# Full wwPDB EM Validation Report

Oct 26, 2026 – 04:15 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 37XW / pdb_000037xw |
| EMDB ID | : | EMD-78610 |
| Title | : | Polynucleotide kinase phosphatase bound to a nucleosome containing a nick with a 3'-phosphate and 5'-OH at SHL-5 (catalytic-FHA, composite) |
| Authors | : | Boesch, D.J.; Evans, J.J.; Weaver, T.M. |
| Deposited on | : | 2026-08-12 |
| Resolution | : | 3.40 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 ⓘ symbol.

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

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

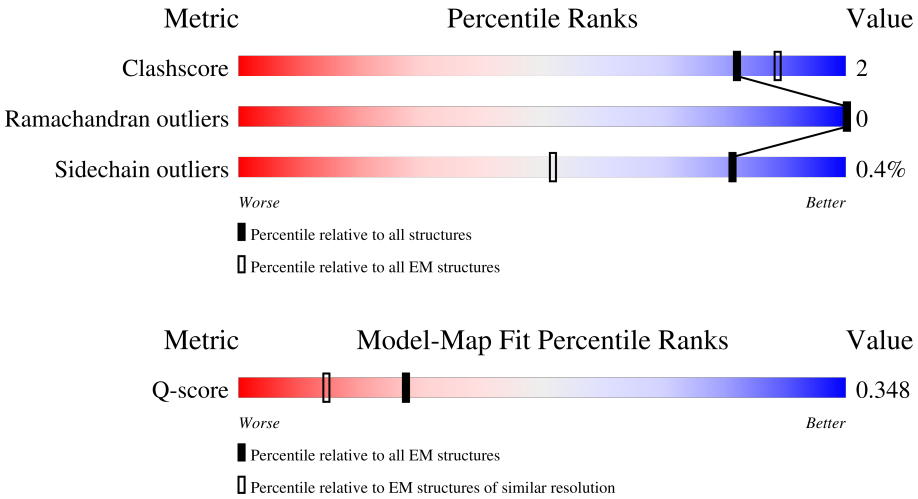
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.2 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.51 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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.







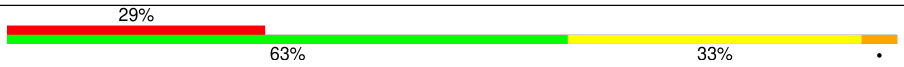
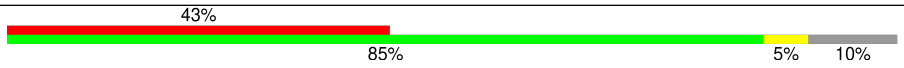
| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 14717 ( 2.90 - 3.90 ) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 135 | 63% 8% 29% |
| 1 | E | 135 | 67% 28% |
| 2 | B | 102 | 76% 20% |
| 2 | F | 102 | 76% 5% 19% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | C | 129 |   |
| 3 | G | 129 |   |
| 4 | D | 125 |   |
| 4 | H | 125 |   |
| 5 | I | 147 |   |
| 6 | J | 24 |   |
| 7 | K | 123 |   |
| 8 | L | 528 |   |

# 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15692 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 789 | 499 | 151 | 137 | 2 | | |
| 1 | E | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 800 | 505 | 155 | 138 | 2 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 110 | ALA | CYS | engineered mutation | UNP Q71DI3 |
| E | 110 | ALA | CYS | engineered mutation | UNP Q71DI3 |

- Molecule 2 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 657 | 416 | 128 | 112 | 1 | | |
| 2 | F | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 668 | 422 | 132 | 113 | 1 | | |

- Molecule 3 is a protein called Histone H2A type 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 3 | C | 109 | Total | C | N | O | 0 | 0 |
| | | | 841 | 532 | 165 | 144 | | |
| 3 | G | 107 | Total | C | N | O | 0 | 0 |
| | | | 823 | 520 | 161 | 142 | | |

- Molecule 4 is a protein called Histone H2B type 1-C/E/F/G/I.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 736 | 461 | 134 | 139 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | H | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 725 | 455 | 130 | 138 | 2 | | |

- Molecule 5 is a DNA chain called 601 I strand (non-damaged strand).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | I | 147 | Total | C | N | O | P | 0 | 0 |
| | | | 2996 | 1423 | 545 | 881 | 147 | | |

- Molecule 6 is a DNA chain called 601 J strand (damaged strand).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | J | 24 | Total | C | N | O | P | 0 | 0 |
| | | | 497 | 236 | 88 | 148 | 25 | | |

- Molecule 7 is a DNA chain called 601 K strand (damaged strand).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | K | 123 | Total | C | N | O | P | 0 | 0 |
| | | | 2535 | 1199 | 478 | 736 | 122 | | |

- Molecule 8 is a protein called Bifunctional polynucleotide phosphatase/kinase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | L | 475 | Total | C | N | O | S | 0 | 0 |
| | | | 3625 | 2314 | 644 | 653 | 14 | | |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| L | -6 | MET | - | initiating methionine | UNP Q96T60 |
| L | -5 | HIS | - | expression tag | UNP Q96T60 |
| L | -4 | HIS | - | expression tag | UNP Q96T60 |
| L | -3 | HIS | - | expression tag | UNP Q96T60 |
| L | -2 | HIS | - | expression tag | UNP Q96T60 |
| L | -1 | HIS | - | expression tag | UNP Q96T60 |
| L | 0 | HIS | - | expression tag | UNP Q96T60 |
| L | 1 | GLY | - | expression tag | UNP Q96T60 |
| L | 171 | ALA | ASP | engineered mutation | UNP Q96T60 |

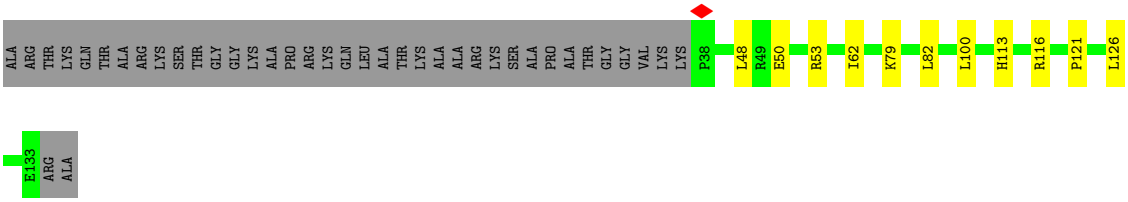
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Histone H3.2

Chain A:

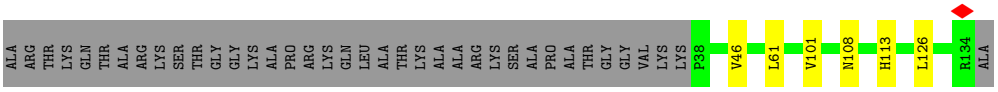



• Molecule 1: Histone H3.2

Chain E:

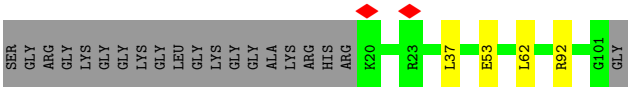



• Molecule 2: Histone H4

Chain B:

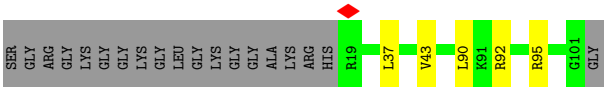



• Molecule 2: Histone H4

Chain F:



