Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 04:23 PM EST

PDB ID	:	7URR
EMDB ID	:	EMD-26717
Title	:	Gea2 closed/open conformation (composite structure)
Authors	:	Muccini, A.; Fromme, J.C.
Deposited on	:	2022-04-22
Resolution	:	4.70 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:

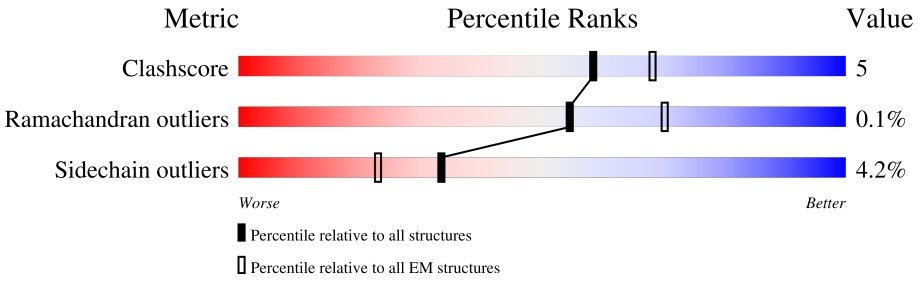
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.70 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	1459	11% 68% 15% 17%
1	B	1459	9% 66% 12% 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 38168 atoms, of which 19331 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 GEA2 isoform 1.

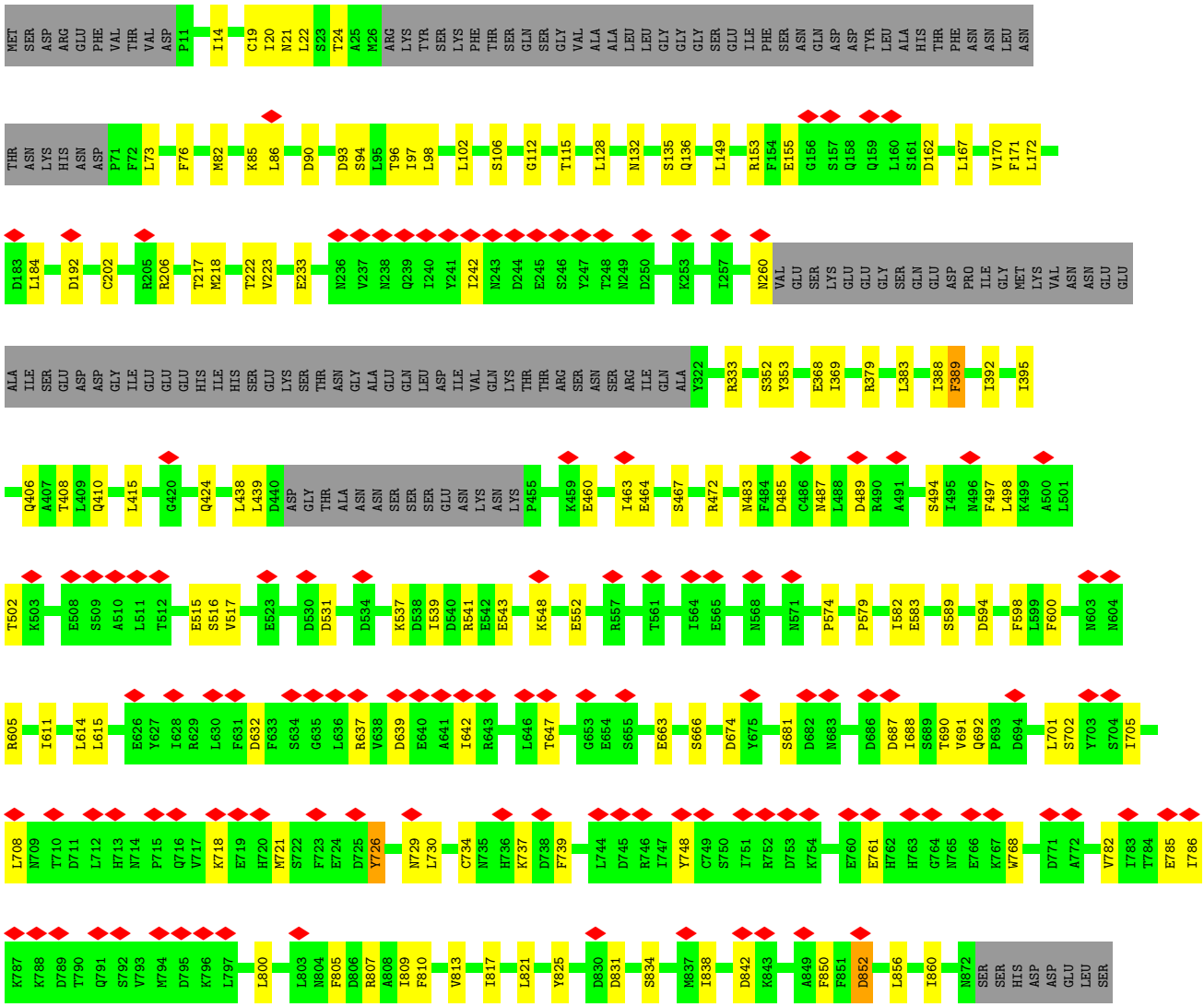
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1216	Total	C	H	N	O	S	0	0
			19748	6272	9985	1590	1864	37		
1	B	1129	Total	C	H	N	O	S	0	0
			18420	5858	9346	1477	1704	35		

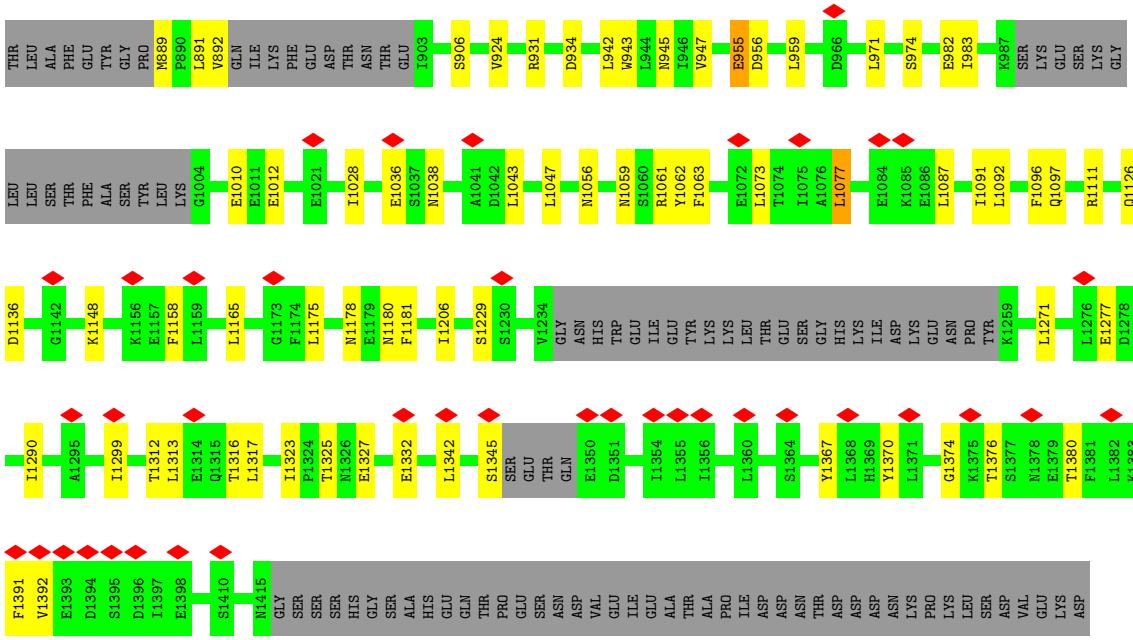
3 Residue-property plots (i)

