# Full wwPDB EM Validation Report ⓘ

Oct 31, 2026 – 09:14 am GMT

| | | |
|---|---|---|
| PDB ID | : | 9TGQ / pdb_00009tgq |
| EMDB ID | : | EMD-55908 |
| Title | : | Cryo-EM structure of tail-engaged TamAB complex |
| Authors | : | Dong, H.; Tang, X.; Luo, Q.; Zerang, Z. |
| Deposited on | : | 2025-12-02 |
| Resolution | : | 3.86 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.

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

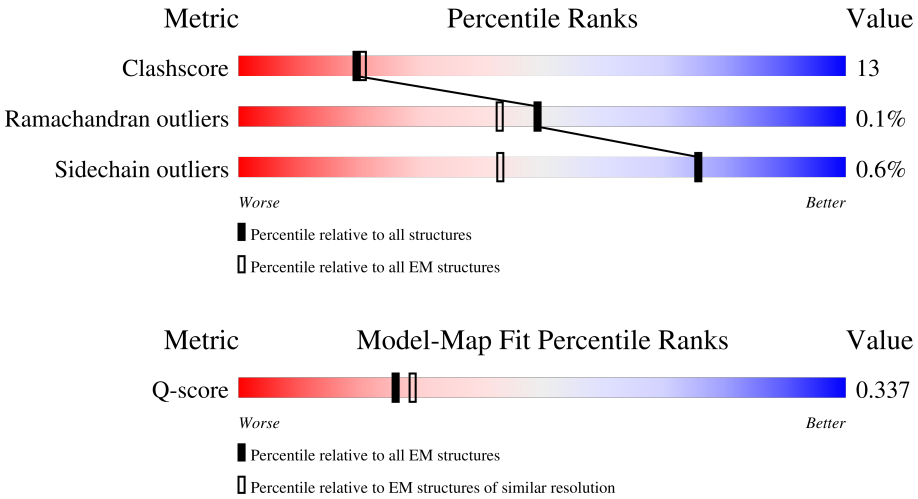
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| MolProbity | : | 4-5-2 with Phenix2.2 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| 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 3.86 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 | 8889 ( 3.36 - 4.35 ) |

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 | 577 | 71% 26% |
| 2 | B | 1259 | 32% 14% 54% |

# 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8851 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 Translocation and assembly module subunit TamA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 556 | 4427 | 2815 | 769 | 838 | 5 | 0 | 0 |

- Molecule 2 is a protein called Translocation and assembly module subunit TamB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 581 | 4424 | 2775 | 776 | 857 | 16 | 0 | 0 |

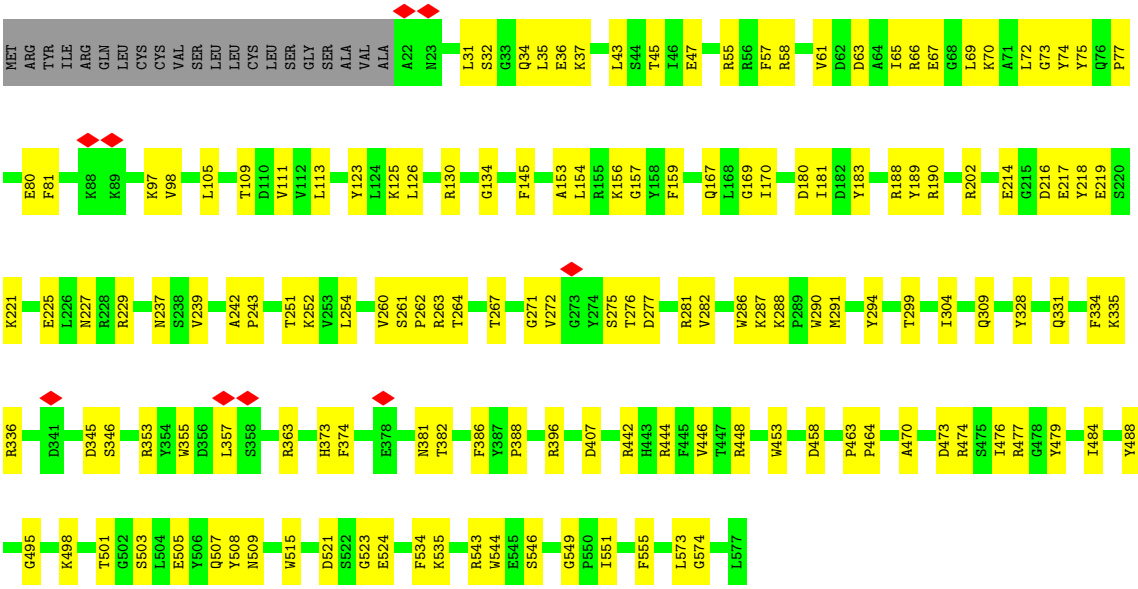
# 3 Residue-property plots (i)

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: Translocation and assembly module subunit TamA

Chain A:

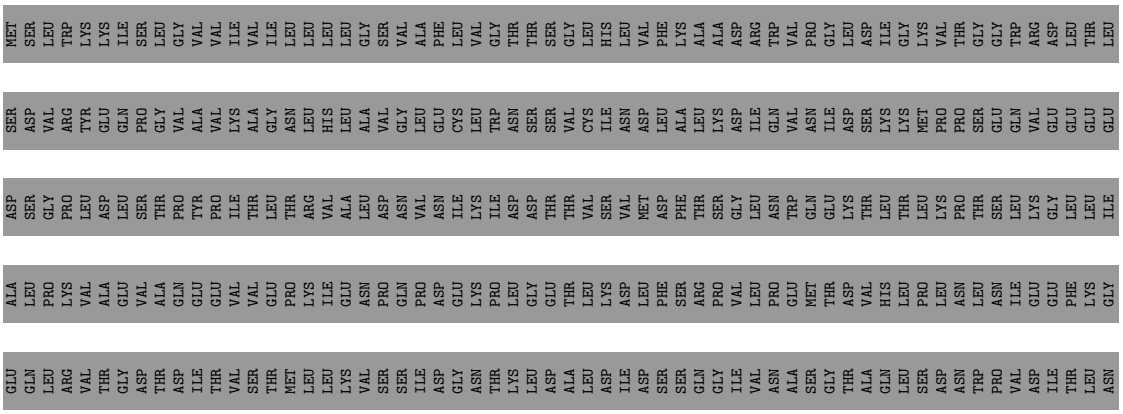


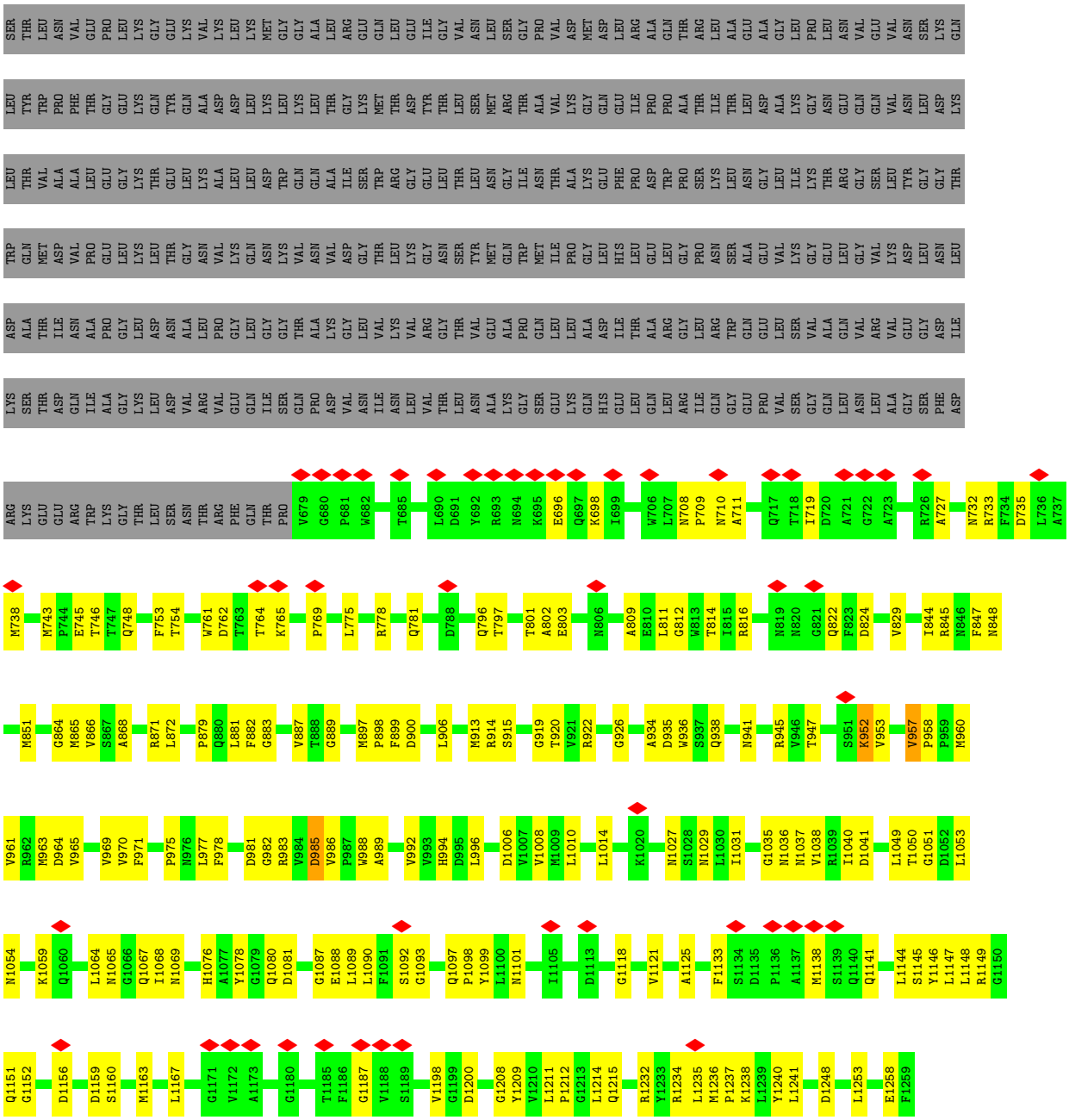




• Molecule 2: Translocation and assembly module subunit TamB

Chain B:




SER THR LEU ASN VAL GLU PRO LEU LYS GLY GLU LYS VAL LYS LEU LYS MET GLY GLY ALA LEU ARG GLU GLN LEU GLU ILE GLY VAL ASN LEU SER GLY PRO VAL ASP MET ASP LEU ARG ALA GLN THR ARG LEU ALA GLU ALA GLY LEU PRO LEU ASN VAL GLU VAL ASN SER LYS GLN
LEU TYR TRP PRO PHE THR GLY GLU LYS GLN TYR GLN ALA ASP ASP LEU LYS LEU LYS LEU THR GLY LYS MET THR ASP TYR THR LEU SER MET ARG THR ALA VAL LYS GLY GLN GLU ILE PRO PRO ALA THR ILE THR LEU ASP ALA LYS GLY ILE GLU GLN GLN VAL ASN LEU ASP LYS
LEU THR VAL ALA ALA LEU GLU GLY LYS THR GLU LEU LYS ALA ALA LEU LEU ASP TRP GLN LEU GLN ALA ILE SER TRP ARG GLY GLU LEU THR LEU ASN SER TYR MET GLN TRP MET ILE PRO GLY GLU PHE PRO ASP PRO PRO ALA THR ALA VAL LYS GLY GLN GLN VAL ASN LEU ASP LYS
TRP GLN MET ASP VAL PRO GLU LEU LYS LEU THR GLY ASN VAL LYS GLN ASN LYS VAL ASN VAL ASP GLY THR LEU LYS GLY ASN SER TYR MET GLN TRP MET ILE PRO GLY GLU HIS LEU GLU GLU LEU GLY PRO ASN SER ALA GLU VAL LYS GLY GLU LEU GLN LEU ASN LEU ARG VAL ASP
ASP ALA THR ILE ASN ALA PRO GLY LEU ASP ASN ALA LEU PRO GLY LEU GLY GLY THR ALA LYS ASN VAL ARG GLY THR VAL LYS VAL LEU ASN ALA LYS GLY LEU ILE THR ALA ARG GLY LEU ARG TRP GLN GLU LEU SER VAL ALA LEU GLN LEU ASN LEU ALA GLY VAL ARG VAL GLU GLY ASP ILE
LYS SER THR ASP GLN ILE ALA GLY LYS LEU ASP VAL ASP VAL ASN ILE ASN LEU VAL THR LEU ASN ALA LYS GLY SER GLU LYS GLN HIS GLU LEU GLN LEU ARG ILE GLN GLY GLU PRO VAL SER GLY GLN LEU ASN LEU ALA GLY SER PHE ASP
ARG LYS GLU GLU ARG TRP LYS GLY THR LEU SER ASN THR ARG PHE GLN THR PRO V679 G680 P681 W682 T685 L690 D691 Y692 R693 N694 K695 E696 Q697 K698 I699 W706 L707 N708 P709 N710 A711 Q717 T718 I719 D720 A721 G722 A723 R726 A727 N732 R733 F734 D735 L736 A737
M738 M743 P744 E745 T746 T747 Q748 F753 T754 W761 D762 T763 T764 K765 P769 L775 R778 Q781 D788 Q796 T797 T801 A802 E803 N806 A809 E810 L811 G812 W813 T814 I815 R816 N819 N820 G821 Q822 F823 D824 V829 I844 R845 N846 F847 N848
M851 G864 M865 V866 S867 A868 R871 L872 P879 Q880 L881 F882 G883 V887 T888 G889 M897 P898 F899 D900 L906 M913 R914 S915 G919 T920 V921 R922 G926 A934 D935 W936 S937 Q938 N941 R945 V946 T947 S951 K952 V953 V957 P958 P959 M960
V961 R962 M963 D964 V965 V969 V970 F971 P975 N976 L977 F978 D981 G982 R983 V984 D985 V986 P987 W988 A989 V992 V993 H994 D995 L996 D1006 V1007 V1008 M1009 L1010 L1014 K1020 N1027 S1028 N1029 L1030 I1031 G1035 N1036 N1037 V1038 R1039 I1040 D1041 L1049 T1050 G1051 D1052 L1053
N1054 K1059 Q1060 L1064 N1065 G1066 Q1067 I1068 N1069 H1076 A1077 Y1078 G1079 Q1080 D1081 G1087 E1088 L1089 L1090 F1091 S1092 G1093 Q1097 P1098 Y1099 L1100 N1101 I1105 D1113 G1118 V1121 A1125 F1133 S1134 D1135 P1136 A1137 M1138 S1139 Q1140 Q1141 L1144 S1145 Y1146 L1147 L1148 R1149 G1150
Q1151 G1152 D1156 D1159 S1160 M1163 L1167 G1171 V1172 A1173 G1180 T1185 F1186 G1187 V1188 S1189 V1198 G1199 D1200 G1208 Y1209 V1210 L1211 P1212 G1213 L1214 Q1215 R1232 Y1233 R1234 L1235 M1236 P1237 K1238 L1239 Y1240 L1241 D1248 L1253 E1258 F1259

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 139788 | 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) | 1500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 1.700 | Depositor |
| Minimum map value | -1.464 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.019 | Depositor |
| Recommended contour level | 0.0976 | Depositor |
| Map size (Å) | 357.12, 357.12, 357.12 | wwPDB |
| Map dimensions | 384, 384, 384 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.93, 0.93, 0.93 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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 | 0.20 | 0/4536 | 0.43 | 0/6151 |
| 2 | B | 0.15 | 0/4503 | 0.43 | 0/6126 |
| All | All | 0.18 | 0/9039 | 0.43 | 0/12277 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | B | 0 | 1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 957 | VAL | Peptide |

## 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 | 4427 | 0 | 4343 | 100 | 0 |
| 2 | B | 4424 | 0 | 4394 | 131 | 0 |
| All | All | 8851 | 0 | 8737 | 221 | 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 13.

