# wwPDB EM Validation Summary Report

Nov 20, 2022 – 05:18 AM EST

| | | |
|---|---|---|
| PDB ID | : | 7M7J |
| EMDB ID | : | EMD-23715 |
| Title | : | 6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: "turnstile closed" state (TE-free) |
| Authors | : | Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C. |
| Deposited on | : | 2021-03-28 |
| Resolution | : | 4.30 Å(reported) |

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

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

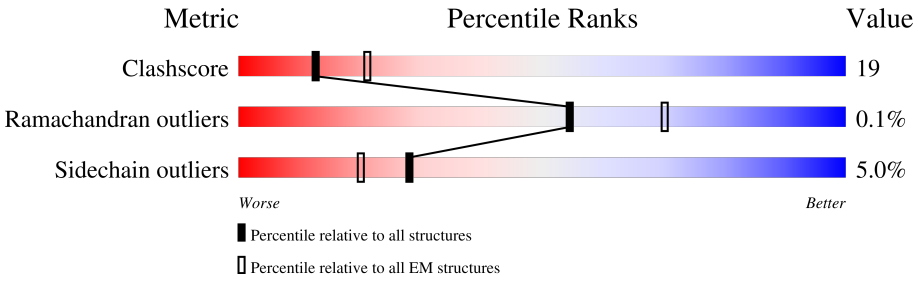
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 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 4.30 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1593 | 18% 57% 30% • 13% |
| 1 | B | 1593 | 14% 35% 21% • 43% |
| 2 | C | 249 | • 46% 35% • 18% |
| 2 | E | 249 | • 49% 31% • 18% |
| 3 | D | 236 | • 49% 35% • 13% |
| 3 | F | 236 | 50% 33% • • 13% |

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23224 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 EryAI.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | B | 912 | Total<br>6741 | C<br>4190 | N<br>1233 | O<br>1291 | S<br>27 | 0 | 0 |
| 1 | A | 1390 | Total<br>10277 | C<br>6381 | N<br>1890 | O<br>1971 | S<br>35 | 0 | 0 |

There are 102 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 1 | MET | - | expression tag | UNP Q5UNP6 |
| B | 2 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 3 | SER | - | expression tag | UNP Q5UNP6 |
| B | 4 | THR | - | expression tag | UNP Q5UNP6 |
| B | 5 | ASP | - | expression tag | UNP Q5UNP6 |
| B | 6 | SER | - | expression tag | UNP Q5UNP6 |
| B | 7 | GLU | - | expression tag | UNP Q5UNP6 |
| B | 8 | LYS | - | expression tag | UNP Q5UNP6 |
| B | 9 | VAL | - | expression tag | UNP Q5UNP6 |
| B | 10 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 11 | GLU | - | expression tag | UNP Q5UNP6 |
| B | 12 | TYR | - | expression tag | UNP Q5UNP6 |
| B | 13 | LEU | - | expression tag | UNP Q5UNP6 |
| B | 14 | ARG | - | expression tag | UNP Q5UNP6 |
| B | 15 | ARG | - | expression tag | UNP Q5UNP6 |
| B | 16 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 17 | THR | - | expression tag | UNP Q5UNP6 |
| B | 18 | LEU | - | expression tag | UNP Q5UNP6 |
| B | 19 | ASP | - | expression tag | UNP Q5UNP6 |
| B | 20 | LEU | - | expression tag | UNP Q5UNP6 |
| B | 21 | ARG | - | expression tag | UNP Q5UNP6 |
| B | 22 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 23 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 24 | ARG | - | expression tag | UNP Q5UNP6 |
| B | 25 | GLN | - | expression tag | UNP Q5UNP6 |
| B | 26 | ARG | - | expression tag | UNP Q5UNP6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 27 | ILE | - | expression tag | UNP Q5UNP6 |
| B | 28 | ARG | - | expression tag | UNP Q5UNP6 |
| B | 29 | GLU | - | expression tag | UNP Q5UNP6 |
| B | 30 | LEU | - | expression tag | UNP Q5UNP6 |
| B | 31 | GLU | - | expression tag | UNP Q5UNP6 |
| B | 1574 | PRO | - | expression tag | UNP Q5UNP6 |
| B | 1575 | ASN | - | expression tag | UNP Q5UNP6 |
| B | 1576 | SER | - | expression tag | UNP Q5UNP6 |
| B | 1577 | SER | - | expression tag | UNP Q5UNP6 |
| B | 1578 | SER | - | expression tag | UNP Q5UNP6 |
| B | 1579 | VAL | - | expression tag | UNP Q5UNP6 |
| B | 1580 | ASP | - | expression tag | UNP Q5UNP6 |
| B | 1581 | LYS | - | expression tag | UNP Q5UNP6 |
| B | 1582 | LEU | - | expression tag | UNP Q5UNP6 |
| B | 1583 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 1584 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 1585 | ALA | - | expression tag | UNP Q5UNP6 |
| B | 1586 | LEU | - | expression tag | UNP Q5UNP6 |
| B | 1587 | GLU | - | expression tag | UNP Q5UNP6 |
| B | 1588 | HIS | - | expression tag | UNP Q5UNP6 |
| B | 1589 | HIS | - | expression tag | UNP Q5UNP6 |
| B | 1590 | HIS | - | expression tag | UNP Q5UNP6 |
| B | 1591 | HIS | - | expression tag | UNP Q5UNP6 |
| B | 1592 | HIS | - | expression tag | UNP Q5UNP6 |
| B | 1593 | HIS | - | expression tag | UNP Q5UNP6 |
| A | 1 | MET | - | expression tag | UNP Q5UNP6 |
| A | 2 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 3 | SER | - | expression tag | UNP Q5UNP6 |
| A | 4 | THR | - | expression tag | UNP Q5UNP6 |
| A | 5 | ASP | - | expression tag | UNP Q5UNP6 |
| A | 6 | SER | - | expression tag | UNP Q5UNP6 |
| A | 7 | GLU | - | expression tag | UNP Q5UNP6 |
| A | 8 | LYS | - | expression tag | UNP Q5UNP6 |
| A | 9 | VAL | - | expression tag | UNP Q5UNP6 |
| A | 10 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 11 | GLU | - | expression tag | UNP Q5UNP6 |
| A | 12 | TYR | - | expression tag | UNP Q5UNP6 |
| A | 13 | LEU | - | expression tag | UNP Q5UNP6 |
| A | 14 | ARG | - | expression tag | UNP Q5UNP6 |
| A | 15 | ARG | - | expression tag | UNP Q5UNP6 |
| A | 16 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 17 | THR | - | expression tag | UNP Q5UNP6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 18 | LEU | - | expression tag | UNP Q5UNP6 |
| A | 19 | ASP | - | expression tag | UNP Q5UNP6 |
| A | 20 | LEU | - | expression tag | UNP Q5UNP6 |
| A | 21 | ARG | - | expression tag | UNP Q5UNP6 |
| A | 22 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 23 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 24 | ARG | - | expression tag | UNP Q5UNP6 |
| A | 25 | GLN | - | expression tag | UNP Q5UNP6 |
| A | 26 | ARG | - | expression tag | UNP Q5UNP6 |
| A | 27 | ILE | - | expression tag | UNP Q5UNP6 |
| A | 28 | ARG | - | expression tag | UNP Q5UNP6 |
| A | 29 | GLU | - | expression tag | UNP Q5UNP6 |
| A | 30 | LEU | - | expression tag | UNP Q5UNP6 |
| A | 31 | GLU | - | expression tag | UNP Q5UNP6 |
| A | 1574 | PRO | - | expression tag | UNP Q5UNP6 |
| A | 1575 | ASN | - | expression tag | UNP Q5UNP6 |
| A | 1576 | SER | - | expression tag | UNP Q5UNP6 |
| A | 1577 | SER | - | expression tag | UNP Q5UNP6 |
| A | 1578 | SER | - | expression tag | UNP Q5UNP6 |
| A | 1579 | VAL | - | expression tag | UNP Q5UNP6 |
| A | 1580 | ASP | - | expression tag | UNP Q5UNP6 |
| A | 1581 | LYS | - | expression tag | UNP Q5UNP6 |
| A | 1582 | LEU | - | expression tag | UNP Q5UNP6 |
| A | 1583 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 1584 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 1585 | ALA | - | expression tag | UNP Q5UNP6 |
| A | 1586 | LEU | - | expression tag | UNP Q5UNP6 |
| A | 1587 | GLU | - | expression tag | UNP Q5UNP6 |
| A | 1588 | HIS | - | expression tag | UNP Q5UNP6 |
| A | 1589 | HIS | - | expression tag | UNP Q5UNP6 |
| A | 1590 | HIS | - | expression tag | UNP Q5UNP6 |
| A | 1591 | HIS | - | expression tag | UNP Q5UNP6 |
| A | 1592 | HIS | - | expression tag | UNP Q5UNP6 |
| A | 1593 | HIS | - | expression tag | UNP Q5UNP6 |

- Molecule 2 is a protein called 1B2 (heavy chain).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1539 | 978 | 257 | 298 | 6 | | |
| 2 | E | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1539 | 978 | 257 | 298 | 6 | | |

- Molecule 3 is a protein called 1B2 (light chain).

