# wwPDB EM Validation Summary Report

Mar 5, 2026 – 07:47 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 9HJM / pdb_00009hjm |
| EMDB ID | : | EMD-52218 |
| Title | : | Porphyromonas gingivalis BAM complex |
| Authors | : | Madej, M.; Silale, A.; van den Berg, B. |
| Deposited on | : | 2024-11-29 |
| Resolution | : | 3.24 Å(reported) |
| Based on initial model | : | . |

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 ⓘ 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 ⓘ) were used in the production of this report:

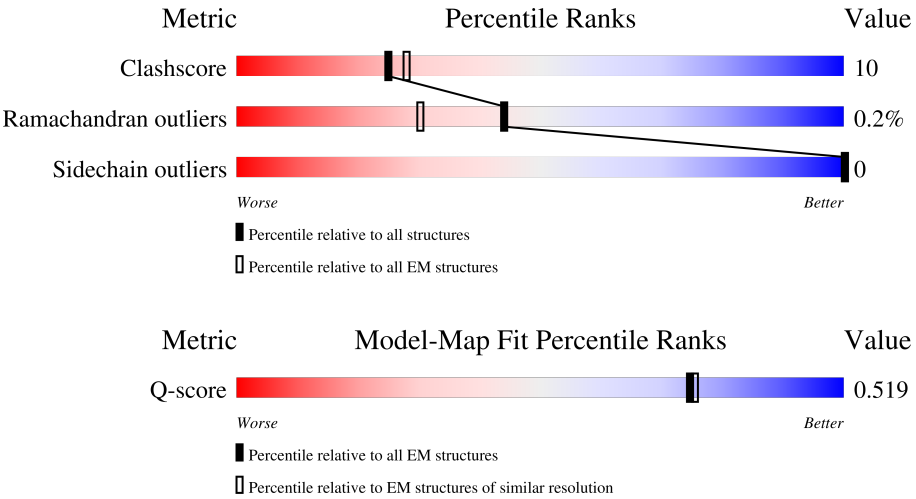
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 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) | : | 2.49 |

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.24 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 | 14594 ( 2.74 - 3.74 ) |

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 | F | 434 | 73% 18% 9% |
| 2 | G | 462 | 76% 19% 5% |
| 3 | H | 456 | 12% 69% 22% 9% |
| 4 | I | 185 | 13% 56% 25% 17% |

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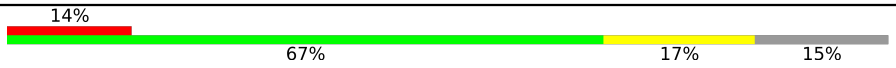
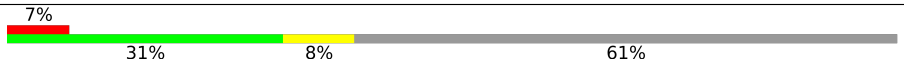
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | J | 203 |   |
| 6 | A | 891 |   |

# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15297 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 Outer membrane protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | F | 393 | Total | C | N | O | S | 0 | 0 |
| | | | 3102 | 1995 | 525 | 571 | 11 | | |

- Molecule 2 is a protein called DUF4270 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | G | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3454 | 2192 | 568 | 682 | 12 | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 456 | HIS | - | expression tag | UNP B2RLK9 |
| G | 457 | HIS | - | expression tag | UNP B2RLK9 |
| G | 458 | HIS | - | expression tag | UNP B2RLK9 |
| G | 459 | HIS | - | expression tag | UNP B2RLK9 |
| G | 460 | HIS | - | expression tag | UNP B2RLK9 |
| G | 461 | HIS | - | expression tag | UNP B2RLK9 |
| G | 462 | HIS | - | expression tag | UNP B2RLK9 |

- Molecule 3 is a protein called DUF6242 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | H | 417 | Total | C | N | O | S | 0 | 0 |
| | | | 3268 | 2099 | 541 | 616 | 12 | | |

- Molecule 4 is a protein called Peptidyl-prolyl cis-trans isomerase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | I | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1218 | 772 | 209 | 233 | 4 | | |

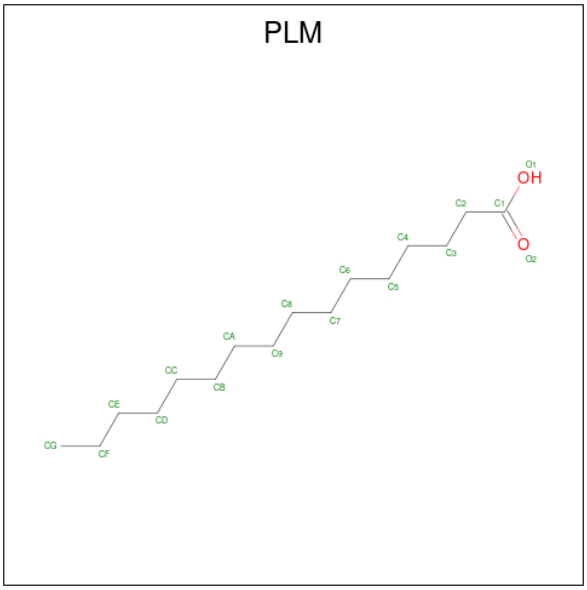
- Molecule 5 is a protein called DUF4827 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | J | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1418 | 908 | 236 | 263 | 11 | | |

- Molecule 6 is a protein called Putative outer membrane protein.

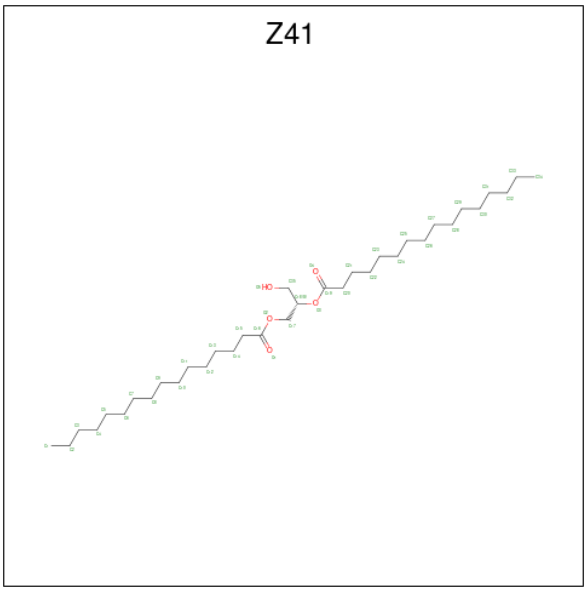
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | A | 344 | Total | C | N | O | S | 0 | 0 |
| | | | 2786 | 1785 | 476 | 513 | 12 | | |

- Molecule 7 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 7 | G | 1 | Total | C | O | | 0 |
| | | | 16 | 15 | 1 | | |

- Molecule 8 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (CCD ID: Z41) (formula: $C_{35}H_{68}O_5$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | C | O | |
| 8 | G | 1 | 35 | 31 | 4 | 0 |

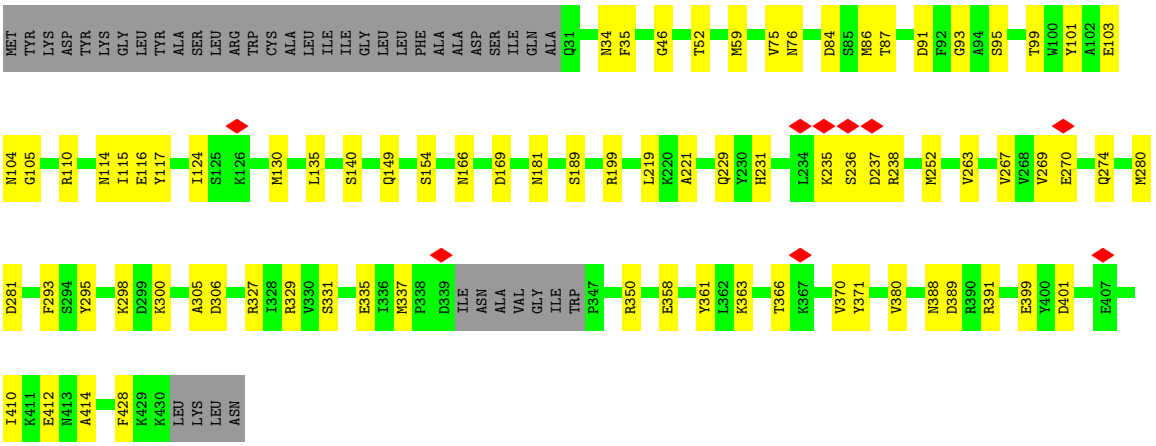
# 3 Residue-property plots (i)

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: Outer membrane protein

Chain F:

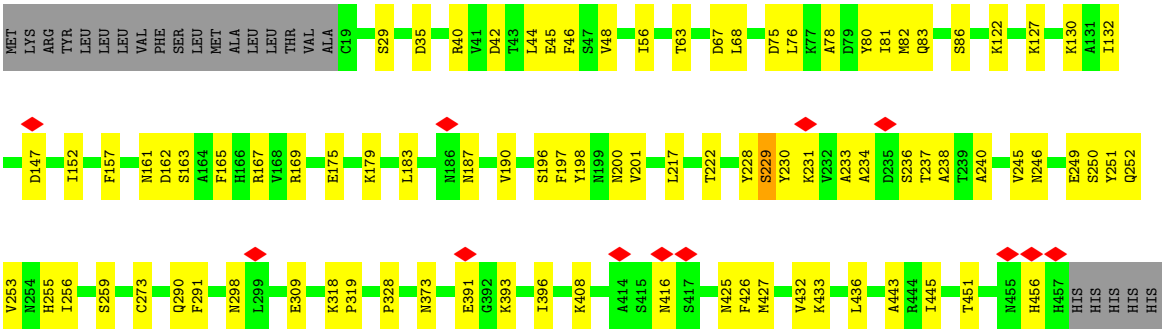



• Molecule 2: DUF4270 domain-containing protein

Chain G:

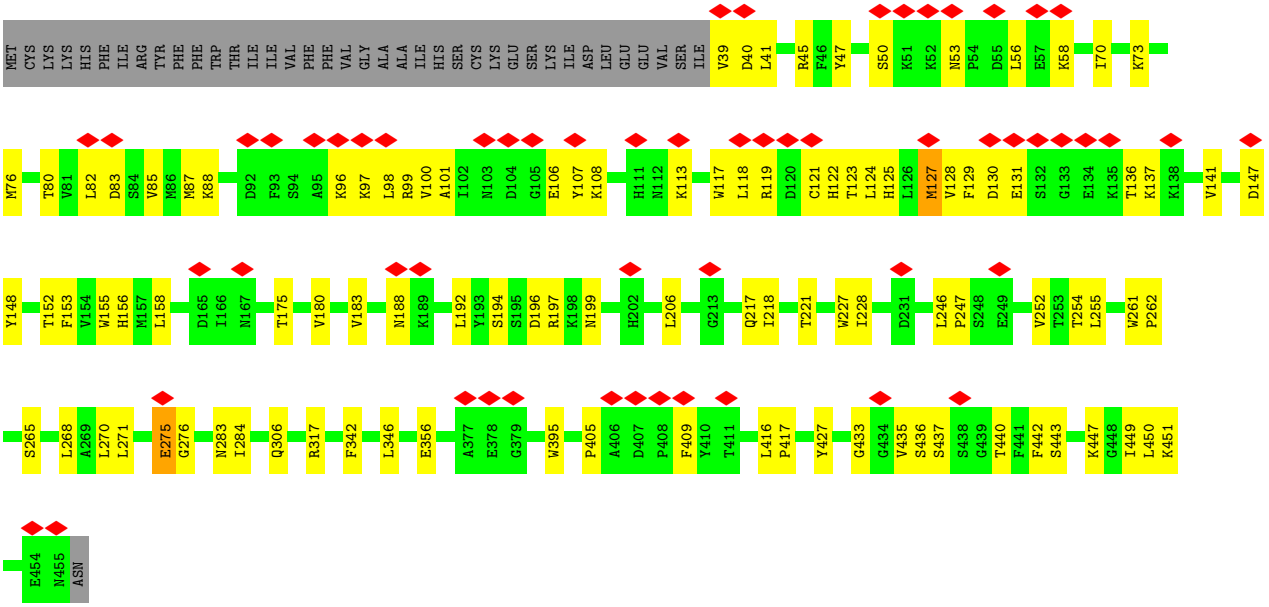



• Molecule 3: DUF6242 domain-containing protein

Chain H:





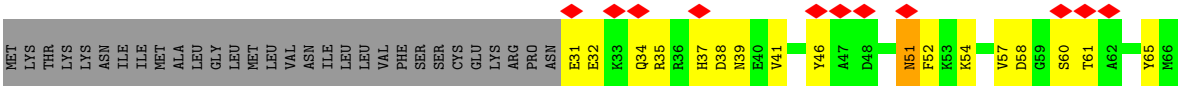


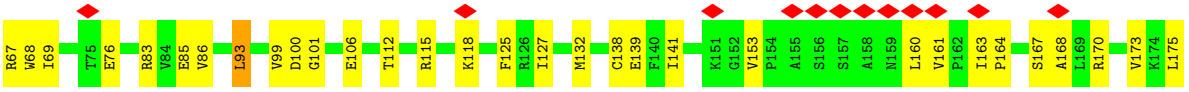


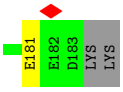
• Molecule 4: Peptidyl-prolyl cis-trans isomerase

Chain I:



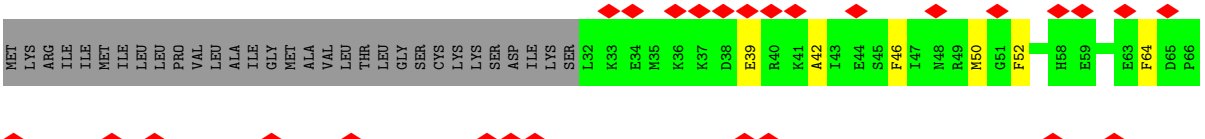




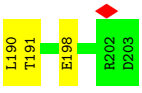
• Molecule 5: DUF4827 domain-containing protein

Chain J:



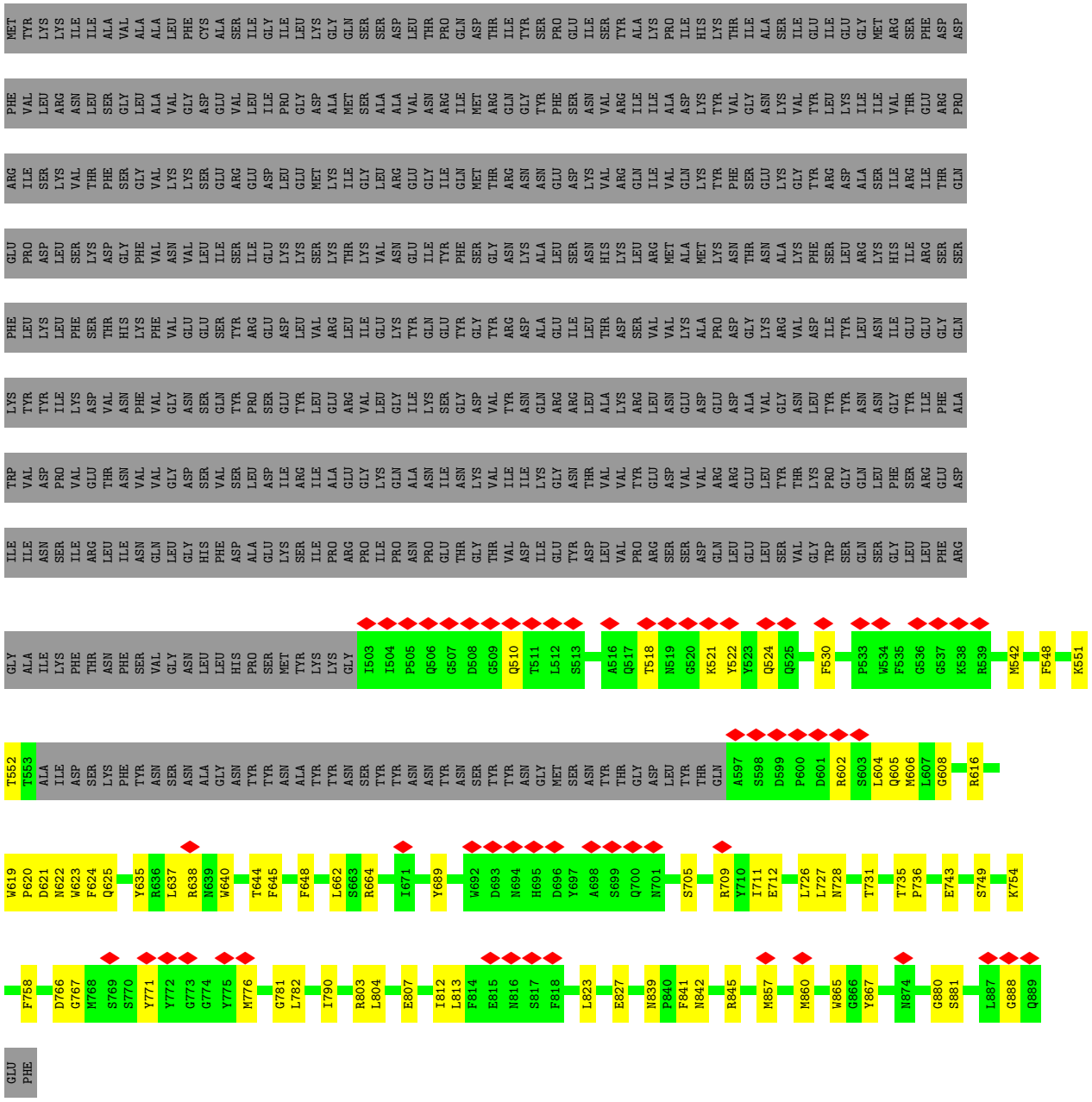




• Molecule 6: Putative outer membrane protein

Chain A:


7%
31%
8%
61%


MET TYR LYS LYS ILE ILE ALA VAL ALA ALA LEU PHE CYS ALA SER ILE GLY ILE LEU LYS GLY GLN SER SER ASP LEU THR PRO GLN ASP THR ILE TYR SER PRO GLU ILE SER TYR ALA LYS PRO ILE HIS LYS THR ILE ALA SER ILE GLU ILE GLU GLY MET ARG SER PHE ASP ASP
PHE VAL LEU ARG ASN LEU SER GLY LEU ALA VAL GLY ASP GLU VAL LEU ILE PRO GLY ASP ALA MET SER ALA ALA VAL ASN ARG ILE MET ARG GLN GLY TYR PHE SER ASN VAL ARG ILE ILE ALA ASP LYS TYR VAL GLY ASN LYS VAL TYR LEU LYS ILE ILE VAL THR GLU ARG PRO
ARG ILE SER LYS VAL THR PHE SER GLY VAL LYS LYS SER GLU ARG GLU ASP LEU GLU MET LYS ILE GLY LEU ARG GLU GLY ILE GLN MET THR ARG ASN ASN GLU ASP LYS VAL ARG GLN ILE ILE VAL GLN LYS TYR PHE SER GLU LYS GLY TYR ARG ASP ALA SER ILE ARG ILE THR GLN
GLU PRO ASP LEU SER LYS ASP GLY PHE VAL ASN VAL LEU ILE SER ILE GLU LYS LYS SER LYS THR LYS VAL ASN GLU ILE TYR PHE SER GLY ASN LYS ALA LEU SER ASN HIS LYS LEU ARG MET ALA MET LYS ASN THR ASN ALA LYS PHE SER LEU ARG LYS HIS ILE ARG SER SER
PHE LEU LYS LEU PHE SER THR HIS LYS PHE VAL GLU GLU SER TYR ARG GLU ASP LEU VAL ARG LEU ILE GLU LYS TYR GLN GLU TYR GLY TYR ARG ASP ALA GLU ILE LEU THR ASP SER VAL VAL LYS ALA PRO ASP GLY LYS ARG VAL ASP ILE TYR LEU ASN ILE GLU GLU GLY GLN
LYS TYR TYR ILE LYS ASP VAL ASN PHE VAL GLY ASN SER GLN TYR PRO SER GLU TYR LEU GLU ARG VAL LEU GLY ILE LYS SER GLY ASP VAL TYR ASN GLN ARG ARG LEU ALA LYS ARG LEU ASN GLU ASP GLU ASP ALA VAL GLY ASN LEU TYR TYR ASN ASN GLY TYR ILE PHE ALA
TRP VAL ASP PRO VAL GLU THR ASN VAL VAL GLY ASP SER VAL SER LEU ASP ILE ARG ILE ALA GLU GLY LYS GLN ALA ASN ILE ASN LYS VAL ILE ILE LYS GLY ASN THR VAL VAL TYR GLU ASP VAL VAL ARG ARG GLU LEU TYR THR LYS PRO GLY GLN LEU PHE SER ARG GLU ASP
ILE ILE ASN SER ILE ARG LEU ILE ASN GLN LEU GLY HIS PHE ASP ALA GLU LYS SER ILE PRO ARG PRO ILE PRO ASN PRO GLU THR GLY THR VAL ASP ILE GLU TYR ASP LEU VAL PRO ARG SER SER ASP GLN LEU GLU LEU SER VAL GLY TRP SER GLN SER GLY LEU LEU PHE ARG
GLY ALA ILE LYS PHE THR ASN PHE SER VAL GLY ASN LEU LEU HIS PRO SER MET TYR LYS LYS GLY I503 I504 P505 Q506 G507 D508 G509 Q510 T511 L512 S513 A516 Q517 T518 N519 G520 K521 Y522 Y523 Q524 Q525 F530 P533 W534 F535 G536 G537 K538 R539 M542 F548 K551
T552 T553 ALA ILE ASP SER LYS PHE TYR ASN SER ASN ALA GLY ASN TYR TYR ASN ALA TYR TYR ASN SER TYR TYR ASN ASN TYR ASN SER TYR TYR ASN GLY MET SER ASN TYR THR GLY ASP LEU TYR THR GLN A597 S598 D599 P600 D601 R602 S603 L604 Q605 M606 L607 G608 R616
W619 P620 D621 N622 W623 F624 Q625 Y635 R636 L637 R638 N639 W640 T644 F645 F648 L662 S663 R664 I671 Y689 W692 D693 N694 H695 D696 Y697 A698 S699 Q700 N701 S705 R709 Y710 I711 E712 L726 L727 N728 T731 T735 P736 E743 S749 K754
F758 D766 G767 M768 S769 S770 Y771 Y772 G773 G774 Y775 M776 G781 L782 I790 R803 L804 E807 I812 L813 F814 E815 N816 S817 F818 L823 E827 N839 P840 F841 N842 R845 M857 M860 W865 G866 Y867 N874 G880 S881 L887 G888 Q889
GLU PHE

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 86584 | 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 ($e^-/Å^2$) | 41.01 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 1500 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 1.161 | Depositor |
| Minimum map value | -0.689 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.028 | Depositor |
| Recommended contour level | 0.189 | Depositor |
| Map size (Å) | 322.56, 322.56, 322.56 | wwPDB |
| Map dimensions | 384, 384, 384 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.84, 0.84, 0.84 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z41, PLM

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 | F | 0.19 | 0/3179 | 0.40 | 0/4285 |
| 2 | G | 0.19 | 0/3529 | 0.48 | 0/4792 |
| 3 | H | 0.18 | 0/3358 | 0.42 | 2/4575 (0.0%) |
| 4 | I | 0.36 | 1/1246 (0.1%) | 0.50 | 0/1691 |
| 5 | J | 0.17 | 0/1450 | 0.43 | 0/1942 |
| 6 | A | 0.19 | 0/2872 | 0.47 | 0/3895 |
| All | All | 0.21 | 1/15634 (0.0%) | 0.45 | 2/21180 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | H | 0 | 1 |
| 6 | A | 0 | 1 |
| All | All | 0 | 2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | I | 93 | LEU | CG-CD2 | -6.46 | 1.31 | 1.52 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | H | 127 | MET | CB-CG-SD | -6.92 | 91.93 | 112.70 |
| 3 | H | 127 | MET | CA-CB-CG | 5.37 | 124.83 | 114.10 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 6 | A | 845 | ARG | Sidechain |
| 3 | H | 45 | ARG | Sidechain |

## 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 | F | 3102 | 0 | 3058 | 64 | 0 |
| 2 | G | 3454 | 0 | 3416 | 64 | 0 |
| 3 | H | 3268 | 0 | 3181 | 78 | 0 |
| 4 | I | 1218 | 0 | 1189 | 50 | 0 |
| 5 | J | 1418 | 0 | 1385 | 28 | 0 |
| 6 | A | 2786 | 0 | 2631 | 64 | 0 |
| 7 | G | 16 | 0 | 26 | 0 | 0 |
| 8 | G | 35 | 0 | 0 | 0 | 0 |
| All | All | 15297 | 0 | 14886 | 316 | 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 10.

The worst 5 of 316 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) |
|---|---|---|---|
| 3:H:127:MET:HE2 | 3:H:129:PHE:CZ | 1.90 | 1.07 |
| 3:H:127:MET:HE2 | 3:H:129:PHE:HZ | 1.24 | 0.97 |
| 1:F:388:ASN:HD21 | 6:A:728:ASN:HB2 | 1.36 | 0.91 |
| 5:J:39:GLU:OE1 | 5:J:191:THR:OG1 | 1.91 | 0.87 |
| 2:G:127:LYS:HB2 | 2:G:152:ILE:HD11 | 1.57 | 0.85 |

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 | F | 389/434 (90%) | 356 (92%) | 33 (8%) | 0 | 100 | 100 |
| 2 | G | 437/462 (95%) | 386 (88%) | 49 (11%) | 2 (0%) | 24 | 56 |
| 3 | H | 415/456 (91%) | 390 (94%) | 24 (6%) | 1 (0%) | 43 | 72 |
| 4 | I | 151/185 (82%) | 137 (91%) | 13 (9%) | 1 (1%) | 18 | 50 |
| 5 | J | 170/203 (84%) | 160 (94%) | 10 (6%) | 0 | 100 | 100 |
| 6 | A | 340/891 (38%) | 316 (93%) | 24 (7%) | 0 | 100 | 100 |
| All | All | 1902/2631 (72%) | 1745 (92%) | 153 (8%) | 4 (0%) | 44 | 72 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | I | 51 | ASN |
| 3 | H | 275 | GLU |
| 2 | G | 229 | SER |
| 2 | G | 234 | ALA |

### 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 | F | 330/362 (91%) | 330 (100%) | 0 | 100 | 100 |
| 2 | G | 396/417 (95%) | 396 (100%) | 0 | 100 | 100 |
| 3 | H | 351/387 (91%) | 351 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | I | 132/162 (82%) | 132 (100%) | 0 | 100 | 100 |
| 5 | J | 155/182 (85%) | 155 (100%) | 0 | 100 | 100 |
| 6 | A | 293/777 (38%) | 293 (100%) | 0 | 100 | 100 |
| All | All | 1657/2287 (72%) | 1657 (100%) | 0 | 100 | 100 |

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

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | A | 517 | GLN |
| 6 | A | 646 | GLN |
| 6 | A | 777 | ASN |
| 2 | G | 155 | GLN |
| 2 | G | 150 | GLN |

