



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 28, 2017 – 12:41 PM EST

PDB ID : 5XTD
EMDB ID: : EMD-6773
Title : Cryo-EM structure of human respiratory complex I
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : unknown
Resolution : 3.70 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-20030345

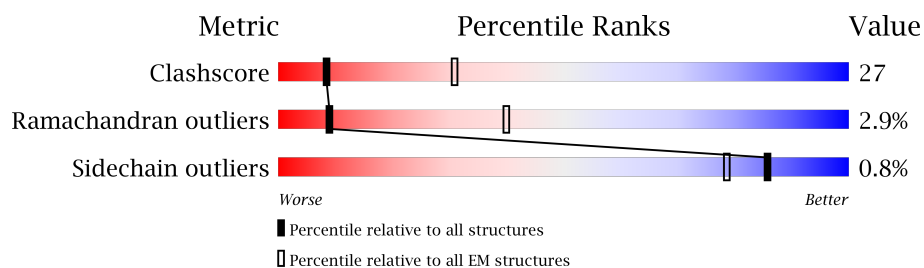
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.






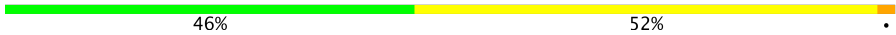

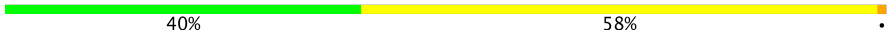
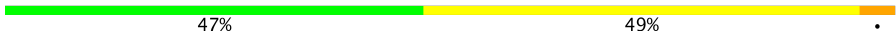






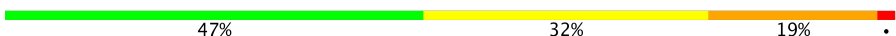

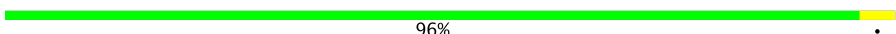

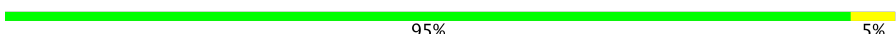
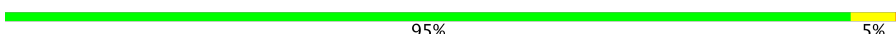
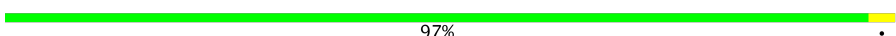
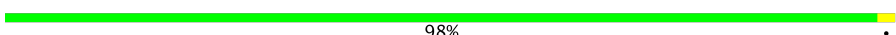
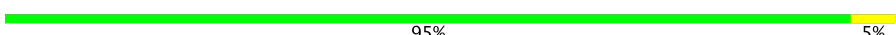
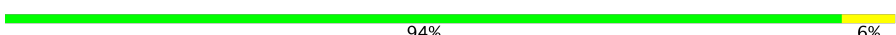
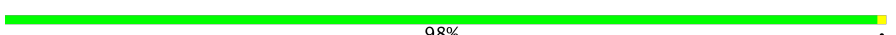

| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |
| Sidechain outliers | 121581 | 1026 |

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 | 431 | 48% 51% . |
| 2 | B | 176 | 50% 49% . |
| 3 | C | 156 | 56% 42% . |
| 4 | E | 113 | 49% 49% . |
| 5 | F | 83 | 51% 49% |
| 6 | G | 85 | 47% 51% . |
| 6 | X | 85 | 58% 40% . |
| 7 | H | 112 | 53% 46% . |
| 8 | I | 110 | 46% 36% . 14% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | J | 337 |  |
| 10 | K | 33 |  |
| 11 | L | 118 |  |
| 12 | M | 687 |  |
| 13 | N | 143 |  |
| 14 | O | 212 |  |
| 15 | P | 208 |  |
| 16 | Q | 430 |  |
| 17 | S | 70 |  |
| 18 | T | 95 |  |
| 19 | U | 83 |  |
| 20 | V | 140 |  |
| 21 | W | 138 |  |
| 22 | Y | 59 |  |
| 23 | Z | 80 |  |
| 24 | a | 138 |  |
| 25 | b | 128 |  |
| 26 | c | 153 |  |
| 27 | d | 171 |  |
| 28 | e | 97 |  |
| 29 | f | 47 |  |
| 30 | g | 119 |  |
| 31 | h | 104 |  |
| 32 | i | 347 |  |
| 33 | j | 115 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 34 | k | 97 |  93% 6% . |
| 35 | l | 603 |  94% 5% . |
| 36 | m | 174 |  94% 6% . |
| 37 | n | 56 |  96% . |
| 38 | o | 128 |  97% . |
| 39 | p | 172 |  98% . |
| 40 | r | 459 |  98% . |
| 41 | s | 318 |  97% . |
| 42 | u | 169 |  97% . |
| 43 | v | 137 |  77% . 19% |
| 44 | w | 320 |  97% . |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 45 | SF4 | A | 501 | - | - | X | - |
| 45 | SF4 | B | 302 | - | - | X | - |
| 45 | SF4 | M | 801 | - | - | X | - |
| 46 | FMN | A | 502 | - | - | X | - |
| 49 | NDP | J | 401 | - | - | X | - |
| 50 | FES | O | 301 | - | - | X | - |

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 66789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3322 | 2096 | 594 | 612 | 20 | | |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2 | B | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1420 | 893 | 243 | 271 | 13 | | |

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3 | C | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1249 | 794 | 227 | 214 | 14 | | |

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | E | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 968 | 623 | 178 | 162 | 5 | | |

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | F | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 422 | 124 | 122 | 2 | | |

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | G | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 672 | 434 | 99 | 134 | 5 | | |
| 6 | X | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 686 | 442 | 101 | 138 | 5 | | |

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | H | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 922 | 593 | 157 | 169 | 3 | | |

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | I | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 769 | 483 | 146 | 138 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9 | J | 337 | Total | C | N | O | S | 0 | 0 |
| | | | 2712 | 1759 | 482 | 463 | 8 | | |

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10 | K | 33 | Total | C | N | O | S | 0 | 0 |
| | | | 274 | 173 | 47 | 53 | 1 | | |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | L | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 964 | 608 | 173 | 179 | 4 | | |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 12 | M | 687 | Total | C | N | O | S | 0 | 0 |
| | | | 5274 | 3310 | 917 | 1009 | 38 | | |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | N | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1195 | 770 | 210 | 212 | 3 | | |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | O | 212 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1047 | 276 | 310 | 10 | | |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15 | P | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1730 | 1117 | 297 | 313 | 3 | | |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16 | Q | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3460 | 2214 | 599 | 624 | 23 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 17 | S | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 568 | 367 | 101 | 96 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | T | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 742 | 459 | 138 | 142 | 3 | | |

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | U | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 427 | 105 | 113 | 2 | | |

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | V | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1038 | 668 | 178 | 187 | 5 | | |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | W | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1135 | 727 | 202 | 200 | 6 | | |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22 | Y | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 533 | 354 | 87 | 91 | 1 | | |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | Z | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 648 | 426 | 110 | 110 | 2 | | |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | a | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1174 | 771 | 199 | 202 | 2 | | |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | b | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1059 | 697 | 181 | 176 | 5 | | |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 26 | c | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1236 | 795 | 208 | 222 | 11 | | |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 27 | d | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1418 | 885 | 262 | 259 | 12 | | |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | e | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 810 | 522 | 132 | 152 | 4 | | |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 29 | f | 47 | Total | C | N | O | 0 | 0 |
| | | | 405 | 269 | 69 | 67 | | |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | g | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 1004 | 658 | 173 | 169 | 4 | | |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | h | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 863 | 546 | 161 | 150 | 6 | | |

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 32 | i | 347 | Total | C | N | O | S | 0 | 0 |
| | | | 2735 | 1819 | 421 | 470 | 25 | | |

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | j | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 919 | 626 | 132 | 152 | 9 | | |

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 34 | k | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 487 | 113 | 127 | 13 | | |

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 35 | l | 603 | Total | C | N | O | S | 0 | 0 |
| | | | 4717 | 3119 | 742 | 823 | 33 | | |

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 36 | m | 174 | Total | C | N | O | S | 0 | 0 |
| | | | 1313 | 879 | 194 | 229 | 11 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37 | n | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 473 | 305 | 85 | 80 | 3 | | |

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

4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | o | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1066 | 685 | 192 | 187 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | p | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1495 | 961 | 265 | 261 | 8 | | |

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40 | r | 459 | Total | C | N | O | S | 0 | 0 |
| | | | 3629 | 2411 | 569 | 619 | 30 | | |

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41 | s | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2509 | 1678 | 380 | 435 | 16 | | |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | u | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1394 | 886 | 247 | 252 | 9 | | |