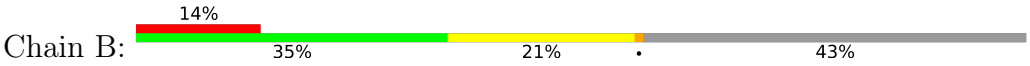
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | D | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1564 | 980 | 261 | 317 | 6 | | |
| 3 | F | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1564 | 981 | 261 | 316 | 6 | | |

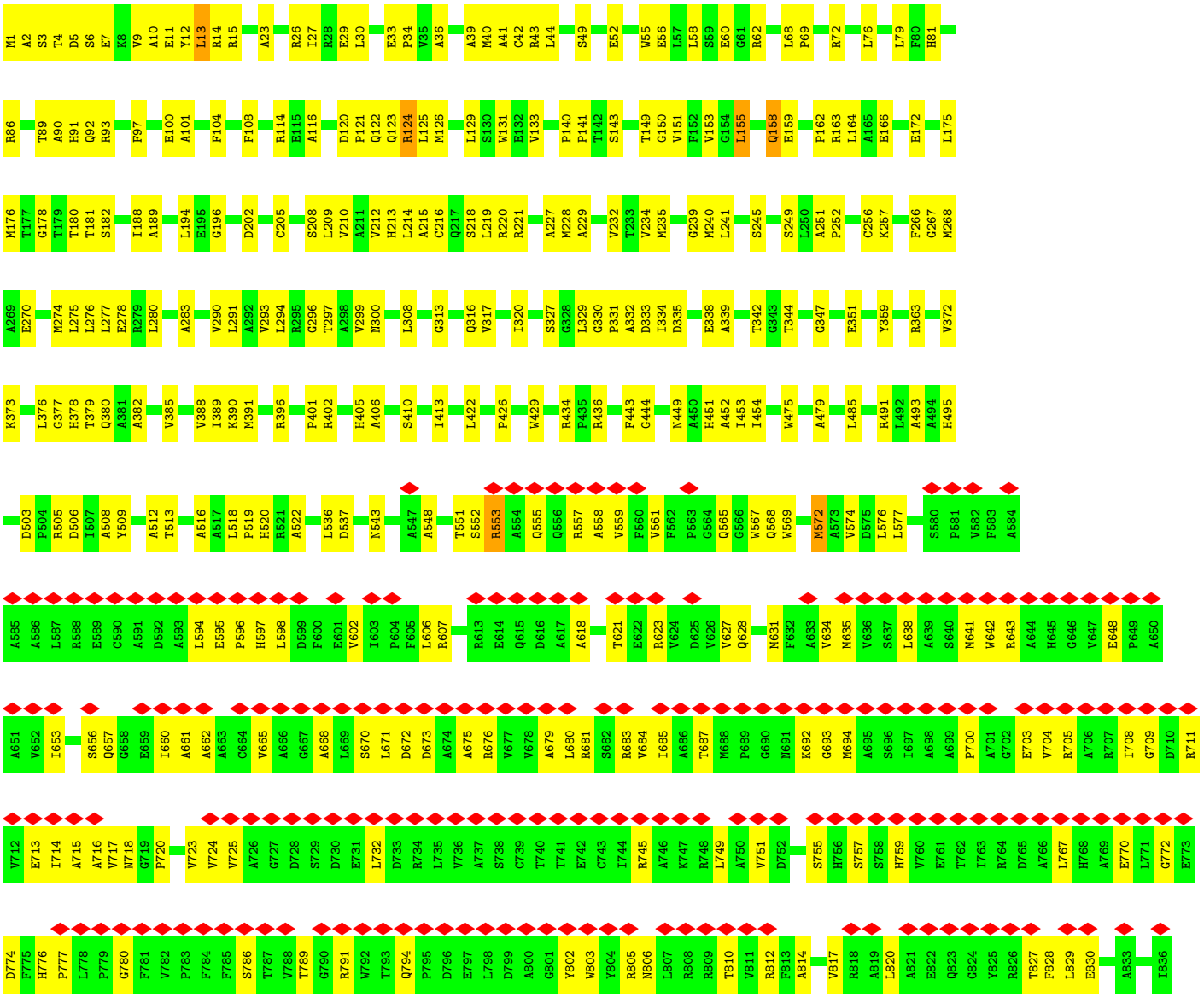
# 3 Residue-property plots (i)

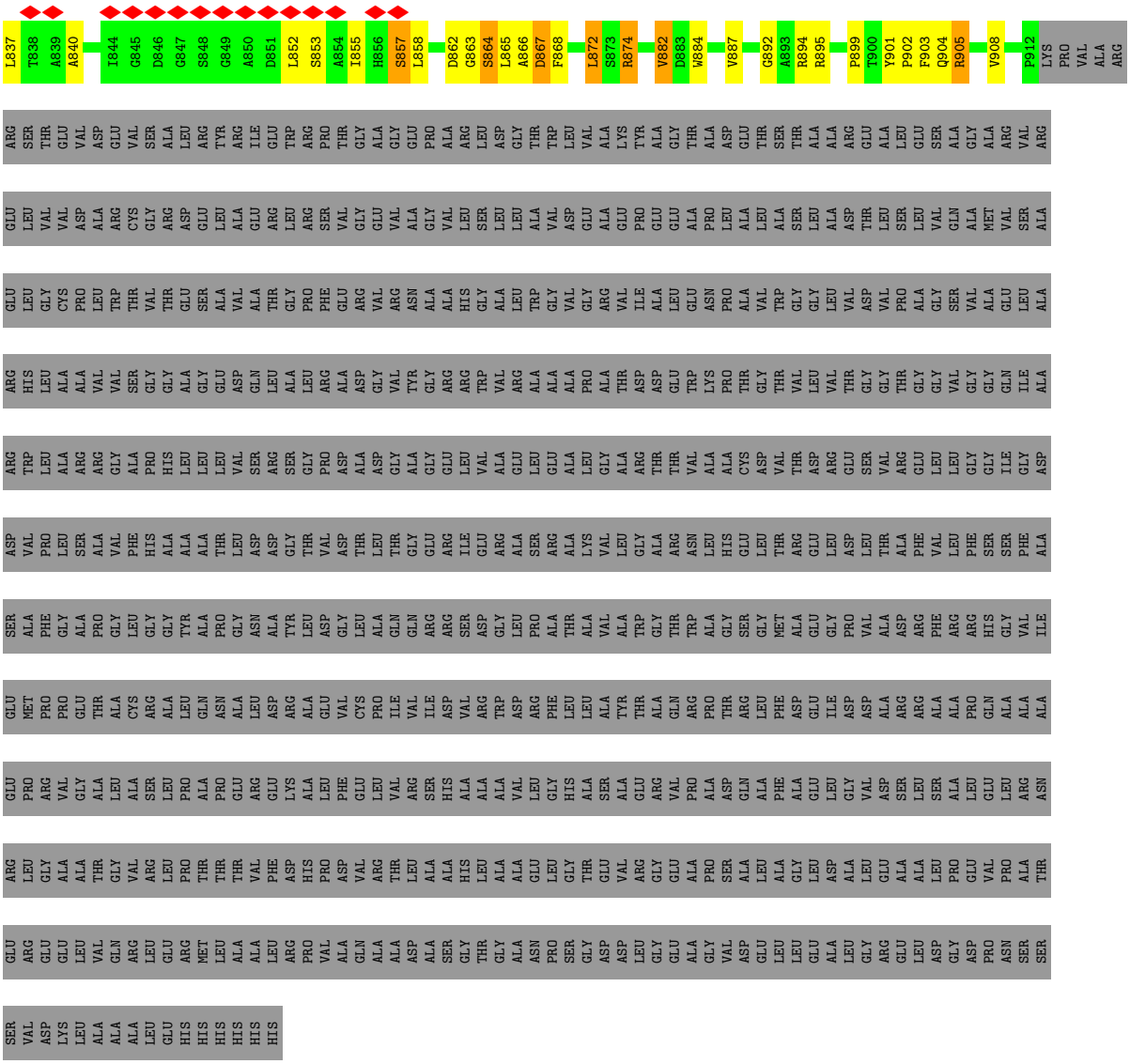
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: EryAI

