



Full wwPDB EM Validation Report ⓘ

Dec 1, 2022 – 12:44 am GMT

PDB ID : 8B6L
EMDB ID : EMD-15870
Title : Subtomogram average of the human Sec61-TRAP-OSTA-translocon
Authors : Gemmer, M.; Fedry, J.M.M.; Forster, F.G.
Deposited on : 2022-09-27
Resolution : 7.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

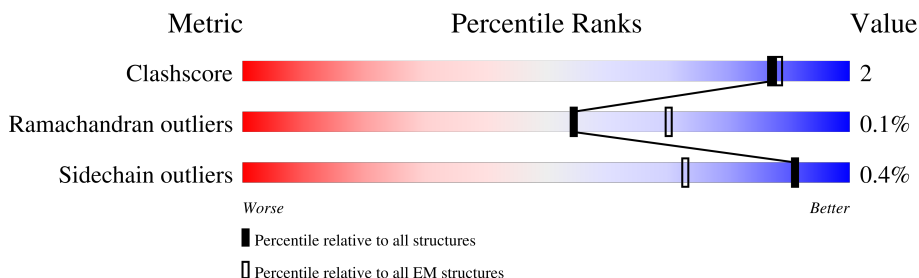
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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

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 $\leq 5\%$. 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	476	<div> <div>20%</div> <div>86%</div> <div>11%</div> </div>
2	B	96	<div> <div>20%</div> <div>78%</div> </div>
3	C	68	<div> <div>22%</div> <div>94%</div> <div>6%</div> </div>
4	D	22	<div> <div>9%</div> <div>100%</div> </div>
5	E	286	<div> <div>45%</div> <div>51%</div> <div>48%</div> </div>
6	F	183	<div> <div>64%</div> <div>81%</div> <div>16%</div> </div>
7	G	185	<div> <div>51%</div> <div>78%</div> <div>20%</div> </div>
8	H	173	<div> <div>71%</div> <div>78%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	705	
10	J	149	
11	K	37	
12	L	79	
13	M	113	
14	N	456	
15	O	607	
16	P	631	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29611 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 transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	425	Total	C	N	O	S	0	0
			3272	2153	518	580	21		

- Molecule 2 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	21	Total	C	N	O	S	0	0
			169	120	24	23	2		

- Molecule 3 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	68	Total	C	N	O	S	0	0
			543	355	94	89	5		

- Molecule 4 is a protein called Signal peptide mix.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 5 is a protein called Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1202	784	195	220	3		

- Molecule 6 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	153	Total	C	N	O	S	0	0
			1192	767	200	223	2		

- Molecule 7 is a protein called Translocon-associated protein subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	148	Total	C	N	O	S	0	0
			1197	795	193	207	2		

- Molecule 8 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	142	Total	C	N	O	S	0	0
			1115	709	188	215	3		

- Molecule 9 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	685	Total	C	N	O	S	0	0
			5515	3614	888	976	37		

- Molecule 10 is a protein called Oligosaccharyltransferase complex subunit OSTC.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	121	Total	C	N	O	S	0	0
			948	631	151	157	9		

- Molecule 11 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			295	196	46	51	2		

- Molecule 12 is a protein called Transmembrane protein 258.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	79	Total	C	N	O	S	0	0
			643	440	92	107	4		

- Molecule 13 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	110	Total	C	N	O	S	0	0
			863	573	135	151	4		

- Molecule 14 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	410	Total	C	N	O	S	0	0
			3224	2079	531	608	6		

- Molecule 15 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	580	Total	C	N	O	S	0	0
			4655	2978	785	883	9		

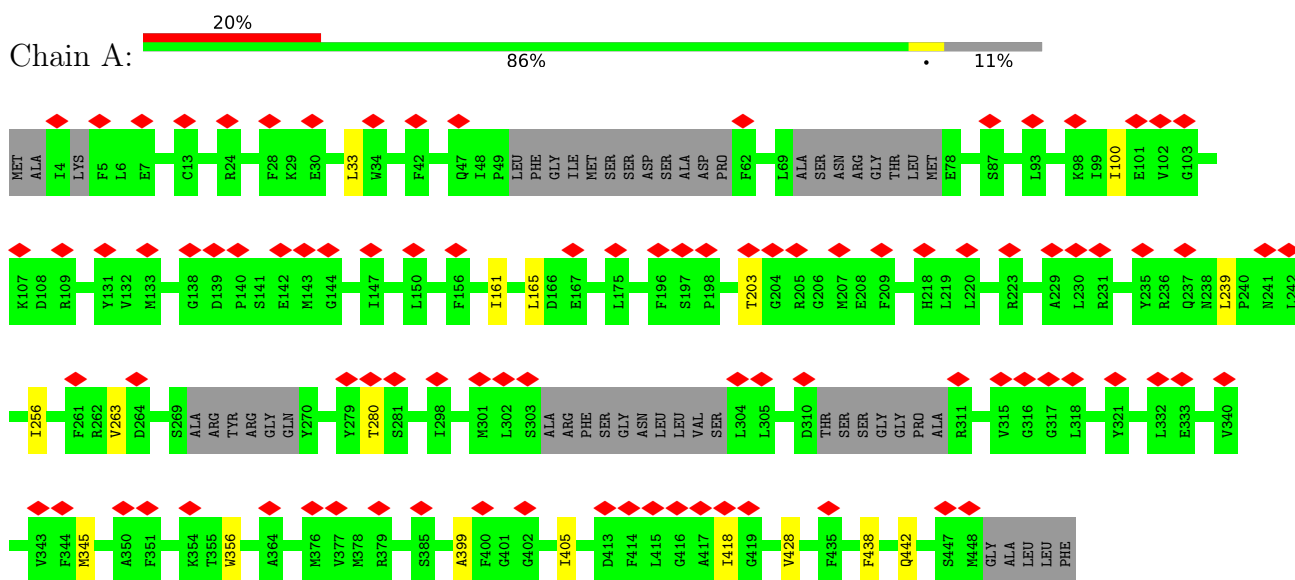
- Molecule 16 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	602	Total	C	N	O	S	0	0
			4668	2984	773	902	9		

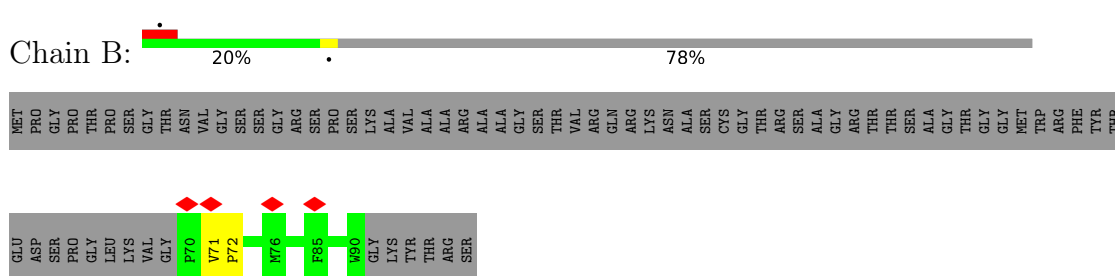
3 Residue-property plots

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.

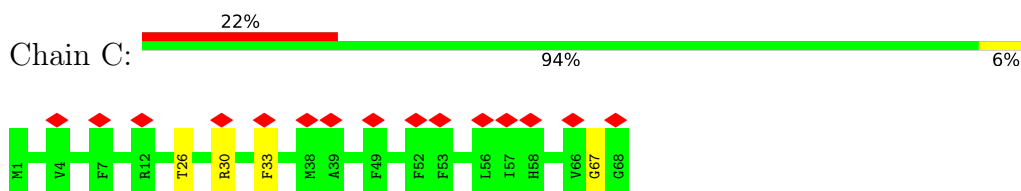
- Molecule 1: Protein transport protein Sec61 subunit alpha isoform 1



- Molecule 2: Protein transport protein Sec61 subunit beta



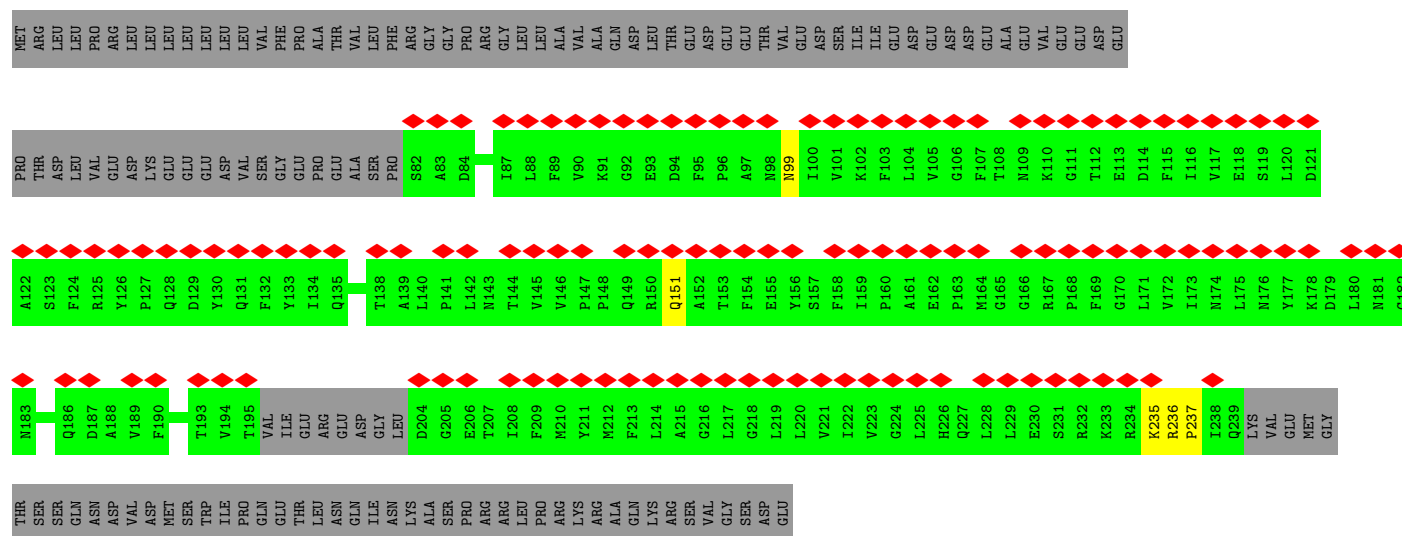
- Molecule 3: Protein transport protein Sec61 subunit gamma