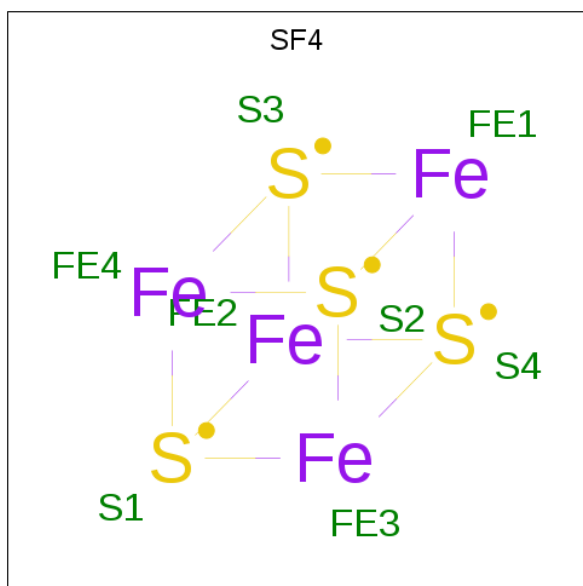
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | v | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 921 | 569 | 187 | 156 | 9 | | |

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

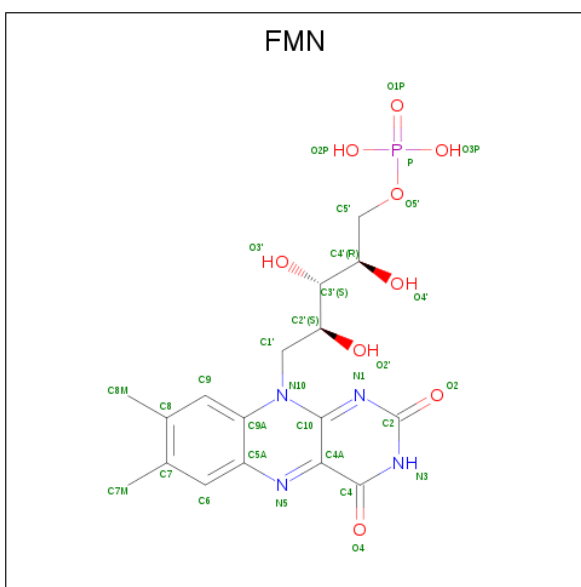
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44 | w | 320 | Total | C | N | O | S | 0 | 0 |
| | | | 2474 | 1573 | 429 | 464 | 8 | | |

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



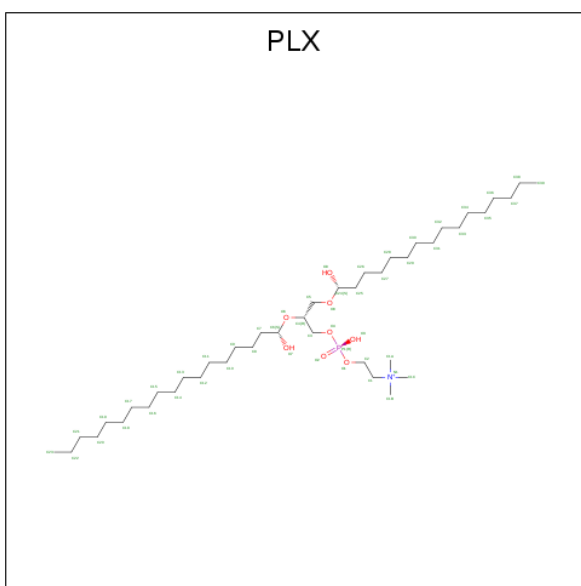
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45 | A | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | B | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 45 | B | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 45 | C | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 45 | M | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |
| 45 | M | 1 | Total | Fe | S | 0 |
| | | | 16 | 8 | 8 | |

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46 | A | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

- Molecule 47 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P).



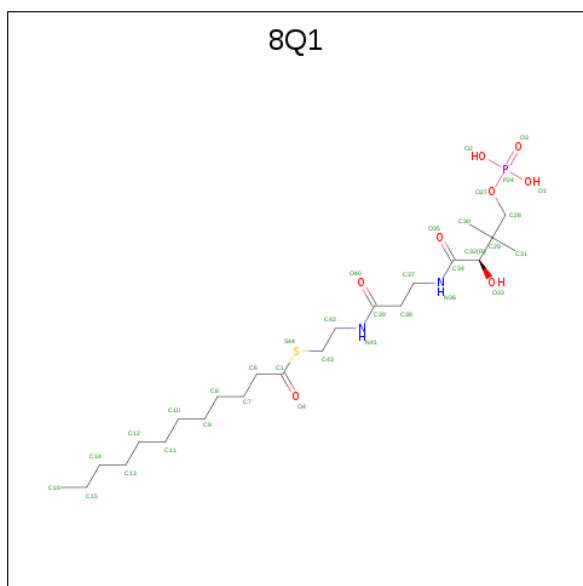
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 47 | B | 1 | Total 52 | C 42 | N 1 | O 8 | P 1 | 0 |
| 47 | U | 1 | Total 52 | C 42 | N 1 | O 8 | P 1 | 0 |

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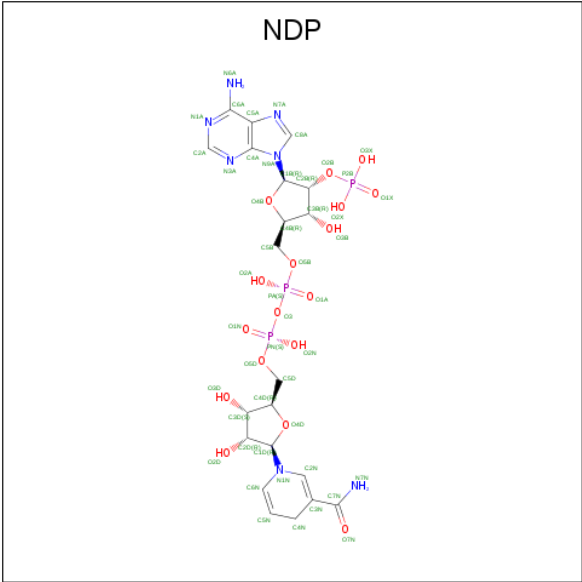
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|---|----|---|---------|
| 47 | V | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 47 | b | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 47 | g | 1 | Total | C | N | O | P | 0 |
| | | | 156 | 126 | 3 | 24 | 3 | |
| 47 | g | 1 | Total | C | N | O | P | 0 |
| | | | 156 | 126 | 3 | 24 | 3 | |
| 47 | g | 1 | Total | C | N | O | P | 0 |
| | | | 156 | 126 | 3 | 24 | 3 | |
| 47 | r | 1 | Total | C | N | O | P | 0 |
| | | | 104 | 84 | 2 | 16 | 2 | |
| 47 | r | 1 | Total | C | N | O | P | 0 |
| | | | 104 | 84 | 2 | 16 | 2 | |

- Molecule 48 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



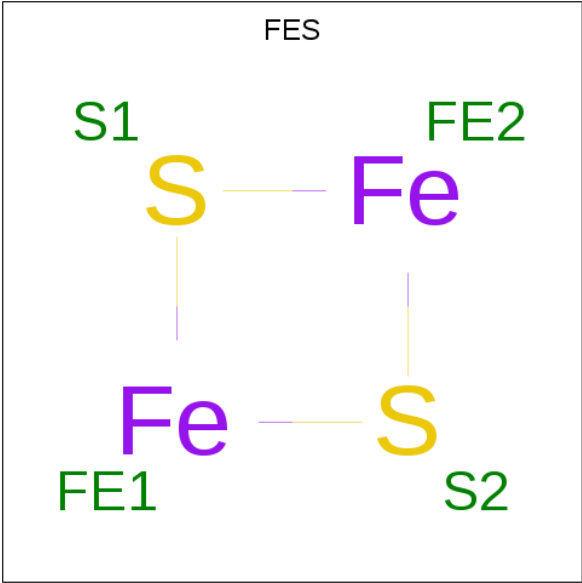
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 48 | E | 1 | Total | C | N | O | P | S | 0 |
| | | | 35 | 23 | 2 | 8 | 1 | 1 | |
| 48 | p | 1 | Total | C | N | O | P | S | 0 |
| | | | 35 | 23 | 2 | 8 | 1 | 1 | |

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



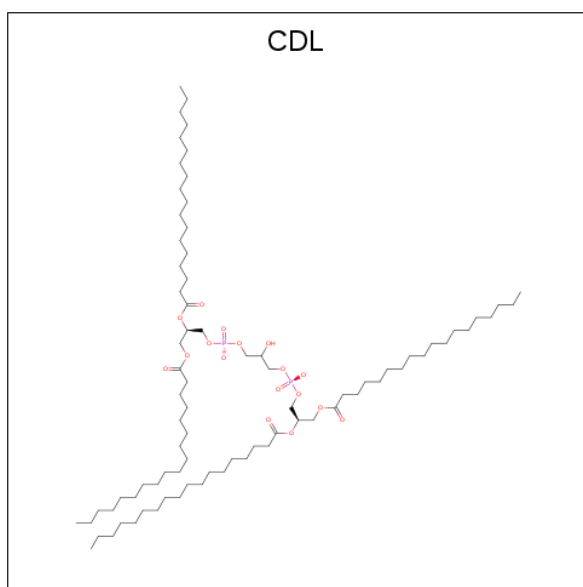
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 49 | J | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



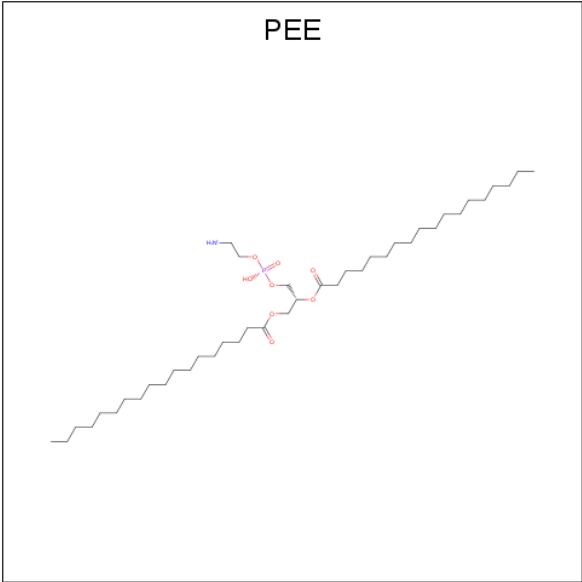
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 50 | M | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 50 | O | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 51 | V | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 51 | i | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 51 | l | 1 | Total | C | O | P | 0 |
| | | | 128 | 90 | 34 | 4 | |
| 51 | l | 1 | Total | C | O | P | 0 |
| | | | 128 | 90 | 34 | 4 | |
| 51 | n | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |

- Molecule 52 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).

