# Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 01:45 am BST

| | | |
|---|---|---|
| PDB ID | : | 8PPU / pdb_00008ppu |
| EMDB ID | : | EMD-17816 |
| Title | : | Pyrococcus abyssi DNA polymerase D (PolD) in its editing mode bound to a primer/template substrate containing three consecutive mismatches |
| Authors | : | Betancurt-Anzola, L.; Martinez-Carranza, M.; Zatopek, K.M.; Gardner, A.F.; Sauguet, L. |
| Deposited on | : | 2023-07-10 |
| Resolution | : | 3.02 Å(reported) |

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

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

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

---

The following versions of software and data (see references (1)) were used in the production of this report:

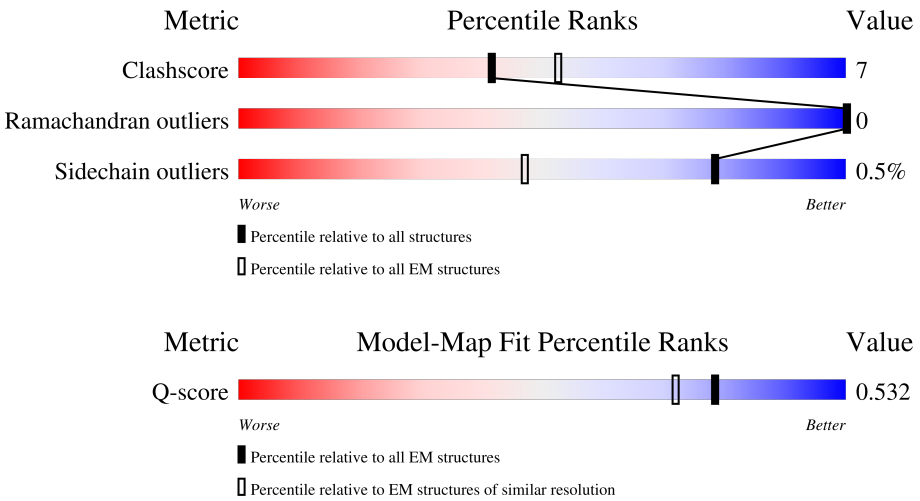
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using 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) | : | 2.50 |

# 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 3.02 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 | 13913 ( 2.52 - 3.52 ) |

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 | P | 21 | 71% 19% 10% |
| 2 | T | 25 | • 8% 60% 32% |
| 3 | A | 662 | 9% 60% 7% 32% |
| 4 | C | 261 | 26% 82% 13% 6% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | D | 261 | 20% 82% 12% • 6% |
| 4 | E | 261 | 30% 79% 16% 6% |
| 5 | B | 1270 | • 82% 11% 6% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 1 | GS | P | 17 | - | - | X | - |
| 1 | PST | P | 19 | - | - | X | - |
| 1 | PST | P | 20 | - | - | X | - |
| 1 | PST | P | 21 | - | - | X | - |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19649 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 DNA chain called DNA (5'-D(P*CP*CP*GP*GP*GP*CP*CP*GP*AP*GP*CP*CP*GP*TP*(GS)P*(C7R)P*(PST)P*(PST)P*(PST))-3').

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | |
| 1 | P | 19 | 388 | 183 | 69 | 112 | 19 | 5 | 0 | 0 |

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*AP*CP*GP*GP*CP*TP*CP*GP*GP*CP*CP*CP*GP*G)-3').

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | T | 17 | 348 | 163 | 65 | 103 | 17 | 0 | 0 |

- Molecule 3 is a protein called DNA polymerase II small subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | A | 447 | 3565 | 2319 | 590 | 649 | 7 | 0 | 0 |

There are 45 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -42 | MET | - | initiating methionine | UNP Q9V2F3 |
| A | -41 | GLY | - | expression tag | UNP Q9V2F3 |
| A | -40 | LYS | - | expression tag | UNP Q9V2F3 |
| A | -39 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -38 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -37 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -36 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -35 | SER | - | expression tag | UNP Q9V2F3 |
| A | -34 | GLY | - | expression tag | UNP Q9V2F3 |
| A | -33 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -32 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -31 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -30 | THR | - | expression tag | UNP Q9V2F3 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -29 | GLY | - | expression tag | UNP Q9V2F3 |
| A | -28 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -27 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -26 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -25 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -24 | SER | - | expression tag | UNP Q9V2F3 |
| A | -23 | GLY | - | expression tag | UNP Q9V2F3 |
| A | -22 | SER | - | expression tag | UNP Q9V2F3 |
| A | -21 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -20 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -19 | HIS | - | expression tag | UNP Q9V2F3 |
| A | -18 | THR | - | expression tag | UNP Q9V2F3 |
| A | -17 | SER | - | expression tag | UNP Q9V2F3 |
| A | -16 | SER | - | expression tag | UNP Q9V2F3 |
| A | -15 | SER | - | expression tag | UNP Q9V2F3 |
| A | -14 | ALA | - | expression tag | UNP Q9V2F3 |
| A | -13 | SER | - | expression tag | UNP Q9V2F3 |
| A | -12 | THR | - | expression tag | UNP Q9V2F3 |
| A | -11 | GLY | - | expression tag | UNP Q9V2F3 |
| A | -10 | GLU | - | expression tag | UNP Q9V2F3 |
| A | -9 | ASN | - | expression tag | UNP Q9V2F3 |
| A | -8 | LEU | - | expression tag | UNP Q9V2F3 |
| A | -7 | TYR | - | expression tag | UNP Q9V2F3 |
| A | -6 | PHE | - | expression tag | UNP Q9V2F3 |
| A | -5 | GLN | - | expression tag | UNP Q9V2F3 |
| A | -4 | GLY | - | expression tag | UNP Q9V2F3 |
| A | -3 | THR | - | expression tag | UNP Q9V2F3 |
| A | -2 | GLY | - | expression tag | UNP Q9V2F3 |
| A | -1 | ASP | - | expression tag | UNP Q9V2F3 |
| A | 0 | GLY | - | expression tag | UNP Q9V2F3 |
| A | 1 | SER | - | expression tag | UNP Q9V2F3 |
| A | 451 | ALA | HIS | engineered mutation | UNP Q9V2F3 |

- Molecule 4 is a protein called DNA polymerase sliding clamp.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | C | 246 | 1939 | 1238 | 308 | 384 | 9 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 4 | D | 246 | 1939 | 1238 | 308 | 384 | 9 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 4 | E | 246 | 1939 | 1238 | 308 | 384 | 9 | 0 | 0 |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | -11 | MET | - | initiating methionine | UNP Q9UYX8 |
| C | -10 | ARG | - | expression tag | UNP Q9UYX8 |
| C | -9 | GLY | - | expression tag | UNP Q9UYX8 |
| C | -8 | SER | - | expression tag | UNP Q9UYX8 |
| C | -7 | HIS | - | expression tag | UNP Q9UYX8 |
| C | -6 | HIS | - | expression tag | UNP Q9UYX8 |
| C | -5 | HIS | - | expression tag | UNP Q9UYX8 |
| C | -4 | HIS | - | expression tag | UNP Q9UYX8 |
| C | -3 | HIS | - | expression tag | UNP Q9UYX8 |
| C | -2 | HIS | - | expression tag | UNP Q9UYX8 |
| C | -1 | GLY | - | expression tag | UNP Q9UYX8 |
| C | 0 | SER | - | expression tag | UNP Q9UYX8 |
| D | -11 | MET | - | initiating methionine | UNP Q9UYX8 |
| D | -10 | ARG | - | expression tag | UNP Q9UYX8 |
| D | -9 | GLY | - | expression tag | UNP Q9UYX8 |
| D | -8 | SER | - | expression tag | UNP Q9UYX8 |
| D | -7 | HIS | - | expression tag | UNP Q9UYX8 |
| D | -6 | HIS | - | expression tag | UNP Q9UYX8 |
| D | -5 | HIS | - | expression tag | UNP Q9UYX8 |
| D | -4 | HIS | - | expression tag | UNP Q9UYX8 |
| D | -3 | HIS | - | expression tag | UNP Q9UYX8 |
| D | -2 | HIS | - | expression tag | UNP Q9UYX8 |
| D | -1 | GLY | - | expression tag | UNP Q9UYX8 |
| D | 0 | SER | - | expression tag | UNP Q9UYX8 |
| E | -11 | MET | - | initiating methionine | UNP Q9UYX8 |
| E | -10 | ARG | - | expression tag | UNP Q9UYX8 |
| E | -9 | GLY | - | expression tag | UNP Q9UYX8 |
| E | -8 | SER | - | expression tag | UNP Q9UYX8 |
| E | -7 | HIS | - | expression tag | UNP Q9UYX8 |
| E | -6 | HIS | - | expression tag | UNP Q9UYX8 |
| E | -5 | HIS | - | expression tag | UNP Q9UYX8 |
| E | -4 | HIS | - | expression tag | UNP Q9UYX8 |
| E | -3 | HIS | - | expression tag | UNP Q9UYX8 |
| E | -2 | HIS | - | expression tag | UNP Q9UYX8 |
| E | -1 | GLY | - | expression tag | UNP Q9UYX8 |
| E | 0 | SER | - | expression tag | UNP Q9UYX8 |

- Molecule 5 is a protein called DP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | B | 1191 | 9525 | 6096 | 1633 | 1755 | 41 | 0 | 0 |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 6 | A | 2 | 2 | 2 | 0 |
| 6 | B | 1 | 1 | 1 | 0 |

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

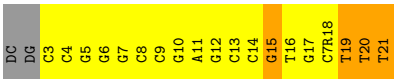
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 7 | B | 3 | 3 | 3 | 0 |

# 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: DNA (5'-D(P*CP*CP*GP*GP*GP*CP*CP*GP*AP*GP*CP*CP*GP*TP*(GS)P*(C7R)P*(PST)P*(PST)P*(PST))-3')

Chain P:

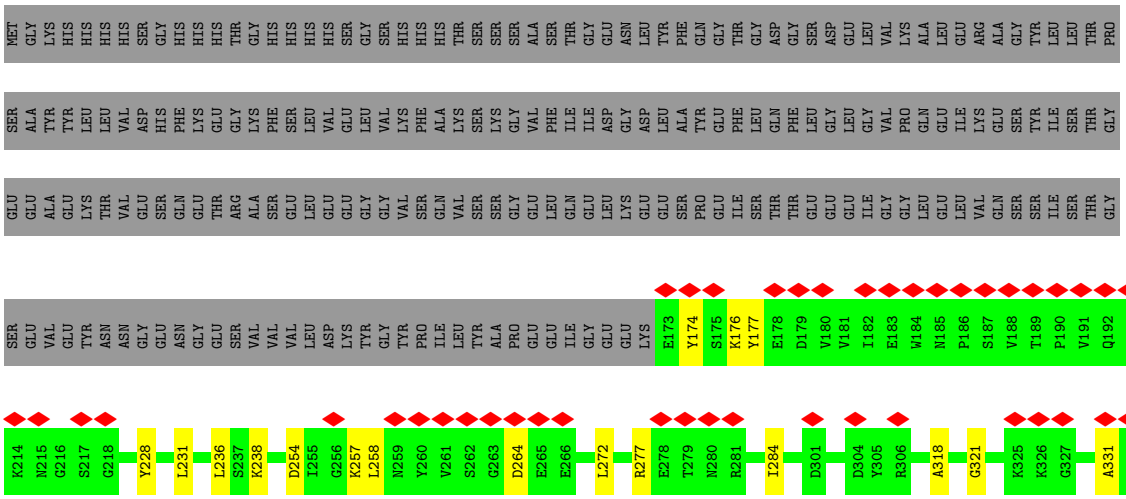



• Molecule 2: DNA (5'-D(P*AP*GP*CP*AP*CP*GP*GP*CP*TP*CP*GP*GP*CP*CP*CP*GP*G)-3')

Chain T:

