# wwPDB EM Validation Summary Report (i)

Oct 7, 2026 – 06:25 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 9ZTF / pdb_00009ztf |
| EMDB ID | : | EMD-74751 |
| Title | : | Nucleosome with an SSB at SHL +5.3 in complex with human PARP2, Class 2 |
| Authors | : | Gregory-Lott, E.; Kim, T.H.; Jayathilake, C.; Virk, R.K. |
| Deposited on | : | 2025-12-23 |
| Resolution | : | 2.67 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:

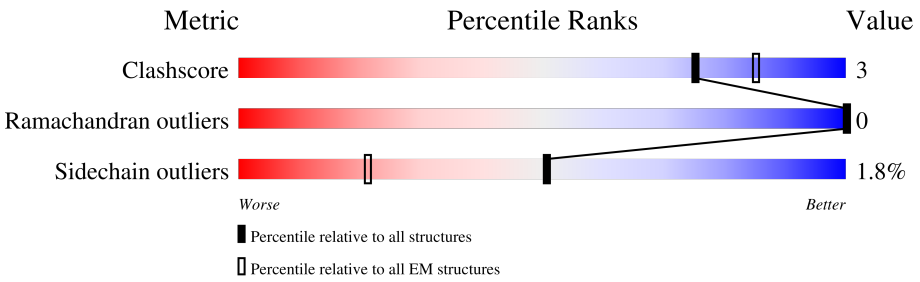
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| MolProbity | : | 4-5-2 with Phenix2.2 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.51 |

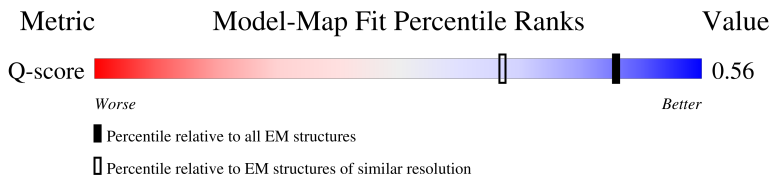
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 9182 ( 2.17 - 3.17 ) |

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 | 124 | 83% • 14% |
| 1 | B | 124 | 83% • 14% |
| 2 | C | 125 | 69% 9% 22% |
| 2 | D | 125 | 72% 6% 22% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | E | 136 | 71% 27% |
| 3 | F | 136 | 69% 27% |
| 4 | G | 104 | 77% 20% |
| 4 | H | 104 | 78% 20% |
| 5 | I | 274 | 77% 7% 16% |
| 5 | J | 274 | 74% 9% 16% |
| 6 | K | 130 | 75% 25% |
| 7 | L | 23 | 78% 22% |
| 8 | M | 153 | 86% 14% |
| 9 | P | 494 | 25% 71% |

# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 31796 atoms, of which 14593 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 Histone H2A.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | A | 107 | 1701 | 518 | 880 | 160 | 142 | 1 | 0 | 0 |
| 1 | B | 107 | 1701 | 518 | 880 | 160 | 142 | 1 | 0 | 0 |

- Molecule 2 is a protein called Histone H2B.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 2 | C | 97 | 1584 | 486 | 813 | 141 | 142 | 2 | 0 | 0 |
| 2 | D | 97 | 1583 | 486 | 812 | 141 | 142 | 2 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 0 | GLY | - | expression tag | UNP P02283 |
| C | 2 | ILE | - | insertion | UNP P02283 |
| D | 0 | GLY | - | expression tag | UNP P02283 |
| D | 2 | ILE | - | insertion | UNP P02283 |

- Molecule 3 is a protein called Histone H3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 3 | E | 99 | 1673 | 514 | 857 | 158 | 142 | 2 | 0 | 0 |
| 3 | F | 99 | 1673 | 514 | 857 | 158 | 142 | 2 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 111 | SER | CYS | engineered mutation | UNP P02299 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 111 | SER | CYS | engineered mutation | UNP P02299 |

- Molecule 4 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 4 | G | 83 | 1372 | 418 | 710 | 129 | 114 | 1 | 0 | 0 |
| 4 | H | 83 | 1372 | 418 | 710 | 129 | 114 | 1 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 2 | ILE | - | insertion | UNP P84040 |
| H | 2 | ILE | - | insertion | UNP P84040 |

- Molecule 5 is a protein called mAb PL2-6 antibody.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 5 | I | 230 | 3543 | 1132 | 1743 | 296 | 363 | 9 | 0 | 0 |
| 5 | J | 230 | 3542 | 1132 | 1742 | 296 | 363 | 9 | 0 | 0 |

- Molecule 6 is a DNA chain called DNA 130-mer.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 6 | K | 130 | 4103 | 1255 | 1458 | 479 | 781 | 130 | 0 | 0 |

- Molecule 7 is a DNA chain called DNA 23-mer.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 7 | L | 23 | 734 | 226 | 262 | 83 | 140 | 23 | 0 | 0 |

- Molecule 8 is a DNA chain called DNA 153-mer.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 8 | M | 153 | 4874 | 1494 | 1717 | 594 | 916 | 153 | 0 | 0 |

- Molecule 9 is a protein called Poly [ADP-ribose] polymerase 2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 9 | P | 145 | 2341 | 751 | 1152 | 210 | 218 | 10 | 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: Histone H2A

Chain A:

- Molecule 1: Histone H2A

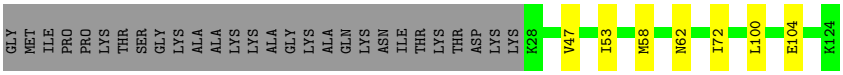
Chain B:

- Molecule 2: Histone H2B

Chain C:

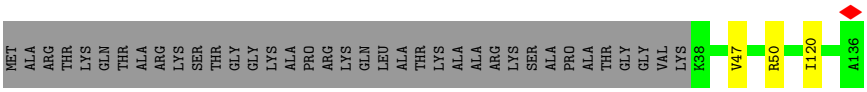
- Molecule 2: Histone H2B

Chain D:




- Molecule 3: Histone H3

Chain E:




- Molecule 3: Histone H3

Chain F: 69% • 27%

MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR GLY GLY VAL LYS K38 T81 D82 Q94 E98 K116 A136

• Molecule 4: Histone H4

Chain G: 77% • 20%

MET ILE THR GLY ARG GLY LYS LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG K22 D26 R37 K93 G104

• Molecule 4: Histone H4

Chain H: 78% • 20%

MET ILE THR GLY ARG GLY LYS LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG K22 R37 R41 G104

• Molecule 5: mAb PL2-6 antibody

Chain I: 77% 7% 16%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY ASN A23 E41 L57 S58 W59 Y60 L78 S84 N101 D105 L113 E129 I130 K131 R132 ALA GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY

SER GLY GLY GLY GLY SER MET E155 G162 L165 T182 K192 I202 Y214 T223 L224 T225 S226 S230 R256 T260 L261 Q266 S273 S274

• Molecule 5: mAb PL2-6 antibody

Chain J: 74% 9% 16%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY ASN A23 I26 T29 S58 I72 Y73 Y74 L78 S91 Q114 E117 L128 E129 I130 K131 R132 ALA GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY

GLY GLY SER GLY GLY GLY GLY SER MET E155 S161 V166 E167 T170 I188 I202 I205 Y208 K217 V233 Y234 M235 E236 L237 L240 T260 L261 S274

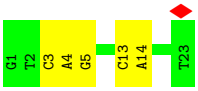
• Molecule 6: DNA 130-mer

Chain K: 75% 25%

A1 T2 T5 G6 G7 A8 G9 C20 C21 T30 C31 T41 A42 C48 T49 C50 T51 C73 G74 T80 C81 C82 C85 G86 T92 A93 A94 A106 T107 T108 C114 T115 A123 G124 C130

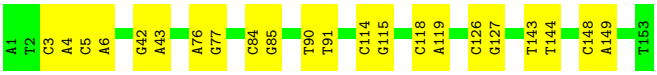
• Molecule 7: DNA 23-mer

Chain L: 78% 22%



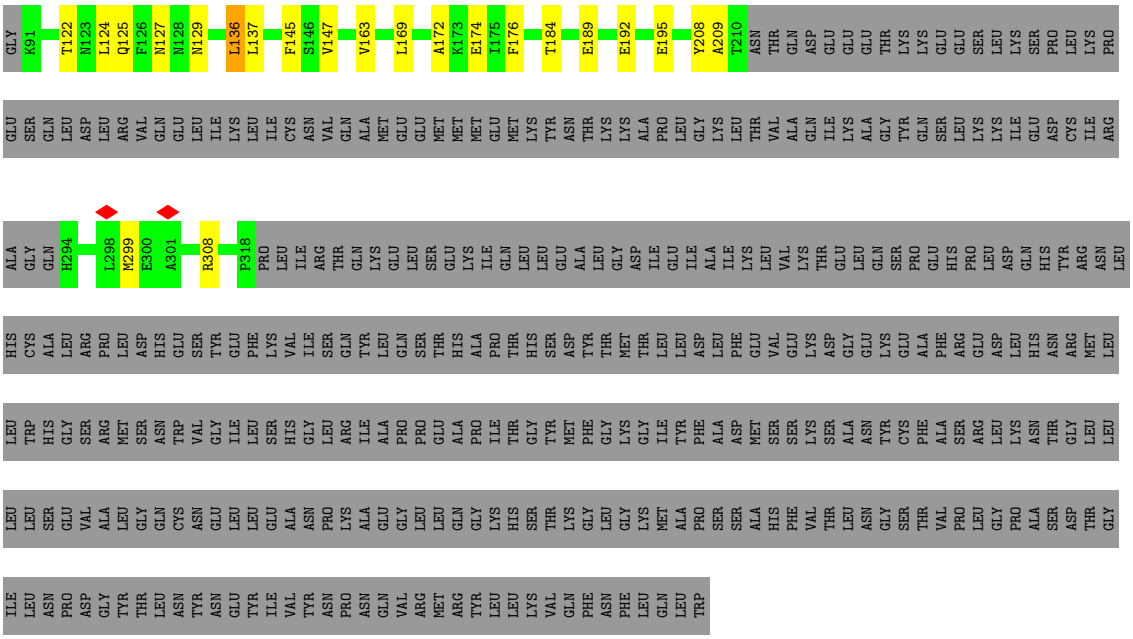

• Molecule 8: DNA 153-mer

Chain M: 86% 14%




• Molecule 9: Poly [ADP-ribose] polymerase 2

Chain P: 25% 71%



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 65386 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 48 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 1.024 | Depositor |
| Minimum map value | -0.251 | Depositor |
| Average map value | 0.004 | Depositor |
| Map value standard deviation | 0.018 | Depositor |
| Recommended contour level | 0.0482 | Depositor |
| Map size (Å) | 331.2, 331.2, 331.2 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.828, 0.828, 0.828 | 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 | 0.14 | 0/831 | 0.27 | 0/1119 |
| 1 | B | 0.15 | 0/831 | 0.27 | 0/1119 |
| 2 | C | 0.15 | 0/782 | 0.24 | 0/1046 |
| 2 | D | 0.16 | 0/782 | 0.29 | 0/1046 |
| 3 | E | 0.15 | 0/828 | 0.25 | 0/1109 |
| 3 | F | 0.16 | 0/828 | 0.28 | 0/1109 |
| 4 | G | 0.16 | 0/669 | 0.27 | 0/894 |
| 4 | H | 0.16 | 0/669 | 0.26 | 0/894 |
| 5 | I | 0.11 | 0/1842 | 0.28 | 0/2493 |
| 5 | J | 0.12 | 0/1842 | 0.29 | 0/2493 |
| 6 | K | 0.76 | 0/2962 | 0.87 | 0/4564 |
| 7 | L | 0.74 | 0/528 | 0.93 | 0/811 |
| 8 | M | 0.73 | 0/3546 | 0.86 | 0/5476 |
| 9 | P | 0.14 | 0/1216 | 0.37 | 0/1635 |
| All | All | 0.48 | 0/18156 | 0.61 | 0/25808 |

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 | 821 | 880 | 879 | 3 | 0 |
| 1 | B | 821 | 880 | 879 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | C | 771 | 813 | 811 | 7 | 0 |
| 2 | D | 771 | 812 | 811 | 4 | 0 |
| 3 | E | 816 | 857 | 856 | 3 | 0 |
| 3 | F | 816 | 857 | 856 | 2 | 0 |
| 4 | G | 662 | 710 | 709 | 3 | 0 |
| 4 | H | 662 | 710 | 709 | 1 | 0 |
| 5 | I | 1800 | 1743 | 1740 | 11 | 0 |
| 5 | J | 1800 | 1742 | 1740 | 14 | 0 |
| 6 | K | 2645 | 1458 | 1458 | 20 | 0 |
| 7 | L | 472 | 262 | 262 | 4 | 0 |
| 8 | M | 3157 | 1717 | 1717 | 11 | 0 |
| 9 | P | 1189 | 1152 | 1150 | 19 | 0 |
| All | All | 17203 | 14593 | 14577 | 99 | 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 3.

The worst 5 of 99 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) |
|---|---|---|---|
| 9:P:124:LEU:HD12 | 9:P:125:GLN:N | 1.99 | 0.76 |
| 5:J:202:ILE:HD13 | 5:J:235:MET:HE1 | 1.78 | 0.64 |
| 6:K:107:DT:H2' | 6:K:108:DT:H71 | 1.82 | 0.62 |
| 9:P:124:LEU:HD11 | 9:P:299:MET:HE1 | 1.85 | 0.58 |
| 6:K:1:DA:H2" | 6:K:2:DT:H71 | 1.86 | 0.57 |