All (221) 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:A:353:ARG:HH21 | 1:A:355:TRP:HE1 | 1.31 | 0.77 |
| 2:B:1010:LEU:HD13 | 2:B:1014:LEU:HA | 1.67 | 0.76 |
| 1:A:69:LEU:HB3 | 1:A:74:TYR:HB2 | 1.67 | 0.75 |
| 2:B:710:ASN:HA | 2:B:735:ASP:HB3 | 1.67 | 0.75 |
| 2:B:844:ILE:HD13 | 2:B:868:ALA:HB3 | 1.71 | 0.73 |
| 2:B:1141:GLN:HG2 | 2:B:1163:MET:HB3 | 1.72 | 0.72 |
| 2:B:906:LEU:HD13 | 2:B:919:GLY:HA3 | 1.74 | 0.70 |
| 1:A:272:VAL:HG22 | 1:A:282:VAL:HG23 | 1.73 | 0.69 |
| 2:B:743:MET:HG3 | 2:B:745:GLU:H | 1.58 | 0.69 |
| 1:A:31:LEU:HB2 | 1:A:36:GLU:HG3 | 1.73 | 0.68 |
| 1:A:111:VAL:HG22 | 1:A:181:ILE:HB | 1.75 | 0.68 |
| 1:A:188:ARG:HD3 | 1:A:217:GLU:HG2 | 1.74 | 0.68 |
| 2:B:864:GLY:HA2 | 2:B:889:GLY:HA3 | 1.75 | 0.68 |
| 2:B:914:ARG:NH1 | 2:B:935:ASP:OD1 | 2.28 | 0.67 |
| 2:B:992:VAL:HG12 | 2:B:1041:ASP:HB3 | 1.79 | 0.65 |
| 2:B:732:ASN:HD21 | 2:B:754:THR:HG23 | 1.60 | 0.64 |
| 2:B:797:THR:HG21 | 2:B:816:ARG:HB2 | 1.78 | 0.64 |
| 1:A:544:TRP:HZ3 | 1:A:546:SER:HB2 | 1.63 | 0.64 |
| 2:B:989:ALA:HB3 | 2:B:1038:VAL:HG13 | 1.80 | 0.63 |
| 2:B:964:ASP:HB2 | 2:B:988:TRP:HB3 | 1.81 | 0.63 |
| 2:B:872:LEU:HD11 | 2:B:879:PRO:HB2 | 1.81 | 0.62 |
| 1:A:105:LEU:HD13 | 1:A:134:GLY:HA2 | 1.79 | 0.62 |
| 2:B:897:MET:SD | 2:B:897:MET:N | 2.69 | 0.62 |
| 2:B:1215:GLN:HB3 | 2:B:1232:ARG:HB3 | 1.82 | 0.61 |
| 1:A:216:ASP:OD1 | 1:A:217:GLU:N | 2.33 | 0.61 |
| 1:A:190:ARG:HG2 | 1:A:217:GLU:HG3 | 1.83 | 0.61 |
| 2:B:748:GLN:OE1 | 2:B:781:GLN:NE2 | 2.34 | 0.61 |
| 2:B:1092:SER:O | 2:B:1097:GLN:NE2 | 2.34 | 0.61 |
| 2:B:796:GLN:OE1 | 2:B:796:GLN:N | 2.34 | 0.60 |
| 1:A:263:ARG:O | 1:A:290:TRP:NE1 | 2.36 | 0.59 |
| 2:B:822:GLN:HB2 | 2:B:845:ARG:HG2 | 1.84 | 0.59 |
| 2:B:915:SER:HB2 | 2:B:934:ALA:HB3 | 1.84 | 0.59 |
| 1:A:446:VAL:HG13 | 1:A:505:GLU:HB3 | 1.83 | 0.59 |
| 1:A:357:LEU:HB2 | 1:A:363:ARG:HH21 | 1.69 | 0.58 |
| 2:B:1148:LEU:HD12 | 2:B:1149:ARG:H | 1.68 | 0.58 |
| 1:A:239:VAL:HG23 | 1:A:260:VAL:HG12 | 1.85 | 0.58 |
| 1:A:61:VAL:O | 1:A:65:ILE:HG12 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:872:LEU:HD13 | 2:B:881:LEU:HB3 | 1.85 | 0.57 |
| 2:B:898:PRO:HG2 | 2:B:899:PHE:HD1 | 1.70 | 0.56 |
| 1:A:63:ASP:O | 1:A:67:GLU:HG3 | 2.05 | 0.56 |
| 1:A:396:ARG:NH1 | 1:A:407:ASP:OD2 | 2.37 | 0.56 |
| 2:B:985:ASP:OD2 | 2:B:985:ASP:N | 2.36 | 0.56 |
| 2:B:969:VAL:HA | 2:B:982:GLY:HA3 | 1.87 | 0.56 |
| 2:B:1080:GLN:N | 2:B:1080:GLN:OE1 | 2.38 | 0.56 |
| 1:A:282:VAL:HG12 | 1:A:304:ILE:HB | 1.87 | 0.56 |
| 2:B:1151:GLN:OE1 | 2:B:1152:GLY:N | 2.38 | 0.56 |
| 2:B:1076:HIS:HA | 2:B:1081:ASP:HA | 1.87 | 0.56 |
| 1:A:75:TYR:CE1 | 1:A:170:ILE:HG21 | 2.41 | 0.56 |
| 2:B:1053:LEU:HD12 | 2:B:1064:LEU:HD11 | 1.87 | 0.55 |
| 2:B:1232:ARG:HG2 | 2:B:1240:TYR:HD1 | 1.71 | 0.55 |
| 1:A:57:PHE:O | 1:A:61:VAL:HG13 | 2.06 | 0.55 |
| 1:A:515:TRP:HB2 | 1:A:543:ARG:HB3 | 1.87 | 0.55 |
| 1:A:448:ARG:HB3 | 1:A:503:SER:HB2 | 1.88 | 0.55 |
| 1:A:334:PHE:HE1 | 1:A:336:ARG:HG3 | 1.71 | 0.55 |
| 1:A:227:ASN:ND2 | 2:B:1160:SER:OG | 2.31 | 0.55 |
| 2:B:1098:PRO:HD2 | 2:B:1125:ALA:H | 1.72 | 0.55 |
| 1:A:442:ARG:NH2 | 1:A:508:TYR:OH | 2.40 | 0.54 |
| 1:A:335:LYS:HB3 | 1:A:346:SER:HB2 | 1.89 | 0.54 |
| 1:A:47:GLU:OE2 | 2:B:994:HIS:NE2 | 2.39 | 0.53 |
| 2:B:938:GLN:HG3 | 2:B:941:ASN:HB3 | 1.89 | 0.53 |
| 1:A:267:THR:HG23 | 1:A:287:LYS:HB2 | 1.90 | 0.53 |
| 2:B:952:LYS:HE3 | 2:B:964:ASP:HB3 | 1.90 | 0.53 |
| 2:B:1211:LEU:HB3 | 2:B:1214:LEU:HB3 | 1.89 | 0.53 |
| 1:A:159:PHE:HB2 | 1:A:189:TYR:CE2 | 2.44 | 0.53 |
| 1:A:153:ALA:HB2 | 1:A:183:TYR:OH | 2.09 | 0.52 |
| 2:B:762:ASP:OD1 | 2:B:765:LYS:NZ | 2.33 | 0.52 |
| 2:B:977:LEU:HD22 | 2:B:1059:LYS:HE3 | 1.92 | 0.52 |
| 2:B:809:ALA:HB3 | 2:B:829:VAL:HB | 1.90 | 0.52 |
| 1:A:458:ASP:N | 1:A:458:ASP:OD1 | 2.43 | 0.52 |
| 2:B:1090:LEU:HB3 | 2:B:1099:TYR:HD2 | 1.74 | 0.52 |
| 2:B:708:ASN:O | 2:B:733:ARG:NH2 | 2.43 | 0.51 |
| 2:B:941:ASN:HA | 2:B:975:PRO:HG3 | 1.91 | 0.51 |
| 1:A:126:LEU:HG | 1:A:145:PHE:CE1 | 2.45 | 0.51 |
| 2:B:1088:GLU:OE2 | 2:B:1101:ASN:HB3 | 2.10 | 0.51 |
| 2:B:981:ASP:HA | 2:B:1029:ASN:O | 2.09 | 0.51 |
| 2:B:965:VAL:HG22 | 2:B:986:VAL:HG12 | 1.92 | 0.51 |
| 2:B:761:TRP:CD1 | 2:B:769:PRO:HA | 2.46 | 0.51 |
| 1:A:286:TRP:HE1 | 1:A:288:LYS:HE2 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1144:LEU:HA | 2:B:1147:LEU:HD12 | 1.93 | 0.51 |
| 1:A:507:GLN:HE22 | 1:A:543:ARG:CZ | 2.24 | 0.50 |
| 1:A:524:GLU:HB2 | 1:A:534:PHE:HA | 1.94 | 0.50 |
| 2:B:816:ARG:HA | 2:B:822:GLN:HE22 | 1.76 | 0.50 |
| 1:A:374:PHE:HB3 | 1:A:381:ASN:HB3 | 1.94 | 0.50 |
| 2:B:1064:LEU:N | 2:B:1093:GLY:O | 2.43 | 0.49 |
| 2:B:738:MET:O | 2:B:738:MET:HG3 | 2.12 | 0.49 |
| 2:B:866:VAL:HG12 | 2:B:887:VAL:HG23 | 1.92 | 0.49 |
| 1:A:488:TYR:OH | 1:A:495:GLY:O | 2.20 | 0.49 |
| 2:B:1215:GLN:N | 2:B:1232:ARG:O | 2.41 | 0.49 |
| 2:B:945:ARG:NH1 | 2:B:947:THR:OG1 | 2.46 | 0.49 |
| 1:A:167:GLN:NE2 | 1:A:180:ASP:OD2 | 2.35 | 0.49 |
| 1:A:573:LEU:HD12 | 1:A:574:GLY:N | 2.28 | 0.49 |
| 1:A:45:THR:HG21 | 2:B:996:LEU:HD23 | 1.95 | 0.49 |
| 1:A:271:GLY:HA3 | 2:B:1253:LEU:O | 2.13 | 0.49 |
| 1:A:214:GLU:OE2 | 1:A:214:GLU:N | 2.46 | 0.49 |
| 2:B:762:ASP:OD2 | 2:B:764:THR:OG1 | 2.21 | 0.49 |
| 2:B:1035:GLY:O | 2:B:1050:THR:OG1 | 2.26 | 0.49 |
| 2:B:871:ARG:HH12 | 2:B:883:GLY:HA2 | 1.78 | 0.48 |
| 2:B:801:THR:O | 2:B:812:GLY:N | 2.45 | 0.48 |
| 2:B:814:THR:HA | 2:B:824:ASP:OD1 | 2.12 | 0.48 |
| 1:A:381:ASN:OD1 | 1:A:382:THR:N | 2.47 | 0.48 |
| 2:B:958:PRO:HB2 | 2:B:960:MET:HG2 | 1.95 | 0.48 |
| 1:A:55:ARG:NH2 | 2:B:900:ASP:OD2 | 2.46 | 0.48 |
| 2:B:848:ASN:O | 2:B:851:MET:HE3 | 2.13 | 0.48 |
| 2:B:1051:GLY:HA3 | 2:B:1068:ILE:HG13 | 1.95 | 0.48 |
| 1:A:479:TYR:CE2 | 1:A:535:LYS:HE2 | 2.49 | 0.48 |
| 2:B:947:THR:HG23 | 2:B:970:VAL:HG12 | 1.95 | 0.48 |
| 2:B:1054:ASN:N | 2:B:1065:ASN:O | 2.34 | 0.48 |
| 2:B:1149:ARG:CZ | 2:B:1149:ARG:HA | 2.43 | 0.48 |
| 1:A:477:ARG:NE | 1:A:521:ASP:OD2 | 2.44 | 0.47 |
| 2:B:971:PHE:CE1 | 2:B:978:PHE:HB3 | 2.49 | 0.47 |
| 2:B:913:MET:HB2 | 2:B:914:ARG:CZ | 2.45 | 0.47 |
| 2:B:1040:ILE:HB | 2:B:1049:LEU:HD11 | 1.96 | 0.47 |
| 1:A:31:LEU:HG | 1:A:98:VAL:HG11 | 1.95 | 0.47 |
| 1:A:546:SER:HB3 | 1:A:549:GLY:O | 2.15 | 0.47 |
| 2:B:1145:SER:HB2 | 2:B:1163:MET:HE3 | 1.97 | 0.47 |