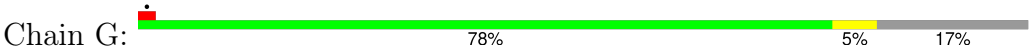

• Molecule 3: Histone H2A type 1

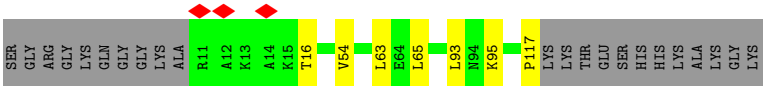
Chain C:





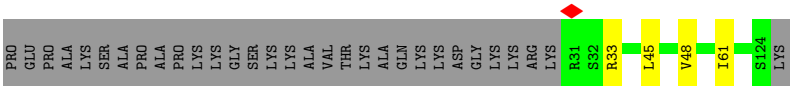

• Molecule 3: Histone H2A type 1



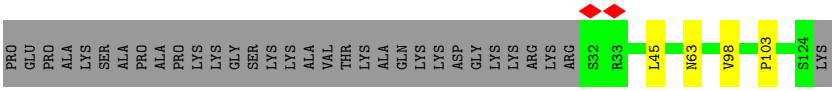

• Molecule 4: Histone H2B type 1-C/E/F/G/I



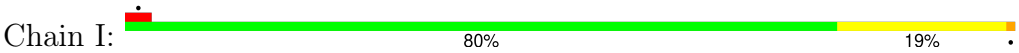



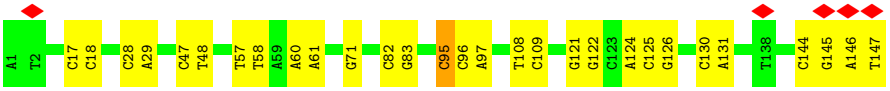

• Molecule 4: Histone H2B type 1-C/E/F/G/I



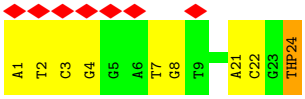

• Molecule 5: 601 I strand (non-damaged strand)



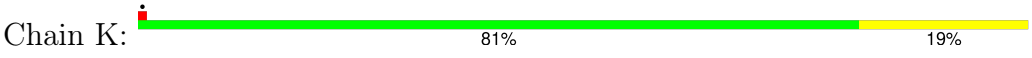



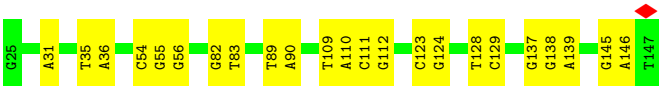

• Molecule 6: 601 J strand (damaged strand)



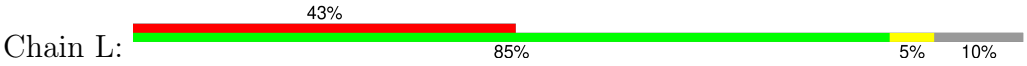

• Molecule 7: 601 K strand (damaged strand)

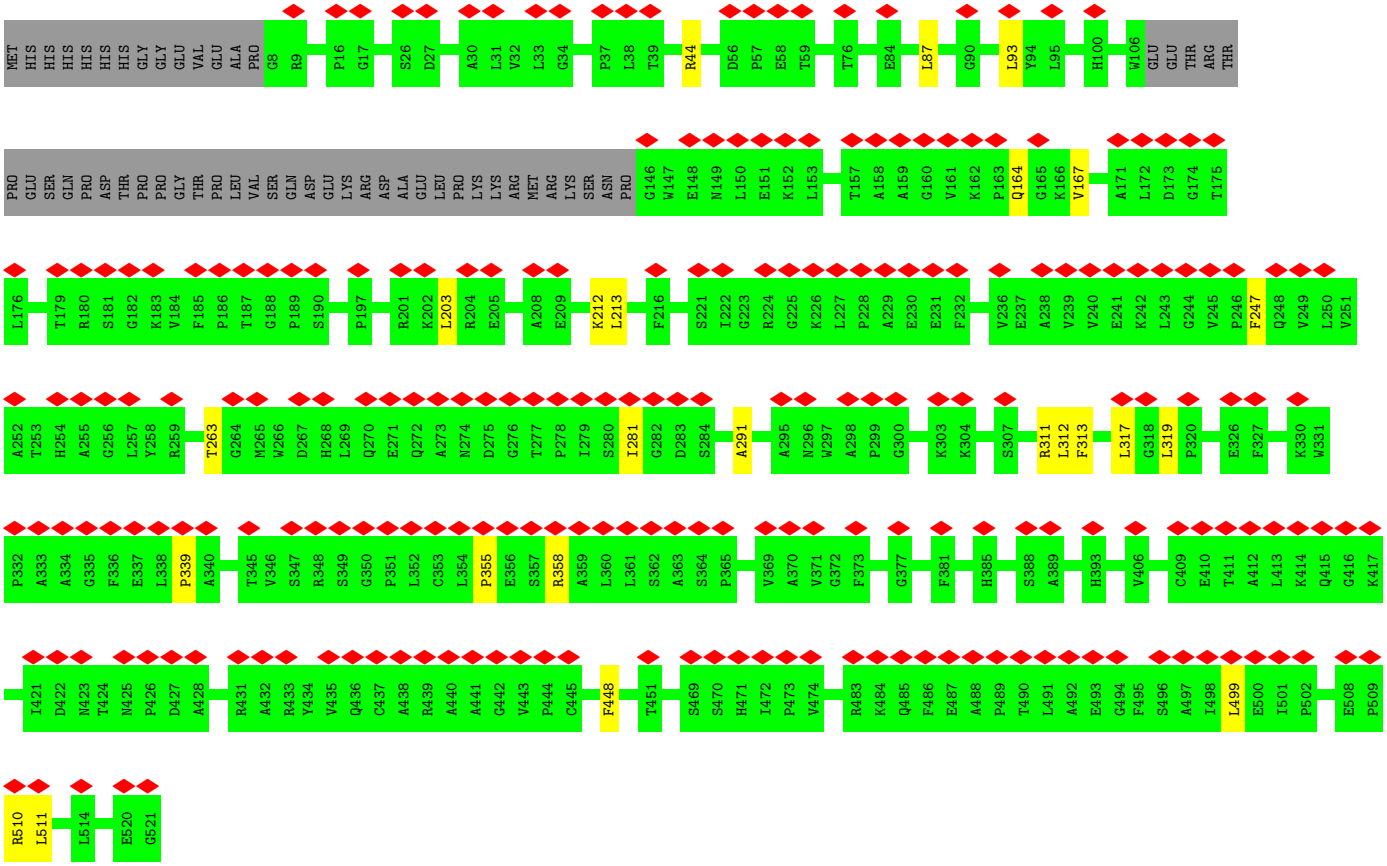



• Molecule 8: Bifunctional polynucleotide phosphatase/kinase

Chain L:


