# WORLDWIDE PDB
## PROTEIN DATA BANK

# wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 11:58 AM EST

|  |  |  |
|---|---|---|
| PDB ID | : | 6XBD |
| EMDB ID | : | EMD-22116 |
| Title | : | Cryo-EM structure of MlaFEDB in nanodiscs with phospholipid substrates |
| Authors | : | Coudray, N.; Isom, G.L.; MacRae, M.R.; Saiduddin, M.; Ekiert, D.C.; Bhabha, G. |
| Deposited on | : | 2020-06-05 |
| Resolution | : | 3.05 Å(reported) |
| Based on initial models | : | 6CM1, 5UW2 |

# 1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.05 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 | Percentile Ranks | Value |
|--------|------------------|-------|
| Clashscore | | 9 |
| Ramachandran outliers | | 0 |
| Sidechain outliers | | 0.1% |

*Worse*        *Better*

▌Percentile relative to all structures

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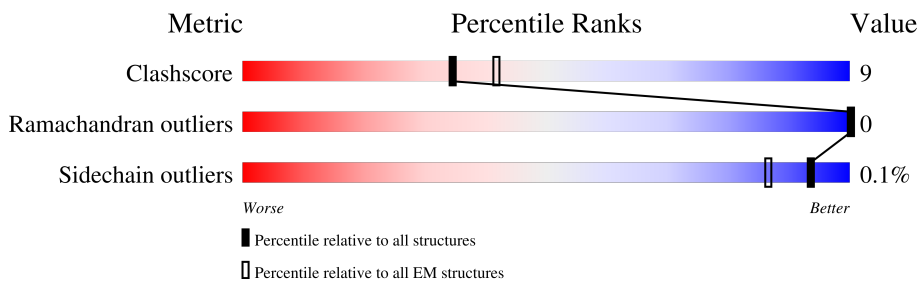
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|--------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | A | 201 | 60% 11% 28% |
| 1 | B | 201 | 55% 14% 31% |
| 1 | C | 201 | 5% 59% 12% 28% |
| 1 | D | 201 | 64% 7% 29% |
| 1 | E | 201 | 61% 11% 28% |
| 1 | F | 201 | 10% 62% 9% 29% |
| 2 | G | 260 | 82% 16% |
| 2 | H | 260 | 81% 17% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | I | 269 | 79% 19% |
| 3 | J | 269 | 79% 19% |
| 4 | K | 97 | 68% 30% |
| 4 | L | 97 | 68% 30% |
| 5 | M | 164 | 34% 75% 25% |
| 5 | N | 164 | 29% 66% 29% 5% |

# 2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 17433 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 Phospholipid ABC transporter-binding protein MlaD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1108 | 715 | 178 | 213 | 2 | | |
| 1 | B | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1063 | 687 | 170 | 204 | 2 | | |
| 1 | C | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1033 | 652 | 172 | 208 | 1 | | |
| 1 | D | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1096 | 707 | 177 | 210 | 2 | | |
| 1 | E | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1112 | 718 | 179 | 213 | 2 | | |
| 1 | F | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1028 | 649 | 171 | 207 | 1 | | |

There are 108 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -17 | MET | - | expression tag | UNP H4UPP8 |
| A | -16 | HIS | - | expression tag | UNP H4UPP8 |
| A | -15 | HIS | - | expression tag | UNP H4UPP8 |
| A | -14 | HIS | - | expression tag | UNP H4UPP8 |
| A | -13 | HIS | - | expression tag | UNP H4UPP8 |
| A | -12 | HIS | - | expression tag | UNP H4UPP8 |
| A | -11 | HIS | - | expression tag | UNP H4UPP8 |
| A | -10 | GLN | - | expression tag | UNP H4UPP8 |
| A | -9 | HIS | - | expression tag | UNP H4UPP8 |
| A | -8 | GLN | - | expression tag | UNP H4UPP8 |
| A | -7 | HIS | - | expression tag | UNP H4UPP8 |
| A | -6 | GLU | - | expression tag | UNP H4UPP8 |
| A | -5 | ASN | - | expression tag | UNP H4UPP8 |
| A | -4 | LEU | - | expression tag | UNP H4UPP8 |
| A | -3 | TYR | - | expression tag | UNP H4UPP8 |
| A | -2 | PHE | - | expression tag | UNP H4UPP8 |
| A | -1 | GLN | - | expression tag | UNP H4UPP8 |
| A | 0 | GLY | - | expression tag | UNP H4UPP8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| B | -17 | MET | - | expression tag | UNP H4UPP8 |
| B | -16 | HIS | - | expression tag | UNP H4UPP8 |
| B | -15 | HIS | - | expression tag | UNP H4UPP8 |
| B | -14 | HIS | - | expression tag | UNP H4UPP8 |
| B | -13 | HIS | - | expression tag | UNP H4UPP8 |
| B | -12 | HIS | - | expression tag | UNP H4UPP8 |
| B | -11 | HIS | - | expression tag | UNP H4UPP8 |
| B | -10 | GLN | - | expression tag | UNP H4UPP8 |
| B | -9 | HIS | - | expression tag | UNP H4UPP8 |
| B | -8 | GLN | - | expression tag | UNP H4UPP8 |
| B | -7 | HIS | - | expression tag | UNP H4UPP8 |
| B | -6 | GLU | - | expression tag | UNP H4UPP8 |
| B | -5 | ASN | - | expression tag | UNP H4UPP8 |
| B | -4 | LEU | - | expression tag | UNP H4UPP8 |
| B | -3 | TYR | - | expression tag | UNP H4UPP8 |
| B | -2 | PHE | - | expression tag | UNP H4UPP8 |
| B | -1 | GLN | - | expression tag | UNP H4UPP8 |
| B | 0 | GLY | - | expression tag | UNP H4UPP8 |
| C | -17 | MET | - | expression tag | UNP H4UPP8 |
| C | -16 | HIS | - | expression tag | UNP H4UPP8 |
| C | -15 | HIS | - | expression tag | UNP H4UPP8 |
| C | -14 | HIS | - | expression tag | UNP H4UPP8 |
| C | -13 | HIS | - | expression tag | UNP H4UPP8 |
| C | -12 | HIS | - | expression tag | UNP H4UPP8 |
| C | -11 | HIS | - | expression tag | UNP H4UPP8 |
| C | -10 | GLN | - | expression tag | UNP H4UPP8 |
| C | -9 | HIS | - | expression tag | UNP H4UPP8 |
| C | -8 | GLN | - | expression tag | UNP H4UPP8 |
| C | -7 | HIS | - | expression tag | UNP H4UPP8 |
| C | -6 | GLU | - | expression tag | UNP H4UPP8 |
| C | -5 | ASN | - | expression tag | UNP H4UPP8 |
| C | -4 | LEU | - | expression tag | UNP H4UPP8 |
| C | -3 | TYR | - | expression tag | UNP H4UPP8 |
| C | -2 | PHE | - | expression tag | UNP H4UPP8 |
| C | -1 | GLN | - | expression tag | UNP H4UPP8 |
| C | 0 | GLY | - | expression tag | UNP H4UPP8 |
| D | -17 | MET | - | expression tag | UNP H4UPP8 |
| D | -16 | HIS | - | expression tag | UNP H4UPP8 |
| D | -15 | HIS | - | expression tag | UNP H4UPP8 |
| D | -14 | HIS | - | expression tag | UNP H4UPP8 |
| D | -13 | HIS | - | expression tag | UNP H4UPP8 |
| D | -12 | HIS | - | expression tag | UNP H4UPP8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| D | -11 | HIS | - | expression tag | UNP H4UPP8 |
| D | -10 | GLN | - | expression tag | UNP H4UPP8 |
| D | -9 | HIS | - | expression tag | UNP H4UPP8 |
| D | -8 | GLN | - | expression tag | UNP H4UPP8 |
| D | -7 | HIS | - | expression tag | UNP H4UPP8 |
| D | -6 | GLU | - | expression tag | UNP H4UPP8 |
| D | -5 | ASN | - | expression tag | UNP H4UPP8 |
| D | -4 | LEU | - | expression tag | UNP H4UPP8 |
| D | -3 | TYR | - | expression tag | UNP H4UPP8 |
| D | -2 | PHE | - | expression tag | UNP H4UPP8 |
| D | -1 | GLN | - | expression tag | UNP H4UPP8 |
| D | 0 | GLY | - | expression tag | UNP H4UPP8 |
| E | -17 | MET | - | expression tag | UNP H4UPP8 |
| E | -16 | HIS | - | expression tag | UNP H4UPP8 |
| E | -15 | HIS | - | expression tag | UNP H4UPP8 |
| E | -14 | HIS | - | expression tag | UNP H4UPP8 |
| E | -13 | HIS | - | expression tag | UNP H4UPP8 |
| E | -12 | HIS | - | expression tag | UNP H4UPP8 |
| E | -11 | HIS | - | expression tag | UNP H4UPP8 |
| E | -10 | GLN | - | expression tag | UNP H4UPP8 |
| E | -9 | HIS | - | expression tag | UNP H4UPP8 |
| E | -8 | GLN | - | expression tag | UNP H4UPP8 |
| E | -7 | HIS | - | expression tag | UNP H4UPP8 |
| E | -6 | GLU | - | expression tag | UNP H4UPP8 |
| E | -5 | ASN | - | expression tag | UNP H4UPP8 |
| E | -4 | LEU | - | expression tag | UNP H4UPP8 |
| E | -3 | TYR | - | expression tag | UNP H4UPP8 |
| E | -2 | PHE | - | expression tag | UNP H4UPP8 |
| E | -1 | GLN | - | expression tag | UNP H4UPP8 |
| E | 0 | GLY | - | expression tag | UNP H4UPP8 |
| F | -17 | MET | - | expression tag | UNP H4UPP8 |
| F | -16 | HIS | - | expression tag | UNP H4UPP8 |
| F | -15 | HIS | - | expression tag | UNP H4UPP8 |
| F | -14 | HIS | - | expression tag | UNP H4UPP8 |
| F | -13 | HIS | - | expression tag | UNP H4UPP8 |
| F | -12 | HIS | - | expression tag | UNP H4UPP8 |
| F | -11 | HIS | - | expression tag | UNP H4UPP8 |
| F | -10 | GLN | - | expression tag | UNP H4UPP8 |
| F | -9 | HIS | - | expression tag | UNP H4UPP8 |
| F | -8 | GLN | - | expression tag | UNP H4UPP8 |
| F | -7 | HIS | - | expression tag | UNP H4UPP8 |
| F | -6 | GLU | - | expression tag | UNP H4UPP8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | -5 | ASN | - | expression tag | UNP H4UPP8 |
| F | -4 | LEU | - | expression tag | UNP H4UPP8 |
| F | -3 | TYR | - | expression tag | UNP H4UPP8 |
| F | -2 | PHE | - | expression tag | UNP H4UPP8 |
| F | -1 | GLN | - | expression tag | UNP H4UPP8 |
| F | 0 | GLY | - | expression tag | UNP H4UPP8 |