| 2:B:1236:MET:HE3 | 2:B:1238:LYS:H | 1.79 | 0.47 |
| 1:A:219:GLU:HG2 | 1:A:221:LYS:HB3 | 1.96 | 0.46 |
| 1:A:328:TYR:CE1 | 1:A:353:ARG:HD2 | 2.50 | 0.46 |
| 1:A:264:THR:OG1 | 2:B:1258:GLU:OE1 | 2.22 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:225:GLU:HG3 | 1:A:229:ARG:HD2 | 1.97 | 0.46 |
| 2:B:1236:MET:SD | 2:B:1237:PRO:HD2 | 2.55 | 0.46 |
| 1:A:507:GLN:HE22 | 1:A:543:ARG:NH1 | 2.13 | 0.46 |
| 1:A:288:LYS:O | 1:A:290:TRP:N | 2.49 | 0.46 |
| 1:A:304:ILE:HD13 | 1:A:309:GLN:HG2 | 1.97 | 0.46 |
| 2:B:1067:GLN:HA | 2:B:1089:LEU:HG | 1.97 | 0.46 |
| 2:B:847:PHE:HB2 | 2:B:866:VAL:HG22 | 1.98 | 0.46 |
| 2:B:926:GLY:HA2 | 2:B:952:LYS:HB3 | 1.97 | 0.46 |
| 1:A:31:LEU:HD23 | 1:A:35:LEU:HB3 | 1.97 | 0.46 |
| 1:A:66:ARG:HH21 | 1:A:77:PRO:HD2 | 1.81 | 0.46 |
| 1:A:251:THR:OG1 | 1:A:252:LYS:N | 2.49 | 0.46 |
| 1:A:113:LEU:HD13 | 1:A:123:TYR:HD2 | 1.80 | 0.46 |
| 1:A:501:THR:HA | 1:A:523:GLY:HA2 | 1.98 | 0.45 |
| 1:A:473:ASP:OD1 | 1:A:474:ARG:N | 2.46 | 0.45 |
| 1:A:501:THR:HG22 | 1:A:523:GLY:HA3 | 1.99 | 0.45 |
| 2:B:802:ALA:HA | 2:B:811:LEU:HA | 1.98 | 0.45 |
| 1:A:80:GLU:HB3 | 1:A:97:LYS:HB2 | 1.99 | 0.45 |
| 2:B:977:LEU:HD21 | 2:B:1027:ASN:HB2 | 1.97 | 0.45 |
| 2:B:983:ARG:HE | 2:B:1031:ILE:HD11 | 1.81 | 0.45 |
| 2:B:1234:ARG:HD2 | 2:B:1236:MET:H | 1.81 | 0.45 |
| 2:B:898:PRO:HG2 | 2:B:899:PHE:CD1 | 2.51 | 0.45 |
| 2:B:1036:ASN:OD1 | 2:B:1037:ASN:N | 2.46 | 0.45 |
| 2:B:1148:LEU:HD13 | 2:B:1149:ARG:HG2 | 1.99 | 0.45 |
| 1:A:113:LEU:HD13 | 1:A:123:TYR:CD2 | 2.51 | 0.45 |
| 1:A:275:SER:OG | 1:A:277:ASP:OD1 | 2.23 | 0.45 |
| 2:B:1148:LEU:HD12 | 2:B:1149:ARG:N | 2.32 | 0.45 |
| 2:B:1241:LEU:HD13 | 2:B:1253:LEU:HD22 | 1.99 | 0.45 |
| 2:B:958:PRO:HG2 | 2:B:961:VAL:H | 1.82 | 0.45 |
| 2:B:1156:ASP:HB3 | 2:B:1159:ASP:OD2 | 2.17 | 0.45 |
| 1:A:237:ASN:N | 1:A:261:SER:O | 2.38 | 0.44 |
| 1:A:479:TYR:HB2 | 1:A:484:ILE:HD11 | 2.00 | 0.44 |
| 2:B:719:ILE:HG23 | 2:B:727:ALA:HB2 | 1.99 | 0.44 |
| 2:B:952:LYS:HA | 2:B:952:LYS:HD2 | 1.69 | 0.44 |
| 1:A:34:GLN:HG2 | 1:A:37:LYS:HE2 | 2.00 | 0.44 |
| 1:A:70:LYS:HG3 | 1:A:75:TYR:CE2 | 2.53 | 0.44 |
| 1:A:43:LEU:O | 1:A:43:LEU:HD23 | 2.17 | 0.43 |
| 1:A:243:PRO:HB2 | 1:A:254:LEU:HD11 | 2.00 | 0.43 |
| 2:B:809:ALA:O | 2:B:829:VAL:N | 2.44 | 0.43 |
| 1:A:286:TRP:CD1 | 1:A:286:TRP:C | 2.95 | 0.43 |
| 2:B:1235:LEU:HD23 | 2:B:1235:LEU:HA | 1.91 | 0.43 |
| 1:A:288:LYS:HD2 | 1:A:291:MET:SD | 2.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:953:VAL:O | 2:B:964:ASP:HA | 2.19 | 0.43 |
| 2:B:978:PHE:CD1 | 2:B:978:PHE:N | 2.86 | 0.43 |
| 2:B:1159:ASP:O | 2:B:1163:MET:SD | 2.77 | 0.43 |
| 1:A:275:SER:HB3 | 1:A:281:ARG:HE | 1.83 | 0.43 |
| 2:B:1144:LEU:O | 2:B:1144:LEU:HD23 | 2.19 | 0.43 |
| 1:A:169:GLY:HA2 | 2:B:1008:VAL:O | 2.19 | 0.43 |
| 1:A:287:LYS:HG2 | 1:A:299:THR:HB | 2.00 | 0.43 |
| 2:B:732:ASN:ND2 | 2:B:754:THR:HG23 | 2.32 | 0.43 |
| 2:B:1078:TYR:C | 2:B:1187:GLY:HA3 | 2.43 | 0.43 |
| 2:B:1234:ARG:NH2 | 2:B:1237:PRO:HA | 2.34 | 0.43 |
| 2:B:753:PHE:HB2 | 2:B:775:LEU:HD21 | 2.01 | 0.42 |
| 2:B:1215:GLN:O | 2:B:1232:ARG:N | 2.48 | 0.42 |
| 2:B:708:ASN:HB3 | 2:B:711:ALA:O | 2.19 | 0.42 |
| 2:B:952:LYS:CE | 2:B:964:ASP:HB3 | 2.49 | 0.42 |
| 1:A:345:ASP:HB3 | 1:A:373:HIS:HB2 | 2.02 | 0.42 |
| 1:A:444:ARG:O | 1:A:507:GLN:N | 2.48 | 0.42 |
| 1:A:551:ILE:HG13 | 1:A:573:LEU:HD13 | 2.01 | 0.42 |
| 2:B:1208:GLY:C | 2:B:1209:TYR:HD1 | 2.28 | 0.42 |
| 1:A:331:GLN:NE2 | 2:B:1200:ASP:OD2 | 2.38 | 0.42 |
| 2:B:963:MET:HA | 2:B:989:ALA:HA | 2.01 | 0.42 |
| 1:A:453:TRP:CZ2 | 1:A:498:LYS:HE3 | 2.54 | 0.42 |
| 2:B:1069:ASN:HA | 2:B:1087:GLY:HA3 | 2.02 | 0.42 |
| 1:A:32:SER:H | 1:A:35:LEU:HD12 | 1.84 | 0.42 |
| 1:A:202:ARG:HE | 1:A:294:TYR:HE1 | 1.67 | 0.42 |
| 1:A:374:PHE:O | 1:A:381:ASN:N | 2.43 | 0.42 |
| 1:A:386:PHE:CD1 | 1:A:388:PRO:HD3 | 2.55 | 0.42 |
| 2:B:1211:LEU:HD22 | 2:B:1214:LEU:HB2 | 2.01 | 0.42 |
| 2:B:745:GLU:O | 2:B:746:THR:OG1 | 2.31 | 0.41 |
| 1:A:154:LEU:HD23 | 1:A:154:LEU:HA | 1.85 | 0.41 |
| 2:B:847:PHE:N | 2:B:847:PHE:CD2 | 2.88 | 0.41 |
| 2:B:934:ALA:HB1 | 2:B:936:TRP:HE1 | 1.84 | 0.41 |
| 1:A:242:ALA:HB1 | 2:B:1167:LEU:HD23 | 2.02 | 0.41 |
| 2:B:1006:ASP:OD1 | 2:B:1006:ASP:N | 2.45 | 0.41 |
| 1:A:276:THR:OG1 | 2:B:1248:ASP:OD1 | 2.29 | 0.41 |
| 2:B:871:ARG:HG2 | 2:B:882:PHE:O | 2.21 | 0.41 |
| 2:B:1118:GLY:HA3 | 2:B:1133:PHE:CZ | 2.55 | 0.41 |
| 2:B:1211:LEU:HG | 2:B:1212:PRO:HD2 | 2.01 | 0.41 |
| 2:B:898:PRO:HA | 2:B:957:VAL:CG2 | 2.50 | 0.41 |
| 1:A:109:THR:HG21 | 1:A:130:ARG:HD2 | 2.01 | 0.41 |
| 1:A:237:ASN:ND2 | 1:A:262:PRO:O | 2.54 | 0.41 |
| 1:A:470:ALA:HB3 | 1:A:484:ILE:HB | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:897:MET:HE3 | 2:B:897:MET:HB3 | 1.91 | 0.41 |
| 1:A:58:ARG:HD3 | 1:A:81:PHE:CE1 | 2.56 | 0.41 |
| 2:B:708:ASN:OD1 | 2:B:709:PRO:HD2 | 2.21 | 0.41 |
| 1:A:125:LYS:HE2 | 1:A:125:LYS:HB2 | 1.87 | 0.40 |
| 1:A:69:LEU:O | 1:A:73:GLY:N | 2.49 | 0.40 |
| 1:A:448:ARG:N | 1:A:503:SER:O | 2.47 | 0.40 |
| 1:A:453:TRP:CH2 | 1:A:498:LYS:HE3 | 2.56 | 0.40 |
| 1:A:463:PRO:HA | 1:A:464:PRO:HD3 | 1.92 | 0.40 |
| 2:B:778:ARG:HD3 | 2:B:796:GLN:HB2 | 2.03 | 0.40 |
| 2:B:879:PRO:O | 2:B:913:MET:HE1 | 2.22 | 0.40 |
| 2:B:881:LEU:HD23 | 2:B:881:LEU:H | 1.85 | 0.40 |
| 1:A:555:PHE:CD1 | 1:A:555:PHE:N | 2.87 | 0.40 |
| 2:B:803:GLU:OE1 | 2:B:803:GLU:N | 2.54 | 0.40 |
| 2:B:920:THR:OG1 | 2:B:922:ARG:NH2 | 2.54 | 0.40 |
| 2:B:989:ALA:HB3 | 2:B:1038:VAL:HG22 | 2.03 | 0.40 |
| 2:B:696:GLU:O | 2:B:698:LYS:HG2 | 2.21 | 0.40 |
| 2:B:1138:MET:HG3 | 2:B:1146:TYR:HE2 | 1.87 | 0.40 |
| 1:A:157:GLY:HA3 | 1:A:218:TYR:HB3 | 2.03 | 0.40 |
| 1:A:442:ARG:HA | 1:A:509:ASN:HB2 | 2.04 | 0.40 |
| 2:B:1101:ASN:HA | 2:B:1121:VAL:O | 2.22 | 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 | 554/577 (96%) | 531 (96%) | 23 (4%) | 0 | 100 | 100 |
| 2 | B | 579/1259 (46%) | 544 (94%) | 34 (6%) | 1 (0%) | 43 | 74 |
| All | All | 1133/1836 (62%) | 1075 (95%) | 57 (5%) | 1 (0%) | 49 | 80 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 1198 | 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 | A | 473/491 (96%) | 470 (99%) | 3 (1%) | 78 | 80 |
| 2 | B | 480/1061 (45%) | 477 (99%) | 3 (1%) | 78 | 80 |
| All | All | 953/1552 (61%) | 947 (99%) | 6 (1%) | 76 | 80 |