43%
85%
5%
10%


MET HIS HIS HIS HIS HIS HIS GLY GLY GLU VAL GLU ALA PRO G8 R9 P16 G17 S26 D27 A30 L31 V32 L33 G34 P37 L38 T39 R44 D56 P57 E58 T59 T76 E84 L87 G90 L93 Y94 L95 H100 W106 GLU GLU THR ARG THR
PRO GLU SER GLN PRO ASP THR PRO PRO GLY THR PRO LEU VAL SER GLN ASP GLU LYS ARG ASP ALA GLU LEU PRO LYS LYS ARG MET ARG LYS SER ASN PRO G146 W147 E148 N149 L150 E151 K152 L153 T157 A158 A159 G160 V161 K162 P163 Q164 G165 K166 V167 A171 L172 D173 G174 T175
L176 T179 R180 S181 G182 K183 V184 F185 P186 T187 G188 P189 S190 P197 R201 K202 L203 R204 E205 A208 E209 K212 L213 F216 S221 I222 G223 R224 G225 K226 L227 P228 A229 E230 E231 F232 V236 E237 A238 V239 V240 E241 K242 L243 G244 V245 P246 F247 Q248 V249 L250 V251
A252 T253 H254 A255 G256 L257 Y258 R259 T263 G264 M265 W266 D267 H268 L269 Q270 E271 Q272 A273 N274 D275 G276 T277 P278 I279 S280 I281 G282 D283 S284 A291 A295 N296 W297 A298 P299 G300 K303 K304 S307 R311 L312 F313 L317 G318 L319 P320 E326 F327 K330 W331
P332 A333 A334 G335 F336 E337 L338 P339 A340 T345 V346 S347 R348 S349 G350 P351 L352 C353 L354 P355 E356 S357 R358 A359 L360 L361 S362 A363 S364 P365 V369 A370 V371 G372 F373 G377 F381 H385 S388 A389 H393 V406 C409 E410 T411 A412 L413 K414 Q415 G416 K417
I421 D422 N423 T424 N425 P426 D427 A428 R431 A432 R433 Y434 V435 Q436 C437 A438 R439 A440 A441 G442 V443 P444 C445 F448 T451 S469 S470 H471 I472 P473 V474 R483 K484 Q485 F486 E487 A488 P489 T490 L491 A492 E493 G494 F495 S496 A497 I498 L499 E500 I501 P502 E508 P509
R510 L511 L514 E520 G521

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 7817 | 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 ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 26.625 | Depositor |
| Minimum map value | -11.398 | Depositor |
| Average map value | 0.006 | Depositor |
| Map value standard deviation | 1.007 | Depositor |
| Recommended contour level | 5 | Depositor |
| Map size (Å) | 260.80002, 260.80002, 260.80002 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.65200007, 0.65200007, 0.65200007 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.16 | 0/801 | 0.30 | 0/1075 |
| 1 | E | 0.15 | 0/812 | 0.27 | 0/1089 |
| 2 | B | 0.16 | 0/664 | 0.32 | 0/889 |
| 2 | F | 0.17 | 0/675 | 0.32 | 0/903 |
| 3 | C | 0.16 | 0/851 | 0.28 | 0/1146 |
| 3 | G | 0.13 | 0/833 | 0.26 | 0/1124 |
| 4 | D | 0.14 | 0/747 | 0.29 | 0/1004 |
| 4 | H | 0.14 | 0/736 | 0.26 | 0/990 |
| 5 | I | 0.73 | 0/3357 | 0.93 | 2/5174 (0.0%) |
| 6 | J | 0.73 | 0/530 | 0.92 | 0/816 |
| 7 | K | 0.70 | 0/2847 | 0.86 | 0/4397 |
| 8 | L | 0.10 | 0/3717 | 0.26 | 0/5054 |
| All | All | 0.47 | 0/16570 | 0.63 | 2/23661 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | I | 126 | DG | O4'-C4'-C3' | -5.48 | 102.71 | 106.00 |
| 5 | I | 95 | DC | O4'-C4'-C3' | -5.33 | 102.80 | 106.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 789 | 0 | 826 | 10 | 0 |
| 1 | E | 800 | 0 | 839 | 6 | 0 |
| 2 | B | 657 | 0 | 706 | 3 | 0 |
| 2 | F | 668 | 0 | 719 | 3 | 0 |
| 3 | C | 841 | 0 | 910 | 4 | 0 |
| 3 | G | 823 | 0 | 884 | 7 | 0 |
| 4 | D | 736 | 0 | 756 | 3 | 0 |
| 4 | H | 725 | 0 | 743 | 3 | 0 |
| 5 | I | 2996 | 0 | 1650 | 16 | 0 |
| 6 | J | 497 | 0 | 272 | 5 | 0 |
| 7 | K | 2535 | 0 | 1380 | 16 | 0 |
| 8 | L | 3625 | 0 | 3612 | 14 | 0 |
| All | All | 15692 | 0 | 13297 | 71 | 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 2.