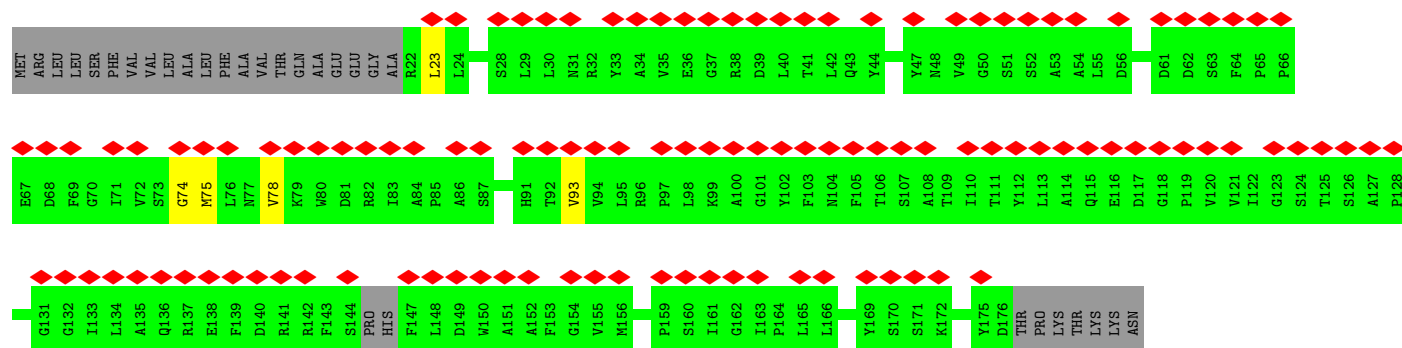
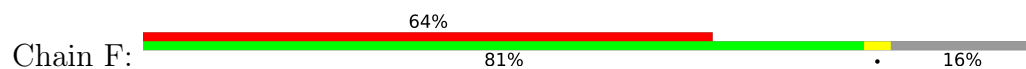
- Molecule 4: Signal peptide mix



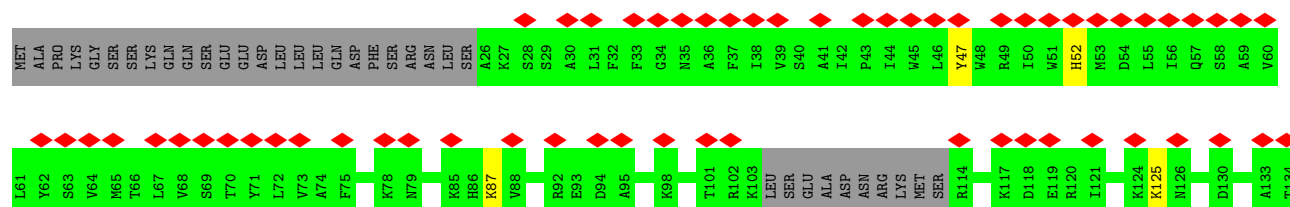
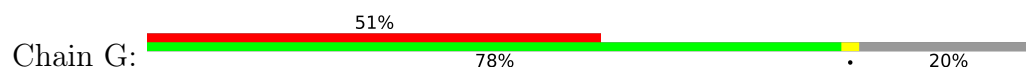
• Molecule 5: Translocon-associated protein subunit alpha

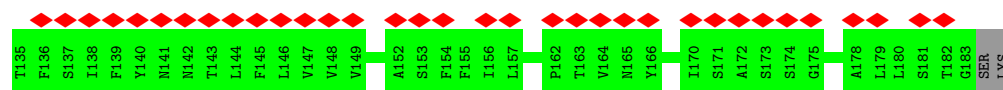


• Molecule 6: Translocon-associated protein subunit beta



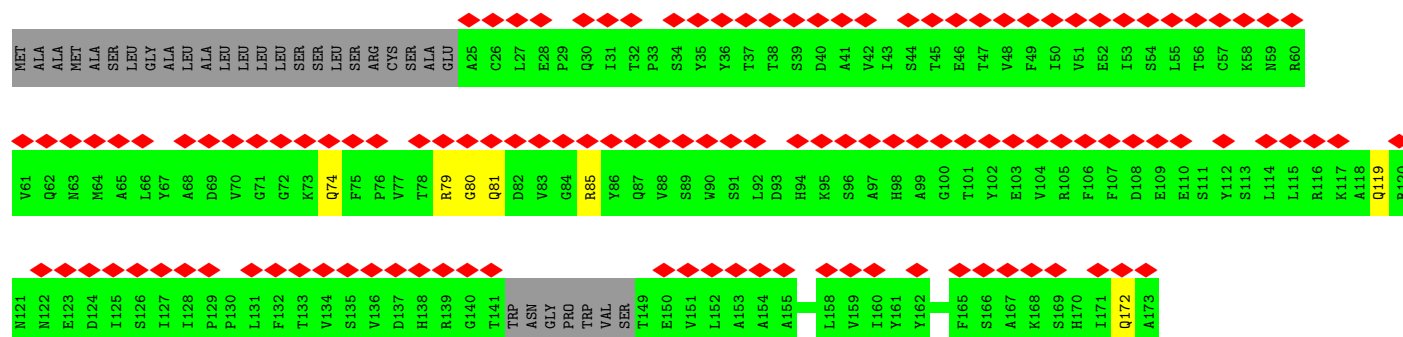
• Molecule 7: Translocon-associated protein subunit gamma





• Molecule 8: Translocon-associated protein subunit delta

Chain H: 71% 78% 18%



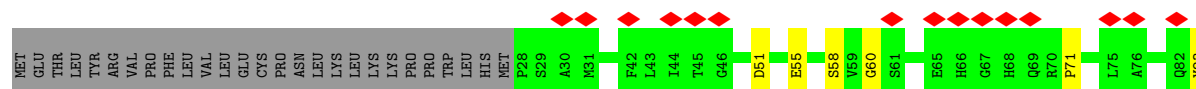
• Molecule 9: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A

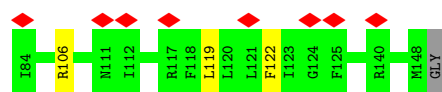
Chain I: 19% 95% 1%



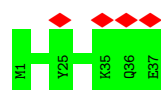
• Molecule 10: Oligosaccharyltransferase complex subunit OSTC

Chain J: 15% 75% 6% 19%

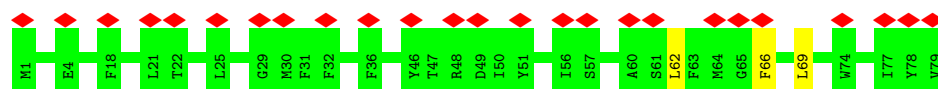




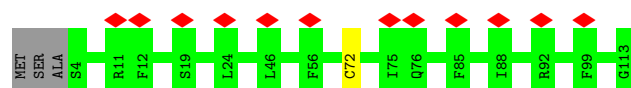
- Molecule 11: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4



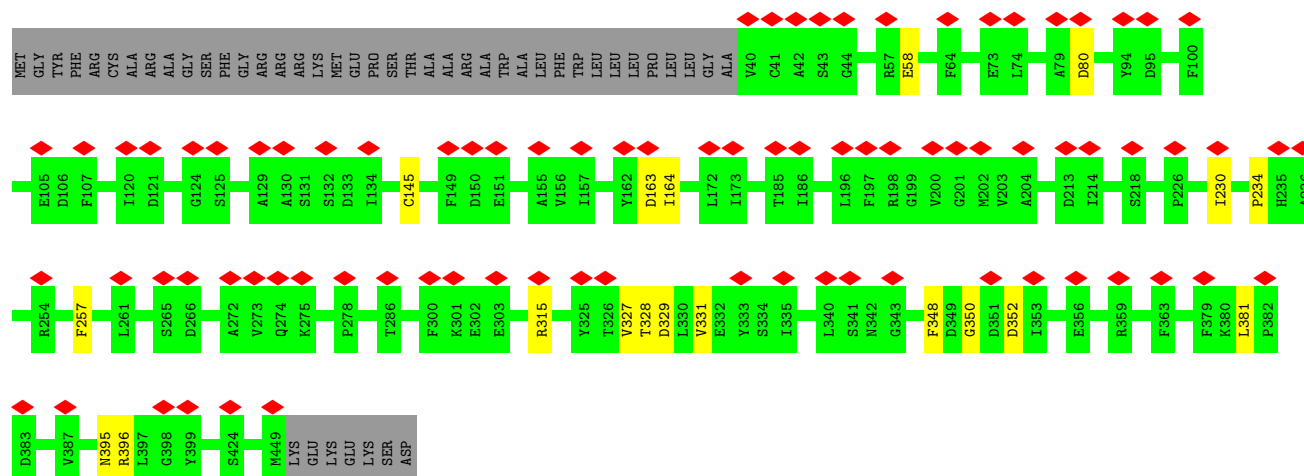
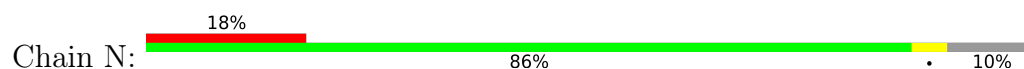
- Molecule 12: Transmembrane protein 258