- Molecule 2 is a protein called Phospholipid ABC transporter permease protein MlaE.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | G | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 1926 | 1261 | 323 | 330 | 12 | | |
| 2 | H | 255 | Total | C | N | O | S | 0 | 0 |
| | | | 1918 | 1257 | 321 | 328 | 12 | | |

- Molecule 3 is a protein called Phospholipid transport system ATP-binding protein MlaF.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | I | 263 | Total | C | N | O | S | 0 | 0 |
| | | | 1996 | 1268 | 352 | 362 | 14 | | |
| 3 | J | 263 | Total | C | N | O | S | 0 | 0 |
| | | | 1996 | 1268 | 352 | 362 | 14 | | |

- Molecule 4 is a protein called Phospholipid ABC transporter-binding protein MlaB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | K | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 734 | 464 | 124 | 143 | 3 | | |
| 4 | L | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 734 | 464 | 124 | 143 | 3 | | |

- Molecule 5 is a protein called MSP1D1.

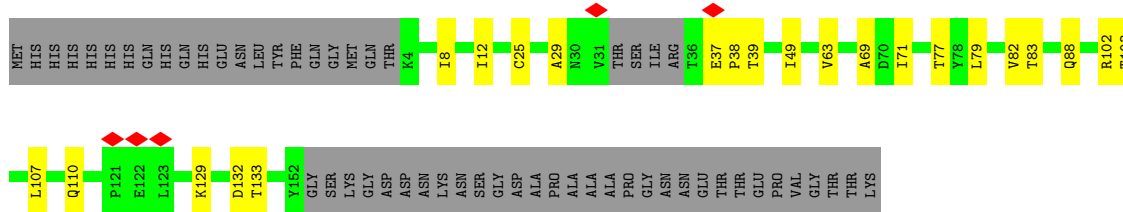| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 5 | M | 164 | Total | C | N | O | 0 | 0 |
| | | | 821 | 492 | 164 | 165 | | |
| 5 | N | 156 | Total | C | N | O | 0 | 0 |
| | | | 780 | 468 | 156 | 156 | | |

- Molecule 6 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$) (labeled as "Ligand of Interest" by depositor).
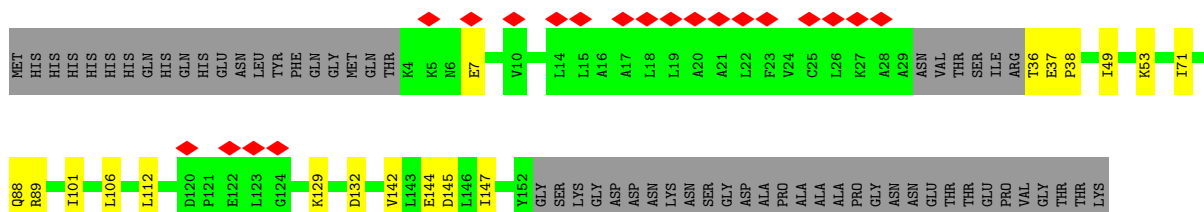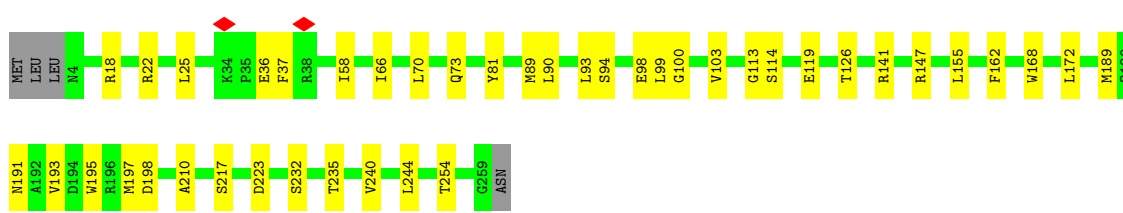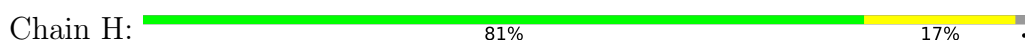
PEF

| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|-----|-----|-----|---------|
| 6 | G | 1 | Total | C | O | P | 0 |
| | | | 44 | 35 | 8 | 1 | |
| 6 | G | 1 | Total | C | O | P | 0 |
| | | | 44 | 35 | 8 | 1 | |

# 3 Residue-property plots ⓘ

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: Phospholipid ABC transporter-binding protein MlaD

Chain A:



- Molecule 1: Phospholipid ABC transporter-binding protein MlaD

Chain B:



- Molecule 1: Phospholipid ABC transporter-binding protein MlaD

Chain C:



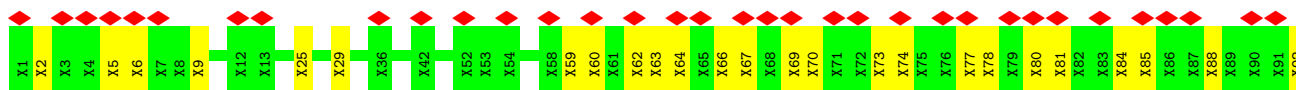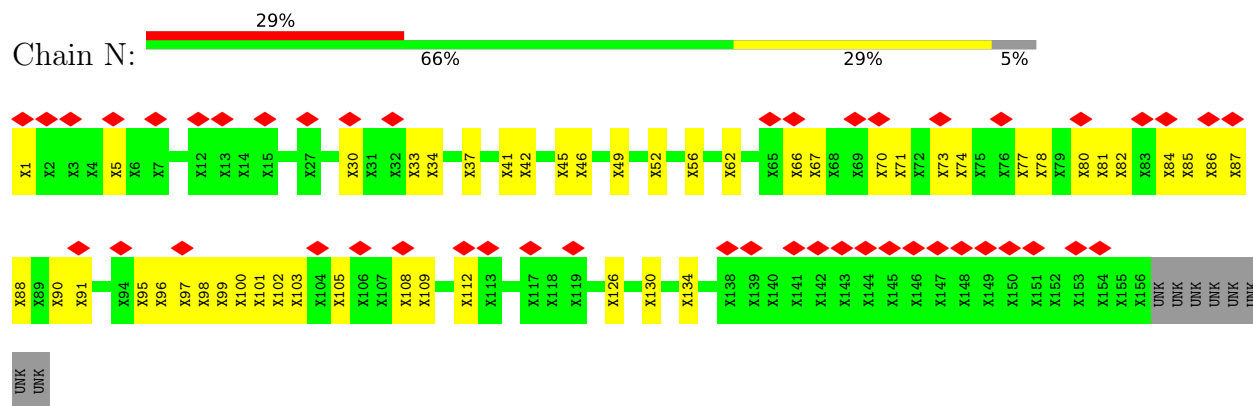- Molecule 1: Phospholipid ABC transporter-binding protein MlaD

Chain D:

64%     7%     29%

MET HIS HIS HIS HIS HIS GLN HIS GLN HIS GLU ASN LEU TYR PHE GLN GLY MET Q2 K5 K27 A28 A29 ASN VAL THR SER ILE ARG T36 E37 I49 A69 D70 I71 T72 L73 T83 R102 P121 GLU LEU G124 D132 T133 V142 Y152 GLY SER

LYS GLY ASP ASP ASN LYS ASN SER GLY ASP ALA PRO ALA ALA PRO GLY ASN ASN GLU THR THR GLU PRO VAL GLY THR THR LYS

• Molecule 1: Phospholipid ABC transporter-binding protein MlaD

Chain E:

61%     11%     28%

MET HIS HIS HIS HIS HIS GLN HIS GLN HIS GLU ASN LEU TYR PHE GLN GLY MET GLN THR K4 I8 I12 C25 A29 N30 V31 THR SER ILE ARG T36 E37 P38 T39 I49 V63 A69 D70 I71 T77 Y78 L79 V82 T83 Q88 R102 T103

L107 Q110 P121 E122 L123 K129 D132 T133 Y152 GLY SER LYS GLY ASP ASN LYS ASN SER GLY ASP ALA PRO ALA ALA PRO GLY ASN ASN GLU THR THR GLU PRO VAL GLY THR THR LYS

• Molecule 1: Phospholipid ABC transporter-binding protein MlaD

Chain F:

10%

62%     9%     29%

MET HIS HIS HIS HIS HIS GLN HIS GLN HIS GLU ASN LEU TYR PHE GLN GLY MET GLN THR K4 K5 N6 E7 V10 L14 L15 A16 A17 L18 L19 A20 A21 L22 F23 V24 C25 L26 K27 A28 A29 ASN VAL THR SER ILE ARG T36 E37 P38 I49 K53 I71

Q88 R89 I101 L106 L112 D120 P121 E122 L123 G124 K129 D132 V142 L143 E144 D145 L146 I147 Y152 GLY SER LYS GLY ASP ASP ASN LYS SER ASN SER GLY ASP ALA PRO ALA ALA ALA PRO GLY ASN ASN GLU THR THR GLU PRO VAL GLY THR THR LYS

• Molecule 2: Phospholipid ABC transporter permease protein MlaE

Chain G:

82%     16%   •

MET LEU LEU N4 R18 R22 L25 K34 P35 E36 F37 R38 I58 I66 L70 Q73 Y81 M89 L90 L93 S94 E98 L99 G100 V103 G113 S114 E119 T126 R141 R147 L155 F162 W168 L172 M189 Q190

N191 A192 V193 D194 W195 R196 M197 D198 A210 S217 D223 S232 T235 V240 L244 T254 G259 ASN

• Molecule 2: Phospholipid ABC transporter permease protein MlaE

Chain H:

81%     17%   •

MET LEU LEU ASN A5 G10 K34 P35 E36 F37 R38 K39 H40 Y49 S55 I58 L70 Y75 S82 L90 L93 E98 L99 G100 F108 G113 S114 A118 E119 M135 P139 L140 R141 R142 V143 I144 S145 P146 R147 F148 W149 L155

F162 W168 L172 W177 V193 D194 K205 A210 I225 P226 T227 G230 T235 V240 L256 M257 F258 G259 ASN

• Molecule 3: Phospholipid transport system ATP-binding protein MlaF

Chain I:

79%    19%    ·

MET GLU GLN SER V5 D13 C22 S28 I39 M40 I45 T49 L50 L51 R52 L53 I58 F67 I72 M87 A95 M100 N101 D104 N105 V106 K128 L129 E130 A131 R135 G136 A137 L140 S146 G147 R151 R157 A160

L165 I166 M167 E170 P171 G181 V184 V201 S202 H203 L209 L218 K221 L232 R241 Q242 V252 R255 G259 D260 L266 P267 GLY SER

• Molecule 3: Phospholipid transport system ATP-binding protein MlaF

Chain J:

79%    19%    ·

MET GLU GLN SER V5 D13 C22 S28 I39 M40 I45 T49 L50 L51 R52 L53 I58 F67 I72 K85 R86 M87 Q92 A95 M100 D104 N105 V106 H113 K128 L129 E130 A131 R135 G136 A137 L140 S146 G147 R151

R157 A160 L165 I166 M167 E170 P171 G181 V184 V201 S202 H203 L209 L218 K221 L232 R241 Q242 V252 R255 D260 P267 GLY SER

• Molecule 4: Phospholipid ABC transporter-binding protein MlaB

Chain K:

68%    30%    ·

MET SER E3 S6 W7 L14 S17 D21 Q22 D23 V24 L25 L26 E30 I39 L44 D51 L55 L59 I62 K66 N70 L74 V77 K80 V81 Y82 A85 Y88 N89 L90 D93 V94 L95 P96 R97

• Molecule 4: Phospholipid ABC transporter-binding protein MlaB

Chain L:

68%    30%    ·

MET SER E3 S6 W7 L14 S17 D21 Q22 D23 V24 L25 L26 E30 I39 L44 D51 L55 L59 I62 D63 K66 N70 L74 V77 K80 V81 A85 Y88 N89 L90 D93 V94 L95 P96 R97

• Molecule 5: MSP1D1

Chain M:

34%

75%    25%

X1 X2 X3 X4 X5 X6 X7 X8 X9 X12 X13 X25 X29 X36 X42 X52 X53 X54 X58 X59 X60 X61 X62 X63 X64 X65 X66 X67 X68 X69 X70 X71 X72 X73 X74 X75 X76 X77 X78 X79 X80 X81 X82 X83 X84 X85 X86 X87 X88 X89 X90 X91 X92

X95 X99 X100 X101 X102 X103 X106 X122 X126 X127 X128 X129 X130 X131 X132 X133 X134 X137 X138 X142 X146 X147 X150 X151 X152 X153 X154 X155 X156 X157 X158 X159 X160 X161 X162 X163 X164

● Molecule 5: MSP1D1

Chain N:

# 4 Experimental information ⓘ

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 731205 | 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 $(e^-/\text{Å}^2)$ | 71 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 29000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 1.904 | Depositor |
| Minimum map value | -0.909 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.071 | Depositor |
| Recommended contour level | 0.27 | Depositor |
| Map size (Å) | 249.6, 249.6, 249.6 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.832, 0.832, 0.832 | 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: PEF