#### 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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 7 | PLM | G | 501 | 2 | 14,15,17 | 0.33 | 0 | 13,14,17 | 0.44 | 0 |
| 8 | Z41 | G | 502 | 2 | 34,34,39 | 1.14 | 3 (8%) | 36,36,41 | 1.12 | 3 (8%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 7 | PLM | G | 501 | 2 | - | 10/13/13/15 | - |
| 8 | Z41 | G | 502 | 2 | - | 13/35/35/41 | - |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | G | 502 | Z41 | O3-C18 | -4.33 | 1.39 | 1.47 |
| 8 | G | 502 | Z41 | O2-C16 | 2.60 | 1.40 | 1.33 |
| 8 | G | 502 | Z41 | O3-C19 | 2.03 | 1.40 | 1.34 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | G | 502 | Z41 | O3-C19-C20 | 3.96 | 120.04 | 111.48 |
| 8 | G | 502 | Z41 | C18-O3-C19 | -2.69 | 113.90 | 117.78 |
| 8 | G | 502 | Z41 | O2-C16-C15 | 2.61 | 119.79 | 111.83 |

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 7 | G | 501 | PLM | O2-C1-C2-C3 |
| 8 | G | 502 | Z41 | C20-C19-O3-C18 |
| 8 | G | 502 | Z41 | O4-C19-O3-C18 |
| 8 | G | 502 | Z41 | C13-C14-C15-C16 |
| 7 | G | 501 | PLM | C4-C5-C6-C7 |

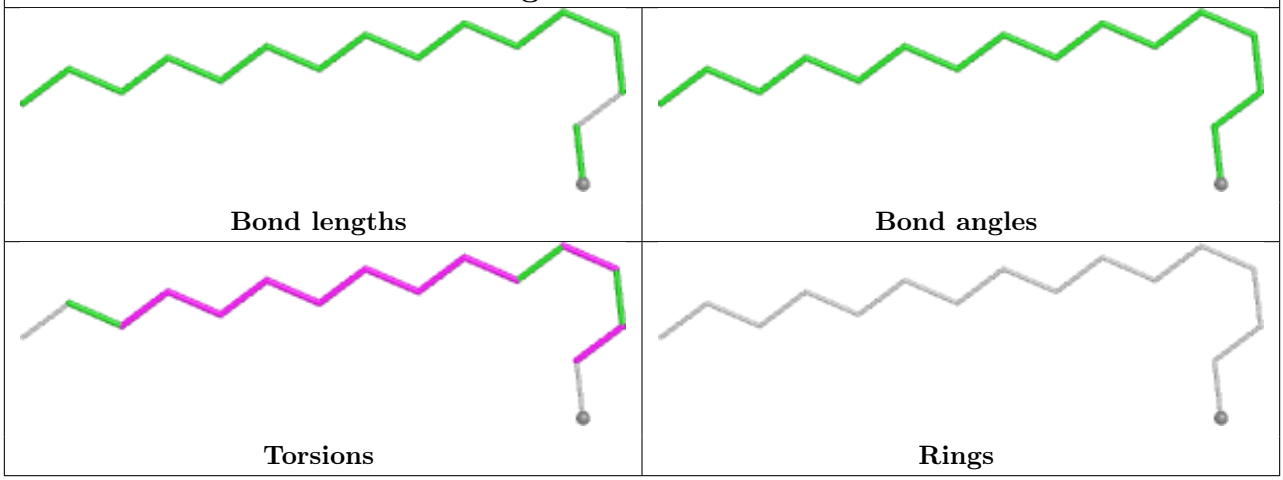
There are no ring outliers.

No monomer is involved in short contacts.

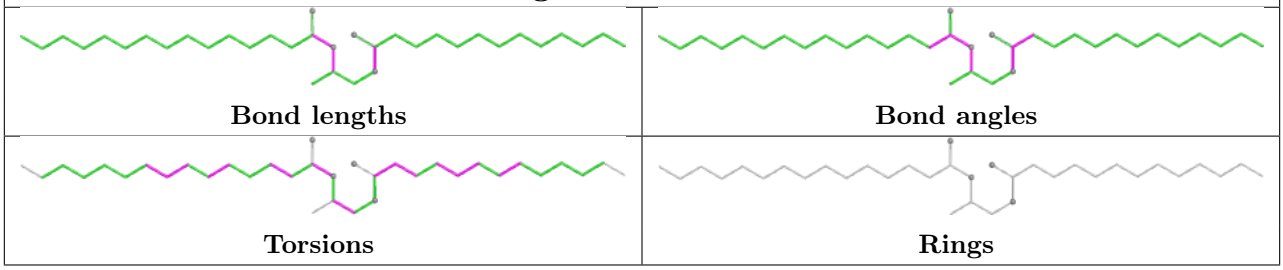
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

**Ligand PLM G 501**




**Ligand Z41 G 502**




## 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.

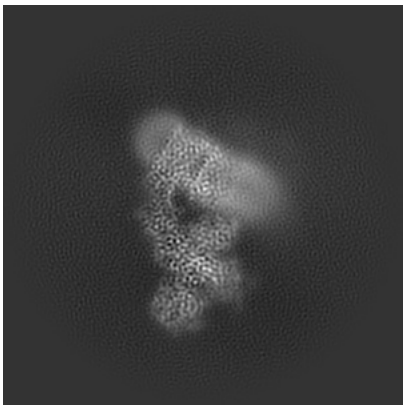
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52218. These allow visual inspection of the internal detail of the map and identification of artifacts.

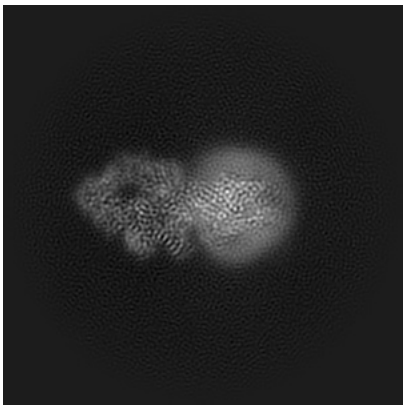
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

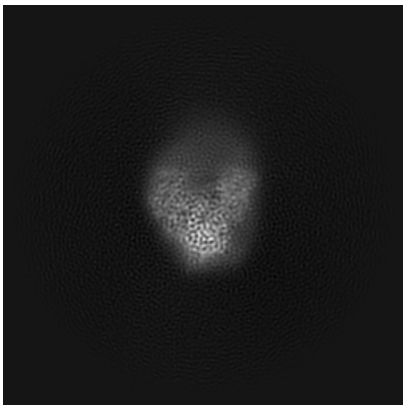
### 6.1.1 Primary map



X

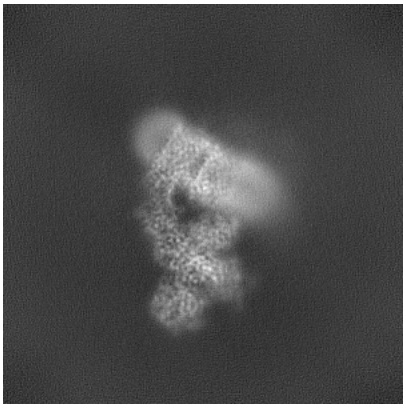


Y

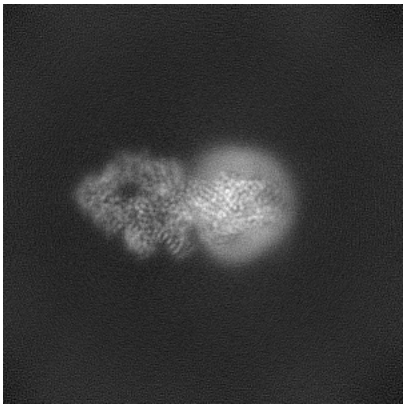


Z

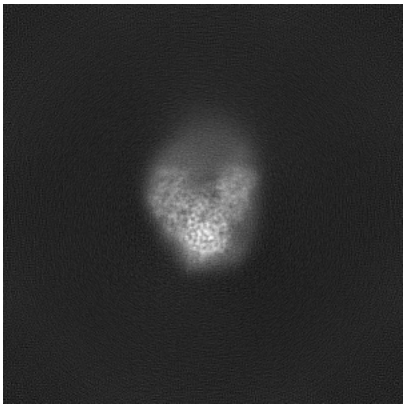
### 6.1.2 Raw map



X



Y

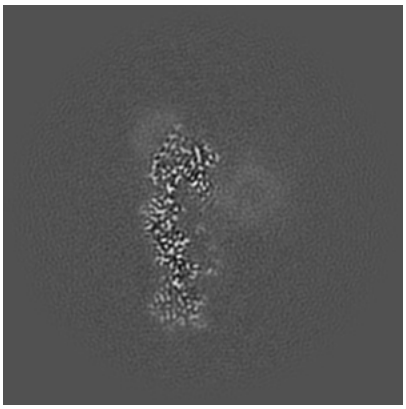


Z

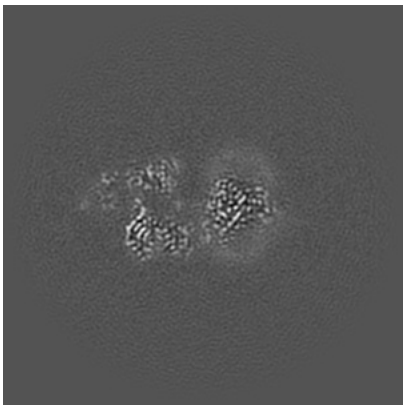
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