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: GEA2 isoform 1

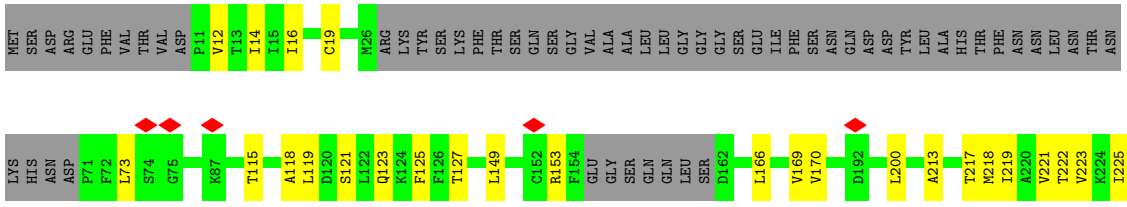
Chain A:

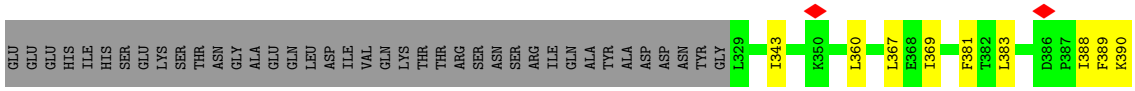


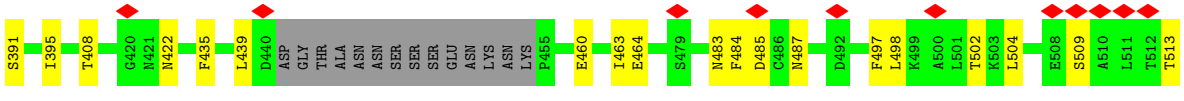


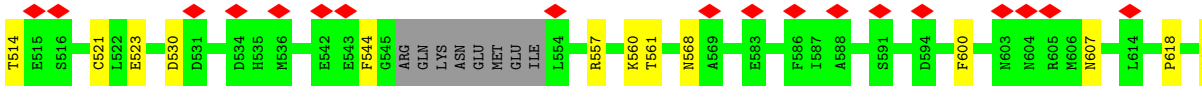
• Molecule 1: GEA2 isoform 1

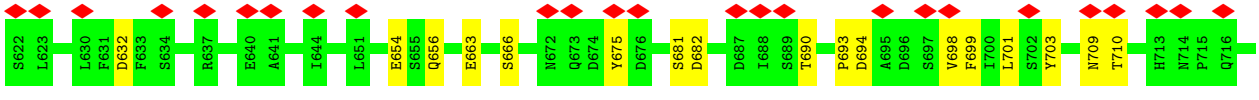
Chain B:

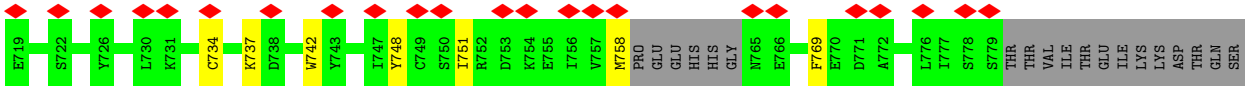


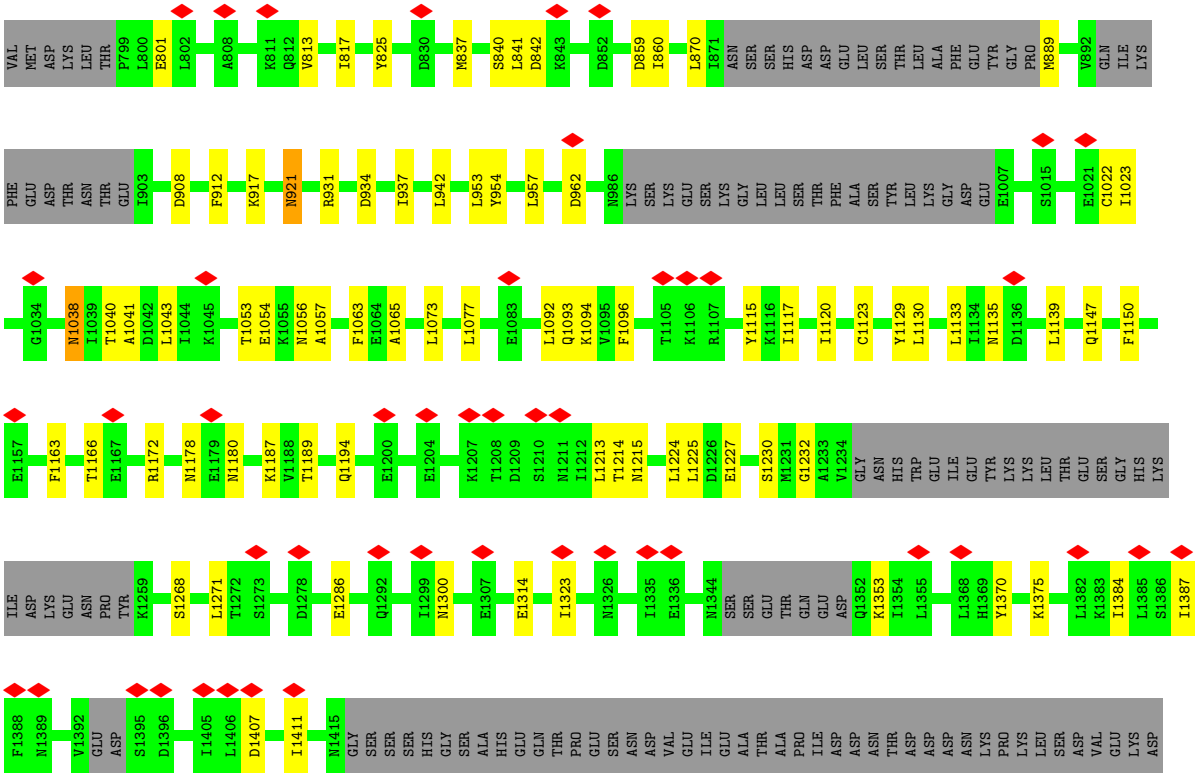











VAL MET ASP LYS LEU THR P799 L800 E801 L802 A808 K811 Q812 V813 I817 Y825 D830 M837 S840 L841 D842 K843 D852 D859 I860 L870 I871 ASN SER SER HIS ASP ASP GLU LEU SER THR LEU ALA PHE GLU TYR GLY PRO M889 V892 GLN ILE LYS
PHE GLU ASP THR ASN THR GLU I903 D908 F912 K917 N921 R931 D934 I937 L942 L953 Y954 L957 D962 N986 LYS SER LYS GLU SER LYS GLY LEU LEU SER THR PHE ALA SER TYR LEU LYS GLY ASP GLU E1007 S1015 E1021 C1022 I1023
G1034 N1038 I1039 T1040 A1041 D1042 L1043 I1044 K1045 T1053 E1054 K1055 N1056 A1057 F1063 E1064 A1065 L1073 L1077 E1083 L1092 Q1093 K1094 V1095 F1096 T1105 K1106 R1107 Y1115 K1116 I1117 I1120 C1123 Y1129 L1130 L1133 I1134 N1135 D1136 L1139 Q1147 F1150
E1157 F1163 T1166 E1167 R1172 N1178 E1179 N1180 K1187 V1188 T1189 Q1194 E1200 E1204 K1207 T1208 D1209 S1210 N1211 I1212 L1213 T1214 N1215 L1224 L1225 D1226 E1227 S1230 M1231 G1232 A1233 V1234 GLY ASN HIS TRP GLU ILE GLU TYR LYS LYS LEU THR GLU SER GLY HIS LYS
ILE ASP LYS GLU ASN PRO TYR K1259 S1268 L1271 T1272 S1273 D1278 E1286 Q1292 I1299 N1300 E1307 E1314 I1323 N1326 I1335 E1336 N1344 SER SER GLU THR GLN GLU ASP Q1352 K1353 I1354 L1355 L1368 H1369 Y1370 K1375 L1382 K1383 I1384 L1385 S1386 I1387
F1388 N1389 V1392 GLU ASP S1395 D1396 I1405 L1406 D1407 I1411 N1415 GLY SER SER SER HIS GLY SER ALA HIS GLU GLN THR PRO GLU SER ASN ASP VAL GLU ILE GLU ALA THR ALA PRO ILE ASP ASP ASN THR ASP ASP ASN LYS PRO LYS LEU SER ASP VAL GLU LYS ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101014	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	131.750	Depositor
Minimum map value	-99.098	Depositor
Average map value	-0.064	Depositor
Map value standard deviation	1.560	Depositor
Recommended contour level	15.0	Depositor
Map size (Å)	499.2, 499.2, 499.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.664, 1.664, 1.664	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	0/9919	0.62	0/13395
1	B	0.32	0/9217	0.62	0/12434
All	All	0.31	0/19136	0.62	0/25829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	9763	9985	9985	106	0
1	B	9074	9346	9346	83	0
All	All	18837	19331	19331	185	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 5.

