# wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 06:20 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 5J4Z |
| EMDB ID | : | EMD-8130 |
| Title | : | Architecture of tight respirasome |
| Authors | : | Letts, J.A.; Fiedorczuk, K.; Sazanov, L.A. |
| Deposited on | : | 2016-04-01 |
| Resolution | : | 5.80 Å(reported) |

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

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

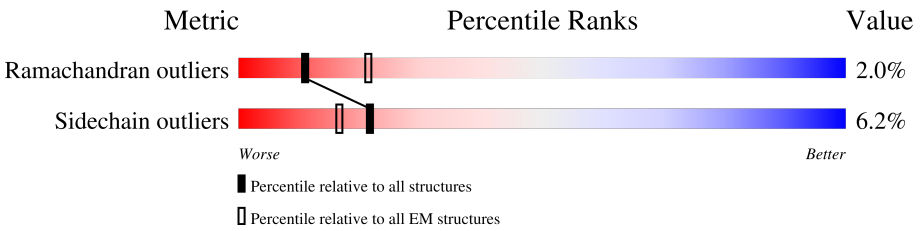
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| 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 5.80 Å.

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




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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 102 | 9% 100% |
| 2 | B | 154 | 7% 98% |
| 3 | C | 194 | 97% |
| 4 | D | 384 | 100% |
| 5 | E | 189 | 100% |
| 6 | F | 429 | 6% 99% |
| 7 | G | 652 | 9% 98% |
| 8 | H | 297 | 100% |
| 9 | I | 171 | 96% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | J | 171 | 81% 19% |
| 11 | K | 93 | 100% |
| 12 | L | 575 | 99% |
| 13 | M | 455 | 99% |
| 14 | N | 345 | 99% |
| 15 | O | 104 | 5% 100% |
| 16 | P | 85 | 5% 100% |
| 17 | Q | 66 | 98% |
| 18 | R | 29 | 21% 97% |
| 19 | S | 80 | 6% 100% |
| 19 | d | 80 | 98% |
| 20 | T | 53 | 100% |
| 21 | U | 96 | 100% |
| 22 | V | 112 | 99% |
| 23 | W | 103 | 99% |
| 24 | X | 309 | 8% 83% 17% |
| 25 | Y | 322 | 98% |
| 26 | Z | 119 | 11% 100% |
| 27 | a | 111 | 100% |
| 28 | b | 92 | 100% |
| 29 | c | 79 | 9% 90% 10% |
| 30 | e | 55 | 100% |
| 31 | f | 59 | 98% |
| 32 | g | 130 | 99% |
| 33 | 9 | 63 | 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | h | 63 | 98% |
| 33 | z | 63 | 40% 59% |
| 34 | i | 70 | 99% |
| 35 | j | 44 | 100% |
| 36 | k | 83 | 96% |
| 37 | 0 | 36 | 100% |
| 38 | 1 | 30 | 97% |
| 39 | 2 | 38 | 5% 100% |
| 40 | 3 | 28 | 100% |
| 40 | 4 | 28 | 100% |
| 41 | 5 | 34 | 100% |
| 42 | 6 | 21 | 100% |
| 43 | 7 | 39 | 100% |
| 44 | 8 | 27 | 100% |
| 45 | y | 46 | 100% |
| 46 | x | 13 | 100% |
| 47 | w | 24 | 100% |
| 48 | v | 18 | 100% |
| 49 | u | 16 | 100% |
| 50 | t | 12 | 100% |
| 51 | AA | 449 | 10% 95% |
| 51 | AL | 449 | 22% 95% |
| 52 | AB | 423 | 12% 95% 5% |
| 52 | AM | 423 | 26% 95% 5% |
| 53 | AC | 378 | 5% 95% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | AN | 378 | 8% 95% 5% |
| 54 | AD | 241 | 11% 94% 6% |
| 54 | AO | 241 | 15% 94% 6% |
| 55 | AE | 196 | 57% 95% |
| 55 | AP | 196 | 46% 94% 5% |
| 56 | AF | 105 | 14% 95% |
| 56 | AQ | 105 | 9% 95% |
| 57 | AG | 75 | 7% 93% 7% |
| 57 | AR | 75 | 8% 93% 7% |
| 58 | AH | 67 | 99% |
| 58 | AS | 67 | 13% 100% |
| 59 | AI | 57 | 72% 74% 23% |
| 59 | AT | 57 | 82% 74% 23% |
| 60 | AJ | 60 | 15% 97% |
| 60 | AU | 60 | 20% 97% |
| 61 | AK | 51 | 12% 96% |
| 61 | AV | 51 | 37% 96% |
| 62 | BN | 514 | 33% 100% |
| 63 | BO | 227 | 53% 100% |
| 64 | BC | 259 | 35% 100% |
| 65 | BD | 144 | 44% 100% |
| 66 | BE | 105 | 34% 100% |
| 67 | BP | 98 | 51% 100% |
| 68 | BG | 84 | 64% 96% |
| 69 | BH | 79 | 61% 99% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 70 | BI | 73 | 56% / 100% |
| 71 | BJ | 58 | 55% / 100% |
| 72 | BK | 49 | 63% / 100% |
| 73 | BL | 46 | 35% / 100% |
| 74 | BM | 43 | 40% / 100% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 79 | HEA | BN | 602 | X | - | - | - |
| 79 | HEA | BN | 603 | X | - | - | - |

# 2 Entry composition (i)

There are 80 unique types of molecules in this entry. The entry contains 64743 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 COMPLEX I ND3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 1 | A | 102 | 510 | 306 | 102 | 102 | 0 | 0 |

- Molecule 2 is a protein called COMPLEX I PSST/NDUFS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 154 | 774 | 462 | 154 | 154 | 4 | 0 | 0 |

- Molecule 3 is a protein called COMPLEX I 30KDA/NDUFS3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | C | 194 | 970 | 582 | 194 | 194 | 0 | 0 |

- Molecule 4 is a protein called COMPLEX I 49KDA/NDUFS2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 4 | D | 384 | 1920 | 1152 | 384 | 384 | 0 | 0 |

- Molecule 5 is a protein called COMPLEX I 24KDA/NDUFV2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 189 | 949 | 567 | 189 | 189 | 4 | 0 | 0 |

- Molecule 6 is a protein called COMPLEX I 51KDA/NDUFV1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 429 | 2149 | 1287 | 429 | 429 | 4 | 0 | 0 |

- Molecule 7 is a protein called COMPLEX I 75KDA/NDUFS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | G | 652 | 3276 | 1959 | 654 | 652 | 11 | 0 | 0 |

- Molecule 8 is a protein called COMPLEX I ND1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 8 | H | 297 | 1485 | 891 | 297 | 297 | 0 | 0 |

- Molecule 9 is a protein called COMPLEX I TYKY/NDUFS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | I | 171 | 863 | 513 | 171 | 171 | 8 | 0 | 0 |

- Molecule 10 is a protein called COMPLEX I ND6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 10 | J | 139 | 695 | 417 | 139 | 139 | 0 | 0 |

- Molecule 11 is a protein called COMPLEX I ND4L.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 11 | K | 93 | 465 | 279 | 93 | 93 | 0 | 0 |

- Molecule 12 is a protein called COMPLEX I ND5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 12 | L | 575 | 2875 | 1725 | 575 | 575 | 0 | 0 |

- Molecule 13 is a protein called COMPLEX I ND4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 13 | M | 455 | 2275 | 1365 | 455 | 455 | 0 | 0 |

- Molecule 14 is a protein called COMPLEX I ND2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 14 | N | 345 | 1725 | 1035 | 345 | 345 | 0 | 0 |

- Molecule 15 is a protein called COMPLEX I 18KDA/NDUFS6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 15 | O | 104 | 520 | 312 | 104 | 104 | 0 | 0 |

- Molecule 16 is a protein called COMPLEX I 13KDA/NDUFS6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 16 | P | 85 | 425 | 255 | 85 | 85 | 0 | 0 |

- Molecule 17 is a protein called COMPLEX I 15KDA/NDUFS5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 17 | Q | 66 | 330 | 198 | 66 | 66 | 0 | 0 |

- Molecule 18 is a protein called COMPLEX I MWFE/NDUFA1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 18 | R | 29 | 145 | 87 | 29 | 29 | 0 | 0 |

- Molecule 19 is a protein called COMPLEX I B8/NDUFA2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 19 | S | 80 | 400 | 240 | 80 | 80 | 0 | 0 |
| 19 | d | 80 | 400 | 240 | 80 | 80 | 0 | 0 |

- Molecule 20 is a protein called COMPLEX I B9/NDUFA3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 20 | T | 53 | 265 | 159 | 53 | 53 | 0 | 0 |

- Molecule 21 is a protein called COMPLEX I B13/NDUFA5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 21 | U | 96 | 480 | 288 | 96 | 96 | 0 | 0 |

- Molecule 22 is a protein called COMPLEX I B14/NDUFA6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 22 | V | 112 | 560 | 336 | 112 | 112 | 0 | 0 |

- Molecule 23 is a protein called COMPLEX I PGIV/NDUFA8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 23 | W | 103 | 515 | 309 | 103 | 103 | 0 | 0 |

- Molecule 24 is a protein called COMPLEX I 39KDA/NDUFA9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 24 | X | 258 | 1290 | 774 | 258 | 258 | 0 | 0 |

- Molecule 25 is a protein called COMPLEX I 42KDA/NDUFA10.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 25 | Y | 322 | 1595 | 951 | 322 | 322 | 0 | 0 |

- Molecule 26 is a protein called COMPLEX I B14.7/NDUFA11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 26 | Z | 119 | 595 | 357 | 119 | 119 | 0 | 0 |

- Molecule 27 is a protein called COMPLEX I B17.2/NDUFA12.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 27 | a | 111 | 555 | 333 | 111 | 111 | 0 | 0 |

- Molecule 28 is a protein called COMPLEX I B16.6/NDUFA13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 28 | b | 92 | 460 | 276 | 92 | 92 | 0 | 0 |

- Molecule 29 is a protein called COMPLEX I SDAP/NDUFAB1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 29 | c | 71 | 355 | 213 | 71 | 71 | 0 | 0 |

- Molecule 30 is a protein called COMPLEX I SDAP/NDUFAB1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 30 | e | 55 | 275 | 165 | 55 | 55 | 0 | 0 |

- Molecule 31 is a protein called COMPLEX I SDAP/NDUFAB1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 31 | f | 58 | 290 | 174 | 58 | 58 | 0 | 0 |

- Molecule 32 is a protein called COMPLEX I B15/NDUFB4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 32 | g | 130 | 650 | 390 | 130 | 130 | 0 | 0 |

- Molecule 33 is a protein called COMPLEX I B18/NDUFB7.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 33 | h | 63 | 315 | 189 | 63 | 63 | 0 | 0 |
| 33 | 9 | 63 | 315 | 189 | 63 | 63 | 0 | 0 |
| 33 | z | 26 | 130 | 78 | 26 | 26 | 0 | 0 |

- Molecule 34 is a protein called COMPLEX I B22/NDUFB9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 34 | i | 70 | 350 | 210 | 70 | 70 | 0 | 0 |

- Molecule 35 is a protein called COMPLEX I PDSW/NDUFB10.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 35 | j | 44 | 220 | 132 | 44 | 44 | 0 | 0 |

- Molecule 36 is a protein called COMPLEX I ESSS/NDUFB11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 36 | k | 80 | 400 | 240 | 80 | 80 | 0 | 0 |

- Molecule 37 is a protein called COMPLEX I KFYI/NDUFC1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 37 | 0 | 36 | 180 | 108 | 36 | 36 | 0 | 0 |

- Molecule 38 is a protein called COMPLEX I B14.5B/NDUFC2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 38 | 1 | 30 | 150 | 90 | 30 | 30 | 0 | 0 |

- Molecule 39 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 39 | 2 | 38 | 190 | 114 | 38 | 38 | 0 | 0 |

- Molecule 40 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 40 | 3 | 28 | 140 | 84 | 28 | 28 | 0 | 0 |
| 40 | 4 | 28 | 140 | 84 | 28 | 28 | 0 | 0 |

- Molecule 41 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 41 | 5 | 34 | 170 | 102 | 34 | 34 | 0 | 0 |

- Molecule 42 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 42 | 6 | 21 | 105 | 63 | 21 | 21 | 0 | 0 |

- Molecule 43 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 43 | 7 | 39 | 195 | 117 | 39 | 39 | 0 | 0 |

- Molecule 44 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 44 | 8 | 27 | 135 | 81 | 27 | 27 | 0 | 0 |

- Molecule 45 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 45 | y | 46 | 230 | 138 | 46 | 46 | 0 | 0 |

- Molecule 46 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 12.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 46 | x | 13 | 65 | 39 | 13 | 13 | 0 | 0 |

- Molecule 47 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 47 | w | 24 | 120 | 72 | 24 | 24 | 0 | 0 |

- Molecule 48 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 14.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 48 | v | 18 | 90 | 54 | 18 | 18 | 0 | 0 |

- Molecule 49 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 15.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 49 | u | 16 | 80 | 48 | 16 | 16 | 0 | 0 |

- Molecule 50 is a protein called COMPLEX I UNKNOWN SUBUNIT FRAGMENT 16.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 50 | t | 12 | 60 | 36 | 12 | 12 | 0 | 0 |

- Molecule 51 is a protein called COMPLEX III SUBUNIT 1 / CORE 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 51 | AA | 446 | 2198 | 1306 | 446 | 446 | 0 | 0 |
| 51 | AL | 446 | 2198 | 1306 | 446 | 446 | 0 | 0 |

There are 26 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AA | 241 | ILE | LEU | conflict | UNP W5Q5G6 |
| AA | 242 | ARG | CYS | conflict | UNP W5Q5G6 |
| AA | 244 | ARG | PRO | conflict | UNP W5Q5G6 |
| AA | 245 | GLU | TRP | conflict | UNP W5Q5G6 |
| AA | 246 | ASP | GLY | conflict | UNP W5Q5G6 |
| AA | 249 | PRO | GLN | conflict | UNP W5Q5G6 |
| AA | 251 | ALA | TRP | conflict | UNP W5Q5G6 |
| AA | 254 | ALA | PRO | conflict | UNP W5Q5G6 |
| AA | 255 | ILE | PHE | conflict | UNP W5Q5G6 |
| AA | 256 | ALA | GLN | conflict | UNP W5Q5G6 |
| AA | 257 | VAL | ILE | conflict | UNP W5Q5G6 |
| AA | 258 | GLU | ARG | conflict | UNP W5Q5G6 |
| AA | 259 | GLY | HIS | conflict | UNP W5Q5G6 |
| AL | 241 | ILE | LEU | conflict | UNP W5Q5G6 |
| AL | 242 | ARG | CYS | conflict | UNP W5Q5G6 |
| AL | 244 | ARG | PRO | conflict | UNP W5Q5G6 |
| AL | 245 | GLU | TRP | conflict | UNP W5Q5G6 |
| AL | 246 | ASP | GLY | conflict | UNP W5Q5G6 |
| AL | 249 | PRO | GLN | conflict | UNP W5Q5G6 |
| AL | 251 | ALA | TRP | conflict | UNP W5Q5G6 |
| AL | 254 | ALA | PRO | conflict | UNP W5Q5G6 |
| AL | 255 | ILE | PHE | conflict | UNP W5Q5G6 |
| AL | 256 | ALA | GLN | conflict | UNP W5Q5G6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AL | 257 | VAL | ILE | conflict | UNP W5Q5G6 |
| AL | 258 | GLU | ARG | conflict | UNP W5Q5G6 |
| AL | 259 | GLY | HIS | conflict | UNP W5Q5G6 |

- Molecule 52 is a protein called COMPLEX III SUBUNIT 2 / CORE 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 52 | AB | 423 | 2081 | 1235 | 423 | 423 | 0 | 0 |
| 52 | AM | 423 | 2081 | 1235 | 423 | 423 | 0 | 0 |

- Molecule 53 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 53 | AC | 378 | 1866 | 1110 | 378 | 378 | 0 | 0 |
| 53 | AN | 378 | 1866 | 1110 | 378 | 378 | 0 | 0 |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AC | 185 | SER | PHE | conflict | UNP P24959 |
| AC | 295 | ILE | VAL | conflict | UNP P24959 |
| AC | 303 | LEU | ILE | conflict | UNP P24959 |
| AC | 359 | ILE | PHE | conflict | UNP P24959 |
| AC | 361 | LEU | ILE | conflict | UNP P24959 |
| AC | 363 | MET | LEU | conflict | UNP P24959 |
| AN | 185 | SER | PHE | conflict | UNP P24959 |
| AN | 295 | ILE | VAL | conflict | UNP P24959 |
| AN | 303 | LEU | ILE | conflict | UNP P24959 |
| AN | 359 | ILE | PHE | conflict | UNP P24959 |
| AN | 361 | LEU | ILE | conflict | UNP P24959 |
| AN | 363 | MET | LEU | conflict | UNP P24959 |

- Molecule 54 is a protein called COMPLEX III SUBUNIT 4 / CYTOCHROME C1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 54 | AD | 241 | 1188 | 706 | 241 | 241 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 54 | AO | 241 | 1188 | 706 | 241 | 241 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AD | 139 | THR | - | insertion | UNP W5Q0A9 |
| AD | 140 | GLY | ARG | conflict | UNP W5Q0A9 |
| AO | 139 | THR | - | insertion | UNP W5Q0A9 |
| AO | 140 | GLY | ARG | conflict | UNP W5Q0A9 |

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 55 | AE | 196 | 967 | 575 | 196 | 196 | 0 | 0 |
| 55 | AP | 196 | 967 | 575 | 196 | 196 | 0 | 0 |

- Molecule 56 is a protein called COMPLEX III SUBUNIT 7 / 14KDA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 56 | AF | 105 | 522 | 312 | 105 | 105 | 0 | 0 |
| 56 | AQ | 105 | 522 | 312 | 105 | 105 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AF | 56 | ASP | ASN | conflict | UNP W5P642 |
| AF | 108 | ALA | THR | conflict | UNP W5P642 |
| AQ | 56 | ASP | ASN | conflict | UNP W5P642 |
| AQ | 108 | ALA | THR | conflict | UNP W5P642 |

- Molecule 57 is a protein called COMPLEX III SUBUNIT 8 / QP-C.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 57 | AG | 75 | 371 | 221 | 75 | 75 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 57 | AR | 75 | 371 | 221 | 75 | 75 | 0 | 0 |

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 58 | AH | 67 | 335 | 201 | 67 | 67 | 0 | 0 |
| 58 | AS | 67 | 335 | 201 | 67 | 67 | 0 | 0 |

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 59 | AI | 57 | 281 | 167 | 57 | 57 | 0 | 0 |
| 59 | AT | 57 | 281 | 167 | 57 | 57 | 0 | 0 |

- Molecule 60 is a protein called COMPLEX III SUBUNIT 9 / 7.2KDA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 60 | AJ | 60 | 297 | 177 | 60 | 60 | 0 | 0 |
| 60 | AU | 60 | 297 | 177 | 60 | 60 | 0 | 0 |

- Molecule 61 is a protein called COMPLEX III SUBUNIT 10 / 6.4KDA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 61 | AK | 51 | 250 | 148 | 51 | 51 | 0 | 0 |
| 61 | AV | 51 | 250 | 148 | 51 | 51 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AK | 22 | GLN | SER | conflict | UNP W5PSD1 |
| AV | 22 | GLN | SER | conflict | UNP W5PSD1 |

- Molecule 62 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 62 | BN | 514 | 2523 | 1495 | 514 | 514 | 0 | 0 |

- Molecule 63 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 63 | BO | 227 | 1127 | 673 | 227 | 227 | 0 | 0 |

- Molecule 64 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 64 | BC | 259 | 1275 | 757 | 259 | 259 | 0 | 0 |

