Full wwPDB EM Validation Report ⓘ

Jul 9, 2022 – 07:23 am BST

PDB ID	:	7ZGR
EMDB ID	:	EMD-14712
Title	:	Polymerase module of yeast CPF in complex with Mpe1, the yPIM of Cft2 and the pre-cleaved CYC1 RNA
Authors	:	Rodriguez-Molina, J.B.; Passmore, L.A.
Deposited on	:	2022-04-04
Resolution	:	2.60 Å(reported)
Based on initial models	:	7ZGP, 1ZGQ

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:

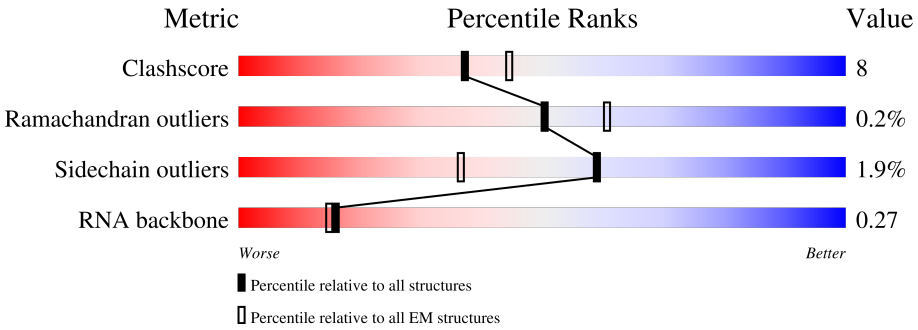
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.60 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	1357	72% 19% • 8%
2	B	208	38% 7% 55%
3	C	720	• • 96%
4	D	465	66% 18% 15%
5	E	42	7% • 90%
6	F	441	7% • 90%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14505 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 Protein CFT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1254	9888	6325	1655	1868	40	0	0

- Molecule 2 is a protein called mRNA 3'-end-processing protein YTH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	94	776	501	136	132	7	0	0

- Molecule 3 is a protein called Cleavage factor two protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	30	236	157	36	41	2	0	0

- Molecule 4 is a protein called Polyadenylation factor subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	395	3164	2008	552	584	20	0	0

- Molecule 5 is a RNA chain called pre-cleaved CYC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	4	65	29	12	21	3	0	0

- Molecule 6 is a protein called MPE1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	46	374	234	67	72	1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

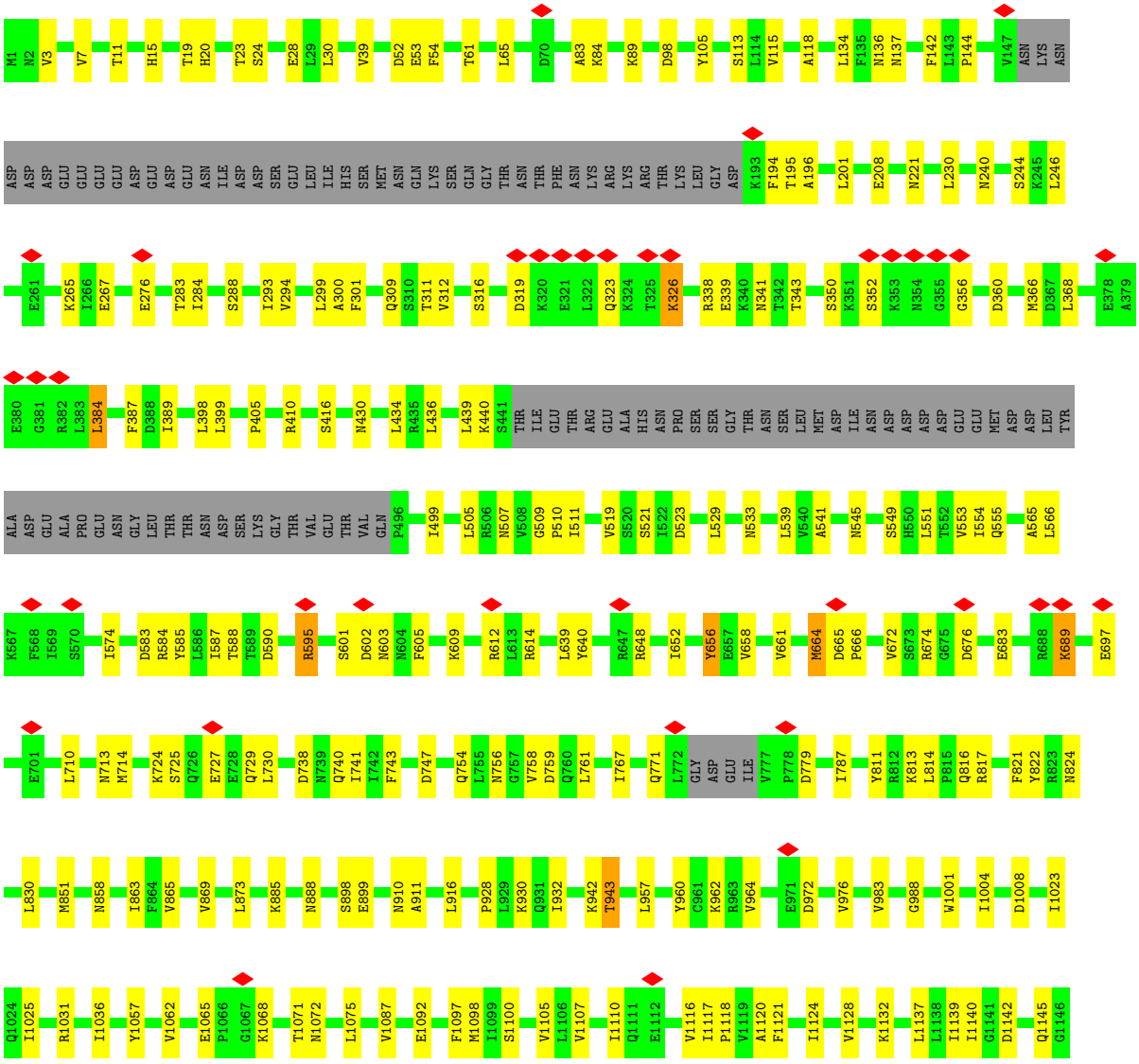
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	B	2	2	2	0

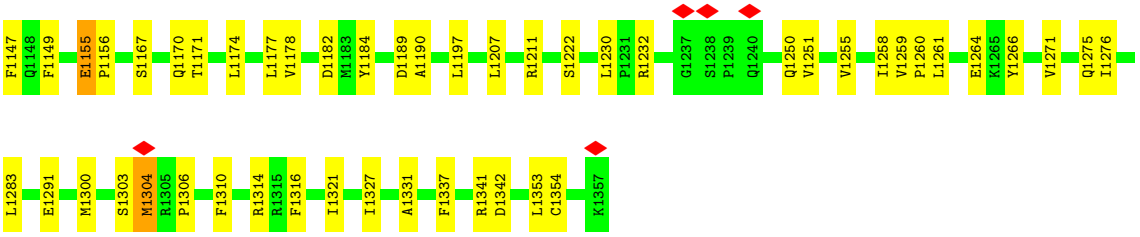
3 Residue-property plots (i)

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: Protein CFT1

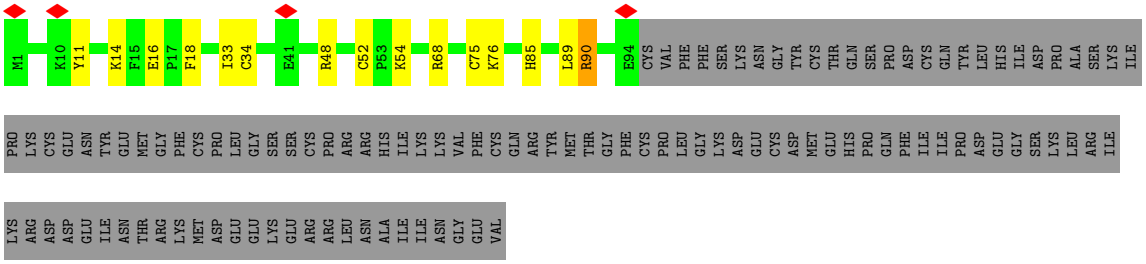
Chain A:





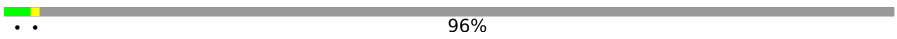
• Molecule 2: mRNA 3'-end-processing protein YTH1