- Molecule 13: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1

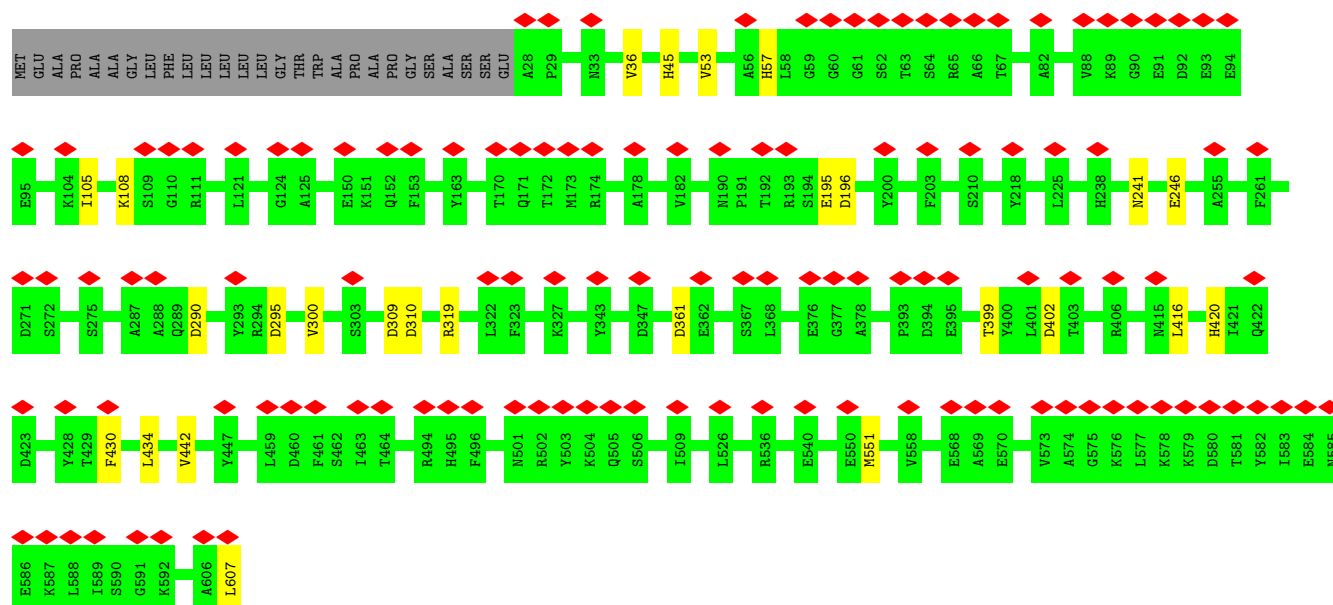


- Molecule 14: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit



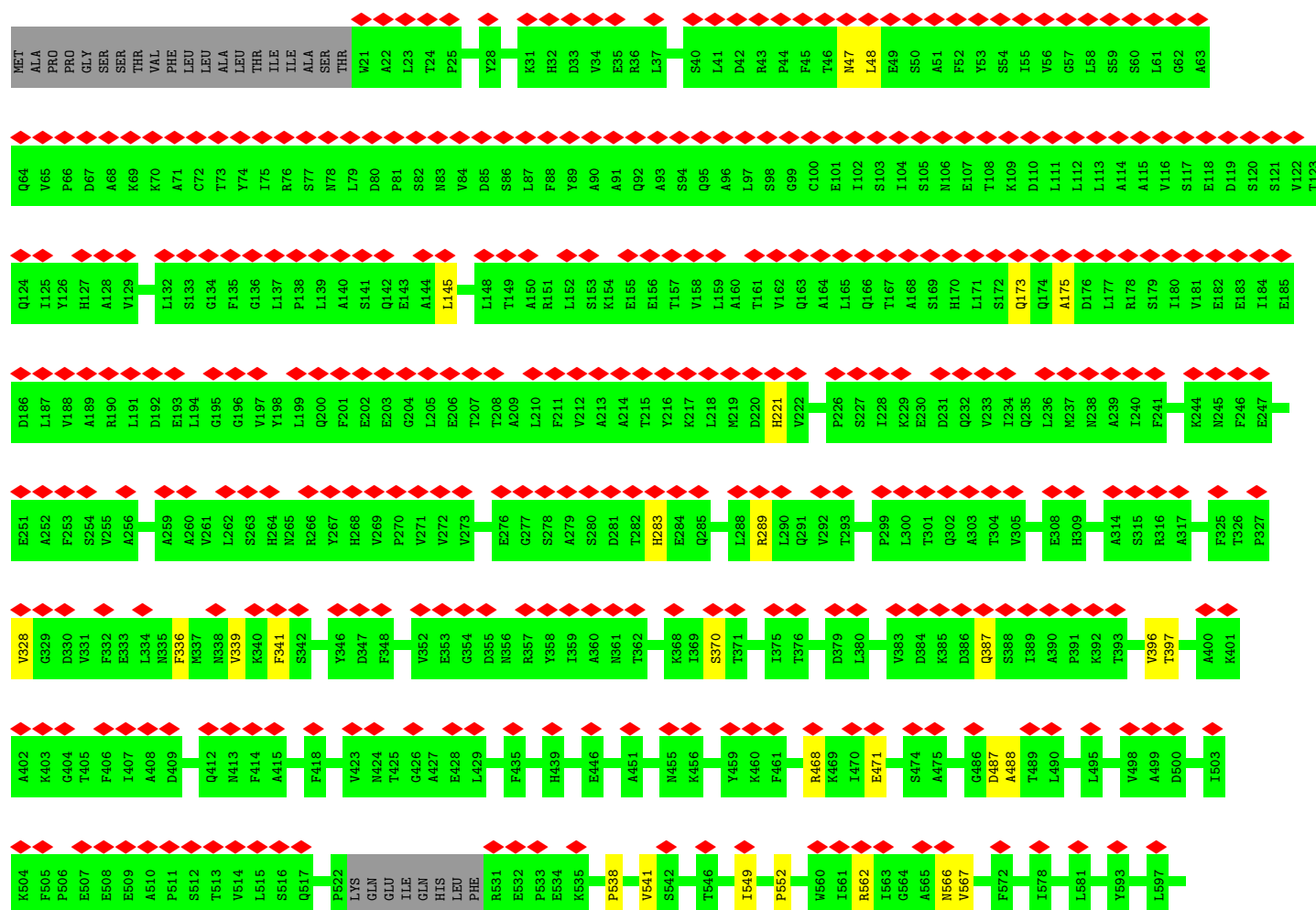
- Molecule 15: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1

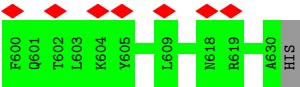




- Molecule 16: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2

Chain P: 58% 91% 5%





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	3D CRYSTAL, $a=600$ Å, $b=600$ Å, $c=600$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, $\gamma=90^\circ$, space group=C1	Depositor
Number of subtomograms used	42215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Estimation and correction in WARP/M	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	79000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	599.95197, 599.95197, 599.95197	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7239999, 1.7239999, 1.7239999	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/3336	0.52	0/4519
2	B	0.26	0/175	0.42	0/239
3	C	0.29	0/553	0.59	0/738
5	E	0.26	0/1231	0.50	0/1670
6	F	0.27	0/1220	0.50	0/1658
7	G	0.27	0/1225	0.46	0/1661
8	H	0.25	0/1138	0.47	0/1547
9	I	0.26	0/5668	0.50	1/7700 (0.0%)
10	J	0.27	0/973	0.54	0/1317
11	K	0.28	0/300	0.40	0/406
12	L	0.29	0/663	0.53	0/903
13	M	0.27	0/883	0.48	0/1197
14	N	0.25	0/3306	0.48	0/4493
15	O	0.24	0/4752	0.51	1/6444 (0.0%)
16	P	0.24	0/4760	0.46	0/6483
All	All	0.26	0/30183	0.49	2/40975 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	675	LEU	CB-CG-CD2	5.82	120.89	111.00
15	O	290	ASP	CB-CG-OD1	5.43	123.19	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	THR	Peptide
1	A	239	LEU	Peptide

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	3272	0	3360	11	0
2	B	169	0	184	1	0
3	C	543	0	577	3	0
4	D	110	0	24	0	0
5	E	1202	0	1186	2	0
6	F	1192	0	1179	7	0
7	G	1197	0	1231	2	0
8	H	1115	0	1091	6	0
9	I	5515	0	5470	9	0
10	J	948	0	975	7	0
11	K	295	0	312	0	0
12	L	643	0	659	2	0
13	M	863	0	880	1	0
14	N	3224	0	3161	13	0
15	O	4655	0	4687	12	0
16	P	4668	0	4670	14	0
All	All	29611	0	29646	79	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 2.