- Molecule 65 is a protein called COMPLEX IV COX4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 65 | BD | 144 | 716 | 428 | 144 | 144 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BD | 97 | ILE | LEU | conflict | UNP W5PPE8 |
| BD | 99 | GLU | GLY | conflict | UNP W5PPE8 |
| BD | 100 | LYS | TRP | conflict | UNP W5PPE8 |
| BD | 101 | HIS | THR | conflict | UNP W5PPE8 |
| BD | 102 | TYR | ALA | conflict | UNP W5PPE8 |

- Molecule 66 is a protein called COMPLEX IV COX5A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 66 | BE | 105 | 520 | 310 | 105 | 105 | 0 | 0 |

- Molecule 67 is a protein called COMPLEX IV COX5B.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 67 | BP | 98 | 481 | 285 | 98 | 98 | 0 | 0 |

- Molecule 68 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 68 | BG | 84 | 412 | 244 | 84 | 84 | 0 | 0 |

- Molecule 69 is a protein called COMPLEX IV COX6B1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 69 | BH | 79 | 391 | 233 | 79 | 79 | 0 | 0 |

- Molecule 70 is a protein called COMPLEX IV COX6C.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 70 | BI | 73 | 361 | 215 | 73 | 73 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BI | 26 | MET | VAL | conflict | UNP W5PXG3 |
| BI | 31 | PHE | SER | conflict | UNP W5PXG3 |
| BI | 36 | LYS | ASN | conflict | UNP W5PXG3 |

- Molecule 71 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 71 | BJ | 58 | 284 | 168 | 58 | 58 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BJ | 1 | PHE | LEU | conflict | UNP W5P5H0 |
| BJ | 36 | LEU | MET | conflict | UNP W5P5H0 |

- Molecule 72 is a protein called COMPLEX IV COX7B.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 72 | BK | 49 | 241 | 143 | 49 | 49 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BK | 9 | PHE | CYS | conflict | UNP W5QE72 |
| BK | 30 | ILE | VAL | conflict | UNP W5QE72 |
| BK | 47 | ARG | THR | conflict | UNP W5QE72 |

- Molecule 73 is a protein called COMPLEX IV COX7C.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 73 | BL | 46 | 226 | 134 | 46 | 46 | 0 | 0 |

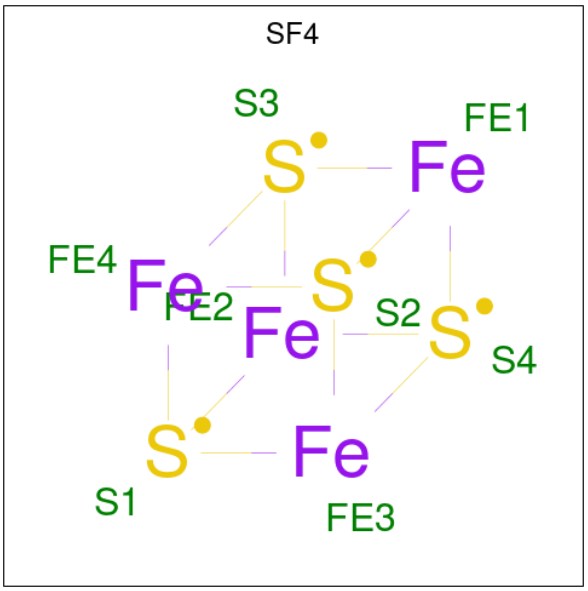
- Molecule 74 is a protein called COMPLEX IV COX8B.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 74 | BM | 43 | 213 | 127 | 43 | 43 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

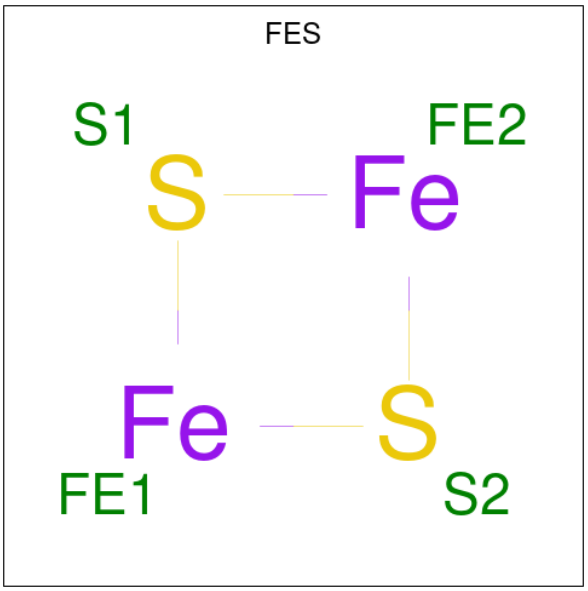
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| BM | ? | - | THR | deletion | UNP W5PFK9 |
| BM | ? | - | GLN | deletion | UNP W5PFK9 |
| BM | 18 | GLY | ALA | conflict | UNP W5PFK9 |
| BM | 21 | VAL | ALA | conflict | UNP W5PFK9 |
| BM | 39 | ASN | HIS | conflict | UNP W5PFK9 |

- Molecule 75 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).



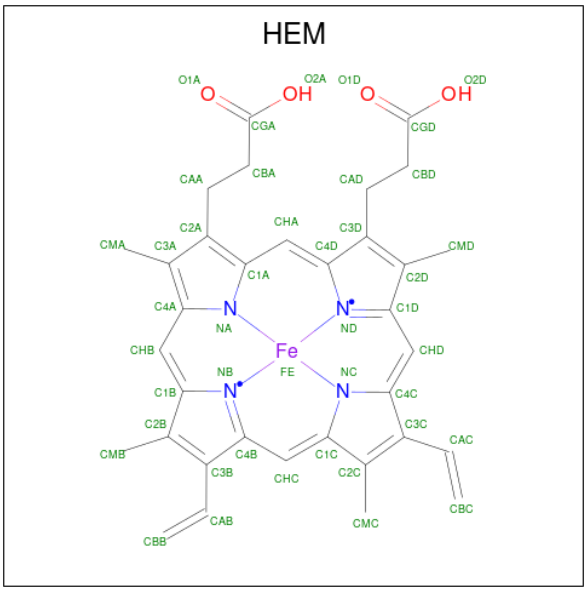

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 75 | B | 1 | 8 | 4 | 4 | 0 |
| 75 | F | 1 | 8 | 4 | 4 | 0 |
| 75 | G | 1 | 16 | 8 | 8 | 0 |
| 75 | G | 1 | 16 | 8 | 8 | 0 |
| 75 | I | 1 | 16 | 8 | 8 | 0 |
| 75 | I | 1 | 16 | 8 | 8 | 0 |

- Molecule 76 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: $Fe_2S_2$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 76 | E | 1 | 4 | 2 | 2 | 0 |
| 76 | G | 1 | 4 | 2 | 2 | 0 |
| 76 | AE | 1 | 4 | 2 | 2 | 0 |
| 76 | AP | 1 | 4 | 2 | 2 | 0 |

- Molecule 77 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

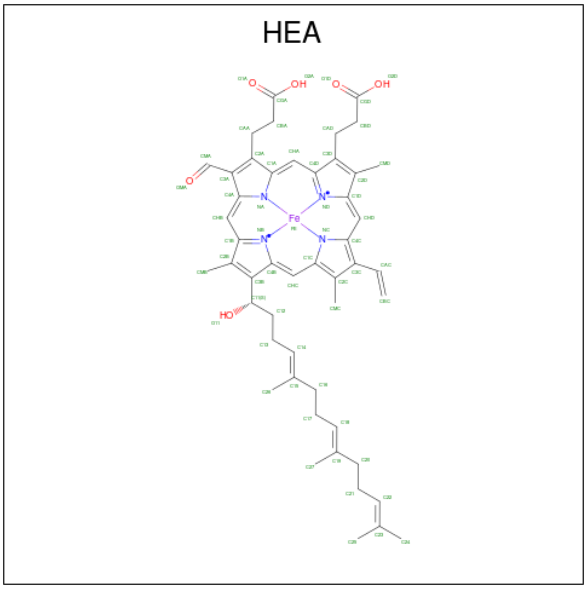


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 77 | AC | 1 | Total<br>86 | C<br>68 | Fe<br>2 | N<br>8 | O<br>8 | 0 |
| 77 | AC | 1 | Total<br>86 | C<br>68 | Fe<br>2 | N<br>8 | O<br>8 | 0 |
| 77 | AD | 1 | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0 |
| 77 | AN | 1 | Total<br>86 | C<br>68 | Fe<br>2 | N<br>8 | O<br>8 | 0 |
| 77 | AN | 1 | Total<br>86 | C<br>68 | Fe<br>2 | N<br>8 | O<br>8 | 0 |
| 77 | AO | 1 | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0 |

- Molecule 78 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

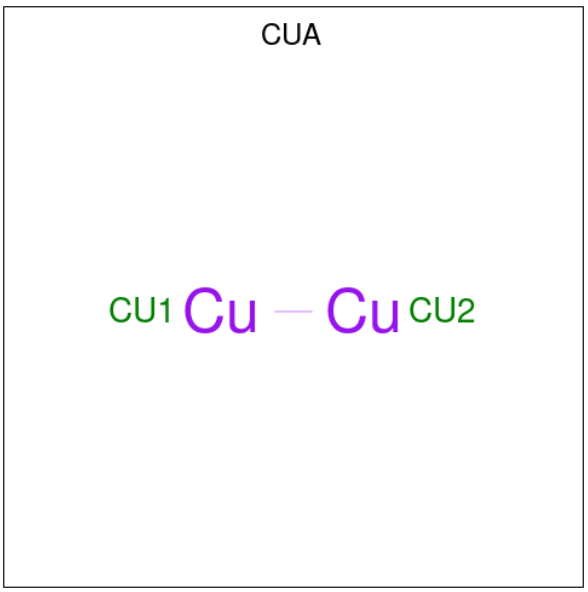
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 78 | BN | 1 | Total<br>1 | Cu<br>1 | 0 |

- Molecule 79 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 79 | BN | 1 | Total<br>120 | C<br>98 | Fe<br>2 | N<br>8 | O<br>12 | 0 |
| 79 | BN | 1 | Total<br>120 | C<br>98 | Fe<br>2 | N<br>8 | O<br>12 | 0 |

- Molecule 80 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: $Cu_2$).



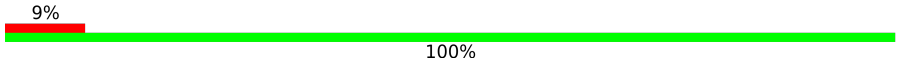

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Cu | |
| 80 | BO | 1 | 2 | 2 | 0 |

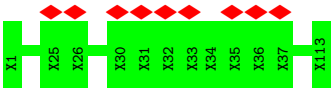
# 3 Residue-property plots (i)

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: COMPLEX I ND3

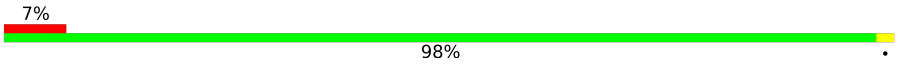
Chain A:

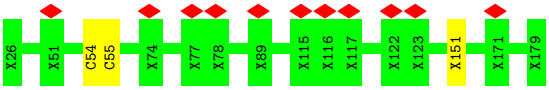



- Molecule 2: COMPLEX I PSST/NDUFS7

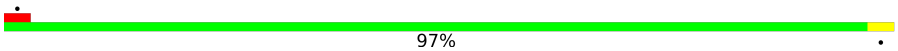
Chain B:



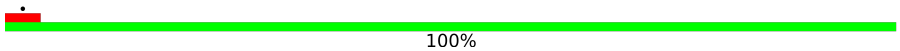

- Molecule 3: COMPLEX I 30KDA/NDUFS3

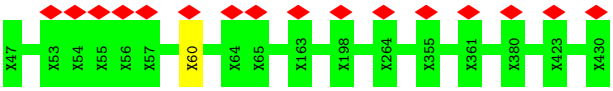
Chain C:



- Molecule 4: COMPLEX I 49KDA/NDUFS2

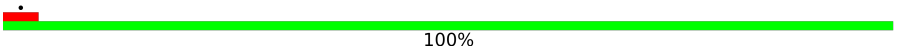
Chain D:

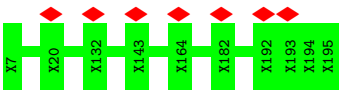



- Molecule 5: COMPLEX I 24KDA/NDUFV2

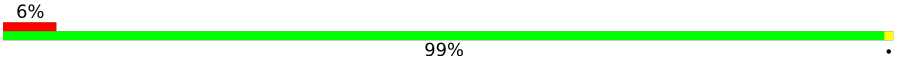
Chain E:

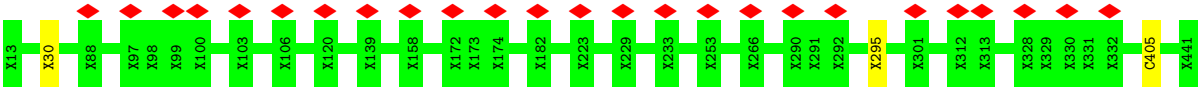


- Molecule 6: COMPLEX I 51KDA/NDUFV1

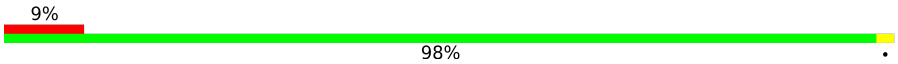
Chain F:

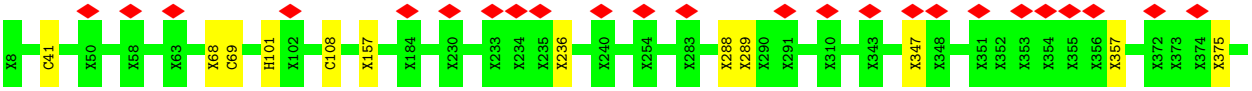


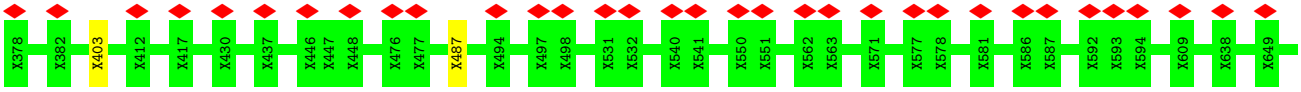




- Molecule 7: COMPLEX I 75KDA/NDUFS1

Chain G:

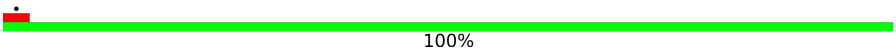


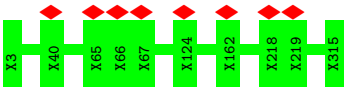



- Molecule 8: COMPLEX I ND1

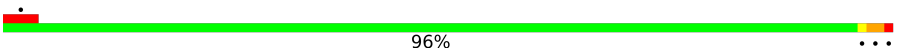
Chain H:

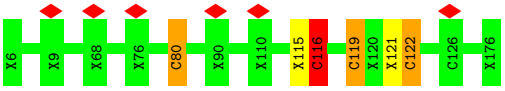



- Molecule 9: COMPLEX I TYKY/NDUFS8

Chain I:



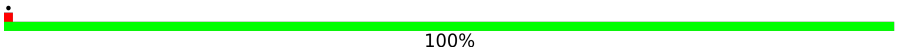




- Molecule 10: COMPLEX I ND6

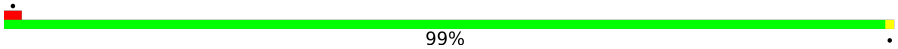
Chain J:

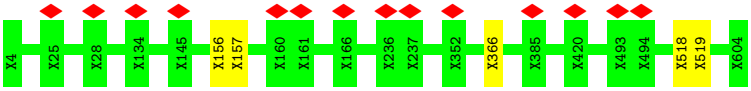
- Molecule 11: COMPLEX I ND4L

Chain K:

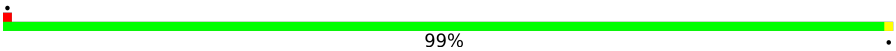


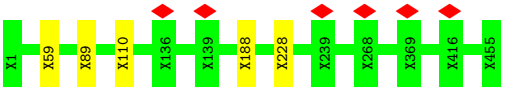
• Molecule 12: COMPLEX I ND5

Chain L: 

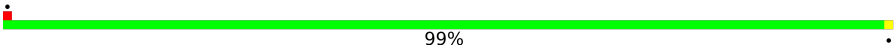



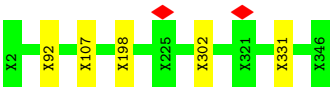

• Molecule 13: COMPLEX I ND4

Chain M: 

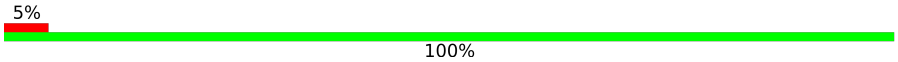



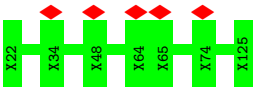

• Molecule 14: COMPLEX I ND2

Chain N: 

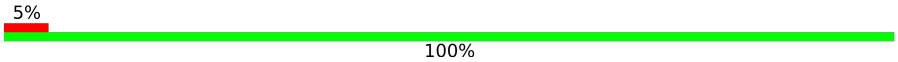



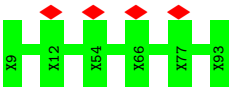

• Molecule 15: COMPLEX I 18KDA/NDUFS6

Chain O: 

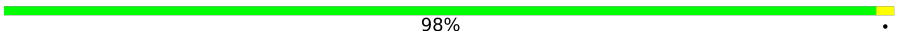




• Molecule 16: COMPLEX I 13KDA/NDUFS6

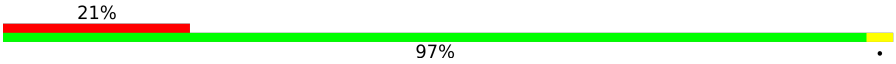
Chain P: 

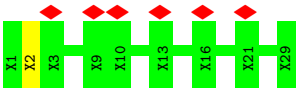




• Molecule 17: COMPLEX I 15KDA/NDUFS5

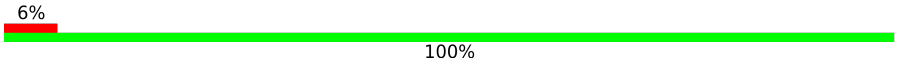
Chain Q: 

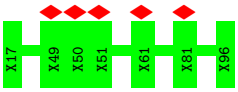
• Molecule 18: COMPLEX I MWFE/NDUFA1

Chain R: 

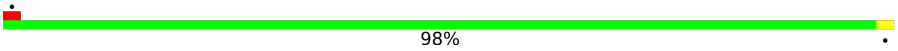



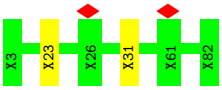

• Molecule 19: COMPLEX I B8/NDUFA2

Chain S: 

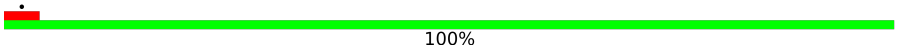



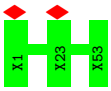

• Molecule 19: COMPLEX I B8/NDUFA2

Chain d: 

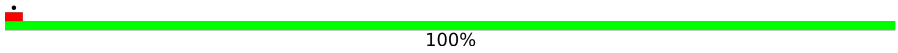



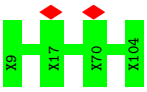

• Molecule 20: COMPLEX I B9/NDUFA3

Chain T: 

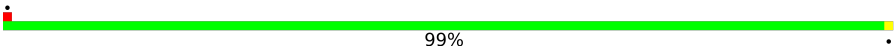



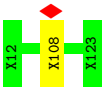

• Molecule 21: COMPLEX I B13/NDUFA5

Chain U: 

