Full wwPDB EM Validation Report

Feb 4, 2024 – 04:00 PM EST

PDB ID	:	7UNE
EMDB ID	:	EMD-26622
Title	:	The V1 region of bovine V-ATPase in complex with human mEAK7 (focused refinement)
Authors	:	Wang, R.; Li, X.
Deposited on	:	2022-04-10
Resolution	:	3.73 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:

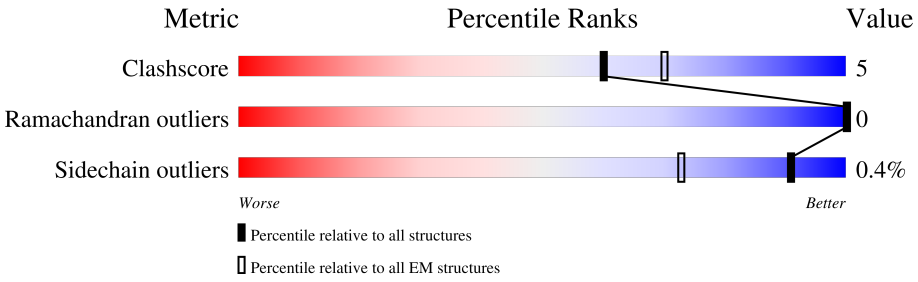
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.73 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	L	617	5% 83% 14% ·
1	M	617	· 84% 12% ·
1	N	617	6% 83% 13% ·
2	D	247	14% 73% 13% 14%
3	U	463	25% 81% 12% 8%
4	b	226	6% 81% 19%
4	c	226	6% 86% 14%
4	d	226	· 99% ·

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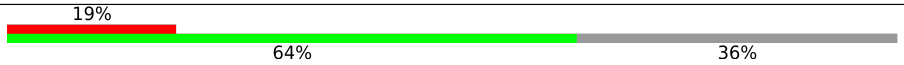
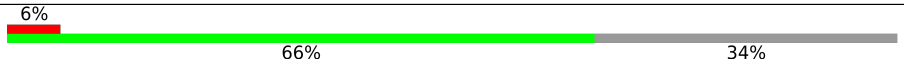
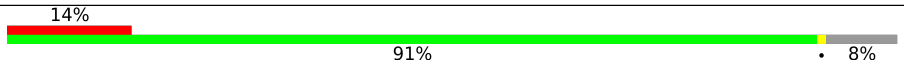
Mol	Chain	Length	Quality of chain
5	O	511	
5	P	511	
5	Q	511	
6	e	118	
6	f	118	
6	g	118	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36209 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 V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	600	Total	C	N	O	S	0	0
			4656	2952	787	889	28		
1	M	594	Total	C	N	O	S	0	0
			4619	2928	781	883	27		
1	N	593	Total	C	N	O	S	0	0
			4613	2925	779	882	27		

- Molecule 2 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	213	Total	C	N	O	S	0	0
			1717	1090	310	312	5		

- Molecule 3 is a protein called KIAA1609 protein, isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	427	Total	C	N	O	S	0	0
			3365	2119	594	631	21		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-6	MET	-	initiating methionine	UNP D3DUL8
U	-5	GLY	-	expression tag	UNP D3DUL8
U	-4	HIS	-	expression tag	UNP D3DUL8
U	-3	HIS	-	expression tag	UNP D3DUL8
U	-2	HIS	-	expression tag	UNP D3DUL8
U	-1	HIS	-	expression tag	UNP D3DUL8
U	0	HIS	-	expression tag	UNP D3DUL8
U	1	HIS	-	expression tag	UNP D3DUL8

- Molecule 4 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	224	Total	C	N	O	S	0	0
			1818	1142	323	344	9		
4	b	182	Total	C	N	O	S	0	0
			1479	934	266	272	7		
4	c	195	Total	C	N	O	S	0	0
			1505	946	273	280	6		

- Molecule 5 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	460	Total	C	N	O	S	0	0
			3604	2286	616	682	20		
5	O	459	Total	C	N	O	S	0	0
			3595	2281	615	679	20		
5	P	455	Total	C	N	O	S	0	0
			3560	2260	608	672	20		

- Molecule 6 is a protein called V-type proton ATPase subunit G.

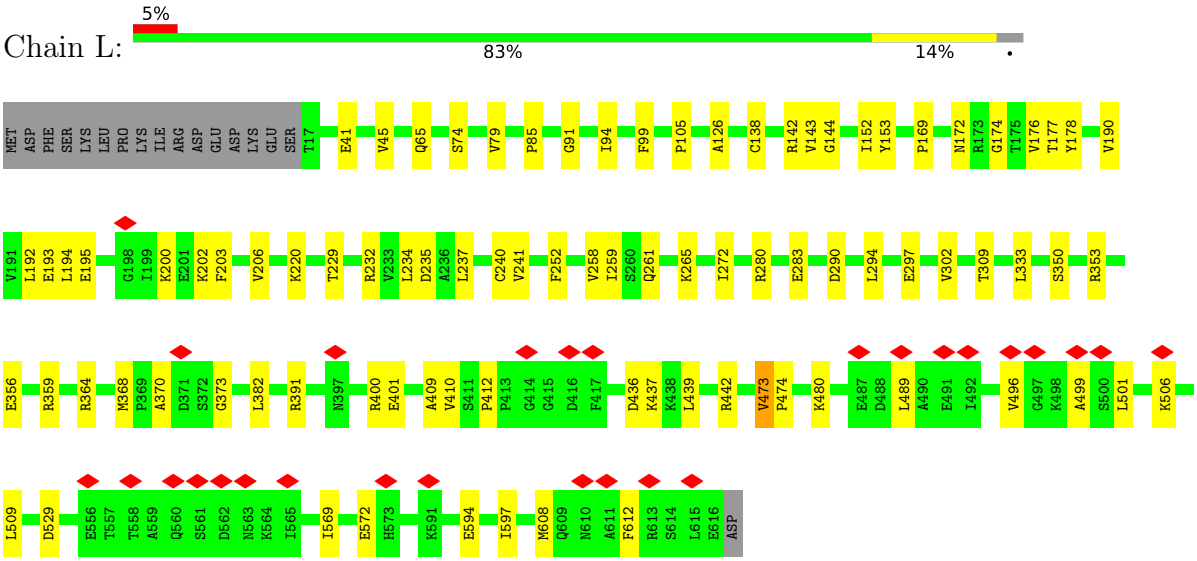
Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	108	Total	C	N	O	S	0	0
			665	395	138	129	3		
6	e	75	Total	C	N	O	S	0	0
			501	297	105	96	3		
6	f	78	Total	C	N	O	S	0	0
			512	304	108	97	3		

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.

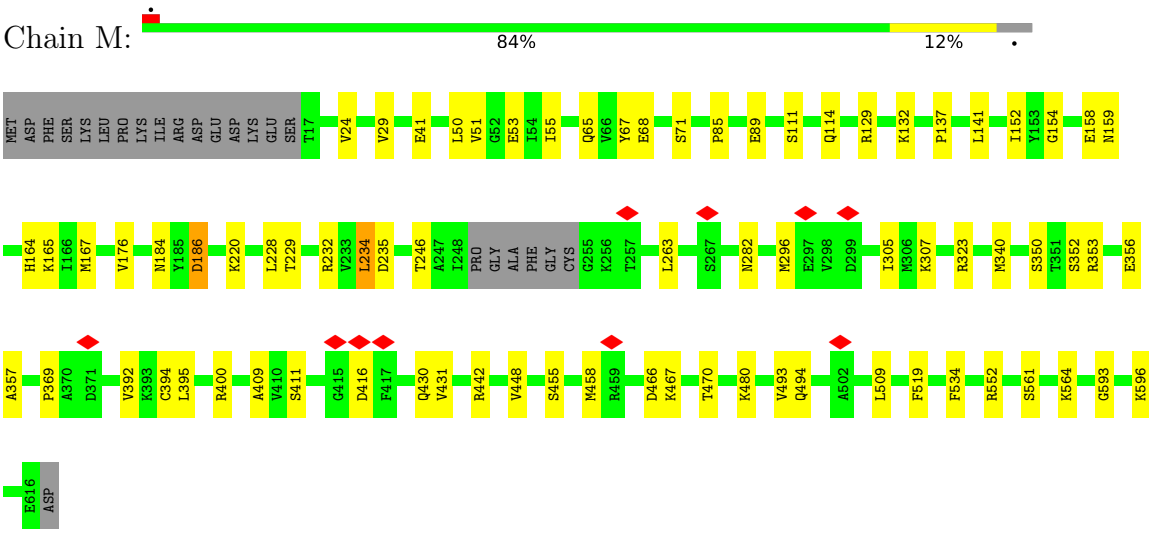
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain L:



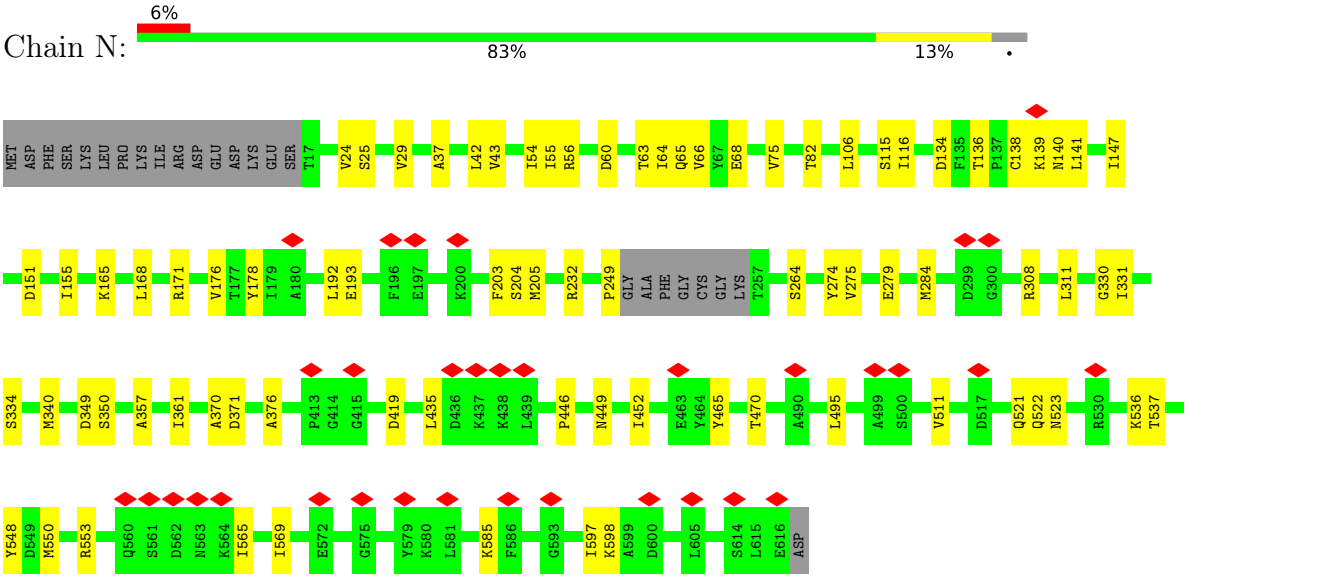
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain M:



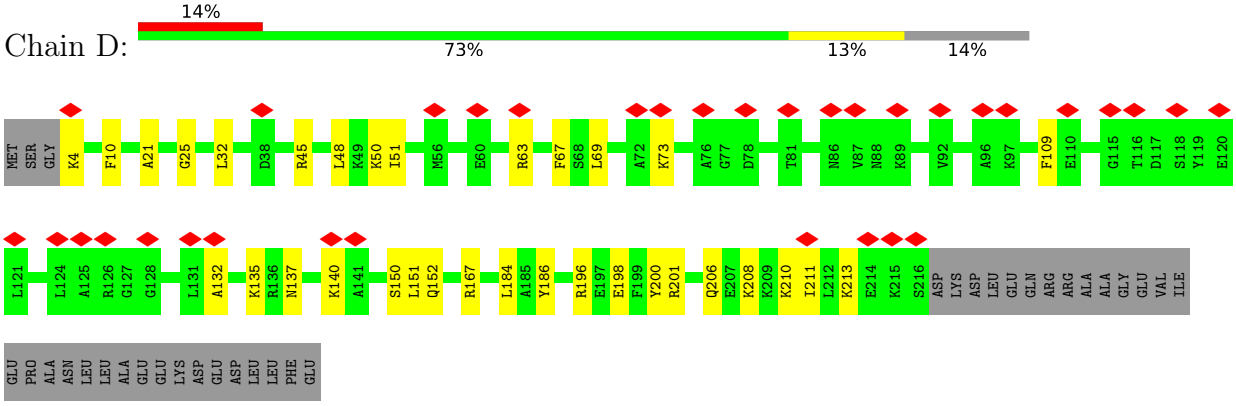
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain N:



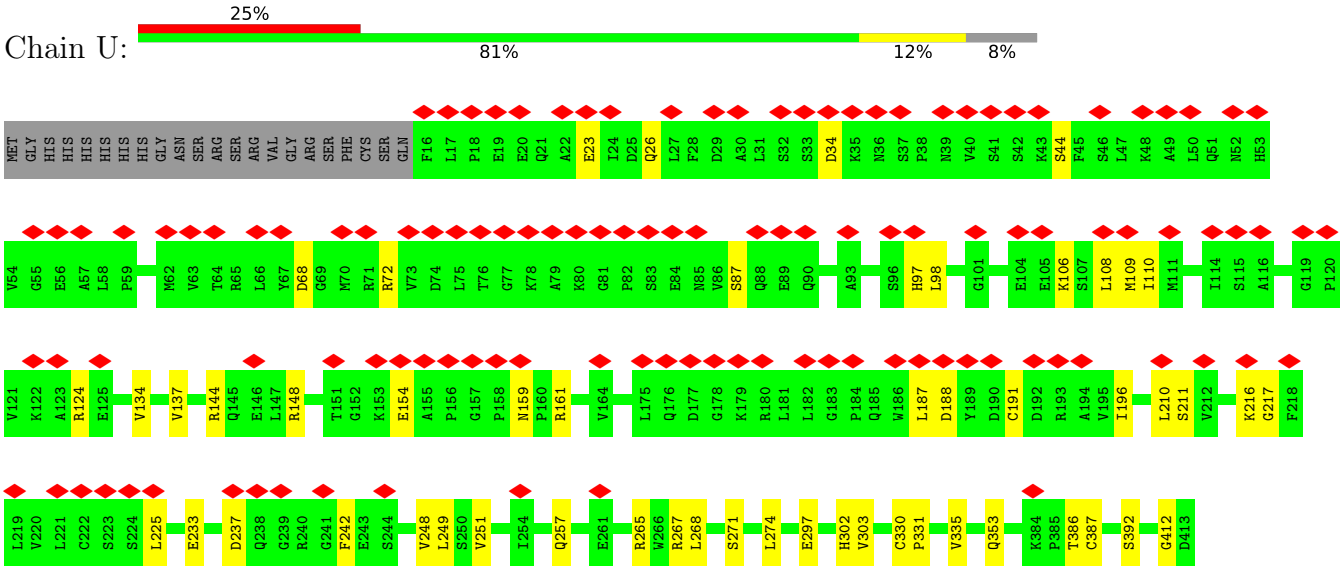
• Molecule 2: V-type proton ATPase subunit D

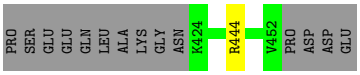
Chain D:



• Molecule 3: KIAA1609 protein, isoform CRA_a

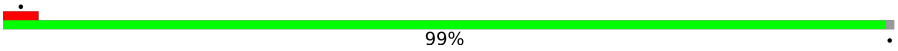
Chain U:

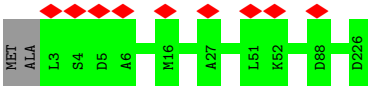




• Molecule 4: V-type proton ATPase subunit E 1

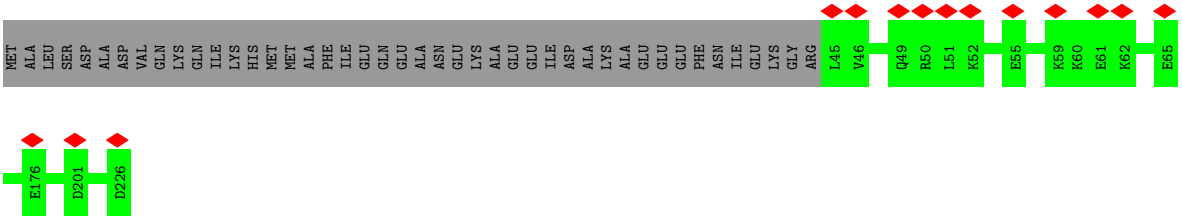
Chain d:





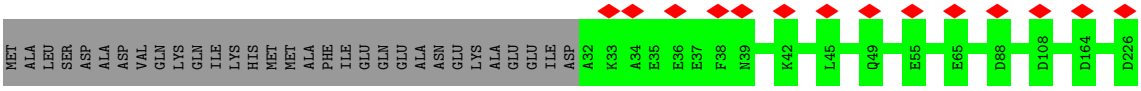
• Molecule 4: V-type proton ATPase subunit E 1

Chain b:



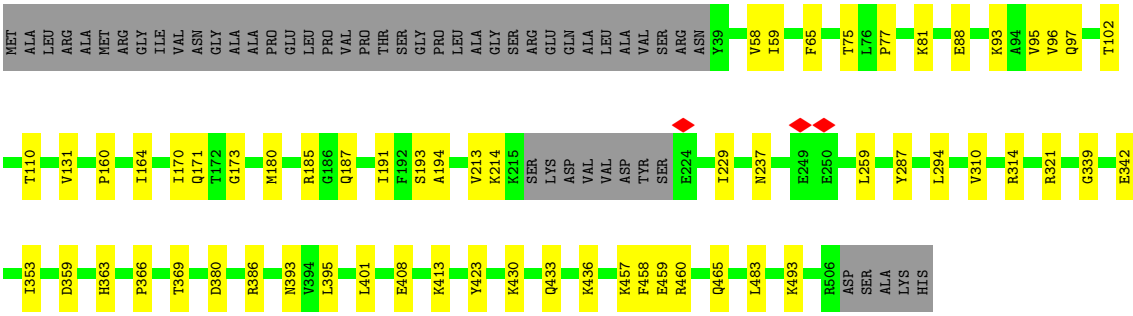
• Molecule 4: V-type proton ATPase subunit E 1

Chain c:



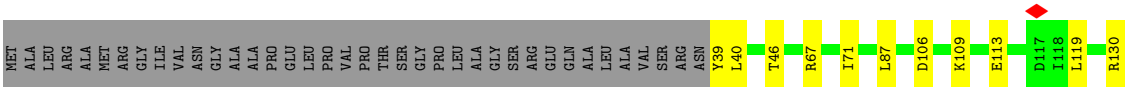
• Molecule 5: V-type proton ATPase subunit B, brain isoform

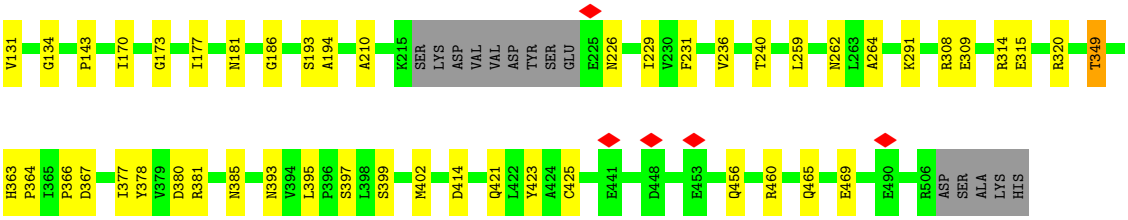
Chain Q:



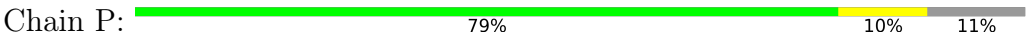
• Molecule 5: V-type proton ATPase subunit B, brain isoform

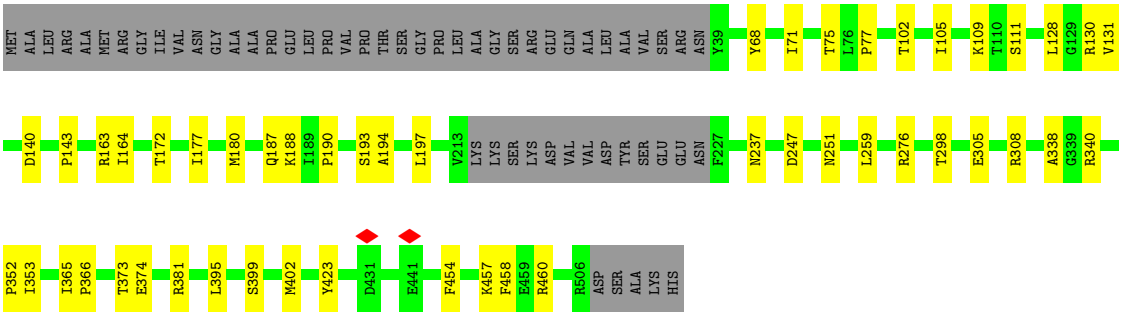
Chain O:



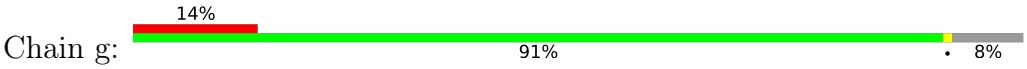


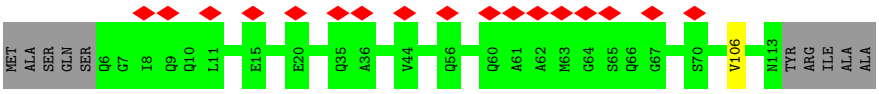
• Molecule 5: V-type proton ATPase subunit B, brain isoform



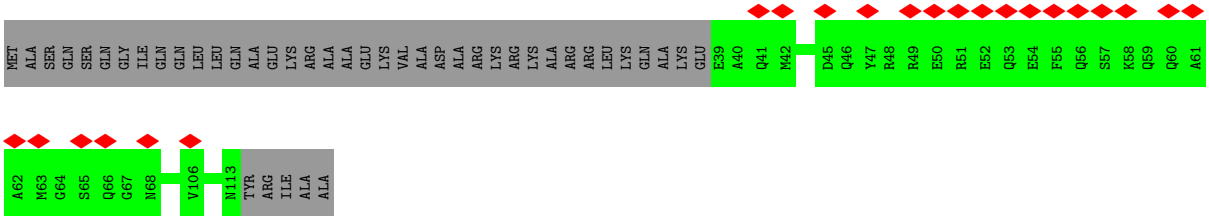


• Molecule 6: V-type proton ATPase subunit G

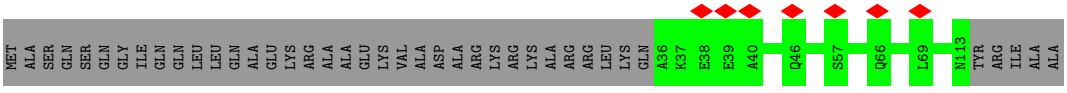




• Molecule 6: V-type proton ATPase subunit G



• Molecule 6: V-type proton ATPase subunit G



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	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)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	L	0.37	0/4752	0.57	2/6435 (0.0%)
1	M	0.40	0/4712	0.57	1/6379 (0.0%)
1	N	0.39	0/4707	0.56	0/6375
2	D	0.30	0/1735	0.55	1/2320 (0.0%)
3	U	0.33	0/3445	0.53	0/4660
4	b	0.32	0/1493	0.52	0/2002
4	c	0.33	0/1519	0.53	0/2044
4	d	0.33	0/1835	0.54	0/2457
5	O	0.41	0/3666	0.55	0/4967
5	P	0.42	0/3631	0.55	0/4922
5	Q	0.42	0/3675	0.56	0/4979
6	e	0.30	0/503	0.51	0/683
6	f	0.29	0/514	0.50	0/699
6	g	0.28	0/667	0.47	0/912
All	All	0.38	0/36854	0.55	4/49834 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	234	LEU	CA-CB-CG	8.12	133.96	115.30
1	L	234	LEU	CA-CB-CG	8.07	133.85	115.30
1	L	509	LEU	CA-CB-CG	5.88	128.82	115.30
2	D	69	LEU	CA-CB-CG	5.60	128.18	115.30

