | O | 355 | 26% 88% 10% |
| 16 | P | 377 | 26% 88% 9% |
| 17 | Q | 175 | 20% 69% 29% |
| 18 | R | 116 | 16% 81% 18% |
| 19 | S | 99 | 44% 83% 16% |
| 20 | T | 156 | 43% 48% 52% |
| 20 | U | 156 | 33% 56% 44% |
| 21 | V | 116 | 29% 94% |
| 22 | W | 131 | 32% 85% 13% |
| 23 | X | 172 | 28% 97% |
| 24 | Y | 143 | 40% 96% |
| 25 | Z | 144 | 29% 92% |
| 26 | a | 67 | 19% 93% 7% |
| 27 | b | 84 | 39% 94% 5% |
| 28 | c | 76 | 37% 59% 38% |
| 29 | d | 120 | 33% 98% |
| 30 | e | 106 | 25% 95% |
| 31 | f | 57 | 42% 84% 11% |
| 32 | g | 151 | 26% 64% 33% |
| 33 | h | 189 | 22% 72% 28% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | i | 128 | 41% 73% 5% 21% |
| 35 | j | 105 | 33% 54% 43% |
| 36 | k | 104 | 49% 68% 31% |
| 37 | l | 186 | 36% 79% 18% |
| 38 | m | 129 | 33% 94% |
| 39 | n | 179 | 46% 98% |
| 40 | o | 137 | 54% 74% 23% |
| 41 | p | 176 | 39% 94% |
| 42 | q | 145 | 26% 96% |
| 43 | r | 113 | 27% 84% 12% |
| 44 | s | 104 | 21% 38% 62% |

# 2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 66810 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 115 | 933 | 633 | 133 | 160 | 7 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 155 | 1241 | 793 | 222 | 212 | 14 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 206 | 1712 | 1105 | 294 | 310 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 430 | 3452 | 2207 | 593 | 628 | 24 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 212 | 1648 | 1048 | 277 | 312 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 428 | 3301 | 2080 | 590 | 609 | 22 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | G | 688 | 5296 | 3321 | 919 | 1015 | 41 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | H | 318 | 2540 | 1706 | 384 | 428 | 22 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | I | 178 | 1408 | 885 | 243 | 268 | 12 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | J | 171 | 1300 | 874 | 185 | 226 | 15 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | K | 98 | 737 | 477 | 112 | 137 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | L | 606 | 4800 | 3182 | 746 | 827 | 45 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | M | 459 | 3632 | 2408 | 567 | 617 | 40 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | N | 344 | 2696 | 1791 | 416 | 452 | 37 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | O | 320 | 2607 | 1674 | 431 | 492 | 10 | 0 | 0 |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | P | 342 | 2748 | 1777 | 483 | 481 | 7 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | Q | 125 | 1015 | 642 | 179 | 190 | 4 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | R | 95 | 748 | 464 | 138 | 143 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | S | 83 | 667 | 419 | 126 | 119 | 3 | 0 | 0 |

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | T | 75 | 604 | 388 | 89 | 122 | 5 | 0 | 0 |
| 20 | U | 88 | 706 | 453 | 104 | 144 | 5 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | V | 112 | 915 | 596 | 152 | 164 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | W | 114 | 970 | 619 | 180 | 165 | 6 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | X | 171 | 1396 | 889 | 250 | 247 | 10 | 0 | 0 |

- Molecule 24 is a protein called MCG5603.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | Y | 140 | 1037 | 662 | 175 | 192 | 8 | 0 | 0 |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | Z | 139 | 1152 | 741 | 204 | 199 | 8 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | a | 67 | 548 | 356 | 97 | 91 | 4 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | b | 83 | 651 | 427 | 105 | 115 | 4 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | c | 47 | 389 | 255 | 67 | 66 | 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | d | 119 | 985 | 645 | 167 | 164 | 9 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | e | 104 | 870 | 550 | 161 | 151 | 8 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | f | 51 | 433 | 278 | 78 | 75 | 2 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | g | 101 | 850 | 549 | 136 | 161 | 4 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | h | 137 | 1154 | 758 | 192 | 201 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | i | 101 | 820 | 534 | 141 | 142 | 3 | 0 | 0 |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | j | 60 | 525 | 345 | 88 | 91 | 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | k | 72 | 582 | 384 | 100 | 97 | 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | l | 152 | 1274 | 821 | 213 | 229 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 38 | m | 124 | 1035 | 667 | 186 | 182 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | n | 176 | 1527 | 976 | 274 | 266 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | o | 105 | 898 | 565 | 167 | 158 | 8 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | p | 170 | 1438 | 903 | 258 | 269 | 8 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 42 | q | 144 | 1203 | 773 | 213 | 212 | 5 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| q | 1 | AME | MET | conflict | UNP Q7TMF3 |

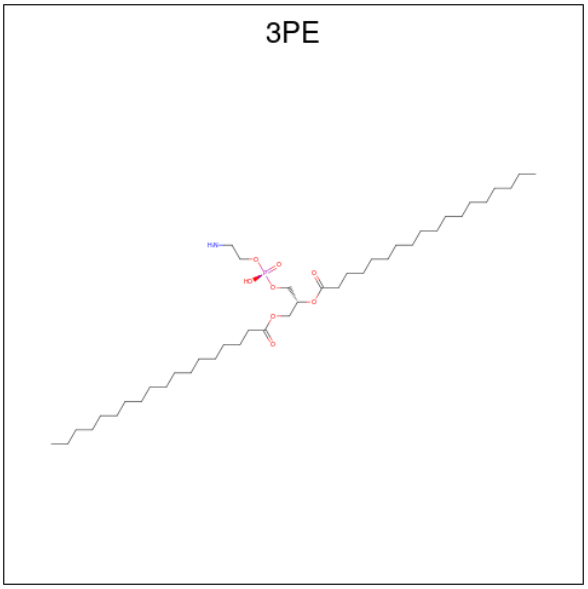
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 43 | r | 99 | 796 | 504 | 148 | 141 | 3 | 0 | 0 |

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

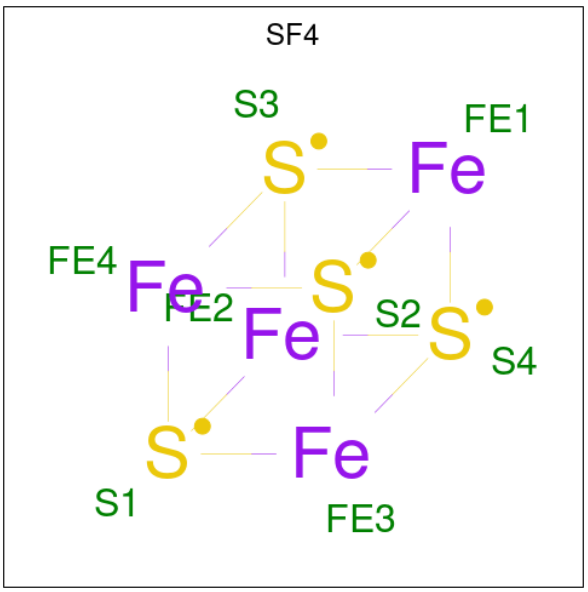
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 44 | s | 40 | 336 | 211 | 60 | 65 | 0 | 0 |

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



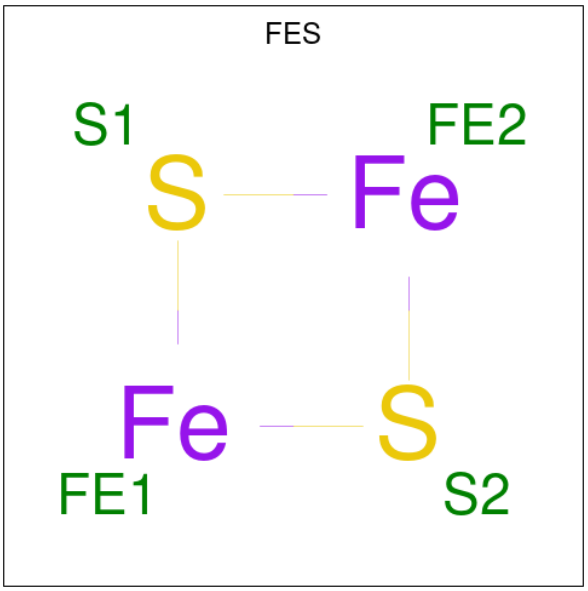

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 45 | A | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 45 | H | 1 | Total | C | N | O | P | 0 |
| | | | 102 | 82 | 2 | 16 | 2 | |
| 45 | H | 1 | Total | C | N | O | P | 0 |
| | | | 102 | 82 | 2 | 16 | 2 | |
| 45 | L | 1 | Total | C | N | O | P | 0 |
| | | | 93 | 73 | 2 | 16 | 2 | |
| 45 | L | 1 | Total | C | N | O | P | 0 |
| | | | 93 | 73 | 2 | 16 | 2 | |
| 45 | M | 1 | Total | C | N | O | P | 0 |
| | | | 277 | 218 | 5 | 48 | 6 | |
| 45 | M | 1 | Total | C | N | O | P | 0 |
| | | | 277 | 218 | 5 | 48 | 6 | |
| 45 | M | 1 | Total | C | N | O | P | 0 |
| | | | 277 | 218 | 5 | 48 | 6 | |
| 45 | M | 1 | Total | C | N | O | P | 0 |
| | | | 277 | 218 | 5 | 48 | 6 | |
| 45 | M | 1 | Total | C | N | O | P | 0 |
| | | | 277 | 218 | 5 | 48 | 6 | |
| 45 | M | 1 | Total | C | N | O | P | 0 |
| | | | 277 | 218 | 5 | 48 | 6 | |
| 45 | N | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |

- Molecule 46 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).



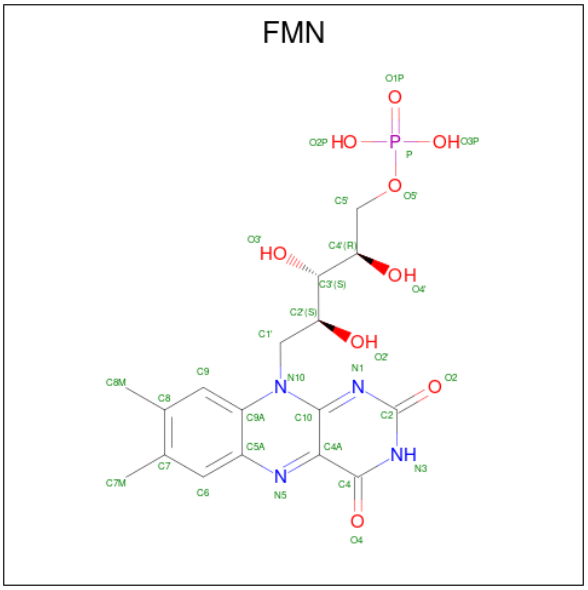

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 46 | B | 1 | 8 | 4 | 4 | 0 |
| 46 | F | 1 | 8 | 4 | 4 | 0 |
| 46 | G | 1 | 16 | 8 | 8 | 0 |
| 46 | G | 1 | 16 | 8 | 8 | 0 |
| 46 | I | 1 | 16 | 8 | 8 | 0 |
| 46 | I | 1 | 16 | 8 | 8 | 0 |

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: $Fe_2S_2$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 47 | E | 1 | 4 | 2 | 2 | 0 |
| 47 | G | 1 | 4 | 2 | 2 | 0 |

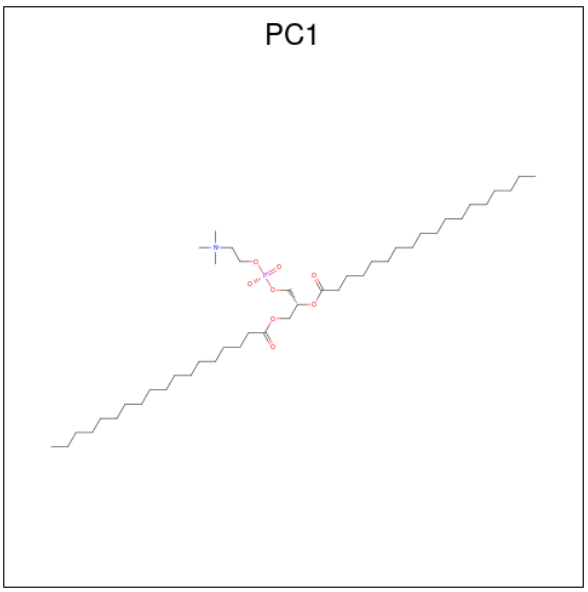
- Molecule 48 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 48 | F | 1 | 31 | 17 | 4 | 9 | 1 | 0 |

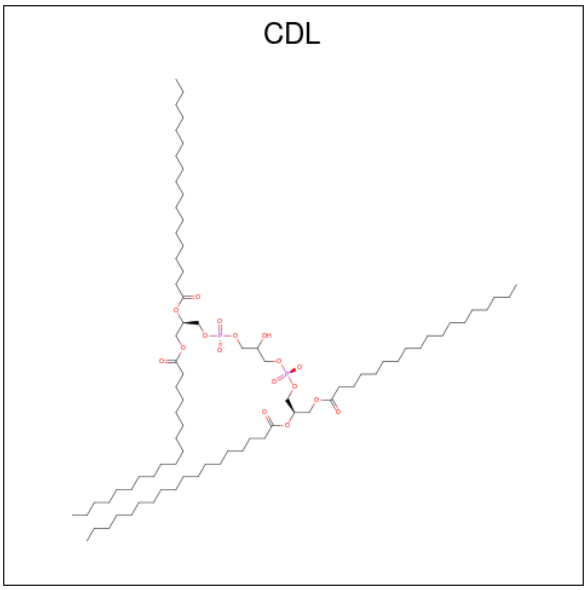
- Molecule 49 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code:

PC1) (formula: $C_{44}H_{88}NO_8P$).



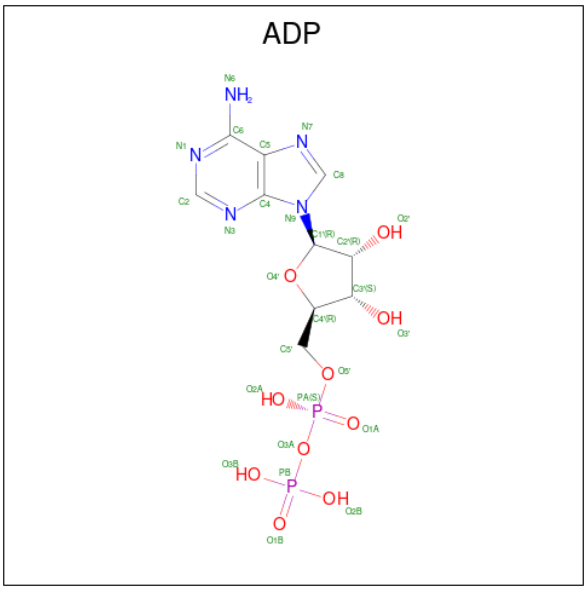

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 49 | H | 1 | Total<br>124 | C<br>94 | N<br>3 | O<br>24 | P<br>3 | 0 |
| 49 | H | 1 | Total<br>124 | C<br>94 | N<br>3 | O<br>24 | P<br>3 | 0 |
| 49 | H | 1 | Total<br>124 | C<br>94 | N<br>3 | O<br>24 | P<br>3 | 0 |
| 49 | P | 1 | Total<br>43 | C<br>33 | N<br>1 | O<br>8 | P<br>1 | 0 |

- Molecule 50 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



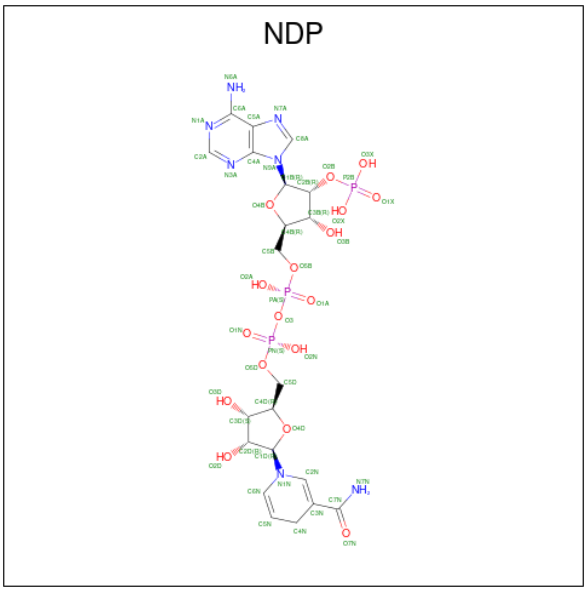
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | P | |
| 50 | H | 1 | 57 | 38 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 50 | L | 1 | 148 | 110 | 34 | 4 | 0 |
| | | | Total | C | O | P | |
| 50 | L | 1 | 148 | 110 | 34 | 4 | 0 |
| | | | Total | C | O | P | |
| 50 | M | 1 | 67 | 48 | 17 | 2 | 0 |

- Molecule 51 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 51 | O | 1 | 27 | 10 | 5 | 10 | 2 | 0 |

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

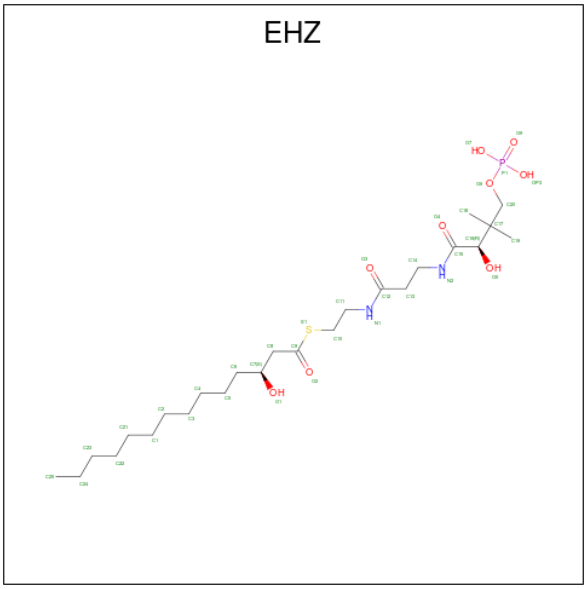



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 52 | P | 1 | 48 | 21 | 7 | 17 | 3 | 0 |

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



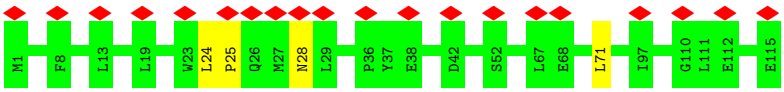
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | |
| 54 | T | 1 | 34 | 22 | 2 | 8 | 1 | 1 | 0 |
| | | | Total | C | N | O | P | S | |
| 54 | U | 1 | 35 | 23 | 2 | 8 | 1 | 1 | 0 |

# 3 Residue-property plots (i)

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

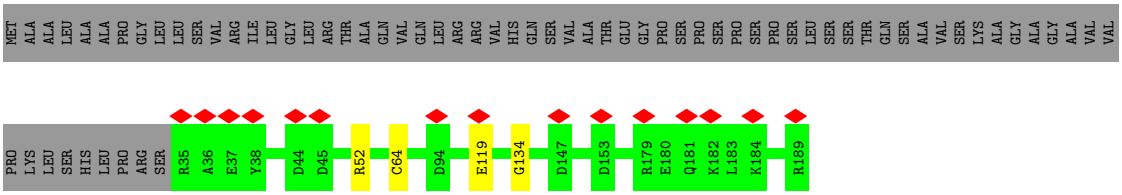
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 17% 97%



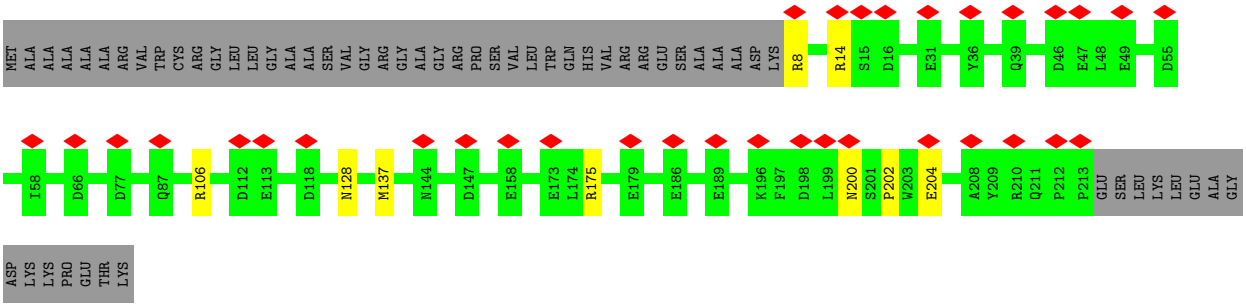

• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 7% 67% 31%



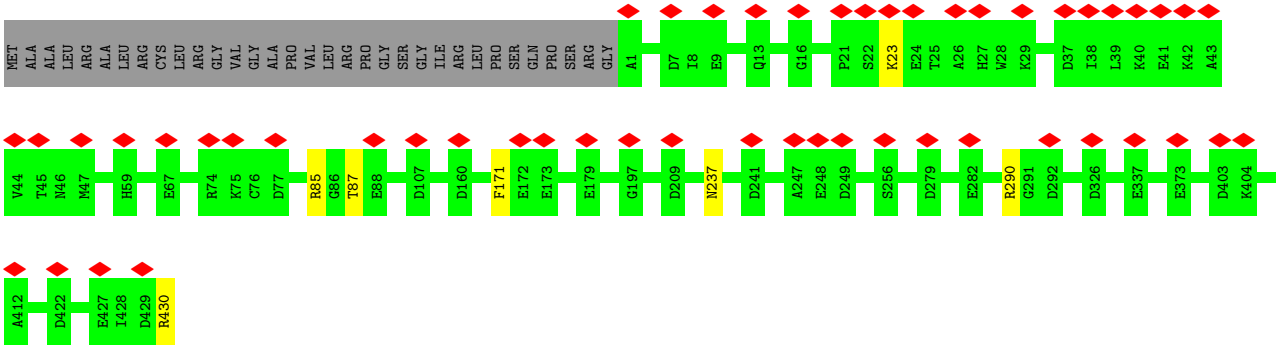

• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 13% 75% 22%



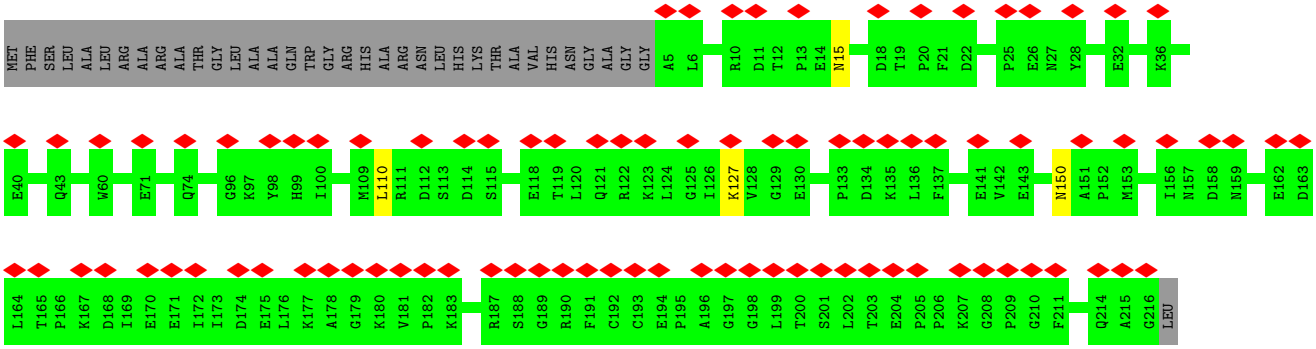

• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 11% 91% 7%



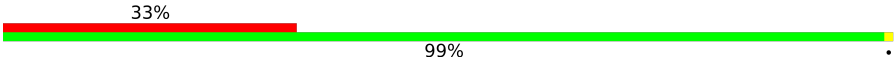

• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

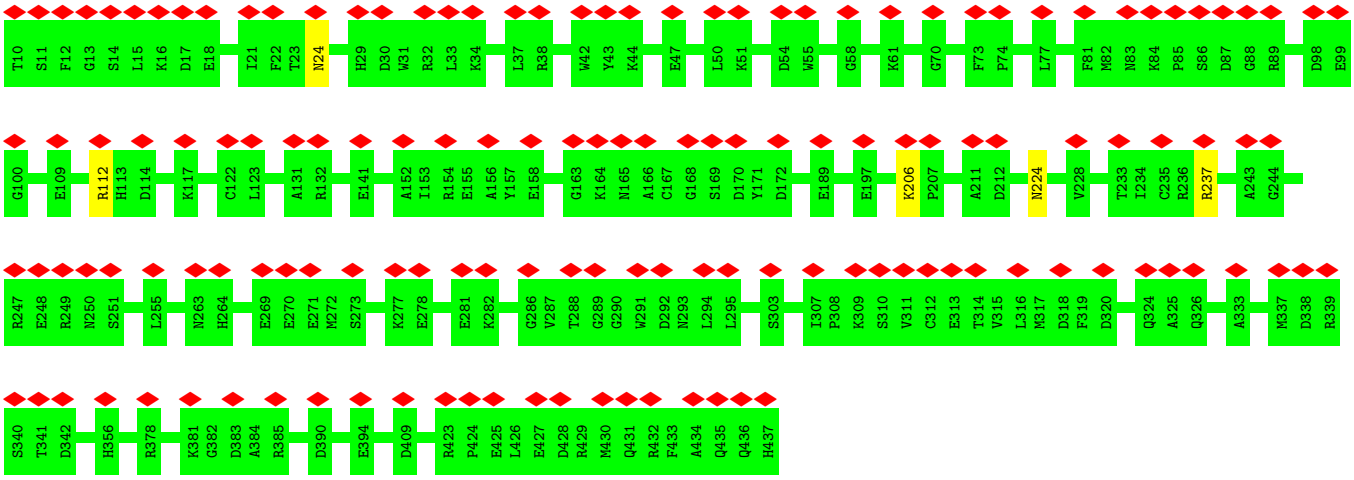
Chain E:




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

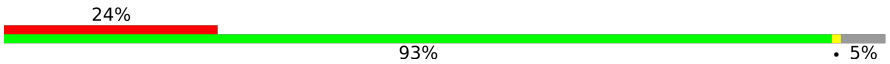
Chain F:

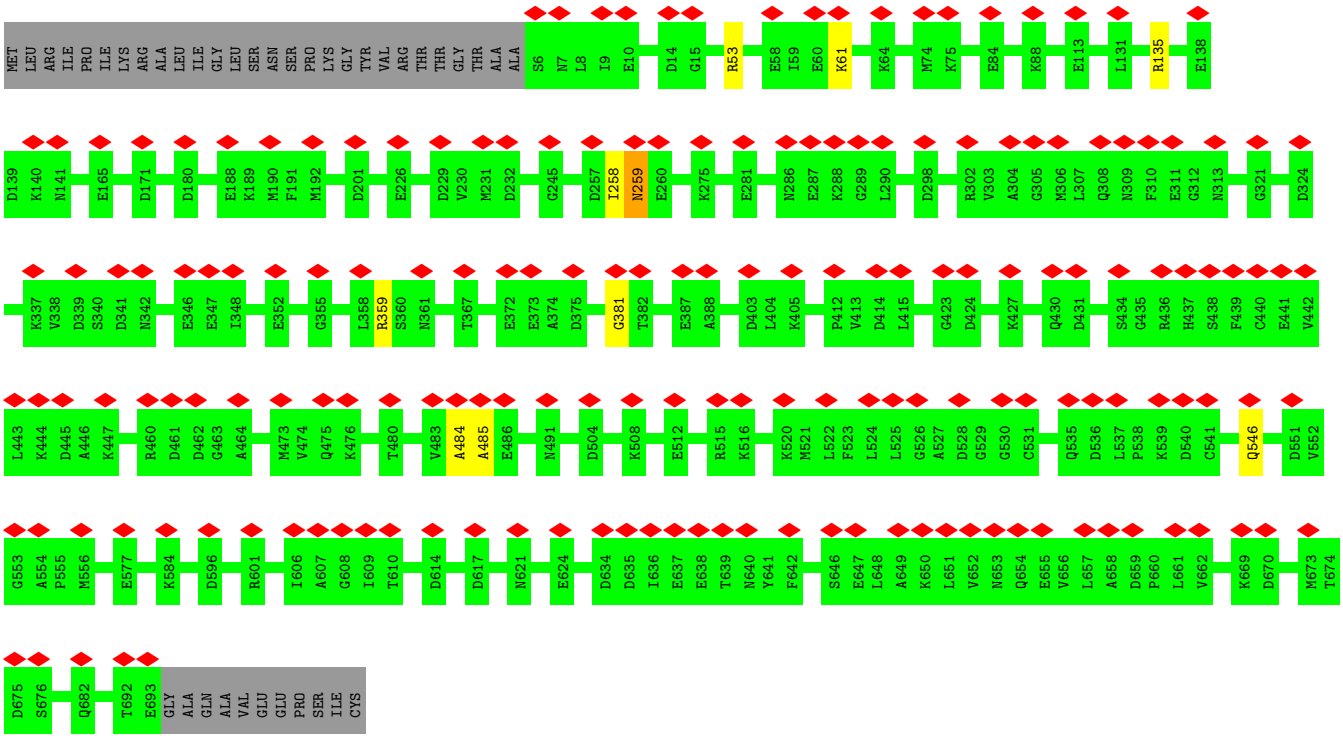



• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

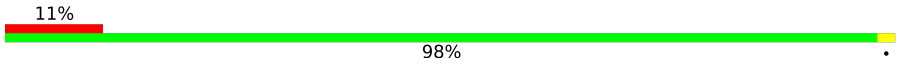
Chain G:

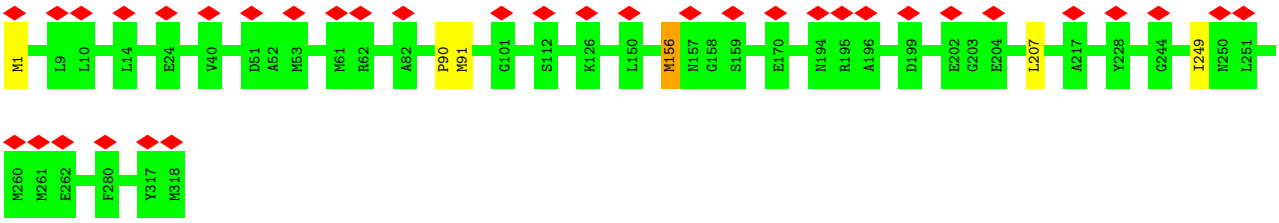





- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

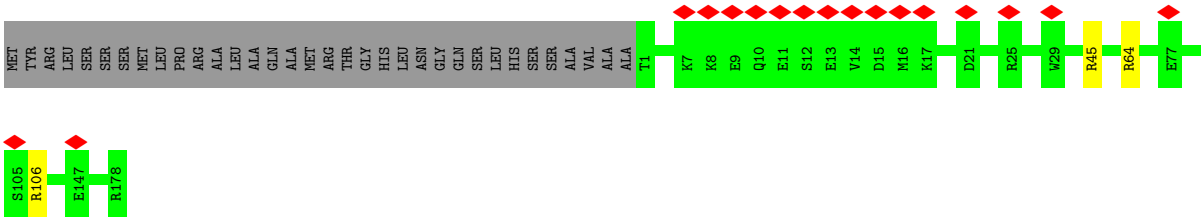
Chain H:



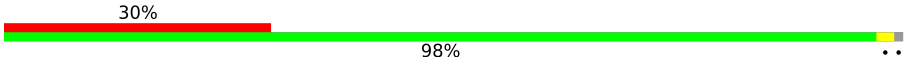

- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

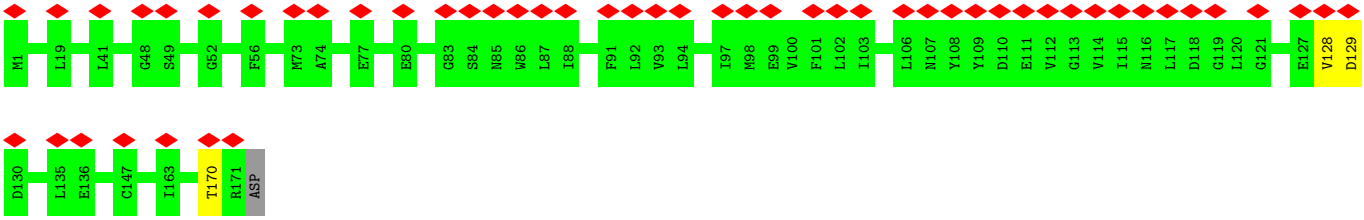
Chain I:




- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

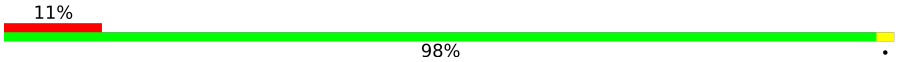
Chain J:

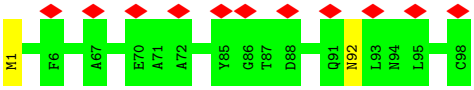





• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

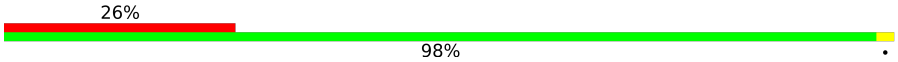
Chain K:

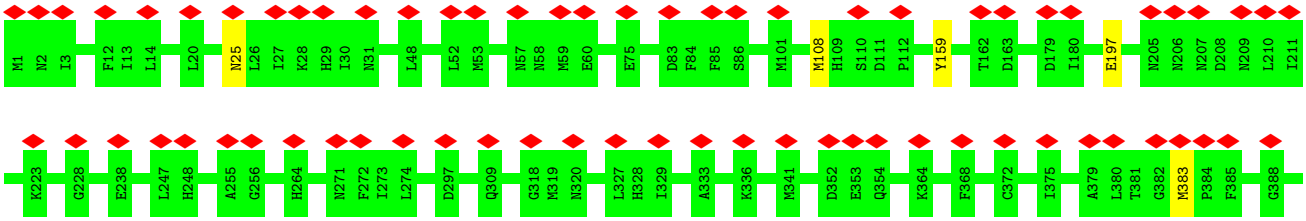



• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

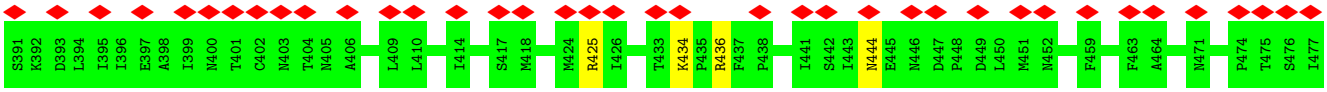
Chain L:

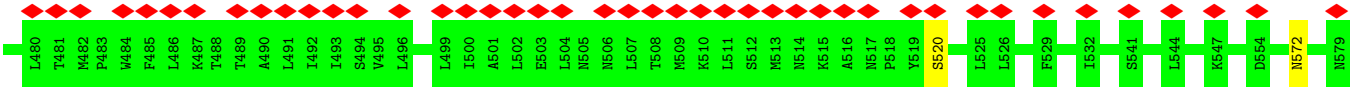


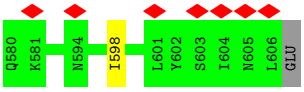







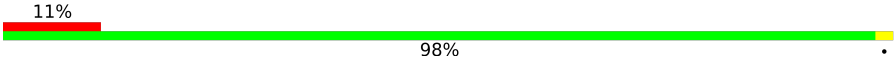


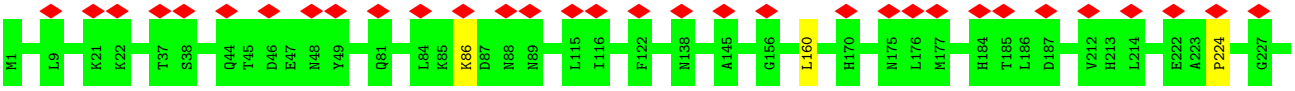



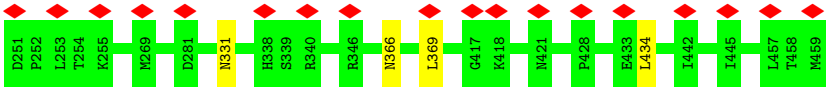




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:

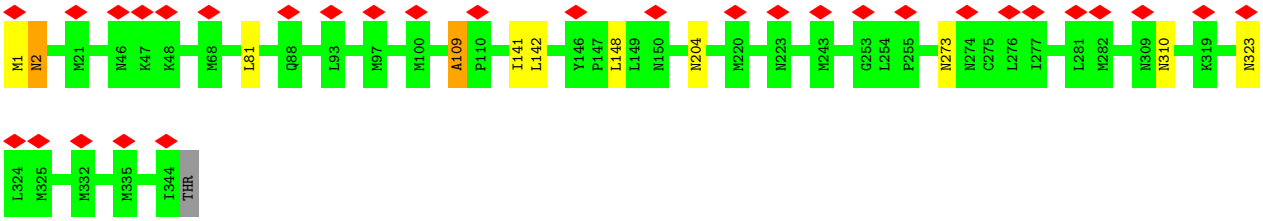


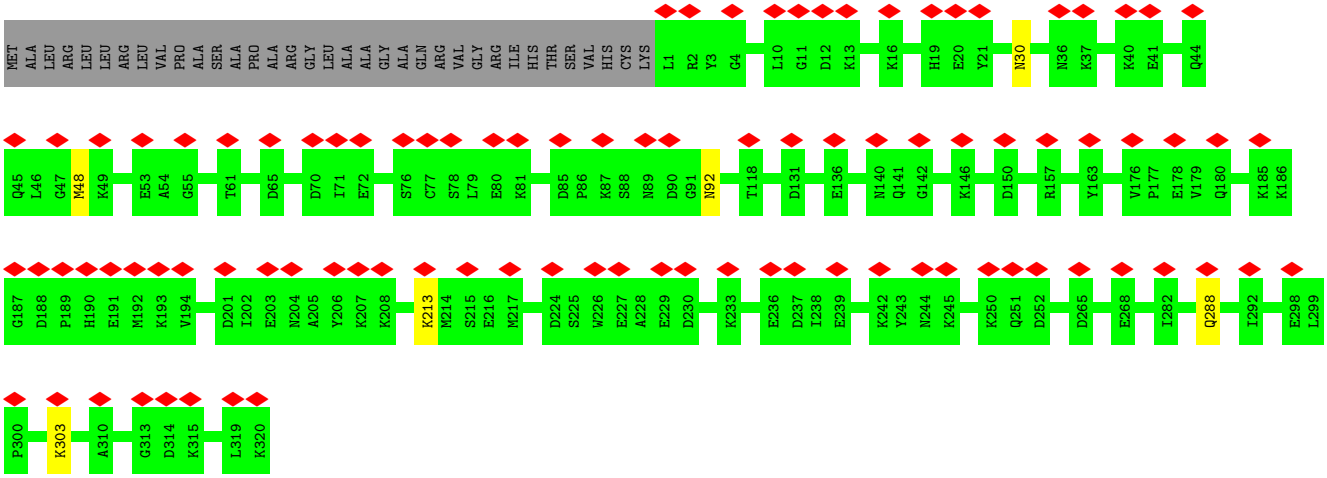

• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 9% 97%



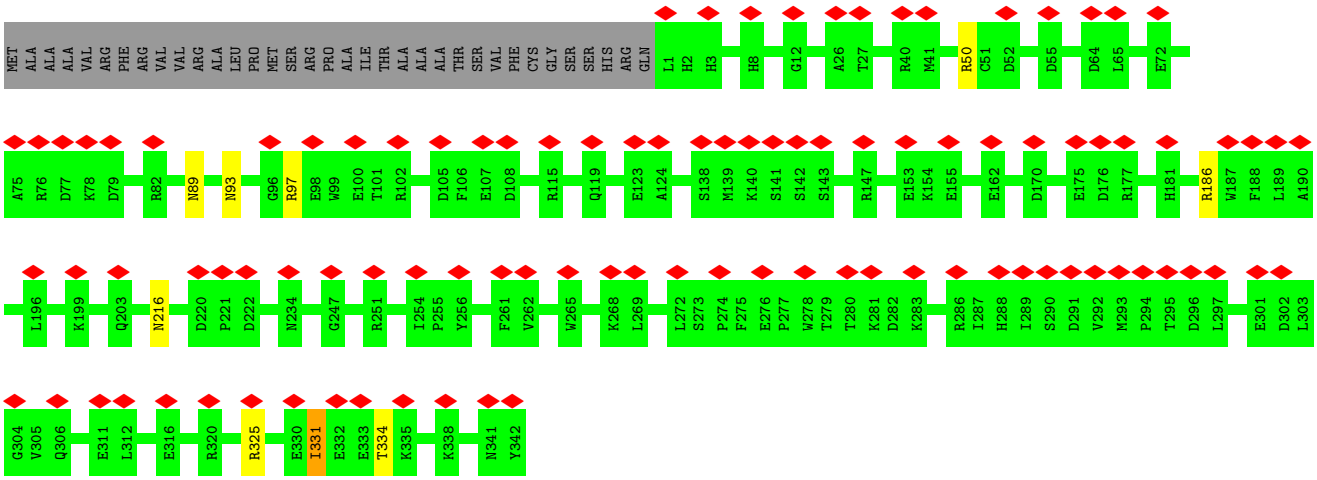

• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 26% 88% 10%



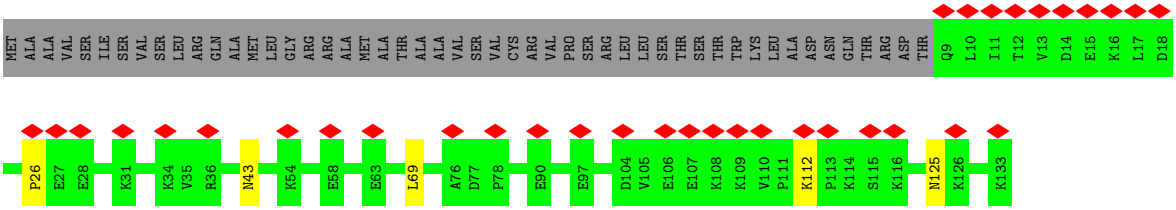

• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 26% 88% 9%



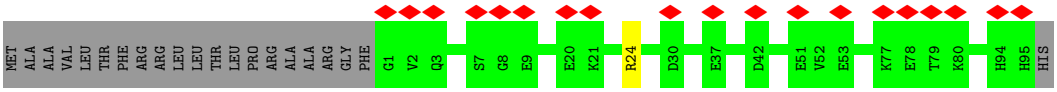

• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



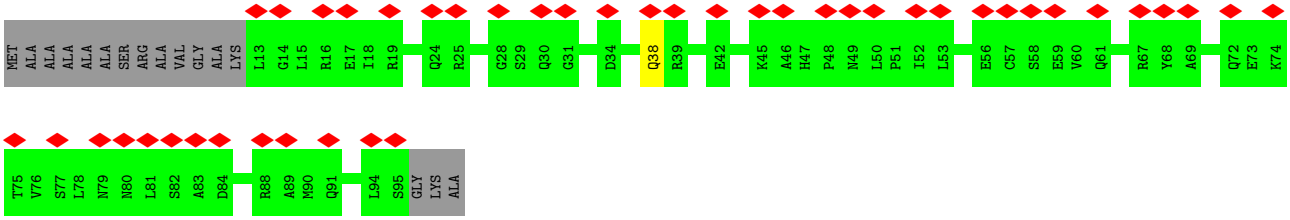

- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



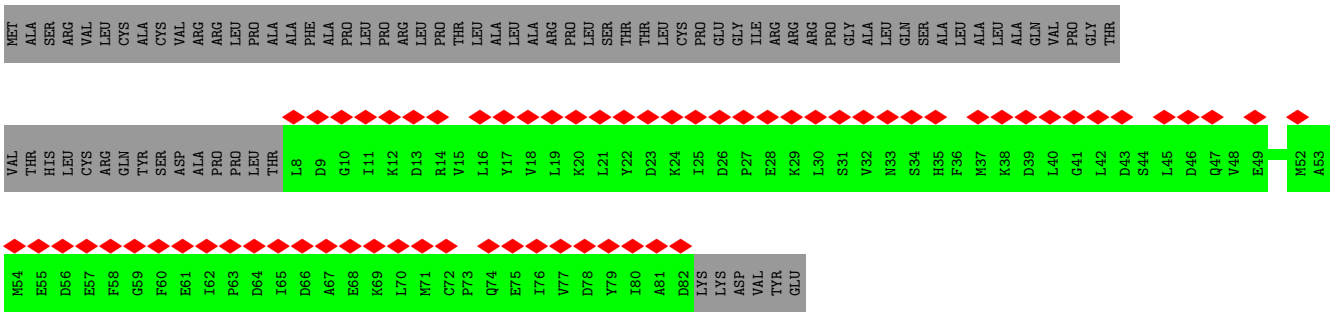

- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



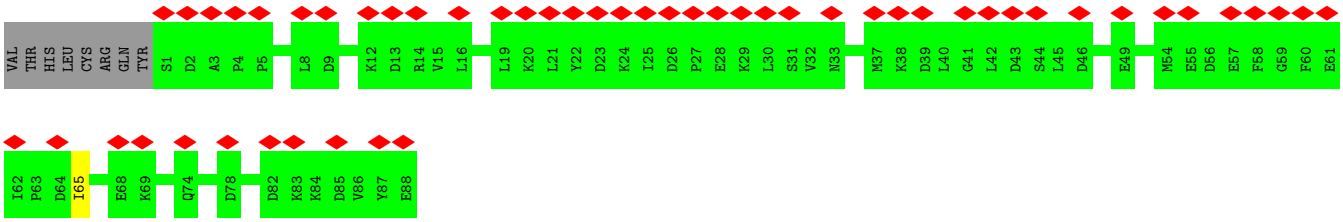

- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



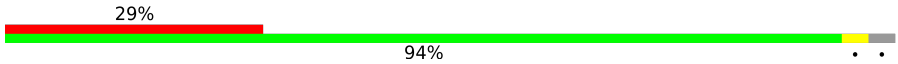

- Molecule 20: Acyl carrier protein, mitochondrial

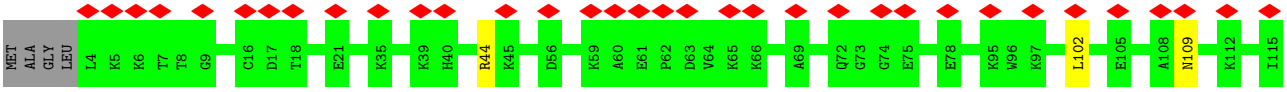
Chain U:




• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

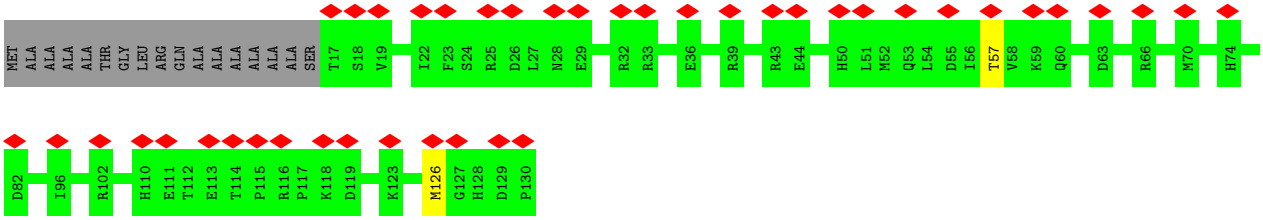
Chain V:



