wwPDB EM Validation Summary Report (i)

May 18, 2024 – 10:30 am BST

PDB ID	:	6YLF
EMDB ID	:	EMD-10837
Title	:	Rix1-Rea1 pre-60S particle - Rea1, body 3 (rigid body refinement, composite structure of Rea1 ring and tail)
Authors	:	Kater, L.; Beckmann, R.
Deposited on	:	2020-04-07
Resolution	:	4.20 Å(reported)
Based on initial models	:	6OR5, 6HYP, 6HYD, 6QTA

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

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

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

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

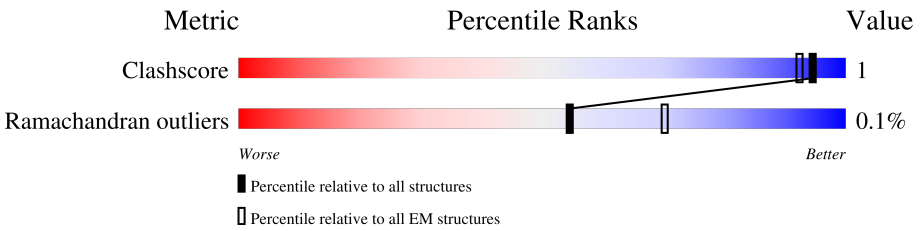
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.20 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

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	AP1	4910	10% 73% • 26%
2	xP1	515	7% 14% 86%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18362 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 Midasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	AP1	3629	18010	10752	3629	3629	0	0

- Molecule 2 is a protein called Ribosome assembly protein 4.

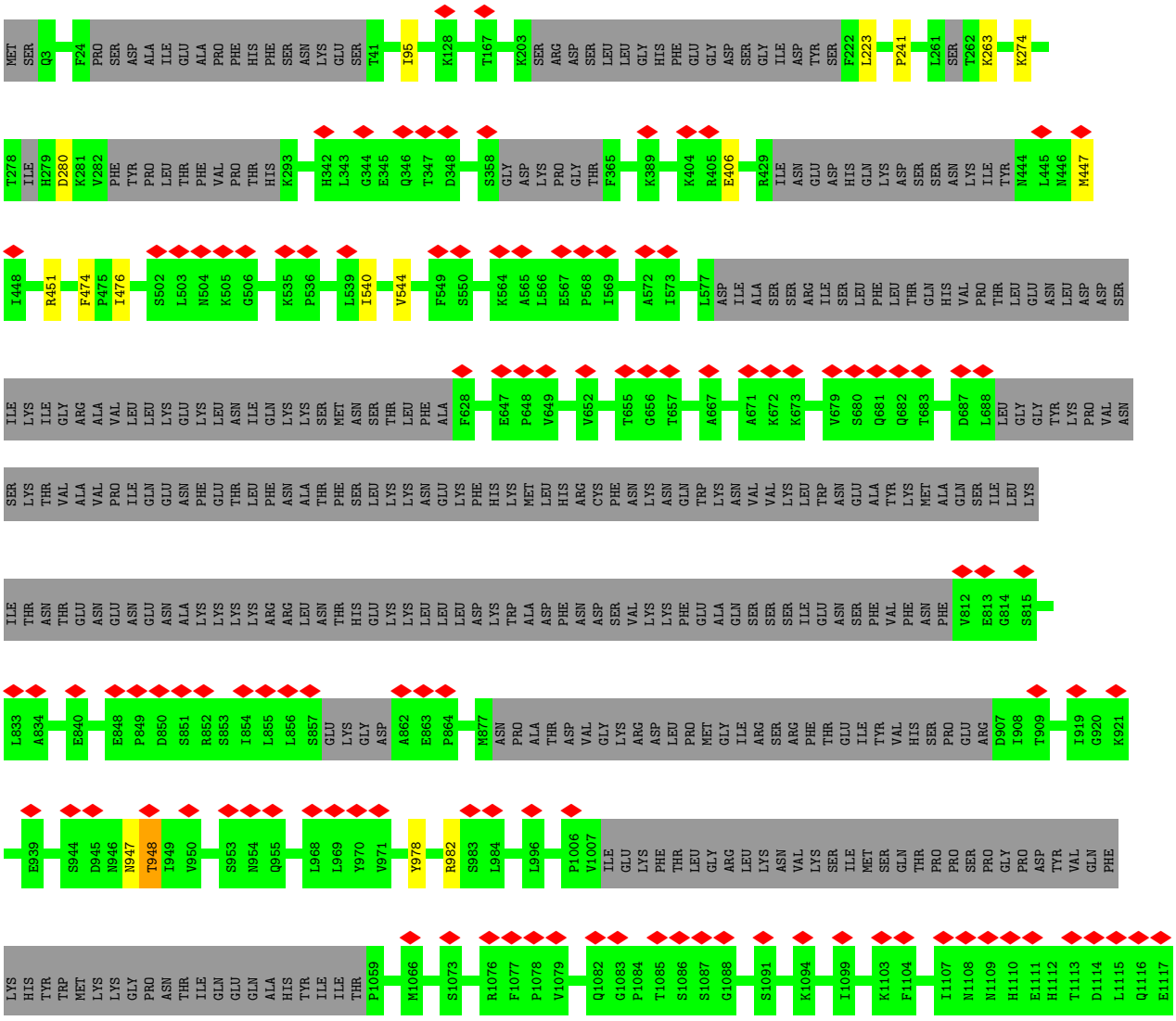
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	xP1	71	352	210	71	71	0	0