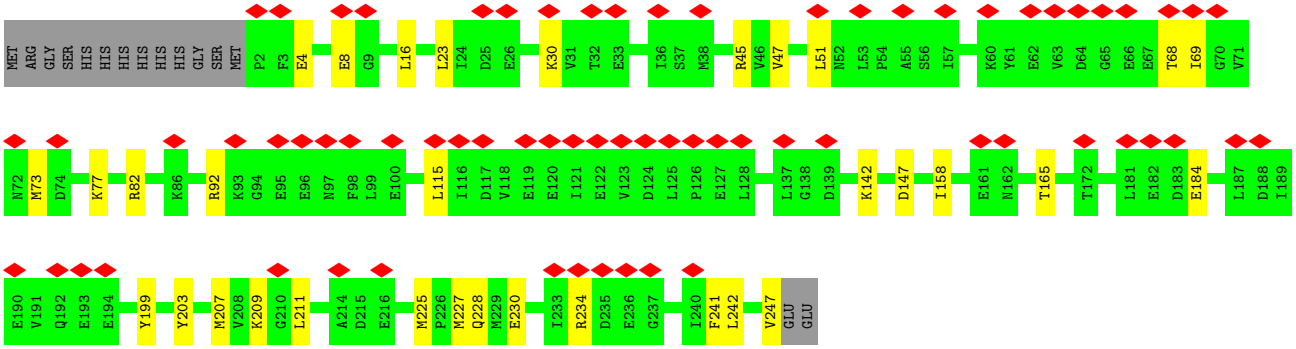
• Molecule 3: DNA polymerase II small subunit

Chain A:



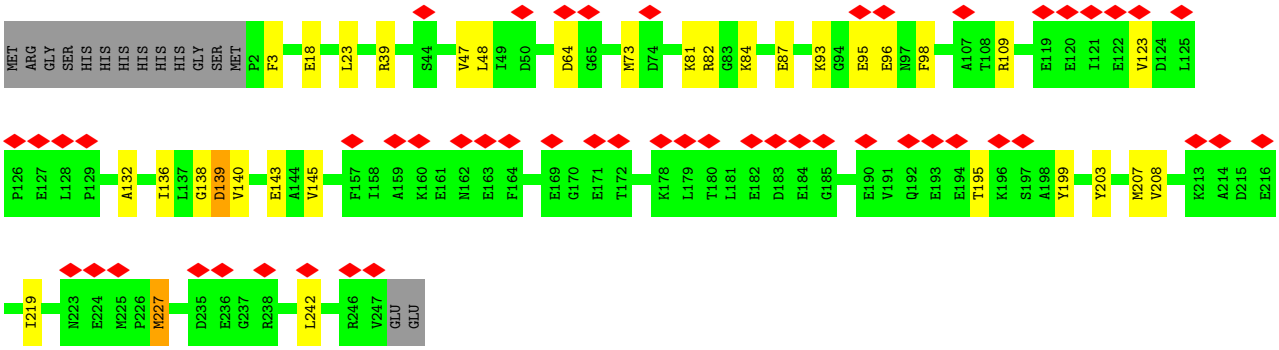
• Molecule 4: DNA polymerase sliding clamp

Chain C:



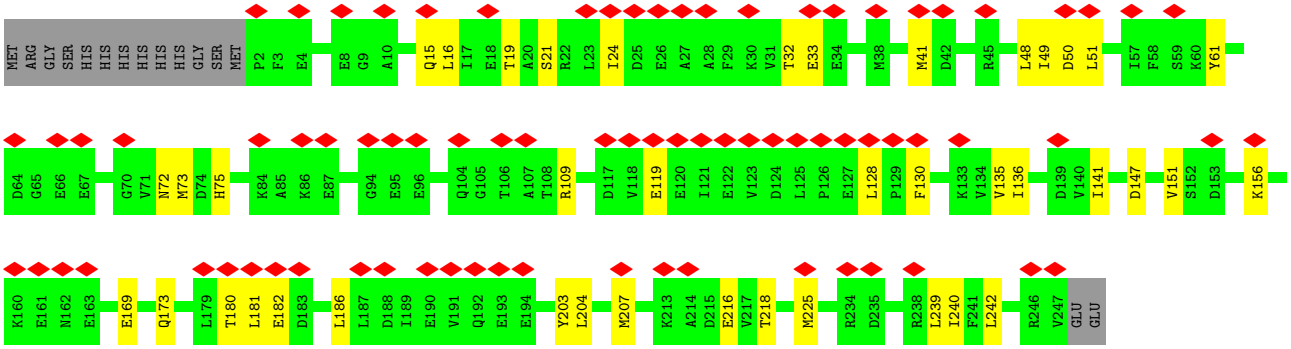

• Molecule 4: DNA polymerase sliding clamp

Chain D:




• Molecule 4: DNA polymerase sliding clamp

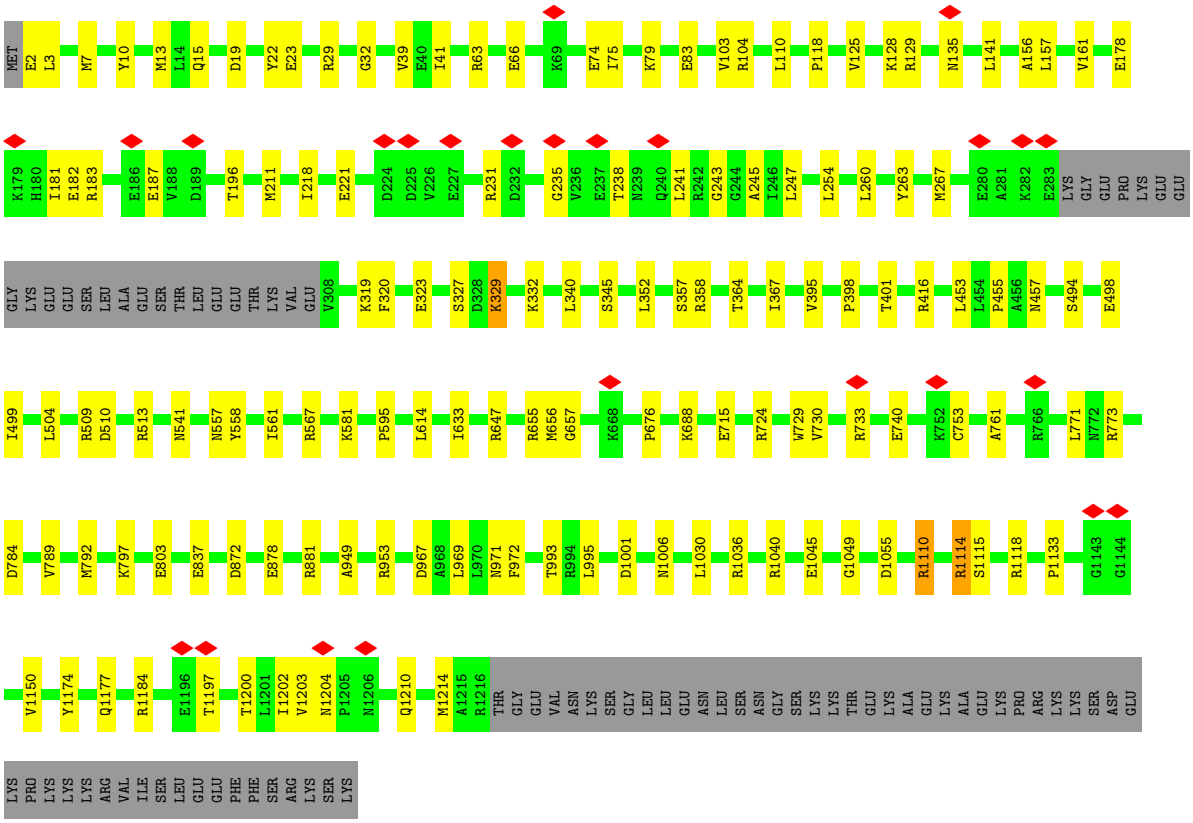
Chain E:




• Molecule 5: DP2

Chain B:

82%
11%
6%


MET E2 L3 M7 Y10 M13 L14 Q15 D19 Y22 E23 R29 G32 V39 E40 I41 R63 E66 K69 E74 I75 K79 E83 V103 R104 L110 P118 V125 K128 R129 N135 L141 A156 L157 V161 E178
K179 H180 I181 E182 R183 E186 E187 V188 D189 T196 M211 I218 E221 D224 D225 V226 E227 R231 D232 G235 V236 E237 T238 N239 Q240 L241 R242 G243 G244 A245 I246 L247 L254 L260 Y263 M267 E280 A281 K282 E283 LYS GLY GLU PRO LYS GLU GLU
GLY LYS GLU GLU SER LEU ALA GLU SER THR LEU GLU GLU THR LYS VAL GLU V308 K319 F320 E323 S327 D328 K329 K332 L340 S345 L352 S357 R358 T364 I367 V395 P398 T401 R416 L453 L454 P455 A456 N457 S494 E498
I499 L504 R509 D510 R513 N541 N557 Y558 I561 R567 K581 P595 L614 I633 R647 R655 M656 G657 K668 P676 K688 E715 R724 W729 V730 R733 E740 K752 C753 A761 R766 L771 N772 R773
D784 V789 M792 K797 E803 E837 D872 E878 R881 A949 R953 D967 A968 L969 L970 N971 F972 T993 R994 L995 D1001 N1006 L1030 R1036 R1040 E1045 G1049 D1055 R1110 R1114 S1115 R1118 P1133 G1143 G1144
V1150 Y1174 Q1177 R1184 E1196 T1197 T1200 L1201 I1202 V1203 N1204 P1205 N1206 Q1210 M1214 A1215 R1216 THR GLY GLU VAL ASN LYS SER GLY LEU LEU GLU ASN LEU SER ASN GLY SER LYS LYS THR GLU LYS ALA GLU LYS ALA GLU LYS PRO ARG LYS LYS SER ASP GLU
LYS PRO LYS LYS LYS ARG VAL ILE SER LEU GLU GLU PHE PHE SER ARG LYS SER LYS

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 306575 | 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 ($e^-/Å^2$) | 40 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 2.058 | Depositor |
| Minimum map value | -1.234 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.037 | Depositor |
| Recommended contour level | 0.2 | Depositor |
| Map size (Å) | 344.0, 344.0, 344.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.86, 0.86, 0.86 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GS, PST, ZN, C7R

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 | P | 0.20 | 0/321 | 0.43 | 1/493 (0.2%) |
| 2 | T | 0.24 | 0/389 | 0.49 | 0/598 |
| 3 | A | 0.13 | 0/3653 | 0.31 | 0/4960 |
| 4 | C | 0.10 | 0/1964 | 0.28 | 0/2642 |
| 4 | D | 0.14 | 0/1964 | 0.34 | 0/2642 |
| 4 | E | 0.12 | 0/1964 | 0.31 | 0/2642 |
| 5 | B | 0.18 | 0/9728 | 0.32 | 0/13146 |
| All | All | 0.16 | 0/19983 | 0.32 | 1/27123 (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 |
|---|---|---|---|
| 5 | B | 0 | 2 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | P | 15 | DG | O3'-P-O5' | 5.89 | 112.83 | 104.00 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | B | 1110 | ARG | Sidechain |
| 5 | B | 1114 | 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 | P | 388 | 0 | 204 | 54 | 0 |
| 2 | T | 348 | 0 | 190 | 30 | 0 |
| 3 | A | 3565 | 0 | 3620 | 36 | 0 |
| 4 | C | 1939 | 0 | 1977 | 23 | 0 |
| 4 | D | 1939 | 0 | 1977 | 20 | 0 |
| 4 | E | 1939 | 0 | 1977 | 28 | 0 |
| 5 | B | 9525 | 0 | 9636 | 89 | 0 |
| 6 | A | 2 | 0 | 0 | 0 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 7 | B | 3 | 0 | 0 | 0 | 0 |
| All | All | 19649 | 0 | 19581 | 265 | 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 7.