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	L	4656	0	4641	51	0
1	M	4619	0	4608	47	0
1	N	4613	0	4599	48	0
2	D	1717	0	1829	23	0
3	U	3365	0	3271	32	0
4	b	1479	0	1563	0	0
4	c	1505	0	1512	0	0
4	d	1818	0	1888	0	0
5	O	3595	0	3600	34	0
5	P	3560	0	3562	31	0
5	Q	3604	0	3606	34	0
6	e	501	0	419	0	0
6	f	512	0	424	0	0
6	g	665	0	507	0	0
All	All	36209	0	36029	278	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (278) 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)
2:D:10:PHE:HB3	5:Q:321:ARG:HH22	1.53	0.73
5:P:365:ILE:HG13	5:P:366:PRO:HD3	1.77	0.66
1:L:195:GLU:HB2	1:L:200:LYS:HE2	1.76	0.65
5:O:399:SER:HB2	5:O:402:MET:HB2	1.78	0.65
2:D:137:ASN:HA	2:D:140:LYS:HE2	1.81	0.63
5:O:421:GLN:NE2	5:O:425:CYS:SG	2.72	0.62
1:L:252:PHE:O	1:L:437:LYS:NZ	2.32	0.61
5:O:170:ILE:HG13	5:O:349:THR:HG21	1.83	0.60
1:L:368:MET:HE1	2:D:200:TYR:HB2	1.84	0.59
1:L:45:VAL:HA	1:L:79:VAL:HG12	1.84	0.59
1:N:138:CYS:O	1:N:140:ASN:ND2	2.36	0.59
3:U:191:CYS:HB3	3:U:196:ILE:HD11	1.85	0.58
1:L:265:LYS:HD2	1:L:294:LEU:HD22	1.84	0.58
1:M:220:LYS:HG2	1:M:392:VAL:HG12	1.86	0.58
1:M:141:LEU:HD21	1:M:176:VAL:HG21	1.86	0.58
1:L:350:SER:H	1:L:409:ALA:HB3	1.68	0.58
5:Q:77:PRO:HD3	5:Q:110:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:97:GLN:HE22	5:Q:310:VAL:HG13	1.68	0.57
1:M:246:THR:HG22	1:M:431:VAL:HB	1.86	0.57
1:M:395:LEU:O	1:M:400:ARG:NH2	2.36	0.57
2:D:4:LYS:HD2	1:M:494:GLN:HE22	1.69	0.57
2:D:167:ARG:O	2:D:167:ARG:HG2	2.03	0.57
1:M:458:MET:SD	1:M:480:LYS:NZ	2.78	0.57
1:M:442:ARG:HH22	5:P:423:TYR:HB3	1.69	0.57
5:O:134:GLY:HA3	5:O:262:ASN:HD22	1.69	0.57
1:L:501:LEU:O	1:L:506:LYS:NZ	2.38	0.56
5:Q:75:THR:OG1	5:Q:81:LYS:NZ	2.38	0.56
1:M:137:PRO:HA	1:M:154:GLY:HA2	1.86	0.56
1:M:152:ILE:HG12	1:M:167:MET:HG2	1.87	0.56
1:N:264:SER:O	1:N:308:ARG:NH2	2.38	0.56
5:P:298:THR:HA	5:P:353:ILE:HB	1.86	0.56
1:L:192:LEU:HB3	1:L:203:PHE:HB2	1.87	0.55
1:L:391:ARG:NH1	1:L:401:GLU:OE2	2.38	0.55
1:N:419:ASP:OD1	1:N:419:ASP:N	2.39	0.55
1:M:159:ASN:ND2	1:M:307:LYS:O	2.37	0.55
5:Q:433:GLN:HA	5:Q:436:LYS:HG2	1.88	0.55
5:O:380:ASP:HB2	5:O:393:ASN:HB2	1.89	0.55
3:U:242:PHE:CD2	3:U:274:LEU:HD11	2.42	0.55
3:U:302:HIS:HA	3:U:331:PRO:HD3	1.89	0.55
3:U:68:ASP:HB2	3:U:72:ARG:HH12	1.73	0.54
3:U:257:GLN:HG2	3:U:335:VAL:HG11	1.88	0.54
2:D:51:ILE:HD11	2:D:152:GLN:HE21	1.71	0.54
1:N:232:ARG:HG2	1:N:537:THR:HG23	1.89	0.54
5:Q:386:ARG:NH2	5:Q:459:GLU:OE1	2.40	0.54
1:L:280:ARG:HB2	1:L:283:GLU:HB2	1.89	0.54
1:M:282:ASN:ND2	5:P:374:GLU:OE1	2.40	0.54
1:N:147:ILE:HG12	1:N:168:LEU:HD22	1.88	0.54
2:D:48:LEU:HA	2:D:51:ILE:HG22	1.89	0.54
2:D:132:ALA:HA	2:D:135:LYS:HB2	1.88	0.54
2:D:201:ARG:NH1	1:M:369:PRO:O	2.41	0.54
5:P:75:THR:HB	5:P:111:SER:HB3	1.90	0.54
1:M:89:GLU:OE2	1:M:129:ARG:NH2	2.40	0.54
5:Q:380:ASP:HB2	5:Q:393:ASN:HB2	1.90	0.54
1:N:178:TYR:HB3	1:N:193:GLU:HB2	1.89	0.53
2:D:206:GLN:NE2	5:O:315:GLU:OE2	2.41	0.53
1:M:158:GLU:OE1	1:M:164:HIS:ND1	2.39	0.53
1:L:258:VAL:HG13	1:L:259:ILE:HG13	1.89	0.53
5:Q:173:GLY:O	5:Q:465:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:147:ILE:HG13	1:N:151:ASP:HB2	1.89	0.53
1:M:353:ARG:NH2	1:M:411:SER:O	2.41	0.53
3:U:23:GLU:HA	3:U:26:GLN:HB2	1.90	0.53
1:N:449:ASN:HD22	1:N:452:ILE:HG12	1.74	0.53
5:P:305:GLU:HG2	5:P:308:ARG:HH21	1.75	0.52
5:O:106:ASP:OD2	5:O:109:LYS:NZ	2.37	0.52
5:P:237:ASN:OD1	5:P:237:ASN:N	2.43	0.52
1:L:473:VAL:HG23	1:L:474:PRO:HD3	1.90	0.52
1:L:436:ASP:HB3	1:L:439:LEU:HB2	1.90	0.52
3:U:34:ASP:OD1	3:U:34:ASP:N	2.40	0.52
1:N:141:LEU:HD21	1:N:147:ILE:HD12	1.91	0.52
1:N:536:LYS:HG3	1:N:597:ILE:HG12	1.90	0.52
5:Q:395:LEU:HA	5:Q:423:TYR:HE2	1.74	0.52
1:N:66:VAL:HG12	1:N:68:GLU:H	1.75	0.52
2:D:50:LYS:HB3	2:D:151:LEU:HD21	1.91	0.52
5:Q:170:ILE:HG12	5:Q:185:ARG:HG2	1.92	0.52
1:N:178:TYR:HD2	1:N:193:GLU:HG3	1.74	0.52
5:Q:164:ILE:HD11	5:Q:342:GLU:HB2	1.90	0.52
1:M:323:ARG:HD2	1:M:357:ALA:HB2	1.91	0.51
3:U:110:ILE:HD11	3:U:210:LEU:HD11	1.92	0.51
1:N:165:LYS:HD2	1:N:340:MET:HB3	1.91	0.51
1:N:550:MET:HG2	1:N:553:ARG:HH22	1.76	0.51
5:O:210:ALA:HB3	5:O:229:ILE:HD11	1.93	0.51
1:L:272:ILE:HB	1:L:309:THR:HG22	1.93	0.51
5:Q:408:GLU:HG2	5:Q:413:LYS:HB3	1.92	0.51
5:O:395:LEU:O	5:O:423:TYR:OH	2.29	0.51
1:L:169:PRO:HB2	1:L:172:ASN:HD22	1.76	0.51
3:U:98:LEU:HA	3:U:106:LYS:HD2	1.93	0.51
1:M:165:LYS:HD2	1:M:340:MET:HB3	1.91	0.51
1:N:56:ARG:HB3	1:N:63:THR:HB	1.93	0.50
1:N:204:SER:OG	1:N:205:MET:N	2.44	0.50
5:Q:131:VAL:HG22	5:Q:259:LEU:HB3	1.94	0.50
1:M:232:ARG:NH1	1:M:519:PHE:O	2.43	0.50
5:P:399:SER:HB3	5:P:402:MET:HB2	1.93	0.50
1:M:55:ILE:HD13	1:M:65:GLN:HB2	1.92	0.50
1:N:376:ALA:HB1	5:O:309:GLU:HA	1.92	0.50
1:N:371:ASP:N	1:N:371:ASP:OD1	2.44	0.50
5:O:231:PHE:HB3	5:O:259:LEU:HD12	1.93	0.49
5:O:381:ARG:O	5:O:385:ASN:ND2	2.44	0.49
5:O:130:ARG:NH2	5:O:143:PRO:O	2.36	0.49
1:M:228:LEU:HD11	1:M:534:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:261:GLN:NE2	1:L:290:ASP:OD2	2.42	0.49
3:U:267:ARG:NH1	3:U:412:GLY:O	2.44	0.49
1:M:561:SER:O	1:M:564:LYS:NZ	2.45	0.49
1:M:111:SER:O	1:M:114:GLN:NE2	2.45	0.49
5:P:102:THR:HA	5:P:105:ILE:HD12	1.93	0.49
5:P:190:PRO:HB3	5:P:352:PRO:HG2	1.95	0.49
3:U:268:LEU:HD11	3:U:271:SER:HB3	1.95	0.49
1:N:115:SER:OG	1:N:116:ILE:N	2.46	0.49
1:N:331:ILE:HD12	1:N:334:SER:HB3	1.95	0.49
5:Q:287:TYR:OH	5:Q:339:GLY:O	2.25	0.49
5:Q:458:PHE:HA	5:Q:483:LEU:HD21	1.94	0.49
5:P:247:ASP:O	5:P:251:ASN:ND2	2.45	0.49
2:D:208:LYS:HA	2:D:211:ILE:HD12	1.94	0.48
1:N:65:GLN:HE22	1:N:361:ILE:HD12	1.77	0.48
1:M:51:VAL:HG23	1:M:67:TYR:HB2	1.95	0.48
1:M:430:GLN:HE21	5:Q:237:ASN:HD21	1.59	0.48
1:M:442:ARG:NH2	5:P:423:TYR:HB3	2.29	0.48
1:M:493:VAL:HG21	1:M:509:LEU:HD21	1.95	0.48
1:L:74:SER:HB3	5:O:67:ARG:HG2	1.94	0.48
1:L:178:TYR:HB3	1:L:193:GLU:HB3	1.94	0.48
3:U:297:GLU:HB2	3:U:303:VAL:HG22	1.96	0.48
1:M:41:GLU:HA	1:M:85:PRO:HA	1.95	0.48
1:M:350:SER:H	1:M:409:ALA:HB3	1.79	0.48
1:N:521:GLN:OE1	1:N:585:LYS:NZ	2.46	0.48
3:U:211:SER:HB3	3:U:225:LEU:HD11	1.95	0.48
5:O:186:GLY:H	5:O:349:THR:HB	1.78	0.48
1:M:229:THR:HB	1:M:263:LEU:HD11	1.96	0.48
1:L:608:MET:O	1:L:612:PHE:N	2.44	0.48
3:U:124:ARG:HB2	3:U:187:LEU:HB3	1.96	0.48
1:M:53:GLU:OE1	1:M:67:TYR:OH	2.32	0.47
5:Q:88:GLU:HB2	5:Q:314:ARG:HH12	1.79	0.47
5:Q:193:SER:OG	5:Q:194:ALA:N	2.47	0.47
2:D:210:LYS:HA	2:D:213:LYS:HG2	1.95	0.47
3:U:237:ASP:OD1	3:U:237:ASP:N	2.46	0.47
1:N:37:ALA:HB1	1:N:54:ILE:HD13	1.96	0.47
1:N:465:TYR:O	1:N:470:THR:N	2.38	0.47
5:P:247:ASP:OD1	5:P:251:ASN:ND2	2.46	0.47
1:L:232:ARG:NH2	1:L:529:ASP:OD1	2.47	0.47
1:N:25:SER:OG	5:Q:314:ARG:NH2	2.48	0.47
1:L:439:LEU:HD23	1:L:442:ARG:HD2	1.96	0.47
1:M:186:ASP:OD1	1:M:186:ASP:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:249:PRO:HG2	1:N:435:LEU:H	1.79	0.47
5:Q:59:ILE:HA	5:Q:95:VAL:HA	1.97	0.47
1:N:43:VAL:HG21	1:N:64:ILE:HD13	1.97	0.46
3:U:148:ARG:HB3	3:U:233:GLU:HG3	1.98	0.46
1:M:353:ARG:NH1	1:M:356:GLU:OE1	2.48	0.46
1:N:275:VAL:HG21	1:N:330:GLY:HA3	1.97	0.46
5:Q:366:PRO:HA	5:Q:369:THR:HG22	1.97	0.46
1:M:71:SER:HA	5:P:68:TYR:HD2	1.81	0.46
1:L:143:VAL:HG13	1:L:177:THR:HA	1.98	0.46
1:L:229:THR:OG1	1:L:235:ASP:OD2	2.33	0.46
