Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 10:51 am BST

PDB ID	:	6FUW
EMDB ID	:	EMD-4225
Title	:	Cryo-EM structure of the human CPSF160-WDR33-CPSF30 complex bound to the PAS AAUAAA motif at 3.1 Angstrom resolution
Authors	:	Clerici, M.; Faini, M.; Jinek, M.
Deposited on	:	2018-02-28
Resolution	:	3.07 Å(reported)
Based on initial model	:	6F9N

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 (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:

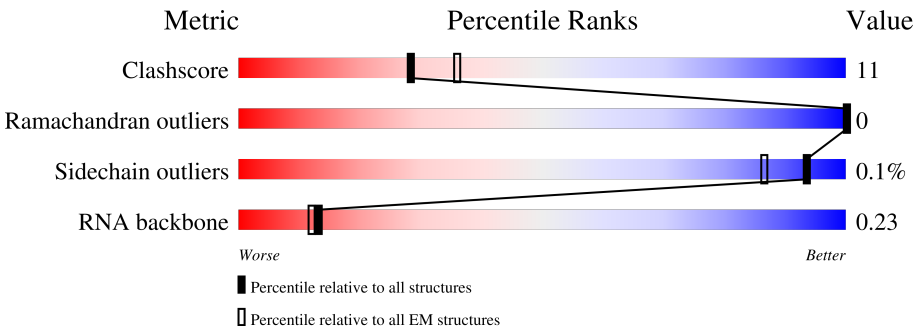
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.07 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
RNA backbone	4643	859

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	1446	• 61% 21% 18%
2	B	413	• 65% 25% 10%
3	C	178	19% 47% 16% • 36%
4	D	10	50% 20% 10% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13421 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 Cleavage and polyadenylation specificity factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1181	9367	6019	1608	1685	55	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q10570
A	-1	ASN	-	expression tag	UNP Q10570
A	0	ALA	-	expression tag	UNP Q10570

- Molecule 2 is a protein called pre-mRNA 3' end processing protein WDR33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	370	2978	1882	544	533	19	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP Q9C0J8
B	-1	ASN	-	expression tag	UNP Q9C0J8
B	0	ALA	-	expression tag	UNP Q9C0J8

- Molecule 3 is a protein called Cleavage and polyadenylation specificity factor subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	114	897	577	148	158	14	0	0

- Molecule 4 is a RNA chain called RNA (5'-R(P*AP*AP*UP*AP*AP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	8	176	79	37	52	8	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

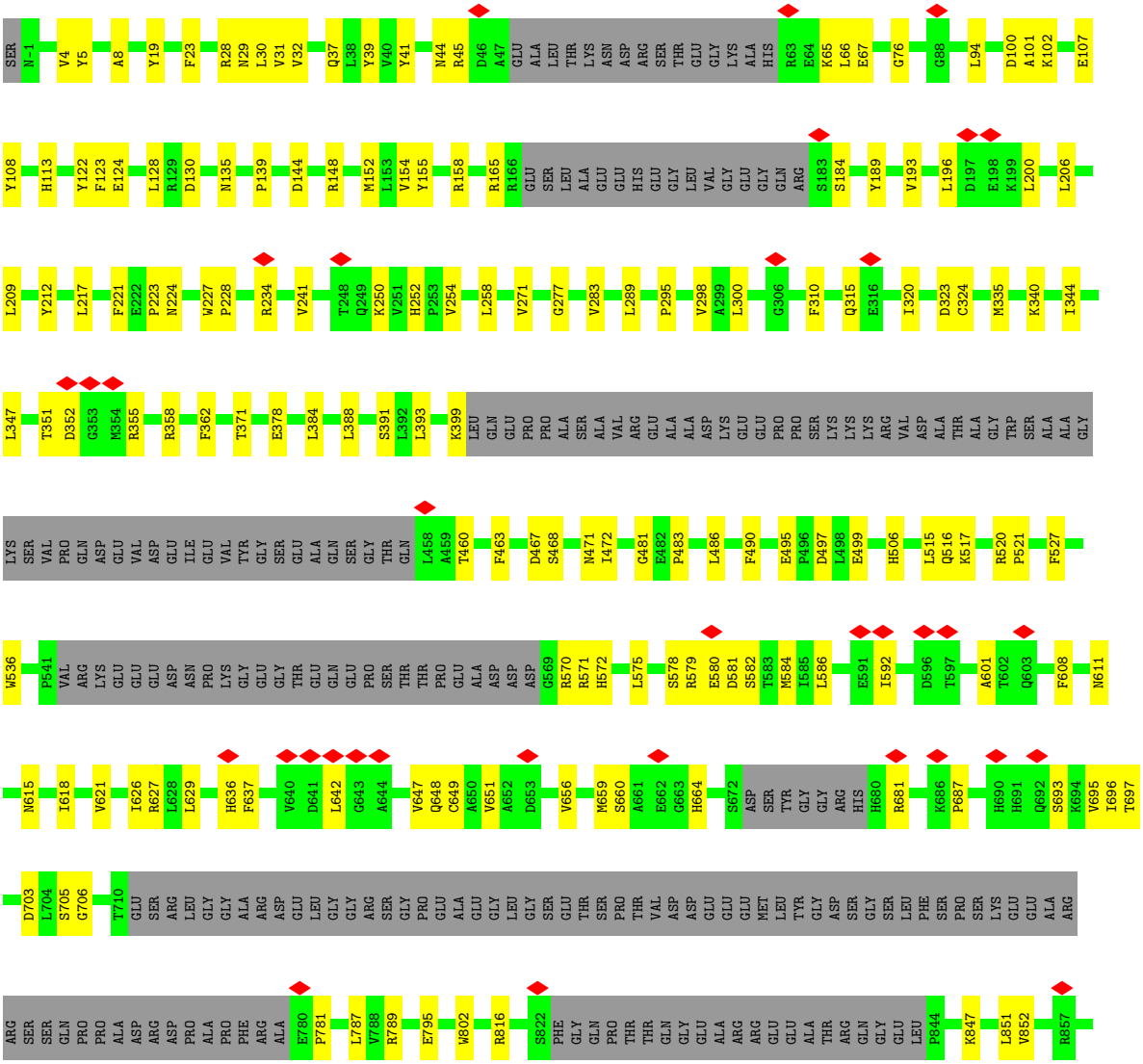
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	C	3	3	3	0

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: Cleavage and polyadenylation specificity factor subunit 1

Chain A:



P861 Y862 L863 L864 V865 H866 V867 D868 I873 A876 F877 D880 SER GLN LEU G884 Q885 K893 F901 R902 E903 LYS LYS PRO LYS PRO SER LYS LYS LYS ALA GLU GLY GLY GLY ALA GLU GLU GLY ALA GLY ALA ARG GLY R927 R932 I937 Y938 P948 W952 L953

A960 L961 R962 M966 A967 I968 P971 S974 F975 H979 C983 P984 R985 G986 F987 L988 Y989 F990 N991 R992 L996 R997 I998 P1010 W1011 P1012 V1013 V1033 Y1034 C1044 A1045 M1050 THR GLY GLU E1054 K1055 E1056 F1057 E1064 R1065 P1069 S1075 L1078

I1087 R1091 Q1095 E1098 H1099 V1100 E1111 E1112 T1113 V1114 T1125 Q1129 V1133 R1138 I1139 L1140 I1141 M1142 D1143 V1144 P1149 GLU PRO GLY GLN P1154 L1155 T1156 Y1164 E1165 K1166 P1171 V1172 S1184 A1185 I1186 I1190 F1191 L1192 W1193 S1194 L1195 R1196 L1200 I1206

D1207 T1208 Q1209 L1210 Q1214 M1215 I1216 K1219 N1220 F1221 A1225 M1228 K1229 S1230 L1234 R1235 Y1236 Q1237 L1245 L1253 V1258 D1259 F1260 D1263 N1264 F1269 L1270 V1271 S1272 R1276 M1277 L1278 M1279 V1280 Y1281 E1286 A1287 K1288 D1301 F1302 H1307 V1308 F1311 W1312 R1313

R1317 GLY ALA THR GLU GLY LEU SER LYS LYS SER VAL V1329 N1332 K1333 H1334 I1335 F1338 A1339 T1340 L1347 L1348 L1349 P1350 M1351 Q1363 N1364 A1365 L1370 R1379 A1380 F1381 R1382 M1383 L1384 H1385 VAL ASP ARG ARG THR LEU GLN N1393 D1400 G1401 E1402 L1403 R1406 Y1409

L1418 A1441 H1442 F1443

- Molecule 2: pre-mRNA 3' end processing protein WDR33

Chain B: 65% 25% 10%

SER ASN ALA MET ALA THR GLU ILE GLY SER PRO PRO ARG PHE PHE HIS MET PRO ARG PHE GLN HIS GLN ALA PRO ARG GLN LEU PHE TYR LYS ARG PRO ASP PHE ALA GLN GLN GLN ALA MET GLN GLN L41 T42 F43 R49 K50 N53 I57 D75 Q76 R77 R80