All (71) 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) |
|---|---|---|---|
| 5:I:17:DC:H2” | 5:I:18:DC:C5 | 2.39 | 0.57 |
| 5:I:96:DC:H2’ | 5:I:97:DA:C8 | 2.42 | 0.55 |
| 1:E:61:LEU:HD12 | 2:F:37:LEU:HD23 | 1.89 | 0.54 |
| 1:A:121:PRO:HB3 | 2:B:53:GLU:HG3 | 1.89 | 0.54 |
| 1:A:50:GLU:HA | 1:A:53:ARG:HB2 | 1.89 | 0.54 |
| 8:L:281:ILE:HG23 | 8:L:319:LEU:HD22 | 1.90 | 0.53 |
| 3:G:63:LEU:HD13 | 4:H:45:LEU:HB2 | 1.92 | 0.52 |
| 6:J:1:DA:H2” | 6:J:2:DT:H5’ | 1.92 | 0.52 |
| 7:K:82:DG:H2’ | 7:K:83:DT:C6 | 2.44 | 0.52 |
| 7:K:89:DT:H2” | 7:K:90:DA:C8 | 2.46 | 0.51 |
| 3:G:16:THR:HA | 7:K:31:DA:H5” | 1.93 | 0.50 |
| 3:G:54:VAL:HG21 | 4:H:98:VAL:HG21 | 1.93 | 0.50 |
| 5:I:130:DC:H2” | 5:I:131:DA:N7 | 2.26 | 0.50 |
| 8:L:510:ARG:HG3 | 8:L:511:LEU:HG | 1.92 | 0.50 |
| 1:E:46:VAL:HG21 | 5:I:83:DG:H3’ | 1.93 | 0.49 |
| 7:K:35:DT:H1’ | 7:K:36:DA:H5’ | 1.95 | 0.49 |
| 8:L:317:LEU:HB3 | 8:L:319:LEU:HD23 | 1.95 | 0.49 |
| 5:I:82:DC:H2” | 5:I:83:DG:C8 | 2.48 | 0.48 |
| 6:J:7:DT:H2’ | 6:J:8:DG:C8 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:I:121:DG:H2" | 5:I:122:DG:C8 | 2.49 | 0.48 |
| 7:K:137:DG:H2" | 7:K:138:DG:C8 | 2.50 | 0.47 |
| 5:I:144:DC:H2" | 5:I:145:DG:C8 | 2.50 | 0.47 |
| 7:K:111:DC:H2" | 7:K:112:DG:C8 | 2.50 | 0.47 |
| 3:G:95:LYS:HD2 | 4:H:103:PRO:HB3 | 1.97 | 0.47 |
| 5:I:124:DA:H2" | 5:I:125:DC:O2 | 2.15 | 0.47 |
| 8:L:263:THR:HA | 8:L:313:PHE:HE1 | 1.81 | 0.46 |
| 5:I:47:DC:H2" | 5:I:48:DT:H72 | 1.98 | 0.46 |
| 5:I:28:DC:H2" | 5:I:29:DA:C8 | 2.51 | 0.45 |
| 3:G:65:LEU:HD21 | 8:L:44:ARG:HH12 | 1.82 | 0.45 |
| 7:K:55:DG:H2" | 7:K:56:DG:C8 | 2.52 | 0.45 |
| 7:K:123:DC:H2" | 7:K:124:DG:C8 | 2.51 | 0.45 |
| 8:L:167:VAL:HG22 | 8:L:212:LYS:HB3 | 1.98 | 0.45 |
| 8:L:312:LEU:HD11 | 8:L:339:PRO:HG2 | 1.98 | 0.45 |
| 3:C:63:LEU:HD13 | 4:D:45:LEU:HB2 | 1.98 | 0.44 |
| 6:J:3:DC:H2" | 6:J:4:DG:C8 | 2.52 | 0.44 |
| 8:L:203:LEU:HD22 | 8:L:213:LEU:HD13 | 1.98 | 0.44 |
| 1:A:113:HIS:CG | 1:E:126:LEU:HD22 | 2.53 | 0.44 |
| 5:I:146:DA:H2" | 5:I:147:DT:H5' | 1.98 | 0.44 |
| 7:K:138:DG:H1' | 7:K:139:DA:H5' | 1.99 | 0.44 |
| 1:A:62:ILE:HD11 | 2:B:37:LEU:HD11 | 2.00 | 0.44 |
| 8:L:291:ALA:HB1 | 8:L:311:ARG:HH21 | 1.83 | 0.44 |
| 1:A:79:LYS:HD3 | 1:A:82:LEU:HD13 | 1.99 | 0.43 |
| 4:D:33:ARG:HG3 | 7:K:123:DC:H4' | 2.00 | 0.43 |
| 7:K:109:DT:H2" | 7:K:110:DA:C8 | 2.54 | 0.43 |
| 7:K:82:DG:C8 | 7:K:83:DT:H72 | 2.54 | 0.43 |
| 5:I:57:DT:H2" | 5:I:58:DT:C6 | 2.53 | 0.43 |
| 1:A:126:LEU:HD22 | 1:E:113:HIS:CG | 2.54 | 0.42 |
| 6:J:24:THP:H2'2 | 6:J:24:THP:H6 | 1.76 | 0.42 |
| 1:E:108:ASN:HB2 | 2:F:43:VAL:HG22 | 2.01 | 0.42 |
| 5:I:95:DC:H2' | 5:I:96:DC:C6 | 2.55 | 0.42 |
| 5:I:60:DA:H2" | 5:I:61:DA:C8 | 2.55 | 0.42 |
| 8:L:213:LEU:HB3 | 8:L:247:PHE:CE1 | 2.54 | 0.42 |
| 1:A:100:LEU:HD23 | 1:A:100:LEU:HA | 1.90 | 0.42 |
| 3:C:107:VAL:HG11 | 1:E:101:VAL:HG11 | 2.02 | 0.42 |
| 1:A:48:LEU:HD11 | 3:G:117:PRO:HD3 | 2.01 | 0.42 |
| 8:L:355:PRO:HD2 | 8:L:358:ARG:HD2 | 2.01 | 0.42 |
| 8:L:87:LEU:HD11 | 8:L:93:LEU:HB2 | 2.01 | 0.42 |
| 6:J:21:DA:H2' | 6:J:22:DC:C5 | 2.55 | 0.41 |
| 8:L:164:GLN:HB2 | 8:L:212:LYS:HB2 | 2.02 | 0.41 |
| 7:K:145:DG:H2" | 7:K:146:DA:H5" | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:K:128:DT:H2" | 7:K:129:DC:C5 | 2.55 | 0.41 |
| 2:F:90:LEU:HB3 | 2:F:95:ARG:HB2 | 2.02 | 0.41 |
| 3:C:44:GLY:HA2 | 7:K:112:DG:H5" | 2.03 | 0.41 |
| 5:I:108:DT:H2" | 5:I:109:DC:C6 | 2.56 | 0.41 |
| 2:B:62:LEU:HD23 | 2:B:62:LEU:HA | 1.85 | 0.41 |
| 1:A:116:ARG:HD3 | 5:I:71:DG:H3' | 2.03 | 0.41 |
| 8:L:448:PHE:CE1 | 8:L:499:LEU:HD12 | 2.56 | 0.40 |
| 3:G:65:LEU:HD12 | 3:G:93:LEU:HD12 | 2.02 | 0.40 |
| 1:A:48:LEU:HD23 | 1:A:48:LEU:HA | 1.92 | 0.40 |
| 7:K:54:DC:H2' | 7:K:55:DG:C8 | 2.56 | 0.40 |
| 3:C:102:ILE:HG23 | 4:D:61:ILE:HD13 | 2.02 | 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 | |
|---|---|---|---|---|---|---|---|
| 1 | A | 94/135 (70%) | 91 (97%) | 3 (3%) | 0 | 100 | 100 |
| 1 | E | 95/135 (70%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | B | 80/102 (78%) | 77 (96%) | 3 (4%) | 0 | 100 | 100 |
| 2 | F | 81/102 (79%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 3 | C | 107/129 (83%) | 107 (100%) | 0 | 0 | 100 | 100 |
| 3 | G | 105/129 (81%) | 105 (100%) | 0 | 0 | 100 | 100 |
| 4 | D | 92/125 (74%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 4 | H | 91/125 (73%) | 88 (97%) | 3 (3%) | 0 | 100 | 100 |
| 8 | L | 471/528 (89%) | 464 (98%) | 7 (2%) | 0 | 100 | 100 |
| All | All | 1216/1510 (80%) | 1193 (98%) | 23 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 83/109 (76%) | 83 (100%) | 0 | 100 100 |
| 1 | E | 84/109 (77%) | 84 (100%) | 0 | 100 100 |
| 2 | B | 68/78 (87%) | 67 (98%) | 1 (2%) | 57 69 |
| 2 | F | 69/78 (88%) | 68 (99%) | 1 (1%) | 59 70 |
| 3 | C | 85/98 (87%) | 85 (100%) | 0 | 100 100 |
| 3 | G | 83/98 (85%) | 83 (100%) | 0 | 100 100 |
| 4 | D | 81/105 (77%) | 80 (99%) | 1 (1%) | 63 72 |
| 4 | H | 80/105 (76%) | 79 (99%) | 1 (1%) | 61 71 |
| 8 | L | 377/435 (87%) | 377 (100%) | 0 | 100 100 |
| All | All | 1010/1215 (83%) | 1006 (100%) | 4 (0%) | 81 83 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 92 | ARG |
| 4 | D | 48 | VAL |
| 2 | F | 92 | ARG |
| 4 | H | 63 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 108 | ASN |
| 1 | E | 108 | ASN |
| 3 | G | 73 | ASN |
| 3 | G | 84 | GLN |
| 4 | H | 95 | GLN |
| 8 | L | 296 | ASN |
| 8 | L | 415 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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 | $\#\|Z\| > 2$ |
| 6 | THP | J | 24 | 6 | 22,25,26 | 0.82 | 0 | 32,37,40 | 0.95 | 2 (6%) |