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 | 0.25 | 0/1126 | 0.47 | 0/1531 |
| 1 | B | 0.25 | 0/1081 | 0.43 | 0/1470 |
| 1 | C | 0.25 | 0/1047 | 0.47 | 0/1429 |
| 1 | D | 0.25 | 0/1113 | 0.43 | 0/1512 |
| 1 | E | 0.25 | 0/1130 | 0.45 | 0/1537 |
| 1 | F | 0.25 | 0/1042 | 0.47 | 0/1422 |
| 2 | G | 0.26 | 0/1964 | 0.45 | 0/2669 |
| 2 | H | 0.26 | 0/1956 | 0.44 | 0/2658 |
| 3 | I | 0.25 | 0/2036 | 0.43 | 0/2764 |
| 3 | J | 0.25 | 0/2036 | 0.43 | 0/2764 |
| 4 | K | 0.26 | 0/743 | 0.44 | 0/1008 |
| 4 | L | 0.26 | 0/743 | 0.44 | 0/1008 |
| All | All | 0.25 | 0/16017 | 0.44 | 0/21772 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1108 | 0 | 1133 | 22 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | B | 1063 | 0 | 1082 | 21 | 0 |
| 1 | C | 1033 | 0 | 973 | 14 | 0 |
| 1 | D | 1096 | 0 | 1120 | 11 | 0 |
| 1 | E | 1112 | 0 | 1138 | 16 | 0 |
| 1 | F | 1028 | 0 | 971 | 21 | 0 |
| 2 | G | 1926 | 0 | 2029 | 46 | 0 |
| 2 | H | 1918 | 0 | 2023 | 37 | 0 |
| 3 | I | 1996 | 0 | 2039 | 30 | 0 |
| 3 | J | 1996 | 0 | 2039 | 32 | 0 |
| 4 | K | 734 | 0 | 755 | 20 | 0 |
| 4 | L | 734 | 0 | 755 | 21 | 0 |
| 5 | M | 821 | 0 | 166 | 22 | 0 |
| 5 | N | 780 | 0 | 158 | 29 | 0 |
| 6 | G | 88 | 0 | 134 | 9 | 0 |
| All | All | 17433 | 0 | 16515 | 298 | 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 9.

The worst 5 of 298 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:F:53:LYS:CD | 2:G:191:ASN:HD22 | 1.61 | 1.13 |
| 1:F:53:LYS:HD3 | 2:G:191:ASN:ND2 | 1.68 | 1.07 |
| 1:F:53:LYS:CD | 2:G:191:ASN:ND2 | 2.30 | 0.91 |
| 1:F:53:LYS:CG | 2:G:191:ASN:HD22 | 1.84 | 0.89 |
| 2:G:89:MET:HG3 | 2:G:193:VAL:HG21 | 1.53 | 0.87 |

There are no symmetry-related clashes.

## 5.3   Torsion angles  ⓘ

### 5.3.1   Protein backbone  ⓘ

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 | 140/201 (70%) | 136 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | B | 134/201 (67%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 1 | C | 140/201 (70%) | 137 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | D | 137/201 (68%) | 134 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | E | 141/201 (70%) | 131 (93%) | 10 (7%) | 0 | 100 | 100 |
| 1 | F | 139/201 (69%) | 132 (95%) | 7 (5%) | 0 | 100 | 100 |
| 2 | G | 254/260 (98%) | 248 (98%) | 6 (2%) | 0 | 100 | 100 |
| 2 | H | 253/260 (97%) | 242 (96%) | 11 (4%) | 0 | 100 | 100 |
| 3 | I | 261/269 (97%) | 253 (97%) | 8 (3%) | 0 | 100 | 100 |
| 3 | J | 261/269 (97%) | 253 (97%) | 8 (3%) | 0 | 100 | 100 |
| 4 | K | 93/97 (96%) | 90 (97%) | 3 (3%) | 0 | 100 | 100 |
| 4 | L | 93/97 (96%) | 90 (97%) | 3 (3%) | 0 | 100 | 100 |
| All | All | 2046/2458 (83%) | 1975 (96%) | 71 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2　Protein sidechains ⓘ

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 | 121/167 (72%) | 121 (100%) | 0 | 100 | 100 |
| 1 | B | 116/167 (70%) | 116 (100%) | 0 | 100 | 100 |
| 1 | C | 100/167 (60%) | 100 (100%) | 0 | 100 | 100 |
| 1 | D | 119/167 (71%) | 119 (100%) | 0 | 100 | 100 |
| 1 | E | 121/167 (72%) | 121 (100%) | 0 | 100 | 100 |
| 1 | F | 100/167 (60%) | 100 (100%) | 0 | 100 | 100 |
| 2 | G | 205/209 (98%) | 204 (100%) | 1 (0%) | 88 | 94 |
| 2 | H | 204/209 (98%) | 204 (100%) | 0 | 100 | 100 |
| 3 | I | 215/220 (98%) | 215 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|-------------|---|
| 3 | J | 215/220 (98%) | 215 (100%) | 0 | 100 | 100 |
| 4 | K | 82/84 (98%) | 82 (100%) | 0 | 100 | 100 |
| 4 | L | 82/84 (98%) | 82 (100%) | 0 | 100 | 100 |
| All | All | 1680/2028 (83%) | 1679 (100%) | 1 (0%) | 93 | 97 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G | 197 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G | 191 | ASN |
| 3 | I | 191 | ASN |
| 3 | J | 226 | HIS |
| 3 | I | 226 | HIS |
| 1 | B | 91 | ASN |

### 5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6　Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| | | | | | Counts | RMSZ | #$|Z| > 2$ | Counts | RMSZ | #$|Z| > 2$ |
| 6 | PEF | G | 301 | - | 43,43,46 | 1.06 | 2 (4%) | 47,48,51 | 0.91 | 2 (4%) |
| 6 | PEF | G | 302 | - | 43,43,46 | 1.06 | 2 (4%) | 47,48,51 | 0.93 | 2 (4%) |

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 | PEF | G | 301 | - | - | 24/45/45/50 | - |
| 6 | PEF | G | 302 | - | - | 27/45/45/50 | - |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 6 | G | 302 | PEF | O2-C10 | 3.68 | 1.44 | 1.34 |
| 6 | G | 301 | PEF | O2-C10 | 3.62 | 1.44 | 1.34 |
| 6 | G | 302 | PEF | O3-C30 | 2.67 | 1.41 | 1.33 |
| 6 | G | 301 | PEF | O3-C30 | 2.67 | 1.41 | 1.33 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 6 | G | 302 | PEF | O2-C10-C11 | 3.88 | 119.87 | 111.50 |
| 6 | G | 301 | PEF | O2-C10-C11 | 3.84 | 119.77 | 111.50 |
| 6 | G | 301 | PEF | O3-C30-C31 | 2.67 | 120.29 | 111.91 |
| 6 | G | 302 | PEF | O3-C30-C31 | 2.64 | 120.20 | 111.91 |

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
| --- | --- | --- | --- | --- |
| 6 | G | 301 | PEF | C31-C30-O3-C3 |
| 6 | G | 301 | PEF | O5-C30-O3-C3 |
| 6 | G | 302 | PEF | C31-C30-O3-C3 |
| 6 | G | 302 | PEF | O5-C30-O3-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 6 | G | 301 | PEF | C34-C35-C36-C37 |

There are no ring outliers.

