# wwPDB EM Validation Summary Report

Dec 11, 2022 – 12:50 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 6SPC |
| EMDB ID | : | EMD-10281 |
| Title | : | Pseudomonas aeruginosa 30s ribosome from an aminoglycoside resistant clinical isolate |
| Authors | : | Halfon, Y.; Jimenez-Fernande, A.; La Ros, R.; Espinos, R.; Krogh Johansen, H.; Matzov, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Belousoff, M.; Molin, S.; Yonath, A. |
| Deposited on | : | 2019-09-01 |
| Resolution | : | 2.95 Å(reported) |

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

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

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

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

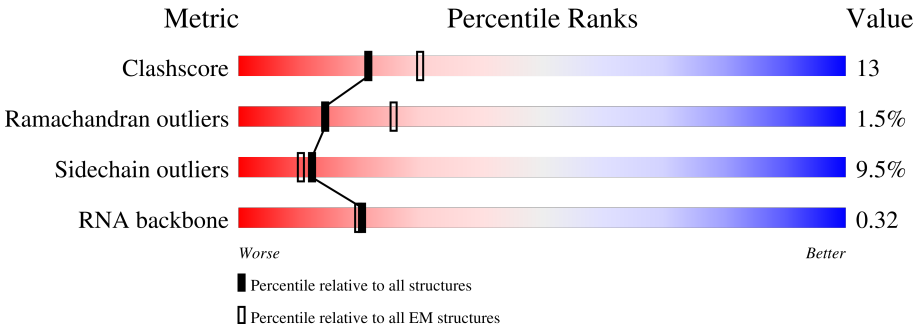
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 2.95 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | a | 1519 | 47% 44% 10% |
| 2 | b | 221 | 68% 31% |
| 3 | c | 203 | 37% 97% |
| 4 | d | 205 | 95% 5% |
| 5 | e | 149 | 90% 9% |
| 6 | f | 100 | 92% 7% |
| 7 | g | 154 | 7% 62% 38% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | h | 125 | 75% 17% 6% |
| 9 | i | 126 | 98% |
| 10 | j | 96 | 18% 97% |
| 11 | k | 115 | 95% 5% |
| 12 | l | 120 | 84% 9% 6% |
| 13 | m | 109 | 19% 94% 6% |
| 14 | n | 98 | 28% 97% |
| 15 | o | 87 | 97% |
| 16 | p | 78 | 94% 6% |
| 17 | q | 76 | 97% |
| 18 | r | 56 | 96% |
| 19 | s | 80 | 10% 94% 6% |
| 20 | t | 86 | 97% |
| 21 | u | 34 | 21% 100% |

# 2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 50569 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 RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | a | 1519 | 32595 | 14540 | 5985 | 10552 | 1518 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| a | 2 | A | - | conflict | GB 1359201046 |
| a | ? | - | C | deletion | GB 1359201046 |
| a | ? | - | G | deletion | GB 1359201046 |
| a | 72 | A | G | conflict | GB 1359201046 |
| a | 101 | A | G | conflict | GB 1359201046 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | b | 221 | 1728 | 1088 | 316 | 314 | 10 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| b | ? | - | THR | deletion | UNP A0A072ZPV8 |
| b | ? | - | PHE | deletion | UNP A0A072ZPV8 |
| b | ? | - | ASP | deletion | UNP A0A072ZPV8 |
| b | ? | - | LYS | deletion | UNP A0A072ZPV8 |
| b | ? | - | LEU | deletion | UNP A0A072ZPV8 |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | c | 203 | 1609 | 1017 | 303 | 284 | 5 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | d | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1600 | 991 | 310 | 294 | 5 | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | e | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1092 | 687 | 202 | 197 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| e | ? | - | ALA | deletion | UNP A0A241XG65 |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | f | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 802 | 497 | 152 | 149 | 4 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| f | 80 | ALA | TYR | conflict | UNP A0A069Q263 |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | g | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1190 | 747 | 227 | 211 | 5 | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | h | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 915 | 575 | 161 | 174 | 5 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| h | 94 | ALA | LYS | conflict | UNP E2RXT9 |
| h | 129 | VAL | LEU | conflict | UNP E2RXT9 |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | i | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 994 | 616 | 198 | 179 | 1 | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | j | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 763 | 479 | 143 | 140 | 1 | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | k | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 828 | 511 | 159 | 156 | 2 | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | l | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 893 | 547 | 184 | 158 | 4 | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | m | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 847 | 515 | 173 | 155 | 4 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| m | ? | - | TYR | deletion | UNP E2RXU3 |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | n | 98 | Total<br>776 | C<br>479 | N<br>163 | O<br>131 | S<br>3 | 0 | 0 |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | o | 86 | Total<br>686 | C<br>425 | N<br>134 | O<br>126 | S<br>1 | 0 | 0 |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 16 | p | 78 | Total<br>606 | C<br>379 | N<br>120 | O<br>107 | 0 | 0 |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | q | 76 | Total<br>619 | C<br>387 | N<br>120 | O<br>110 | S<br>2 | 0 | 0 |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 18 | r | 56 | Total<br>443 | C<br>283 | N<br>79 | O<br>81 | 0 | 0 |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | s | 80 | Total<br>635 | C<br>405 | N<br>121 | O<br>106 | S<br>3 | 0 | 0 |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | t | 85 | Total<br>653 | C<br>404 | N<br>135 | O<br>112 | S<br>2 | 0 | 0 |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 21 | u | 34 | Total | C | N | O | 0 | 0 |
| | | | 295 | 178 | 70 | 47 | | |

There is a discrepancy between the modelled and reference sequences:

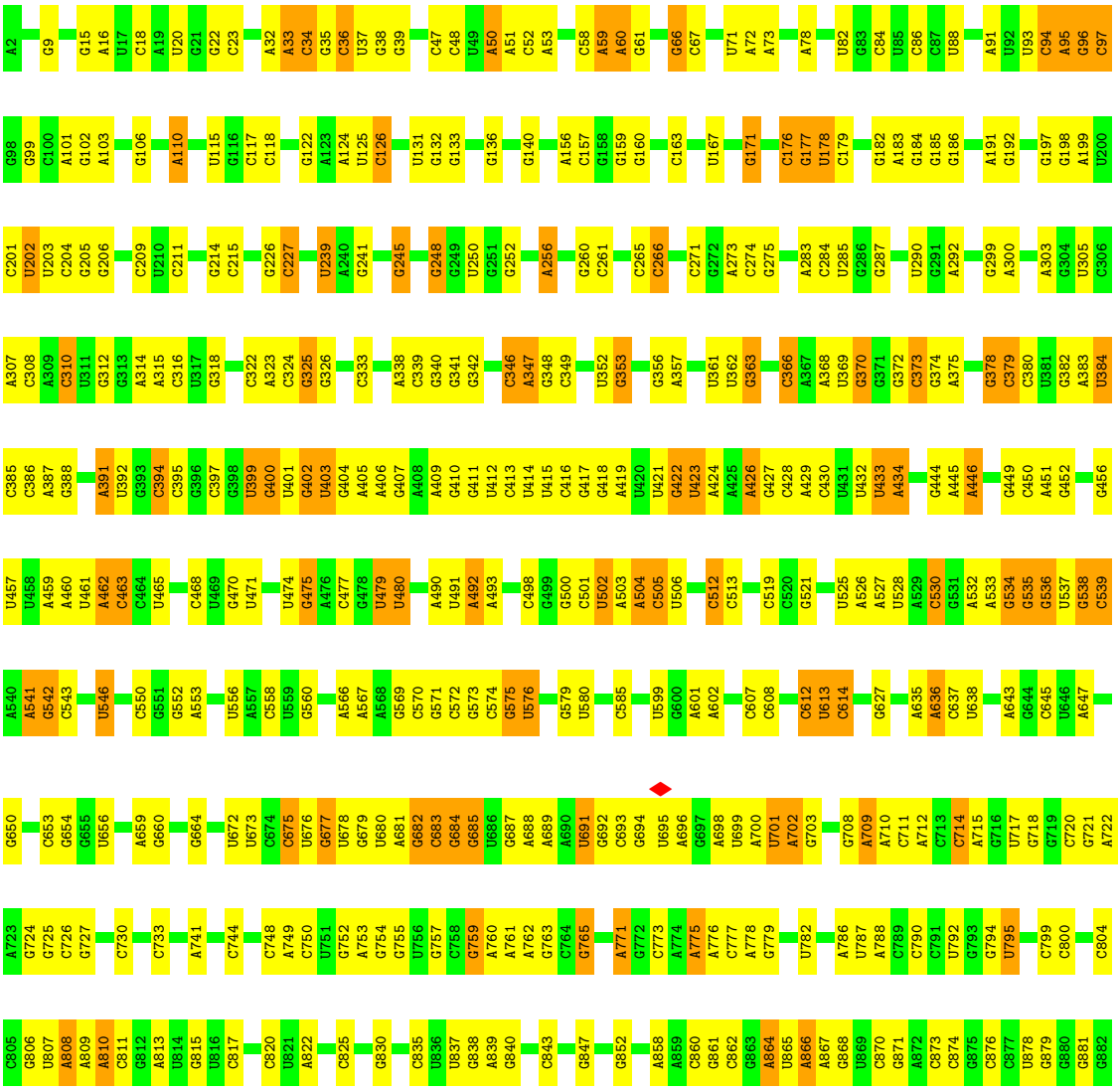
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| u | 46 | ARG | LYS | conflict | UNP A0A069QC99 |

