# wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:08 PM BST

| | | |
|---|---|---|
| PDB ID | : | 4V1A |
| EMDB ID: | : | EMD-2787 |
| Title | : | Structure of the large subunit of the mammalian mitoribosome, part 2 of 2 |
| Authors | : | Greber, B.J.; Boehringer, D.; Leibundgut, M.; Bieri, P.; Leitner, A.; Schmitz, N.; Aebersold, R.; Ban, N. |
| Deposited on | : | 2014-09-25 |
| Resolution | : | 3.40 Å(reported) |

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

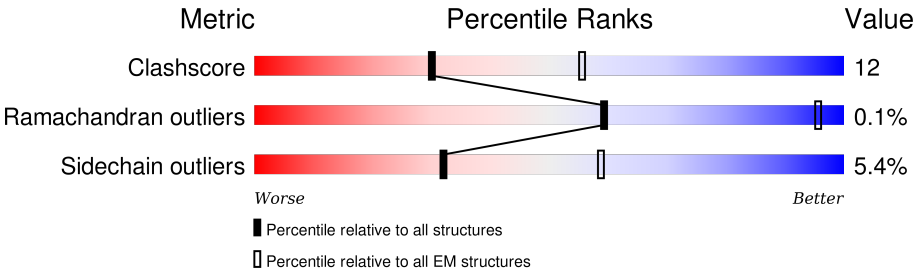
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk27241 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | a | 423 | 89% · 7% |
| 2 | b | 380 | 89% · 7% |
| 3 | c | 334 | 85% · 12% |
| 4 | d | 206 | 45% · 52% |
| 5 | e | 135 | 85% · 10% |
| 6 | f | 142 | 70% 6% 24% |
| 7 | g | 159 | 84% 9% 7% |
| 8 | h | 332 | 82% 5% 13% |
| 9 | i | 312 | 75% · 22% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | j | 279 | 73% 5% 22% |
| 11 | k | 212 | 60% 38% |
| 12 | l | 166 | 76% 20% |
| 13 | m | 159 | 67% 31% |
| 14 | n | 128 | 70% 6% 24% |
| 15 | o | 124 | 71% 5% 24% |
| 16 | p | 112 | 86% 13% |
| 17 | q | 138 | 27% 73% |
| 18 | t | 102 | 84% 8% 8% |
| 19 | u | 205 | 71% 26% |
| 20 | v | 222 | 58% 41% |
| 21 | w | 433 | 84% 6% 11% |
| 22 | x | 196 | 77% 6% 17% |
| 23 | z | 47 | 100% |

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 31917 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 MITORIBOSOMAL PROTEIN ML37, MRPL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | a | 393 | 3173 | 2040 | 556 | 565 | 12 | 0 | 0 |

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | b | 354 | 2952 | 1876 | 542 | 525 | 9 | 0 | 0 |

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | c | 295 | 2408 | 1541 | 410 | 441 | 16 | 0 | 0 |

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | d | 99 | 832 | 528 | 148 | 155 | 1 | 0 | 0 |

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | e | 121 | 968 | 626 | 167 | 172 | 3 | 0 | 0 |

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | f | 108 | 852 | 544 | 154 | 150 | 4 | 0 | 0 |

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | g | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1167 | 727 | 225 | 212 | 3 | | |

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | h | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2319 | 1486 | 399 | 426 | 8 | | |

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | i | 242 | Total | C | N | O | S | 0 | 0 |
| | | | 1979 | 1266 | 352 | 351 | 10 | | |

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | j | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1775 | 1137 | 311 | 321 | 6 | | |

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | k | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1050 | 671 | 178 | 196 | 5 | | |

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | l | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1097 | 709 | 192 | 194 | 2 | | |

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | m | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 893 | 568 | 160 | 162 | 3 | | |

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | n | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 837 | 539 | 166 | 128 | 4 | | |

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | o | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 747 | 466 | 143 | 136 | 2 | | |

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | p | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 742 | 459 | 143 | 134 | 6 | | |