2 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6 | G | 301 | PEF | 3 | 0 |
| 6 | G | 302 | PEF | 6 | 0 |

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

**Ligand PEF G 301**



Bond lengths

Bond angles

Torsions

Rings

**Ligand PEF G 302**



Bond lengths

Bond angles

Torsions

Rings
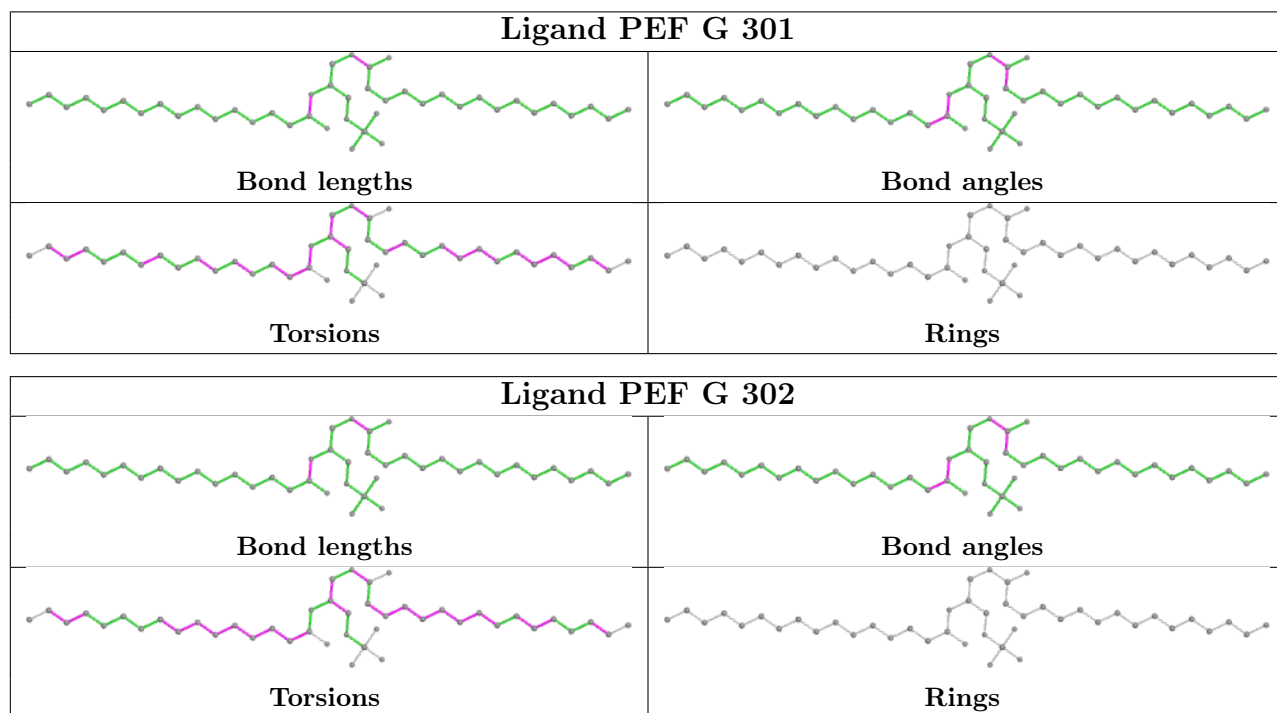
## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-22116. 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  |
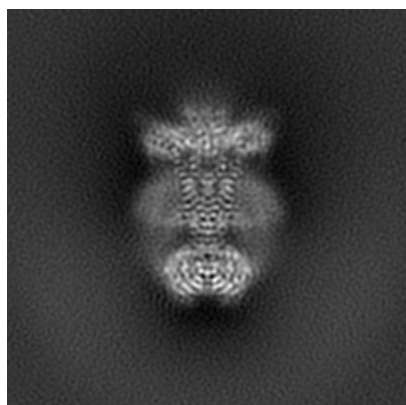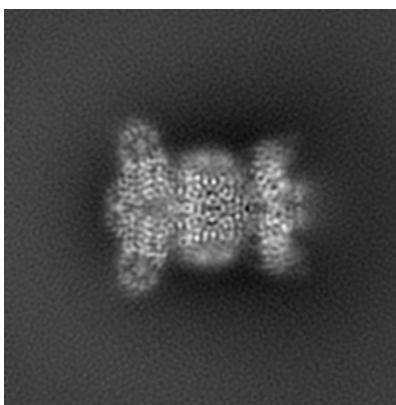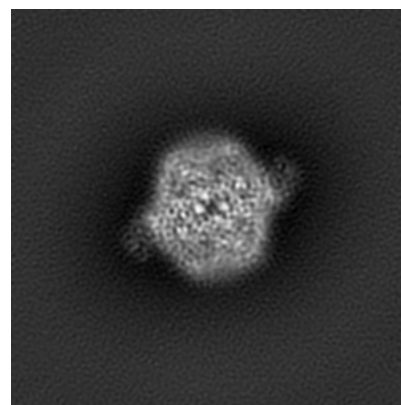
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices ⓘ
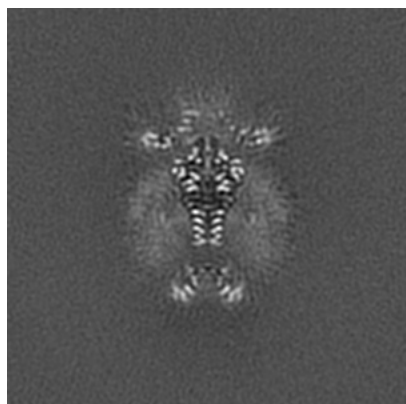
### 6.2.1 Primary map
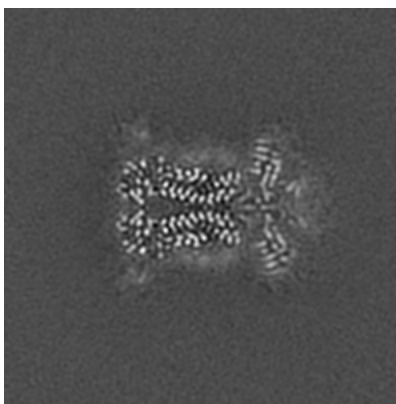


| X Index: 150 | Y Index: 150 | Z Index: 150 |
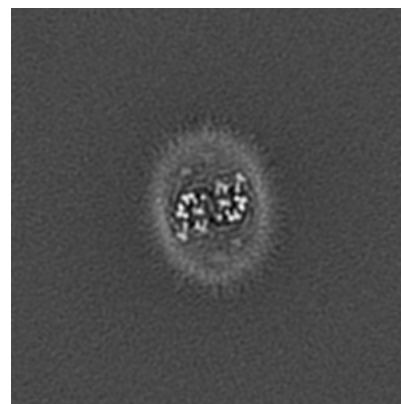
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

### 6.3.1 Primary map
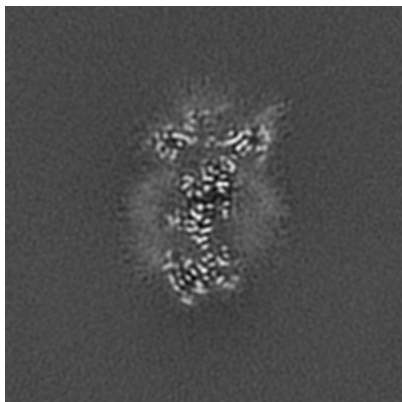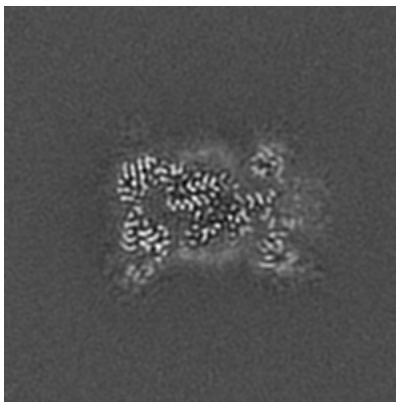


| X Index: 162 | Y Index: 144 | Z Index: 198 |
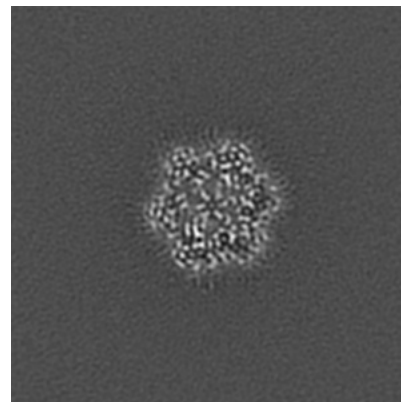
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