N100 N104 A105 K117 V125 R133 L134 V135 T136 L145 W146 N147 G148 E154 T155 H160 D161 S162 P163 A166 H171 W175 M176 A179 D180 H181 G182 K186 Y187 W188 N191 M192 N193 N194 V195 K196 M197 H201 A204 I205 S211 P212 T213 D214

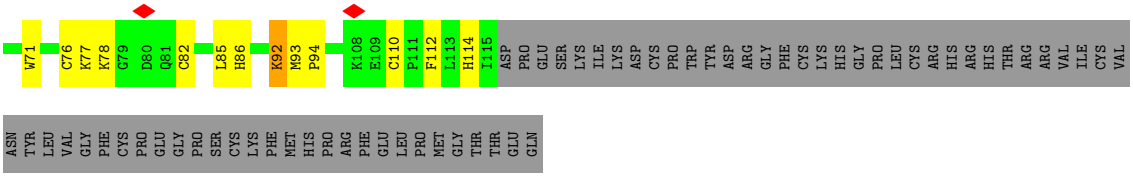
N215 K216 S221 D222 D223 G224 T225 V226 R227 D230 F231 L232 L240 H243 H253 P254 V259 G262 S263 K264 D265 S266 Q267 Q268 P269 I270 W273 D274 P275 T283 L284 H285 V294 N297 L298 N299 W302 L303 L304 T305 L311 C312 K313 L314 F315 K321

E322 E323 L324 Q325 V326 F327 R328 K332 E333 V337 E344 G345 L356 L357 V361 K365 G369 H374 C391 S394 N395 D396 R406 D409 K410

- Molecule 3: Cleavage and polyadenylation specificity factor subunit 4

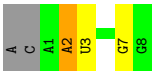
Chain C: 19% 47% 16% 36%

M1 Q2 E3 I4 I5 A6 S7 V8 D9 H10 I11 K12 F13 D14 L15 E16 E20 L23 G24 A25 Q26 P27 L28 P31 G32 M33 ASP K35 S36 G37 A38 A39 V40 C41 E42 F43 F44 L45 K46 A47 A48 C49 G50 K51 G52 G53 M54 C55 P56 F57 S61 G62 E63 K64 V67



• Molecule 4: RNA (5'-R(P*AP*AP*UP*AP*AP*AP*GP*G)-3')

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	137000	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47259	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.329	Depositor
Minimum map value	-0.208	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.058	Depositor
Map size (Å)	211.59999, 211.59999, 211.59999	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.51	0/9581	0.59	0/13000
2	B	0.51	0/3062	0.61	1/4146 (0.0%)
3	C	0.39	0/920	0.53	1/1231 (0.1%)
4	D	0.73	0/198	0.87	0/307
All	All	0.51	0/13761	0.60	2/18684 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	92	LYS	C-N-CA	5.73	136.01	121.70
2	B	356	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9367	0	9420	188	0
2	B	2978	0	2895	78	0
3	C	897	0	872	25	0
4	D	176	0	88	1	0
5	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13421	0	13275	281	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 11.