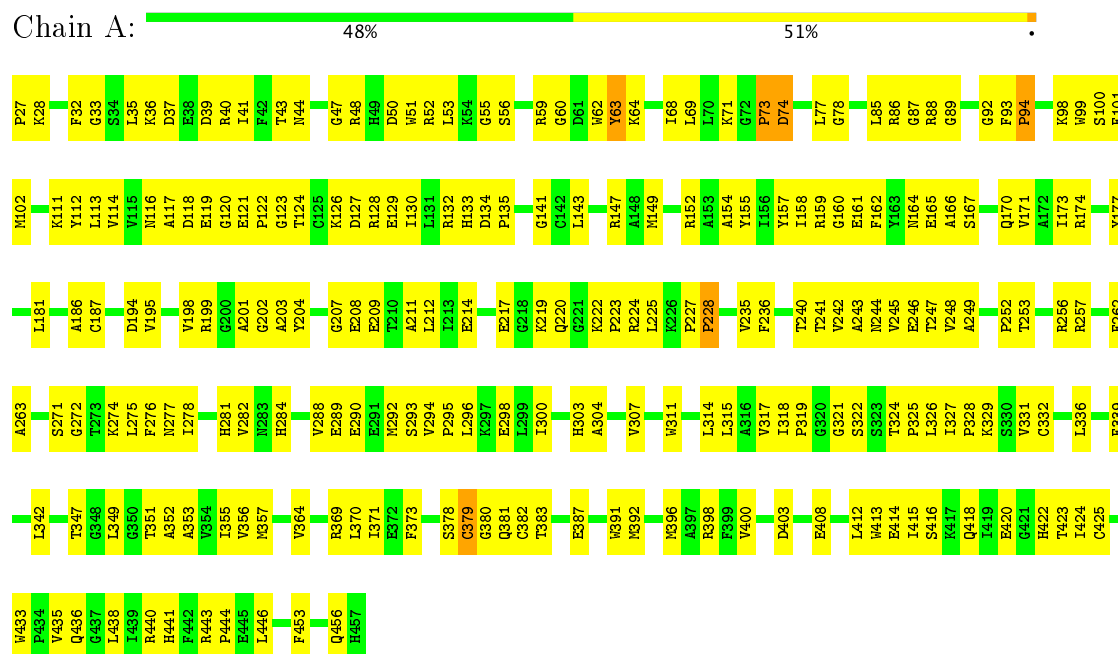


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 52 | V | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 52 | W | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 52 | l | 1 | Total | C | N | O | P | 0 |
| | | | 100 | 80 | 2 | 16 | 2 | |
| 52 | l | 1 | Total | C | N | O | P | 0 |
| | | | 100 | 80 | 2 | 16 | 2 | |

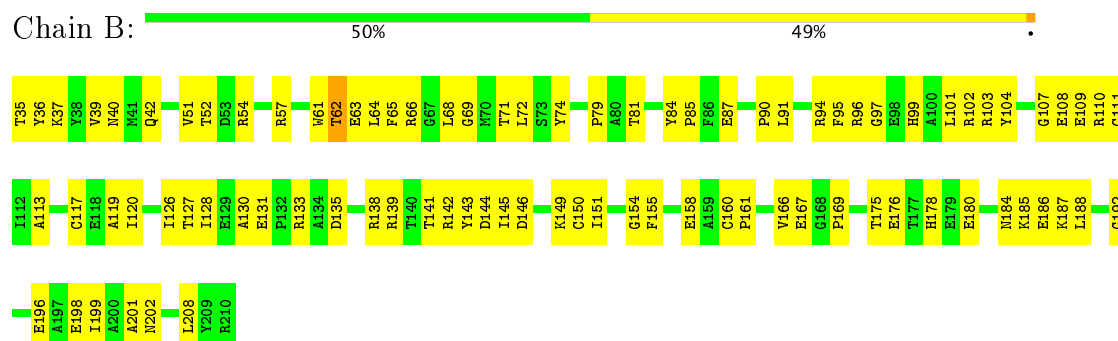
3 Residue-property plots

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: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



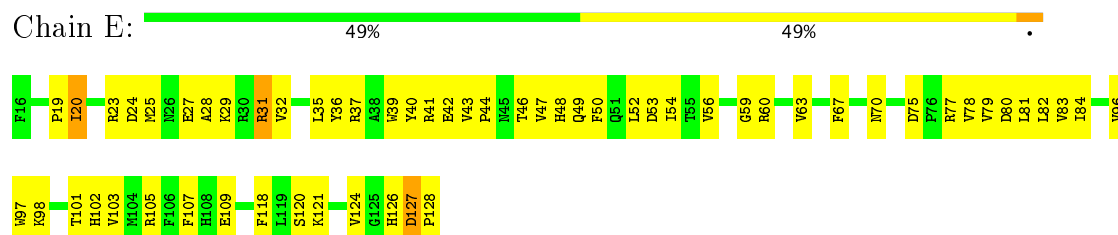
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



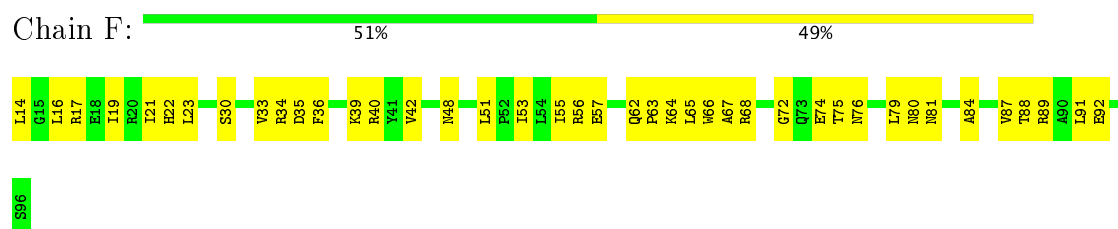
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



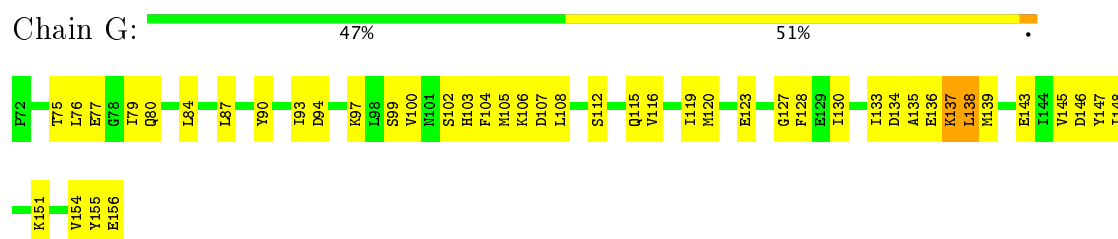
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



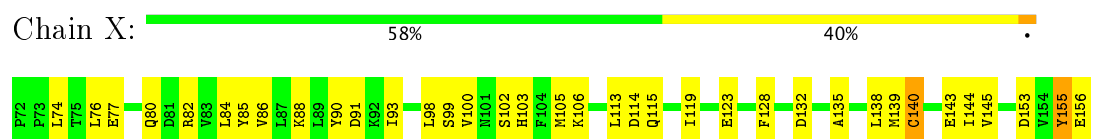
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



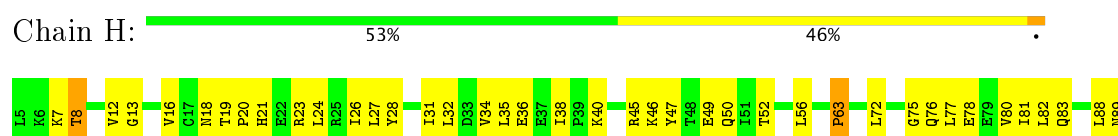
- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



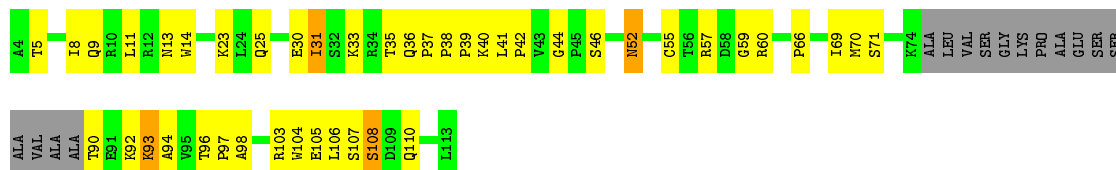
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5