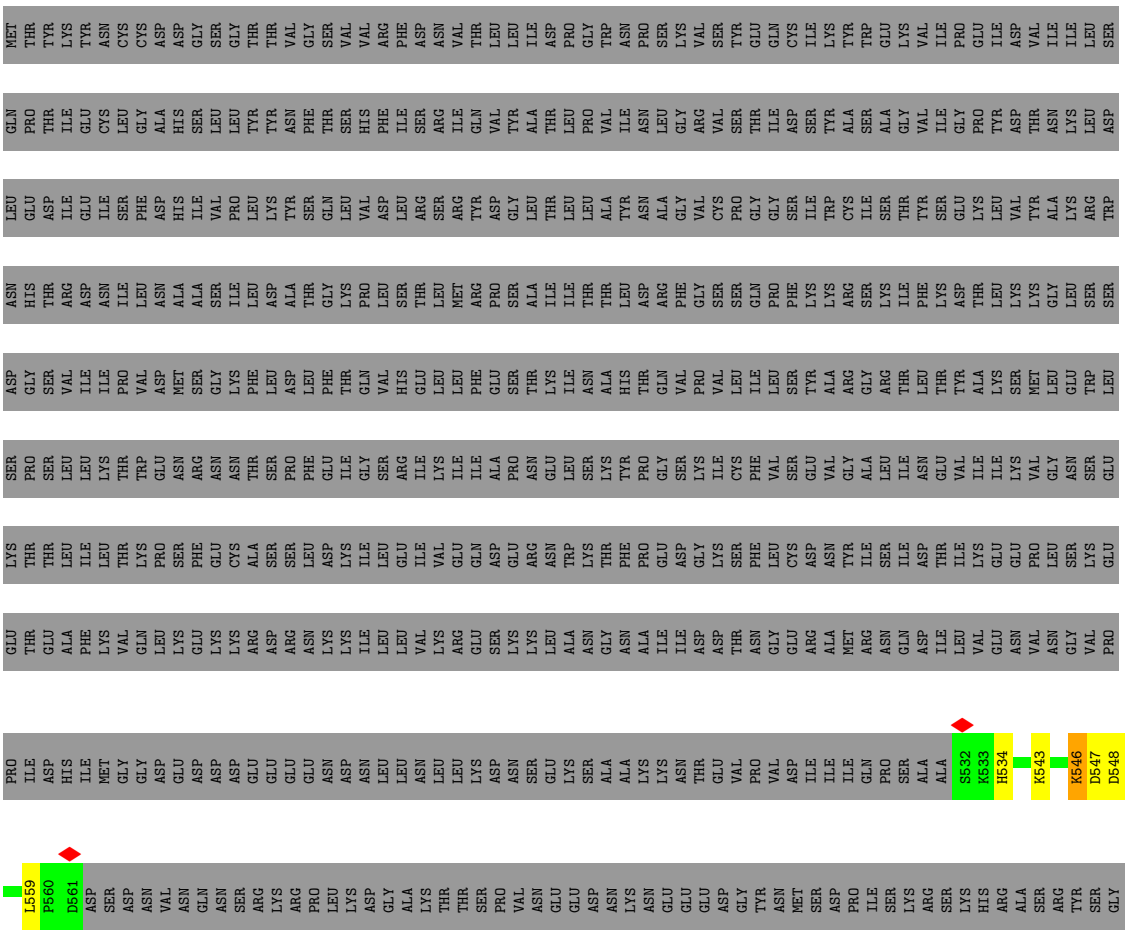
Chain B:

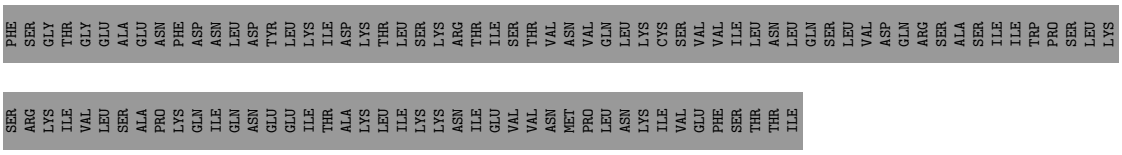


• Molecule 3: Cleavage factor two protein 2

Chain C:

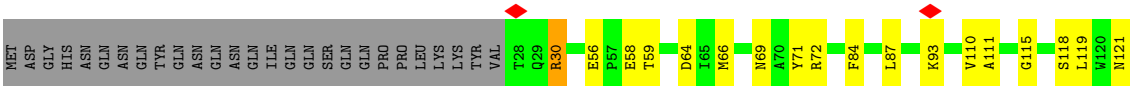


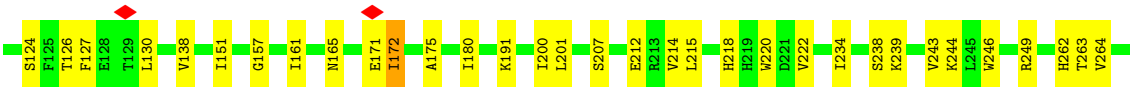


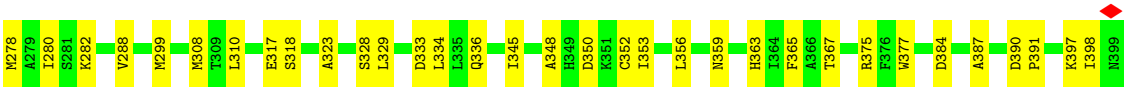


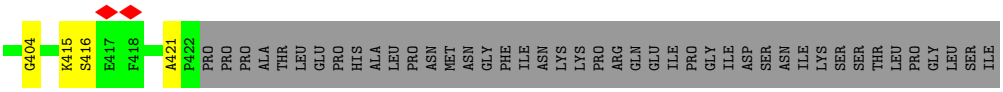
• Molecule 4: Polyadenylation factor subunit 2

Chain D:







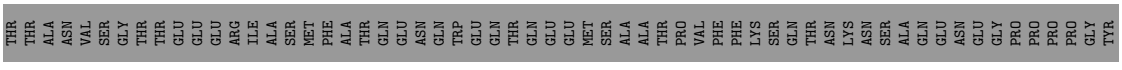


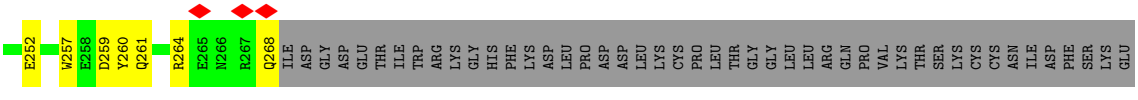
• Molecule 5: pre-cleaved CYC1

Chain E:

• Molecule 6: MPE1 isoform 1

Chain F:





MET LYS LEU MET ASP PRO THR GLY THR ALA GLY LEU ASN ASN THR SER LEU PRO THR SER VAL ASN ASN GLY GLY THR PRO VAL PRO PRO VAL PRO LEU PRO PHE GLY ILE PRO PRO PHE PRO MET PHE PRO MET PRO PHE MET PRO PRO THR ALA THR ILE THR ASN PRO HIS GLN

ALA ASP ALA SER PRO LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	846349	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

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	0.27	0/10082	0.49	0/13667
2	B	0.26	0/803	0.46	0/1087
3	C	0.29	0/244	0.55	0/330
4	D	0.28	0/3251	0.50	0/4413
5	E	0.18	0/72	0.63	0/111
6	F	0.27	0/378	0.55	0/505
All	All	0.27	0/14830	0.49	0/20113

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	9888	0	9912	169	0
2	B	776	0	746	11	0
3	C	236	0	220	4	0
4	D	3164	0	3059	55	0
5	E	65	0	33	1	0
6	F	374	0	356	10	0
7	B	2	0	0	0	0
All	All	14505	0	14326	236	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 8.