All (281) 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:1365:ALA:HB1	1:A:1418:LEU:HD11	1.65	0.79
1:A:575:LEU:HD23	1:A:586:LEU:HD12	1.66	0.78
1:A:481:GLY:O	1:A:499:GLU:HB3	1.85	0.77
1:A:648:GLN:HB3	1:A:659:MET:HB3	1.68	0.76
1:A:1184:SER:HG	1:A:1193:TRP:HE1	1.27	0.76
1:A:130:ASP:OD1	1:A:158:ARG:NH2	2.19	0.75
1:A:1370:LEU:HD23	1:A:1406:ARG:HH21	1.51	0.75
1:A:19:TYR:O	1:A:28:ARG:NH2	2.20	0.74
2:B:147:ASN:OD1	2:B:148:GLY:N	2.23	0.71
2:B:325:GLN:NE2	2:B:361:VAL:O	2.22	0.71
2:B:304:LEU:HD22	2:B:337:VAL:HG11	1.72	0.71
1:A:66:LEU:HD11	1:A:393:LEU:HD22	1.72	0.70
1:A:1263:ASP:OD1	1:A:1264:ASN:N	2.21	0.70
1:A:693:SER:HB2	1:A:789:ARG:HD3	1.74	0.70
2:B:294:VAL:HG23	2:B:305:THR:HG22	1.74	0.69
1:A:108:TYR:HH	1:A:113:HIS:HD1	1.39	0.69
1:A:937:ILE:HD11	1:A:987:PHE:HB3	1.72	0.69
1:A:516:GLN:OE1	1:A:520:ARG:NH1	2.26	0.68
2:B:182:GLY:H	2:B:204:ALA:HA	1.58	0.67
1:A:579:ARG:HG2	1:A:580:GLU:H	1.58	0.67
1:A:1276:ARG:HE	1:A:1307:HIS:CE1	2.12	0.67
1:A:224:ASN:HB3	1:A:234:ARG:HH11	1.59	0.66
2:B:315:PHE:HE1	2:B:323:GLU:HG2	1.61	0.66
1:A:221:PHE:HE2	1:A:223:PRO:HG3	1.60	0.65
1:A:1317:ARG:NH1	1:A:1441:ALA:O	2.30	0.65
1:A:320:ILE:HD11	1:A:362:PHE:HE2	1.61	0.65
1:A:847:LYS:HB2	1:A:866:HIS:HD2	1.62	0.64
1:A:1230:SER:HB3	1:A:1253:LEU:HB3	1.79	0.64
1:A:1301:ASP:HB2	1:A:1384:LEU:HD21	1.79	0.64
3:C:28:LEU:HD11	3:C:35:LYS:HD3	1.80	0.64
2:B:125:VAL:HG12	2:B:136:THR:HG22	1.79	0.64
1:A:1364:ASN:OD1	1:A:1379:ARG:NH1	2.31	0.63
1:A:4:VAL:HG13	1:A:1351:MET:SD	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:HD11	1:A:362:PHE:CE2	2.35	0.62
1:A:627:ARG:HB3	1:A:637:PHE:HD1	1.65	0.61
1:A:517:LYS:N	1:A:1443:PHE:OXT	2.24	0.61
1:A:1313:ARG:O	3:C:1:MET:N	2.33	0.61
1:A:1138:ARG:HG3	1:A:1166:LYS:C	2.21	0.61
1:A:953:LEU:HG	1:A:961:LEU:HD11	1.83	0.60
1:A:1195:LEU:HD13	1:A:1200:LEU:HD12	1.83	0.60
1:A:344:ILE:HG21	1:A:463:PHE:HE2	1.66	0.60
1:A:971:PRO:HG2	1:A:992:ARG:HD2	1.83	0.59
1:A:45:ARG:NH2	1:A:378:GLU:OE1	2.35	0.58
1:A:1190:ILE:HD12	1:A:1208:THR:HG21	1.84	0.58
2:B:75:ASP:OD2	2:B:77:ARG:NH1	2.35	0.58
1:A:196:LEU:HD21	1:A:252:HIS:CD2	2.38	0.58
2:B:186:LYS:NZ	2:B:197:MET:SD	2.77	0.58
1:A:227:TRP:CD1	1:A:228:PRO:HD2	2.38	0.58
1:A:695:VAL:HG22	1:A:787:LEU:HD21	1.86	0.58
3:C:93:MET:SD	3:C:94:PRO:HD2	2.43	0.58
2:B:145:LEU:HD12	2:B:155:THR:OG1	2.04	0.58
2:B:43:PHE:CD2	2:B:117:LYS:HG3	2.39	0.57
2:B:175:TRP:HZ3	2:B:195:VAL:HG21	1.68	0.57
2:B:297:ASN:HD22	2:B:302:TRP:HE3	1.52	0.57
1:A:864:LEU:HD23	1:A:873:ILE:HG12	1.86	0.57
2:B:394:SER:OG	2:B:396:ASP:OD1	2.22	0.57
2:B:201:HIS:CG	2:B:221:SER:HB2	2.39	0.57
1:A:154:VAL:HG12	1:A:155:TYR:CD2	2.40	0.57
1:A:1075:SER:HB3	1:A:1091:ARG:HE	1.71	0.56
1:A:1286:GLU:OE2	3:C:23:LEU:HB3	2.05	0.56
1:A:324:CYS:SG	2:B:80:ARG:NH1	2.79	0.56
1:A:515:LEU:HG	1:A:1013:VAL:HG12	1.87	0.56
1:A:647:VAL:HG22	1:A:927:ARG:HD3	1.86	0.55
1:A:101:ALA:HB3	1:A:124:GLU:HG3	1.87	0.55
1:A:44:ASN:HB2	1:A:67:GLU:OE1	2.07	0.55
1:A:983:CYS:SG	1:A:998:ILE:HG22	2.46	0.55
1:A:1140:LEU:HG	1:A:1142:MET:SD	2.47	0.55
1:A:497:ASP:OD1	1:A:520:ARG:NH2	2.33	0.55
1:A:636:HIS:ND1	1:A:681:ARG:HD2	2.21	0.54
2:B:187:TYR:CD2	2:B:196:LYS:HB3	2.42	0.54
1:A:867:VAL:HG12	1:A:868:ASP:H	1.72	0.54
3:C:64:LYS:HE2	3:C:85:LEU:HA	1.90	0.54
1:A:224:ASN:HB3	1:A:234:ARG:NH1	2.22	0.54
1:A:932:ARG:HG3	1:A:975:PHE:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:SER:OG	2:B:222:ASP:N	2.41	0.54
1:A:300:LEU:O	1:A:1065:ARG:NH1	2.41	0.53
1:A:601:ALA:HB2	1:A:627:ARG:CZ	2.39	0.53
1:A:31:VAL:HG11	1:A:94:LEU:HD21	1.90	0.53
1:A:703:ASP:O	1:A:781:PRO:HA	2.09	0.53
1:A:1234:LEU:HD23	1:A:1245:LEU:HA	1.91	0.53
2:B:104:ASN:OD1	2:B:105:ALA:N	2.42	0.53
3:C:82:CYS:HB3	3:C:86:HIS:HE1	1.74	0.53
1:A:165:ARG:HB3	1:A:184:SER:HA	1.91	0.53
1:A:1363:GLN:HG3	1:A:1403:LEU:HD23	1.92	0.52
2:B:192:MET:O	3:C:77:LYS:HE3	2.10	0.52
3:C:71:TRP:CD1	3:C:86:HIS:HD2	2.26	0.52
2:B:299:ASN:ND2	2:B:344:GLU:OE2	2.42	0.52
1:A:340:LYS:HE3	2:B:80:ARG:HG2	1.91	0.52
1:A:988:LEU:HD13	1:A:996:LEU:HD11	1.92	0.52
2:B:267:GLN:O	2:B:285:HIS:NE2	2.43	0.52
1:A:642:LEU:HD11	1:A:660:SER:OG	2.09	0.52
1:A:1138:ARG:HG3	1:A:1166:LYS:O	2.09	0.52
2:B:176:MET:HB3	2:B:188:TRP:HB2	1.92	0.51
2:B:262:GLY:HA2	2:B:269:PRO:O	2.11	0.51
2:B:57:ILE:HD12	2:B:406:ARG:HH22	1.75	0.51
2:B:75:ASP:OD1	2:B:75:ASP:N	2.40	0.51
1:A:516:GLN:O	1:A:1012:PRO:HD2	2.11	0.51
2:B:357:LEU:HD23	2:B:369:GLY:HA3	1.93	0.51
1:A:298:VAL:CG1	1:A:315:GLN:HB2	2.41	0.51
3:C:39:ALA:O	3:C:57:PHE:HB3	2.10	0.51
1:A:193:VAL:HG22	1:A:200:LEU:HD22	1.91	0.50
1:A:139:PRO:HB3	1:A:152:MET:HE2	1.93	0.50
1:A:1216:ILE:HG22	1:A:1260:PHE:HE2	1.76	0.50
1:A:209:LEU:HD12	1:A:212:TYR:HE2	1.76	0.50
1:A:1100:VAL:HG22	1:A:1125:THR:HG22	1.93	0.50
2:B:160:HIS:CG	2:B:180:ASP:HB3	2.47	0.50
1:A:221:PHE:CE2	1:A:223:PRO:HG3	2.44	0.50
2:B:270:ILE:HB	2:B:284:LEU:HB3	1.94	0.50
2:B:315:PHE:CE1	2:B:323:GLU:HG2	2.45	0.50
1:A:283:VAL:HG22	1:A:323:ASP:HB3	1.94	0.50
2:B:133:ARG:NE	2:B:154:GLU:OE1	2.42	0.50
2:B:160:HIS:CE1	2:B:186:LYS:HD3	2.47	0.50
2:B:259:VAL:HG23	2:B:275:PRO:HG3	1.93	0.49
2:B:201:HIS:HD2	2:B:205:ILE:HG12	1.78	0.49
1:A:579:ARG:NH1	1:A:584:MET:SD	2.82	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:VAL:HG22	1:A:1340:THR:HG22	1.94	0.49
1:A:816:ARG:HD3	1:A:1409:TYR:O	2.12	0.49
1:A:527:PHE:HE2	1:A:592:ILE:HG21	1.78	0.49
2:B:374:HIS:CG	2:B:394:SER:HG	2.30	0.49
1:A:852:VAL:O	1:A:861:PRO:HA	2.12	0.49
1:A:861:PRO:HG2	1:A:876:ALA:HB3	1.95	0.49
2:B:240:LEU:HD22	2:B:273:TRP:CE3	2.48	0.48
2:B:75:ASP:OD1	2:B:77:ARG:HG2	2.12	0.48
2:B:186:LYS:HG2	2:B:197:MET:HG3	1.95	0.48
1:A:258:LEU:HD12	1:A:289:LEU:HD23	1.96	0.48
2:B:243:HIS:CG	2:B:263:SER:HG	2.30	0.48
1:A:352:ASP:OD1	1:A:358:ARG:NE	2.46	0.48
1:A:37:GLN:HG2	1:A:39:TYR:OH	2.14	0.48
2:B:133:ARG:HB2	2:B:146:TRP:O	2.13	0.48
2:B:212:PRO:HB3	2:B:254:PRO:O	2.14	0.48
3:C:78:LYS:O	3:C:82:CYS:N	2.47	0.48
1:A:371:THR:HG22	1:A:384:LEU:HB3	1.95	0.48
1:A:642:LEU:HD13	1:A:664:HIS:HB2	1.96	0.48
1:A:128:LEU:HD23	1:A:158:ARG:NH1	2.29	0.47
1:A:1044:CYS:HB3	1:A:1069:PRO:HB2	1.96	0.47
1:A:1219:LYS:NZ	3:C:11:ILE:O	2.47	0.47
2:B:191:ASN:ND2	3:C:76:CYS:O	2.46	0.47
1:A:471:ASN:OD1	1:A:472:ILE:N	2.48	0.47
1:A:651:VAL:HG22	1:A:656:VAL:HG22	1.94	0.47
1:A:1143:ASP:OD1	1:A:1144:VAL:N	2.48	0.47
1:A:29:ASN:HB2	1:A:41:TYR:O	2.14	0.47
1:A:144:ASP:OD2	1:A:148:ARG:HG2	2.15	0.47
1:A:536:TRP:HZ3	1:A:578:SER:HB2	1.79	0.47
1:A:1210:LEU:HD22	1:A:1228:MET:HE2	1.97	0.47
2:B:201:HIS:CE1	2:B:227:ARG:HD2	2.50	0.47
1:A:467:ASP:OD1	1:A:468:SER:N	2.44	0.47
3:C:51:LYS:HG3	3:C:56:PRO:HD2	1.96	0.47
1:A:847:LYS:HB2	1:A:866:HIS:CD2	2.47	0.46
1:A:1095:GLN:HB3	1:A:1098:GLU:OE1	2.15	0.46
2:B:204:ALA:HB3	2:B:222:ASP:OD2	2.14	0.46