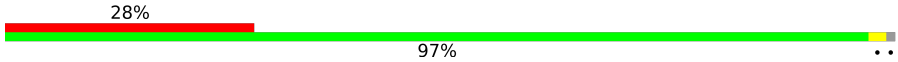

• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

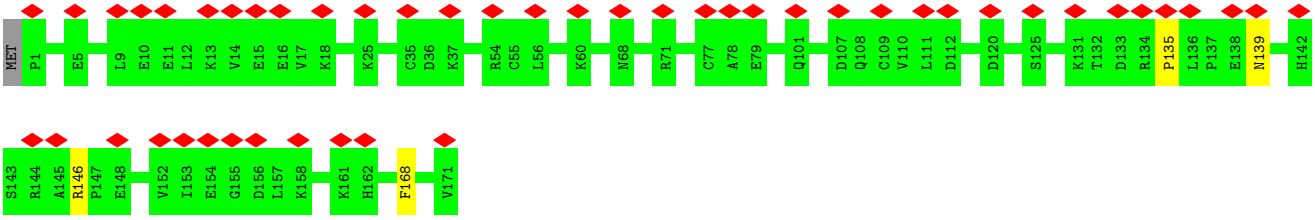
Chain W:




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

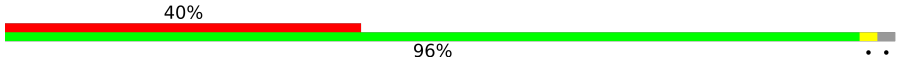
Chain X:

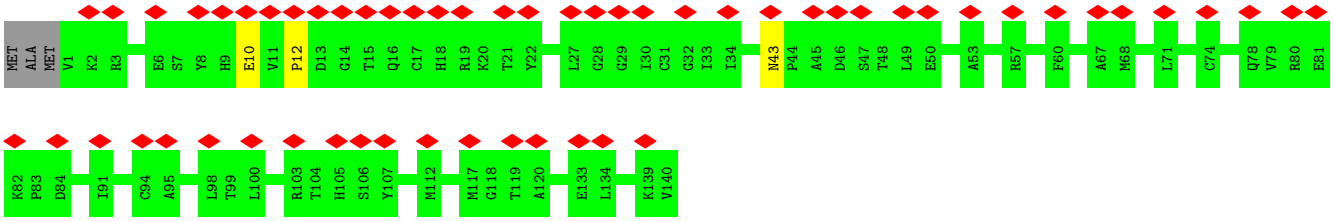



• Molecule 24: MCG5603

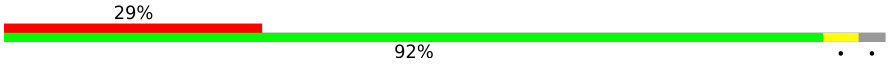
Chain Y:

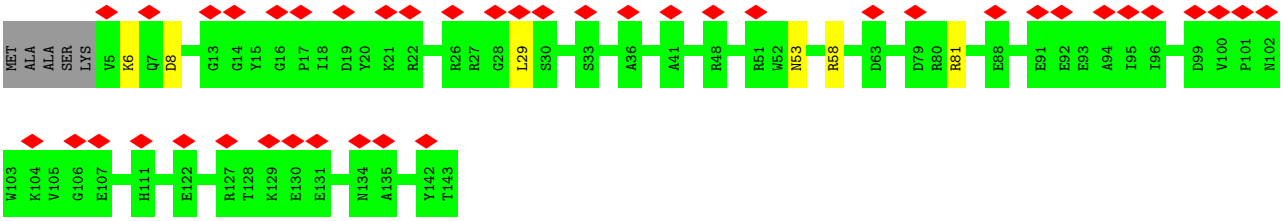



• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

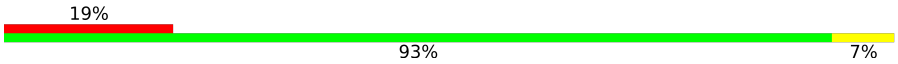
Chain Z:

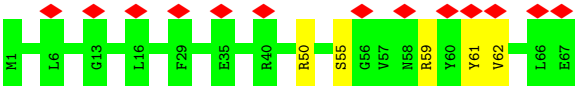



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

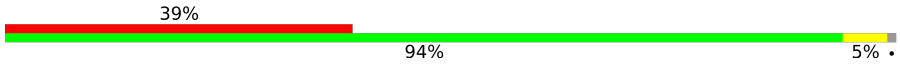
Chain a:

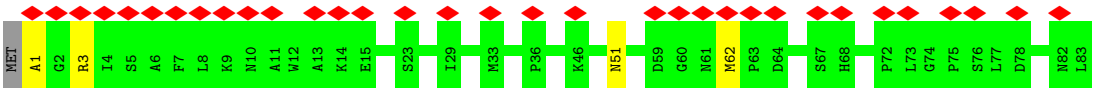



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

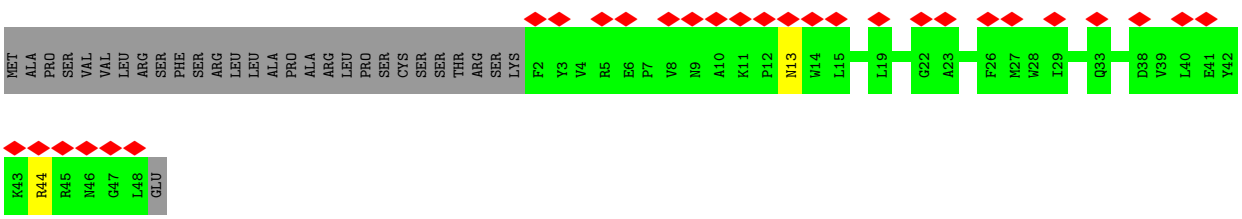
Chain b:



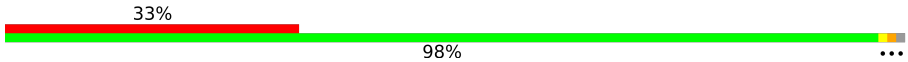

- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

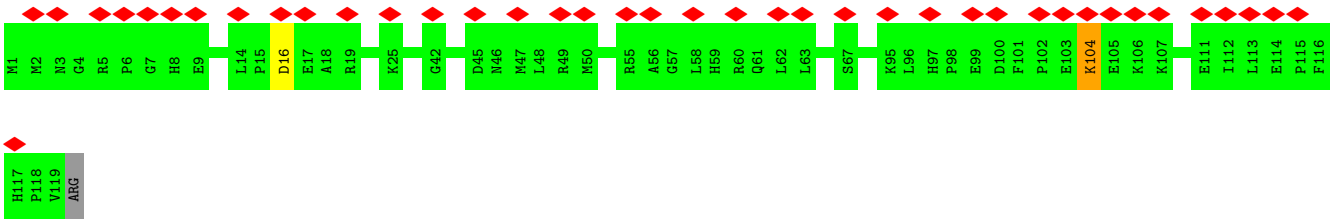
Chain c:




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

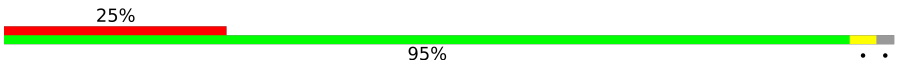
Chain d:



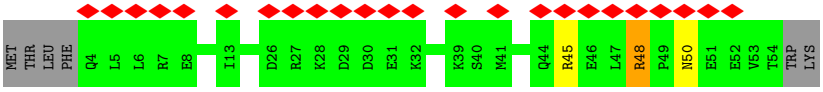

- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



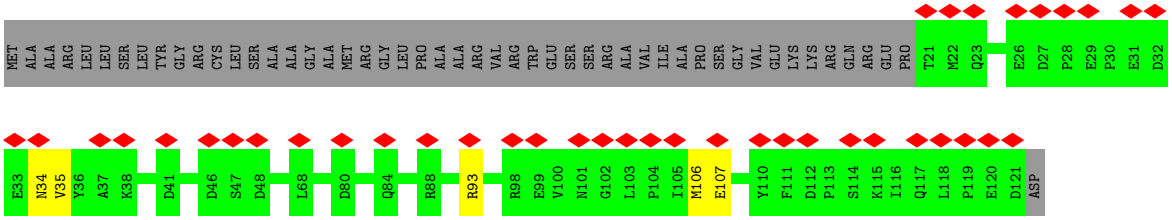
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



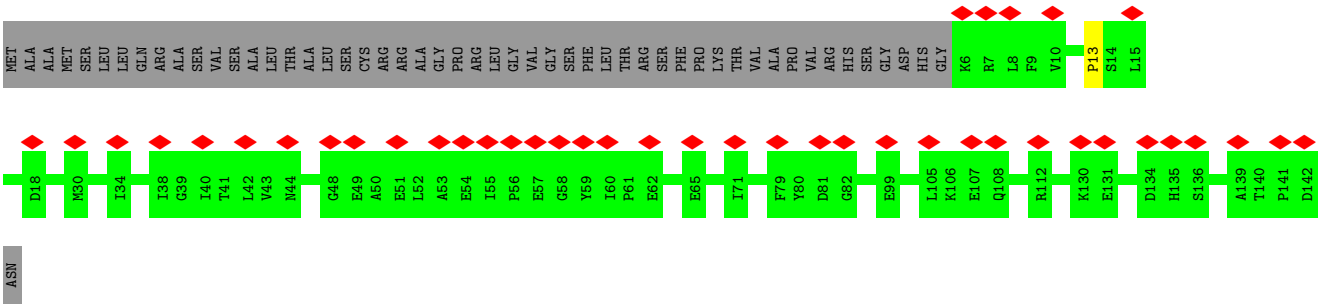

• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



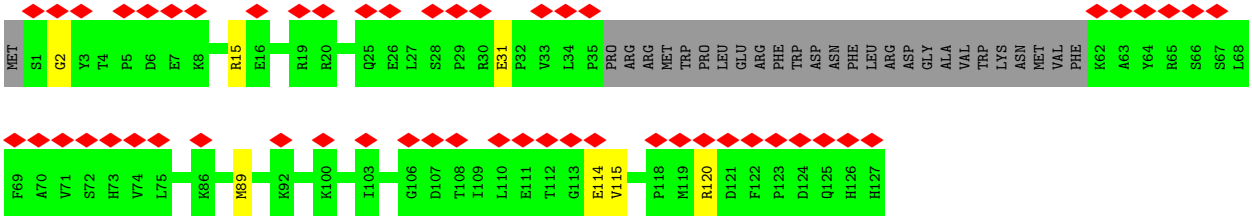

• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



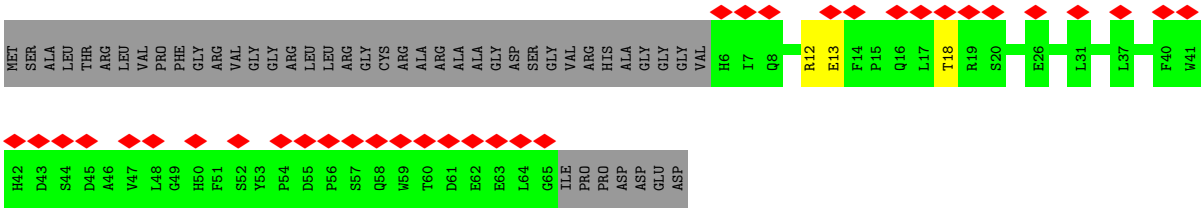

• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



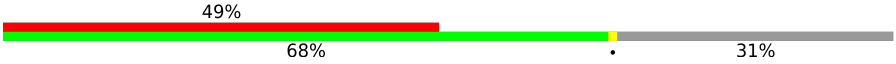
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

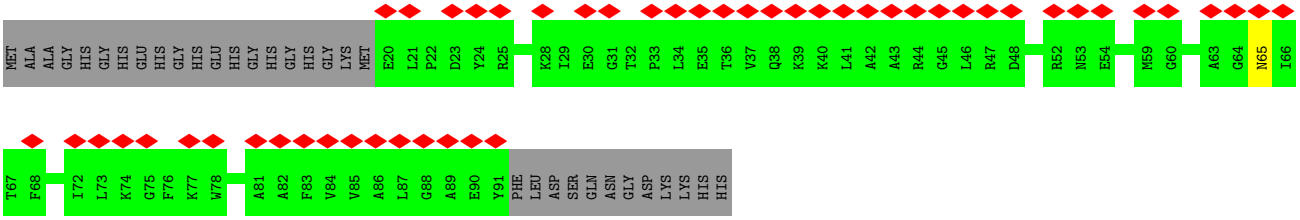
Chain j:




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

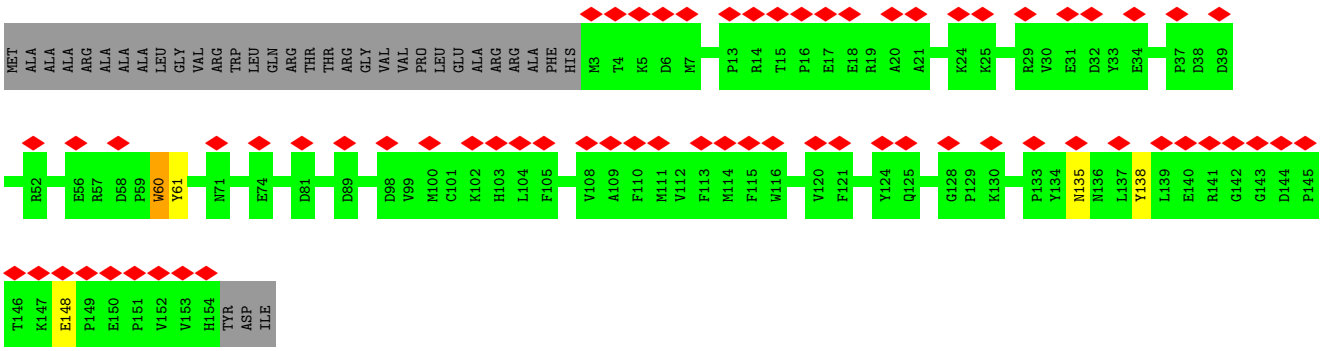
Chain k:



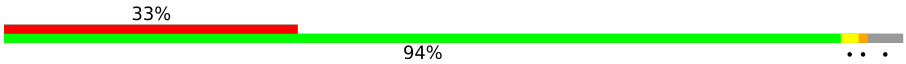

• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

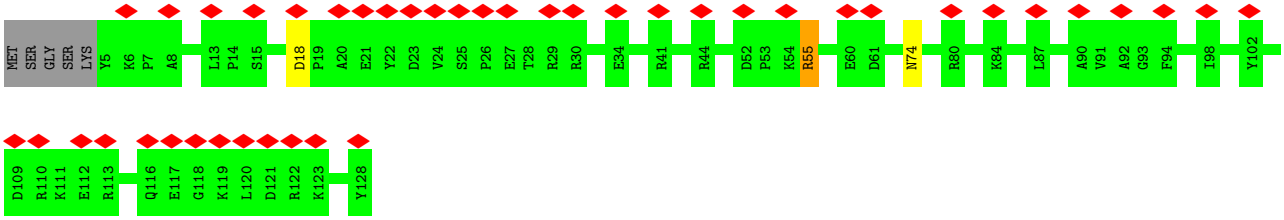
Chain l:




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

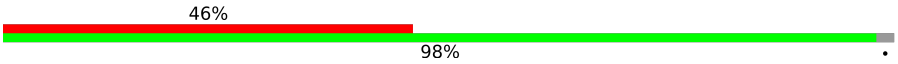
Chain m:

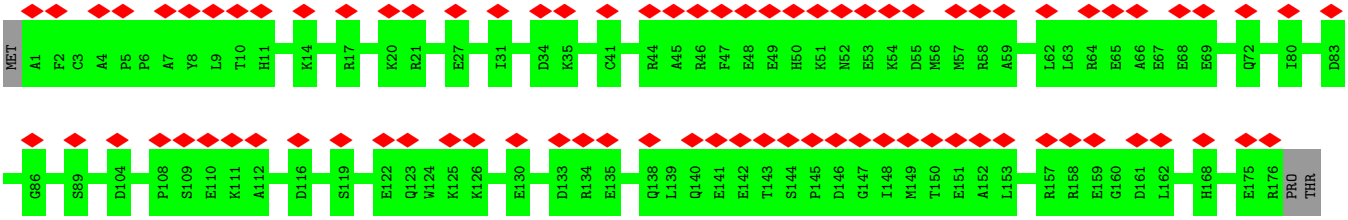


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

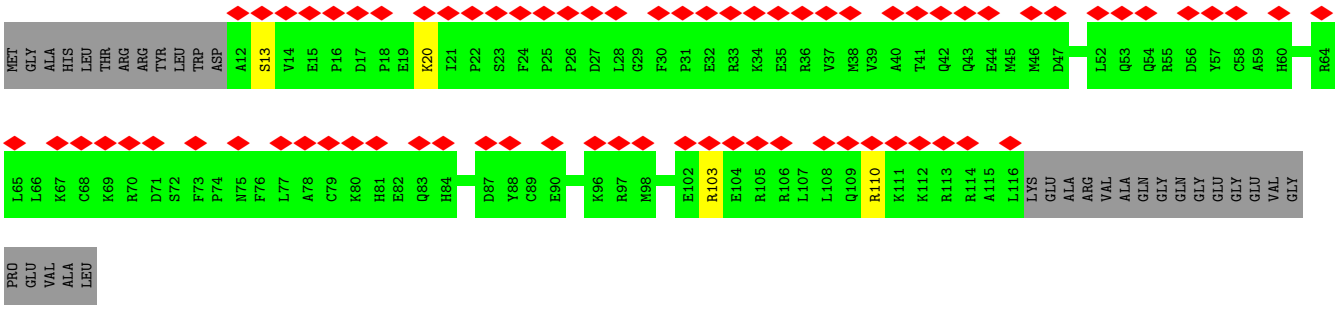
Chain n:



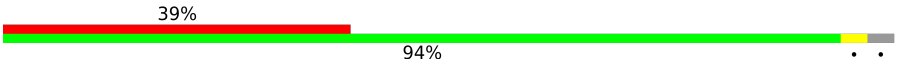

• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

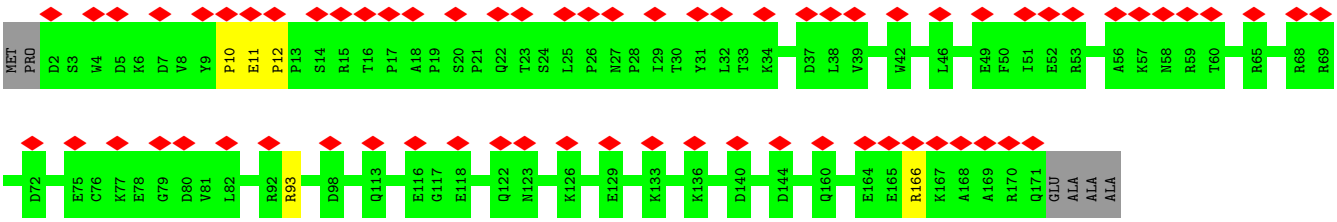
Chain o:




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

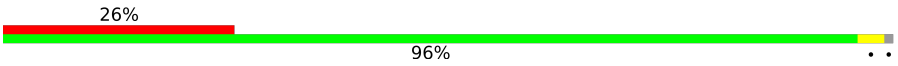
Chain p:

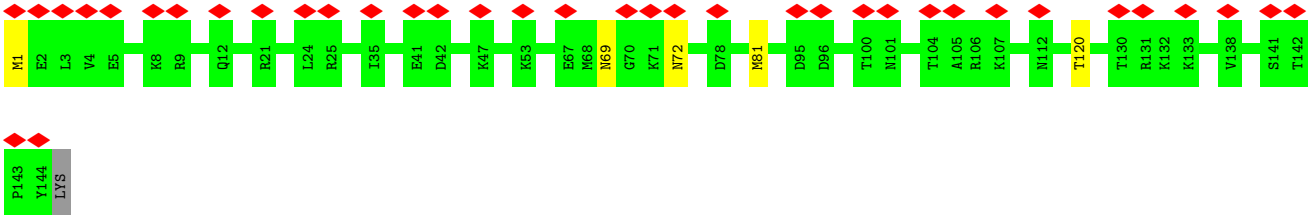



• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

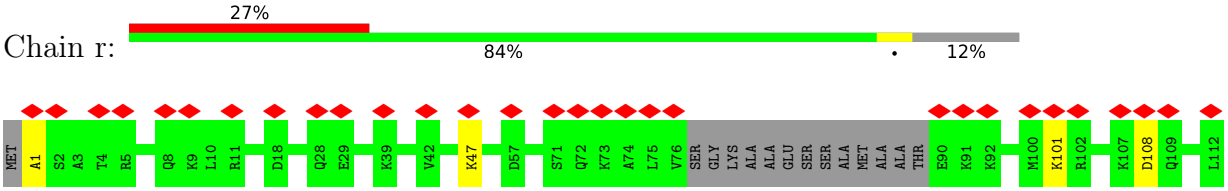
Chain q:



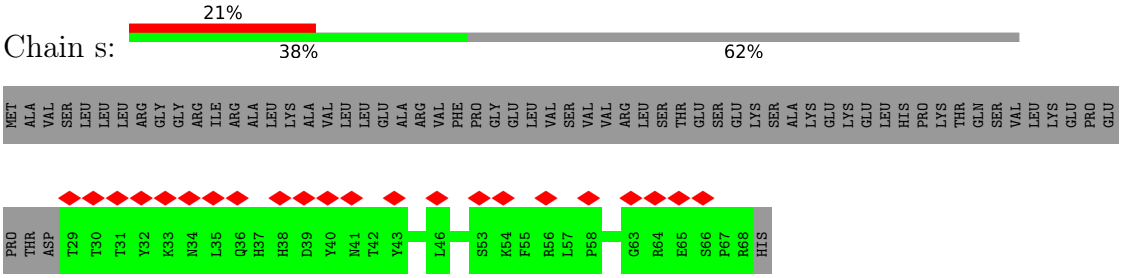

• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:




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

Chain s:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 20370 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50.0 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3100 | Depositor |
| Magnification | 47600 | Depositor |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 0.450 | Depositor |
| Minimum map value | -0.156 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.013 | Depositor |
| Recommended contour level | 0.075 | Depositor |
| Map size (Å) | 472.49997, 472.49997, 472.49997 | wwPDB |
| Map dimensions | 450, 450, 450 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.05, 1.05, 1.05 | 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: SAC, ADP, 2MR, FME, ZN, NDP, FES, CDL, AYA, EHZ, PC1, FMN, SF4, AME, 3PE