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 17 | q | 37 | Total | C | N | O | 0 | 0 |
| | | | 336 | 214 | 69 | 53 | | |

- Molecule 18 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | t | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 780 | 485 | 168 | 126 | 1 | | |

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | u | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1208 | 748 | 233 | 222 | 5 | | |

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | v | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1068 | 662 | 206 | 195 | 5 | | |

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | w | 387 | Total | C | N | O | S | 0 | 0 |
| | | | 3126 | 2011 | 548 | 555 | 12 | | |

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | x | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1325 | 845 | 249 | 224 | 7 | | |

- Molecule 23 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 23 | z | 47 | Total | C | N | O | 0 | 0 |
| | | | 282 | 188 | 47 | 47 | | |

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

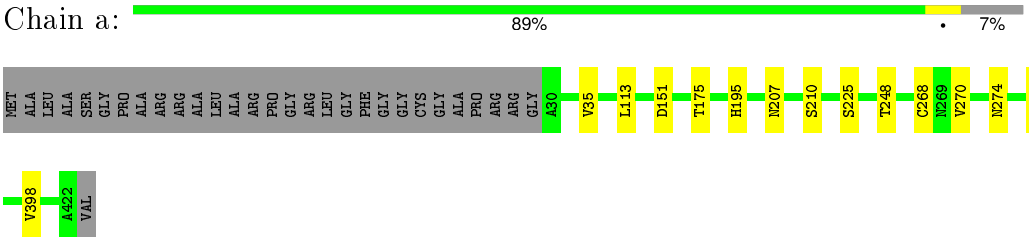
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 24 | x | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

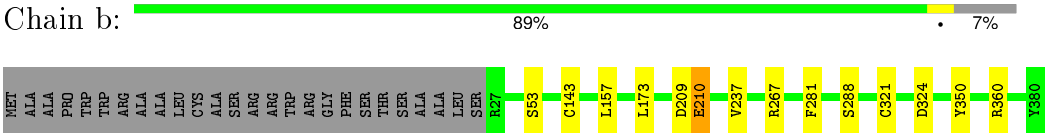
- Molecule 1: MITORIBOSOMAL PROTEIN ML37, MRPL37

Chain a:



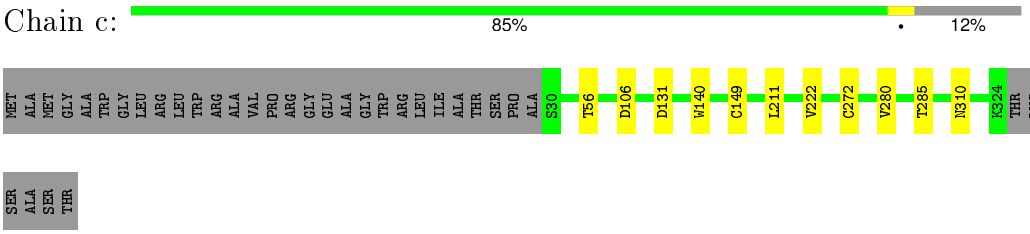

- Molecule 2: MITORIBOSOMAL PROTEIN ML38, MRPL38

Chain b:



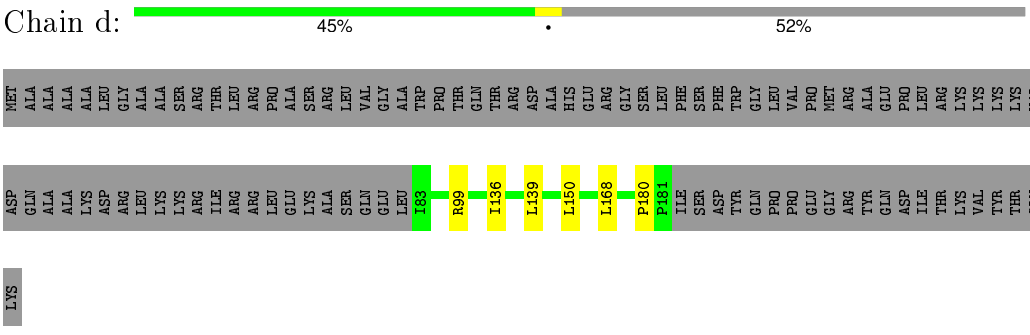

- Molecule 3: MITORIBOSOMAL PROTEIN ML39, MRPL39

Chain c:



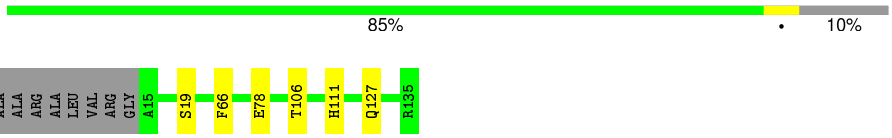

- Molecule 4: MITORIBOSOMAL PROTEIN ML40, MRPL40

Chain d:



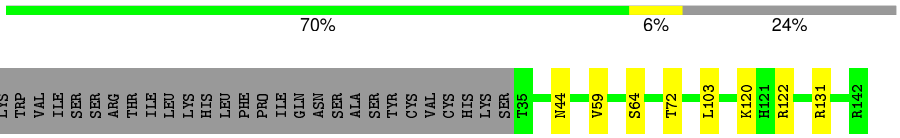

- Molecule 5: MITORIBOSOMAL PROTEIN ML41, MRPL41

Chain e:



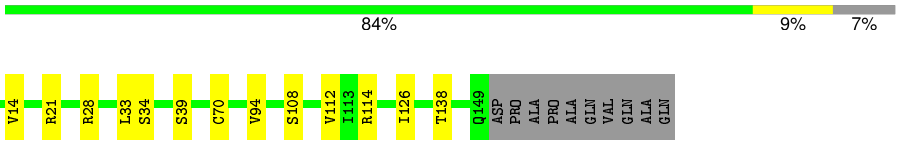

• Molecule 6: MITORIBOSOMAL PROTEIN ML42, MRPL42

Chain f:



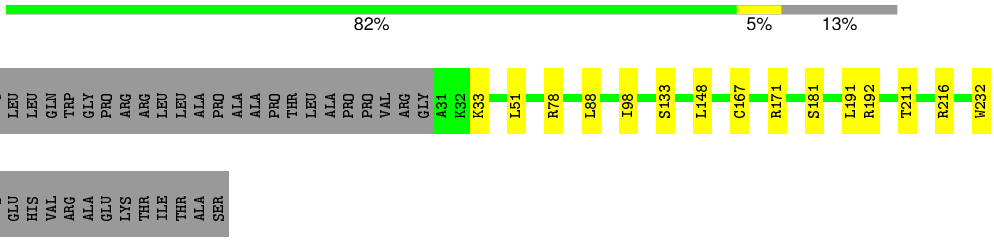

• Molecule 7: MITORIBOSOMAL PROTEIN ML43, MRPL43

Chain g:



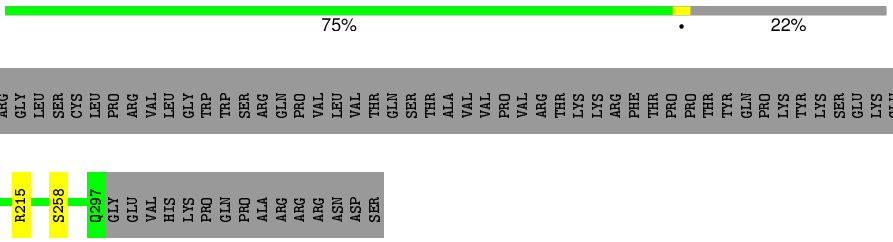

• Molecule 8: MITORIBOSOMAL PROTEIN ML44, MRPL44

Chain h:



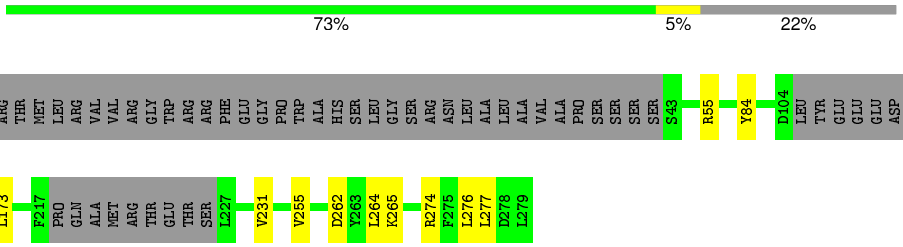

• Molecule 9: MITORIBOSOMAL PROTEIN ML45, MRPL45

Chain i:



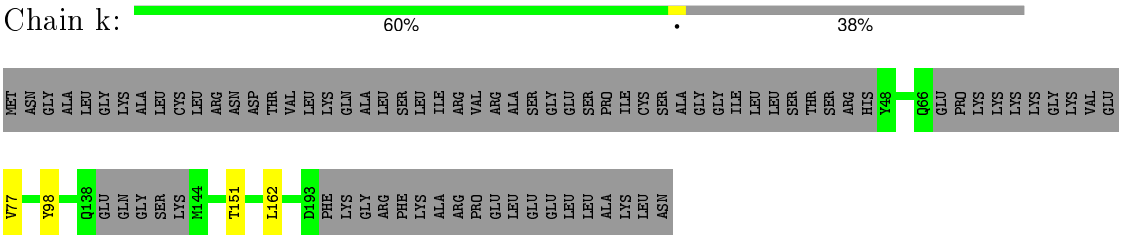

• Molecule 10: MITORIBOSOMAL PROTEIN ML46, MRPL46

Chain j:



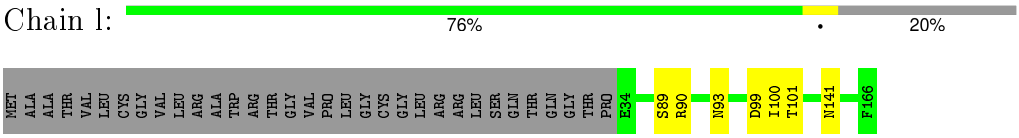

• Molecule 11: MITORIBOSOMAL PROTEIN ML48, MRPL48

Chain k:



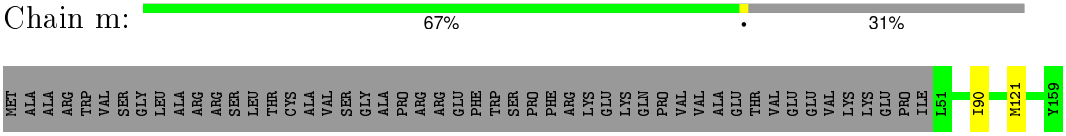

• Molecule 12: MITORIBOSOMAL PROTEIN ML49, MRPL49

Chain l:



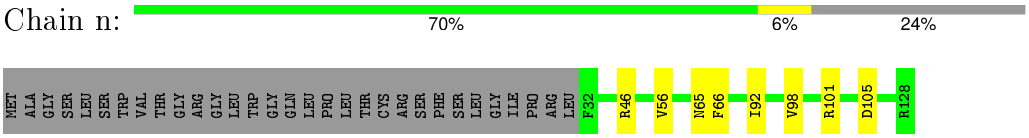

• Molecule 13: MITORIBOSOMAL PROTEIN ML50, MRPL50

Chain m:



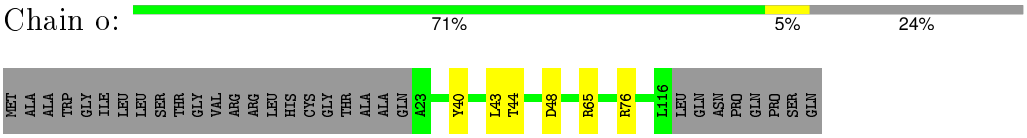

• Molecule 14: MITORIBOSOMAL PROTEIN ML51, MRPL51

Chain n:



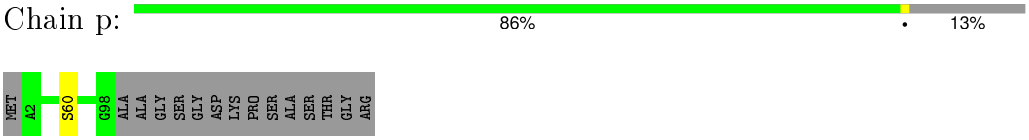

• Molecule 15: MITORIBOSOMAL PROTEIN ML52, MRPL52

Chain o:



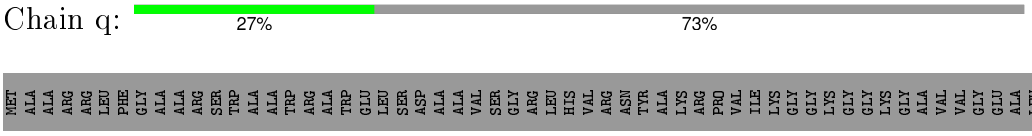

• Molecule 16: MITORIBOSOMAL PROTEIN ML53, MRPL53

Chain p:



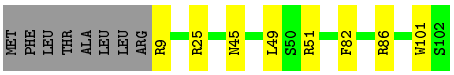

• Molecule 17: MITORIBOSOMAL PROTEIN ML54, MRPL54

Chain q:




- Molecule 18: MITORIBOSOMAL PROTEIN ML63, MRPL57, MRP63

Chain t:

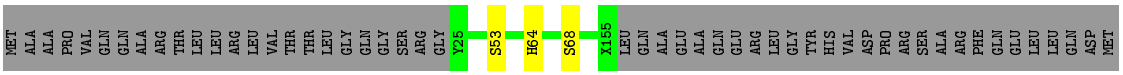

- Molecule 19: MITORIBOSOMAL PROTEIN ML62, MRPL58, ICT1

Chain u:




- Molecule 20: MITORIBOSOMAL PROTEIN ML64, MRPL59, CRIF1

Chain v:



- Molecule 21: MITORIBOSOMAL PROTEIN ML65, MRPS30

Chain w:



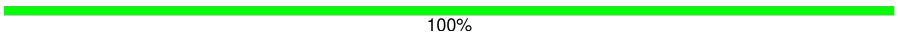

- Molecule 22: MITORIBOSOMAL PROTEIN ML66, MRPS18A

Chain x:



- Molecule 23: UNASSIGNED SECONDARY STRUCTURE ELEMENTS

Chain z:




There are no outlier residues recorded for this chain.

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | PER DETECTOR FRAME | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 2000 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | 59000 | Depositor |
| Image detector | FEI FALCON II | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.34 | 0/3267 | 0.53 | 0/4455 |
| 10 | j | 0.34 | 0/1811 | 0.56 | 0/2436 |
| 11 | k | 0.35 | 0/1070 | 0.55 | 0/1448 |
| 12 | l | 0.38 | 0/1135 | 0.53 | 0/1549 |
| 13 | m | 0.30 | 0/917 | 0.49 | 0/1248 |
| 14 | n | 0.44 | 0/860 | 0.60 | 0/1150 |
| 15 | o | 0.39 | 0/762 | 0.52 | 0/1022 |
| 16 | p | 0.34 | 0/752 | 0.53 | 0/1013 |
| 17 | q | 0.29 | 0/346 | 0.47 | 0/463 |
| 18 | t | 0.41 | 0/798 | 0.61 | 0/1073 |
| 19 | u | 0.31 | 0/1163 | 0.49 | 0/1557 |
| 2 | b | 0.36 | 0/3047 | 0.55 | 0/4139 |
| 20 | v | 0.33 | 0/1022 | 0.44 | 0/1382 |
| 21 | w | 0.39 | 0/3206 | 0.55 | 0/4354 |
| 22 | x | 0.36 | 0/1364 | 0.62 | 0/1849 |
| 3 | c | 0.33 | 0/2464 | 0.50 | 0/3330 |
| 4 | d | 0.38 | 0/853 | 0.56 | 1/1153 (0.1%) |
| 5 | e | 0.37 | 0/996 | 0.56 | 0/1340 |
| 6 | f | 0.38 | 0/731 | 0.54 | 0/990 |
| 7 | g | 0.38 | 0/1191 | 0.58 | 0/1614 |
| 8 | h | 0.35 | 0/2372 | 0.53 | 0/3211 |
| 9 | i | 0.32 | 0/2034 | 0.52 | 0/2759 |
| All | All | 0.36 | 0/32161 | 0.54 | 1/43535 (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 |
|---|---|---|---|
| 10 | j | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 14 | n | 0 | 1 |
| 2 | b | 0 | 1 |
| 21 | w | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | d | 180 | PRO | C-N-CD | -5.25 | 109.05 | 120.60 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | b | 210 | GLU | Peptide |
| 10 | j | 173 | LEU | Peptide |
| 14 | n | 65 | ASN | Peptide |
| 21 | w | 357 | ASP | Peptide |