1:A:1098:GLU:OE1	1:A:1138:ARG:NH2	2.49	0.46
1:A:490:PHE:CZ	1:A:521:PRO:HG2	2.50	0.46
1:A:23:PHE:HD2	1:A:29:ASN:HD21	1.63	0.46
1:A:948:PRO:HA	1:A:971:PRO:HB3	1.96	0.46
1:A:570:ARG:HD2	1:A:985:ARG:HH22	1.79	0.46
1:A:705:SER:OG	1:A:706:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:VAL:HG12	3:C:11:ILE:HD12	1.98	0.46
1:A:344:ILE:CG2	1:A:463:PHE:HE2	2.27	0.46
1:A:388:LEU:HD22	1:A:506:HIS:HB3	1.98	0.46
1:A:618:ILE:HB	1:A:629:LEU:HB2	1.97	0.46
1:A:209:LEU:HD12	1:A:212:TYR:CE2	2.51	0.46
1:A:1311:PHE:CD1	1:A:1338:PHE:HB3	2.51	0.46
2:B:225:THR:OG1	2:B:227:ARG:NH1	2.49	0.46
1:A:101:ALA:HB1	1:A:123:PHE:HB2	1.98	0.46
1:A:1370:LEU:HD23	1:A:1406:ARG:NH2	2.26	0.46
2:B:253:HIS:CG	2:B:254:PRO:HD2	2.51	0.46
1:A:271:VAL:HB	1:A:277:GLY:H	1.80	0.45
1:A:867:VAL:HG12	1:A:868:ASP:N	2.31	0.45
1:A:1335:ILE:HG12	1:A:1349:LEU:HD13	1.99	0.45
1:A:344:ILE:HG21	1:A:463:PHE:CE2	2.49	0.45
2:B:163:PRO:HD2	2:B:181:HIS:HB3	1.98	0.45
2:B:186:LYS:HE3	2:B:194:ASN:ND2	2.30	0.45
2:B:43:PHE:HD2	2:B:117:LYS:HG3	1.81	0.45
1:A:571:ARG:HA	1:A:979:HIS:HD2	1.82	0.45
1:A:789:ARG:NH1	1:A:795:GLU:OE1	2.47	0.45
3:C:71:TRP:CG	3:C:86:HIS:HD2	2.34	0.45
3:C:82:CYS:HB3	3:C:86:HIS:CE1	2.51	0.45
3:C:110:CYS:HB3	3:C:114:HIS:HE1	1.81	0.45
1:A:877:PHE:CE1	1:A:893:LYS:HB2	2.51	0.45
1:A:1033:VAL:HG12	1:A:1034:TYR:N	2.31	0.45
1:A:1221:PHE:HE2	3:C:15:LEU:HB3	1.82	0.45
1:A:1235:ARG:HH22	1:A:1237:GLN:HE21	1.63	0.45
1:A:1258:VAL:HG23	1:A:1271:VAL:HG22	1.99	0.45
1:A:851:LEU:HD12	1:A:862:TYR:O	2.17	0.45
1:A:76:GLY:HA2	1:A:1381:PHE:CE1	2.52	0.45
1:A:952:TRP:HE1	1:A:966:MET:CE	2.29	0.45
2:B:201:HIS:CD2	2:B:205:ILE:HG12	2.52	0.44
2:B:201:HIS:CE1	2:B:227:ARG:HH11	2.36	0.44
2:B:171:HIS:ND1	2:B:214:ASP:OD1	2.45	0.44
2:B:211:SER:O	2:B:214:ASP:N	2.40	0.44
1:A:1186:ILE:HD12	1:A:1191:PHE:CD2	2.51	0.44
2:B:240:LEU:HD13	2:B:273:TRP:CD2	2.52	0.44
4:D:2:A:O2'	4:D:3:U:H5'	2.17	0.44
1:A:636:HIS:CE1	1:A:681:ARG:HD2	2.52	0.44
1:A:1078:LEU:HB3	1:A:1087:ILE:HD12	1.98	0.44
2:B:294:VAL:HG22	2:B:303:LEU:HD11	2.00	0.44
3:C:51:LYS:HB2	3:C:55:CYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD12	1:A:217:LEU:HD21	1.99	0.44
1:A:241:VAL:HG13	1:A:254:VAL:HG13	1.99	0.44
1:A:1334:HIS:CD2	3:C:6:ALA:HB1	2.52	0.44
1:A:107:GLU:HG2	1:A:108:TYR:H	1.82	0.44
1:A:608:PHE:HB3	1:A:621:VAL:HB	2.00	0.44
1:A:1214:GLN:HB3	1:A:1225:ALA:HB3	2.00	0.44
1:A:1302:PHE:CZ	1:A:1382:ARG:HD2	2.53	0.44
1:A:1279:MET:HB3	1:A:1281:TYR:HE1	1.83	0.44
1:A:579:ARG:HH22	1:A:584:MET:HB2	1.82	0.43
1:A:1171:PRO:O	1:A:1186:ILE:HA	2.18	0.43
1:A:1206:ILE:HG23	1:A:1208:THR:HG23	2.00	0.43
2:B:221:SER:HB3	2:B:223:ASP:OD1	2.18	0.43
2:B:268:GLN:HG2	2:B:283:THR:HG21	2.00	0.43
1:A:335:MET:HE2	1:A:347:LEU:HD23	1.99	0.43
1:A:611:ASN:HB3	1:A:615:ASN:HA	2.00	0.43
1:A:5:TYR:O	1:A:1401:GLY:HA3	2.19	0.43
2:B:43:PHE:CE2	2:B:117:LYS:HG3	2.53	0.43
2:B:311:LEU:CD2	2:B:328:ARG:HG2	2.48	0.43
1:A:621:VAL:HG13	1:A:626:ILE:HG22	2.00	0.43
3:C:27:PRO:HG3	3:C:51:LYS:HD2	2.00	0.43
1:A:687:PRO:HB3	1:A:802:TRP:CE2	2.53	0.43
1:A:1235:ARG:HH22	1:A:1237:GLN:NE2	2.16	0.43
1:A:696:ILE:HG22	1:A:697:THR:HG23	2.01	0.43
1:A:1129:GLN:HG3	1:A:1133:VAL:HG11	1.99	0.43
2:B:134:LEU:HD21	2:B:391:CYS:SG	2.59	0.43
2:B:135:VAL:HG22	2:B:145:LEU:CD2	2.49	0.43
1:A:65:LYS:HG3	1:A:467:ASP:OD2	2.18	0.43
1:A:391:SER:O	1:A:468:SER:HA	2.19	0.43
1:A:490:PHE:HZ	1:A:521:PRO:HG2	1.84	0.43
1:A:960:ALA:HB1	1:A:962:ARG:NH1	2.33	0.43
1:A:1164:TYR:CZ	1:A:1166:LYS:HB3	2.53	0.43
2:B:43:PHE:CE2	2:B:117:LYS:HE3	2.54	0.43
1:A:903:GLU:HG2	1:A:948:PRO:HB3	2.00	0.43
1:A:974:SER:HB2	1:A:990:PHE:HB2	2.00	0.42
1:A:1156:THR:O	1:A:1156:THR:HG22	2.20	0.42
1:A:1400:ASP:O	1:A:1402:GLU:N	2.47	0.42
2:B:216:LYS:HG2	2:B:230:ASP:HA	2.02	0.42
1:A:100:ASP:OD1	1:A:135:ASN:ND2	2.39	0.42
1:A:572:HIS:HD2	1:A:979:HIS:N	2.17	0.42
1:A:621:VAL:HG21	1:A:649:CYS:SG	2.59	0.42
1:A:323:ASP:OD1	1:A:340:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:GLU:OE1	1:A:1111:GLU:N	2.49	0.42
2:B:57:ILE:HD12	2:B:406:ARG:NH2	2.35	0.42
2:B:76:GLN:OE1	2:B:100:ASN:HB2	2.20	0.42
2:B:312:CYS:HB2	2:B:327:PHE:HB2	2.02	0.42
3:C:67:VAL:HG23	3:C:92:LYS:O	2.20	0.42
1:A:206:LEU:HD12	1:A:217:LEU:HD11	2.01	0.42
2:B:49:ARG:HD2	2:B:50:LYS:O	2.19	0.42
1:A:1113:THR:HG22	1:A:1114:VAL:N	2.35	0.42
2:B:187:TYR:HD2	2:B:196:LYS:HB3	1.82	0.42
1:A:399:LYS:N	1:A:460:THR:O	2.53	0.41
1:A:1184:SER:OG	1:A:1193:TRP:NE1	2.23	0.41
1:A:1332:ASN:OD1	3:C:10:HIS:NE2	2.38	0.41
1:A:581:ASP:OD1	1:A:582:SER:N	2.53	0.41
2:B:303:LEU:O	2:B:314:LEU:HD12	2.20	0.41
1:A:527:PHE:HB2	1:A:996:LEU:HB3	2.02	0.41
1:A:1055:LYS:HE3	1:A:1057:PHE:HZ	1.85	0.41
2:B:332:LYS:HB3	2:B:333:GLU:H	1.77	0.41
1:A:351:THR:HB	1:A:355:ARG:HA	2.02	0.41
1:A:1259:ASP:OD1	1:A:1260:PHE:N	2.53	0.41
2:B:240:LEU:HD13	2:B:273:TRP:CG	2.55	0.41
1:A:298:VAL:HG11	1:A:315:GLN:NE2	2.36	0.41
2:B:345:GLY:O	2:B:361:VAL:HG23	2.21	0.41
1:A:30:LEU:HG	1:A:32:VAL:HG13	2.01	0.41
1:A:938:TYR:O	1:A:938:TYR:CG	2.72	0.41
1:A:8:ALA:HB2	1:A:1347:LEU:HD23	2.03	0.41
1:A:139:PRO:HB3	1:A:152:MET:CE	2.50	0.41
1:A:1269:PHE:O	1:A:1280:VAL:HA	2.20	0.41
1:A:1272:SER:HB3	1:A:1278:LEU:HD23	2.03	0.41
3:C:94:PRO:HG2	3:C:112:PHE:CE1	2.56	0.41
1:A:189:TYR:CD1	1:A:250:LYS:HE2	2.56	0.41
1:A:486:LEU:HD11	1:A:968:ILE:HD11	2.03	0.41
2:B:232:LEU:HD23	2:B:232:LEU:HA	1.95	0.40
1:A:1010:PRO:O	1:A:1011:TRP:HD1	2.04	0.40
2:B:135:VAL:HG22	2:B:145:LEU:HD23	2.03	0.40
2:B:162:SER:OG	2:B:181:HIS:O	2.22	0.40
1:A:234:ARG:HH22	2:B:365:LYS:NZ	2.20	0.40
3:C:71:TRP:CD1	3:C:86:HIS:CD2	3.09	0.40
1:A:102:LYS:HE3	1:A:122:TYR:HE1	1.87	0.40
1:A:1172:VAL:HG22	1:A:1186:ILE:HG12	2.04	0.40
2:B:166:ALA:HB3	2:B:179:ALA:HB3	2.03	0.40
1:A:295:PRO:HB2	1:A:310:PHE:HZ	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PRO:HG3	1:A:516:GLN:NE2	2.36	0.40
1:A:495:GLU:HG2	1:A:495:GLU:O	2.20	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	1153/1446 (80%)	1010 (88%)	143 (12%)	0	100	100
2	B	368/413 (89%)	336 (91%)	32 (9%)	0	100	100
3	C	110/178 (62%)	92 (84%)	18 (16%)	0	100	100
All	All	1631/2037 (80%)	1438 (88%)	193 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	1032/1237 (83%)	1031 (100%)	1 (0%)	93	97
2	B	320/357 (90%)	319 (100%)	1 (0%)	92	96
3	C	97/156 (62%)	97 (100%)	0	100	100
All	All	1449/1750 (83%)	1447 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	901	PHE
2	B	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	85	GLN
1	A	202	ASN
1	A	225	GLN
1	A	291	GLN
1	A	315	GLN
1	A	572	HIS
1	A	1237	GLN
1	A	1307	HIS
2	B	69	ASN
2	B	194	ASN
2	B	343	HIS
2	B	405	ASN
3	C	86	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	7/10 (70%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	2	A
4	D	7	G