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 |
|---|---|---|---|---|---|---|---|
| 6 | THP | J | 24 | 6 | - | 7/12/26/27 | 0/2/2/2 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | J | 24 | THP | O2P-P1-O1P | 2.54 | 120.72 | 110.83 |
| 6 | J | 24 | THP | O4-C4-C5 | -2.26 | 122.33 | 124.92 |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | J | 24 | THP | O4'-C1'-N1-C2 |
| 6 | J | 24 | THP | O4'-C1'-N1-C6 |
| 6 | J | 24 | THP | O4'-C4'-C5'-O5' |
| 6 | J | 24 | THP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | J | 24 | THP | C2'-C1'-N1-C6 |
| 6 | J | 24 | THP | C4'-C5'-O5'-P2 |
| 6 | J | 24 | THP | C2'-C1'-N1-C2 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 6 | J | 24 | THP | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

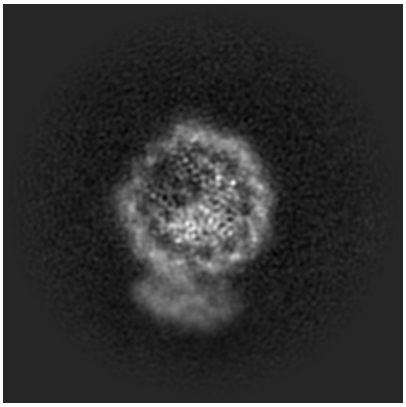
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-78610. These allow visual inspection of the internal detail of the map and identification of artifacts.

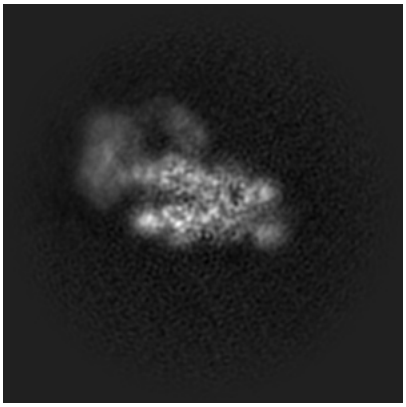
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

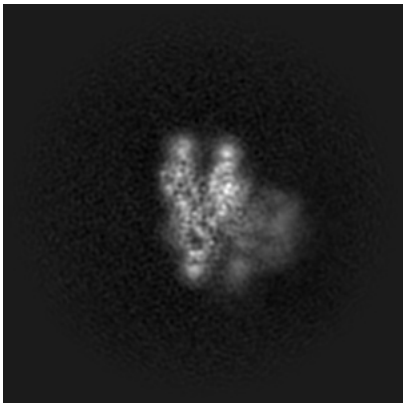
### 6.1.1 Primary map



X



Y

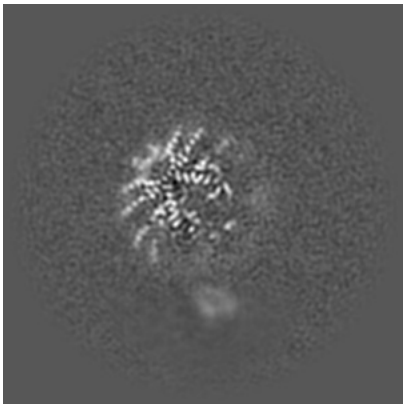


Z

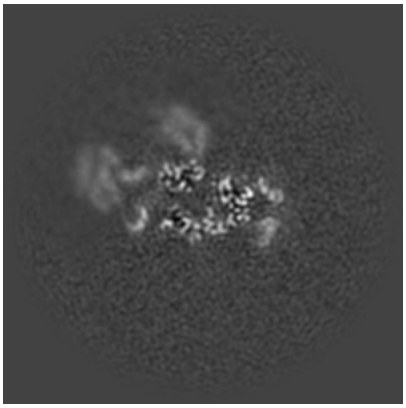
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

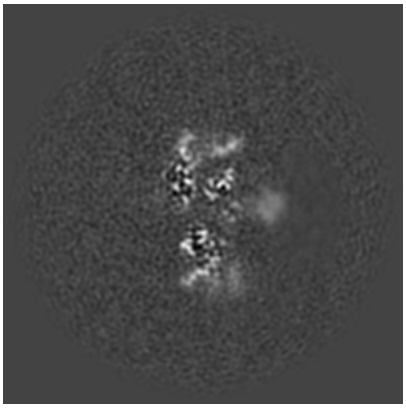
### 6.2.1 Primary map



X Index: 200



Y Index: 200

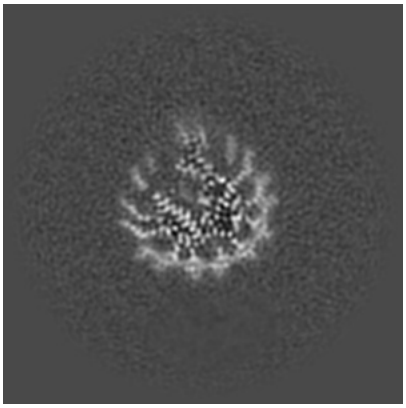


Z Index: 200

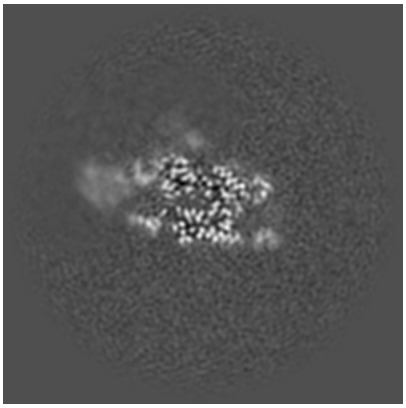
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

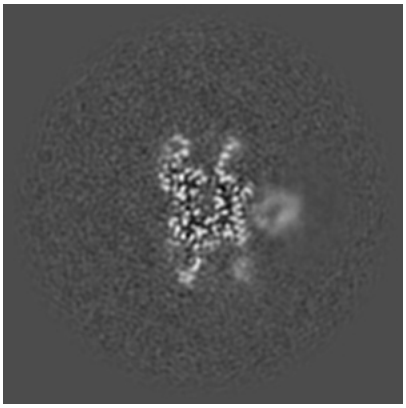
### 6.3.1 Primary map



X Index: 183



Y Index: 215

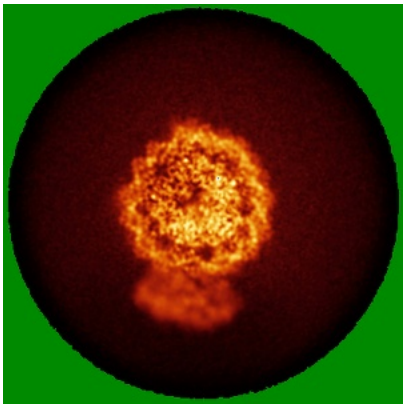


Z Index: 178

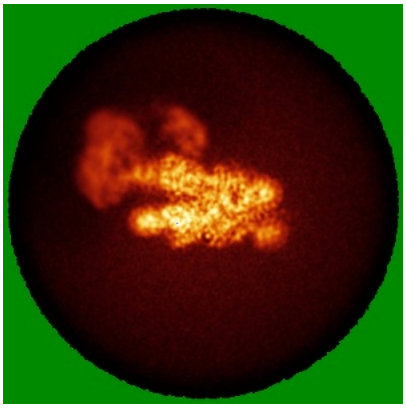
The images above show the largest variance slices of the map in three orthogonal directions.