All (236) 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)
4:D:318:SER:HB2	4:D:334:LEU:HB2	1.64	0.80
1:A:366:MET:HG2	1:A:405:PRO:HG2	1.67	0.75
1:A:1124:ILE:HD13	1:A:1128:VAL:HG23	1.69	0.74
1:A:1264:GLU:OE1	1:A:1264:GLU:N	2.18	0.74
1:A:19:THR:HB	1:A:65:LEU:HD21	1.68	0.73
1:A:54:PHE:HB3	1:A:1283:LEU:HD21	1.75	0.69
1:A:84:LYS:NZ	1:A:1291:GLU:OE2	2.25	0.69
1:A:683:GLU:HB2	1:A:689:LYS:HB2	1.75	0.68
1:A:697:GLU:OE1	1:A:697:GLU:N	2.21	0.67
1:A:1232:ARG:NH1	1:A:1260:PRO:O	2.27	0.67
1:A:343:THR:HG21	1:A:405:PRO:HB2	1.76	0.67
1:A:1276:ILE:HD11	1:A:1316:PHE:HB2	1.77	0.65
4:D:384:ASP:HB3	4:D:387:ALA:HB2	1.78	0.65
1:A:574:ILE:HG22	1:A:588:THR:HG22	1.78	0.65
1:A:1271:VAL:HG21	1:A:1331:ALA:HB3	1.77	0.64
1:A:430:ASN:HA	1:A:507:ASN:HB3	1.79	0.64
1:A:1118:PRO:HG2	2:B:89:LEU:HD21	1.78	0.64
1:A:1304:MET:SD	1:A:1304:MET:N	2.67	0.63
1:A:384:LEU:HD21	1:A:387:PHE:HB2	1.78	0.63
1:A:1155:GLU:HB2	1:A:1156:PRO:HD2	1.80	0.63
1:A:519:VAL:HG13	1:A:1001:TRP:HZ2	1.63	0.63
4:D:278:MET:HB2	4:D:288:VAL:HG22	1.81	0.63
4:D:333:ASP:HB3	4:D:336:GLN:HB2	1.81	0.62
2:B:75:CYS:O	4:D:165:ASN:ND2	2.32	0.62
1:A:566:LEU:HB2	1:A:911:ALA:HB3	1.80	0.62
1:A:553:VAL:HB	1:A:930:LYS:HB3	1.81	0.62
4:D:234:ILE:HB	4:D:246:TRP:HB2	1.81	0.62
1:A:1232:ARG:HD2	1:A:1259:VAL:HG13	1.82	0.61
1:A:888:ASN:ND2	1:A:1354:CYS:O	2.32	0.61
1:A:511:ILE:HG23	1:A:541:ALA:HB1	1.83	0.61
1:A:316:SER:HB2	1:A:983:VAL:HG23	1.83	0.60
1:A:300:ALA:HA	1:A:311:THR:HG22	1.82	0.60
4:D:110:VAL:HB	4:D:118:SER:HB2	1.82	0.60
1:A:761:LEU:HD12	1:A:1321:ILE:HD11	1.83	0.60
1:A:11:THR:HB	1:A:507:ASN:HA	1.84	0.59
1:A:1023:ILE:HG21	1:A:1110:ILE:HD12	1.85	0.59
2:B:34:CYS:HA	2:B:54:LYS:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ILE:HD12	2:B:33:ILE:H	1.68	0.58
1:A:230:LEU:HB2	1:A:284:ILE:HD11	1.85	0.58
1:A:583:ASP:O	1:A:601:SER:OG	2.22	0.58
1:A:144:PRO:HB2	1:A:196:ALA:HB3	1.85	0.58
1:A:1117:ILE:HD12	2:B:90:ARG:HH22	1.69	0.57
1:A:676:ASP:N	1:A:676:ASP:OD1	2.34	0.57
1:A:727:GLU:O	1:A:729:GLN:NE2	2.37	0.57
1:A:23:THR:HG22	1:A:28:GLU:OE2	2.03	0.57
1:A:976:VAL:HB	4:D:59:THR:HG21	1.85	0.57
1:A:740:GLN:OE1	1:A:754:GLN:NE2	2.37	0.57
4:D:280:ILE:HG23	4:D:310:LEU:HD23	1.86	0.57
4:D:323:ALA:HB2	4:D:356:LEU:HD21	1.87	0.57
1:A:434:LEU:HD13	1:A:499:ILE:HD11	1.86	0.56
1:A:656:TYR:CZ	1:A:674:ARG:HD3	2.41	0.56
1:A:1266:TYR:OH	1:A:1306:PRO:O	2.21	0.56
1:A:713:ASN:ND2	1:A:725:SER:O	2.26	0.56
1:A:1107:VAL:HB	1:A:1120:ALA:HB3	1.87	0.55
1:A:1065:GLU:OE2	1:A:1068:LYS:NZ	2.29	0.55
4:D:329:LEU:HD11	4:D:367:THR:HG21	1.88	0.55
1:A:664:MET:HG2	1:A:730:LEU:HD11	1.89	0.54
4:D:69:ASN:O	4:D:72:ARG:NH1	2.41	0.54
1:A:1025:ILE:HD11	1:A:1031:ARG:HD2	1.88	0.54
4:D:263:THR:CG2	4:D:282:LYS:HE2	2.38	0.54
4:D:130:LEU:HB2	6:F:212:THR:HG21	1.89	0.54
1:A:658:VAL:HA	1:A:672:VAL:HA	1.89	0.54
1:A:311:THR:HG23	1:A:326:LYS:HE3	1.90	0.53
1:A:858:ASN:ND2	1:A:916:LEU:O	2.39	0.53
3:C:547:ASP:OD2	4:D:249:ARG:NE	2.29	0.53
1:A:1098:MET:HB2	1:A:1107:VAL:HG22	1.91	0.53
1:A:713:ASN:OD1	1:A:813:LYS:NZ	2.42	0.52
1:A:555:GLN:HB2	1:A:928:PRO:HG2	1.91	0.52
4:D:115:GLY:HA2	4:D:138:VAL:HG23	1.91	0.52
4:D:415:LYS:NZ	4:D:416:SER:O	2.38	0.52
1:A:83:ALA:HB1	1:A:105:TYR:HB2	1.91	0.52
1:A:1310:PHE:O	1:A:1314:ARG:HG3	2.10	0.52
1:A:1110:ILE:HG12	1:A:1116:VAL:HG22	1.91	0.52
1:A:957:LEU:HD22	1:A:1036:ILE:HG21	1.92	0.52
4:D:218:HIS:CE1	4:D:238:SER:HG	2.27	0.52
1:A:747:ASP:OD1	1:A:747:ASP:N	2.40	0.52
1:A:738:ASP:OD1	1:A:738:ASP:N	2.40	0.51
4:D:398:ILE:O	4:D:398:ILE:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:257:TRP:O	6:F:261:GLN:HG2	2.10	0.51
1:A:221:ASN:ND2	1:A:288:SER:O	2.41	0.51
1:A:338:ARG:NH2	4:D:64:ASP:OD2	2.28	0.51
4:D:390:ASP:OD1	4:D:391:PRO:HD2	2.11	0.51
4:D:151:ILE:HG22	4:D:161:ILE:HG12	1.92	0.51
1:A:584:ARG:HG2	1:A:602:ASP:OD2	2.12	0.50
1:A:614:ARG:NH1	1:A:640:TYR:OH	2.44	0.50
1:A:942:LYS:HG2	1:A:962:LYS:HG2	1.94	0.50
1:A:1036:ILE:HB	1:A:1057:TYR:HB2	1.92	0.50
4:D:200:ILE:HG23	4:D:214:VAL:HG13	1.93	0.50
1:A:240:ASN:O	1:A:244:SER:OG	2.30	0.50
1:A:39:VAL:HB	1:A:52:ASP:OD1	2.11	0.50
1:A:265:LYS:NZ	1:A:267:GLU:OE1	2.45	0.50
1:A:343:THR:HG23	1:A:366:MET:HB3	1.93	0.50
1:A:410:ARG:NH2	1:A:416:SER:O	2.44	0.50
4:D:348:ALA:O	4:D:375:ARG:NH1	2.45	0.49
6:F:260:TYR:O	6:F:264:ARG:HG3	2.12	0.49
1:A:118:ALA:N	1:A:136:ASN:OD1	2.43	0.49
1:A:246:LEU:HD13	1:A:276:GLU:HB3	1.93	0.49
4:D:157:GLY:HA2	4:D:180:ILE:HG12	1.94	0.49
1:A:863:ILE:HB	1:A:873:LEU:HB2	1.93	0.49
1:A:811:TYR:HB3	1:A:821:PHE:HB3	1.95	0.49
1:A:743:PHE:HZ	1:A:767:ILE:HD12	1.77	0.49
1:A:326:LYS:HD3	1:A:326:LYS:N	2.28	0.49
1:A:710:LEU:HD11	1:A:787:ILE:HB	1.95	0.49
1:A:1105:VAL:HG11	1:A:1140:ILE:HD13	1.95	0.49
1:A:1222:SER:OG	1:A:1250:GLN:HB3	2.13	0.49
4:D:262:HIS:ND1	4:D:263:THR:HG22	2.28	0.49
2:B:76:LYS:HD2	5:E:2:A:C2	2.48	0.48
4:D:262:HIS:ND1	4:D:282:LYS:HB3	2.28	0.48
3:C:546:LYS:HG3	3:C:546:LYS:O	2.14	0.48
1:A:584:ARG:NH2	1:A:585:TYR:OH	2.46	0.48
4:D:119:LEU:O	4:D:127:PHE:HB3	2.13	0.48
1:A:551:LEU:HB2	1:A:932:ILE:HB	1.94	0.48
1:A:590:ASP:N	1:A:595:ARG:O	2.46	0.48
1:A:851:MET:HG2	1:A:865:VAL:HG22	1.95	0.48
1:A:964:VAL:O	1:A:988:GLY:N	2.36	0.48
1:A:957:LEU:HD21	1:A:1075:LEU:HD21	1.95	0.47
2:B:75:CYS:SG	2:B:85:HIS:CE1	3.07	0.47
1:A:1087:VAL:HA	1:A:1100:SER:O	2.14	0.47
1:A:352:SER:HB3	1:A:356:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:TYR:O	1:A:587:ILE:HD12	2.14	0.47
1:A:1337:PHE:CE2	1:A:1341:ARG:HD2	2.50	0.47
2:B:48:ARG:NE	2:B:52:CYS:SG	2.83	0.47
