Full wwPDB EM Validation Report

Dec 17, 2023 – 12:13 AM JST

PDB ID	:	8HCO
EMDB ID	:	EMD-34660
Title	:	Substrate-engaged TOM complex from yeast
Authors	:	Zhou, X.Y.; Yang, Y.Q.; Wang, G.P.; Wang, S.S.
Deposited on	:	2022-11-02
Resolution	:	4.10 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:

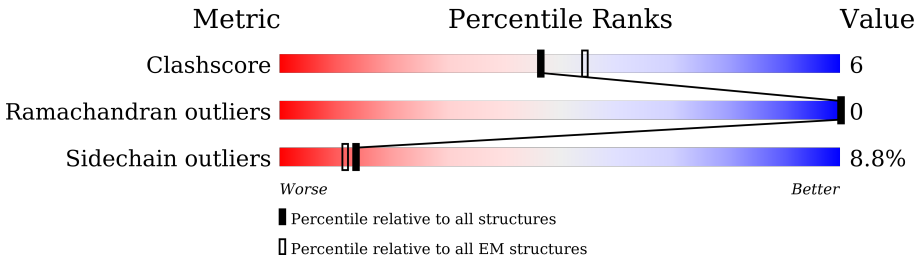
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



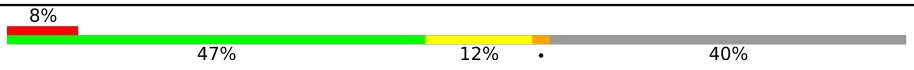
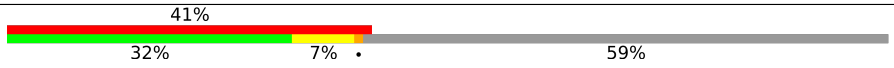
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	387	10% 59% 22% · 16%
1	I	387	17% 67% 16% · 15%
2	B	152	7% 30% · 67%
2	J	152	11% 29% · 67%
3	C	50	14% 64% 10% 26%
3	K	50	20% 68% 6% 26%
4	D	61	13% 48% 8% · 43%
4	L	61	21% 49% 7% · 43%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	60	
5	M	60	
6	G	553	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9330 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 Mitochondrial import receptor subunit TOM40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	326	Total	C	N	O	S	0	0
			2507	1581	426	492	8		
1	I	329	Total	C	N	O	S	0	0
			2528	1594	429	497	8		

- Molecule 2 is a protein called Mitochondrial import receptor subunit TOM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	50	Total	C	N	O	S	0	0
			387	249	61	76	1		
2	J	50	Total	C	N	O	S	0	0
			387	249	61	76	1		

- Molecule 3 is a protein called Mitochondrial import receptor subunit TOM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	37	Total	C	N	O	S	0	0
			303	201	52	49	1		
3	K	37	Total	C	N	O	S	0	0
			303	201	52	49	1		

- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	35	Total	C	N	O	S	0	0
			267	180	39	46	2		
4	L	35	Total	C	N	O	S	0	0
			267	180	39	46	2		

- Molecule 5 is a protein called Mitochondrial import receptor subunit TOM7.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	36	Total 295	C 198	N 51	O 46	0	0
5	M	36	Total 295	C 198	N 51	O 46	0	0

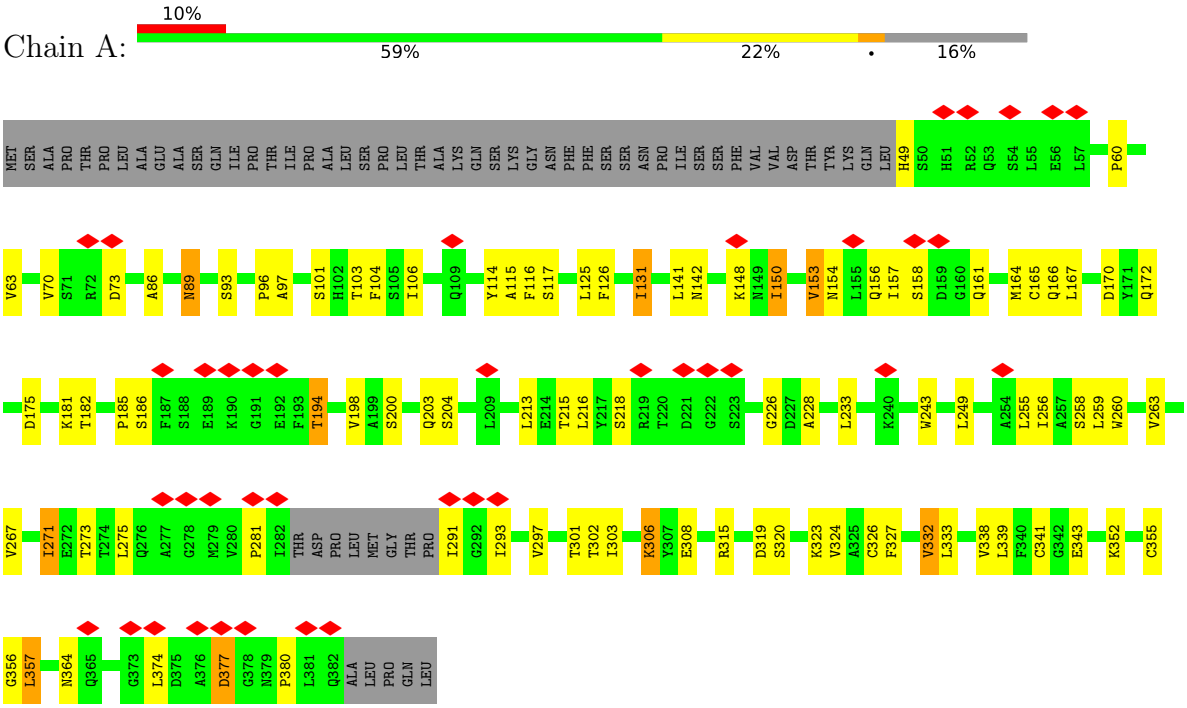
- Molecule 6 is a protein called sfGFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	224	Total 1791	C 1135	N 307	O 344	S 5	1	0

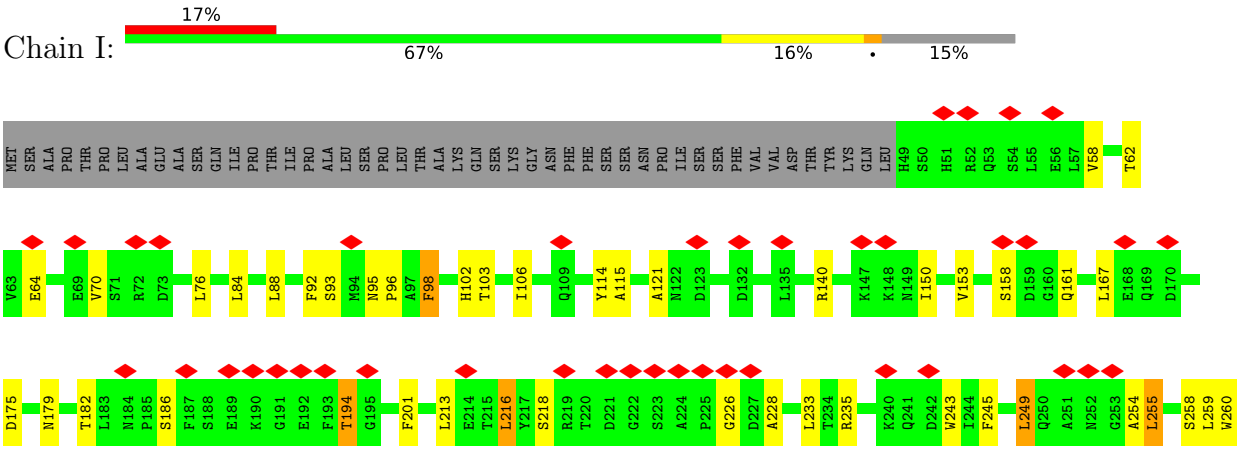
3 Residue-property plots

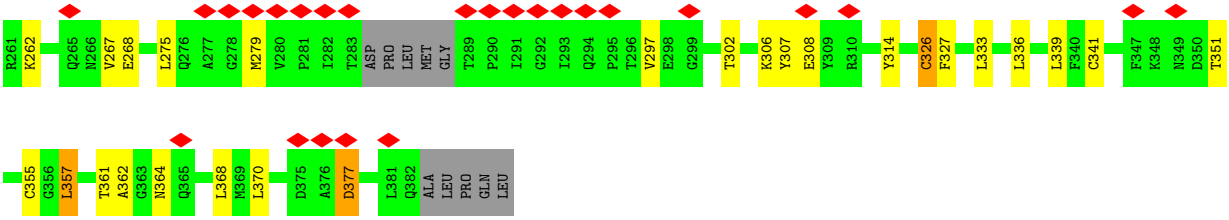
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mitochondrial import receptor subunit TOM40