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

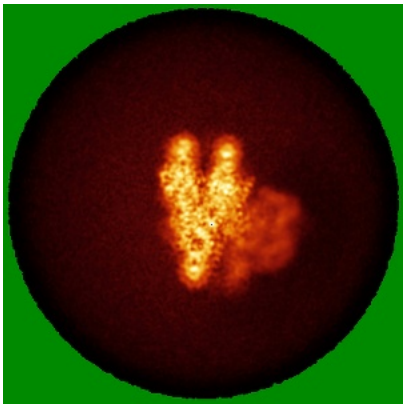
### 6.4.1 Primary map



X



Y



Z

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

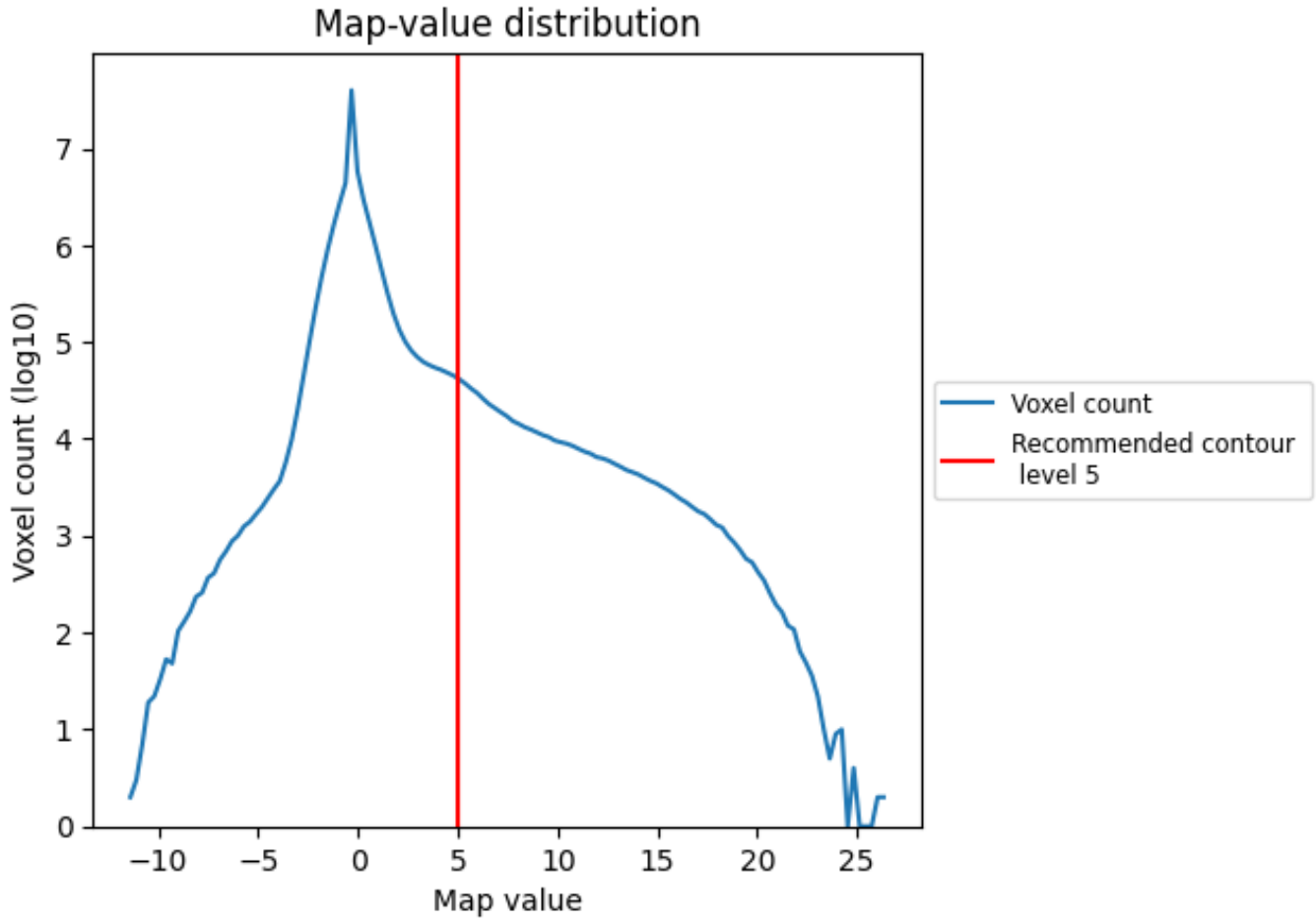
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

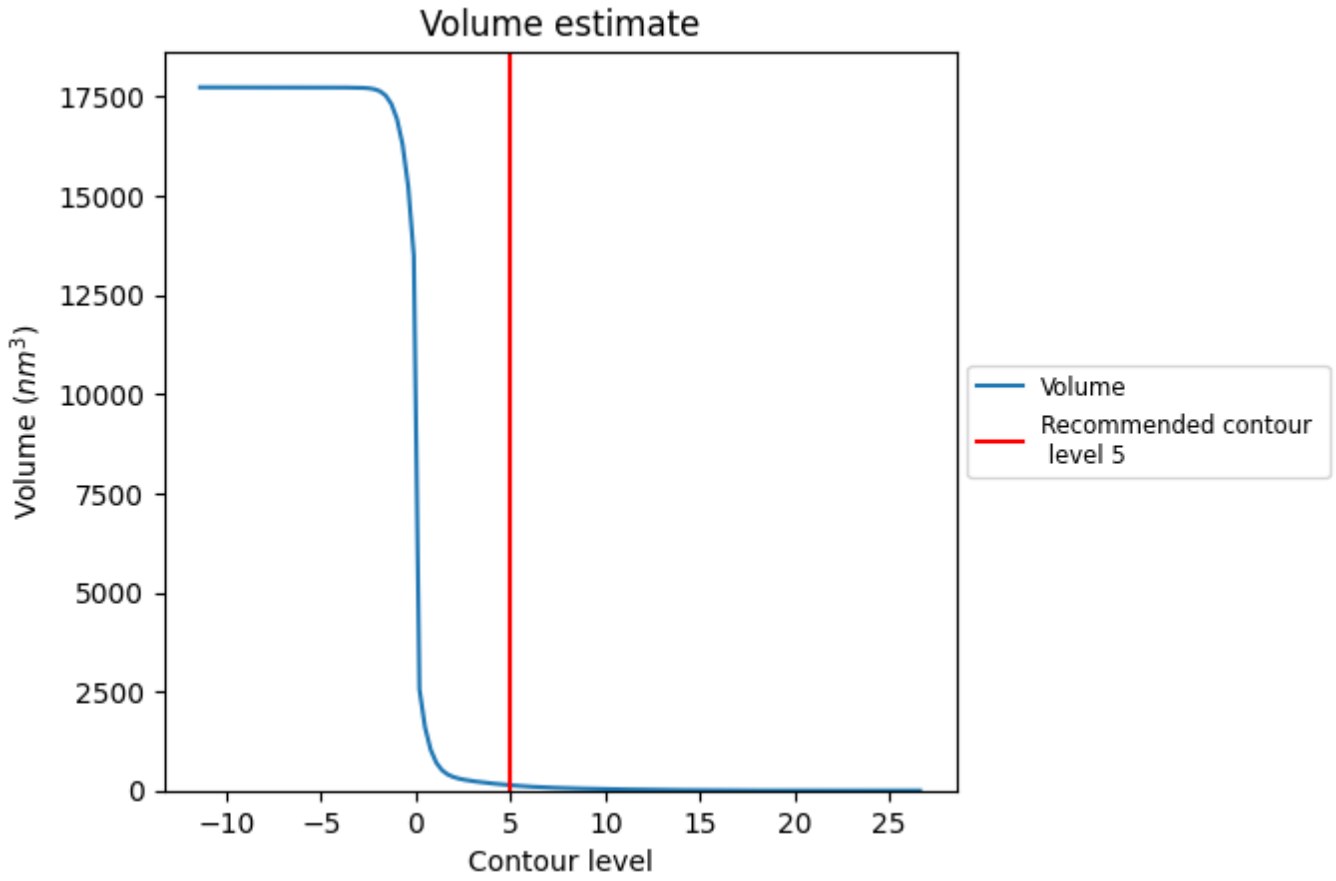
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

