

Feb 11, 2024 – 05:50 PM EST

PDB ID : 3EQ4EMDB ID : EMD-1564 Title : Model of tRNA(Leu)-EF-Tu in the ribosomal pre-accommodated state revealed by cryo-EM Frank, J.; Li, W.; Agirrezabala, X. Authors : 2008-09-30 Deposited on : : 12.00 Å(reported)Resolution Based on initial models 1QZA, 2AVY, 2AW4, 10B2 :

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. dev70 |
|--------------------------------|---|--|
| 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) | : | 2.36 |

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 12.00 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 | Percentile | Ranks | Value |
|--------------|-----------------------------------|----------------------|-------|
| Clashscore | | | 1 |
| RNA backbone | | | 0.00 |
| Worse | | Bett | er |
| Percent | ile relative to all structures | | |
| Percent | ile relative to all EM structures | | |
| Metric | Whole archive | EM structures | |
| Metric | $(\# {\rm Entries})$ | $(\# {\rm Entries})$ | |
| Clashscore | 158937 | 4297 | |
| 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 $\geq=3, 2, 1$ 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 $\leq=5\%$ 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 |
|-----|-------|--------|------------------|
| | | | 82% |
| 1 | Х | 393 | 100% |
| | | | 37% |
| 2 | L | 123 | 100% |
| | | | 57% |
| 3 | Ι | 141 | 100% |
| | | | 73% |
| 4 | Y | 85 | 98% • |
| | | | 100% |
| 5 | A | 9 | 100% |
| | ~ | | 55% |
| 6 | С | 11 | 100% |
| _ | D | 10 | 12% |
| 7 | В | 48 | 100% |
| | | | 32% |
| 8 | D | 28 | 100% |
| | E | 1 17 | 29% |
| 9 | Е | 17 | 100% |



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 855 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 Elongation factor Tu.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|-----|-------|----------|-------------------|---------|-------|
| 1 | Х | 393 | Total C 393 393 | 0 | 393 |

• Molecule 2 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|-----|-------|----------|-------------------|---------|-------|
| 2 | L | 123 | Total C 123 123 | 0 | 123 |

• Molecule 3 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | 5 | AltConf | Trace |
|-----|-------|----------|-------------------|---------|---------|-------|
| 3 | Ι | 141 | Total (141 1- | C 41 | 0 | 141 |

• Molecule 4 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|-----|-------|----------|-----------------|---------|-------|
| 4 | Y | 85 | Total P 85 85 | 0 | 85 |

• Molecule 5 is a RNA chain called Fragment h18 of the 16S rRNA.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|-----|-------|----------|----------------|---------|-------|
| 5 | А | 9 | Total P 9 9 | 0 | 9 |

• Molecule 6 is a RNA chain called Fragment h44 of the 16S rRNA.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|-----|-------|----------|------------------|---------|-------|
| 6 | С | 11 | Total P 11 11 | 0 | 11 |



• Molecule 7 is a RNA chain called Fragment H43-44 of the 23S rRNA.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|-----|-------|----------|-----------------|---------|-------|
| 7 | В | 48 | Total P 48 48 | 0 | 48 |

• Molecule 8 is a RNA chain called Fragment H95 of the 23S rRNA.

| Mol | Chain | Residues | Aton | ns | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|-------|
| 8 | D | 28 | Total 28 | Р 28 | 0 | 28 |

• Molecule 9 is a RNA chain called Fragment H69 of the 23S rRNA.