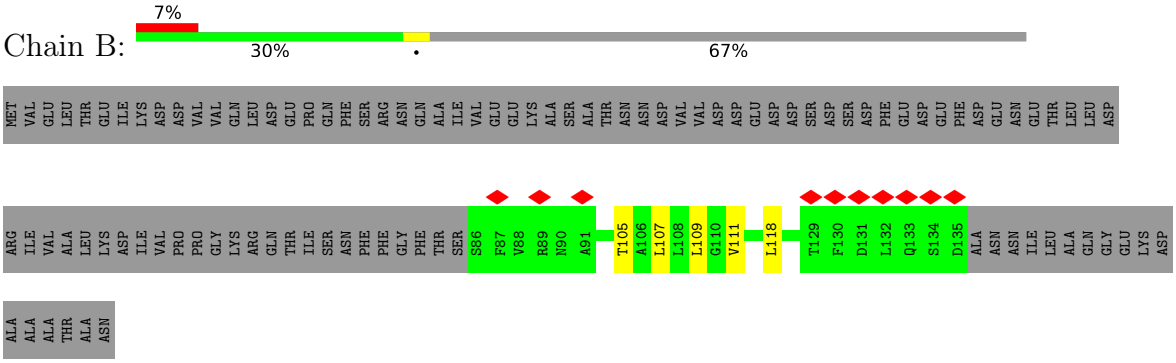


• Molecule 1: Mitochondrial import receptor subunit TOM40

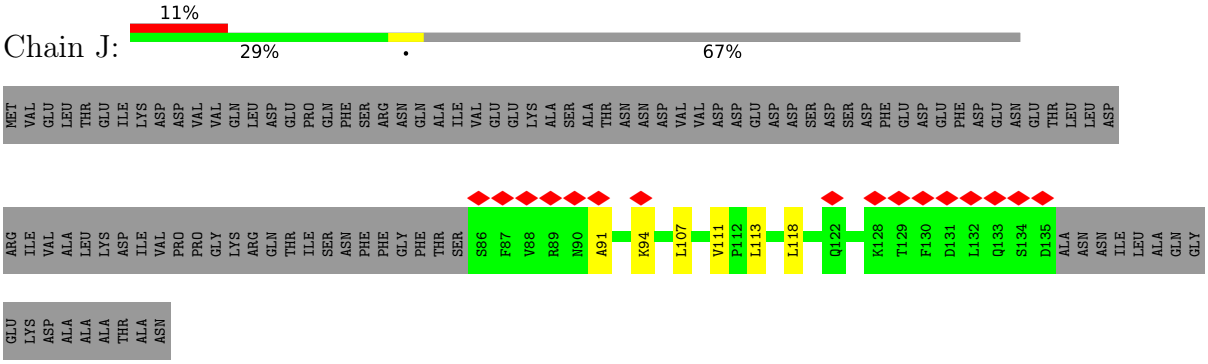




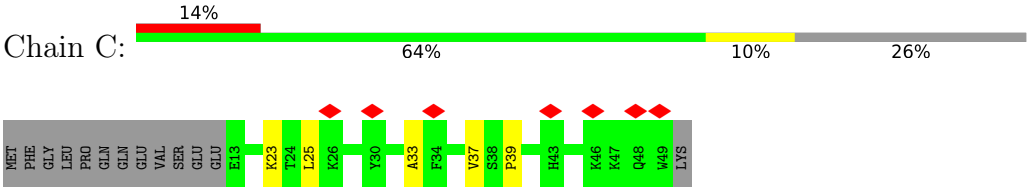
• Molecule 2: Mitochondrial import receptor subunit TOM22



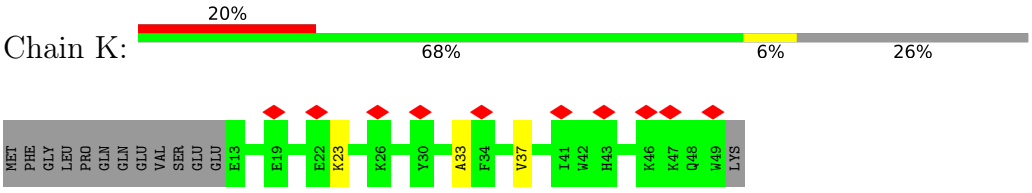
• Molecule 2: Mitochondrial import receptor subunit TOM22



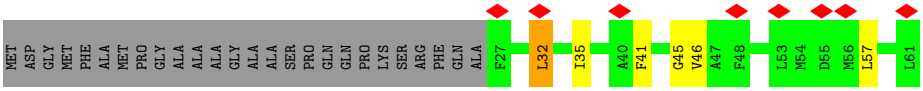
• Molecule 3: Mitochondrial import receptor subunit TOM5



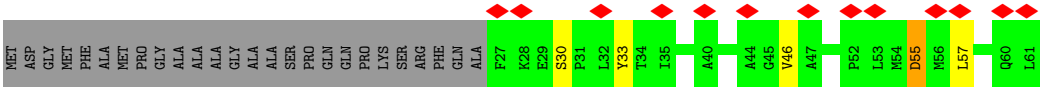
• Molecule 3: Mitochondrial import receptor subunit TOM5



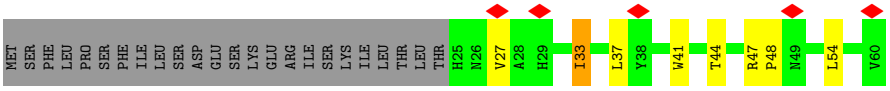
• Molecule 4: Mitochondrial import receptor subunit TOM6



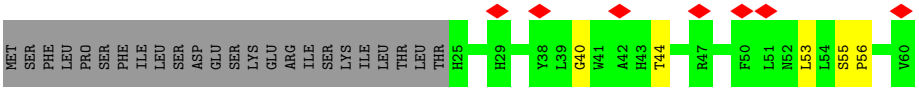
• Molecule 4: Mitochondrial import receptor subunit TOM6



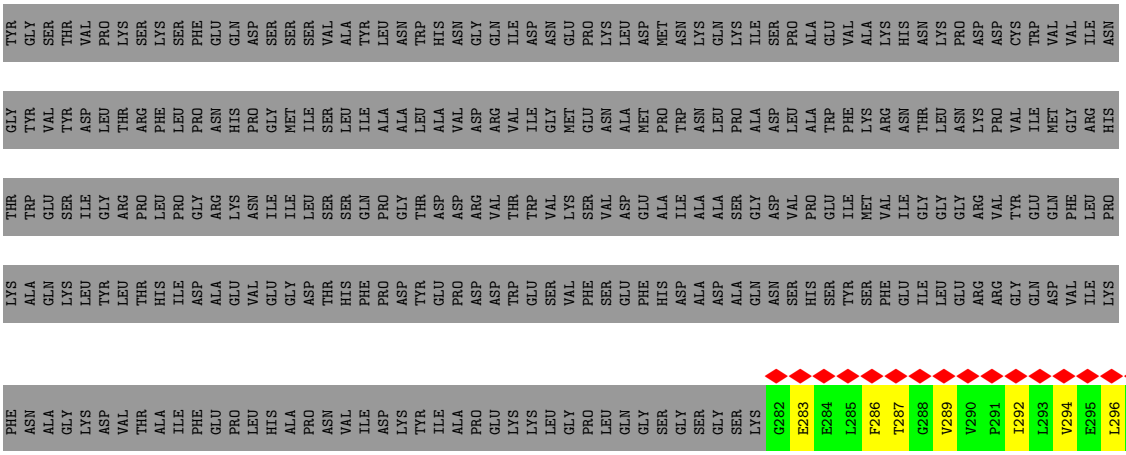
• Molecule 5: Mitochondrial import receptor subunit TOM7

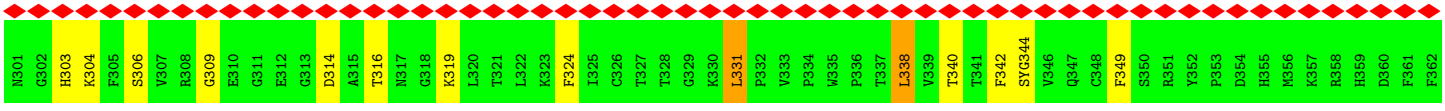


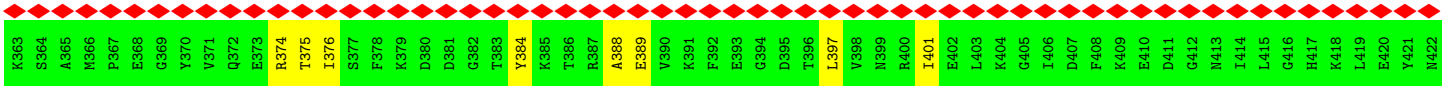
• Molecule 5: Mitochondrial import receptor subunit TOM7