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 | 105/124 (85%) | 103 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | B | 105/124 (85%) | 102 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | C | 95/125 (76%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 2 | D | 95/125 (76%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | E | 97/136 (71%) | 96 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | F | 97/136 (71%) | 96 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | G | 81/104 (78%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | H | 81/104 (78%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 5 | I | 226/274 (82%) | 217 (96%) | 9 (4%) | 0 | 100 | 100 |
| 5 | J | 226/274 (82%) | 219 (97%) | 7 (3%) | 0 | 100 | 100 |
| 9 | P | 141/494 (28%) | 133 (94%) | 8 (6%) | 0 | 100 | 100 |
| All | All | 1349/2020 (67%) | 1313 (97%) | 36 (3%) | 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 | 83/94 (88%) | 82 (99%) | 1 (1%) | 63 | 82 |
| 1 | B | 83/94 (88%) | 82 (99%) | 1 (1%) | 63 | 82 |
| 2 | C | 84/105 (80%) | 83 (99%) | 1 (1%) | 63 | 82 |
| 2 | D | 84/105 (80%) | 82 (98%) | 2 (2%) | 43 | 70 |
| 3 | E | 86/111 (78%) | 86 (100%) | 0 | 100 | 100 |
| 3 | F | 86/111 (78%) | 85 (99%) | 1 (1%) | 63 | 82 |
| 4 | G | 68/80 (85%) | 67 (98%) | 1 (2%) | 57 | 79 |
| 4 | H | 68/80 (85%) | 68 (100%) | 0 | 100 | 100 |
| 5 | I | 202/226 (89%) | 197 (98%) | 5 (2%) | 42 | 69 |
| 5 | J | 202/226 (89%) | 196 (97%) | 6 (3%) | 36 | 63 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 9 | P | 127/433 (29%) | 124 (98%) | 3 (2%) | 43 | 70 |
| All | All | 1173/1665 (70%) | 1152 (98%) | 21 (2%) | 51 | 76 |

5 of 21 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | J | 91 | SER |
| 5 | J | 205 | ILE |
| 9 | P | 184 | THR |
| 9 | P | 127 | ASN |
| 5 | J | 166 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | J | 266 | GLN |
| 9 | P | 129 | ASN |
| 9 | P | 170 | ASN |
| 9 | P | 135 | GLN |
| 4 | G | 77 | 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 oligosaccharides 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.

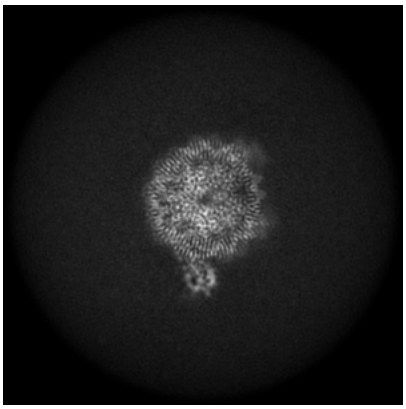
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-74751. These allow visual inspection of the internal detail of the map and identification of artifacts.

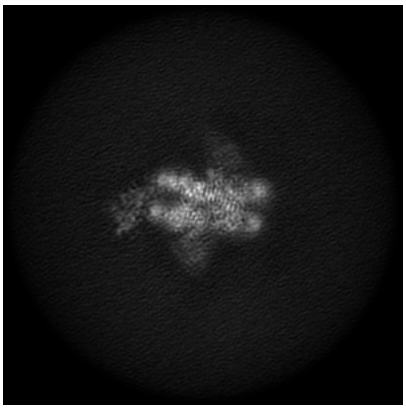
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

