# wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 08:14 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 6T8H |
| EMDB ID | : | EMD-10401 |
| Title | : | Cryo-EM structure of the DNA-bound PolD-PCNA processive complex from P. abyssi |
| Authors | : | Madru, C.; Raia, P.; Hugonneau Beaufet, I.; Pehau-Arnaudet, G.; England, P.; Lindhal, E.; Delarue, M.; Carroni, M.; Sauguet, L. |
| Deposited on | : | 2019-10-24 |
| Resolution | : | 3.77 Å(reported) |

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

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

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

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

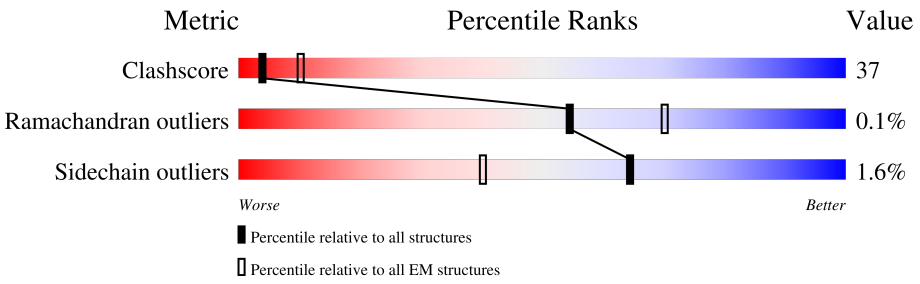
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | C | 261 | 8%, 37%, 57%, • 6% |
| 1 | D | 261 | 11%, 36%, 57%, • 6% |
| 1 | E | 261 | 22%, 36%, 57%, • 6% |
| 2 | A | 619 | 10%, 30%, 38%, 32% |
| 3 | B | 1275 | 8%, 41%, 50%, • 7% |
| 4 | P | 18 | 17%, 72%, 6%, 6% |
| 5 | T | 25 | •, 60%, •, 32% |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19398 atoms, of which 33 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 DNA polymerase sliding clamp.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | E | 246 | 1950 | 1238 | 11 | 308 | 384 | 9 | 0 | 0 |
| 1 | C | 246 | 1950 | 1238 | 11 | 308 | 384 | 9 | 0 | 0 |
| 1 | D | 246 | 1950 | 1238 | 11 | 308 | 384 | 9 | 0 | 0 |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 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 |
| 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 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 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 |

- Molecule 2 is a protein called DNA polymerase II small subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | A | 420 | 3345 | 2178 | 556 | 604 | 7 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 451 | ALA | HIS | engineered mutation | UNP Q9V2F3 |

- Molecule 3 is a protein called DP2 subunit of D-family DNA-polymerase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | B | 1188 | 9501 | 6080 | 1630 | 1750 | 41 | 0 | 0 |

- Molecule 4 is a DNA chain called DNA primer.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | P | 17 | 350 | 163 | 68 | 102 | 17 | 0 | 0 |

- Molecule 5 is a DNA chain called DNA template.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | T | 17 | 347 | 162 | 66 | 102 | 17 | 0 | 0 |

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Fe | |
| 6 | A | 1 | 1 | 1 | 0 |

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

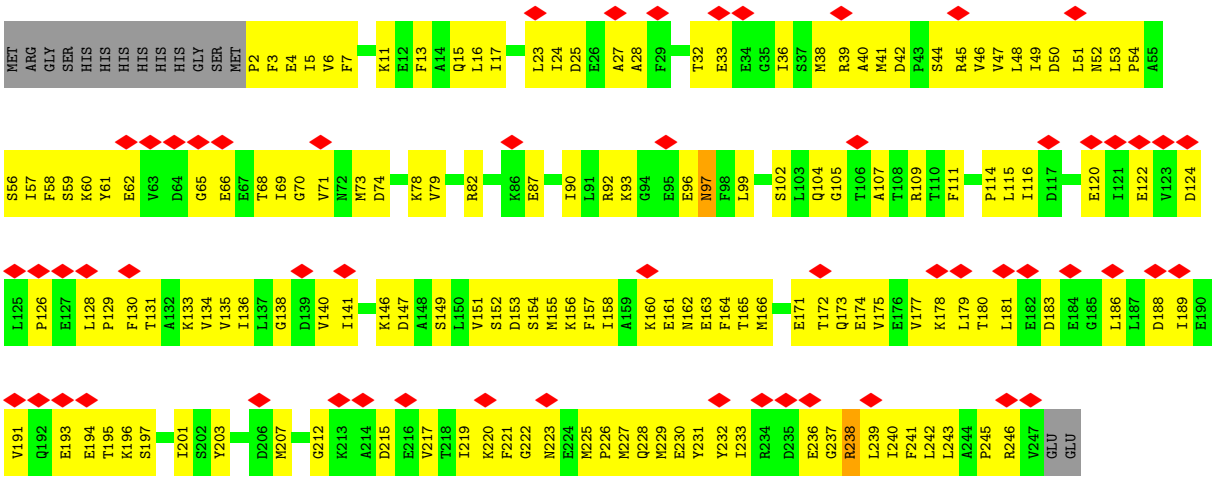
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 7 | A | 1 | 1 | 1 | 0 |
| 7 | B | 3 | 3 | 3 | 0 |

# 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.

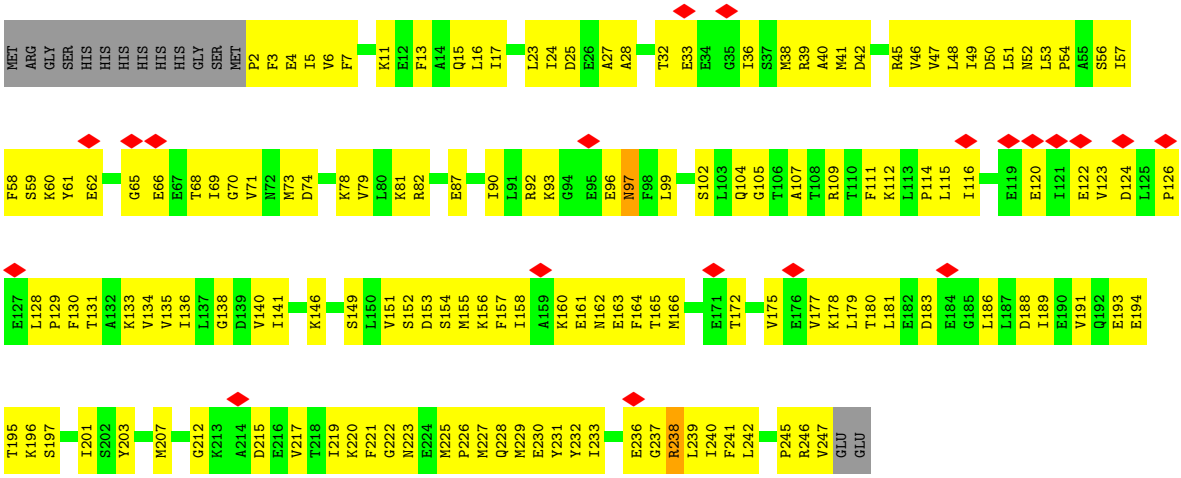
- Molecule 1: DNA polymerase sliding clamp

Chain E:




- Molecule 1: DNA polymerase sliding clamp

Chain C:




- Molecule 1: DNA polymerase sliding clamp

Chain D: 11% 36% 57% • 6%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER MET P2 F3 E4 I5 V6 F7 K11 E12 F13 A14 Q15 L16 I17 L23 I24 D25 E26 A27 A28 T32 E33 I36 S37 M38 R39 A40 M41 D42 P43 S44 R45 V46 V47 L48 I49 D50 L51 N52 L53 P54 A55 S56 I57

F58 S59 K60 Y61 E62 V63 D64 G65 E66 E67 T68 I69 G70 V71 N72 M73 D74 K78 V79 R82 E87 I90 L91 R92 K93 G94 E95 E96 N97 F98 L99 S102 L103 Q104 G105 T106 A107 T108 R109 T110 F111 K112 L113 P114 L115 I116 E119 E120 I121 E122 V123 D124 L125 P126

