# wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 04:57 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 7AXZ |
| EMDB ID | : | EMD-11933 |
| Title | : | Ku70/80 complex apo form |
| Authors | : | Hnizda, A.; Tesina, P.; Novak, P.; Blundell, T.L. |
| Deposited on | : | 2020-11-10 |
| Resolution | : | 3.20 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.

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

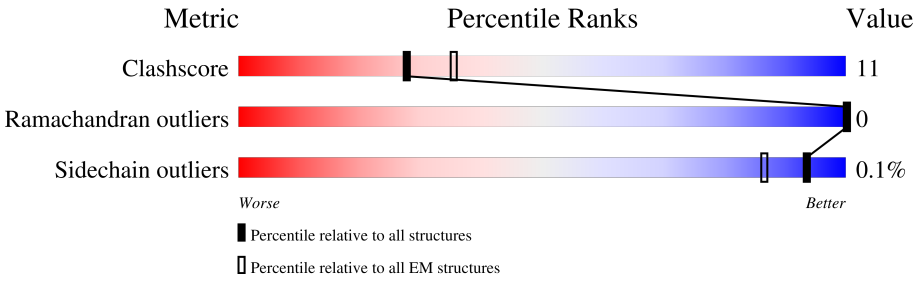
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 3.20 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 |

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 | 609 | 5% 63% 19% 18% |
| 2 | B | 732 | 6% 53% 18% 28% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8225 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 X-ray repair cross-complementing protein 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 499 | 4033 | 2583 | 685 | 747 | 18 | 0 | 0 |

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

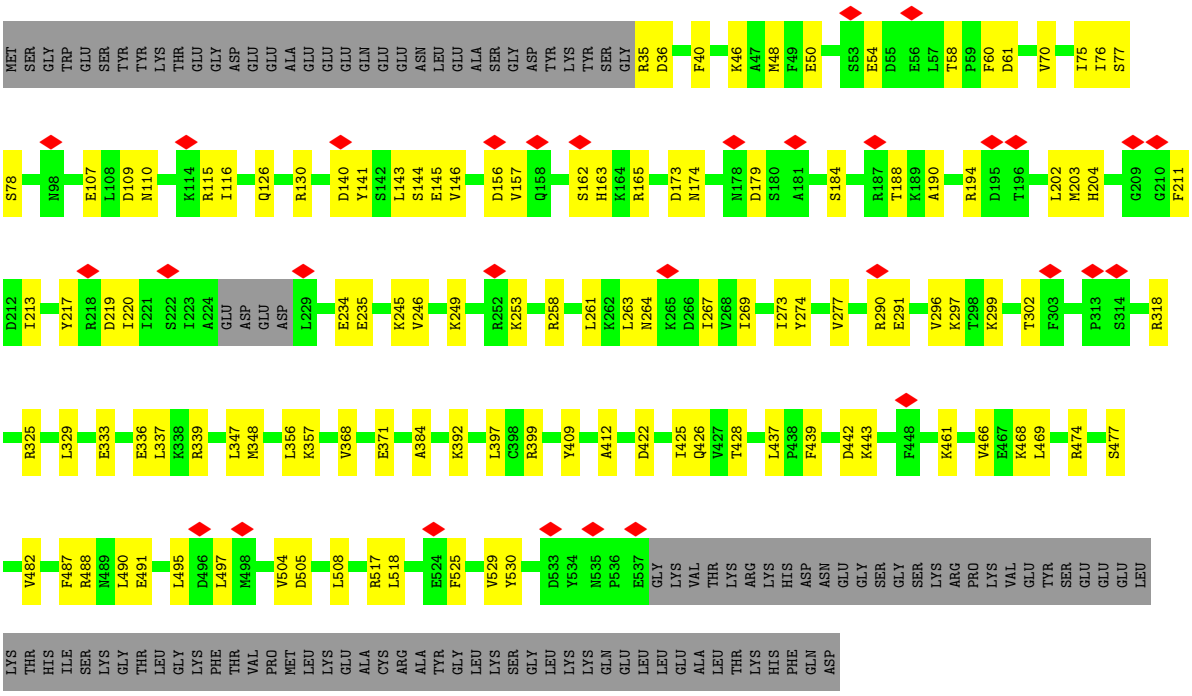
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 524 | 4192 | 2683 | 704 | 782 | 23 | 0 | 0 |

# 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.

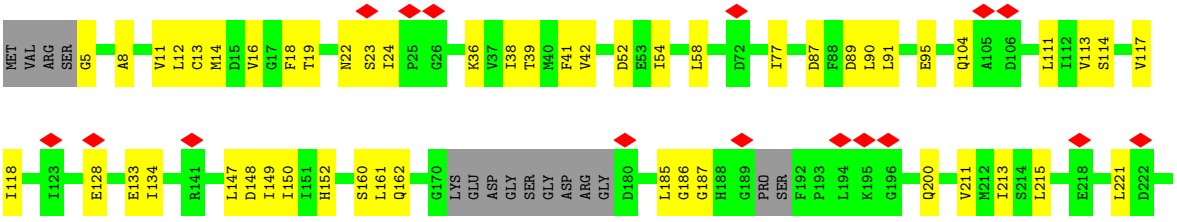
• Molecule 1: X-ray repair cross-complementing protein 6