All (6) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 72 | LEU |
| 1 | A | 156 | LYS |
| 1 | A | 476 | ILE |
| 2 | B | 865 | MET |
| 2 | B | 952 | LYS |
| 2 | B | 985 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 237 | ASN |
| 1 | A | 568 | GLN |
| 2 | B | 732 | ASN |
| 2 | B | 880 | GLN |
| 2 | B | 1065 | ASN |
| 2 | B | 1069 | 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 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.

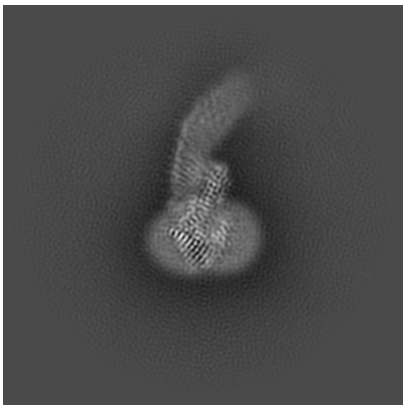
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55908. These allow visual inspection of the internal detail of the map and identification of artifacts.

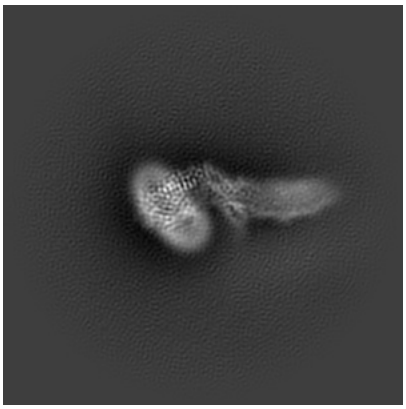
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

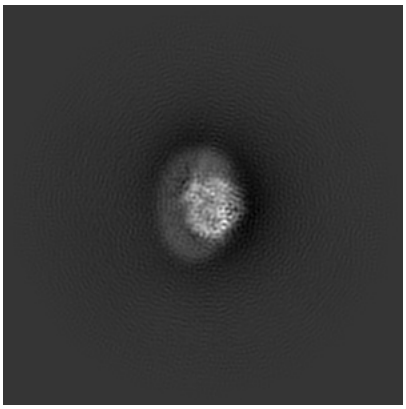
### 6.1.1 Primary map



X

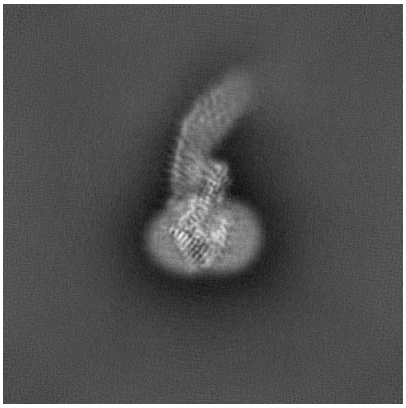


Y

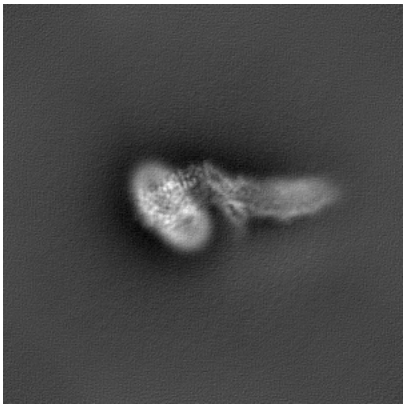


Z

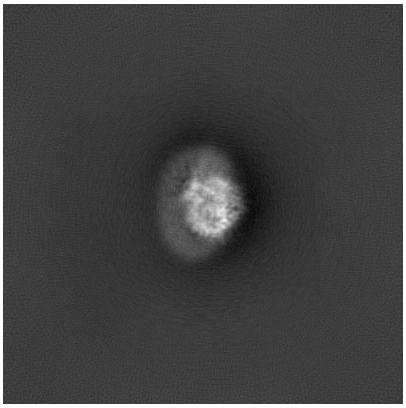
### 6.1.2 Raw map



X



Y

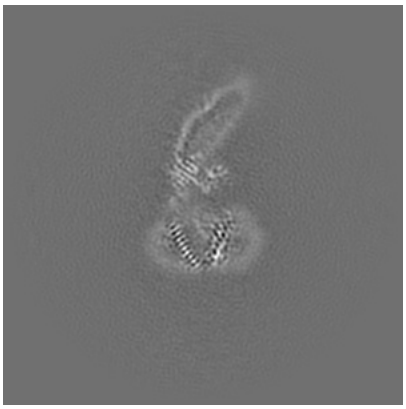


Z

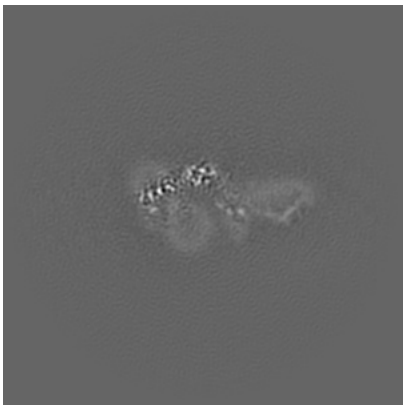
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

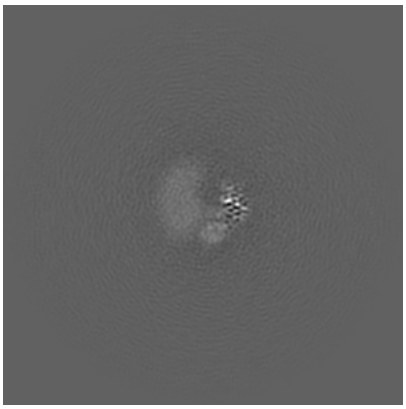
### 6.2.1 Primary map



X Index: 192

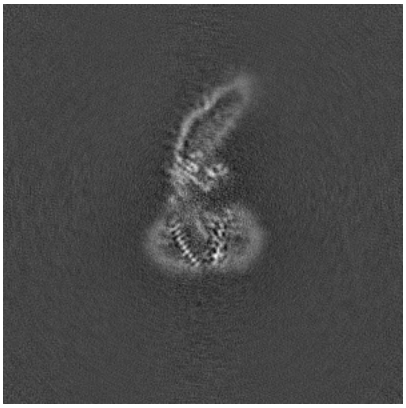


Y Index: 192

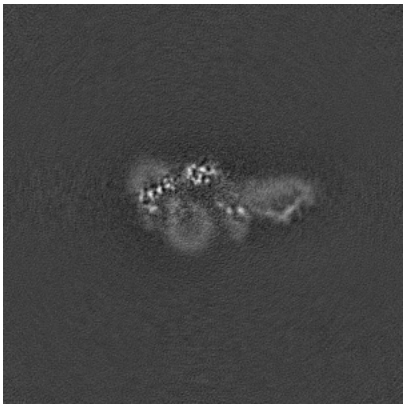


Z Index: 192

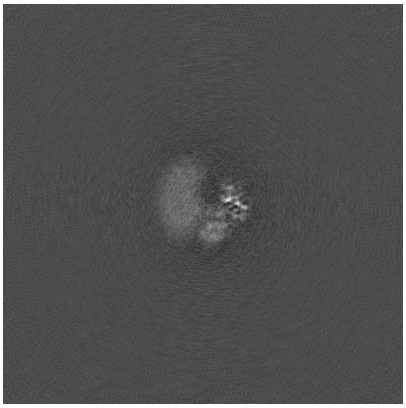
### 6.2.2 Raw map



X Index: 192



Y Index: 192

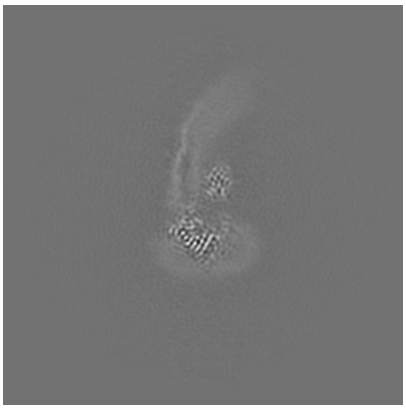


Z Index: 192

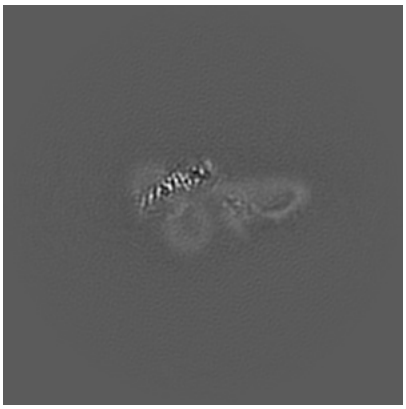
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

