

Dec 10, 2022 – 09:31 am GMT

| PDB ID | : | 4UQ8 |
|--------------|---|--|
| EMDB ID | : | EMD-2676 |
| Title | : | Electron cryo-microscopy of bovine Complex I |
| Authors | : | Vinothkumar, K.R.; Zhu, J.; Hirst, J. |
| Deposited on | : | 2014-06-21 |
| Resolution | : | 4.95 Å(reported) |
| | | |

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

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

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

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

| EMDB validation analysis | : | 0.0.1. dev 43 |
|--------------------------------|---|--|
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.95 Å.

Ramachandran outliers

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 | Percentile Ranks | Value |
|-----------------------|--------------------------|--|
| Ramachandran outliers | | 12.5% |
| Sidechain outliers | | 25.0% |
| Worse | Better | |
| Percentile relation | ive to all structures | |
| Percentile relat | ive to all EM structures | |
| Metric | [| ${f EM\ structures}\ (\#{ m Entries})$ |

154571

| Sidechain outliers | 154315 | 3826 | |
|-----------------------------|-------------------------|-------------------------|---------------------------------|
| | | | |
| The table below summaris | es the geometric issue | es observed across the | polymeric chains and their fit |
| to the map. The red, oran | ge, yellow and green | segments of the bar in | dicate the fraction of residues |
| that contain outliers for > | >=3, 2, 1 and 0 type | s of geometric quality | criteria respectively. A grey |
| segment represents the fr | action of residues th | at are not modelled. | The numeric value for each |
| fraction is indicated below | w the corresponding | segment, with a dot | representing fractions $<=5\%$ |
| The upper red bar (where | present) indicates th | ne fraction of residues | that have poor fit to the EM |
| map (all-atom inclusion < | (40%). The numeric | value is given above t | the bar. |

4023

| Mol | Chain | Length | Quality of chain | |
|-----|-------|--------|------------------|-----|
| 1 | А | 111 | • 75% 25% | |
| 2 | В | 143 | 97% | ••• |
| 3 | С | 154 | 99% | • |
| 4 | D | 384 | 100% | |
| 5 | Е | 159 | 100% | |
| 6 | F | 411 | <u>8%</u> 99% | - |
| 7 | G | 538 | 96% | •• |
| 8 | Н | 313 | 91% | % |
| 9 | Ι | 162 | 97% | • |

Continued on next page...



Continued from previous page... Chain Length Quality of chain Mol 10% 10 J 17177% 23% Κ 11 84 100% 7% 12L 601 92% • 7% М 1345397% • 6% 14Ν 34594% • 6% • 15Ο 22081% 18% 6% Р 16303 82% 17% • 17Q 85• 80% 19% R 18 47100% \mathbf{S} 1980 99% 13% Т 20755% 95% • 79U 2195% 5% ÷ 22V 71100% 7% 23W 7299% . Х 792499% 15% 25Υ 106100% Ζ 2665100% 17% 2927 \mathbf{a} 100% 5% 28b 42 100% 2927 \mathbf{c} 100% 2927W 100% 30 39 d 100% 10% 31 20е 100% 32f 30 100% 7% 32 h 30 100%

Continued on next page...



| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 32 | i | 30 | 7%100% |
| 33 | g | 22 | 100% |
| 34 | j | 24 | 100% |
| 34 | 1 | 24 | 100% |
| 35 | k | 28 | 100% |
| 35 | р | 28 | 100% |
| 35 | s | 28 | 100% |
| 36 | m | 34 | 100% |
| 37 | n | 59 | 100% |
| 38 | 0 | 21 | 100% |
| 39 | q | 25 | 100% |
| 40 | r | 26 | 100% |
| 41 | t | 57 | 100% |
| 42 | u | 43 | 35% 65% |
| 43 | V | 32 | 100% |

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2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 28647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 1 | А | 83 | Total 415 | C 249 | N 83 | O 83 | 0 | 0 |

• Molecule 2 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 2 | В | 143 | Total 719 | C 429 | N 143 | 0 143 | $\frac{S}{4}$ | 0 | 0 |

• Molecule 3 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 3 | С | 154 | Total 770 | C 462 | N 154 | O 154 | 0 | 0 |

• Molecule 4 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 2, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 4 | Л | 384 | Total | С | N | Ō | 0 | 0 |
| 4 | D | 304 | 1920 | 1152 | 384 | 384 | 0 | 0 |

• Molecule 5 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPRO-TEIN 2, MITOCHONDRIAL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 5 | Е | 159 | Total 799 | C 477 | N 159 | O 159 | ${S \atop 4}$ | 0 | 0 |