All (79) 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)
16:P:283:HIS:ND1	16:P:370:SER:O	2.19	0.74
15:O:295:ASP:OD2	15:O:319:ARG:NH1	2.22	0.73
5:E:151:GLN:NE2	6:F:23:LEU:O	2.22	0.71
14:N:327:VAL:O	14:N:328:THR:HG22	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:47:TYR:O	7:G:52:HIS:N	2.31	0.64
1:A:280:THR:HG22	1:A:356:TRP:CH2	2.32	0.64
1:A:256:ILE:HD11	1:A:428:VAL:CG1	2.31	0.60
14:N:352:ASP:O	14:N:352:ASP:OD1	2.20	0.60
12:L:69:LEU:HD21	15:O:442:VAL:HG21	1.84	0.58
15:O:399:THR:N	15:O:402:ASP:OD2	2.38	0.56
15:O:195:GLU:HG3	15:O:196:ASP:H	1.70	0.56
14:N:80:ASP:OD1	14:N:80:ASP:O	2.24	0.55
6:F:75:MET:SD	8:H:81:GLN:N	2.80	0.54
6:F:75:MET:SD	8:H:80:GLY:HA2	2.48	0.53
9:I:675:LEU:HD22	9:I:678:LEU:HD21	1.89	0.52
14:N:230:ILE:HD11	14:N:234:PRO:HG3	1.92	0.52
1:A:33:LEU:HD22	10:J:119:LEU:HD13	1.91	0.51
14:N:145:CYS:HG	14:N:257:PHE:HZ	1.57	0.51
9:I:154:VAL:O	9:I:154:VAL:HG13	2.10	0.51
16:P:538:PRO:O	16:P:541:VAL:HG12	2.11	0.50
16:P:47:ASN:OD1	16:P:48:LEU:N	2.44	0.50
1:A:100:ILE:HG22	1:A:100:ILE:O	2.11	0.49
9:I:365:GLN:HG2	9:I:366:LEU:N	2.26	0.49
16:P:487:ASP:OD1	16:P:488:ALA:N	2.45	0.49
8:H:80:GLY:N	8:H:85:ARG:O	2.30	0.49
6:F:75:MET:CE	8:H:79:ARG:O	2.61	0.49
2:B:71:VAL:N	2:B:72:PRO:CD	2.77	0.47
1:A:33:LEU:CD2	10:J:119:LEU:HD13	2.44	0.47
1:A:418:ILE:HD12	1:A:418:ILE:H	1.79	0.47
16:P:468:ARG:O	16:P:471:GLU:N	2.47	0.47
9:I:56:THR:HB	9:I:93:MET:SD	2.54	0.47
9:I:88:ILE:HD13	9:I:93:MET:HE1	1.96	0.47
10:J:119:LEU:O	10:J:122:PHE:N	2.46	0.47
15:O:309:ASP:OD1	15:O:310:ASP:N	2.48	0.47
1:A:438:PHE:CE1	1:A:442:GLN:HG3	2.50	0.46
9:I:675:LEU:HD22	9:I:678:LEU:HD11	1.98	0.46
14:N:327:VAL:O	14:N:328:THR:CG2	2.62	0.46
14:N:58:GLU:HA	14:N:58:GLU:OE1	2.16	0.46
14:N:315:ARG:NE	14:N:329:ASP:OD2	2.47	0.46
14:N:230:ILE:HG23	14:N:230:ILE:O	2.16	0.46
1:A:161:ILE:O	1:A:165:LEU:HG	2.16	0.46
15:O:36:VAL:HG22	15:O:53:VAL:HG12	1.98	0.46
15:O:430:PHE:CZ	15:O:434:LEU:HB2	2.51	0.45
9:I:678:LEU:H	9:I:678:LEU:HD23	1.81	0.45
14:N:395:ASN:O	14:N:396:ARG:NH1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:MET:HE3	6:F:75:MET:HB2	1.89	0.44
1:A:100:ILE:O	1:A:100:ILE:CG2	2.66	0.44
3:C:30:ARG:O	3:C:33:PHE:HB3	2.18	0.43
15:O:295:ASP:OD2	15:O:300:VAL:CG2	2.67	0.43
15:O:551:MET:HE1	15:O:607:LEU:HD11	2.01	0.43
10:J:51:ASP:O	10:J:55:GLU:HA	2.19	0.43
5:E:236:ARG:N	5:E:237:PRO:CD	2.82	0.42
15:O:105:ILE:HG23	15:O:108:LYS:HB2	2.01	0.42
1:A:263:VAL:CG1	3:C:26:THR:HB	2.49	0.42
9:I:192:ILE:HD11	13:M:72:CYS:HB3	2.01	0.42
10:J:58:SER:O	10:J:83:TYR:HB3	2.20	0.42
16:P:173:GLN:NE2	16:P:221:HIS:O	2.43	0.42
16:P:549:ILE:O	16:P:552:PRO:HD2	2.20	0.42
16:P:566:ASN:OD1	16:P:567:VAL:N	2.52	0.42
7:G:87:LYS:NZ	8:H:172:GLN:O	2.50	0.42
8:H:74:GLN:NE2	8:H:119:GLN:OE1	2.53	0.42
1:A:405:ILE:H	1:A:405:ILE:HD12	1.84	0.41
6:F:74:GLY:HA3	6:F:93:VAL:HA	2.02	0.41
16:P:387:GLN:O	16:P:387:GLN:HG3	2.20	0.41
14:N:331:VAL:HG21	14:N:381:LEU:HD21	2.02	0.41
16:P:339:VAL:HG23	16:P:341:PHE:CE2	2.55	0.41
3:C:67:GLY:HA2	10:J:71:PRO:O	2.20	0.41
12:L:62:LEU:O	12:L:66:PHE:HD2	2.03	0.41
15:O:416:LEU:HG	15:O:420:HIS:ND1	2.35	0.41
16:P:396:VAL:HG12	16:P:397:THR:N	2.35	0.41
9:I:676:ASP:OD1	9:I:676:ASP:N	2.54	0.41
16:P:145:LEU:HD22	16:P:175:ALA:HB1	2.02	0.41
16:P:328:VAL:O	16:P:328:VAL:HG23	2.21	0.41
16:P:562:ARG:O	16:P:562:ARG:CG	2.68	0.41
6:F:75:MET:HE1	6:F:78:VAL:HG23	2.03	0.40
10:J:60:GLY:O	10:J:71:PRO:HA	2.21	0.40
14:N:163:ASP:OD1	14:N:164:ILE:N	2.54	0.40
14:N:348:PHE:CE2	14:N:350:GLY:HA3	2.56	0.40
15:O:246:GLU:HG3	15:O:246:GLU:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	412/476 (87%)	377 (92%)	34 (8%)	1 (0%)	47	81
2	B	19/96 (20%)	17 (90%)	2 (10%)	0	100	100
3	C	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
5	E	146/286 (51%)	140 (96%)	6 (4%)	0	100	100
6	F	149/183 (81%)	149 (100%)	0	0	100	100
7	G	144/185 (78%)	139 (96%)	5 (4%)	0	100	100
8	H	138/173 (80%)	138 (100%)	0	0	100	100
9	I	681/705 (97%)	664 (98%)	16 (2%)	1 (0%)	51	86
10	J	119/149 (80%)	117 (98%)	2 (2%)	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
12	L	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
13	M	108/113 (96%)	107 (99%)	1 (1%)	0	100	100
14	N	408/456 (90%)	394 (97%)	14 (3%)	0	100	100
15	O	578/607 (95%)	554 (96%)	23 (4%)	1 (0%)	47	81
16	P	598/631 (95%)	569 (95%)	29 (5%)	0	100	100
All	All	3678/4244 (87%)	3534 (96%)	141 (4%)	3 (0%)	54	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ALA
15	O	45	HIS
9	I	646	ARG

5.3.2 Protein sidechains ⓘ

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	353/398 (89%)	352 (100%)	1 (0%)	92	95
2	B	20/74 (27%)	20 (100%)	0	100	100
3	C	59/59 (100%)	59 (100%)	0	100	100
5	E	131/253 (52%)	129 (98%)	2 (2%)	65	80
6	F	128/153 (84%)	128 (100%)	0	100	100
7	G	130/165 (79%)	129 (99%)	1 (1%)	81	89
8	H	122/145 (84%)	122 (100%)	0	100	100
9	I	596/615 (97%)	594 (100%)	2 (0%)	92	95
10	J	103/130 (79%)	102 (99%)	1 (1%)	76	86
11	K	33/33 (100%)	33 (100%)	0	100	100
12	L	70/70 (100%)	70 (100%)	0	100	100
13	M	96/98 (98%)	96 (100%)	0	100	100
14	N	356/391 (91%)	356 (100%)	0	100	100
15	O	519/537 (97%)	516 (99%)	3 (1%)	86	92
16	P	516/541 (95%)	514 (100%)	2 (0%)	91	94
All	All	3232/3662 (88%)	3220 (100%)	12 (0%)	91	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	MET
5	E	99	ASN
5	E	235	LYS
7	G	125	LYS
9	I	664	ARG
9	I	700	ARG
10	J	106	ARG
15	O	57	HIS
15	O	241	ASN
15	O	361	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	289	ARG
16	P	336	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

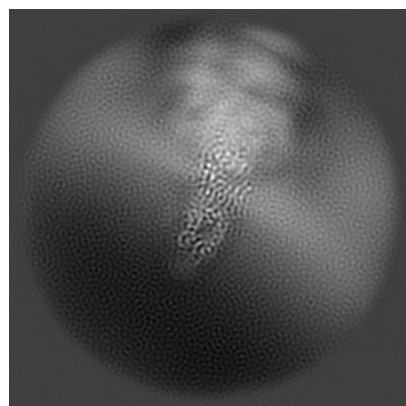
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15870. These allow visual inspection of the internal detail of the map and identification of artifacts.