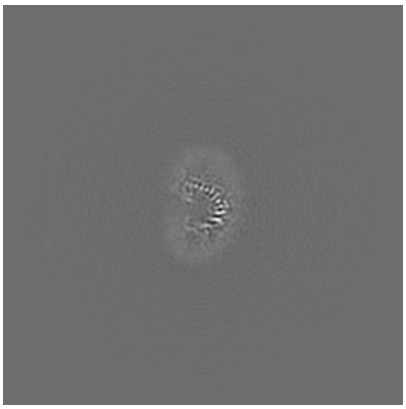
### 6.3.1 Primary map



X Index: 207

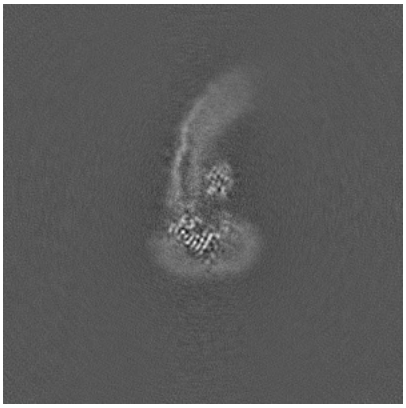


Y Index: 186

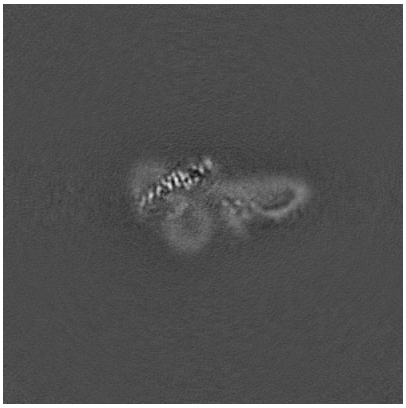


Z Index: 155

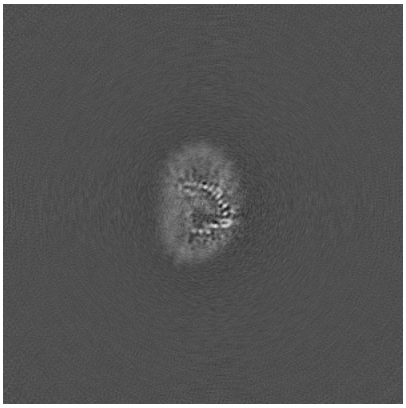
### 6.3.2 Raw map



X Index: 207



Y Index: 186

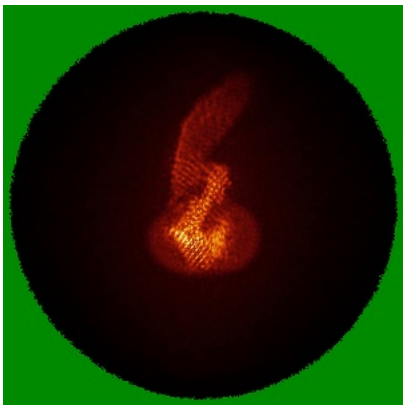


Z Index: 162

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

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

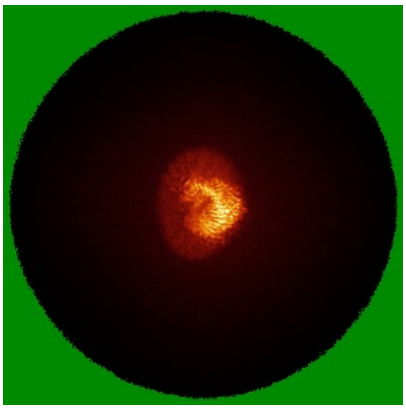
### 6.4.1 Primary map



X

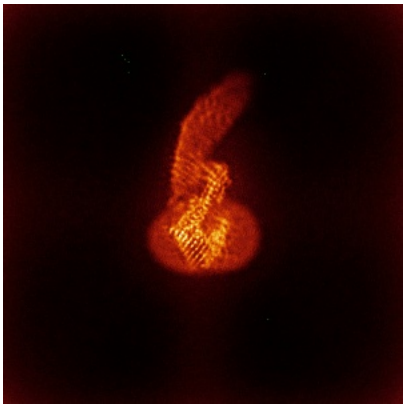


Y

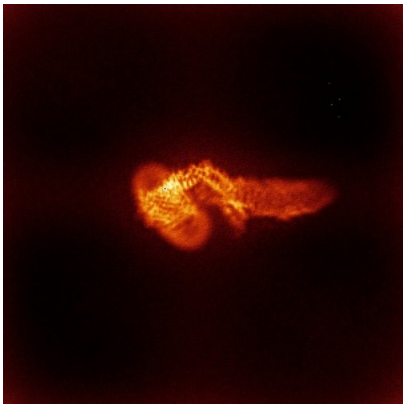


Z

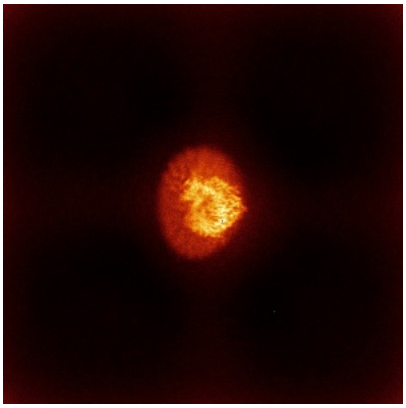
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0976. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

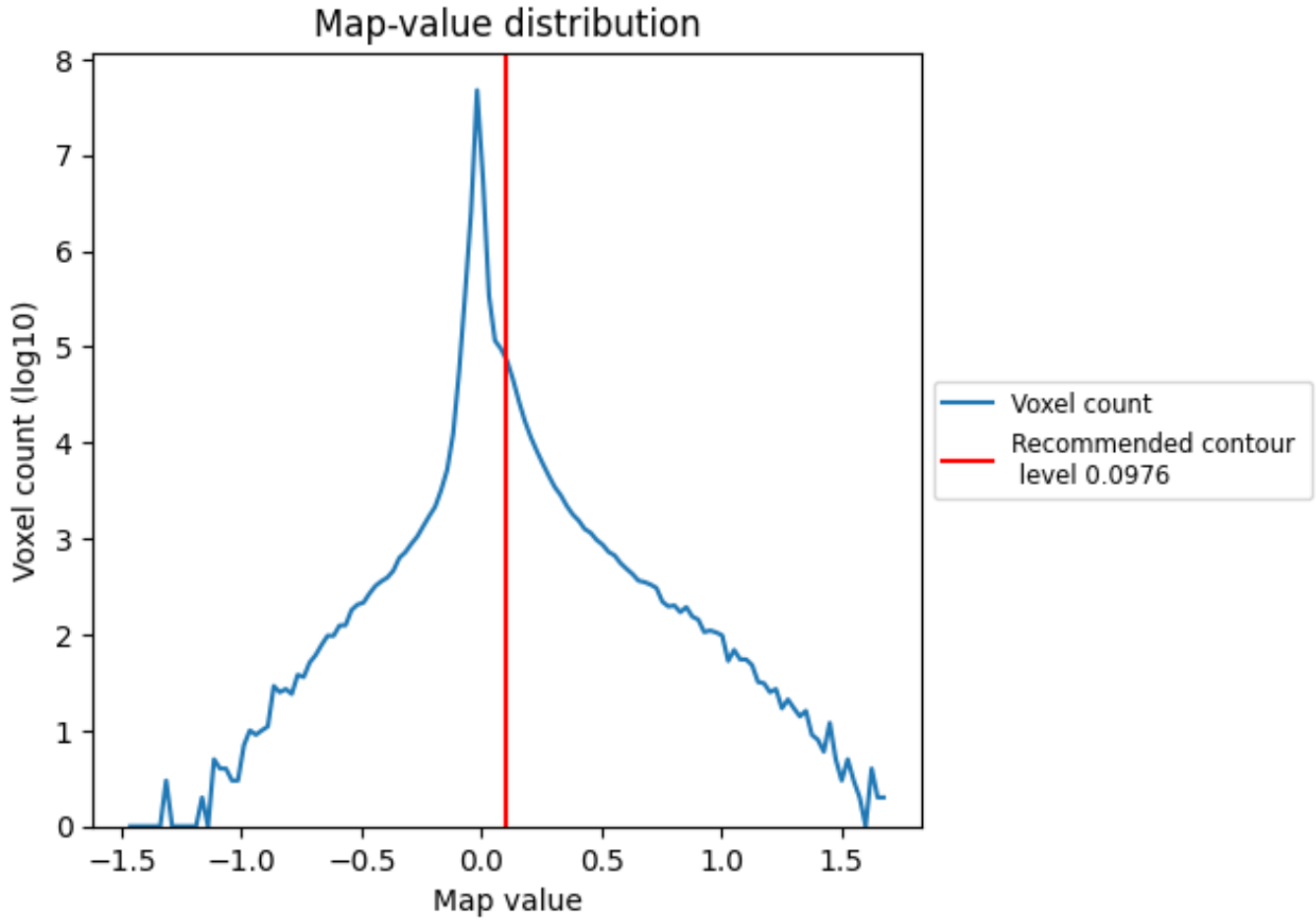
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