Chain B:

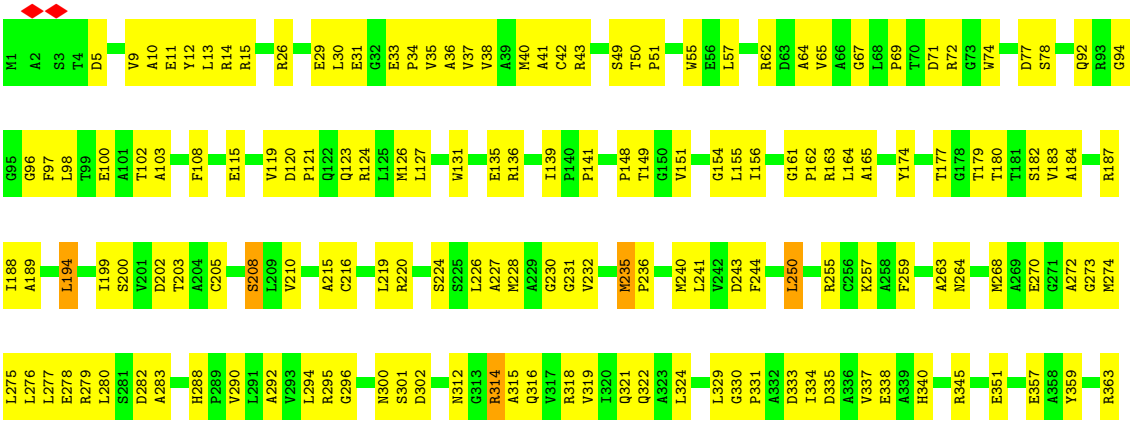


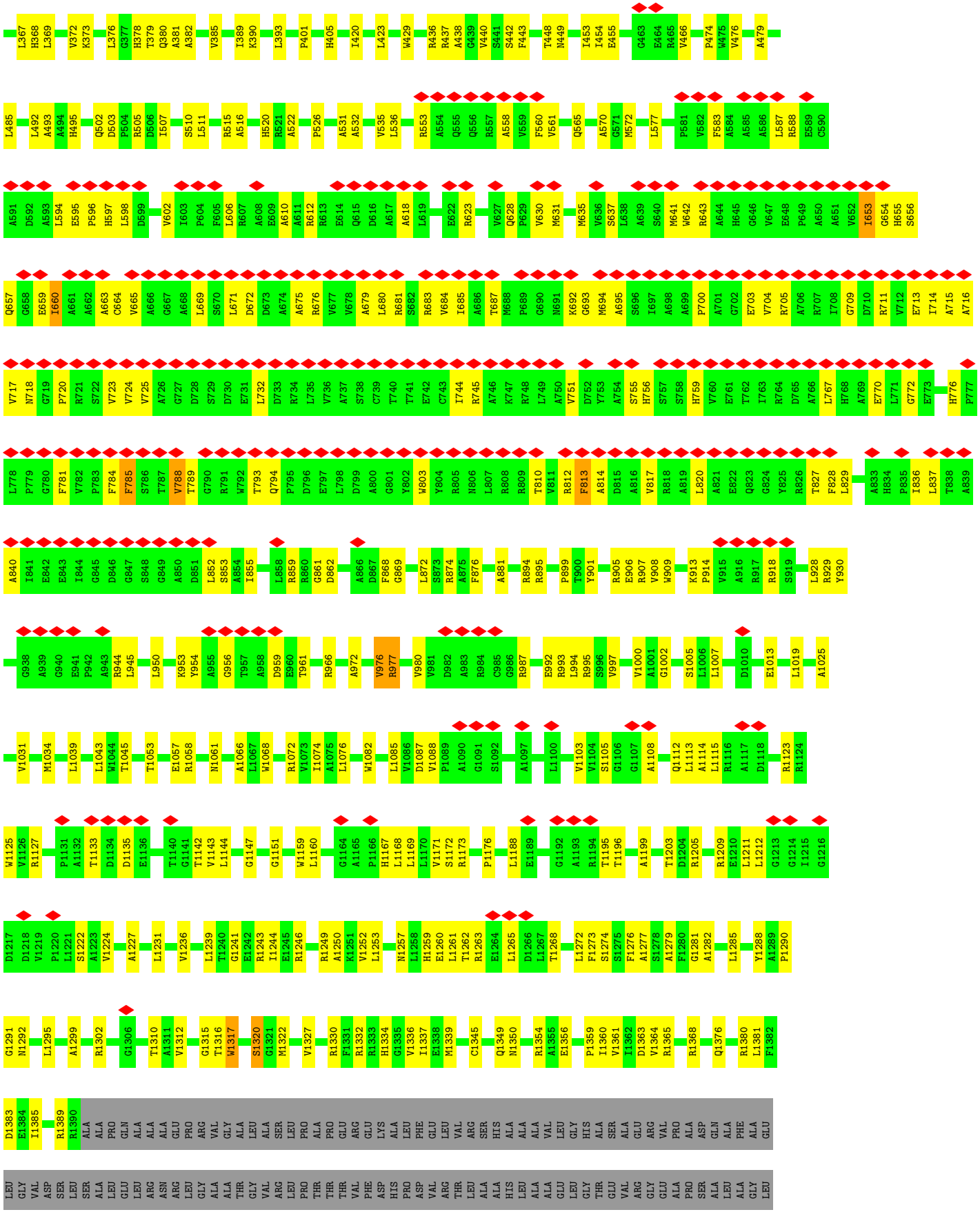



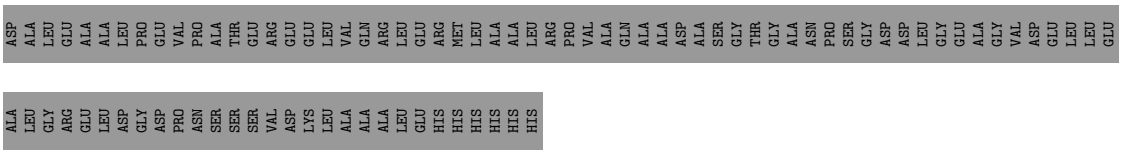


• Molecule 1: EryAI

Chain A:

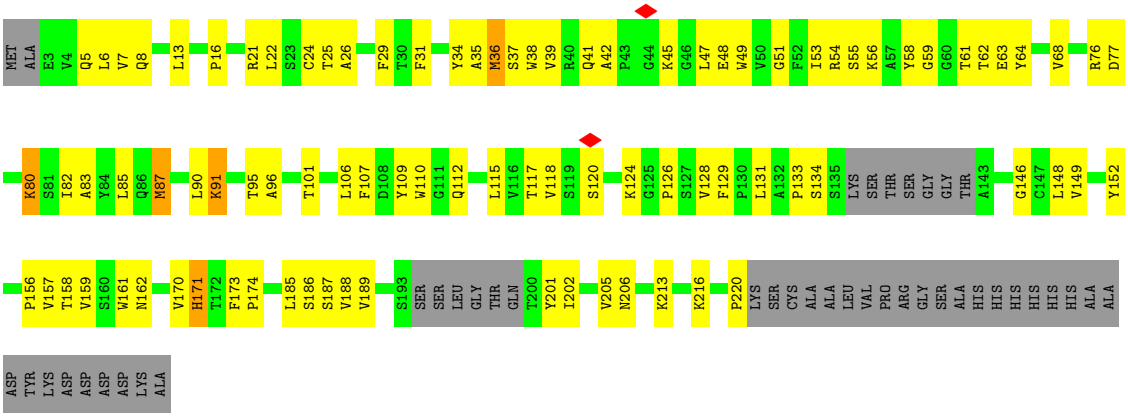




L367 H368 L369 V372 K373 L376 G377 H378 T379 Q380 A381 A382 V385 I389 K390 L393 P401 H405 I420 L423 W429 R436 R437 A438 G439 V440 S441 S442 F443 T448 N449 I453 I454 E455 G463 E464 R465 V466 P474 W475 V476 A479
L485 L492 A493 A494 H495 Q502 D503 P504 R505 D506 I507 S510 L511 R515 A516 H520 R521 A522 P526 A531 A532 V535 L536 R553 A554 Q555 Q556 R557 A558 V559 F560 V561 Q565 A570 G571 M572 L577 P581 V582 F583 A584 A585 A586 L587 R588 E589 C590
A591 D592 A593 L594 E595 P596 H597 L598 D599 V602 I603 P604 F605 L606 R607 A608 E609 A610 A611 R612 R613 E614 Q615 D616 A617 A618 L619 E622 R623 V627 Q628 P629 V630 M631 M635 V636 S637 L638 A639 S640 M641 W642 R643 A644 H645 G646 V647 E648 P649 A650 A651 V652 I653 G654 H655 S656
Q657 G658 E659 I660 A661 A662 A663 C664 V665 A666 G667 A668 L669 S670 L671 D672 D673 A674 A675 R676 V677 V678 A679 L680 R681 S682 R683 V684 I685 A686 T687 M688 P689 G690 N691 K692 G693 M694 A695 S696 I697 A698 A699 P700 A701 G702 E703 V704 R705 A706 R707 I708 G709 D710 R711 V712 E713 I714 A715 A716
V717 N718 G719 P720 R721 S722 V723 V724 V725 A726 G727 D728 S729 D730 E731 L732 D733 R734 L735 V736 A737 S738 C739 T740 T741 E742 C743 I744 R745 A746 K747 R748 L749 A750 V751 D752 Y753 A754 S755 H756 S757 S758 H759 V760 E761 T762 I763 R764 D765 A766 L767 H768 A769 E770 L771 G772 E773 H776 P777
L778 P779 G780 F781 V782 P783 F784 F785 S786 T787 V788 T789 G790 R791 W792 T793 Q794 P795 D796 E797 L798 D799 A800 G801 Y802 W803 Y804 R805 N806 L807 R808 R809 T810 V811 R812 F813 A814 D815 A816 V817 R818 A819 L820 A821 E822 Q823 G824 Y825 R826 T827 F828 L829 A833 H834 P835 I836 L837 T838 A839
A840 I841 E842 E843 I844 G845 D846 G847 S848 G849 A850 D851 L852 S853 A854 I855 L858 R859 R860 G861 D862 A866 D867 F868 G869 L872 S873 R874 A875 F876 A881 R894 R895 P899 T900 Y901 R905 E906 R907 V908 W909 K913 P914 V915 A916 R917 R918 S919 L928 R929 Y930
G938 A939 G940 E941 P942 A943 R944 L945 L950 K953 Y954 A955 G956 T957 A958 D959 E960 T961 R966 A972 V976 R977 V980 V981 D982 A983 R984 C985 G986 R987 E992 R993 L994 R995 S996 V997 V1000 A1001 G1002 S1005 L1006 L1007 D1010 E1013 L1019 A1025
V1031 M1034 L1039 L1043 W1044 T1045 T1053 E1057 R1058 N1061 A1066 L1067 W1068 R1072 V1073 I1074 A1075 L1076 W1082 L1085 V1086 D1087 V1088 P1089 A1090 G1091 S1092 A1097 L1100 V1103 V1104 S1105 G1106 G1107 A1108 Q1112 L1113 A1114 L1115 R1116 A1117 D1118 R1123 R1124
W1125 V1126 R1127 P1131 A1132 T1133 D1134 D1135 E1136 T1140 G1141 T1142 V1143 L1144 G1147 G1151 W1159 L1160 G1164 A1165 P1166 H1167 L1168 L1169 L1170 V1171 S1172 R1173 P1176 L1188 E1189 G1192 A1193 R1194 T1195 T1196 A1199 T1203 D1204 R1205 R1209 E1210 L1211 L1212 G1213 G1214 I1215 G1216
D1217 D1218 V1219 P1220 L1221 S1222 A1223 V1224 A1227 L1231 V1236 L1239 T1240 G1241 E1242 R1243 I1244 E1245 R1246 R1249 A1250 K1251 V1252 L1253 N1257 L1258 H1259 E1260 L1261 T1262 R1263 E1264 L1265 D1266 L1267 T1268 L1272 F1273 S1274 S1275 F1276 A1277 S1278 A1279 F1280 G1281 A1282 L1285 Y1288 A1289 P1290
G1291 N1292 L1295 A1299 R1302 G1306 T1310 A1311 V1312 G1315 T1316 W1317 S1320 G1321 M1322 V1327 R1330 F1331 R1332 R1333 H1334 G1335 V1336 I1337 E1338 M1339 C1345 Q1349 N1350 R1354 A1355 E1356 P1359 I1360 V1361 I1362 D1363 V1364 R1365 R1368 Q1376 R1380 L1381 F1382
D1383 E1384 I1385 R1389 R1390 ALA ALA PRO GLN ALA ALA ALA GLU PRO ARG VAL GLY ALA LEU ALA SER LEU PRO ALA PRO GLU ARG GLU PHE LYS ALA LEU PRO HIS PRO ASP VAL ARG THR LEU ALA ALA HIS LEU ALA ALA ALA VAL LEU GLU LEU GLY HIS ALA SER ALA GLU VAL ARG GLY GLU ALA PRO ALA ASP GLN ALA LEU ALA PHE ALA GLU
LEU GLY VAL ASP SER LEU SER ALA LEU GLU LEU ARG ASN ARG LEU GLY ALA ALA THR GLY VAL ARG LEU PRO THR THR THR VAL PHE ASP HIS PRO ASP VAL ARG THR LEU ALA ALA HIS LEU ALA ALA ALA GLU LEU GLY HIS ALA SER ALA GLU VAL ARG GLY GLU ALA PRO ALA SER ALA LEU ALA GLY LEU



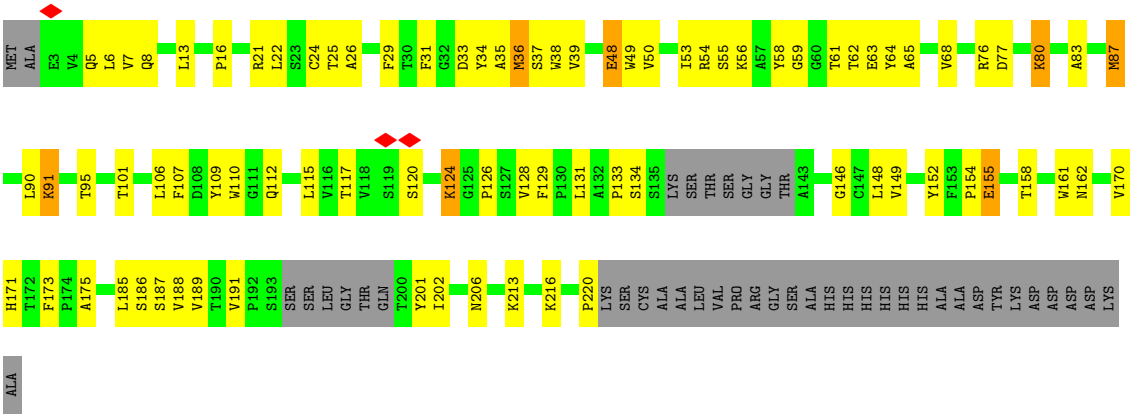
• Molecule 2: 1B2 (heavy chain)

Chain C:

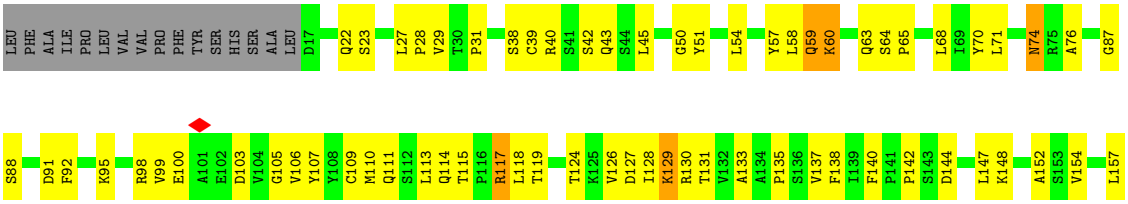
• Molecule 2: 1B2 (heavy chain)

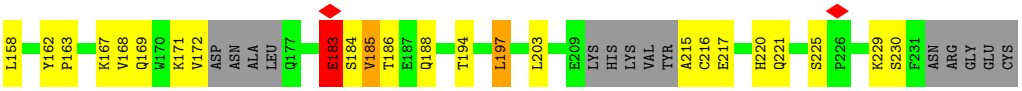
Chain E:

• Molecule 3: 1B2 (light chain)

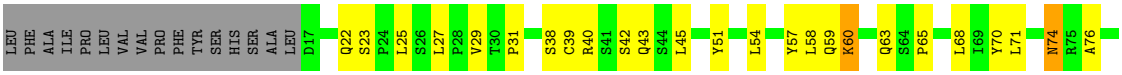
Chain D:

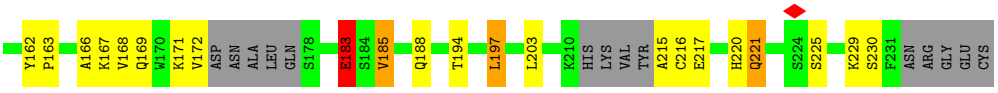



• Molecule 3: 1B2 (light chain)

Chain F:





# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 102772 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 1.481 | Depositor |
| Minimum map value | -0.533 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.061 | Depositor |
| Recommended contour level | 0.28 | Depositor |
| Map size (Å) | 336.0, 336.0, 336.0 | wwPDB |
| Map dimensions | 336, 336, 336 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.0, 1.0, 1.0 | 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 | 0.31 | 0/10473 | 0.59 | 1/14255 (0.0%) |
| 1 | B | 0.32 | 0/6875 | 0.59 | 1/9353 (0.0%) |
| 2 | C | 0.32 | 0/1575 | 0.61 | 0/2141 |
| 2 | E | 0.32 | 0/1575 | 0.59 | 0/2141 |
| 3 | D | 0.32 | 0/1597 | 0.60 | 1/2171 (0.0%) |
| 3 | F | 0.36 | 0/1597 | 0.63 | 2/2170 (0.1%) |
| All | All | 0.32 | 0/23692 | 0.60 | 5/32231 (0.0%) |

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 250 | LEU | C-N-CA | 7.61 | 140.73 | 121.70 |
| 1 | B | 13 | LEU | CA-CB-CG | 5.87 | 128.81 | 115.30 |
| 3 | F | 183 | GLU | CA-CB-CG | 5.41 | 125.30 | 113.40 |
| 3 | D | 183 | GLU | CA-CB-CG | 5.40 | 125.28 | 113.40 |
| 3 | F | 125 | LYS | CA-CB-CG | 5.24 | 124.92 | 113.40 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 905 | ARG | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 10277 | 0 | 10118 | 363 | 0 |
| 1 | B | 6741 | 0 | 6618 | 271 | 0 |
| 2 | C | 1539 | 0 | 1511 | 71 | 0 |
| 2 | E | 1539 | 0 | 1511 | 72 | 0 |
| 3 | D | 1564 | 0 | 1517 | 73 | 0 |
| 3 | F | 1564 | 0 | 1522 | 72 | 0 |
| All | All | 23224 | 0 | 22797 | 862 | 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 19.

The worst 5 of 862 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:125:LYS:H | 3:F:125:LYS:HD3 | 1.23 | 1.02 |
| 1:B:151:VAL:HA | 1:B:228:MET:HB2 | 1.62 | 0.82 |
| 1:B:121:PRO:HB2 | 1:B:234:VAL:HG11 | 1.61 | 0.81 |
| 1:A:966:ARG:HG2 | 1:A:976:VAL:HG11 | 1.62 | 0.80 |
| 1:A:235:MET:HG2 | 1:A:240:MET:HG3 | 1.68 | 0.76 |

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 | 1388/1593 (87%) | 1300 (94%) | 88 (6%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | B | 910/1593 (57%) | 844 (93%) | 65 (7%) | 1 (0%) | 51 85 |
| 2 | C | 199/249 (80%) | 193 (97%) | 5 (2%) | 1 (0%) | 29 68 |
| 2 | E | 199/249 (80%) | 191 (96%) | 7 (4%) | 1 (0%) | 29 68 |
| 3 | D | 200/236 (85%) | 187 (94%) | 13 (6%) | 0 | 100 100 |
| 3 | F | 200/236 (85%) | 181 (90%) | 19 (10%) | 0 | 100 100 |
| All | All | 3096/4156 (74%) | 2896 (94%) | 197 (6%) | 3 (0%) | 54 85 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 156 | PRO |
| 2 | E | 154 | PRO |
| 1 | B | 864 | SER |

### 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 | 1022/1173 (87%) | 989 (97%) | 33 (3%) | 39 62 |
| 1 | B | 675/1173 (58%) | 646 (96%) | 29 (4%) | 29 55 |
| 2 | C | 170/203 (84%) | 157 (92%) | 13 (8%) | 13 40 |
| 2 | E | 170/203 (84%) | 157 (92%) | 13 (8%) | 13 40 |
| 3 | D | 181/208 (87%) | 164 (91%) | 17 (9%) | 8 30 |
| 3 | F | 181/208 (87%) | 165 (91%) | 16 (9%) | 10 34 |
| All | All | 2399/3168 (76%) | 2278 (95%) | 121 (5%) | 28 51 |

5 of 121 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1317 | TRP |
| 3 | F | 112 | SER |
| 2 | C | 134 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 110 | MET |
| 3 | F | 197 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1112 | GLN |
| 3 | F | 221 | GLN |
| 1 | A | 340 | HIS |
| 1 | A | 718 | ASN |
| 1 | A | 794 | GLN |

#### 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

There are no ligands in this entry.

### 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.

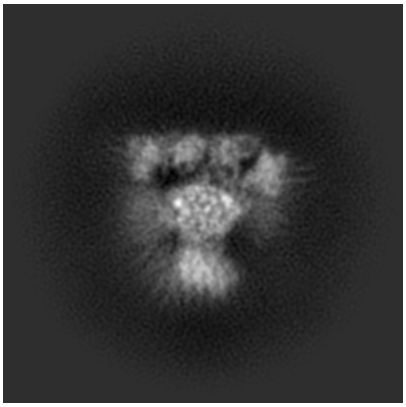
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23715. These allow visual inspection of the internal detail of the map and identification of artifacts.

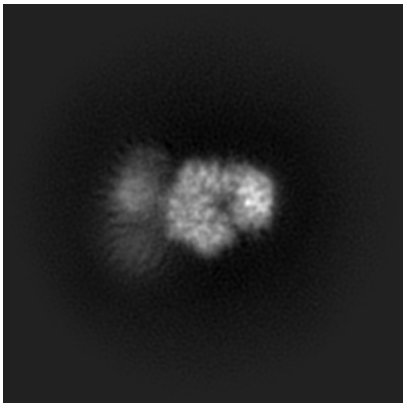
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

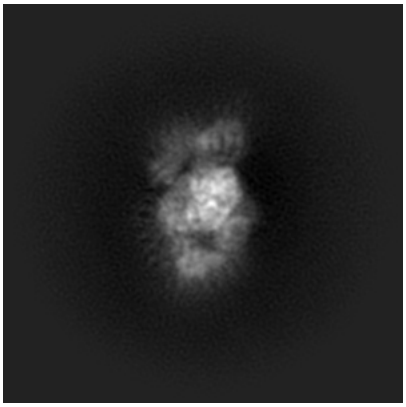
### 6.1.1 Primary map



X



Y

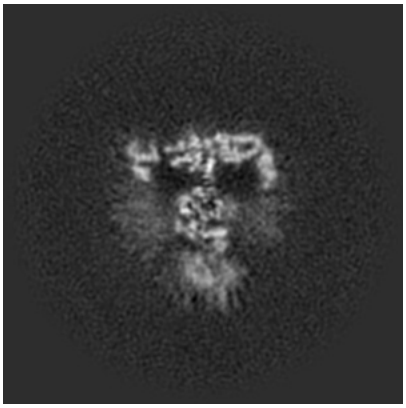


Z

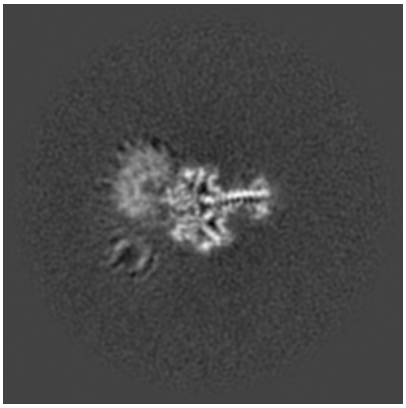
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