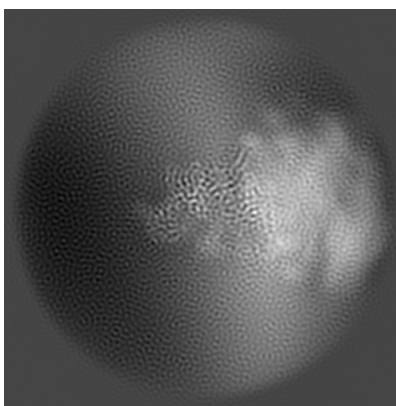
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

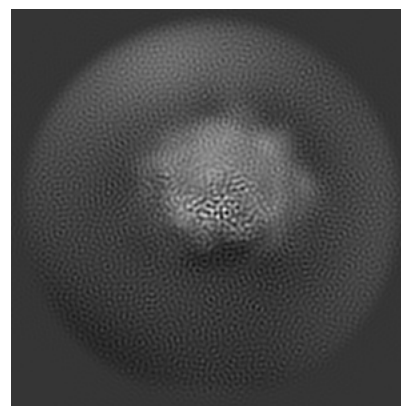
6.1.1 Primary map



X

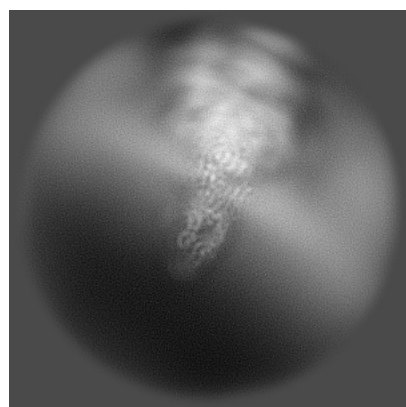


Y

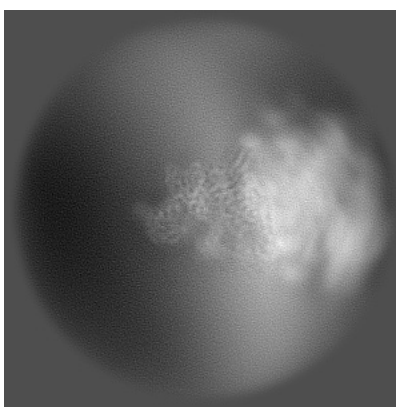


Z

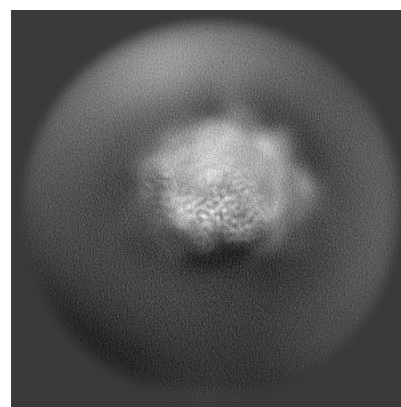
6.1.2 Raw map



X



Y

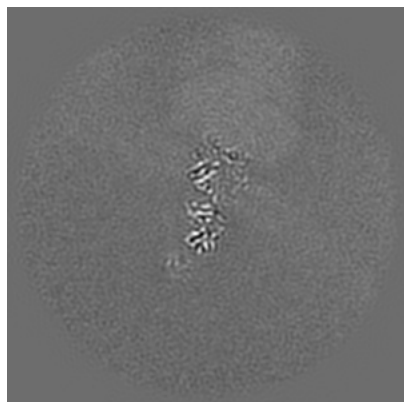


Z

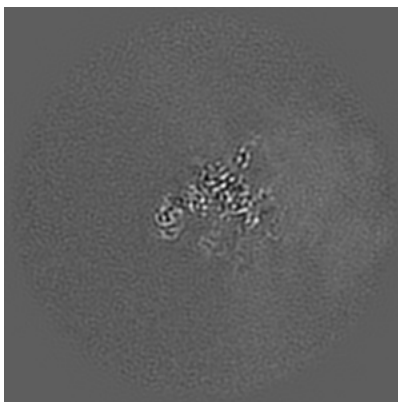
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

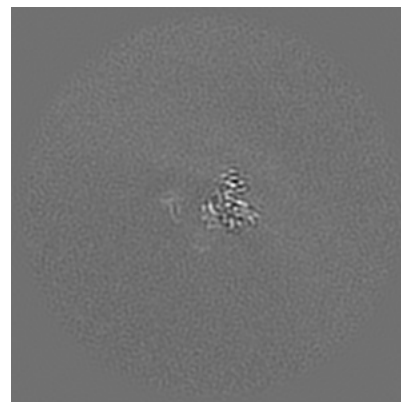
6.2.1 Primary map



X Index: 174

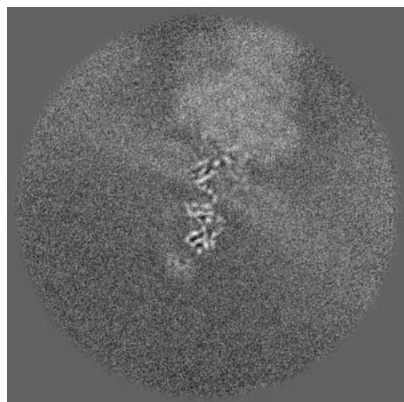


Y Index: 174

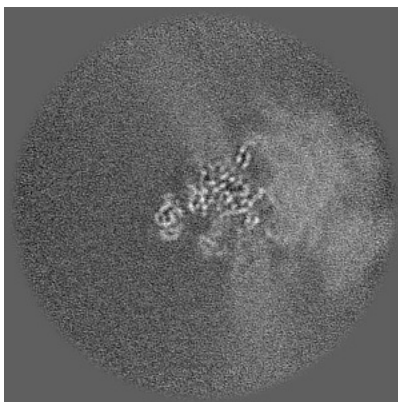


Z Index: 174

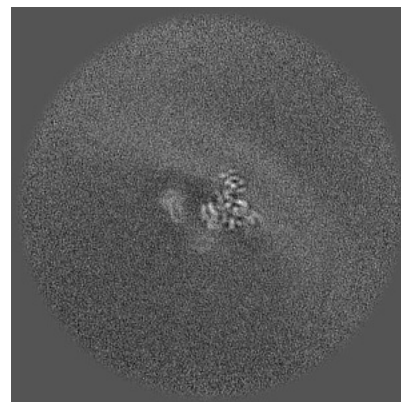
6.2.2 Raw map



X Index: 174



Y Index: 174

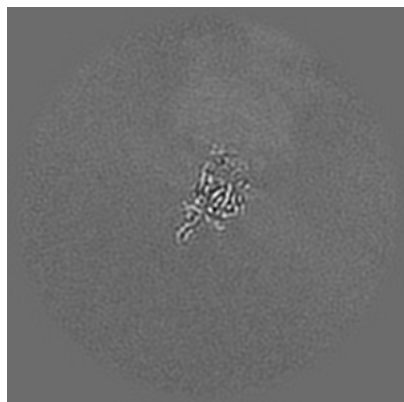


Z Index: 174

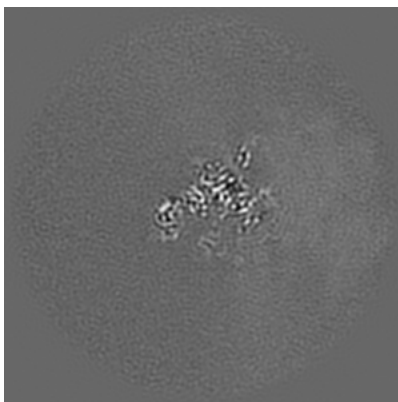
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