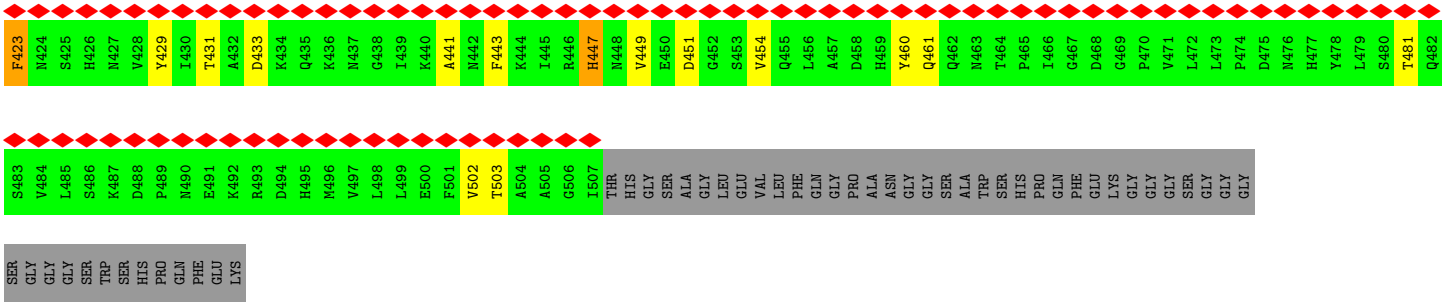


• Molecule 6: sfGFP








F423 N424 S425 H426 N427 V428 Y429 I430 T431 A432 D433 K434 Q435 K436 N437 G438 I439 K440 A441 N442 F443 K444 I445 R446 H447 N448 V449 E450 D451 G452 S453 V454 Q455 L456 A457 D458 H459 Y460 Q461 Q462 N463 T464 P465 I466 G467 D468 G469 P470 V471 L472 L473 P474 D475 N476 H477 Y478 L479 S480 T481 Q482
S483 V484 L485 S486 K487 D488 P489 N490 E491 K492 R493 D494 H495 M496 V497 L498 L499 E500 F501 V502 T503 A504 A505 G506 I507 THR HIS GLY SER ALA GLY LEU GLU VAL LEU PHE GLN GLY PRO ALA ASN GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY
SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103262	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.35	0/2554	0.58	0/3459
1	I	0.37	0/2576	0.60	0/3491
2	B	0.38	0/392	0.58	0/532
2	J	0.35	0/392	0.53	0/532
3	C	0.39	0/313	0.47	0/426
3	K	0.37	0/313	0.47	0/426
4	D	0.41	0/274	0.47	0/372
4	L	0.40	0/274	0.48	0/372
5	E	0.35	0/309	0.59	0/427
5	M	0.36	0/309	0.63	0/427
6	G	0.41	0/1808	0.59	0/2443
All	All	0.38	0/9514	0.58	0/12907

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	2507	0	2449	50	0
1	I	2528	0	2470	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	387	0	396	3	0
2	J	387	0	396	2	0
3	C	303	0	294	2	0
3	K	303	0	294	1	0
4	D	267	0	271	5	0
4	L	267	0	271	3	0
5	E	295	0	283	2	0
5	M	295	0	283	3	0
6	G	1791	0	1732	26	0
All	All	9330	0	9139	119	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 6.

All (119) 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)
6:G:296:LEU:HD22	6:G:342:PHE:CE1	1.72	1.23
6:G:296:LEU:CD2	6:G:342:PHE:HE1	1.68	1.06
6:G:296:LEU:HD22	6:G:342:PHE:HE1	1.02	0.98
6:G:296:LEU:CD2	6:G:342:PHE:CE1	2.46	0.97
6:G:309:GLY:HA3	6:G:324:PHE:HD1	1.57	0.70
6:G:338:LEU:HB3	6:G:342:PHE:CE2	2.31	0.66
1:I:98:PHE:CZ	5:M:53:LEU:HD11	2.31	0.65
1:A:93:SER:O	1:A:97:ALA:HA	1.96	0.64
1:A:198:VAL:HA	1:A:215:THR:O	2.00	0.60
1:I:93:SER:HB2	1:I:96:PRO:HD2	1.84	0.59
1:I:84:LEU:HA	1:I:355:CYS:O	2.03	0.58
6:G:449:VAL:HG12	6:G:451:ASP:OD1	2.05	0.56
1:A:218:SER:O	1:A:226:GLY:HA2	2.05	0.55
1:A:103:THR:O	1:A:114:TYR:HA	2.07	0.55
1:A:259:LEU:HD22	4:D:46:VAL:HG22	1.89	0.55
6:G:449:VAL:CG1	6:G:451:ASP:OD1	2.54	0.55
1:I:96:PRO:HA	1:I:121:ALA:O	2.07	0.54
1:A:158:SER:HB2	1:A:161:GLN:HB2	1.90	0.54
1:A:126:PHE:HB3	1:A:142:ASN:HB2	1.90	0.54
1:I:254:ALA:HA	1:I:275:LEU:O	2.06	0.54
1:A:271:ILE:HD13	4:D:45:GLY:HA3	1.89	0.54
1:I:307:TYR:HB2	1:I:314:TYR:HB3	1.89	0.54
6:G:340:THR:HB	6:G:374:ARG:HH12	1.73	0.53
6:G:375:THR:HB	6:G:460:TYR:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:441:ALA:HB3	6:G:461:GLN:HB3	1.90	0.53
1:A:203:GLN:HE21	3:C:39:PRO:HG2	1.74	0.52
1:A:70:VAL:HG22	1:A:260:TRP:HB2	1.91	0.52
6:G:309:GLY:HA3	6:G:324:PHE:CD1	2.42	0.52
1:I:259:LEU:HD22	4:L:46:VAL:HG22	1.91	0.51
6:G:376:ILE:HB	6:G:384:TYR:HB2	1.91	0.51
1:I:327:PHE:HD1	1:I:341:CYS:HB3	1.76	0.51
1:A:355:CYS:SG	1:A:356:GLY:N	2.84	0.51
1:A:86:ALA:HB3	1:A:104:PHE:HB2	1.93	0.51
1:A:216:LEU:O	1:A:228:ALA:HA	2.11	0.50
1:A:141:LEU:HB3	1:A:153:VAL:HG12	1.93	0.50
1:A:186:SER:HB3	1:A:194:THR:HG23	1.93	0.50
1:A:364:ASN:N	1:A:364:ASN:OD1	2.46	0.49
1:A:306:LYS:HE3	1:A:308:GLU:HB2	1.94	0.49
1:A:175:ASP:N	1:A:175:ASP:OD1	2.46	0.48
2:B:111:VAL:HG11	1:I:357:LEU:HD22	1.94	0.48
6:G:433:ASP:OD1	6:G:433:ASP:N	2.46	0.48
1:A:150:ILE:HG13	1:A:170:ASP:HB3	1.95	0.48
1:I:95:ASN:HB3	1:I:96:PRO:HD3	1.94	0.48
1:A:165:CYS:HB2	1:A:185:PRO:HD2	1.94	0.48
2:B:118:LEU:HG	1:I:333:LEU:HD21	1.95	0.48
1:A:357:LEU:HD22	2:J:111:VAL:HG11	1.96	0.48
1:I:103:THR:HB	1:I:115:ALA:HB3	1.96	0.48
1:A:116:PHE:HB3	1:A:131:ILE:HG23	1.95	0.48
1:I:216:LEU:O	1:I:228:ALA:HA	2.14	0.48
1:A:70:VAL:HG11	1:A:258:SER:HB2	1.96	0.48
1:I:70:VAL:HG22	1:I:260:TRP:HB2	1.95	0.48
1:I:326:CYS:SG	1:I:327:PHE:N	2.87	0.48
1:A:271:ILE:HD12	1:A:303:ILE:HB	1.96	0.48
1:A:374:LEU:HA	1:A:380:PRO:HA	1.96	0.48
5:E:41:TRP:NE1	5:E:48:PRO:O	2.47	0.48
1:A:154:ASN:HB3	1:A:166:GLN:HB3	1.95	0.47
6:G:283:GLU:HG2	6:G:286:PHE:HB2	1.97	0.47
1:A:327:PHE:HD1	1:A:341:CYS:HB3	1.80	0.47
1:A:343:GLU:HB3	1:A:352:LYS:HG3	1.96	0.47
1:A:89:ASN:HA	1:A:101:SER:HA	1.96	0.47
1:A:156:GLN:HB3	1:A:164:MET:HB2	1.96	0.47
1:A:101:SER:HB3	1:A:117:SER:HB3	1.96	0.47
1:A:243:TRP:HA	1:A:260:TRP:O	2.15	0.47
1:I:243:TRP:HA	1:I:260:TRP:O	2.14	0.47
1:A:73:ASP:O	1:A:315:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:GLU:OE2	1:I:179:ASN:ND2	2.47	0.47
1:I:249:LEU:HG	1:I:255:LEU:HD12	1.97	0.46
1:I:186:SER:HB3	1:I:194:THR:HG23	1.98	0.46
1:I:364:ASN:N	1:I:364:ASN:OD1	2.48	0.46
1:I:279:MET:SD	1:I:279:MET:N	2.89	0.46
1:A:377:ASP:OD1	1:A:377:ASP:N	2.48	0.46
4:L:30:SER:H	4:L:33:TYR:HB3	1.81	0.46
4:L:55:ASP:N	4:L:55:ASP:OD1	2.49	0.46
1:I:377:ASP:OD1	1:I:377:ASP:N	2.47	0.46
1:I:262:LYS:HG3	1:I:268:GLU:HG2	1.97	0.45
1:A:256:ILE:HA	1:A:273:THR:O	2.17	0.45
1:A:275:LEU:HD22	4:D:35:ILE:HG22	1.98	0.45
1:I:98:PHE:CE1	5:M:40:GLY:HA3	2.52	0.45
1:A:181:LYS:HG2	1:A:198:VAL:HG22	1.99	0.45
1:A:218:SER:O	1:A:226:GLY:CA	2.65	0.45
1:A:301:THR:HG21	4:D:41:PHE:HB3	1.99	0.44
1:A:324:VAL:O	1:A:343:GLU:HA	2.17	0.44
1:I:218:SER:O	1:I:226:GLY:CA	2.66	0.44
1:A:332:VAL:HG22	1:A:333:LEU:HD22	1.99	0.44
1:A:93:SER:HB3	1:A:96:PRO:HD2	1.99	0.44
6:G:423:PHE:HE1	6:G:447:HIS:CE1	2.35	0.43
1:A:60:PRO:HG3	1:A:204:SER:HB3	2.00	0.43
1:A:63:VAL:HG21	1:A:200:SER:HB2	2.00	0.43
1:I:92:PHE:HB2	1:I:98:PHE:CD2	2.54	0.43
1:I:362:ALA:HB3	1:I:368:LEU:HG	2.00	0.43
6:G:449:VAL:HG12	6:G:451:ASP:H	1.84	0.43
6:G:331:LEU:HD13	6:G:331:LEU:HA	1.85	0.43
1:I:235:ARG:HA	1:I:245:PHE:O	2.18	0.43
5:E:33:ILE:O	5:E:37:LEU:HB2	2.19	0.42
6:G:292:ILE:HG23	6:G:397:LEU:HD12	1.99	0.42
1:A:148:LYS:HD2	1:A:172:GLN:HB2	2.01	0.42
1:I:175:ASP:N	1:I:175:ASP:OD1	2.52	0.42
6:G:429:TYR:H	6:G:443:PHE:HB3	1.85	0.42
3:K:33:ALA:O	3:K:37:VAL:HG23	2.20	0.42
1:A:319:ASP:HB3	1:A:323:LYS:H	1.85	0.42
1:I:158:SER:HB2	1:I:161:GLN:HB2	2.00	0.42
6:G:314:ASP:O	6:G:349:PHE:HB3	2.19	0.41
1:A:281:PRO:HG3	1:A:293:ILE:HG13	2.02	0.41
6:G:423:PHE:HE1	6:G:447:HIS:HE1	1.69	0.41
1:A:301:THR:HB	1:A:320:SER:HB2	2.02	0.41
6:G:481:THR:HG22	6:G:502:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:PHE:HD1	1:I:98:PHE:HA	1.69	0.41
6:G:319:LYS:HE3	6:G:319:LYS:HB2	1.92	0.41
6:G:388:ALA:HB2	6:G:401:ILE:HG23	2.01	0.41
2:J:91:ALA:HA	2:J:94:LYS:HE2	2.02	0.41
6:G:304:LYS:NZ	6:G:306:SER:OG	2.45	0.41
1:I:70:VAL:HG11	1:I:258:SER:HB2	2.02	0.41
1:I:306:LYS:HE3	1:I:308:GLU:HB2	2.03	0.41
1:A:103:THR:HB	1:A:115:ALA:HB3	2.03	0.40
1:A:324:VAL:HG11	2:B:105:THR:HG23	2.03	0.40
4:D:32:LEU:HA	4:D:35:ILE:HG12	2.03	0.40
3:C:33:ALA:O	3:C:37:VAL:HG23	2.20	0.40
1:I:88:LEU:O	1:I:102:HIS:N	2.47	0.40
5:M:55:SER:HA	5:M:56:PRO:HD3	1.94	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	322/387 (83%)	313 (97%)	9 (3%)	0	100	100
1	I	325/387 (84%)	316 (97%)	9 (3%)	0	100	100
2	B	48/152 (32%)	48 (100%)	0	0	100	100
2	J	48/152 (32%)	48 (100%)	0	0	100	100
3	C	35/50 (70%)	35 (100%)	0	0	100	100
3	K	35/50 (70%)	35 (100%)	0	0	100	100
4	D	33/61 (54%)	33 (100%)	0	0	100	100
4	L	33/61 (54%)	33 (100%)	0	0	100	100
5	E	34/60 (57%)	33 (97%)	1 (3%)	0	100	100
5	M	34/60 (57%)	33 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	219/553 (40%)	211 (96%)	8 (4%)	0	100	100
All	All	1166/1973 (59%)	1138 (98%)	28 (2%)	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	273/327 (84%)	245 (90%)	28 (10%)	7	28
1	I	276/327 (84%)	247 (90%)	29 (10%)	7	27
2	B	44/133 (33%)	42 (96%)	2 (4%)	27	54
2	J	44/133 (33%)	41 (93%)	3 (7%)	16	44
3	C	29/44 (66%)	27 (93%)	2 (7%)	15	43
3	K	29/44 (66%)	28 (97%)	1 (3%)	37	61
4	D	28/44 (64%)	26 (93%)	2 (7%)	14	42
4	L	28/44 (64%)	26 (93%)	2 (7%)	14	42
5	E	32/56 (57%)	27 (84%)	5 (16%)	2	16
5	M	32/56 (57%)	31 (97%)	1 (3%)	40	63
6	G	195/467 (42%)	181 (93%)	14 (7%)	14	42
All	All	1010/1675 (60%)	921 (91%)	89 (9%)	13	34