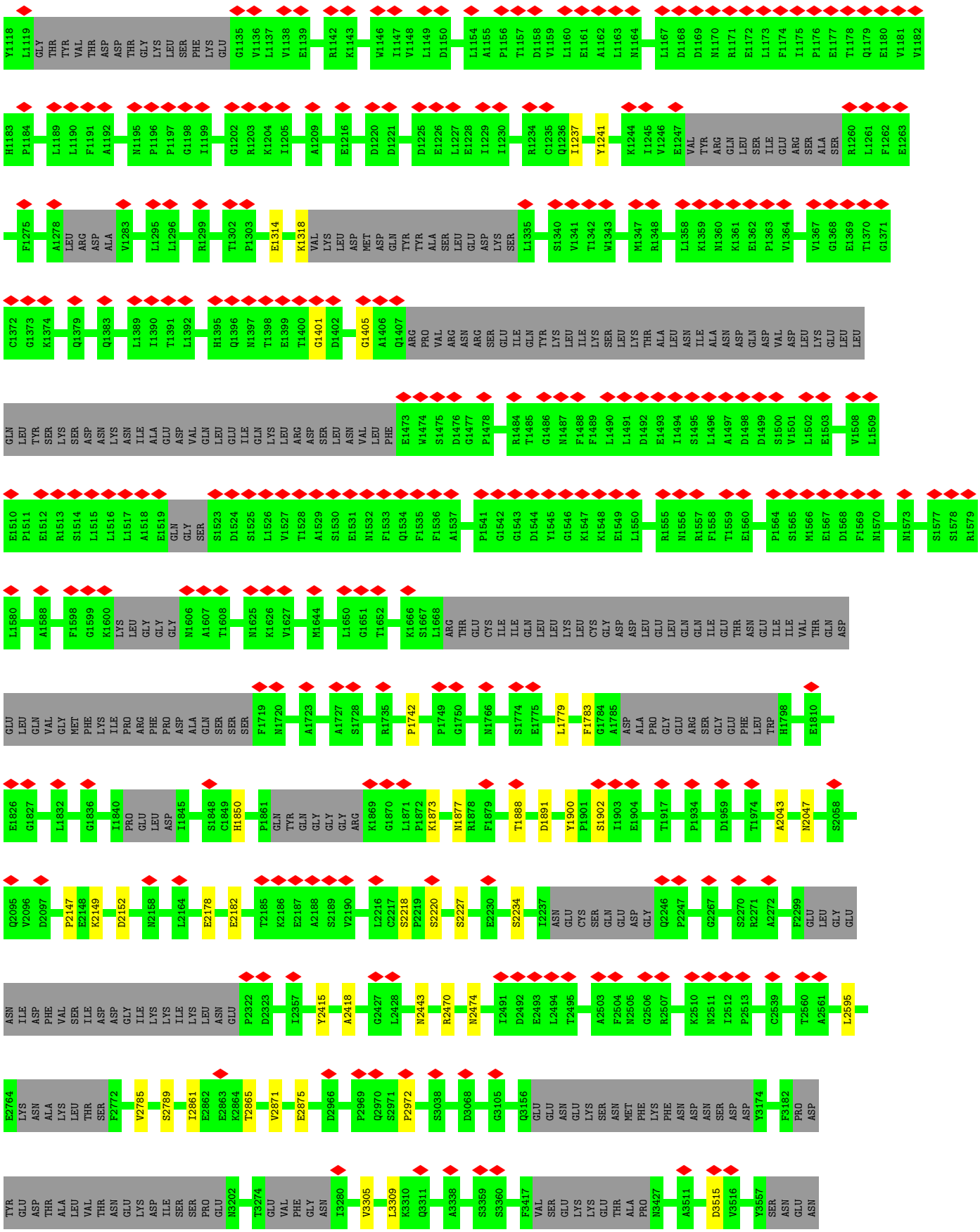
3 Residue-property plots (i)

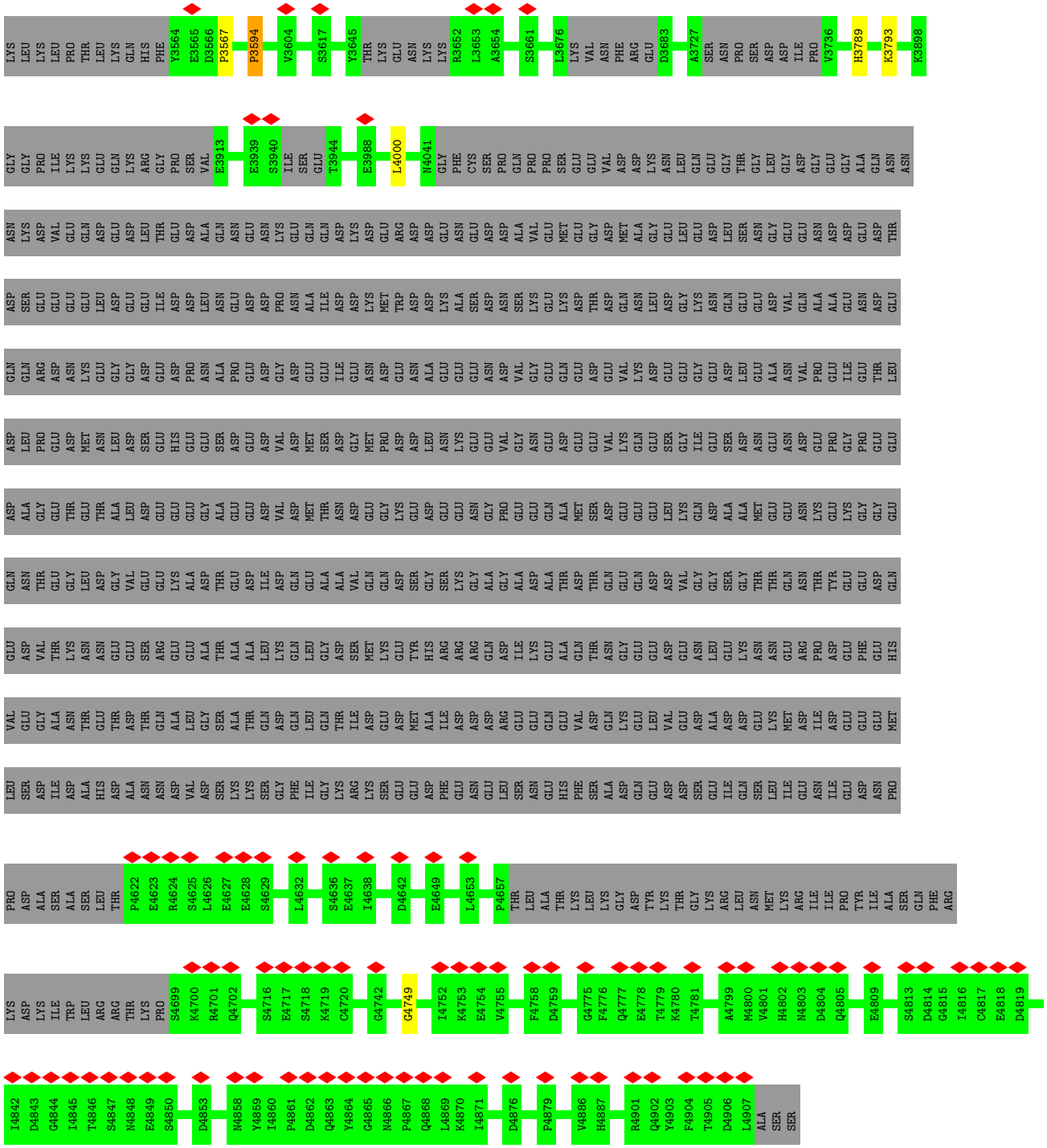
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain AP1:

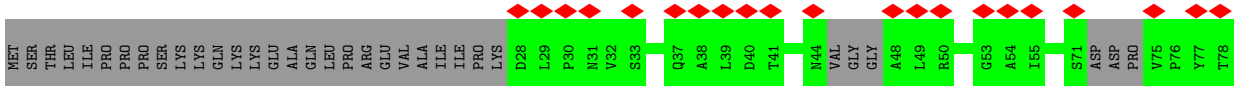


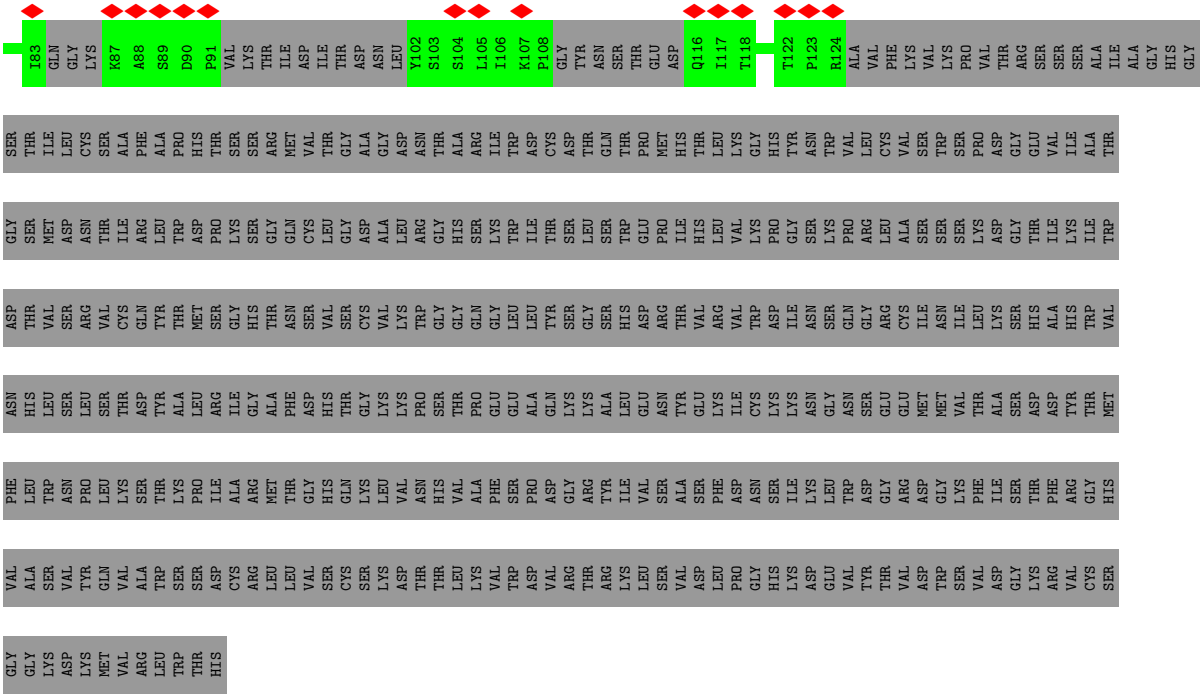

Y1118 L1119 GLY THR TYR VAL THR ASP ASP THR GLY LYS LEU SER PHE LYS GLU G1135 V1136 L1137 V1138 E1139 R1142 K1143 W1146 I1147 V1148 L1149 D1150 L1154 A1155 P1156 T1157 D1158 V1159 L1160 E1161 A1162 L1163 M1164 L1167 D1168 D1169 N1170 R1171 E1172 L1173 F1174 I1175 P1176 E1177 T1178 Q1179 E1180 V1181 V1182
H1183 P1184 L1189 L1190 F1191 A1192 N1195 P1196 P1197 G1198 I1199 G1202 R1203 K1204 I1205 A1209 E1216 D1220 D1221 D1225 E1226 L1227 E1228 I1229 I1230 R1234 C1235 Q1236 I1237 Y1241 K1244 I1245 V1246 E1247 VAL TYR ARG GLN LEU SER ILE GLU ARG SER ALA SER R1260 L1261 F1262 E1263
T1275 A1278 LEU ARG ASP ALA V1283 L1295 L1296 R1299 T1302 P1303 E1314 K1318 VAL LYS LEU ASP MET ASP GLN TYR TYR ALA SER LEU GLU ASP LYS SER L1335 S1340 V1341 T1342 W1343 M1347 R1348 L1358 K1359 N1360 K1361 E1362 P1363 V1364 V1367 G1368 E1369 T1370 G1371
C1372 G1373 K1374 Q1379 Q1383 L1389 I1390 T1391 L1392 H1395 Q1396 N1397 T1398 E1399 T1400 G1401 D1402 G1405 A1406 Q1407 ARG PRO VAL ARG ASN ARG SER GLU ILE GLN TYR LYS LEU ILE LYS SER LEU LYS THR ALA LEU ASN ILE ALA ASN ASP GLN ASP VAL ASP LEU LYS GLU LEU LEU
GLN LEU TYR SER LYS SER ASP ASN LYS ASN ILE ALA GLU ASP VAL GLN LEU GLU ILE GLN LYS LEU ARG ASP SER LEU ASN VAL LEU PHE E1473 W1474 S1475 D1476 G1477 P1478 R1484 T1485 G1486 N1487 F1488 F1489 L1490 L1491 D1492 E1493 I1494 S1495 L1496 A1497 D1498 D1499 S1500 V1501 L1502 E1503 V1508 L1509
E1510 P1511 E1512 R1513 S1514 L1515 L1516 L1517 A1518 E1519 GLN GLY SER S1523 D1524 S1525 L1526 V1527 T1528 A1529 S1530 E1531 N1532 F1533 Q1534 F1535 F1536 A1537 P1541 G1542 G1543 D1544 Y1545 G1546 K1547 K1548 E1549 L1550 R1555 N1556 R1557 F1558 T1559 E1560 P1564 S1565 M1566 E1567 D1568 F1569 N1570 N1573 S1577 S1578 R1579
L1580 A1588 F1598 G1599 K1600 LYS LEU GLY GLY GLY N1606 A1607 T1608 N1625 K1626 V1627 M1644 L1650 G1651 T1652 K1666 S1667 L1668 ARG THR GLU CYS ILE ILE GLN LEU LEU LYS LEU CYS GLY ASP ASP LEU GLU LEU GLN GLN ILE ILE GLU THR ASN GLU ILE ILE VAL THR GLN ASP
GLU LEU GLN VAL GLY MET PHE LYS ILE PRO ARG PHE PRO ASP ALA GLN SER SER SER F1719 N1720 A1723 A1727 S1728 R1735 P1742 P1749 G1750 N1766 S1774 E1775 L1779 F1783 G1784 A1785 ASP ALA PRO GLY GLU ARG SER GLY GLU PHE LEU TRP H1798 E1810
E1826 G1827 L1832 G1836 I1840 PRO GLU LEU ASP I1845 S1848 C1849 H1850 P1861 GLN TYR GLN GLY GLY GLY ARG K1869 G1870 L1871 P1872 K1873 N1877 R1878 F1879 T1888 D1891 Y1900 P1901 S1902 I1903 E1904 T1917 P1934 D1959 T1974 A2043 N2047 S2058
Q2095 V2096 D2097 P2147 E2148 K2149 D2152 N2158 L2164 E2178 E2182 T2185 K2186 E2187 A2188 S2189 V2190 L2216 C2217 S2218 P2219 S2220 S2227 E2230 S2234 I2237 ASN GLU CYS SER GLN GLU ASP GLY Q2246 P2247 G2267 S2270 R2271 A2272 F2299 GLU LEU GLY GLU
ASN ILE ASP PHE VAL SER ILE ASP ASP GLY ILE LYS LYS ILE LYS LEU ASN GLU P2322 D2323 I2357 Y2415 A2418 G2427 L2428 N2443 R2470 N2474 I2491 D2492 E2493 L2494 T2495 A2503 F2504 N2505 G2506 R2507 K2510 N2511 I2512 P2513 C2539 T2560 A2561 L2595
E2764 LYS ASN ALA LYS LEU THR SER F2772 V2785 S2789 I2861 E2862 E2863 K2864 T2865 V2871 E2875 D2966 P2969 Q2970 S2971 P2972 S3038 D3068 G3105 Q3156 GLU GLU ASN GLU LYS SER ASN MET PHE LYS PHE ASN ASP ASN SER ASP ASP Y3174 F3182 PRO ASP
TYR GLU ASP THR ALA LEU VAL THR ASN GLU LYS ASP ILE SER SER PRO GLU N3202 T3274 GLU VAL PHE GLY ASN I3280 V3305 L3309 K3310 Q3311 A3338 S3359 S3360 F3417 VAL SER GLU LYS LYS GLU THR ALA PRO N3427 A3511 D3515 V3516 Y3557 SER ASN GLU ASN