1:A:612:ARG:HG3	1:A:612:ARG:HH11	1.80	0.47
1:A:1092:GLU:HA	1:A:1097:PHE:HA	1.97	0.47
4:D:111:ALA:HB1	4:D:138:VAL:HB	1.96	0.47
4:D:220:TRP:HB3	4:D:239:LYS:HB2	1.97	0.47
1:A:83:ALA:HA	1:A:134:LEU:HD21	1.97	0.47
1:A:293:ILE:HB	1:A:300:ALA:HB3	1.97	0.47
4:D:328:SER:HA	4:D:345:ILE:O	2.15	0.47
4:D:365:PHE:HB3	4:D:377:TRP:HB2	1.97	0.47
1:A:1167:SER:HB3	1:A:1300:MET:HE1	1.97	0.46
1:A:771:GLN:N	1:A:771:GLN:OE1	2.49	0.46
4:D:359:ASN:HD22	4:D:363:HIS:CE1	2.33	0.46
1:A:15:HIS:NE2	1:A:61:THR:O	2.49	0.46
4:D:121:ASN:ND2	4:D:126:THR:O	2.47	0.46
4:D:404:GLY:H	4:D:421:ALA:CB	2.29	0.46
1:A:208:GLU:H	1:A:208:GLU:CD	2.19	0.45
1:A:339:GLU:HB3	1:A:368:LEU:HD11	1.98	0.45
1:A:529:LEU:HD13	1:A:910:ASN:HB3	1.98	0.45
1:A:1178:VAL:HG11	2:B:11:TYR:CZ	2.52	0.45
4:D:308:MET:HG3	4:D:352:CYS:SG	2.57	0.45
1:A:1004:ILE:HD12	1:A:1071:THR:HG22	1.97	0.45
1:A:1207:LEU:HB2	1:A:1211:ARG:CZ	2.46	0.45
1:A:23:THR:N	1:A:28:GLU:OE2	2.49	0.45
1:A:20:HIS:ND1	1:A:24:SER:HA	2.32	0.45
1:A:830:LEU:O	1:A:1314:ARG:NH2	2.48	0.45
4:D:30:ARG:HD2	4:D:124:SER:HB2	1.98	0.45
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.84	0.45
4:D:84:PHE:HZ	4:D:87:LEU:HB2	1.81	0.45
1:A:436:LEU:HD23	1:A:439:LEU:HD21	1.98	0.45
4:D:243:VAL:HG23	4:D:264:VAL:HG21	1.99	0.45
1:A:510:PRO:HG3	1:A:545:ASN:ND2	2.32	0.45
1:A:972:ASP:OD1	1:A:972:ASP:N	2.50	0.45
1:A:323:GLN:HG2	1:A:326:LYS:NZ	2.31	0.44
1:A:603:ASN:OD1	1:A:603:ASN:N	2.50	0.44
4:D:222:VAL:HA	4:D:238:SER:HA	1.98	0.44
1:A:283:THR:HB	1:A:294:VAL:HB	2.00	0.44
2:B:18:PHE:HE1	6:F:268:GLN:HA	1.81	0.44
4:D:218:HIS:NE2	4:D:244:LYS:HB2	2.33	0.44
4:D:323:ALA:HB1	4:D:353:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:SER:CB	1:A:943:THR:HA	2.48	0.44
1:A:639:LEU:HB3	1:A:652:ILE:HB	1.98	0.44
1:A:350:SER:OG	1:A:360:ASP:OD2	2.34	0.44
1:A:113:SER:OG	1:A:115:VAL:O	2.26	0.43
4:D:350:ASP:OD1	4:D:397:LYS:NZ	2.46	0.43
1:A:724:LYS:HE3	1:A:724:LYS:HB2	1.89	0.43
1:A:1177:LEU:HD11	1:A:1258:ILE:HG21	2.00	0.43
1:A:399:LEU:HD21	1:A:434:LEU:HD11	2.00	0.43
1:A:869:VAL:HG13	1:A:885:LYS:HE2	2.01	0.43
1:A:1155:GLU:HB2	1:A:1156:PRO:CD	2.48	0.43
1:A:1147:PHE:HE1	1:A:1197:LEU:HD13	1.83	0.43
4:D:171:GLU:HB2	6:F:252:GLU:OE1	2.17	0.43
4:D:218:HIS:CD2	4:D:246:TRP:HZ2	2.37	0.43
1:A:741:ILE:HD12	1:A:758:VAL:HG21	1.99	0.42
1:A:858:ASN:HB2	1:A:916:LEU:HB3	2.01	0.42
1:A:529:LEU:HD12	1:A:565:ALA:HB1	2.01	0.42
4:D:404:GLY:H	4:D:421:ALA:HB1	1.84	0.42
1:A:7:VAL:N	1:A:1255:VAL:O	2.53	0.42
1:A:519:VAL:HG11	1:A:553:VAL:HG21	2.02	0.42
1:A:566:LEU:HD11	1:A:605:PHE:CD2	2.54	0.42
1:A:779:ASP:N	1:A:779:ASP:OD1	2.52	0.42
1:A:898:SER:OG	1:A:899:GLU:N	2.51	0.42
1:A:1142:ASP:O	1:A:1171:THR:HG22	2.20	0.42
6:F:260:TYR:CZ	6:F:264:ARG:HD2	2.54	0.42
1:A:612:ARG:O	1:A:648:ARG:NH2	2.43	0.42
1:A:1142:ASP:OD2	1:A:1145:GLN:N	2.50	0.42
4:D:191:LYS:NZ	4:D:212:GLU:OE2	2.40	0.42
1:A:519:VAL:HG13	1:A:1001:TRP:CZ2	2.49	0.42
1:A:1137:LEU:HD13	1:A:1149:PHE:HZ	1.85	0.42
4:D:207:SER:OG	6:F:264:ARG:NE	2.53	0.42
1:A:98:ASP:OD1	1:A:98:ASP:N	2.53	0.42
1:A:323:GLN:HG2	1:A:326:LYS:HZ2	1.85	0.42
1:A:639:LEU:HD22	1:A:652:ILE:HD12	2.01	0.42
1:A:1275:GLN:HB3	1:A:1327:ILE:HD12	2.02	0.42
6:F:240:MET:HG3	6:F:241:ILE:HG22	2.01	0.42
1:A:816:GLN:O	1:A:817:ARG:HG2	2.20	0.41
1:A:1139:ILE:HD12	1:A:1174:LEU:HB3	2.01	0.41
1:A:1189:ASP:OD1	1:A:1190:ALA:N	2.53	0.41
4:D:66:MET:HB2	4:D:71:TYR:CZ	2.55	0.41
4:D:93:LYS:HE2	4:D:93:LYS:HB3	1.96	0.41
1:A:814:LEU:HD11	1:A:822:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:ASP:OD1	2:B:14:LYS:HD2	2.20	0.41
1:A:759:ASP:OD1	1:A:759:ASP:N	2.50	0.41
3:C:543:LYS:HD3	3:C:543:LYS:HA	1.80	0.41
1:A:510:PRO:HA	1:A:1251:VAL:O	2.20	0.41
1:A:1132:LYS:NZ	1:A:1174:LEU:O	2.52	0.41
6:F:214:ILE:HA	6:F:215:PRO:HD3	1.90	0.41
1:A:115:VAL:HG12	4:D:317:GLU:HB2	2.02	0.41
1:A:539:LEU:HB2	1:A:554:ILE:HB	2.03	0.41
4:D:172:ILE:HG22	4:D:175:ALA:HB2	2.03	0.41
1:A:53:GLU:O	1:A:824:ASN:ND2	2.54	0.41
1:A:326:LYS:HD3	1:A:326:LYS:H	1.85	0.41
1:A:814:LEU:HB2	1:A:816:GLN:O	2.21	0.41
1:A:1230:LEU:HD11	1:A:1353:LEU:HD21	2.03	0.41
1:A:1177:LEU:O	1:A:1184:TYR:HB2	2.21	0.41
1:A:505:LEU:HD23	1:A:505:LEU:HA	1.94	0.41
1:A:1062:VAL:N	1:A:1072:ASN:O	2.51	0.41
4:D:201:LEU:HB2	4:D:215:LEU:HB2	2.03	0.41
6:F:216:LYS:HA	6:F:219:LEU:HD12	2.03	0.41
1:A:30:LEU:HD22	1:A:39:VAL:HG22	2.02	0.41
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.87	0.41
1:A:665:ASP:HB3	1:A:666:PRO:HD3	2.03	0.41
1:A:194:PHE:CD2	1:A:195:THR:HG23	2.56	0.40
1:A:1170:GLN:HG3	1:A:1190:ALA:HB3	2.03	0.40
3:C:559:LEU:HD22	3:C:559:LEU:H	1.85	0.40
1:A:3:VAL:HB	1:A:1261:LEU:HD11	2.03	0.40
1:A:960:TYR:OH	1:A:1008:ASP:OD1	2.35	0.40
1:A:312:VAL:HG11	1:A:389:ILE:HG22	2.03	0.40
4:D:56:GLU:O	4:D:58:GLU:N	2.53	0.40
1:A:142:PHE:HE2	1:A:201:LEU:HD11	1.86	0.40
1:A:294:VAL:HA	1:A:299:LEU:HD23	2.03	0.40
1:A:521:SER:HB3	1:A:533:ASN:O	2.21	0.40
1:A:89:LYS:HB3	1:A:89:LYS:HE3	1.93	0.40
1:A:301:PHE:HD2	1:A:309:GLN:HB2	1.87	0.40
1:A:507:ASN:C	1:A:509:GLY:H	2.24	0.40
4:D:278:MET:HG2	4:D:310:LEU:HD22	2.04	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	1246/1357 (92%)	1175 (94%)	70 (6%)	1 (0%)	51 75
2	B	92/208 (44%)	88 (96%)	4 (4%)	0	100 100
3	C	28/720 (4%)	25 (89%)	2 (7%)	1 (4%)	3 4
4	D	393/465 (84%)	370 (94%)	22 (6%)	1 (0%)	41 64
6	F	42/441 (10%)	37 (88%)	5 (12%)	0	100 100
All	All	1801/3191 (56%)	1695 (94%)	103 (6%)	3 (0%)	50 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1155	GLU
3	C	534	HIS
4	D	172	ILE