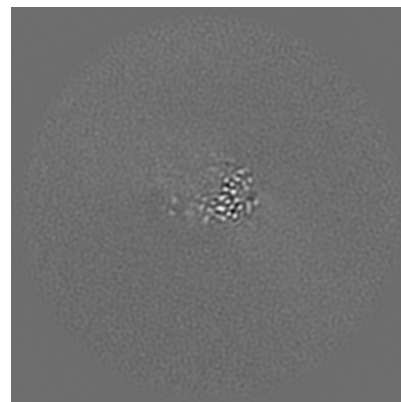
6.3.1 Primary map



X Index: 191

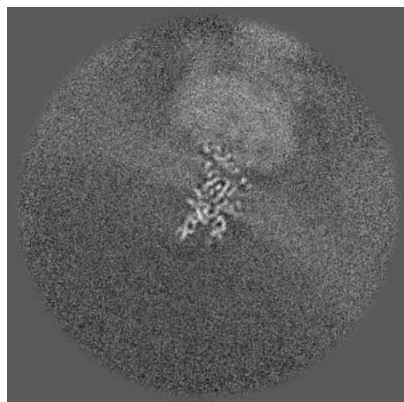


Y Index: 173

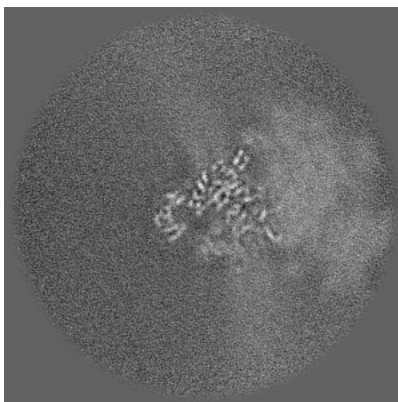


Z Index: 189

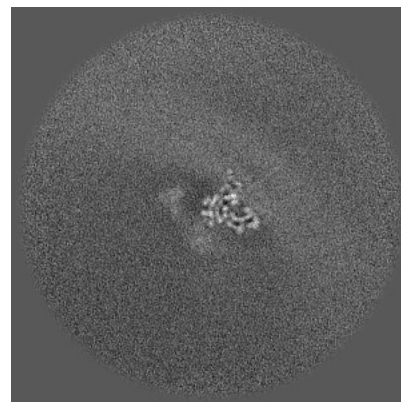
6.3.2 Raw map



X Index: 186



Y Index: 177

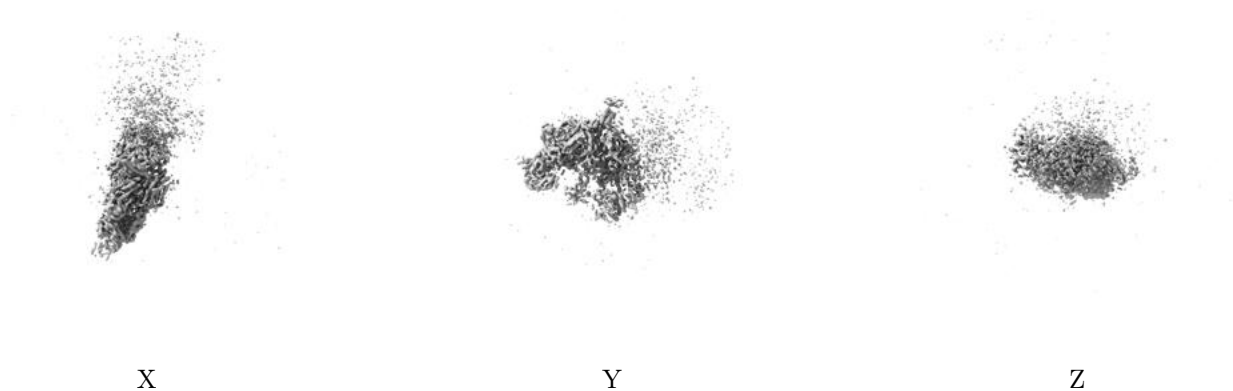


Z Index: 169

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

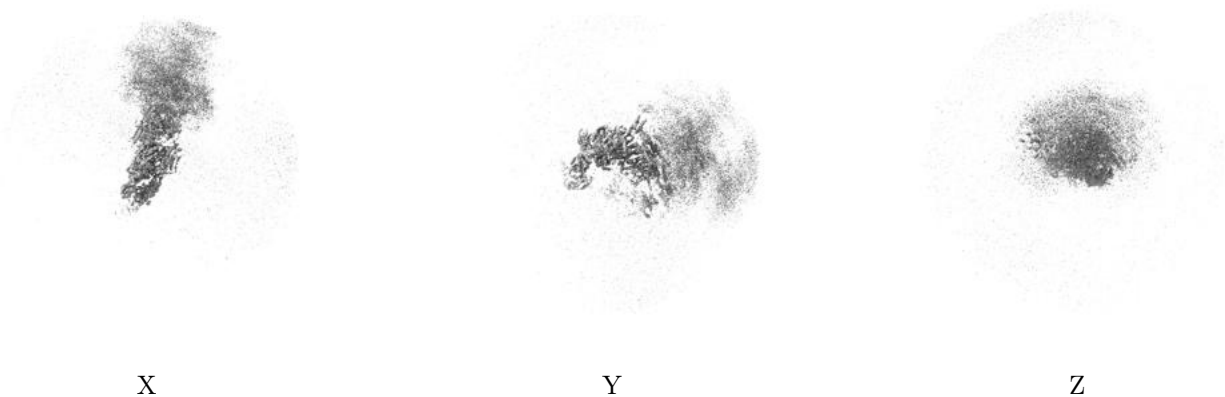
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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.

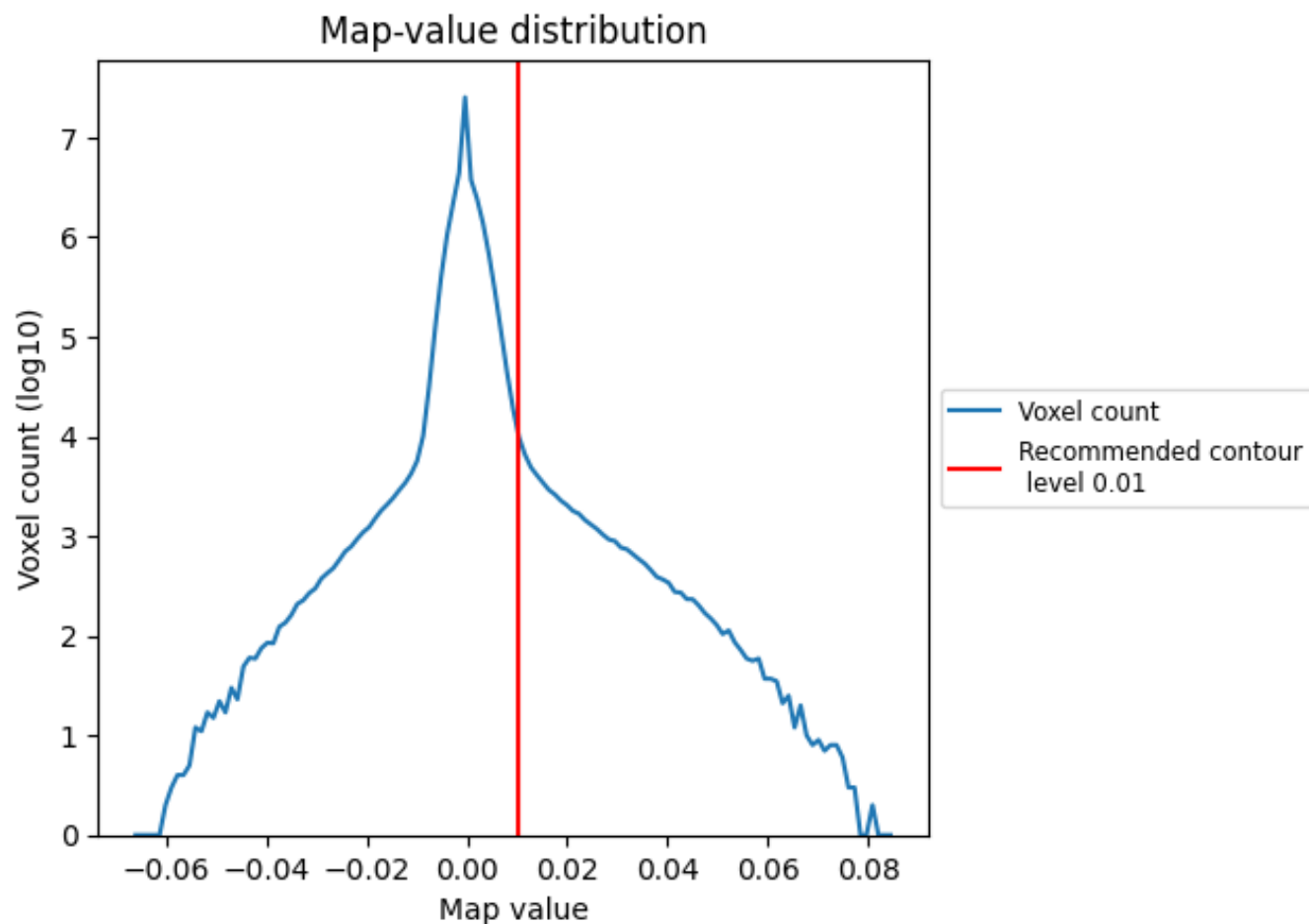
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

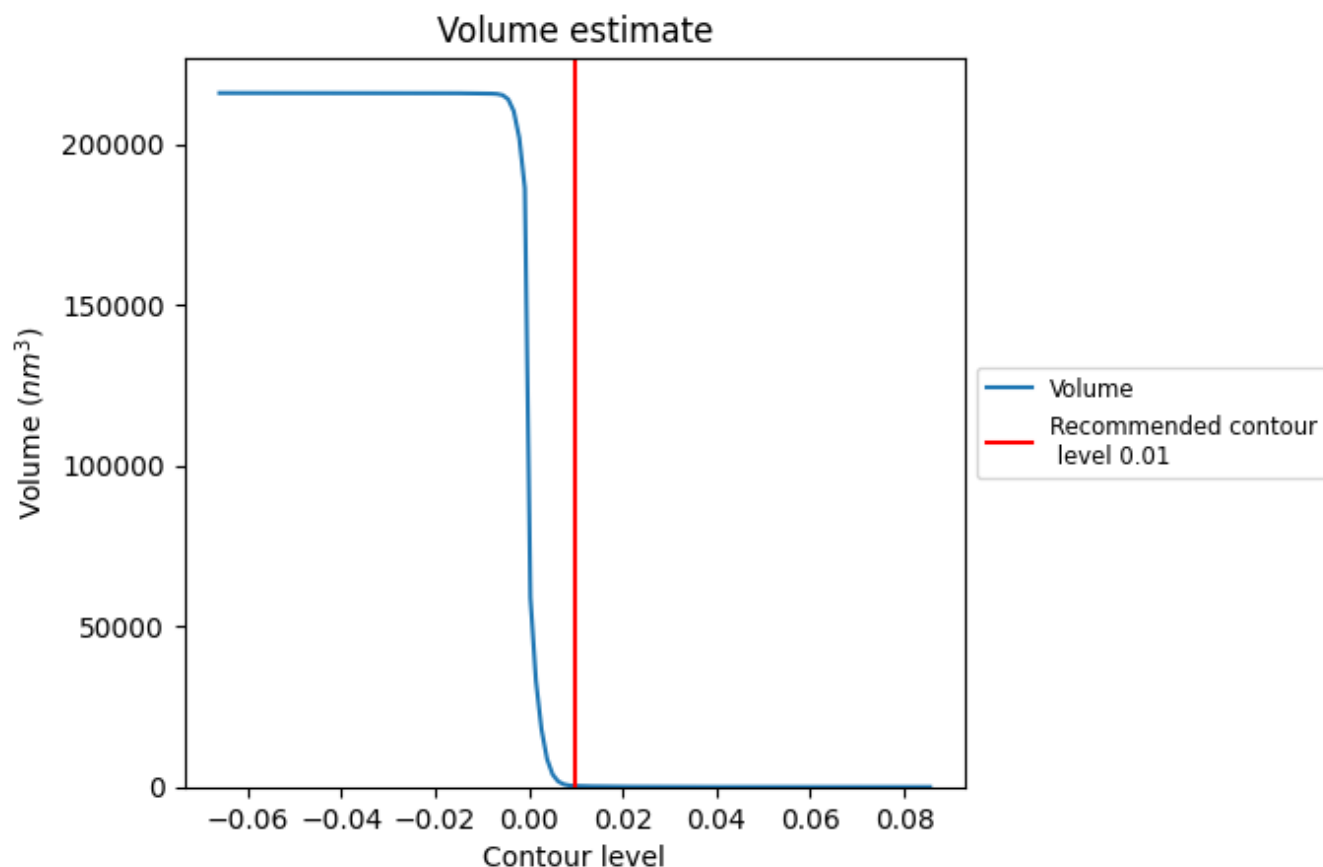
This section contains the results of statistical analysis of the map.