• Molecule 6 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPRO-TEIN 1, MITOCHONDRIAL.



| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------------|---------|-------|
| 6 | F | 411 | Total 2059 | C 1233 | N 411 | 0 411 | $\frac{S}{4}$ | 0 | 0 |

• Molecule 7 is a protein called NADH-UBIQUINONE OXIDOREDUCTASE 75 KDA SUB-UNIT, MITOCHONDRIAL.

| Mol | Chain | Residues | | At | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---|---|
| 7 | G | 527 | Total 2651 | C 1584 | N 529 | O 527 | S 11 | 0 | 0 |

• Molecule 8 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|-------|
| 8 | Н | 285 | Total 1425 | C 855 | N 285 | O 285 | 0 | 0 |

• Molecule 9 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|
| 9 | Ι | 162 | Total 818 | C 486 | N 162 | 0 162 | S 8 | 0 | 0 |

• Molecule 10 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 10 | J | 131 | Total 655 | C 393 | N 131 | 0 131 | 0 | 0 |

• Molecule 11 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4L.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 11 | Κ | 84 | Total 420 | C 252 | N 84 | O 84 | 0 | 0 |

• Molecule 12 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 5.

| Mol | Chain | Residues | | Aton | AltConf | Trace | | |
|-----|-------|----------|---------------|-----------|----------|----------|---|---|
| 12 | L | 558 | Total 2790 | C 1674 | N 558 | O 558 | 0 | 0 |

• Molecule 13 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4.



| Mol | Chain | Residues | | Ator | AltConf | Trace | | |
|-----|-------|----------|---------------|-----------|----------|----------|---|---|
| 13 | М | 439 | Total 2195 | C 1317 | N 439 | O 439 | 0 | 0 |

• Molecule 14 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 2.

| Mol | Chain | Residues | | Ato | ms | AltConf | Trace | |
|-----|-------|----------|---------------|----------|----------|----------|-------|---|
| 14 | Ν | 326 | Total 1630 | C 978 | N 326 | O 326 | 0 | 0 |

• Molecule 15 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 10.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 15 | О | 181 | Total 905 | C 543 | N 181 | 0 181 | 0 | 0 |

• Molecule 16 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 9, MITOCHONDRIAL.

| Mol | Chain | Residues | | Ato | ms | AltConf | Trace | |
|-----|-------|----------|---------------|----------|----------|----------|-------|---|
| 16 | Р | 252 | Total 1260 | C 756 | N 252 | O 252 | 0 | 0 |

• Molecule 17 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 4.

| Mol | Chain | Residues | | Aton | ıs | AltConf | Trace | |
|-----|-------|----------|--------------|----------|---------|---------|-------|---|
| 17 | Q | 69 | Total 345 | C 207 | N 69 | O 69 | 0 | 0 |

• Molecule 18 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 18 | R | 47 | Total 235 | C 141 | N 47 | O 47 | 0 | 0 |

• Molecule 19 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 2.

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

• Molecule 20 is a protein called ACYL CARRIER PROTEIN, MITOCHONDRIAL.



| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 20 | Т | 71 | Total 355 | C 213 | N 71 | 0 71 | 0 | 0 |

• Molecule 21 is a protein called NADH UBIQUINONE DEHYDROGENASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 21 | U | 75 | Total 375 | C 225 | N 75 | O 75 | 0 | 0 |

• Molecule 22 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 22 | V | 71 | Total 355 | C 213 | N 71 | 0 71 | 0 | 0 |

• Molecule 23 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 23 | W | 72 | Total 360 | C 216 | N 72 | О 72 | 0 | 0 |

• Molecule 24 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 24 | Х | 79 | Total 395 | C 237 | N 79 | O 79 | 0 | 0 |

• Molecule 25 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 11.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 25 | Y | 106 | Total 530 | C 318 | N 106 | O 106 | 0 | 0 |

• Molecule 26 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 26 | Z | 65 | Total 325 | C 195 | N 65 | O 65 | 0 | 0 |



• Molecule 27 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|-------|
| 27 | a | 29 | Total 145 | C 87 | N 29 | O 29 | 0 | 0 |

• Molecule 28 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 28 | b | 42 | Total 210 | C 126 | N 42 | O 42 | 0 | 0 |

• Molecule 29 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 29 | с | 27 | Total | С | Ν | 0 | 0 | 0 |
| | | | 135 | 81 | 27 | 27 | Ŭ | |
| 20 | 117 | 27 | Total | С | Ν | 0 | 0 | 0 |
| 29 | W | 21 | 135 | 81 | 27 | 27 | 0 | 0 |