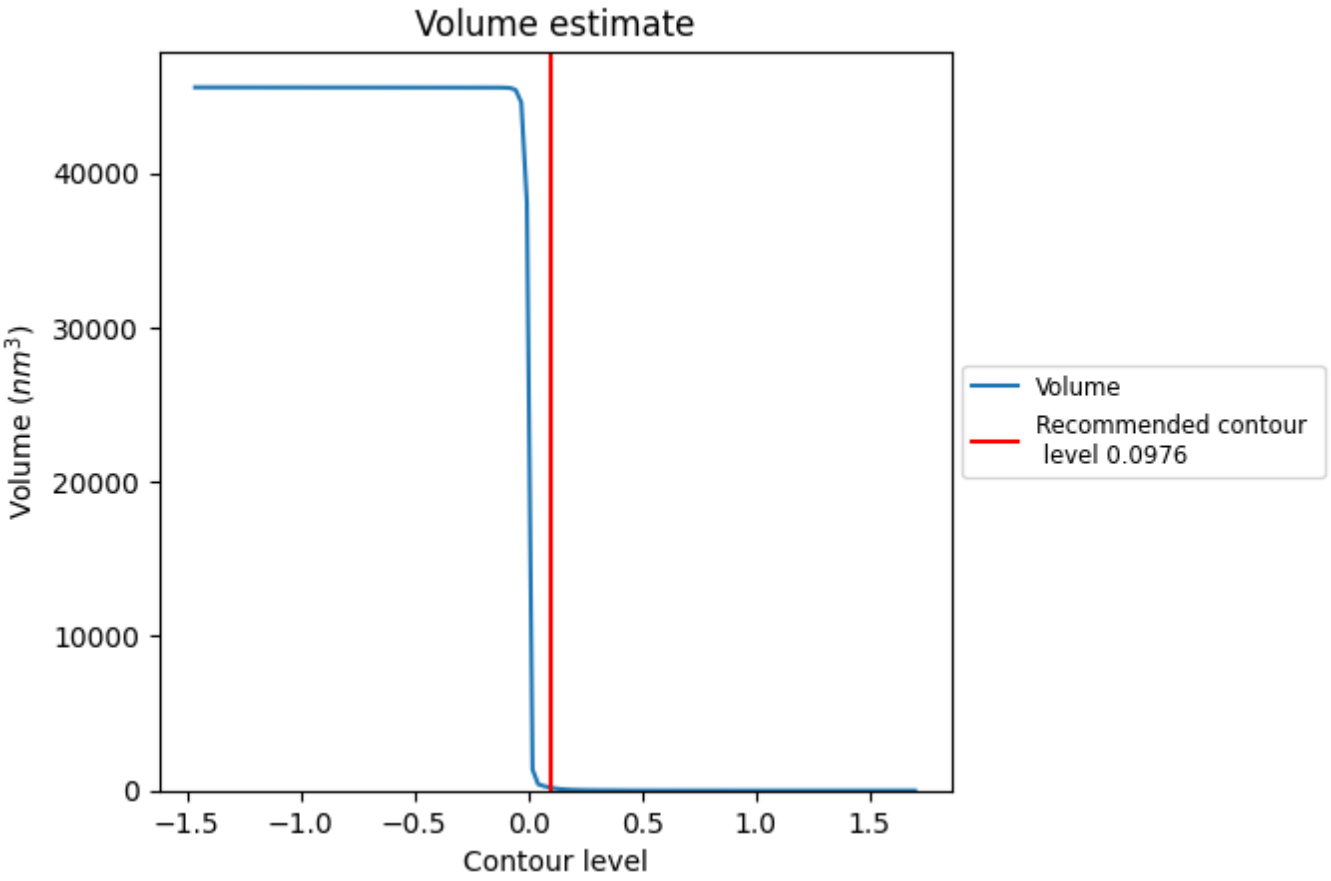
This section contains the results of statistical analysis of the map.

## 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.

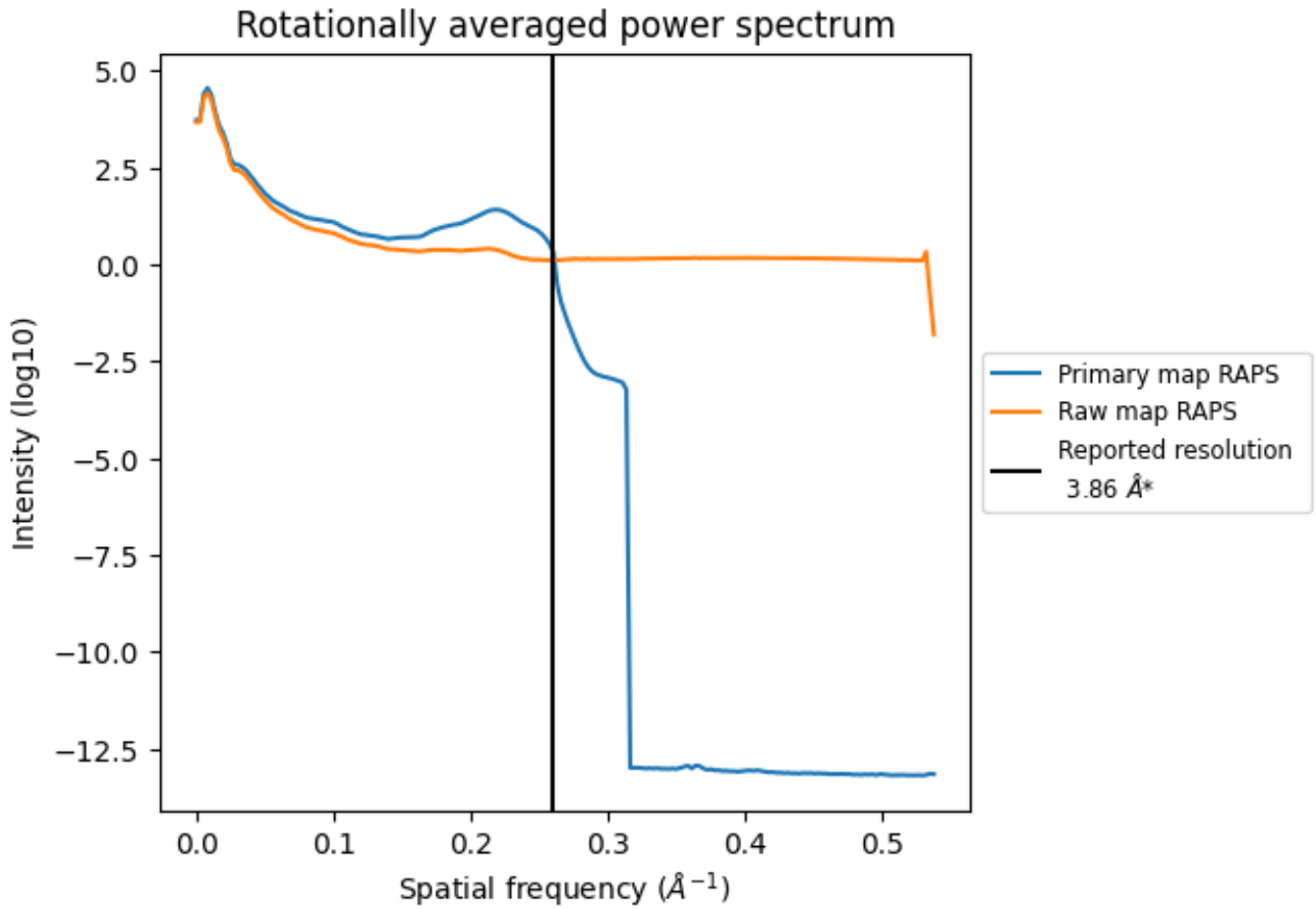
## 7.2 Volume estimate




The volume at the recommended contour level is 197 $nm^3$; this corresponds to an approximate mass of 178 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)