• Molecule 2: Ribosome assembly protein 4

Chain xP1:




I83 GLN GLY LYS K87 A88 S89 D90 P91 VAL LYS THR ILE ASP ILE THR ASP ASN LEU Y102 S103 S104 L105 I106 K107 P108 GLY TYR ASN SER THR GLU ASP Q116 I117 T118 T122 P123 R124 ALA VAL PHE LYS VAL LYS PRO VAL THR ARG SER SER SER ALA ILE ALA GLY HIS GLY
SER THR ILE LEU CYS SER ALA PHE ALA PRO HIS THR SER SER ARG MET VAL THR GLY ALA GLY ASP ASN THR ALA ARG ILE TRP ASP CYS ASP THR GLN THR PRO MET HIS THR LEU LYS GLY HIS TYR ASN TRP VAL LEU CYS VAL SER TRP SER PRO ASP GLY GLU VAL ILE ALA THR
GLY SER MET ASP ASN THR ILE ARG LEU TRP ASP PRO LYS SER GLY GLN CYS LEU GLY ASP ALA LEU ARG GLY HIS SER LYS TRP ILE THR SER LEU SER TRP GLU PRO ILE HIS LEU VAL LYS PRO GLY SER LYS PRO ARG LEU ALA SER SER SER LYS ASP GLY THR ILE LYS ILE TRP
ASP THR VAL SER ARG VAL CYS GLN TYR THR MET SER GLY HIS THR ASN SER VAL SER CYS VAL LYS TRP GLY GLY GLN GLY LEU LEU TYR SER GLY SER HIS ASP ARG THR VAL ARG VAL TRP ASP ILE ASN SER GLN GLY ARG CYS ILE ASN ILE LEU LYS SER HIS ALA HIS TRP VAL
ASN HIS LEU SER LEU SER THR ASP TYR ALA LEU ARG ILE GLY ALA PHE ASP HIS THR GLY LYS LYS PRO SER THR PRO GLU GLU ALA GLN LYS LYS ALA LEU GLU ASN TYR GLU LYS ILE CYS LYS LYS ASN GLY ASN SER GLU GLU MET MET VAL THR ALA SER ASP ASP TYR THR MET
PHE LEU TRP ASN PRO LEU LYS LYS SER THR LYS PRO ILE ALA ARG MET THR GLY HIS GLN LYS LEU VAL ASN HIS VAL ALA PHE SER PRO ASP GLY ARG TYR ILE VAL SER ALA SER PHE ASP ASN SER ILE LYS LEU TRP ASP GLY ARG ASP GLY LYS PHE ILE SER THR PHE ARG GLY HIS
VAL ALA SER VAL TYR GLN VAL ALA TRP SER SER ASP CYS ARG LEU LEU VAL SER CYS SER LYS ASP THR THR LEU LYS VAL TRP ASP VAL ARG THR ARG LYS LEU SER VAL ASP LEU PRO GLY HIS LYS ASP GLU VAL TYR THR VAL ASP TRP SER VAL ASP GLY LYS ARG VAL CYS SER
GLY GLY LYS ASP LYS MET VAL ARG LEU TRP THR HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55397	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	370.65, 370.65, 370.65	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	AP1	0.27	0/17970	0.50	2/25013 (0.0%)
2	xP1	0.24	0/346	0.51	0/473
All	All	0.27	0/18316	0.50	2/25486 (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	AP1	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AP1	3567	PRO	N-CA-CB	6.53	111.14	103.30
1	AP1	3594	PRO	N-CA-CB	6.18	110.72	103.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AP1	223	LEU	Peptide
1	AP1	406	GLU	Peptide
1	AP1	947	ASN	Peptide
1	AP1	948	THR	Peptide
1	AP1	95	ILE	Peptide

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	AP1	18010	0	7839	27	0
2	xP1	352	0	145	0	0
All	All	18362	0	7984	27	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 1.