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	89	ASN
1	A	106	ILE
1	A	125	LEU
1	A	131	ILE
1	A	150	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	153	VAL
1	A	157	ILE
1	A	167	LEU
1	A	182	THR
1	A	194	THR
1	A	213	LEU
1	A	233	LEU
1	A	249	LEU
1	A	255	LEU
1	A	263	VAL
1	A	267	VAL
1	A	271	ILE
1	A	291	ILE
1	A	297	VAL
1	A	302	THR
1	A	306	LYS
1	A	326	CYS
1	A	332	VAL
1	A	338	VAL
1	A	339	LEU
1	A	357	LEU
1	A	377	ASP
2	B	107	LEU
2	B	109	LEU
3	C	23	LYS
3	C	25	LEU
4	D	32	LEU
4	D	57	LEU
5	E	27	VAL
5	E	33	ILE
5	E	44	THR
5	E	47	ARG
5	E	54	LEU
6	G	287	THR
6	G	289	VAL
6	G	294	VAL
6	G	300	VAL
6	G	303	HIS
6	G	316	THR
6	G	331	LEU
6	G	338	LEU
6	G	389	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	G	423	PHE
6	G	431	THR
6	G	447	HIS
6	G	454	VAL
6	G	503	THR
1	I	58	VAL
1	I	62	THR
1	I	76	LEU
1	I	98	PHE
1	I	106	ILE
1	I	114	TYR
1	I	140	ARG
1	I	150	ILE
1	I	153	VAL
1	I	167	LEU
1	I	182	THR
1	I	194	THR
1	I	201	PHE
1	I	213	LEU
1	I	216	LEU
1	I	233	LEU
1	I	249	LEU
1	I	255	LEU
1	I	267	VAL
1	I	297	VAL
1	I	302	THR
1	I	326	CYS
1	I	336	LEU
1	I	339	LEU
1	I	351	THR
1	I	357	LEU
1	I	361	THR
1	I	370	LEU
1	I	377	ASP
2	J	107	LEU
2	J	113	LEU
2	J	118	LEU
3	K	23	LYS
4	L	55	ASP
4	L	57	LEU
5	M	44	THR

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

sidechains are listed below:

Mol	Chain	Res	Type
6	G	317	ASN
6	G	424	ASN
6	G	448	ASN
1	I	89	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GYS	G	344[B]	-	22,22,23	1.84	4 (18%)	27,30,32	1.36	4 (14%)
6	GYS	G	344[A]	-	22,22,23	1.56	3 (13%)	27,30,32	1.18	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GYS	G	344[B]	-	-	0/9/29/30	0/2/2/2
6	GYS	G	344[A]	-	-	0/9/29/30	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	344[A]	GYS	CB2-CA2	5.09	1.39	1.35
6	G	344[B]	GYS	CB2-CA2	5.09	1.39	1.35
6	G	344[B]	GYS	OG1-CB1	4.55	1.61	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	344[A]	GYS	OH-CZ	-2.19	1.31	1.37
6	G	344[B]	GYS	OH-CZ	-2.19	1.31	1.37
6	G	344[A]	GYS	CE1-CZ	2.08	1.42	1.38
6	G	344[B]	GYS	CE1-CZ	2.08	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	344[B]	GYS	OG1-CB1-CA1	3.59	120.34	110.85
6	G	344[A]	GYS	CA1-C1-N3	-3.00	120.94	124.85
6	G	344[B]	GYS	CA1-C1-N3	-3.00	120.94	124.85
6	G	344[A]	GYS	O2-C2-CA2	2.45	132.34	130.96
6	G	344[B]	GYS	O2-C2-CA2	2.45	132.34	130.96
6	G	344[A]	GYS	O3-C3-CA3	-2.43	119.05	126.39
6	G	344[B]	GYS	O3-C3-CA3	-2.43	119.05	126.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

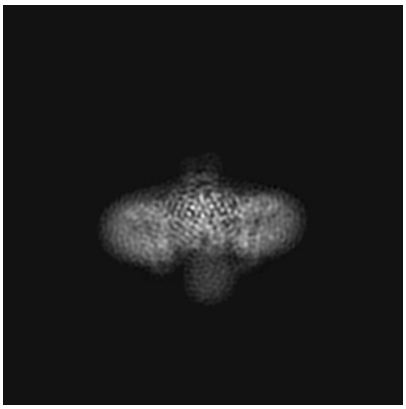
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34660. These allow visual inspection of the internal detail of the map and identification of artifacts.