E127 L128 P129 F130 T131 A132 K133 V134 V135 I136 L137 G138 D139 V140 I141 K146 S149 L150 V151 S152 D153 S154 M155 K156 F157 I158 A159 K160 E161 N162 E163 F164 T165 M166 R167 A168 E171 T172 Q173 E174 V175 E176 V177 K178 L179 T180 L181 E182 D183 E184 G185 L186 L187 D188 I189 E190 V191

Q192 E193 E194 T195 K196 S197 I201 S202 Y203 M207 G212 K213 A214 D215 E216 V217 T218 I219 K220 F221 G222 N223 E224 M225 P226 M227 Q228 M229 E230 Y231 Y232 I233 E236 G237 R238 L239 I240 F241 L242 L243 A244 P245 R246 V247 GLU GLU

• Molecule 2: DNA polymerase II small subunit

Chain A: 10% 30% 38% 32%

MET ASP GLU LEU VAL LYS ALA LEU GLU ARG ALA GLY TYR LEU LEU THR PRO SER ALA TYR TYR LEU LEU VAL ASP HIS PHE LYS GLU GLY LYS PHE SER LEU VAL GLU LEU VAL LYS PHE ALA LYS SER LYS GLY VAL PHE ILE ILE ASP GLY ASP LEU ALA TYR GLU PHE LEU GLN PHE

LEU GLY LEU GLY VAL PRO GLN GLU ILE LYS SER TYR ILE SER THR GLY GLU GLU ALA GLU LYS THR VAL GLU SER GLN GLU THR ARG ALA SER GLU LEU GLU GLU GLY GLY VAL SER GLN VAL SER SER GLY GLU GLU LEU GLN GLU LEU LYS GLU GLU SER PRO GLU ILE SER THR THR

GLU GLU GLU ILE GLY GLY LEU GLU LEU VAL GLN SER SER ILE SER THR GLY SER GLU VAL GLU TYR ASN ASN GLY GLU ASN GLY GLU SER VAL VAL VAL LEU ASP LYS TYR GLY TYR PRO ILE LEU TYR ALA PRO GLU GLU ILE GLY GLU GLU LYS GLU TYR SER LYS TYR GLU ASP VAL

VAL ILE GLU TRP ASN PRO SER VAL THR PRO VAL GLN ILE GLU LYS N196 Y197 K200 F201 D202 V203 R204 Q205 L208 R209 P210 P211 K212 V213 LYS ASN GLY SER G218 K219 E220 I223 I224 V225 E226 A227 Y228 L231 F232 K233 S234 R235 L236 L239 K240 L243 R244 E245 N246

I249 S250 N251 V252 I255 G256 K257 L258 N259 Y260 V261 S262 G263 D264 E265 E266 V267 T268 I269 I270 G271 L272 V273 N274 S275 K276 R277 E278 T279 N280 R281 G282 L283 I284 F285 E286 V287 E288 F297 L298 P299 K300 D301 S302 E303 D304 Y305 R306 E307 A308 F309 K310 V311 L312 A315 V316

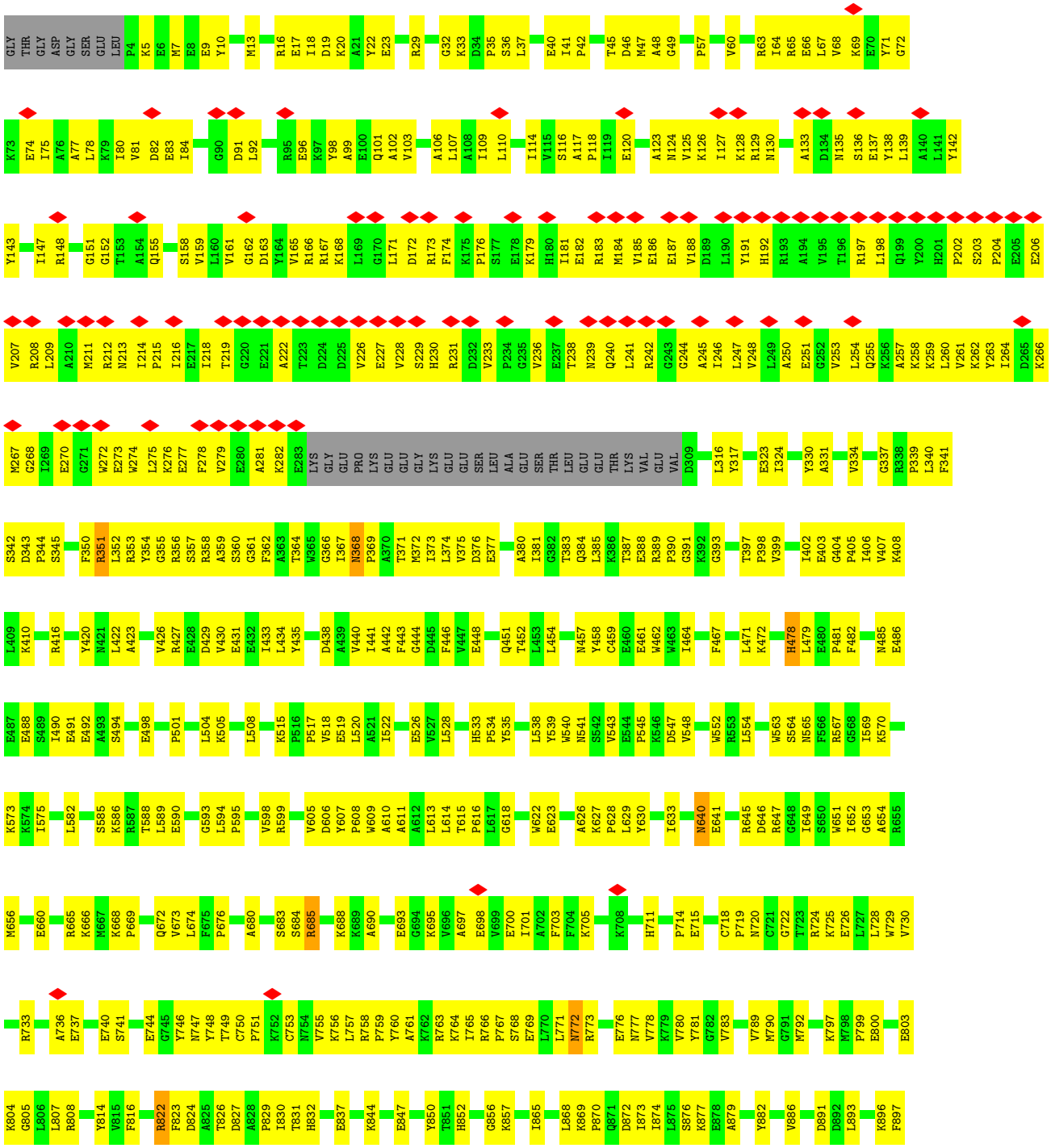
V317 A318 F319 K320 Y323 S324 K325 K326 G327 F330 K333 F334 Y335 L336 P337 D338 V339 P340 L341 Y342 R343 K344 Q345 K346 P347 P348 L349 E350 E351 K352 V353 Y354 A355 I356 L357 I358 S359 D360 I361 H362 V363 G364 S365 R366 E370 L374 K375 F376 L377 E378 W379 L380 N381 V384