All (265) 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:P:20:PST:P | 1:P:20:PST:SP | 1.48 | 1.47 |
| 1:P:21:PST:P | 1:P:21:PST:SP | 1.48 | 1.47 |
| 1:P:19:PST:SP | 1:P:19:PST:P | 1.48 | 1.47 |
| 1:P:17:GS:S2P | 1:P:17:GS:P | 1.48 | 1.46 |
| 1:P:18:C7R:SP2 | 1:P:18:C7R:P | 1.48 | 1.46 |
| 2:T:7:DT:H73 | 2:T:8:DG:O4' | 1.62 | 0.98 |
| 2:T:7:DT:H73 | 2:T:8:DG:C5' | 1.97 | 0.94 |
| 2:T:7:DT:H6 | 2:T:8:DG:H5" | 1.35 | 0.90 |
| 2:T:7:DT:H73 | 2:T:8:DG:C4' | 2.02 | 0.87 |
| 3:A:369:CYS:HG | 3:A:619:CYS:HG | 1.01 | 0.87 |
| 2:T:7:DT:C6 | 2:T:8:DG:H5" | 2.14 | 0.83 |
| 1:P:8:DC:H4' | 1:P:9:DC:OP1 | 1.83 | 0.79 |
| 3:A:369:CYS:CB | 3:A:619:CYS:HG | 1.96 | 0.78 |
| 1:P:9:DC:H5" | 1:P:9:DC:H6 | 1.49 | 0.77 |
| 2:T:8:DG:H4' | 2:T:8:DG:OP1 | 1.84 | 0.76 |
| 4:E:48:LEU:HB2 | 4:E:242:LEU:HB3 | 1.71 | 0.73 |
| 1:P:18:C7R:O3' | 1:P:19:PST:SP | 2.48 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:19:PST:H3' | 1:P:20:PST:SP | 2.29 | 0.72 |
| 1:P:20:PST:O3' | 1:P:21:PST:SP | 2.49 | 0.71 |
| 1:P:12:DG:H2' | 1:P:13:DC:C6 | 2.26 | 0.71 |
| 2:T:7:DT:C7 | 2:T:8:DG:C5' | 2.68 | 0.70 |
| 1:P:18:C7R:SP2 | 1:P:18:C7R:O5' | 2.49 | 0.70 |
| 5:B:729:TRP:NE1 | 5:B:740:GLU:OE1 | 2.23 | 0.70 |
| 1:P:19:PST:O3' | 1:P:20:PST:SP | 2.50 | 0.70 |
| 1:P:16:DT:O3' | 1:P:17:GS:S2P | 2.49 | 0.70 |
| 2:T:15:DT:H2" | 2:T:16:DC:O5' | 1.91 | 0.70 |
| 1:P:17:GS:S2P | 1:P:17:GS:O5' | 2.49 | 0.69 |
| 5:B:498:GLU:O | 5:B:567:ARG:NH2 | 2.25 | 0.69 |
| 5:B:1040:ARG:NH1 | 5:B:1049:GLY:O | 2.26 | 0.68 |
| 1:P:17:GS:O3' | 1:P:18:C7R:SP2 | 2.49 | 0.68 |
| 4:C:45:ARG:NH1 | 5:B:1202:ILE:O | 2.27 | 0.68 |
| 2:T:22:DG:H2" | 2:T:23:DG:C8 | 2.28 | 0.67 |
| 1:P:21:PST:SP | 1:P:21:PST:O5' | 2.49 | 0.67 |
| 1:P:19:PST:SP | 1:P:19:PST:O5' | 2.50 | 0.67 |
| 1:P:20:PST:SP | 1:P:20:PST:O5' | 2.50 | 0.66 |
| 2:T:7:DT:C7 | 2:T:8:DG:O4' | 2.41 | 0.66 |
| 1:P:16:DT:C3' | 1:P:17:GS:S2P | 2.84 | 0.65 |
| 2:T:7:DT:H73 | 2:T:8:DG:H5' | 1.78 | 0.65 |
| 1:P:14:DC:H5" | 1:P:14:DC:H6 | 1.61 | 0.65 |
| 3:A:466:GLU:OE2 | 5:B:1184:ARG:NH1 | 2.28 | 0.65 |
| 5:B:688:LYS:HG2 | 5:B:771:LEU:HD21 | 1.79 | 0.64 |
| 1:P:9:DC:H5" | 1:P:9:DC:C6 | 2.33 | 0.64 |
| 1:P:7:DG:C8 | 1:P:7:DG:H5' | 2.32 | 0.64 |
| 1:P:19:PST:C3' | 1:P:20:PST:SP | 2.85 | 0.64 |
| 4:D:82:ARG:HD2 | 4:E:147:ASP:OD1 | 1.98 | 0.64 |
| 1:P:13:DC:H2" | 1:P:14:DC:H5" | 1.79 | 0.63 |
| 5:B:32:GLY:O | 5:B:724:ARG:NH1 | 2.32 | 0.63 |
| 5:B:803:GLU:N | 5:B:803:GLU:OE1 | 2.31 | 0.63 |
| 4:C:184:GLU:N | 4:C:184:GLU:OE2 | 2.32 | 0.63 |
| 2:T:15:DT:H4' | 2:T:16:DC:OP1 | 1.98 | 0.61 |
| 4:C:228:GLN:NE2 | 4:C:230:GLU:OE2 | 2.23 | 0.61 |
| 3:A:318:ALA:HB3 | 3:A:335:TYR:HB2 | 1.81 | 0.61 |
| 1:P:13:DC:C2' | 1:P:14:DC:H5" | 2.30 | 0.61 |
| 4:C:16:LEU:HD21 | 4:C:51:LEU:HD21 | 1.81 | 0.61 |
| 4:E:182:GLU:OE1 | 4:E:182:GLU:N | 2.25 | 0.60 |
| 4:E:15:GLN:O | 4:E:19:THR:HG23 | 2.01 | 0.60 |
| 5:B:352:LEU:O | 5:B:457:ASN:ND2 | 2.35 | 0.60 |
| 5:B:401:THR:CG2 | 5:B:1055:ASP:O | 2.50 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:16:DT:H3' | 1:P:17:GS:S2P | 2.42 | 0.60 |
| 4:E:203:TYR:O | 4:E:207:MET:HG3 | 2.02 | 0.59 |
| 2:T:7:DT:C7 | 2:T:8:DG:H5' | 2.33 | 0.59 |
| 4:C:147:ASP:OD2 | 4:E:109:ARG:NH1 | 2.28 | 0.59 |
| 2:T:17:DG:H2" | 2:T:18:DG:C8 | 2.38 | 0.59 |
| 1:P:21:PST:H1' | 3:A:592:ILE:CD1 | 2.33 | 0.59 |
| 5:B:75:ILE:O | 5:B:79:LYS:HG2 | 2.02 | 0.59 |
| 3:A:321:GLY:HA3 | 3:A:331:ALA:HA | 1.84 | 0.59 |
| 4:C:142:LYS:NZ | 4:C:211:LEU:O | 2.27 | 0.58 |
| 5:B:792:MET:O | 5:B:797:LYS:NZ | 2.36 | 0.58 |
| 4:E:151:VAL:HG23 | 4:E:173:GLN:HB2 | 1.86 | 0.58 |
| 4:D:84:LYS:HB2 | 4:D:87:GLU:HG3 | 1.85 | 0.58 |
| 4:E:41:MET:HA | 4:E:41:MET:HE2 | 1.86 | 0.58 |
| 1:P:9:DC:H2" | 1:P:10:DG:C8 | 2.39 | 0.58 |
| 2:T:7:DT:H3' | 2:T:8:DG:H5" | 1.85 | 0.58 |
| 2:T:18:DG:H1' | 2:T:19:DC:H5" | 1.84 | 0.58 |
| 3:A:423:ASP:OD1 | 5:B:1177:GLN:NE2 | 2.31 | 0.58 |
| 3:A:254:ASP:HB3 | 3:A:257:LYS:HG2 | 1.86 | 0.58 |
| 5:B:401:THR:HG23 | 5:B:1055:ASP:O | 2.04 | 0.58 |
| 1:P:14:DC:H2' | 1:P:15:DG:C8 | 2.38 | 0.57 |
| 4:D:145:VAL:HG11 | 4:D:208:VAL:HG21 | 1.85 | 0.57 |
| 3:A:228:TYR:HB3 | 5:B:1133:PRO:HG3 | 1.86 | 0.57 |
| 4:C:82:ARG:NH2 | 4:D:143:GLU:OE1 | 2.36 | 0.57 |
| 1:P:6:DG:H2" | 1:P:7:DG:C8 | 2.39 | 0.57 |
| 2:T:11:DC:H2" | 2:T:12:DG:O5' | 2.04 | 0.57 |
| 4:D:73:MET:HA | 4:D:73:MET:HE2 | 1.86 | 0.57 |
| 4:E:181:LEU:HD13 | 4:E:186:LEU:HD23 | 1.85 | 0.57 |
| 5:B:541:ASN:OD1 | 5:B:633:ILE:HG13 | 2.05 | 0.57 |
| 4:E:33:GLU:OE2 | 4:E:33:GLU:N | 2.32 | 0.57 |
| 4:E:48:LEU:HD13 | 4:E:242:LEU:HD22 | 1.87 | 0.57 |
| 4:D:23:LEU:HD22 | 4:D:47:VAL:HG21 | 1.87 | 0.56 |
| 4:D:132:ALA:HB2 | 4:D:195:THR:HG21 | 1.87 | 0.56 |
| 1:P:5:DG:H2" | 1:P:6:DG:C8 | 2.40 | 0.56 |
| 3:A:384:VAL:HG21 | 3:A:390:GLU:HB2 | 1.88 | 0.55 |
| 5:B:358:ARG:NH2 | 5:B:837:GLU:OE2 | 2.30 | 0.55 |
| 5:B:221:GLU:N | 5:B:221:GLU:OE1 | 2.40 | 0.55 |
| 3:A:520:MET:HE2 | 3:A:574:LEU:HB3 | 1.89 | 0.54 |
| 1:P:16:DT:H4' | 5:B:1150:VAL:HG22 | 1.89 | 0.54 |
| 4:C:203:TYR:O | 4:C:207:MET:HG2 | 2.08 | 0.54 |
| 1:P:5:DG:H2" | 1:P:6:DG:H8 | 1.73 | 0.54 |
| 5:B:340:LEU:HD12 | 5:B:655:ARG:HB2 | 1.90 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:E:119:GLU:OE1 | 4:E:119:GLU:N | 2.27 | 0.54 |
| 4:D:109:ARG:NH1 | 4:E:147:ASP:OD2 | 2.32 | 0.54 |
| 5:B:104:ARG:NH1 | 5:B:118:PRO:O | 2.40 | 0.53 |
| 5:B:1210:GLN:O | 5:B:1214:MET:HG2 | 2.08 | 0.53 |
| 2:T:19:DC:H2" | 2:T:20:DC:O5' | 2.08 | 0.53 |
| 5:B:730:VAL:HG11 | 5:B:761:ALA:HB2 | 1.90 | 0.53 |
| 1:P:8:DC:H2" | 1:P:9:DC:O5' | 2.09 | 0.53 |
| 1:P:20:PST:H3' | 1:P:21:PST:H73 | 1.91 | 0.53 |
| 5:B:187:GLU:HG2 | 5:B:241:LEU:HD23 | 1.91 | 0.52 |
| 4:C:73:MET:O | 4:C:77:LYS:HG2 | 2.09 | 0.52 |
| 4:E:136:ILE:HD11 | 4:E:141:ILE:HB | 1.90 | 0.52 |
| 5:B:329:LYS:HA | 5:B:332:LYS:HE2 | 1.91 | 0.52 |
| 3:A:174:TYR:HE1 | 3:A:421:ILE:HG23 | 1.74 | 0.52 |
| 1:P:8:DC:H2" | 1:P:9:DC:C5' | 2.39 | 0.52 |
| 1:P:8:DC:H2" | 1:P:9:DC:H5" | 1.91 | 0.51 |
| 3:A:476:ASN:OD1 | 3:A:476:ASN:N | 2.43 | 0.51 |
| 4:C:4:GLU:OE1 | 4:C:92:ARG:NH1 | 2.37 | 0.51 |
| 5:B:967:ASP:OD1 | 5:B:971:ASN:ND2 | 2.41 | 0.51 |
| 5:B:1203:VAL:HG22 | 5:B:1204:ASN:H | 1.76 | 0.51 |
| 4:D:199:TYR:CZ | 4:D:227:MET:HB2 | 2.46 | 0.51 |
| 1:P:17:GS:S2P | 1:P:17:GS:H8 | 2.51 | 0.50 |
| 5:B:243:GLY:O | 5:B:247:LEU:HB2 | 2.11 | 0.50 |
| 5:B:558:TYR:CD1 | 5:B:581:LYS:HD2 | 2.45 | 0.50 |
| 3:A:497:HIS:O | 3:A:559:GLY:N | 2.38 | 0.50 |
| 4:C:199:TYR:CE2 | 4:C:227:MET:HB2 | 2.46 | 0.50 |
| 3:A:579:THR:OG1 | 3:A:580:TRP:N | 2.43 | 0.50 |
| 5:B:110:LEU:HB3 | 5:B:157:LEU:HD23 | 1.93 | 0.50 |
| 5:B:63:ARG:NH2 | 5:B:83:GLU:OE2 | 2.44 | 0.50 |
| 1:P:17:GS:H8 | 1:P:17:GS:C5' | 2.42 | 0.50 |
| 1:P:11:DA:H2" | 1:P:12:DG:O4' | 2.12 | 0.50 |
| 1:P:8:DC:H2' | 1:P:9:DC:C5 | 2.47 | 0.49 |
| 2:T:14:DC:C6 | 2:T:15:DT:H72 | 2.47 | 0.49 |
| 4:E:216:GLU:OE1 | 4:E:216:GLU:N | 2.45 | 0.49 |
| 3:A:231:LEU:HB2 | 3:A:542:ASP:O | 2.13 | 0.49 |
| 5:B:128:LYS:NZ | 5:B:235:GLY:O | 2.41 | 0.49 |
| 2:T:8:DG:H2" | 2:T:9:DC:O5' | 2.13 | 0.49 |
| 4:D:23:LEU:HD11 | 4:D:207:MET:HG2 | 1.95 | 0.49 |
| 5:B:457:ASN:HB3 | 5:B:647:ARG:O | 2.12 | 0.49 |
| 1:P:19:PST:O2 | 1:P:19:PST:C2' | 2.61 | 0.49 |
| 4:C:30:LYS:HD3 | 4:C:68:THR:HG22 | 1.95 | 0.49 |
| 4:C:45:ARG:HH12 | 5:B:1200:THR:HG21 | 1.77 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:B:509:ARG:HH11 | 5:B:509:ARG:HG2 | 1.78 | 0.49 |
| 1:P:14:DC:H2' | 1:P:15:DG:H8 | 1.78 | 0.48 |
| 2:T:19:DC:H2" | 2:T:20:DC:C6 | 2.48 | 0.48 |
| 4:E:32:THR:O | 4:E:61:TYR:OH | 2.29 | 0.48 |
| 3:A:177:TYR:CD2 | 3:A:430:ALA:HB1 | 2.48 | 0.48 |
| 3:A:369:CYS:HB2 | 3:A:619:CYS:SG | 2.54 | 0.48 |
| 4:D:95:GLU:OE1 | 4:D:95:GLU:N | 2.46 | 0.48 |
| 3:A:538:PRO:HB3 | 5:B:1118:ARG:HH21 | 1.79 | 0.48 |
| 1:P:14:DC:H6 | 1:P:14:DC:C5' | 2.26 | 0.47 |
| 3:A:370:GLU:O | 3:A:374:LEU:HG | 2.14 | 0.47 |
| 1:P:21:PST:H1' | 3:A:592:ILE:HD12 | 1.95 | 0.47 |
| 3:A:358:ILE:HG23 | 3:A:580:TRP:HE1 | 1.79 | 0.47 |
| 4:E:130:PHE:HA | 4:E:225:MET:HE1 | 1.96 | 0.47 |
| 5:B:39:VAL:HG11 | 5:B:969:LEU:HD22 | 1.96 | 0.47 |
| 5:B:63:ARG:NE | 5:B:66:GLU:OE2 | 2.48 | 0.47 |
| 5:B:499:ILE:HD11 | 5:B:504:LEU:HD13 | 1.95 | 0.47 |
| 3:A:176:LYS:HB2 | 3:A:430:ALA:HB2 | 1.97 | 0.47 |
| 5:B:715:GLU:OE1 | 5:B:773:ARG:NH2 | 2.48 | 0.47 |
| 4:D:136:ILE:HD11 | 4:D:219:ILE:HD12 | 1.96 | 0.47 |
| 1:P:3:DC:H2" | 1:P:4:DC:C6 | 2.51 | 0.46 |
| 5:B:125:VAL:HG13 | 5:B:141:LEU:HD23 | 1.98 | 0.46 |
| 5:B:156:ALA:HB1 | 5:B:260:LEU:HD22 | 1.98 | 0.46 |
| 5:B:178:GLU:O | 5:B:182:GLU:HG2 | 2.16 | 0.46 |
| 5:B:181:ILE:HA | 5:B:211:MET:HE2 | 1.97 | 0.46 |
| 2:T:21:DC:H2" | 2:T:22:DG:C8 | 2.50 | 0.46 |
| 3:A:369:CYS:CB | 3:A:619:CYS:SG | 3.01 | 0.46 |
| 4:E:16:LEU:HD11 | 4:E:239:LEU:HD13 | 1.98 | 0.46 |
| 5:B:22:TYR:OH | 5:B:41:ILE:O | 2.32 | 0.46 |
| 5:B:878:GLU:OE2 | 5:B:881:ARG:NH2 | 2.43 | 0.46 |
| 5:B:3:LEU:HD23 | 5:B:7:MET:HB3 | 1.98 | 0.46 |
| 1:P:20:PST:O5' | 1:P:20:PST:H6 | 2.15 | 0.46 |
| 2:T:18:DG:C2' | 2:T:19:DC:H5" | 2.45 | 0.46 |
| 5:B:63:ARG:NH1 | 5:B:83:GLU:OE1 | 2.49 | 0.46 |
| 2:T:22:DG:H2" | 2:T:23:DG:N7 | 2.31 | 0.45 |
| 4:C:242:LEU:HD23 | 4:C:242:LEU:HA | 1.86 | 0.45 |
| 1:P:18:C7R:C3' | 1:P:19:PST:SP | 3.04 | 0.45 |
| 4:D:203:TYR:O | 4:D:207:MET:HG3 | 2.16 | 0.45 |
| 5:B:10:TYR:OH | 5:B:872:ASP:OD1 | 2.30 | 0.45 |
| 5:B:453:LEU:HD11 | 5:B:1030:LEU:HD21 | 1.98 | 0.45 |
| 5:B:1040:ARG:HD3 | 5:B:1045:GLU:O | 2.17 | 0.45 |
| 5:B:129:ARG:NH1 | 5:B:135:ASN:O | 2.48 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:B:949:ALA:HB1 | 5:B:1001:ASP:HB2 | 1.99 | 0.45 |
| 3:A:518:LEU:HB2 | 3:A:519:PRO:HD3 | 1.98 | 0.45 |
| 3:A:236:LEU:HD12 | 3:A:272:LEU:HG | 1.98 | 0.44 |
| 4:C:69:ILE:HG23 | 4:C:115:LEU:HD11 | 1.99 | 0.44 |
| 4:C:225:MET:HE3 | 4:C:225:MET:HB2 | 1.83 | 0.44 |
| 4:E:51:LEU:HD23 | 4:E:51:LEU:HA | 1.79 | 0.44 |
| 5:B:2:GLU:HB3 | 5:B:3:LEU:H | 1.58 | 0.44 |
| 2:T:21:DC:H2" | 2:T:22:DG:H8 | 1.82 | 0.44 |
| 3:A:264:ASP:OD1 | 3:A:264:ASP:N | 2.48 | 0.44 |
| 5:B:733:ARG:HD2 | 5:B:753:CYS:SG | 2.58 | 0.44 |
| 4:D:18:GLU:OE2 | 4:D:81:LYS:NZ | 2.47 | 0.44 |
| 3:A:395:ARG:HA | 3:A:395:ARG:HD3 | 1.78 | 0.44 |
| 4:E:156:LYS:NZ | 4:E:169:GLU:OE2 | 2.38 | 0.44 |
| 4:D:64:ASP:OD1 | 4:D:64:ASP:N | 2.48 | 0.44 |
| 2:T:7:DT:C7 | 2:T:8:DG:H5" | 2.46 | 0.43 |
| 4:D:96:GLU:HG3 | 4:D:98:PHE:H | 1.82 | 0.43 |
| 5:B:231:ARG:HG3 | 5:B:231:ARG:HH11 | 1.83 | 0.43 |
| 5:B:784:ASP:OD1 | 5:B:784:ASP:N | 2.37 | 0.43 |
| 3:A:177:TYR:HD2 | 3:A:430:ALA:HB1 | 1.82 | 0.43 |
| 3:A:195:LYS:NZ | 3:A:441:HIS:O | 2.52 | 0.43 |
| 5:B:401:THR:HG21 | 5:B:1055:ASP:O | 2.18 | 0.43 |
| 2:T:18:DG:H2" | 2:T:19:DC:H5" | 1.99 | 0.43 |
| 4:C:158:ILE:HB | 4:C:165:THR:HG23 | 1.99 | 0.43 |
| 5:B:416:ARG:HG3 | 5:B:595:PRO:HG3 | 2.00 | 0.43 |
| 5:B:1110:ARG:HA | 5:B:1110:ARG:HD2 | 1.91 | 0.43 |
| 1:P:16:DT:H2' | 1:P:17:GS:C8 | 2.47 | 0.43 |
| 4:E:24:ILE:HD12 | 4:E:41:MET:H | 1.83 | 0.43 |
| 5:B:345:SER:O | 5:B:345:SER:OG | 2.30 | 0.43 |
| 1:P:17:GS:O5' | 1:P:17:GS:H8 | 2.18 | 0.43 |
| 3:A:238:LYS:NZ | 3:A:545:ASP:O | 2.47 | 0.43 |
| 4:D:48:LEU:HB3 | 4:D:242:LEU:HB3 | 2.00 | 0.43 |
| 5:B:263:TYR:O | 5:B:267:MET:HB2 | 2.19 | 0.43 |
| 5:B:995:LEU:HD23 | 5:B:995:LEU:HA | 1.89 | 0.43 |
| 2:T:20:DC:H4' | 2:T:20:DC:OP1 | 2.18 | 0.43 |
| 4:E:21:SER:HB2 | 4:E:73:MET:HB3 | 2.01 | 0.43 |
| 4:E:135:VAL:HG12 | 4:E:218:THR:HA | 2.01 | 0.43 |
| 4:E:72:ASN:HD21 | 4:E:75:HIS:CG | 2.37 | 0.43 |
| 2:T:18:DG:C1' | 2:T:19:DC:H5" | 2.49 | 0.42 |
| 4:C:247:VAL:N | 5:B:1197:THR:O | 2.52 | 0.42 |
| 5:B:231:ARG:HG3 | 5:B:231:ARG:NH1 | 2.35 | 0.42 |
| 5:B:364:THR:HG22 | 5:B:395:VAL:HB | 2.00 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:B:103:VAL:HG23 | 5:B:161:VAL:HG12 | 2.01 | 0.42 |
| 4:E:180:THR:OG1 | 4:E:181:LEU:N | 2.53 | 0.42 |
| 3:A:277:ARG:HD3 | 3:A:284:ILE:HD12 | 2.01 | 0.42 |
| 5:B:319:LYS:O | 5:B:323:GLU:HG2 | 2.18 | 0.42 |
| 5:B:367:ILE:O | 5:B:398:PRO:HA | 2.19 | 0.42 |
| 3:A:369:CYS:HB2 | 3:A:619:CYS:HG | 1.76 | 0.42 |
| 5:B:13:MET:HE3 | 5:B:13:MET:HB3 | 1.98 | 0.42 |
| 5:B:1030:LEU:HD23 | 5:B:1030:LEU:H | 1.85 | 0.42 |
| 1:P:21:PST:O5' | 1:P:21:PST:H6 | 2.20 | 0.42 |
| 4:E:50:ASP:HB2 | 4:E:240:ILE:HB | 2.02 | 0.42 |
| 4:E:204:LEU:HD23 | 4:E:207:MET:HE2 | 2.01 | 0.42 |
| 5:B:211:MET:HE3 | 5:B:211:MET:HB3 | 1.91 | 0.42 |
| 5:B:557:ASN:HB3 | 5:B:558:TYR:CD2 | 2.55 | 0.42 |
| 5:B:561:ILE:HD13 | 5:B:614:LEU:HD11 | 2.01 | 0.42 |
| 5:B:656:MET:HG2 | 5:B:657:GLY:N | 2.35 | 0.42 |
| 3:A:452:ASP:N | 3:A:452:ASP:OD1 | 2.52 | 0.41 |
| 5:B:254:LEU:HD23 | 5:B:254:LEU:HA | 1.90 | 0.41 |
| 5:B:74:GLU:HB3 | 5:B:267:MET:HG2 | 2.02 | 0.41 |
| 4:C:23:LEU:HG | 4:C:47:VAL:HG11 | 2.01 | 0.41 |
| 4:E:128:LEU:HB2 | 4:E:130:PHE:CE1 | 2.56 | 0.41 |
| 5:B:357:SER:OG | 5:B:358:ARG:N | 2.52 | 0.41 |
| 5:B:320:PHE:CE1 | 5:B:455:PRO:HD2 | 2.55 | 0.41 |
| 4:D:138:GLY:O | 4:D:139:ASP:C | 2.64 | 0.41 |
| 5:B:15:GLN:OE1 | 5:B:993:THR:HG21 | 2.21 | 0.41 |
| 5:B:29:ARG:NH2 | 5:B:972:PHE:O | 2.53 | 0.41 |
| 5:B:218:ILE:HG22 | 5:B:245:ALA:HB1 | 2.02 | 0.41 |
| 5:B:510:ASP:OD2 | 5:B:513:ARG:HD2 | 2.21 | 0.41 |
| 4:C:209:LYS:HB3 | 4:C:209:LYS:HE2 | 1.90 | 0.41 |
| 1:P:7:DG:H5' | 1:P:7:DG:H8 | 1.83 | 0.41 |
| 4:C:8:GLU:O | 4:C:234:ARG:NH2 | 2.54 | 0.41 |
| 1:P:12:DG:H2' | 1:P:13:DC:H6 | 1.83 | 0.40 |
| 2:T:8:DG:H2" | 2:T:9:DC:C6 | 2.56 | 0.40 |
| 4:D:39:ARG:HD3 | 4:D:123:VAL:O | 2.21 | 0.40 |
| 5:B:953:ARG:HA | 5:B:953:ARG:HD2 | 1.76 | 0.40 |
| 5:B:1006:ASN:OD1 | 5:B:1036:ARG:NH1 | 2.54 | 0.40 |
| 3:A:409:ILE:HG13 | 5:B:1174:TYR:CE1 | 2.57 | 0.40 |
| 4:C:47:VAL:HA | 4:C:242:LEU:O | 2.21 | 0.40 |
| 5:B:19:ASP:O | 5:B:23:GLU:HG2 | 2.22 | 0.40 |
| 3:A:258:LEU:HD23 | 3:A:258:LEU:HA | 1.89 | 0.40 |
| 4:C:228:GLN:HA | 4:C:241:PHE:O | 2.22 | 0.40 |
| 5:B:676:PRO:HA | 5:B:789:VAL:O | 2.22 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:3:PHE:CE2 | 4:D:93:LYS:HB3 | 2.57 | 0.40 |
| 5:B:183:ARG:NH2 | 5:B:238:THR:O | 2.55 | 0.40 |