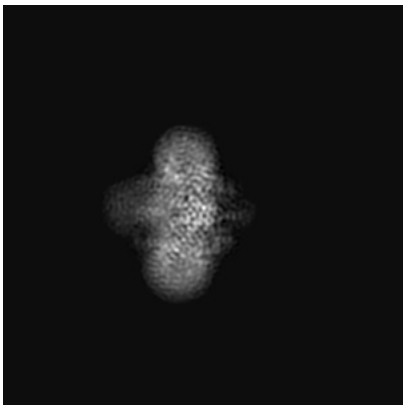
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

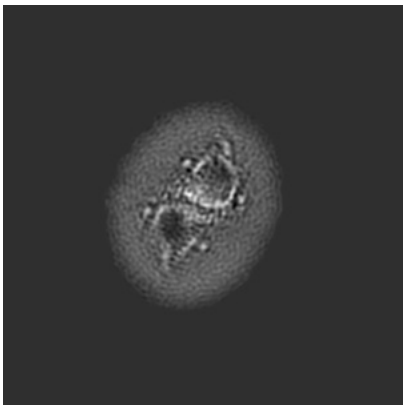
6.1.1 Primary map



X

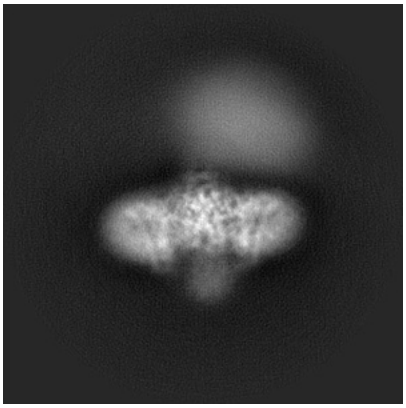


Y

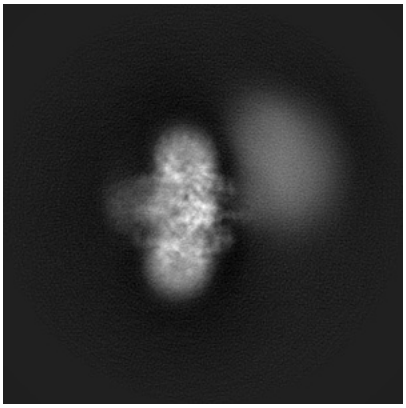


Z

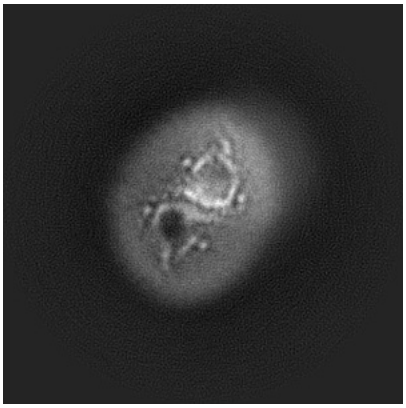
6.1.2 Raw map



X



Y

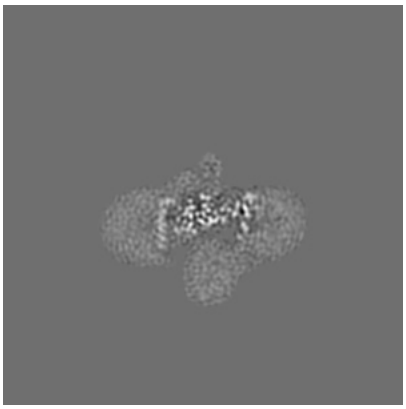


Z

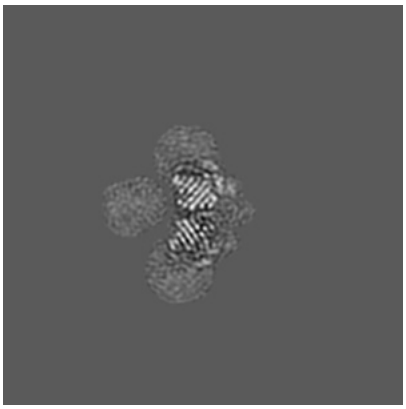
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

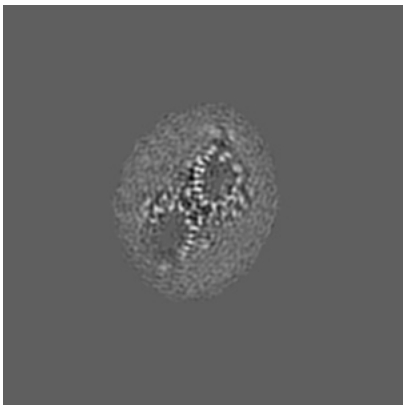
6.2.1 Primary map



X Index: 140

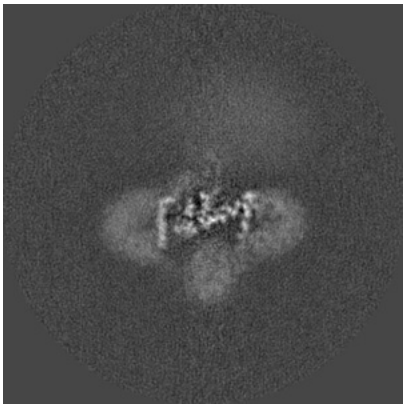


Y Index: 140

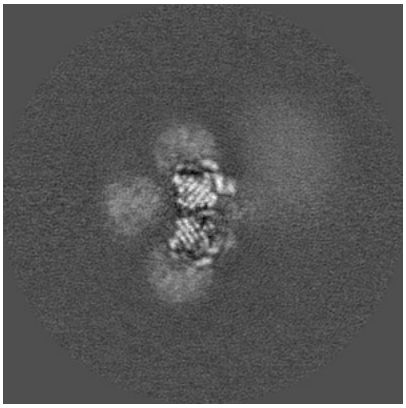


Z Index: 140

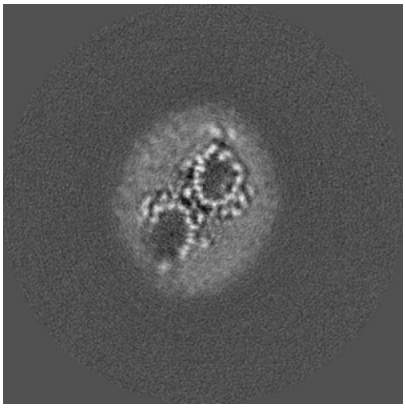
6.2.2 Raw map



X Index: 140



Y Index: 140



Z Index: 140

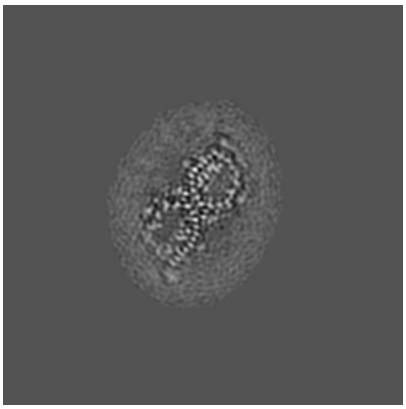
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

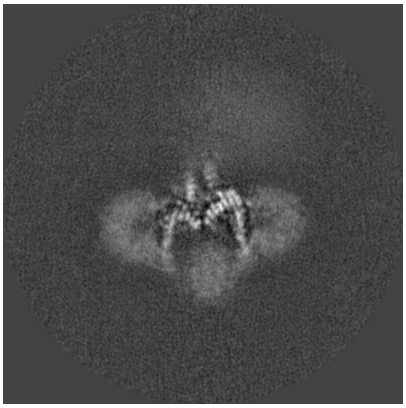
X Index: 134

Y Index: 139

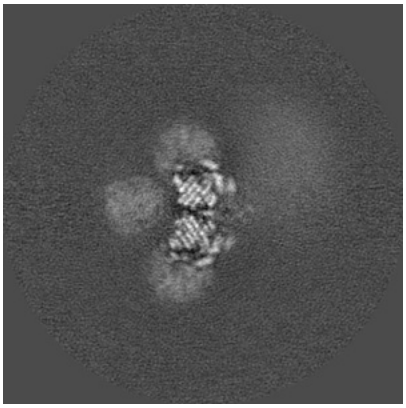


Z Index: 132

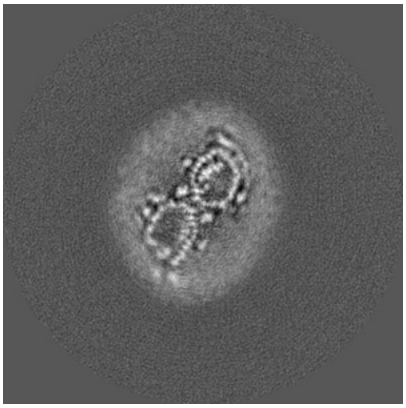
6.3.2 Raw map



X Index: 135



Y Index: 139

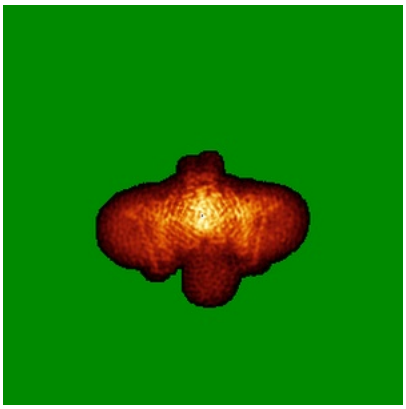


Z Index: 134

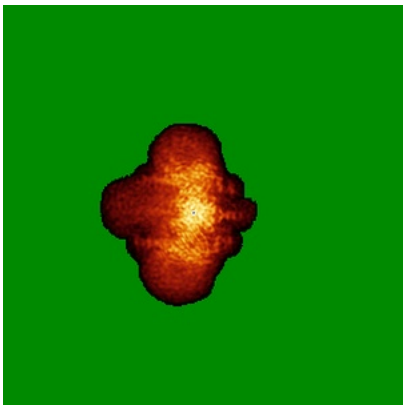
The images above show the largest variance slices of the map in three orthogonal directions.