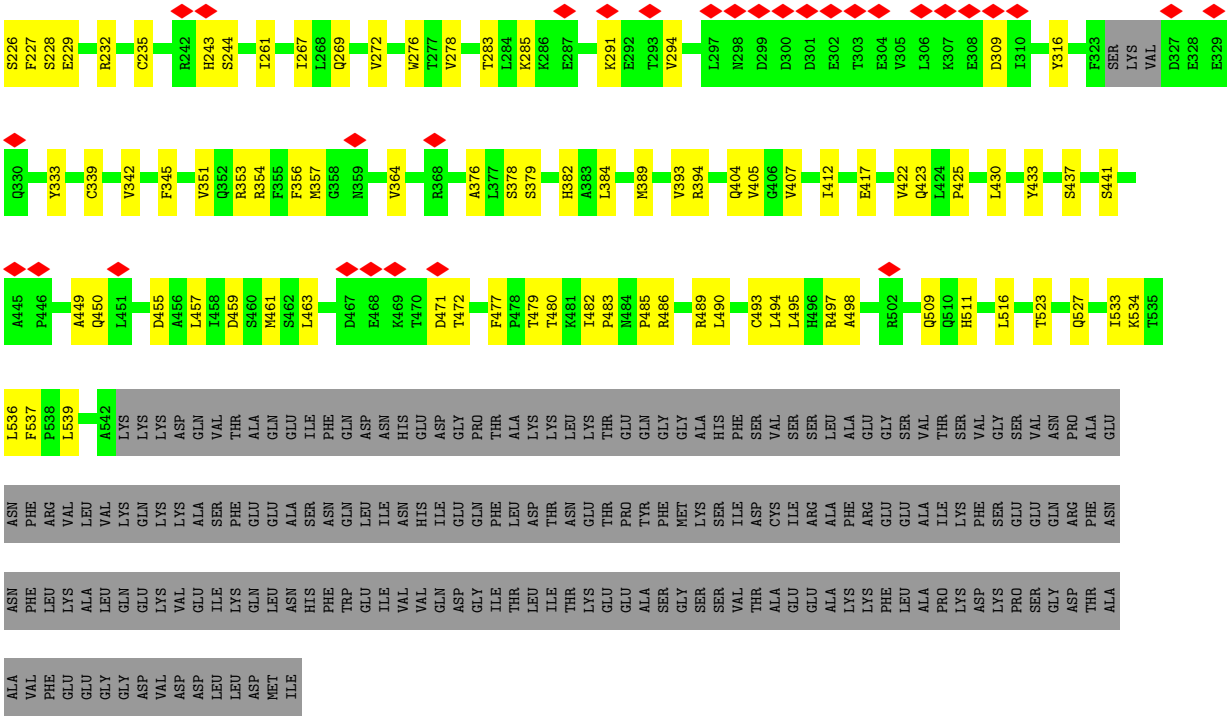
Chain A: 5% 63% 19% 18%




• Molecule 2: X-ray repair cross-complementing protein 5

Chain B: 6% 53% 18% 28%




S226 F227 S228 E229 R232 C235 R242 H243 S244 I261 I267 L268 Q269 V272 W276 T277 V278 T283 L284 K285 K286 E287 K291 E292 T293 V294 L297 N298 D299 D300 D301 E302 T303 E304 V305 L306 K307 E308 D309 I310 Y316 F323 SER LYS VAL D327 E328 E329
Q330 Y333 C339 V342 F345 V351 Q352 R353 R354 F355 F356 M357 G358 N359 V364 R368 A376 L377 S378 S379 H382 A383 L384 M389 V393 R394 Q404 V405 G406 V407 I412 E417 V422 Q423 L424 P425 L430 Y433 S437 S441
A445 P446 A449 Q450 L451 D455 A456 L457 I458 D459 S460 M461 S462 L463 D467 E468 K469 T470 D471 T472 F477 P478 T479 T480 K481 I482 P483 N484 P485 R486 R489 L490 C493 L494 L495 H496 R497 A498 R502 Q509 Q510 H511 L516 T523 Q527 I533 K534 T535
L536 F537 P538 L539 A542 LYS LYS LYS ASP GLN VAL THR ALA GLN GLU ILE PHE GLN ASP ASN HIS GLU ASP GLY PRO THR ALA LYS LYS LEU LYS THR GLU GLN GLY GLY ALA HIS PHE SER VAL SER SER LEU ALA GLU GLY SER VAL THR SER VAL GLY SER VAL ASN PRO ALA GLU
ASN PHE ARG VAL LEU VAL LYS GLN LYS LYS ALA SER PHE GLU GLU ALA SER ASN GLN LEU ILE ASN HIS ILE GLU GLN PHE LEU ASP THR ASN GLU THR PRO TYR PHE MET LYS SER ILE ASP CYS ILE ARG ALA PHE ARG GLU GLU ALA ILE LYS PHE SER GLU GLU GLN ARG PHE ASN
ASN PHE LEU LYS ALA LEU GLN GLU LYS VAL GLU ILE LYS GLN LEU ASN HIS PHE TRP GLU ILE VAL VAL GLN ASP GLY ILE THR LEU ILE THR LYS GLU GLU ALA SER GLY SER SER VAL THR ALA GLU GLU ALA LYS LYS PHE LEU ALA PRO LYS ASP LYS PRO SER GLY ASP THR ALA
ALA VAL PHE GLU GLU GLY GLY ASP VAL ASP ASP LEU LEU ASP MET ILE