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 | |
|---|---|---|---|---|---|---|---|
| 3 | A | 445/662 (67%) | 429 (96%) | 16 (4%) | 0 | 100 | 100 |
| 4 | C | 244/261 (94%) | 238 (98%) | 6 (2%) | 0 | 100 | 100 |
| 4 | D | 244/261 (94%) | 236 (97%) | 8 (3%) | 0 | 100 | 100 |
| 4 | E | 244/261 (94%) | 236 (97%) | 8 (3%) | 0 | 100 | 100 |
| 5 | B | 1187/1270 (94%) | 1135 (96%) | 52 (4%) | 0 | 100 | 100 |
| All | All | 2364/2715 (87%) | 2274 (96%) | 90 (4%) | 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 | |
|---|---|---|---|---|---|---|
| 3 | A | 392/573 (68%) | 392 (100%) | 0 | 100 | 100 |
| 4 | C | 214/227 (94%) | 214 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | D | 214/227 (94%) | 211 (99%) | 3 (1%) | 59 | 79 |
| 4 | E | 214/227 (94%) | 213 (100%) | 1 (0%) | 81 | 88 |
| 5 | B | 1022/1094 (93%) | 1016 (99%) | 6 (1%) | 78 | 87 |
| All | All | 2056/2348 (88%) | 2046 (100%) | 10 (0%) | 78 | 88 |