| X | Y | Z |
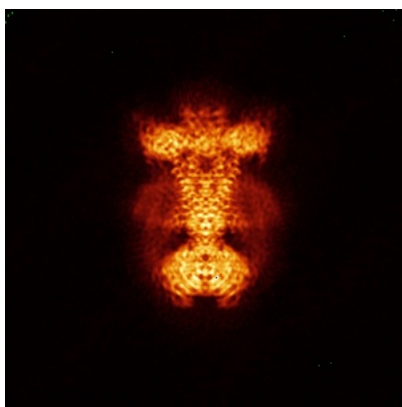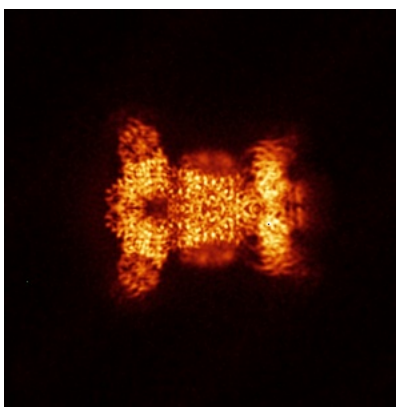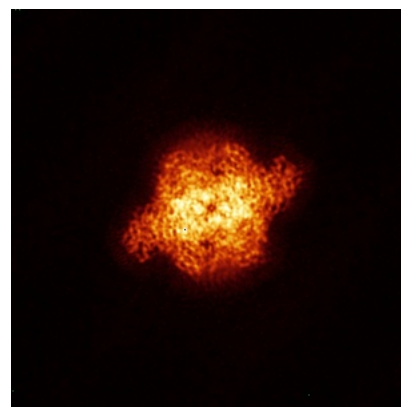
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5    Orthogonal surface views (i)

### 6.5.1    Primary map
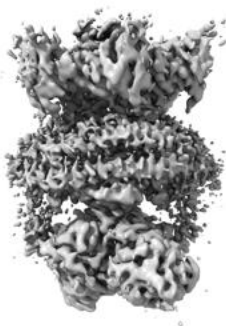


X                      Y                      Z
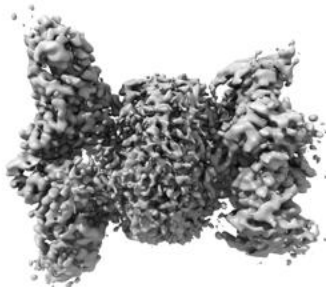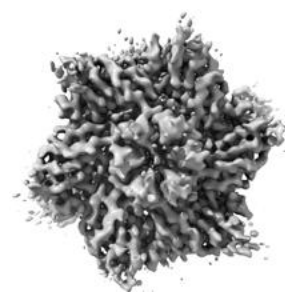
The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 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 ⓘ
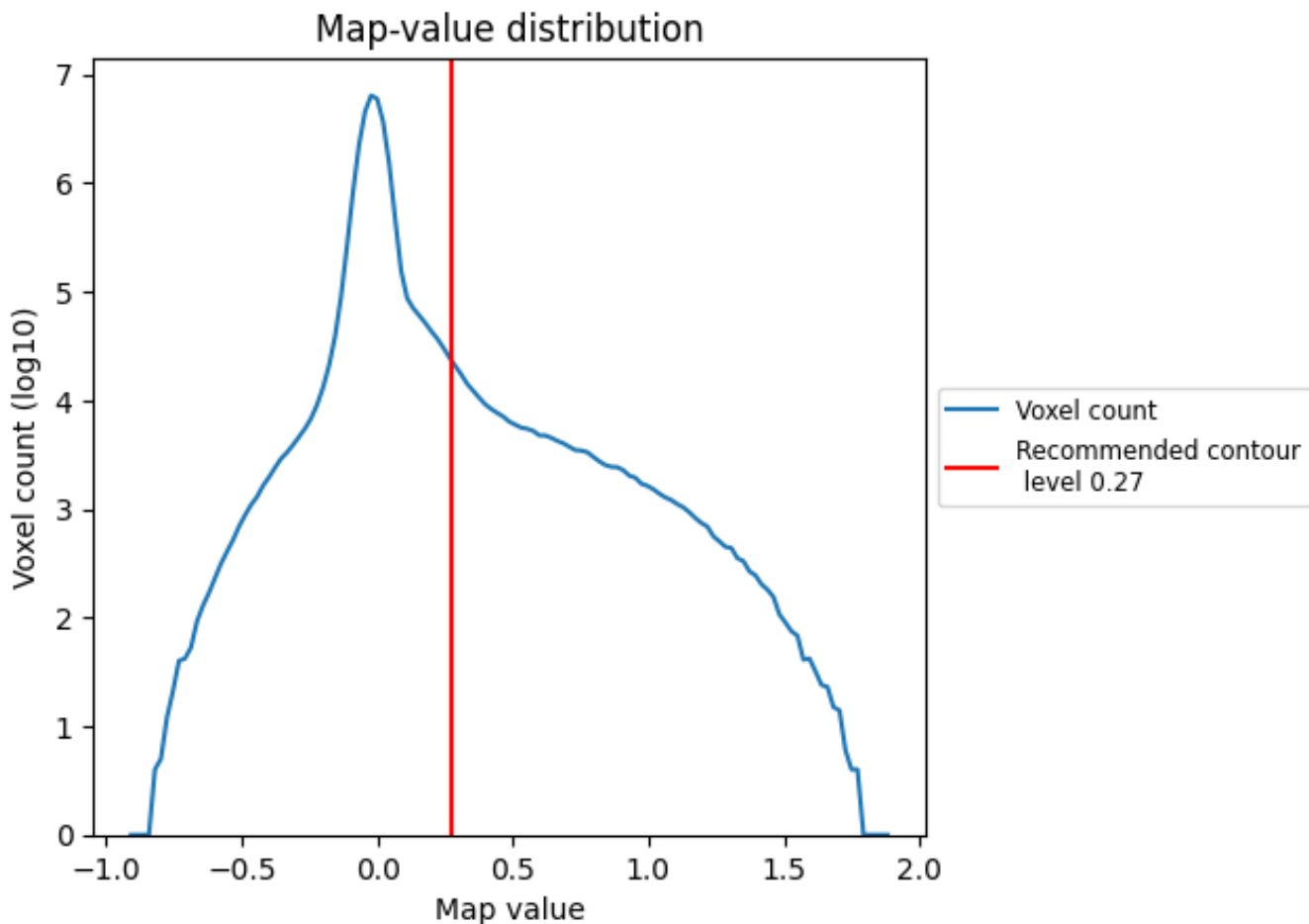


The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2   Volume estimate ⓘ
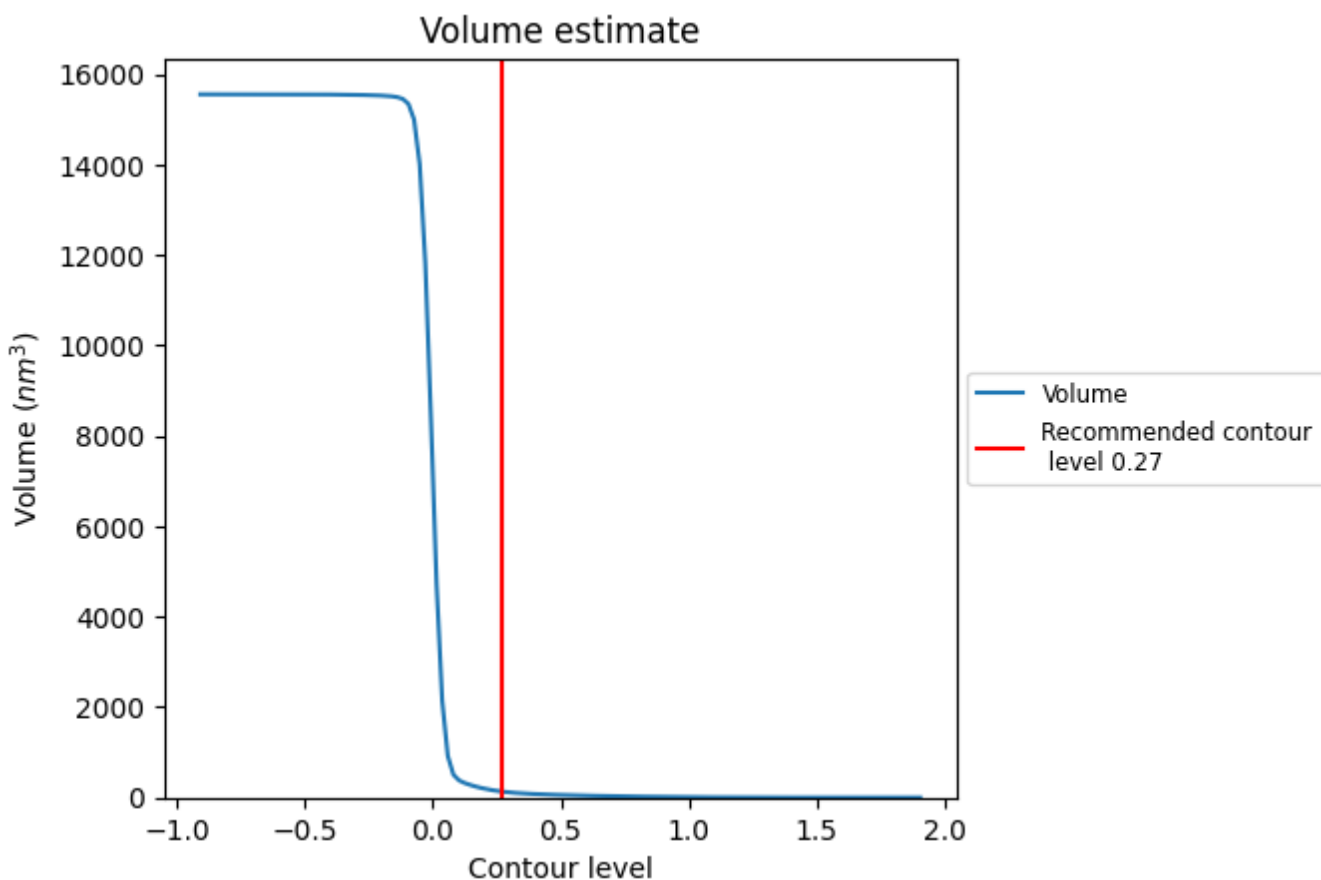