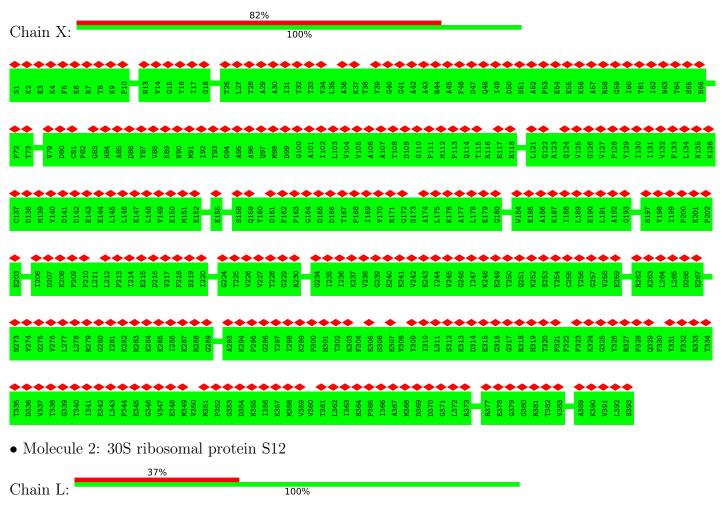
| Mol | Chain | Residues | Ator | ns | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|-------|
| 9 | Е | 17 | Total 17 | Р 17 | 0 | 17 |



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: Elongation factor Tu





• Molecule 3: 50S ribosomal protein L11

57%

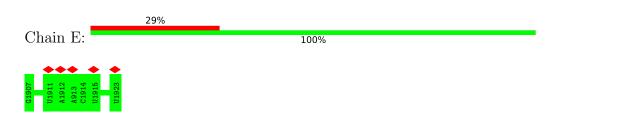
Chain I:

100%

| <u> </u> | ••••• •• •••• | ** ** **** | ••••• | ********* |
|---|--|---|---|--|
| A1 K2 K3 V4 Q5 A6 Q1 1 V12 V12 V12 A13 | 615 A17 A17 P19 820 624 628 628 628 629 631 | M35 E36 F37 C38 K39 N42 A43 K44 T45 | D46 S47 I48 E49 K50 G51 L52 L52 F53 I54 | A76 A76 L78 L78 K80 K81 A82 A83 G84 C84 K86 |
| ••• | *** * ** ** ** | • •••• | | |
| 887 688 889 889 889 895 895 895 895 895 895 8 | 8101 R102 A103 Q104 E107 E107 E107 A112 A113 A113 A113 1120 D120 | E122 L137 V138 V139 E140 D141 | | |
| • Molecule 4: tRNA | | | | |
| Chain Y: | 73% 98% | | <u> </u> | |
| ••••• | | | | |
| C2 63 64 A5 A5 A5 A5 C1 C11 C11 C11 C13 C13 A14 | G15 U16 G18 G18 G19 G20 G22 G22 G26 G26 G26 G26 G26 G26 G26 G26 | A29 G30 U39 U41 G42 G42 C48 C48 | u50 G51 U52 G53 G53 G53 A58 U59 C60 C60 C61 | C63 A64 G85 A66 A67 A67 U68 U68 U69 C70 C70 C72 C72 C74 |
| | •• | | | |
| C75 C76 U77 C78 C79 C80 C81 U82 C81 G84 G85 C86 C87 C87 | 880 M | | | |
| • Molecule 5: Fragme | ent h18 of the 16S rRNA | | | |
| | 100% | | | |
| Chain A: | 100% | | | |
| C526 G527 C528 G529 G530 U531 A532 A533 A533 U534 | | | | |
| • Molecule 6: Fragme | ent h44 of the 16S rRNA | | | |
| | 55% | | | |
| Chain C: | 100% | | | |
| G1487 G1488 G1489 G1490 G1491 A1492 A1492 A1492 G1497 | | | | |
| • Molecule 7: Fragme | ent H43-44 of the 23S rR | NA | | |
| Chain B: | 100% | | | |
| A1054 U1066 A1067 C1079 G1091 C1092 C1092 U1101 | | | | |
| • Molecule 8: Fragme | ent H95 of the 23S rRNA $$ | L. | | |
| Chain D: | 5 | | | |
| | 100% | | | |
| 12847 12849 12850 12850 12850 12850 12855 12855 12865 12865 12865 12865 12865 | C3874 | | | |
| | | | | |