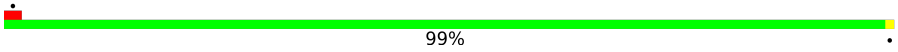



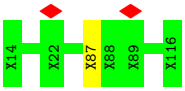

• Molecule 22: COMPLEX I B14/NDUFA6

Chain V: 

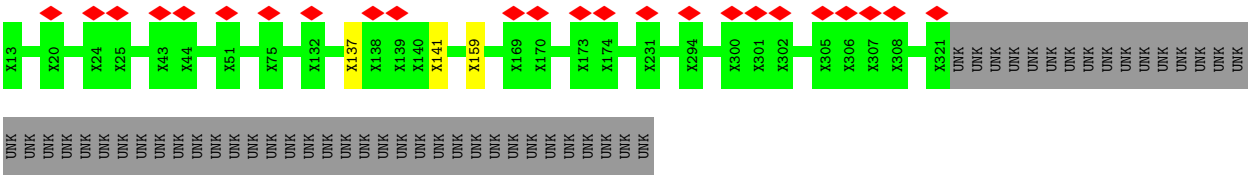

• Molecule 23: COMPLEX I PGIV/NDUFA8

Chain W: 



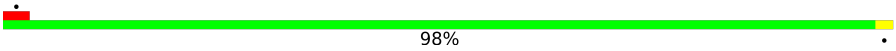

• Molecule 24: COMPLEX I 39KDA/NDUFA9

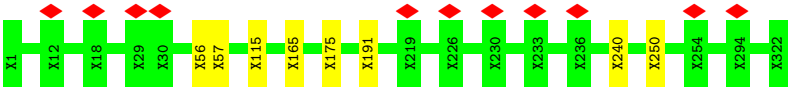
Chain X:




• Molecule 25: COMPLEX I 42KDA/NDUFA10

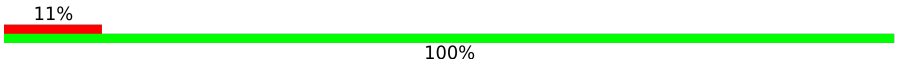
Chain Y:

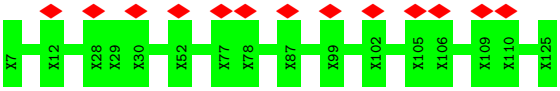



• Molecule 26: COMPLEX I B14.7/NDUFA11

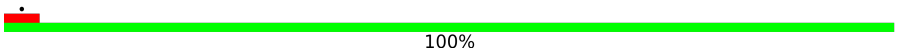
Chain Z:

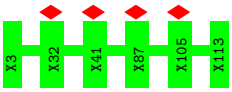



• Molecule 27: COMPLEX I B17.2/NDUFA12

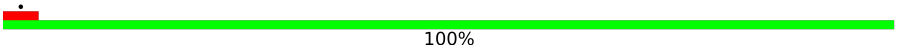
Chain a:

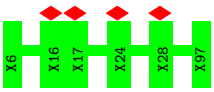



• Molecule 28: COMPLEX I B16.6/NDUFA13

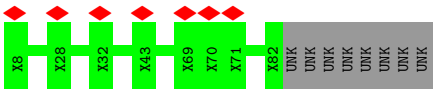
Chain b:




• Molecule 29: COMPLEX I SDAP/NDUFAB1

Chain c:




• Molecule 30: COMPLEX I SDAP/NDUFAB1

Chain e: 100%

There are no outlier residues recorded for this chain.

• Molecule 31: COMPLEX I SDAP/NDUFAB1

Chain f: 98%

• Molecule 32: COMPLEX I B15/NDUFB4

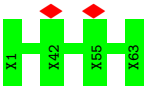
Chain g: 99%

• Molecule 33: COMPLEX I B18/NDUFB7

Chain h: 98%

• Molecule 33: COMPLEX I B18/NDUFB7

Chain 9: 100%



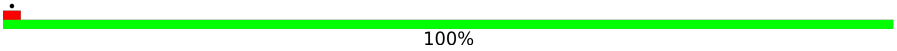

• Molecule 33: COMPLEX I B18/NDUFB7

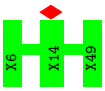
Chain z: 40% 59%

• Molecule 34: COMPLEX I B22/NDUFB9

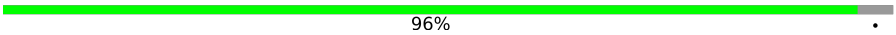
Chain i: 99%

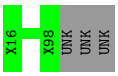
• Molecule 35: COMPLEX I PDSW/NDUFB10

Chain j: 

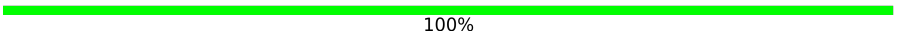




• Molecule 36: COMPLEX I ESSS/NDUFB11

Chain k: 

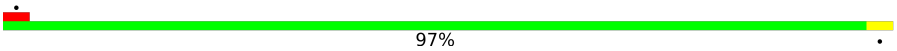



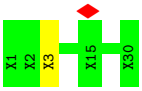

• Molecule 37: COMPLEX I KFYI/NDUFC1

Chain 0: 

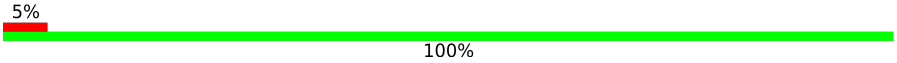

There are no outlier residues recorded for this chain.

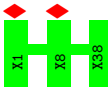
• Molecule 38: COMPLEX I B14.5B/NDUFC2

Chain 1: 

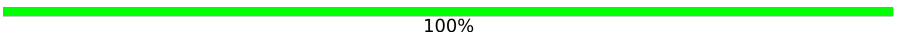




• Molecule 39: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 1

Chain 2: 

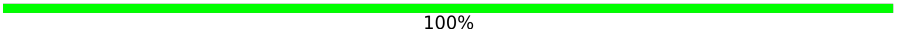




• Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2

Chain 3: 


There are no outlier residues recorded for this chain.

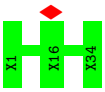
• Molecule 40: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 2

Chain 4: 


There are no outlier residues recorded for this chain.

• Molecule 41: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 3

Chain 5: 100%




• Molecule 42: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 4

Chain 6: 100%

There are no outlier residues recorded for this chain.

• Molecule 43: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 5

Chain 7: 100%

There are no outlier residues recorded for this chain.

• Molecule 44: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 6

Chain 8: 100%

There are no outlier residues recorded for this chain.

• Molecule 45: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 11

Chain y: 100%

There are no outlier residues recorded for this chain.

• Molecule 46: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 12

Chain x: 100%

There are no outlier residues recorded for this chain.

• Molecule 47: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 13

Chain w: 100%

There are no outlier residues recorded for this chain.

• Molecule 48: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 14

Chain v: 100%

There are no outlier residues recorded for this chain.

• Molecule 49: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 15

Chain u: 100%

There are no outlier residues recorded for this chain.

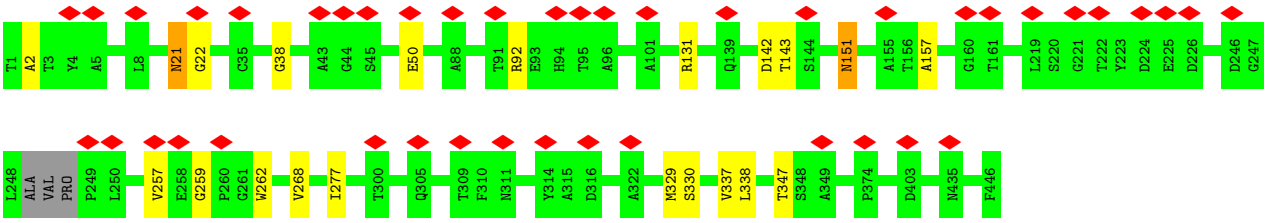
• Molecule 50: COMPLEX I UNKNOWN SUBUNIT FRAGMENT 16

Chain t: 100%

There are no outlier residues recorded for this chain.

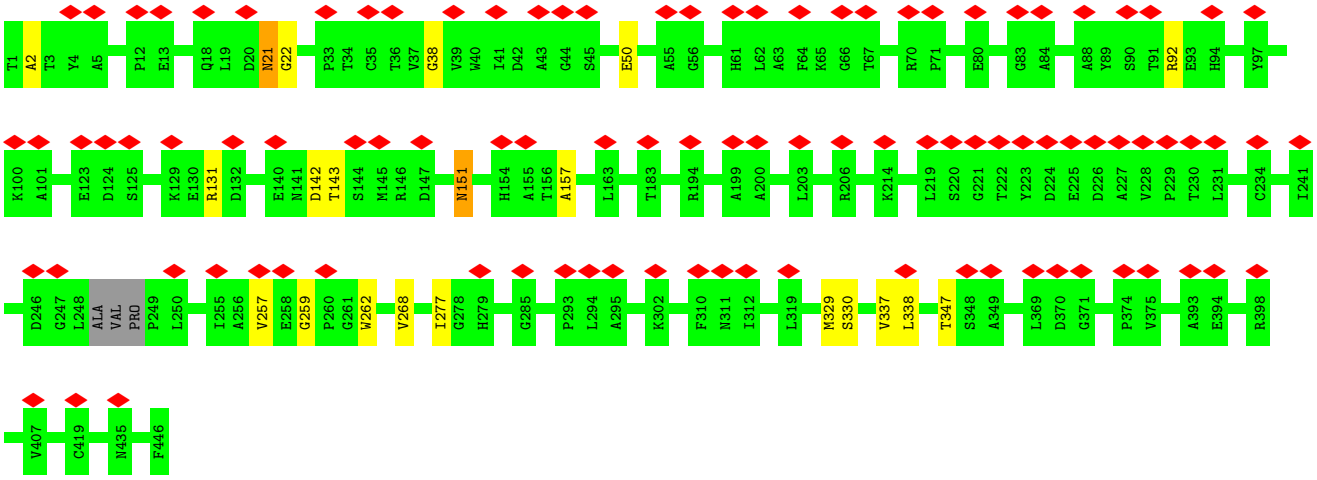
• Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1

Chain AA: 10% 95%



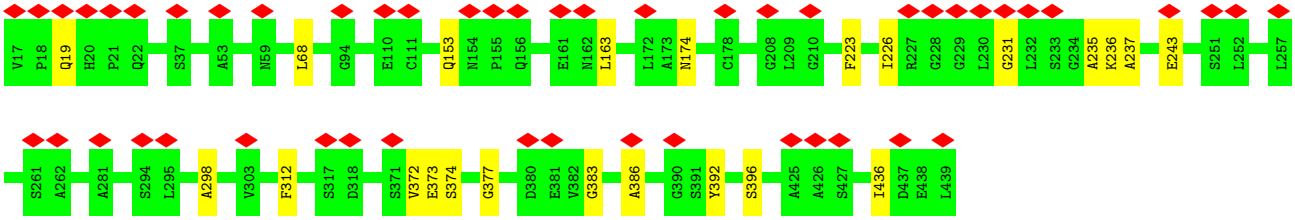

• Molecule 51: COMPLEX III SUBUNIT 1 / CORE 1

Chain AL: 22% 95%



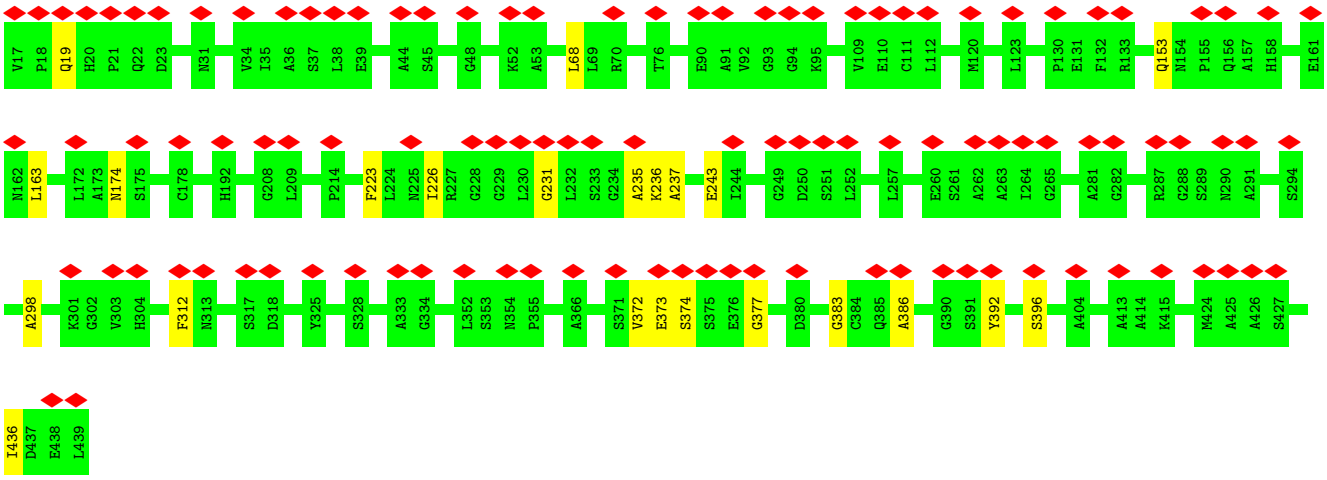

• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

Chain AB: 12% 95% 5%



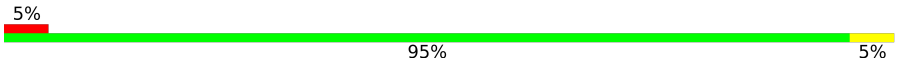

• Molecule 52: COMPLEX III SUBUNIT 2 / CORE 2

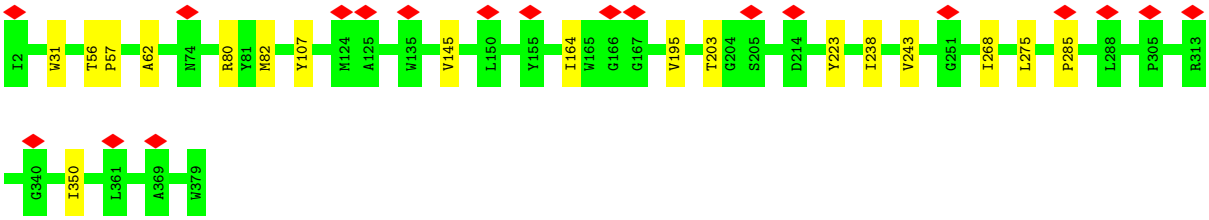
Chain AM: 26% 95% 5%




- Molecule 53: Cytochrome b

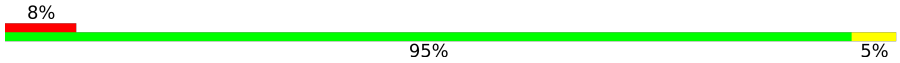
Chain AC:

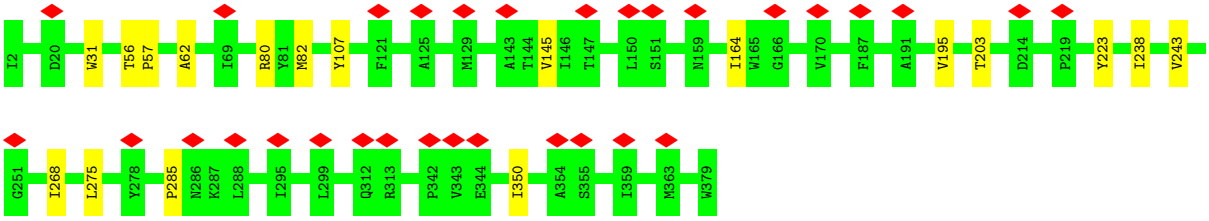



- Molecule 53: Cytochrome b

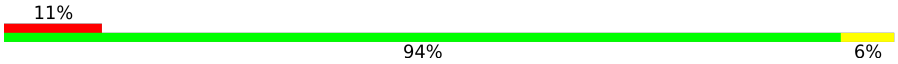
Chain AN:

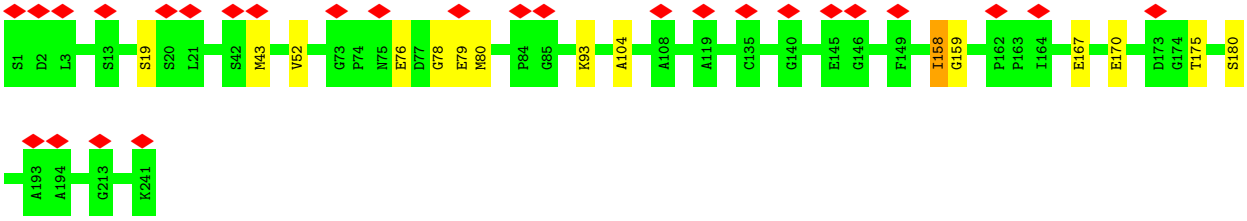



- Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

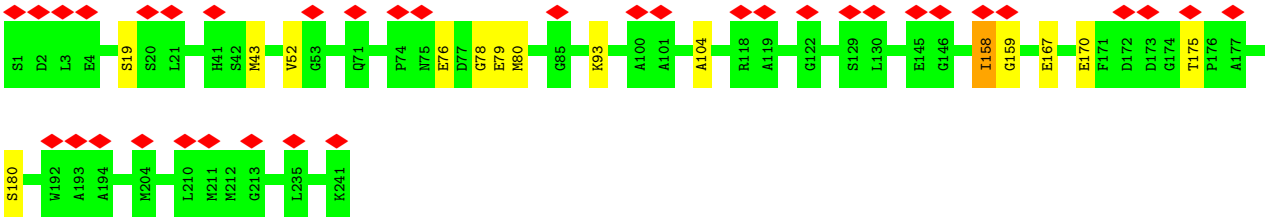
Chain AD:



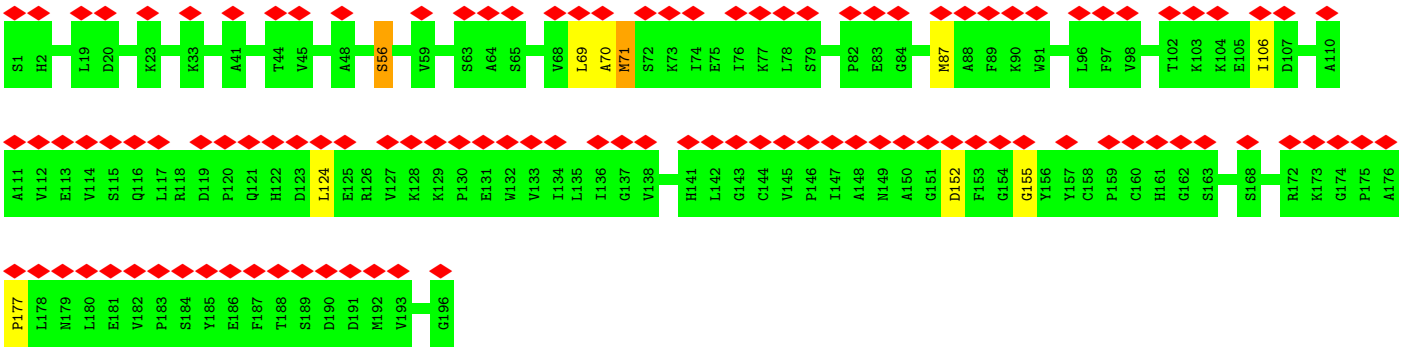

- Molecule 54: COMPLEX III SUBUNIT 4 / CYTOCHROME C1

Chain AO: 15% 94% 6%



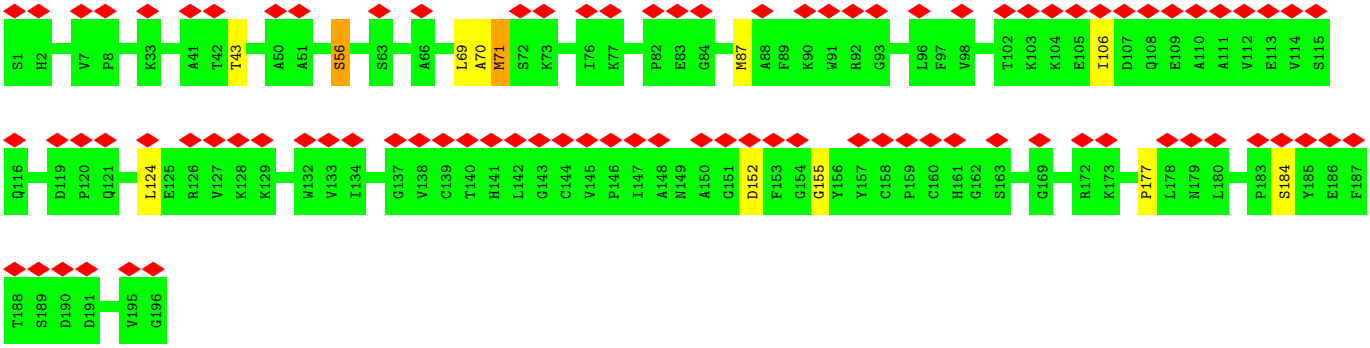

- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AE: 57% 95%



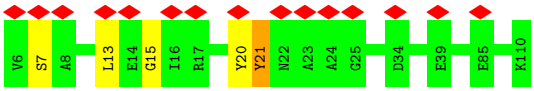

- Molecule 55: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AP: 46% 94% 5%