## 5.2 Too-close contacts (i)

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 | 3173 | 0 | 3153 | 0 | 0 |
| 2 | b | 2952 | 0 | 2840 | 0 | 0 |
| 3 | c | 2408 | 0 | 2415 | 0 | 0 |
| 4 | d | 832 | 0 | 828 | 0 | 0 |
| 5 | e | 968 | 0 | 968 | 0 | 0 |
| 6 | f | 852 | 0 | 834 | 0 | 0 |
| 7 | g | 1167 | 0 | 1173 | 0 | 0 |
| 8 | h | 2319 | 0 | 2332 | 0 | 0 |
| 9 | i | 1979 | 0 | 1974 | 0 | 0 |
| 10 | j | 1775 | 0 | 1797 | 0 | 0 |
| 11 | k | 1050 | 0 | 1044 | 0 | 0 |
| 12 | l | 1097 | 0 | 1080 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 13 | m | 893 | 0 | 878 | 0 | 0 |
| 14 | n | 837 | 0 | 860 | 0 | 0 |
| 15 | o | 747 | 0 | 748 | 0 | 0 |
| 16 | p | 742 | 0 | 749 | 0 | 0 |
| 17 | q | 336 | 0 | 342 | 0 | 0 |
| 18 | t | 780 | 0 | 792 | 0 | 0 |
| 19 | u | 1208 | 0 | 1227 | 0 | 0 |
| 20 | v | 1068 | 0 | 1034 | 0 | 0 |
| 21 | w | 3126 | 0 | 3153 | 0 | 0 |
| 22 | x | 1325 | 0 | 1354 | 0 | 0 |
| 23 | z | 282 | 0 | 294 | 0 | 0 |
| 24 | x | 1 | 0 | 0 | 0 | 0 |
| All | All | 31917 | 0 | 31869 | 0 | 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 12.

There are no clashes within the asymmetric unit.