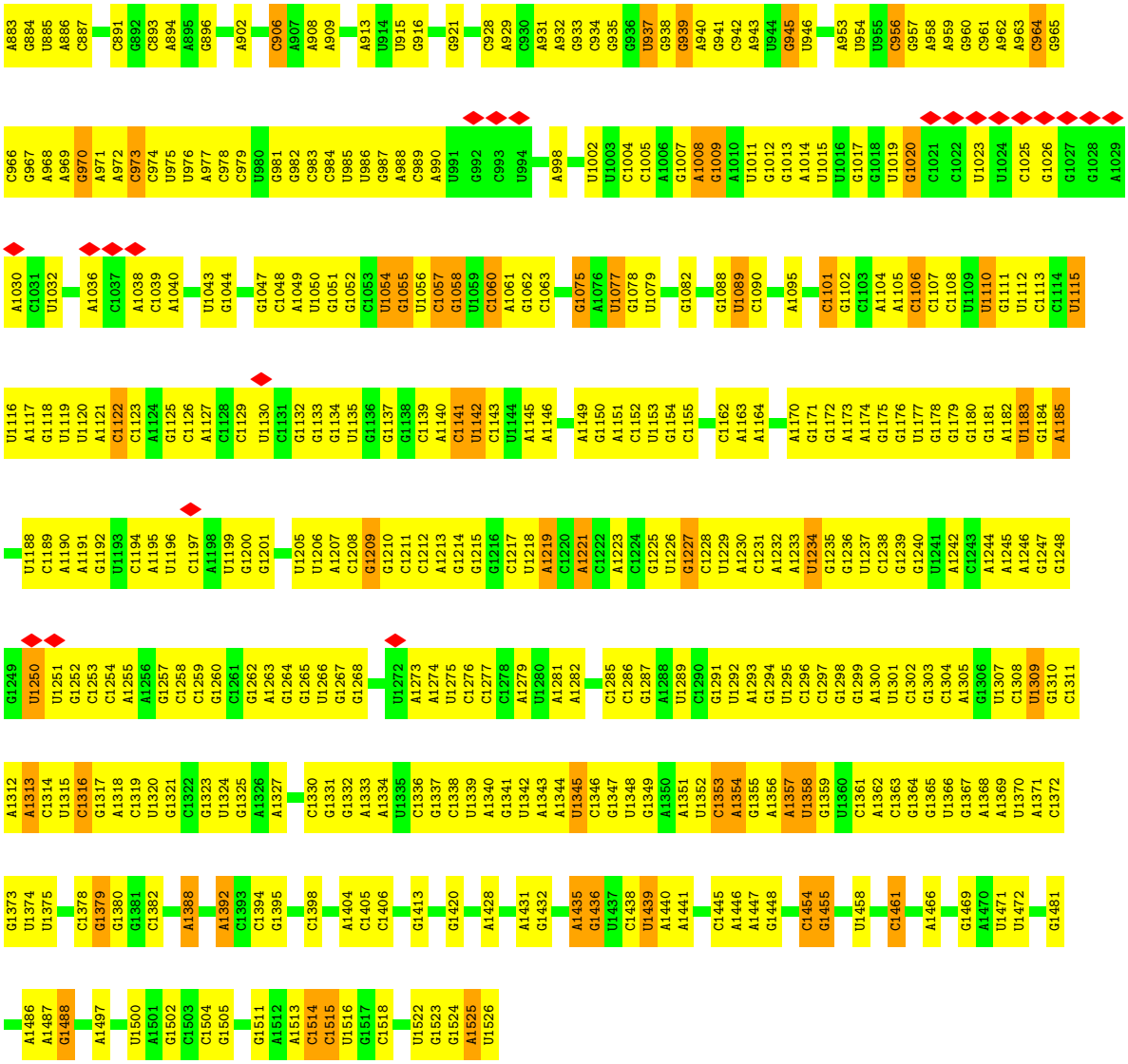
# 3 Residue-property plots (i)

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: 16S rRNA

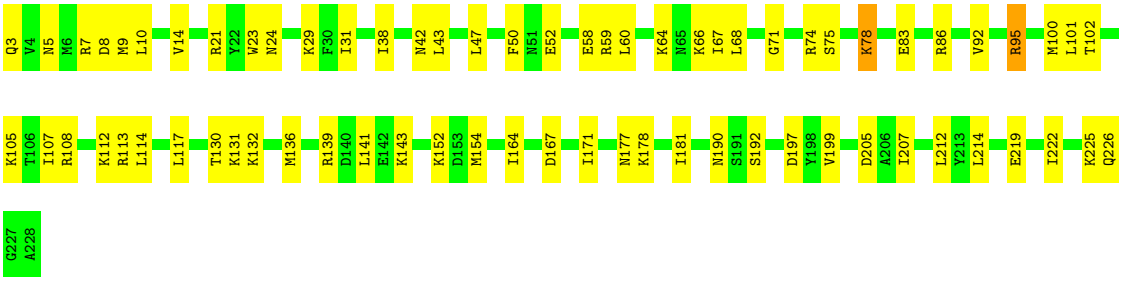
Chain a:



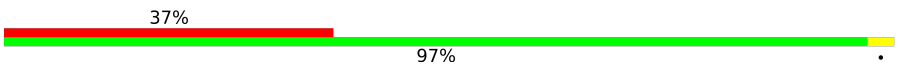
• Molecule 2: 30S ribosomal protein S2

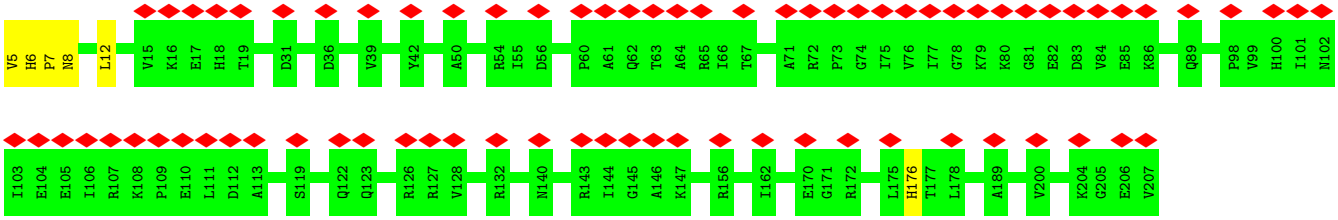
Chain b:

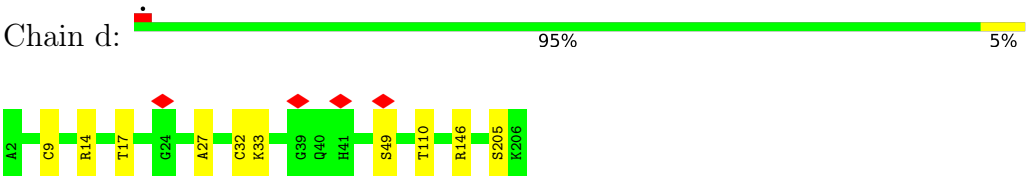
• Molecule 3: 30S ribosomal protein S3

Chain c:

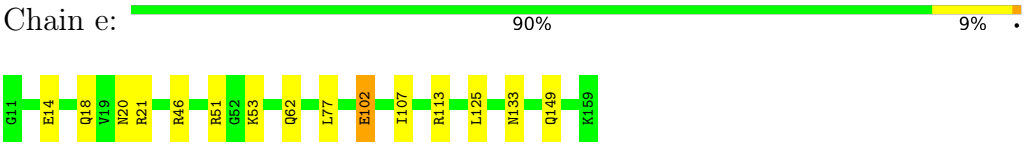




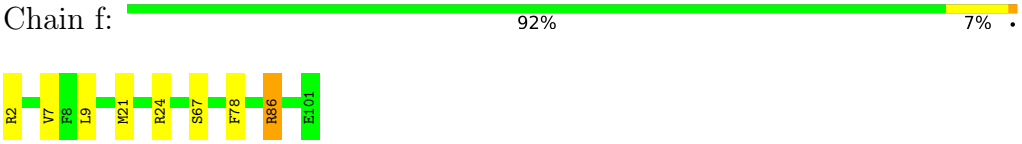

• Molecule 4: 30S ribosomal protein S4



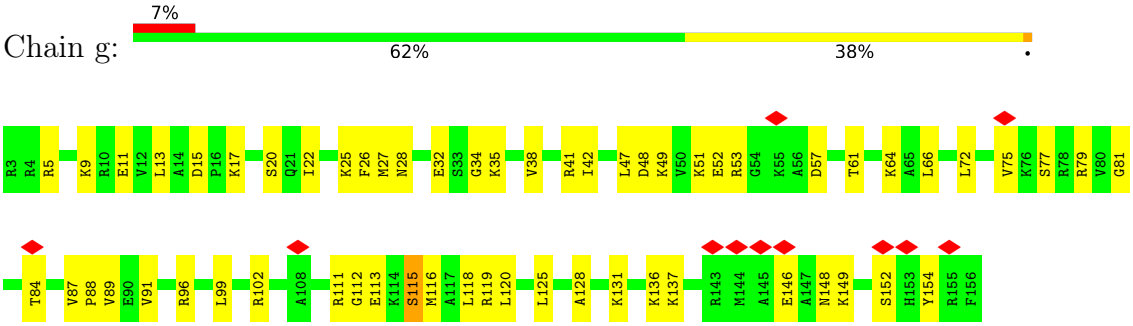

• Molecule 5: 30S ribosomal protein S5



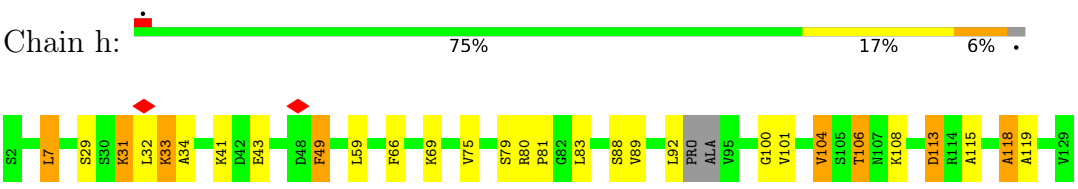

• Molecule 6: 30S ribosomal protein S6




• Molecule 7: 30S ribosomal protein S7

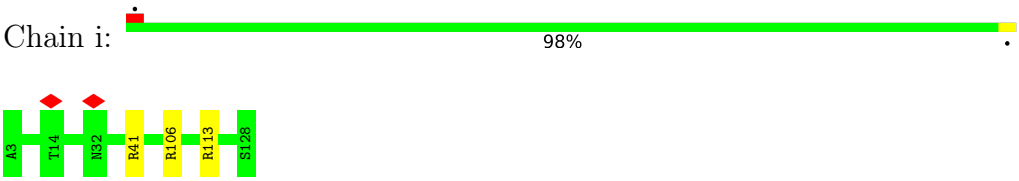



• Molecule 8: 30S ribosomal protein S8



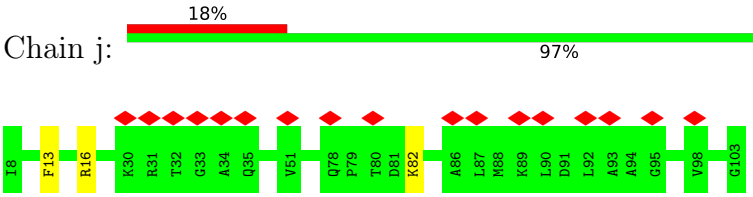

• Molecule 9: 30S ribosomal protein S9

Chain i:



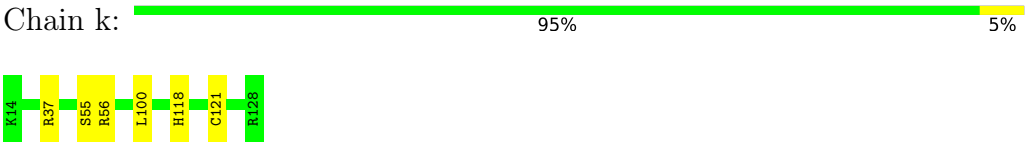

• Molecule 10: 30S ribosomal protein S10

Chain j:



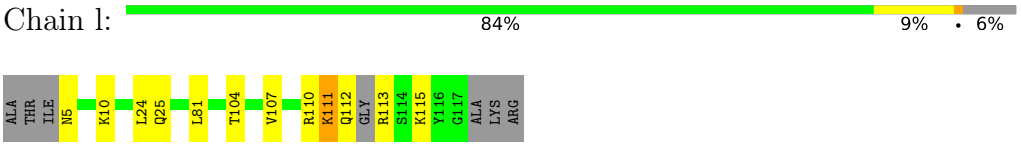

• Molecule 11: 30S ribosomal protein S11

Chain k:



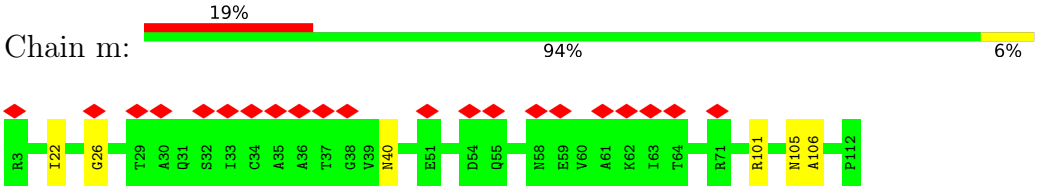

• Molecule 12: 30S ribosomal protein S12

Chain l:



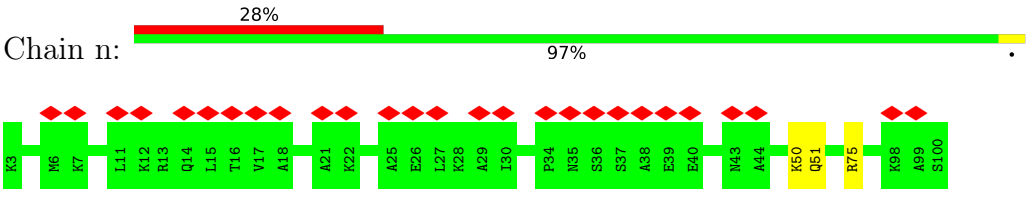

• Molecule 13: 30S ribosomal protein S13

Chain m:



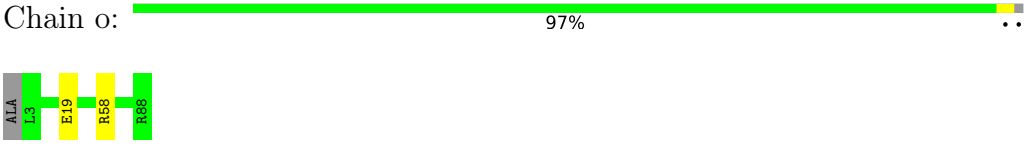

• Molecule 14: 30S ribosomal protein S14

Chain n:



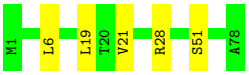

• Molecule 15: 30S ribosomal protein S15

Chain o:



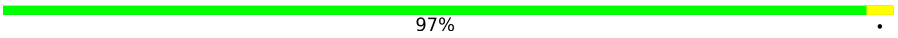
• Molecule 16: 30S ribosomal protein S16

Chain p:


• Molecule 17: 30S ribosomal protein S17

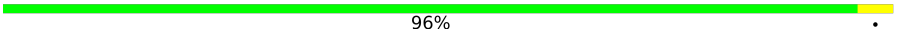
Chain q:

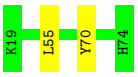




• Molecule 18: 30S ribosomal protein S18

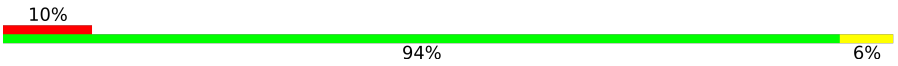
Chain r:

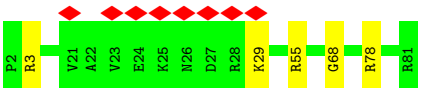



• Molecule 19: 30S ribosomal protein S19

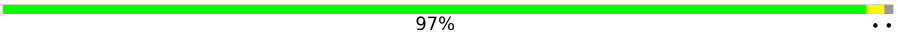
Chain s:

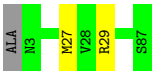



• Molecule 20: 30S ribosomal protein S20

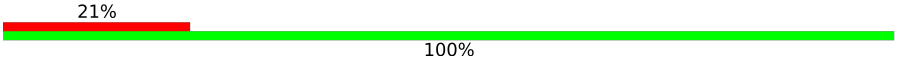
Chain t:

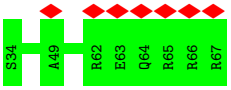



• Molecule 21: 30S ribosomal protein S21

Chain u:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 319022 | 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 ($e^-/Å^2$) | 1.0 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.603 | Depositor |
| Minimum map value | -0.352 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.009 | Depositor |
| Recommended contour level | 0.00936 | Depositor |
| Map size (Å) | 440.0, 440.0, 440.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1, 1.1, 1.1 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | a | 1.40 | 78/36497 (0.2%) | 1.83 | 689/56927 (1.2%) |
| 2 | b | 0.35 | 0/1754 | 0.57 | 0/2355 |
| 3 | c | 0.30 | 0/1638 | 0.60 | 0/2209 |
| 4 | d | 0.48 | 1/1619 (0.1%) | 0.76 | 1/2168 (0.0%) |
| 5 | e | 0.53 | 0/1106 | 0.72 | 0/1488 |
| 6 | f | 0.49 | 0/815 | 0.71 | 1/1098 (0.1%) |
| 7 | g | 0.24 | 0/1207 | 0.50 | 0/1616 |
| 8 | h | 0.73 | 1/924 (0.1%) | 1.14 | 6/1243 (0.5%) |
| 9 | i | 0.32 | 0/1006 | 0.68 | 0/1347 |
| 10 | j | 0.29 | 0/773 | 0.63 | 0/1045 |
| 11 | k | 0.47 | 0/844 | 0.66 | 1/1148 (0.1%) |
| 12 | l | 0.57 | 0/906 | 0.91 | 2/1215 (0.2%) |
| 13 | m | 0.31 | 0/853 | 0.71 | 0/1144 |
| 14 | n | 0.31 | 0/786 | 0.68 | 0/1047 |
| 15 | o | 0.61 | 0/693 | 0.75 | 0/926 |
| 16 | p | 0.77 | 0/617 | 0.89 | 2/832 (0.2%) |
| 17 | q | 0.59 | 0/627 | 0.67 | 0/844 |
| 18 | r | 0.62 | 0/450 | 0.76 | 1/608 (0.2%) |
| 19 | s | 4.73 | 1/649 (0.2%) | 0.75 | 1/874 (0.1%) |
| 20 | t | 0.56 | 0/660 | 0.67 | 0/880 |
| 21 | u | 0.43 | 0/298 | 0.60 | 0/391 |
| All | All | 1.28 | 81/54722 (0.1%) | 1.58 | 704/81405 (0.9%) |

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 |
|---|---|---|---|
| 3 | c | 0 | 2 |
| 4 | d | 0 | 2 |
| 8 | h | 0 | 15 |
| 11 | k | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 12 | l | 0 | 6 |
| 13 | m | 0 | 4 |
| 14 | n | 0 | 2 |
| 16 | p | 0 | 1 |
| All | All | 0 | 34 |

The worst 5 of 81 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | s | 3 | ARG | CB-CG | 120.10 | 4.76 | 1.52 |
| 1 | a | 1313 | A | N3-C4 | 57.70 | 1.69 | 1.34 |
| 1 | a | 1313 | A | C6-N1 | 51.87 | 1.71 | 1.35 |
| 1 | a | 1219 | A | N9-C4 | 44.11 | 1.64 | 1.37 |
| 1 | a | 1313 | A | C5-C4 | 41.51 | 1.67 | 1.38 |

The worst 5 of 704 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | a | 1219 | A | N7-C8-N9 | -144.78 | 41.41 | 113.80 |
| 1 | a | 1219 | A | C4-C5-N7 | -137.11 | 42.15 | 110.70 |
| 1 | a | 1219 | A | C8-N9-C4 | -133.34 | 52.46 | 105.80 |
| 1 | a | 1219 | A | C5-N7-C8 | 57.27 | 132.53 | 103.90 |
| 1 | a | 1219 | A | C6-C5-N7 | 38.34 | 159.14 | 132.30 |

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | c | 12 | LEU | Peptide |
| 3 | c | 176 | HIS | Peptide |
| 4 | d | 205 | SER | Peptide |
| 4 | d | 49 | SER | Peptide |
| 8 | h | 29 | SER | 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 | 32595 | 0 | 16400 | 0 | 0 |
| 2 | b | 1728 | 0 | 1766 | 0 | 0 |
| 3 | c | 1609 | 0 | 1636 | 0 | 0 |
| 4 | d | 1600 | 0 | 1620 | 0 | 0 |
| 5 | e | 1092 | 0 | 1139 | 0 | 0 |
| 6 | f | 802 | 0 | 769 | 0 | 0 |
| 7 | g | 1190 | 0 | 1227 | 0 | 0 |
| 8 | h | 915 | 0 | 952 | 0 | 0 |
| 9 | i | 994 | 0 | 1031 | 0 | 0 |
| 10 | j | 763 | 0 | 801 | 0 | 0 |
| 11 | k | 828 | 0 | 808 | 0 | 0 |
| 12 | l | 893 | 0 | 932 | 0 | 0 |
| 13 | m | 847 | 0 | 888 | 0 | 0 |
| 14 | n | 776 | 0 | 818 | 0 | 0 |
| 15 | o | 686 | 0 | 709 | 0 | 0 |
| 16 | p | 606 | 0 | 606 | 0 | 0 |
| 17 | q | 619 | 0 | 659 | 0 | 0 |
| 18 | r | 443 | 0 | 460 | 0 | 0 |
| 19 | s | 635 | 0 | 662 | 0 | 0 |
| 20 | t | 653 | 0 | 699 | 0 | 0 |
| 21 | u | 295 | 0 | 313 | 0 | 0 |
| All | All | 50569 | 0 | 34895 | 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 13.