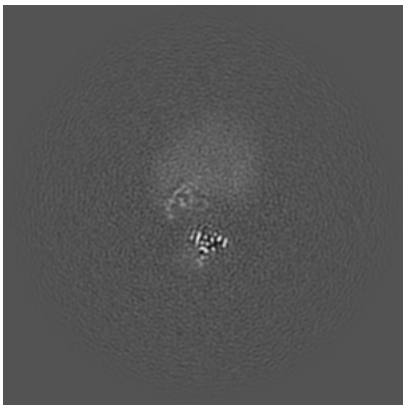
### 6.2.1 Primary map



X Index: 192

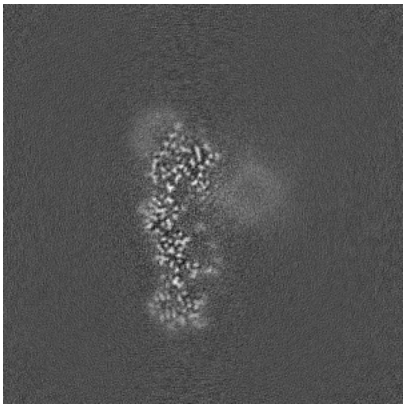


Y Index: 192

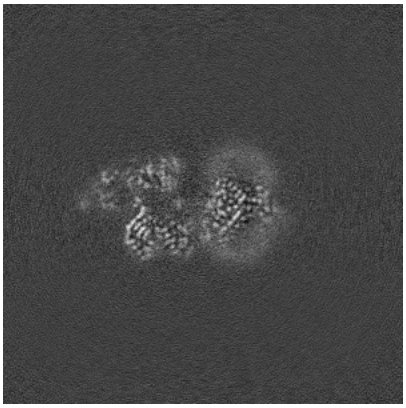


Z Index: 192

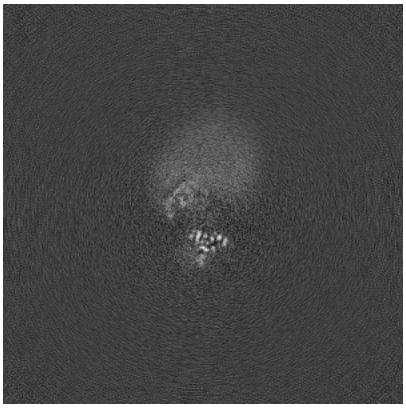
### 6.2.2 Raw map



X Index: 192



Y Index: 192

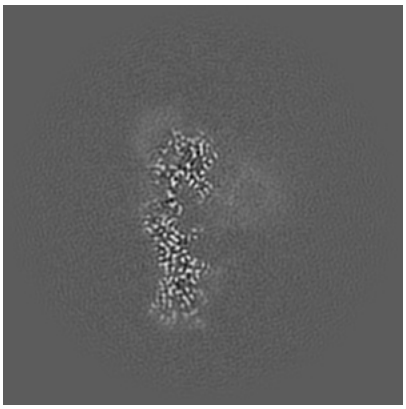


Z Index: 192

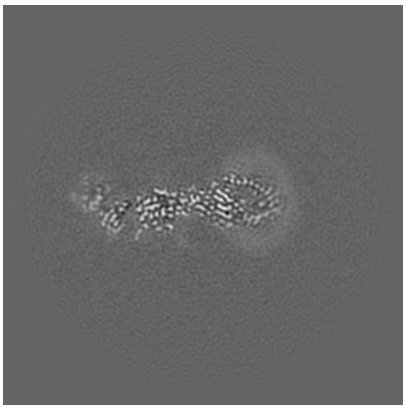
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

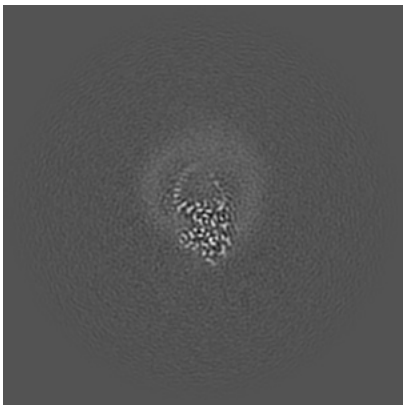
### 6.3.1 Primary map



X Index: 188

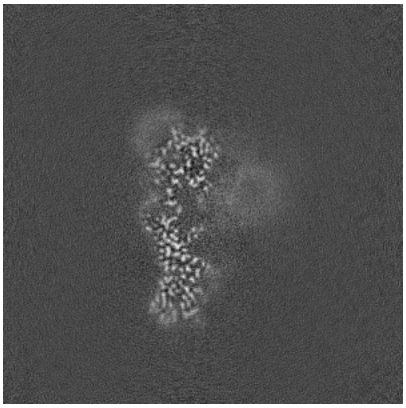


Y Index: 163

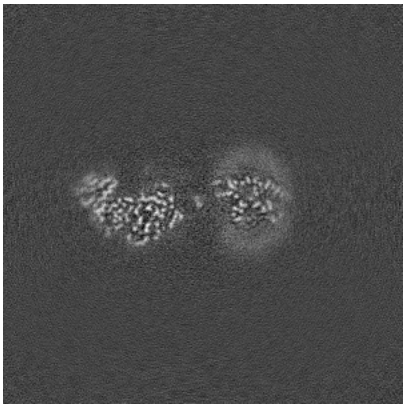


Z Index: 217

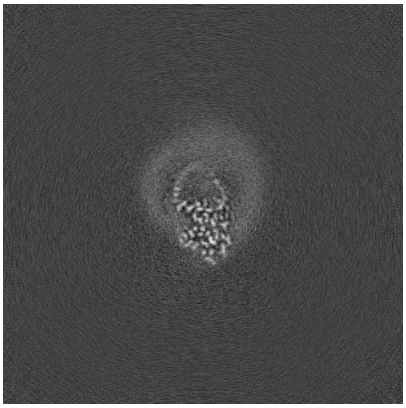
### 6.3.2 Raw map



X Index: 187



Y Index: 172

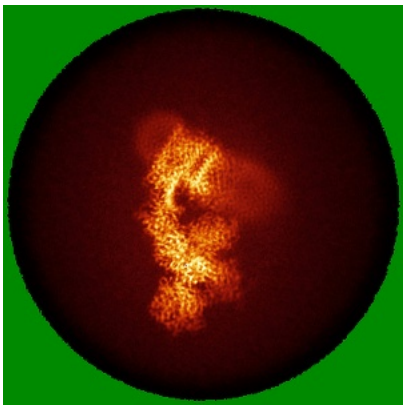


Z Index: 217

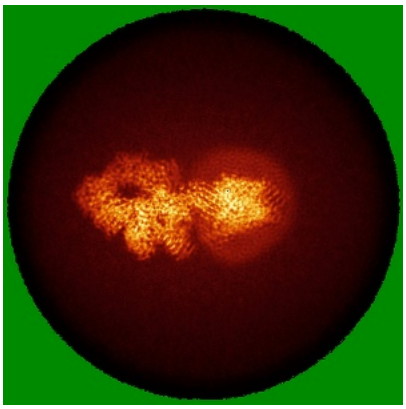
The images above show the largest variance slices of the map in three orthogonal directions.

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

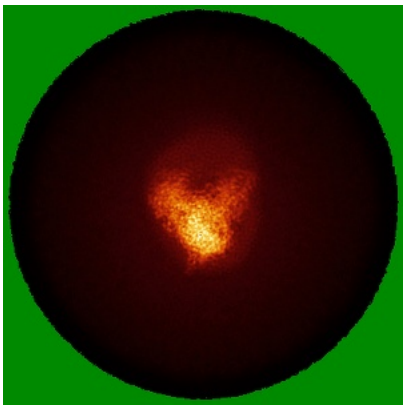
### 6.4.1 Primary map



X

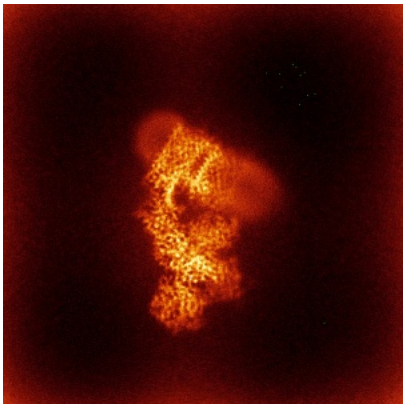


Y

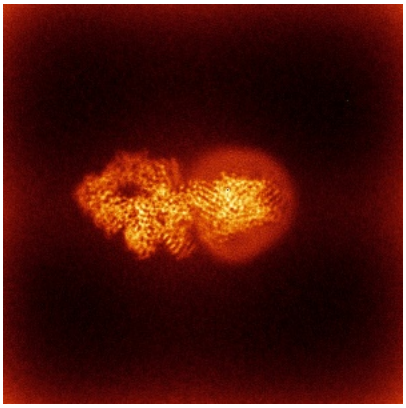


Z

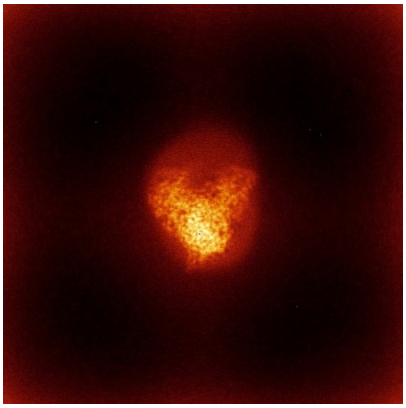
### 6.4.2 Raw map



X



Y

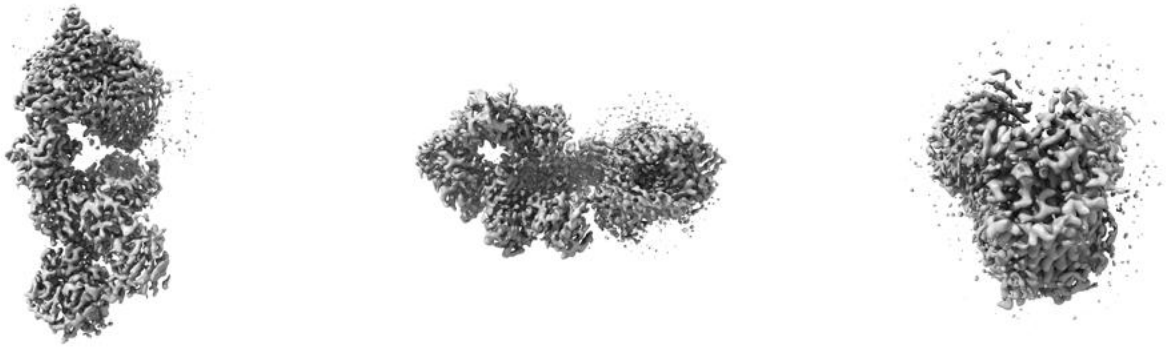


Z

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 0.189. 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.