There are no RNA pucker outliers to report.

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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

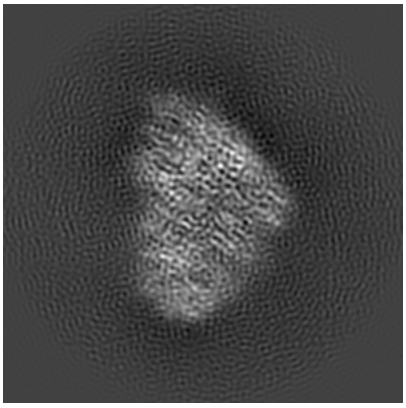
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4225. These allow visual inspection of the internal detail of the map and identification of artifacts.

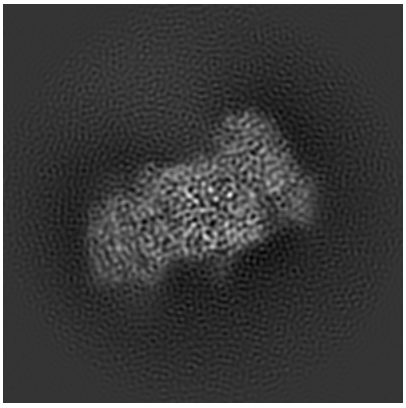
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

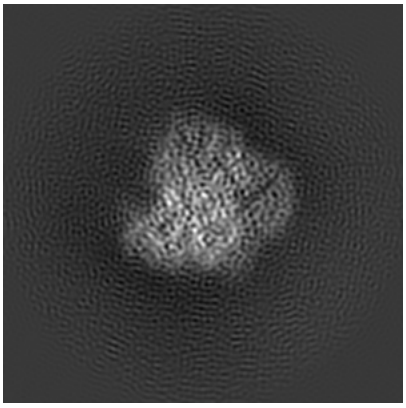
6.1.1 Primary map



X



Y

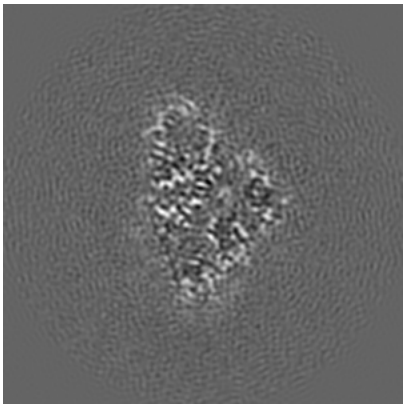


Z

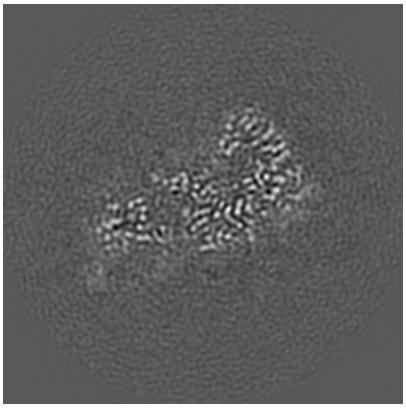
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

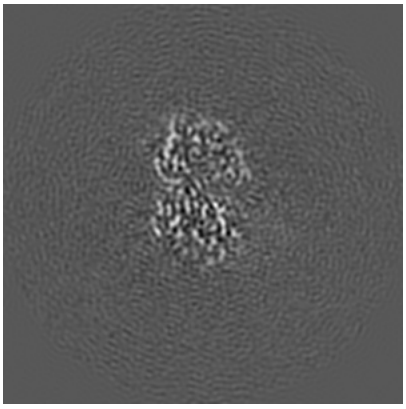
6.2.1 Primary map



X Index: 100



Y Index: 100

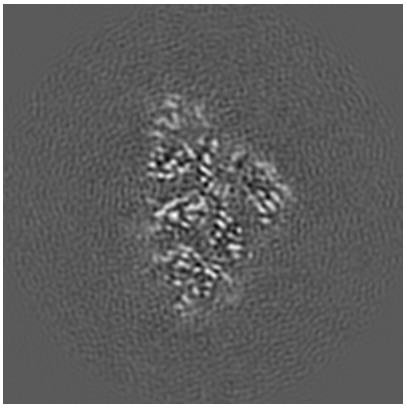


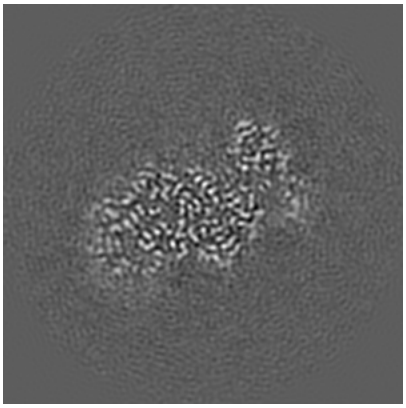
Z Index: 100

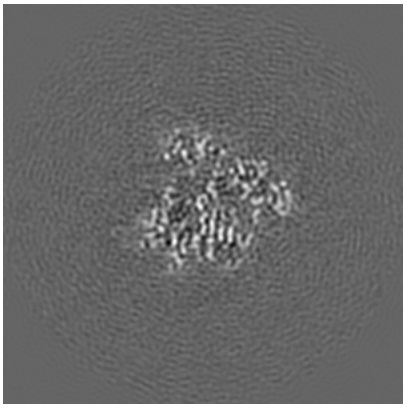
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 96

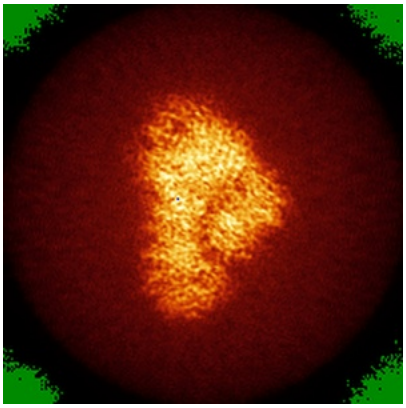

Y Index: 91

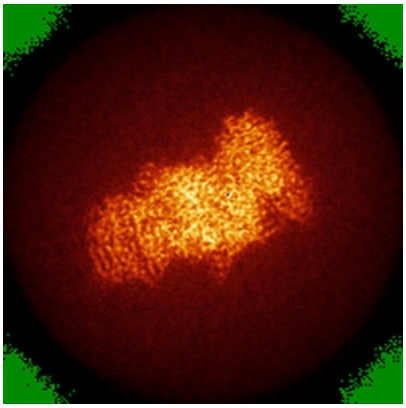

Z Index: 113

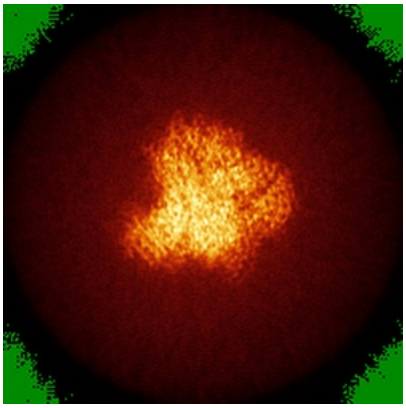
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.058. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