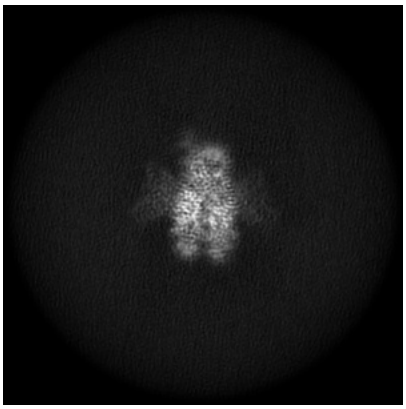
### 6.1.1 Primary map



X

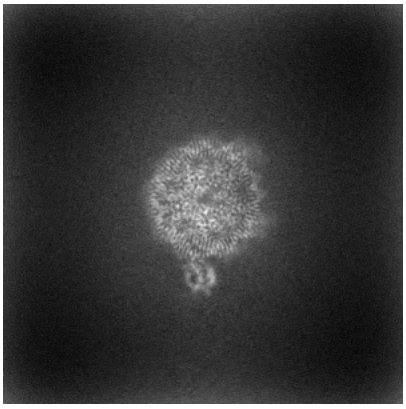


Y

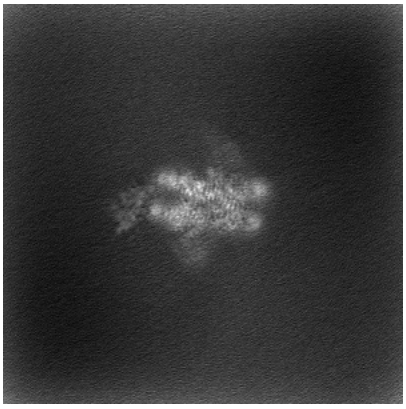


Z

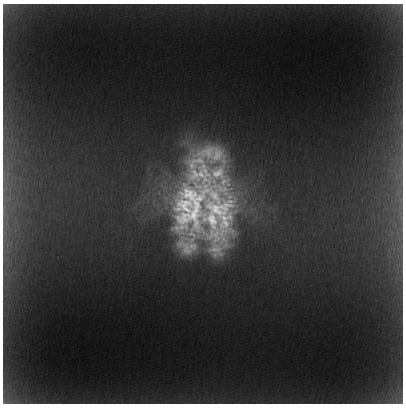
### 6.1.2 Raw map



X



Y

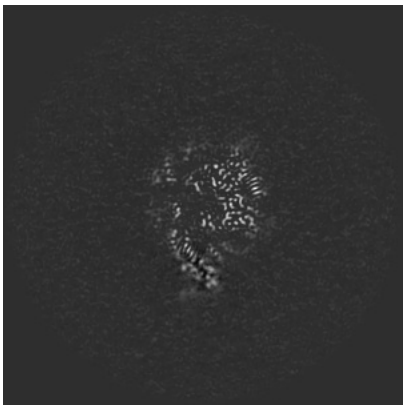


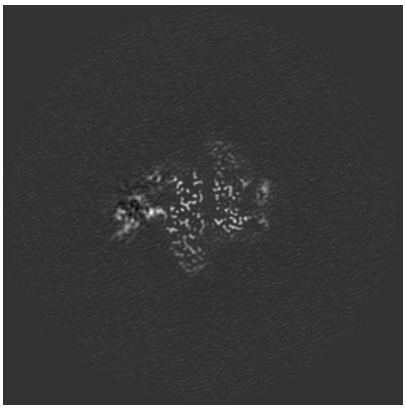
Z

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

## 6.2 Central slices (i)

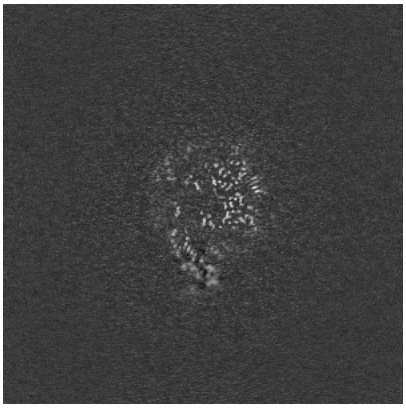
### 6.2.1 Primary map

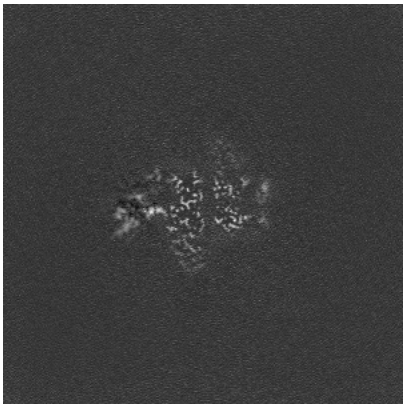

X Index: 200


Y Index: 200

Z Index: 200

### 6.2.2 Raw map


X Index: 200

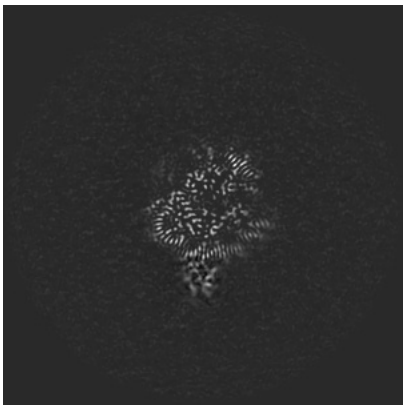

Y Index: 200

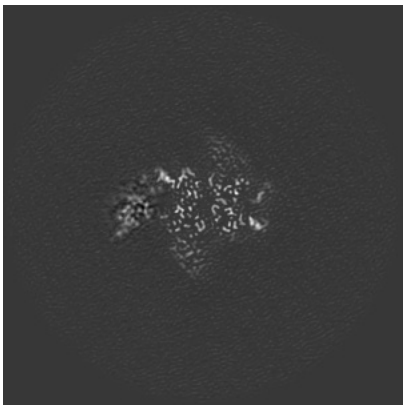
Z Index: 200

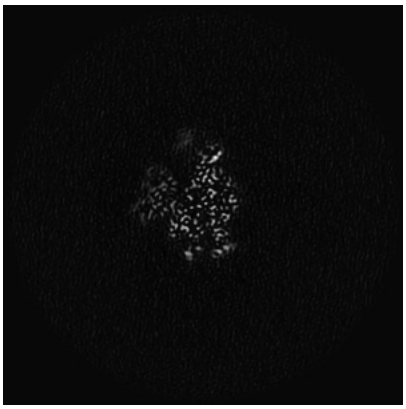
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

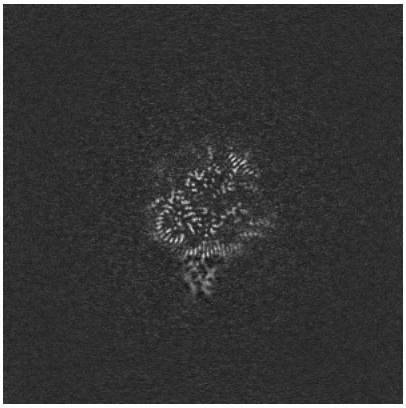
### 6.3.1 Primary map

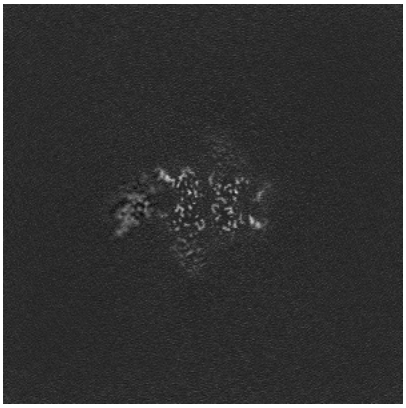

X Index: 191

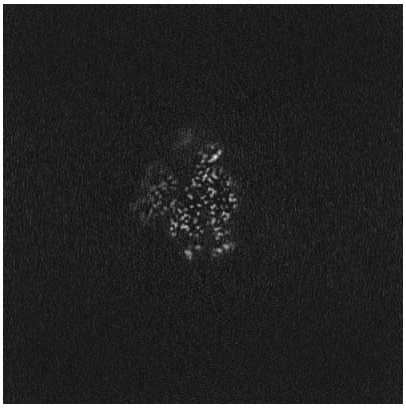

Y Index: 198


Z Index: 187

### 6.3.2 Raw map


X Index: 191

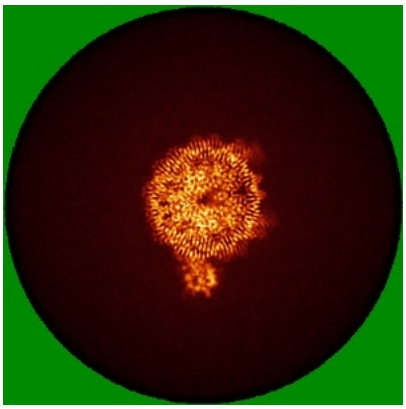

Y Index: 198

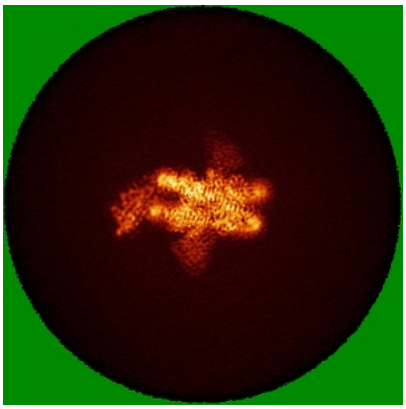

Z Index: 187

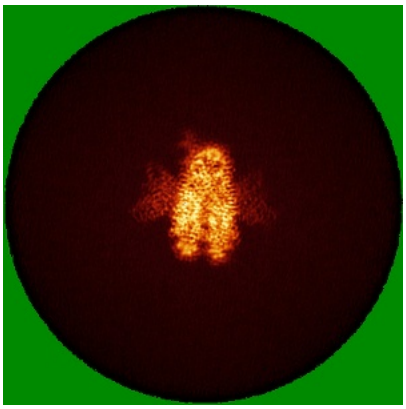
The images above show the largest variance slices of the map in three orthogonal directions.