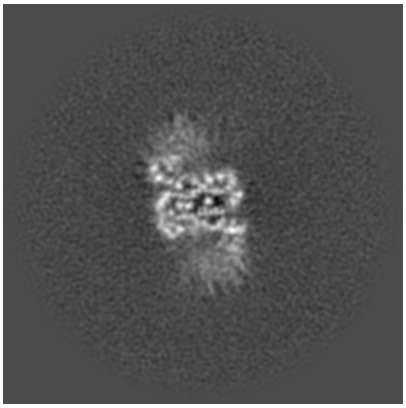
### 6.2.1 Primary map



X Index: 168



Y Index: 168

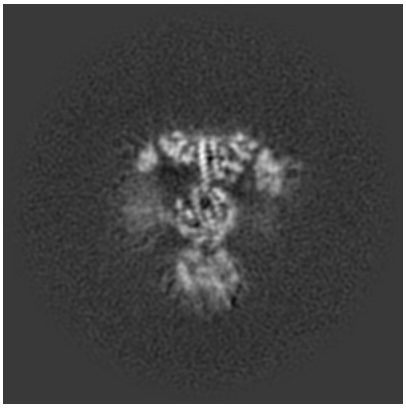


Z Index: 168

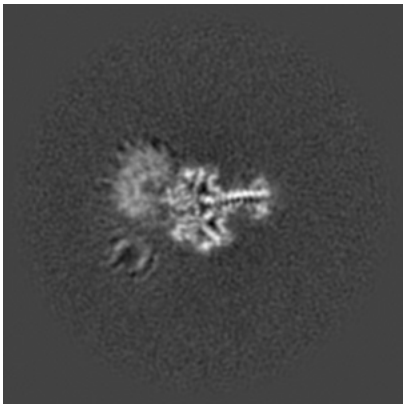
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

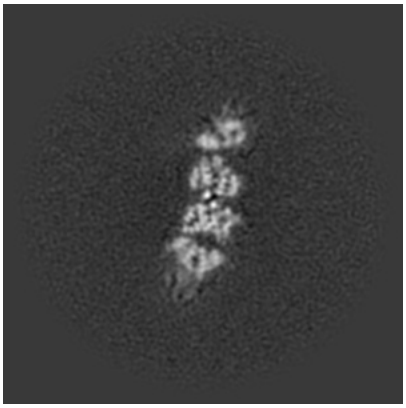
### 6.3.1 Primary map



X Index: 177



Y Index: 168

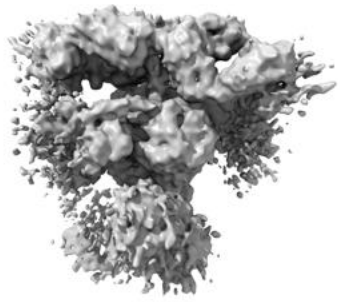


Z Index: 206

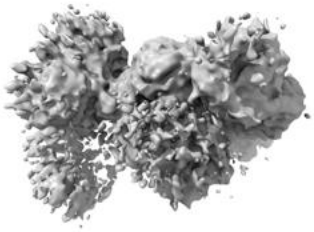
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

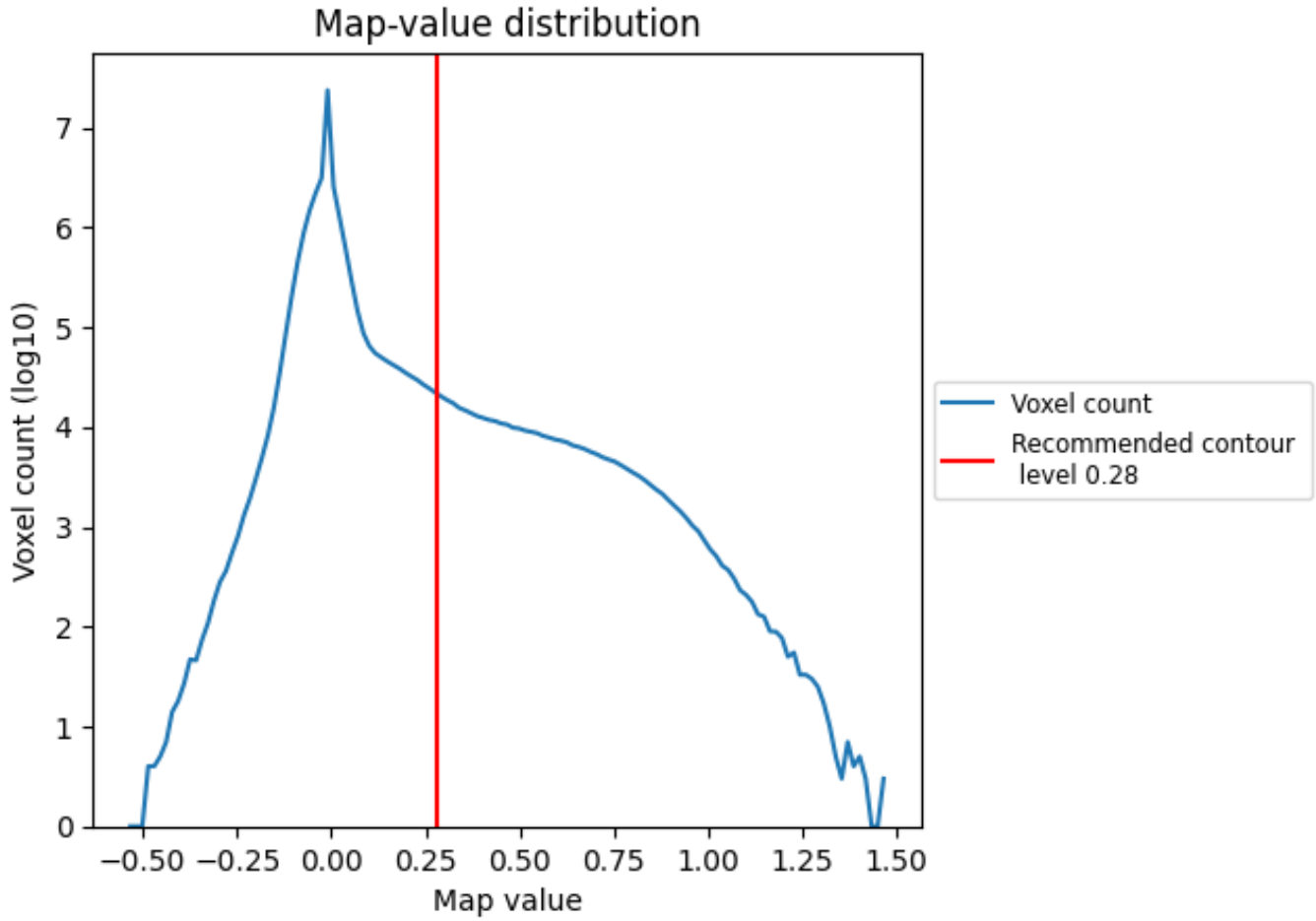
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