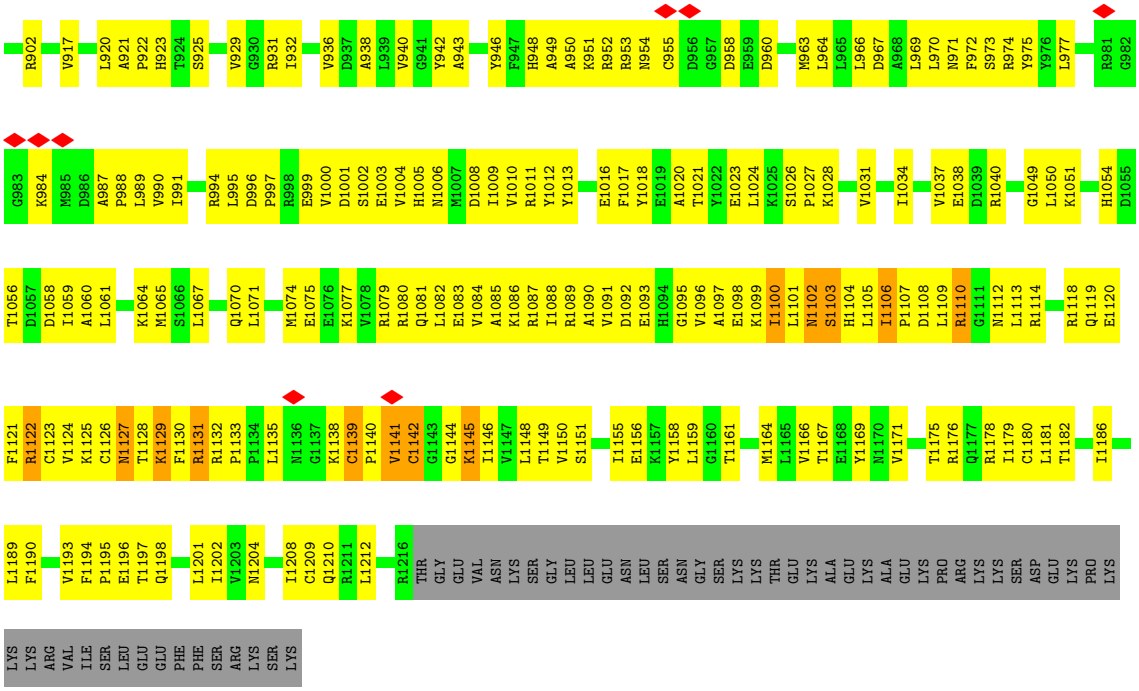
E385 S386 K387 E388 E389 E390 E391 I392 R395 V396 K397 Y398 L399 I400 I401 A402 G403 D404 V405 V406 D407 G408 I409 Q415 D418 L419 V420 I424 F425 D426 Q427 Y428 L431 P439 E440 H441 I442 T443 M444 F445 I446 G447 P448 D452 A453 A457 I458 F463 Y464 K465 E466

Y467 A468 Y472 N476 A477 I478 I479 I480 S481 N482 P483 A484 V485 I486 R487 L488 H489 G490 R491 D492 F493 L494 I495 A496 H497 G498 R499 G500 I501 E502 D503 V504 V505 S506 F507 V508 P509 G510 L511 T512 H513 H514 K515 P516 G517 L518 P519 M520 V521 L524 K525 M526 R527 H528 L529 V537

P538 I539 A540 P541 D542 P543 E544 D545 L546 L547 V548 I549 E550 E551 V552 P553 D554 L555 V556 Q557 M558 G559 H562 V563 Y564 D565 A566 V567 V568 G571 V572 Q573 L574 V575 N576 S577 A578 T579 W580 Q581 A582 Q583 T584 E585 F586 Q587 K588 M589 V590 N591 I592 V593 P594 T595 P596 A597 K598 V599

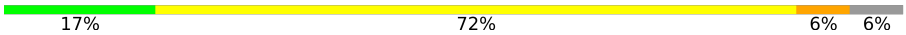
• Molecule 3: DP2 subunit of D-family DNA-polymerase

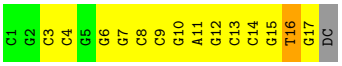





- Molecule 4: DNA primer

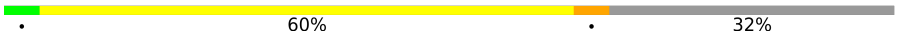
Chain P:

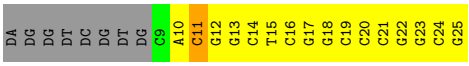



- Molecule 5: DNA template

Chain T:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 149200 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 40 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 3500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 0.108 | Depositor |
| Minimum map value | -0.061 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.014 | Depositor |
| Map size (Å) | 249.0, 249.0, 249.0 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.83, 0.83, 0.83 | 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: FE, ZN

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 | C | 0.40 | 0/1964 | 0.52 | 0/2642 |
| 1 | D | 0.40 | 0/1964 | 0.52 | 0/2642 |
| 1 | E | 0.40 | 0/1964 | 0.52 | 0/2642 |
| 2 | A | 0.50 | 1/3426 (0.0%) | 0.55 | 0/4647 |
| 3 | B | 0.70 | 2/9704 (0.0%) | 0.65 | 2/13112 (0.0%) |
| 4 | P | 1.00 | 0/392 | 1.05 | 2/603 (0.3%) |
| 5 | T | 0.98 | 0/388 | 1.23 | 3/596 (0.5%) |
| All | All | 0.61 | 3/19802 (0.0%) | 0.63 | 7/26884 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 345 | GLN | C-N | -7.33 | 1.17 | 1.34 |
| 3 | B | 882 | TYR | CE1-CZ | -5.25 | 1.31 | 1.38 |
| 3 | B | 1142 | CYS | CB-SG | -5.14 | 1.73 | 1.81 |

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | T | 10 | DA | OP1-P-O3' | -11.69 | 79.47 | 105.20 |
| 5 | T | 10 | DA | OP2-P-O3' | -8.64 | 86.19 | 105.20 |
| 5 | T | 11 | DC | OP1-P-OP2 | 7.95 | 131.52 | 119.60 |
| 4 | P | 16 | DT | N3-C4-O4 | 5.98 | 123.49 | 119.90 |
| 4 | P | 16 | DT | C5-C4-O4 | -5.35 | 121.15 | 124.90 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | C | 1939 | 11 | 1977 | 151 | 0 |
| 1 | D | 1939 | 11 | 1977 | 152 | 0 |
| 1 | E | 1939 | 11 | 1977 | 154 | 0 |
| 2 | A | 3345 | 0 | 3406 | 274 | 0 |
| 3 | B | 9501 | 0 | 9613 | 721 | 0 |
| 4 | P | 350 | 0 | 189 | 27 | 0 |
| 5 | T | 347 | 0 | 189 | 14 | 0 |
| 6 | A | 1 | 0 | 0 | 0 | 0 |
| 7 | A | 1 | 0 | 0 | 0 | 0 |
| 7 | B | 3 | 0 | 0 | 0 | 0 |
| All | All | 19365 | 33 | 19328 | 1445 | 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 37.

The worst 5 of 1445 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:B:1106:ILE:HD11 | 3:B:1179:ILE:CD1 | 1.21 | 1.63 |
| 2:A:223:ILE:HD11 | 3:B:1194:PHE:CE1 | 1.36 | 1.59 |
| 3:B:1103:SER:O | 3:B:1107:PRO:CD | 1.70 | 1.39 |
| 3:B:1106:ILE:CD1 | 3:B:1179:ILE:HD11 | 0.91 | 1.39 |
| 3:B:1106:ILE:CD1 | 3:B:1179:ILE:CD1 | 1.82 | 1.37 |

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 | C | 244/261 (94%) | 232 (95%) | 12 (5%) | 0 | 100 | 100 |
| 1 | D | 244/261 (94%) | 233 (96%) | 11 (4%) | 0 | 100 | 100 |
| 1 | E | 244/261 (94%) | 233 (96%) | 11 (4%) | 0 | 100 | 100 |
| 2 | A | 416/619 (67%) | 381 (92%) | 34 (8%) | 1 (0%) | 47 | 78 |
| 3 | B | 1184/1275 (93%) | 1049 (89%) | 133 (11%) | 2 (0%) | 47 | 78 |
| All | All | 2332/2677 (87%) | 2128 (91%) | 201 (9%) | 3 (0%) | 54 | 83 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 1131 | ARG |
| 3 | B | 1127 | ASN |
| 2 | A | 225 | VAL |