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | A | 0.39 | 0/949 | 0.71 | 2/1297 (0.2%) |
| 2 | B | 0.52 | 0/1272 | 0.72 | 0/1722 |
| 3 | C | 0.46 | 0/1762 | 0.69 | 1/2401 (0.0%) |
| 4 | D | 0.46 | 0/3528 | 0.64 | 0/4782 |
| 5 | E | 0.39 | 0/1688 | 0.63 | 1/2300 (0.0%) |
| 6 | F | 0.39 | 0/3376 | 0.63 | 0/4561 |
| 7 | G | 0.39 | 0/5383 | 0.64 | 1/7293 (0.0%) |
| 8 | H | 0.42 | 0/2607 | 0.64 | 0/3564 |
| 9 | I | 0.52 | 0/1438 | 0.77 | 1/1946 (0.1%) |
| 10 | J | 0.41 | 0/1322 | 0.61 | 0/1799 |
| 11 | K | 0.39 | 0/738 | 0.65 | 0/1002 |
| 12 | L | 0.39 | 0/4913 | 0.62 | 0/6686 |
| 13 | M | 0.39 | 0/3709 | 0.64 | 2/5052 (0.0%) |
| 14 | N | 0.40 | 0/2748 | 0.65 | 3/3741 (0.1%) |
| 15 | O | 0.40 | 0/2674 | 0.61 | 0/3626 |
| 16 | P | 0.38 | 0/2823 | 0.66 | 0/3828 |
| 17 | Q | 0.39 | 0/1038 | 0.64 | 0/1401 |
| 18 | R | 0.40 | 0/762 | 0.63 | 1/1026 (0.1%) |
| 19 | S | 0.34 | 0/678 | 0.65 | 0/915 |
| 20 | T | 0.30 | 0/613 | 0.51 | 0/826 |
| 20 | U | 0.38 | 0/718 | 0.55 | 0/970 |
| 21 | V | 0.35 | 0/937 | 0.66 | 1/1270 (0.1%) |
| 22 | W | 0.38 | 0/993 | 0.68 | 0/1335 |
| 23 | X | 0.37 | 0/1434 | 0.61 | 0/1937 |
| 24 | Y | 0.35 | 0/1061 | 0.61 | 0/1439 |
| 25 | Z | 0.39 | 0/1183 | 0.67 | 1/1597 (0.1%) |
| 26 | a | 0.39 | 0/561 | 0.64 | 0/755 |
| 27 | b | 0.39 | 0/666 | 0.60 | 0/914 |
| 28 | c | 0.34 | 0/400 | 0.55 | 0/544 |
| 29 | d | 0.40 | 0/1017 | 0.67 | 0/1373 |
| 30 | e | 0.36 | 0/892 | 0.65 | 0/1187 |
| 31 | f | 0.36 | 0/443 | 0.65 | 0/596 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 32 | g | 0.38 | 0/878 | 0.60 | 0/1196 |
| 33 | h | 0.39 | 0/1189 | 0.60 | 0/1610 |
| 34 | i | 0.36 | 0/836 | 0.63 | 1/1138 (0.1%) |
| 35 | j | 0.36 | 0/548 | 0.67 | 0/748 |
| 36 | k | 0.35 | 0/601 | 0.61 | 0/814 |
| 37 | l | 0.40 | 0/1327 | 0.62 | 0/1811 |
| 38 | m | 0.38 | 0/1064 | 0.71 | 1/1444 (0.1%) |
| 39 | n | 0.39 | 0/1581 | 0.64 | 0/2140 |
| 40 | o | 0.35 | 0/919 | 0.63 | 0/1232 |
| 41 | p | 0.39 | 0/1471 | 0.64 | 1/1988 (0.1%) |
| 42 | q | 0.45 | 0/1234 | 0.68 | 0/1681 |
| 43 | r | 0.38 | 0/806 | 0.71 | 1/1090 (0.1%) |
| 44 | s | 0.32 | 0/345 | 0.56 | 0/468 |
| All | All | 0.40 | 0/67125 | 0.64 | 18/91045 (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 |
|---|---|---|---|
| 2 | B | 0 | 2 |
| 3 | C | 0 | 1 |
| 4 | D | 0 | 2 |
| 5 | E | 0 | 1 |
| 6 | F | 0 | 1 |
| 7 | G | 0 | 5 |
| 8 | H | 0 | 5 |
| 10 | J | 0 | 2 |
| 12 | L | 0 | 7 |
| 13 | M | 0 | 1 |
| 14 | N | 0 | 2 |
| 16 | P | 0 | 3 |
| 17 | Q | 0 | 1 |
| 20 | U | 0 | 1 |
| 22 | W | 0 | 1 |
| 23 | X | 0 | 1 |
| 25 | Z | 0 | 1 |
| 26 | a | 0 | 2 |
| 29 | d | 0 | 2 |
| 30 | e | 0 | 1 |
| 31 | f | 0 | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 32 | g | 0 | 2 |
| 34 | i | 0 | 3 |
| 35 | j | 0 | 2 |
| 37 | l | 0 | 3 |
| 38 | m | 0 | 1 |
| 40 | o | 0 | 2 |
| 41 | p | 0 | 3 |
| 42 | q | 0 | 1 |
| All | All | 0 | 60 |

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 24 | LEU | CA-CB-CG | 7.87 | 133.40 | 115.30 |
| 38 | m | 18 | ASP | CB-CG-OD1 | 7.04 | 124.64 | 118.30 |
| 21 | V | 102 | LEU | CB-CG-CD2 | 6.87 | 122.67 | 111.00 |
| 43 | r | 108 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 14 | N | 148 | LEU | CA-CB-CG | 5.75 | 128.53 | 115.30 |

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 119 | GLU | Peptide |
| 2 | B | 134 | GLY | Peptide |
| 3 | C | 8 | ARG | Peptide |
| 4 | D | 171 | PHE | Peptide |
| 4 | D | 87 | THR | Peptide |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 113/115 (98%) | 90 (80%) | 22 (20%) | 1 (1%) | 17 | 48 |
| 2 | B | 153/224 (68%) | 134 (88%) | 19 (12%) | 0 | 100 | 100 |
| 3 | C | 204/263 (78%) | 172 (84%) | 30 (15%) | 2 (1%) | 15 | 46 |
| 4 | D | 427/463 (92%) | 372 (87%) | 55 (13%) | 0 | 100 | 100 |
| 5 | E | 210/248 (85%) | 169 (80%) | 40 (19%) | 1 (0%) | 29 | 61 |
| 6 | F | 426/428 (100%) | 360 (84%) | 66 (16%) | 0 | 100 | 100 |
| 7 | G | 686/727 (94%) | 593 (86%) | 90 (13%) | 3 (0%) | 34 | 66 |
| 8 | H | 316/318 (99%) | 272 (86%) | 44 (14%) | 0 | 100 | 100 |
| 9 | I | 176/212 (83%) | 145 (82%) | 31 (18%) | 0 | 100 | 100 |
| 10 | J | 169/172 (98%) | 148 (88%) | 20 (12%) | 1 (1%) | 25 | 57 |
| 11 | K | 96/98 (98%) | 89 (93%) | 7 (7%) | 0 | 100 | 100 |
| 12 | L | 604/607 (100%) | 508 (84%) | 96 (16%) | 0 | 100 | 100 |
| 13 | M | 457/459 (100%) | 413 (90%) | 43 (9%) | 1 (0%) | 47 | 77 |
| 14 | N | 342/345 (99%) | 309 (90%) | 31 (9%) | 2 (1%) | 25 | 57 |
| 15 | O | 318/355 (90%) | 273 (86%) | 44 (14%) | 1 (0%) | 41 | 71 |
| 16 | P | 340/377 (90%) | 280 (82%) | 59 (17%) | 1 (0%) | 41 | 71 |
| 17 | Q | 123/175 (70%) | 109 (89%) | 13 (11%) | 1 (1%) | 19 | 51 |
| 18 | R | 93/116 (80%) | 80 (86%) | 13 (14%) | 0 | 100 | 100 |
| 19 | S | 81/99 (82%) | 69 (85%) | 12 (15%) | 0 | 100 | 100 |
| 20 | T | 73/156 (47%) | 66 (90%) | 7 (10%) | 0 | 100 | 100 |
| 20 | U | 86/156 (55%) | 69 (80%) | 17 (20%) | 0 | 100 | 100 |
| 21 | V | 110/116 (95%) | 92 (84%) | 18 (16%) | 0 | 100 | 100 |
| 22 | W | 112/131 (86%) | 101 (90%) | 11 (10%) | 0 | 100 | 100 |
| 23 | X | 169/172 (98%) | 140 (83%) | 27 (16%) | 2 (1%) | 13 | 42 |
| 24 | Y | 138/143 (96%) | 120 (87%) | 16 (12%) | 2 (1%) | 11 | 38 |
| 25 | Z | 137/144 (95%) | 114 (83%) | 22 (16%) | 1 (1%) | 22 | 54 |
| 26 | a | 65/67 (97%) | 55 (85%) | 9 (14%) | 1 (2%) | 10 | 38 |
| 27 | b | 81/84 (96%) | 63 (78%) | 18 (22%) | 0 | 100 | 100 |
| 28 | c | 45/76 (59%) | 42 (93%) | 3 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 29 | d | 117/120 (98%) | 98 (84%) | 19 (16%) | 0 | 100 | 100 |
| 30 | e | 102/106 (96%) | 84 (82%) | 17 (17%) | 1 (1%) | 15 | 46 |
| 31 | f | 49/57 (86%) | 37 (76%) | 11 (22%) | 1 (2%) | 7 | 32 |
| 32 | g | 99/151 (66%) | 76 (77%) | 22 (22%) | 1 (1%) | 15 | 46 |
| 33 | h | 135/189 (71%) | 113 (84%) | 21 (16%) | 1 (1%) | 22 | 54 |
| 34 | i | 97/128 (76%) | 76 (78%) | 19 (20%) | 2 (2%) | 7 | 31 |
| 35 | j | 58/105 (55%) | 41 (71%) | 16 (28%) | 1 (2%) | 9 | 35 |
| 36 | k | 70/104 (67%) | 54 (77%) | 16 (23%) | 0 | 100 | 100 |
| 37 | l | 150/186 (81%) | 112 (75%) | 35 (23%) | 3 (2%) | 7 | 32 |
| 38 | m | 122/129 (95%) | 102 (84%) | 20 (16%) | 0 | 100 | 100 |
| 39 | n | 174/179 (97%) | 149 (86%) | 25 (14%) | 0 | 100 | 100 |
| 40 | o | 103/137 (75%) | 85 (82%) | 18 (18%) | 0 | 100 | 100 |
| 41 | p | 168/176 (96%) | 142 (84%) | 26 (16%) | 0 | 100 | 100 |
| 42 | q | 142/145 (98%) | 108 (76%) | 32 (22%) | 2 (1%) | 11 | 38 |
| 43 | r | 95/113 (84%) | 77 (81%) | 18 (19%) | 0 | 100 | 100 |
| 44 | s | 38/104 (36%) | 32 (84%) | 6 (16%) | 0 | 100 | 100 |
| All | All | 8069/9175 (88%) | 6833 (85%) | 1204 (15%) | 32 (0%) | 38 | 66 |

5 of 32 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | g | 107 | GLU |
| 35 | j | 13 | GLU |
| 37 | l | 61 | TYR |
| 7 | G | 259 | ASN |
| 15 | O | 303 | LYS |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 103/103 (100%) | 102 (99%) | 1 (1%) | 76 | 86 |
| 2 | B | 131/185 (71%) | 129 (98%) | 2 (2%) | 65 | 81 |
| 3 | C | 188/227 (83%) | 183 (97%) | 5 (3%) | 44 | 71 |
| 4 | D | 367/394 (93%) | 363 (99%) | 4 (1%) | 73 | 85 |
| 5 | E | 183/206 (89%) | 182 (100%) | 1 (0%) | 88 | 93 |
| 6 | F | 343/343 (100%) | 339 (99%) | 4 (1%) | 71 | 83 |
| 7 | G | 580/610 (95%) | 578 (100%) | 2 (0%) | 92 | 96 |
| 8 | H | 279/279 (100%) | 278 (100%) | 1 (0%) | 91 | 95 |
| 9 | I | 145/178 (82%) | 143 (99%) | 2 (1%) | 67 | 82 |
| 10 | J | 136/137 (99%) | 136 (100%) | 0 | 100 | 100 |
| 11 | K | 87/87 (100%) | 86 (99%) | 1 (1%) | 73 | 85 |
| 12 | L | 548/549 (100%) | 543 (99%) | 5 (1%) | 78 | 87 |
| 13 | M | 414/414 (100%) | 411 (99%) | 3 (1%) | 84 | 90 |
| 14 | N | 306/307 (100%) | 301 (98%) | 5 (2%) | 62 | 79 |
| 15 | O | 284/309 (92%) | 279 (98%) | 5 (2%) | 59 | 78 |
| 16 | P | 299/325 (92%) | 293 (98%) | 6 (2%) | 55 | 76 |
| 17 | Q | 112/153 (73%) | 109 (97%) | 3 (3%) | 44 | 71 |
| 18 | R | 80/96 (83%) | 80 (100%) | 0 | 100 | 100 |
| 19 | S | 74/80 (92%) | 73 (99%) | 1 (1%) | 67 | 82 |
| 20 | T | 69/135 (51%) | 69 (100%) | 0 | 100 | 100 |
| 20 | U | 81/135 (60%) | 81 (100%) | 0 | 100 | 100 |
| 21 | V | 100/102 (98%) | 98 (98%) | 2 (2%) | 55 | 76 |
| 22 | W | 108/114 (95%) | 107 (99%) | 1 (1%) | 78 | 87 |
| 23 | X | 153/154 (99%) | 152 (99%) | 1 (1%) | 84 | 90 |
| 24 | Y | 105/107 (98%) | 104 (99%) | 1 (1%) | 76 | 86 |
| 25 | Z | 120/123 (98%) | 117 (98%) | 3 (2%) | 47 | 72 |
| 26 | a | 57/57 (100%) | 55 (96%) | 2 (4%) | 36 | 64 |
| 27 | b | 72/73 (99%) | 69 (96%) | 3 (4%) | 30 | 60 |
| 28 | c | 41/67 (61%) | 39 (95%) | 2 (5%) | 25 | 56 |
| 29 | d | 106/107 (99%) | 105 (99%) | 1 (1%) | 78 | 87 |
| 30 | e | 92/94 (98%) | 91 (99%) | 1 (1%) | 73 | 85 |
| 31 | f | 47/53 (89%) | 45 (96%) | 2 (4%) | 29 | 59 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 32 | g | 92/129 (71%) | 90 (98%) | 2 (2%) | 52 | 74 |
| 33 | h | 122/162 (75%) | 122 (100%) | 0 | 100 | 100 |
| 34 | i | 87/119 (73%) | 86 (99%) | 1 (1%) | 73 | 85 |
| 35 | j | 56/87 (64%) | 56 (100%) | 0 | 100 | 100 |
| 36 | k | 55/78 (70%) | 54 (98%) | 1 (2%) | 59 | 78 |
| 37 | l | 137/161 (85%) | 137 (100%) | 0 | 100 | 100 |
| 38 | m | 110/114 (96%) | 108 (98%) | 2 (2%) | 59 | 78 |
| 39 | n | 161/164 (98%) | 161 (100%) | 0 | 100 | 100 |
| 40 | o | 98/121 (81%) | 96 (98%) | 2 (2%) | 55 | 76 |
| 41 | p | 155/158 (98%) | 154 (99%) | 1 (1%) | 86 | 91 |
| 42 | q | 129/130 (99%) | 128 (99%) | 1 (1%) | 81 | 89 |
| 43 | r | 88/96 (92%) | 86 (98%) | 2 (2%) | 50 | 73 |
| 44 | s | 39/95 (41%) | 39 (100%) | 0 | 100 | 100 |
| All | All | 7139/7917 (90%) | 7057 (99%) | 82 (1%) | 74 | 85 |

5 of 82 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 25 | Z | 53 | ASN |
| 32 | g | 93 | ARG |
| 26 | a | 50 | ARG |
| 28 | c | 44 | ARG |
| 38 | m | 74 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | M | 139 | GLN |
| 37 | l | 103 | HIS |
| 14 | N | 323 | ASN |
| 36 | k | 65 | ASN |
| 42 | q | 72 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 34 | SAC | i | 1 | 34 | 7,8,9 | 1.03 | 0 | 8,9,11 | 0.93 | 0 |
| 43 | AYA | r | 1 | 43 | 6,7,8 | 1.22 | 1 (16%) | 5,8,10 | 1.25 | 1 (20%) |
| 14 | FME | N | 1 | 14 | 8,9,10 | 0.94 | 0 | 7,9,11 | 1.32 | 1 (14%) |
| 10 | FME | J | 1 | 10 | 8,9,10 | 0.91 | 0 | 7,9,11 | 0.63 | 0 |
| 8 | FME | H | 1 | 8 | 8,9,10 | 0.94 | 0 | 7,9,11 | 1.31 | 1 (14%) |
| 4 | 2MR | D | 85 | 4 | 10,12,13 | 2.53 | 3 (30%) | 5,13,15 | 1.68 | 1 (20%) |
| 27 | AYA | b | 1 | 27 | 6,7,8 | 1.24 | 1 (16%) | 5,8,10 | 1.16 | 1 (20%) |
| 42 | AME | q | 1 | 42 | 9,10,11 | 1.76 | 2 (22%) | 9,11,13 | 2.00 | 4 (44%) |
| 1 | FME | A | 1 | 1 | 8,9,10 | 0.97 | 0 | 7,9,11 | 0.83 | 0 |
| 13 | FME | M | 1 | 13 | 8,9,10 | 0.97 | 0 | 7,9,11 | 0.76 | 0 |
| 12 | FME | L | 1 | 12 | 8,9,10 | 0.95 | 0 | 7,9,11 | 0.71 | 0 |
| 11 | FME | K | 1 | 11 | 8,9,10 | 1.06 | 0 | 7,9,11 | 1.39 | 1 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 34 | SAC | i | 1 | 34 | - | 2/7/8/10 | - |
| 43 | AYA | r | 1 | 43 | - | 0/4/6/8 | - |
| 14 | FME | N | 1 | 14 | - | 3/7/9/11 | - |
| 10 | FME | J | 1 | 10 | - | 2/7/9/11 | - |
| 8 | FME | H | 1 | 8 | - | 4/7/9/11 | - |
| 4 | 2MR | D | 85 | 4 | - | 3/10/13/15 | - |
| 27 | AYA | b | 1 | 27 | - | 1/4/6/8 | - |
| 42 | AME | q | 1 | 42 | - | 4/9/10/12 | - |
| 1 | FME | A | 1 | 1 | - | 3/7/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 13 | FME | M | 1 | 13 | - | 1/7/9/11 | - |
| 12 | FME | L | 1 | 12 | - | 3/7/9/11 | - |
| 11 | FME | K | 1 | 11 | - | 5/7/9/11 | - |

The worst 5 of 7 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | D | 85 | 2MR | CZ-NE | 5.58 | 1.46 | 1.34 |
| 4 | D | 85 | 2MR | CZ-NH2 | 4.92 | 1.44 | 1.33 |
| 42 | q | 1 | AME | CT1-N | 3.89 | 1.47 | 1.34 |
| 43 | r | 1 | AYA | CA-N | -2.42 | 1.44 | 1.46 |
| 27 | b | 1 | AYA | CA-N | -2.30 | 1.44 | 1.46 |

The worst 5 of 10 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | D | 85 | 2MR | CD-NE-CZ | 3.51 | 129.97 | 123.41 |
| 42 | q | 1 | AME | CE-SD-CG | 3.47 | 112.33 | 100.40 |
| 42 | q | 1 | AME | CT2-CT1-N | 3.08 | 121.31 | 116.10 |
| 8 | H | 1 | FME | C-CA-N | 3.04 | 115.21 | 109.73 |
| 14 | N | 1 | FME | C-CA-N | 2.70 | 114.60 | 109.73 |

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | A | 1 | FME | CA-CB-CG-SD |
| 8 | H | 1 | FME | N-CA-CB-CG |
| 8 | H | 1 | FME | O-C-CA-CB |
| 11 | K | 1 | FME | O1-CN-N-CA |
| 13 | M | 1 | FME | CB-CA-N-CN |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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 | $\#\|Z\| > 2$ |
| 49 | PC1 | P | 401 | - | 42,42,53 | 1.06 | 4 (9%) | 48,50,61 | 1.03 | 2 (4%) |
| 46 | SF4 | I | 201 | 9 | 0,12,12 | - | - | - | | |
| 46 | SF4 | I | 202 | 9 | 0,12,12 | - | - | - | | |
| 49 | PC1 | H | 402 | - | 41,41,53 | 1.07 | 3 (7%) | 47,49,61 | 0.92 | 2 (4%) |
| 47 | FES | E | 301 | 5 | 0,4,4 | - | - | - | | |
| 45 | 3PE | M | 506 | - | 30,30,50 | 1.10 | 4 (13%) | 33,35,55 | 1.13 | 2 (6%) |
| 49 | PC1 | H | 406 | - | 34,34,53 | 1.17 | 4 (11%) | 40,42,61 | 1.09 | 2 (5%) |
| 45 | 3PE | L | 704 | - | 41,41,50 | 0.95 | 4 (9%) | 44,46,55 | 1.01 | 2 (4%) |
| 45 | 3PE | M | 504 | - | 50,50,50 | 0.86 | 4 (8%) | 53,55,55 | 1.10 | 2 (3%) |
| 45 | 3PE | M | 502 | - | 41,41,50 | 1.04 | 4 (9%) | 45,46,55 | 1.20 | 3 (6%) |
| 45 | 3PE | N | 401 | - | 50,50,50 | 0.89 | 4 (8%) | 53,55,55 | 1.09 | 2 (3%) |
| 46 | SF4 | G | 802 | 7 | 0,12,12 | - | - | - | | |
| 52 | NDP | P | 501 | - | 45,52,52 | 2.28 | 8 (17%) | 53,80,80 | 1.57 | 9 (16%) |
| 46 | SF4 | F | 502 | 6 | 0,12,12 | - | - | - | | |
| 50 | CDL | L | 702 | - | 77,77,99 | 0.99 | 6 (7%) | 83,89,111 | 1.12 | 4 (4%) |
| 50 | CDL | H | 405 | - | 56,56,99 | 1.13 | 7 (12%) | 62,68,111 | 1.11 | 4 (6%) |
| 45 | 3PE | M | 501 | - | 50,50,50 | 0.87 | 4 (8%) | 53,55,55 | 0.98 | 2 (3%) |
| 45 | 3PE | M | 503 | - | 50,50,50 | 0.87 | 3 (6%) | 53,55,55 | 1.06 | 2 (3%) |
| 45 | 3PE | H | 401 | - | 50,50,50 | 0.85 | 4 (8%) | 53,55,55 | 0.98 | 2 (3%) |
| 54 | EHZ | T | 201 | 20 | 26,33,37 | 1.80 | 5 (19%) | 32,41,47 | 1.34 | 2 (6%) |
| 50 | CDL | M | 507 | - | 66,66,99 | 1.05 | 8 (12%) | 72,78,111 | 1.22 | 5 (6%) |
| 45 | 3PE | M | 505 | - | 50,50,50 | 0.86 | 3 (6%) | 53,55,55 | 1.01 | 3 (5%) |
| 47 | FES | G | 803 | 7 | 0,4,4 | - | - | - | | |
| 45 | 3PE | A | 201 | - | 40,40,50 | 0.96 | 4 (10%) | 43,45,55 | 1.06 | 2 (4%) |
| 49 | PC1 | H | 404 | - | 46,46,53 | 1.02 | 4 (8%) | 52,54,61 | 1.02 | 2 (3%) |
| 50 | CDL | L | 703 | - | 69,69,99 | 1.02 | 8 (11%) | 75,81,111 | 1.08 | 4 (5%) |
| 46 | SF4 | B | 201 | 2 | 0,12,12 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 46 | SF4 | G | 801 | 7 | 0,12,12 | - | - | - | | |
| 45 | 3PE | L | 701 | - | 50,50,50 | 0.85 | 4 (8%) | 53,55,55 | 1.01 | 2 (3%) |
| 51 | ADP | O | 401 | - | 24,29,29 | 0.96 | 1 (4%) | 29,45,45 | 1.42 | 4 (13%) |
| 45 | 3PE | H | 403 | - | 50,50,50 | 0.87 | 3 (6%) | 53,55,55 | 1.10 | 2 (3%) |
| 54 | EHZ | U | 201 | 20 | 27,34,37 | 1.79 | 6 (22%) | 33,42,47 | 1.18 | 3 (9%) |
| 48 | FMN | F | 501 | - | 33,33,33 | 1.12 | 2 (6%) | 48,50,50 | 1.42 | 8 (16%) |

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 |
|---|---|---|---|---|---|---|---|
| 49 | PC1 | P | 401 | - | - | 27/46/46/57 | - |
| 46 | SF4 | I | 201 | 9 | - | - | 0/6/5/5 |
| 46 | SF4 | I | 202 | 9 | - | - | 0/6/5/5 |
| 49 | PC1 | H | 402 | - | - | 26/45/45/57 | - |
| 47 | FES | E | 301 | 5 | - | - | 0/1/1/1 |
| 45 | 3PE | M | 506 | - | - | 16/34/34/54 | - |
| 49 | PC1 | H | 406 | - | - | 19/38/38/57 | - |
| 45 | 3PE | L | 704 | - | - | 18/45/45/54 | - |
| 45 | 3PE | M | 504 | - | - | 23/54/54/54 | - |
| 45 | 3PE | M | 502 | - | - | 17/43/43/54 | - |
| 45 | 3PE | N | 401 | - | - | 25/54/54/54 | - |
| 52 | NDP | P | 501 | - | - | 4/30/77/77 | 0/5/5/5 |
| 46 | SF4 | G | 802 | 7 | - | - | 0/6/5/5 |
| 46 | SF4 | F | 502 | 6 | - | - | 0/6/5/5 |
| 50 | CDL | L | 702 | - | - | 43/88/88/110 | - |
| 50 | CDL | H | 405 | - | - | 39/67/67/110 | - |
| 45 | 3PE | M | 501 | - | - | 29/54/54/54 | - |
| 45 | 3PE | M | 503 | - | - | 21/54/54/54 | - |
| 45 | 3PE | H | 401 | - | - | 27/54/54/54 | - |
| 54 | EHZ | T | 201 | 20 | - | 7/39/41/45 | - |
| 50 | CDL | M | 507 | - | - | 32/77/77/110 | - |
| 45 | 3PE | M | 505 | - | - | 25/54/54/54 | - |
| 47 | FES | G | 803 | 7 | - | - | 0/1/1/1 |
| 45 | 3PE | A | 201 | - | - | 19/44/44/54 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 49 | PC1 | H | 404 | - | - | 21/50/50/57 | - |
| 50 | CDL | L | 703 | - | - | 39/80/80/110 | - |
| 46 | SF4 | B | 201 | 2 | - | - | 0/6/5/5 |
| 46 | SF4 | G | 801 | 7 | - | - | 0/6/5/5 |
| 45 | 3PE | L | 701 | - | - | 20/54/54/54 | - |
| 51 | ADP | O | 401 | - | - | 5/12/32/32 | 0/3/3/3 |
| 45 | 3PE | H | 403 | - | - | 26/54/54/54 | - |
| 54 | EHZ | U | 201 | 20 | - | 16/40/42/45 | - |
| 48 | FMN | F | 501 | - | - | 7/18/18/18 | 0/3/3/3 |

The worst 5 of 111 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 52 | P | 501 | NDP | P2B-O2B | 12.21 | 1.82 | 1.59 |
| 54 | U | 201 | EHZ | C15-N2 | 5.53 | 1.45 | 1.33 |
| 54 | T | 201 | EHZ | C15-N2 | 5.51 | 1.45 | 1.33 |
| 54 | U | 201 | EHZ | C12-N1 | 5.32 | 1.45 | 1.33 |
| 54 | T | 201 | EHZ | C12-N1 | 5.31 | 1.45 | 1.33 |

The worst 5 of 77 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | P | 501 | NDP | PN-O3-PA | -5.92 | 112.52 | 132.83 |
| 54 | T | 201 | EHZ | C8-C9-S1 | 5.04 | 119.86 | 113.63 |
| 45 | M | 502 | 3PE | O31-C31-C32 | 4.61 | 126.36 | 111.91 |
| 50 | M | 507 | CDL | OB6-CB5-C51 | 4.60 | 121.42 | 111.50 |
| 45 | M | 504 | 3PE | O21-C21-C22 | 4.53 | 121.26 | 111.50 |

There are no chirality outliers.