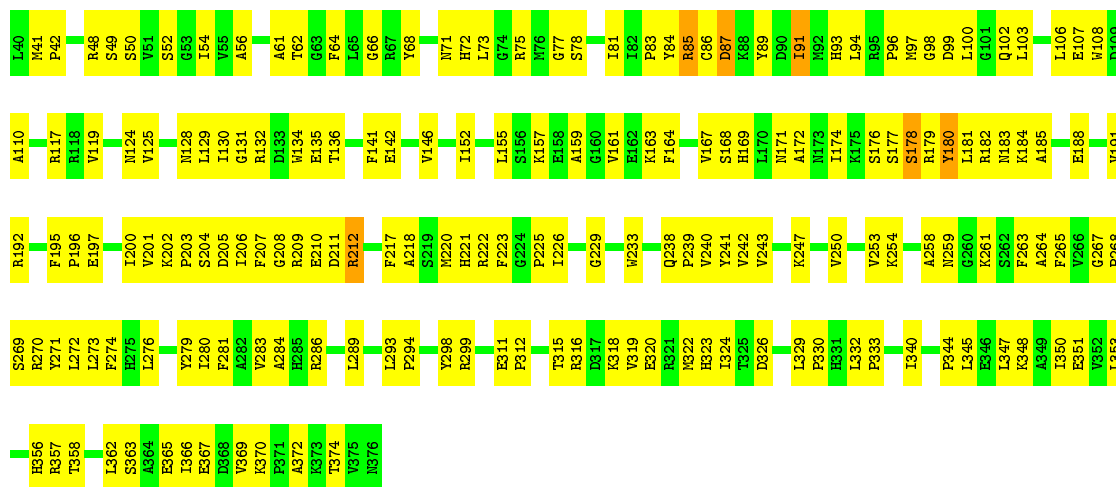
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain I: 46% 36% 14%



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

Chain J: 47% 51%



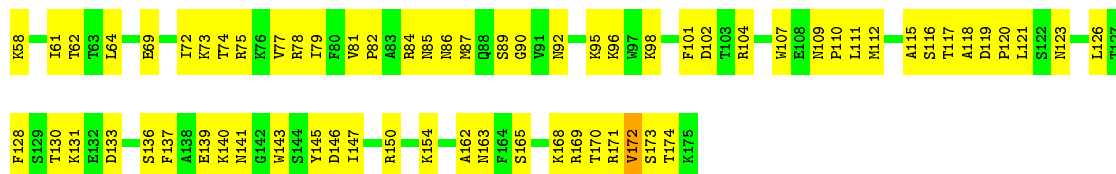
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K: 45% 45% 9%



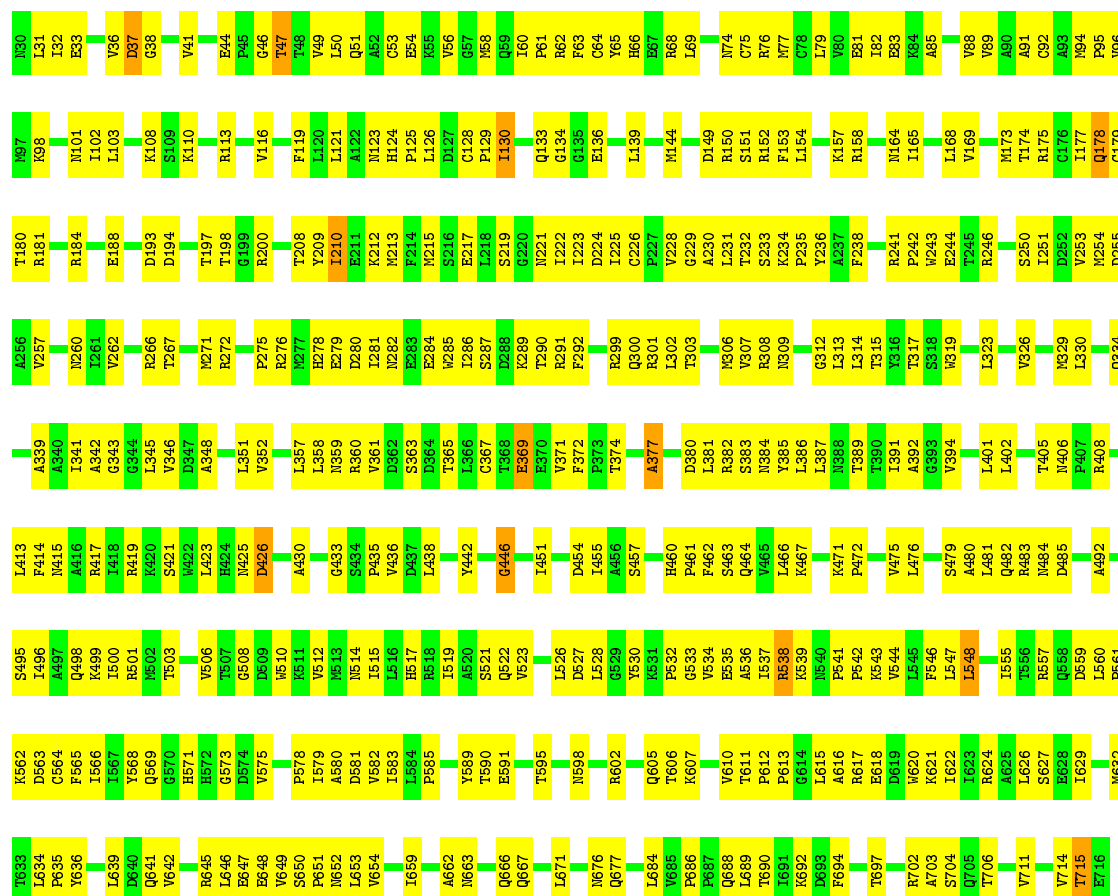
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L: 44% 55%



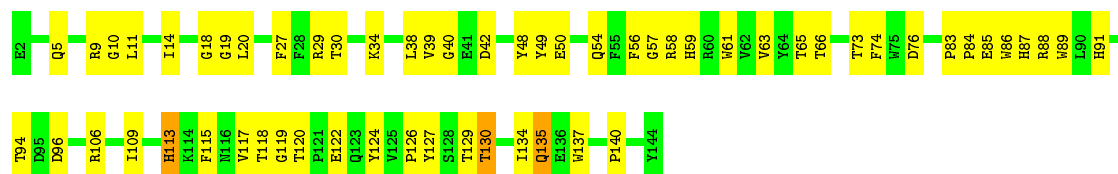
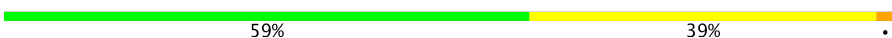
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:

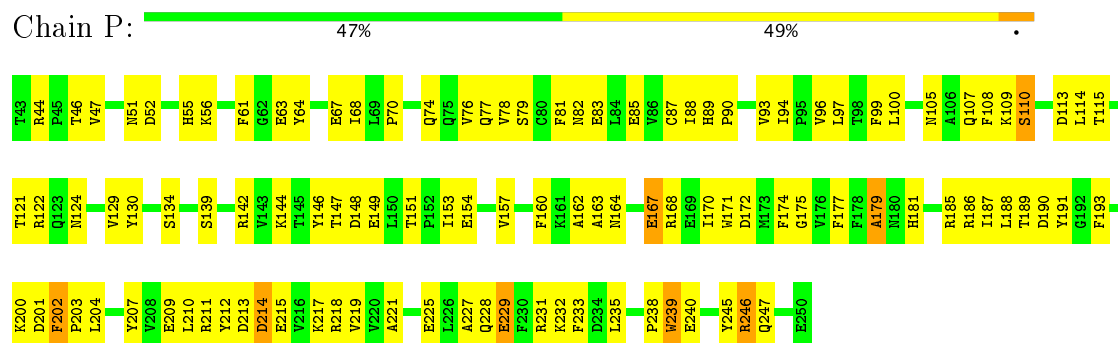


- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

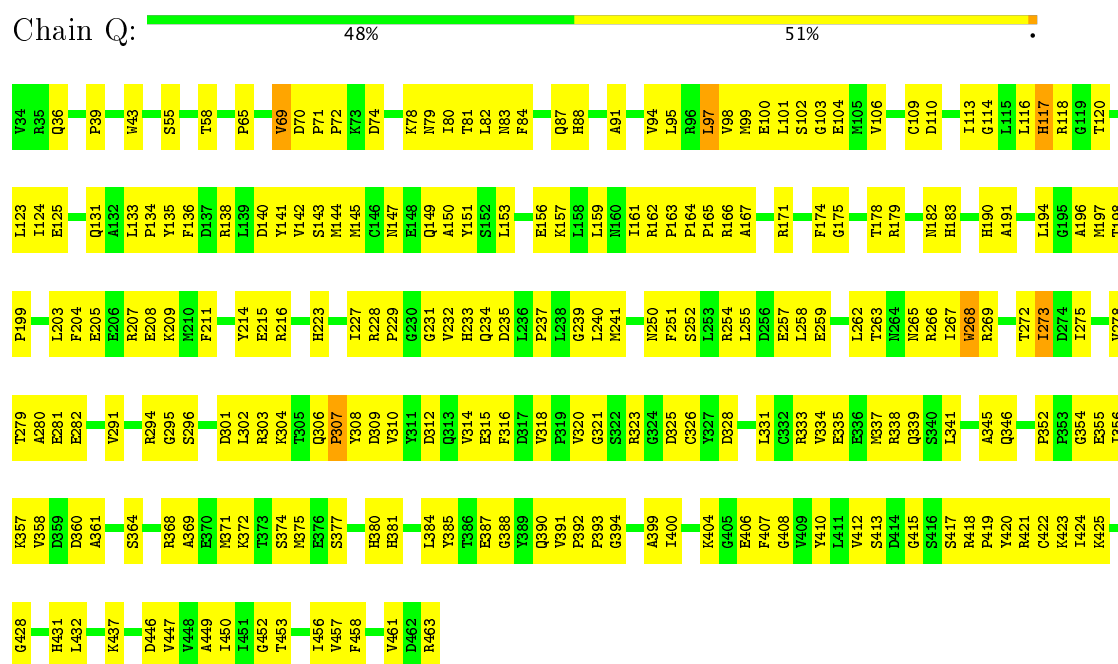
Chain 0:



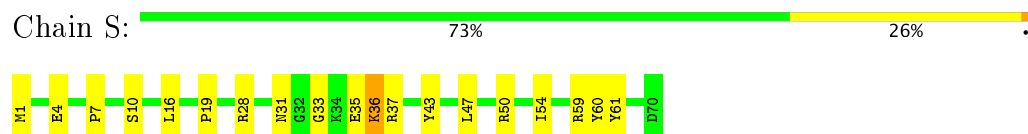
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



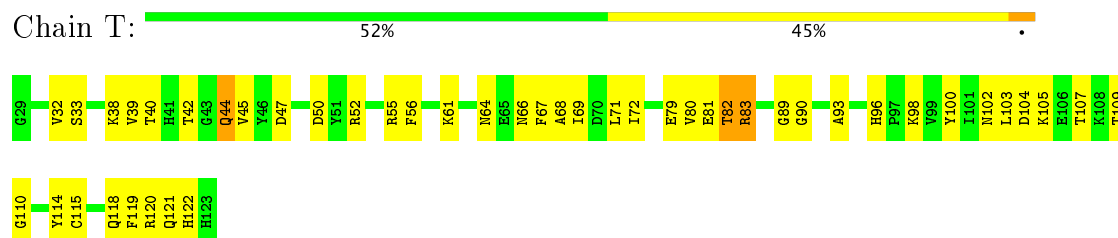
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



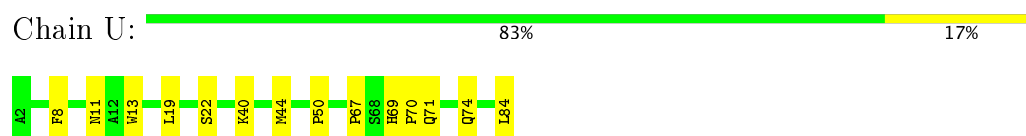
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



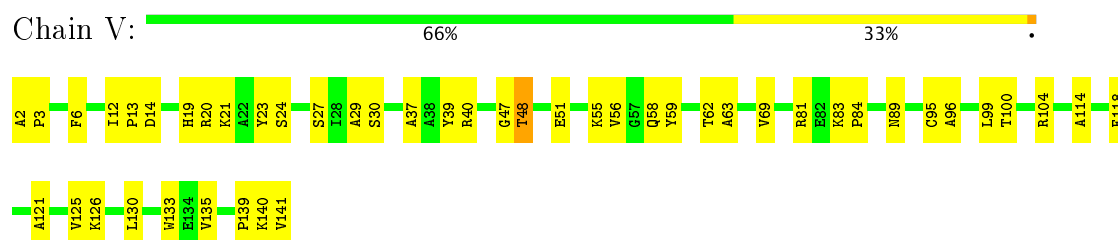
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



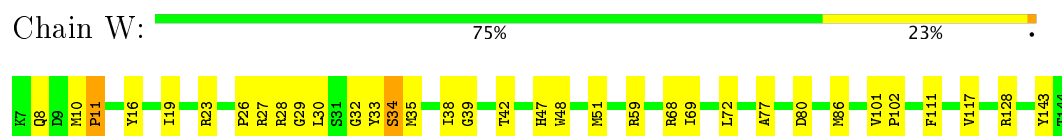
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



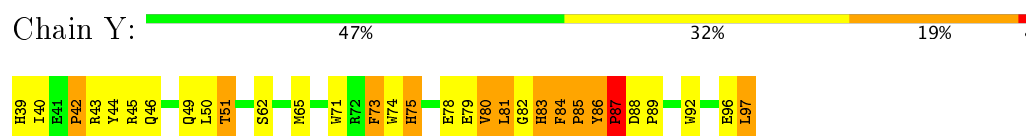
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



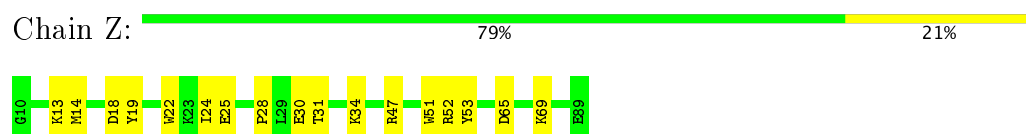
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



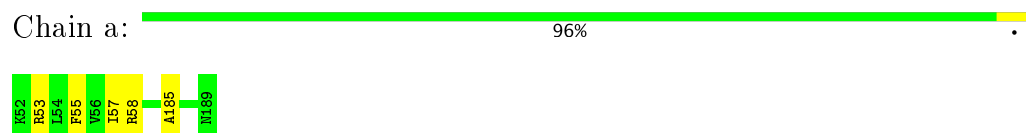
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



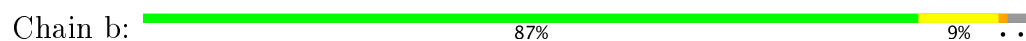
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6





- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 95% 5%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 95% 5%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 97%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 98%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 95% 5%



- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 94% 6%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i: 98%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 97%



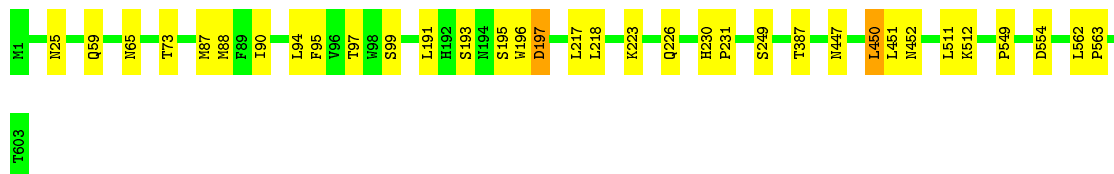
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 93%



- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l: 94%



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m: 94%



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 96%



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

Chain o: 97%



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

Chain p: 98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 98%



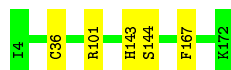
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 97%



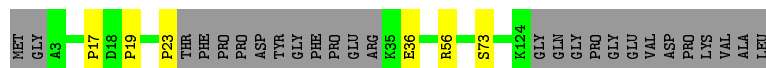
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 97%



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 77% 19%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w: 97%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 167761 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.25 | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, SF4, PLX, FMN, FES, 8Q1, PEE, NDP