All (185) 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:223:VAL:HG22	1:A:369:ILE:HD11	1.65	0.78
1:B:343:ILE:HD11	1:B:360:LEU:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ILE:HG21	1:A:517:VAL:HG13	1.74	0.69
1:B:1135:ASN:OD1	1:B:1180:ASN:ND2	2.26	0.69
1:B:1189:THR:HG21	1:B:1224:LEU:HD11	1.75	0.68
1:A:94:SER:OG	1:A:136:GLN:O	2.11	0.68
1:B:842:ASP:OD1	1:B:931:ARG:NH2	2.26	0.68
1:B:1093:GLN:OE1	1:B:1129:TYR:OH	2.12	0.66
1:B:218:MET:O	1:B:222:THR:OG1	2.10	0.66
1:B:460:GLU:OE1	1:B:514:THR:OG1	2.11	0.66
1:A:132:ASN:O	1:A:135:SER:OG	2.13	0.65
1:A:472:ARG:NH2	1:B:12:VAL:O	2.29	0.65
1:B:1163:PHE:O	1:B:1166:THR:OG1	2.14	0.65
1:B:123:GLN:OE1	1:B:127:THR:OG1	2.14	0.64
1:A:842:ASP:OD1	1:A:931:ARG:NH2	2.31	0.64
1:A:498:LEU:O	1:A:502:THR:OG1	2.16	0.64
1:B:509:SER:O	1:B:513:THR:OG1	2.16	0.63
1:A:1073:LEU:O	1:A:1077:LEU:HD12	1.98	0.63
1:A:424:GLN:OE1	1:A:483:ASN:ND2	2.32	0.63
1:B:813:VAL:HG22	1:B:817:ILE:HD11	1.81	0.62
1:A:943:TRP:O	1:A:947:VAL:HG23	2.00	0.62
1:B:654:GLU:N	1:B:654:GLU:OE1	2.33	0.62
1:B:1120:ILE:HG21	1:B:1130:LEU:HD13	1.82	0.61
1:A:674:ASP:O	1:A:692:GLN:NE2	2.33	0.61
1:B:934:ASP:OD2	1:B:937:ILE:N	2.34	0.61
1:A:153:ARG:NH1	1:A:260:ASN:OD1	2.33	0.61
1:A:388:ILE:O	1:A:392:ILE:HD12	2.01	0.60
1:B:388:ILE:O	1:B:391:SER:OG	2.15	0.60
1:A:1206:ILE:HG21	1:A:1271:LEU:HD11	1.82	0.60
1:B:1407:ASP:OD1	1:B:1411:ILE:HD12	2.01	0.60
1:A:102:LEU:O	1:A:106:SER:OG	2.14	0.60
1:A:831:ASP:O	1:A:834:SER:OG	2.19	0.59
1:A:701:LEU:O	1:A:705:ILE:HG22	2.01	0.59
1:A:1313:LEU:HD12	1:A:1317:LEU:HD23	1.84	0.59
1:A:856:LEU:O	1:A:860:ILE:HG23	2.02	0.59
1:A:333:ARG:NH2	1:A:379:ARG:O	2.35	0.59
1:A:20:ILE:HG23	1:B:464:GLU:OE2	2.01	0.59
1:A:543:GLU:N	1:A:543:GLU:OE2	2.37	0.58
1:A:1312:THR:O	1:A:1316:THR:HG22	2.04	0.58
1:A:552:GLU:N	1:A:552:GLU:OE1	2.36	0.58
1:A:785:GLU:OE1	1:A:786:ILE:N	2.37	0.58
1:A:1087:LEU:O	1:A:1091:ILE:HG22	2.03	0.58
1:B:219:ILE:O	1:B:223:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:SER:O	1:A:690:THR:OG1	2.22	0.57
1:A:218:MET:O	1:A:222:THR:HG23	2.05	0.57
1:A:233:GLU:OE1	1:A:233:GLU:N	2.38	0.57
1:A:541:ARG:NH2	1:A:852:ASP:OD2	2.37	0.56
1:A:589:SER:OG	1:A:594:ASP:OD2	2.21	0.56
1:A:955:GLU:OE1	1:A:1061:ARG:NH2	2.38	0.56
1:A:223:VAL:HG22	1:A:369:ILE:CD1	2.33	0.56
1:A:242:ILE:HD13	1:A:782:VAL:O	2.06	0.56
1:B:1092:LEU:HD11	1:B:1120:ILE:HD13	1.87	0.56
1:A:974:SER:OG	1:A:1111:ARG:NH2	2.39	0.55
1:A:368:GLU:OE2	1:B:14:ILE:HD12	2.06	0.55
1:B:1130:LEU:HD12	1:B:1133:LEU:HD23	1.89	0.55
1:A:889:MET:SD	1:A:889:MET:N	2.80	0.54
1:B:221:VAL:O	1:B:225:ILE:HG22	2.06	0.54
1:A:891:LEU:N	1:A:982:GLU:OE2	2.39	0.54
1:A:838:ILE:HG23	1:A:924:VAL:HG21	1.88	0.54
1:B:825:TYR:OH	1:B:921:ASN:OD1	2.11	0.54
1:B:801:GLU:N	1:B:801:GLU:OE1	2.38	0.54
1:B:908:ASP:N	1:B:908:ASP:OD1	2.41	0.54
1:B:166:LEU:HD12	1:B:200:LEU:HD11	1.89	0.53
1:B:223:VAL:HG13	1:B:369:ILE:CD1	2.39	0.53
1:A:1380:THR:HG22	1:A:1384:ILE:HD12	1.90	0.53
1:A:1036:GLU:N	1:A:1036:GLU:OE1	2.42	0.53
1:B:1022:CYS:SG	1:B:1023:ILE:N	2.80	0.53
1:B:1178:ASN:OD1	1:B:1180:ASN:N	2.42	0.53
1:B:487:ASN:O	1:B:560:LYS:NZ	2.42	0.52
1:B:118:ALA:O	1:B:121:SER:OG	2.24	0.52
1:A:642:ILE:HG21	1:A:705:ILE:HD13	1.92	0.52
1:B:734:CYS:N	1:B:737:LYS:O	2.41	0.52
1:B:1056:ASN:OD1	1:B:1057:ALA:N	2.42	0.52
1:A:637:ARG:NE	1:A:639:ASP:OD2	2.43	0.52
1:A:464:GLU:O	1:A:467:SER:OG	2.25	0.52
1:A:721:MET:O	1:A:748:TYR:OH	2.25	0.52
1:B:1150:PHE:O	1:B:1194:GLN:NE2	2.43	0.52
1:A:943:TRP:CZ3	1:A:1043:LEU:HD12	2.45	0.51
1:B:917:LYS:O	1:B:921:ASN:ND2	2.43	0.51
1:B:383:LEU:HD23	1:B:383:LEU:O	2.11	0.51
1:A:93:ASP:O	1:A:96:THR:OG1	2.24	0.51
1:A:389:PHE:HE1	1:A:415:LEU:HD13	1.74	0.51
1:B:1286:GLU:N	1:B:1286:GLU:OE1	2.44	0.51
1:A:395:ILE:HG21	1:A:408:THR:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:ILE:O	1:A:813:VAL:HG22	2.12	0.50
1:B:395:ILE:HG21	1:B:408:THR:HG21	1.91	0.50
1:A:701:LEU:HD13	1:A:739:PHE:HE1	1.77	0.49
1:A:1010:GLU:N	1:A:1012:GLU:OE2	2.45	0.49
1:B:954:TYR:OH	1:B:1065:ALA:HB1	2.12	0.49
1:A:1175:LEU:HD21	1:A:1181:PHE:CE2	2.47	0.49
1:A:170:VAL:HG13	1:A:217:THR:HG21	1.95	0.49
1:A:734:CYS:O	1:A:737:LYS:N	2.42	0.49
1:A:167:LEU:HD21	1:B:213:ALA:HB2	1.95	0.49
1:A:1175:LEU:HD21	1:A:1181:PHE:CZ	2.48	0.48
1:A:1206:ILE:CG2	1:A:1271:LEU:HD11	2.43	0.48
1:B:1225:LEU:HD11	1:B:1271:LEU:HD23	1.96	0.48
1:A:959:LEU:HD13	1:A:1028:ILE:HG21	1.96	0.48
1:B:1147:GLN:N	1:B:1147:GLN:OE1	2.46	0.48
1:B:675:TYR:OH	1:B:693:PRO:O	2.21	0.48
1:A:170:VAL:CG1	1:A:217:THR:HG21	2.44	0.48
1:A:515:GLU:N	1:A:515:GLU:OE1	2.46	0.48
1:B:666:SER:HB2	1:B:698:VAL:HG23	1.95	0.48
1:B:498:LEU:O	1:B:502:THR:HG22	2.14	0.47
1:B:1117:ILE:CD1	1:B:1133:LEU:HD21	2.44	0.47
1:A:22:LEU:HD23	1:A:76:PHE:CZ	2.50	0.47
1:A:541:ARG:NH1	1:A:850:PHE:O	2.47	0.47
1:A:85:LYS:O	1:A:86:LEU:HD23	2.14	0.47
1:A:690:THR:HG23	1:A:691:VAL:HG23	1.96	0.47
1:A:90:ASP:OD1	1:A:90:ASP:N	2.47	0.47
1:A:149:LEU:HD11	1:A:172:LEU:HD23	1.97	0.47
1:A:729:ASN:O	1:A:730:LEU:HD22	2.14	0.47
1:B:1227:GLU:O	1:B:1230:SER:N	2.48	0.47
1:B:557:ARG:O	1:B:561:THR:HG23	2.15	0.46
1:A:574:PRO:HG2	1:A:614:LEU:HD21	1.97	0.46
1:B:709:ASN:OD1	1:B:710:THR:N	2.47	0.46
1:A:112:GLY:O	1:A:115:THR:OG1	2.30	0.46
1:B:149:LEU:HD13	1:B:169:VAL:HG22	1.98	0.46
1:B:681:SER:O	1:B:690:THR:OG1	2.30	0.46
1:A:489:ASP:O	1:A:605:ARG:NH1	2.49	0.46
1:A:906:SER:OG	1:A:956:ASP:OD2	2.16	0.46
1:A:1178:ASN:OD1	1:A:1180:ASN:N	2.49	0.46
1:B:170:VAL:HG13	1:B:217:THR:HG21	1.97	0.46
1:B:870:LEU:HD11	1:B:912:PHE:CD2	2.51	0.46
1:B:942:LEU:HD12	1:B:942:LEU:O	2.16	0.46
1:B:1225:LEU:HD11	1:B:1271:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:THR:HG23	1:A:1327:GLU:H	1.81	0.45
1:B:1073:LEU:O	1:B:1077:LEU:HD23	2.17	0.45
1:A:611:ILE:HG22	1:A:615:LEU:HD23	1.99	0.45
1:A:1370:TYR:O	1:A:1374:GLY:N	2.48	0.45
1:A:838:ILE:CG2	1:A:924:VAL:HG21	2.47	0.45
1:A:460:GLU:OE2	1:A:516:SER:OG	2.33	0.45
1:A:687:ASP:OD1	1:A:688:ILE:N	2.50	0.45
1:B:485:ASP:O	1:B:560:LYS:NZ	2.36	0.45
1:A:352:SER:OG	1:A:353:TYR:N	2.50	0.44
1:A:438:LEU:HD21	1:A:463:ILE:HD13	1.98	0.44
1:B:841:LEU:HD22	1:B:860:ILE:HD11	2.00	0.44
1:B:343:ILE:CD1	1:B:360:LEU:HD13	2.43	0.44
1:A:817:ILE:O	1:A:821:LEU:HD23	2.18	0.44
1:A:1316:THR:HG23	1:A:1317:LEU:HD22	2.00	0.44
1:B:1214:THR:OG1	1:B:1215:ASN:N	2.50	0.44
1:B:1139:LEU:O	1:B:1187:LYS:NZ	2.51	0.44
1:B:1323:ILE:HD11	1:B:1375:LYS:HE2	1.99	0.44
1:A:708:LEU:HD22	1:A:726:TYR:HE2	1.82	0.43
1:A:1323:ILE:HD11	1:A:1370:TYR:CE1	2.53	0.43
1:B:632:ASP:N	1:B:632:ASP:OD1	2.51	0.43
1:B:360:LEU:HD21	1:B:408:THR:HG23	2.00	0.43
1:A:942:LEU:O	1:A:942:LEU:HD12	2.18	0.43
1:B:1040:THR:OG1	1:B:1041:ALA:N	2.51	0.43
1:A:1165:LEU:O	1:A:1165:LEU:HD23	2.19	0.43
1:B:16:ILE:H	1:B:16:ILE:HD12	1.84	0.43
1:B:115:THR:O	1:B:119:LEU:HD23	2.19	0.43
1:A:541:ARG:NH2	1:A:934:ASP:OD2	2.49	0.43
1:A:1313:LEU:HD12	1:A:1317:LEU:CD2	2.46	0.43
1:A:647:THR:HG21	1:A:782:VAL:HG11	2.01	0.42
1:A:663:GLU:O	1:A:666:SER:OG	2.31	0.42
1:B:463:ILE:HD11	1:B:504:LEU:HD13	2.02	0.42
1:B:953:LEU:HD13	1:B:1023:ILE:HD11	2.00	0.42
1:A:1056:ASN:N	1:A:1059:ASN:OD1	2.48	0.42
1:A:14:ILE:HG21	1:A:128:LEU:HD22	2.01	0.42
1:B:1053:THR:OG1	1:B:1054:GLU:N	2.52	0.42
1:A:947:VAL:HG13	1:A:1047:LEU:HD12	2.02	0.41
1:B:1166:THR:O	1:B:1172:ARG:NH2	2.52	0.41
1:B:694:ASP:O	1:B:698:VAL:HG22	2.20	0.41
1:B:1384:ILE:HA	1:B:1387:ILE:HD12	2.02	0.41
1:A:1092:LEU:HD23	1:A:1126:GLN:HG2	2.02	0.41
1:B:223:VAL:HG13	1:B:369:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASN:O	1:A:24:THR:OG1	2.33	0.41
1:B:748:TYR:HA	1:B:751:ILE:HG22	2.01	0.41
1:B:435:PHE:O	1:B:439:LEU:N	2.50	0.41
1:B:483:ASN:OD1	1:B:484:PHE:N	2.54	0.41
1:A:539:ILE:HD11	1:A:800:LEU:HD21	2.02	0.41
1:B:698:VAL:HA	1:B:701:LEU:HD12	2.02	0.41
1:A:162:ASP:N	1:A:162:ASP:OD1	2.54	0.41
1:A:579:PRO:HA	1:A:582:ILE:HG22	2.02	0.41
1:A:1290:ILE:H	1:A:1290:ILE:HD12	1.86	0.41
1:A:1299:ILE:HD11	1:A:1342:LEU:HD21	2.03	0.41
1:A:1376:THR:HG22	1:A:1380:THR:HG21	2.03	0.41
1:B:618:PRO:O	1:B:621:VAL:HG23	2.21	0.41
1:B:682:ASP:OD1	1:B:742:TRP:NE1	2.52	0.41
1:A:892:VAL:HG23	1:A:983:ILE:HG23	2.03	0.40
1:A:82:MET:O	1:A:86:LEU:HD21	2.21	0.40
1:A:97:ILE:HG23	1:A:98:LEU:HD13	2.04	0.40
1:B:1038:ASN:OD1	1:B:1038:ASN:N	2.54	0.40
1:A:406:GLN:O	1:A:410:GLN:NE2	2.55	0.40
1:B:1232:GLY:O	1:B:1300:ASN:ND2	2.52	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	1198/1459 (82%)	1126 (94%)	70 (6%)	2 (0%)	47 81
1	B	1101/1459 (76%)	1035 (94%)	65 (6%)	1 (0%)	51 85
All	All	2299/2918 (79%)	2161 (94%)	135 (6%)	3 (0%)	54 85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	LYS
1	B	663	GLU
1	A	1392	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	1130/1346 (84%)	1080 (96%)	50 (4%)	28	54
1	B	1050/1346 (78%)	1009 (96%)	41 (4%)	32	57
All	All	2180/2692 (81%)	2089 (96%)	91 (4%)	33	55