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

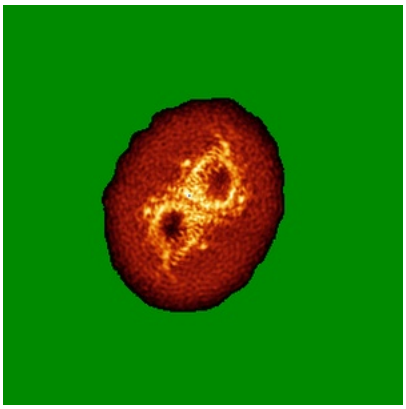
6.4.1 Primary map



X

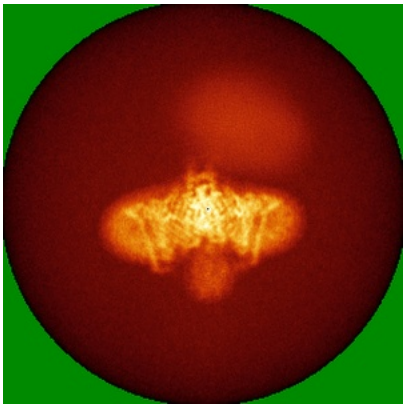


Y

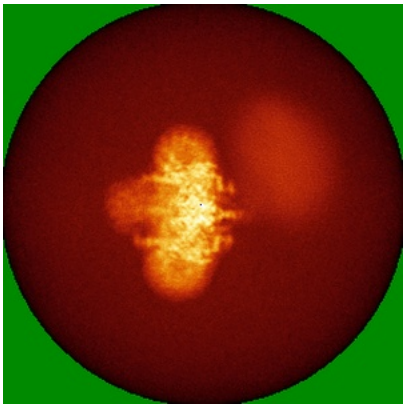


Z

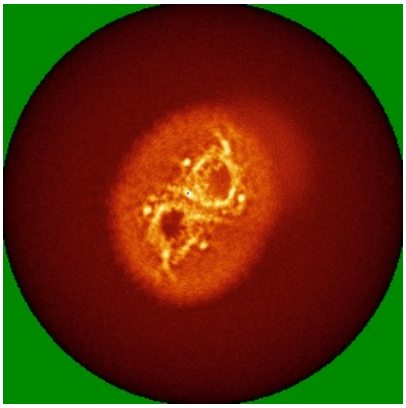
6.4.2 Raw map



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

6.5.2 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.

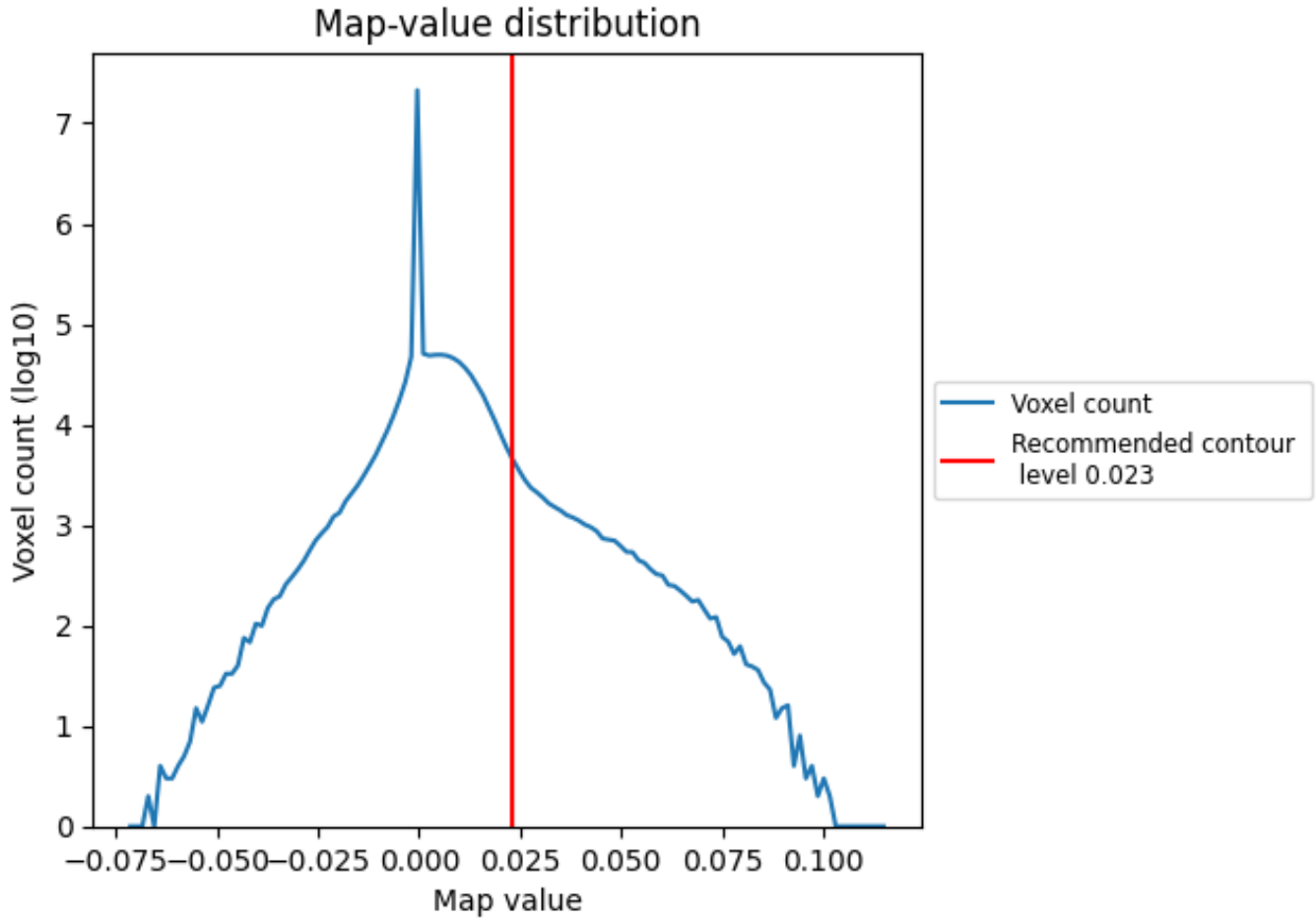
6.6 Mask visualisation (i)

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

7 Map analysis

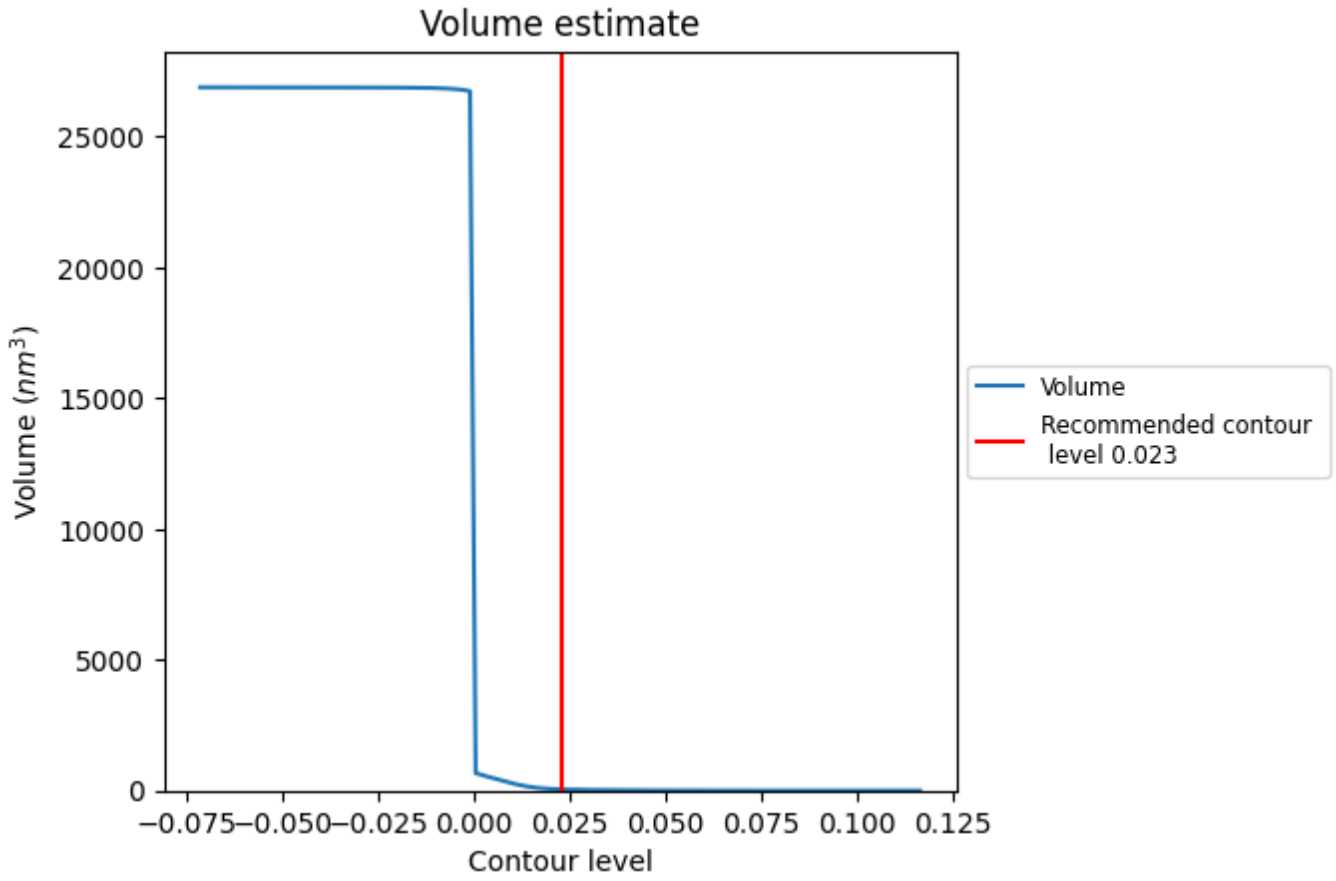
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