All (10) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 139 | ASP |
| 4 | D | 140 | VAL |
| 4 | D | 227 | MET |
| 4 | E | 49 | ILE |
| 5 | B | 196 | THR |
| 5 | B | 327 | SER |
| 5 | B | 329 | LYS |
| 5 | B | 494 | SER |
| 5 | B | 1114 | ARG |
| 5 | B | 1115 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | C | 162 | ASN |
| 4 | D | 173 | GLN |
| 4 | E | 72 | ASN |
| 4 | E | 75 | HIS |
| 4 | E | 192 | GLN |
| 5 | B | 130 | ASN |
| 5 | B | 239 | ASN |
| 5 | B | 639 | ASN |
| 5 | B | 777 | ASN |
| 5 | B | 832 | HIS |
| 5 | B | 852 | 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)

5 non-standard protein/DNA/RNA residues 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 | $\#\|Z\| > 2$ |
| 1 | PST | P | 20 | 1 | 18,21,22 | 0.35 | 0 | 26,30,33 | 0.66 | 1 (3%) |
| 1 | PST | P | 19 | 1 | 18,21,22 | 0.42 | 0 | 26,30,33 | 0.74 | 1 (3%) |
| 1 | C7R | P | 18 | 1 | 17,20,21 | 0.34 | 0 | 24,28,31 | 0.38 | 0 |
| 1 | PST | P | 21 | 1,6 | 18,21,22 | 0.33 | 0 | 26,30,33 | 0.64 | 1 (3%) |
| 1 | GS | P | 17 | 2,1 | 21,24,25 | 0.40 | 0 | 31,35,38 | 0.28 | 0 |

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 |
|---|---|---|---|---|---|---|---|
| 1 | PST | P | 20 | 1 | - | 2/7/21/22 | 0/2/2/2 |
| 1 | PST | P | 19 | 1 | - | 2/7/21/22 | 0/2/2/2 |
| 1 | C7R | P | 18 | 1 | - | 0/6/21/22 | 0/2/2/2 |
| 1 | PST | P | 21 | 1,6 | - | 2/7/21/22 | 0/2/2/2 |
| 1 | GS | P | 17 | 2,1 | - | 2/6/21/22 | 0/3/3/3 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | P | 20 | PST | O4-C4-C5 | -2.25 | 122.29 | 124.90 |
| 1 | P | 21 | PST | O4-C4-C5 | -2.17 | 122.39 | 124.90 |
| 1 | P | 19 | PST | O4-C4-C5 | -2.16 | 122.39 | 124.90 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | P | 17 | GS | O4'-C4'-C5'-O5' |
| 1 | P | 17 | GS | C3'-C4'-C5'-O5' |
| 1 | P | 19 | PST | C2'-C1'-N1-C2 |
| 1 | P | 20 | PST | O4'-C4'-C5'-O5' |
| 1 | P | 20 | PST | C3'-C4'-C5'-O5' |
| 1 | P | 19 | PST | C2'-C1'-N1-C6 |
| 1 | P | 21 | PST | O4'-C4'-C5'-O5' |
| 1 | P | 21 | PST | C3'-C4'-C5'-O5' |

There are no ring outliers.

5 monomers are involved in 30 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | P | 20 | PST | 8 | 0 |
| 1 | P | 19 | PST | 8 | 0 |
| 1 | P | 18 | C7R | 5 | 0 |
| 1 | P | 21 | PST | 7 | 0 |
| 1 | P | 17 | GS | 10 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

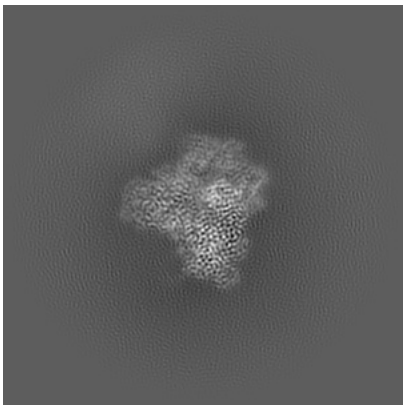
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-17816. These allow visual inspection of the internal detail of the map and identification of artifacts.

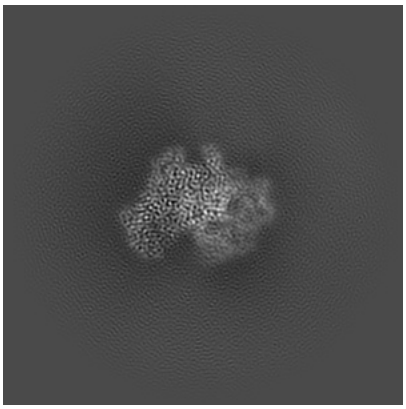
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

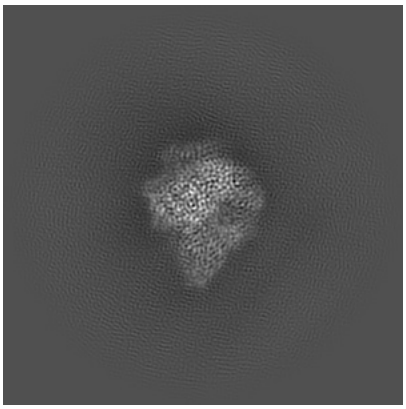
### 6.1.1 Primary map



X

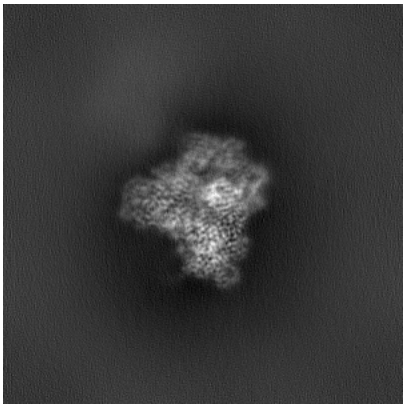


Y

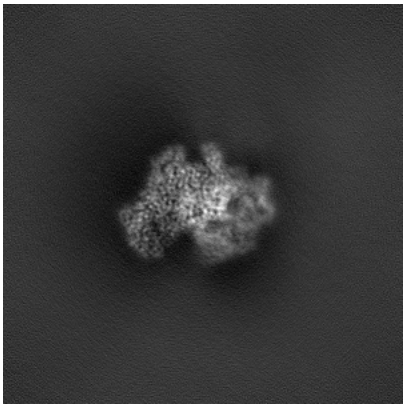


Z

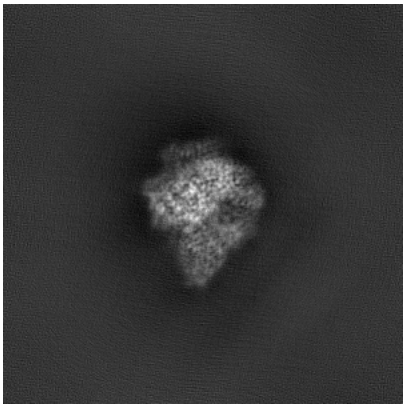
### 6.1.2 Raw map



X



Y

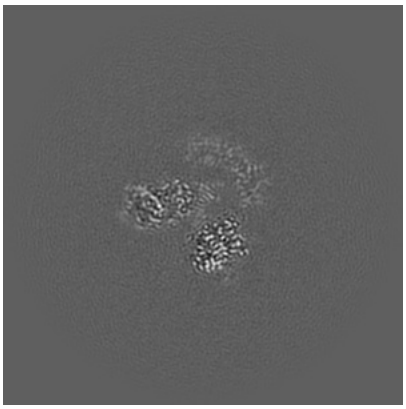


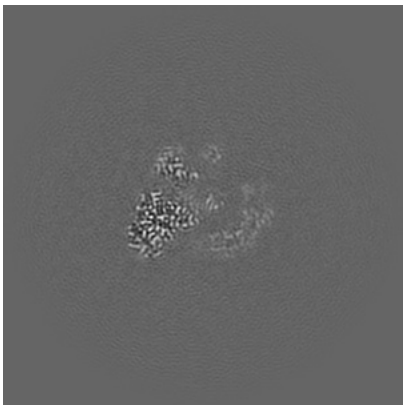
Z

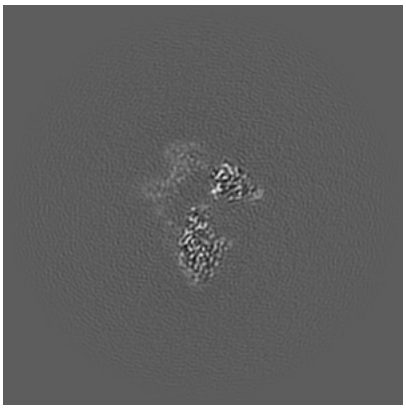
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