The worst 5 of 27 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:AP1:263:LYS:HA	1:AP1:274:LYS:O	1.74	0.87
1:AP1:263:LYS:CA	1:AP1:274:LYS:O	2.40	0.69
1:AP1:263:LYS:CB	1:AP1:274:LYS:O	2.45	0.65
1:AP1:1779:LEU:O	1:AP1:1783:PHE:N	2.30	0.64
1:AP1:2178:GLU:O	1:AP1:2182:GLU:N	2.37	0.57

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	AP1	3549/4910 (72%)	3232 (91%)	313 (9%)	4 (0%)	51 85
2	xP1	59/515 (12%)	53 (90%)	6 (10%)	0	100 100
All	All	3608/5425 (66%)	3285 (91%)	319 (9%)	4 (0%)	54 85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AP1	241	PRO
1	AP1	3594	PRO
1	AP1	280	ASP
1	AP1	948	THR

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AP1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AP1	3595:LEU	C	3599:ARG	N	4.97
1	AP1	3575:LEU	C	3579:VAL	N	3.43
1	AP1	3587:MET	C	3591:ARG	N	3.23

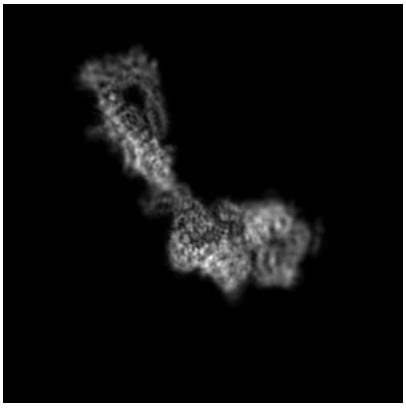
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10837. These allow visual inspection of the internal detail of the map and identification of artifacts.

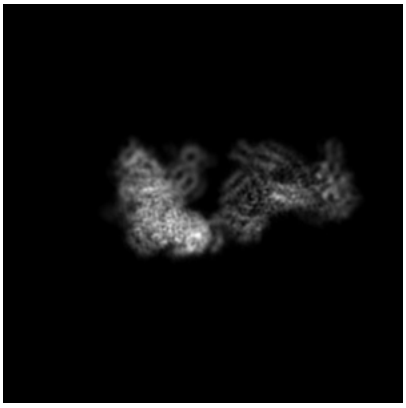
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

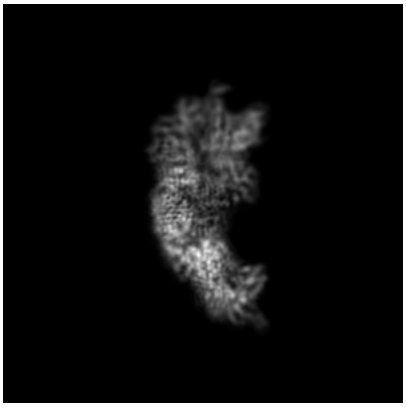
6.1.1 Primary map



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: 175

Y Index: 175

Z Index: 175

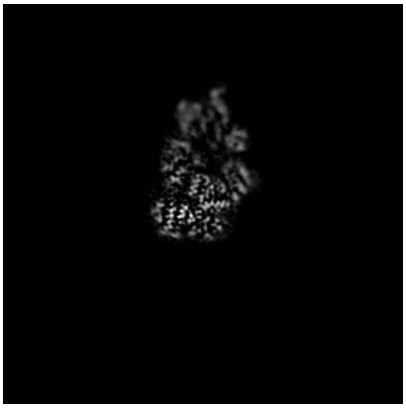
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 188

Y Index: 132

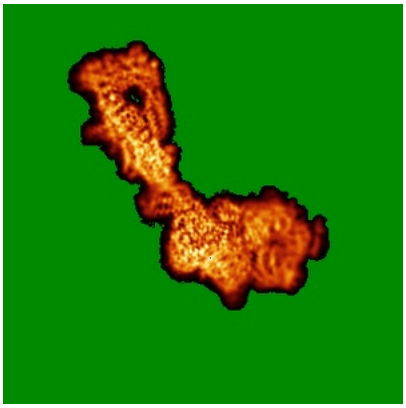


Z Index: 133

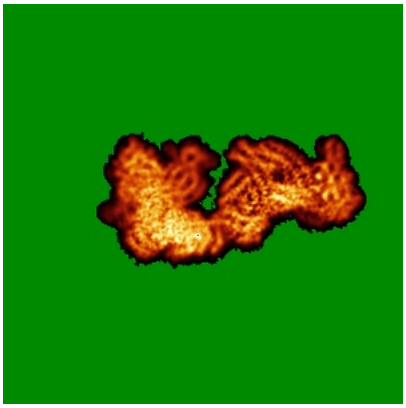
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