5:O:87:LEU:HD11	5:O:314:ARG:HG2	1.98	0.46
5:O:363:HIS:HB3	5:O:366:PRO:HD2	1.98	0.46
1:L:138:CYS:HB2	1:L:153:TYR:HA	1.97	0.46
1:L:190:VAL:HG21	1:L:202:LYS:HD3	1.97	0.46
3:U:154:GLU:HB3	3:U:159:ASN:HD21	1.80	0.46
1:M:352:SER:HB2	1:M:411:SER:HB2	1.96	0.46
3:U:44:SER:OG	3:U:87:SER:OG	2.34	0.46
1:M:593:GLY:H	1:M:596:LYS:HB3	1.81	0.46
5:Q:229:ILE:HD12	5:Q:294:LEU:HD23	1.97	0.46
5:P:164:ILE:HB	5:P:340:ARG:HB2	1.98	0.46
1:L:410:VAL:HG13	1:L:412:PRO:HD3	1.97	0.45
3:U:144:ARG:HG3	3:U:216:LYS:HG2	1.98	0.45
3:U:444:ARG:HA	3:U:444:ARG:HD2	1.74	0.45
5:Q:58:VAL:O	5:Q:96:VAL:N	2.48	0.45
5:P:163:ARG:NH2	5:P:338:ALA:O	2.45	0.45
1:M:296:MET:HB2	1:M:305:ILE:HG22	1.98	0.45
1:M:394:CYS:HB2	1:M:400:ARG:HB2	1.98	0.45
1:L:91:GLY:HA3	1:L:206:VAL:HG12	1.97	0.45
1:M:466:ASP:HA	1:M:470:THR:HA	1.98	0.45
5:P:187:GLN:NE2	5:P:374:GLU:O	2.50	0.45
1:N:134:ASP:OD1	1:N:134:ASP:N	2.42	0.45
1:L:569:ILE:HA	1:L:572:GLU:HG2	1.97	0.45
1:N:106:LEU:HD13	5:Q:160:PRO:HD2	1.99	0.45
5:P:197:LEU:HD21	5:P:381:ARG:HG3	1.98	0.45
5:P:77:PRO:HG3	5:P:109:LYS:HG3	1.98	0.45
5:P:131:VAL:HG22	5:P:259:LEU:HD13	1.99	0.45
5:P:180:MET:O	5:P:423:TYR:OH	2.31	0.45
3:U:242:PHE:CG	3:U:274:LEU:HD11	2.51	0.45
5:O:236:VAL:HB	5:O:240:THR:HG23	1.99	0.45
1:L:240:CYS:SG	1:L:241:VAL:N	2.90	0.45
5:Q:191:ILE:HB	5:Q:353:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:173:GLY:O	5:O:465:GLN:NE2	2.36	0.45
1:N:279:GLU:HB3	1:N:284:MET:HG2	1.99	0.44
1:L:594:GLU:HA	1:L:597:ILE:HB	1.98	0.44
1:N:511:VAL:HG11	1:N:548:TYR:HB2	1.99	0.44
1:N:523:ASN:OD1	1:N:523:ASN:N	2.50	0.44
1:L:237:LEU:HD22	1:L:480:LYS:HZ3	1.83	0.44
1:M:467:LYS:HE3	1:M:467:LYS:HB2	1.78	0.44
1:L:373:GLY:HA3	5:O:320:ARG:HD2	1.99	0.44
1:N:24:VAL:HG12	1:N:29:VAL:HG13	2.00	0.44
1:L:370:ALA:O	2:D:196:ARG:NH2	2.48	0.44
1:L:350:SER:HB3	1:L:353:ARG:HG2	2.00	0.44
3:U:387:CYS:N	3:U:392:SER:O	2.51	0.44
5:Q:395:LEU:HD11	5:Q:430:LYS:HG3	2.00	0.44
1:N:370:ALA:HB1	5:O:308:ARG:HD2	1.99	0.44
5:O:414:ASP:OD1	5:O:414:ASP:N	2.48	0.44
2:D:73:LYS:HE2	2:D:73:LYS:HB3	1.83	0.43
1:L:105:PRO:HD3	1:L:126:ALA:HA	2.00	0.43
2:D:63:ARG:O	2:D:67:PHE:N	2.51	0.43
1:M:442:ARG:HD3	5:P:395:LEU:HD22	1.99	0.43
1:N:42:LEU:O	1:N:82:THR:OG1	2.35	0.43
1:N:274:TYR:HB3	1:N:311:LEU:HD22	2.01	0.43
1:L:174:GLY:HA3	1:L:194:LEU:HD13	2.01	0.43
1:L:220:LYS:HE3	1:L:220:LYS:HB3	1.82	0.43
5:P:71:ILE:HD13	5:P:71:ILE:HA	1.88	0.43
1:L:297:GLU:HG3	1:L:302:VAL:HG23	2.00	0.43
3:U:161:ARG:NH1	3:U:330:CYS:SG	2.92	0.43
1:N:141:LEU:HD23	1:N:176:VAL:HG21	2.00	0.43
1:N:446:PRO:HD3	1:N:522:GLN:HB2	2.00	0.43
5:O:377:ILE:O	5:O:397:SER:OG	2.35	0.43
1:L:94:ILE:HG23	1:L:99:PHE:HE1	1.82	0.43
2:D:109:PHE:HB2	2:D:150:SER:HB3	2.01	0.43
3:U:248:VAL:HA	3:U:251:VAL:HG22	2.00	0.43
1:N:55:ILE:HD13	1:N:65:GLN:HB2	2.00	0.43
5:O:226:ASN:HB2	5:O:291:LYS:HA	2.01	0.43
1:N:75:VAL:HG22	5:Q:65:PHE:HA	2.01	0.43
5:Q:171:GLN:HB3	5:Q:213:VAL:HG22	2.00	0.43
5:O:71:ILE:HD11	5:O:119:LEU:HB2	2.01	0.43
5:P:454:PHE:O	5:P:458:PHE:N	2.51	0.43
3:U:144:ARG:HH21	3:U:217:GLY:HA2	1.84	0.42
5:O:46:THR:HA	5:O:113:GLU:HA	2.01	0.42
1:L:496:VAL:HG13	1:L:499:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:98:LEU:HD21	3:U:109:MET:HB2	2.01	0.42
1:N:349:ASP:OD1	1:N:350:SER:OG	2.37	0.42
1:L:382:LEU:HD23	1:L:382:LEU:HA	1.90	0.42
1:N:192:LEU:HB3	1:N:203:PHE:HB2	2.00	0.42
1:M:132:LYS:HD2	1:M:184:ASN:HB3	2.01	0.42
5:O:193:SER:OG	5:O:194:ALA:N	2.51	0.42
1:M:229:THR:OG1	1:M:235:ASP:OD1	2.33	0.42
5:Q:363:HIS:HB3	5:Q:366:PRO:HD2	2.01	0.42
5:O:465:GLN:NE2	5:O:469:GLU:O	2.50	0.42
5:P:172:THR:HG21	5:P:177:ILE:HG13	2.01	0.42
5:Q:93:LYS:HB2	5:Q:93:LYS:HE2	1.77	0.42
5:Q:457:LYS:HB3	5:Q:483:LEU:HD11	2.00	0.42
1:L:65:GLN:HE22	1:L:364:ARG:HD2	1.85	0.42
1:L:144:GLY:N	1:L:176:VAL:O	2.50	0.42
5:O:236:VAL:O	5:O:264:ALA:N	2.53	0.42
1:L:496:VAL:HG22	1:L:499:ALA:HB3	2.02	0.42
1:L:237:LEU:O	1:L:480:LYS:NZ	2.42	0.42
2:D:198:GLU:OE1	2:D:201:ARG:NH2	2.46	0.42
3:U:233:GLU:HB3	3:U:265:ARG:HG2	2.02	0.42
1:M:431:VAL:HG13	1:M:455:SER:HB2	2.00	0.41
5:P:457:LYS:HD3	5:P:460:ARG:HH12	1.84	0.41
2:D:32:LEU:HD13	1:N:495:LEU:HD22	2.02	0.41
5:P:140:ASP:OD1	5:P:140:ASP:N	2.46	0.41
1:L:94:ILE:HG21	1:L:333:LEU:HD22	2.02	0.41
1:L:489:LEU:HD12	1:L:489:LEU:HA	1.90	0.41
2:D:186:TYR:OH	1:M:416:ASP:OD1	2.33	0.41
1:M:50:LEU:HD23	1:M:68:GLU:HB3	2.03	0.41
5:Q:187:GLN:HG3	5:Q:401:LEU:HD12	2.03	0.41
5:P:130:ARG:NH2	5:P:143:PRO:O	2.35	0.41
3:U:249:LEU:HD23	3:U:249:LEU:HA	1.85	0.41
5:P:128:LEU:HD23	5:P:128:LEU:HA	1.90	0.41
1:L:437:LYS:HE2	1:L:437:LYS:HB2	1.95	0.41
2:D:21:ALA:O	2:D:25:GLY:N	2.45	0.41
5:Q:460:ARG:HA	5:Q:460:ARG:HD3	1.82	0.41
5:Q:493:LYS:HE2	5:Q:493:LYS:HB3	1.90	0.41
5:O:177:ILE:HA	5:O:181:ASN:HB2	2.01	0.41
1:N:357:ALA:O	1:N:361:ILE:HG12	2.21	0.41
2:D:45:ARG:HD3	2:D:45:ARG:HA	1.92	0.41
1:N:136:THR:O	1:N:155:ILE:N	2.53	0.41
1:M:24:VAL:HG12	1:M:29:VAL:HG22	2.03	0.41
2:D:184:LEU:HD23	2:D:184:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:188:ASP:OD1	3:U:188:ASP:N	2.49	0.40
5:O:39:TYR:HB2	5:O:40:LEU:H	1.63	0.40
1:L:41:GLU:HA	1:L:85:PRO:HA	2.04	0.40
1:L:152:ILE:HD11	1:L:400:ARG:HD3	2.02	0.40
5:O:364:PRO:HA	5:O:367:ASP:HB3	2.03	0.40
5:P:188:LYS:HG3	5:P:373:THR:HA	2.04	0.40
1:N:565:ILE:HB	1:N:569:ILE:HG21	2.04	0.40
1:L:356:GLU:OE1	1:L:359:ARG:NH2	2.55	0.40
3:U:97:HIS:CD2	3:U:108:LEU:HD22	2.57	0.40
3:U:353:GLN:OE1	1:M:552:ARG:NH2	2.53	0.40
5:O:131:VAL:HG13	5:O:259:LEU:HD23	2.02	0.40
3:U:134:VAL:HA	3:U:137:VAL:HG12	2.04	0.40
1:N:60:ASP:OD1	1:N:60:ASP:N	2.47	0.40
5:O:456:GLN:O	5:O:460:ARG:NE	2.54	0.40
5:P:193:SER:OG	5:P:194:ALA:N	2.55	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	L	598/617 (97%)	559 (94%)	39 (6%)	0	100	100
1	M	590/617 (96%)	554 (94%)	36 (6%)	0	100	100
1	N	589/617 (96%)	551 (94%)	38 (6%)	0	100	100
2	D	211/247 (85%)	202 (96%)	9 (4%)	0	100	100
3	U	423/463 (91%)	390 (92%)	33 (8%)	0	100	100
4	b	180/226 (80%)	176 (98%)	4 (2%)	0	100	100
4	c	193/226 (85%)	182 (94%)	11 (6%)	0	100	100
4	d	222/226 (98%)	218 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	455/511 (89%)	431 (95%)	24 (5%)	0	100	100
5	P	451/511 (88%)	426 (94%)	25 (6%)	0	100	100
5	Q	456/511 (89%)	436 (96%)	20 (4%)	0	100	100
6	e	73/118 (62%)	69 (94%)	4 (6%)	0	100	100
6	f	76/118 (64%)	71 (93%)	5 (7%)	0	100	100
6	g	106/118 (90%)	102 (96%)	4 (4%)	0	100	100
All	All	4623/5126 (90%)	4367 (94%)	256 (6%)	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	L	507/524 (97%)	505 (100%)	2 (0%)	91	95
1	M	504/524 (96%)	501 (99%)	3 (1%)	86	92
1	N	504/524 (96%)	501 (99%)	3 (1%)	86	92
2	D	184/212 (87%)	184 (100%)	0	100	100
3	U	371/402 (92%)	370 (100%)	1 (0%)	92	96
4	b	162/198 (82%)	162 (100%)	0	100	100
4	c	151/198 (76%)	151 (100%)	0	100	100
4	d	197/198 (100%)	197 (100%)	0	100	100
5	O	392/432 (91%)	390 (100%)	2 (0%)	88	94
5	P	388/432 (90%)	387 (100%)	1 (0%)	92	96
5	Q	393/432 (91%)	389 (99%)	4 (1%)	76	86
6	e	38/97 (39%)	38 (100%)	0	100	100
6	f	37/97 (38%)	37 (100%)	0	100	100
6	g	38/97 (39%)	37 (97%)	1 (3%)	46	69
All	All	3866/4367 (88%)	3849 (100%)	17 (0%)	91	95