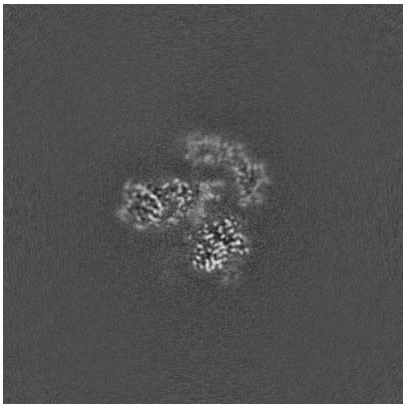
### 6.2.1 Primary map

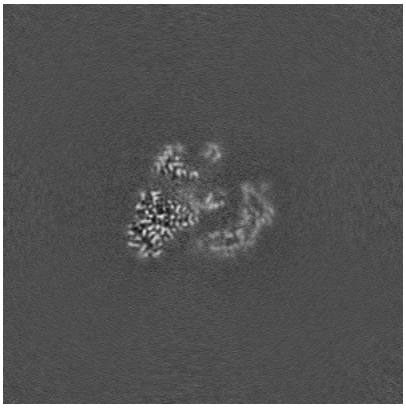

X Index: 200


Y Index: 200


Z Index: 200

### 6.2.2 Raw map


X Index: 200

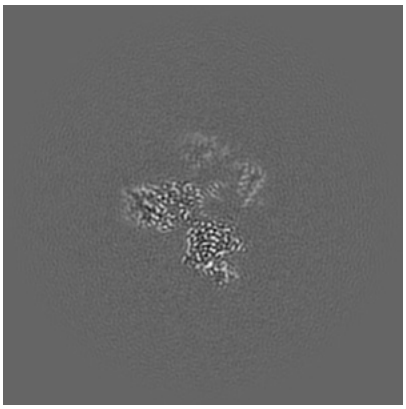

Y Index: 200

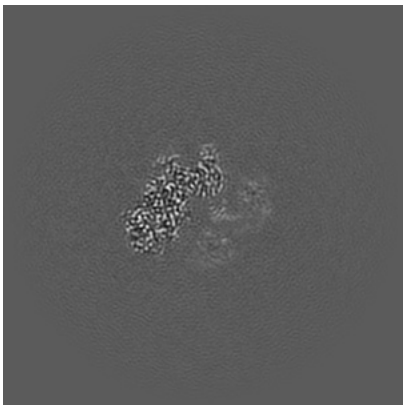
Z Index: 200

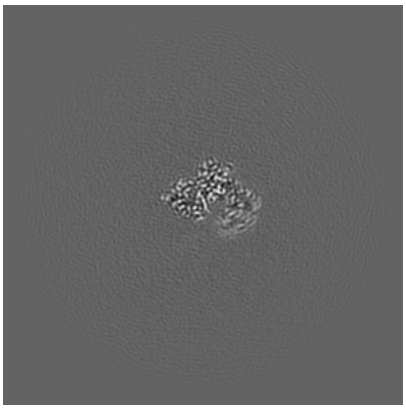
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

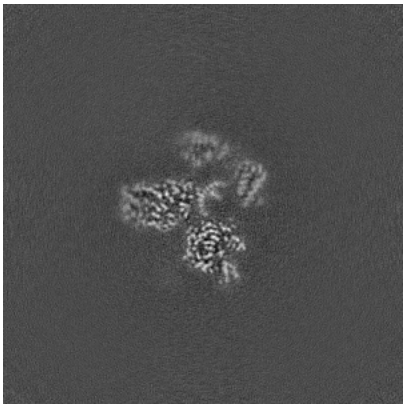
### 6.3.1 Primary map

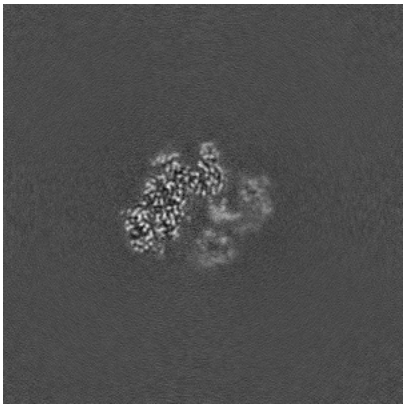

X Index: 195

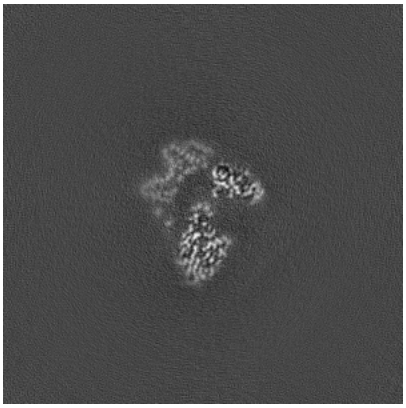

Y Index: 212


Z Index: 166

### 6.3.2 Raw map


X Index: 196

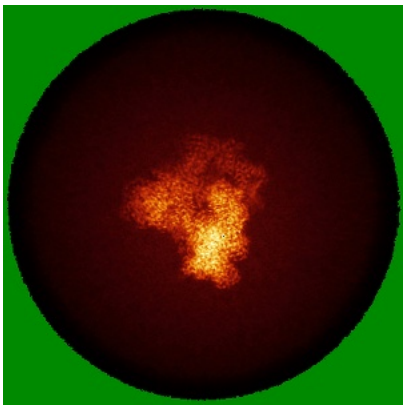

Y Index: 212

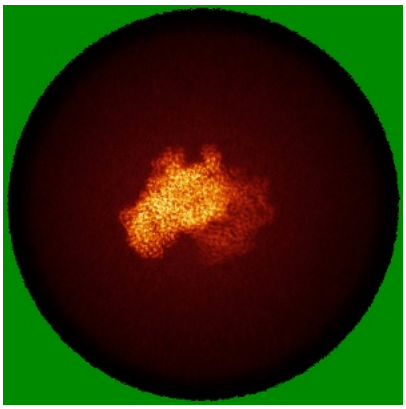

Z Index: 202

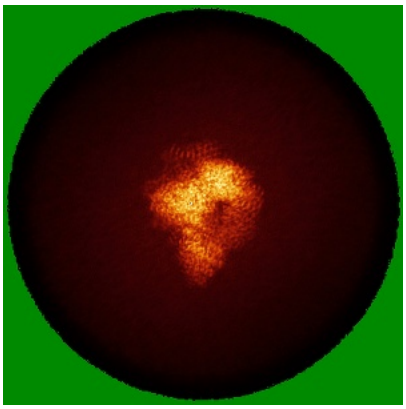
The images above show the largest variance slices of the map in three orthogonal directions.

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

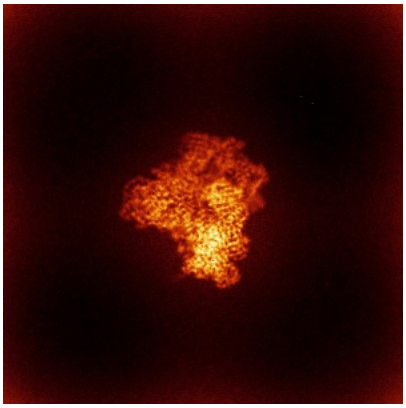
### 6.4.1 Primary map

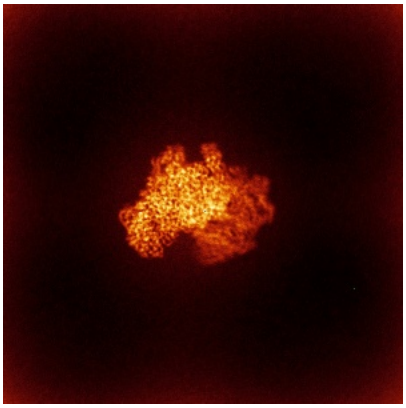

X

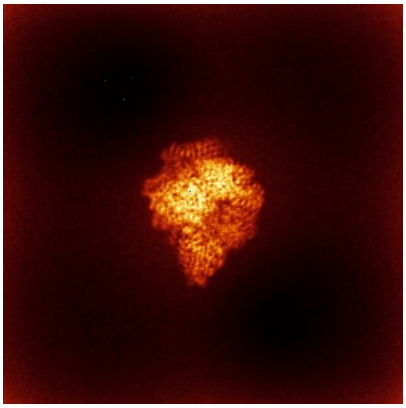

Y


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 0.2. 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.

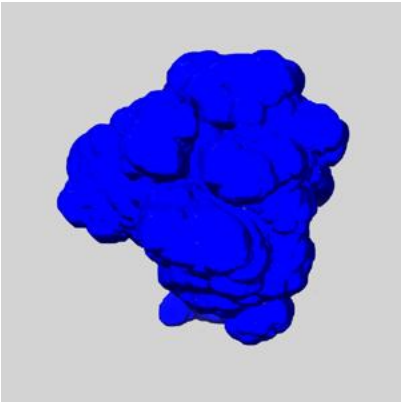
## 6.6 Mask visualisation (i)

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

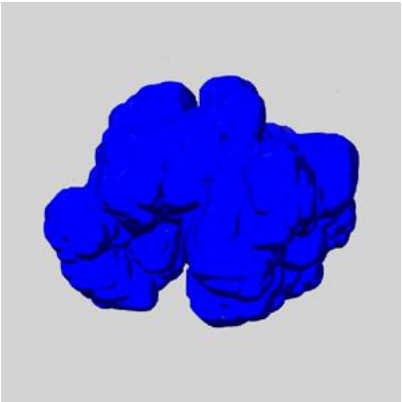
A mask typically either:

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

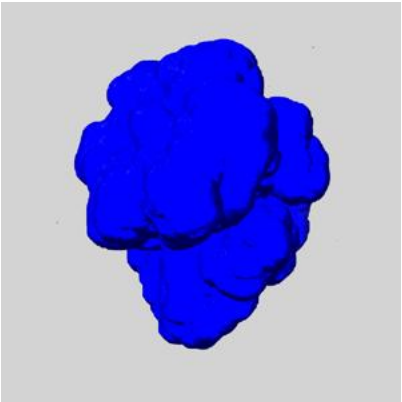
### 6.6.1 emd_17816_msk_1.map (i)