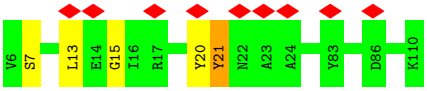

- Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA

Chain AF: 14% 95%



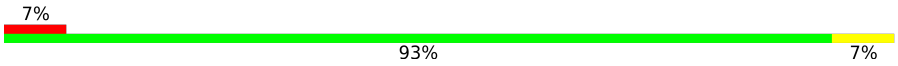

- Molecule 56: COMPLEX III SUBUNIT 7 / 14KDA

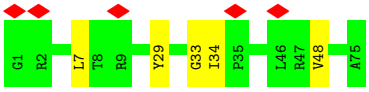
Chain AQ: 9% 95%




• Molecule 57: COMPLEX III SUBUNIT 8 / QP-C

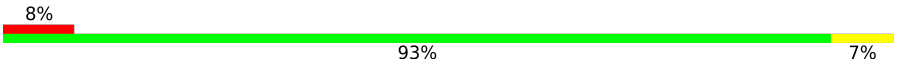
Chain AG:

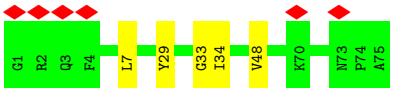



• Molecule 57: COMPLEX III SUBUNIT 8 / QP-C

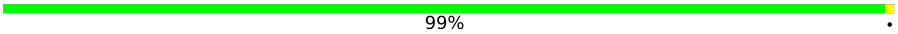
Chain AR:



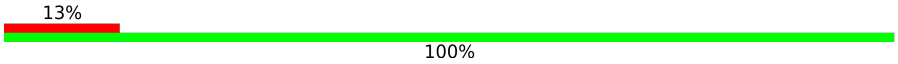

• Molecule 58: Cytochrome b-c1 complex subunit 6

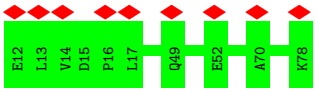
Chain AH:



• Molecule 58: Cytochrome b-c1 complex subunit 6

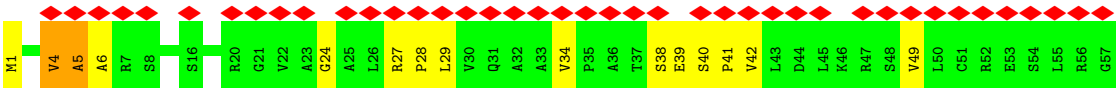
Chain AS:



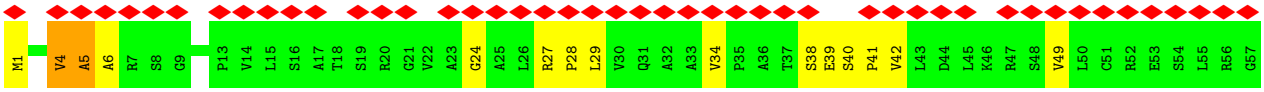

• Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



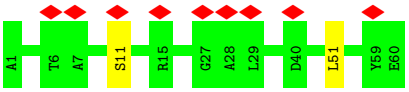

• Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AT:



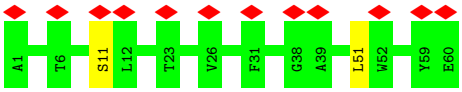

• Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA

Chain AJ: 15% 97%



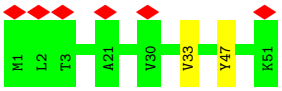

• Molecule 60: COMPLEX III SUBUNIT 9 / 7.2KDA

Chain AU: 20% 97%



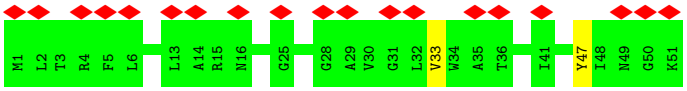

• Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA

Chain AK: 12% 96%



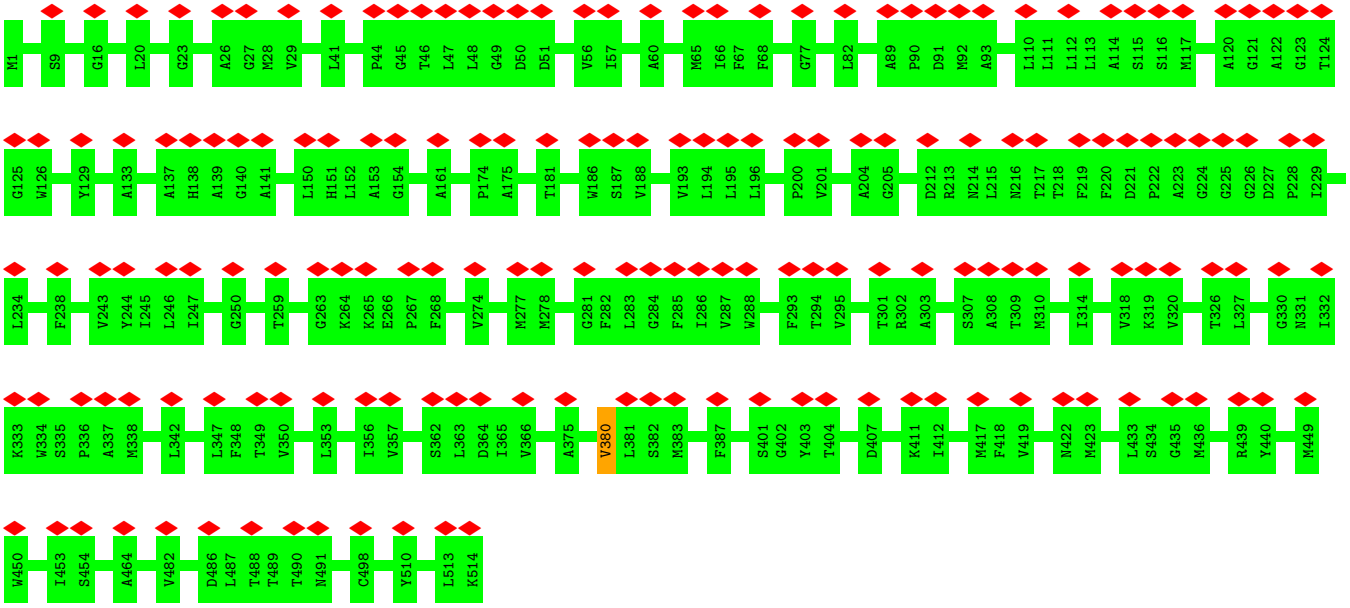

• Molecule 61: COMPLEX III SUBUNIT 10 / 6.4KDA

Chain AV: 37% 96%



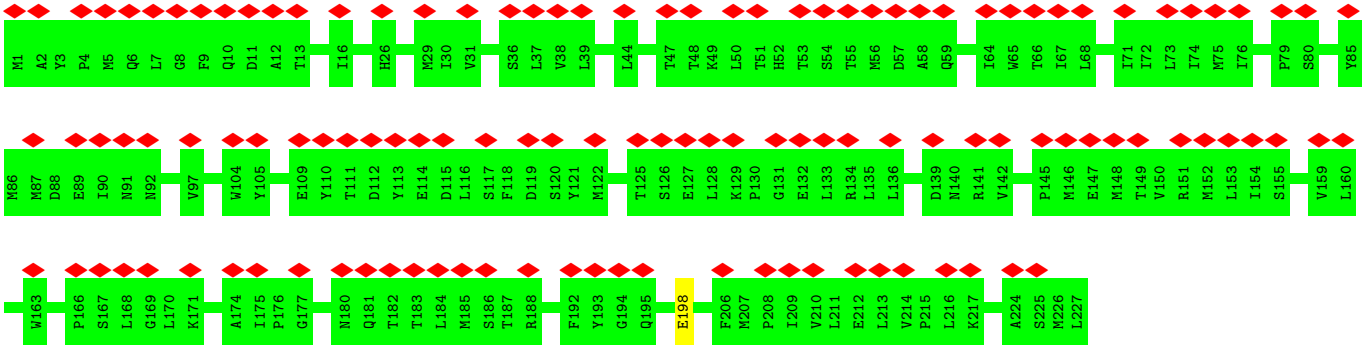

• Molecule 62: Cytochrome c oxidase subunit 1

Chain BN: 33% 100%



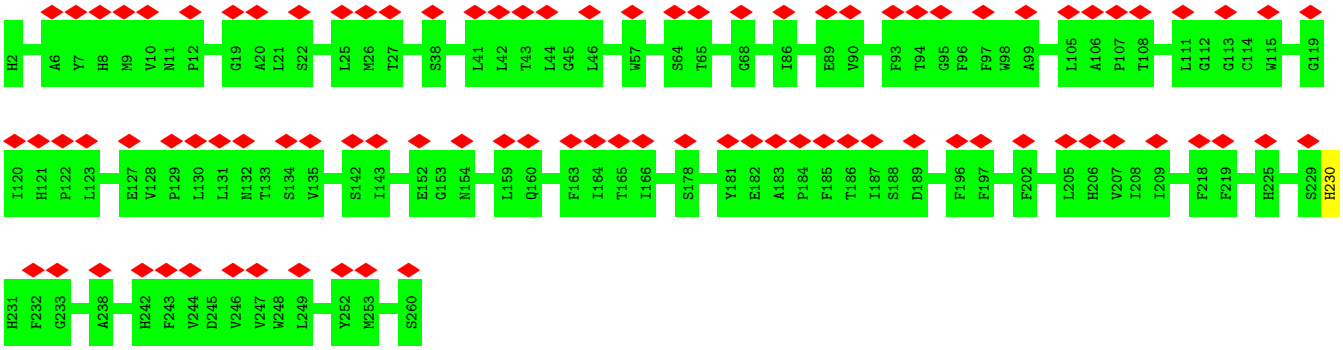
- Molecule 63: Cytochrome c oxidase subunit 2

Chain BO: 53% 100%



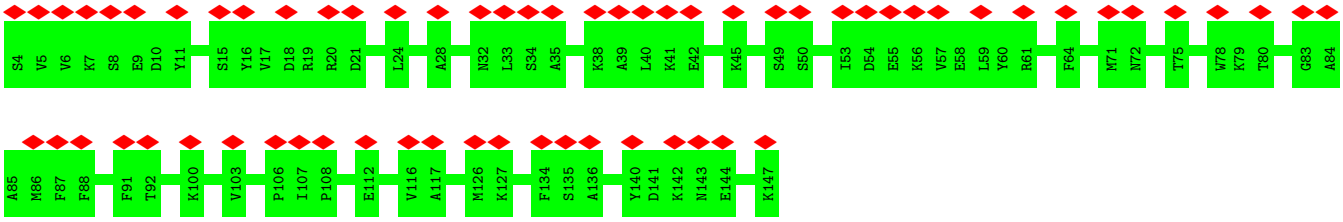

- Molecule 64: Cytochrome c oxidase subunit 3

Chain BC: 35% 100%



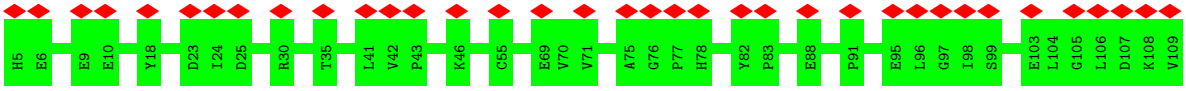

- Molecule 65: COMPLEX IV COX4

Chain BD: 44% 100%



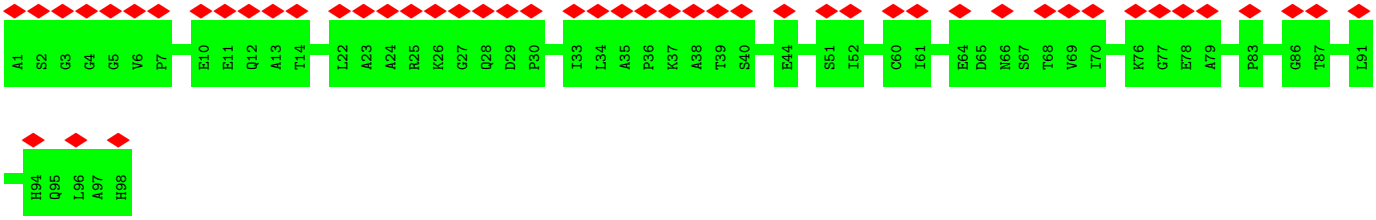

- Molecule 66: COMPLEX IV COX5A

Chain BE: 34% 100%




- Molecule 67: COMPLEX IV COX5B

Chain BP: 51% 100%

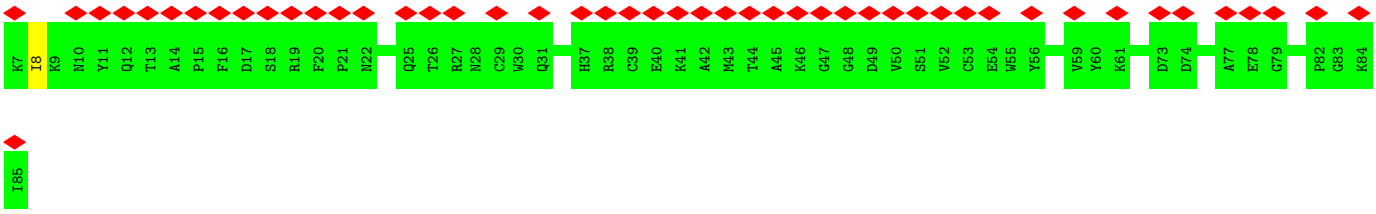



- Molecule 68: Cytochrome c oxidase subunit 6A, mitochondrial

Chain BG: 64% 96%

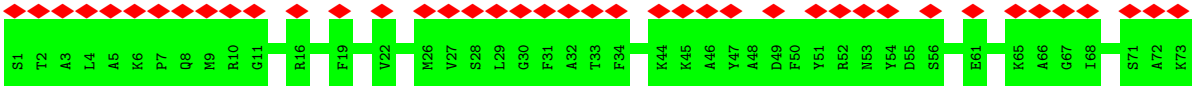
- Molecule 69: COMPLEX IV COX6B1

Chain BH: 61% 99%



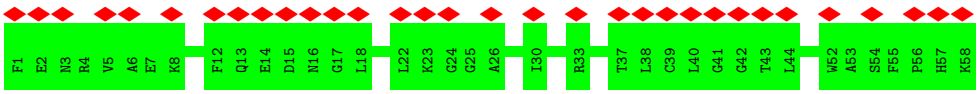

- Molecule 70: COMPLEX IV COX6C

Chain BI: 56% 100%



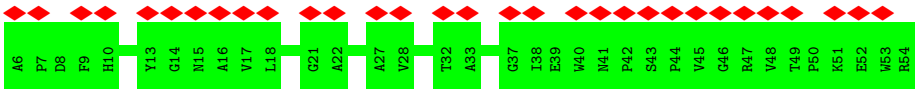

- Molecule 71: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain BJ: 55% 100%



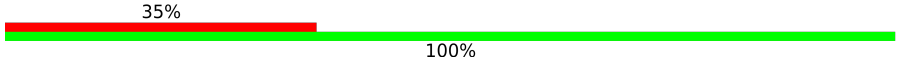

- Molecule 72: COMPLEX IV COX7B

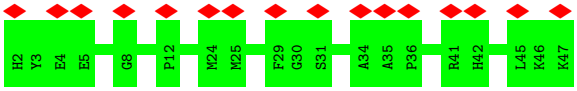
Chain BK: 63% 100%




- Molecule 73: COMPLEX IV COX7C

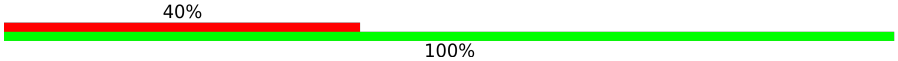
Chain BL:

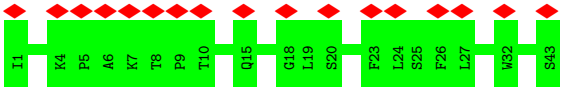



- Molecule 74: COMPLEX IV COX8B

Chain BM:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 18379 | 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 ($e^-/Å^2$) | 34 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 5000 | Depositor |
| Magnification | 81935 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.694 | Depositor |
| Minimum map value | -0.214 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.019 | Depositor |
| Recommended contour level | 0.12 | Depositor |
| Map size (Å) | 853.12, 853.12, 853.12 | wwPDB |
| Map dimensions | 496, 496, 496 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.72, 1.72, 1.72 | 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: CU, FES, HEA, HEM, SF4, CUA