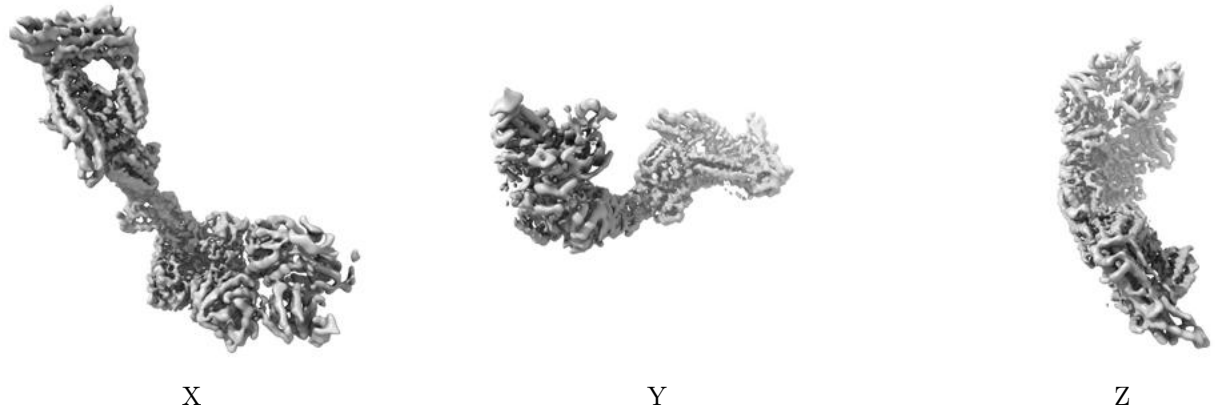
Y

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



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

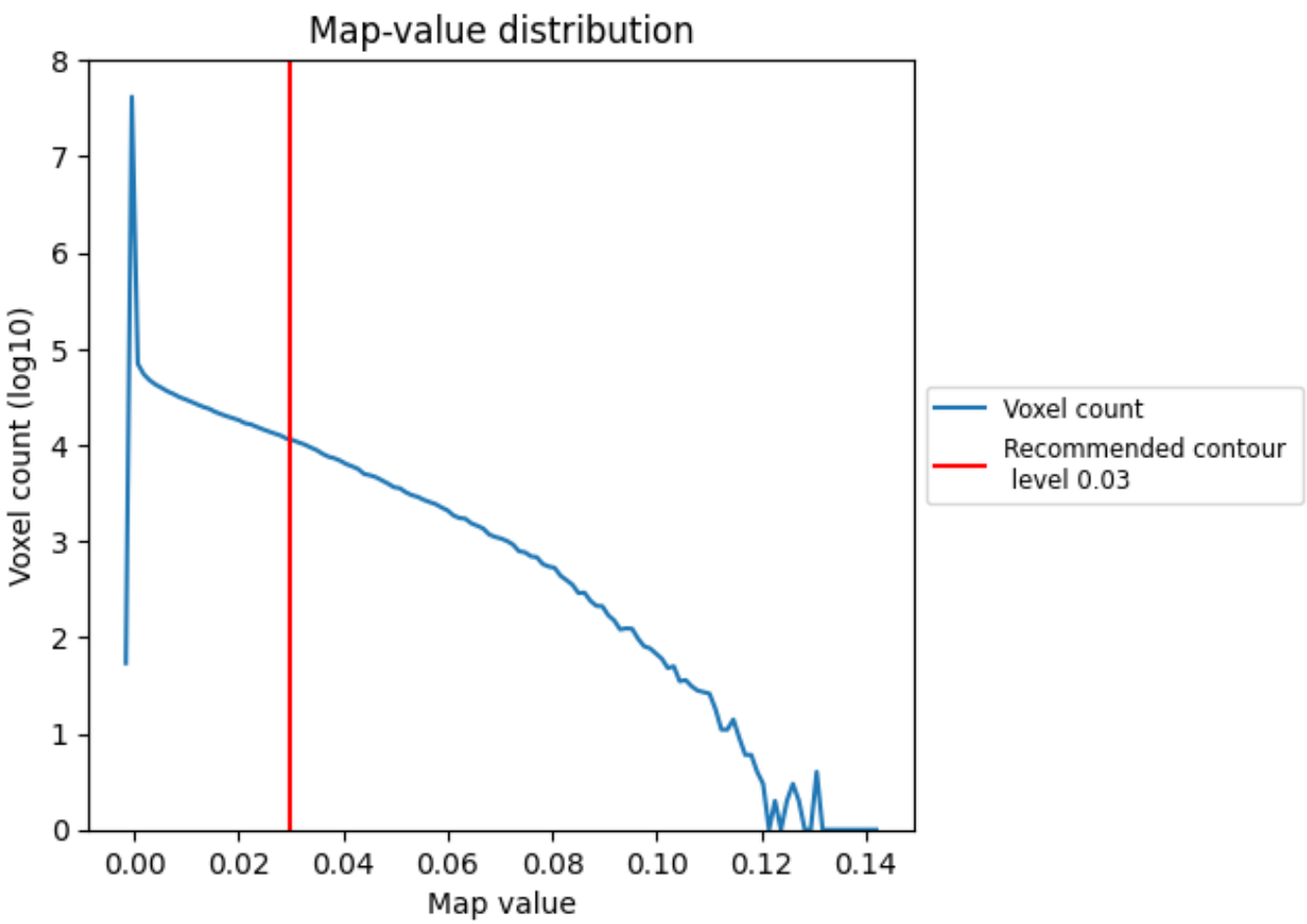
6.6 Mask visualisation (i)

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

7 Map analysis (i)

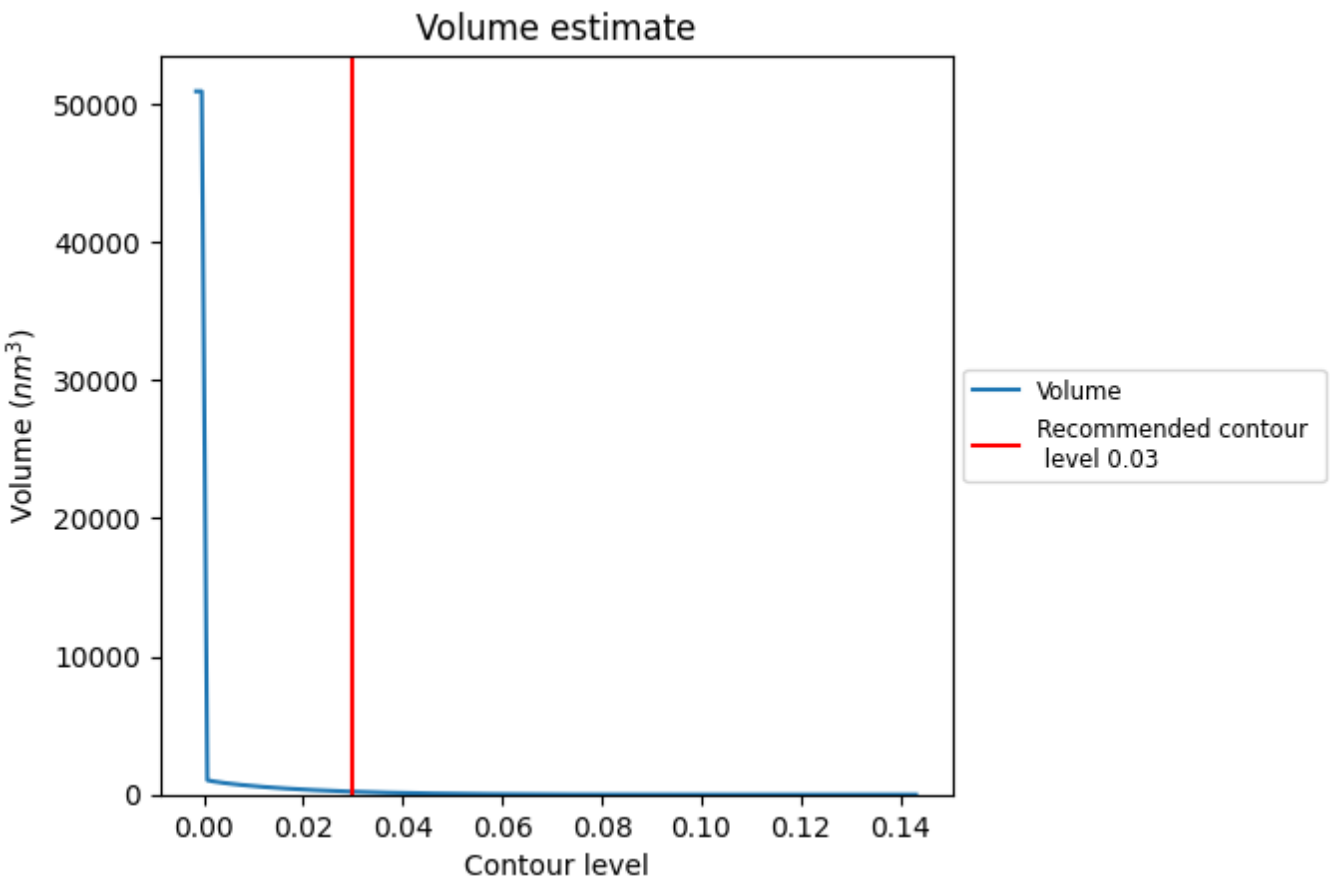
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