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 |
|---|---|---|---|---|---|---|
| 2 | b | 217/221 (98%) | 179 (82%) | 34 (16%) | 4 (2%) | 8 33 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | c | 201/203 (99%) | 170 (85%) | 29 (14%) | 2 (1%) | 15 48 |
| 4 | d | 203/205 (99%) | 161 (79%) | 39 (19%) | 3 (2%) | 10 38 |
| 5 | e | 147/149 (99%) | 130 (88%) | 15 (10%) | 2 (1%) | 11 39 |
| 6 | f | 98/100 (98%) | 86 (88%) | 10 (10%) | 2 (2%) | 7 30 |
| 7 | g | 152/154 (99%) | 115 (76%) | 27 (18%) | 10 (7%) | 1 5 |
| 8 | h | 121/125 (97%) | 84 (69%) | 29 (24%) | 8 (7%) | 1 5 |
| 9 | i | 124/126 (98%) | 104 (84%) | 20 (16%) | 0 | 100 100 |
| 10 | j | 94/96 (98%) | 82 (87%) | 12 (13%) | 0 | 100 100 |
| 11 | k | 113/115 (98%) | 93 (82%) | 20 (18%) | 0 | 100 100 |
| 12 | l | 111/120 (92%) | 91 (82%) | 18 (16%) | 2 (2%) | 8 33 |
| 13 | m | 105/109 (96%) | 86 (82%) | 19 (18%) | 0 | 100 100 |
| 14 | n | 96/98 (98%) | 80 (83%) | 16 (17%) | 0 | 100 100 |
| 15 | o | 84/87 (97%) | 79 (94%) | 4 (5%) | 1 (1%) | 13 43 |
| 16 | p | 76/78 (97%) | 64 (84%) | 12 (16%) | 0 | 100 100 |
| 17 | q | 74/76 (97%) | 71 (96%) | 3 (4%) | 0 | 100 100 |
| 18 | r | 54/56 (96%) | 52 (96%) | 2 (4%) | 0 | 100 100 |
| 19 | s | 78/80 (98%) | 63 (81%) | 15 (19%) | 0 | 100 100 |
| 20 | t | 83/86 (96%) | 83 (100%) | 0 | 0 | 100 100 |
| 21 | u | 32/34 (94%) | 25 (78%) | 7 (22%) | 0 | 100 100 |
| All | All | 2263/2318 (98%) | 1898 (84%) | 331 (15%) | 34 (2%) | 14 38 |

5 of 34 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | c | 8 | ASN |
| 4 | d | 14 | ARG |
| 4 | d | 33 | LYS |
| 5 | e | 14 | GLU |
| 6 | f | 86 | ARG |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | b | 182/183 (100%) | 114 (63%) | 68 (37%) | 0 0 |
| 3 | c | 163/169 (96%) | 161 (99%) | 2 (1%) | 71 88 |
| 4 | d | 166/173 (96%) | 162 (98%) | 4 (2%) | 49 77 |
| 5 | e | 108/109 (99%) | 94 (87%) | 14 (13%) | 4 16 |
| 6 | f | 81/85 (95%) | 75 (93%) | 6 (7%) | 13 41 |
| 7 | g | 116/120 (97%) | 66 (57%) | 50 (43%) | 0 0 |
| 8 | h | 98/103 (95%) | 90 (92%) | 8 (8%) | 11 36 |
| 9 | i | 102/102 (100%) | 99 (97%) | 3 (3%) | 42 73 |
| 10 | j | 85/85 (100%) | 82 (96%) | 3 (4%) | 36 68 |
| 11 | k | 82/87 (94%) | 79 (96%) | 3 (4%) | 34 66 |
| 12 | l | 100/104 (96%) | 97 (97%) | 3 (3%) | 41 72 |
| 13 | m | 91/91 (100%) | 89 (98%) | 2 (2%) | 52 79 |
| 14 | n | 78/80 (98%) | 77 (99%) | 1 (1%) | 69 87 |
| 15 | o | 73/73 (100%) | 72 (99%) | 1 (1%) | 67 86 |
| 16 | p | 60/63 (95%) | 58 (97%) | 2 (3%) | 38 70 |
| 17 | q | 70/70 (100%) | 68 (97%) | 2 (3%) | 42 73 |
| 18 | r | 46/48 (96%) | 45 (98%) | 1 (2%) | 52 79 |
| 19 | s | 69/71 (97%) | 66 (96%) | 3 (4%) | 29 62 |
| 20 | t | 67/68 (98%) | 65 (97%) | 2 (3%) | 41 72 |
| 21 | u | 28/28 (100%) | 28 (100%) | 0 | 100 100 |
| All | All | 1865/1912 (98%) | 1687 (90%) | 178 (10%) | 12 29 |

5 of 178 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | g | 61 | THR |
| 7 | g | 154 | TYR |
| 7 | g | 75 | VAL |
| 7 | g | 113 | GLU |
| 8 | h | 106 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | n | 71 | HIS |
| 15 | o | 42 | HIS |
| 19 | s | 14 | HIS |
| 5 | e | 123 | ASN |
| 5 | e | 90 | HIS |

#### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | a | 1514/1519 (99%) | 677 (44%) | 0 |

5 of 677 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | a | 9 | G |
| 1 | a | 15 | G |
| 1 | a | 22 | G |
| 1 | a | 32 | A |
| 1 | a | 33 | A |

There are no RNA pucker outliers to report.

### 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)

There are no ligands in this entry.

### 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 |
|---|---|---|
| 1 | a | 4 |
| 2 | b | 1 |
| 13 | m | 1 |

The worst 5 of 6 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | a | 2:A | O3' | 7:A | P | 21.37 |
| 1 | a | 63:C | O3' | 65:A | P | 7.46 |
| 1 | b | 124:GLY | C | 130:THR | N | 5.42 |
| 1 | m | 20:THR | C | 22:ILE | N | 3.27 |
| 1 | a | 1376:C | O3' | 1377:C | P | 3.24 |

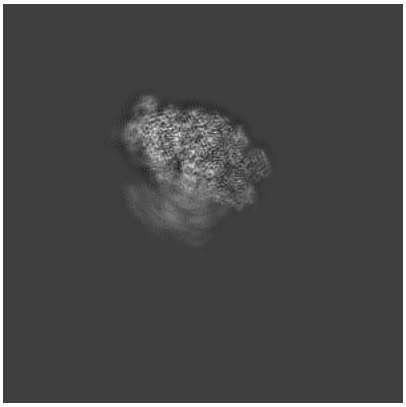
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10281. These allow visual inspection of the internal detail of the map and identification of artifacts.

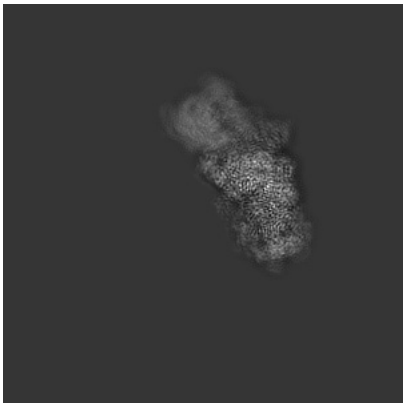
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

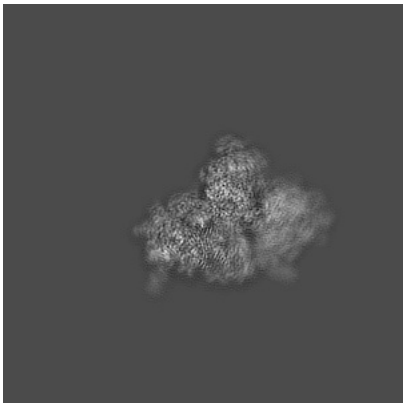
### 6.1.1 Primary map



X



Y



Z

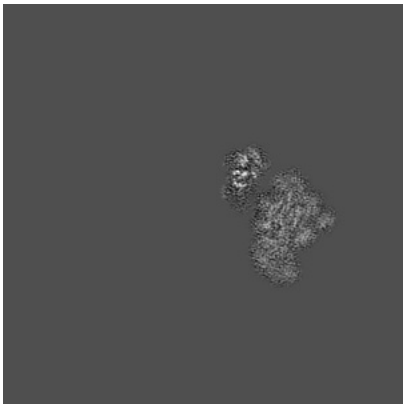
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