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	CYS
1	A	73	LEU
1	A	155	GLU
1	A	171	PHE
1	A	184	LEU
1	A	192	ASP
1	A	202	CYS
1	A	206	ARG
1	A	383	LEU
1	A	389	PHE
1	A	439	LEU
1	A	485	ASP
1	A	487	ASN
1	A	494	SER
1	A	497	PHE
1	A	531	ASP
1	A	548	LYS
1	A	583	GLU
1	A	598	PHE
1	A	600	PHE
1	A	632	ASP

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Mol	Chain	Res	Type
1	A	702	SER
1	A	718	LYS
1	A	726	TYR
1	A	761	GLU
1	A	768	TRP
1	A	805	PHE
1	A	807	ARG
1	A	810	PHE
1	A	825	TYR
1	A	852	ASP
1	A	945	ASN
1	A	955	GLU
1	A	971	LEU
1	A	1038	ASN
1	A	1062	TYR
1	A	1063	PHE
1	A	1077	LEU
1	A	1096	PHE
1	A	1097	GLN
1	A	1136	ASP
1	A	1148	LYS
1	A	1158	PHE
1	A	1229	SER
1	A	1277	GLU
1	A	1279	ASN
1	A	1332	GLU
1	A	1345	SER
1	A	1367	TYR
1	A	1391	PHE
1	B	19	CYS
1	B	73	LEU
1	B	125	PHE
1	B	153	ARG
1	B	367	LEU
1	B	381	PHE
1	B	389	PHE
1	B	390	LYS
1	B	422	ASN
1	B	497	PHE
1	B	521	CYS
1	B	523	GLU
1	B	530	ASP

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Mol	Chain	Res	Type
1	B	544	PHE
1	B	568	ASN
1	B	600	PHE
1	B	607	ASN
1	B	656	GLN
1	B	699	PHE
1	B	703	TYR
1	B	758	MET
1	B	769	PHE
1	B	837	MET
1	B	840	SER
1	B	859	ASP
1	B	889	MET
1	B	921	ASN
1	B	957	LEU
1	B	962	ASP
1	B	1038	ASN
1	B	1043	LEU
1	B	1063	PHE
1	B	1094	LYS
1	B	1096	PHE
1	B	1115	TYR
1	B	1123	CYS
1	B	1213	LEU
1	B	1268	SER
1	B	1314	GLU
1	B	1353	LYS
1	B	1370	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	692	GLN
1	B	347	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 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)

There are no chain breaks in this entry.

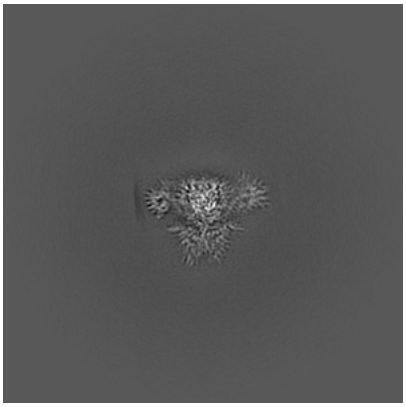
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26717. These allow visual inspection of the internal detail of the map and identification of artifacts.

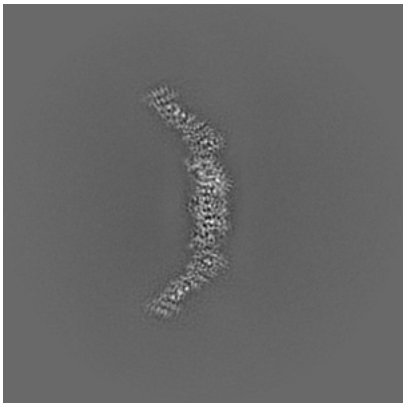
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