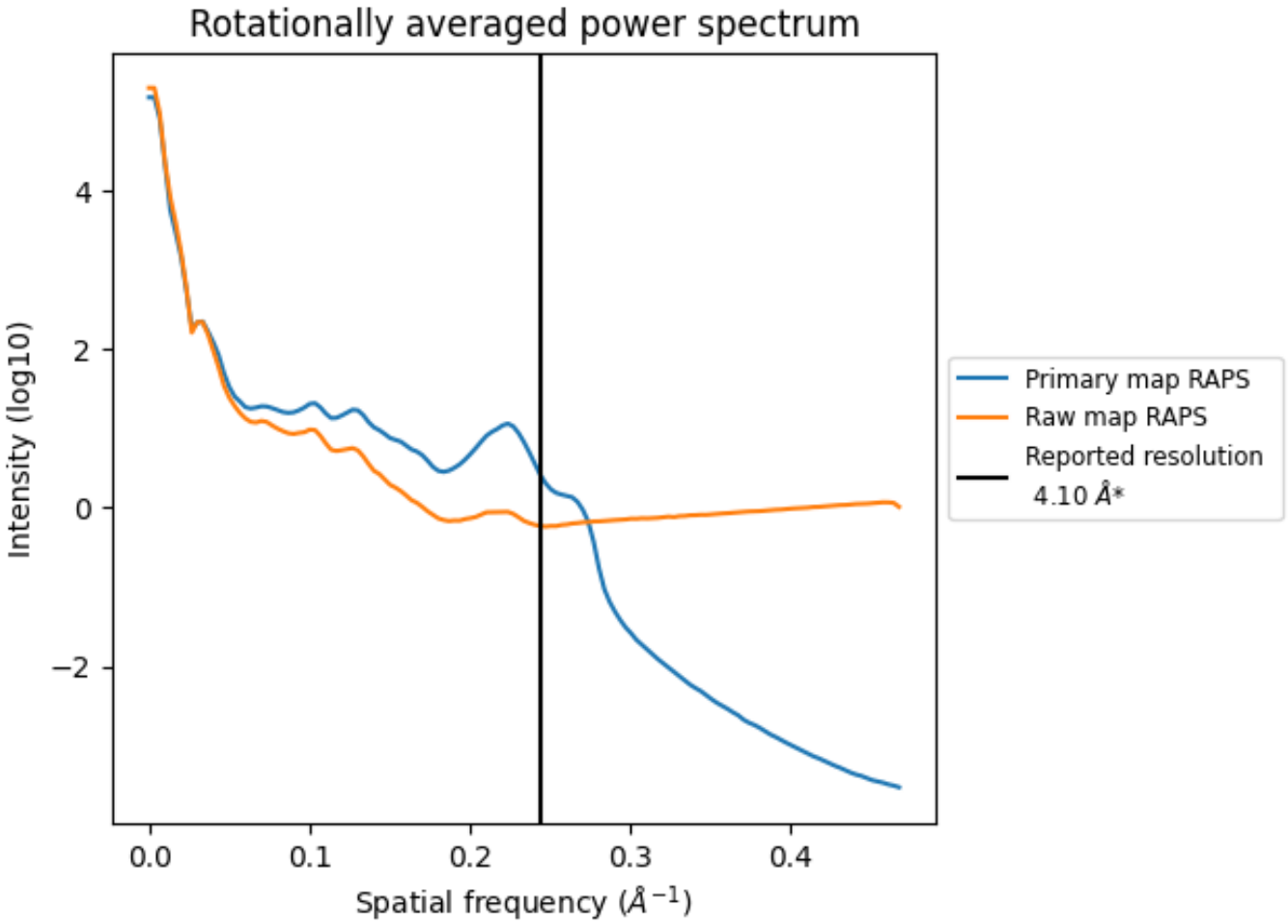
7.2 Volume estimate (i)



The volume at the recommended contour level is 45 nm^3; this corresponds to an approximate mass of 41 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)

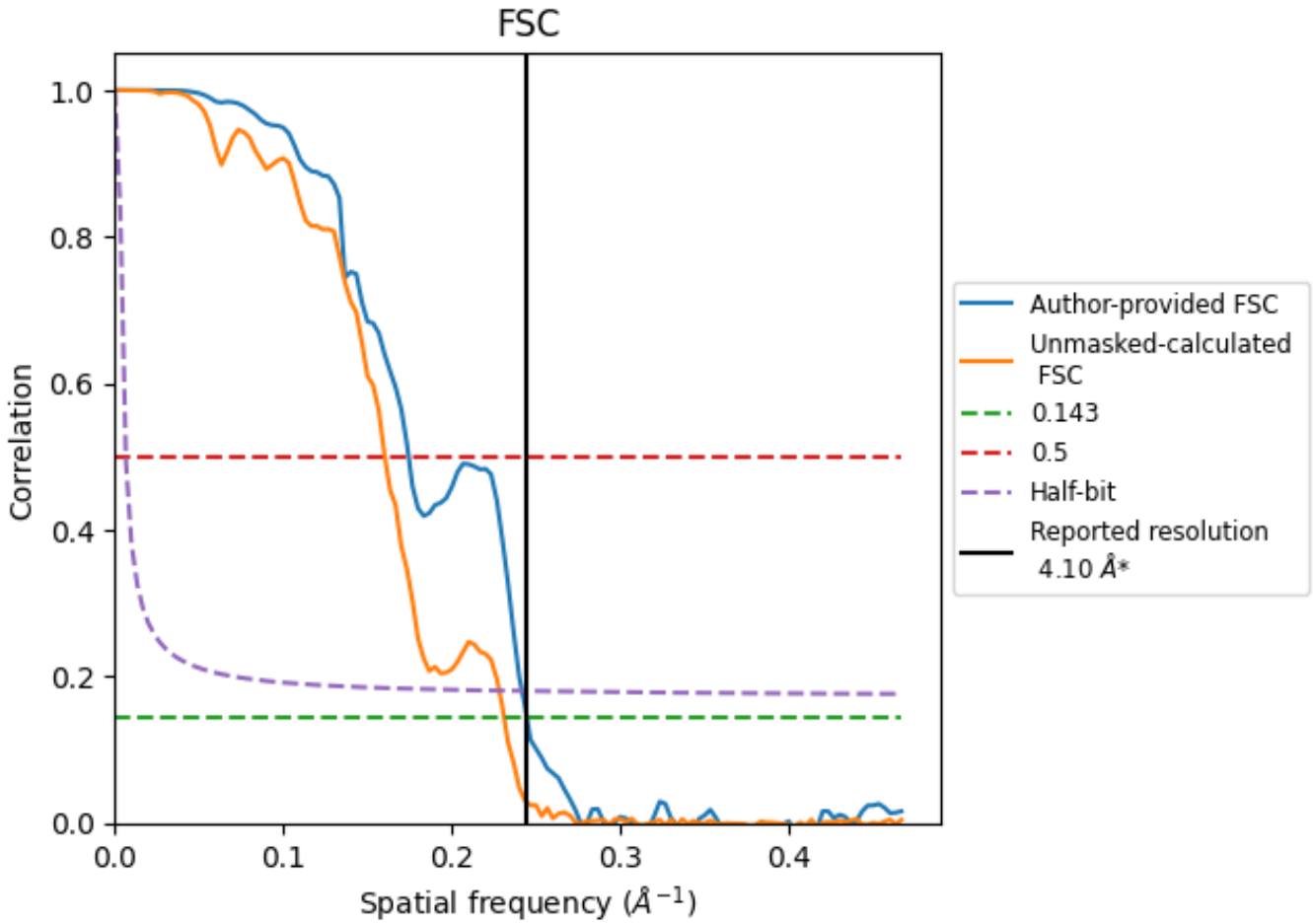


*Reported resolution corresponds to spatial frequency of 0.244 $Å^{-1}$

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 0.244 Å^{-1}

8.2 Resolution estimates (i)

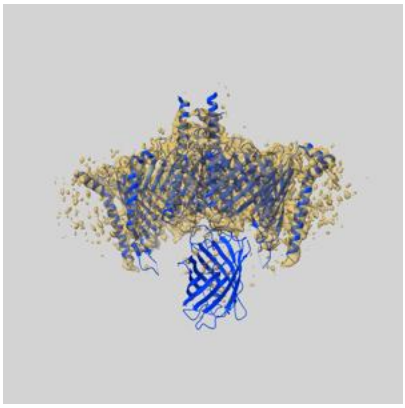
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	5.73	4.13
Unmasked-calculated*	4.32	6.23	4.38

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

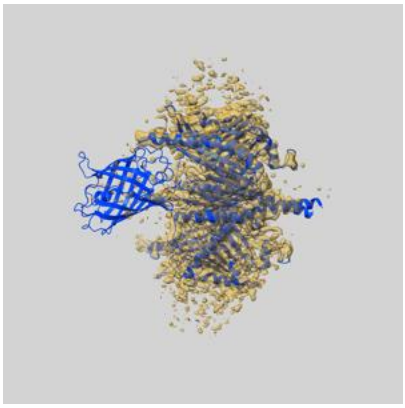
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34660 and PDB model 8HCO. Per-residue inclusion information can be found in section 3 on page 6.