5 of 551 torsion outliers are listed below:

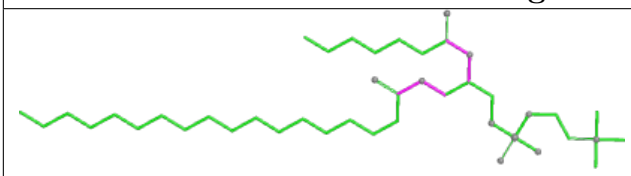
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 45 | A | 201 | 3PE | C1-O11-P-O14 |
| 45 | H | 401 | 3PE | O13-C11-C12-N |
| 45 | H | 401 | 3PE | C22-C21-O21-C2 |
| 45 | H | 403 | 3PE | C1-O11-P-O12 |
| 45 | H | 403 | 3PE | C1-O11-P-O13 |

There are no ring outliers.

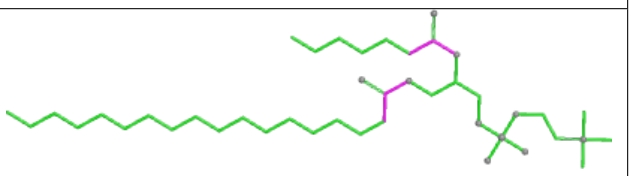
No monomer is involved in short contacts.

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

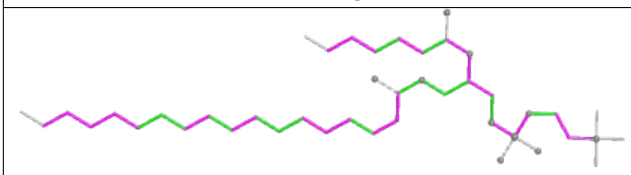
**Ligand PC1 P 401**



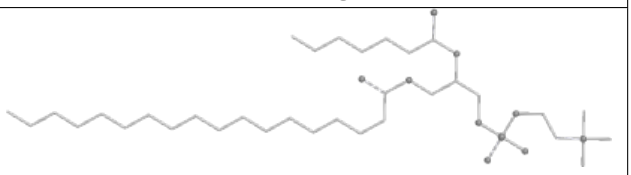
**Bond lengths**



**Bond angles**

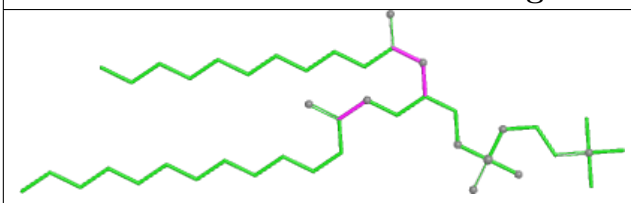


**Torsions**

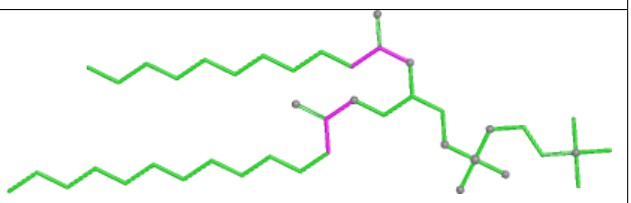


**Rings**

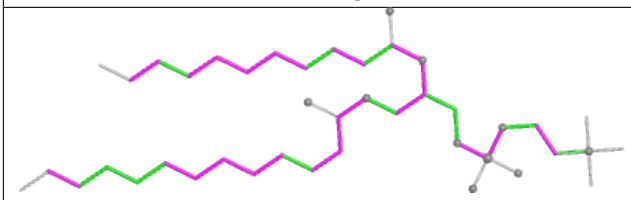
**Ligand PC1 H 402**



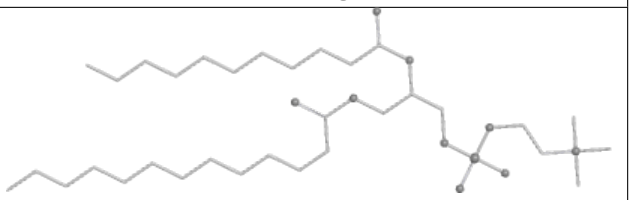
**Bond lengths**



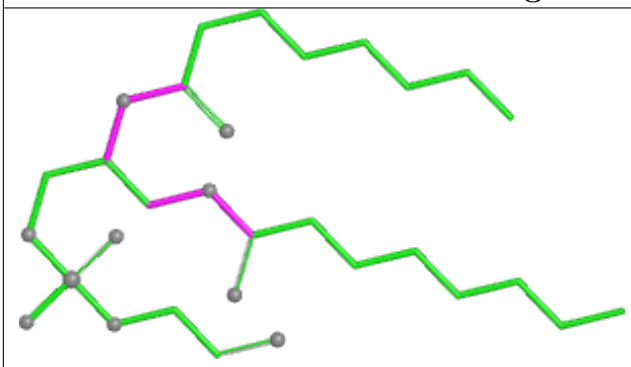
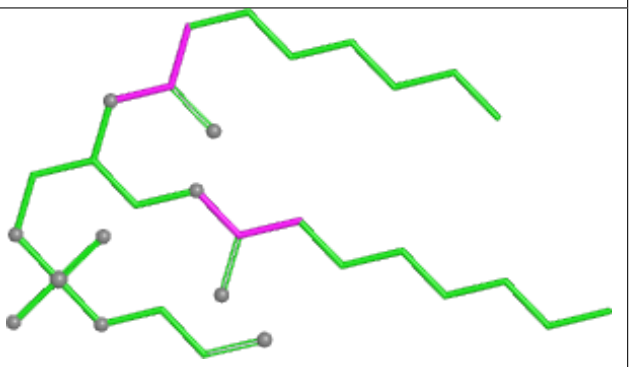
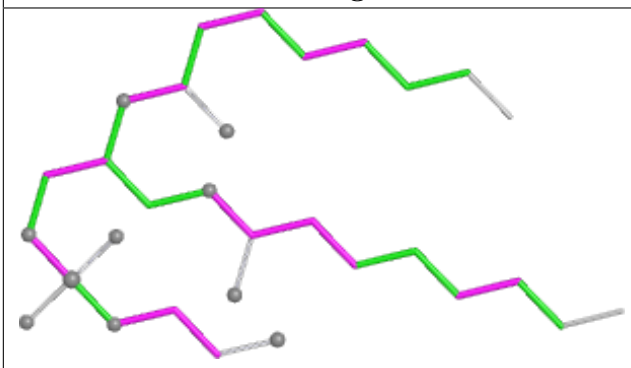
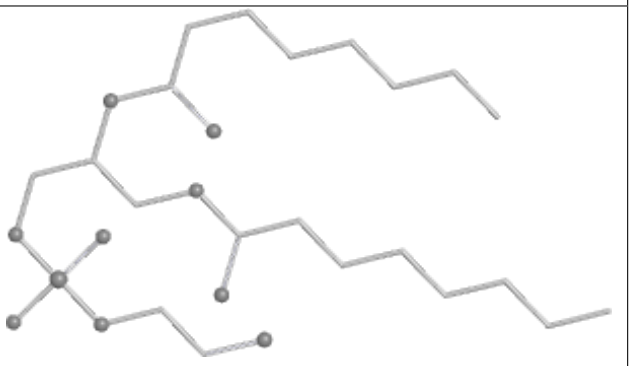
**Bond angles**

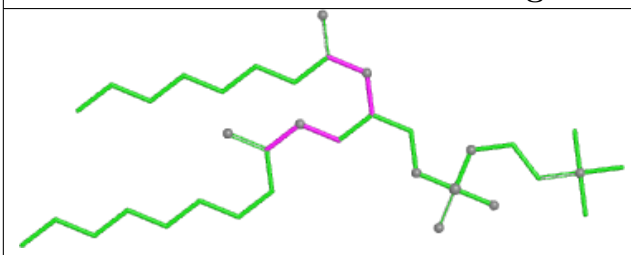
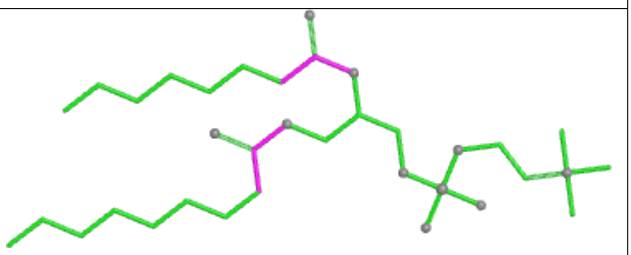
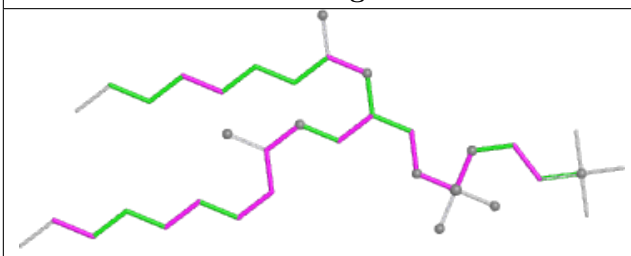
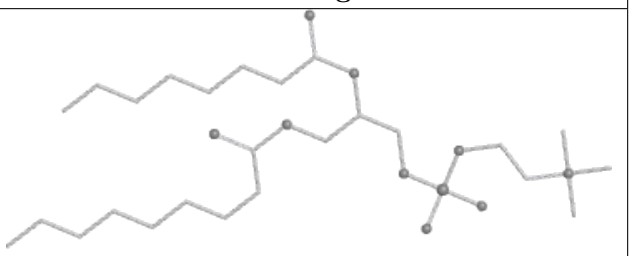


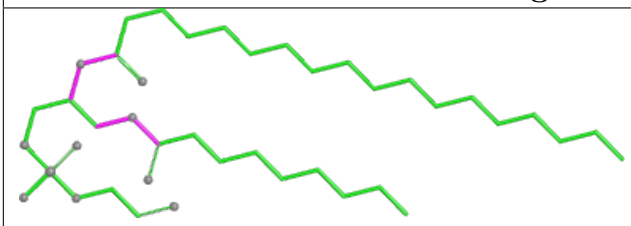
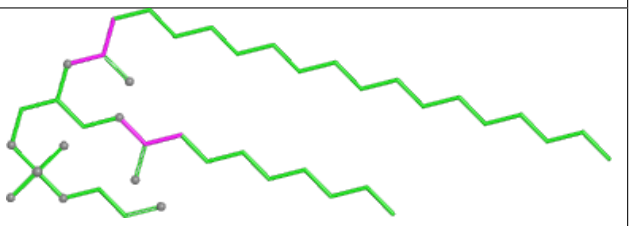
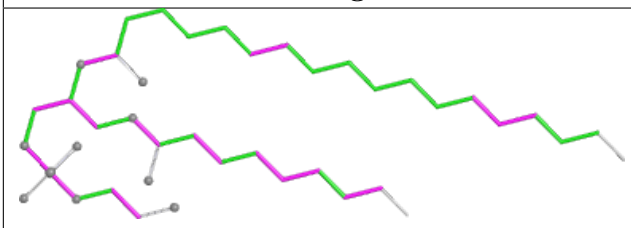
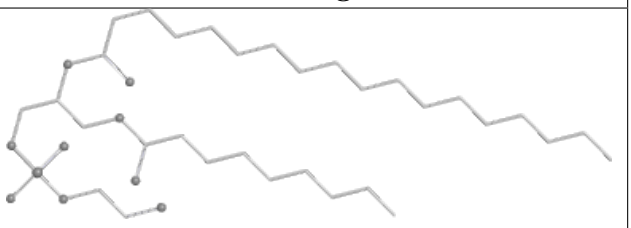
**Torsions**



**Rings**

| Ligand 3PE M 506 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand PC1 H 406 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE L 704 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE M 504 | |
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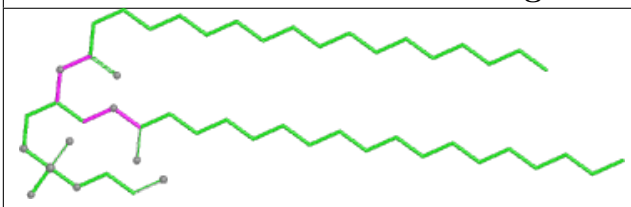
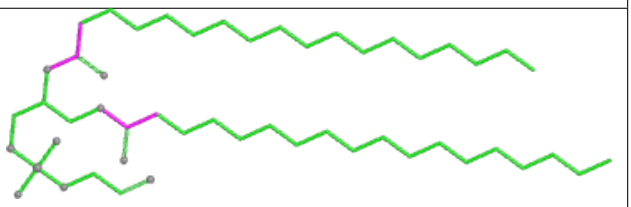
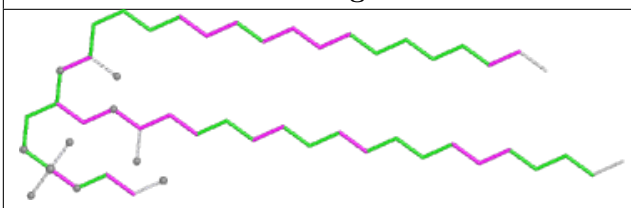
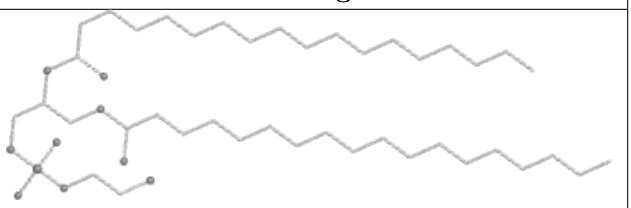
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE M 502 | |
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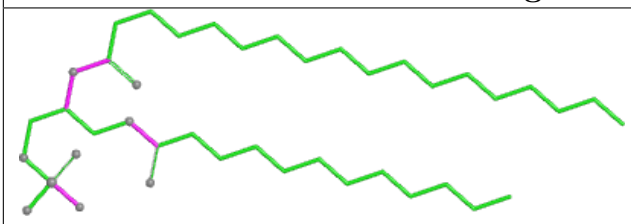
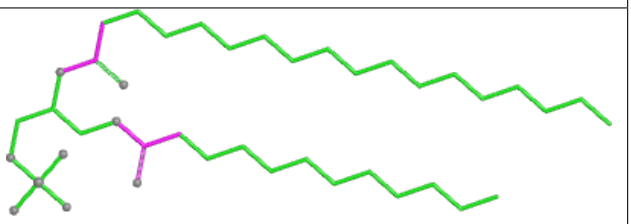
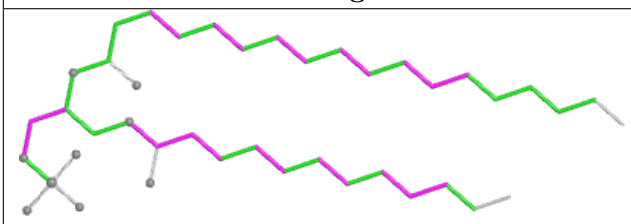
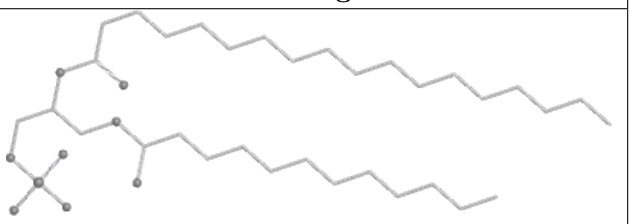
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE N 401 | |
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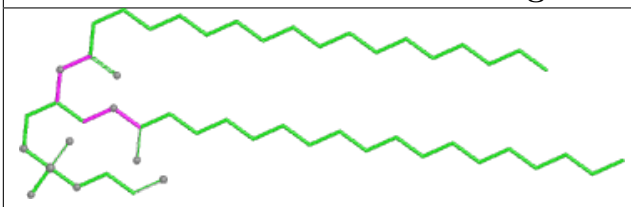
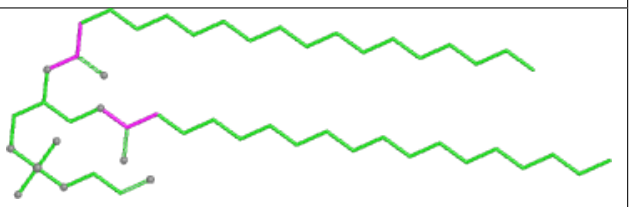
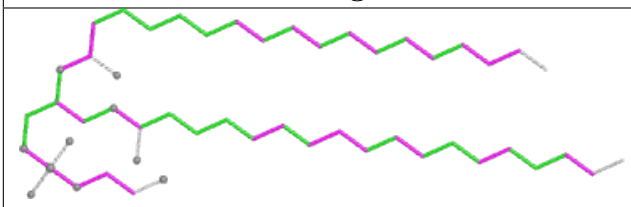
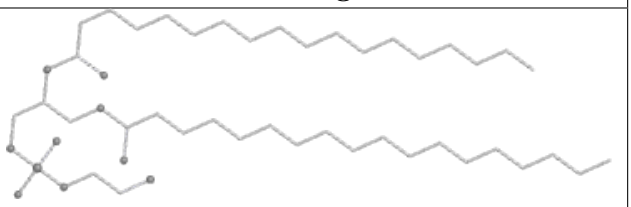
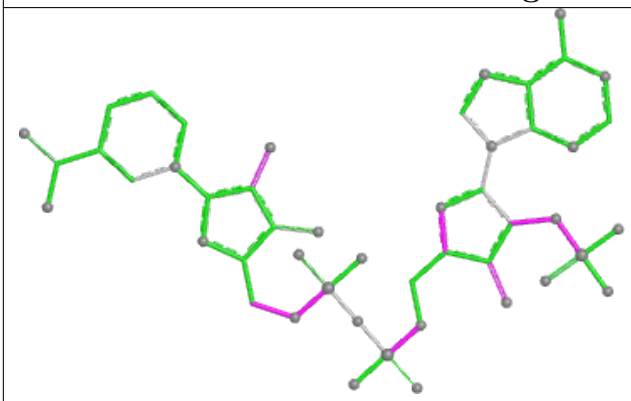
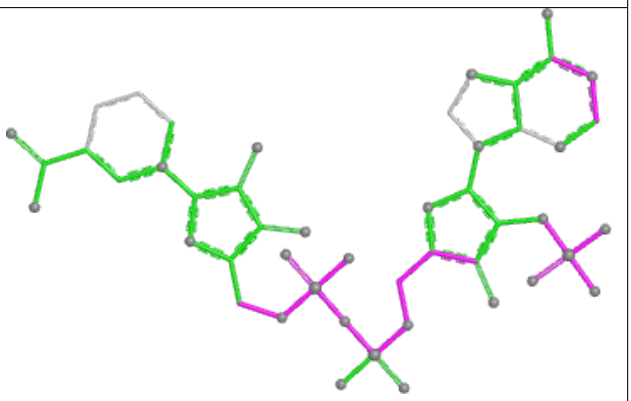
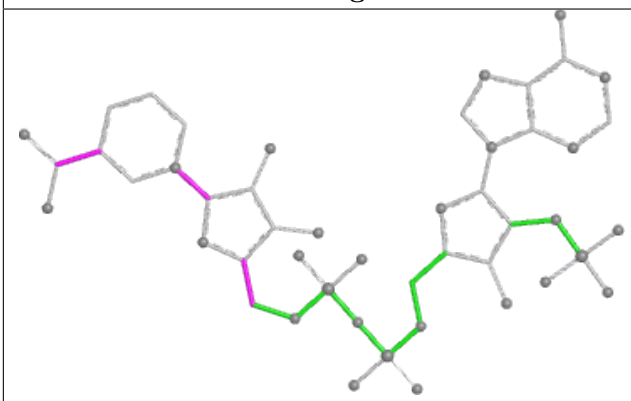
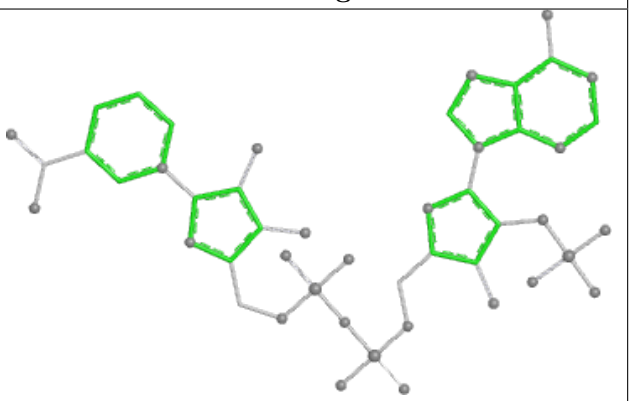
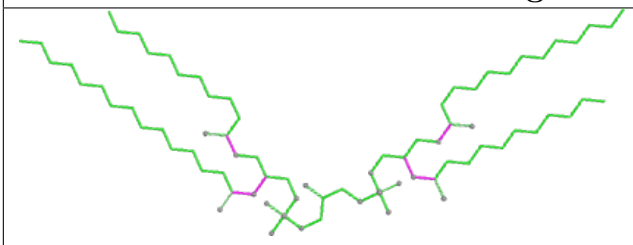
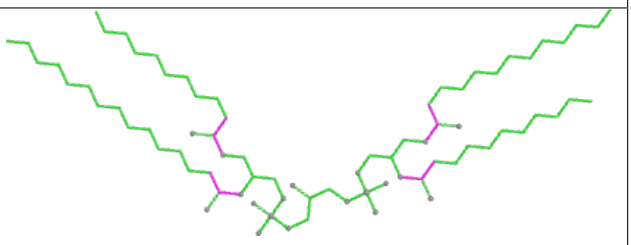
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand NDP P 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