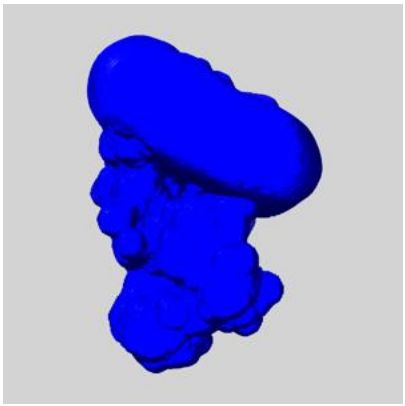
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

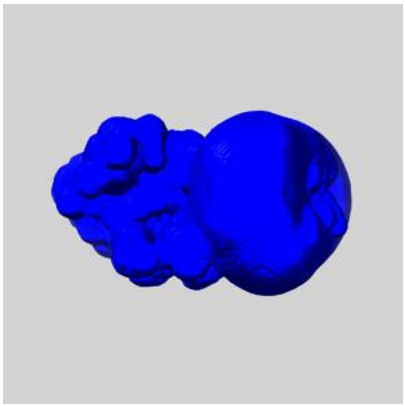
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

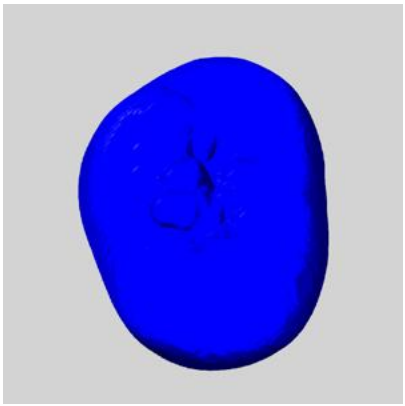
### 6.6.1 emd_52218_msk_1.map (i)



X



Y

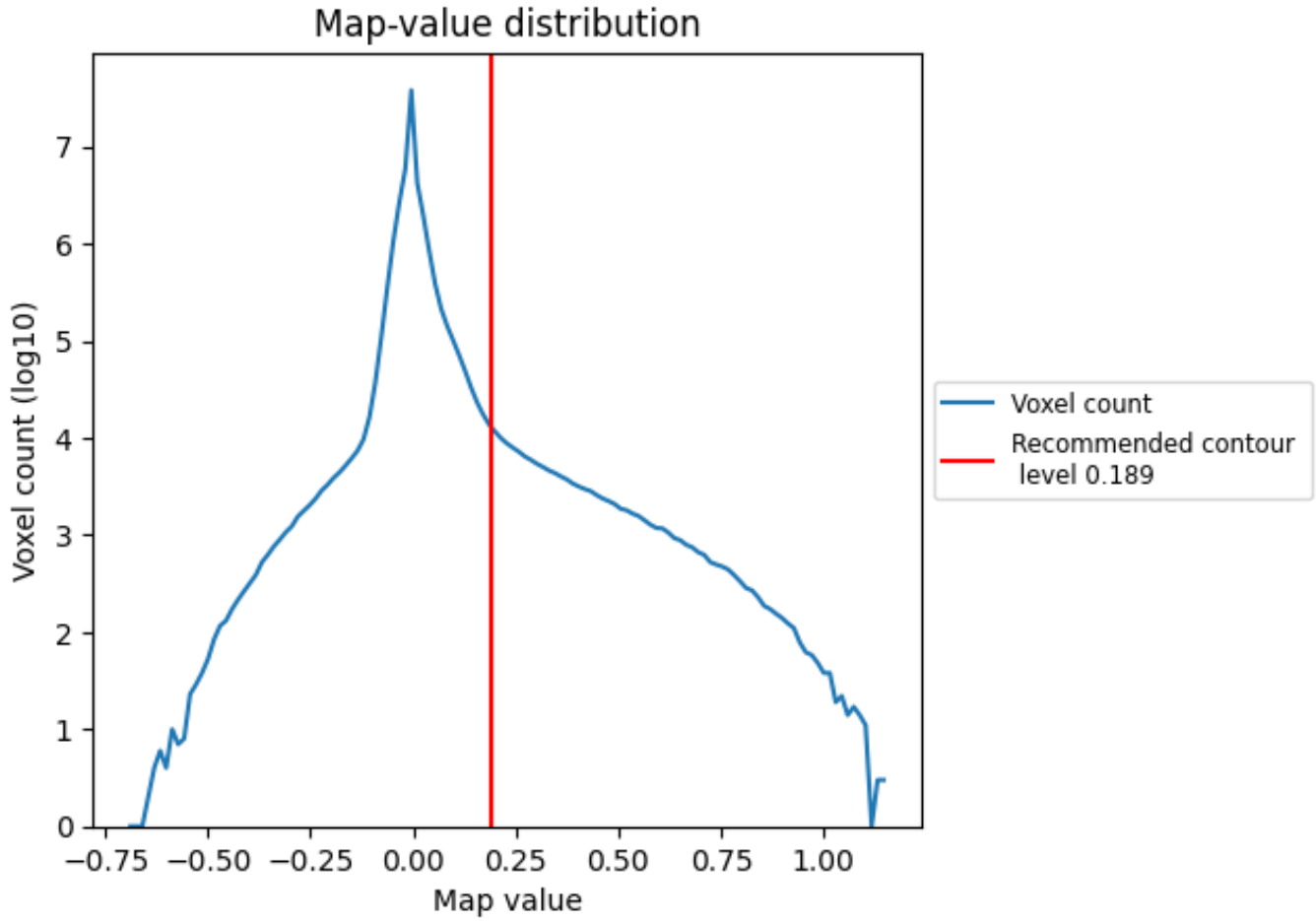


Z

# 7 Map analysis

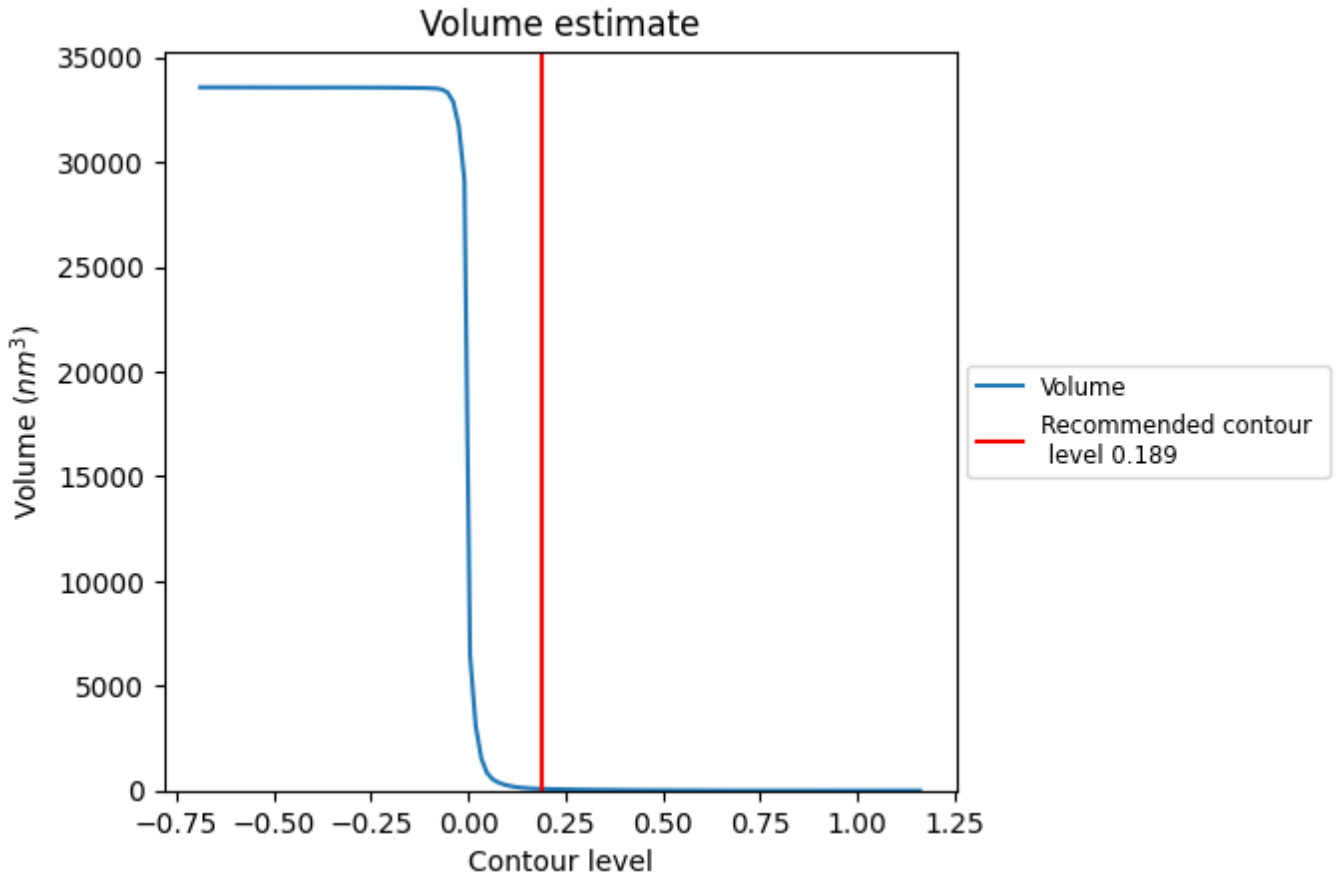
This section contains the results of statistical analysis of the map.