• Molecule 9: Fragment H69 of the 23S rRNA







4 Experimental information (i)

| Property | Value | Source |
|------------------------------------|---------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 80000 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | FEI TECNAI F20 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{\AA}^2)$ | 15 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 50000 | Depositor |
| Image detector | GENERIC CCD | Depositor |
| Maximum map value | 0.001 | Depositor |
| Minimum map value | -0.000 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.000 | Depositor |
| Recommended contour level | 0.00045 | Depositor |
| Map size (Å) | 366.6, 366.6, 366.6 | wwPDB |
| Map dimensions | 130, 130, 130 | wwPDB |
| Map angles (°) | 90, 90, 90 | wwPDB |
| Pixel spacing (Å) | 2.82, 2.82, 2.82 | 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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 | Х | 393 | 0 | 0 | 0 | 0 |
| 2 | L | 123 | 0 | 0 | 0 | 0 |
| 3 | Ι | 141 | 0 | 0 | 0 | 0 |
| 4 | Y | 85 | 0 | 0 | 1 | 0 |
| 5 | А | 9 | 0 | 0 | 0 | 0 |
| 6 | С | 11 | 0 | 0 | 0 | 0 |
| 7 | В | 48 | 0 | 0 | 0 | 0 |
| 8 | D | 28 | 0 | 0 | 0 | 0 |
| 9 | Е | 17 | 0 | 0 | 0 | 0 |
| All | All | 855 | 0 | 0 | 1 | 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 1.

All (1) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------|------------|-----------------------------|----------------------|
| 4:Y:10:G:P | 4:Y:79:C:P | 1.57 | 1.55 |

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|----------|-------------------|-----------------|
| 4 | Y | 0/85 | - | - |
| 5 | А | 0/9 | - | - |
| 6 | С | 0/11 | - | - |
| 7 | В | 0/48 | - | - |
| 8 | D | 0/28 | - | - |
| 9 | Е | 0/17 | - | - |
| All | All | 0/198 | - | - |

There are no RNA backbone outliers to report.

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)

There are no chain breaks in this entry.



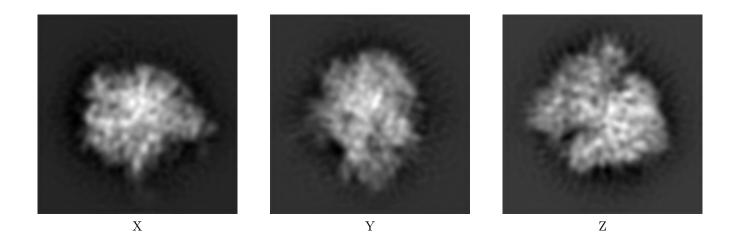
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1564. 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)

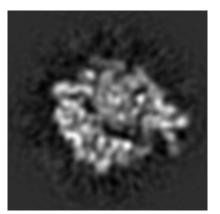
6.1.1 Primary map



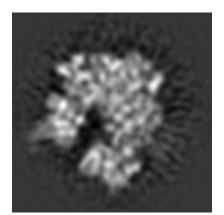
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