The volume at the recommended contour level is 132 nm$^3$; this corresponds to an approximate mass of 120 kDa.

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 ⓘ
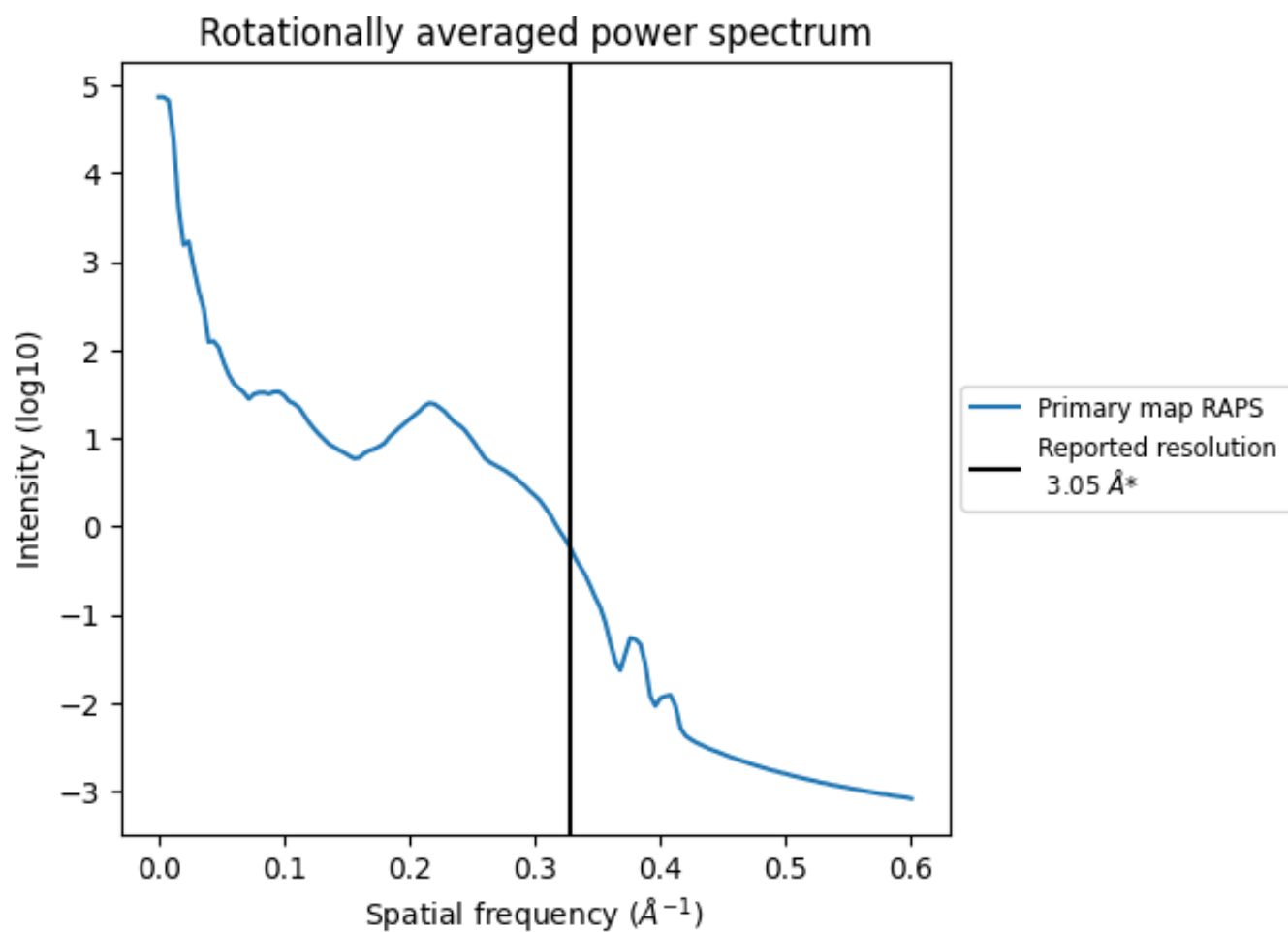


*Reported resolution corresponds to spatial frequency of 0.328 $\text{Å}^{-1}$

# 8 Fourier-Shell correlation ⓘ

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

# 9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22116 and PDB model 6XBD. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1   Map-model overlay (i)



|  |  |  |
| --- | --- | --- |
| X | Y | Z |
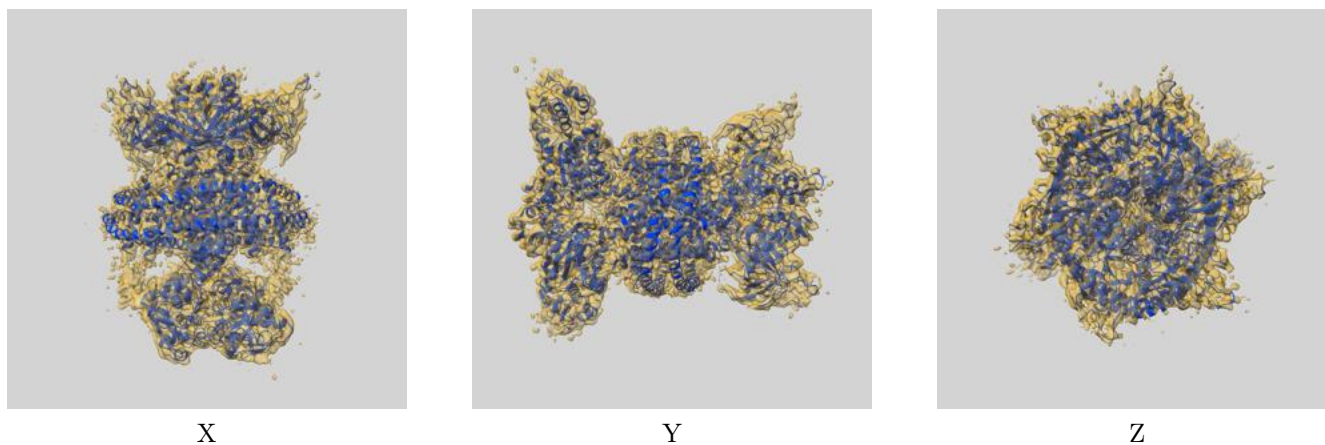
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2　Q-score mapped to coordinate model ⓘ