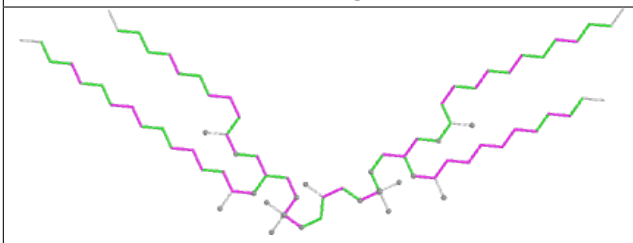
## Ligand CDL L 702



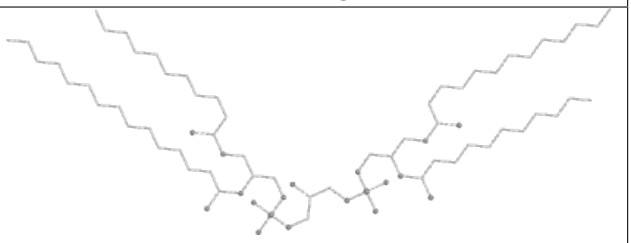
Bond lengths



Bond angles

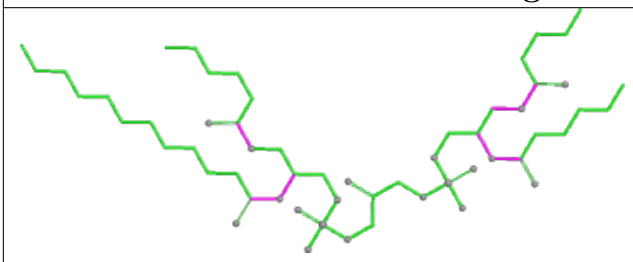


Torsions

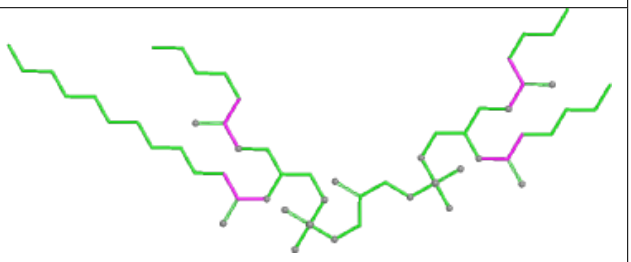


Rings

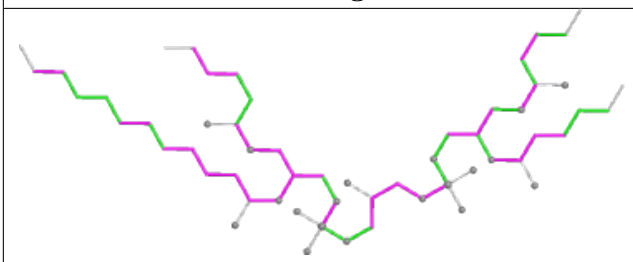
## Ligand CDL H 405



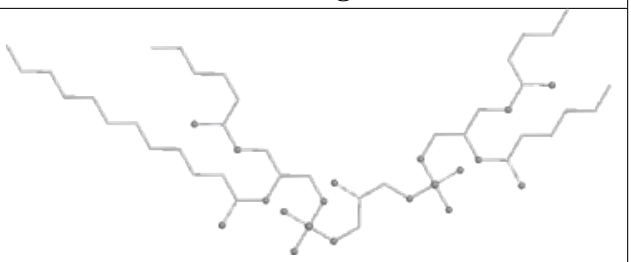
Bond lengths



Bond angles

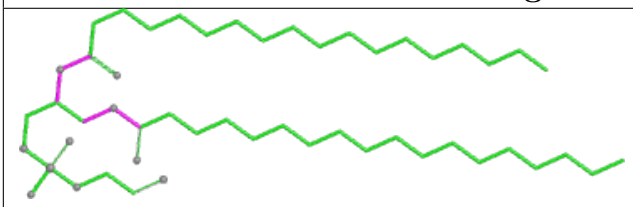


Torsions

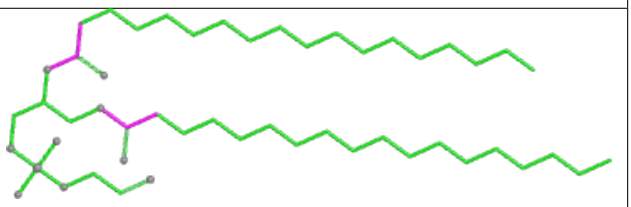


Rings

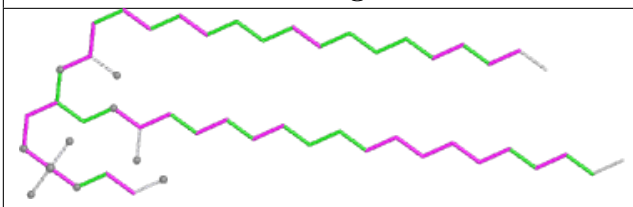
## Ligand 3PE M 501



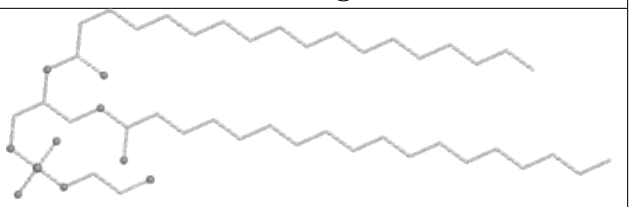
Bond lengths



Bond angles

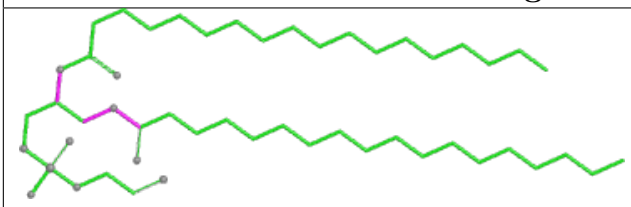


Torsions



Rings

## Ligand 3PE M 503



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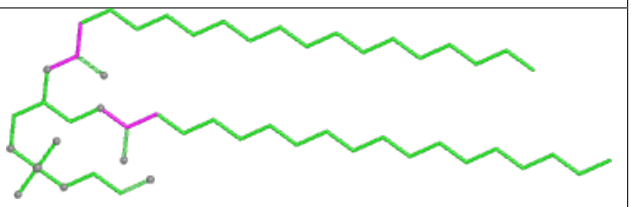
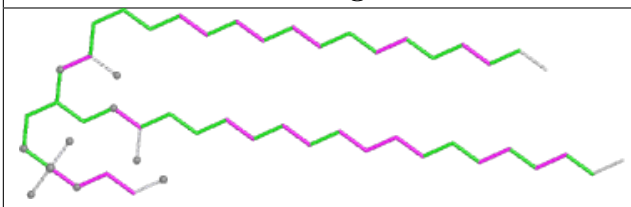
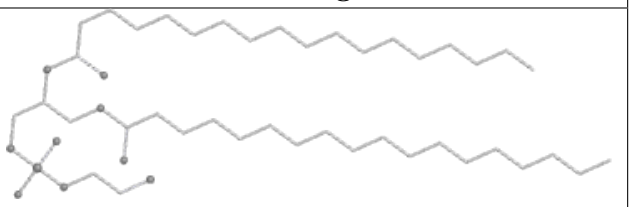


Bond angles

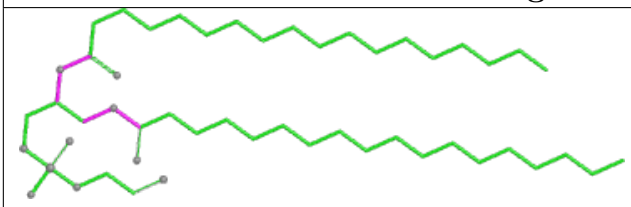


Torsions

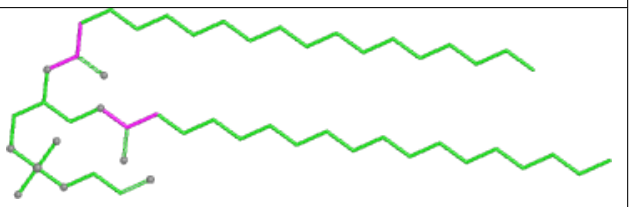


Rings

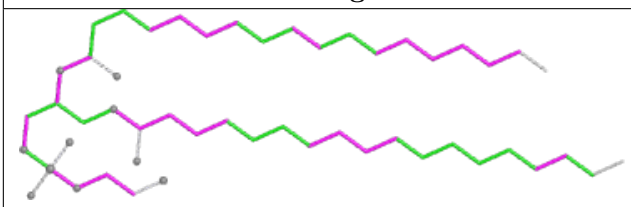
## Ligand 3PE H 401



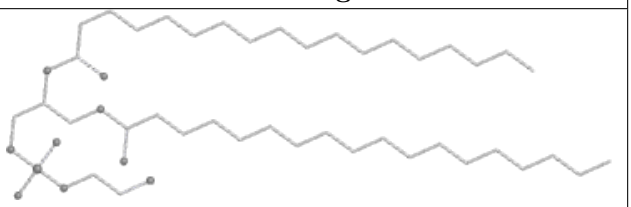
Bond lengths



Bond angles

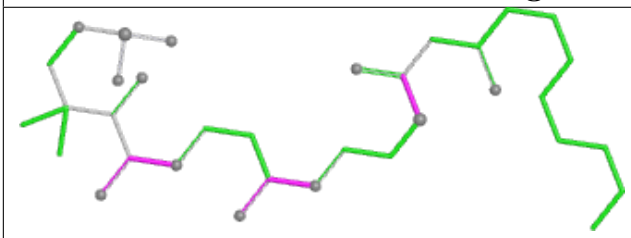


Torsions

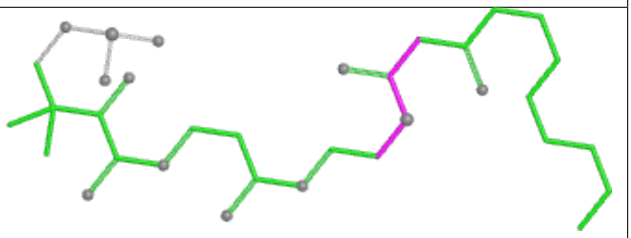


Rings

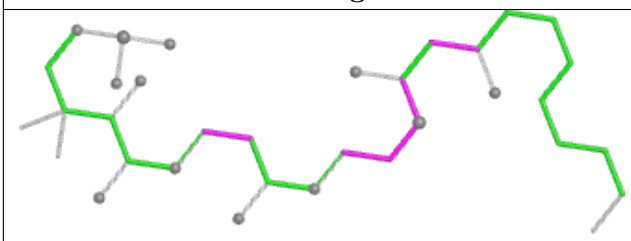
## Ligand EHZ T 201



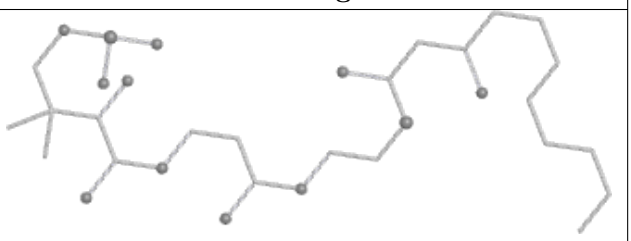
Bond lengths



Bond angles

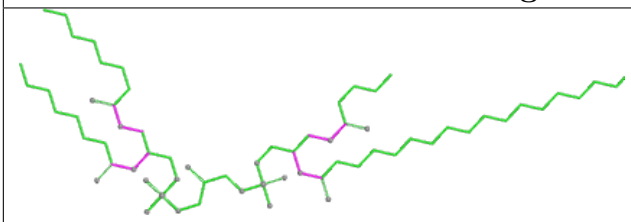


Torsions

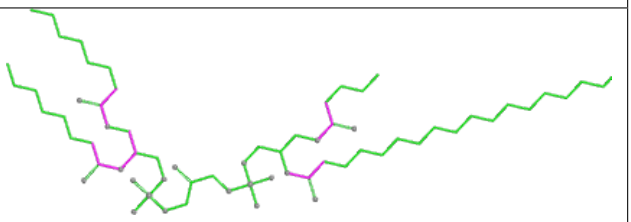


Rings

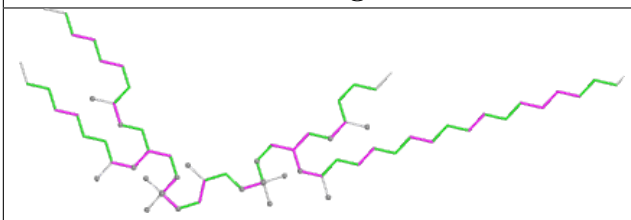
## Ligand CDL M 507



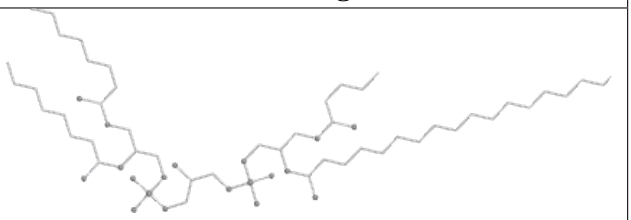
Bond lengths



Bond angles

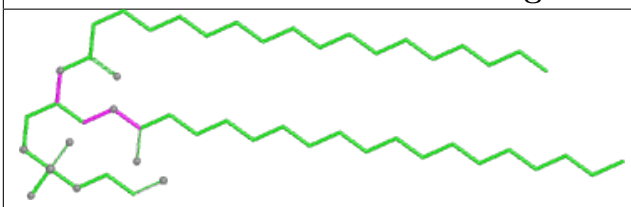


Torsions

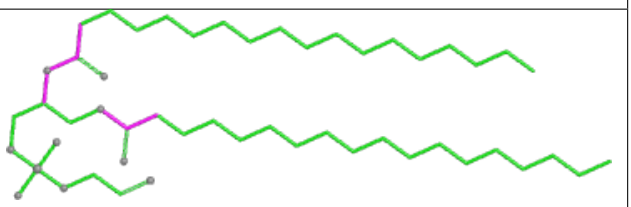


Rings

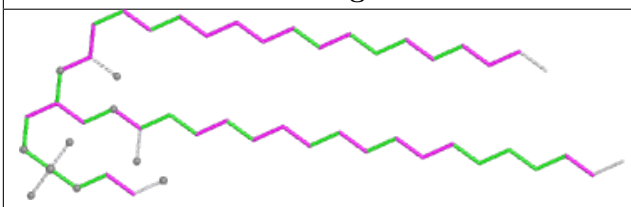
## Ligand 3PE M 505



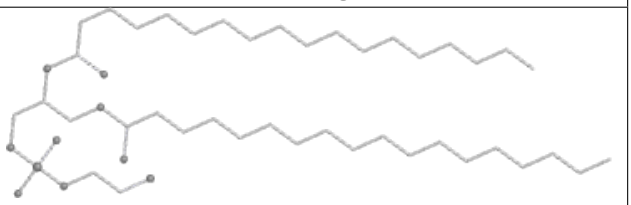
Bond lengths



Bond angles

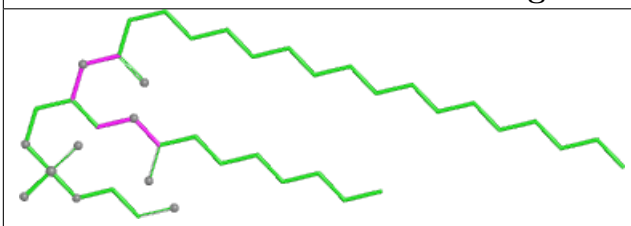


Torsions

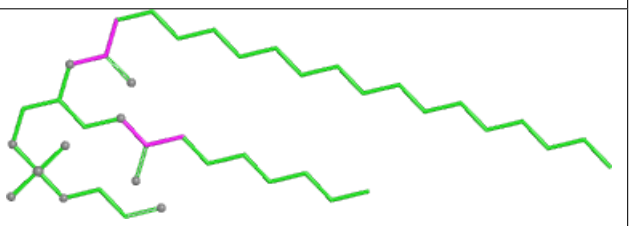


Rings

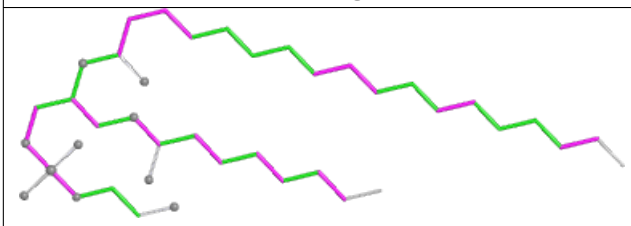
## Ligand 3PE A 201



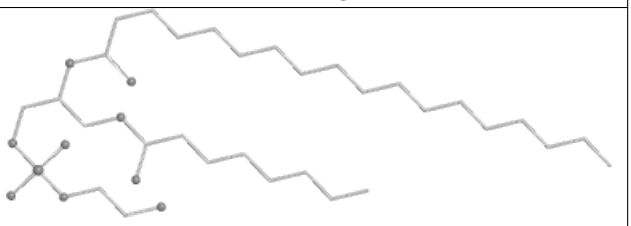
Bond lengths



Bond angles

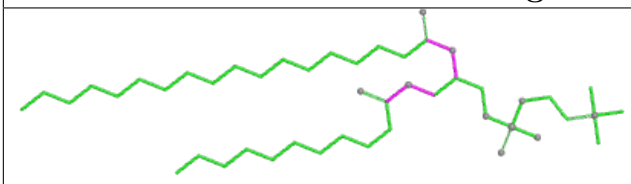


Torsions

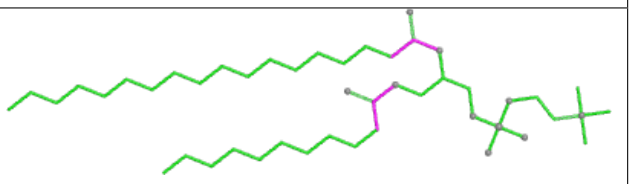


Rings

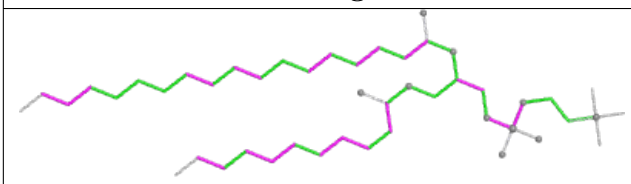
## Ligand PC1 H 404



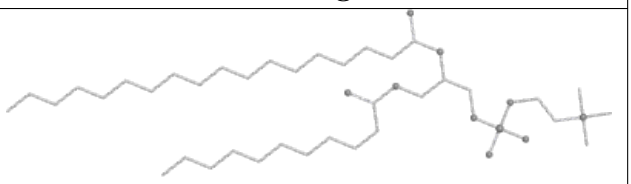
Bond lengths



Bond angles

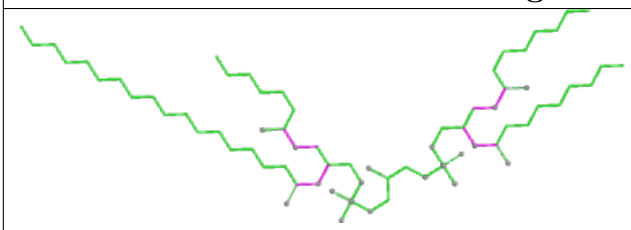


Torsions

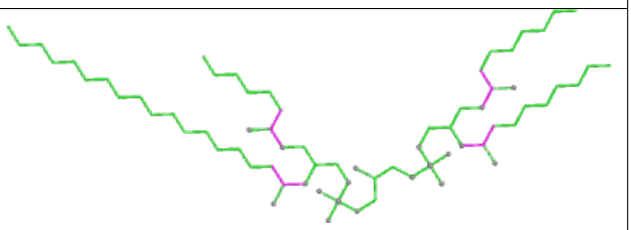


Rings

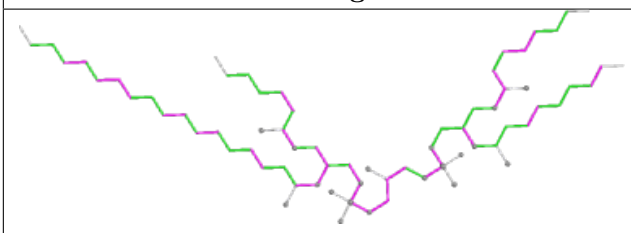
## Ligand CDL L 703



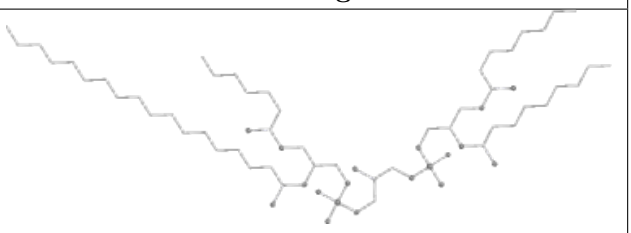
Bond lengths



Bond angles

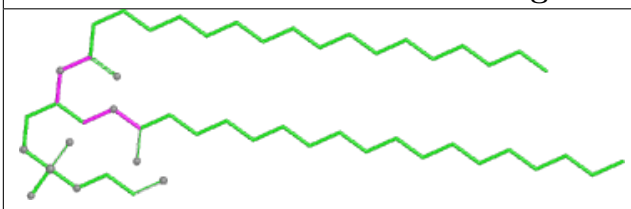


Torsions

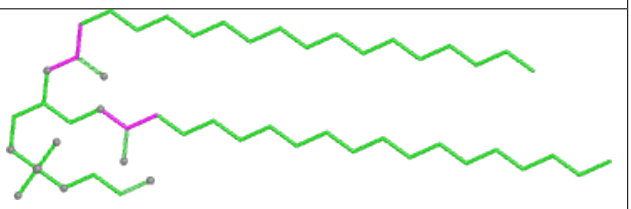


Rings

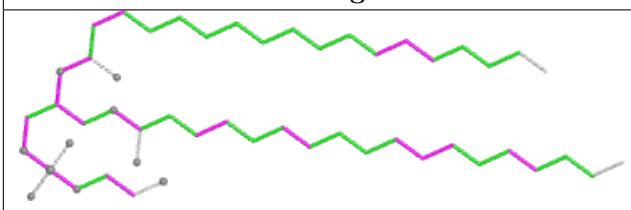
## Ligand 3PE L 701



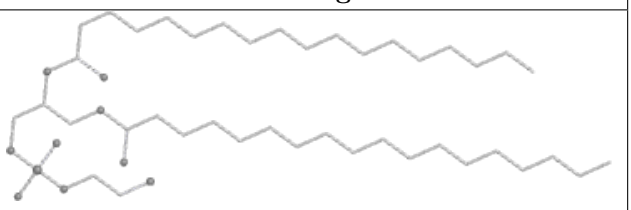
Bond lengths



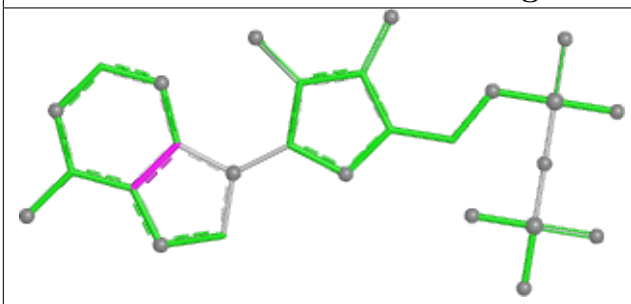
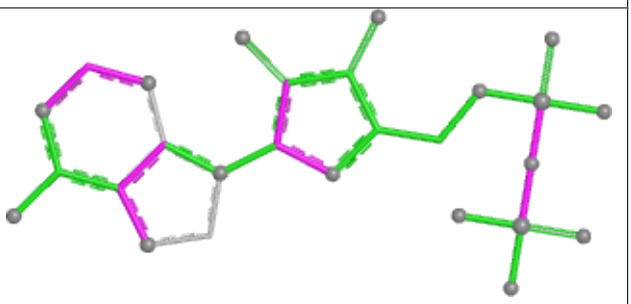
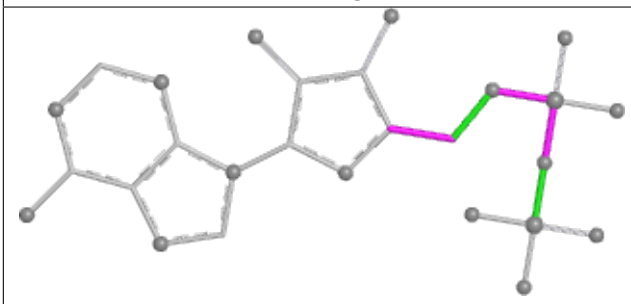
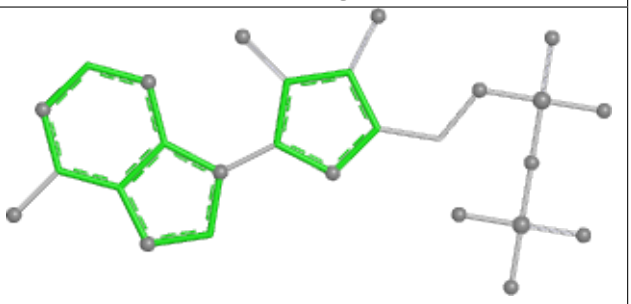
Bond angles