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 | 0.30 | 0/3398 | 0.49 | 0/4590 |
| 10 | K | 0.27 | 0/282 | 0.47 | 0/381 |
| 11 | L | 0.33 | 0/987 | 0.53 | 0/1331 |
| 12 | M | 0.32 | 0/5362 | 0.53 | 0/7266 |
| 13 | N | 0.37 | 0/1236 | 0.55 | 0/1681 |
| 14 | O | 0.29 | 0/1682 | 0.51 | 0/2289 |
| 15 | P | 0.38 | 0/1780 | 0.59 | 0/2424 |
| 16 | Q | 0.43 | 0/3552 | 0.59 | 1/4815 (0.0%) |
| 17 | S | 0.60 | 0/583 | 0.64 | 0/785 |
| 18 | T | 0.31 | 0/755 | 0.47 | 0/1017 |
| 19 | U | 0.52 | 0/670 | 0.63 | 0/920 |
| 2 | B | 0.50 | 0/1452 | 0.57 | 0/1964 |
| 20 | V | 0.51 | 0/1065 | 0.61 | 0/1450 |
| 21 | W | 0.57 | 0/1166 | 0.66 | 0/1579 |
| 22 | Y | 0.52 | 0/559 | 0.73 | 3/763 (0.4%) |
| 23 | Z | 0.45 | 0/669 | 0.53 | 0/899 |
| 24 | a | 0.68 | 0/1209 | 0.65 | 0/1639 |
| 25 | b | 0.59 | 1/1095 (0.1%) | 0.69 | 4/1480 (0.3%) |
| 26 | c | 0.58 | 0/1287 | 0.58 | 0/1761 |
| 27 | d | 0.63 | 0/1445 | 0.65 | 1/1945 (0.1%) |
| 28 | e | 0.61 | 0/835 | 0.62 | 0/1134 |
| 29 | f | 0.48 | 0/418 | 0.58 | 0/566 |
| 3 | C | 0.58 | 0/1280 | 0.57 | 0/1732 |
| 30 | g | 0.64 | 0/1035 | 0.63 | 0/1398 |
| 31 | h | 0.62 | 0/884 | 0.65 | 0/1182 |
| 32 | i | 0.67 | 0/2808 | 0.77 | 2/3843 (0.1%) |
| 33 | j | 0.55 | 0/945 | 0.69 | 1/1292 (0.1%) |
| 34 | k | 0.68 | 1/751 (0.1%) | 0.79 | 1/1019 (0.1%) |
| 35 | l | 0.61 | 1/4840 (0.0%) | 0.69 | 3/6611 (0.0%) |
| 36 | m | 0.68 | 0/1346 | 0.67 | 0/1832 |
| 37 | n | 0.49 | 0/484 | 0.62 | 0/652 |
| 38 | o | 0.54 | 0/1093 | 0.61 | 0/1479 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 39 | p | 0.59 | 0/1549 | 0.59 | 0/2098 |
| 4 | E | 0.34 | 0/993 | 0.54 | 0/1335 |
| 40 | r | 0.70 | 0/3723 | 0.76 | 2/5089 (0.0%) |
| 41 | s | 0.62 | 0/2580 | 0.73 | 0/3539 |
| 42 | u | 0.57 | 0/1433 | 0.61 | 0/1937 |
| 43 | v | 0.48 | 0/934 | 0.67 | 3/1241 (0.2%) |
| 44 | w | 0.44 | 0/2533 | 0.56 | 0/3440 |
| 5 | F | 0.28 | 0/682 | 0.52 | 0/922 |
| 6 | G | 0.33 | 0/684 | 0.53 | 0/926 |
| 6 | X | 0.57 | 0/698 | 0.61 | 0/942 |
| 7 | H | 0.33 | 0/941 | 0.59 | 0/1275 |
| 8 | I | 0.29 | 0/788 | 0.54 | 0/1066 |
| 9 | J | 0.34 | 0/2785 | 0.52 | 0/3771 |
| All | All | 0.51 | 3/67276 (0.0%) | 0.62 | 21/91300 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 44 | w | 0 | 1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 25 | b | 118 | PRO | N-CD | 5.18 | 1.55 | 1.47 |
| 34 | k | 2 | PRO | N-CD | 5.14 | 1.55 | 1.47 |
| 35 | l | 231 | PRO | N-CD | 5.05 | 1.54 | 1.47 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32 | i | 323 | THR | C-N-CD | -7.37 | 104.38 | 120.60 |
| 22 | Y | 92 | TRP | N-CA-C | -7.00 | 92.10 | 111.00 |
| 27 | d | 2 | PRO | N-CA-CB | 6.79 | 111.44 | 103.30 |
| 22 | Y | 87 | PRO | CA-N-CD | -6.57 | 102.30 | 111.50 |
| 25 | b | 36 | PRO | C-N-CD | 6.22 | 141.46 | 128.40 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 44 | w | 338 | LYS | Peptide |

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 | 3322 | 0 | 3289 | 210 | 0 |
| 2 | B | 1420 | 0 | 1371 | 100 | 0 |
| 3 | C | 1249 | 0 | 1253 | 68 | 0 |
| 4 | E | 968 | 0 | 982 | 61 | 0 |
| 5 | F | 670 | 0 | 679 | 37 | 0 |
| 6 | G | 672 | 0 | 650 | 30 | 0 |
| 6 | X | 686 | 0 | 676 | 23 | 0 |
| 7 | H | 922 | 0 | 950 | 58 | 0 |
| 8 | I | 769 | 0 | 788 | 45 | 0 |
| 9 | J | 2712 | 0 | 2757 | 232 | 0 |
| 10 | K | 274 | 0 | 257 | 24 | 0 |
| 11 | L | 964 | 0 | 962 | 65 | 0 |
| 12 | M | 5274 | 0 | 5312 | 331 | 0 |
| 13 | N | 1195 | 0 | 1155 | 49 | 0 |
| 14 | O | 1643 | 0 | 1646 | 111 | 0 |
| 15 | P | 1730 | 0 | 1685 | 118 | 0 |
| 16 | Q | 3460 | 0 | 3419 | 252 | 0 |
| 17 | S | 568 | 0 | 567 | 15 | 0 |
| 18 | T | 742 | 0 | 723 | 40 | 0 |
| 19 | U | 647 | 0 | 653 | 10 | 0 |
| 20 | V | 1038 | 0 | 1027 | 34 | 0 |
| 21 | W | 1135 | 0 | 1129 | 33 | 0 |
| 22 | Y | 533 | 0 | 475 | 46 | 0 |
| 23 | Z | 648 | 0 | 627 | 13 | 0 |
| 24 | a | 1174 | 0 | 1177 | 0 | 0 |
| 25 | b | 1059 | 0 | 1079 | 0 | 0 |
| 26 | c | 1236 | 0 | 1092 | 0 | 0 |
| 27 | d | 1418 | 0 | 1375 | 0 | 0 |
| 28 | e | 810 | 0 | 772 | 0 | 0 |
| 29 | f | 405 | 0 | 407 | 0 | 0 |
| 30 | g | 1004 | 0 | 1008 | 0 | 0 |
| 31 | h | 863 | 0 | 861 | 0 | 0 |
| 32 | i | 2735 | 0 | 2893 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33 | j | 919 | 0 | 968 | 0 | 0 |
| 34 | k | 740 | 0 | 792 | 0 | 0 |
| 35 | l | 4717 | 0 | 4893 | 0 | 0 |
| 36 | m | 1313 | 0 | 1330 | 0 | 0 |
| 37 | n | 473 | 0 | 480 | 0 | 0 |
| 38 | o | 1066 | 0 | 1086 | 0 | 0 |
| 39 | p | 1495 | 0 | 1440 | 0 | 0 |
| 40 | r | 3629 | 0 | 3825 | 0 | 0 |
| 41 | s | 2509 | 0 | 2617 | 0 | 0 |
| 42 | u | 1394 | 0 | 1367 | 0 | 0 |
| 43 | v | 921 | 0 | 892 | 0 | 0 |
| 44 | w | 2474 | 0 | 2304 | 0 | 0 |
| 45 | A | 8 | 0 | 0 | 6 | 0 |
| 45 | B | 16 | 0 | 0 | 3 | 0 |
| 45 | C | 8 | 0 | 0 | 0 | 0 |
| 45 | M | 16 | 0 | 0 | 3 | 0 |
| 46 | A | 31 | 0 | 19 | 17 | 0 |
| 47 | B | 52 | 0 | 88 | 3 | 0 |
| 47 | U | 52 | 0 | 88 | 1 | 0 |
| 47 | V | 52 | 0 | 88 | 2 | 0 |
| 47 | b | 52 | 0 | 88 | 0 | 0 |
| 47 | g | 156 | 0 | 264 | 0 | 0 |
| 47 | r | 104 | 0 | 176 | 0 | 0 |
| 48 | E | 35 | 0 | 0 | 4 | 0 |
| 48 | p | 35 | 0 | 0 | 0 | 0 |
| 49 | J | 48 | 0 | 26 | 26 | 0 |
| 50 | M | 4 | 0 | 0 | 1 | 0 |
| 50 | O | 4 | 0 | 0 | 2 | 0 |
| 51 | V | 63 | 0 | 68 | 8 | 0 |
| 51 | i | 64 | 0 | 72 | 0 | 0 |
| 51 | l | 128 | 0 | 144 | 0 | 0 |
| 51 | n | 64 | 0 | 72 | 0 | 0 |
| 52 | V | 51 | 0 | 82 | 12 | 0 |
| 52 | W | 51 | 0 | 82 | 5 | 0 |
| 52 | l | 100 | 0 | 157 | 0 | 0 |
| All | All | 66789 | 0 | 67204 | 1752 | 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 27.