### 6.2.1 Primary map

X Index: 200

Y Index: 200

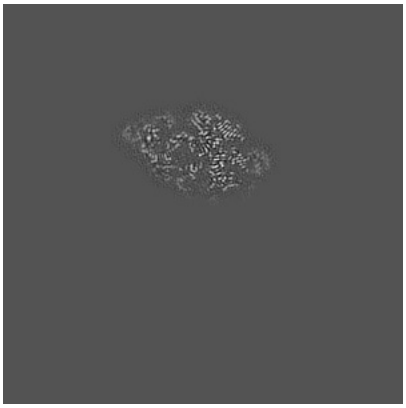


Z Index: 200

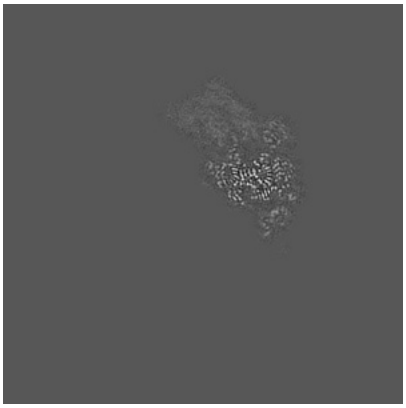
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

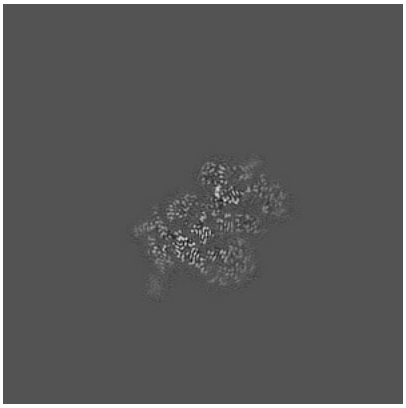
### 6.3.1 Primary map



X Index: 218



Y Index: 207

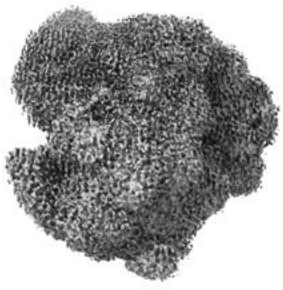


Z Index: 268

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.00936. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

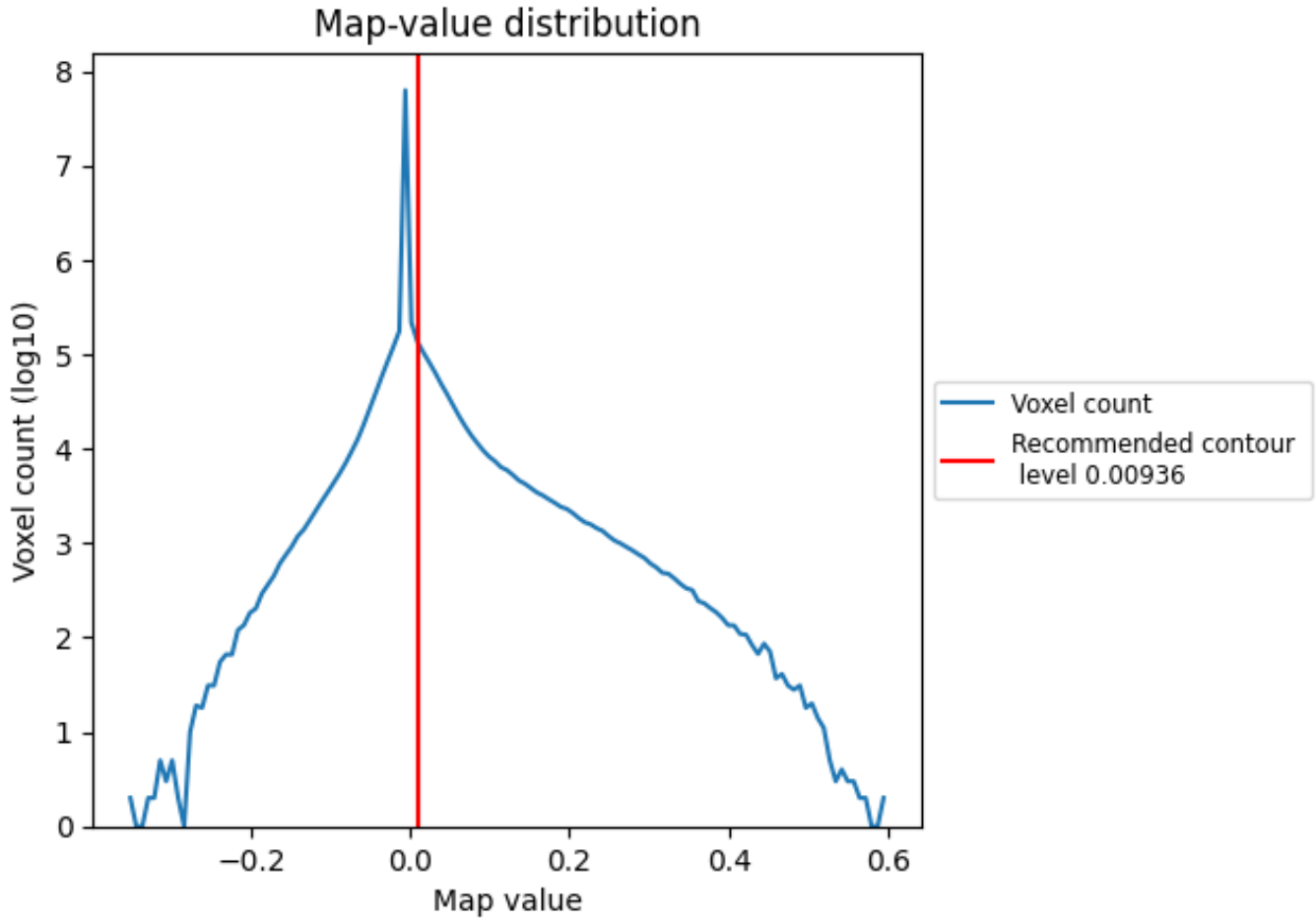
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