X



Y

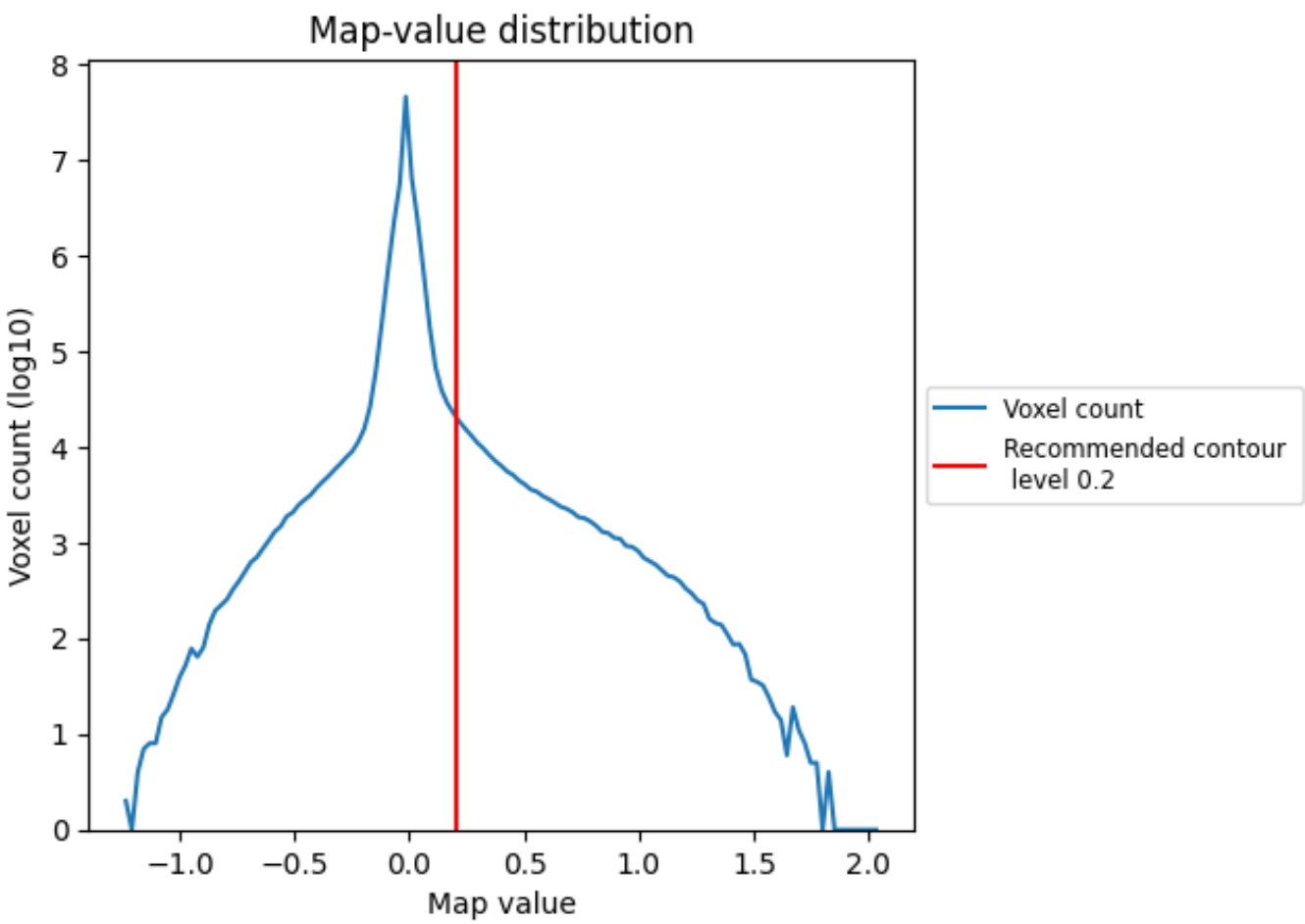


Z

# 7 Map analysis (i)

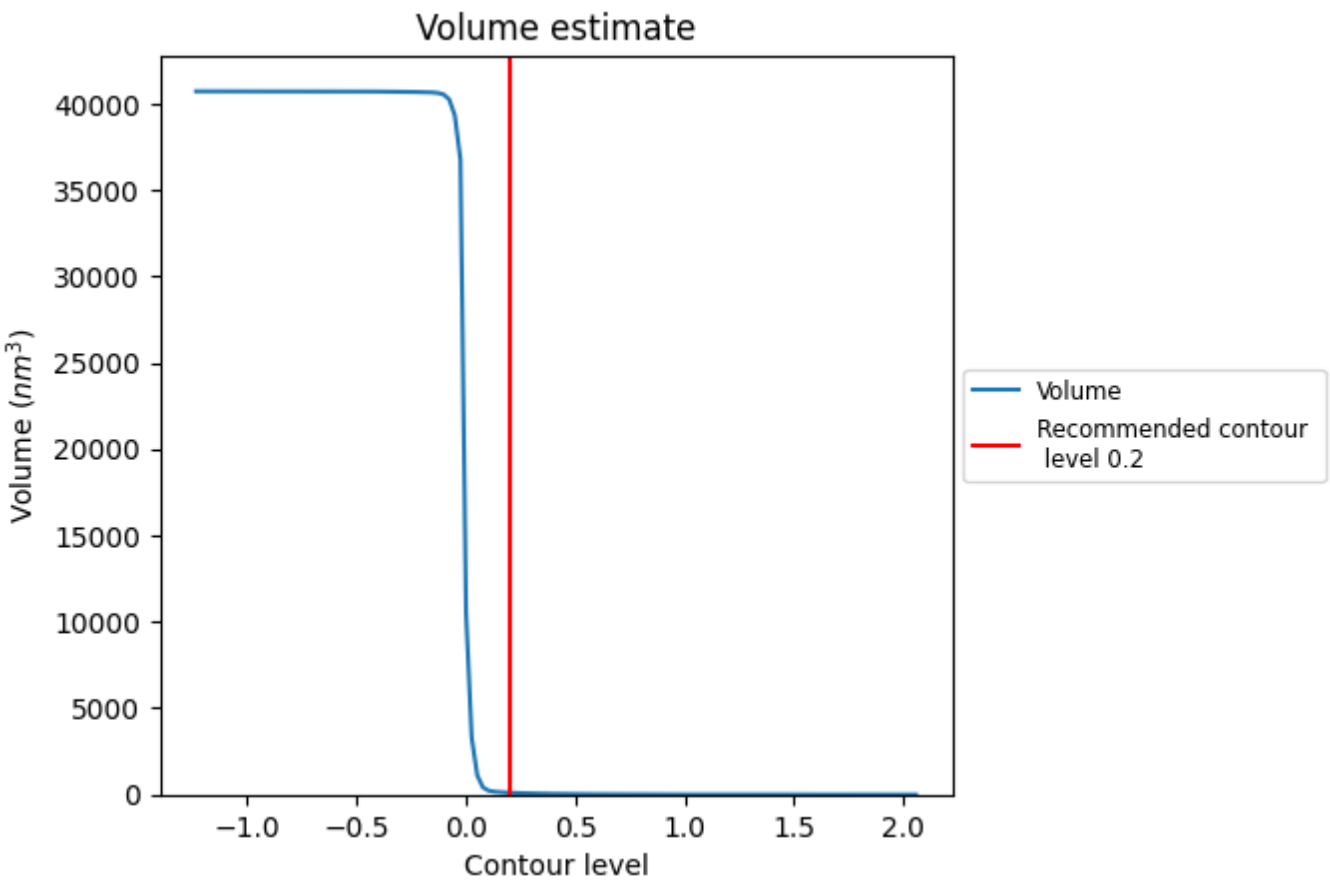
This section contains the results of statistical analysis of the map.

## 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.

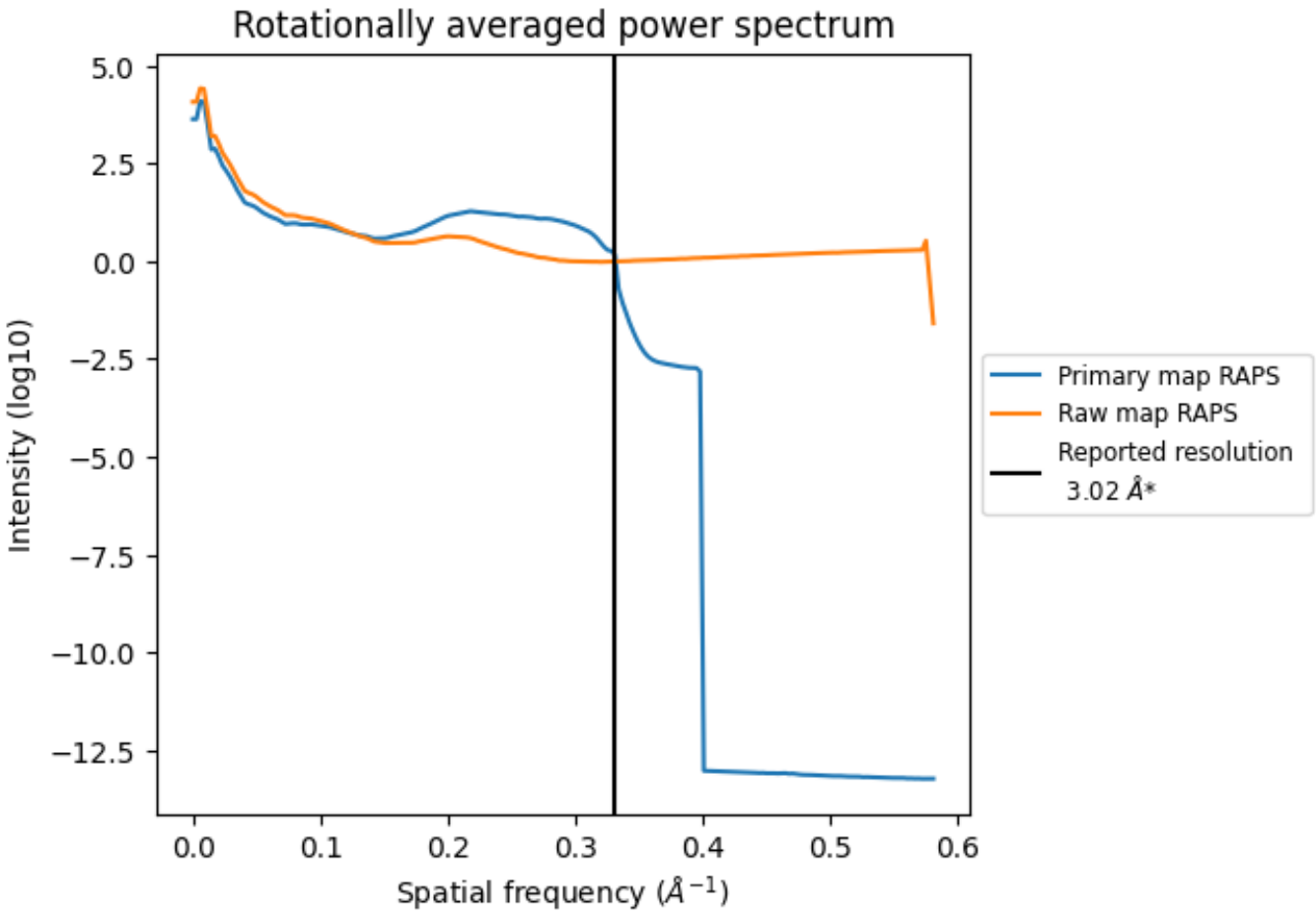
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 105 $nm^3$; this corresponds to an approximate mass of 95 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)