The worst 5 of 1752 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) |
|-------------------|------------------|--------------------------|-------------------|
| 9:J:130:ILE:HG23 | 49:J:401:NDP:C8A | 1.46 | 1.46 |
| 12:M:134:GLY:HA2 | 45:M:801:SF4:S3 | 1.57 | 1.42 |
| 16:Q:262:LEU:HD22 | 16:Q:268:TRP:CD1 | 1.64 | 1.32 |
| 9:J:206:ILE:HA | 9:J:240:VAL:O | 1.35 | 1.27 |
| 16:Q:82:LEU:O | 16:Q:98:VAL:HG13 | 1.25 | 1.26 |

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 | 429/431 (100%) | 396 (92%) | 24 (6%) | 9 (2%) | 8 | 49 |
| 2 | B | 174/176 (99%) | 163 (94%) | 10 (6%) | 1 (1%) | 28 | 70 |
| 3 | C | 154/156 (99%) | 136 (88%) | 13 (8%) | 5 (3%) | 5 | 40 |
| 4 | E | 111/113 (98%) | 101 (91%) | 8 (7%) | 2 (2%) | 10 | 52 |
| 5 | F | 81/83 (98%) | 74 (91%) | 7 (9%) | 0 | 100 | 100 |
| 6 | G | 83/85 (98%) | 78 (94%) | 3 (4%) | 2 (2%) | 7 | 46 |
| 6 | X | 83/85 (98%) | 73 (88%) | 6 (7%) | 4 (5%) | 2 | 29 |
| 7 | H | 110/112 (98%) | 100 (91%) | 5 (4%) | 5 (4%) | 3 | 31 |
| 8 | I | 91/110 (83%) | 79 (87%) | 6 (7%) | 6 (7%) | 1 | 22 |
| 9 | J | 335/337 (99%) | 314 (94%) | 14 (4%) | 7 (2%) | 8 | 49 |
| 10 | K | 31/33 (94%) | 27 (87%) | 1 (3%) | 3 (10%) | 1 | 12 |
| 11 | L | 116/118 (98%) | 104 (90%) | 8 (7%) | 4 (3%) | 4 | 39 |
| 12 | M | 685/687 (100%) | 608 (89%) | 54 (8%) | 23 (3%) | 4 | 39 |
| 13 | N | 141/143 (99%) | 119 (84%) | 15 (11%) | 7 (5%) | 2 | 28 |
| 14 | O | 210/212 (99%) | 188 (90%) | 15 (7%) | 7 (3%) | 4 | 39 |
| 15 | P | 206/208 (99%) | 173 (84%) | 22 (11%) | 11 (5%) | 2 | 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 16 | Q | 428/430 (100%) | 397 (93%) | 24 (6%) | 7 (2%) | 11 | 54 |
| 17 | S | 68/70 (97%) | 61 (90%) | 5 (7%) | 2 (3%) | 5 | 42 |
| 18 | T | 93/95 (98%) | 87 (94%) | 2 (2%) | 4 (4%) | 3 | 32 |
| 19 | U | 81/83 (98%) | 76 (94%) | 4 (5%) | 1 (1%) | 15 | 59 |
| 20 | V | 138/140 (99%) | 129 (94%) | 6 (4%) | 3 (2%) | 8 | 48 |
| 21 | W | 136/138 (99%) | 127 (93%) | 5 (4%) | 4 (3%) | 5 | 42 |
| 22 | Y | 57/59 (97%) | 50 (88%) | 1 (2%) | 6 (10%) | 0 | 10 |
| 23 | Z | 78/80 (98%) | 73 (94%) | 5 (6%) | 0 | 100 | 100 |
| 24 | a | 136/138 (99%) | 121 (89%) | 12 (9%) | 3 (2%) | 8 | 48 |
| 25 | b | 122/128 (95%) | 107 (88%) | 10 (8%) | 5 (4%) | 3 | 33 |
| 26 | c | 151/153 (99%) | 129 (85%) | 15 (10%) | 7 (5%) | 3 | 30 |
| 27 | d | 169/171 (99%) | 165 (98%) | 3 (2%) | 1 (1%) | 28 | 70 |
| 28 | e | 95/97 (98%) | 83 (87%) | 9 (10%) | 3 (3%) | 5 | 40 |
| 29 | f | 45/47 (96%) | 43 (96%) | 1 (2%) | 1 (2%) | 8 | 48 |
| 30 | g | 117/119 (98%) | 105 (90%) | 6 (5%) | 6 (5%) | 2 | 28 |
| 31 | h | 102/104 (98%) | 86 (84%) | 10 (10%) | 6 (6%) | 2 | 24 |
| 32 | i | 345/347 (99%) | 324 (94%) | 15 (4%) | 6 (2%) | 11 | 53 |
| 33 | j | 113/115 (98%) | 103 (91%) | 7 (6%) | 3 (3%) | 6 | 43 |
| 34 | k | 95/97 (98%) | 88 (93%) | 4 (4%) | 3 (3%) | 5 | 40 |
| 35 | l | 601/603 (100%) | 551 (92%) | 38 (6%) | 12 (2%) | 9 | 50 |
| 36 | m | 172/174 (99%) | 150 (87%) | 12 (7%) | 10 (6%) | 2 | 24 |
| 37 | n | 54/56 (96%) | 50 (93%) | 2 (4%) | 2 (4%) | 4 | 36 |
| 38 | o | 126/128 (98%) | 113 (90%) | 9 (7%) | 4 (3%) | 5 | 40 |
| 39 | p | 170/172 (99%) | 158 (93%) | 9 (5%) | 3 (2%) | 10 | 52 |
| 40 | r | 457/459 (100%) | 420 (92%) | 28 (6%) | 9 (2%) | 9 | 50 |
| 41 | s | 316/318 (99%) | 286 (90%) | 21 (7%) | 9 (3%) | 6 | 43 |
| 42 | u | 167/169 (99%) | 152 (91%) | 10 (6%) | 5 (3%) | 5 | 41 |
| 43 | v | 107/137 (78%) | 90 (84%) | 14 (13%) | 3 (3%) | 6 | 43 |
| 44 | w | 318/320 (99%) | 281 (88%) | 28 (9%) | 9 (3%) | 6 | 43 |
| All | All | 8097/8236 (98%) | 7338 (91%) | 526 (6%) | 233 (3%) | 9 | 42 |

5 of 233 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 63 | TYR |
| 1 | A | 73 | PRO |
| 1 | A | 379 | CYS |
| 2 | B | 62 | THR |
| 12 | M | 37 | ASP |

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 | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 346/346 (100%) | 346 (100%) | 0 | 100 | 100 |
| 2 | B | 151/151 (100%) | 151 (100%) | 0 | 100 | 100 |
| 3 | C | 132/132 (100%) | 132 (100%) | 0 | 100 | 100 |
| 4 | E | 106/106 (100%) | 105 (99%) | 1 (1%) | 82 | 92 |
| 5 | F | 74/74 (100%) | 74 (100%) | 0 | 100 | 100 |
| 6 | G | 74/79 (94%) | 74 (100%) | 0 | 100 | 100 |
| 6 | X | 78/79 (99%) | 78 (100%) | 0 | 100 | 100 |
| 7 | H | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 8 | I | 87/96 (91%) | 87 (100%) | 0 | 100 | 100 |
| 9 | J | 292/292 (100%) | 288 (99%) | 4 (1%) | 71 | 89 |
| 10 | K | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 11 | L | 107/107 (100%) | 107 (100%) | 0 | 100 | 100 |
| 12 | M | 576/577 (100%) | 574 (100%) | 2 (0%) | 94 | 98 |
| 13 | N | 129/129 (100%) | 129 (100%) | 0 | 100 | 100 |
| 14 | O | 181/181 (100%) | 181 (100%) | 0 | 100 | 100 |
| 15 | P | 190/190 (100%) | 190 (100%) | 0 | 100 | 100 |
| 16 | Q | 371/371 (100%) | 369 (100%) | 2 (0%) | 91 | 96 |
| 17 | S | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 18 | T | 79/79 (100%) | 79 (100%) | 0 | 100 | 100 |
| 19 | U | 72/72 (100%) | 72 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 20 | V | 102/102 (100%) | 102 (100%) | 0 | 100 | 100 |
| 21 | W | 119/119 (100%) | 119 (100%) | 0 | 100 | 100 |
| 22 | Y | 57/57 (100%) | 49 (86%) | 8 (14%) | 4 | 27 |
| 23 | Z | 62/63 (98%) | 62 (100%) | 0 | 100 | 100 |
| 24 | a | 124/124 (100%) | 122 (98%) | 2 (2%) | 68 | 88 |
| 25 | b | 118/122 (97%) | 114 (97%) | 4 (3%) | 42 | 75 |
| 26 | c | 124/137 (90%) | 124 (100%) | 0 | 100 | 100 |
| 27 | d | 145/154 (94%) | 137 (94%) | 8 (6%) | 25 | 64 |
| 28 | e | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 29 | f | 43/43 (100%) | 43 (100%) | 0 | 100 | 100 |
| 30 | g | 105/105 (100%) | 105 (100%) | 0 | 100 | 100 |
| 31 | h | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 32 | i | 314/314 (100%) | 314 (100%) | 0 | 100 | 100 |
| 33 | j | 102/103 (99%) | 102 (100%) | 0 | 100 | 100 |
| 34 | k | 85/85 (100%) | 82 (96%) | 3 (4%) | 41 | 75 |
| 35 | l | 531/532 (100%) | 511 (96%) | 20 (4%) | 38 | 73 |
| 36 | m | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 37 | n | 53/53 (100%) | 53 (100%) | 0 | 100 | 100 |
| 38 | o | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 39 | p | 157/157 (100%) | 156 (99%) | 1 (1%) | 89 | 95 |
| 40 | r | 416/416 (100%) | 416 (100%) | 0 | 100 | 100 |
| 41 | s | 278/278 (100%) | 278 (100%) | 0 | 100 | 100 |
| 42 | u | 153/153 (100%) | 153 (100%) | 0 | 100 | 100 |
| 43 | v | 89/121 (74%) | 89 (100%) | 0 | 100 | 100 |
| 44 | w | 249/288 (86%) | 249 (100%) | 0 | 100 | 100 |
| All | All | 7093/7209 (98%) | 7038 (99%) | 55 (1%) | 86 | 93 |

5 of 55 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | d | 55 | TYR |
| 27 | d | 117 | GLN |
| 35 | l | 226 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | d | 57 | TYR |
| 27 | d | 61 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | W | 112 | HIS |
| 27 | d | 113 | GLN |
| 42 | u | 104 | GLN |
| 22 | Y | 75 | HIS |
| 25 | b | 126 | GLN |