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	1113/1230 (90%)	1092 (98%)	21 (2%)	57 79
2	B	86/195 (44%)	83 (96%)	3 (4%)	36 62
3	C	25/654 (4%)	23 (92%)	2 (8%)	12 24
4	D	348/420 (83%)	346 (99%)	2 (1%)	86 95
6	F	39/394 (10%)	37 (95%)	2 (5%)	24 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1611/2893 (56%)	1581 (98%)	30 (2%)	59 79

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	319	ASP
1	A	326	LYS
1	A	341	ASN
1	A	384	LEU
1	A	398	LEU
1	A	440	LYS
1	A	523	ASP
1	A	595	ARG
1	A	609	LYS
1	A	656	TYR
1	A	661	VAL
1	A	664	MET
1	A	689	LYS
1	A	714	MET
1	A	756	ASN
1	A	943	THR
1	A	1121	PHE
1	A	1303	SER
1	A	1304	MET
1	A	1342	ASP
2	B	16	GLU
2	B	68	ARG
2	B	90	ARG
3	C	546	LYS
3	C	548	ASP
4	D	30	ARG
4	D	299	MET
6	F	207	ARG
6	F	259	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	740	GLN
1	A	754	GLN

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Mol	Chain	Res	Type
1	A	1250	GLN
4	D	363	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	E	2/42 (4%)	0	0

There are no RNA backbone outliers to report.

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 2 ligands modelled in this entry, 2 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.

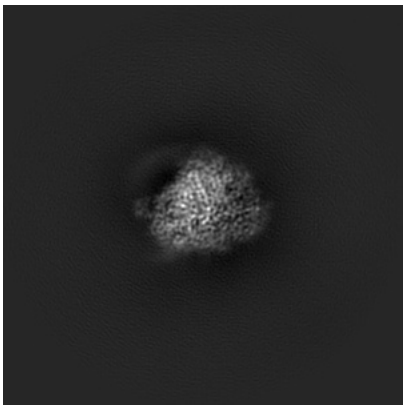
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14712. These allow visual inspection of the internal detail of the map and identification of artifacts.

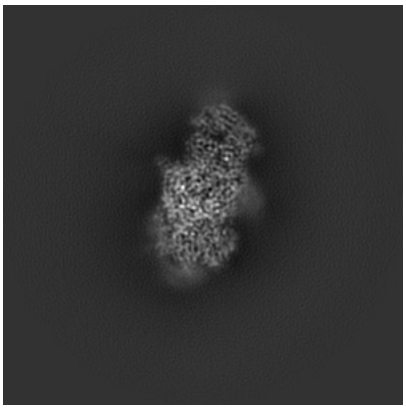
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

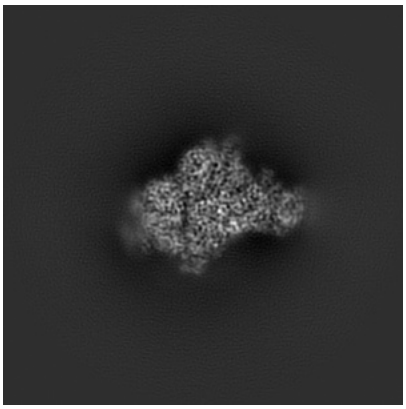
6.1.1 Primary map



X

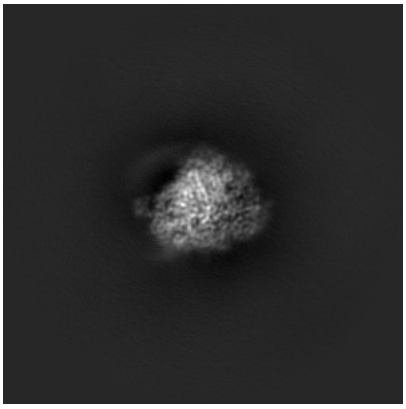


Y

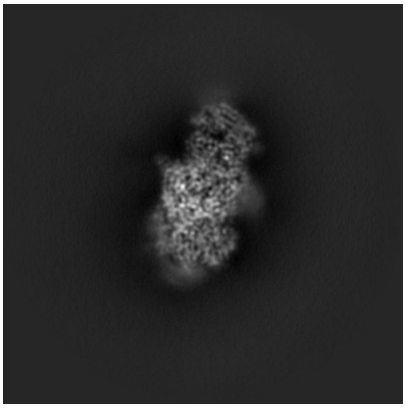


Z

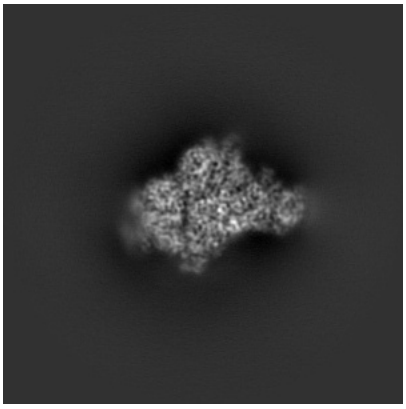
6.1.2 Raw map



X



Y

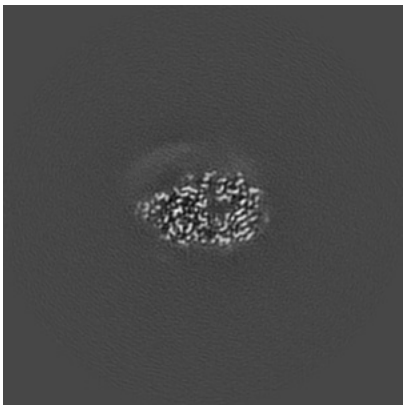


Z

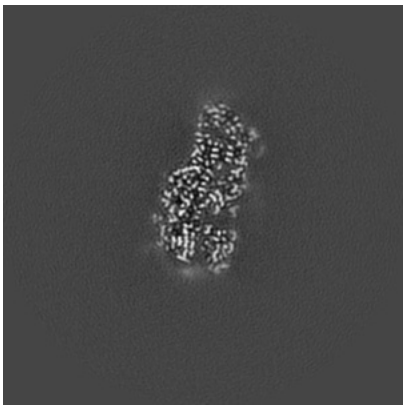
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

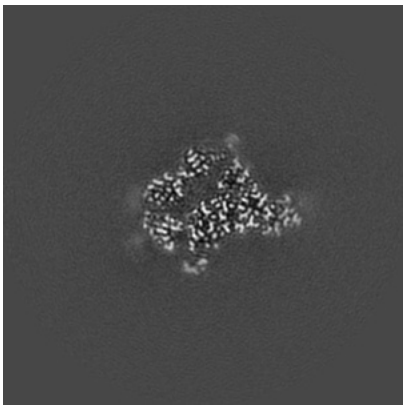
6.2.1 Primary map



X Index: 180

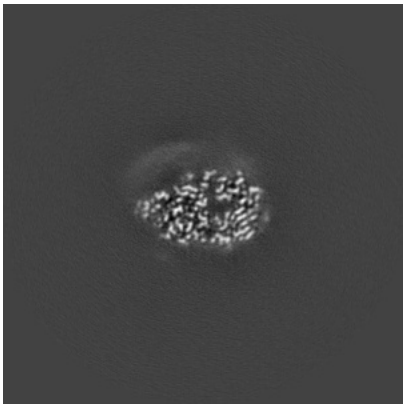


Y Index: 180

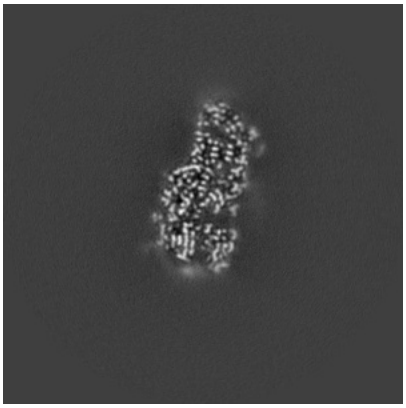


Z Index: 180

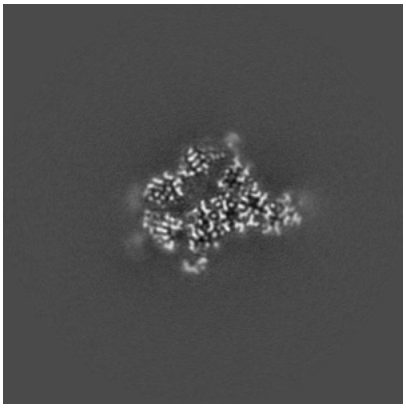
6.2.2 Raw map



X Index: 180



Y Index: 180

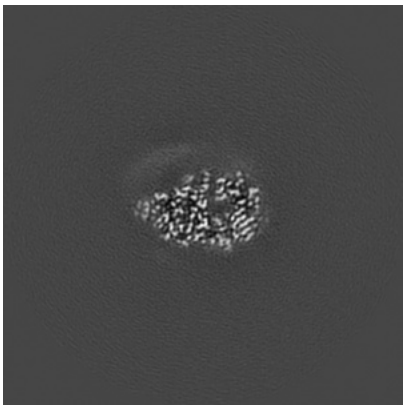


Z Index: 180

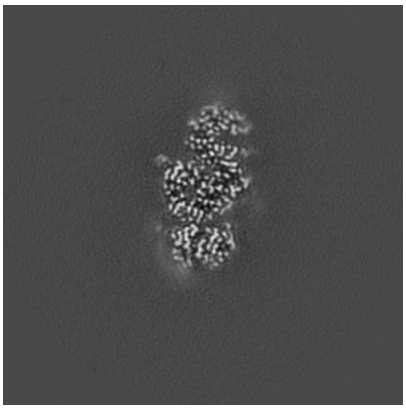
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