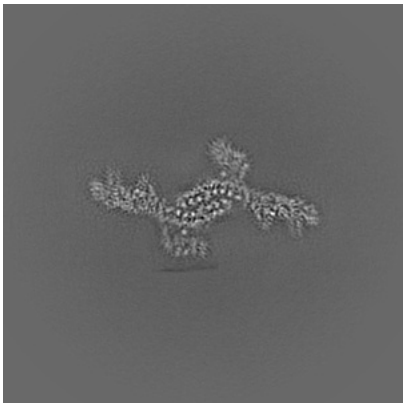
6.1.1 Primary map



X



Y

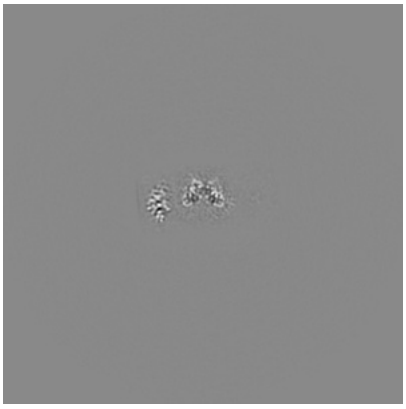


Z

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

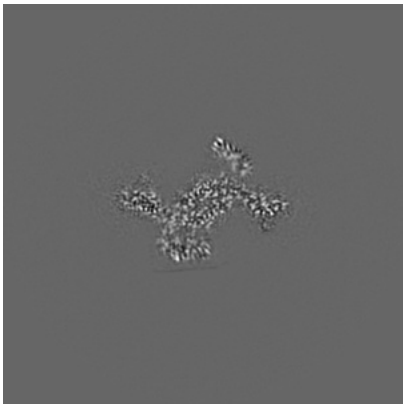
6.2 Central slices

6.2.1 Primary map



X Index: 150

Y Index: 150



Z Index: 150

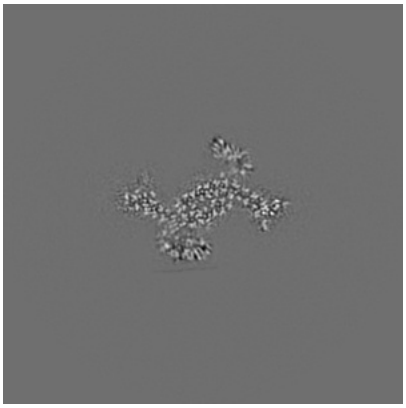
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 149

Y Index: 148



Z Index: 151

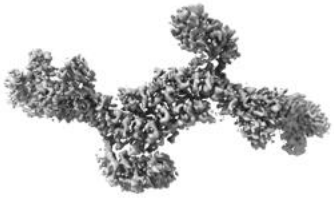
The images above show the largest variance slices of the map in three orthogonal directions.

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

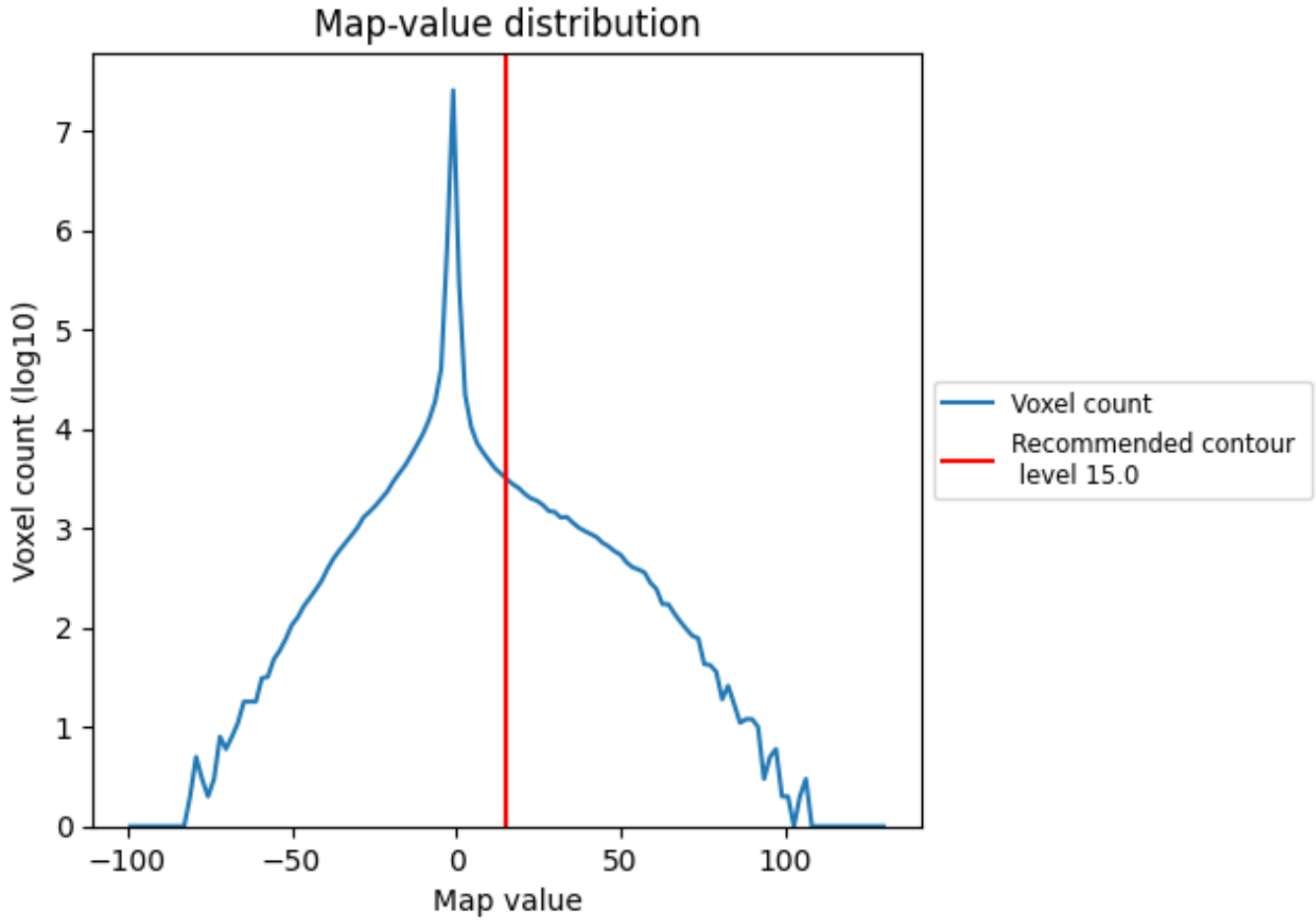
6.5 Mask visualisation (i)