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 | $\#\|Z\|>5$ |
| 2 | B | 1.51 | 1/21 (4.8%) | 0.85 | 0/23 |
| 5 | E | 0.76 | 0/20 | 0.79 | 0/20 |
| 6 | F | 1.42 | 0/20 | 1.20 | 0/20 |
| 7 | G | 0.82 | 0/65 | 1.24 | 2/67 (3.0%) |
| 9 | I | 1.64 | 2/40 (5.0%) | 2.15 | 2/40 (5.0%) |
| 51 | AA | 0.41 | 0/2197 | 0.68 | 3/3055 (0.1%) |
| 51 | AL | 0.41 | 0/2197 | 0.67 | 3/3055 (0.1%) |
| 52 | AB | 0.42 | 0/2080 | 0.66 | 1/2890 (0.0%) |
| 52 | AM | 0.42 | 0/2080 | 0.65 | 1/2890 (0.0%) |
| 53 | AC | 0.75 | 1/1865 (0.1%) | 0.55 | 0/2595 |
| 53 | AN | 0.75 | 1/1865 (0.1%) | 0.55 | 0/2595 |
| 54 | AD | 0.42 | 0/1187 | 0.69 | 1/1650 (0.1%) |
| 54 | AO | 0.42 | 0/1187 | 0.69 | 1/1650 (0.1%) |
| 55 | AE | 0.55 | 1/965 (0.1%) | 1.17 | 2/1340 (0.1%) |
| 55 | AP | 0.76 | 2/966 (0.2%) | 1.21 | 4/1343 (0.3%) |
| 56 | AF | 0.43 | 0/521 | 0.62 | 1/726 (0.1%) |
| 56 | AQ | 0.43 | 0/521 | 0.62 | 1/726 (0.1%) |
| 57 | AG | 0.38 | 0/370 | 0.52 | 0/514 |
| 57 | AR | 0.37 | 0/370 | 0.52 | 0/514 |
| 58 | AH | 0.37 | 0/334 | 0.47 | 0/466 |
| 58 | AS | 0.37 | 0/334 | 0.47 | 0/466 |
| 59 | AI | 0.50 | 0/280 | 1.17 | 4/388 (1.0%) |
| 59 | AT | 0.49 | 0/280 | 1.17 | 4/388 (1.0%) |
| 60 | AJ | 0.37 | 0/296 | 0.53 | 0/411 |
| 60 | AU | 0.37 | 0/296 | 0.53 | 0/411 |
| 61 | AK | 0.37 | 0/249 | 0.45 | 0/344 |
| 61 | AV | 0.38 | 0/249 | 0.45 | 0/344 |
| 62 | BN | 0.27 | 0/2522 | 0.46 | 0/3501 |
| 63 | BO | 0.28 | 0/1126 | 0.53 | 0/1570 |
| 64 | BC | 0.25 | 0/1274 | 0.39 | 0/1770 |
| 65 | BD | 0.25 | 0/715 | 0.41 | 0/997 |
| 66 | BE | 0.27 | 0/519 | 0.46 | 0/722 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 67 | BP | 0.30 | 0/480 | 0.51 | 0/665 |
| 68 | BG | 0.31 | 0/411 | 0.55 | 0/569 |
| 69 | BH | 0.26 | 0/390 | 0.43 | 0/542 |
| 70 | BI | 0.29 | 0/360 | 0.41 | 0/500 |
| 71 | BJ | 0.26 | 0/283 | 0.41 | 0/391 |
| 72 | BK | 0.29 | 0/240 | 0.47 | 0/332 |
| 73 | BL | 0.26 | 0/225 | 0.38 | 0/311 |
| 74 | BM | 0.27 | 0/212 | 0.45 | 0/294 |
| All | All | 0.47 | 8/29612 (0.0%) | 0.65 | 30/41095 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | B | 0 | 2 |
| 3 | C | 0 | 5 |
| 4 | D | 0 | 1 |
| 6 | F | 0 | 3 |
| 7 | G | 0 | 10 |
| 9 | I | 0 | 5 |
| 12 | L | 0 | 5 |
| 13 | M | 0 | 5 |
| 14 | N | 0 | 5 |
| 17 | Q | 0 | 1 |
| 18 | R | 0 | 1 |
| 19 | d | 0 | 2 |
| 22 | V | 0 | 1 |
| 23 | W | 0 | 1 |
| 24 | X | 0 | 3 |
| 25 | Y | 0 | 8 |
| 32 | g | 0 | 1 |
| 33 | h | 0 | 1 |
| 33 | z | 0 | 1 |
| 34 | i | 0 | 1 |
| 38 | 1 | 0 | 1 |
| 51 | AA | 0 | 13 |
| 51 | AL | 0 | 13 |
| 52 | AB | 0 | 17 |
| 52 | AM | 0 | 17 |
| 53 | AC | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 53 | AN | 0 | 2 |
| 54 | AD | 0 | 8 |
| 54 | AO | 0 | 8 |
| 55 | AE | 0 | 3 |
| 55 | AP | 0 | 4 |
| 56 | AF | 0 | 5 |
| 56 | AQ | 0 | 5 |
| 57 | AG | 0 | 2 |
| 57 | AR | 0 | 2 |
| 59 | AI | 0 | 6 |
| 59 | AT | 0 | 6 |
| 60 | AJ | 0 | 1 |
| 60 | AU | 0 | 1 |
| 61 | AK | 0 | 1 |
| 61 | AV | 0 | 1 |
| 62 | BN | 0 | 1 |
| 64 | BC | 0 | 1 |
| 68 | BG | 0 | 1 |
| All | All | 0 | 183 |

The worst 5 of 8 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 53 | AC | 56 | THR | C-N | -26.52 | 0.83 | 1.34 |
| 53 | AN | 56 | THR | C-N | -26.50 | 0.83 | 1.34 |
| 55 | AP | 43 | THR | C-N | -16.36 | 0.96 | 1.34 |
| 9 | I | 122 | CYS | CB-SG | -6.14 | 1.71 | 1.82 |
| 55 | AP | 56 | SER | C-O | 5.40 | 1.33 | 1.23 |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | I | 122 | CYS | CA-CB-SG | -10.08 | 95.85 | 114.00 |
| 54 | AO | 159 | GLY | N-CA-C | 9.60 | 137.09 | 113.10 |
| 54 | AD | 159 | GLY | N-CA-C | 9.57 | 137.01 | 113.10 |
| 52 | AB | 231 | GLY | N-CA-C | 8.66 | 134.75 | 113.10 |
| 52 | AM | 231 | GLY | N-CA-C | 8.64 | 134.70 | 113.10 |

There are no chirality outliers.

5 of 183 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 151 | UNK | Peptide |
| 2 | B | 54 | CYS | Peptide |
| 3 | C | 115 | UNK | Peptide |
| 3 | C | 150 | UNK | Peptide |
| 3 | C | 68 | UNK | 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 | |
|---|---|---|---|---|---|---|---|
| 2 | B | 4/154 (3%) | 4 (100%) | 0 | 0 | 100 | 100 |
| 5 | E | 4/189 (2%) | 2 (50%) | 2 (50%) | 0 | 100 | 100 |
| 6 | F | 4/429 (1%) | 4 (100%) | 0 | 0 | 100 | 100 |
| 7 | G | 12/652 (2%) | 6 (50%) | 4 (33%) | 2 (17%) | 0 | 3 |
| 9 | I | 8/171 (5%) | 4 (50%) | 3 (38%) | 1 (12%) | 0 | 5 |
| 51 | AA | 444/449 (99%) | 369 (83%) | 68 (15%) | 7 (2%) | 9 | 43 |
| 51 | AL | 444/449 (99%) | 370 (83%) | 67 (15%) | 7 (2%) | 9 | 43 |
| 52 | AB | 421/423 (100%) | 369 (88%) | 47 (11%) | 5 (1%) | 13 | 49 |
| 52 | AM | 421/423 (100%) | 369 (88%) | 47 (11%) | 5 (1%) | 13 | 49 |
| 53 | AC | 376/378 (100%) | 288 (77%) | 73 (19%) | 15 (4%) | 3 | 23 |
| 53 | AN | 376/378 (100%) | 289 (77%) | 72 (19%) | 15 (4%) | 3 | 23 |
| 54 | AD | 239/241 (99%) | 180 (75%) | 52 (22%) | 7 (3%) | 4 | 29 |
| 54 | AO | 239/241 (99%) | 180 (75%) | 52 (22%) | 7 (3%) | 4 | 29 |
| 55 | AE | 192/196 (98%) | 148 (77%) | 36 (19%) | 8 (4%) | 3 | 22 |
| 55 | AP | 194/196 (99%) | 151 (78%) | 35 (18%) | 8 (4%) | 3 | 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 56 | AF | 103/105 (98%) | 86 (84%) | 17 (16%) | 0 | 100 | 100 |
| 56 | AQ | 103/105 (98%) | 86 (84%) | 17 (16%) | 0 | 100 | 100 |
| 57 | AG | 73/75 (97%) | 59 (81%) | 11 (15%) | 3 (4%) | 3 | 22 |
| 57 | AR | 73/75 (97%) | 59 (81%) | 11 (15%) | 3 (4%) | 3 | 22 |
| 58 | AH | 65/67 (97%) | 53 (82%) | 11 (17%) | 1 (2%) | 10 | 45 |
| 58 | AS | 65/67 (97%) | 52 (80%) | 13 (20%) | 0 | 100 | 100 |
| 59 | AI | 55/57 (96%) | 31 (56%) | 17 (31%) | 7 (13%) | 0 | 5 |
| 59 | AT | 55/57 (96%) | 31 (56%) | 17 (31%) | 7 (13%) | 0 | 5 |
| 60 | AJ | 58/60 (97%) | 47 (81%) | 10 (17%) | 1 (2%) | 9 | 42 |
| 60 | AU | 58/60 (97%) | 47 (81%) | 10 (17%) | 1 (2%) | 9 | 42 |
| 61 | AK | 49/51 (96%) | 44 (90%) | 4 (8%) | 1 (2%) | 7 | 37 |
| 61 | AV | 49/51 (96%) | 44 (90%) | 4 (8%) | 1 (2%) | 7 | 37 |
| 62 | BN | 512/514 (100%) | 485 (95%) | 26 (5%) | 1 (0%) | 47 | 81 |
| 63 | BO | 225/227 (99%) | 200 (89%) | 24 (11%) | 1 (0%) | 34 | 72 |
| 64 | BC | 257/259 (99%) | 249 (97%) | 8 (3%) | 0 | 100 | 100 |
| 65 | BD | 142/144 (99%) | 136 (96%) | 6 (4%) | 0 | 100 | 100 |
| 66 | BE | 103/105 (98%) | 97 (94%) | 6 (6%) | 0 | 100 | 100 |
| 67 | BP | 96/98 (98%) | 89 (93%) | 7 (7%) | 0 | 100 | 100 |
| 68 | BG | 82/84 (98%) | 70 (85%) | 10 (12%) | 2 (2%) | 6 | 33 |
| 69 | BH | 77/79 (98%) | 68 (88%) | 8 (10%) | 1 (1%) | 12 | 48 |
| 70 | BI | 71/73 (97%) | 65 (92%) | 6 (8%) | 0 | 100 | 100 |
| 71 | BJ | 56/58 (97%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 72 | BK | 47/49 (96%) | 43 (92%) | 4 (8%) | 0 | 100 | 100 |
| 73 | BL | 44/46 (96%) | 42 (96%) | 2 (4%) | 0 | 100 | 100 |
| 74 | BM | 41/43 (95%) | 39 (95%) | 2 (5%) | 0 | 100 | 100 |
| All | All | 5937/7578 (78%) | 5010 (84%) | 810 (14%) | 117 (2%) | 11 | 37 |

5 of 117 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | AA | 143 | THR |
| 52 | AB | 436 | ILE |
| 54 | AD | 79 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | AE | 70 | ALA |
| 55 | AE | 177 | PRO |

### 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 | |
|---|---|---|---|---|---|---|
| 2 | B | 4/4 (100%) | 4 (100%) | 0 | 100 | 100 |
| 5 | E | 4/4 (100%) | 4 (100%) | 0 | 100 | 100 |
| 6 | F | 4/4 (100%) | 4 (100%) | 0 | 100 | 100 |
| 7 | G | 12/12 (100%) | 12 (100%) | 0 | 100 | 100 |
| 9 | I | 8/8 (100%) | 6 (75%) | 2 (25%) | 0 | 3 |
| All | All | 32/32 (100%) | 30 (94%) | 2 (6%) | 21 | 42 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | I | 116 | CYS |
| 9 | I | 119 | CYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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 | $\#\|Z\| > 2$ |
| 80 | CUA | BO | 301 | 63 | 0,1,1 | - | - | - | | |
| 77 | HEM | AC | 401 | - | 41,50,50 | 3.05 | 20 (48%) | 45,82,82 | 2.91 | 14 (31%) |
| 76 | FES | E | 201 | 5 | 0,4,4 | - | - | - | | |
| 76 | FES | G | 803 | 7 | 0,4,4 | - | - | - | | |
| 75 | SF4 | I | 201 | 9 | 0,12,12 | - | - | - | | |
| 77 | HEM | AN | 401 | - | 41,50,50 | 3.05 | 19 (46%) | 45,82,82 | 2.91 | 14 (31%) |
| 75 | SF4 | F | 500 | 6 | 0,12,12 | - | - | - | | |
| 79 | HEA | BN | 602 | - | 57,67,67 | 1.06 | 2 (3%) | 61,103,103 | 1.32 | 7 (11%) |
| 77 | HEM | AD | 301 | - | 41,50,50 | 3.02 | 19 (46%) | 45,82,82 | 2.66 | 19 (42%) |
| 75 | SF4 | B | 201 | 2 | 0,12,12 | - | - | - | | |
| 75 | SF4 | G | 802 | 7 | 0,12,12 | - | - | - | | |
| 75 | SF4 | G | 801 | 7 | 0,12,12 | - | - | - | | |
| 77 | HEM | AN | 402 | - | 41,50,50 | 2.90 | 19 (46%) | 45,82,82 | 2.48 | 16 (35%) |
| 75 | SF4 | I | 202 | 9 | 0,12,12 | - | - | - | | |
| 77 | HEM | AO | 301 | - | 41,50,50 | 3.02 | 19 (46%) | 45,82,82 | 2.66 | 20 (44%) |
| 76 | FES | AP | 201 | - | 0,4,4 | - | - | - | | |
| 76 | FES | AE | 201 | - | 0,4,4 | - | - | - | | |
| 79 | HEA | BN | 603 | - | 57,67,67 | 1.19 | 4 (7%) | 61,103,103 | 1.25 | 6 (9%) |
| 77 | HEM | AC | 402 | - | 41,50,50 | 2.90 | 19 (46%) | 45,82,82 | 2.48 | 16 (35%) |

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 |
|---|---|---|---|---|---|---|---|
| 77 | HEM | AD | 301 | - | - | 2/12/54/54 | - |
| 76 | FES | AP | 201 | - | - | - | 0/1/1/1 |
| 76 | FES | AE | 201 | - | - | - | 0/1/1/1 |
| 79 | HEA | BN | 603 | - | 3/3/7/16 | 7/32/76/76 | - |
| 75 | SF4 | B | 201 | 2 | - | - | 0/6/5/5 |
| 76 | FES | G | 803 | 7 | - | - | 0/1/1/1 |
| 75 | SF4 | I | 202 | 9 | - | - | 0/6/5/5 |
| 75 | SF4 | I | 201 | 9 | - | - | 0/6/5/5 |
| 77 | HEM | AN | 401 | - | - | 6/12/54/54 | - |
| 77 | HEM | AN | 402 | - | - | 8/12/54/54 | - |
| 77 | HEM | AC | 402 | - | - | 7/12/54/54 | - |
| 75 | SF4 | G | 801 | 7 | - | - | 0/6/5/5 |
| 77 | HEM | AC | 401 | - | - | 6/12/54/54 | - |
| 75 | SF4 | G | 802 | 7 | - | - | 0/6/5/5 |
| 75 | SF4 | F | 500 | 6 | - | - | 0/6/5/5 |
| 79 | HEA | BN | 602 | - | 3/3/7/16 | 7/32/76/76 | - |
| 77 | HEM | AO | 301 | - | - | 2/12/54/54 | - |
| 76 | FES | E | 201 | 5 | - | - | 0/1/1/1 |

The worst 5 of 121 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 77 | AC | 401 | HEM | C4D-C3D | -7.64 | 1.31 | 1.45 |
| 77 | AN | 401 | HEM | C4D-C3D | -7.61 | 1.31 | 1.45 |
| 77 | AD | 301 | HEM | C4D-C3D | -6.78 | 1.33 | 1.45 |
| 77 | AO | 301 | HEM | C4D-C3D | -6.78 | 1.33 | 1.45 |
| 77 | AD | 301 | HEM | C1B-C2B | -6.62 | 1.31 | 1.44 |

The worst 5 of 112 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 77 | AC | 402 | HEM | C4C-CHD-C1D | -8.91 | 110.80 | 122.56 |
| 77 | AN | 402 | HEM | C4C-CHD-C1D | -8.89 | 110.82 | 122.56 |
| 77 | AN | 401 | HEM | C4B-CHC-C1C | -8.51 | 111.32 | 122.56 |
| 77 | AC | 401 | HEM | C4B-CHC-C1C | -8.51 | 111.32 | 122.56 |
| 77 | AO | 301 | HEM | C4B-CHC-C1C | -7.94 | 112.08 | 122.56 |

5 of 6 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 79 | BN | 602 | HEA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 79 | BN | 602 | HEA | NB |
| 79 | BN | 602 | HEA | NA |
| 79 | BN | 603 | HEA | ND |
| 79 | BN | 603 | HEA | NB |

5 of 45 torsion outliers are listed below:

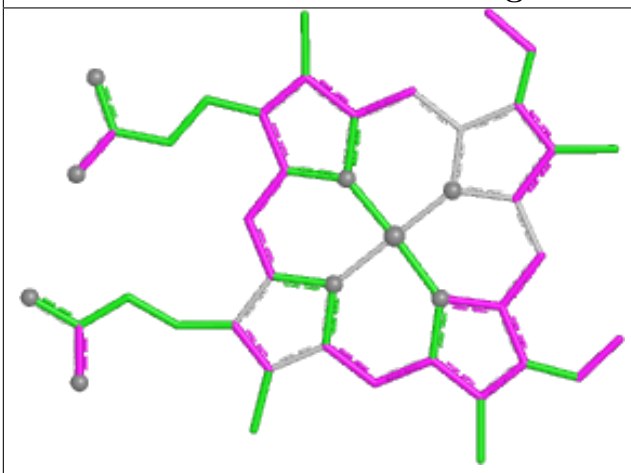
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | AC | 401 | HEM | C2B-C3B-CAB-CBB |
| 77 | AC | 401 | HEM | C4B-C3B-CAB-CBB |
| 77 | AC | 402 | HEM | C1A-C2A-CAA-CBA |
| 77 | AC | 402 | HEM | C3A-C2A-CAA-CBA |
| 77 | AC | 402 | HEM | C2B-C3B-CAB-CBB |

There are no ring outliers.

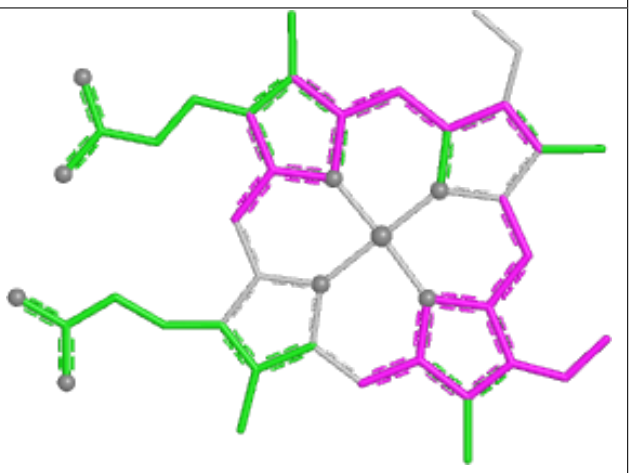
No monomer is involved in short contacts.

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.