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	142	ARG
1	L	473	VAL
3	U	386	THR
1	M	186	ASP
1	M	234	LEU
1	M	448	VAL
1	N	139	LYS
1	N	171	ARG
1	N	598	LYS
5	Q	102	THR
5	Q	180	MET
5	Q	214	LYS
5	Q	359	ASP
5	O	349	THR
5	O	378	TYR
5	P	276	ARG
6	g	106	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	172	ASN
1	L	231	GLN
2	D	31	ASN
2	D	137	ASN
2	D	152	GLN
3	U	139	HIS
3	U	145	GLN
3	U	257	GLN
3	U	434	GLN
4	d	139	GLN
1	M	65	GLN
1	M	123	ASN
1	M	261	GLN
1	M	430	GLN
1	M	468	HIS
1	M	494	GLN
1	N	65	GLN
1	N	430	GLN
1	N	449	ASN
1	N	573	HIS

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Mol	Chain	Res	Type
5	Q	97	GLN
5	Q	199	HIS
5	Q	256	ASN
5	Q	421	GLN
5	O	199	HIS
5	O	262	ASN
5	O	288	GLN
5	O	292	HIS
5	O	385	ASN
5	O	433	GLN
5	P	199	HIS
5	P	256	ASN
5	P	421	GLN
4	b	67	GLN
4	b	78	GLN
4	b	206	GLN
4	c	77	ASN
4	c	113	GLN
4	c	166	GLN
6	f	82	GLN
6	f	85	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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.