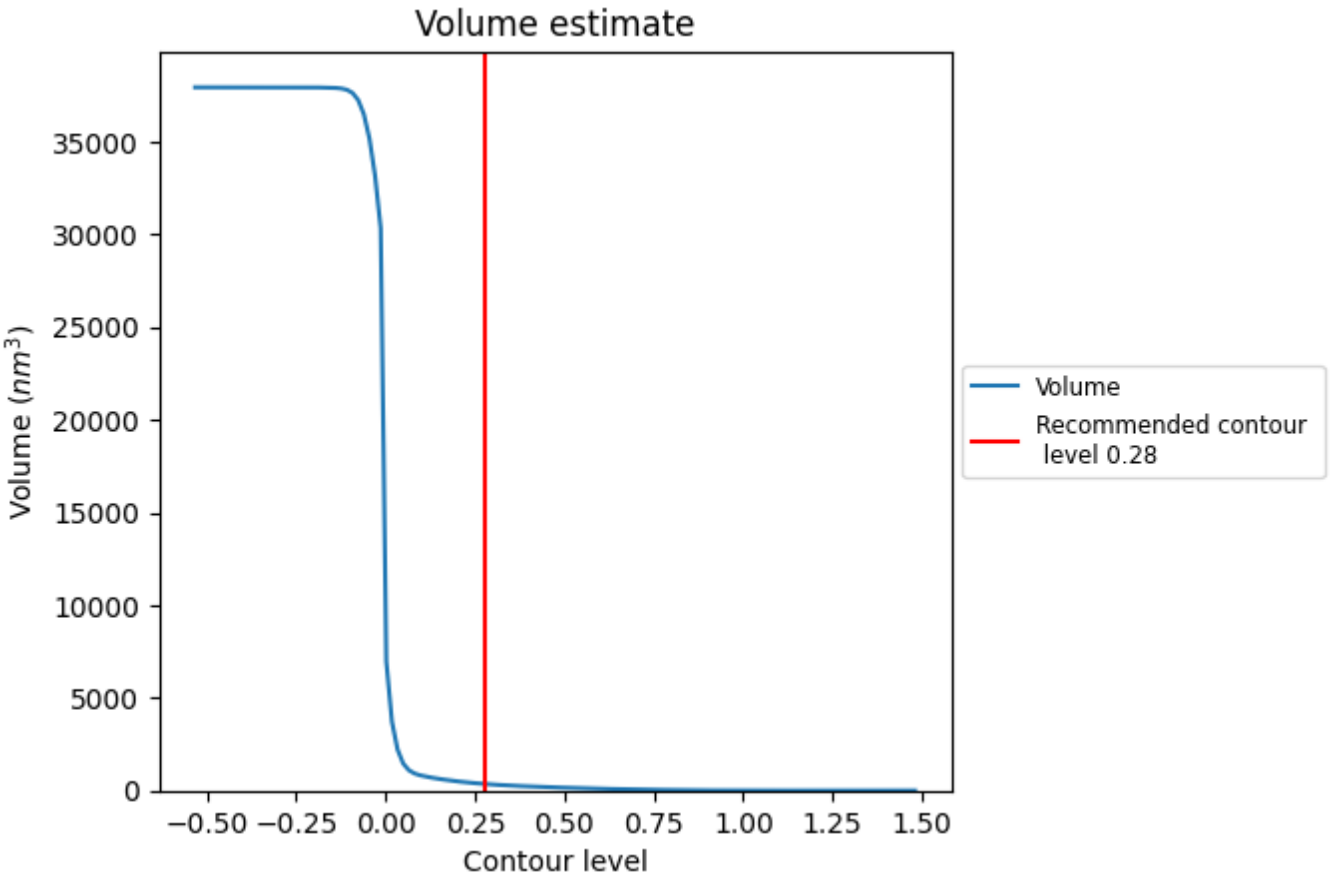
This section contains the results of statistical analysis of the map.

## 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.

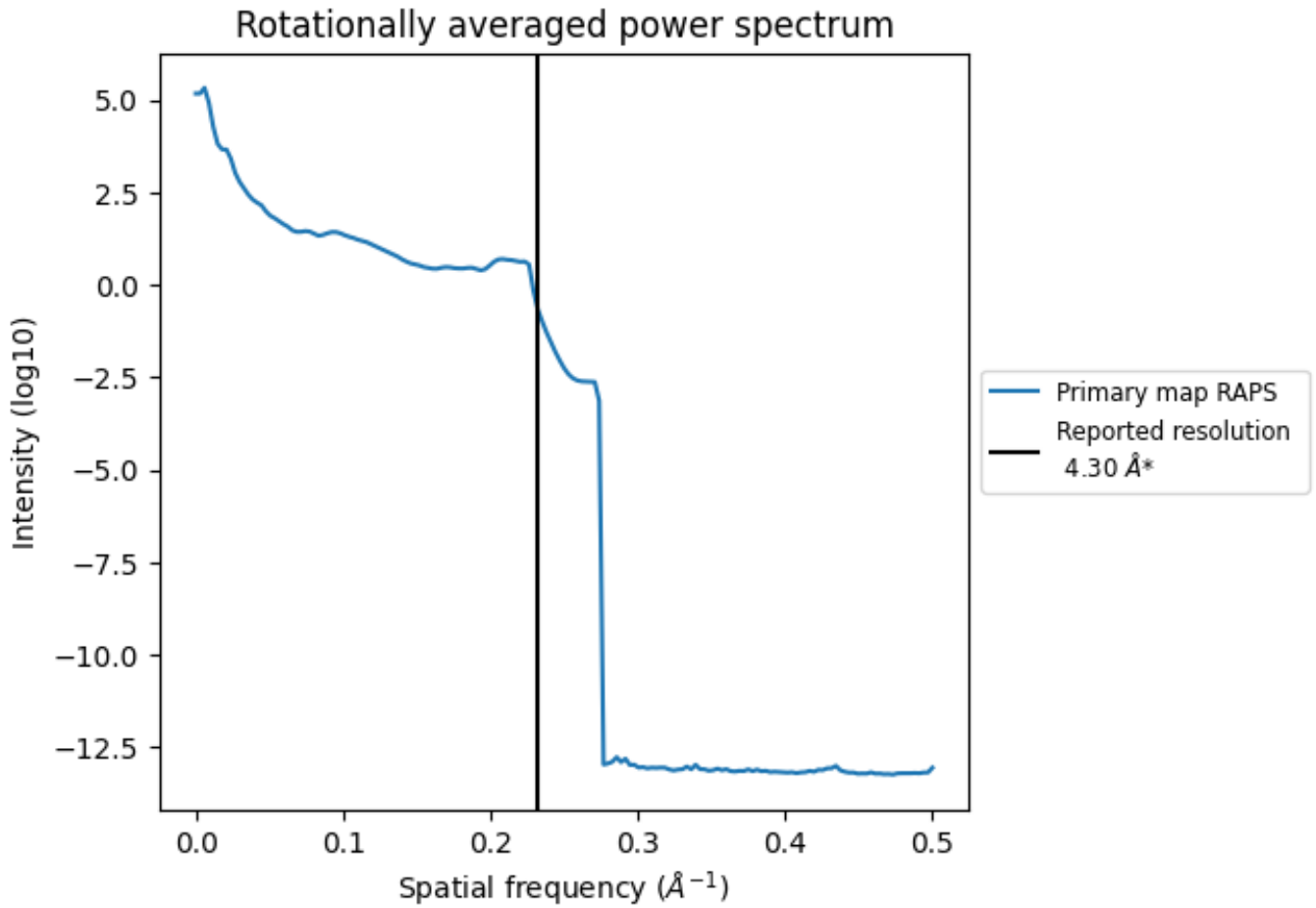
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 352 $nm^3$; this corresponds to an approximate mass of 318 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 0.233 $Å^{-1}$

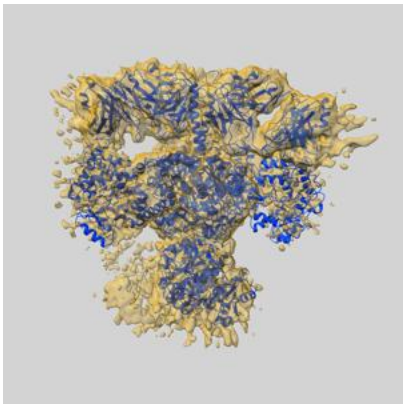
# 8 Fourier-Shell correlation

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

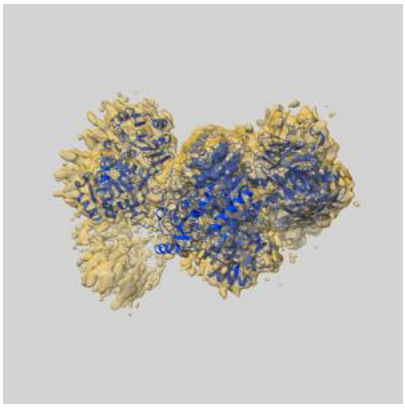
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23715 and PDB model 7M7J. Per-residue inclusion information can be found in section 3 on page 7.