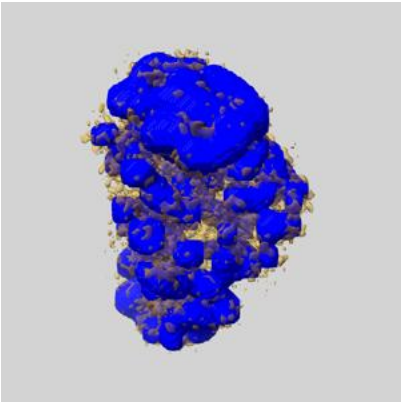
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

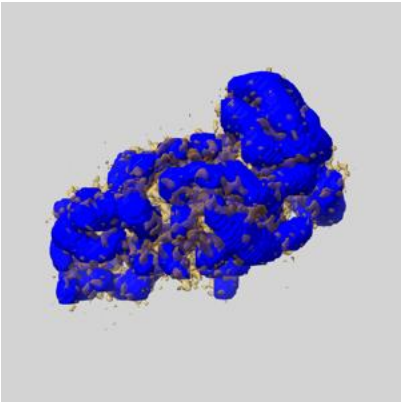
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

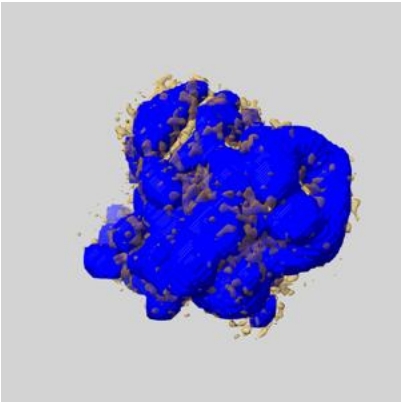
6.6.1 emd_4225_msk_1.map (i)



X



Y

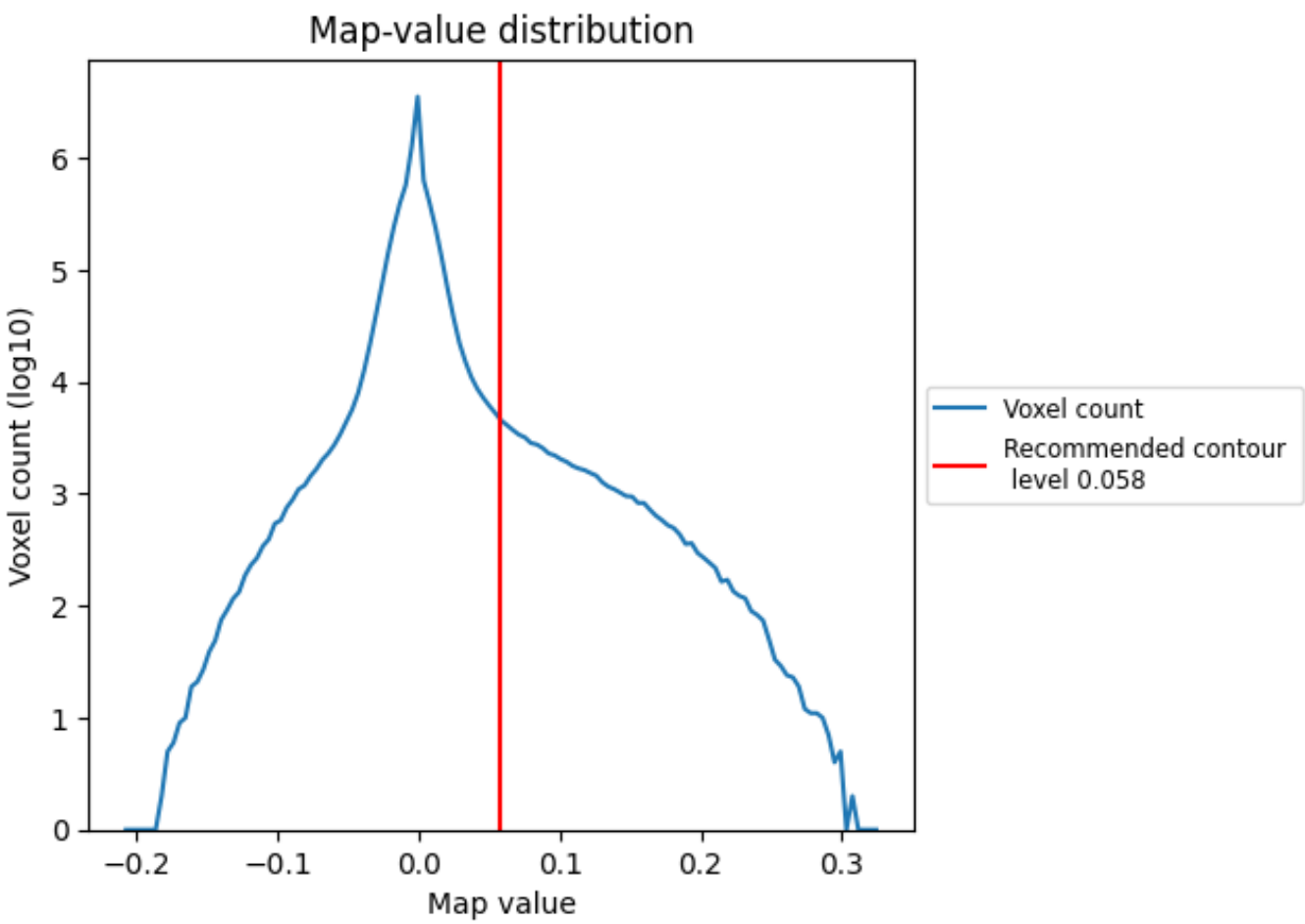


Z

7 Map analysis (i)

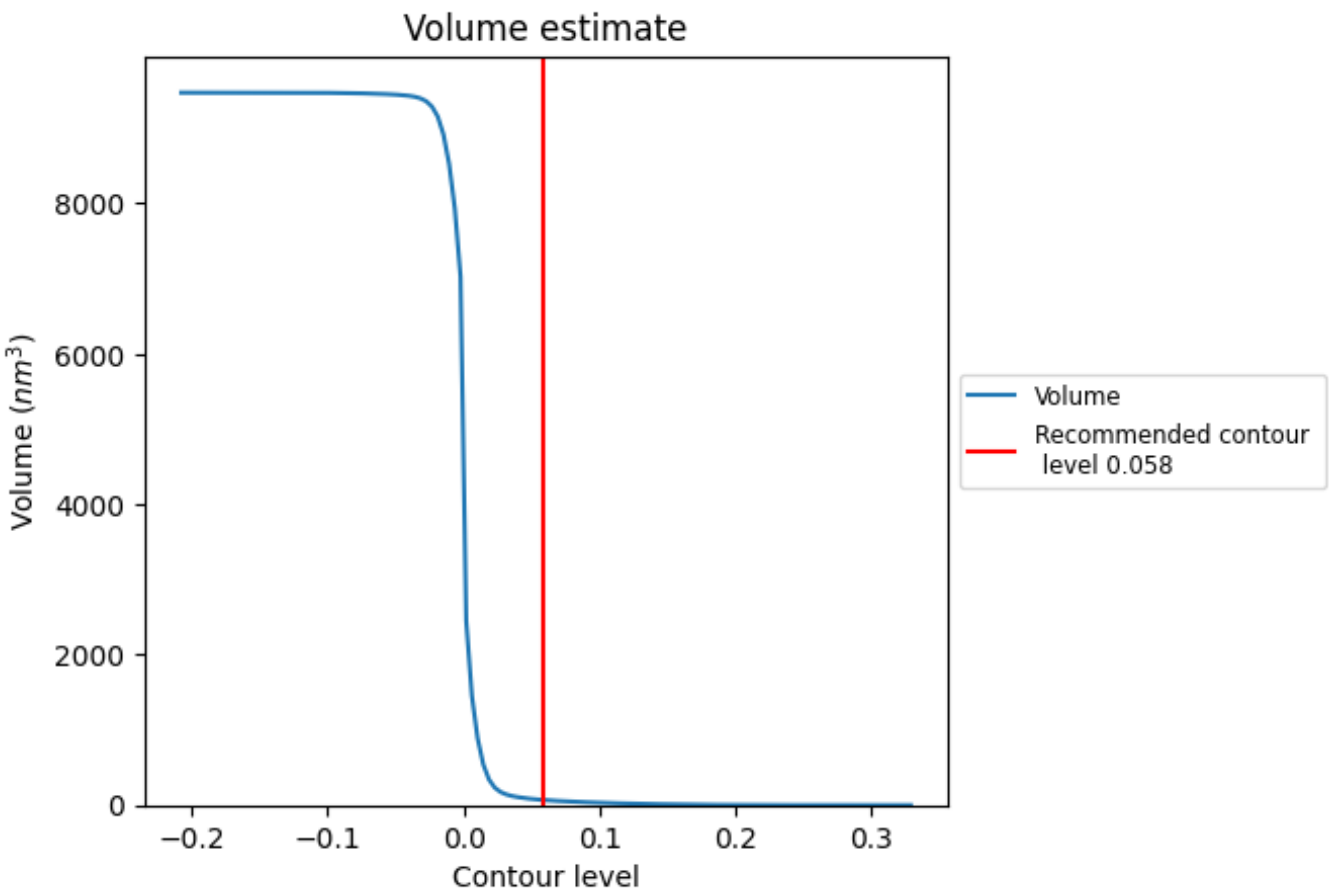
This section contains the results of statistical analysis of the map.