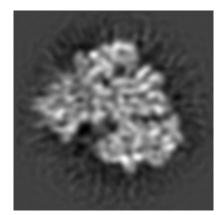
6.2.1 Primary map



X Index: 65



Y Index: 65

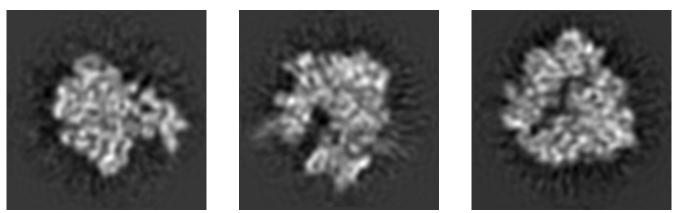


Z Index: 65

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: 70

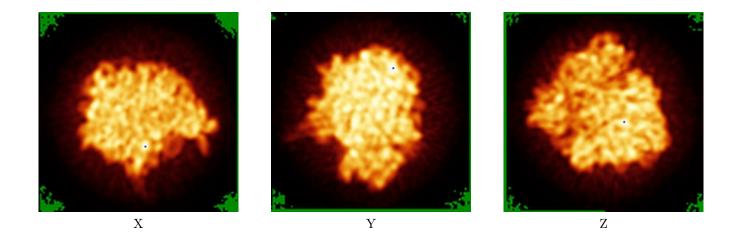
Y Index: 67

Z Index: 58

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

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

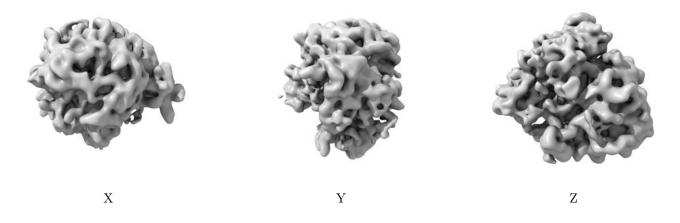


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

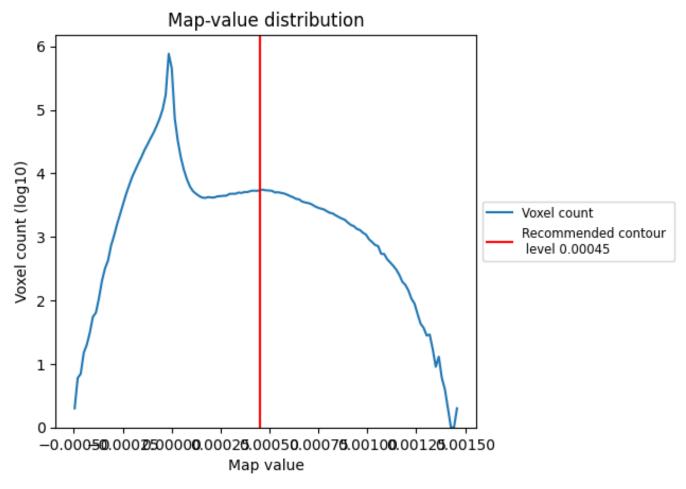
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

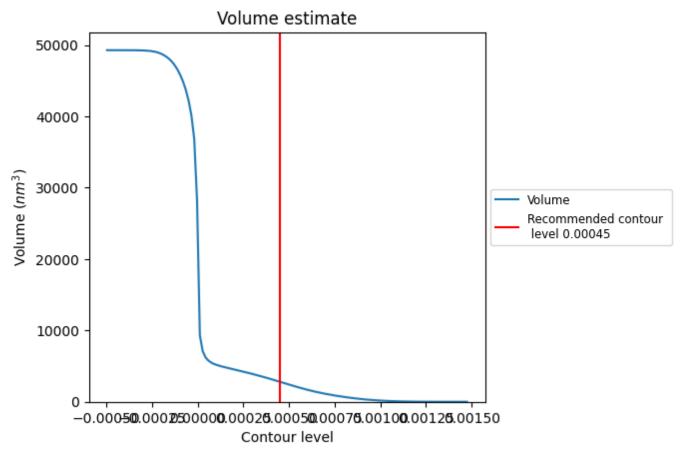
7.1 Map-value distribution (i)



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)

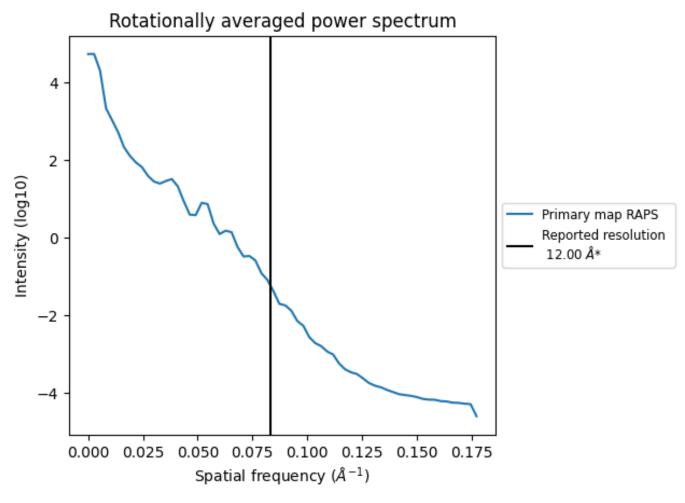


The volume at the recommended contour level is 2808 $\rm nm^3;$ this corresponds to an approximate mass of 2537 kDa.