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

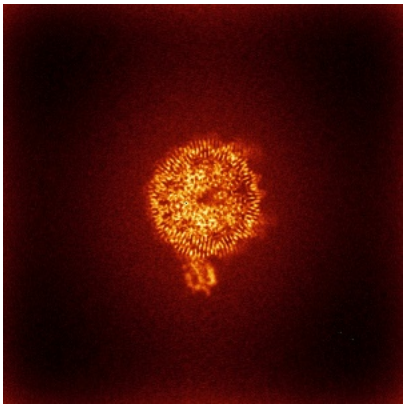
### 6.4.1 Primary map

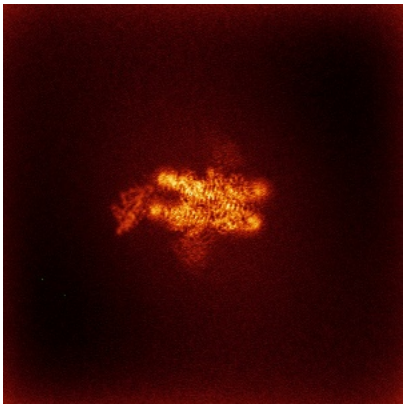

X

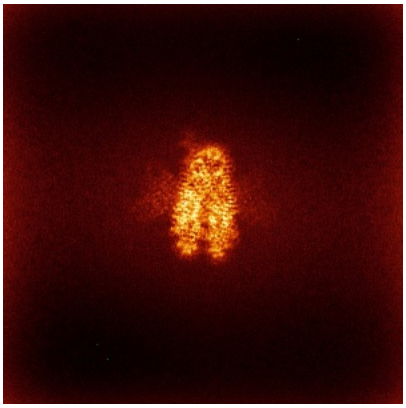

Y


Z

### 6.4.2 Raw map


X

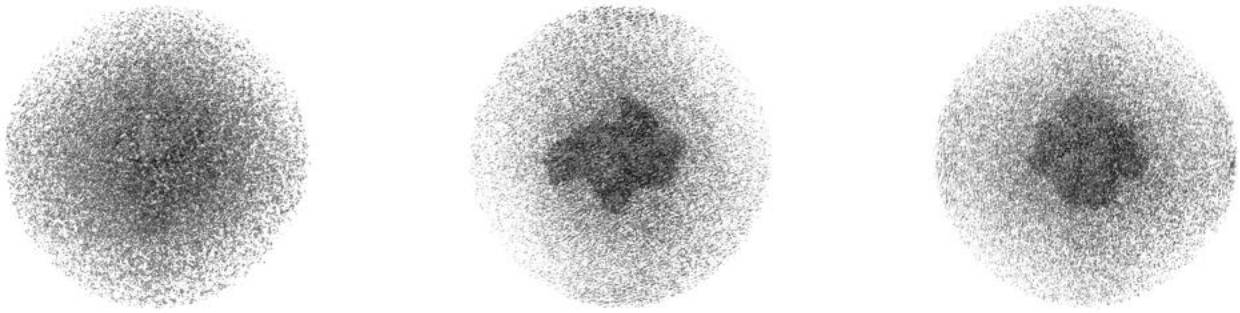

Y


Z

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)

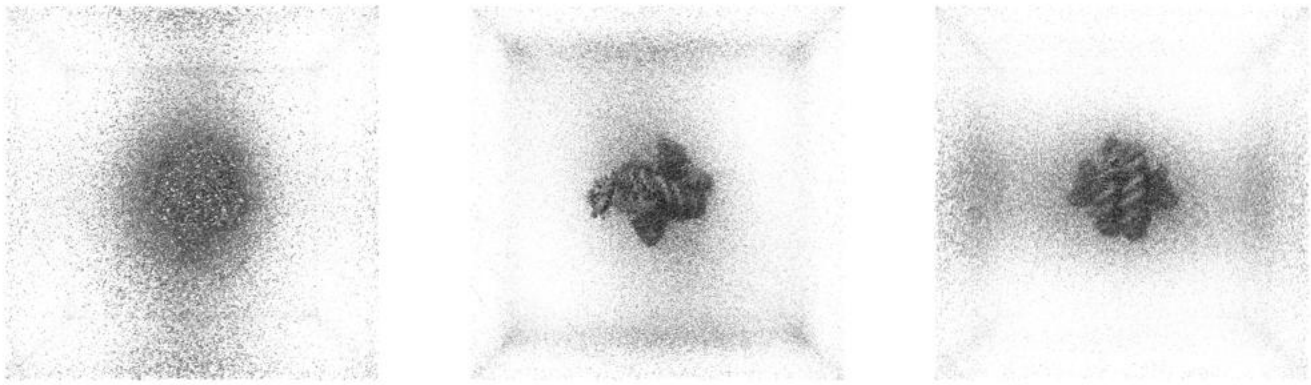
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0482. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

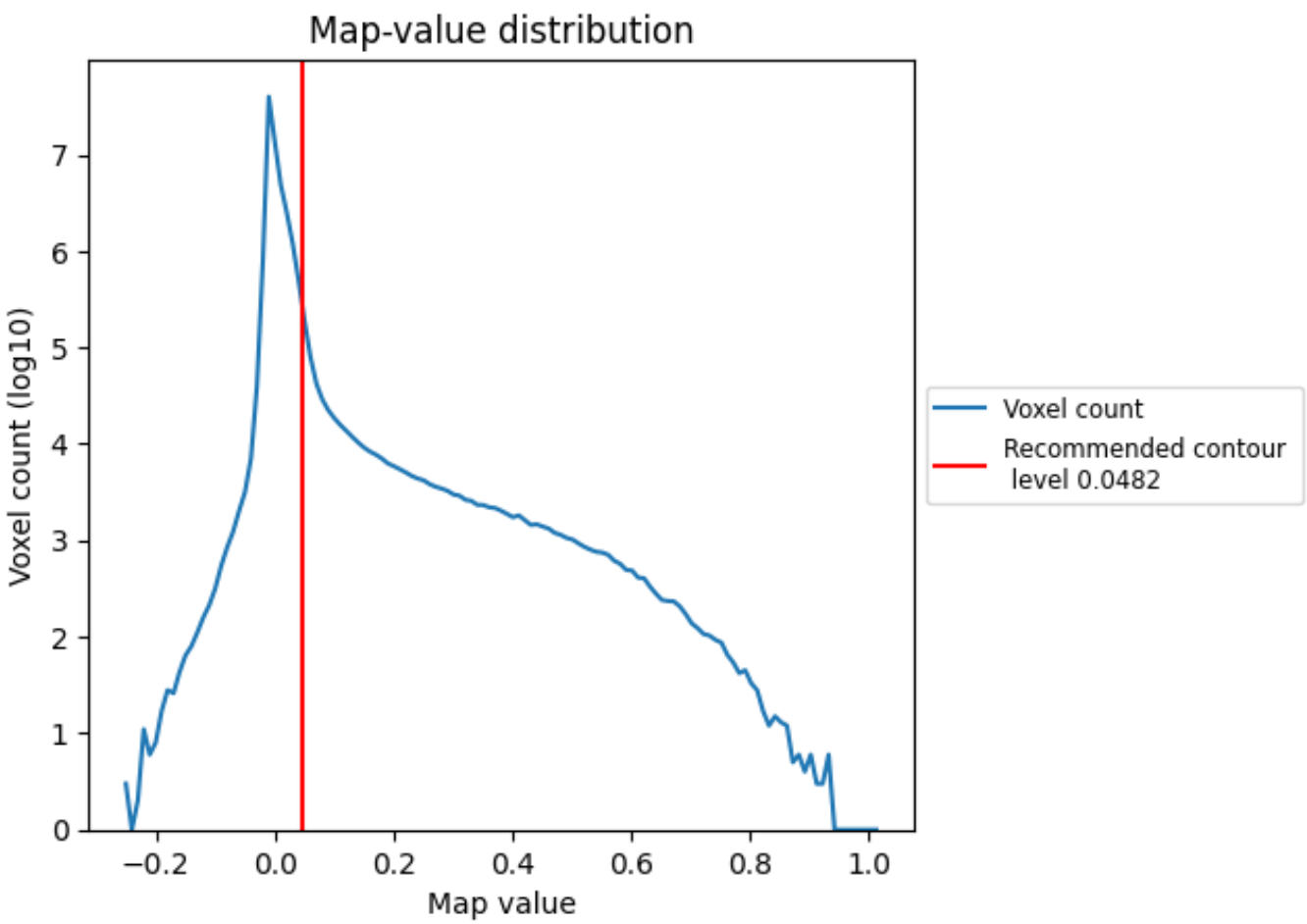
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