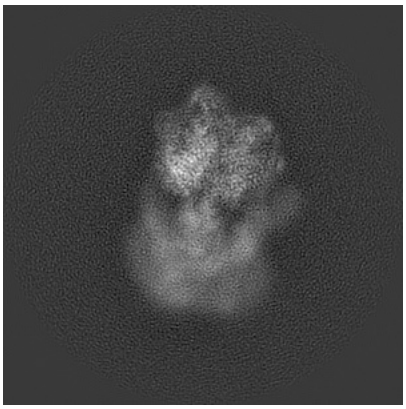
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26622. These allow visual inspection of the internal detail of the map and identification of artifacts.

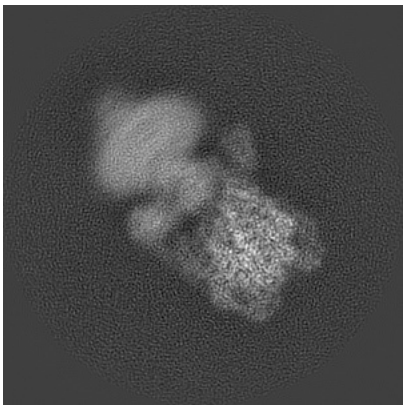
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

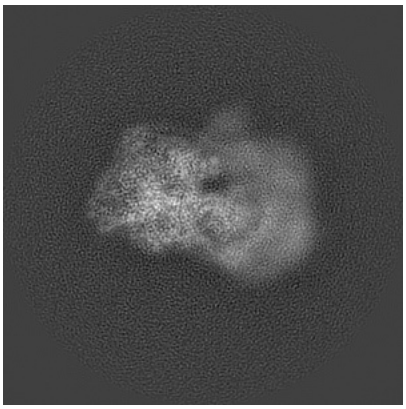
6.1.1 Primary map



X

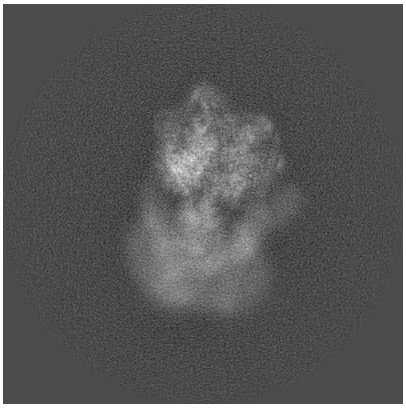


Y

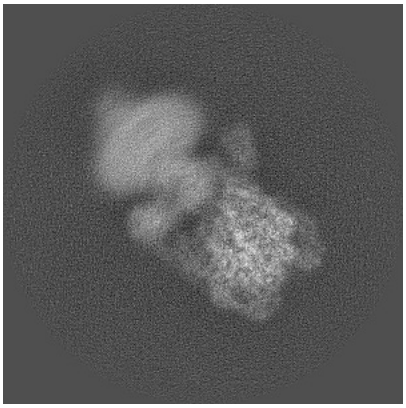


Z

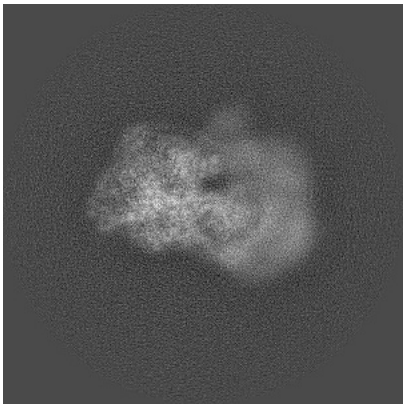
6.1.2 Raw map



X



Y

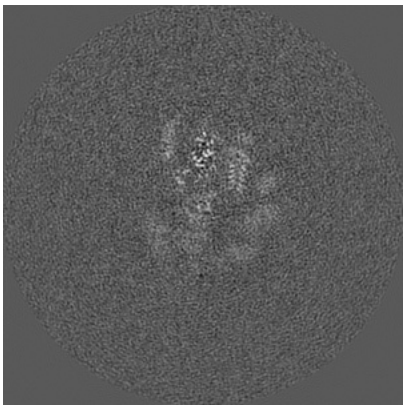


Z

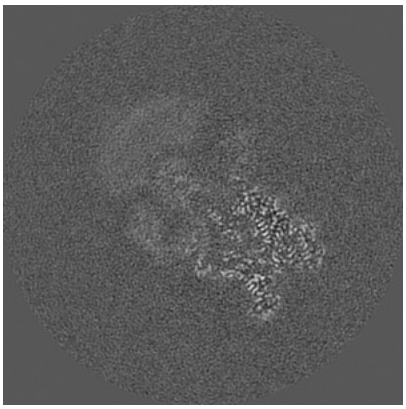
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

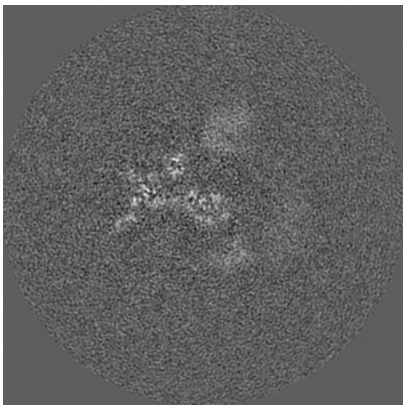
6.2.1 Primary map



X Index: 240

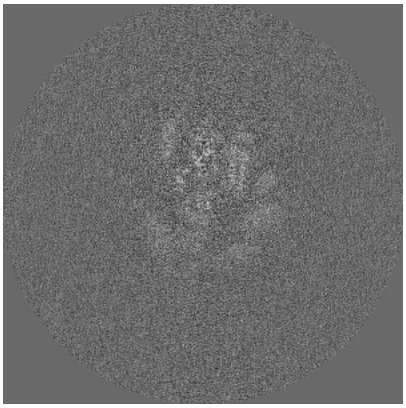


Y Index: 240

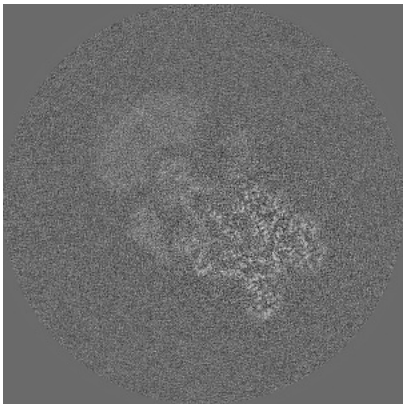


Z Index: 240

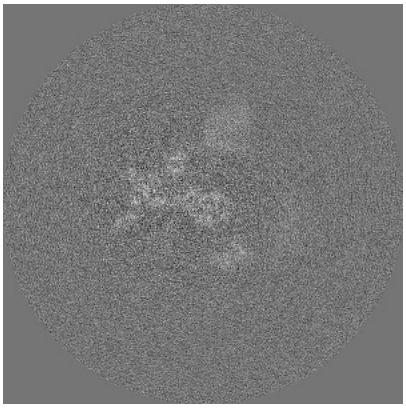
6.2.2 Raw map



X Index: 240



Y Index: 240

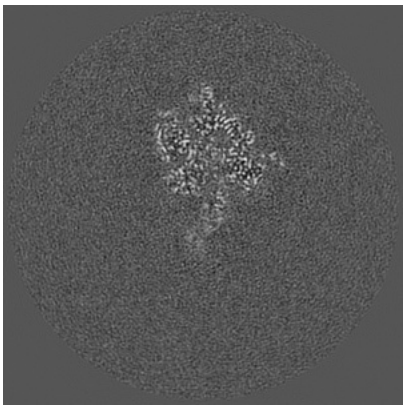


Z Index: 240

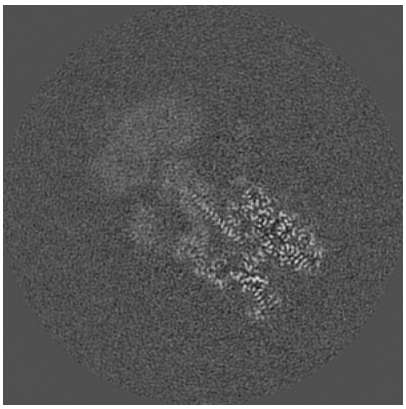
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