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 226000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 39.3 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.111 | Depositor |
| Minimum map value | -0.050 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.004 | Depositor |
| Recommended contour level | 0.0203 | Depositor |
| Map size (Å) | 209.59999, 209.59999, 209.59999 | wwPDB |
| Map dimensions | 200, 200, 200 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.048, 1.048, 1.048 | 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 | 0.46 | 0/4112 | 0.57 | 0/5540 |
| 2 | B | 0.45 | 0/4276 | 0.54 | 0/5766 |
| All | All | 0.45 | 0/8388 | 0.55 | 0/11306 |

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 | A | 4033 | 0 | 4117 | 97 | 0 |
| 2 | B | 4192 | 0 | 4221 | 111 | 0 |
| All | All | 8225 | 0 | 8338 | 177 | 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 11.

The worst 5 of 177 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) |
|---|---|---|---|
| 1:A:274:TYR:OH | 1:A:371:GLU:OE2 | 1.91 | 0.88 |
| 2:B:509:GLN:OE1 | 2:B:511:HIS:NE2 | 2.10 | 0.85 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:489:ARG:NH1 | 2:B:493:CYS:SG | 2.50 | 0.84 |
| 1:A:469:LEU:HD21 | 1:A:518:LEU:HD21 | 1.60 | 0.84 |
| 1:A:325:ARG:NH2 | 2:B:498:ALA:O | 2.13 | 0.81 |

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 | 495/609 (81%) | 451 (91%) | 44 (9%) | 0 | 100 | 100 |
| 2 | B | 516/732 (70%) | 457 (89%) | 59 (11%) | 0 | 100 | 100 |
| All | All | 1011/1341 (75%) | 908 (90%) | 103 (10%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 453/548 (83%) | 452 (100%) | 1 (0%) | 93 | 98 |
| 2 | B | 470/649 (72%) | 470 (100%) | 0 | 100 | 100 |
| All | All | 923/1197 (77%) | 922 (100%) | 1 (0%) | 93 | 98 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 488 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 204 | HIS |

#### 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)

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.

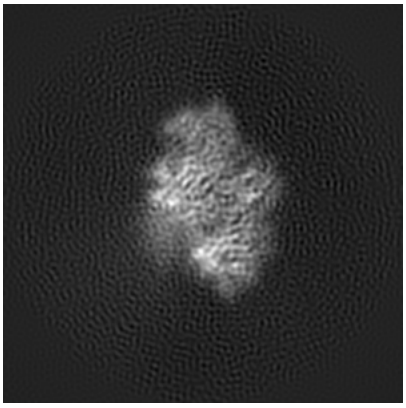
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11933. These allow visual inspection of the internal detail of the map and identification of artifacts.

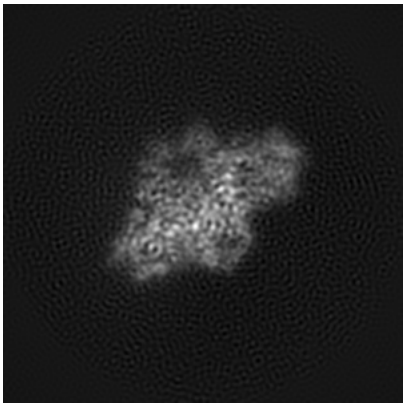
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