## 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.

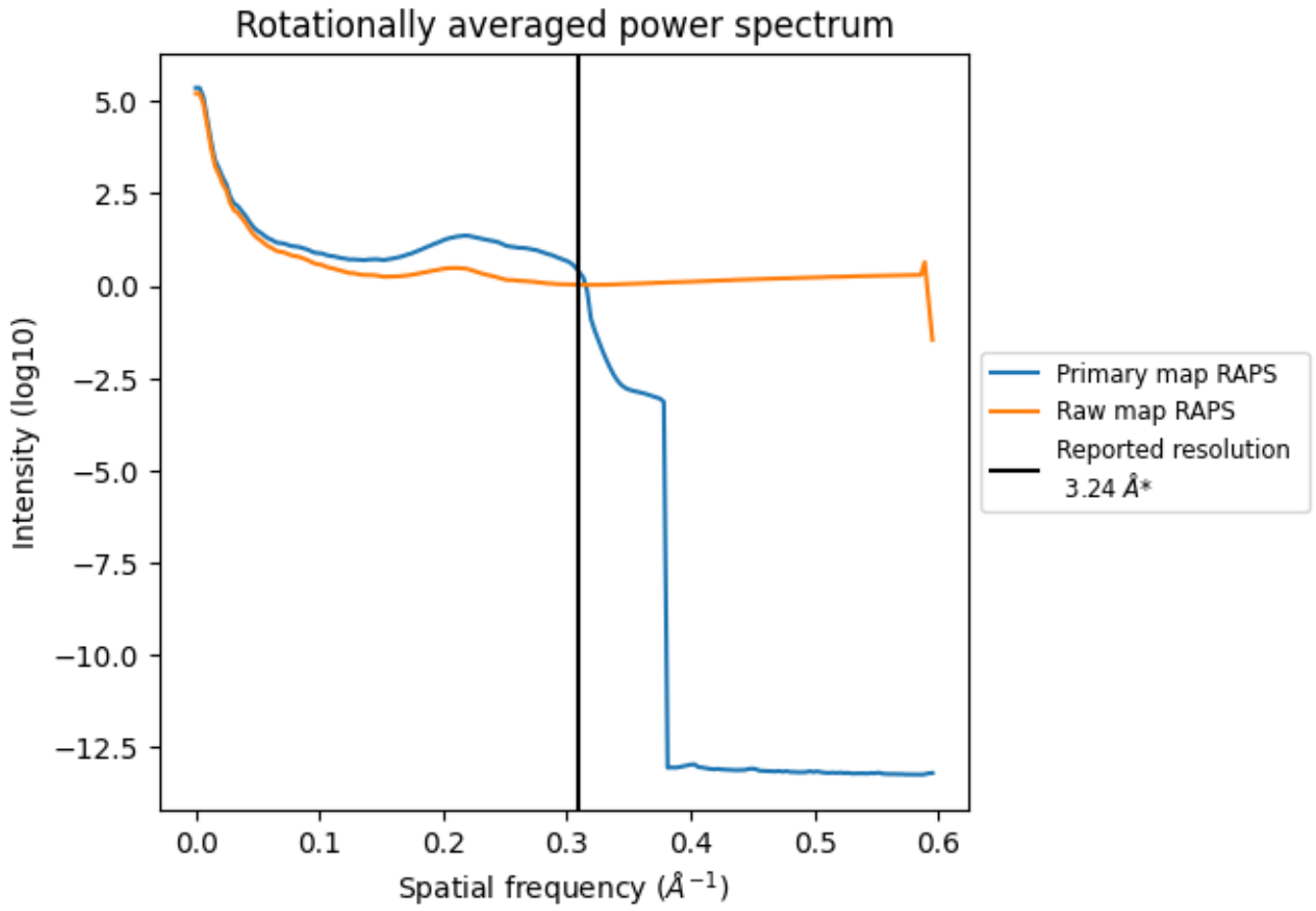
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 82 $nm^3$; this corresponds to an approximate mass of 75 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)

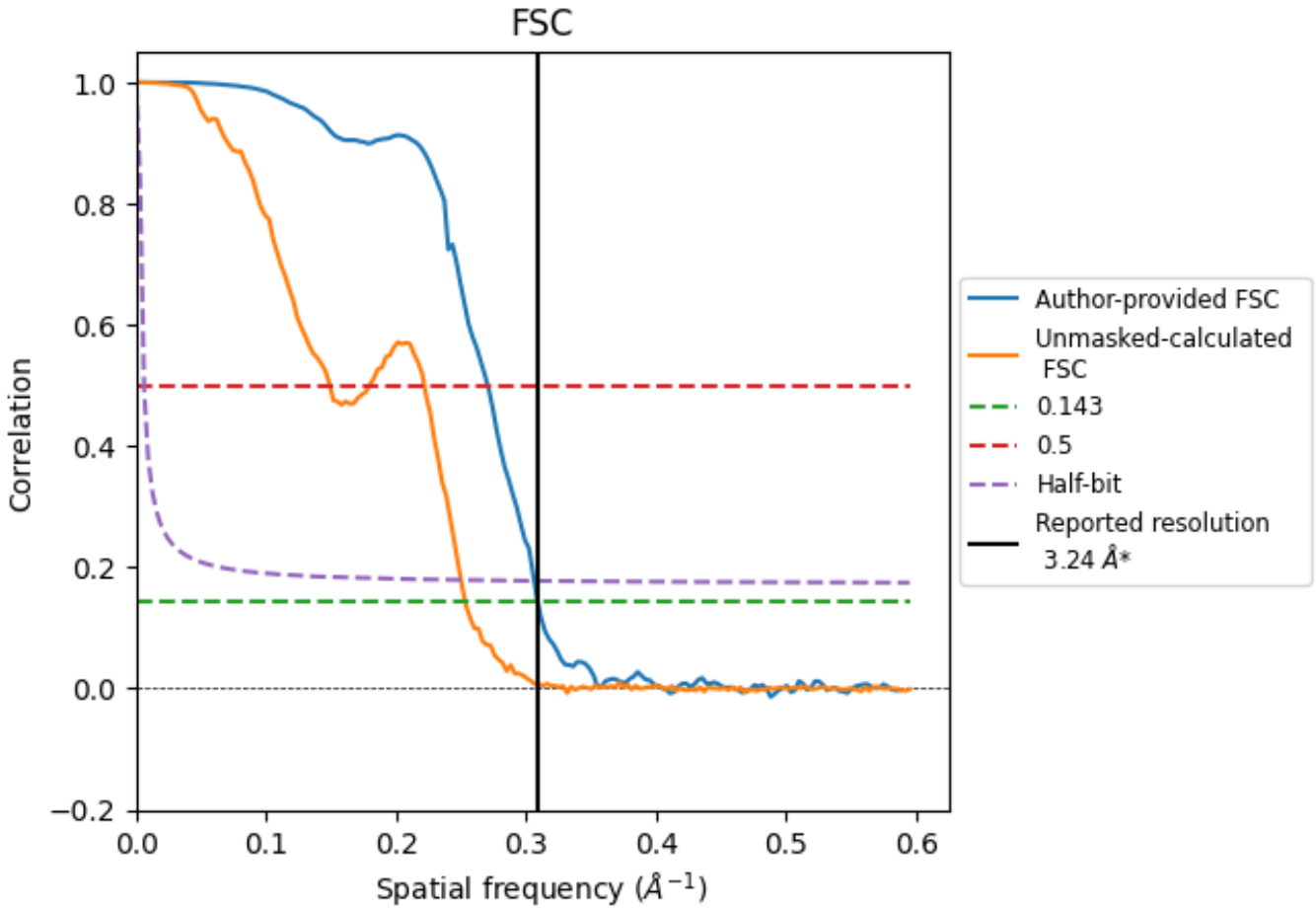



*Reported resolution corresponds to spatial frequency of 0.309 $Å^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.309 Å$^{-1}$