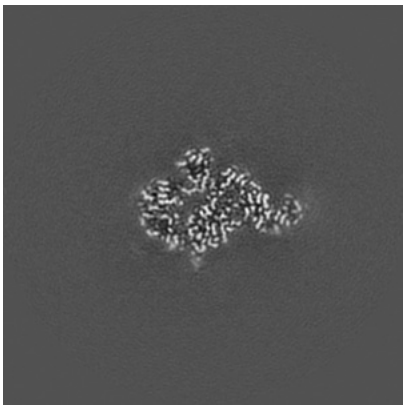
6.3.1 Primary map



X Index: 179

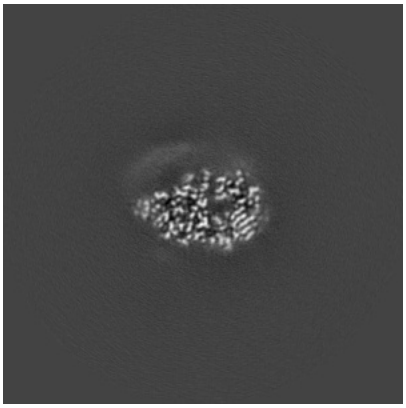


Y Index: 168

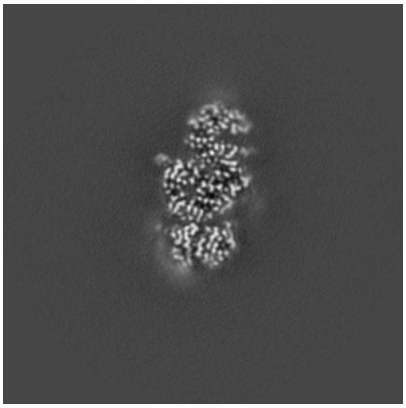


Z Index: 186

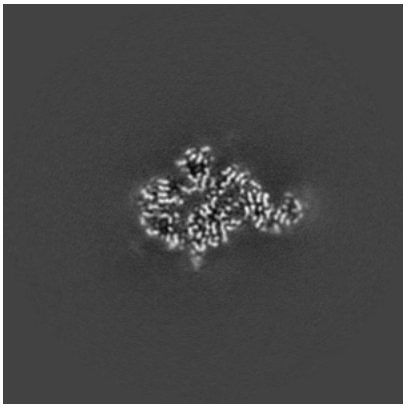
6.3.2 Raw map



X Index: 179



Y Index: 168

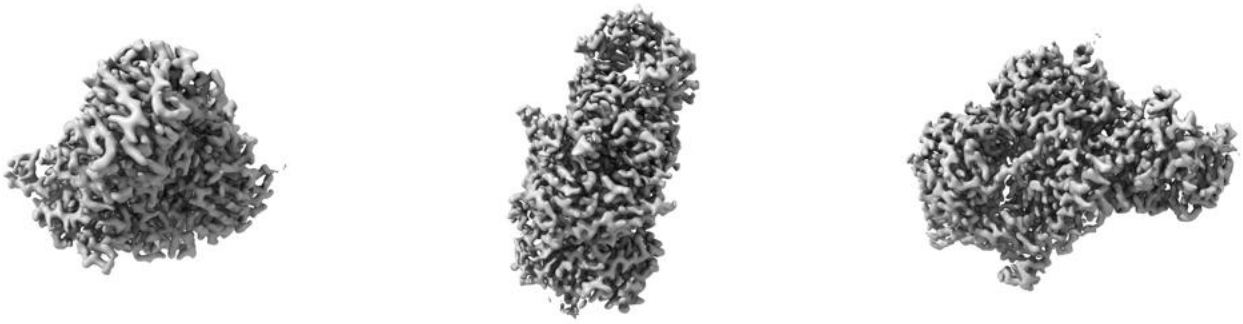


Z Index: 186

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

6.4 Orthogonal surface views (i)

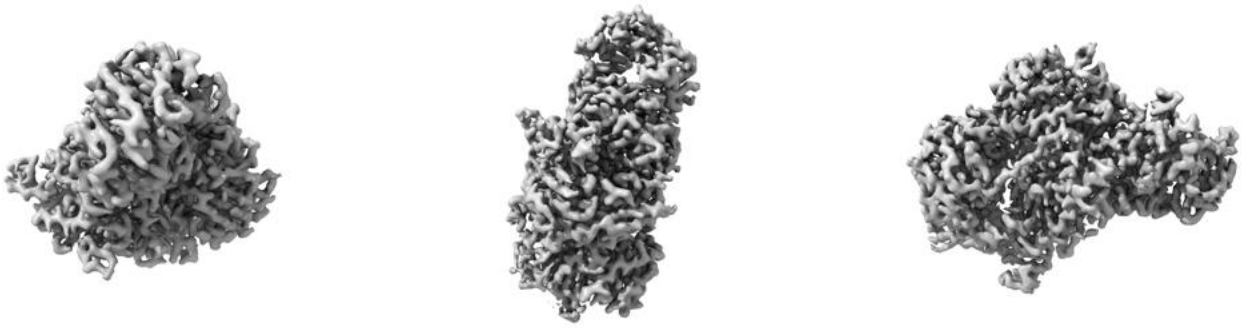
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

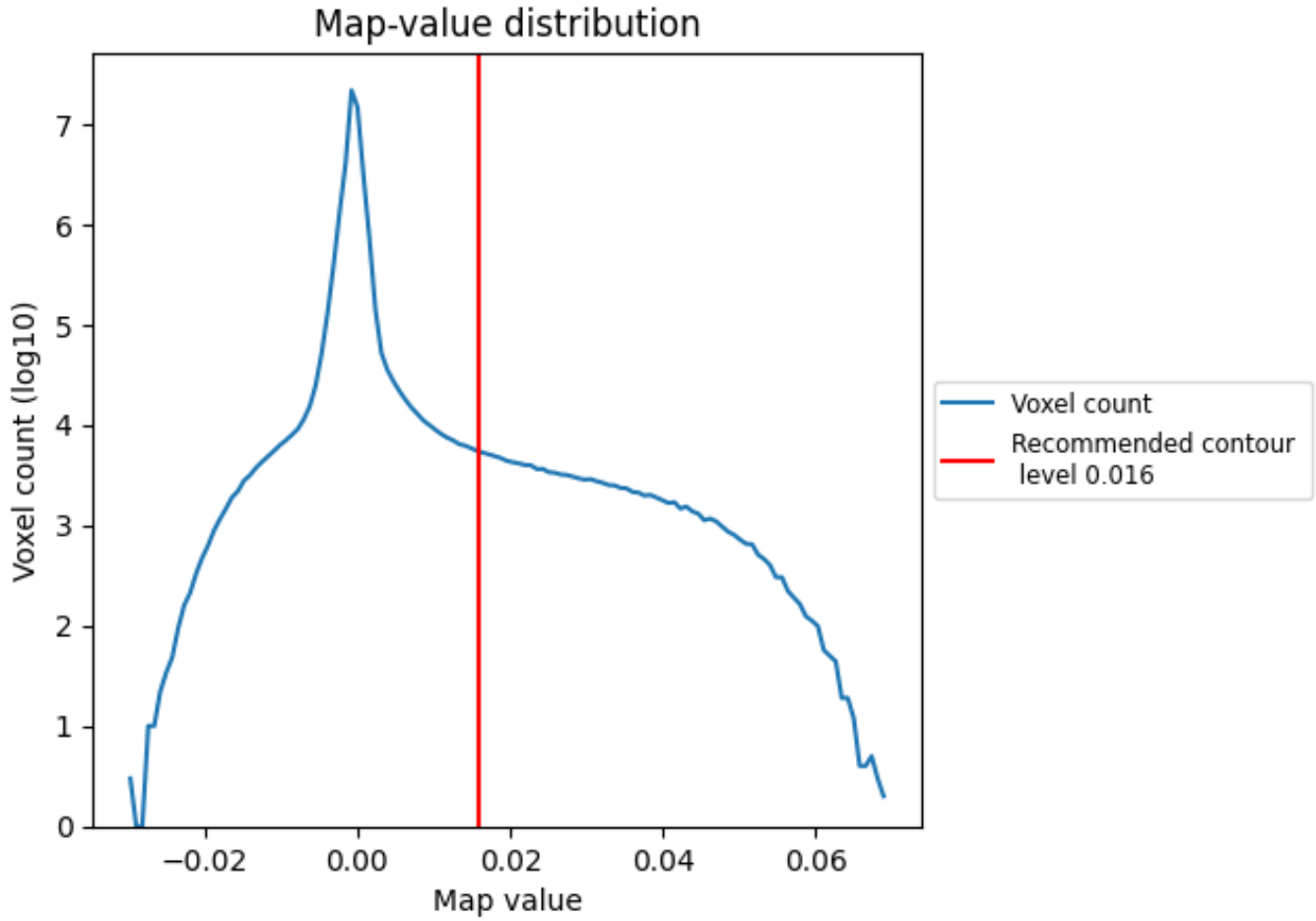
6.5 Mask visualisation (i)