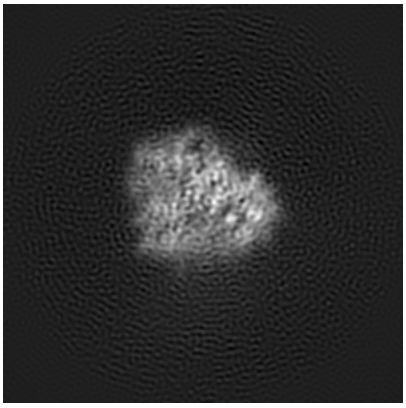
### 6.1.1 Primary map



X



Y

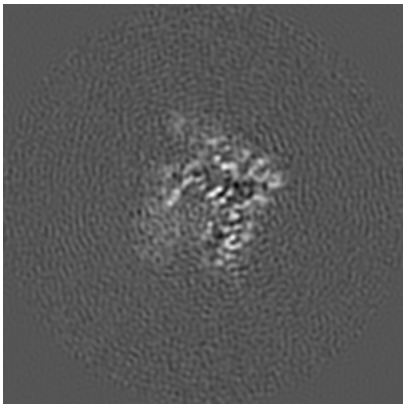


Z

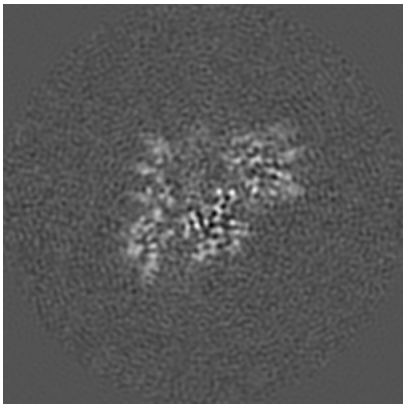
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

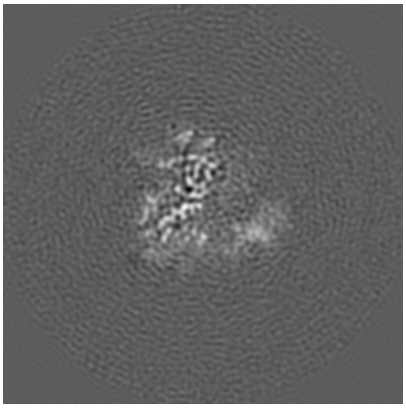
### 6.2.1 Primary map



X Index: 100



Y Index: 100

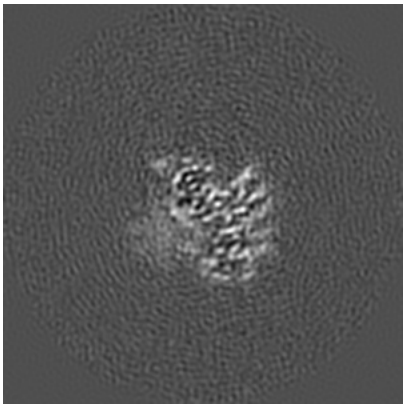


Z Index: 100

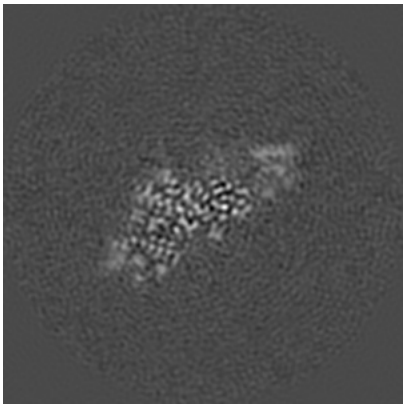
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

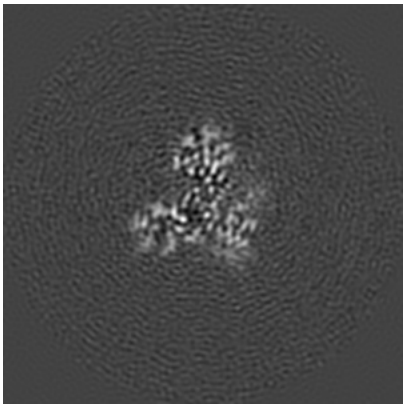
### 6.3.1 Primary map



X Index: 87



Y Index: 113



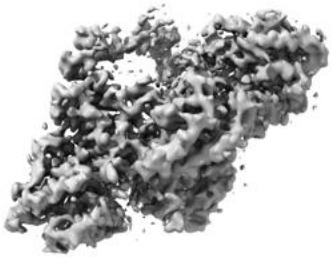
Z Index: 113

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 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

