



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Apr 5, 2017 – 12:22 PM EDT

PDB ID : 5GPN
EMDB ID: : EMD-9534
Title : Architecture of mammalian respirasome
Authors : Gu, J.; Wu, M.; Guo, R.; Yang, M.
Deposited on : 2016-08-03
Resolution : 5.40 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

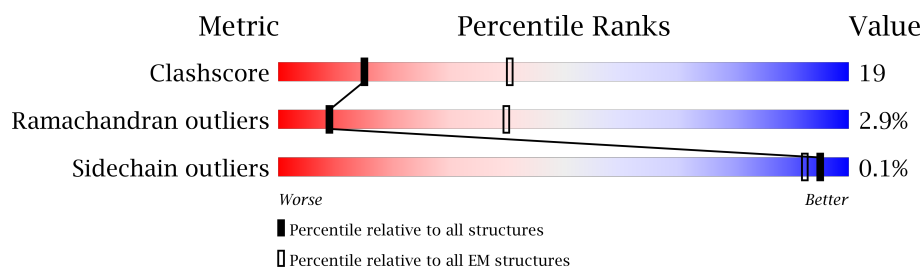
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 Å.

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
















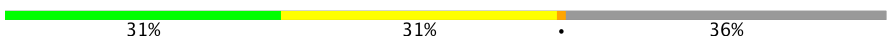






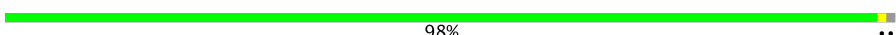
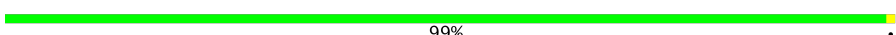



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 446 | |
| 1 | M | 446 | |
| 2 | B | 439 | |
| 2 | N | 439 | |
| 3 | C | 379 | |
| 3 | O | 379 | |
| 4 | D | 241 | |
| 4 | P | 241 | |
| 5 | E | 274 | |

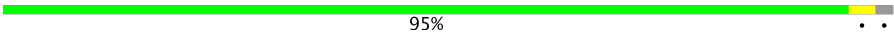









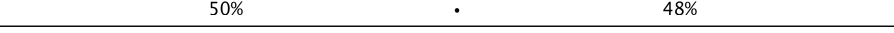
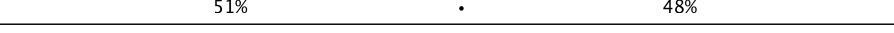
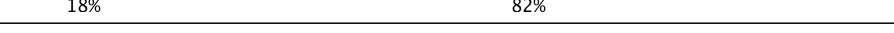


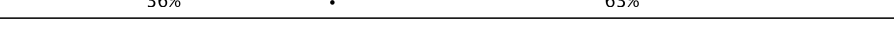
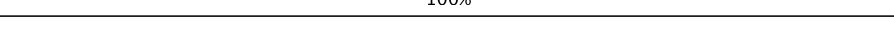
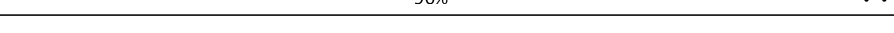
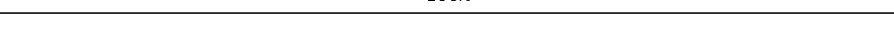






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | Q | 274 |  |
| 6 | F | 110 |  |
| 6 | R | 110 |  |
| 7 | G | 81 |  |
| 7 | S | 81 |  |
| 8 | H | 78 |  |
| 8 | T | 78 |  |
| 9 | I | 78 |  |
| 9 | U | 78 |  |
| 10 | J | 62 |  |
| 10 | L | 62 |  |
| 11 | K | 56 |  |
| 11 | V | 56 |  |
| 12 | W | 264 |  |
| 13 | Y | 727 |  |
| 14 | Z | 463 |  |
| 15 | a | 216 |  |
| 16 | b | 212 |  |
| 17 | c | 464 |  |
| 18 | d | 249 |  |
| 19 | e | 318 |  |
| 20 | f | 347 |  |
| 21 | g | 115 |  |
| 22 | h | 459 |  |
| 23 | i | 98 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 24 | j | 606 |  |
| 25 | k | 175 |  |
| 25 | l | 175 |  |
| 26 | m | 84 |  |
| 27 | n | 99 |  |
| 28 | o | 106 |  |
| 29 | p | 377 |  |
| 30 | q | 357 |  |
| 30 | v | 357 |  |
| 31 | r | 144 |  |
| 32 | Aa | 156 |  |
| 32 | t | 156 |  |
| 33 | Ai | 189 |  |
| 33 | u | 189 |  |
| 34 | w | 175 |  |
| 35 | x | 123 |  |
| 36 | 0 | 261 |  |
| 37 | 1 | 147 |  |
| 38 | 2 | 109 |  |
| 39 | 3 | 98 |  |
| 40 | 4 | 84 |  |
| 41 | 5 | 85 |  |
| 42 | 6 | 73 |  |
| 43 | 7 | 59 |  |
| 44 | 8 | 56 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 45 | 9 | 47 | 100% |
| 46 | s | 46 | 93% 7% |
| 47 | y | 514 | 99% . |
| 48 | z | 227 | 99% . |
| 49 | Ab | 134 | 96% . |
| 49 | Ah | 134 | 79% 21% |
| 50 | Ac | 70 | 76% . 21% |
| 51 | Ad | 43 | 100% |
| 51 | Ao | 43 | 95% 5% |
| 51 | Ap | 43 | 81% 19% |
| 51 | Av | 43 | 91% 9% |
| 52 | Ae | 116 | 74% . 24% |
| 53 | Af | 128 | 68% .. 30% |
| 54 | Ag | 141 | 87% 6% 7% |
| 55 | Aj | 176 | 72% . 24% |
| 56 | Ak | 178 | 80% . . 15% |
| 57 | Al | 122 | 75% . 21% |
| 58 | Am | 76 | 36% 64% |
| 59 | An | 172 | 55% . 44% |
| 60 | Aq | 76 | 88% 12% |
| 60 | As | 76 | 86% 14% |
| 60 | Aw | 76 | 100% |
| 61 | Ar | 34 | 100% |
| 62 | At | 17 | 100% |
| 63 | Au | 13 | 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 64 | HEM | C | 402 | - | - | X | - |
| 67 | SF4 | Y | 801 | - | - | X | - |
| 71 | HEA | y | 601 | X | - | - | - |
| 71 | HEA | y | 602 | X | - | - | - |

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 75545 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 1 | A | 446 | Total | C | N | O | 0 | 0 |
| | | | 2198 | 1306 | 446 | 446 | | |
| 1 | M | 446 | Total | C | N | O | 0 | 0 |
| | | | 2198 | 1306 | 446 | 446 | | |

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 2 | B | 419 | Total | C | N | O | 0 | 0 |
| | | | 2061 | 1223 | 419 | 419 | | |
| 2 | N | 419 | Total | C | N | O | 0 | 0 |
| | | | 2061 | 1223 | 419 | 419 | | |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 3 | C | 379 | Total | C | N | O | 0 | 0 |
| | | | 1870 | 1112 | 379 | 379 | | |
| 3 | O | 379 | Total | C | N | O | 0 | 0 |
| | | | 1870 | 1112 | 379 | 379 | | |

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 4 | D | 241 | Total | C | N | O | 0 | 0 |
| | | | 1188 | 706 | 241 | 241 | | |
| 4 | P | 241 | Total | C | N | O | 0 | 0 |
| | | | 1188 | 706 | 241 | 241 | | |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5 | E | 196 | Total | C | N | O | 0 | 0 |
| | | | 967 | 575 | 196 | 196 | | |
| 5 | Q | 196 | Total | C | N | O | 0 | 0 |
| | | | 966 | 574 | 196 | 196 | | |

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6 | F | 106 | Total | C | N | O | 0 | 0 |
| | | | 527 | 315 | 106 | 106 | | |
| 6 | R | 106 | Total | C | N | O | 0 | 0 |
| | | | 527 | 315 | 106 | 106 | | |

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 7 | G | 81 | Total | C | N | O | 0 | 0 |
| | | | 401 | 239 | 81 | 81 | | |
| 7 | S | 78 | Total | C | N | O | 0 | 0 |
| | | | 386 | 230 | 78 | 78 | | |

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 8 | H | 64 | Total | C | N | O | 0 | 0 |
| | | | 320 | 192 | 64 | 64 | | |
| 8 | T | 64 | Total | C | N | O | 0 | 0 |
| | | | 320 | 192 | 64 | 64 | | |

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 9 | I | 33 | Total | C | N | O | 0 | 0 |
| | | | 163 | 97 | 33 | 33 | | |
| 9 | U | 33 | Total | C | N | O | 0 | 0 |
| | | | 163 | 97 | 33 | 33 | | |

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10 | J | 62 | Total | C | N | O | 0 | 0 |
| | | | 307 | 183 | 62 | 62 | | |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10 | L | 62 | Total | C | N | O | 0 | 0 |
| | | | 307 | 183 | 62 | 62 | | |

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11 | K | 43 | Total | C | N | O | 0 | 0 |
| | | | 211 | 125 | 43 | 43 | | |
| 11 | V | 37 | Total | C | N | O | 0 | 0 |
| | | | 182 | 108 | 37 | 37 | | |

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | W | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1366 | 884 | 234 | 246 | 2 | | |

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13 | Y | 672 | Total | C | N | O | S | 0 | 0 |
| | | | 4998 | 3128 | 874 | 958 | 38 | | |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | Z | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 3003 | 1917 | 515 | 548 | 23 | | |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15 | a | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1146 | 730 | 204 | 198 | 14 | | |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16 | b | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1189 | 746 | 205 | 228 | 10 | | |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17 | c | 410 | Total | C | N | O | S | 0 | 0 |
| | | | 3125 | 1974 | 558 | 573 | 20 | | |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | d | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1324 | 852 | 218 | 245 | 9 | | |

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19 | e | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2486 | 1665 | 381 | 419 | 21 | | |

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20 | f | 346 | Total | C | N | O | S | 0 | 0 |
| | | | 2698 | 1774 | 418 | 461 | 45 | | |

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | g | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 829 | 559 | 120 | 144 | 6 | | |

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22 | h | 457 | Total | C | N | O | S | 0 | 0 |
| | | | 3610 | 2396 | 570 | 606 | 38 | | |

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23 | i | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 677 | 448 | 101 | 115 | 13 | | |

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24 | j | 594 | Total | C | N | O | S | 0 | 0 |
| | | | 4705 | 3120 | 729 | 807 | 49 | | |

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 25 | k | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1059 | 712 | 152 | 183 | 12 | | |
| 25 | l | 15 | Total | C | N | O | | 0 | 0 |
| | | | 73 | 43 | 15 | 15 | | | |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 26 | m | 53 | Total | C | N | O | 0 | 0 |
| | | | 263 | 157 | 53 | 53 | | |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 27 | n | 83 | Total | C | N | O | 0 | 0 |
| | | | 411 | 245 | 83 | 83 | | |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28 | o | 51 | Total | C | N | O | 0 | 0 |
| | | | 251 | 149 | 51 | 51 | | |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 29 | p | 314 | Total | C | N | O | 0 | 0 |
| | | | 1546 | 918 | 314 | 314 | | |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 30 | q | 196 | Total | C | N | O | 0 | 0 |
| | | | 967 | 575 | 196 | 196 | | |
| 30 | v | 51 | Total | C | N | O | 0 | 0 |
| | | | 252 | 150 | 51 | 51 | | |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 31 | r | 63 | Total | C | N | O | 0 | 0 |
| | | | 311 | 185 | 63 | 63 | | |