## 8.2 Resolution estimates (i)

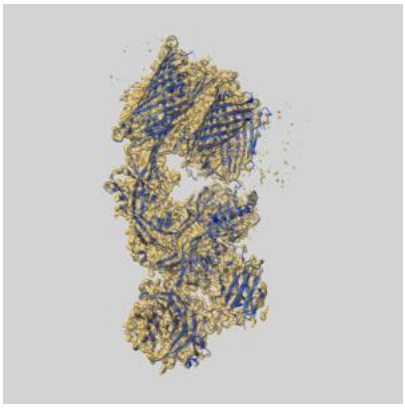
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.24 | - | - |
| Author-provided FSC curve | 3.24 | 3.70 | 3.26 |
| Unmasked-calculated* | 3.95 | 6.71 | 4.00 |

*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 3.95 differs from the reported value 3.24 by more than 10 %

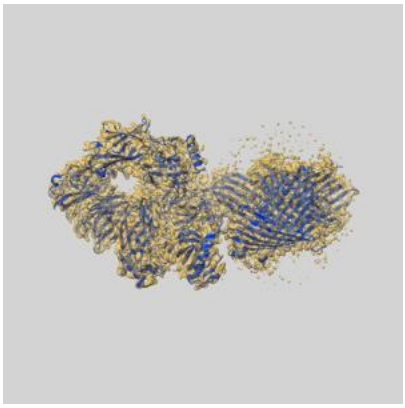
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52218 and PDB model 9HJM. Per-residue inclusion information can be found in section 3 on page 7.

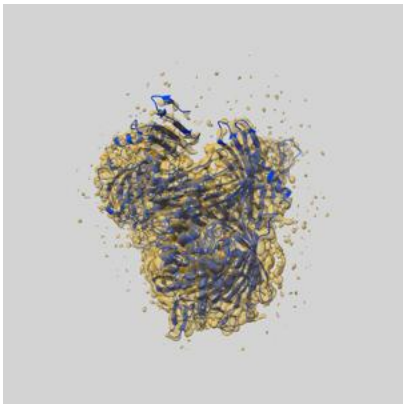
## 9.1 Map-model overlay



X



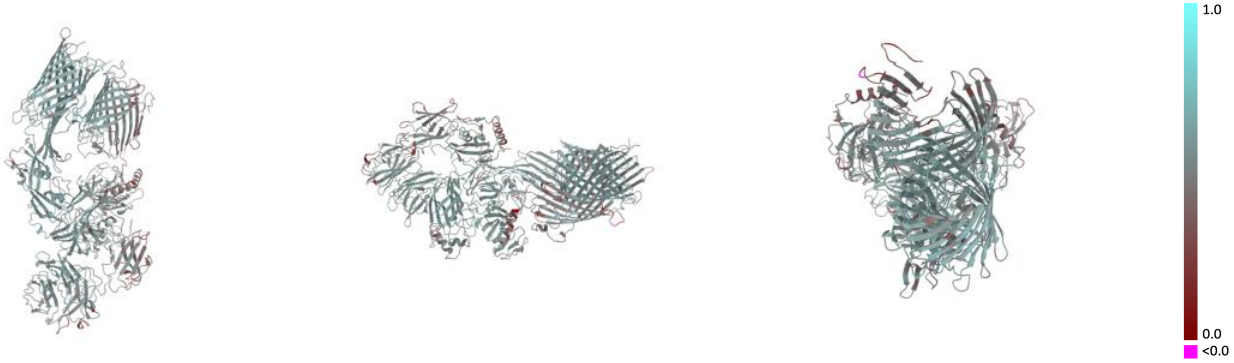
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.189 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.

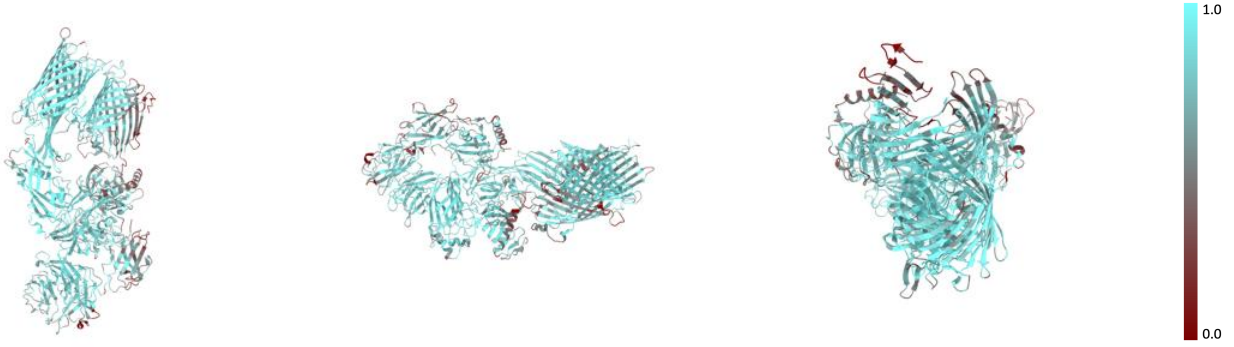
## 9.2 Q-score mapped to coordinate model




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.

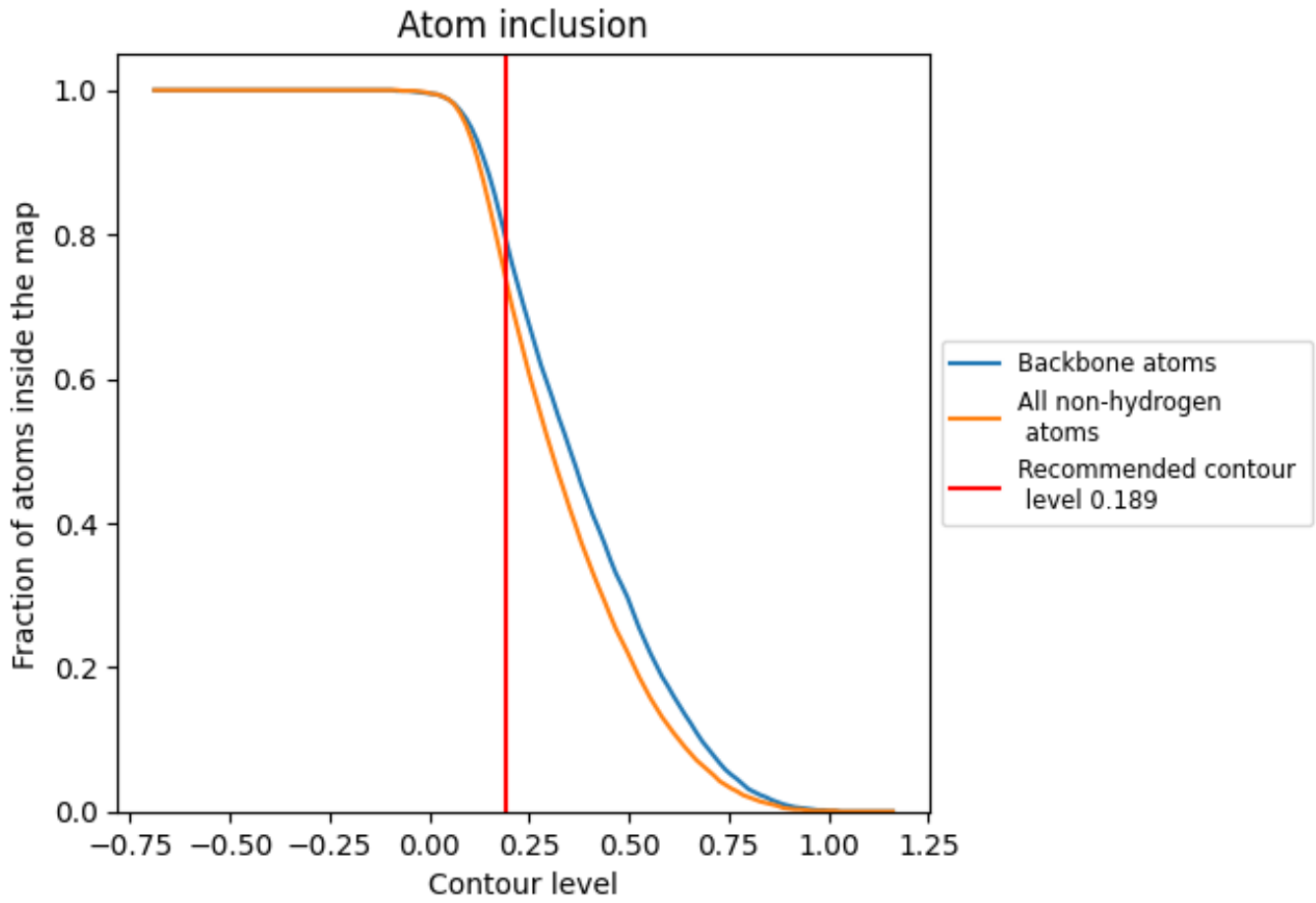
## 9.3 Atom inclusion mapped to coordinate model




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 (0.189).

## 9.4 Atom inclusion (i)




At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.189) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7430 | 0.5190 |
| A | 0.6730 | 0.4940 |
| F | 0.8200 | 0.5510 |
| G | 0.8400 | 0.5470 |
| H | 0.6830 | 0.4950 |
| I | 0.6540 | 0.4880 |
| J | 0.6880 | 0.5140 |