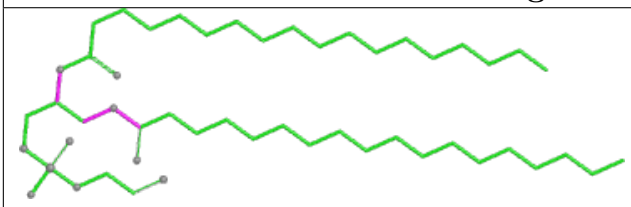
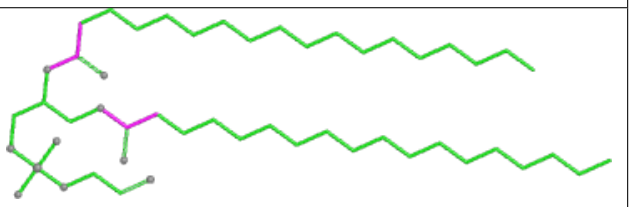
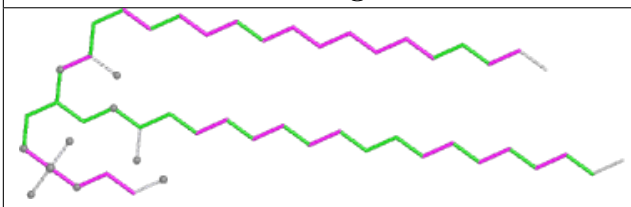
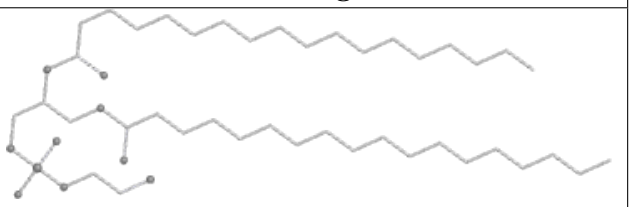


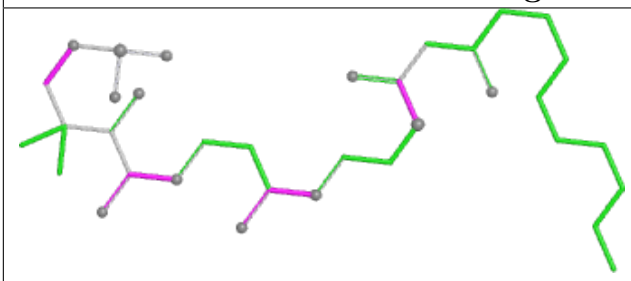
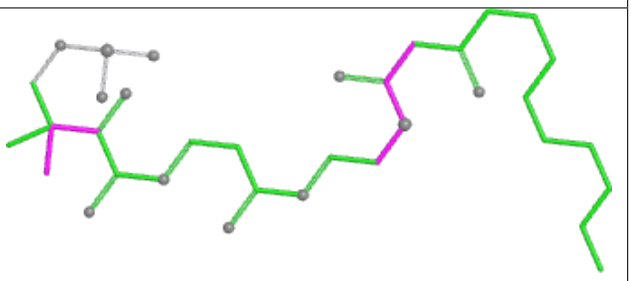
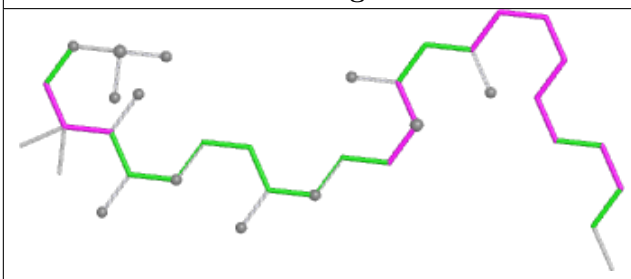
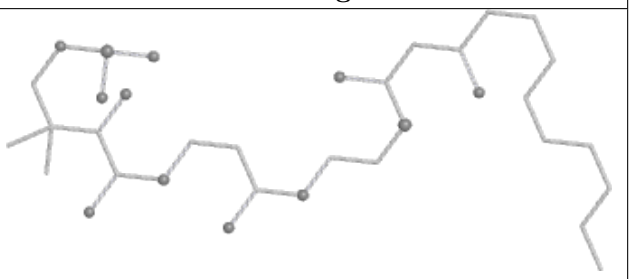
Torsions

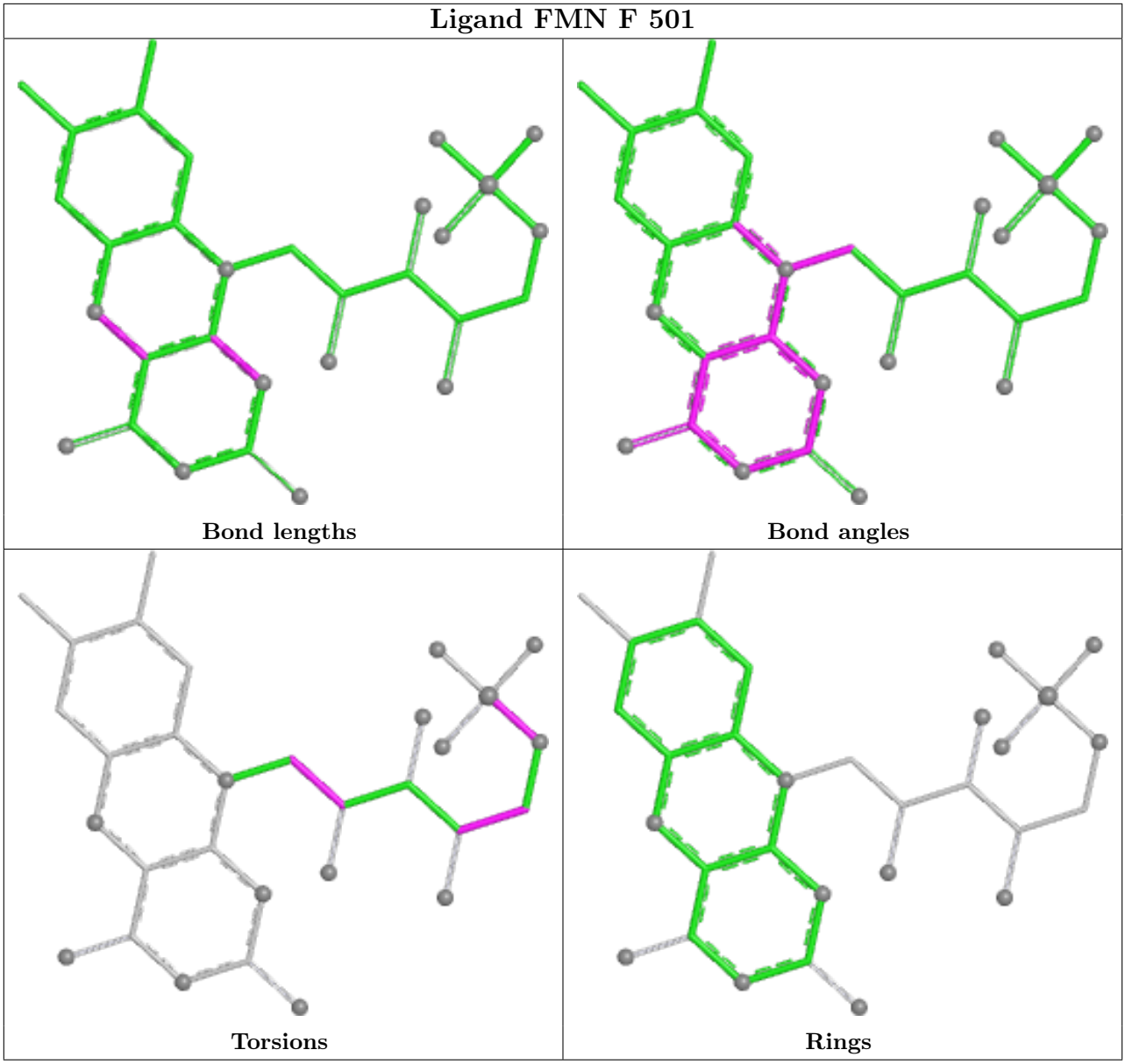


Rings

| Ligand ADP O 401 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE H 403 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand EHZ U 201 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

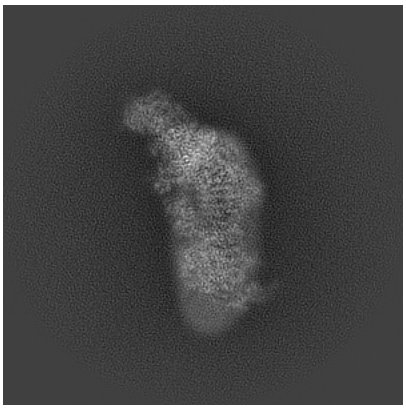
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4345. These allow visual inspection of the internal detail of the map and identification of artifacts.

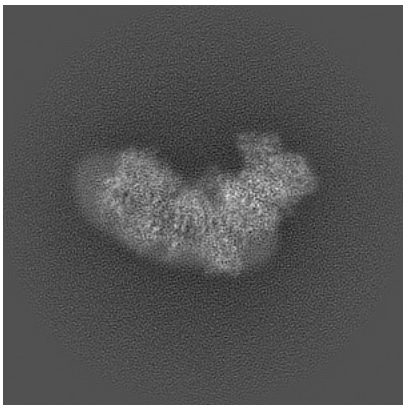
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

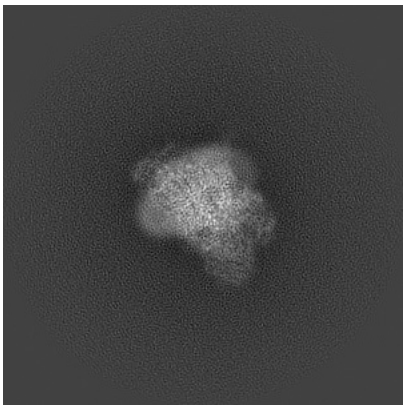
### 6.1.1 Primary map



X

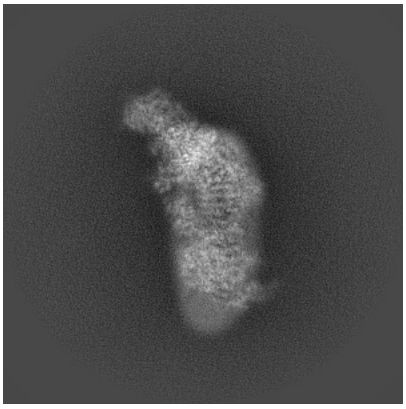


Y



Z

### 6.1.2 Raw map



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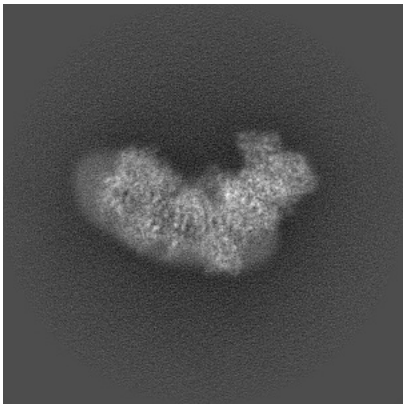
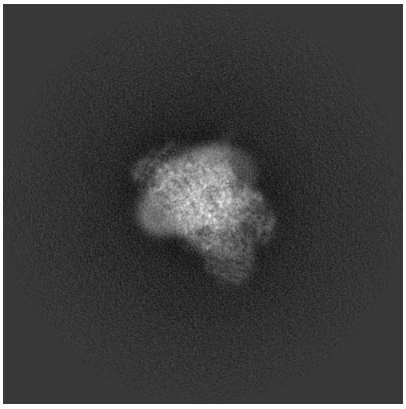


Y

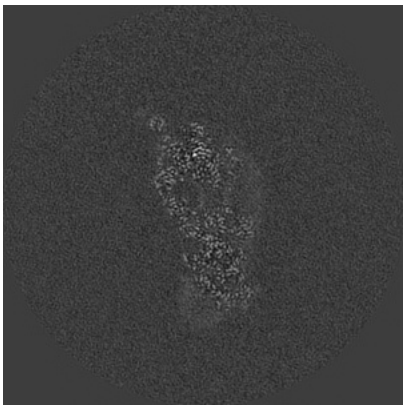


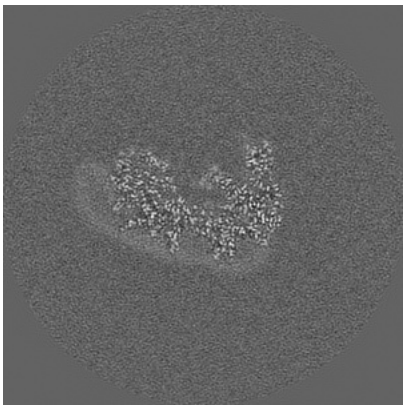
Z

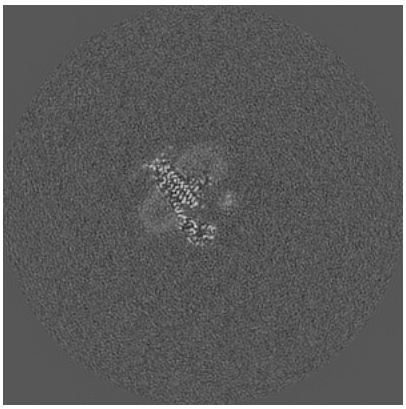
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

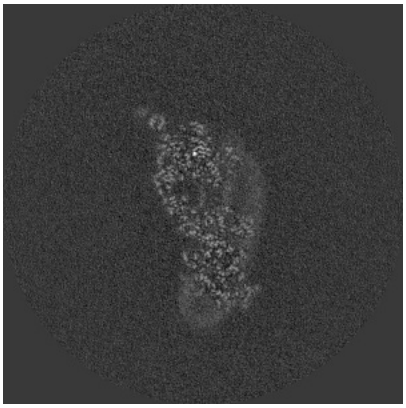
### 6.2.1 Primary map

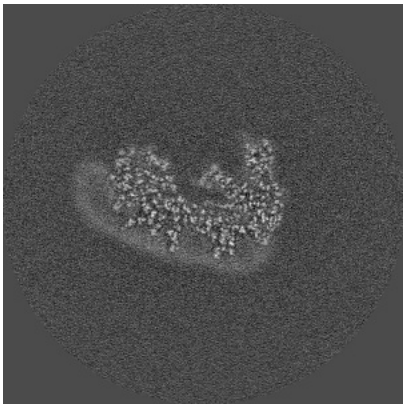

X Index: 225

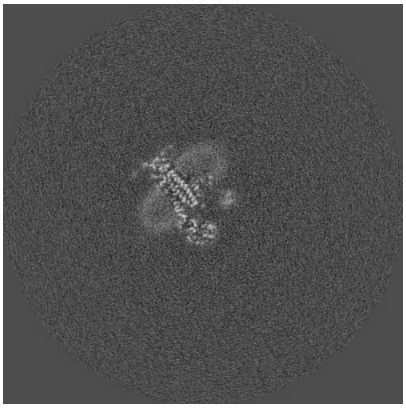

Y Index: 225


Z Index: 225

### 6.2.2 Raw map


X Index: 225

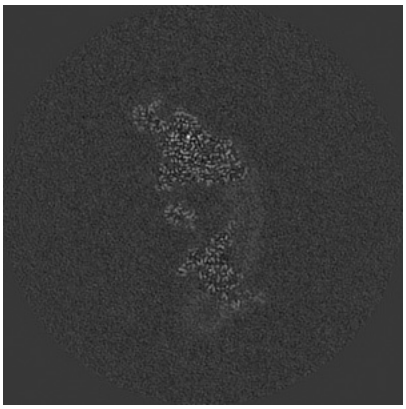

Y Index: 225

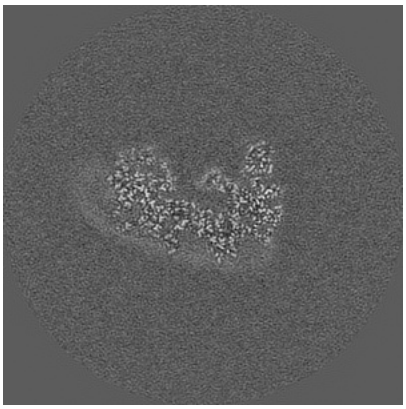

Z Index: 225

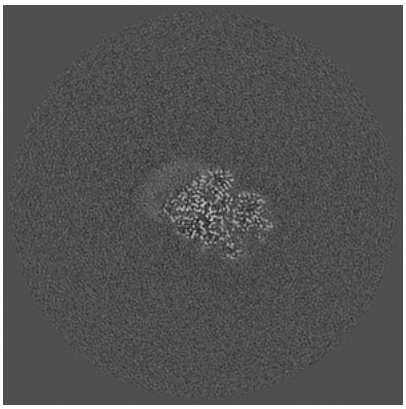
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

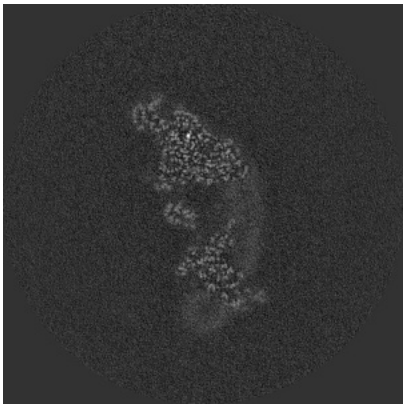
### 6.3.1 Primary map

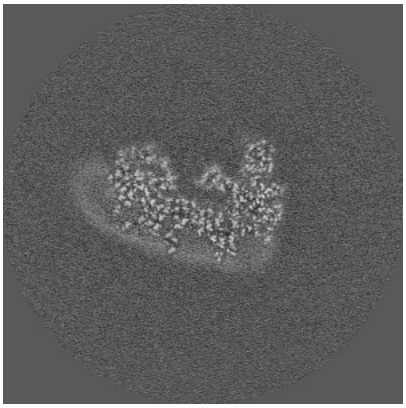

X Index: 237

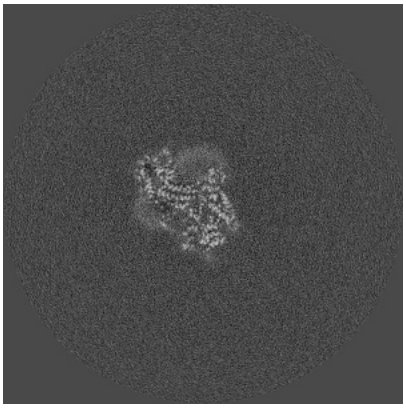

Y Index: 227


Z Index: 287

### 6.3.2 Raw map


X Index: 237

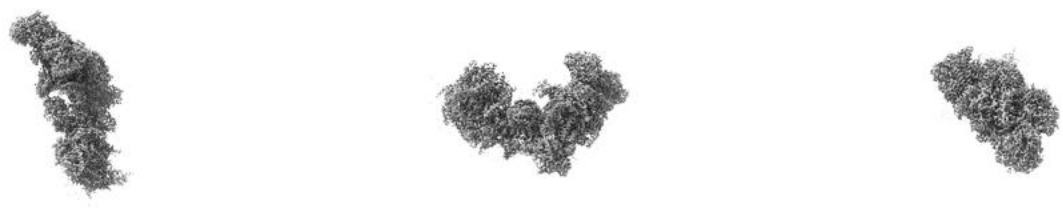

Y Index: 227


Z Index: 252

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

## 6.4 Orthogonal surface views (i)

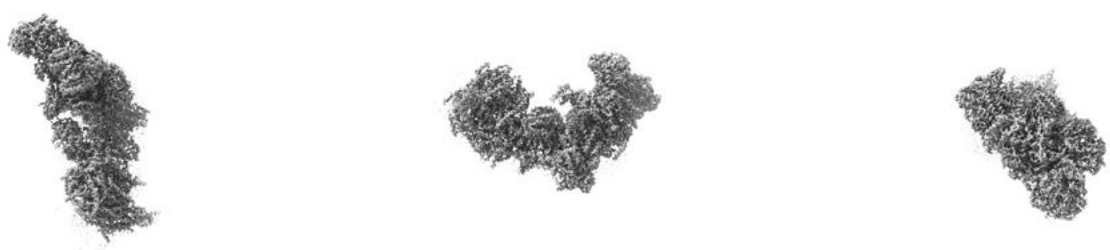
### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

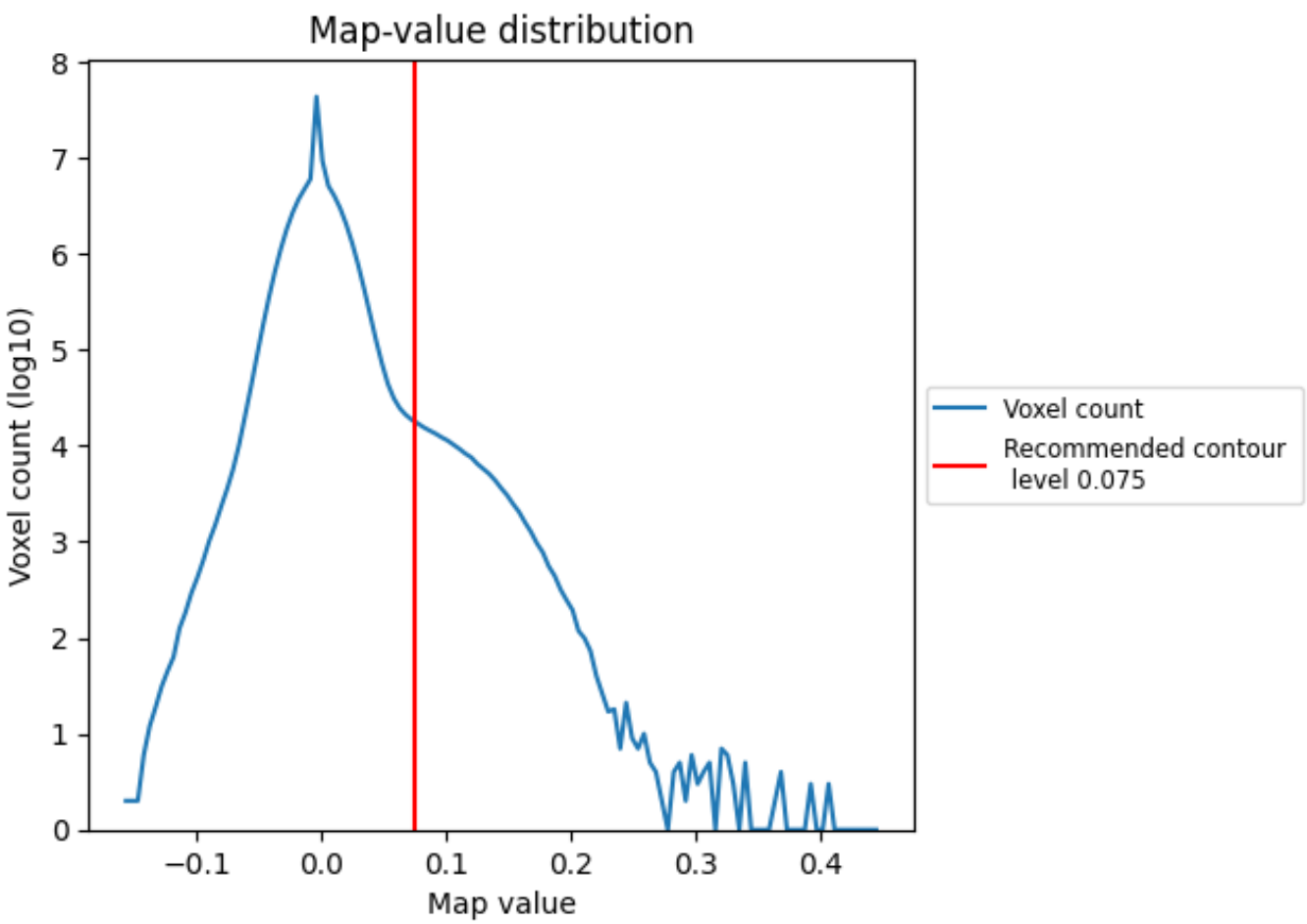
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