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.

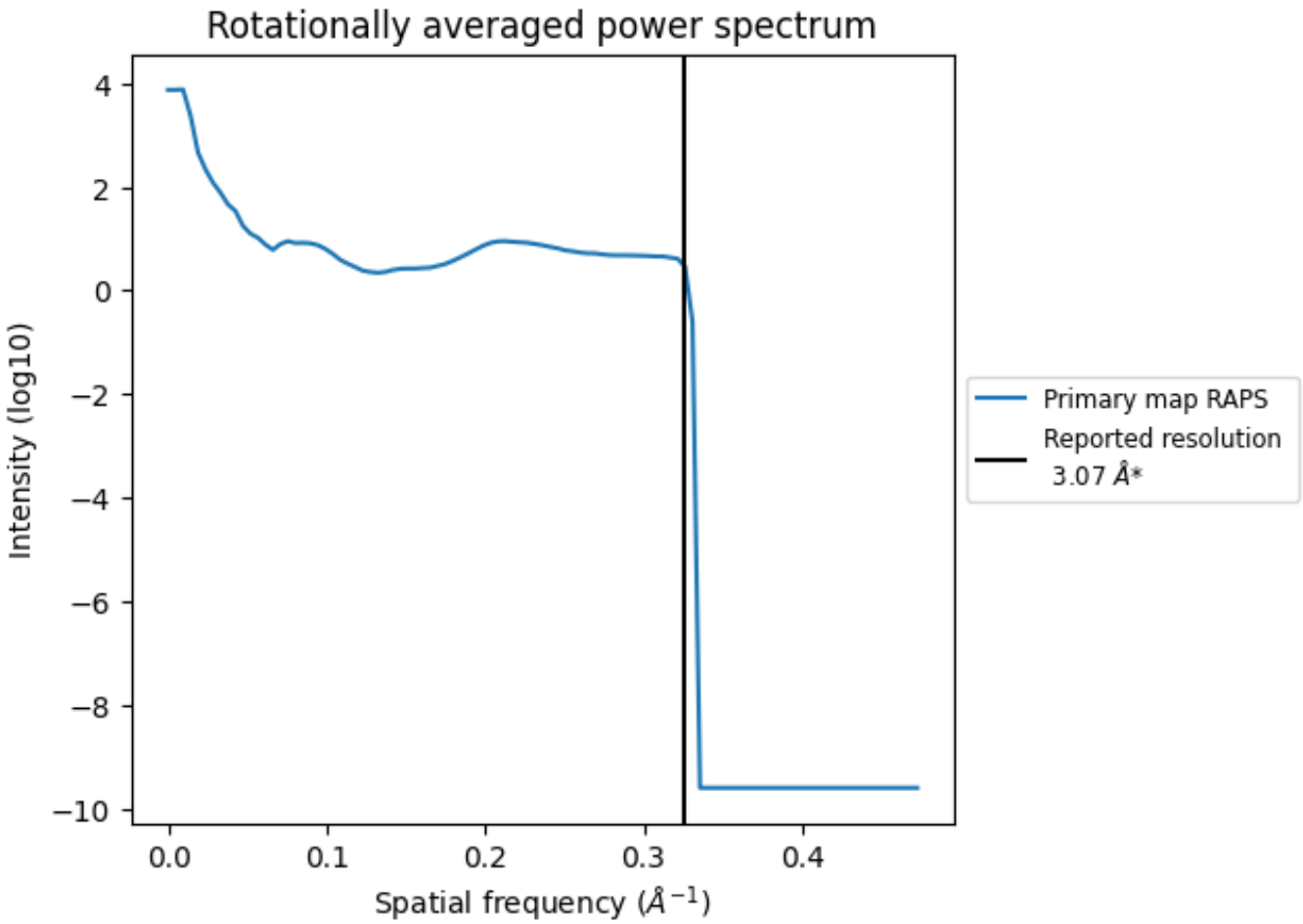
7.2 Volume estimate (i)



The volume at the recommended contour level is 70 nm^3; this corresponds to an approximate mass of 63 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)

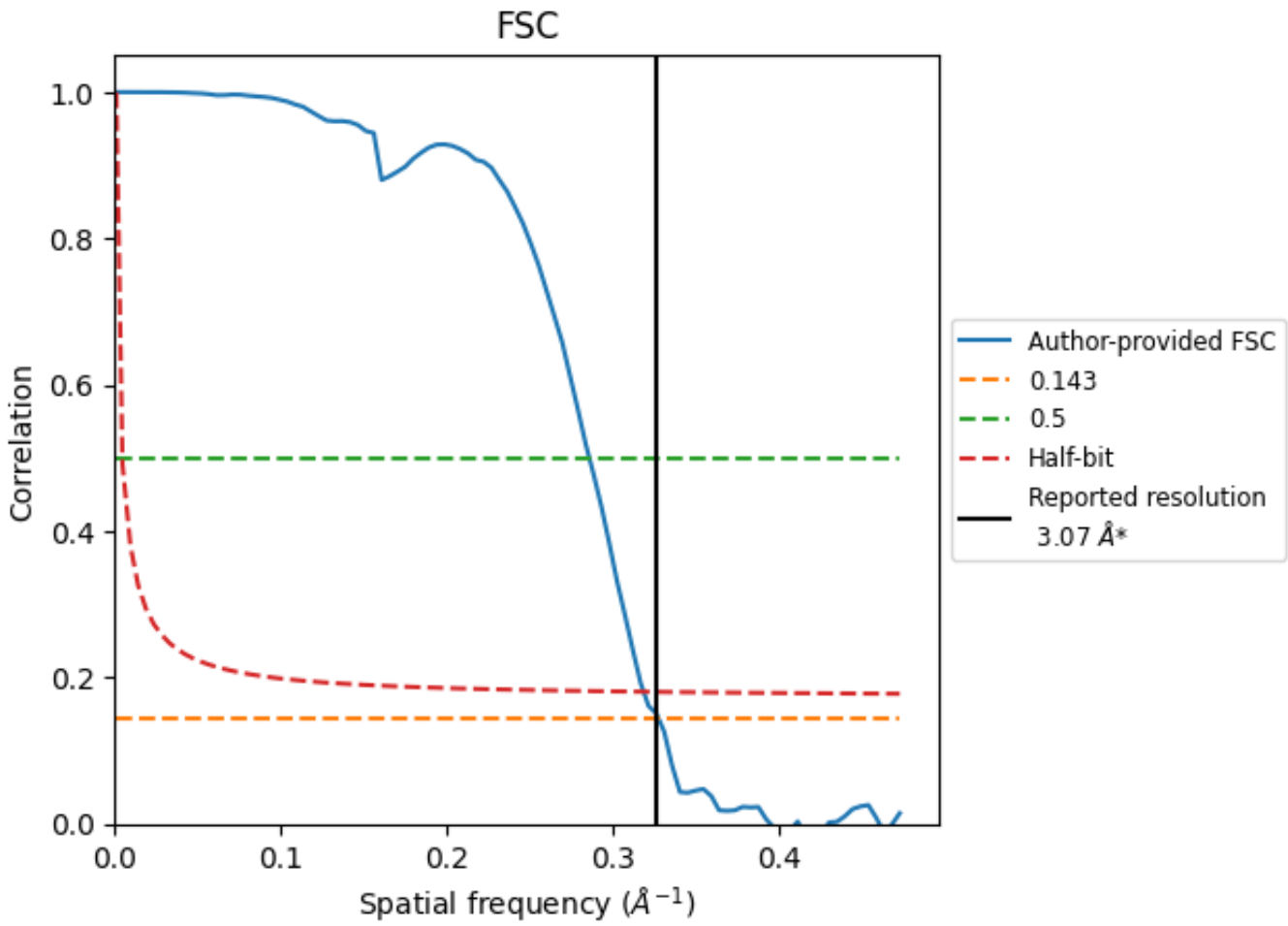


*Reported resolution corresponds to spatial frequency of 0.326 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.326 Å^{-1}

8.2 Resolution estimates (i)

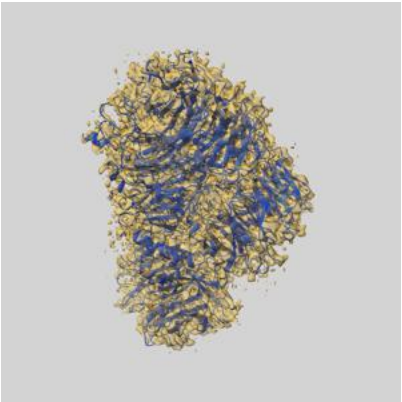
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.07	-	-
Author-provided FSC curve	3.05	3.50	3.14
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

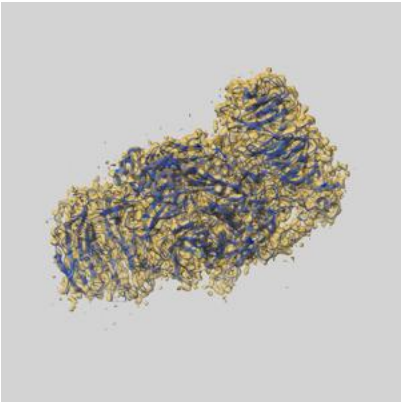
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4225 and PDB model 6FUW. Per-residue inclusion information can be found in section 3 on page 5.