- Molecule 32 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 32 | t | 81 | Total | C | N | O | 0 | 0 |
| | | | 403 | 241 | 81 | 81 | | |
| 32 | Aa | 81 | Total | C | N | O | 0 | 0 |
| | | | 403 | 241 | 81 | 81 | | |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 33 | u | 54 | Total | C | N | O | 0 | 0 |
| | | | 267 | 159 | 54 | 54 | | |
| 33 | Ai | 34 | Total | C | N | O | 0 | 0 |
| | | | 167 | 99 | 34 | 34 | | |

- Molecule 34 is a protein called Mitochondrial NADH dehydrogenase Fe-S protein 4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 34 | w | 107 | Total | C | N | O | 0 | 0 |
| | | | 530 | 316 | 107 | 107 | | |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 35 | x | 46 | Total | C | N | O | 0 | 0 |
| | | | 221 | 129 | 46 | 46 | | |

- Molecule 36 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 36 | 0 | 261 | Total | C | N | O | 0 | 0 |
| | | | 1284 | 762 | 261 | 261 | | |

- Molecule 37 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 37 | 1 | 144 | Total | C | N | O | 0 | 0 |
| | | | 716 | 428 | 144 | 144 | | |

- Molecule 38 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 38 | 2 | 109 | Total | C | N | O | 0 | 0 |
| | | | 539 | 321 | 109 | 109 | | |

- Molecule 39 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 39 | 3 | 98 | Total | C | N | O | 0 | 0 |
| | | | 481 | 285 | 98 | 98 | | |

- Molecule 40 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 40 | 4 | 84 | Total | C | N | O | 0 | 0 |
| | | | 411 | 243 | 84 | 84 | | |

- Molecule 41 is a protein called Cytochrome c oxidase subunit 6B1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 41 | 5 | 75 | Total | C | N | O | 0 | 0 |
| | | | 371 | 221 | 75 | 75 | | |

- Molecule 42 is a protein called Cytochrome c oxidase subunit 6C.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 42 | 6 | 73 | Total | C | N | O | 0 | 0 |
| | | | 361 | 215 | 73 | 73 | | |

- Molecule 43 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 43 | 7 | 56 | Total | C | N | O | 0 | 0 |
| | | | 274 | 162 | 56 | 56 | | |

- Molecule 44 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 44 | 8 | 49 | Total | C | N | O | 0 | 0 |
| | | | 241 | 143 | 49 | 49 | | |

- Molecule 45 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 45 | 9 | 47 | Total | C | N | O | 0 | 0 |
| | | | 231 | 137 | 47 | 47 | | |

- Molecule 46 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 46 | s | 43 | Total | C | N | O | 0 | 0 |
| | | | 213 | 127 | 43 | 43 | | |

- Molecule 47 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 47 | y | 514 | Total | C | N | O | 0 | 0 |
| | | | 2523 | 1495 | 514 | 514 | | |

- Molecule 48 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 48 | z | 227 | Total | C | N | O | 0 | 0 |
| | | | 1127 | 673 | 227 | 227 | | |

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 49 | Ab | 129 | Total | C | N | O | 0 | 0 |
| | | | 637 | 379 | 129 | 129 | | |
| 49 | Ah | 106 | Total | C | N | O | 0 | 0 |
| | | | 526 | 314 | 106 | 106 | | |

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 50 | Ac | 55 | Total | C | N | O | 0 | 0 |
| | | | 271 | 161 | 55 | 55 | | |

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 51 | Ad | 43 | Total | C | N | O | 0 | 0 |
| | | | 211 | 125 | 43 | 43 | | |
| 51 | Ao | 41 | Total | C | N | O | 0 | 0 |
| | | | 205 | 123 | 41 | 41 | | |
| 51 | Ap | 35 | Total | C | N | O | 0 | 0 |
| | | | 173 | 103 | 35 | 35 | | |
| 51 | Av | 39 | Total | C | N | O | 0 | 0 |
| | | | 193 | 115 | 39 | 39 | | |

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52 | Ae | 88 | Total | C | N | O | 0 | 0 |
| | | | 435 | 259 | 88 | 88 | | |

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 53 | Af | 90 | Total | C | N | O | 0 | 0 |
| | | | 448 | 268 | 90 | 90 | | |

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 54 | Ag | 131 | Total | C | N | O | 0 | 0 |
| | | | 637 | 375 | 131 | 131 | | |

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 55 | Aj | 133 | Total | C | N | O | 0 | 0 |
| | | | 663 | 397 | 133 | 133 | | |

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 56 | Ak | 151 | Total | C | N | O | 0 | 0 |
| | | | 750 | 448 | 151 | 151 | | |

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 57 | Al | 96 | Total | C | N | O | 0 | 0 |
| | | | 473 | 281 | 96 | 96 | | |

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 58 | Am | 27 | Total | C | N | O | 0 | 0 |
| | | | 134 | 80 | 27 | 27 | | |

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 59 | An | 97 | Total | C | N | O | 0 | 0 |
| | | | 482 | 288 | 97 | 97 | | |

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 60 | Aq | 67 | Total | C | N | O | 0 | 0 |
| | | | 335 | 201 | 67 | 67 | | |
| 60 | As | 65 | Total | C | N | O | 0 | 0 |
| | | | 322 | 192 | 65 | 65 | | |
| 60 | Aw | 76 | Total | C | N | O | 0 | 0 |
| | | | 376 | 224 | 76 | 76 | | |

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 61 | Ar | 34 | Total | C | N | O | 0 | 0 |
| | | | 169 | 101 | 34 | 34 | | |

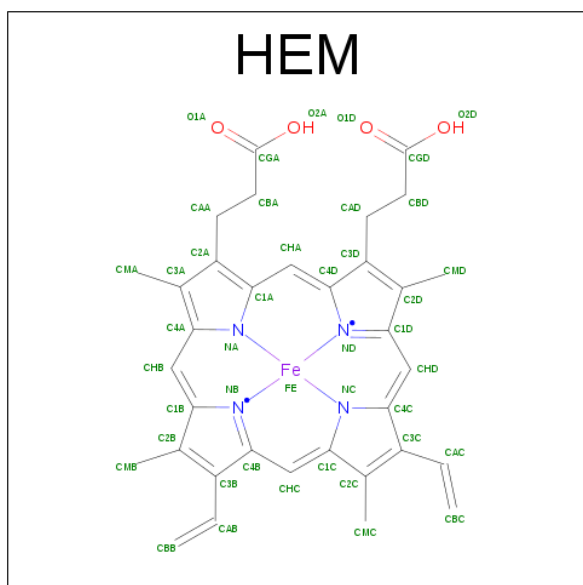
- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 62 | At | 17 | Total | C | N | O | 0 | 0 |
| | | | 84 | 50 | 17 | 17 | | |

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 63 | Au | 13 | Total | C | N | O | 0 | 0 |
| | | | 62 | 36 | 13 | 13 | | |

- Molecule 64 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



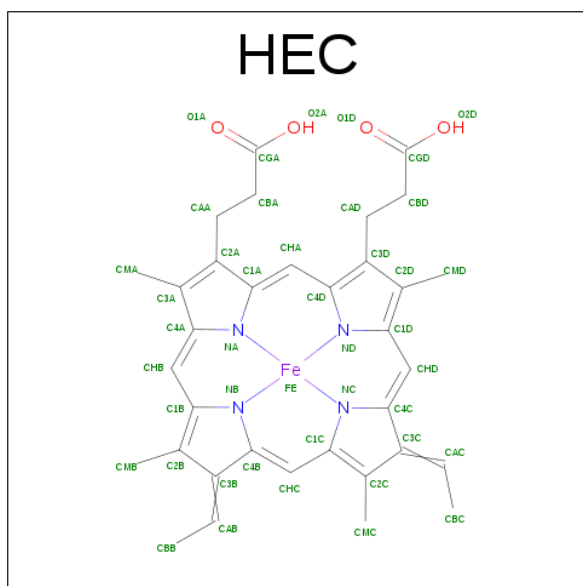
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 64 | C | 1 | Total | C | Fe | N | O | 0 |
| | | | 86 | 68 | 2 | 8 | 8 | |
| 64 | C | 1 | Total | C | Fe | N | O | 0 |
| | | | 86 | 68 | 2 | 8 | 8 | |
| 64 | O | 1 | Total | C | Fe | N | O | 0 |
| | | | 86 | 68 | 2 | 8 | 8 | |

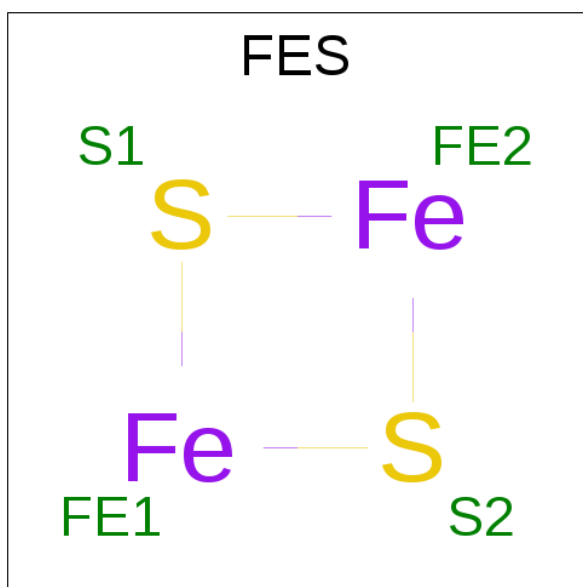
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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 64 | O | 1 | Total | C | Fe | N | O | 0 |
| | | | 86 | 68 | 2 | 8 | 8 | |

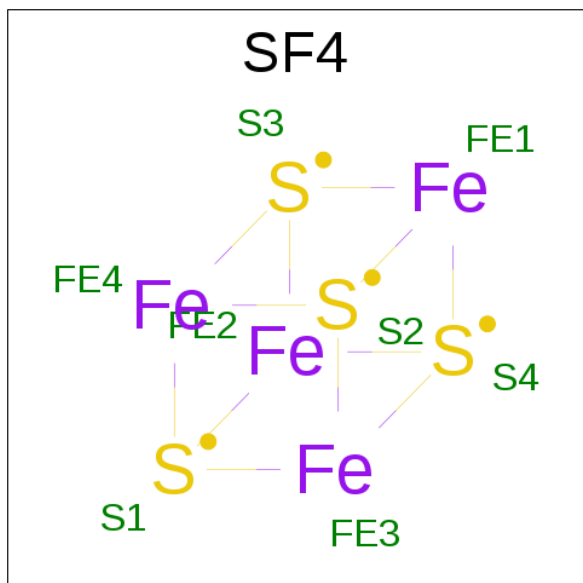
- Molecule 65 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).