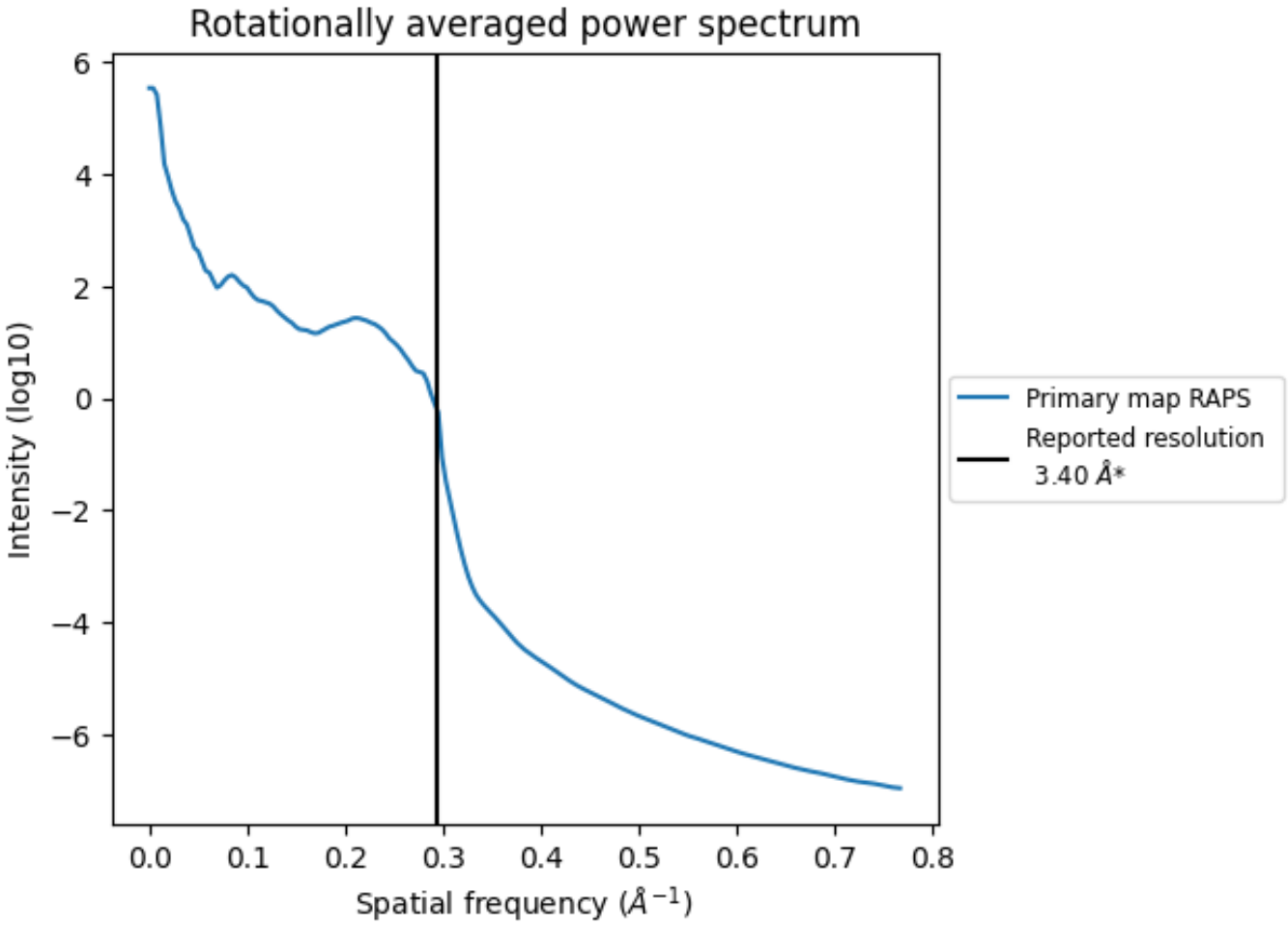
## 7.2 Volume estimate




The volume at the recommended contour level is 135 $nm^3$; this corresponds to an approximate mass of 122 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 0.294 Å$^{-1}$

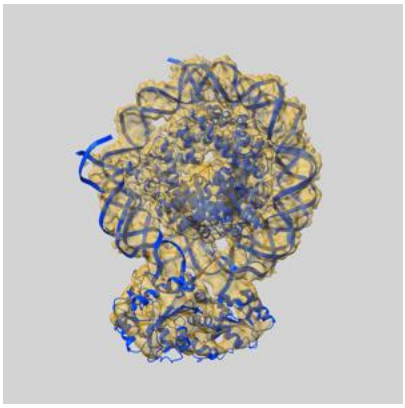
# 8 Fourier-Shell correlation (i)

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

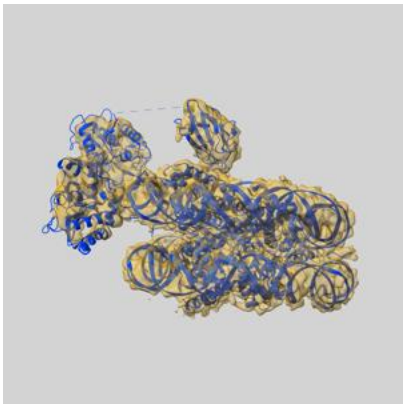
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-78610 and PDB model 37XW. Per-residue inclusion information can be found in section 3 on page 6.