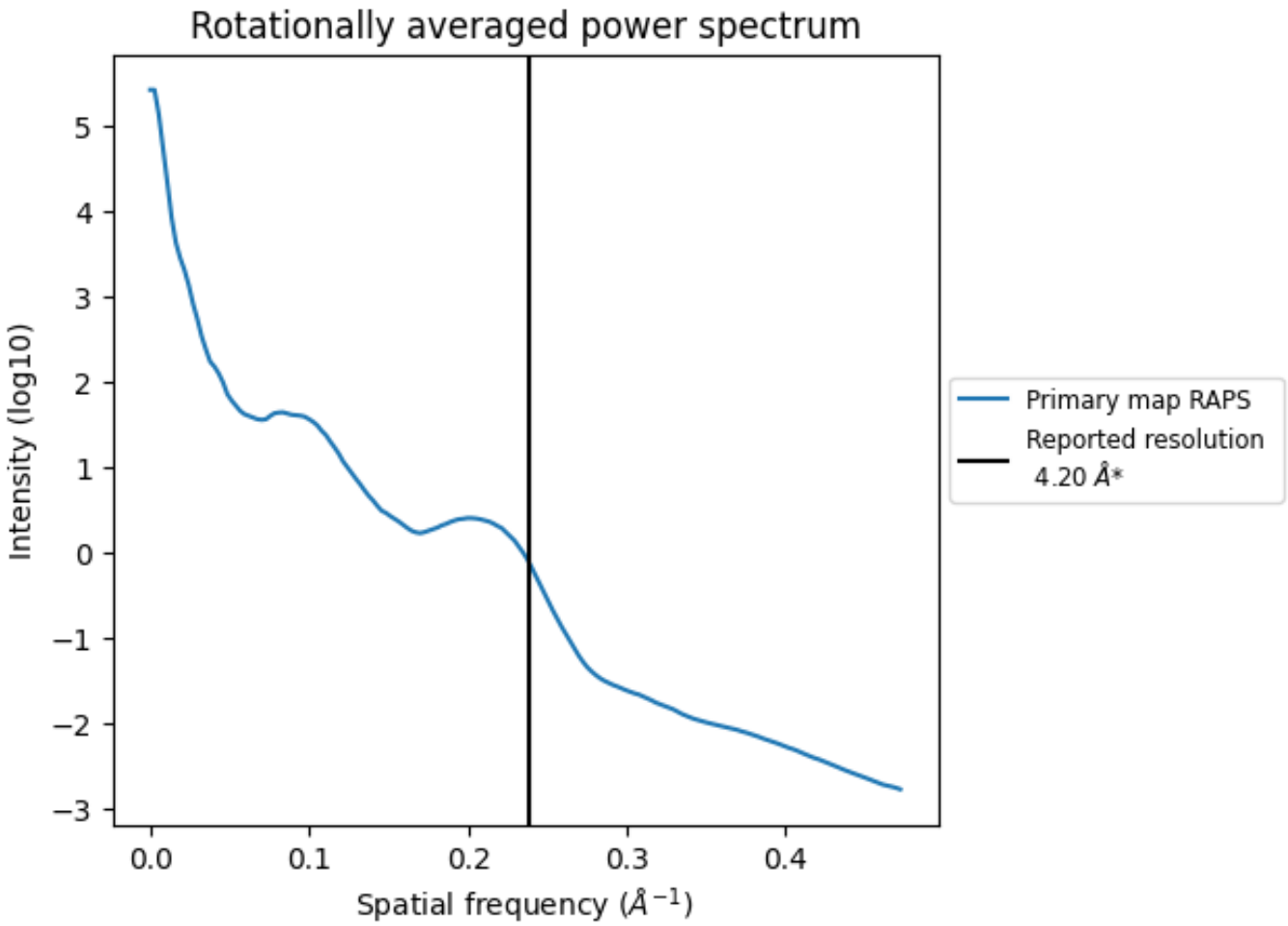
7.2 Volume estimate (i)



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 189 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 0.238 Å^{-1}

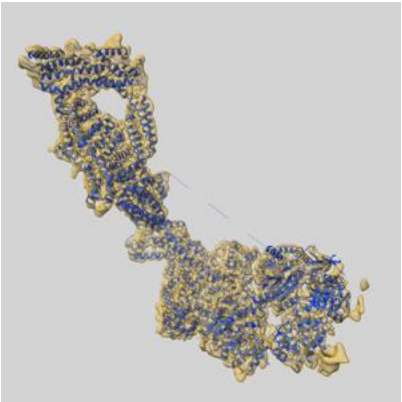
8 Fourier-Shell correlation (i)

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

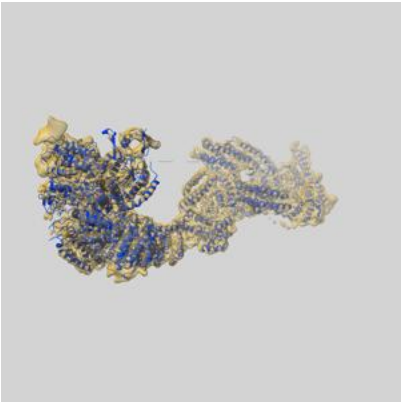
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10837 and PDB model 6YLF. Per-residue inclusion information can be found in section 3 on page 4.

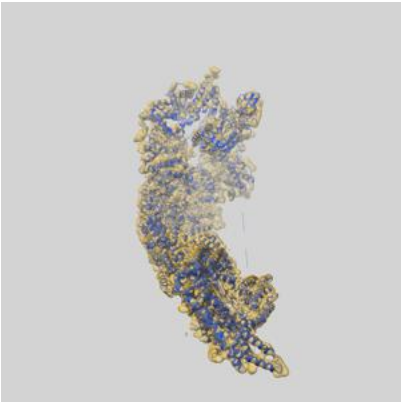
9.1 Map-model overlay (i)