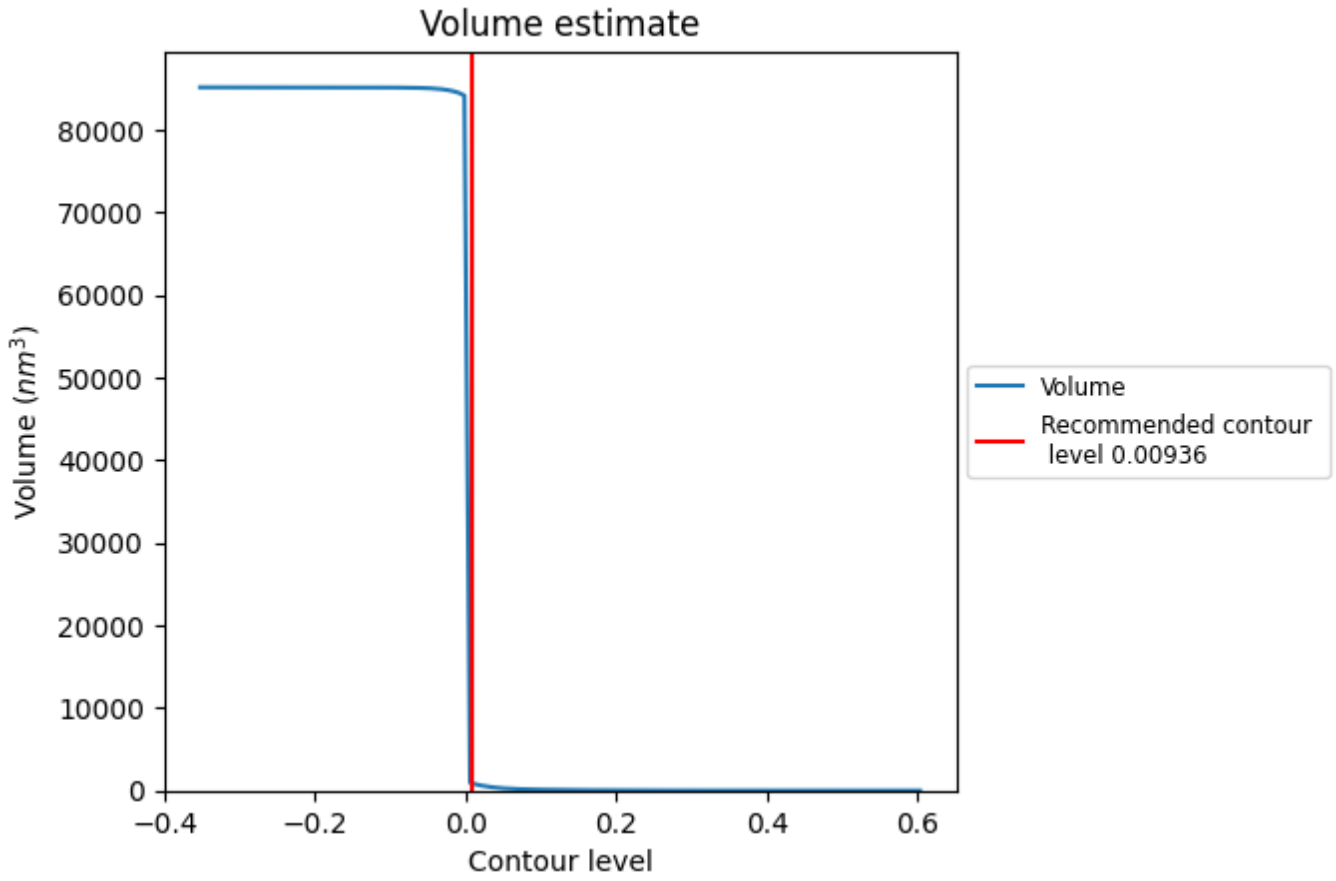
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

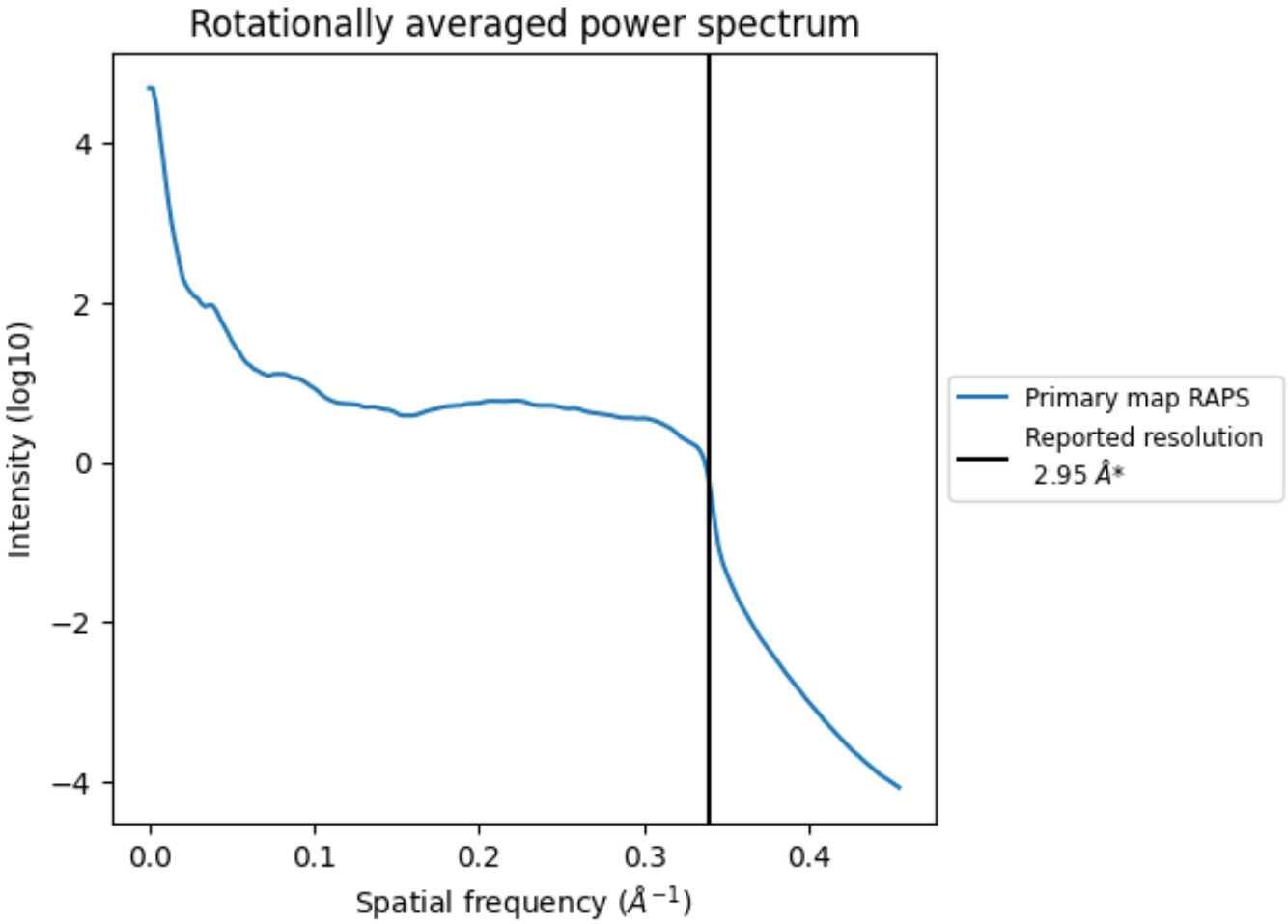
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 868 $nm^3$; this corresponds to an approximate mass of 784 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 0.339 $Å^{-1}$

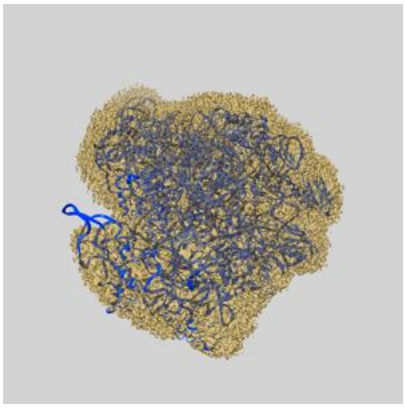
# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

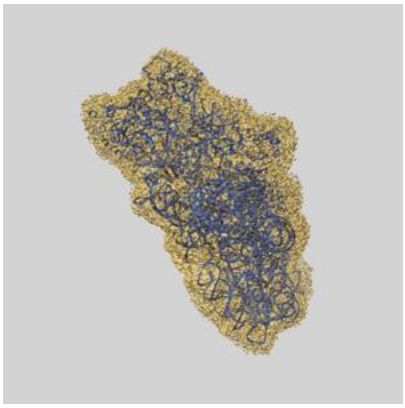
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10281 and PDB model 6SPC. Per-residue inclusion information can be found in section 3 on page 9.