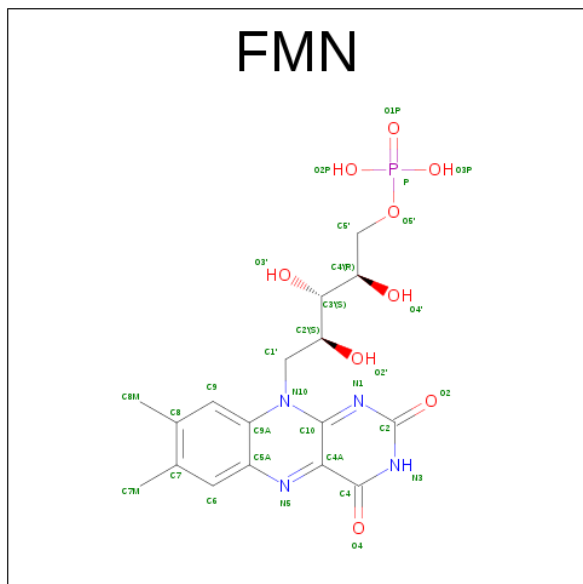
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 66 | E | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 66 | Q | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 66 | Y | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 66 | d | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 67 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



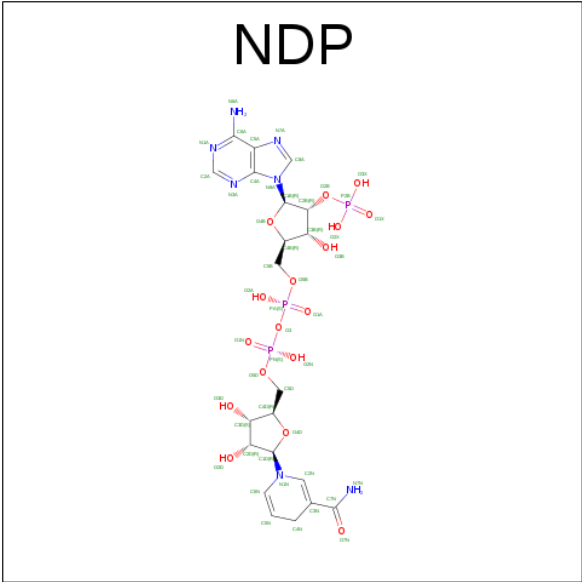
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 67 | Y | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 67 | Y | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 67 | a | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 67 | b | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 67 | b | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 67 | c | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 68 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 68 | c | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

- Molecule 69 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

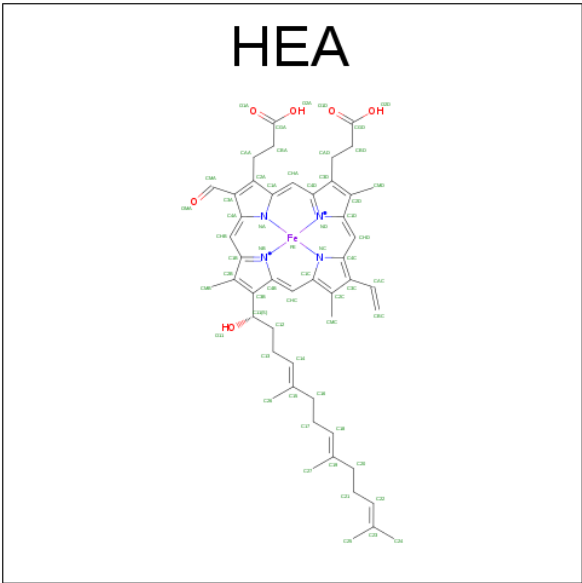


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | p | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 70 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 70 | 3 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 71 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|----|---------|
| 71 | y | 1 | Total | C | Fe | N | O | 0 |
| | | | 120 | 98 | 2 | 8 | 12 | |
| 71 | y | 1 | Total | C | Fe | N | O | 0 |
| | | | 120 | 98 | 2 | 8 | 12 | |

- Molecule 72 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 72 | z | 2 | Total | Cu | 0 |
| | | | 2 | 2 | |
| 72 | y | 1 | Total | Cu | 0 |
| | | | 1 | 1 | |

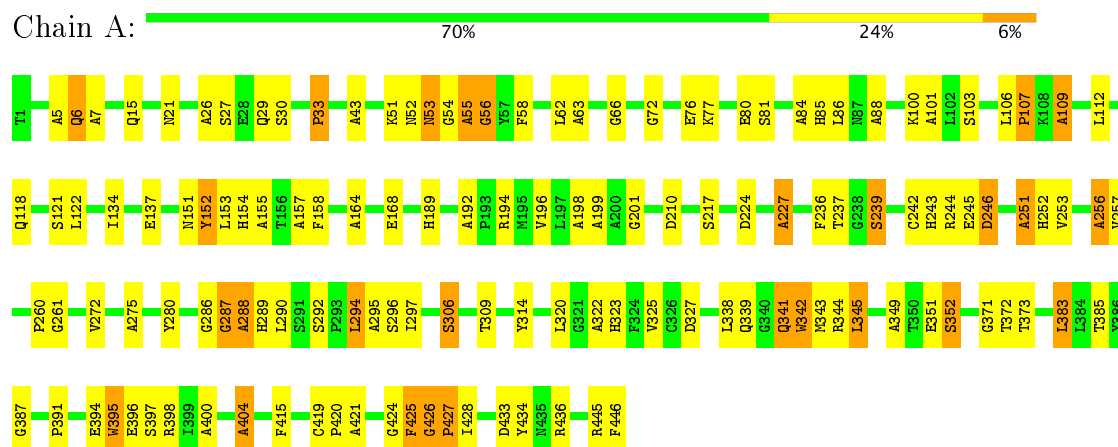
- Molecule 73 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 73 | y | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

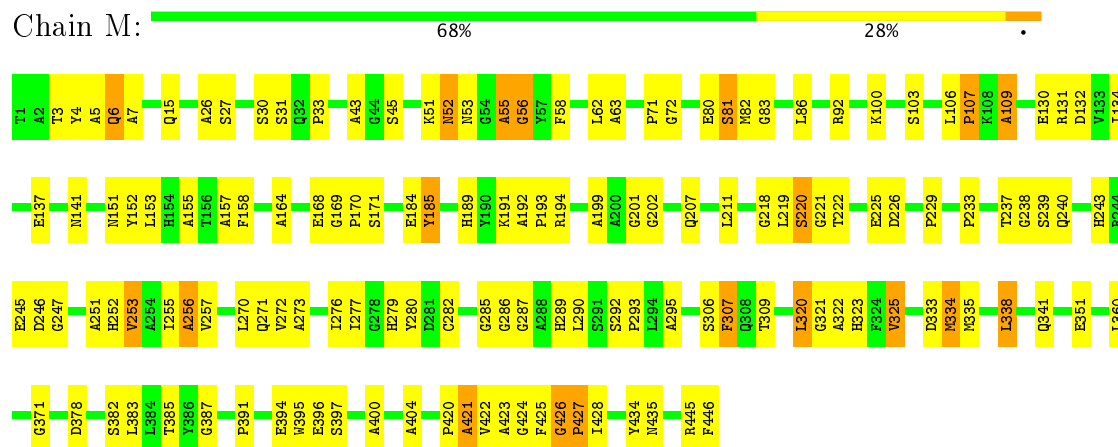
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

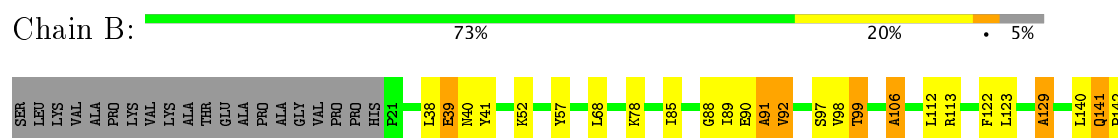
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

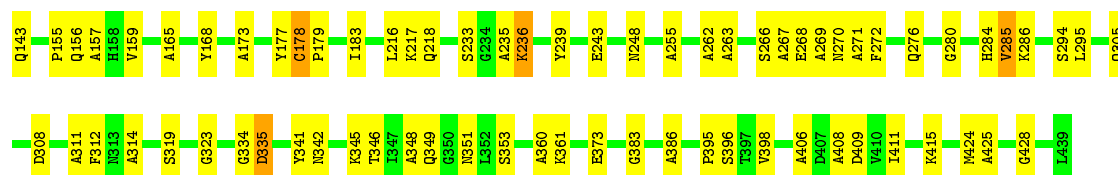


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

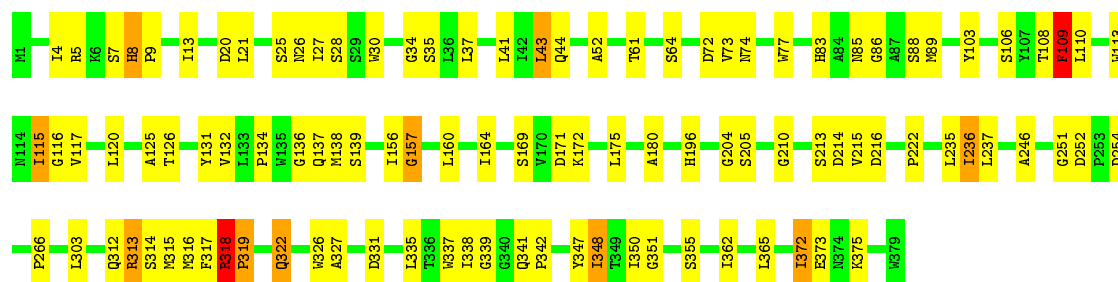




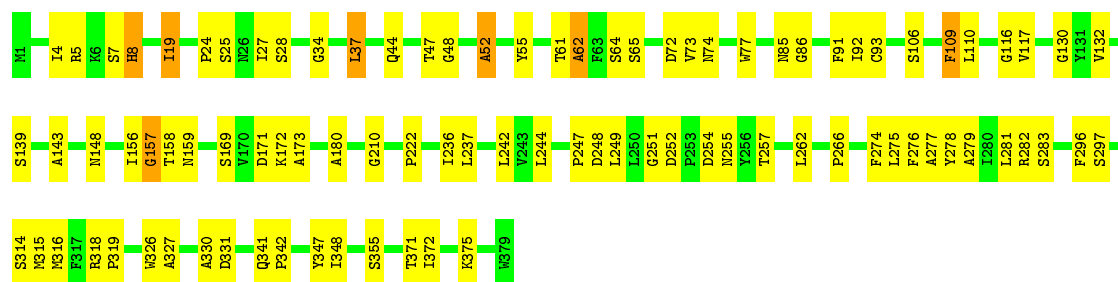
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 3: Cytochrome b



- Molecule 3: Cytochrome b

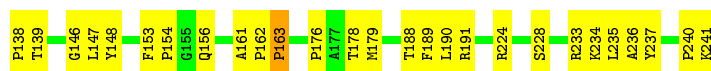
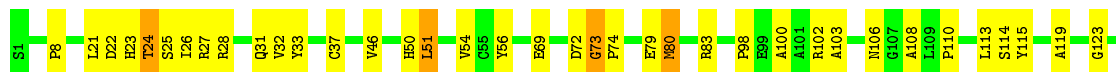