X



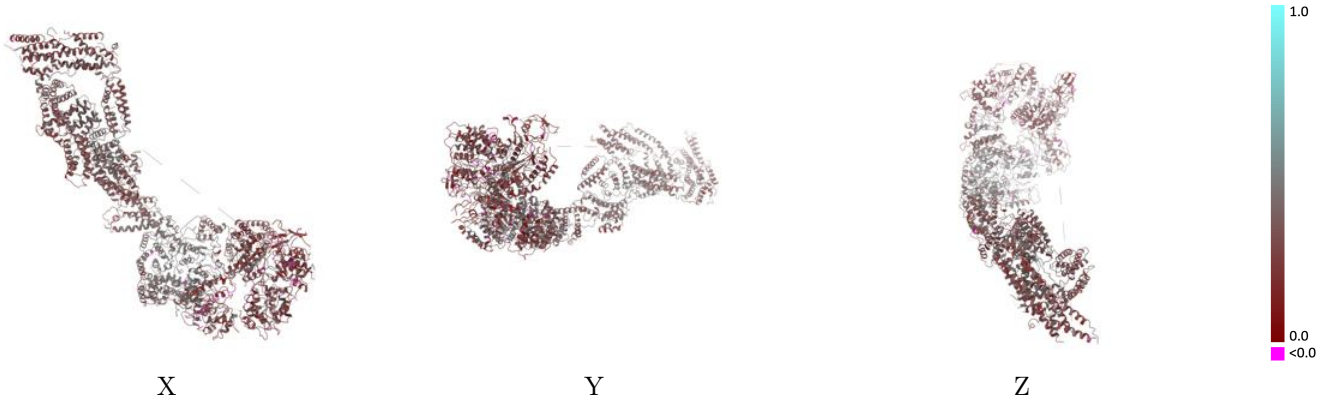
Y



Z

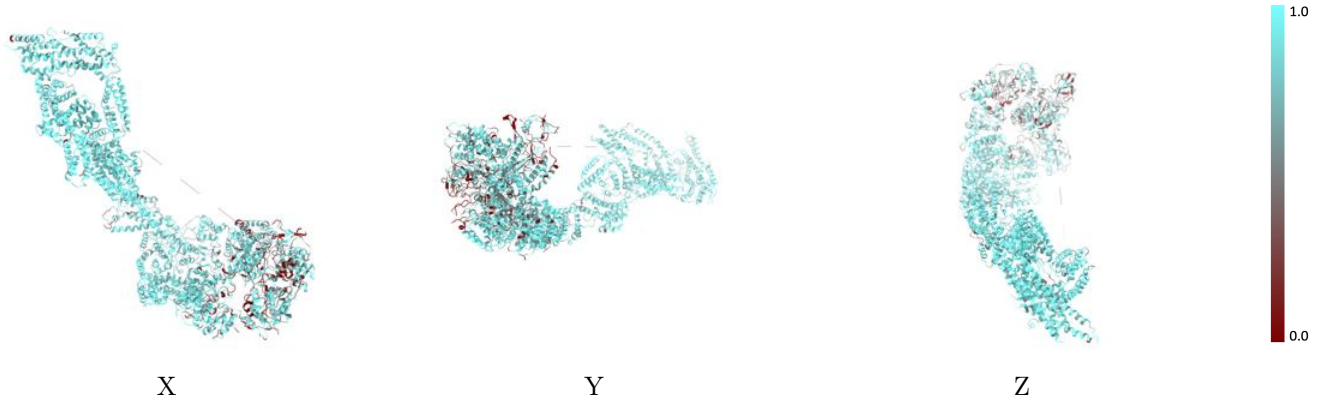
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



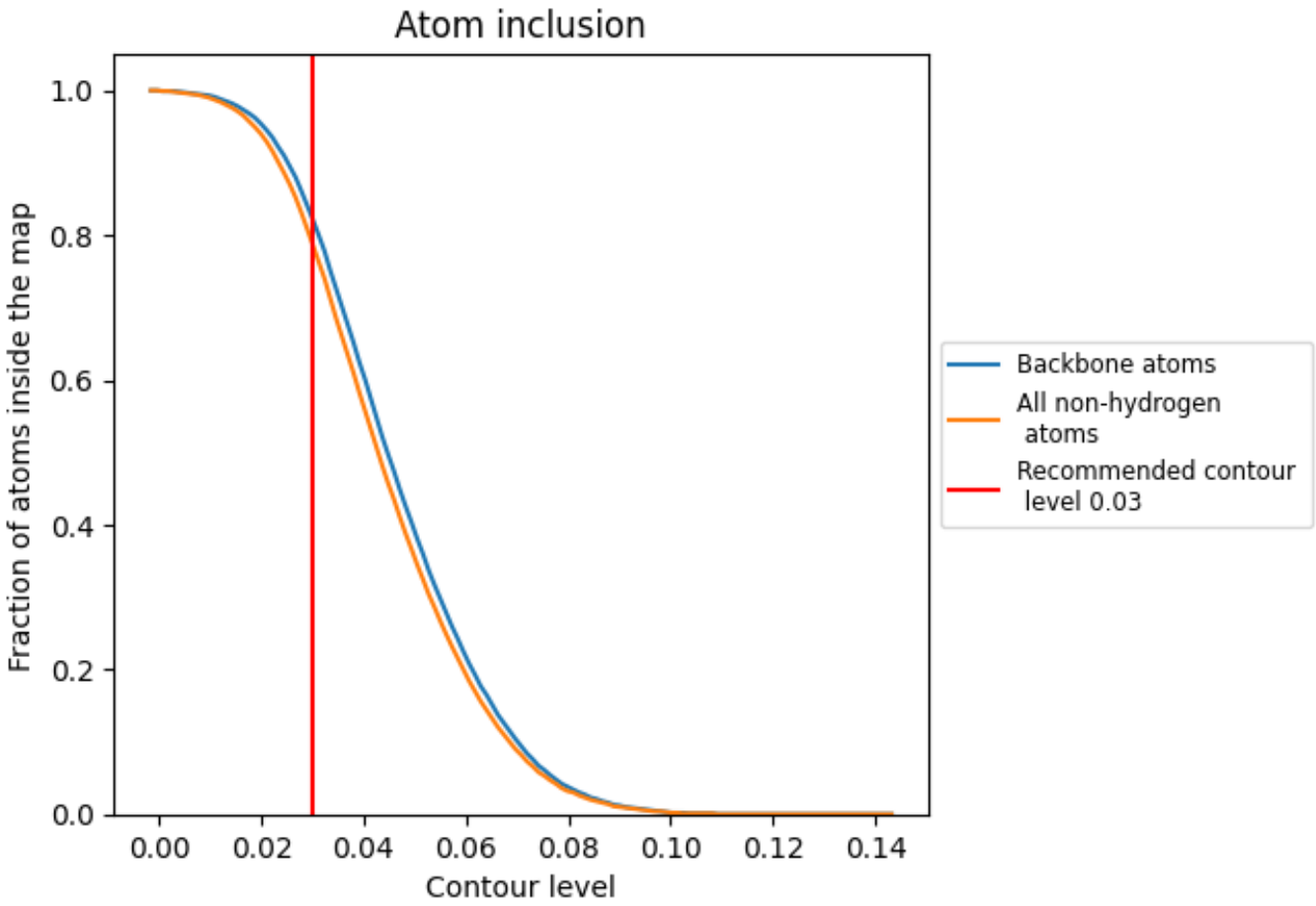
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.3360
AP1	0.7950	0.3380
xP1	0.4800	0.2400