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.

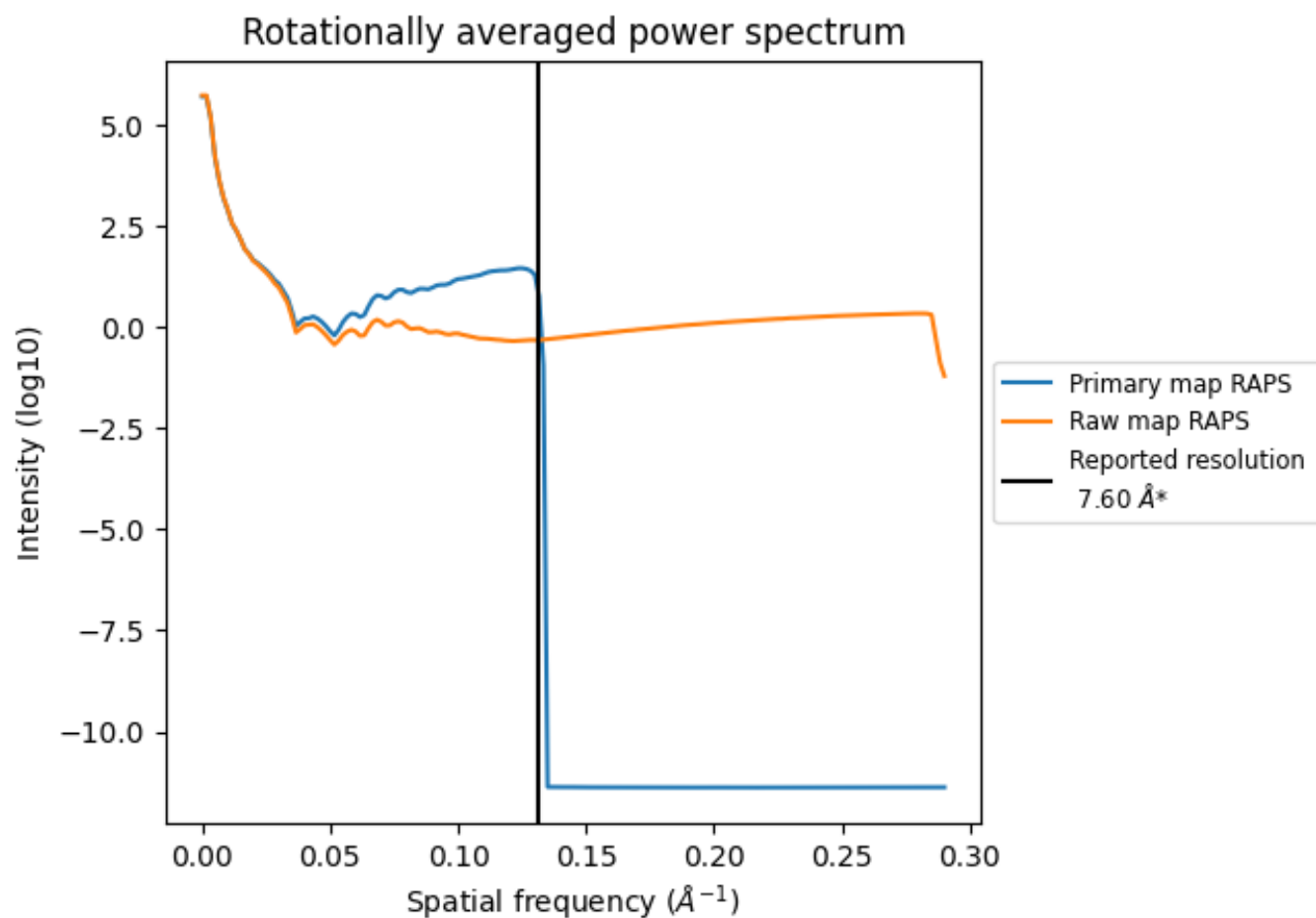
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm^3 ; this corresponds to an approximate mass of 284 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 ⓘ