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](#)

30 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 45 | SF4 | A | 501 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 46 | FMN | A | 502 | - | 31,33,33 | 1.46 | 5 (16%) | 38,50,50 | 1.95 | 8 (21%) |
| 45 | SF4 | B | 301 | 2 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 45 | SF4 | B | 302 | 2 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 47 | PLX | B | 303 | - | 51,51,51 | 0.75 | 1 (1%) | 54,59,59 | 0.69 | 1 (1%) |
| 45 | SF4 | C | 301 | 3 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 48 | 8Q1 | E | 201 | - | 32,34,34 | 1.64 | 6 (18%) | 39,43,43 | 1.54 | 8 (20%) |
| 49 | NDP | J | 401 | - | 43,52,52 | 0.98 | 2 (4%) | 49,80,80 | 1.41 | 3 (6%) |
| 45 | SF4 | M | 801 | 12 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 45 | SF4 | M | 802 | 12 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 50 | FES | M | 803 | - | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 50 | FES | O | 301 | 14 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 47 | PLX | U | 101 | - | 51,51,51 | 0.73 | 1 (1%) | 54,59,59 | 0.74 | 2 (3%) |
| 51 | CDL | V | 201 | - | 61,61,99 | 1.24 | 5 (8%) | 60,71,111 | 0.99 | 3 (5%) |
| 52 | PEE | V | 202 | - | 50,50,50 | 0.87 | 4 (8%) | 52,55,55 | 0.85 | 2 (3%) |
| 47 | PLX | V | 203 | - | 51,51,51 | 0.77 | 1 (1%) | 54,59,59 | 0.61 | 1 (1%) |
| 52 | PEE | W | 201 | - | 50,50,50 | 0.86 | 4 (8%) | 52,55,55 | 0.92 | 2 (3%) |
| 47 | PLX | b | 201 | - | 51,51,51 | 0.60 | 0 | 54,59,59 | 0.64 | 0 |
| 47 | PLX | g | 201 | - | 51,51,51 | 0.81 | 1 (1%) | 54,59,59 | 0.69 | 1 (1%) |
| 47 | PLX | g | 202 | - | 51,51,51 | 0.74 | 1 (1%) | 54,59,59 | 0.62 | 1 (1%) |
| 47 | PLX | g | 203 | - | 51,51,51 | 0.77 | 1 (1%) | 54,59,59 | 0.59 | 1 (1%) |
| 51 | CDL | i | 401 | - | 63,63,99 | 1.19 | 5 (7%) | 65,75,111 | 1.10 | 5 (7%) |
| 52 | PEE | l | 701 | - | 48,48,50 | 1.02 | 2 (4%) | 50,53,55 | 0.89 | 2 (4%) |
| 52 | PEE | l | 702 | - | 50,50,50 | 0.88 | 4 (8%) | 52,55,55 | 0.93 | 2 (3%) |
| 51 | CDL | l | 703 | - | 63,63,99 | 1.19 | 5 (7%) | 65,75,111 | 1.12 | 4 (6%) |
| 51 | CDL | l | 704 | - | 63,63,99 | 1.24 | 5 (7%) | 65,75,111 | 1.06 | 4 (6%) |
| 51 | CDL | n | 101 | - | 63,63,99 | 1.22 | 5 (7%) | 65,75,111 | 1.12 | 4 (6%) |
| 48 | 8Q1 | p | 201 | - | 32,34,34 | 1.67 | 5 (15%) | 39,43,43 | 1.80 | 5 (12%) |
| 47 | PLX | r | 501 | - | 51,51,51 | 0.74 | 1 (1%) | 54,59,59 | 0.66 | 1 (1%) |
| 47 | PLX | r | 502 | - | 51,51,51 | 0.67 | 0 | 54,59,59 | 0.67 | 1 (1%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 45 | SF4 | A | 501 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 46 | FMN | A | 502 | - | - | 0/16/18/18 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 45 | SF4 | B | 301 | 2 | - | 0/0/48/48 | 0/6/5/5 |
| 45 | SF4 | B | 302 | 2 | - | 0/0/48/48 | 0/6/5/5 |
| 47 | PLX | B | 303 | - | - | 0/54/55/55 | 0/0/0/0 |
| 45 | SF4 | C | 301 | 3 | - | 0/0/48/48 | 0/6/5/5 |
| 48 | 8Q1 | E | 201 | - | - | 2/41/41/41 | 0/0/0/0 |
| 49 | NDP | J | 401 | - | - | 0/30/77/77 | 0/5/5/5 |
| 45 | SF4 | M | 801 | 12 | - | 0/0/48/48 | 0/6/5/5 |
| 45 | SF4 | M | 802 | 12 | - | 0/0/48/48 | 0/6/5/5 |
| 50 | FES | M | 803 | - | - | 0/0/4/4 | 0/1/1/1 |
| 50 | FES | O | 301 | 14 | - | 0/0/4/4 | 0/1/1/1 |
| 47 | PLX | U | 101 | - | - | 0/54/55/55 | 0/0/0/0 |
| 51 | CDL | V | 201 | - | - | 0/69/69/110 | 0/0/0/0 |
| 52 | PEE | V | 202 | - | - | 0/54/54/54 | 0/0/0/0 |
| 47 | PLX | V | 203 | - | - | 0/54/55/55 | 0/0/0/0 |
| 52 | PEE | W | 201 | - | - | 0/54/54/54 | 0/0/0/0 |
| 47 | PLX | b | 201 | - | - | 0/54/55/55 | 0/0/0/0 |
| 47 | PLX | g | 201 | - | - | 0/54/55/55 | 0/0/0/0 |
| 47 | PLX | g | 202 | - | - | 0/54/55/55 | 0/0/0/0 |
| 47 | PLX | g | 203 | - | - | 0/54/55/55 | 0/0/0/0 |
| 51 | CDL | i | 401 | - | - | 0/74/74/110 | 0/0/0/0 |
| 52 | PEE | l | 701 | - | - | 0/52/52/54 | 0/0/0/0 |
| 52 | PEE | l | 702 | - | - | 0/54/54/54 | 0/0/0/0 |
| 51 | CDL | l | 703 | - | - | 0/74/74/110 | 0/0/0/0 |
| 51 | CDL | l | 704 | - | - | 0/74/74/110 | 0/0/0/0 |
| 51 | CDL | n | 101 | - | - | 2/74/74/110 | 0/0/0/0 |
| 48 | 8Q1 | p | 201 | - | - | 2/41/41/41 | 0/0/0/0 |
| 47 | PLX | r | 501 | - | - | 0/54/55/55 | 0/0/0/0 |
| 47 | PLX | r | 502 | - | - | 0/54/55/55 | 0/0/0/0 |

The worst 5 of 64 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 47 | B | 303 | PLX | O6-C4 | -2.89 | 1.40 | 1.44 |
| 47 | g | 203 | PLX | O6-C4 | -2.85 | 1.40 | 1.44 |
| 47 | V | 203 | PLX | O6-C4 | -2.75 | 1.40 | 1.44 |
| 47 | g | 201 | PLX | O6-C4 | -2.72 | 1.40 | 1.44 |
| 51 | n | 101 | CDL | OB6-CB4 | -2.64 | 1.39 | 1.46 |

The worst 5 of 61 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 49 | J | 401 | NDP | N3A-C2A-N1A | -6.95 | 122.81 | 128.86 |
| 48 | p | 201 | 8Q1 | O4-C1-C6 | -4.85 | 119.70 | 123.95 |
| 46 | A | 502 | FMN | C4-C4A-C10 | -3.94 | 116.78 | 119.96 |
| 46 | A | 502 | FMN | C4A-C4-N3 | -3.39 | 118.66 | 123.48 |
| 48 | E | 201 | 8Q1 | O4-C1-C6 | -3.37 | 121.00 | 123.95 |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 48 | E | 201 | 8Q1 | C29-C32-C34-N36 |
| 48 | E | 201 | 8Q1 | O35-C34-C32-C29 |
| 51 | n | 101 | CDL | CA4-OA6-CA5-OA7 |
| 51 | n | 101 | CDL | CA4-OA6-CA5-C11 |
| 48 | p | 201 | 8Q1 | C6-C1-S44-C43 |

There are no ring outliers.

15 monomers are involved in 93 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 45 | A | 501 | SF4 | 6 | 0 |
| 46 | A | 502 | FMN | 17 | 0 |
| 45 | B | 301 | SF4 | 1 | 0 |
| 45 | B | 302 | SF4 | 2 | 0 |
| 47 | B | 303 | PLX | 3 | 0 |
| 48 | E | 201 | 8Q1 | 4 | 0 |
| 49 | J | 401 | NDP | 26 | 0 |
| 45 | M | 801 | SF4 | 3 | 0 |
| 50 | M | 803 | FES | 1 | 0 |
| 50 | O | 301 | FES | 2 | 0 |
| 47 | U | 101 | PLX | 1 | 0 |
| 51 | V | 201 | CDL | 8 | 0 |
| 52 | V | 202 | PEE | 12 | 0 |
| 47 | V | 203 | PLX | 2 | 0 |
| 52 | W | 201 | PEE | 5 | 0 |

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.