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

7 Map analysis

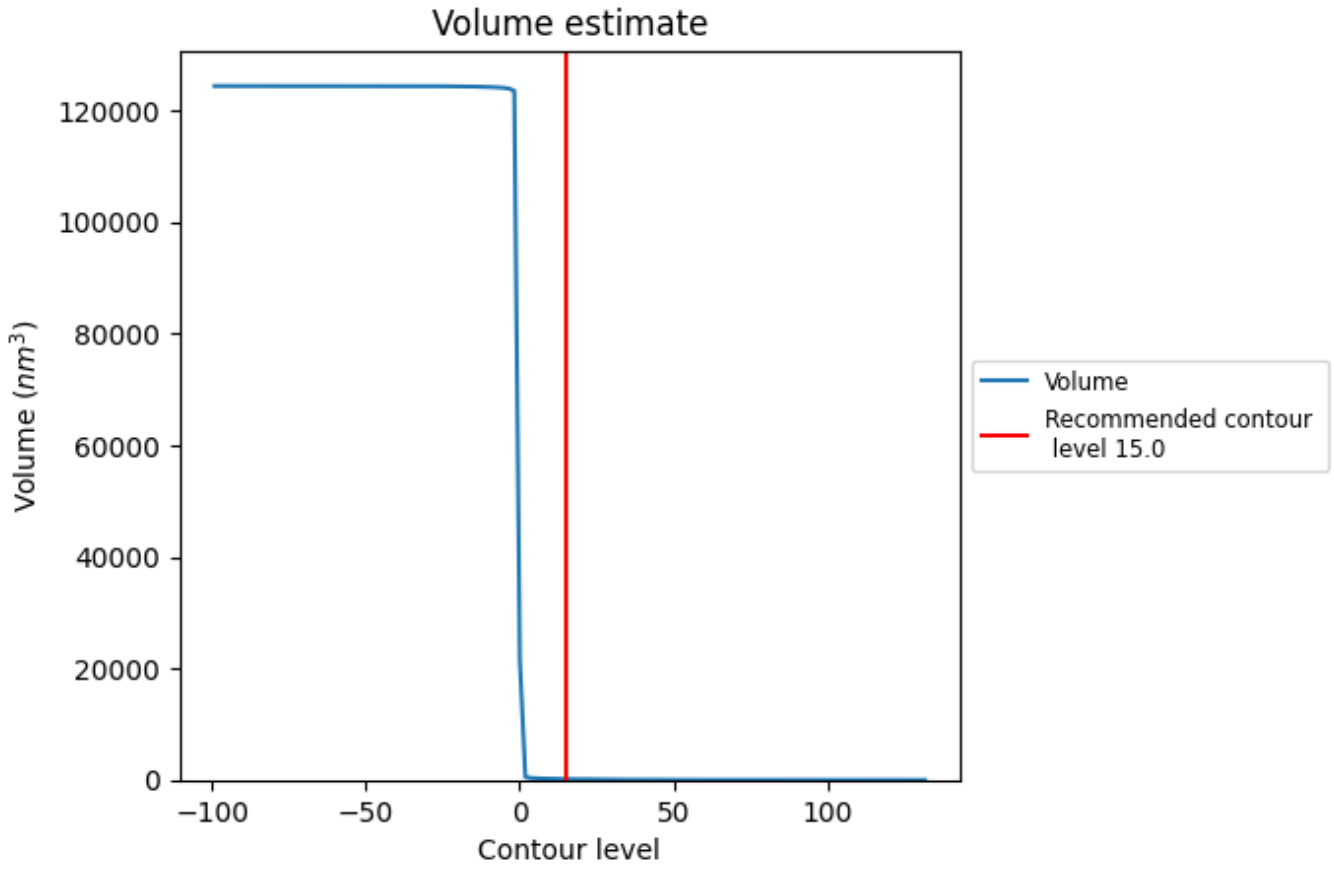
This section contains the results of statistical analysis of the map.

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.

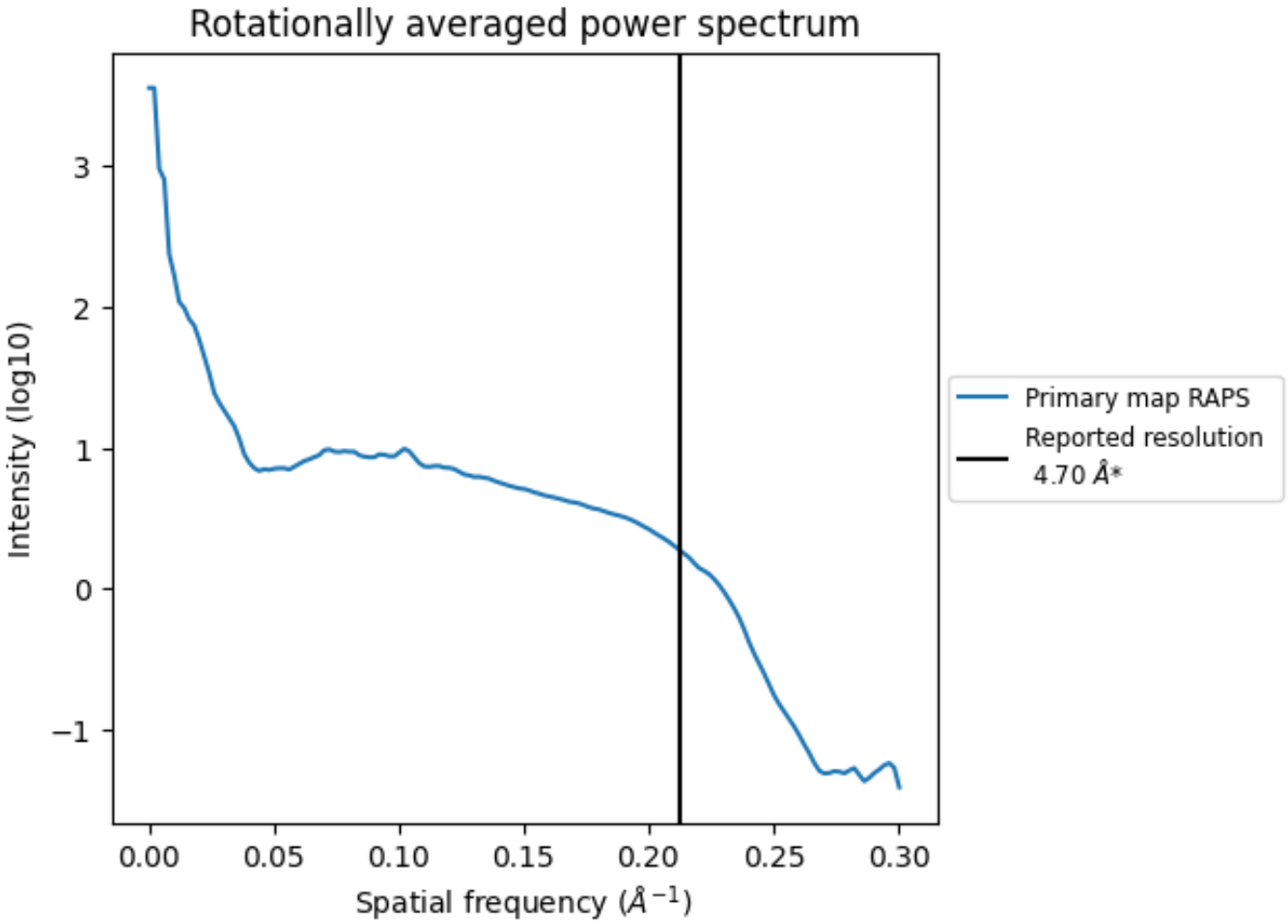
7.2 Volume estimate



The volume at the recommended contour level is 153 nm^3; this corresponds to an approximate mass of 138 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 0.213 Å^{-1}

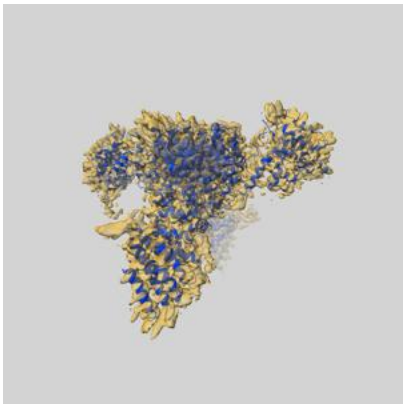
8 Fourier-Shell correlation

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

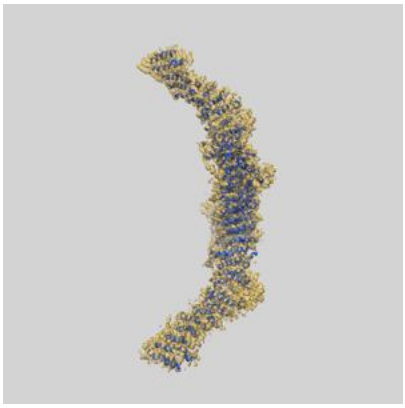
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26717 and PDB model 7URR. Per-residue inclusion information can be found in section 3 on page 4.