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 | 391/423 (92%) | 375 (96%) | 16 (4%) | 0 | 100 | 100 |
| 2 | b | 352/380 (93%) | 329 (94%) | 23 (6%) | 0 | 100 | 100 |
| 3 | c | 293/334 (88%) | 279 (95%) | 14 (5%) | 0 | 100 | 100 |
| 4 | d | 97/206 (47%) | 92 (95%) | 5 (5%) | 0 | 100 | 100 |
| 5 | e | 119/135 (88%) | 115 (97%) | 4 (3%) | 0 | 100 | 100 |
| 6 | f | 82/142 (58%) | 81 (99%) | 1 (1%) | 0 | 100 | 100 |
| 7 | g | 146/159 (92%) | 141 (97%) | 5 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 8 | h | 287/332 (86%) | 270 (94%) | 17 (6%) | 0 | 100 | 100 |
| 9 | i | 240/312 (77%) | 230 (96%) | 10 (4%) | 0 | 100 | 100 |
| 10 | j | 211/279 (76%) | 200 (95%) | 9 (4%) | 2 (1%) | 21 | 65 |
| 11 | k | 125/212 (59%) | 119 (95%) | 6 (5%) | 0 | 100 | 100 |
| 12 | l | 131/166 (79%) | 127 (97%) | 4 (3%) | 0 | 100 | 100 |
| 13 | m | 107/159 (67%) | 101 (94%) | 6 (6%) | 0 | 100 | 100 |
| 14 | n | 95/128 (74%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 15 | o | 92/124 (74%) | 87 (95%) | 5 (5%) | 0 | 100 | 100 |
| 16 | p | 95/112 (85%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 17 | q | 35/138 (25%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 18 | t | 92/102 (90%) | 88 (96%) | 4 (4%) | 0 | 100 | 100 |
| 19 | u | 137/205 (67%) | 130 (95%) | 7 (5%) | 0 | 100 | 100 |
| 20 | v | 118/222 (53%) | 116 (98%) | 2 (2%) | 0 | 100 | 100 |
| 21 | w | 385/433 (89%) | 363 (94%) | 20 (5%) | 2 (0%) | 34 | 75 |
| 22 | x | 160/196 (82%) | 155 (97%) | 4 (2%) | 1 (1%) | 30 | 72 |
| All | All | 3790/4899 (77%) | 3612 (95%) | 173 (5%) | 5 (0%) | 59 | 89 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | w | 159 | VAL |
| 22 | x | 93 | ILE |
| 10 | j | 84 | TYR |
| 10 | j | 151 | ARG |
| 21 | w | 358 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | a | 348/365 (95%) | 332 (95%) | 16 (5%) | 33 72 |
| 2 | b | 310/328 (94%) | 296 (96%) | 14 (4%) | 34 73 |
| 3 | c | 271/299 (91%) | 260 (96%) | 11 (4%) | 37 75 |
| 4 | d | 92/181 (51%) | 87 (95%) | 5 (5%) | 27 67 |
| 5 | e | 100/108 (93%) | 94 (94%) | 6 (6%) | 24 64 |
| 6 | f | 80/110 (73%) | 72 (90%) | 8 (10%) | 9 38 |
| 7 | g | 128/136 (94%) | 113 (88%) | 15 (12%) | 7 30 |
| 8 | h | 251/284 (88%) | 234 (93%) | 17 (7%) | 20 60 |
| 9 | i | 218/281 (78%) | 211 (97%) | 7 (3%) | 46 80 |
| 10 | j | 190/242 (78%) | 180 (95%) | 10 (5%) | 28 67 |
| 11 | k | 115/181 (64%) | 111 (96%) | 4 (4%) | 43 78 |
| 12 | l | 122/147 (83%) | 115 (94%) | 7 (6%) | 25 65 |
| 13 | m | 103/145 (71%) | 101 (98%) | 2 (2%) | 65 87 |
| 14 | n | 88/113 (78%) | 81 (92%) | 7 (8%) | 15 51 |
| 15 | o | 74/97 (76%) | 68 (92%) | 6 (8%) | 15 51 |
| 16 | p | 79/88 (90%) | 78 (99%) | 1 (1%) | 76 91 |
| 17 | q | 36/114 (32%) | 36 (100%) | 0 | 100 100 |
| 18 | t | 75/82 (92%) | 67 (89%) | 8 (11%) | 8 35 |
| 19 | u | 126/169 (75%) | 121 (96%) | 5 (4%) | 38 75 |
| 20 | v | 102/173 (59%) | 99 (97%) | 3 (3%) | 50 82 |
| 21 | w | 340/373 (91%) | 318 (94%) | 22 (6%) | 21 61 |
| 22 | x | 149/173 (86%) | 139 (93%) | 10 (7%) | 20 60 |
| All | All | 3397/4189 (81%) | 3213 (95%) | 184 (5%) | 32 67 |

5 of 184 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | h | 171 | ARG |
| 10 | j | 255 | VAL |
| 21 | w | 404 | VAL |
| 8 | h | 191 | LEU |
| 9 | i | 100 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | h | 260 | GLN |
| 11 | k | 61 | HIS |
| 21 | w | 234 | GLN |
| 9 | i | 115 | ASN |
| 9 | i | 193 | GLN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no carbohydrates in this entry.

### 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.