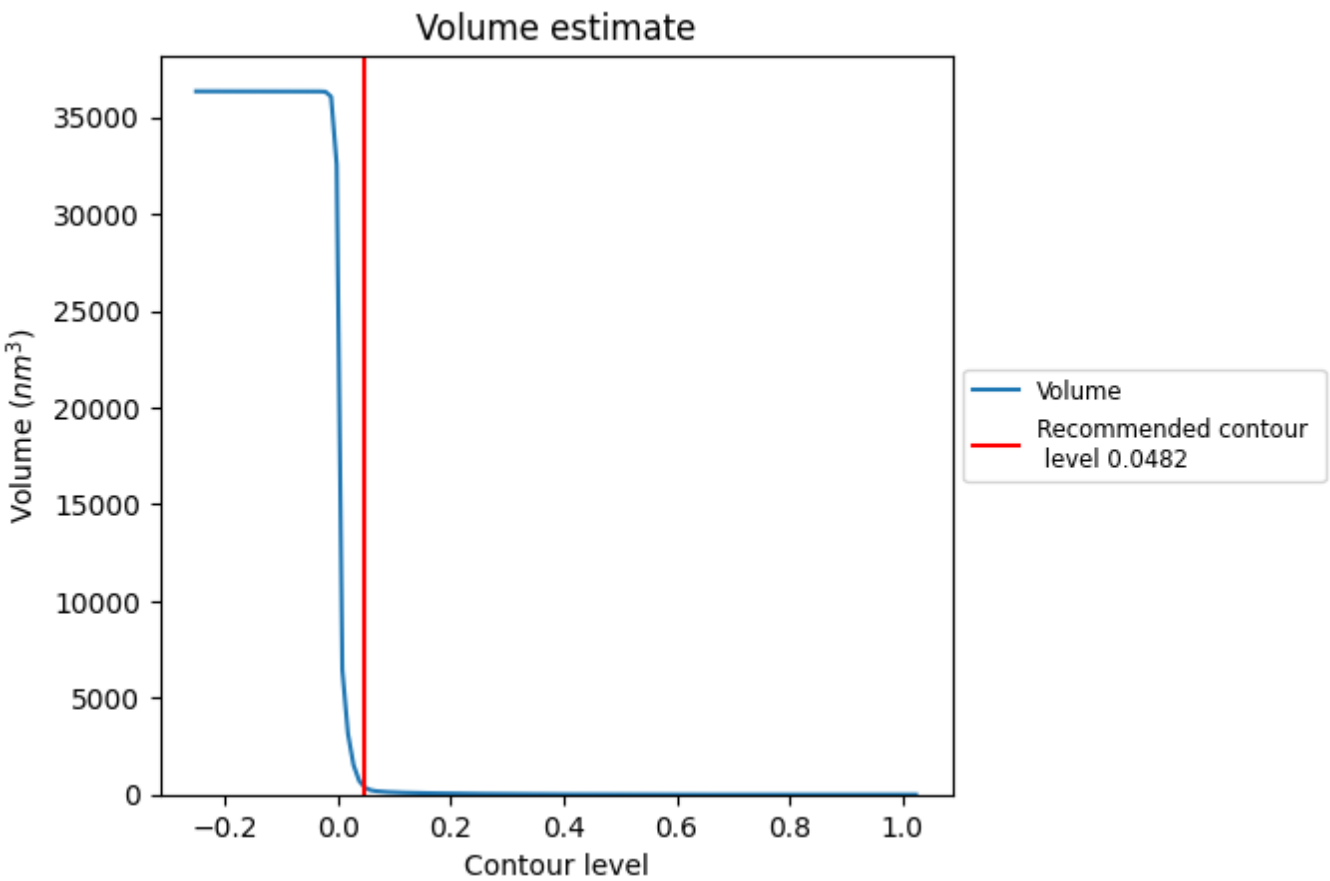
This section contains the results of statistical analysis of the map.

## 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.

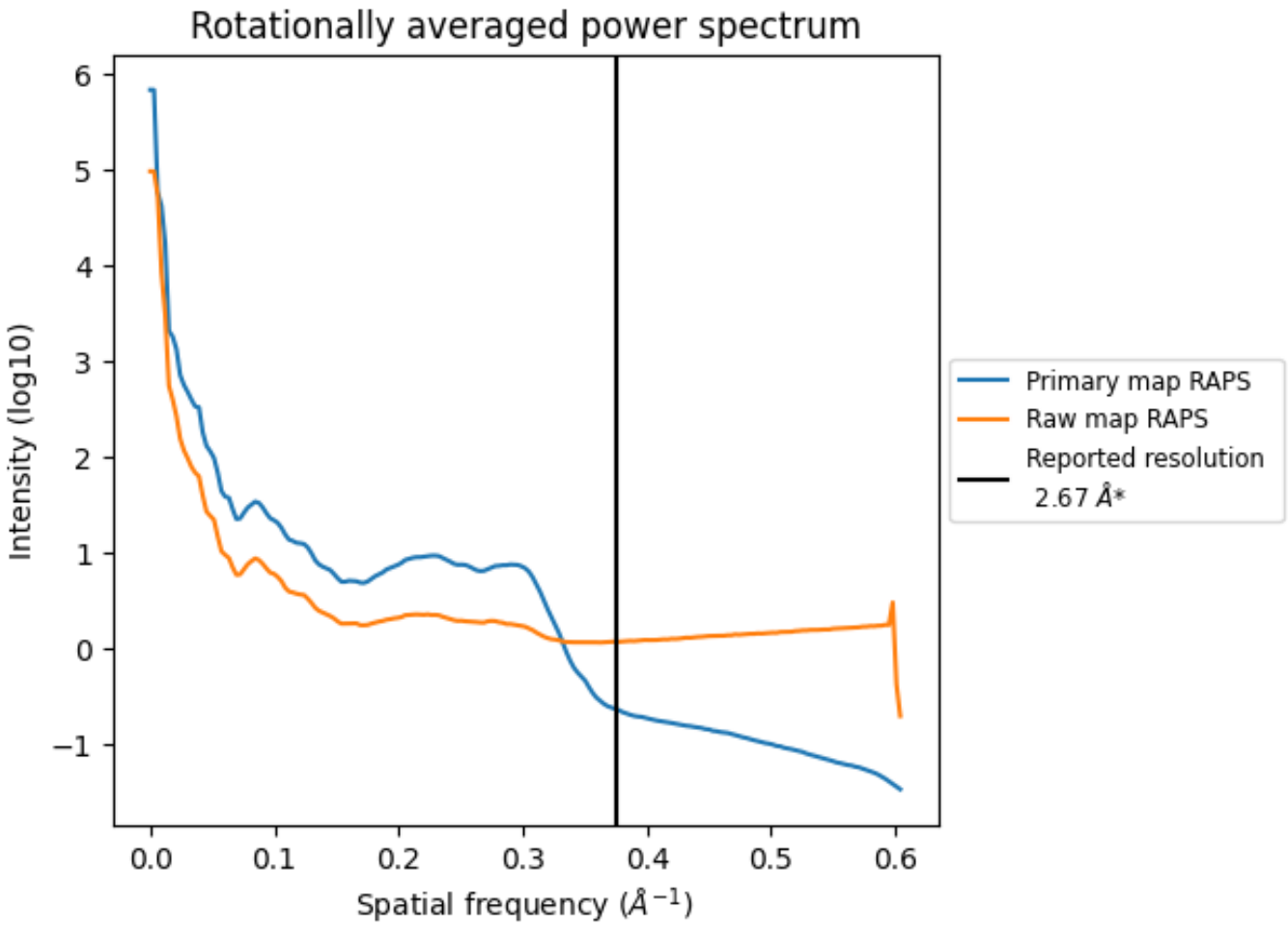
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 361 $nm^3$; this corresponds to an approximate mass of 326 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)