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 0.083 \AA^{-1}



8 Fourier-Shell correlation (i)

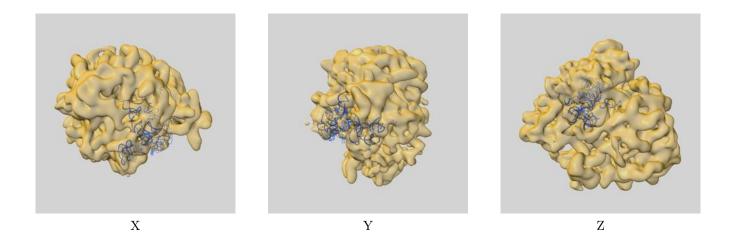
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1564 and PDB model 3EQ4. Per-residue inclusion information can be found in section 3 on page 5.

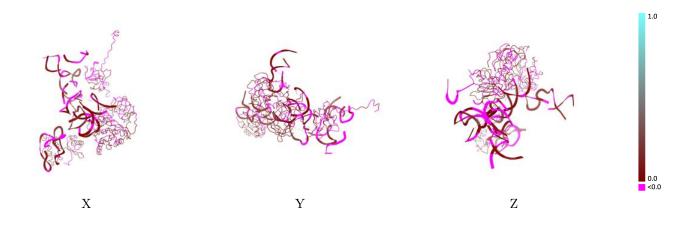
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.00045 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.

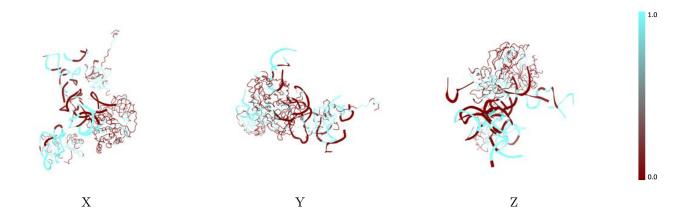


9.2 Q-score mapped to coordinate model (i)



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.

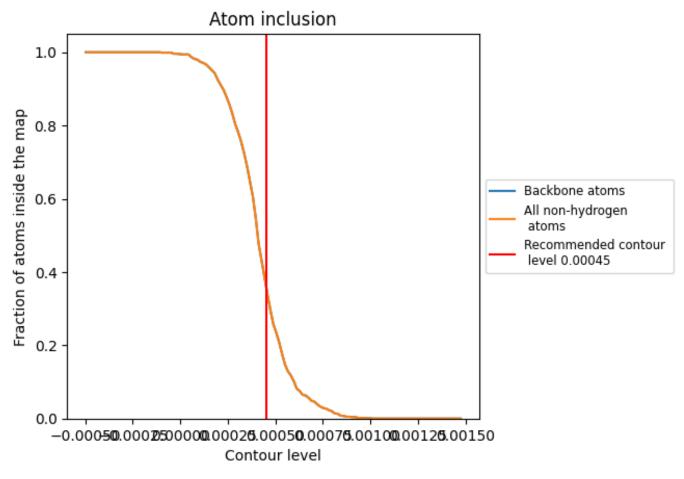
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00045).



9.4 Atom inclusion (i)



At the recommended contour level, 36% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00045) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score | 1.0 |
|-------|----------------|---------|-------------|
| All | 0.3650 | 0.0350 | |
| А | 0.0000 | -0.1370 | |
| В | 0.8750 | 0.0200 | |
| C | 0.4550 | -0.0630 | |
| D | 0.6790 | 0.0400 | |
| E | 0.7060 | 0.0200 | |
| Ι | 0.4330 | 0.0580 | |
| L | 0.6340 | 0.0010 | |
| X | 0.1830 | 0.0480 | 0.0 <0.0 |
| Y | 0.2710 | 0.0300 | |