X　　　　　　　　　　　Y　　　　　　　　　　　Z
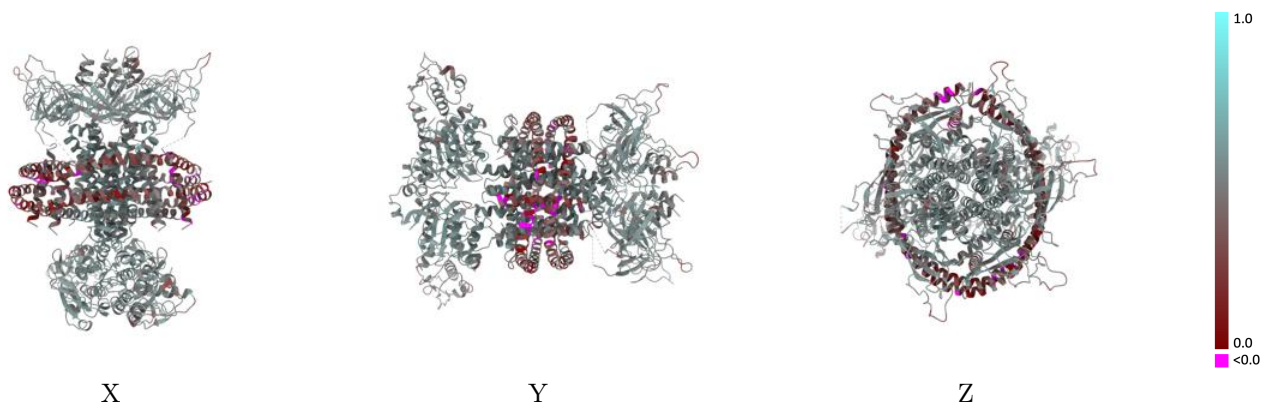
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3　Atom inclusion mapped to coordinate model ⓘ



X　　　　　　　　　　　Y　　　　　　　　　　　Z
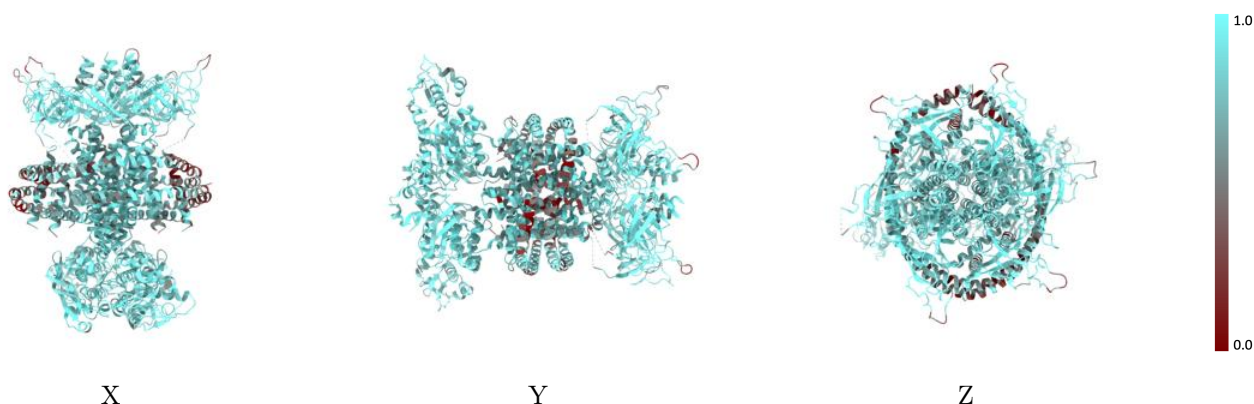
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.27).

## 9.4   Atom inclusion ⓘ
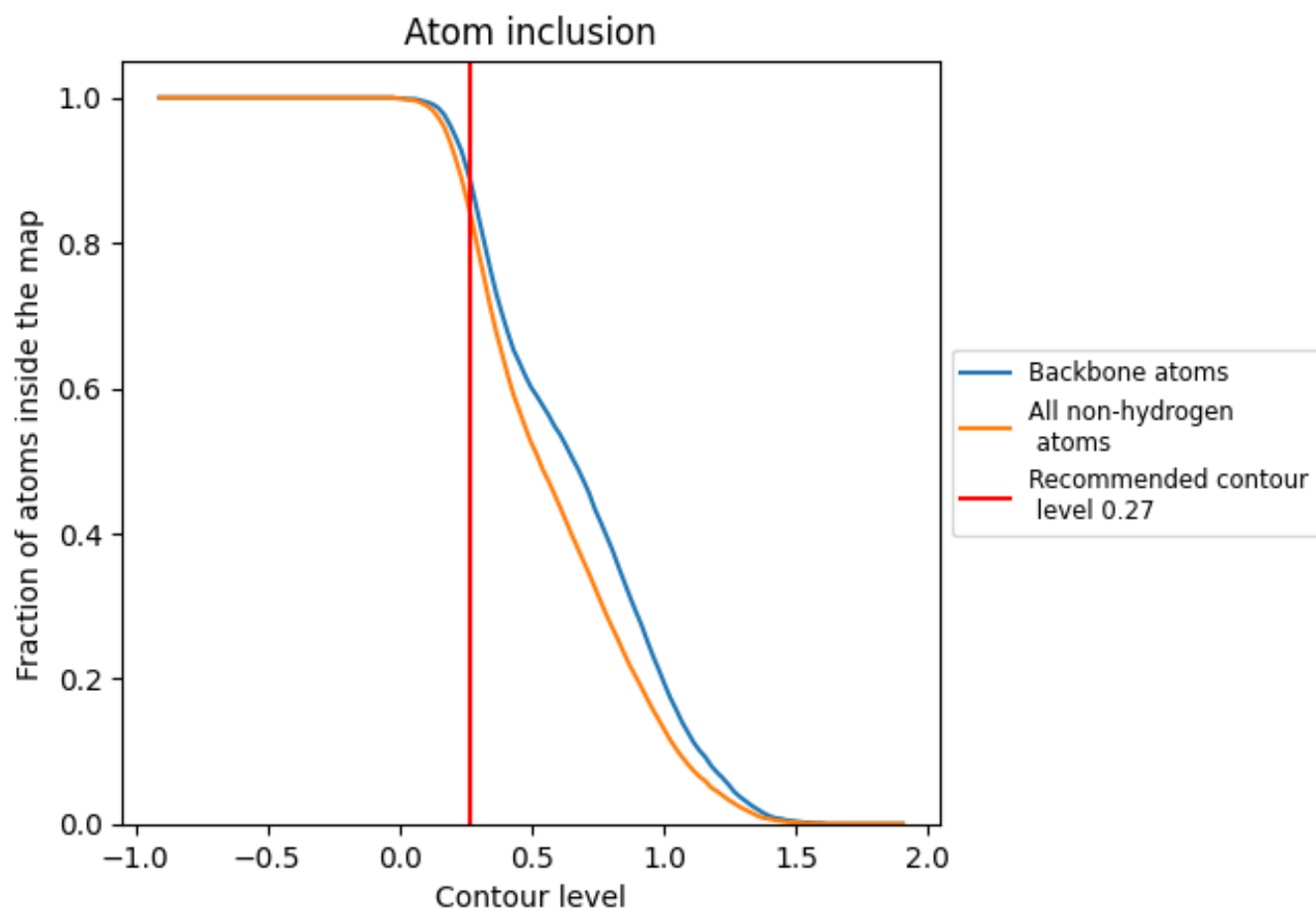


At the recommended contour level, 88% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.27) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.8370 | 0.4890 |
| A | 0.8480 | 0.5030 |
| B | 0.8270 | 0.4930 |
| C | 0.8510 | 0.4950 |
| D | 0.8650 | 0.5060 |
| E | 0.8310 | 0.4940 |
| F | 0.8040 | 0.4680 |
| G | 0.8660 | 0.5350 |
| H | 0.8700 | 0.5330 |
| I | 0.9010 | 0.5360 |
| J | 0.8940 | 0.5360 |
| K | 0.8300 | 0.4880 |
| L | 0.8380 | 0.4710 |
| M | 0.6050 | 0.2450 |
| N | 0.6310 | 0.2680 |

1.0

0.0
<0.0