### 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 | C | 214/227 (94%) | 211 (99%) | 3 (1%) | 67 | 82 |
| 1 | D | 214/227 (94%) | 210 (98%) | 4 (2%) | 57 | 76 |
| 1 | E | 214/227 (94%) | 211 (99%) | 3 (1%) | 67 | 82 |
| 2 | A | 366/539 (68%) | 365 (100%) | 1 (0%) | 92 | 96 |
| 3 | B | 1019/1096 (93%) | 997 (98%) | 22 (2%) | 52 | 73 |
| All | All | 2027/2316 (88%) | 1994 (98%) | 33 (2%) | 64 | 80 |

5 of 33 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 238 | ARG |
| 1 | D | 52 | ASN |
| 1 | D | 238 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 772 | ASN |
| 3 | B | 747 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 747 | ASN |
| 1 | D | 52 | ASN |
| 3 | B | 852 | HIS |
| 1 | D | 223 | ASN |
| 1 | C | 97 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 2 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 345:GLN | C | 346:LYS | N | 1.17 |

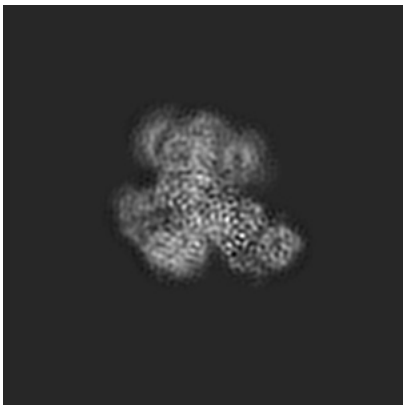
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10401. These allow visual inspection of the internal detail of the map and identification of artifacts.

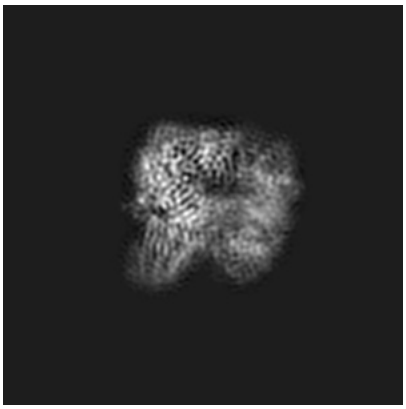
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

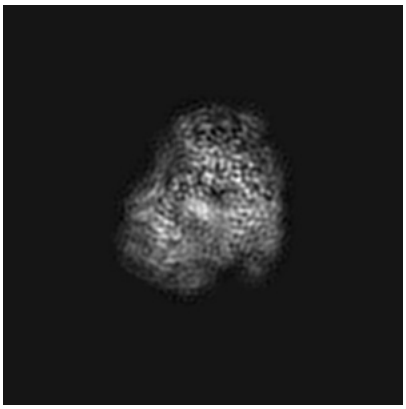
### 6.1.1 Primary map



X

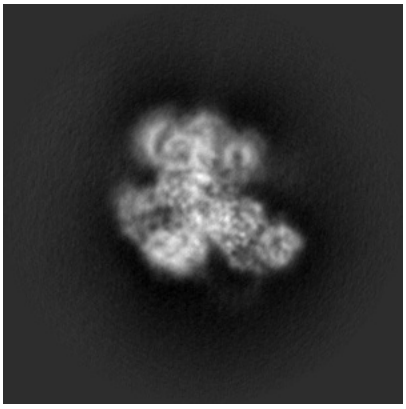


Y

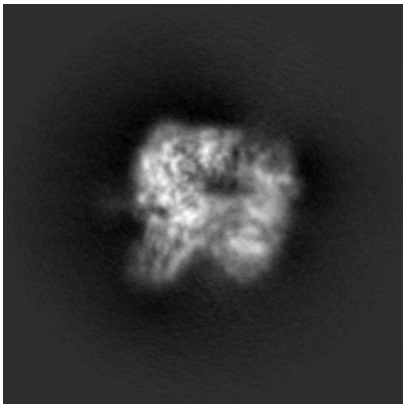


Z

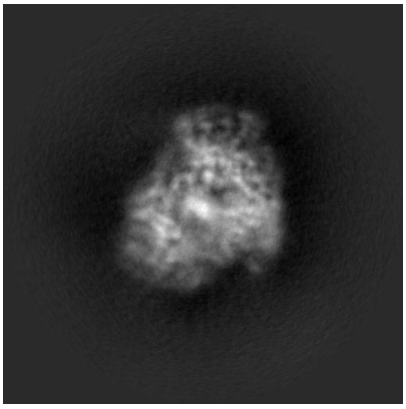
### 6.1.2 Raw map



X



Y

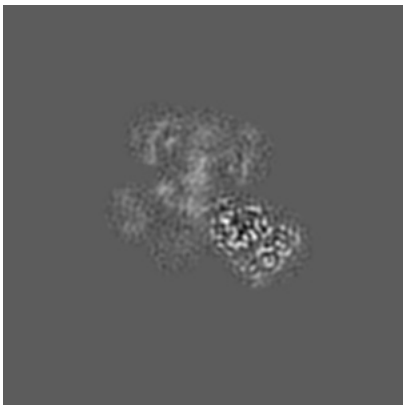


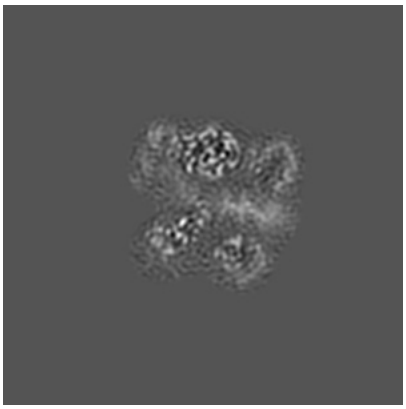
Z

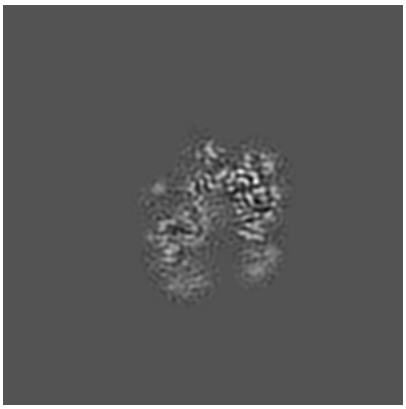
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

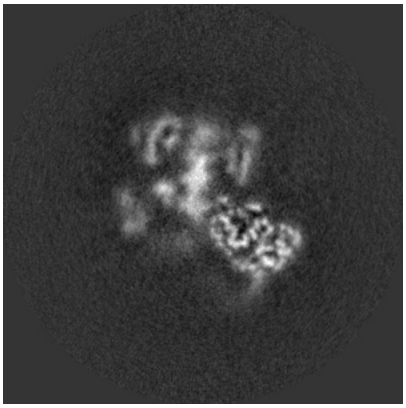
### 6.2.1 Primary map

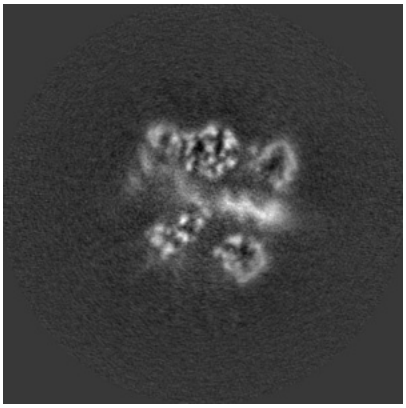

X Index: 150

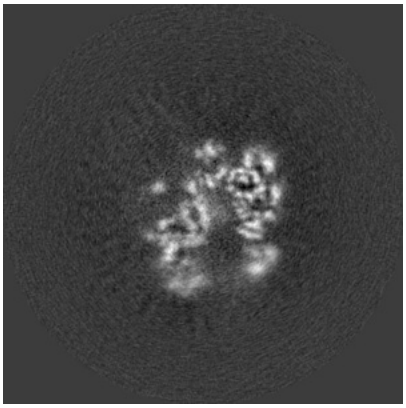

Y Index: 150


Z Index: 150

### 6.2.2 Raw map


X Index: 150

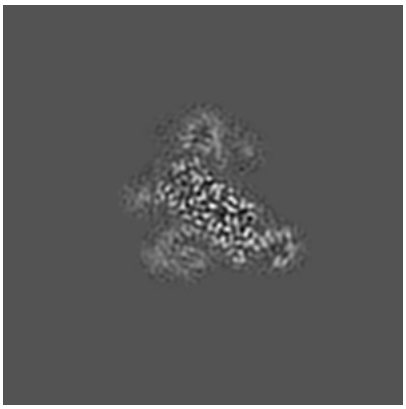

Y Index: 150


Z Index: 150

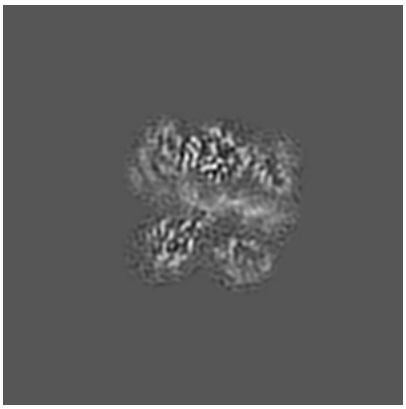
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