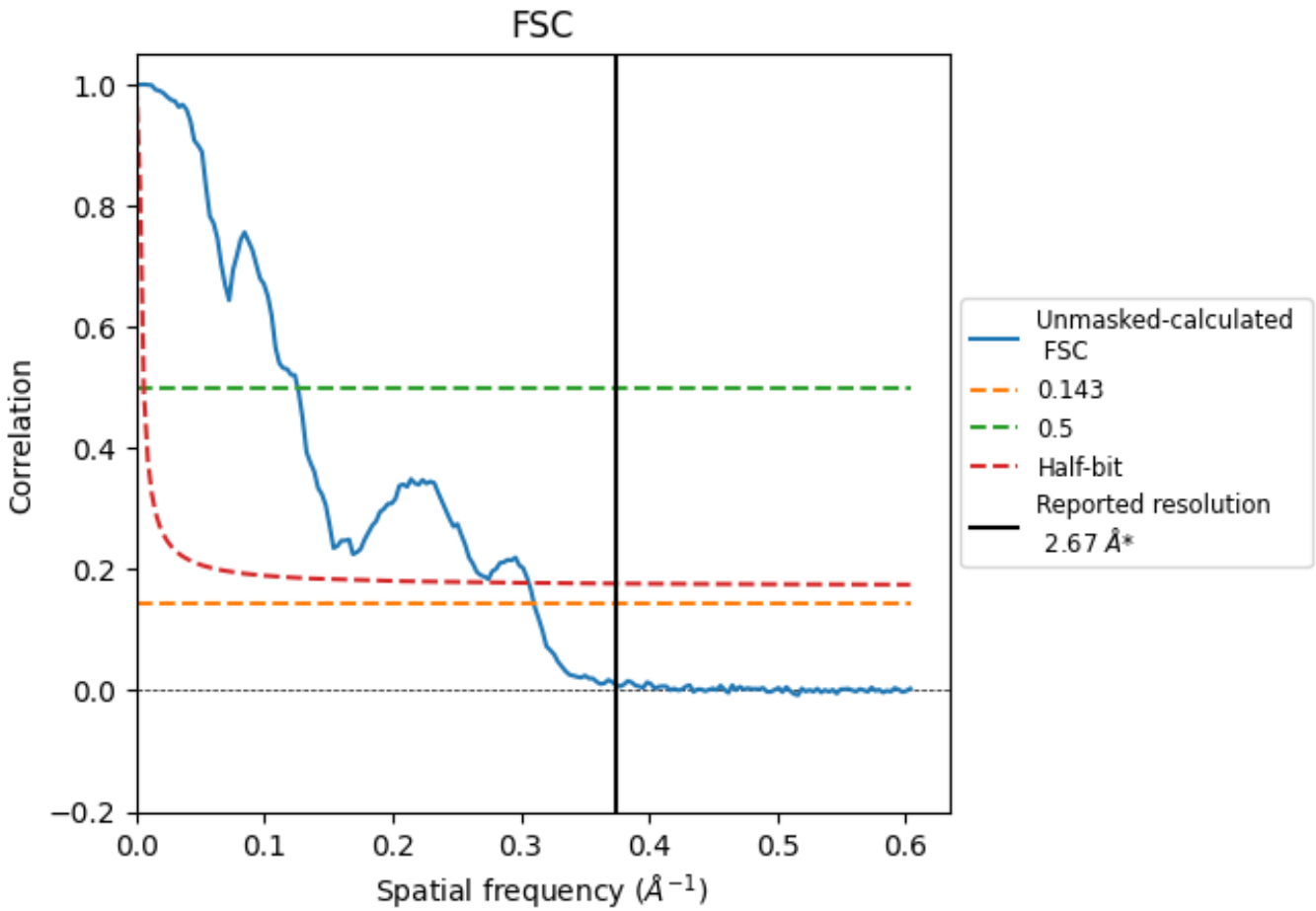



*Reported resolution corresponds to spatial frequency of 0.375 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.375 Å$^{-1}$

## 8.2 Resolution estimates (i)

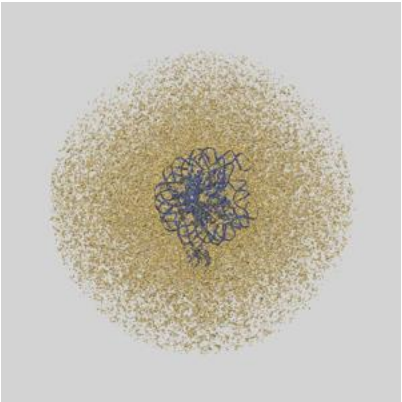
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.67 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.22 | 7.94 | 3.27 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.67 by more than 10 %

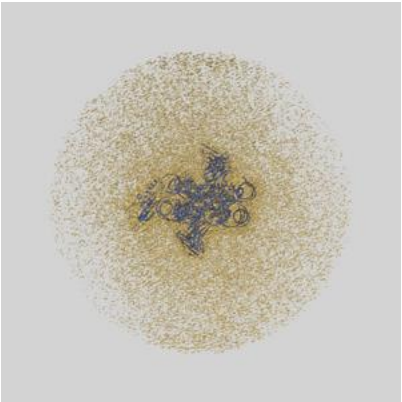
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-74751 and PDB model 9ZTF. Per-residue inclusion information can be found in section 3 on page 7.

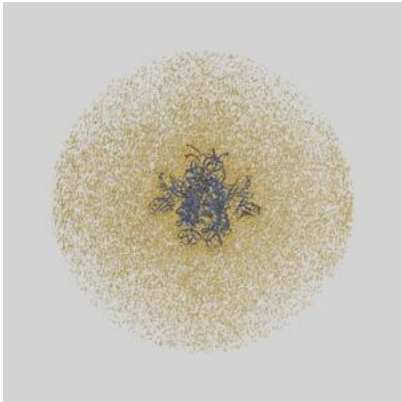
## 9.1 Map-model overlay (i)



X



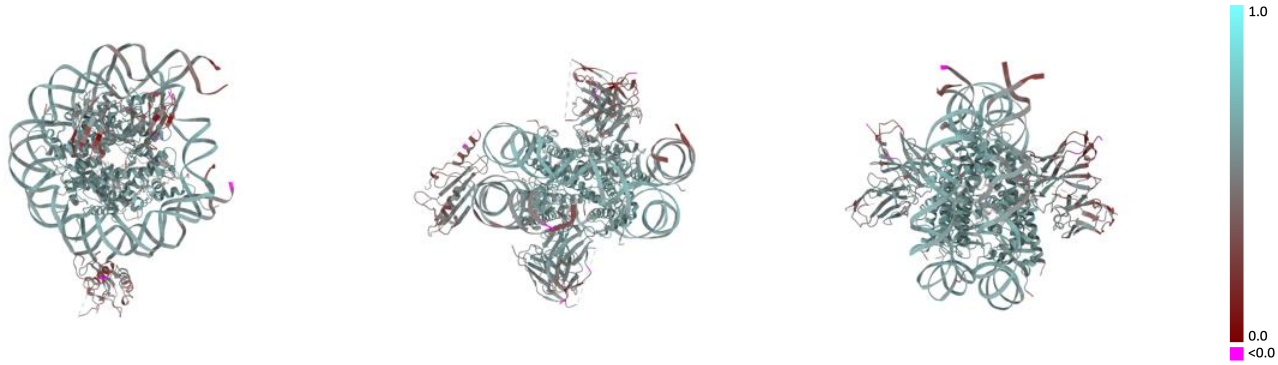
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0482 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.