• Molecule 30 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 30 | d | 39 | Total 195 | C 117 | N 39 | O 39 | 0 | 0 |

• Molecule 31 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|-------|
| 31 | е | 20 | Total 100 | C 60 | N 20 | O 20 | 0 | 0 |

• Molecule 32 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|-----|-------|----------|-----------------|---------|-------|
| 30 | f | 30 | Total C N O | 0 | 0 |
| 52 | 1 | 50 | 150 90 30 30 | 0 | 0 |
| 30 | h | 30 | Total C N O | 0 | 0 |
| 52 | 11 | 50 | 150 90 30 30 | 0 | 0 |
| 20 | ; | 20 | Total C N O | 0 | 0 |
| 02 | | 50 | 150 90 30 30 | | 0 |

• Molecule 33 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.



| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|-------|
| 33 | g | 22 | Total 110 | C 66 | N 22 | O 22 | 0 | 0 |

• Molecule 34 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|------|-------|----------|-------|----|----|----|---------|-------|
| 24 | ; | 24 | Total | С | Ν | 0 | 0 | 0 |
| - 34 | J | 24 | 120 | 72 | 24 | 24 | 0 | 0 |
| 24 | 1 | 24 | Total | С | Ν | 0 | 0 | 0 |
| 04 | 1 | 24 | 120 | 72 | 24 | 24 | 0 | 0 |

• Molecule 35 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atom | s | AltConf | Trace |
|-----|-------|----------|---------------------|--------------|---------|-------|
| 35 | k | 28 | Total C 140 84 2 | N O 28 28 | 0 | 0 |
| 35 | р | 28 | Total C 140 84 2 | N O 28 28 | 0 | 0 |
| 35 | S | 28 | Total C 140 84 2 | N O 28 28 | 0 | 0 |

• Molecule 36 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | | Aton | ıs | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 36 | m | 34 | Total 170 | C 102 | N 34 | O 34 | 0 | 0 |

• Molecule 37 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 37 | n | 59 | Total 295 | C 177 | N 59 | O 59 | 0 | 0 |

• Molecule 38 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|-------|
| 38 | 0 | 21 | Total 105 | C 63 | N 21 | O 21 | 0 | 0 |

• Molecule 39 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.



| Mol | Chain | Residues | L | Ator | \mathbf{ns} | | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------------|---------|---------|-------|
| 39 | q | 25 | Total 125 | C 75 | N 25 | O 25 | 0 | 0 |

• Molecule 40 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|-------|
| 40 | r | 26 | Total 130 | C 78 | N 26 | O 26 | 0 | 0 |

• Molecule 41 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|
| 41 | t | 57 | Total 285 | C 171 | N 57 | O 57 | 0 | 0 |

• Molecule 42 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | 1 | Ator | ns | | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|---------|---------|-------|
| 42 | u | 15 | Total 75 | C 45 | N 15 | O 15 | 0 | 0 |

• Molecule 43 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms | | AltConf | Trace | | |
|-----|-------|----------|--------------|---------|---------|---------|---|---|
| 43 | V | 32 | Total 160 | C 96 | N 32 | O 32 | 0 | 0 |

• Molecule 44 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).





| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|----------------------|---------|
| 44 | В | 1 | Total Fe S 8 4 4 | 0 |
| 44 | F | 1 | TotalFeS844 | 0 |
| 44 | G | 1 | TotalFeS1688 | 0 |
| 44 | G | 1 | Total Fe S 16 8 8 | 0 |
| 44 | Ι | 1 | Total Fe S 16 8 8 | 0 |
| 44 | Ι | 1 | TotalFeS1688 | 0 |

• Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).





| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------|---------|
| 45 | Е | 1 | Total Fe S | 0 |
| | | | 4 2 2 | |
| 45 | C | C 1 | Total Fe S | 0 |
| 40 | G | I | 4 2 2 | 0 |



3 Residue-property plots (i)

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

• Molecule 1: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 3



 \bullet Molecule 2: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL



 \bullet Molecule 3: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL



Chain E:

100%



X20 X101 X130 X130 X146 X158

 \bullet Molecule 6: NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 1, MITOCHONDRIAL



 \bullet Molecule 7: NADH-UBIQUINONE OXIDOREDUCTASE 75 KDA SUBUNIT, MITOCHONDRIAL



• Molecule 8: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1

| Chain H: | 91% | 9% |
|---|---|---|
| X3 X47 X47 X50 X64 X65 X65 X65 X65 X65 X65 X65 X65 X65 X75 X10 X105 | X127 X128 X128 X158 X158 X158 X158 X158 V100 V100 V100 V100 V100 V100 V100 V10 | 0.0.0K 0.01K 0.01K 0.01K 0.01K 0.01K 0.01K 0.01K 0.01K 0.01K |