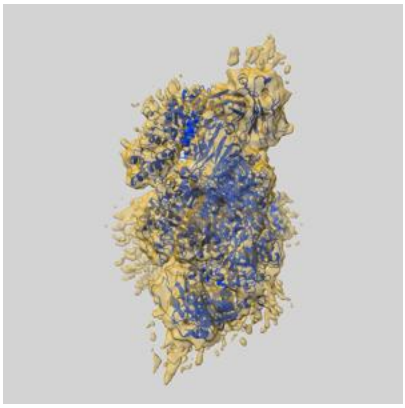
## 9.1 Map-model overlay



X



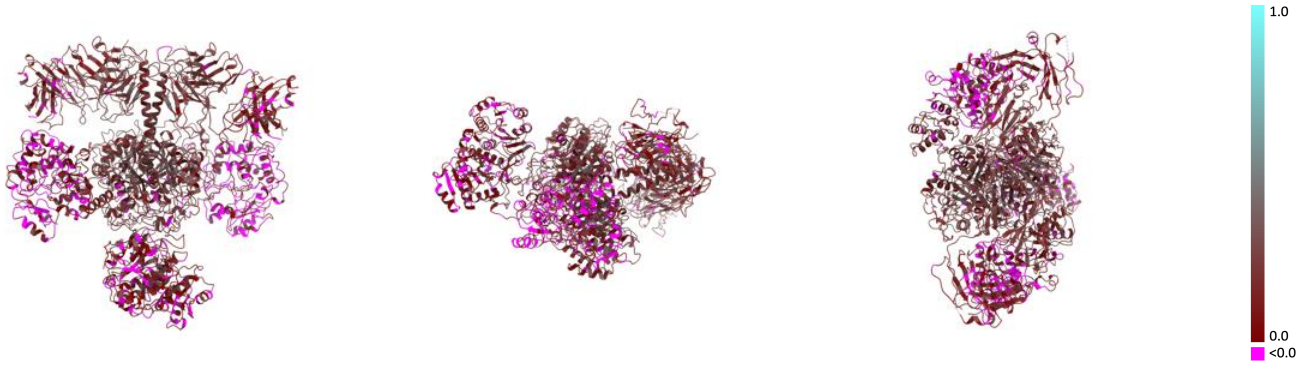
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

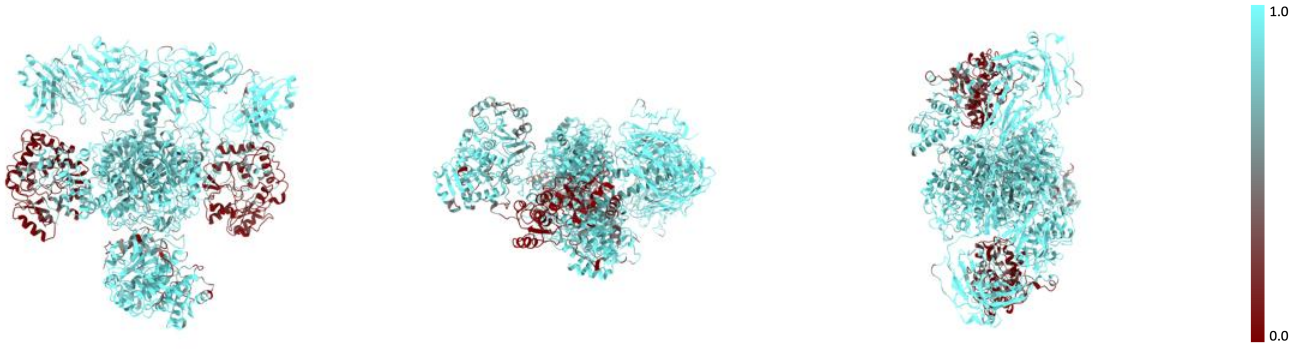
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

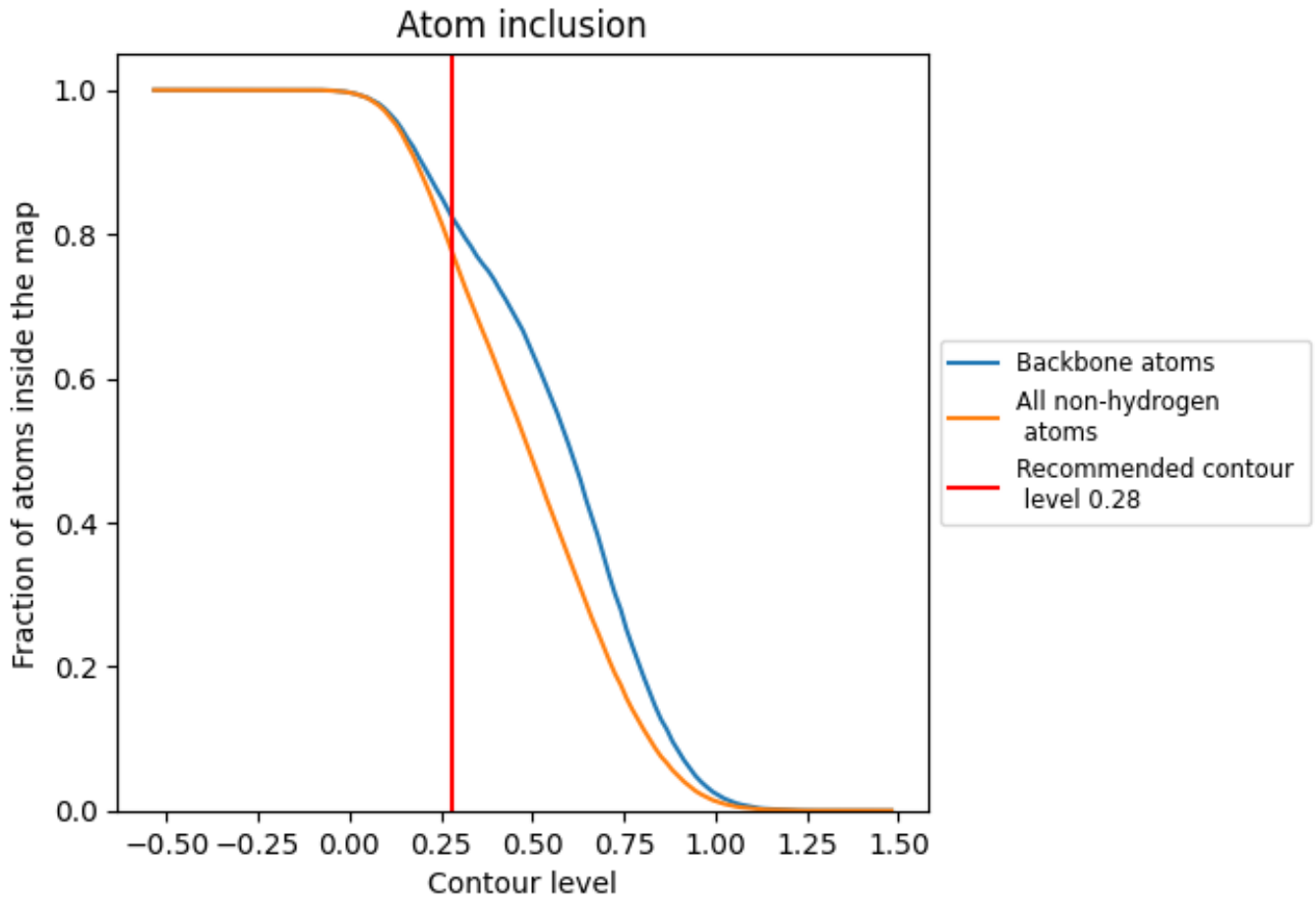
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

## 9.4 Atom inclusion (i)




At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.28) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7761 | 0.1660 |
| A | 0.7351 | 0.1410 |
| B | 0.6879 | 0.1610 |
| C | 0.9345 | 0.2010 |
| D | 0.9370 | 0.2120 |
| E | 0.9444 | 0.2050 |
| F | 0.9370 | 0.2280 |