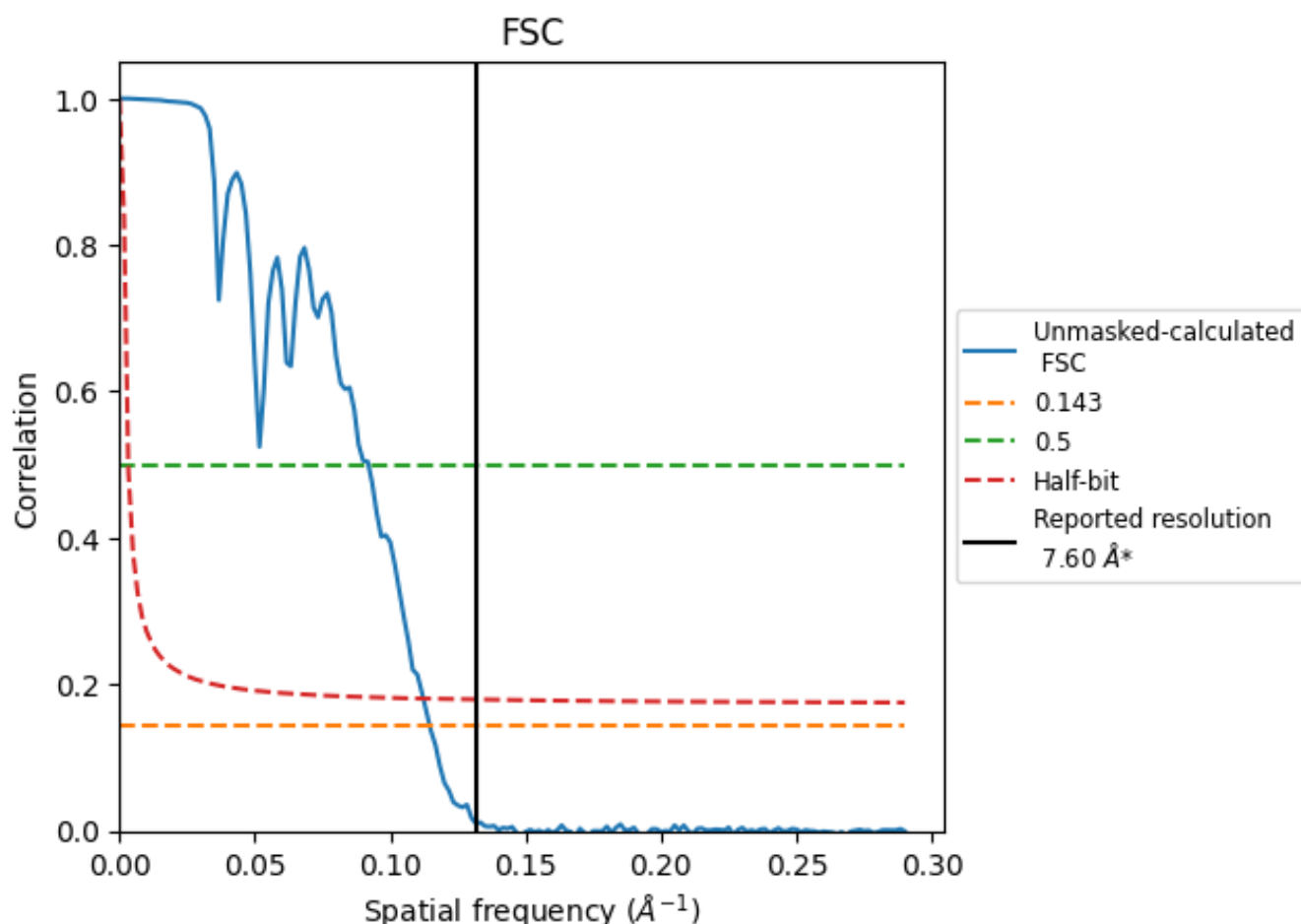


*Reported resolution corresponds to spatial frequency of 0.132 \AA^{-1}

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 0.132 \AA^{-1}

8.2 Resolution estimates [i](#)

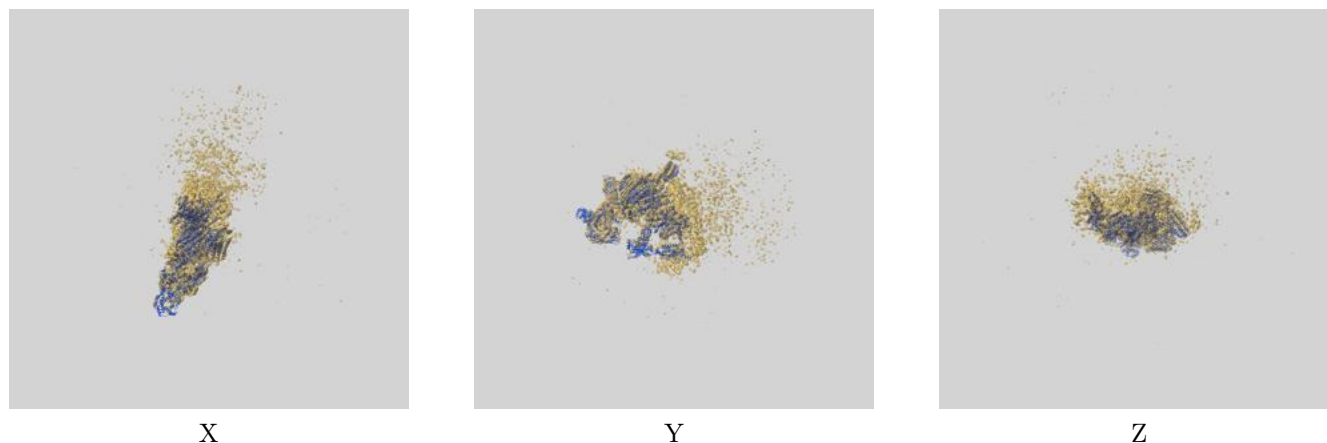
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.73	10.88	8.91

*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 8.73 differs from the reported value 7.6 by more than 10 %

9 Map-model fit [i](#)

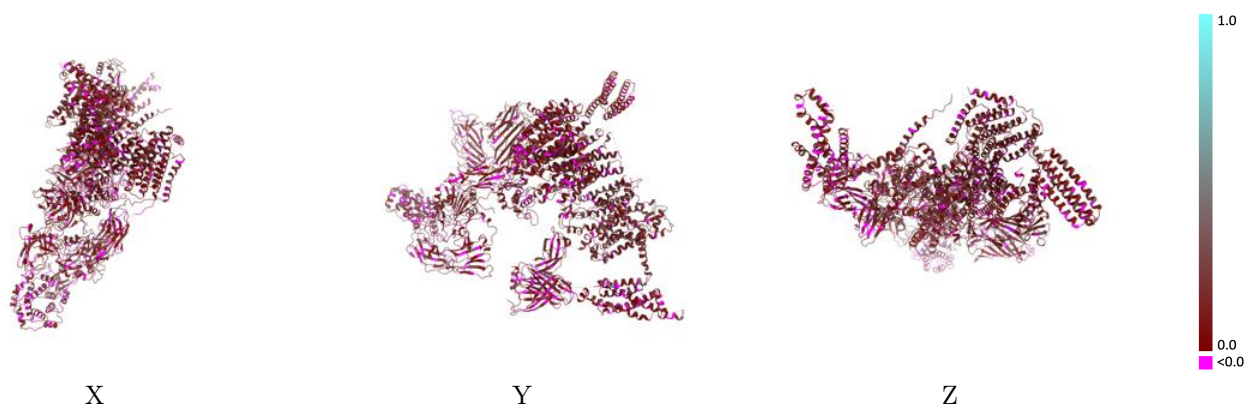
This section contains information regarding the fit between EMDB map EMD-15870 and PDB model 8B6L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



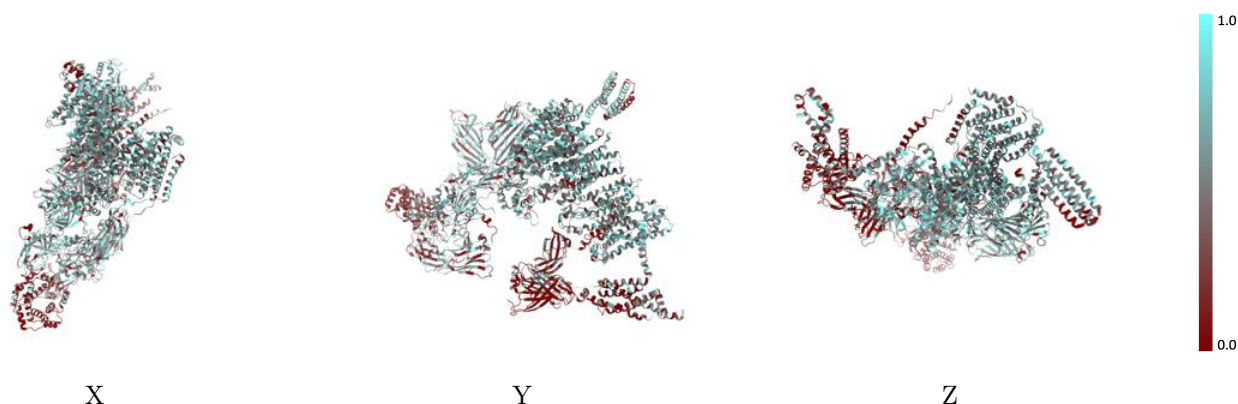
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



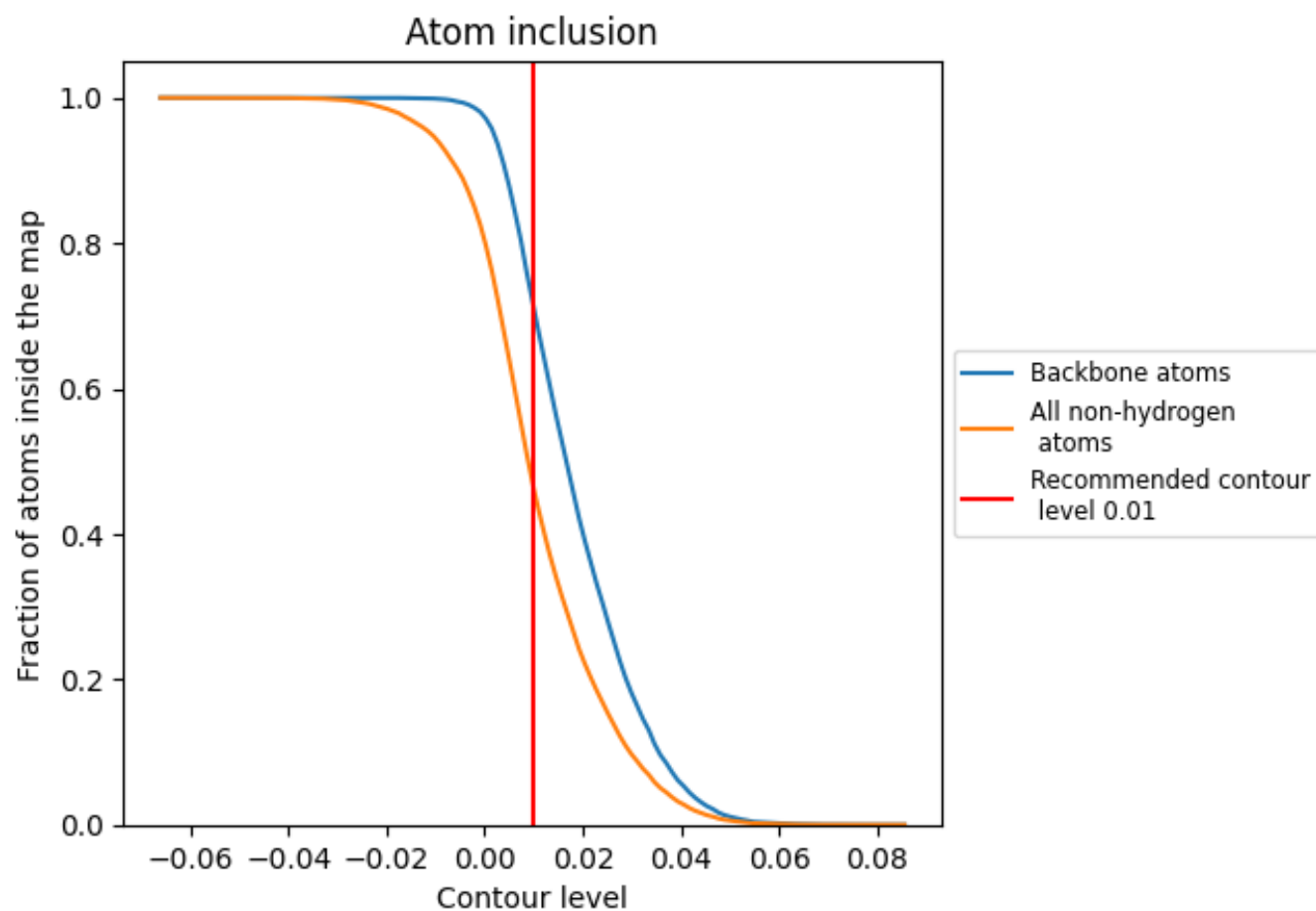
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4630	 0.1330
A	 0.5629	 0.1860
B	 0.5833	 0.1790
C	 0.5551	 0.1760
D	 0.7818	 0.3170
E	 0.1934	 0.1350
F	 0.2259	 0.1110
G	 0.3061	 0.0930
H	 0.1392	 0.0950
I	 0.5522	 0.1280
J	 0.5473	 0.1350
K	 0.5427	 0.1110
L	 0.5032	 0.1440
M	 0.5899	 0.1330
N	 0.5672	 0.1320
O	 0.5442	 0.1340
P	 0.3086	 0.1180