 \bullet Molecule 9: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL



UNK UNK UNK UNK UNK UNK UNK UNK

• Molecule 11: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4L

| Chain K: | 100% | • |
|---|--|--|
| X1 X56 X74 X74 X75 X75 | | |
| • Molecule 12: N | ADH UBIQUINONE OXIDOREDUCTASE CHAIN 5 | |
| Chain L: | 92% · 7% | 1 |
| X4 X9 X47 X133 X133 | x143 x146 x146 x211 x227 x224 x225 x255 x255 x254 x254 x254 x254 x255 x254 x254 x255 x254 x255 x254 x255 x256 x256 x256 x256 x257 x257 x257 x257 x257 x256 x257 x257 x256 x257 x256 x256 x256 x257 x256 x276 x277 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x276 x277 x276 x277 x277 x276 x277 | X385 X388 X388 X389 X399 X399 |
| X415 X416 X417 X417 X418 X418 X416 X496 X493 | X530 X546 X546 X562 X562 X564 X562 X564 X604 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK | UNK UNK UNK UNK UNK UNK UNK |
| UNK UNK UNK UNK UNK UNK UNK | | |
| • Molecule 13: N | ADH UBIQUINONE OXIDOREDUCTASE CHAIN 4 | |
| Chain M: | 97% | - |
| X3 X86 X87 X88 X88 X88 X88 X88 X88 X88 X83 X13 | x224 x257 x258 x276 x276 x281 x311 x311 x311 x332 x332 x312 x311 x332 x312 x31 | |
| • Molecule 14: N | ADH UBIQUINONE OXIDOREDUCTASE CHAIN 2 | |
| Chain N: | 94% • 6% |) |
| X2 X46 X81 X81 X87 X91 X92 | x125 x126 x157 x129 x157 x228 x225 x225 x225 x225 x233 x233 x233 x233 | UNK UNK UNK UNK UNK UNK UNK UNK |
| UNK UNK | | |
| • Molecule 15: N UNIT 10 | NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA | SUBCOMPLEX SUB- |
| Chain O: | 81% • 18% | |





 \bullet Molecule 16: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 9, MITOCHONDRIAL

| Chain P: | 82% | • 17% | _ |
|---|--|--|---|
| X19 X25 X39 X42 X60 X60 X100 X100 | x130 x138 x138 x139 x140 x140 x160 x160 x173 x173 x223 x223 x225 x225 | X226 X227 X228 X2296 X296 X313 X317 X313 X317 X317 X317 VUK | UNK UNK UNK UNK UNK UNK UNK UNK UNK |
| UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK | UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK | | |
| • Molecule 17: NADI | H DEHYDROGENASE [UBI | QUINONE] SUBUNIT | · 4 |
| Chain Q: | 80% | • 19% | _ |
| X32 X40 UNK UNK UNK UNK UNK UNK UNK UNK | UNK UNK UNK UNK UNK | | |
| • Molecule 18: NADI | H DEHYDROGENASE [UBI | QUINONE] SUBUNIT | 6 |
| Chain R: | 100% | | - |
| There are no outlier | residues recorded for this chai | n. | |
| • Molecule 19: NAD UNIT 2 | H DEHYDROGENASE [UB] | IQUINONE] 1 ALPHA | A SUBCOMPLEX SUB- |
| Chain S: | 99% | | - |
| X17 X51 X71 X75 X75 X75 X96 | | | |
| • Molecule 20: ACYI | CARRIER PROTEIN, MIT | OCHONDRIAL | |
| Chain T: | 95% | 5 | 5% |
| X8 X13 X20 X40 X40 X60 X60 | X63 X63 X82 WWK UNK UNK | | |
| • Molecule 21: NADI | H UBIQUINONE DEHYDRC | GENASE | |
| Chain U: | 95% | | 5% |
| UNK UNK UNK VNK X8 X27 X27 X69 X69 A82 | | | |

 \bullet Molecule 22: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 5



| Chain V: | 100% | |
|--|---|-----------------|
| X1 X23 X43 X53 X53 | | |
| • Molecule 23: UNIT; 6 | NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA | SUBCOMPLEX SUB- |
| Chain W: | 99% | - |
| X1 X13 X13 X38 X38 X40 X41 X41 X42 | x61 x772 | |
| • Molecule 24: UNIT 8 | NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA | SUBCOMPLEX SUB- |
| Chain X: | 99% | |
| X35 X56 X73 | | |
| • Molecule 25: UNIT; 11 | NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA | SUBCOMPLEX SUB- |
| Chain Y: | 100% | • |
| X1 X14 X15 X17 X17 X18 X19 X19 | x62 x63 x64 x72 x77 x77 x86 x93 x93 x93 x93 | |
| • Molecule 26: UNIT 13 | NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA | SUBCOMPLEX SUB- |
| Chain Z: | 100% | • |
| X33 X41 X97 | | |
| • Molecule 27: | NADH UBIQUINONE OXIDOREDUCTASE | |
| Chain a: | % 100% | • |
| X1 X18 X19 X22 X23 X28 | | |