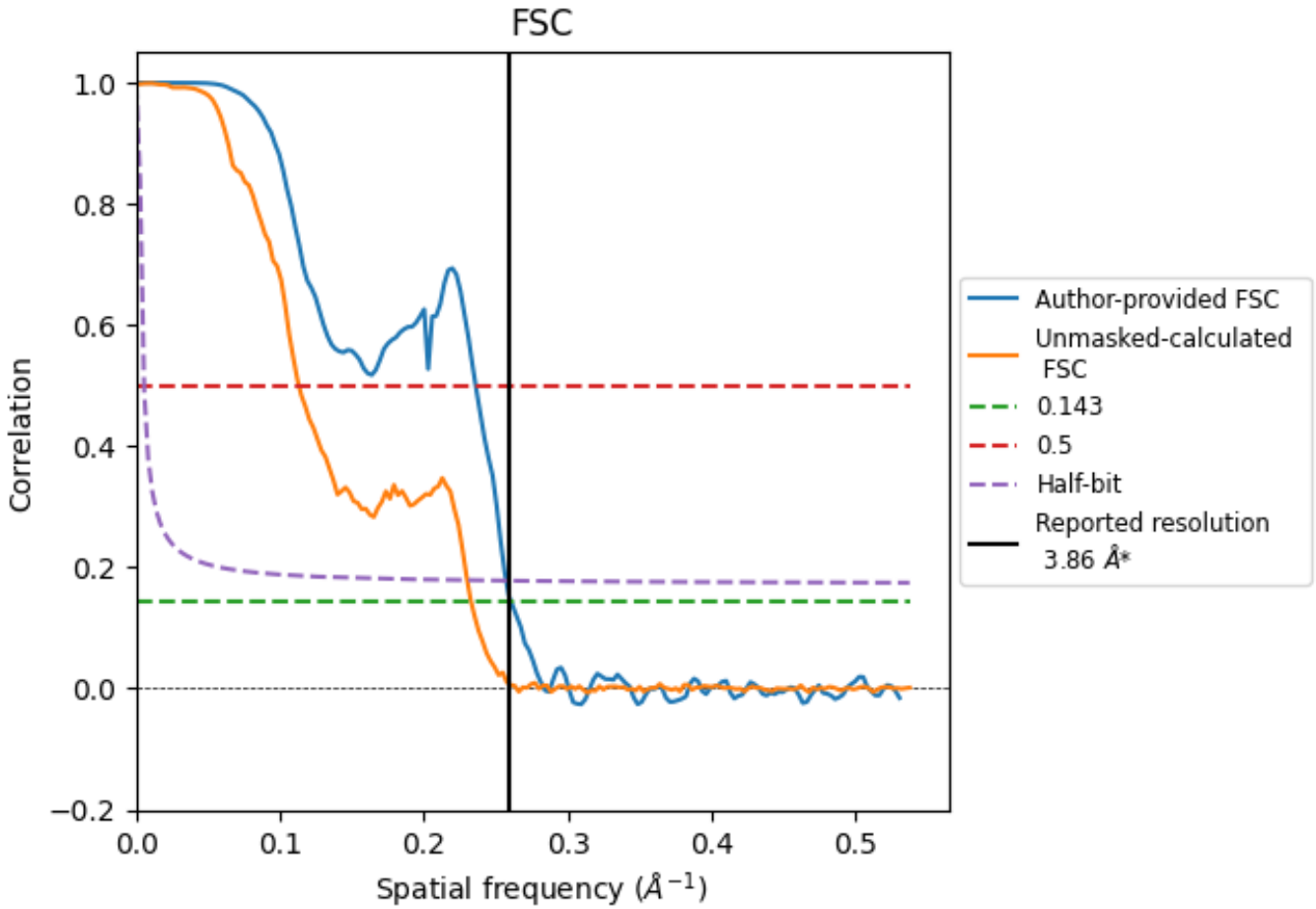



*Reported resolution corresponds to spatial frequency of 0.259 $Å^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.259 Å$^{-1}$

## 8.2 Resolution estimates (i)

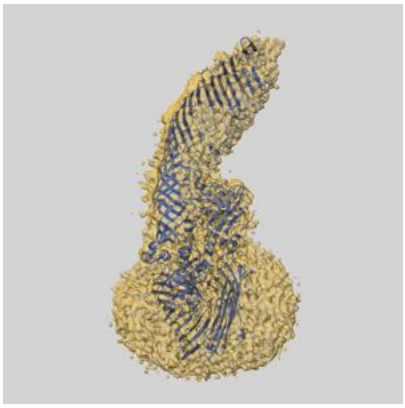
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.86 | - | - |
| Author-provided FSC curve | 3.84 | 4.24 | 3.89 |
| Unmasked-calculated* | 4.29 | 8.83 | 4.34 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.29 differs from the reported value 3.86 by more than 10 %

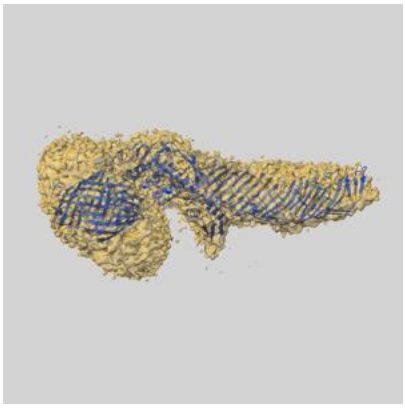
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55908 and PDB model 9TGQ. Per-residue inclusion information can be found in section 3 on page 4.

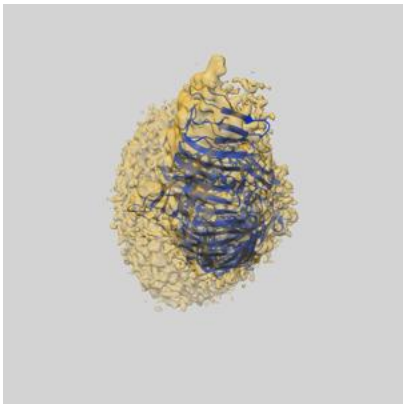
## 9.1 Map-model overlay



X



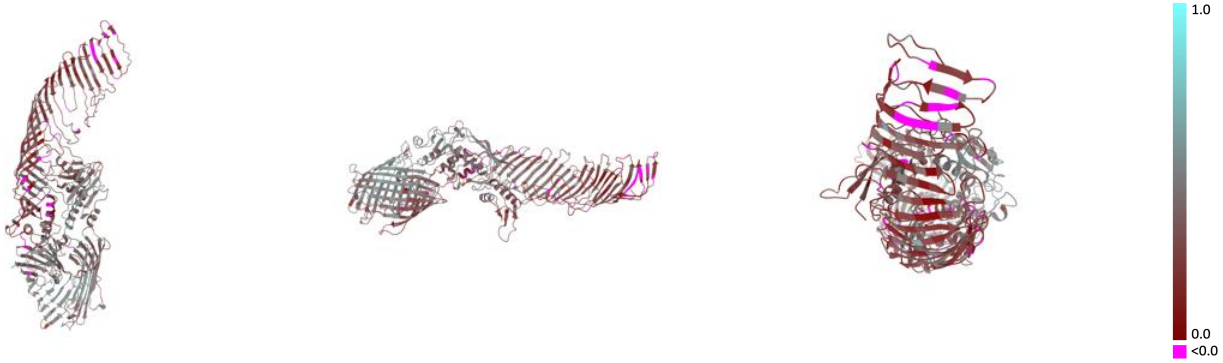
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0976 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.

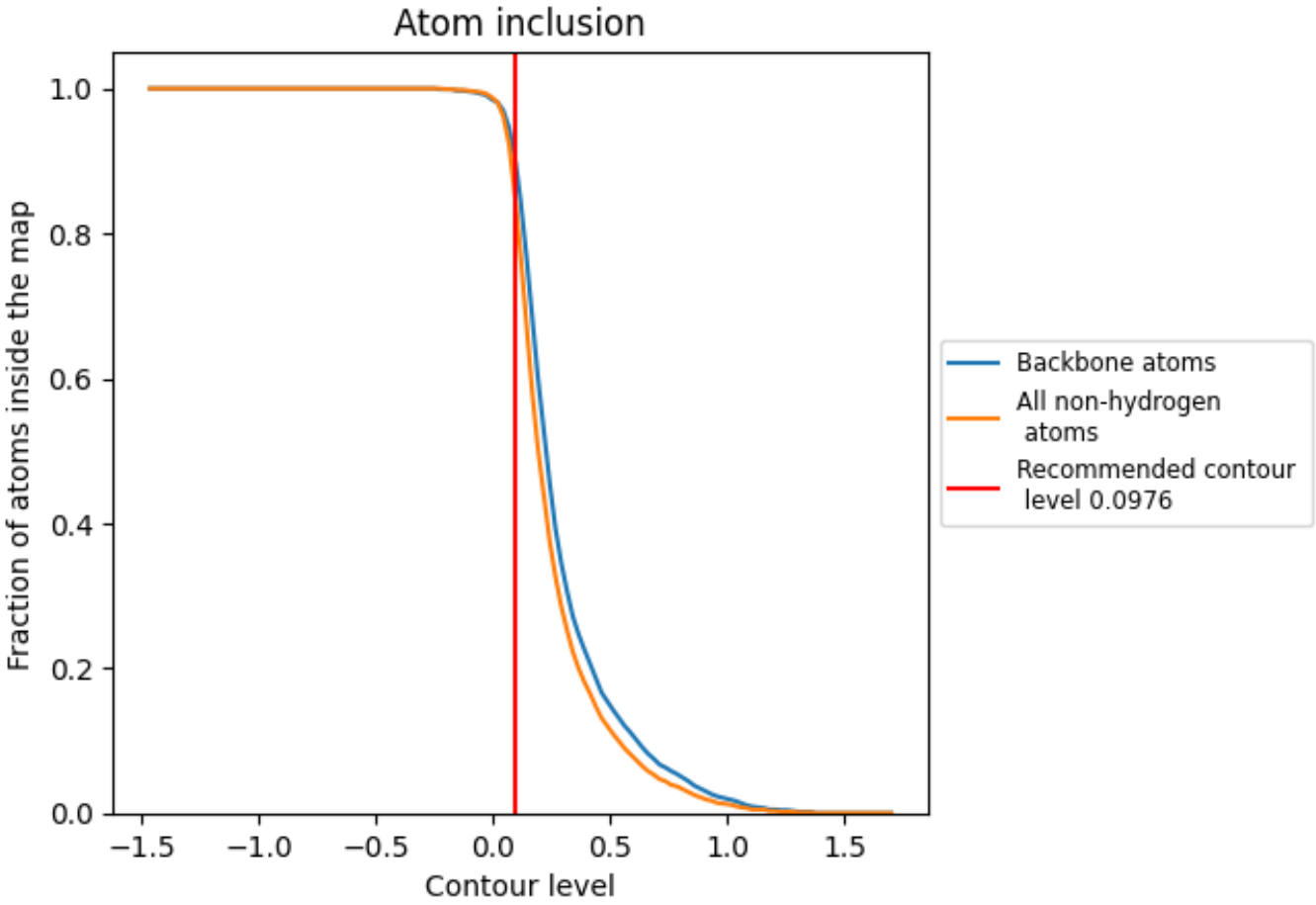
## 9.3 Atom inclusion mapped to coordinate model




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 (0.0976).

## 9.4 Atom inclusion (i)




At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.0976) and Q-score for the entire model and for each chain.




| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8420 | 0.3370 |
| A | 0.9030 | 0.4140 |
| B | 0.7810 | 0.2610 |