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

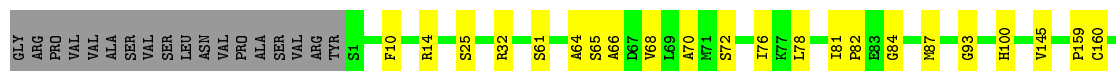




- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



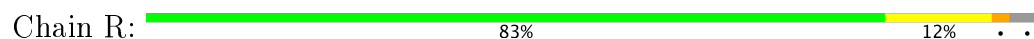
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 7

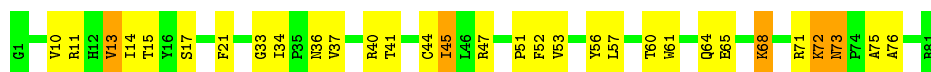


- Molecule 6: Cytochrome b-c1 complex subunit 7

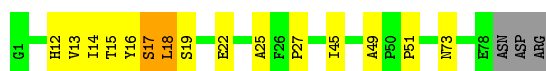
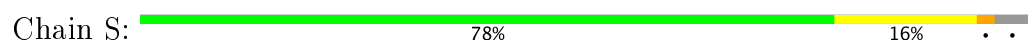




- Molecule 7: Cytochrome b-c1 complex subunit 8



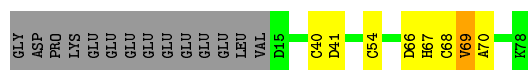
- Molecule 7: Cytochrome b-c1 complex subunit 8



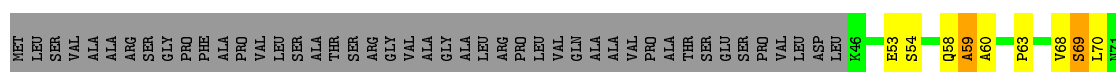
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



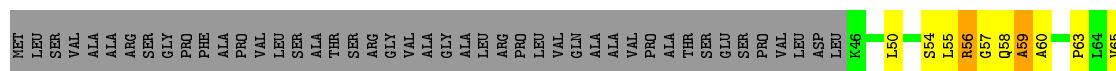
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial




- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain J:  74% 21% 5%



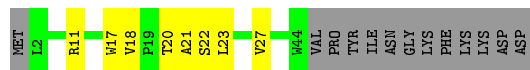
- Molecule 10: Cytochrome b-c1 complex subunit 9

Chain L:  66% 26% 8%



- Molecule 11: Cytochrome b-c1 complex subunit 10

Chain K:  63% 14% 23%



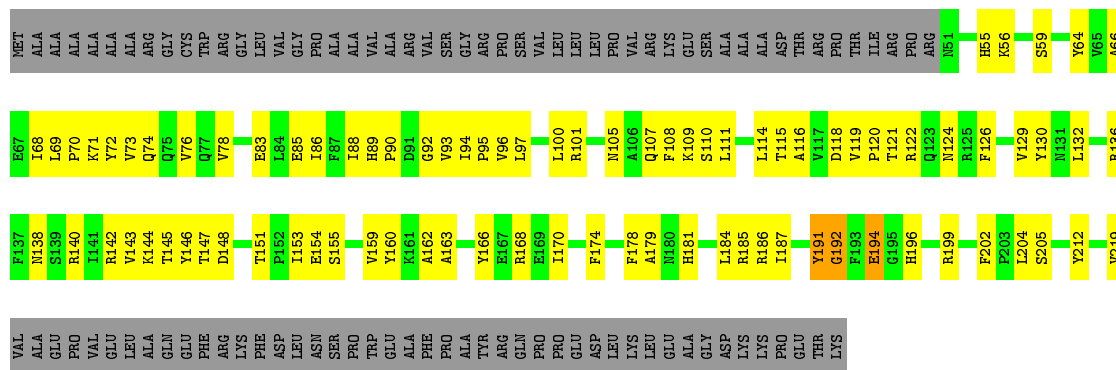
- Molecule 11: Cytochrome b-c1 complex subunit 10

Chain V:  57% 9% 34%



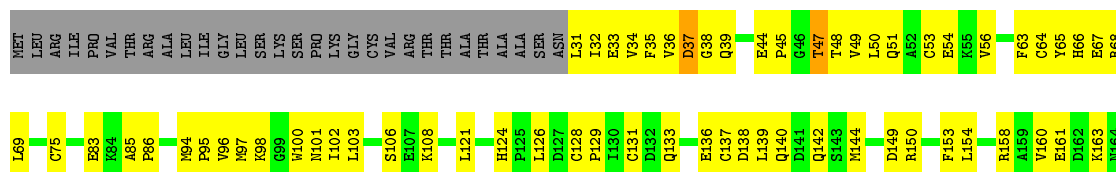
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

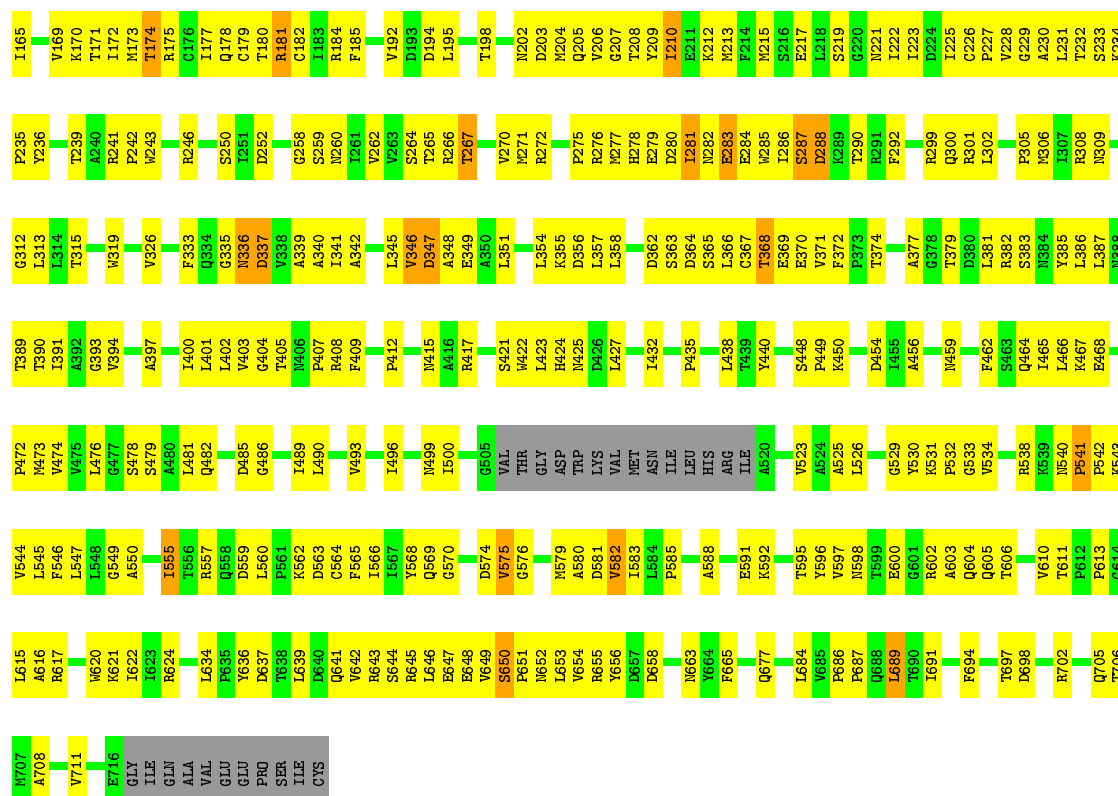
Chain W:  31% 31% 36%



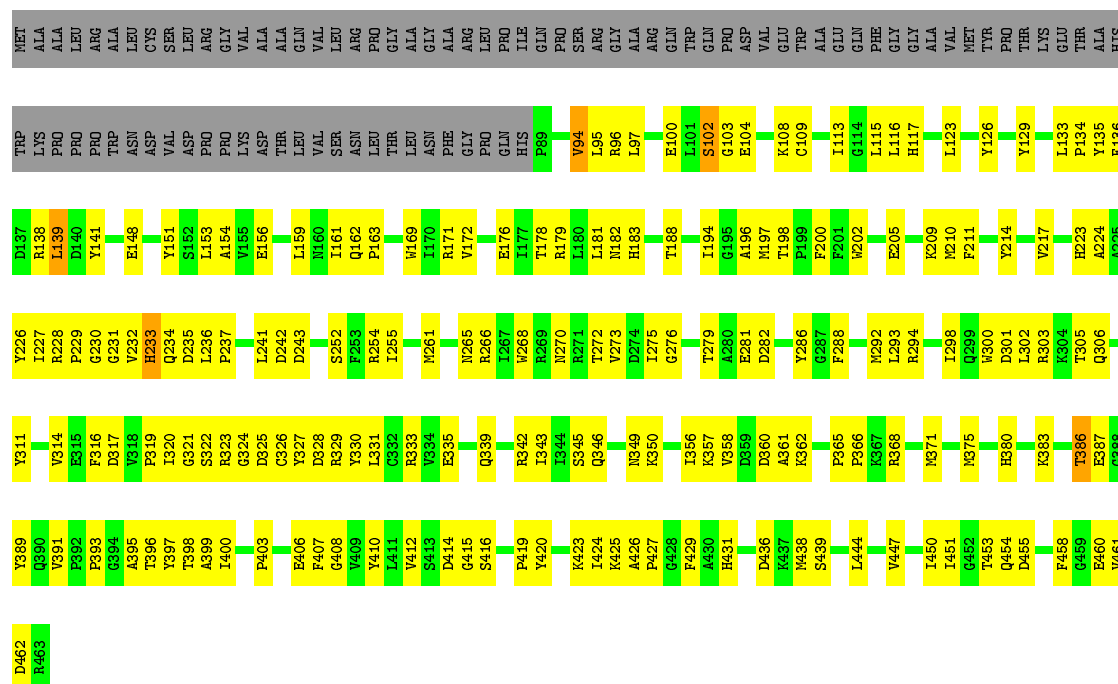
- Molecule 13: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain Y:  44% 46% 8%

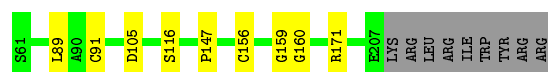




- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2



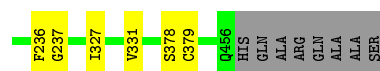
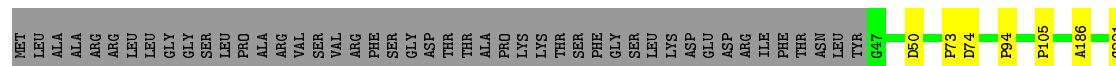
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7



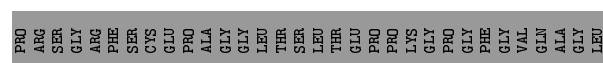
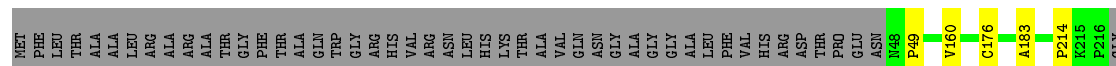
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8



- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 18: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 19: NADH-ubiquinone oxidoreductase chain 1

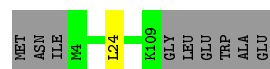


- Molecule 20: NADH-ubiquinone oxidoreductase chain 2



- Molecule 21: NADH-ubiquinone oxidoreductase chain 3

Chain g: 91% • 8%



- Molecule 22: NADH-ubiquinone oxidoreductase chain 4

Chain h: 97%



- Molecule 23: NADH-ubiquinone oxidoreductase chain 4L

Chain i: 90% • 8%



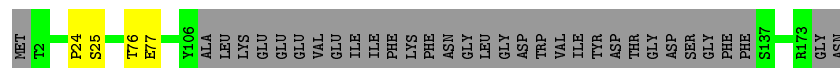
- Molecule 24: NADH-ubiquinone oxidoreductase chain 5

Chain j:  95%



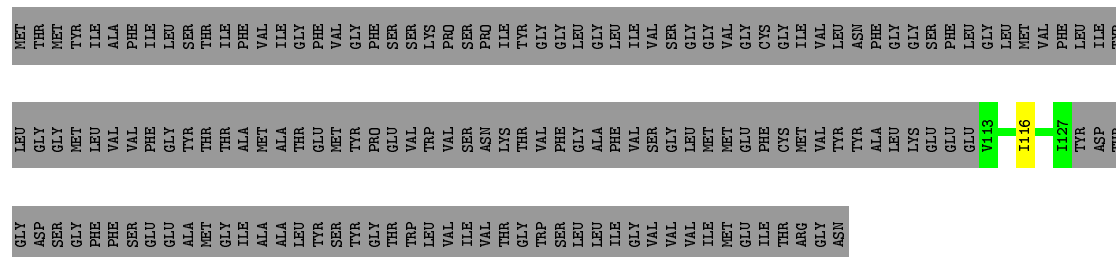
- Molecule 25: NADH-ubiquinone oxidoreductase chain 6

Chain k: 79% 19%



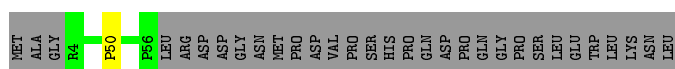
- Molecule 25: NADH-ubiquinone oxidoreductase chain 6

Chain 1:  8% 91%

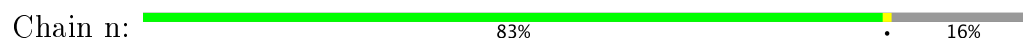


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain m: 62% . 37%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9

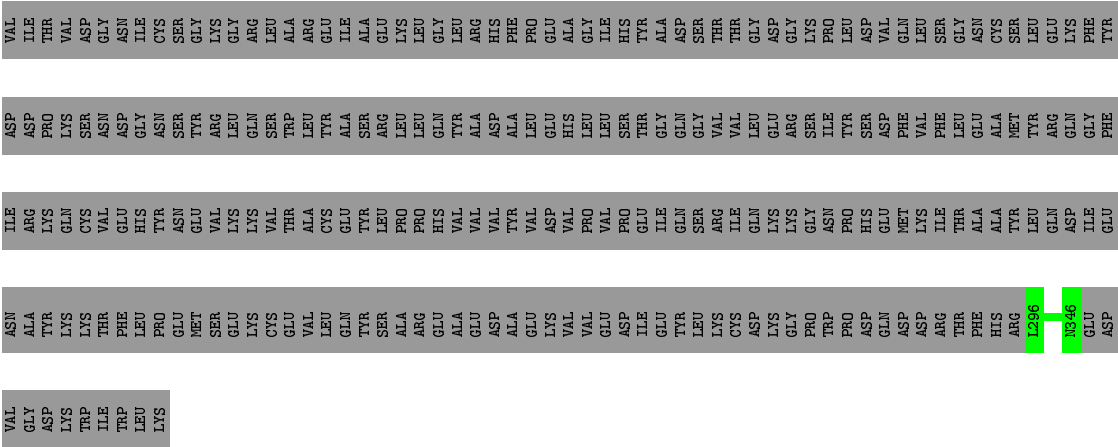


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

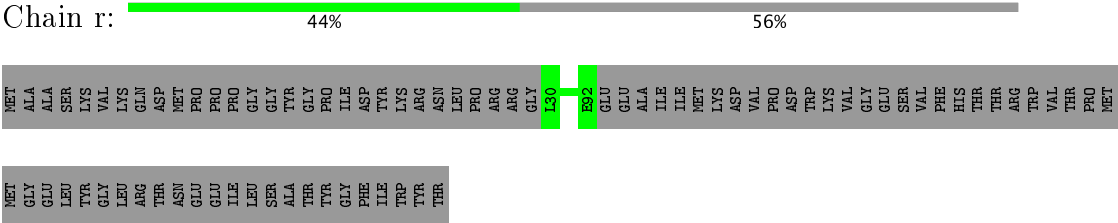


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

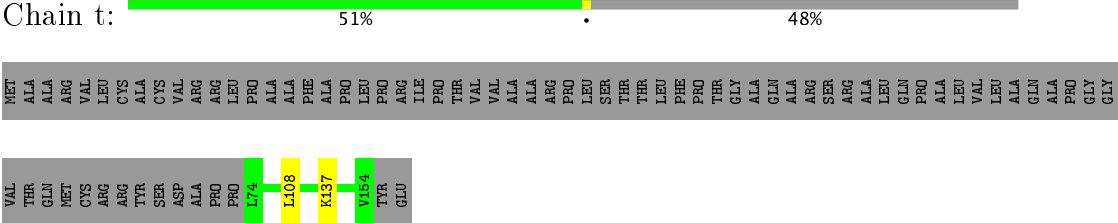




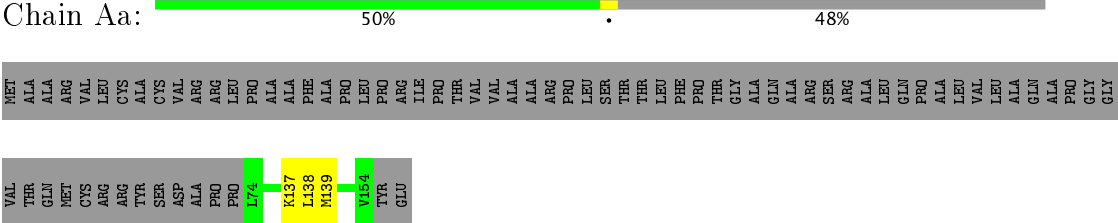
● Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



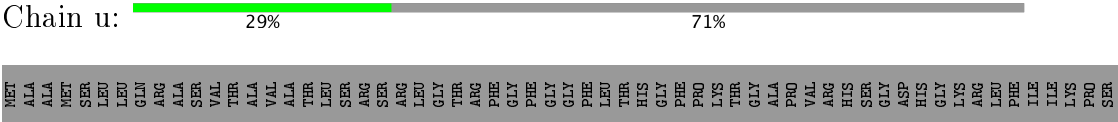
● Molecule 32: Acyl carrier protein

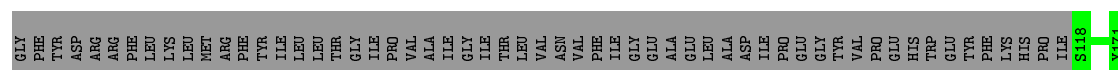


● Molecule 32: Acyl carrier protein

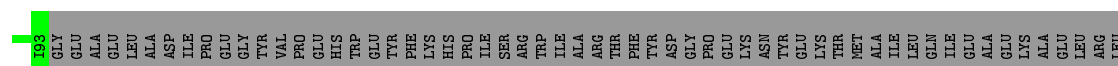


● Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5

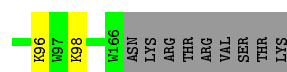
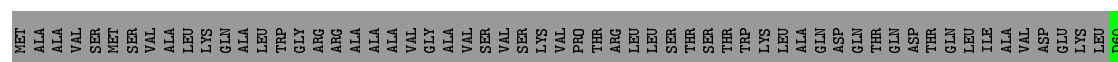




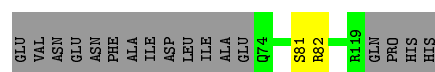
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5



- Molecule 34: Mitochondrial NADH dehydrogenase Fe-S protein 4



- Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 36: Cytochrome c oxidase subunit 3



There are no outlier residues recorded for this chain.

- Molecule 37: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



- Molecule 38: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 3:  92% 7%



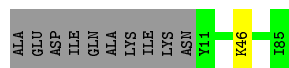
- Molecule 40: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain 4:  88% 10%



- Molecule 41: Cytochrome c oxidase subunit 6B1

Chain 5:  87% 12%



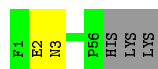
- Molecule 42: Cytochrome c oxidase subunit 6C

Chain 6:  100%


There are no outlier residues recorded for this chain.

- Molecule 43: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 7:  92% 5%



- Molecule 44: Cytochrome c oxidase subunit 7B, mitochondrial

Chain 8:  88% 13%



- Molecule 45: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 9:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: Cytochrome c oxidase subunit 8B, mitochondrial

Chain s:  93% 7%



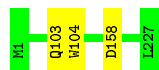
- Molecule 47: Cytochrome c oxidase subunit 1

Chain v: 99%



- Molecule 48: Cytochrome c oxidase subunit 2

Chain z: 



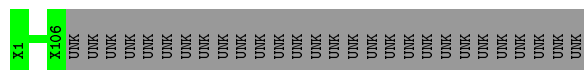
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ab:  96%



- Molecule 49: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ah: 79% 21%



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain Ac: 76% . 21%



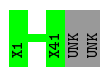
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ad: 100%

There are no outlier residues recorded for this chain.

- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ao: 95% 5%



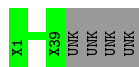
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Ap: 81% 19%



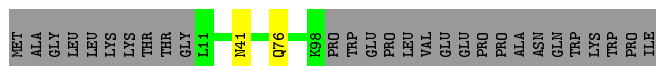
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Av: 91% 9%



- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain Ae: 74% 24%



- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Af: 68% 30%



- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Ag: 87% 6% 7%



- Molecule 55: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain Aj: 72% 24%

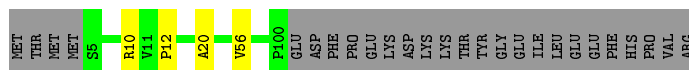
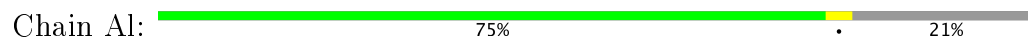


- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

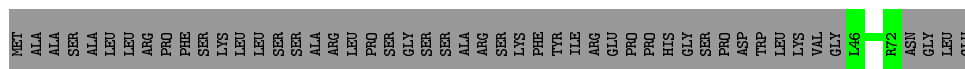
Chain Ak: 80% 15%



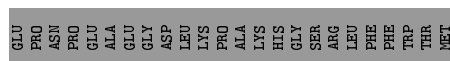
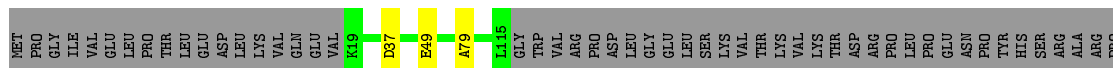
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 58: NADH dehydrogenase [ubiquinone] 1 subunit C1



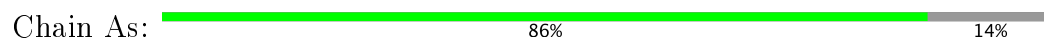
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



- Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



- Molecule 60: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



There are no outlier residues recorded for this chain.