• Molecule 28: NADH UBIQUINONE OXIDOREDUCTASE



| Chain b: | 100% |
|------------------------|---|
| | |
| X1 X12 X42 | |
| • Molecule 29 | : NADH UBIQUINONE OXIDOREDUCTASE |
| Chain c: | 100% |
| | |
| X1 X22 X27 | |
| • Molecule 29 | : NADH UBIQUINONE OXIDOREDUCTASE |
| Chain w: | 100% |
| There are no | outlier residues recorded for this chain. |
| • Molecule 30 | : NADH UBIQUINONE OXIDOREDUCTASE |
| Chain d: | 100% |
| There are no | outlier residues recorded for this chain. |
| • Molecule 31 | : NADH UBIQUINONE OXIDOREDUCTASE |
| Chain at | |
| Chain e: | 100% |
| X1 X9 X17 | |
| • Molecule 20 | . NADU UDIOUINONE OVIDODEDUCTASE |
| • Wrotecute 52 | . NADII UDIQUINONE OAIDOREDUCTASE |
| Chain f: | 100% |
| X1 X13 | |
| • Molecule 32 | : NADH UBIQUINONE OXIDOREDUCTASE |
| Chain h: | 100% |
| | 10070 |
| X1 X6 X17 X30 | |
| • Molecule 32 | : NADH UBIQUINONE OXIDOREDUCTASE |
| Chain i: | 100% |
| | PROTEIN DATA BANK |

| | ٠ | • | |
|---|----|----|-----|
| L | | | |
| X | X5 | XI | X3(|
| | | | - |

| • Molecule 33: NADH UBIQUINONE OXIDOREDUCTA | SE |
|---|----|
|---|----|

| Chain g: | 100% |
|-------------------------------|---|
| There are no ou | tlier residues recorded for this chain. |
| • Molecule 34: | NADH UBIQUINONE OXIDOREDUCTASE |
| Chain j: | 100% |
| There are no ou | tlier residues recorded for this chain. |
| • Molecule 34: | NADH UBIQUINONE OXIDOREDUCTASE |
| Chain l: | 100% |
| X1 X9 X24 | |
| • Molecule 35: | NADH UBIQUINONE OXIDOREDUCTASE |
| Chain k: | 100% |
| X1 X8 X20 X20 X28 | |
| • Molecule 35: | NADH UBIQUINONE OXIDOREDUCTASE |
| Chain p: | 100% |
| There are no ou | tlier residues recorded for this chain. |
| • Molecule 35: | NADH UBIQUINONE OXIDOREDUCTASE |
| Chain s: | 100% |
| There are no ou | tlier residues recorded for this chain. |
| • Molecule 36: | NADH UBIQUINONE OXIDOREDUCTASE |
| Chain m: | 100% |
| There are no ou | tlier residues recorded for this chain. |
| • Molecule 37: | NADH UBIQUINONE OXIDOREDUCTASE |
| Chain n: | 100% |



| There are no outlier residues recorded for this chain. |
|--|
| • Molecule 38: NADH UBIQUINONE OXIDOREDUCTASE |
| Chain o: 100% |
| There are no outlier residues recorded for this chain. |
| • Molecule 39: NADH UBIQUINONE OXIDOREDUCTASE |
| Chain q: 100% |
| There are no outlier residues recorded for this chain. |
| • Molecule 40: NADH UBIQUINONE OXIDOREDUCTASE |
| Chain r: 100% |
| There are no outlier residues recorded for this chain. |
| • Molecule 41: NADH UBIQUINONE OXIDOREDUCTASE |
| Chain t: 100% |
| There are no outlier residues recorded for this chain. |
| • Molecule 42: NADH UBIQUINONE OXIDOREDUCTASE |
| Chain u: 35% 65% |
| х1 х15 10 мк 10 мк |
| • Molecule 43: NADH UBIQUINONE OXIDOREDUCTASE |

Chain v:

100%

There are no outlier residues recorded for this chain.