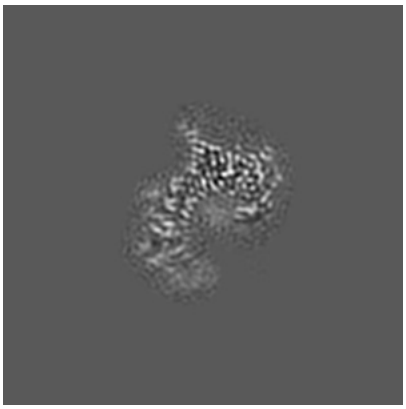
### 6.3.1 Primary map



X Index: 183

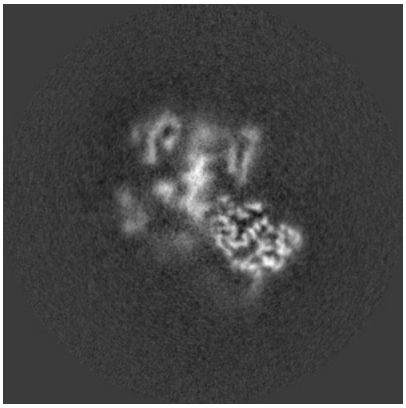


Y Index: 145

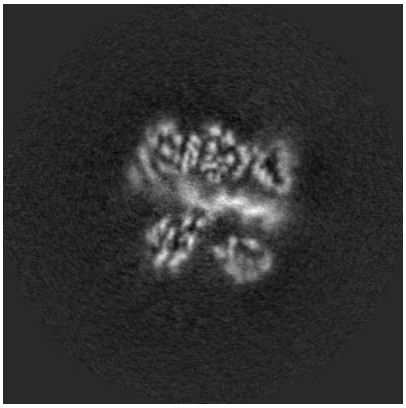


Z Index: 137

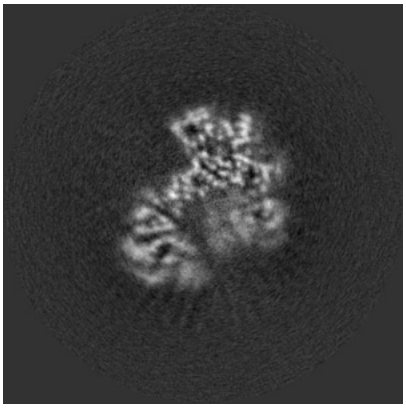
### 6.3.2 Raw map



X Index: 151



Y Index: 145

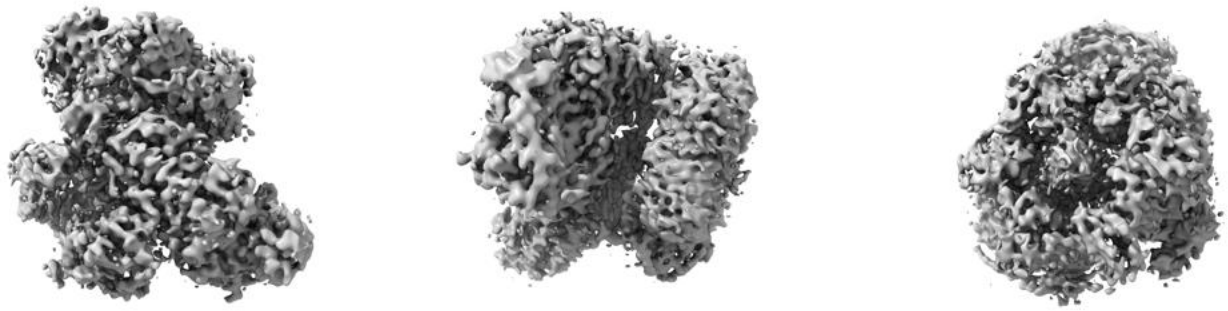


Z Index: 128

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

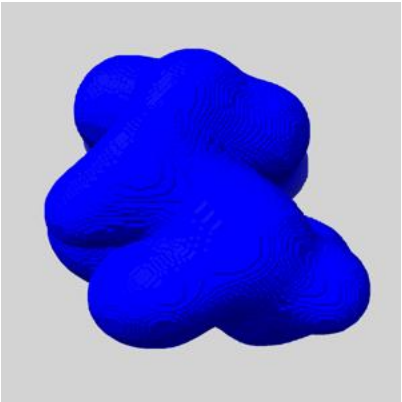
## 6.5 Mask visualisation (i)

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

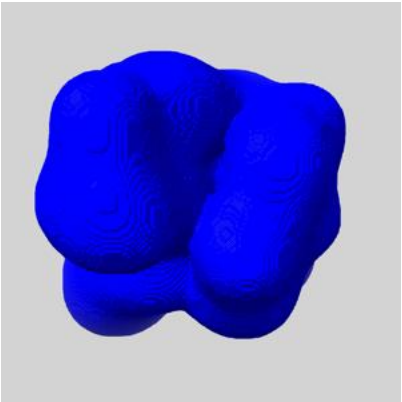
A mask typically either:

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

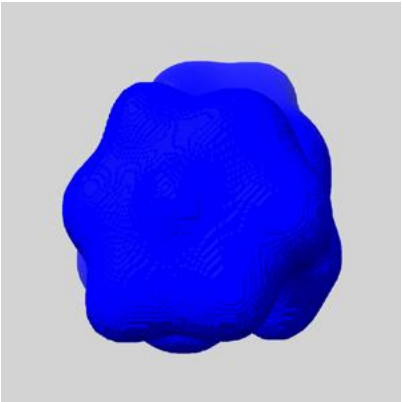
### 6.5.1 emd_10401_msk_1.map (i)