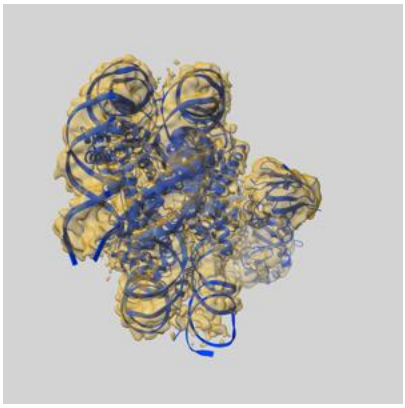
## 9.1 Map-model overlay



X



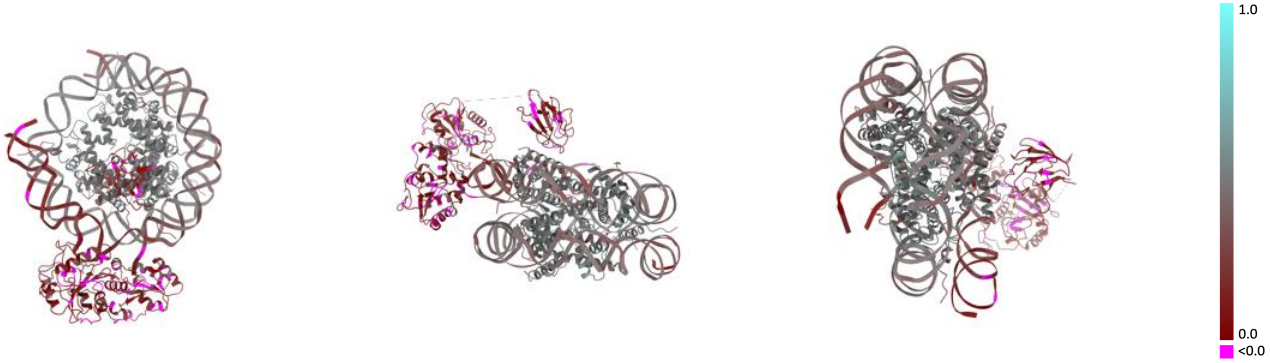
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0 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.

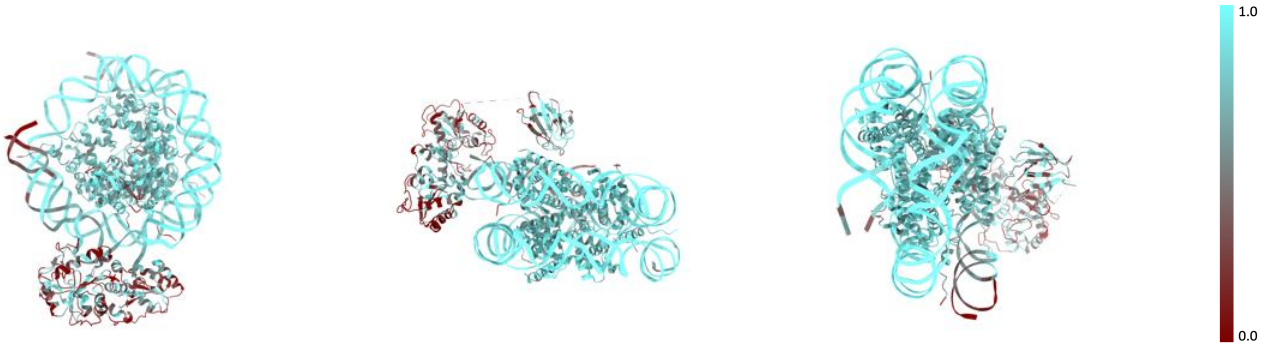
## 9.2 Q-score mapped to coordinate model (i)




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.

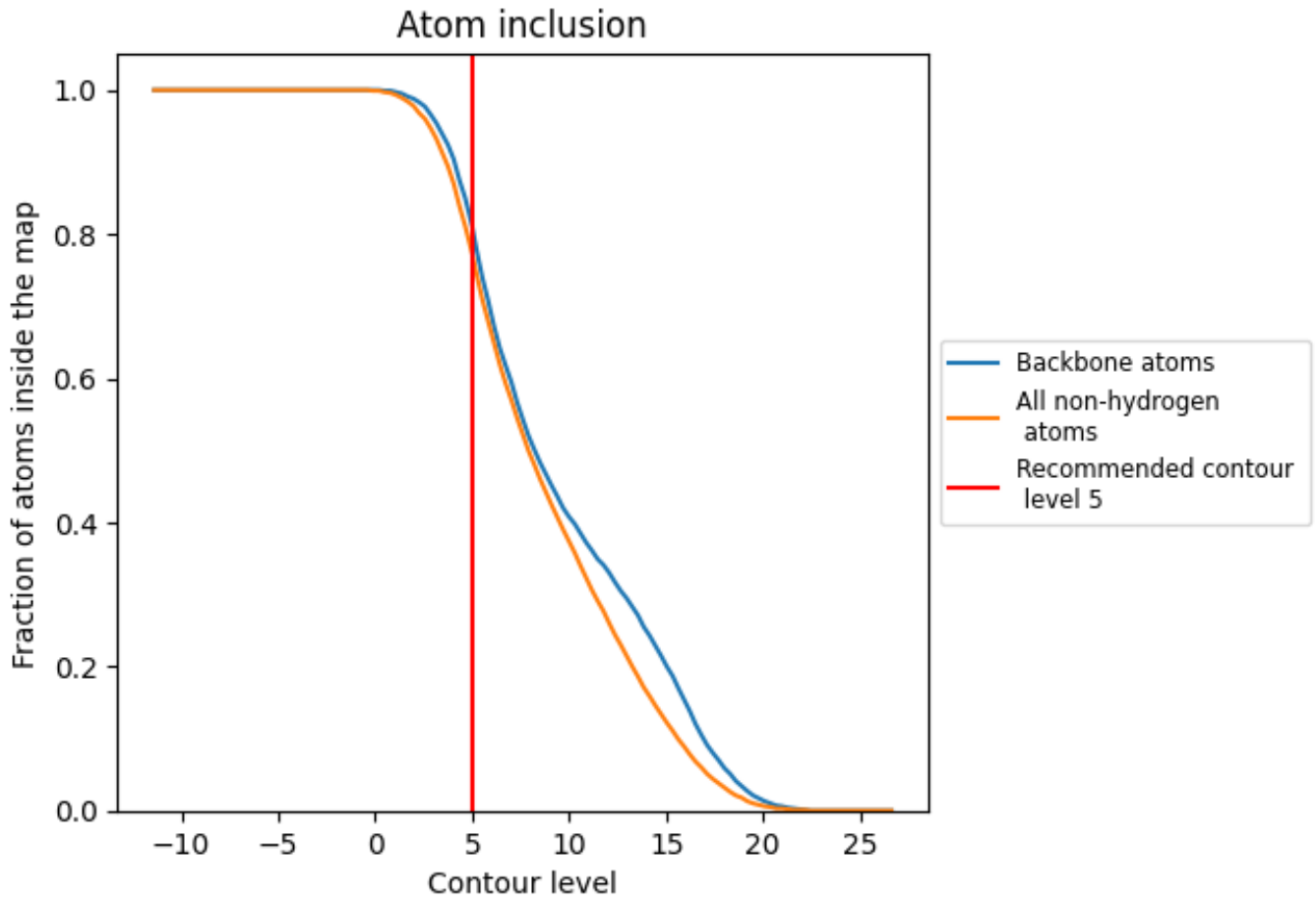
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (5).

## 9.4 Atom inclusion (i)




At the recommended contour level, 81% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7730 | 0.3480 |
| A | 0.8400 | 0.4820 |
| B | 0.8780 | 0.4890 |
| C | 0.8660 | 0.4900 |
| D | 0.8580 | 0.4710 |
| E | 0.8710 | 0.4970 |
| F | 0.8640 | 0.4880 |
| G | 0.8160 | 0.4670 |
| H | 0.8250 | 0.4570 |
| I | 0.8890 | 0.3610 |
| J | 0.5330 | 0.1620 |
| K | 0.9550 | 0.3910 |
| L | 0.4470 | 0.1110 |