4 Experimental information (i)

| Property | Value | Source |
|------------------------------------|-------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 25492 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | EACH PARTICLE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{\AA}^2)$ | 64 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 5000 | Depositor |
| Magnification | 81495 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 2.635 | Depositor |
| Minimum map value | -0.698 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.065 | Depositor |
| Recommended contour level | 0.32 | Depositor |
| Map size (Å) | 480.76, 480.76, 480.76 | wwPDB |
| Map dimensions | 280, 280, 280 | wwPDB |
| Map angles $(^{\circ})$ | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.717, 1.717, 1.717 | Depositor |



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES

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 | | Bon | d lengths | Bond angles | | |
|-----------|-------|------|--------------|-------------|--------------|--|
| MIOI | Unain | RMSZ | # Z > 5 | RMSZ | # Z > 5 | |
| 2 | В | 1.57 | 1/21~(4.8%) | 2.68 | 2/23~(8.7%) | |
| 5 | Е | 0.77 | 0/20 | 1.59 | 0/20 | |
| 6 | F | 2.57 | 1/20~(5.0%) | 2.24 | 0/20 | |
| 7 | G | 1.04 | 0/65 | 1.60 | 0/67 | |
| 9 | Ι | 2.32 | 2/40~(5.0%) | 1.47 | 0/40 | |
| 21 | U | 0.08 | 0/4 | 0.20 | 0/4 | |
| All | All | 1.68 | 4/170~(2.4%) | 1.82 | 2/174~(1.1%) | |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | В | 0 | 2 |
| 3 | С | 0 | 1 |
| 4 | D | 0 | 1 |
| 6 | F | 0 | 2 |
| 7 | G | 0 | 6 |
| 9 | Ι | 0 | 1 |
| 12 | L | 0 | 4 |
| 14 | Ν | 0 | 2 |
| 15 | 0 | 0 | 2 |
| 16 | Р | 0 | 3 |
| 17 | Q | 0 | 1 |
| 19 | S | 0 | 1 |
| 23 | W | 0 | 1 |
| 24 | Х | 0 | 1 |
| All | All | 0 | 28 |

All (4) bond length outliers are listed below:



| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | $\operatorname{Ideal}(\operatorname{\AA})$ |
|-----|-------|-----|------|-------|-------|-------------|--|
| 6 | F | 405 | CYS | CA-CB | -8.99 | 1.34 | 1.53 |
| 9 | Ι | 87 | CYS | CA-CB | 7.91 | 1.71 | 1.53 |
| 9 | Ι | 77 | CYS | CA-CB | 6.99 | 1.69 | 1.53 |
| 2 | В | 55 | CYS | CA-CB | 5.36 | 1.65 | 1.53 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|----------|-------|------------------|---------------|
| 2 | В | 55 | CYS | CA-CB-SG | -9.60 | 96.72 | 114.00 |
| 2 | В | 55 | CYS | CB-CA-C | -5.16 | 100.09 | 110.40 |

There are no chirality outliers.

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | В | 120 | UNK | Peptide |
| 2 | В | 130 | UNK | Peptide |
| 3 | С | 56 | UNK | Peptide |
| 4 | D | 195 | UNK | Peptide |
| 6 | F | 166 | UNK | Mainchain |
| 6 | F | 96 | UNK | Peptide |
| 7 | G | 177 | UNK | Peptide |
| 7 | G | 178 | UNK | Mainchain |
| 7 | G | 206 | UNK | Peptide |
| 7 | G | 289 | UNK | Peptide |
| 7 | G | 399 | UNK | Mainchain |
| 7 | G | 565 | UNK | Mainchain |
| 9 | Ι | 160 | UNK | Mainchain |
| 12 | L | 133 | UNK | Peptide |
| 12 | L | 366 | UNK | Peptide |
| 12 | L | 446 | UNK | Peptide |
| 12 | L | 546 | UNK | Mainchain |
| 14 | Ν | 276 | UNK | Peptide |
| 14 | Ν | 91 | UNK | Peptide |
| 15 | 0 | 229 | UNK | Peptide |
| 15 | 0 | 92 | UNK | Peptide |
| 16 | Р | 223 | UNK | Peptide |
| 16 | Р | 225 | UNK | Peptide |
| 16 | Р | 42 | UNK | Peptide |
| 17 | Q | 40 | UNK | Peptide |
| 19 | S | 75 | UNK | Mainchain |
| 23 | W | 40 | UNK | Peptide |
| 24 | Х | 56 | UNK | Peptide |

All (28) planarity outliers are listed below:



5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Perce | ntiles |
|-----|-------|--------------|----------|---------|----------|-------|--------|
| 2 | В | 4/143~(3%) | 3~(75%) | 0 | 1 (25%) | 0 | 1 |
| 5 | Ε | 4/159~(2%) | 3~(75%) | 1 (25%) | 0 | 100 | 100 |
| 6 | F | 4/411~(1%) | 4 (100%) | 0 | 0 | 100 | 100 |
| 7 | G | 12/538~(2%) | 9~(75%) | 1 (8%) | 2(17%) | 0 | 3 |
| 9 | Ι | 8/162~(5%) | 7 (88%) | 0 | 1 (12%) | 0 | 5 |
| All | All | 32/1413~(2%) | 26 (81%) | 2~(6%) | 4 (12%) | 1 | 5 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 2 | В | 119 | CYS |
| 7 | G | 105 | CYS |
| 9 | Ι | 116 | CYS |
| 7 | G | 156 | CYS |

5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|------------|-----------|----------|-------------|
| 2 | В | 4/4 (100%) | 2 (50%) | 2 (50%) | 0 0 |

Continued on next page...



| Mol | Chain | Analysed | Analysed Rotameric Outliers | | Percentiles | | |
|-----|-------|--------------|-----------------------------|---------|-------------|-----|--|
| 5 | Ε | 4/4~(100%) | 4 (100%) | 0 | 100 | 100 | |
| 6 | F | 4/4~(100%) | 3~(75%) | 1 (25%) | 0 | 4 | |
| 7 | G | 12/12~(100%) | 8~(67%) | 4(33%) | 0 | 2 | |
| 9 | Ι | 8/8~(100%) | 7~(88%) | 1 (12%) | 4 | 21 | |
| All | All | 32/32~(100%) | 24~(75%) | 8 (25%) | 2 | 4 | |

Continued from previous page...

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 2 | В | 54 | CYS |
| 2 | В | 55 | CYS |
| 6 | F | 405 | CYS |
| 7 | G | 41 | CYS |
| 7 | G | 52 | CYS |
| 7 | G | 55 | CYS |
| 7 | G | 69 | CYS |
| 9 | Ι | 119 | CYS |

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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).

| Mal | Turne | Chain | Dec | Tink | B | ond leng | gths | B | ond angles |
|-----|-------|-------|-----|------|---------|----------|----------|--------|------------------|
| | туре | Unain | nes | | Counts | RMSZ | # Z > 2 | Counts | RMSZ # Z > 2 |
| 44 | SF4 | Ι | 222 | 9 | 0,12,12 | - | - | - | |
| 44 | SF4 | В | 201 | 2 | 0,12,12 | - | - | - | |
| 44 | SF4 | G | 802 | 7 | 0,12,12 | - | - | - | |
| 45 | FES | Е | 201 | 5 | 0,4,4 | - | - | - | |
| 44 | SF4 | G | 801 | 7 | 0,12,12 | - | - | - | |
| 44 | SF4 | Ι | 223 | 9 | 0,12,12 | - | - | - | |
| 44 | SF4 | F | 508 | 6 | 0,12,12 | - | - | - | |
| 45 | FES | G | 804 | 7 | 0,4,4 | - | - | - | |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 44 | SF4 | Ι | 222 | 9 | - | - | 0/6/5/5 |
| 44 | SF4 | В | 201 | 2 | - | - | 0/6/5/5 |
| 44 | SF4 | G | 802 | 7 | - | - | 0/6/5/5 |
| 45 | FES | Е | 201 | 5 | - | - | 0/1/1/1 |
| 44 | SF4 | G | 801 | 7 | - | - | 0/6/5/5 |
| 44 | SF4 | Ι | 223 | 9 | - | - | 0/6/5/5 |
| 44 | SF4 | F | 508 | 6 | - | - | 0/6/5/5 |
| 45 | FES | G | 804 | 7 | - | - | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 7 | G | 6 |
| 12 | L | 5 |
| 15 | 0 | 3 |
| 10 | J | 2 |
| 16 | Р | 2 |
| 8 | Н | 2 |
| 20 | Т | 2 |
| 1 | А | 1 |
| 14 | Ν | 1 |
| 13 | М | 1 |
| 17 | Q | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | А | 23:UNK | С | 52:UNK | N | 39.81 |
| 1 | J | 107:UNK | С | 140:UNK | N | 30.90 |
| 1 | Ν | 300:UNK | С | 320:UNK | N | 26.56 |
| 1 | Р | 250:UNK | С | 285:UNK | N | 26.48 |
| 1 | L | 466:UNK | С | 487:UNK | N | 23.59 |
| 1 | G | 347:UNK | С | 367:UNK | N | 22.81 |
| 1 | М | 415:UNK | С | 430:UNK | N | 22.06 |
| 1 | Р | 185:UNK | С | 203:UNK | N | 21.21 |
| 1 | Н | 200:UNK | С | 219:UNK | N | 20.56 |
| 1 | J | 76:UNK | С | 85:UNK | N | 19.66 |
| 1 | Н | 242:UNK | С | 253:UNK | N | 18.95 |
| 1 | G | 495:UNK | С | 525:UNK | N | 18.00 |
| 1 | L | 513:UNK | С | 520:UNK | N | 17.41 |
| 1 | G | 530:UNK | С | 542:UNK | N | 16.15 |
| 1 | L | 400:UNK | С | 408:UNK | N | 14.38 |
| 1 | Q | 59:UNK | С | 76:UNK | N | 13.51 |
| 1 | 0 | 54:UNK | С | 79:UNK | N | 12.62 |
| 1 | G | 318:UNK | С | 326:UNK | N | 12.59 |
| 1 | L | 22:UNK | С | 28:UNK | N | 11.17 |
| 1 | 0 | 167:UNK | С | 172:UNK | N | 11.08 |