X



Y

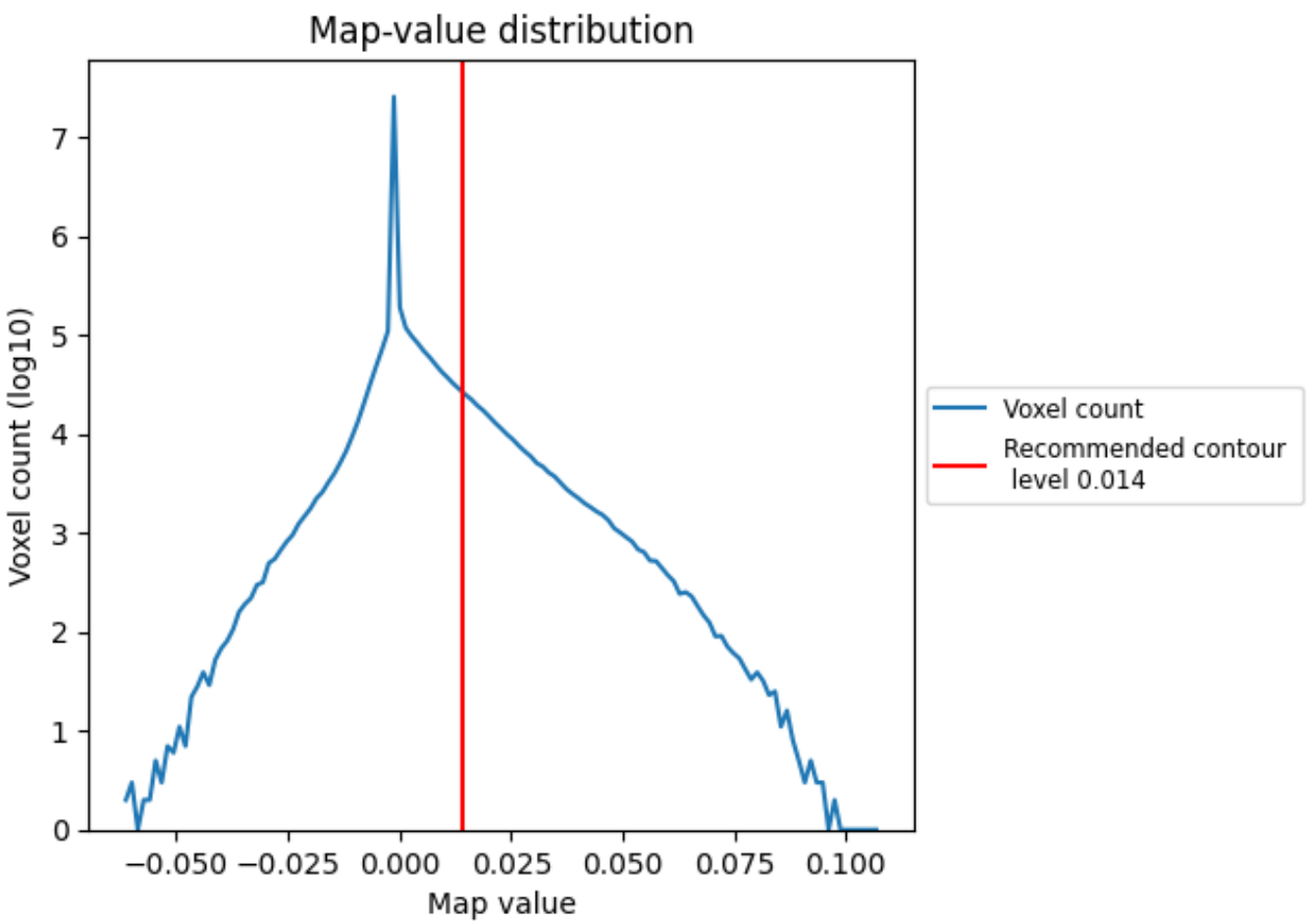


Z

# 7 Map analysis (i)

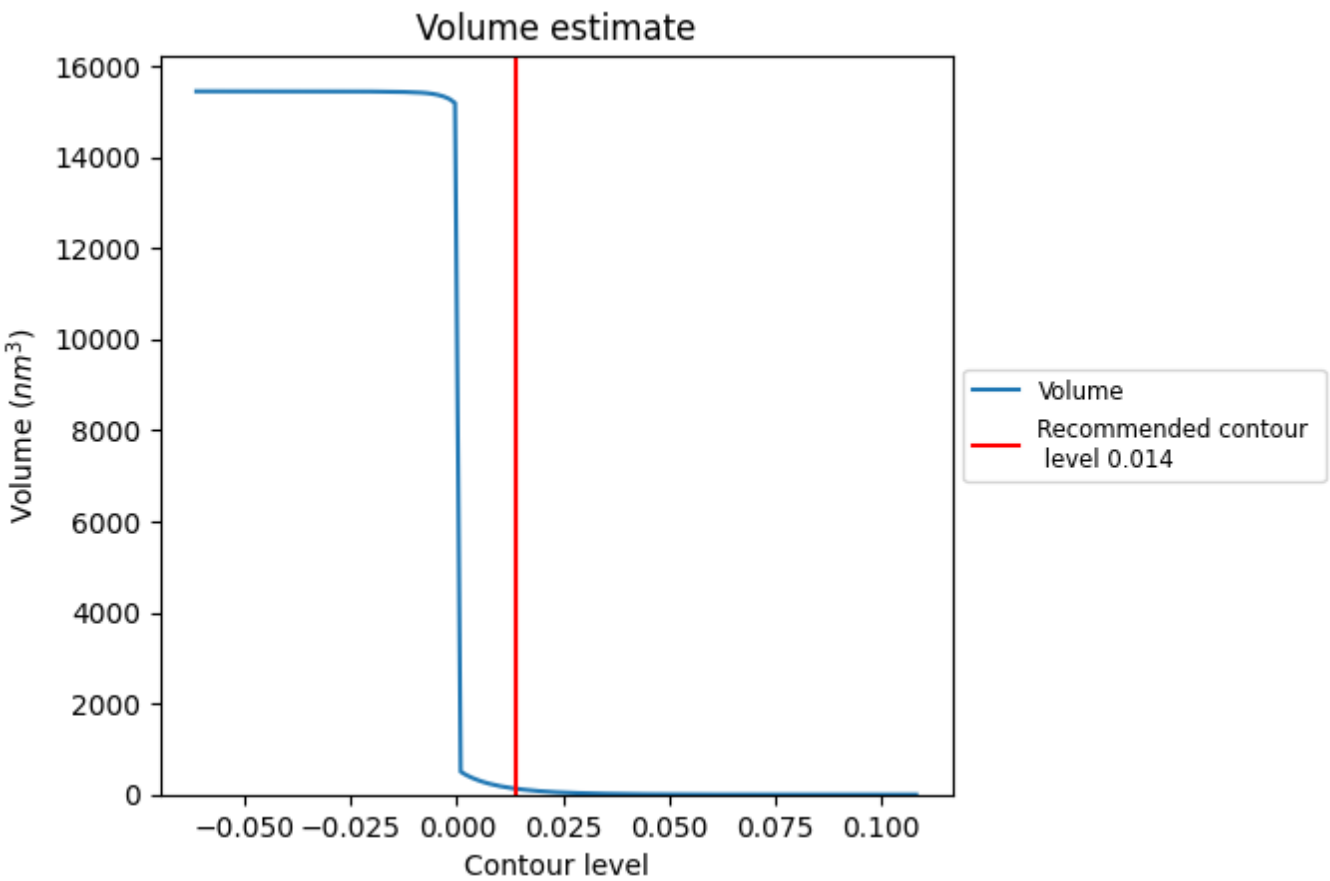
This section contains the results of statistical analysis of the map.