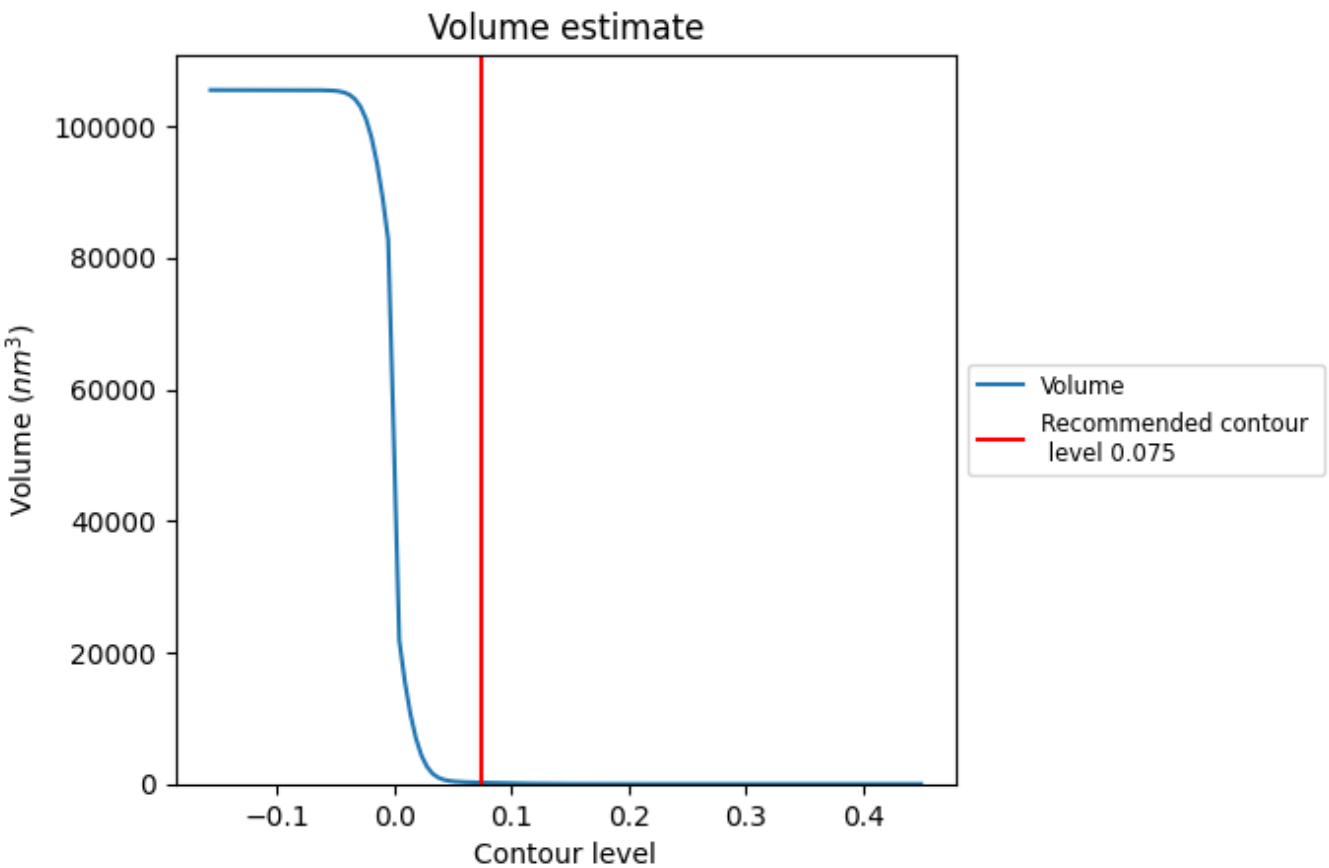
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

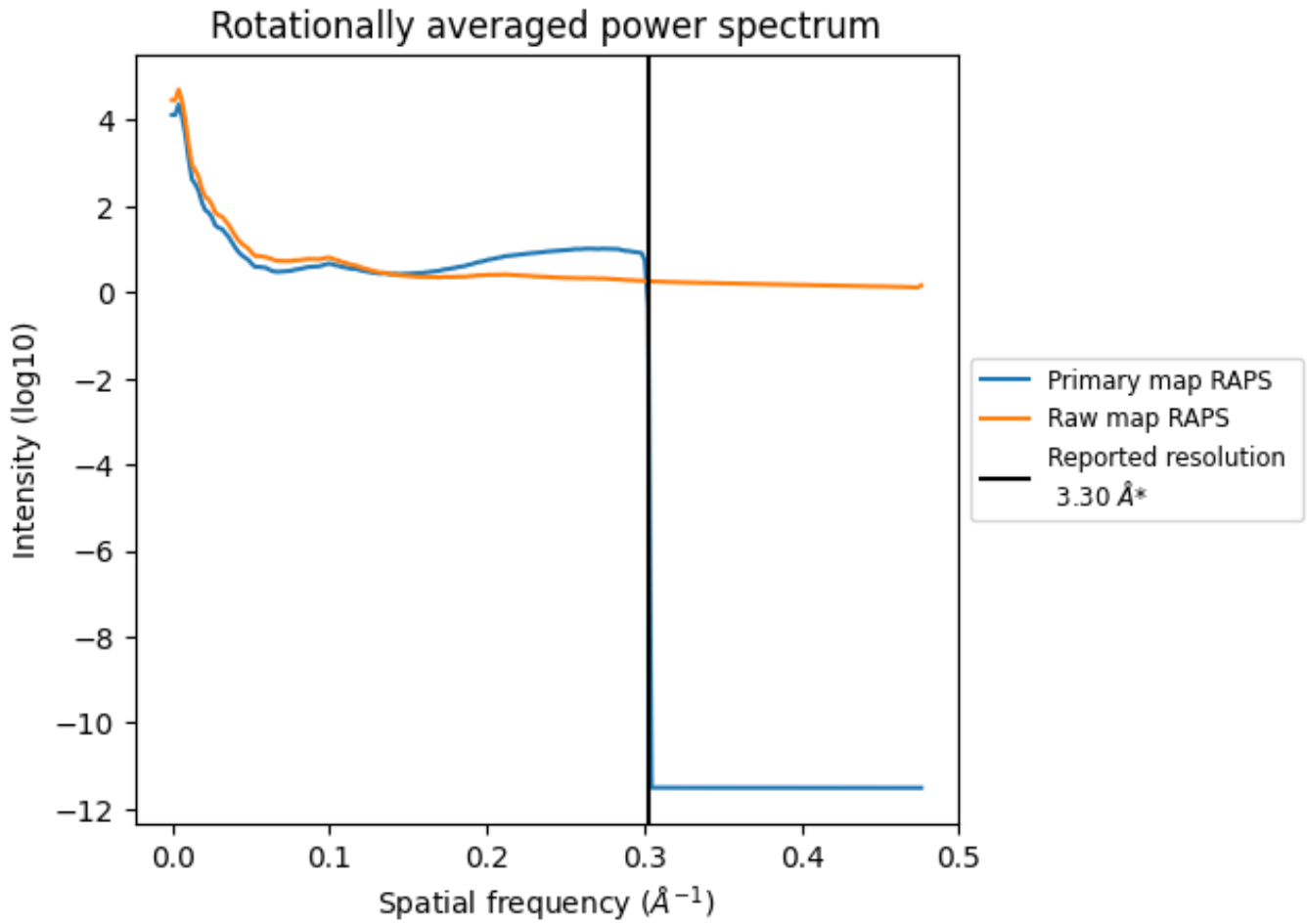
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 195 $nm^3$; this corresponds to an approximate mass of 176 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)

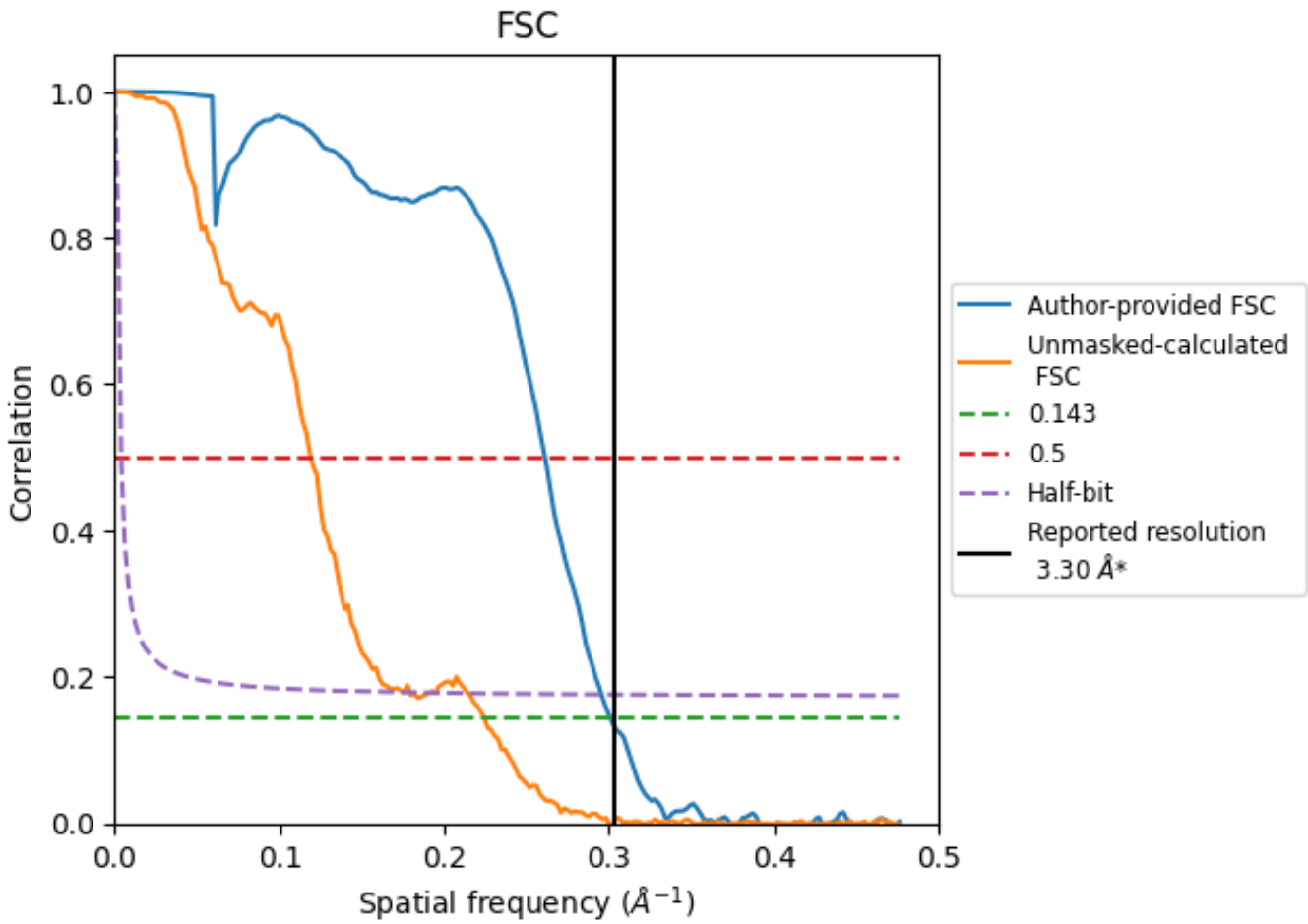



*Reported resolution corresponds to spatial frequency of 0.303 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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

## 8.1 FSC (i)




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

## 8.2 Resolution estimates (i)

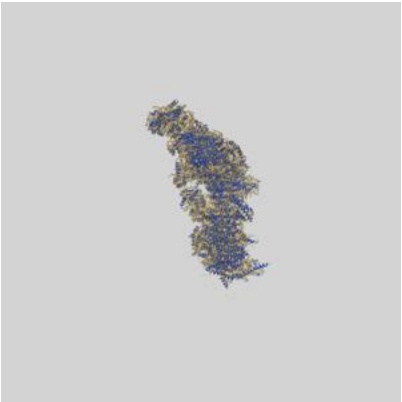
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.30 | - | - |
| Author-provided FSC curve | 3.32 | 3.83 | 3.38 |
| Unmasked-calculated* | 4.45 | 8.39 | 5.70 |

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

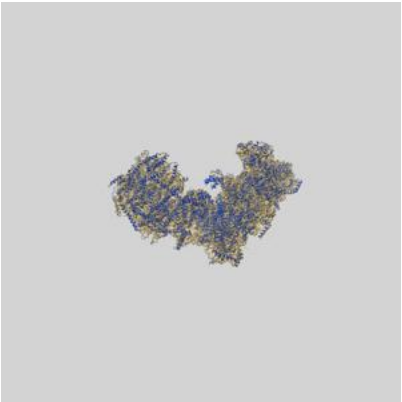
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4345 and PDB model 6G2J. Per-residue inclusion information can be found in section 3 on page 19.

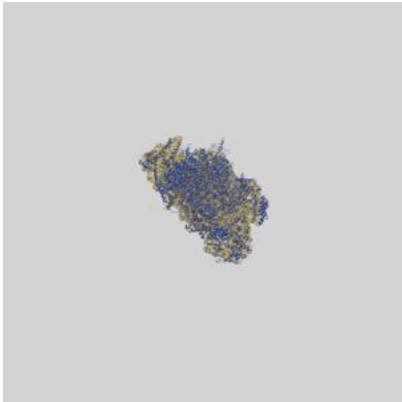
## 9.1 Map-model overlay (i)



X



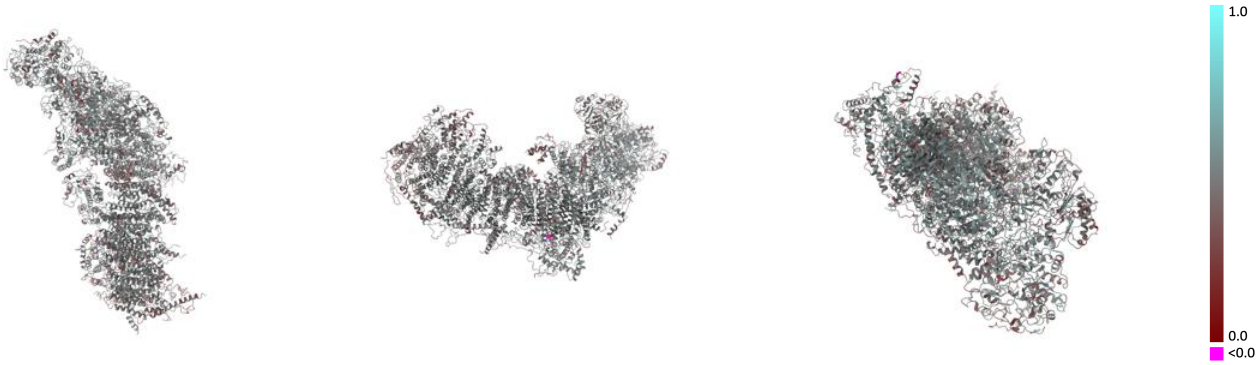
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

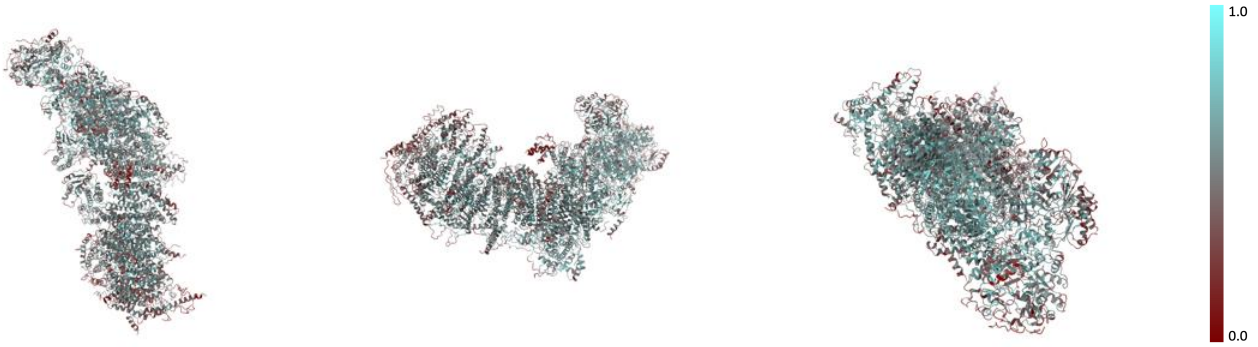
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

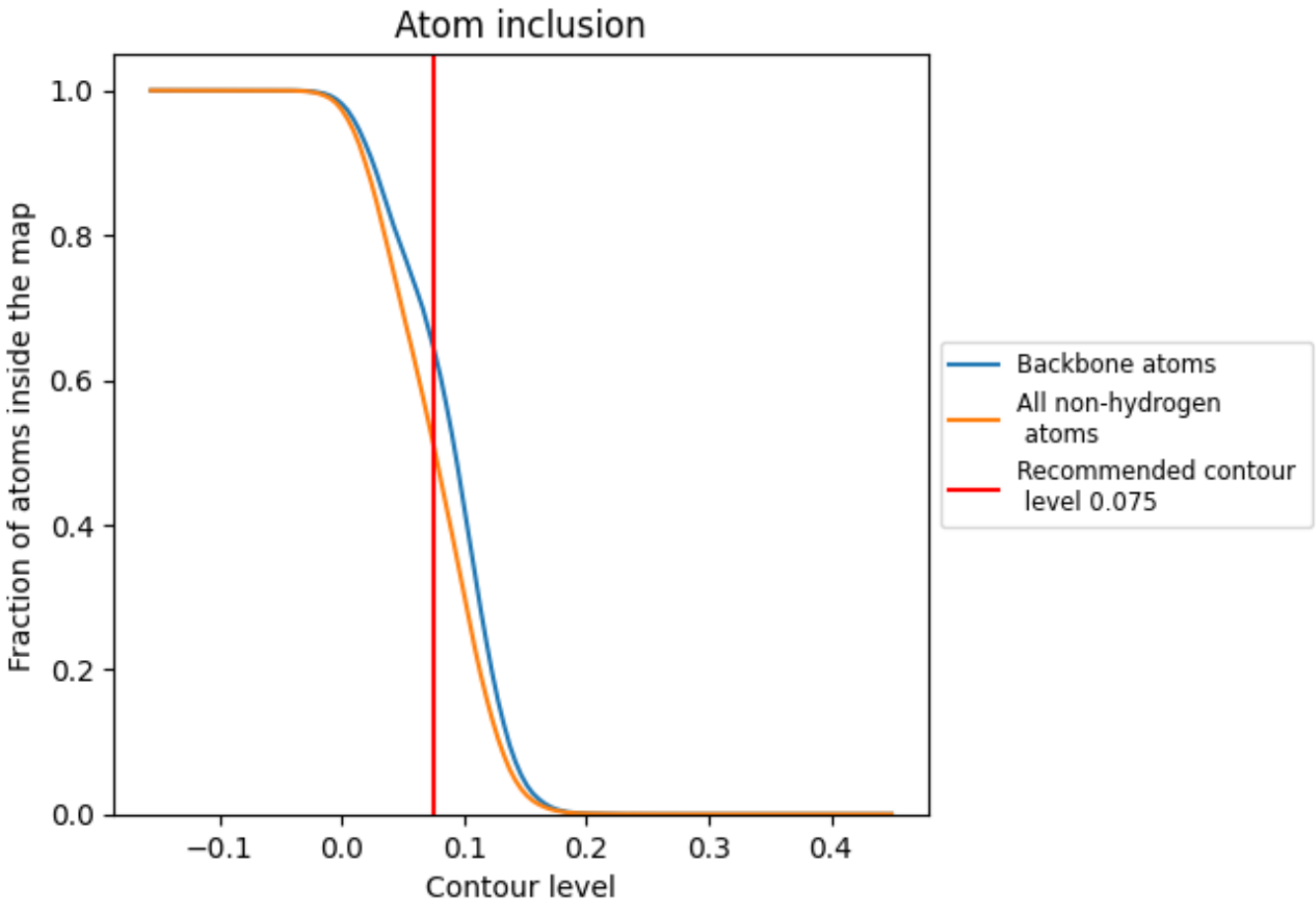
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).

## 9.4 Atom inclusion (i)




At the recommended contour level, 64% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5095 | 0.4690 |
| A | 0.5088 | 0.4820 |
| B | 0.6556 | 0.5030 |
| C | 0.6026 | 0.4980 |
| D | 0.6179 | 0.5020 |
| E | 0.4468 | 0.4570 |
| F | 0.4943 | 0.4600 |
| G | 0.5383 | 0.4760 |
| H | 0.5596 | 0.4960 |
| I | 0.6522 | 0.5070 |
| J | 0.4829 | 0.4650 |
| K | 0.5648 | 0.4900 |
| L | 0.4968 | 0.4760 |
| M | 0.5579 | 0.5020 |
| N | 0.5771 | 0.4920 |
| O | 0.5033 | 0.4640 |
| P | 0.5175 | 0.4680 |
| Q | 0.5332 | 0.4850 |
| R | 0.5401 | 0.4850 |
| S | 0.4136 | 0.4400 |
| T | 0.1785 | 0.3630 |
| U | 0.3537 | 0.4140 |
| V | 0.4734 | 0.4550 |
| W | 0.4952 | 0.4640 |
| X | 0.5176 | 0.4720 |
| Y | 0.4346 | 0.4490 |
| Z | 0.5157 | 0.4500 |
| a | 0.5671 | 0.4960 |
| b | 0.4625 | 0.4310 |
| c | 0.3810 | 0.4180 |
| d | 0.4964 | 0.4650 |
| e | 0.5200 | 0.4630 |
| f | 0.4181 | 0.4250 |
| g | 0.4331 | 0.4570 |
| h | 0.5143 | 0.4690 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| i | 0.3726 | 0.4220 |
| j | 0.3510 | 0.3870 |
| k | 0.3257 | 0.4250 |
| l | 0.4564 | 0.4470 |
| m | 0.4629 | 0.4640 |
| n | 0.4236 | 0.4110 |
| o | 0.3222 | 0.3870 |
| p | 0.4597 | 0.4440 |
| q | 0.5573 | 0.4780 |
| r | 0.4948 | 0.4560 |
| s | 0.3853 | 0.4410 |