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

7 Map analysis

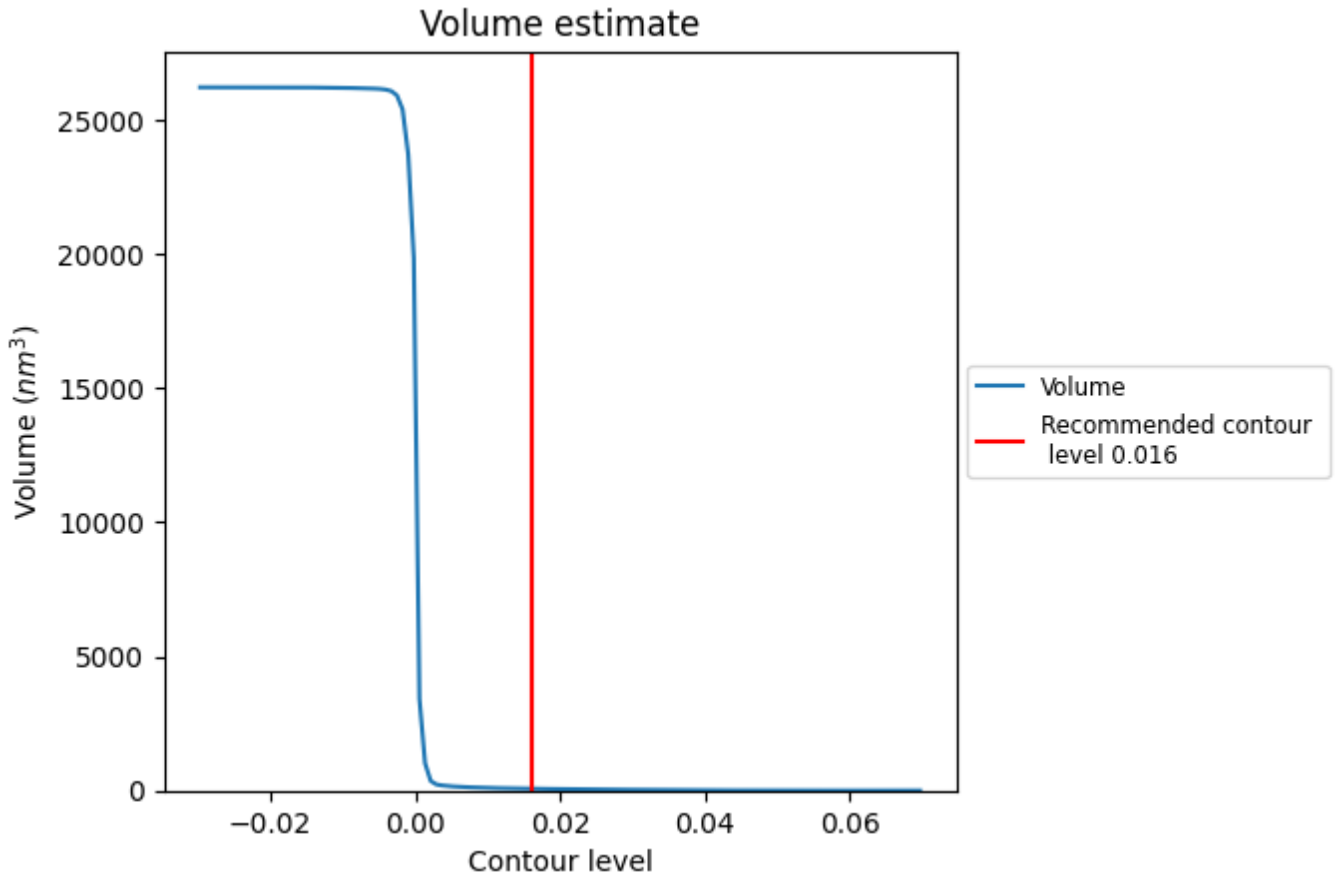
This section contains the results of statistical analysis of the map.

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.

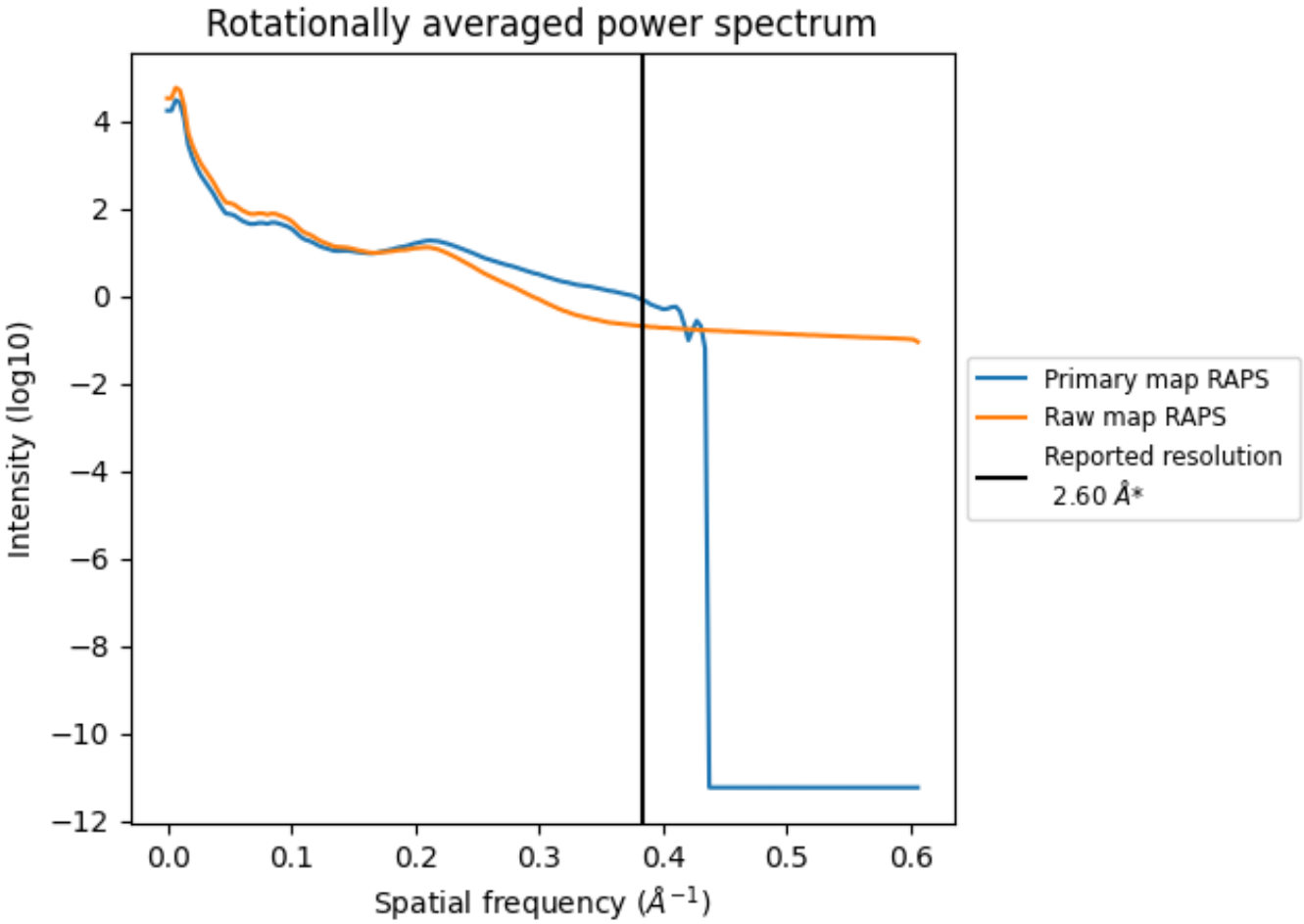
7.2 Volume estimate



The volume at the recommended contour level is 69 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)