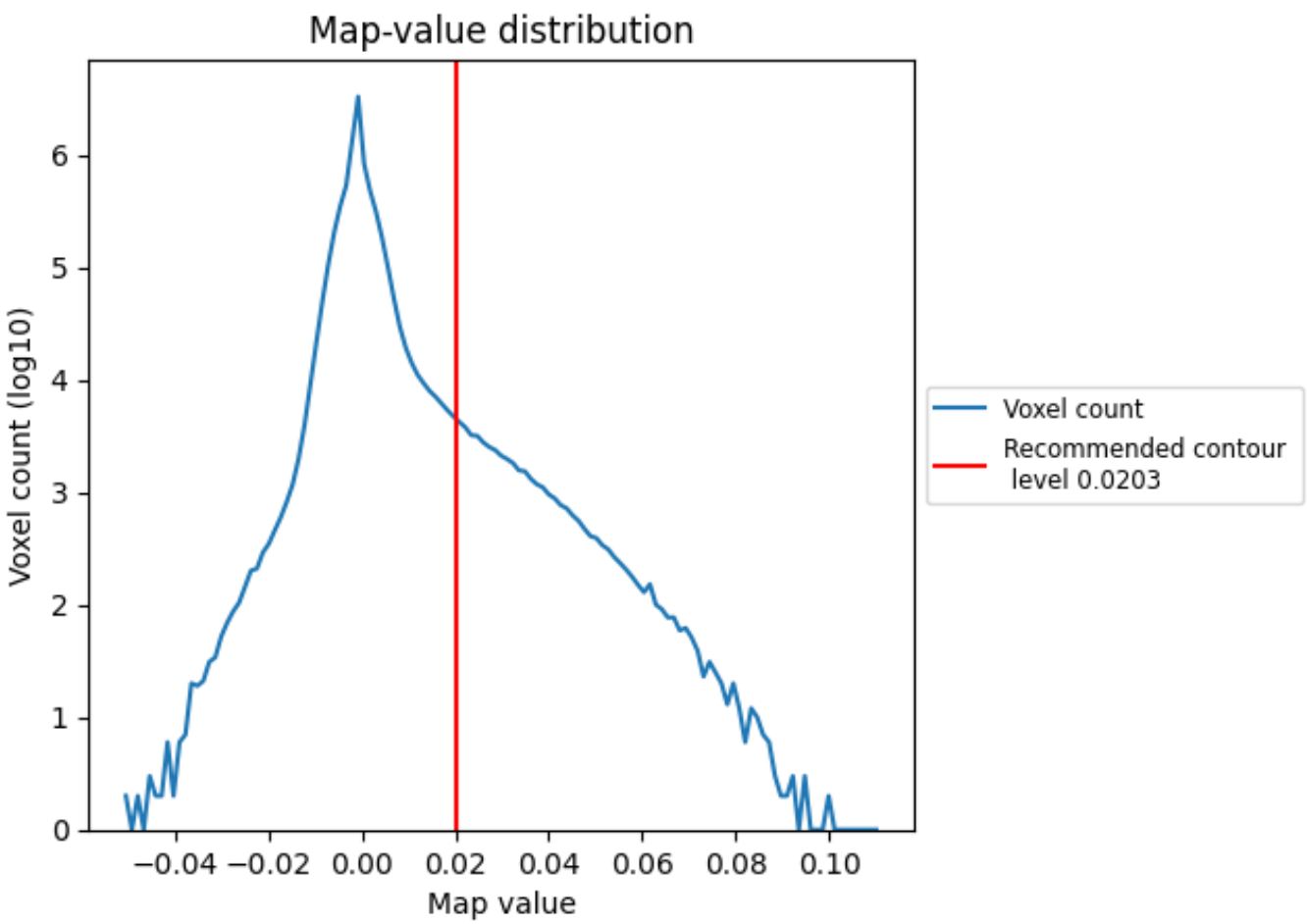
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

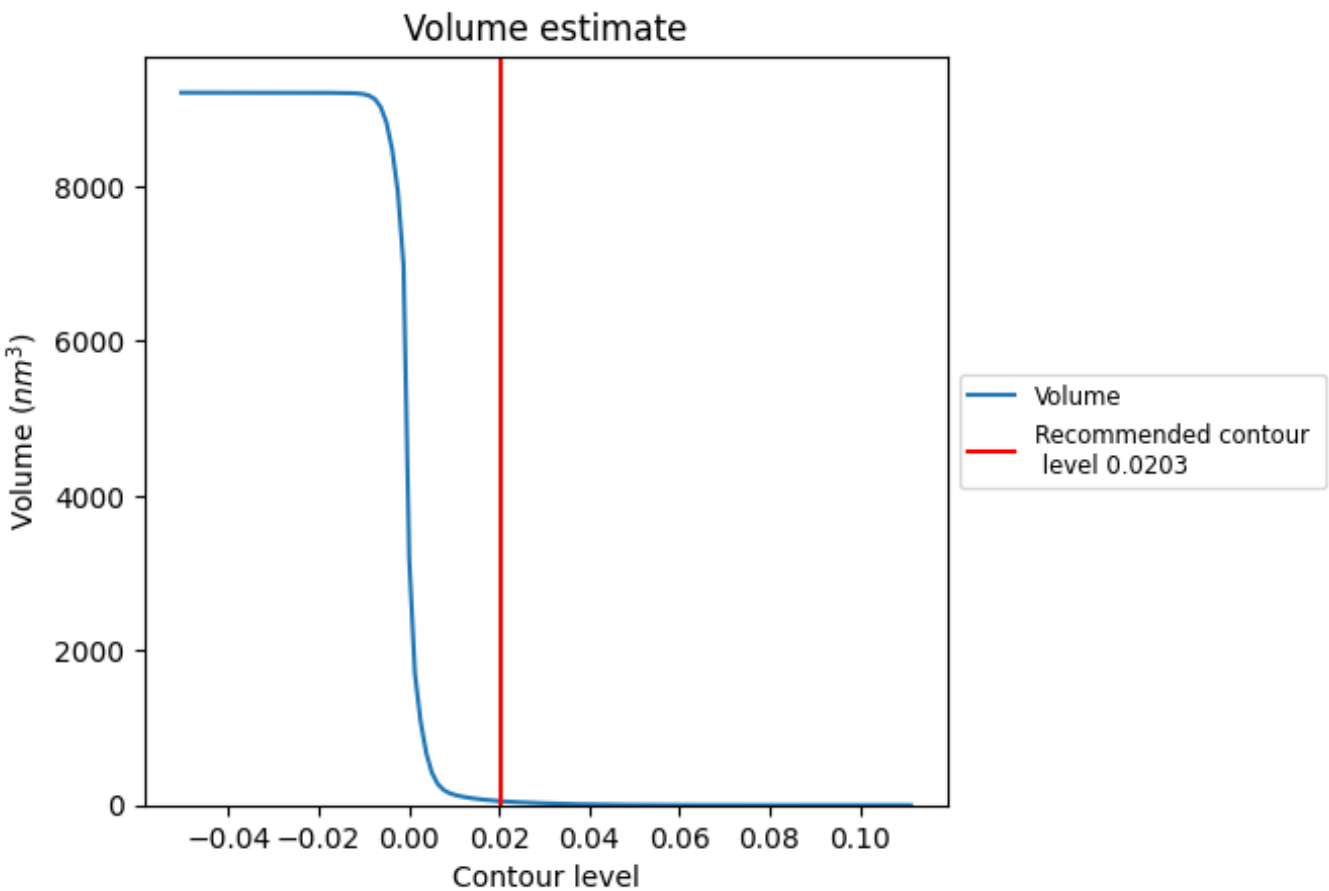
This section contains the results of statistical analysis of the map.