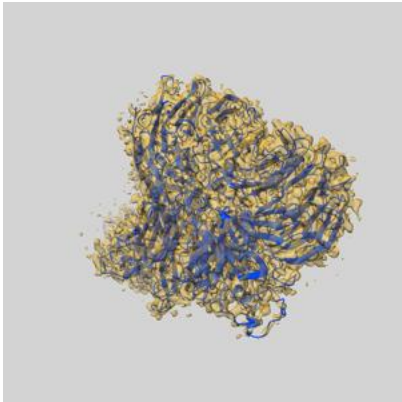
9.1 Map-model overlay (i)



X



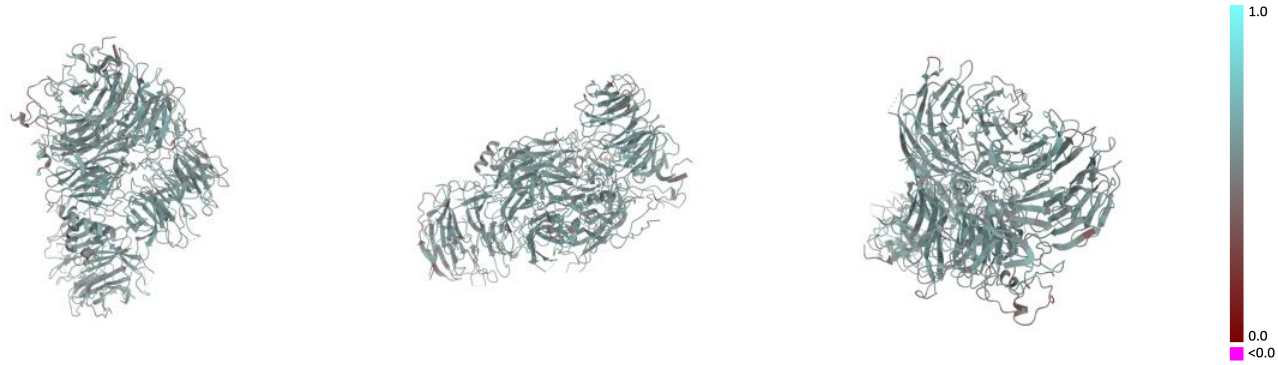
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.058 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.

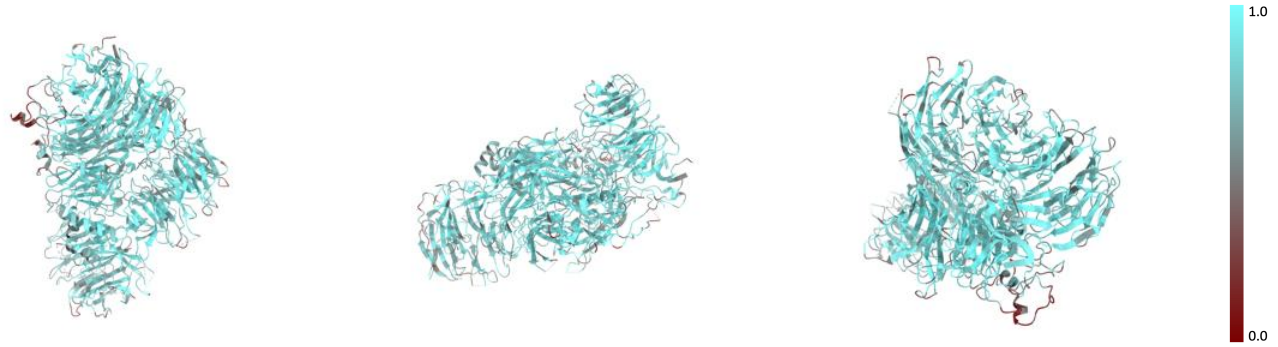
9.2 Q-score mapped to coordinate model (i)



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.

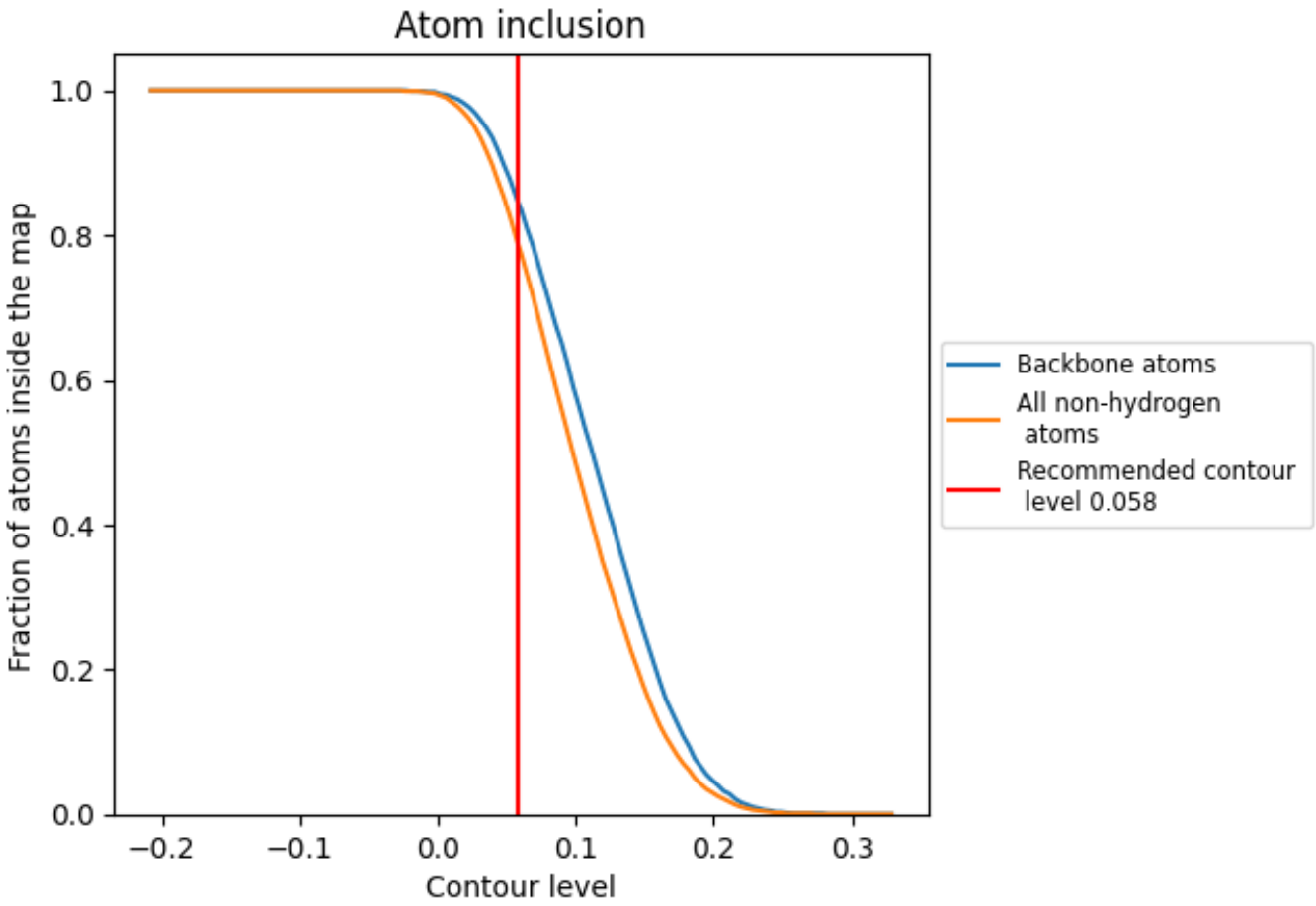
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.058).

9.4 Atom inclusion (i)



At the recommended contour level, 85% 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 (0.058) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7880	0.5560
A	0.7950	0.5590
B	0.8240	0.5630
C	0.5960	0.5040
D	0.7840	0.5340