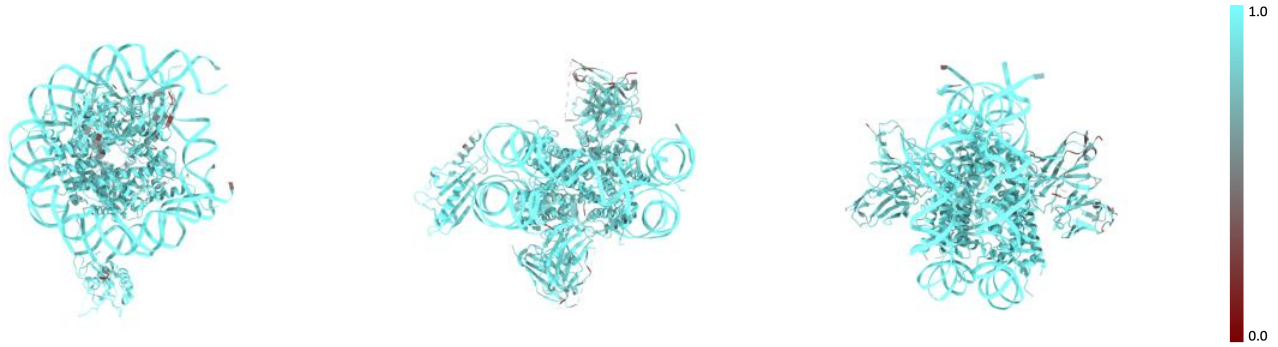
## 9.2 Q-score mapped to coordinate model (i)




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.

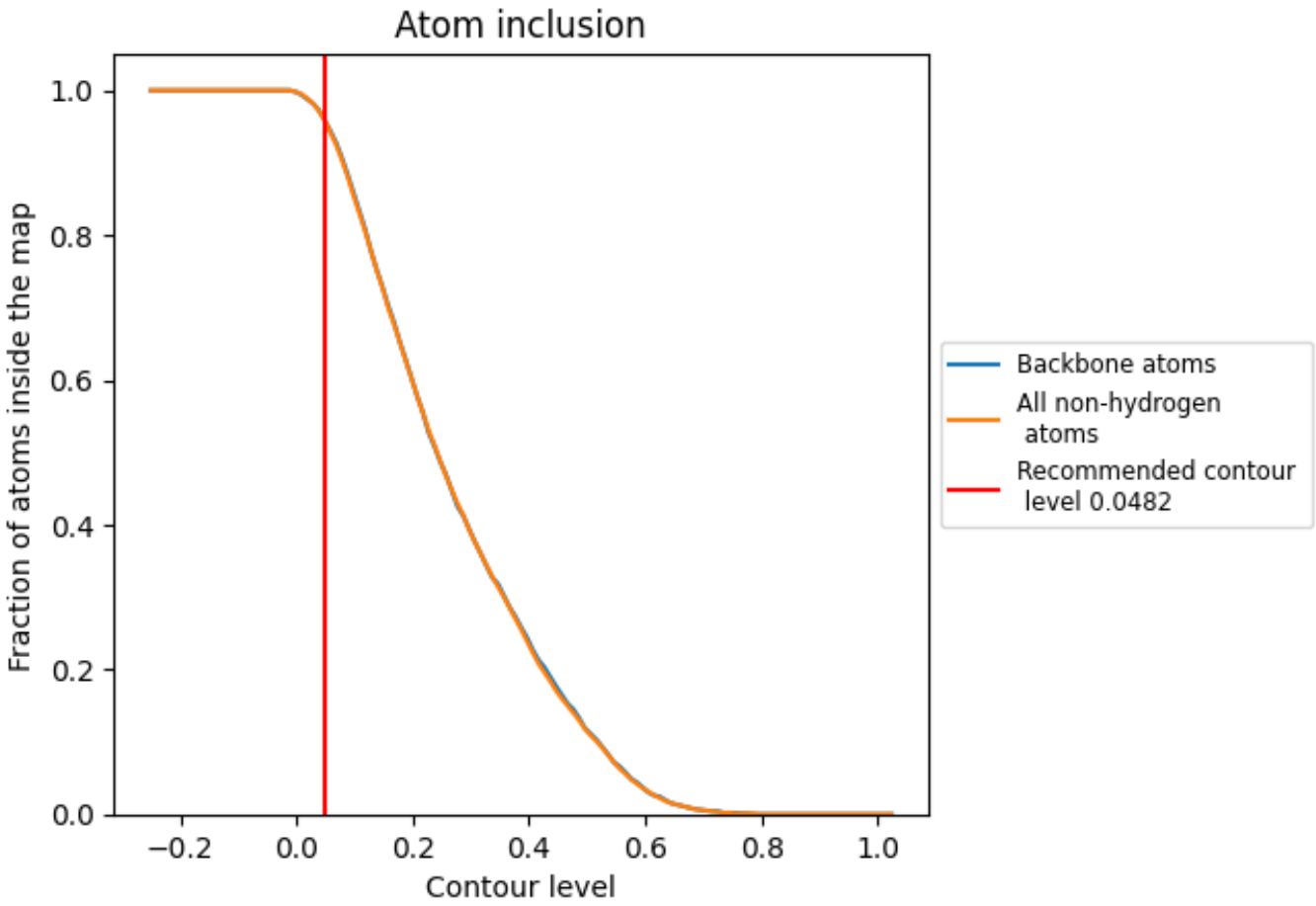
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.0482).

## 9.4 Atom inclusion (i)




At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.0482) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9590 | 0.5600 |
| A | 0.9840 | 0.6150 |
| B | 0.9840 | 0.6210 |
| C | 0.9840 | 0.5960 |
| D | 0.9890 | 0.6160 |
| E | 0.9780 | 0.6230 |
| F | 0.9800 | 0.6170 |
| G | 0.9890 | 0.6290 |
| H | 0.9840 | 0.6190 |
| I | 0.8150 | 0.4540 |
| J | 0.9180 | 0.5210 |
| K | 0.9950 | 0.5830 |
| L | 0.9560 | 0.4950 |
| M | 0.9910 | 0.5740 |
| P | 0.9610 | 0.4190 |