## 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.

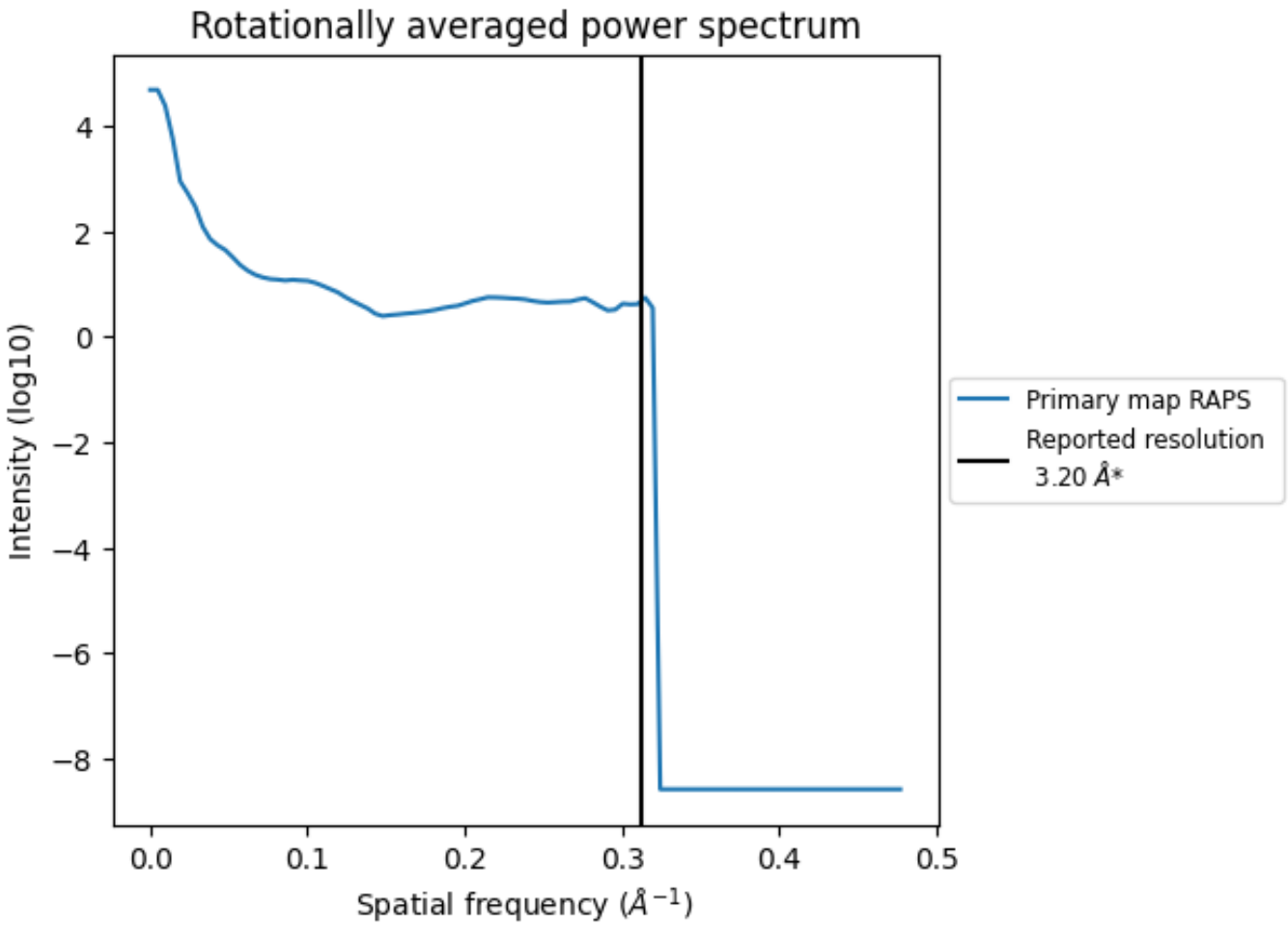
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 52 $nm^3$; this corresponds to an approximate mass of 47 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 0.312 Å$^{-1}$