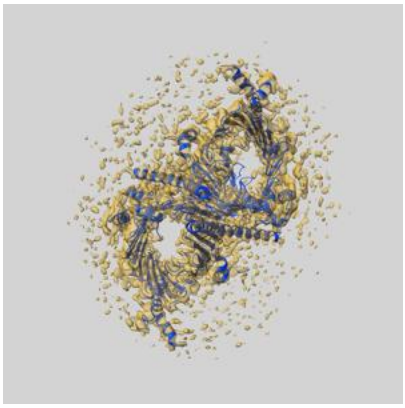
9.1 Map-model overlay



X



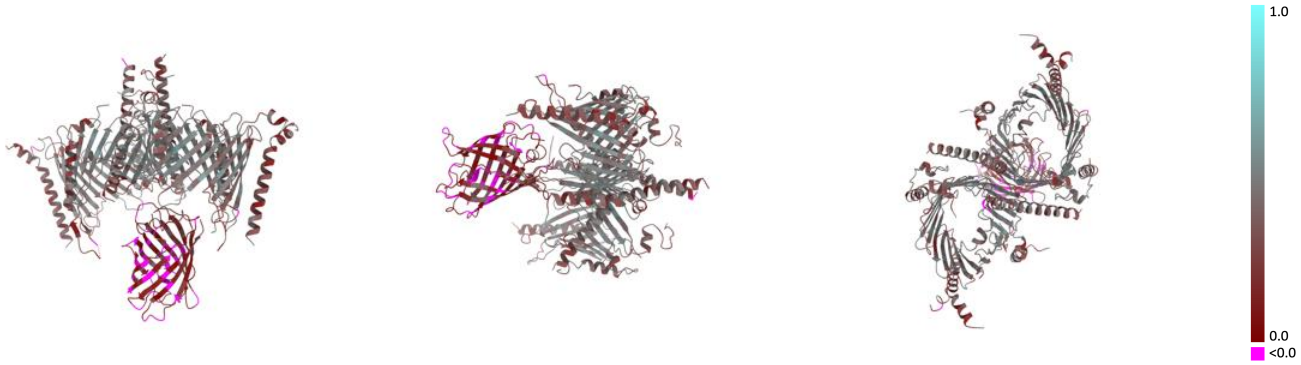
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 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.

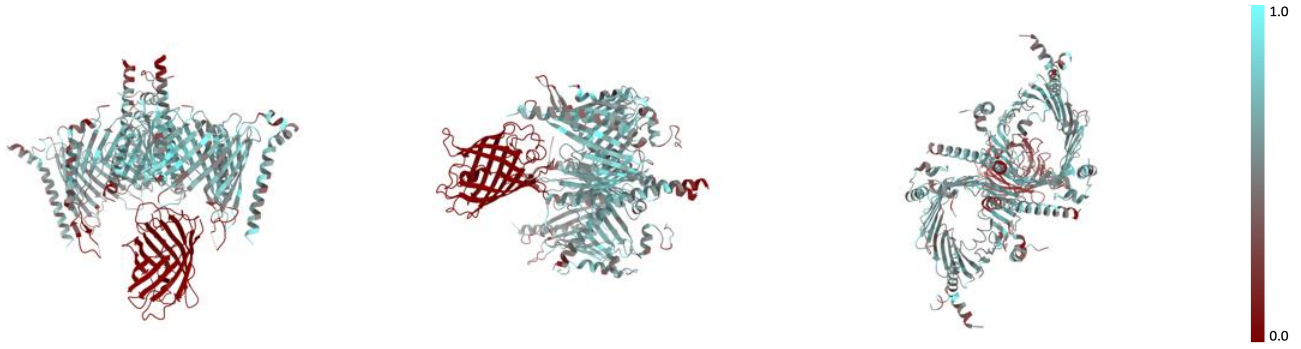
9.2 Q-score mapped to coordinate model (i)



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.

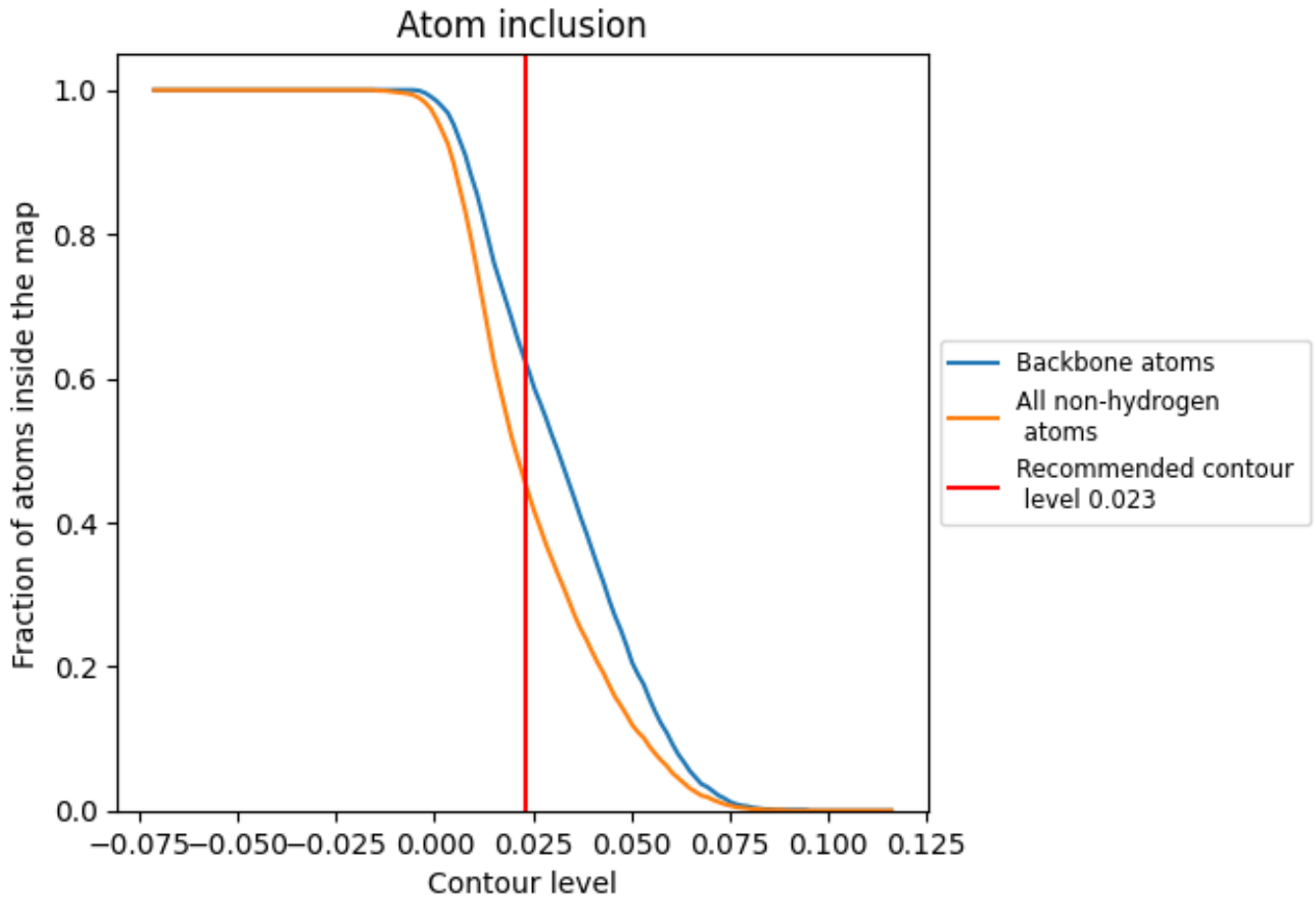
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4560	0.3400
A	0.6070	0.4290
B	0.4950	0.3710
C	0.5380	0.3080
D	0.5530	0.3600
E	0.6400	0.3990
G	0.0030	0.1110
I	0.5550	0.4060
J	0.4740	0.3480
K	0.4920	0.2720
L	0.4620	0.3590
M	0.5950	0.3770