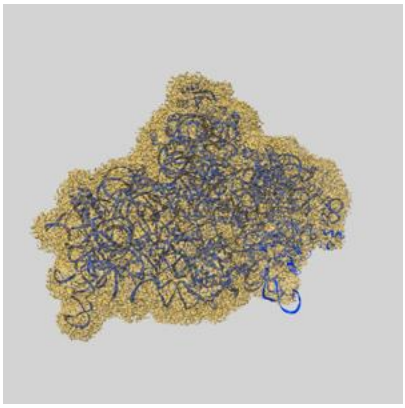
## 9.1 Map-model overlay



X



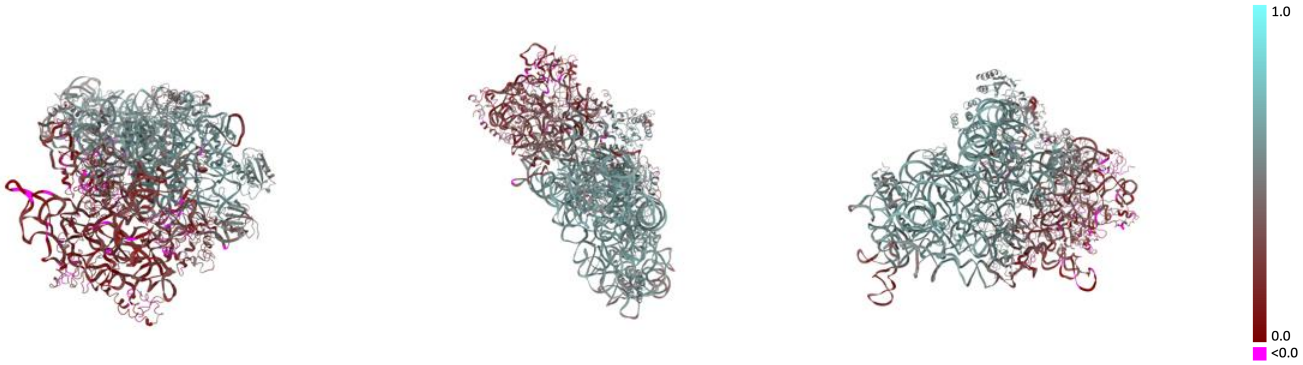
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00936 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.

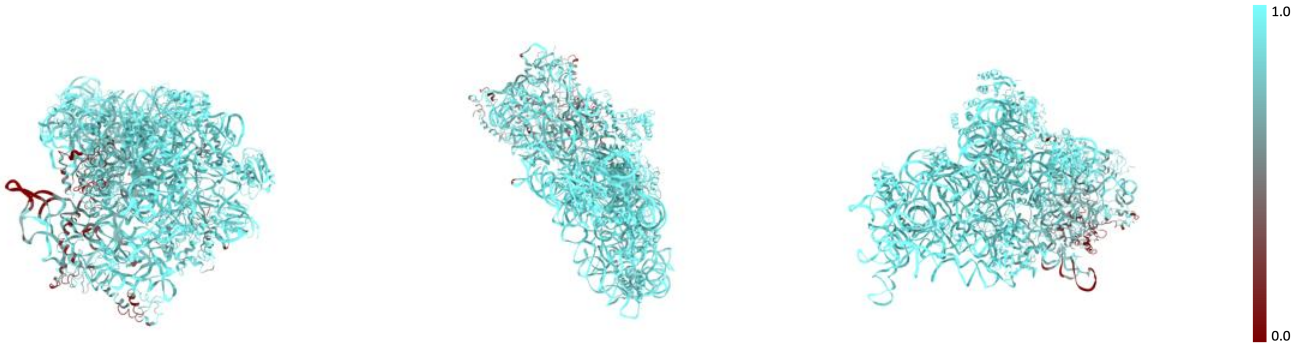
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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.

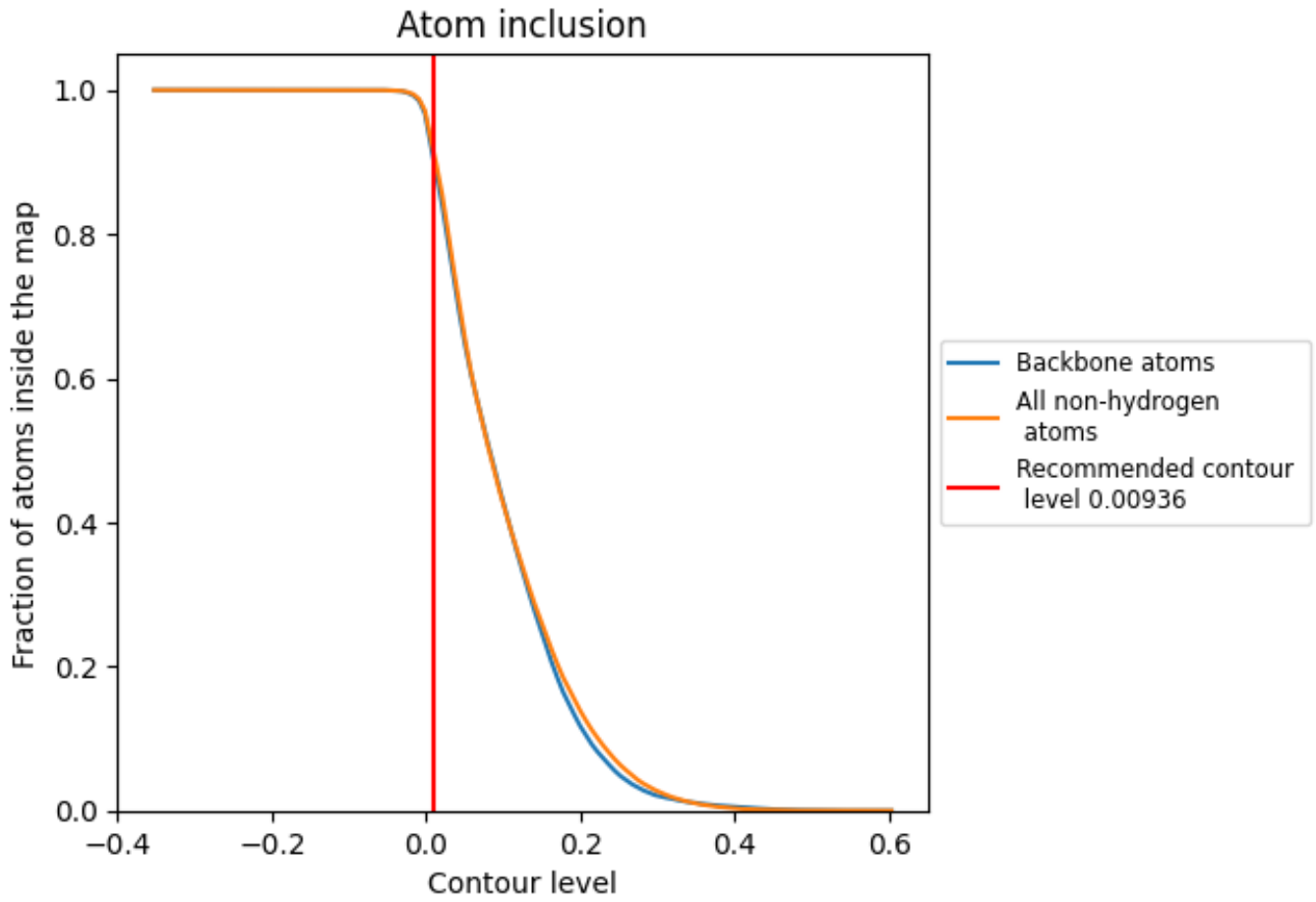
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (0.00936).

## 9.4 Atom inclusion (i)




At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00936) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9146 | 0.4440 |
| a | 0.9445 | 0.4710 |
| b | 0.9769 | 0.5140 |
| c | 0.5423 | 0.1890 |
| d | 0.9276 | 0.4220 |
| e | 0.9729 | 0.5630 |
| f | 0.9820 | 0.5190 |
| g | 0.8147 | 0.3130 |
| h | 0.8831 | 0.4250 |
| i | 0.8249 | 0.1150 |
| j | 0.7151 | 0.2080 |
| k | 0.9679 | 0.4590 |
| l | 0.9406 | 0.5120 |
| m | 0.7197 | 0.1780 |
| n | 0.6121 | 0.2090 |
| o | 0.9955 | 0.5860 |
| p | 0.9880 | 0.5980 |
| q | 0.9766 | 0.5740 |
| r | 0.9860 | 0.5670 |
| s | 0.7617 | 0.2050 |
| t | 0.9890 | 0.5810 |
| u | 0.7283 | 0.4130 |