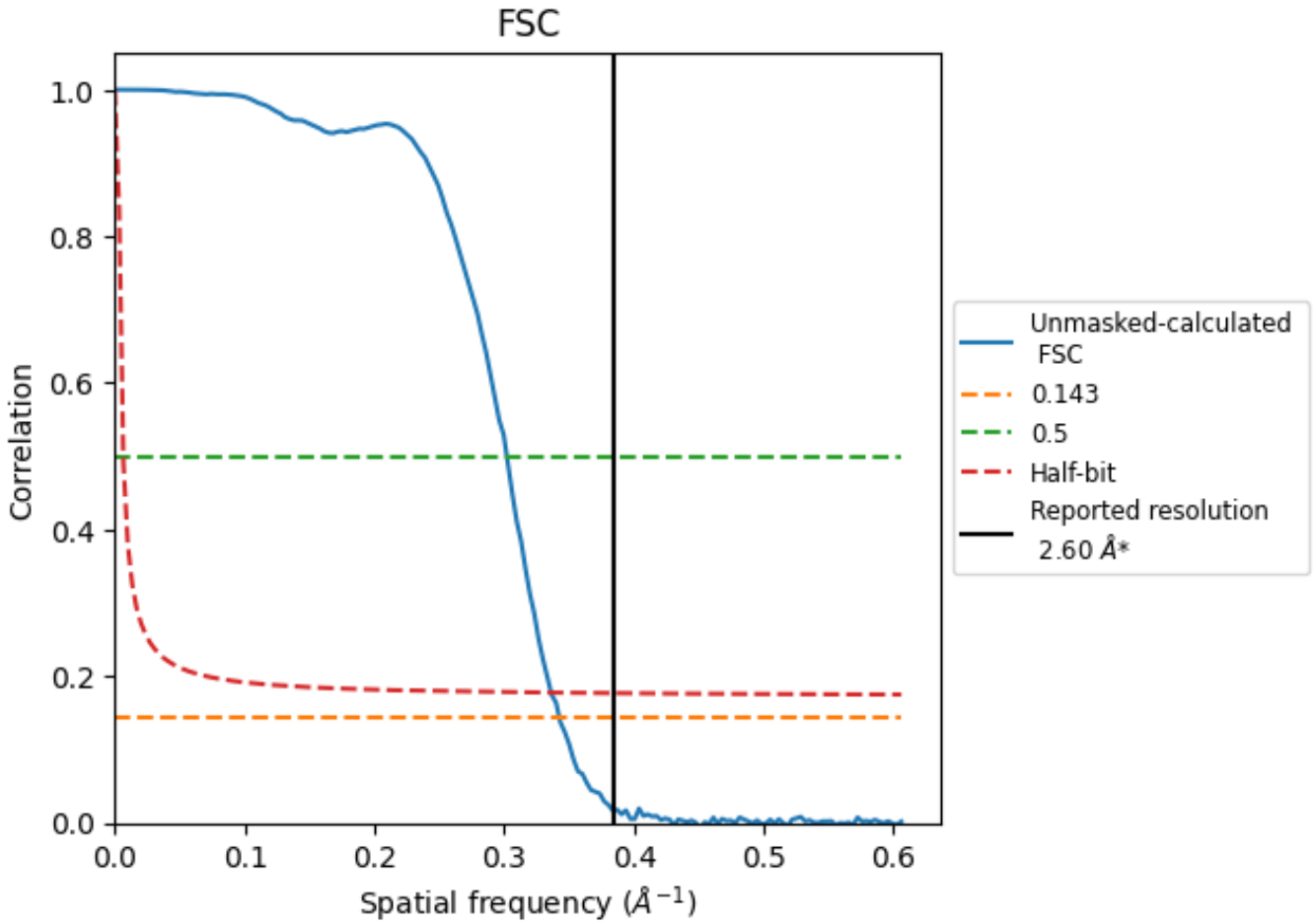


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

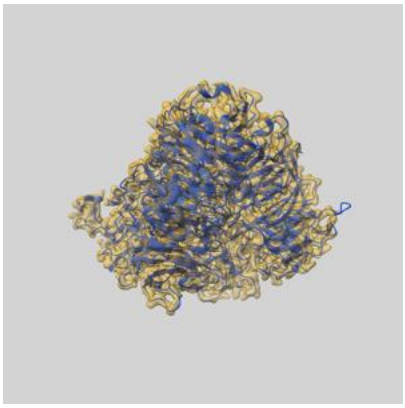
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.92	3.31	2.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.92 differs from the reported value 2.6 by more than 10 %

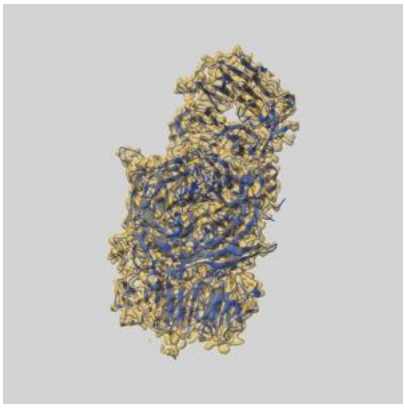
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14712 and PDB model 7ZGR. Per-residue inclusion information can be found in section 3 on page 5.

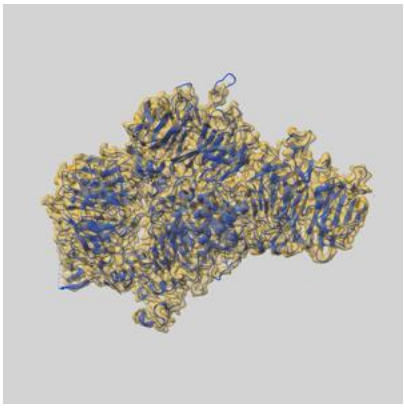
9.1 Map-model overlay



X



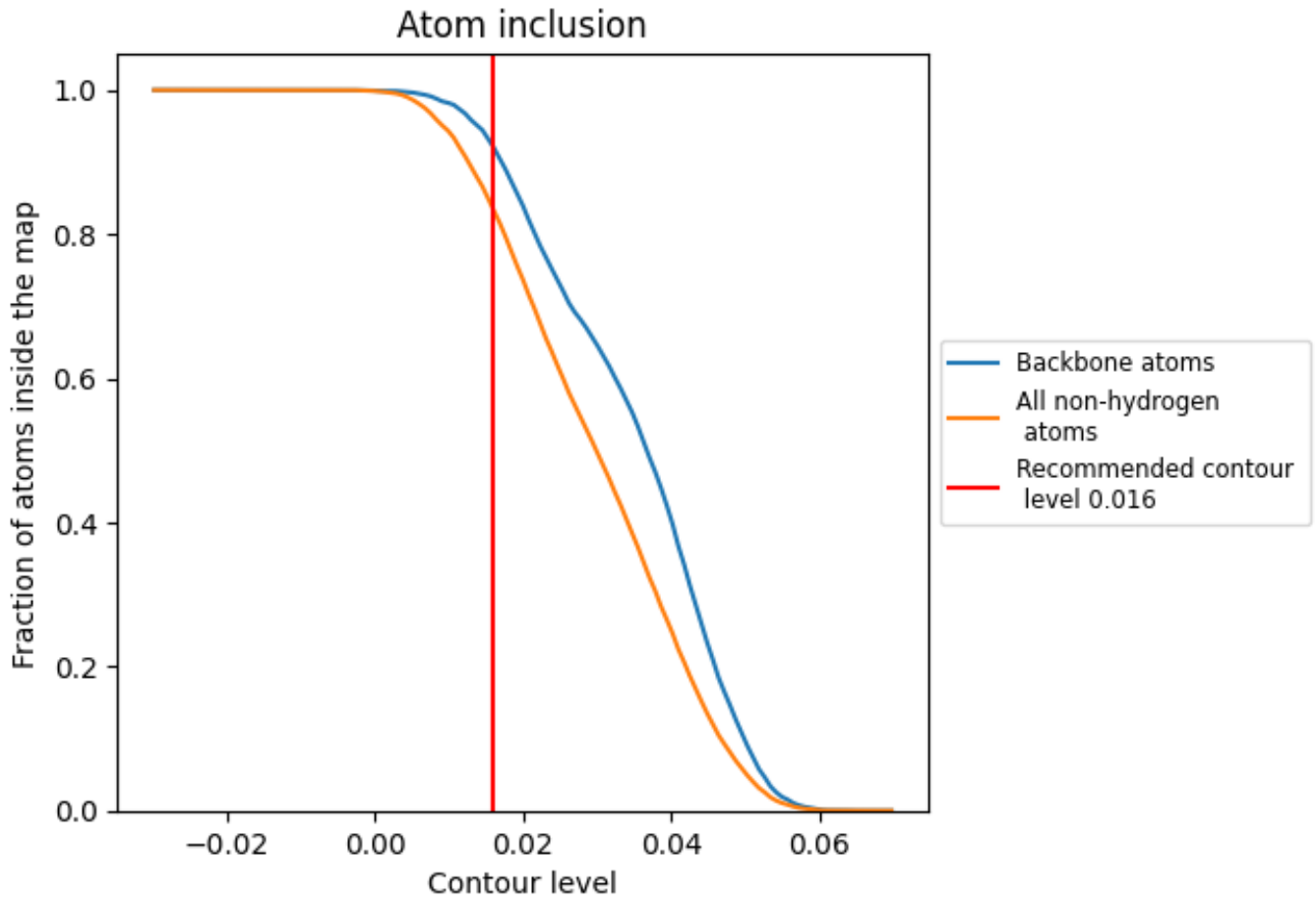
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.