## 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.

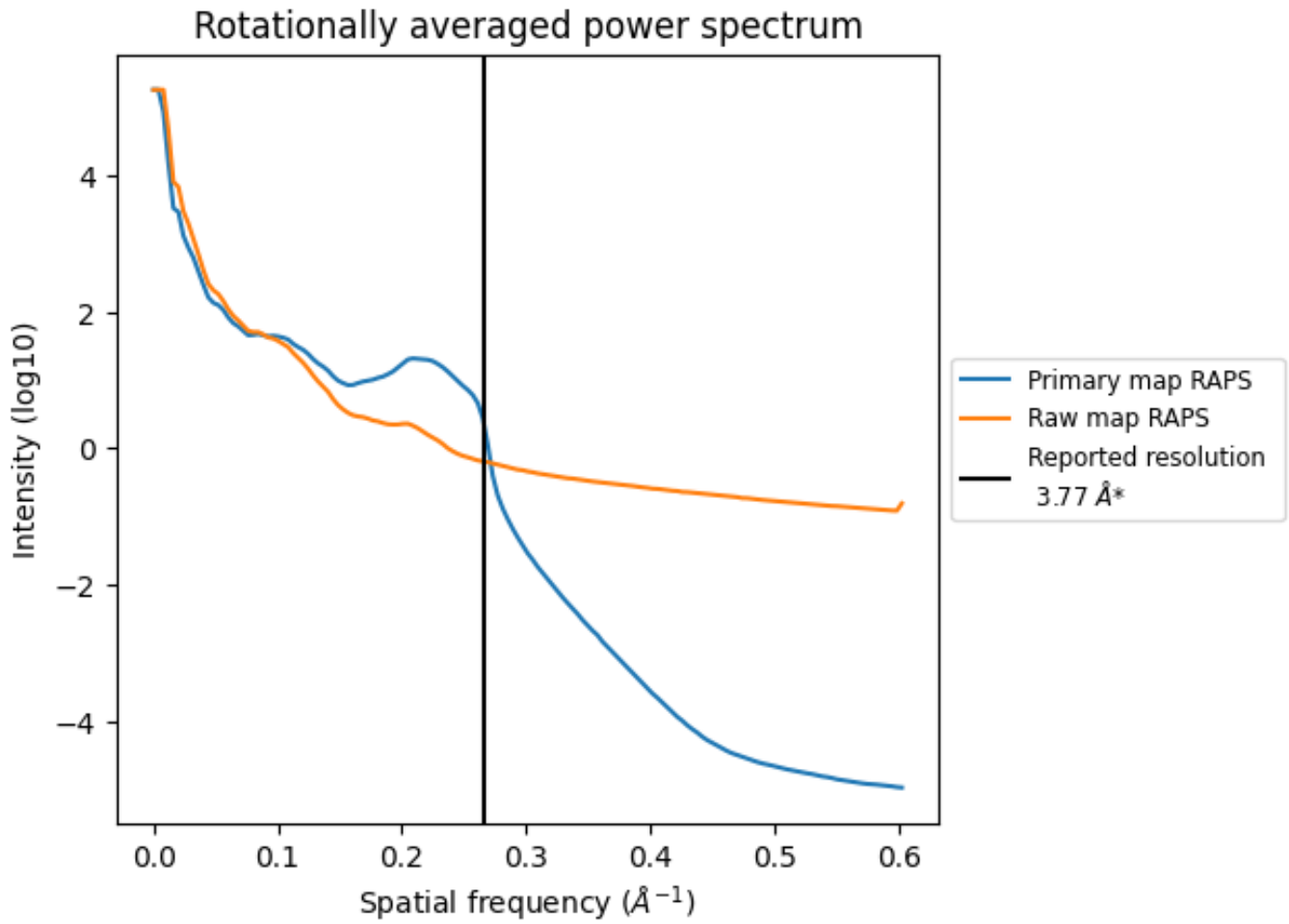
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 128 $nm^3$; this corresponds to an approximate mass of 115 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)

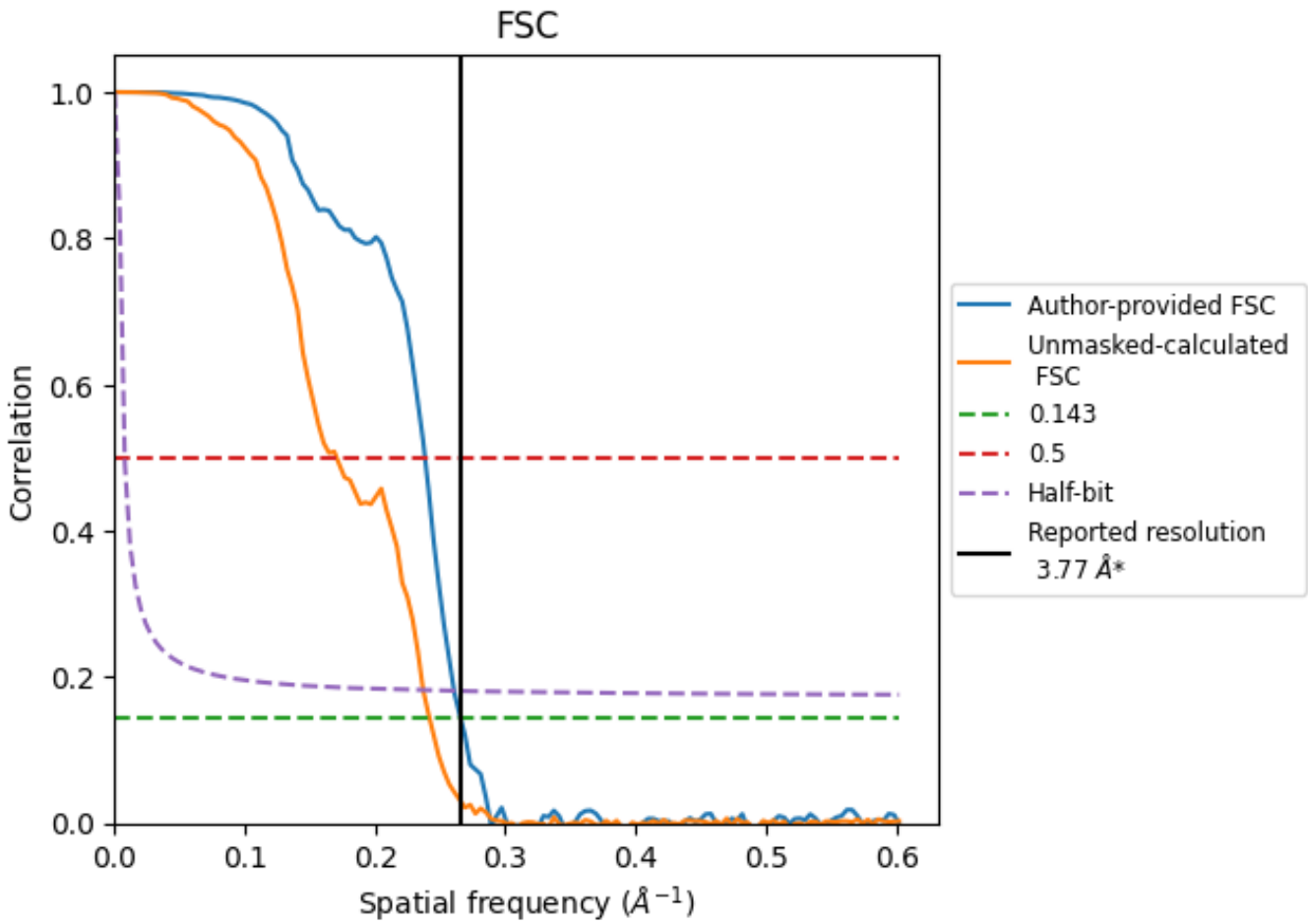



*Reported resolution corresponds to spatial frequency of 0.265 Å$^{-1}$

# 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 0.265 Å$^{-1}$

## 8.2 Resolution estimates (i)

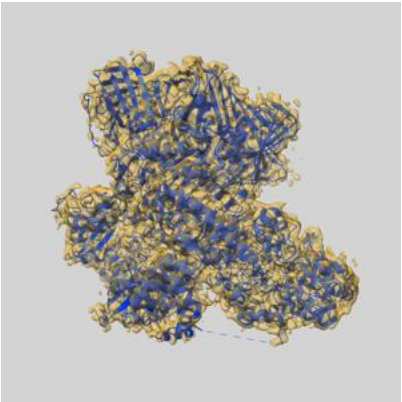
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.77 | - | - |
| Author-provided FSC curve | 3.76 | 4.19 | 3.83 |
| Unmasked-calculated* | 4.13 | 5.87 | 4.22 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

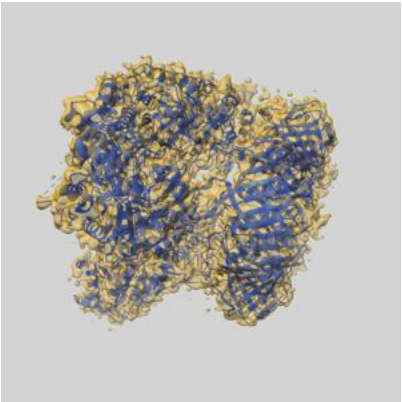
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10401 and PDB model 6T8H. Per-residue inclusion information can be found in section 3 on page 6.