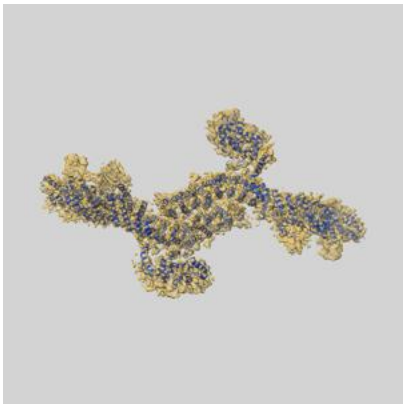
9.1 Map-model overlay



X



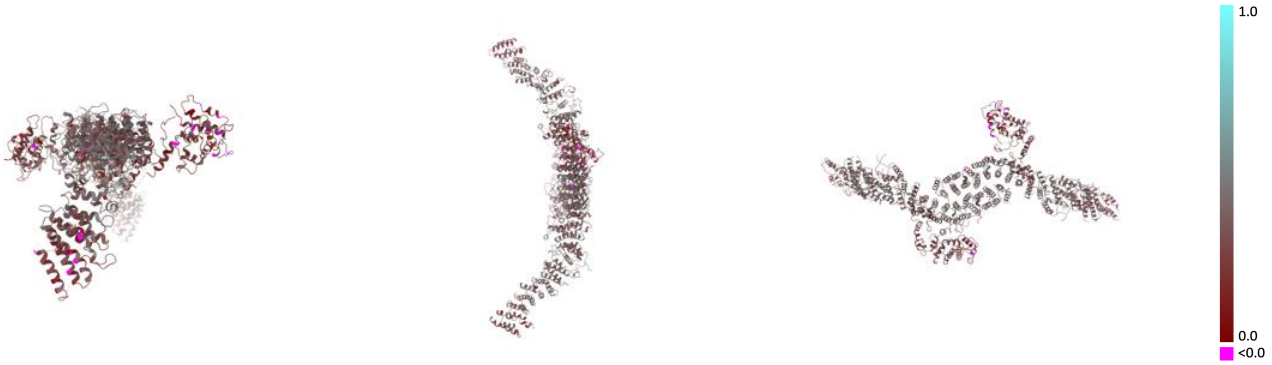
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 15.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

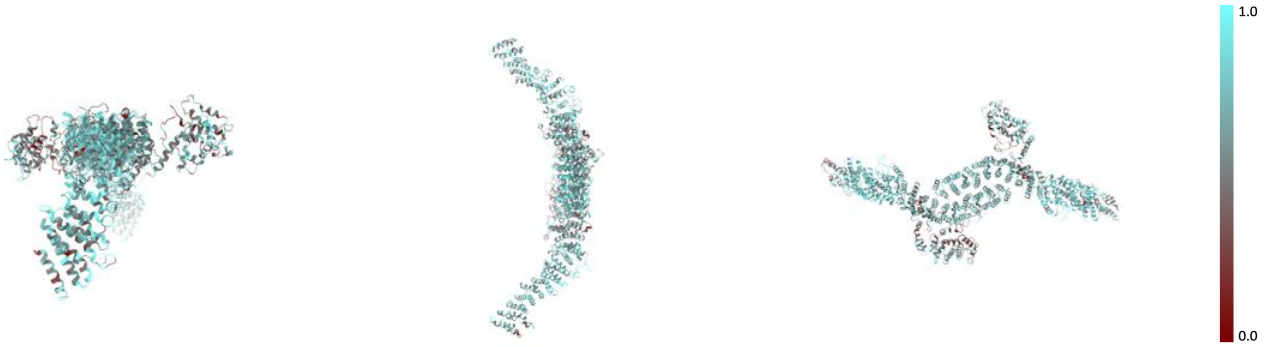
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

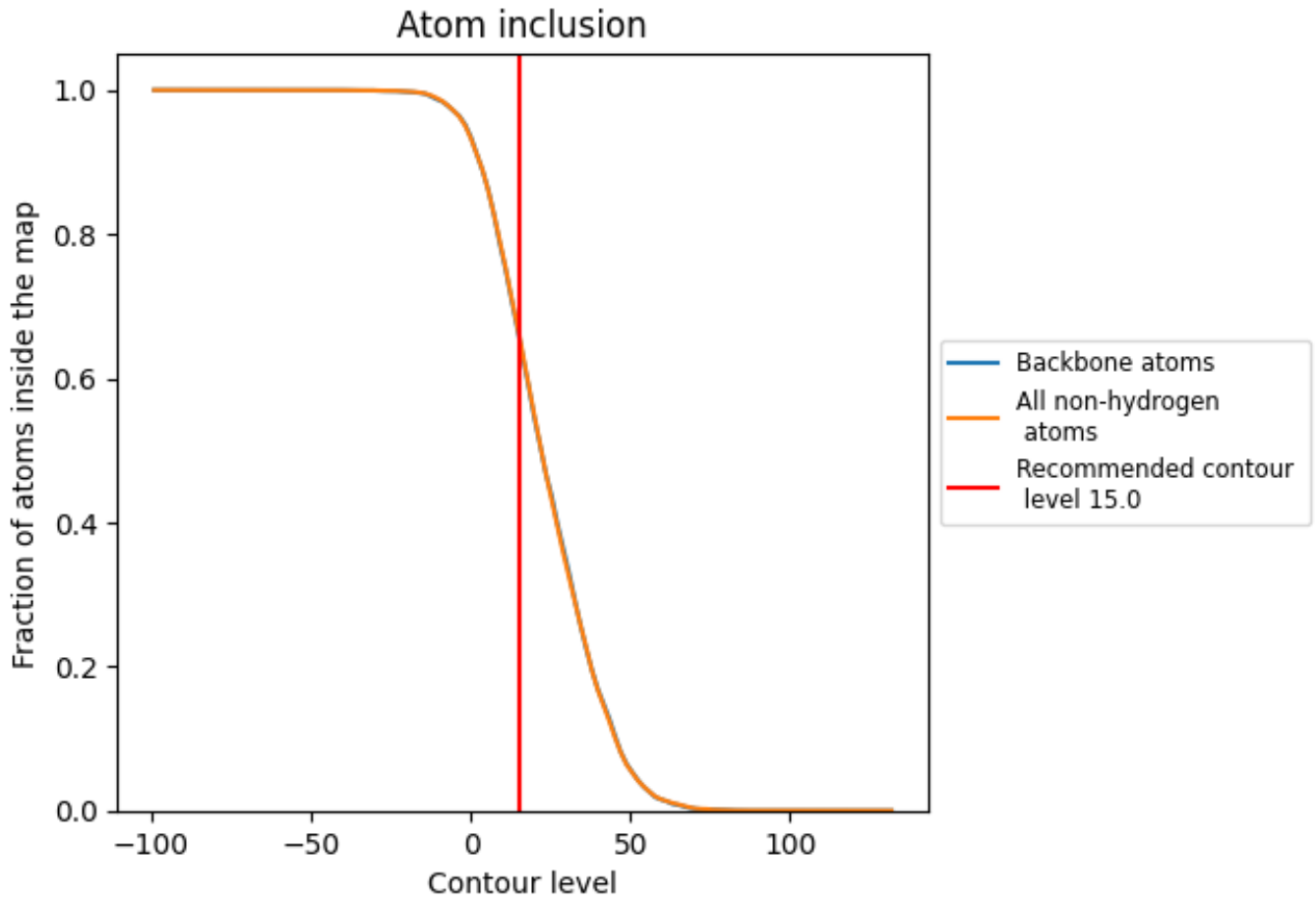
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (15.0).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (15.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6644	0.3530
A	0.6567	0.3630
B	0.6725	0.3420