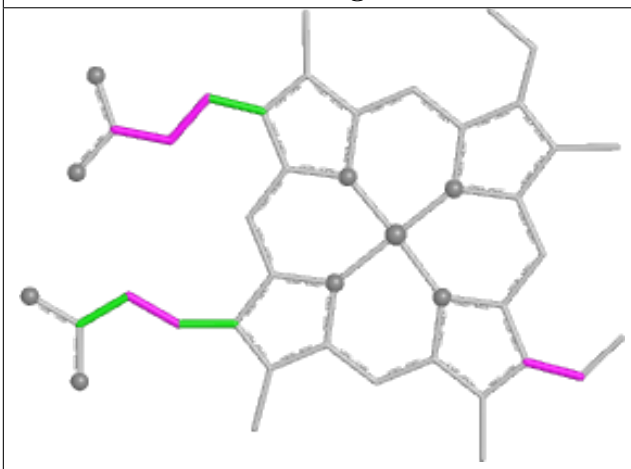
**Ligand HEM AC 401**



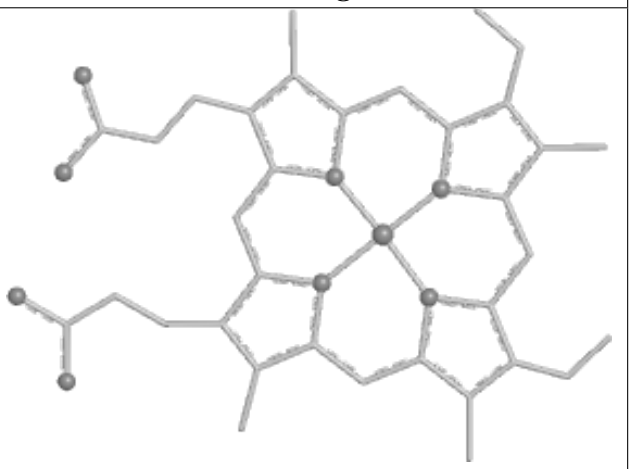
**Bond lengths**



**Bond angles**

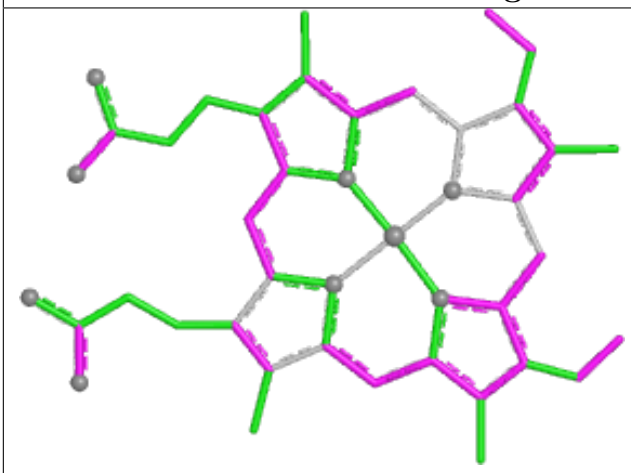


**Torsions**

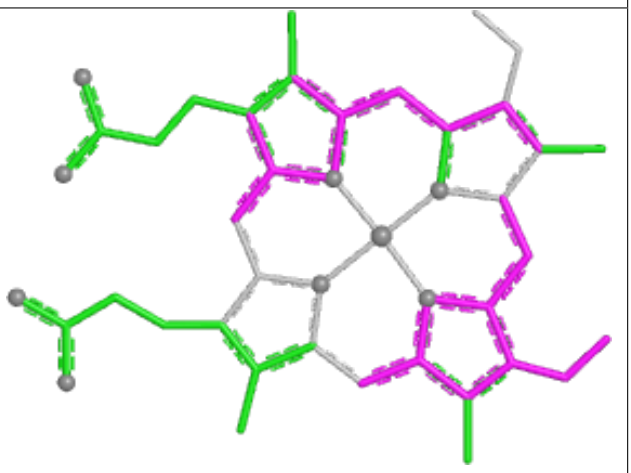


**Rings**

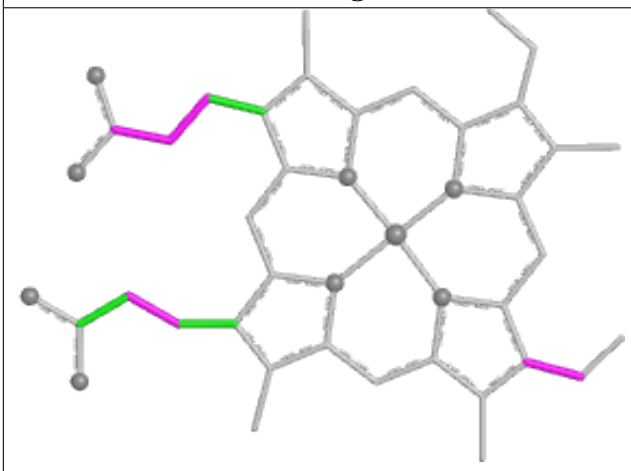
## Ligand HEM AN 401



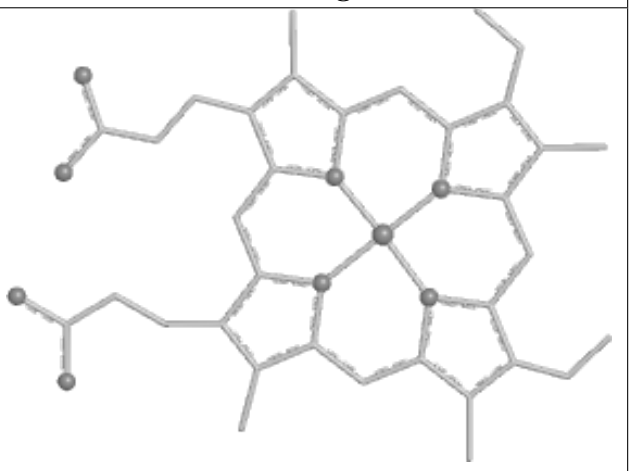
Bond lengths



Bond angles

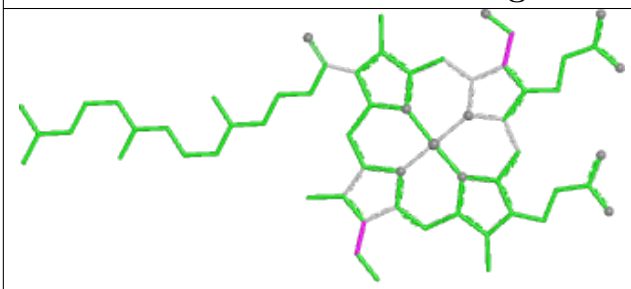


Torsions

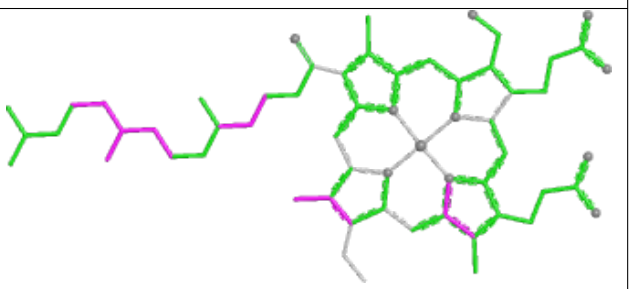


Rings

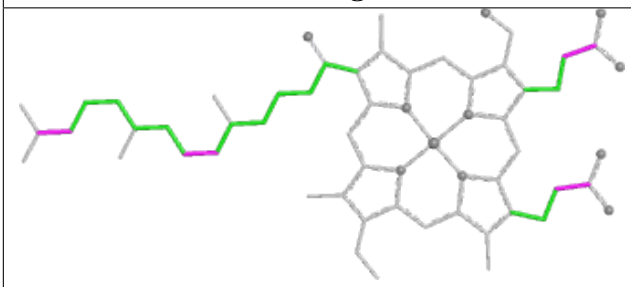
## Ligand HEA BN 602



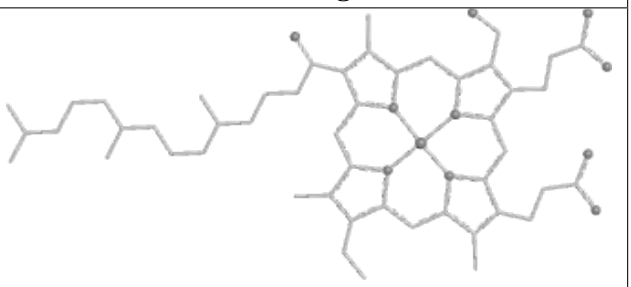
Bond lengths



Bond angles

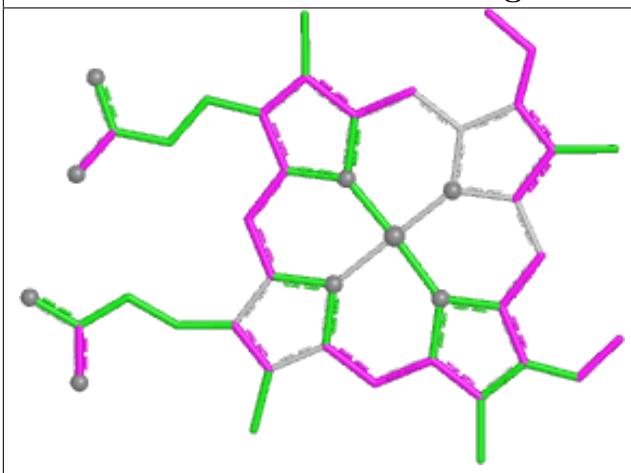


Torsions

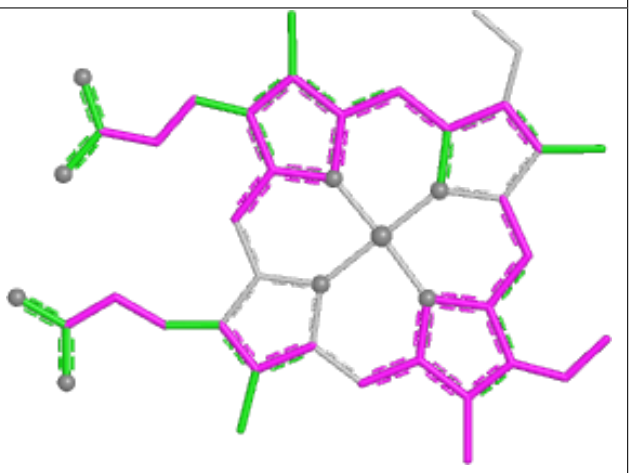


Rings

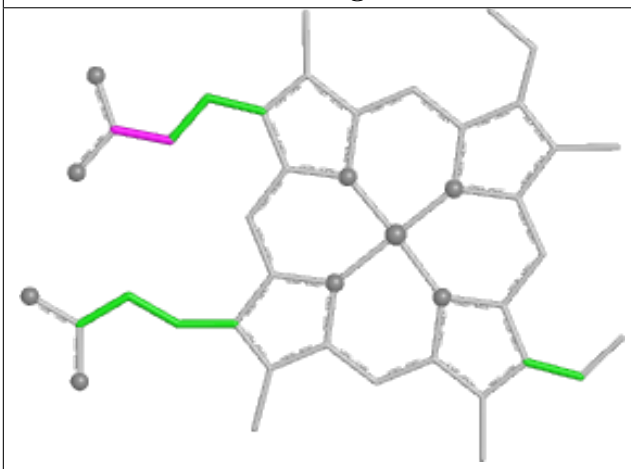
**Ligand HEM AD 301**



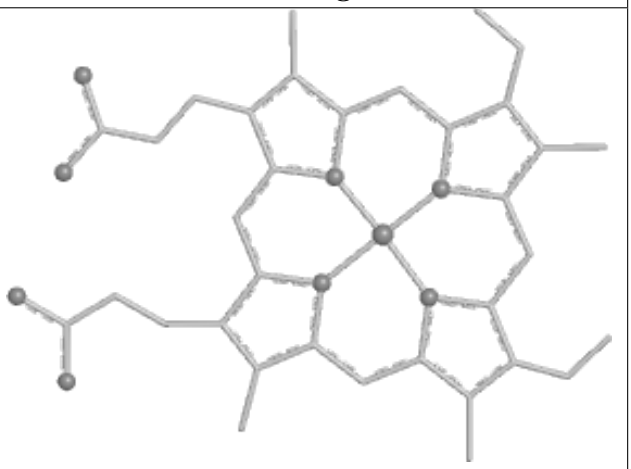
**Bond lengths**



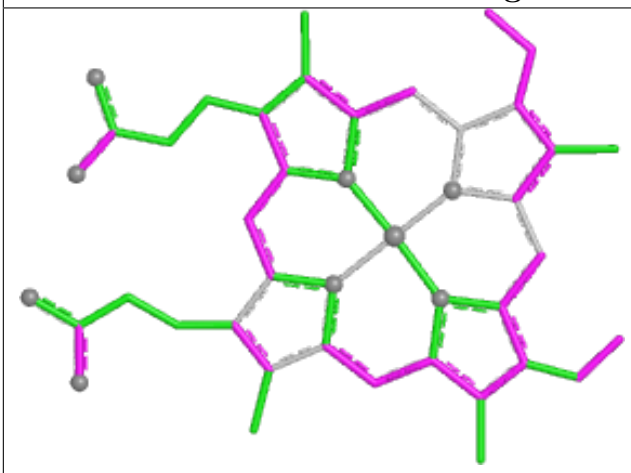
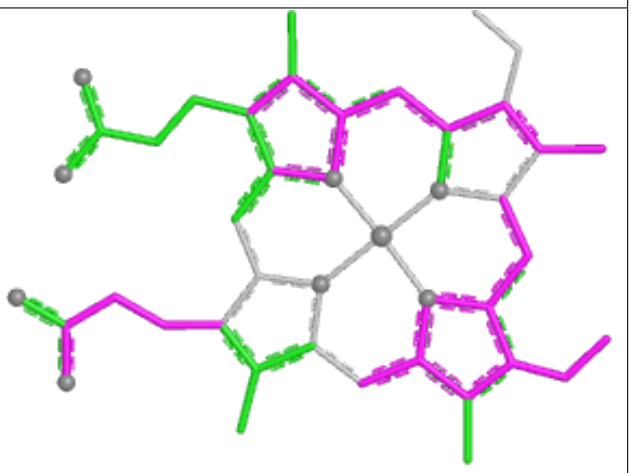
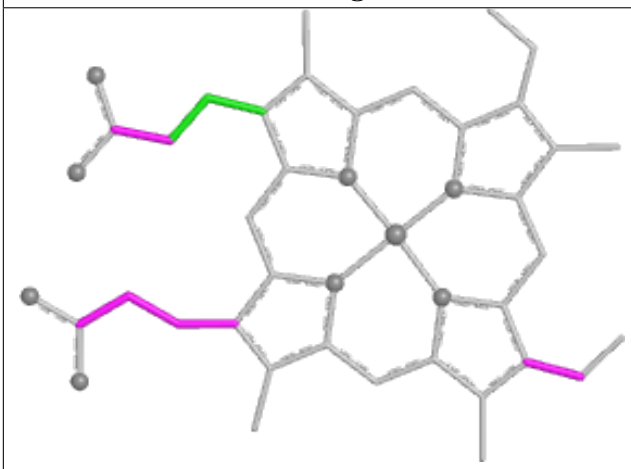
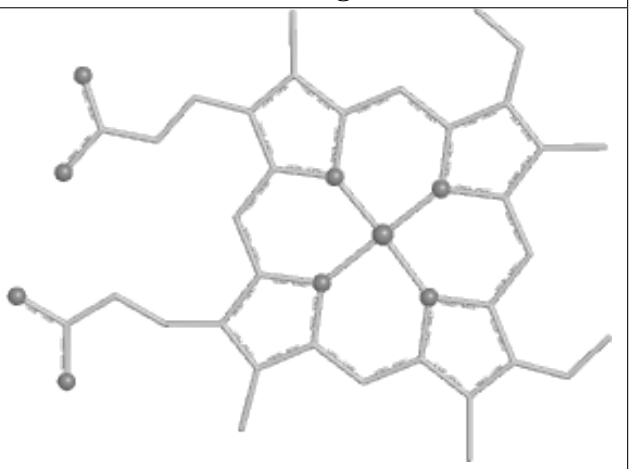
**Bond angles**