- Molecule 61: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment



There are no outlier residues recorded for this chain.

- Molecule 62: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain At:  100%

There are no outlier residues recorded for this chain.

- Molecule 63: NADH dehydrogenase [ubiquinone] 1 unknown subunit fragment

Chain Au:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 139996 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, HEM, ZN, FMN, FES, HEC, NDP, CU, HEA

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 > 2$ | RMSZ | # $ Z > 2$ |
| 1 | A | 0.61 | 0/2197 | 1.43 | 13/3055 (0.4%) |
| 1 | M | 0.66 | 2/2197 (0.1%) | 1.48 | 17/3055 (0.6%) |
| 10 | J | 0.48 | 0/306 | 1.18 | 0/425 |
| 10 | L | 0.50 | 0/306 | 1.24 | 2/425 (0.5%) |
| 11 | K | 0.23 | 0/210 | 0.52 | 0/290 |
| 11 | V | 0.21 | 0/181 | 0.51 | 0/250 |
| 12 | W | 0.46 | 0/1401 | 0.66 | 0/1906 |
| 13 | Y | 0.43 | 0/5077 | 0.61 | 3/6888 (0.0%) |
| 14 | Z | 0.61 | 0/3075 | 0.64 | 0/4155 |
| 15 | a | 0.70 | 0/1174 | 0.65 | 0/1591 |
| 16 | b | 0.65 | 0/1215 | 0.62 | 0/1644 |
| 17 | c | 0.37 | 0/3196 | 0.56 | 0/4323 |
| 18 | d | 0.39 | 0/1353 | 0.58 | 1/1841 (0.1%) |
| 19 | e | 0.57 | 0/2558 | 0.68 | 0/3497 |
| 2 | B | 0.53 | 0/2060 | 1.33 | 8/2862 (0.3%) |
| 2 | N | 0.51 | 0/2060 | 1.28 | 3/2862 (0.1%) |
| 20 | f | 0.63 | 0/2761 | 0.70 | 0/3754 |
| 21 | g | 0.51 | 0/850 | 0.60 | 0/1163 |
| 22 | h | 0.59 | 0/3700 | 0.70 | 0/5045 |
| 23 | i | 0.62 | 0/687 | 0.71 | 0/931 |
| 24 | j | 0.50 | 0/4831 | 0.63 | 1/6572 (0.0%) |
| 25 | k | 0.59 | 0/1084 | 0.64 | 0/1470 |
| 25 | l | 0.41 | 0/72 | 0.59 | 0/98 |
| 26 | m | 0.44 | 0/262 | 0.58 | 0/364 |
| 27 | n | 0.32 | 0/410 | 0.57 | 0/570 |
| 28 | o | 0.50 | 0/250 | 0.63 | 0/346 |
| 29 | p | 0.34 | 0/1545 | 0.55 | 0/2147 |
| 3 | C | 0.70 | 1/1869 (0.1%) | 1.57 | 15/2600 (0.6%) |
| 3 | O | 0.69 | 1/1869 (0.1%) | 1.49 | 12/2600 (0.5%) |
| 30 | q | 0.38 | 0/966 | 0.61 | 1/1343 (0.1%) |
| 30 | v | 0.45 | 0/251 | 0.61 | 0/348 |
| 31 | r | 0.48 | 0/310 | 0.62 | 0/430 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 32 | Aa | 0.32 | 0/402 | 0.52 | 0/560 |
| 32 | t | 0.44 | 0/402 | 0.57 | 0/560 |
| 33 | Ai | 0.52 | 0/166 | 0.60 | 0/229 |
| 33 | u | 0.57 | 0/266 | 0.60 | 0/369 |
| 34 | w | 0.39 | 0/529 | 0.59 | 0/736 |
| 35 | x | 0.39 | 0/220 | 0.56 | 0/301 |
| 36 | 0 | 0.50 | 0/1283 | 0.70 | 0/1782 |
| 37 | 1 | 0.51 | 0/715 | 0.67 | 1/997 (0.1%) |
| 38 | 2 | 0.47 | 0/538 | 0.62 | 0/748 |
| 39 | 3 | 0.52 | 0/480 | 0.80 | 0/665 |
| 4 | D | 0.49 | 0/1187 | 1.12 | 0/1650 |
| 4 | P | 0.48 | 0/1187 | 1.07 | 0/1650 |
| 40 | 4 | 0.50 | 0/410 | 0.78 | 1/567 (0.2%) |
| 41 | 5 | 0.49 | 0/370 | 0.77 | 0/514 |
| 42 | 6 | 0.51 | 0/360 | 0.65 | 0/500 |
| 43 | 7 | 0.51 | 0/273 | 0.78 | 0/377 |
| 44 | 8 | 0.51 | 0/240 | 0.69 | 0/332 |
| 45 | 9 | 0.52 | 0/230 | 0.64 | 0/318 |
| 46 | s | 0.49 | 0/212 | 0.61 | 0/294 |
| 47 | y | 0.52 | 0/2522 | 0.76 | 1/3501 (0.0%) |
| 48 | z | 0.56 | 0/1126 | 0.81 | 0/1570 |
| 5 | E | 0.27 | 0/966 | 0.70 | 0/1343 |
| 5 | Q | 0.51 | 0/965 | 1.27 | 3/1341 (0.2%) |
| 50 | Ac | 0.50 | 0/270 | 0.56 | 0/374 |
| 52 | Ae | 0.38 | 0/434 | 0.58 | 0/603 |
| 53 | Af | 0.40 | 0/447 | 0.66 | 1/623 (0.2%) |
| 54 | Ag | 0.45 | 0/636 | 0.62 | 0/878 |
| 55 | Aj | 0.51 | 0/662 | 0.61 | 1/924 (0.1%) |
| 56 | Ak | 0.48 | 0/749 | 0.69 | 3/1044 (0.3%) |
| 57 | Al | 0.48 | 0/472 | 0.65 | 0/655 |
| 58 | Am | 0.48 | 0/133 | 0.54 | 0/184 |
| 59 | An | 0.44 | 0/481 | 0.60 | 0/670 |
| 6 | F | 0.52 | 0/526 | 1.17 | 2/733 (0.3%) |
| 6 | R | 0.56 | 0/526 | 1.22 | 3/733 (0.4%) |
| 7 | G | 0.61 | 0/400 | 1.35 | 2/556 (0.4%) |
| 7 | S | 0.52 | 0/385 | 0.96 | 0/535 |
| 8 | H | 0.45 | 0/319 | 1.04 | 0/445 |
| 8 | T | 0.42 | 0/319 | 0.96 | 0/445 |
| 9 | I | 0.52 | 0/162 | 1.32 | 1/224 (0.4%) |
| 9 | U | 0.42 | 0/162 | 1.08 | 0/224 |
| All | All | 0.53 | 4/72415 (0.0%) | 0.89 | 95/99604 (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 |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 13 |
| 1 | M | 0 | 3 |
| 10 | J | 0 | 1 |
| 17 | c | 0 | 1 |
| 2 | B | 0 | 9 |
| 2 | N | 0 | 5 |
| 3 | C | 0 | 14 |
| 3 | O | 0 | 6 |
| 34 | w | 0 | 1 |
| 4 | D | 0 | 1 |
| 4 | P | 0 | 2 |
| 5 | Q | 0 | 5 |
| 54 | Ag | 0 | 1 |
| 6 | F | 0 | 1 |
| 7 | G | 0 | 2 |
| 7 | S | 0 | 2 |
| 8 | T | 0 | 1 |
| 9 | I | 0 | 1 |
| All | All | 0 | 69 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | M | 253 | VAL | C-O | 6.79 | 1.36 | 1.23 |
| 1 | M | 169 | GLY | N-CA | -6.51 | 1.36 | 1.46 |
| 3 | C | 318 | ARG | C-N | -5.57 | 1.23 | 1.34 |
| 3 | O | 37 | LEU | C-N | -5.02 | 1.24 | 1.33 |

The worst 5 of 95 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | M | 253 | VAL | O-C-N | -14.87 | 98.92 | 122.70 |
| 1 | M | 256 | ALA | CB-CA-C | -11.05 | 93.52 | 110.10 |
| 1 | M | 168 | GLU | C-N-CA | 10.51 | 144.36 | 122.30 |
| 1 | M | 253 | VAL | CA-C-O | 8.21 | 137.34 | 120.10 |
| 3 | C | 204 | GLY | C-N-CA | 8.16 | 142.10 | 121.70 |

There are no chirality outliers.