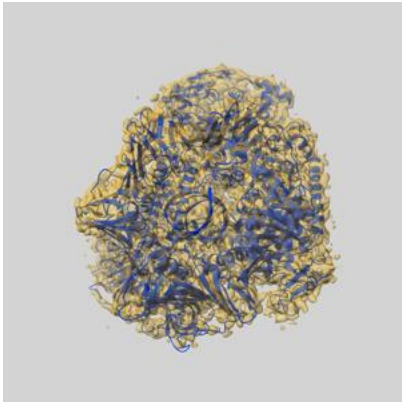
## 9.1 Map-model overlay (i)



X



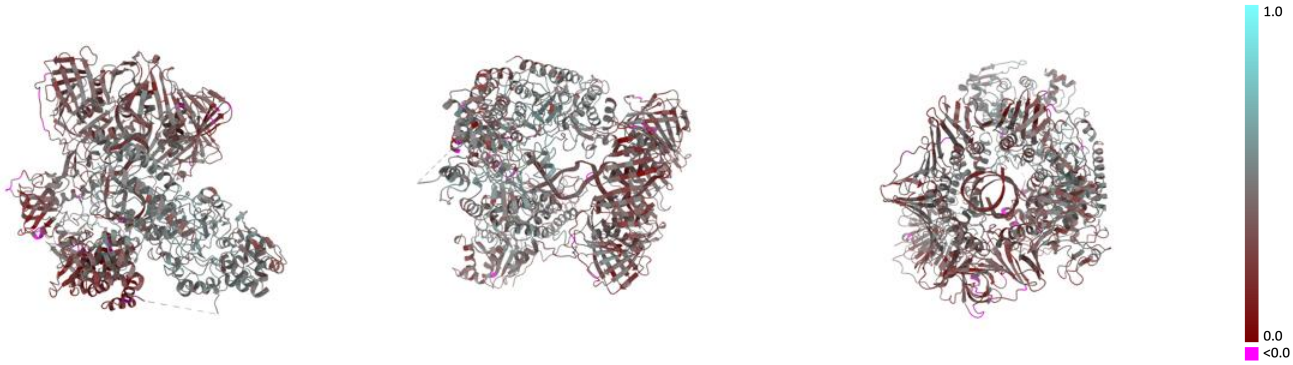
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

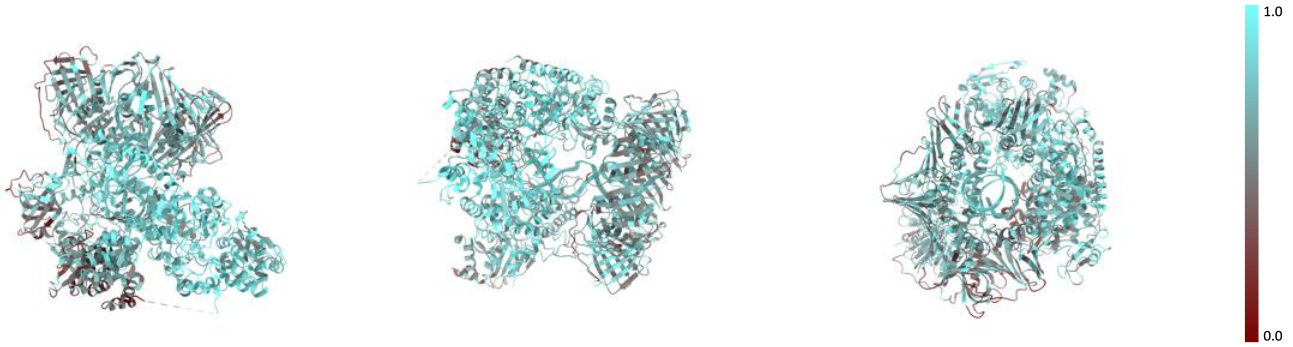
## 9.2 Q-score mapped to coordinate model (i)




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.

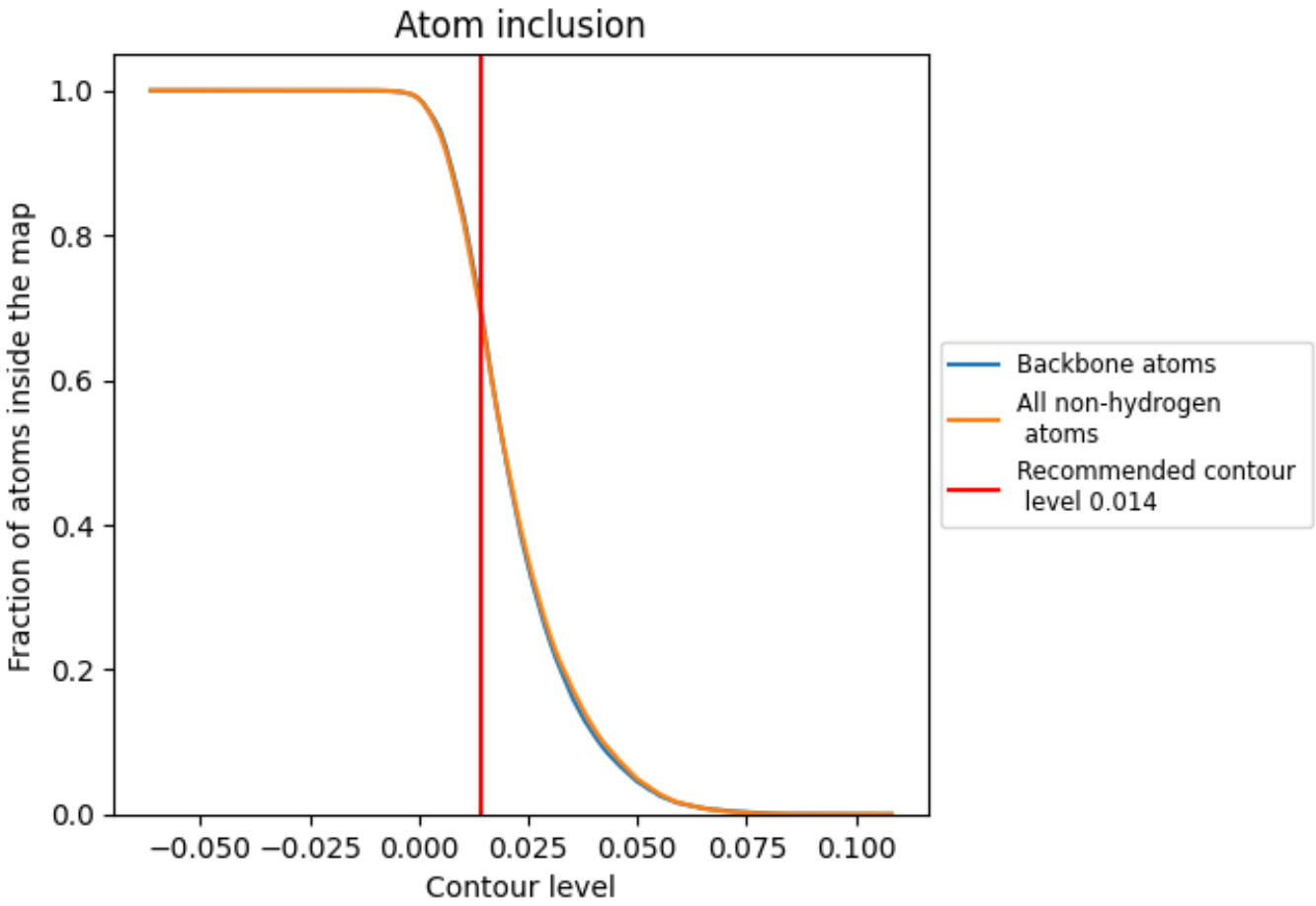
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.014).

## 9.4 Atom inclusion (i)




At the recommended contour level, 71% of all backbone atoms, 70% 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 (0.014) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6968 | 0.3860 |
| A | 0.6545 | 0.3660 |
| B | 0.7679 | 0.4270 |
| C | 0.6395 | 0.3520 |
| D | 0.6327 | 0.3470 |
| E | 0.5517 | 0.3270 |
| P | 0.8429 | 0.2680 |
| T | 0.8559 | 0.2840 |