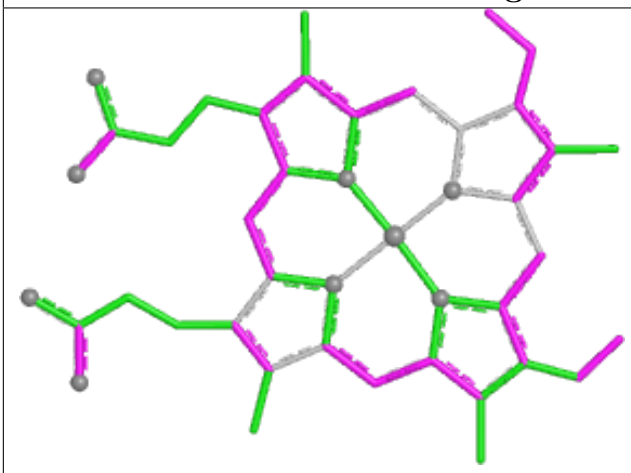
**Torsions**



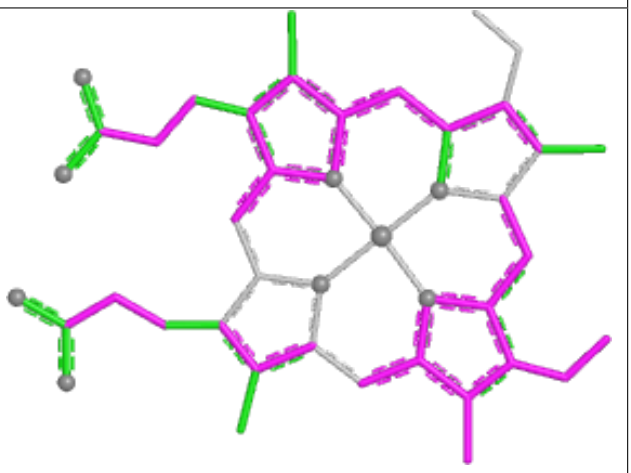
**Rings**

| Ligand HEM AN 402 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

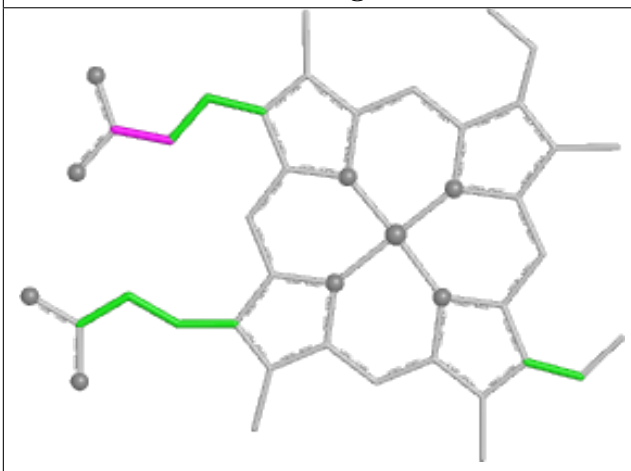
## Ligand HEM AO 301



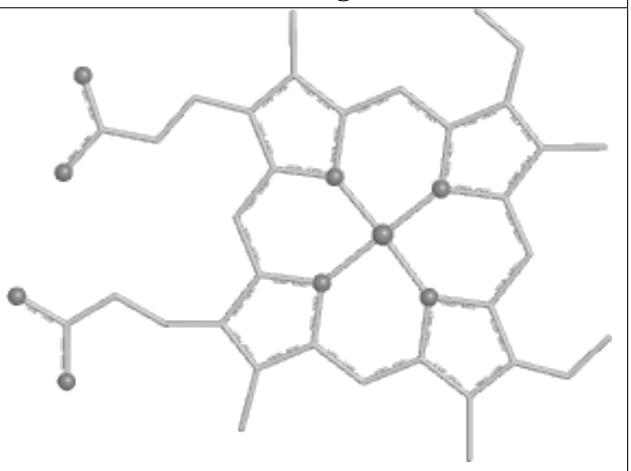
Bond lengths



Bond angles

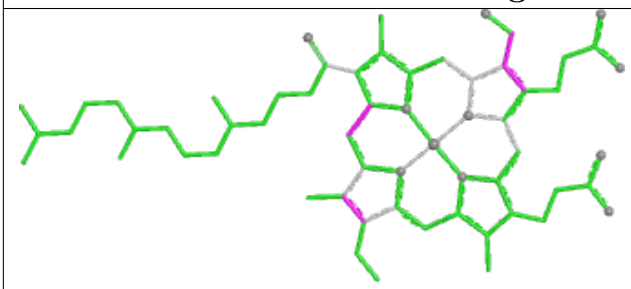


Torsions

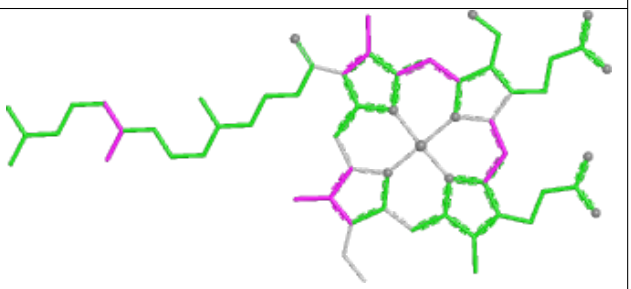


Rings

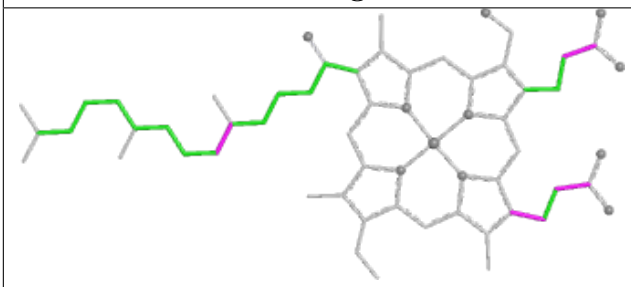
## Ligand HEA BN 603



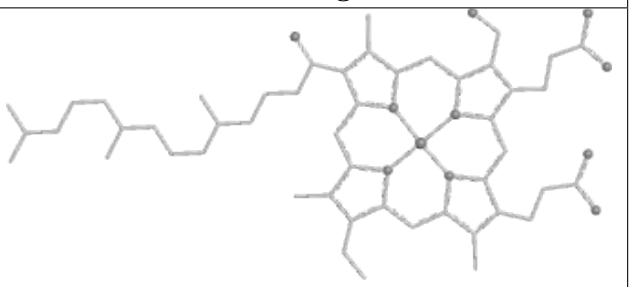
Bond lengths



Bond angles

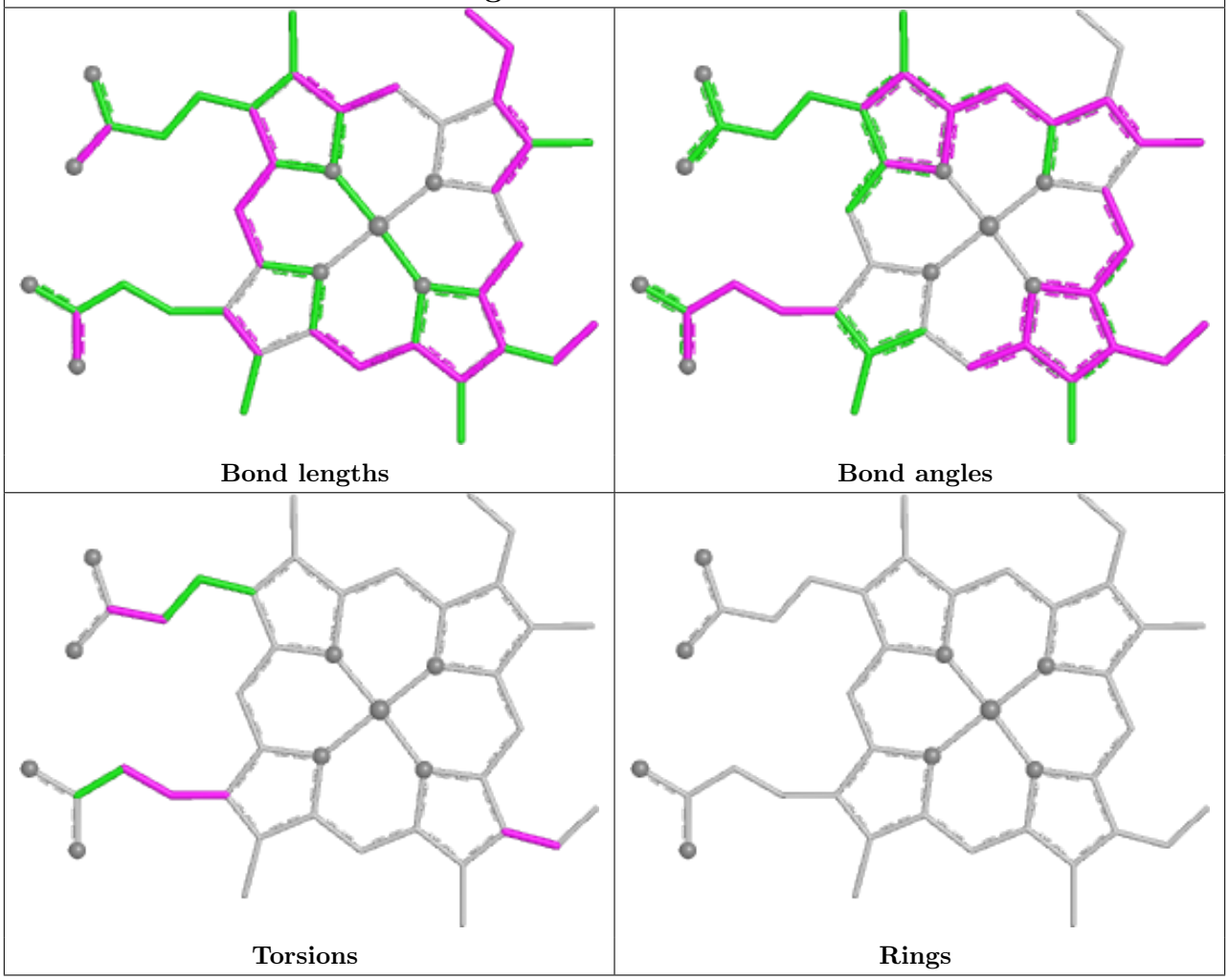


Torsions



Rings

**Ligand HEM AC 402**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 7 | G | 3 |
| 12 | L | 3 |
| 24 | X | 2 |
| 10 | J | 1 |
| 1 | A | 1 |
| 36 | k | 1 |
| 8 | H | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Number of breaks |
|---|---|---|
| 29 | c | 1 |
| 55 | AE | 1 |
| 55 | AP | 1 |
| 53 | AC | 1 |
| 53 | AN | 1 |

The worst 5 of 17 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | J | 107:UNK | C | 140:UNK | N | 31.95 |
| 1 | X | 250:UNK | C | 285:UNK | N | 27.39 |
| 1 | G | 632:UNK | C | 637:UNK | N | 21.00 |
| 1 | X | 185:UNK | C | 203:UNK | N | 20.68 |
| 1 | A | 37:UNK | C | 49:UNK | N | 20.22 |

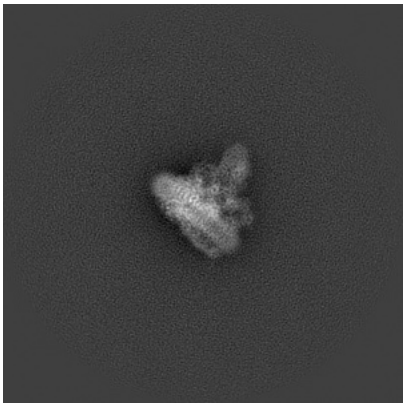
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8130. These allow visual inspection of the internal detail of the map and identification of artifacts.

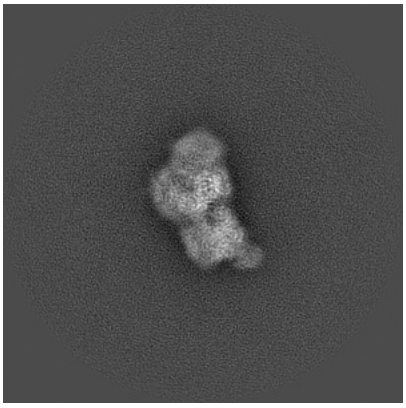
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

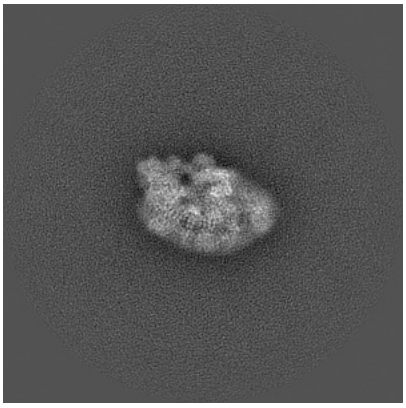
### 6.1.1 Primary map



X



Y

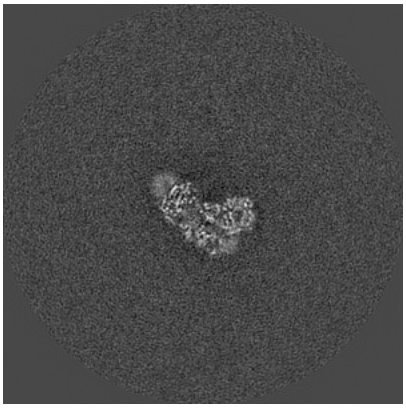


Z

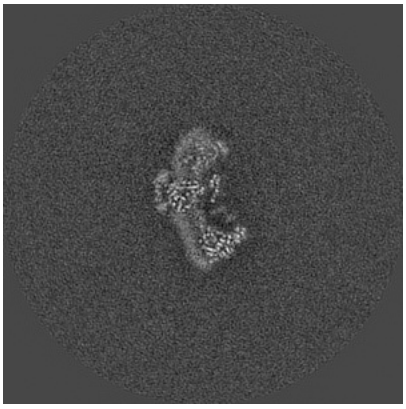
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

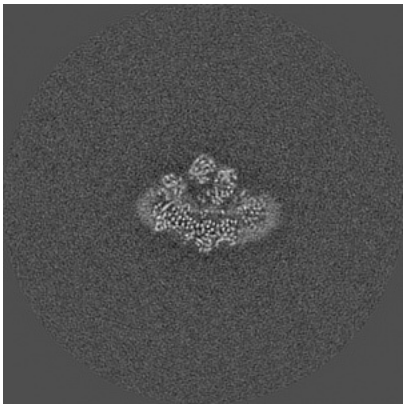
### 6.2.1 Primary map



X Index: 248



Y Index: 248

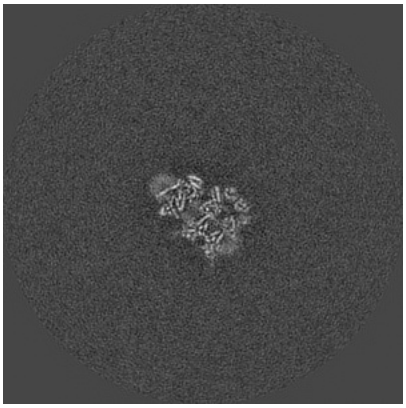


Z Index: 248

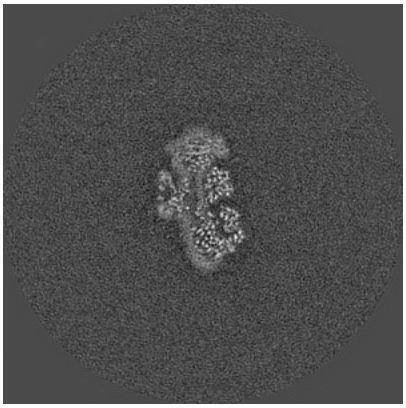
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

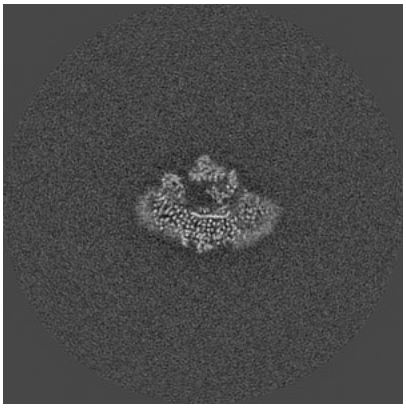
### 6.3.1 Primary map



X Index: 260



Y Index: 241



Z Index: 251

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 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

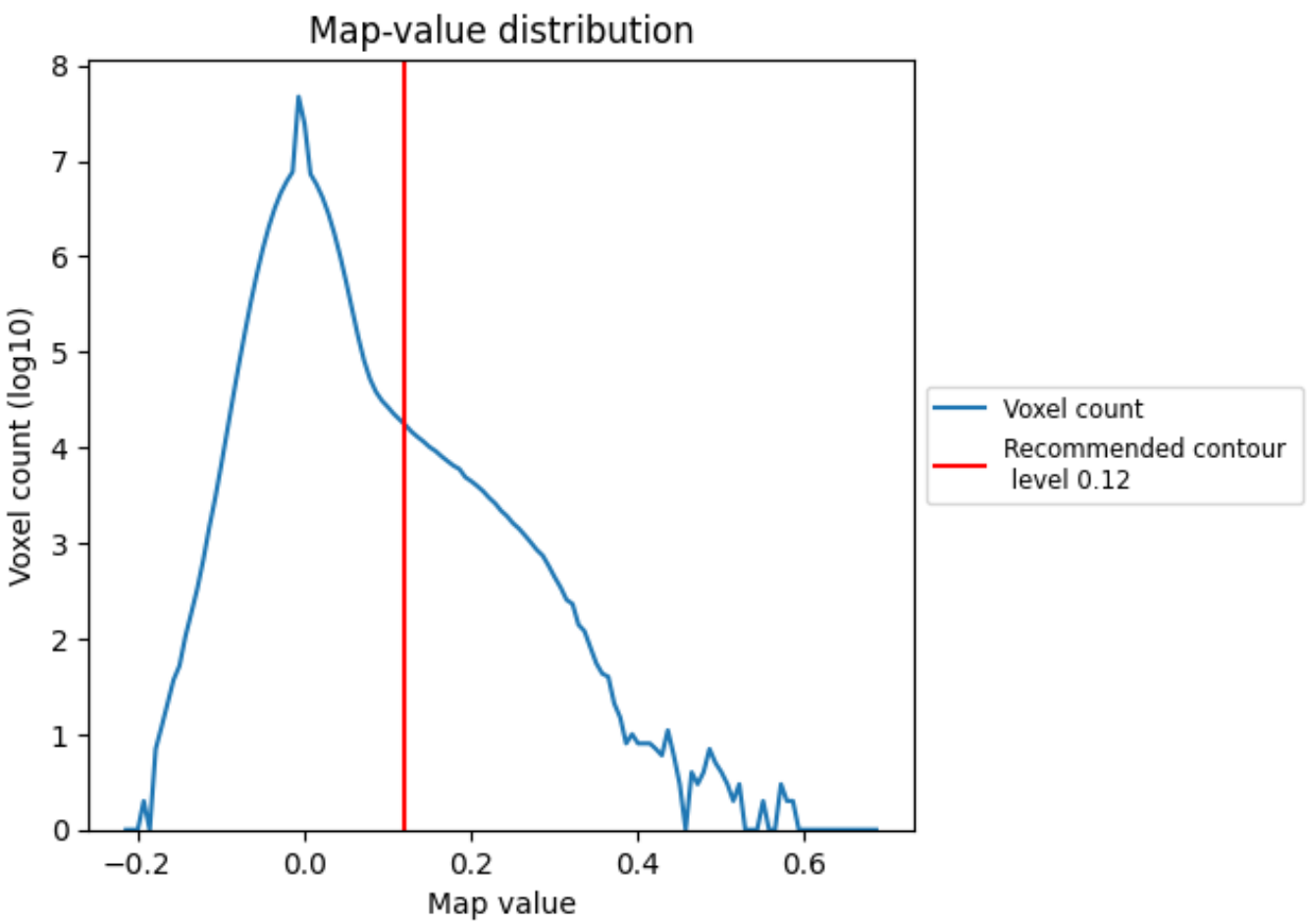
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

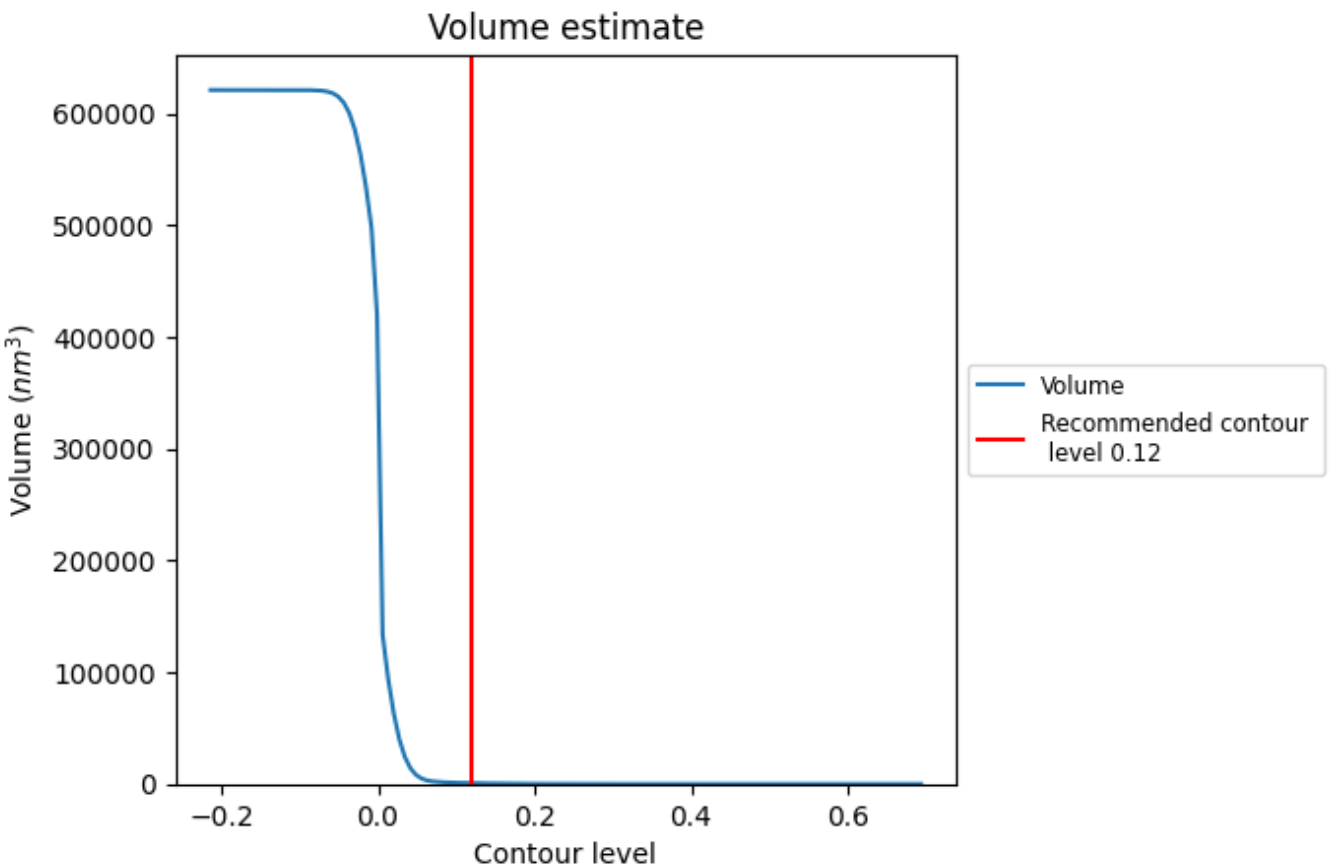
This section contains the results of statistical analysis of the map.