5 of 69 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 118 | GLN | Mainchain |
| 1 | A | 122 | LEU | Mainchain |
| 1 | A | 196 | VAL | Mainchain |
| 1 | A | 210 | ASP | Mainchain |
| 1 | A | 53 | ASN | Mainchain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2198 | 0 | 1040 | 96 | 0 |
| 1 | M | 2198 | 0 | 1039 | 102 | 0 |
| 2 | B | 2061 | 0 | 1028 | 61 | 0 |
| 2 | N | 2061 | 0 | 1028 | 90 | 0 |
| 3 | C | 1870 | 0 | 843 | 101 | 0 |
| 3 | O | 1870 | 0 | 843 | 63 | 0 |
| 4 | D | 1188 | 0 | 533 | 33 | 0 |
| 4 | P | 1188 | 0 | 533 | 59 | 0 |
| 5 | E | 967 | 0 | 441 | 34 | 0 |
| 5 | Q | 966 | 0 | 440 | 40 | 0 |
| 6 | F | 527 | 0 | 232 | 18 | 0 |
| 6 | R | 527 | 0 | 232 | 7 | 0 |
| 7 | G | 401 | 0 | 180 | 21 | 0 |
| 7 | S | 386 | 0 | 174 | 30 | 0 |
| 8 | H | 320 | 0 | 135 | 7 | 0 |
| 8 | T | 320 | 0 | 135 | 7 | 0 |
| 9 | I | 163 | 0 | 77 | 8 | 0 |
| 9 | U | 163 | 0 | 77 | 28 | 0 |
| 10 | J | 307 | 0 | 149 | 9 | 0 |
| 10 | L | 307 | 0 | 149 | 17 | 0 |
| 11 | K | 211 | 0 | 102 | 9 | 0 |
| 11 | V | 182 | 0 | 90 | 6 | 0 |
| 12 | W | 1366 | 0 | 1316 | 79 | 0 |
| 13 | Y | 4998 | 0 | 4891 | 336 | 0 |
| 14 | Z | 3003 | 0 | 2971 | 145 | 0 |
| 15 | a | 1146 | 0 | 1143 | 0 | 0 |
| 16 | b | 1189 | 0 | 1144 | 0 | 0 |
| 17 | c | 3125 | 0 | 3087 | 0 | 0 |
| 18 | d | 1324 | 0 | 1338 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | e | 2486 | 0 | 2587 | 0 | 0 |
| 20 | f | 2698 | 0 | 2851 | 0 | 0 |
| 21 | g | 829 | 0 | 863 | 0 | 0 |
| 22 | h | 3610 | 0 | 3816 | 0 | 0 |
| 23 | i | 677 | 0 | 726 | 0 | 0 |
| 24 | j | 4705 | 0 | 4848 | 0 | 0 |
| 25 | k | 1059 | 0 | 1077 | 0 | 0 |
| 25 | l | 73 | 0 | 31 | 0 | 0 |
| 26 | m | 263 | 0 | 125 | 0 | 0 |
| 27 | n | 411 | 0 | 177 | 0 | 0 |
| 28 | o | 251 | 0 | 115 | 0 | 0 |
| 29 | p | 1546 | 0 | 688 | 0 | 0 |
| 30 | q | 967 | 0 | 431 | 0 | 0 |
| 30 | v | 252 | 0 | 103 | 0 | 0 |
| 31 | r | 311 | 0 | 140 | 0 | 0 |
| 32 | Aa | 403 | 0 | 172 | 0 | 0 |
| 32 | t | 403 | 0 | 172 | 0 | 0 |
| 33 | Ai | 167 | 0 | 72 | 0 | 0 |
| 33 | u | 267 | 0 | 123 | 0 | 0 |
| 34 | w | 530 | 0 | 230 | 0 | 0 |
| 35 | x | 221 | 0 | 101 | 0 | 0 |
| 36 | 0 | 1284 | 0 | 575 | 0 | 0 |
| 37 | 1 | 716 | 0 | 321 | 1 | 0 |
| 38 | 2 | 539 | 0 | 243 | 0 | 0 |
| 39 | 3 | 481 | 0 | 224 | 3 | 0 |
| 40 | 4 | 411 | 0 | 193 | 3 | 0 |
| 41 | 5 | 371 | 0 | 161 | 0 | 0 |
| 42 | 6 | 361 | 0 | 184 | 0 | 0 |
| 43 | 7 | 274 | 0 | 127 | 0 | 0 |
| 44 | 8 | 241 | 0 | 115 | 0 | 0 |
| 45 | 9 | 231 | 0 | 106 | 0 | 0 |
| 46 | s | 213 | 0 | 98 | 0 | 0 |
| 47 | y | 2523 | 0 | 1169 | 0 | 0 |
| 48 | z | 1127 | 0 | 475 | 0 | 0 |
| 49 | Ab | 637 | 0 | 132 | 0 | 0 |
| 49 | Ah | 526 | 0 | 107 | 0 | 0 |
| 50 | Ac | 271 | 0 | 132 | 0 | 0 |
| 51 | Ad | 211 | 0 | 42 | 0 | 0 |
| 51 | Ao | 205 | 0 | 46 | 0 | 0 |
| 51 | Ap | 173 | 0 | 36 | 0 | 0 |
| 51 | Av | 193 | 0 | 40 | 0 | 0 |
| 52 | Ae | 435 | 0 | 195 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 53 | Af | 448 | 0 | 190 | 0 | 0 |
| 54 | Ag | 637 | 0 | 331 | 0 | 0 |
| 55 | Aj | 663 | 0 | 292 | 0 | 0 |
| 56 | Ak | 750 | 0 | 321 | 0 | 0 |
| 57 | Al | 473 | 0 | 204 | 0 | 0 |
| 58 | Am | 134 | 0 | 54 | 0 | 0 |
| 59 | An | 482 | 0 | 214 | 0 | 0 |
| 60 | Aq | 335 | 0 | 69 | 0 | 0 |
| 60 | As | 322 | 0 | 65 | 0 | 0 |
| 60 | Aw | 376 | 0 | 76 | 0 | 0 |
| 61 | Ar | 169 | 0 | 37 | 0 | 0 |
| 62 | At | 84 | 0 | 18 | 0 | 0 |
| 63 | Au | 62 | 0 | 12 | 0 | 0 |
| 64 | C | 86 | 0 | 60 | 41 | 0 |
| 64 | O | 86 | 0 | 60 | 9 | 0 |
| 65 | D | 43 | 0 | 32 | 3 | 0 |
| 65 | P | 43 | 0 | 32 | 2 | 0 |
| 66 | E | 4 | 0 | 0 | 0 | 0 |
| 66 | Q | 4 | 0 | 0 | 0 | 0 |
| 66 | Y | 4 | 0 | 0 | 0 | 0 |
| 66 | d | 4 | 0 | 0 | 0 | 0 |
| 67 | Y | 16 | 0 | 0 | 5 | 0 |
| 67 | a | 8 | 0 | 0 | 0 | 0 |
| 67 | b | 16 | 0 | 0 | 0 | 0 |
| 67 | c | 8 | 0 | 0 | 0 | 0 |
| 68 | c | 31 | 0 | 19 | 0 | 0 |
| 69 | p | 48 | 0 | 26 | 0 | 0 |
| 70 | 3 | 1 | 0 | 0 | 0 | 0 |
| 71 | y | 120 | 0 | 108 | 0 | 0 |
| 72 | y | 1 | 0 | 0 | 0 | 0 |
| 72 | z | 2 | 0 | 0 | 0 | 0 |
| 73 | y | 1 | 0 | 0 | 0 | 0 |
| All | All | 75545 | 0 | 51779 | 1253 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 1253 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:A:84:ALA:CB | 1:A:101:ALA:HB2 | 1.51 | 1.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:117:VAL:N | 64:C:402:HEM:HBC2 | 1.43 | 1.34 |
| 1:M:83:GLY:CA | 2:N:363:LYS:HA | 1.57 | 1.33 |
| 3:C:116:GLY:HA3 | 64:C:402:HEM:C3C | 1.63 | 1.33 |
| 12:W:162:ALA:HB2 | 14:Z:286:TYR:CA | 1.61 | 1.28 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1 | A | 444/446 (100%) | 359 (81%) | 63 (14%) | 22 (5%) | 2 | 27 |
| 1 | M | 444/446 (100%) | 377 (85%) | 47 (11%) | 20 (4%) | 3 | 29 |
| 2 | B | 417/439 (95%) | 342 (82%) | 66 (16%) | 9 (2%) | 8 | 45 |
| 2 | N | 417/439 (95%) | 345 (83%) | 60 (14%) | 12 (3%) | 5 | 38 |
| 3 | C | 377/379 (100%) | 307 (81%) | 56 (15%) | 14 (4%) | 4 | 33 |
| 3 | O | 377/379 (100%) | 316 (84%) | 50 (13%) | 11 (3%) | 5 | 38 |
| 4 | D | 239/241 (99%) | 199 (83%) | 28 (12%) | 12 (5%) | 2 | 27 |
| 4 | P | 239/241 (99%) | 201 (84%) | 26 (11%) | 12 (5%) | 2 | 27 |
| 5 | E | 194/274 (71%) | 178 (92%) | 12 (6%) | 4 (2%) | 8 | 46 |
| 5 | Q | 194/274 (71%) | 158 (81%) | 28 (14%) | 8 (4%) | 3 | 31 |
| 6 | F | 104/110 (94%) | 90 (86%) | 11 (11%) | 3 (3%) | 5 | 38 |
| 6 | R | 104/110 (94%) | 89 (86%) | 12 (12%) | 3 (3%) | 5 | 38 |
| 7 | G | 79/81 (98%) | 63 (80%) | 13 (16%) | 3 (4%) | 4 | 33 |
| 7 | S | 76/81 (94%) | 72 (95%) | 2 (3%) | 2 (3%) | 6 | 41 |
| 8 | H | 62/78 (80%) | 52 (84%) | 10 (16%) | 0 | 100 | 100 |
| 8 | T | 62/78 (80%) | 51 (82%) | 10 (16%) | 1 (2%) | 11 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9 | I | 31/78 (40%) | 19 (61%) | 10 (32%) | 2 (6%) | 1 | 22 |
| 9 | U | 31/78 (40%) | 20 (64%) | 7 (23%) | 4 (13%) | 0 | 6 |
| 10 | J | 60/62 (97%) | 41 (68%) | 13 (22%) | 6 (10%) | 1 | 12 |
| 10 | L | 60/62 (97%) | 44 (73%) | 12 (20%) | 4 (7%) | 1 | 21 |
| 11 | K | 41/56 (73%) | 40 (98%) | 0 | 1 (2%) | 7 | 42 |
| 11 | V | 35/56 (62%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 12 | W | 167/264 (63%) | 136 (81%) | 23 (14%) | 8 (5%) | 2 | 28 |
| 13 | Y | 668/727 (92%) | 575 (86%) | 65 (10%) | 28 (4%) | 3 | 30 |
| 14 | Z | 373/463 (81%) | 343 (92%) | 20 (5%) | 10 (3%) | 6 | 40 |
| 15 | a | 145/216 (67%) | 126 (87%) | 11 (8%) | 8 (6%) | 2 | 25 |
| 16 | b | 147/212 (69%) | 140 (95%) | 6 (4%) | 1 (1%) | 25 | 68 |
| 17 | c | 408/464 (88%) | 369 (90%) | 27 (7%) | 12 (3%) | 5 | 38 |
| 18 | d | 167/249 (67%) | 152 (91%) | 11 (7%) | 4 (2%) | 7 | 42 |
| 19 | e | 313/318 (98%) | 282 (90%) | 27 (9%) | 4 (1%) | 14 | 56 |
| 20 | f | 344/347 (99%) | 324 (94%) | 17 (5%) | 3 (1%) | 20 | 63 |
| 21 | g | 104/115 (90%) | 96 (92%) | 7 (7%) | 1 (1%) | 18 | 61 |
| 22 | h | 455/459 (99%) | 424 (93%) | 21 (5%) | 10 (2%) | 8 | 45 |
| 23 | i | 88/98 (90%) | 82 (93%) | 4 (4%) | 2 (2%) | 7 | 43 |
| 24 | j | 592/606 (98%) | 534 (90%) | 40 (7%) | 18 (3%) | 5 | 38 |
| 25 | k | 138/175 (79%) | 126 (91%) | 8 (6%) | 4 (3%) | 5 | 38 |
| 25 | l | 13/175 (7%) | 11 (85%) | 1 (8%) | 1 (8%) | 1 | 17 |
| 26 | m | 51/84 (61%) | 48 (94%) | 2 (4%) | 1 (2%) | 9 | 47 |
| 27 | n | 81/99 (82%) | 74 (91%) | 6 (7%) | 1 (1%) | 15 | 58 |
| 28 | o | 49/106 (46%) | 42 (86%) | 3 (6%) | 4 (8%) | 1 | 16 |
| 29 | p | 312/377 (83%) | 281 (90%) | 19 (6%) | 12 (4%) | 4 | 33 |
| 30 | q | 194/357 (54%) | 172 (89%) | 16 (8%) | 6 (3%) | 5 | 37 |
| 30 | v | 49/357 (14%) | 46 (94%) | 3 (6%) | 0 | 100 | 100 |
| 31 | r | 61/144 (42%) | 60 (98%) | 1 (2%) | 0 | 100 | 100 |
| 32 | Aa | 79/156 (51%) | 75 (95%) | 1 (1%) | 3 (4%) | 4 | 33 |
| 32 | t | 79/156 (51%) | 74 (94%) | 3 (4%) | 2 (2%) | 6 | 41 |
| 33 | Ai | 32/189 (17%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 33 | u | 52/189 (28%) | 48 (92%) | 4 (8%) | 0 | 100 | 100 |
| 34 | w | 105/175 (60%) | 93 (89%) | 11 (10%) | 1 (1%) | 18 | 61 |
| 35 | x | 44/123 (36%) | 41 (93%) | 1 (2%) | 2 (4%) | 3 | 29 |
| 36 | 0 | 259/261 (99%) | 249 (96%) | 10 (4%) | 0 | 100 | 100 |
| 37 | 1 | 142/147 (97%) | 135 (95%) | 7 (5%) | 0 | 100 | 100 |
| 38 | 2 | 107/109 (98%) | 104 (97%) | 3 (3%) | 0 | 100 | 100 |
| 39 | 3 | 96/98 (98%) | 86 (90%) | 6 (6%) | 4 (4%) | 3 | 30 |
| 40 | 4 | 82/84 (98%) | 67 (82%) | 10 (12%) | 5 (6%) | 2 | 22 |
| 41 | 5 | 73/85 (86%) | 64 (88%) | 8 (11%) | 1 (1%) | 13 | 54 |
| 42 | 6 | 71/73 (97%) | 65 (92%) | 6 (8%) | 0 | 100 | 100 |
| 43 | 7 | 54/59 (92%) | 48 (89%) | 4 (7%) | 2 (4%) | 4 | 33 |
| 44 | 8 | 47/56 (84%) | 41 (87%) | 6 (13%) | 0 | 100 | 100 |
| 45 | 9 | 45/47 (96%) | 42 (93%) | 3 (7%) | 0 | 100 | 100 |
| 46 | s | 41/46 (89%) | 39 (95%) | 2 (5%) | 0 | 100 | 100 |
| 47 | y | 512/514 (100%) | 479 (94%) | 29 (6%) | 4 (1%) | 22 | 66 |
| 48 | z | 225/227 (99%) | 203 (90%) | 19 (8%) | 3 (1%) | 14 | 56 |
| 50 | Ac | 53/70 (76%) | 49 (92%) | 2 (4%) | 2 (4%) | 4 | 33 |
| 52 | Ae | 86/116 (74%) | 82 (95%) | 2 (2%) | 2 (2%) | 7 | 43 |
| 53 | Af | 88/128 (69%) | 81 (92%) | 4 (4%) | 3 (3%) | 4 | 36 |
| 54 | Ag | 129/141 (92%) | 120 (93%) | 2 (2%) | 7 (5%) | 2 | 25 |
| 55 | Aj | 131/176 (74%) | 124 (95%) | 2 (2%) | 5 (4%) | 4 | 33 |
| 56 | Ak | 149/178 (84%) | 131 (88%) | 11 (7%) | 7 (5%) | 3 | 28 |
| 57 | Al | 94/122 (77%) | 83 (88%) | 7 (7%) | 4 (4%) | 3 | 30 |
| 58 | Am | 25/76 (33%) | 23 (92%) | 2 (8%) | 0 | 100 | 100 |
| 59 | An | 95/172 (55%) | 87 (92%) | 5 (5%) | 3 (3%) | 5 | 36 |
| All | All | 12001/14873 (81%) | 10603 (88%) | 1047 (9%) | 351 (3%) | 9 | 38 |