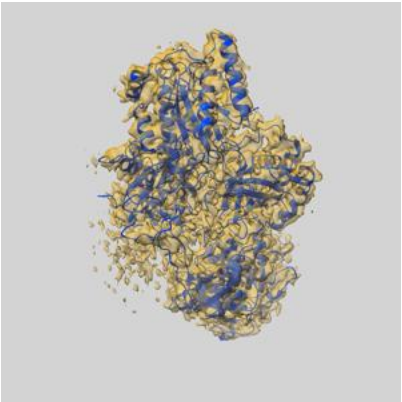
# 8 Fourier-Shell correlation (i)

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

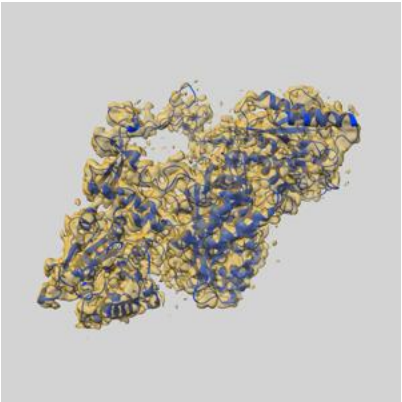
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11933 and PDB model 7AXZ. Per-residue inclusion information can be found in section 3 on page 4.

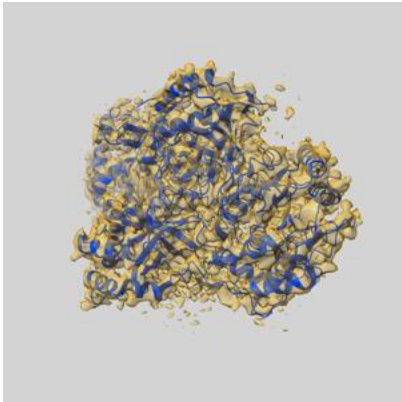
## 9.1 Map-model overlay (i)



X



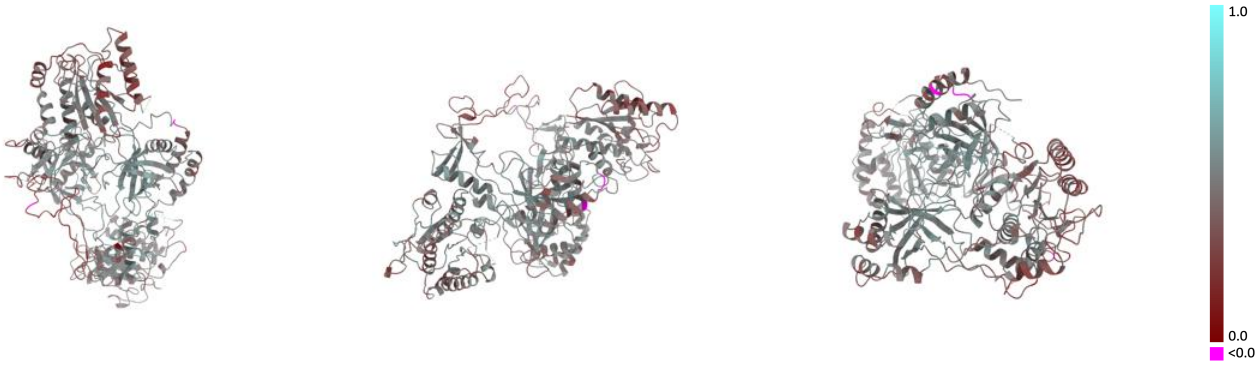
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0203 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.