## 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.

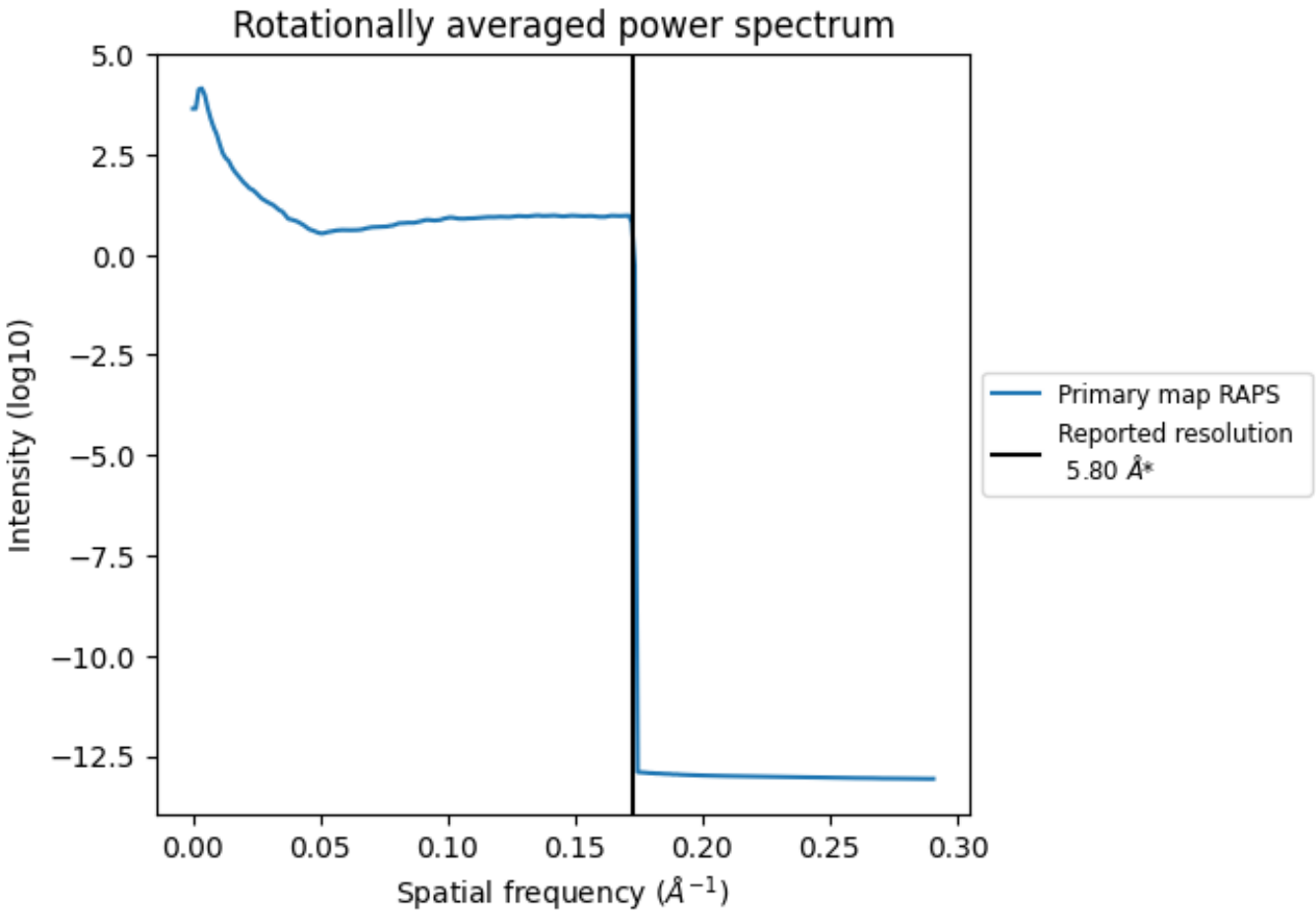
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 734 $nm^3$; this corresponds to an approximate mass of 663 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)

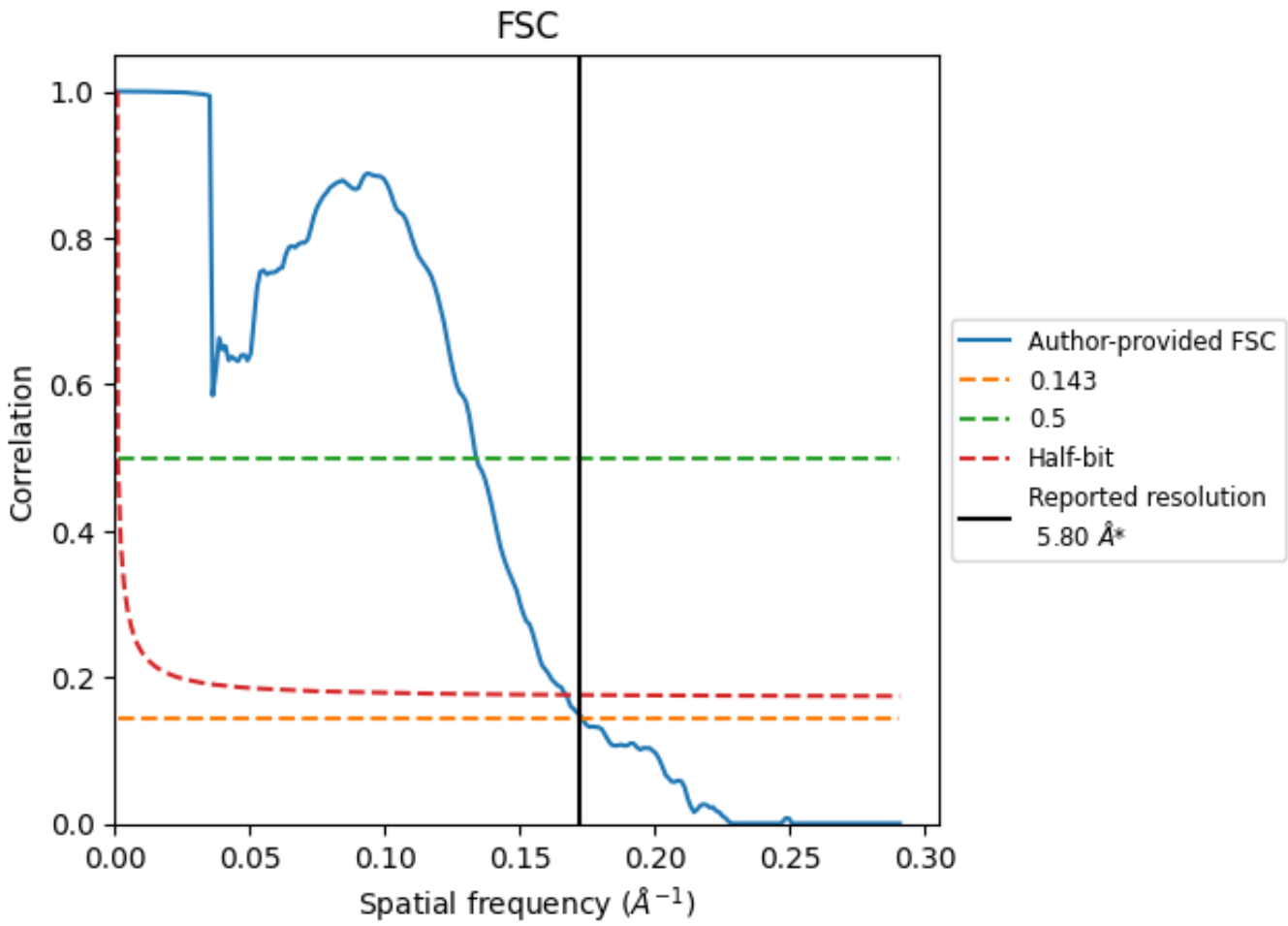



*Reported resolution corresponds to spatial frequency of 0.172 Å$^{-1}$

# 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 0.172 Å$^{-1}$

## 8.2 Resolution estimates (i)

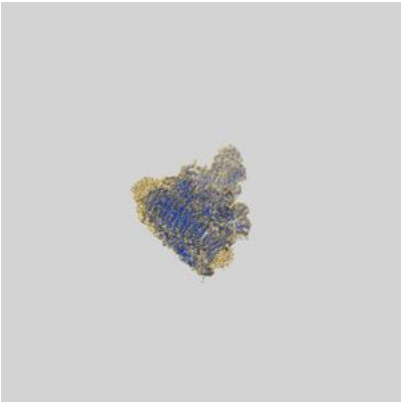
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 5.80 | - | - |
| Author-provided FSC curve | 5.78 | 7.47 | 5.99 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

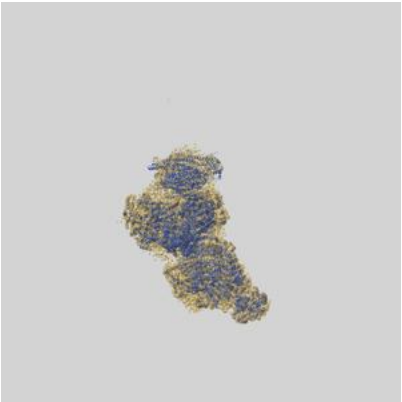
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8130 and PDB model 5J4Z. Per-residue inclusion information can be found in section 3 on page 25.

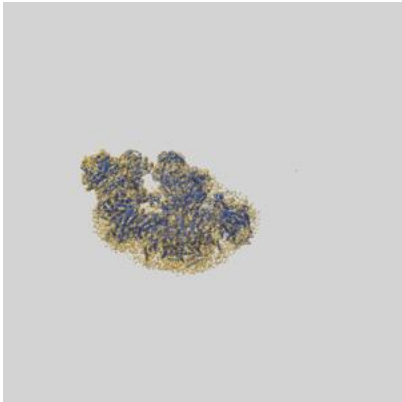
## 9.1 Map-model overlay (i)



X



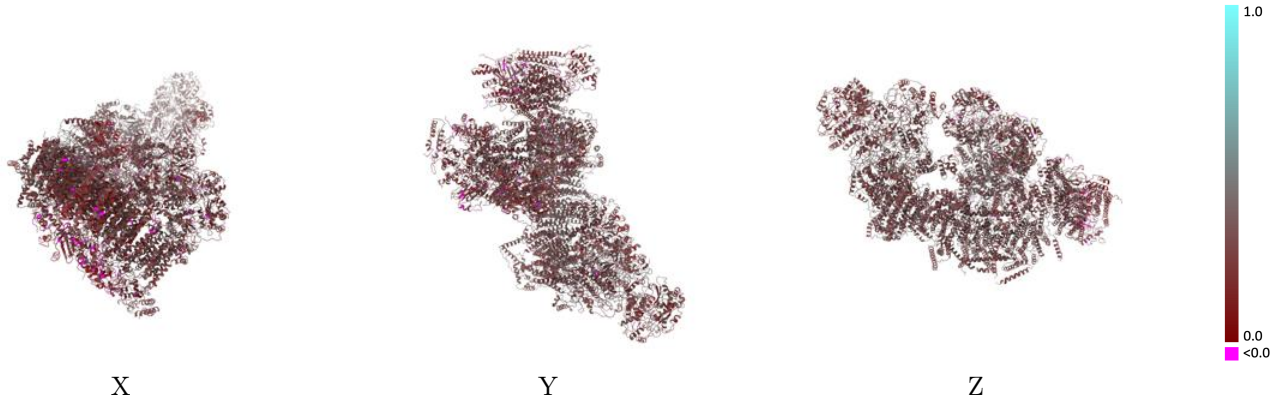
Y



Z

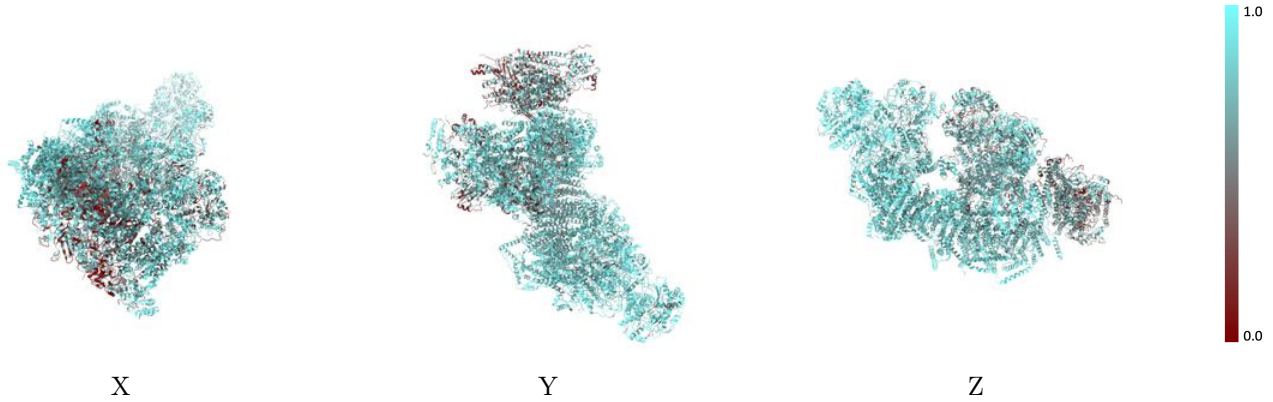
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



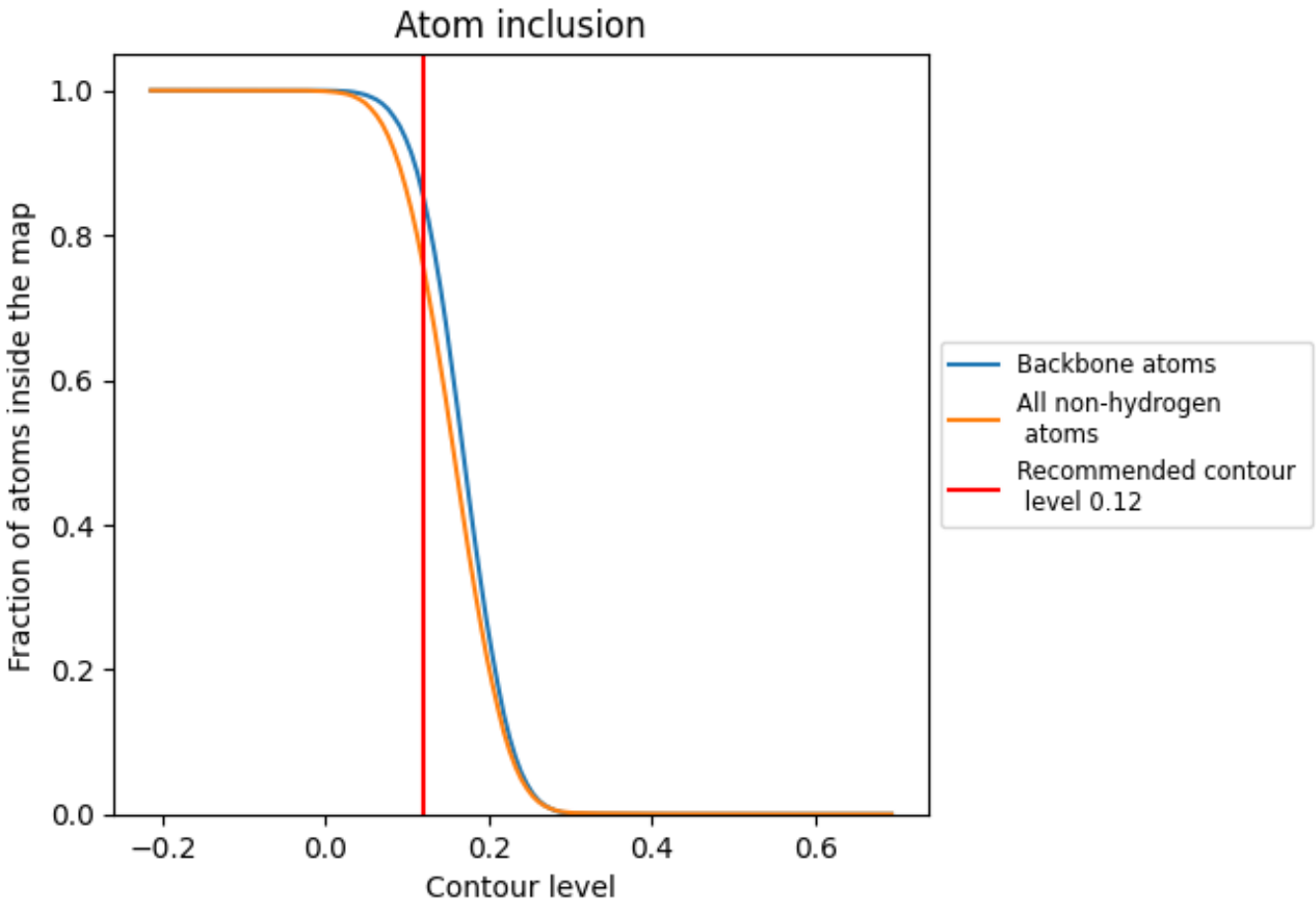

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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




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

## 9.4 Atom inclusion (i)




At the recommended contour level, 85% of all backbone atoms, 76% 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 (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7561 | 0.2980 |
| 0 | 0.8556 | 0.3200 |
| 1 | 0.8000 | 0.2910 |
| 2 | 0.8842 | 0.3430 |
| 3 | 0.8714 | 0.3510 |
| 4 | 0.8286 | 0.3190 |
| 5 | 0.8824 | 0.3480 |
| 6 | 0.9429 | 0.2940 |
| 7 | 0.9026 | 0.3310 |
| 8 | 0.9185 | 0.3200 |
| 9 | 0.8698 | 0.3540 |
| A | 0.7745 | 0.3360 |
| AA | 0.8085 | 0.2990 |
| AB | 0.7799 | 0.2980 |
| AC | 0.7942 | 0.3130 |
| AD | 0.7734 | 0.2920 |
| AE | 0.4171 | 0.1770 |
| AF | 0.7701 | 0.2920 |
| AG | 0.7951 | 0.3300 |
| AH | 0.8418 | 0.3030 |
| AI | 0.2776 | 0.2220 |
| AJ | 0.7205 | 0.2900 |
| AK | 0.7520 | 0.3290 |
| AL | 0.6934 | 0.2740 |
| AM | 0.6689 | 0.2720 |
| AN | 0.7726 | 0.3070 |
| AO | 0.7579 | 0.2850 |
| AP | 0.4985 | 0.2130 |
| AQ | 0.7989 | 0.2920 |
| AR | 0.7951 | 0.3170 |
| AS | 0.7761 | 0.2940 |
| AT | 0.2064 | 0.1870 |
| AU | 0.7239 | 0.2690 |
| AV | 0.5960 | 0.2880 |
| B | 0.8248 | 0.3180 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| BC | 0.5647 | 0.2490 |
| BD | 0.4874 | 0.2330 |
| BE | 0.5846 | 0.2190 |
| BG | 0.3617 | 0.2160 |
| BH | 0.3657 | 0.1910 |
| BI | 0.4515 | 0.2130 |
| BJ | 0.4331 | 0.2320 |
| BK | 0.4025 | 0.2040 |
| BL | 0.6150 | 0.2800 |
| BM | 0.5258 | 0.2510 |
| BN | 0.5774 | 0.2440 |
| BO | 0.4269 | 0.1880 |
| BP | 0.4636 | 0.2430 |
| C | 0.8680 | 0.3480 |
| D | 0.8365 | 0.3360 |
| E | 0.8604 | 0.3010 |
| F | 0.8493 | 0.2980 |
| G | 0.8152 | 0.3160 |
| H | 0.8202 | 0.3260 |
| I | 0.8510 | 0.3180 |
| J | 0.7885 | 0.3150 |
| K | 0.8344 | 0.3370 |
| L | 0.8264 | 0.3180 |
| M | 0.8334 | 0.3170 |
| N | 0.8301 | 0.3200 |
| O | 0.8615 | 0.3600 |
| P | 0.8706 | 0.3640 |
| Q | 0.9152 | 0.3270 |
| R | 0.7241 | 0.2980 |
| S | 0.8300 | 0.2820 |
| T | 0.8528 | 0.3200 |
| U | 0.8729 | 0.3360 |
| V | 0.8482 | 0.3400 |
| W | 0.9010 | 0.3260 |
| X | 0.7992 | 0.3140 |
| Y | 0.8571 | 0.3220 |
| Z | 0.7664 | 0.3160 |
| a | 0.8883 | 0.3690 |
| b | 0.8609 | 0.3290 |
| c | 0.7859 | 0.3130 |
| d | 0.8775 | 0.3410 |
| e | 0.8691 | 0.3370 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| f | 0.9310 | 0.3050 |
| g | 0.9185 | 0.3540 |
| h | 0.9079 | 0.3280 |
| i | 0.9229 | 0.3530 |
| j | 0.8727 | 0.3290 |
| k | 0.8775 | 0.3290 |
| t | 0.9000 | 0.3370 |
| u | 0.9625 | 0.4090 |
| v | 0.9667 | 0.3480 |
| w | 0.8917 | 0.3260 |
| x | 0.8923 | 0.3600 |
| y | 0.9174 | 0.3170 |
| z | 0.8846 | 0.3430 |