5 of 351 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 327 | ASP |
| 1 | A | 426 | GLY |
| 1 | A | 427 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 141 | GLN |
| 2 | B | 183 | ILE |

5.3.2 Protein sidechains ⓘ

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 | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 12 | W | 145/228 (64%) | 145 (100%) | 0 | 100 | 100 |
| 13 | Y | 517/610 (85%) | 516 (100%) | 1 (0%) | 94 | 96 |
| 14 | Z | 322/393 (82%) | 322 (100%) | 0 | 100 | 100 |
| 15 | a | 120/177 (68%) | 119 (99%) | 1 (1%) | 85 | 92 |
| 16 | b | 126/176 (72%) | 126 (100%) | 0 | 100 | 100 |
| 17 | c | 321/368 (87%) | 321 (100%) | 0 | 100 | 100 |
| 18 | d | 145/207 (70%) | 145 (100%) | 0 | 100 | 100 |
| 19 | e | 272/275 (99%) | 272 (100%) | 0 | 100 | 100 |
| 20 | f | 309/311 (99%) | 309 (100%) | 0 | 100 | 100 |
| 21 | g | 91/100 (91%) | 91 (100%) | 0 | 100 | 100 |
| 22 | h | 407/409 (100%) | 406 (100%) | 1 (0%) | 94 | 96 |
| 23 | i | 76/85 (89%) | 76 (100%) | 0 | 100 | 100 |
| 24 | j | 527/540 (98%) | 526 (100%) | 1 (0%) | 94 | 96 |
| 25 | k | 112/141 (79%) | 112 (100%) | 0 | 100 | 100 |
| All | All | 3490/4020 (87%) | 3486 (100%) | 4 (0%) | 95 | 97 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | Y | 478 | SER |
| 15 | a | 91 | CYS |
| 22 | h | 96 | ILE |
| 24 | j | 283 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | d | 153 | GLN |
| 19 | e | 230 | ASN |
| 24 | j | 332 | HIS |
| 18 | d | 189 | ASN |
| 19 | e | 235 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 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 | $\# Z > 2$ |
| 64 | HEM | C | 401 | - | 28,50,50 | 2.09 | 4 (14%) | 17,82,82 | 2.63 | 7 (41%) |
| 64 | HEM | C | 402 | - | 28,50,50 | 1.86 | 6 (21%) | 17,82,82 | 3.00 | 6 (35%) |
| 65 | HEC | D | 301 | - | 28,50,50 | 2.33 | 5 (17%) | 16,82,82 | 2.13 | 8 (50%) |
| 66 | FES | E | 201 | - | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 64 | HEM | O | 401 | - | 28,50,50 | 2.18 | 8 (28%) | 17,82,82 | 3.23 | 9 (52%) |
| 64 | HEM | O | 402 | - | 28,50,50 | 2.06 | 6 (21%) | 17,82,82 | 2.43 | 9 (52%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 65 | HEC | P | 301 | - | 28,50,50 | 2.33 | 4 (14%) | 16,82,82 | 2.12 | 8 (50%) |
| 66 | FES | Q | 201 | - | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 67 | SF4 | Y | 801 | 13 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 67 | SF4 | Y | 802 | 13 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 66 | FES | Y | 803 | 13 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 67 | SF4 | a | 301 | 15 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 67 | SF4 | b | 301 | 16 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 67 | SF4 | b | 302 | 16 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 67 | SF4 | c | 501 | 17 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 68 | FMN | c | 502 | - | 31,33,33 | 1.50 | 7 (22%) | 38,50,50 | 1.90 | 8 (21%) |
| 66 | FES | d | 301 | - | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 69 | NDP | p | 401 | - | 43,52,52 | 0.99 | 2 (4%) | 49,80,80 | 1.41 | 3 (6%) |
| 71 | HEA | y | 601 | - | 44,67,67 | 1.63 | 8 (18%) | 37,103,103 | 1.85 | 10 (27%) |
| 71 | HEA | y | 602 | - | 44,67,67 | 1.52 | 4 (9%) | 37,103,103 | 1.36 | 7 (18%) |

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 |
|-----|------|-------|-----|------|----------|------------|---------|
| 64 | HEM | C | 401 | - | - | 0/6/54/54 | 0/0/8/8 |
| 64 | HEM | C | 402 | - | - | 0/6/54/54 | 0/0/8/8 |
| 65 | HEC | D | 301 | - | - | 0/6/54/54 | 0/0/8/8 |
| 66 | FES | E | 201 | - | - | 0/0/4/4 | 0/1/1/1 |
| 64 | HEM | O | 401 | - | - | 0/6/54/54 | 0/0/8/8 |
| 64 | HEM | O | 402 | - | - | 0/6/54/54 | 0/0/8/8 |
| 65 | HEC | P | 301 | - | - | 0/6/54/54 | 0/0/8/8 |
| 66 | FES | Q | 201 | - | - | 0/0/4/4 | 0/1/1/1 |
| 67 | SF4 | Y | 801 | 13 | - | 0/0/48/48 | 0/6/5/5 |
| 67 | SF4 | Y | 802 | 13 | - | 0/0/48/48 | 0/6/5/5 |
| 66 | FES | Y | 803 | 13 | - | 0/0/4/4 | 0/1/1/1 |
| 67 | SF4 | a | 301 | 15 | - | 0/0/48/48 | 0/6/5/5 |
| 67 | SF4 | b | 301 | 16 | - | 0/0/48/48 | 0/6/5/5 |
| 67 | SF4 | b | 302 | 16 | - | 0/0/48/48 | 0/6/5/5 |
| 67 | SF4 | c | 501 | 17 | - | 0/0/48/48 | 0/6/5/5 |
| 68 | FMN | c | 502 | - | - | 0/16/18/18 | 0/3/3/3 |
| 66 | FES | d | 301 | - | - | 0/0/4/4 | 0/1/1/1 |
| 69 | NDP | p | 401 | - | - | 0/30/77/77 | 0/5/5/5 |
| 71 | HEA | y | 601 | - | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 71 | HEA | y | 602 | - | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |

The worst 5 of 54 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 65 | P | 301 | HEC | C3C-C2C | -7.04 | 1.33 | 1.40 |
| 64 | C | 401 | HEM | C3B-C2B | -6.98 | 1.31 | 1.40 |
| 65 | D | 301 | HEC | C3B-C2B | -6.95 | 1.33 | 1.40 |
| 65 | P | 301 | HEC | C3B-C2B | -6.74 | 1.33 | 1.40 |
| 71 | y | 602 | HEA | C3A-C2A | -6.66 | 1.31 | 1.40 |

The worst 5 of 75 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 69 | p | 401 | NDP | N3A-C2A-N1A | -6.96 | 122.79 | 128.86 |
| 64 | O | 401 | HEM | CMA-C3A-C4A | -6.90 | 117.87 | 128.46 |
| 64 | C | 402 | HEM | CMA-C3A-C4A | -5.39 | 120.19 | 128.46 |
| 64 | O | 401 | HEM | CMD-C2D-C1D | -5.01 | 120.76 | 128.46 |
| 71 | y | 601 | HEA | C4B-C3B-C2B | -4.52 | 103.71 | 106.87 |

5 of 6 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 71 | y | 602 | HEA | ND |
| 71 | y | 602 | HEA | NA |
| 71 | y | 602 | HEA | NB |
| 71 | y | 601 | HEA | ND |
| 71 | y | 601 | HEA | NA |

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 60 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 64 | C | 401 | HEM | 3 | 0 |
| 64 | C | 402 | HEM | 38 | 0 |
| 65 | D | 301 | HEC | 3 | 0 |
| 64 | O | 401 | HEM | 6 | 0 |
| 64 | O | 402 | HEM | 3 | 0 |
| 65 | P | 301 | HEC | 2 | 0 |
| 67 | Y | 801 | SF4 | 4 | 0 |
| 67 | Y | 802 | SF4 | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.