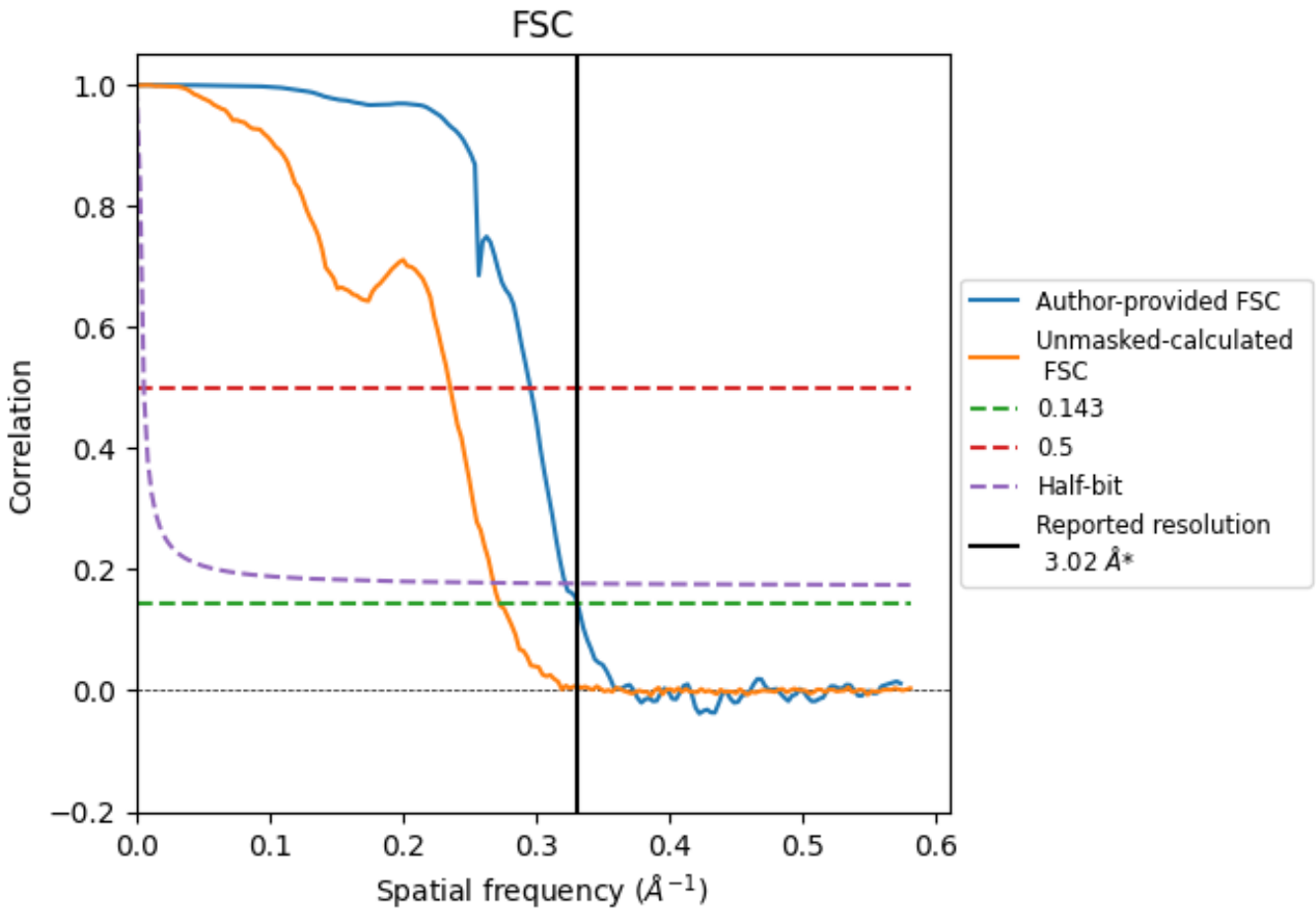



*Reported resolution corresponds to spatial frequency of 0.331 Å$^{-1}$

# 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 0.331 Å$^{-1}$

## 8.2 Resolution estimates (i)

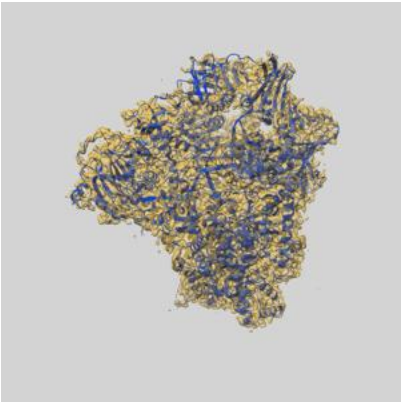
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.02 | - | - |
| Author-provided FSC curve | 3.02 | 3.38 | 3.10 |
| Unmasked-calculated* | 3.67 | 4.24 | 3.72 |

*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 3.67 differs from the reported value 3.02 by more than 10 %

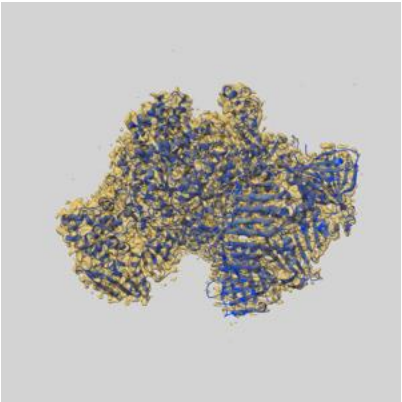
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17816 and PDB model 8PPU. Per-residue inclusion information can be found in section 3 on page 8.

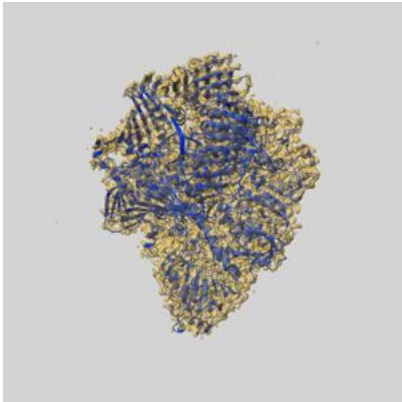
## 9.1 Map-model overlay (i)



X



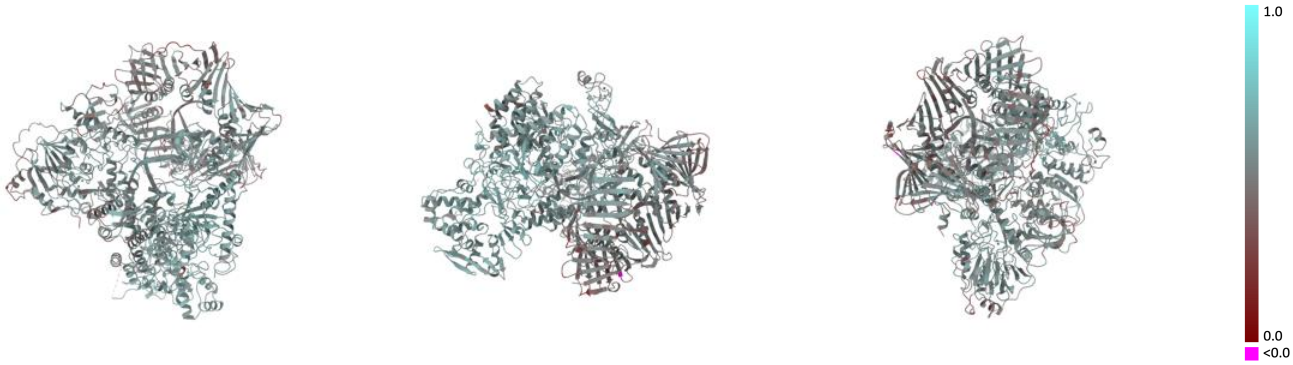
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

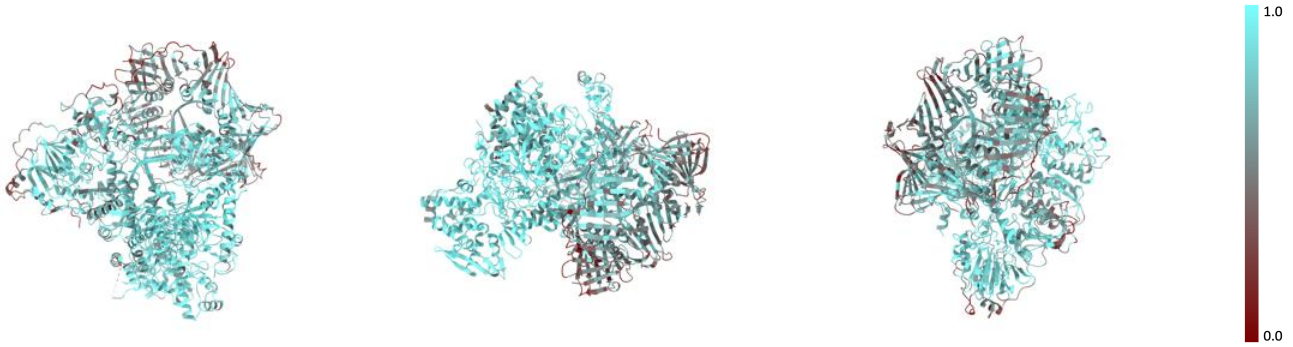
## 9.2 Q-score mapped to coordinate model (i)




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.

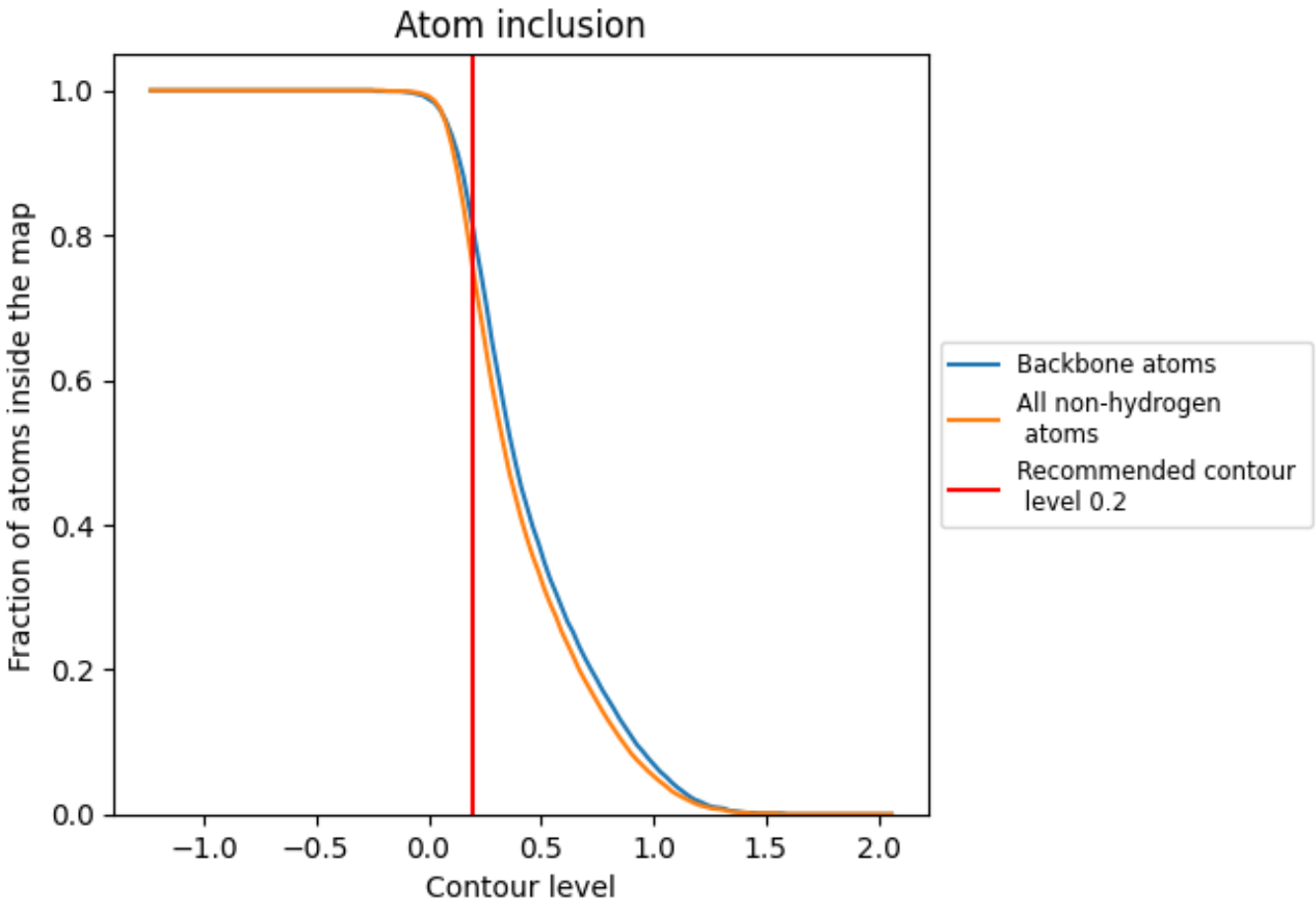
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.2).

## 9.4 Atom inclusion (i)




At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7480 | 0.5320 |
| A | 0.7380 | 0.5240 |
| B | 0.8750 | 0.5730 |
| C | 0.5400 | 0.4760 |
| D | 0.6030 | 0.4890 |
| E | 0.4990 | 0.4590 |
| P | 0.7650 | 0.5090 |
| T | 0.7610 | 0.5020 |