Continued on next page...



| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 0 | 210:UNK | С | 222:UNK | Ν | 10.93 |
| 1 | Т | 23:UNK | С | 28:UNK | Ν | 9.73 |
| 1 | L | 358:UNK | С | 363:UNK | Ν | 8.92 |
| 1 | G | 410:UNK | С | 425:UNK | Ν | 7.45 |
| 1 | G | 400:UNK | С | 404:UNK | N | 6.25 |
| 1 | Т | 8:UNK | С | 9:UNK | Ν | 1.65 |

Continued from previous page...



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2676. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 140

Y Index: 140



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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 148

Y Index: 144

Z Index: 160

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 480 $\rm nm^3;$ this corresponds to an approximate mass of 433 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.202 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.202 \AA^{-1}



8.2 Resolution estimates (i)

| B osolution ostimato $(\hat{\lambda})$ | Estimation criterion (FSC cut-off) | | | |
|---|------------------------------------|------|----------|--|
| Resolution estimate (A) | 0.143 | 0.5 | Half-bit | |
| Reported by author | - | - | - | |
| Author-provided FSC curve | 4.91 | 7.02 | 5.11 | |
| Unmasked-calculated* | - | - | - | |

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2676 and PDB model 4UQ8. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).



9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.32) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All | 0.8495 | 0.3380 |
| А | 0.8265 | 0.3350 |
| В | 0.8514 | 0.3690 |
| С | 0.8831 | 0.3740 |
| D | 0.8589 | 0.3640 |
| Е | 0.8842 | 0.3210 |
| F | 0.8326 | 0.3090 |
| G | 0.8577 | 0.3450 |
| Η | 0.8379 | 0.3480 |
| Ι | 0.8813 | 0.3560 |
| J | 0.7588 | 0.3100 |
| K | 0.8286 | 0.3460 |
| L | 0.8201 | 0.3330 |
| М | 0.8601 | 0.3680 |
| Ν | 0.8301 | 0.3350 |
| О | 0.8519 | 0.3390 |
| Р | 0.8135 | 0.3160 |
| Q | 0.8928 | 0.3930 |
| R | 0.8809 | 0.3670 |
| S | 0.8675 | 0.2910 |
| Т | 0.7831 | 0.2790 |
| U | 0.8320 | 0.3170 |
| V | 0.8930 | 0.3260 |
| W | 0.8361 | 0.3030 |
| Х | 0.9165 | 0.3250 |
| Y | 0.7509 | 0.2980 |
| Z | 0.9046 | 0.3250 |
| a | 0.7793 | 0.3300 |
| b | 0.8571 | 0.3410 |
| с | 0.8741 | 0.3360 |
| d | 0.9077 | 0.3510 |
| е | 0.7700 | 0.3010 |
| f | 0.8667 | 0.3110 |
| g | 0.9273 | 0.3790 |
| h | 0.8333 | 0.3380 |

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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| i | 0.8667 | 0.3190 |
| j | 0.8917 | 0.3340 |
| k | 0.7929 | 0.2940 |
| 1 | 0.8750 | 0.3140 |
| m | 0.8706 | 0.3350 |
| n | 0.9119 | 0.3390 |
| 0 | 0.9333 | 0.3190 |
| р | 0.9357 | 0.3420 |
| q | 0.8960 | 0.3080 |
| r | 0.9615 | 0.3830 |
| S | 0.9429 | 0.3610 |
| t | 0.9298 | 0.3620 |
| u | 0.9600 | 0.3750 |
| V | 0.9375 | 0.3070 |
| W | 0.9111 | 0.3270 |