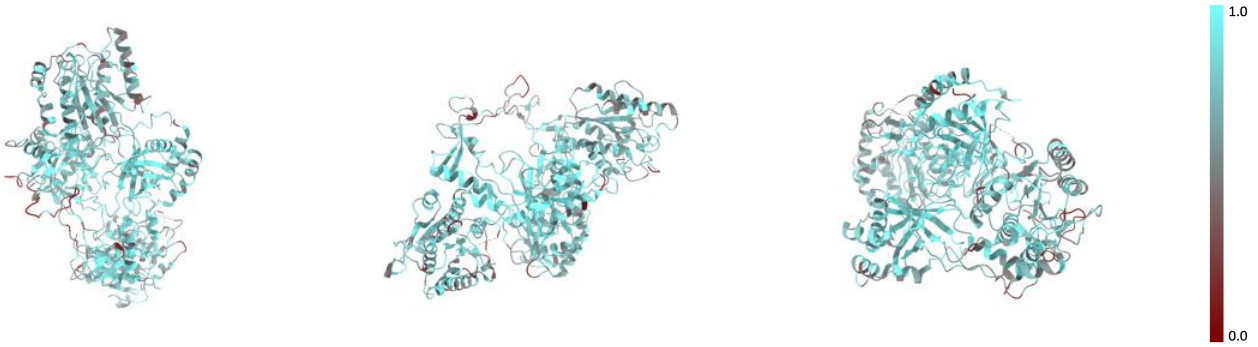
## 9.2 Q-score mapped to coordinate model (i)




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.

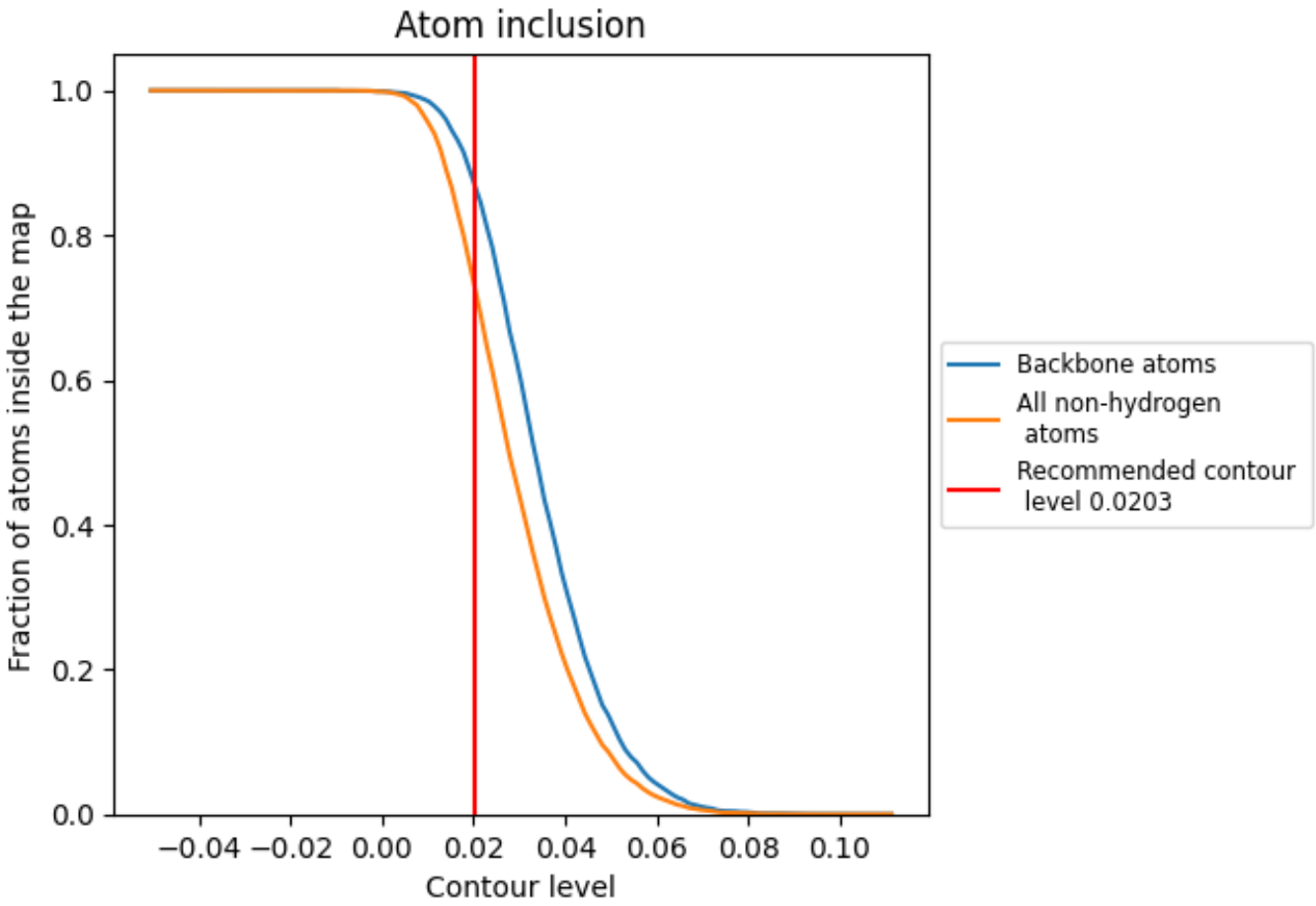
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.0203).

## 9.4 Atom inclusion (i)




At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.0203) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7263 | 0.4460 |
| A | 0.7270 | 0.4390 |
| B | 0.7258 | 0.4520 |