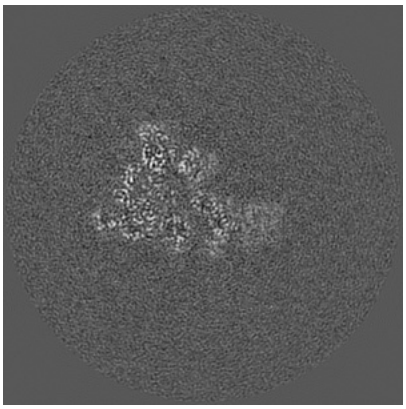
6.3.1 Primary map



X Index: 181

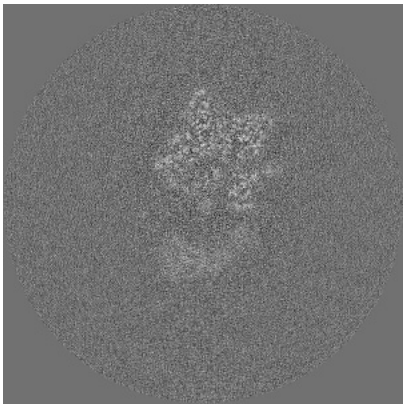


Y Index: 245

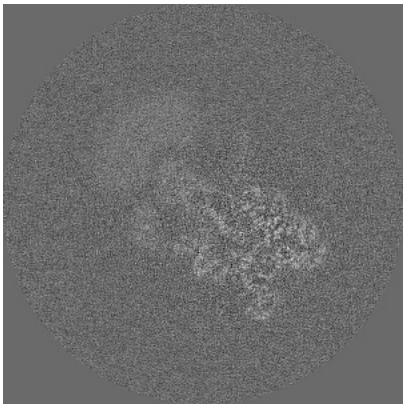


Z Index: 290

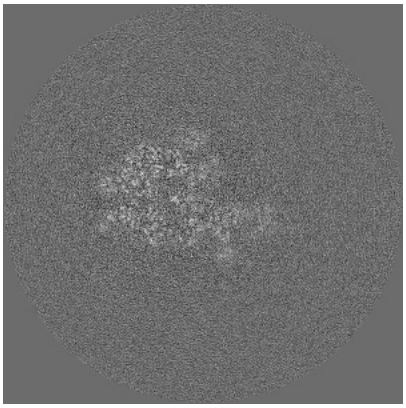
6.3.2 Raw map



X Index: 210



Y Index: 242

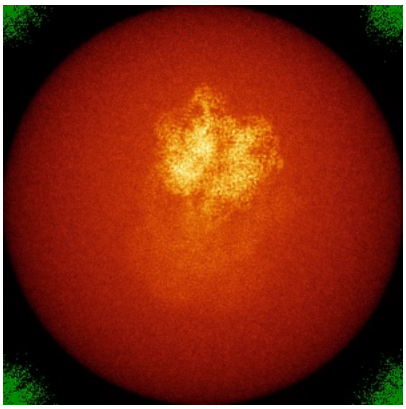


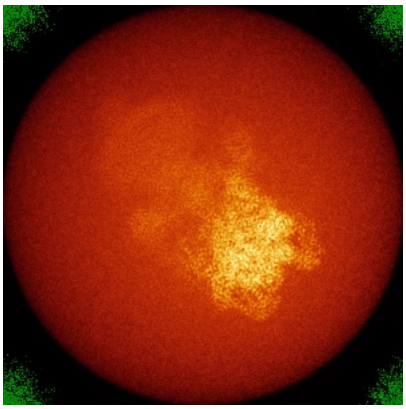
Z Index: 272

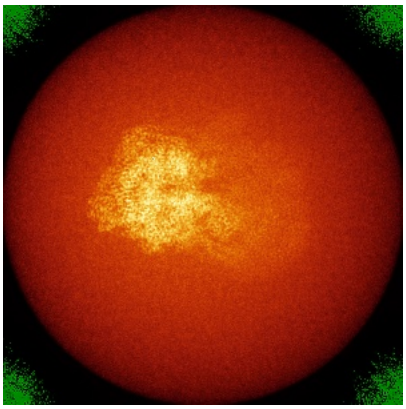
The images above show the largest variance slices of the map in three orthogonal directions.

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

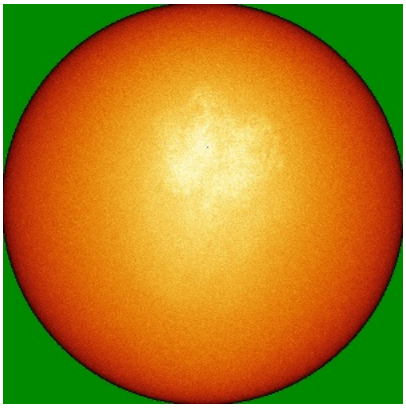
6.4.1 Primary map

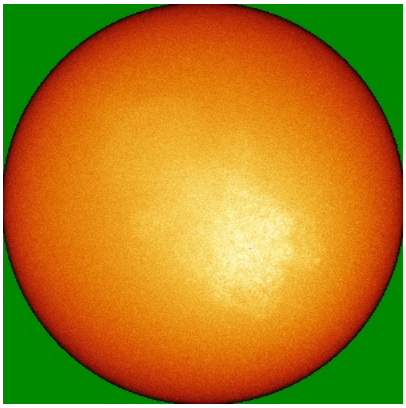

X

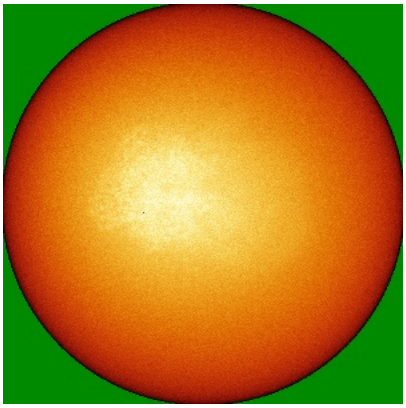

Y


Z

6.4.2 Raw map


X

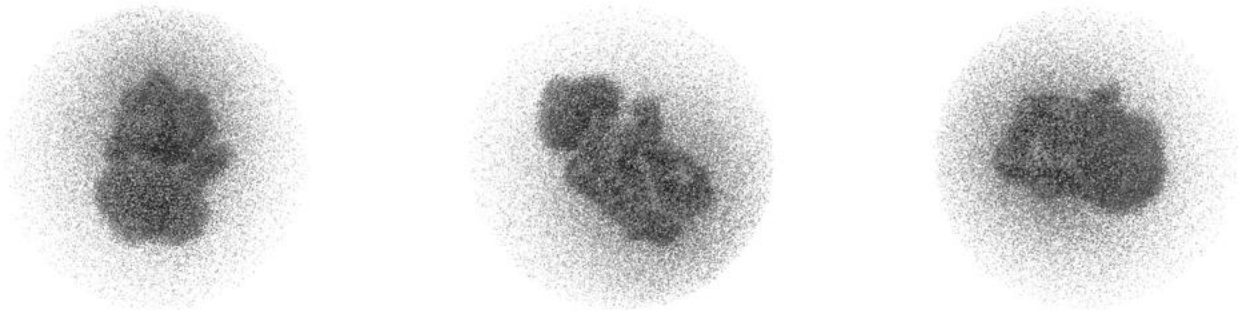

Y


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)

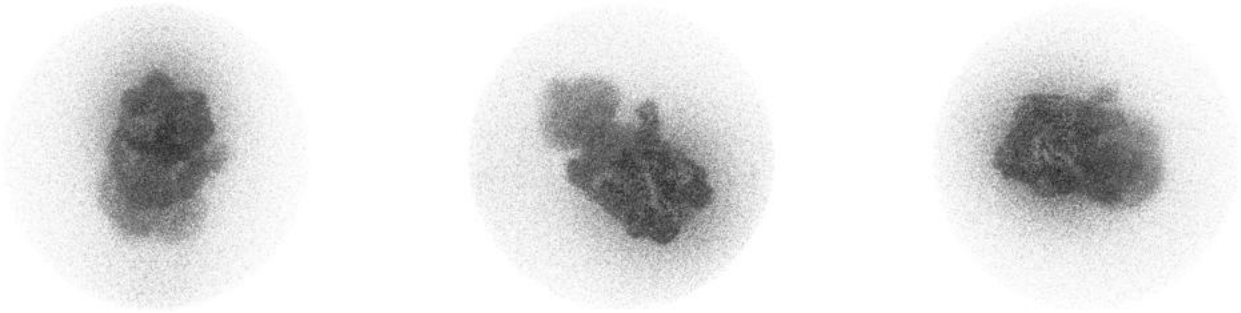
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

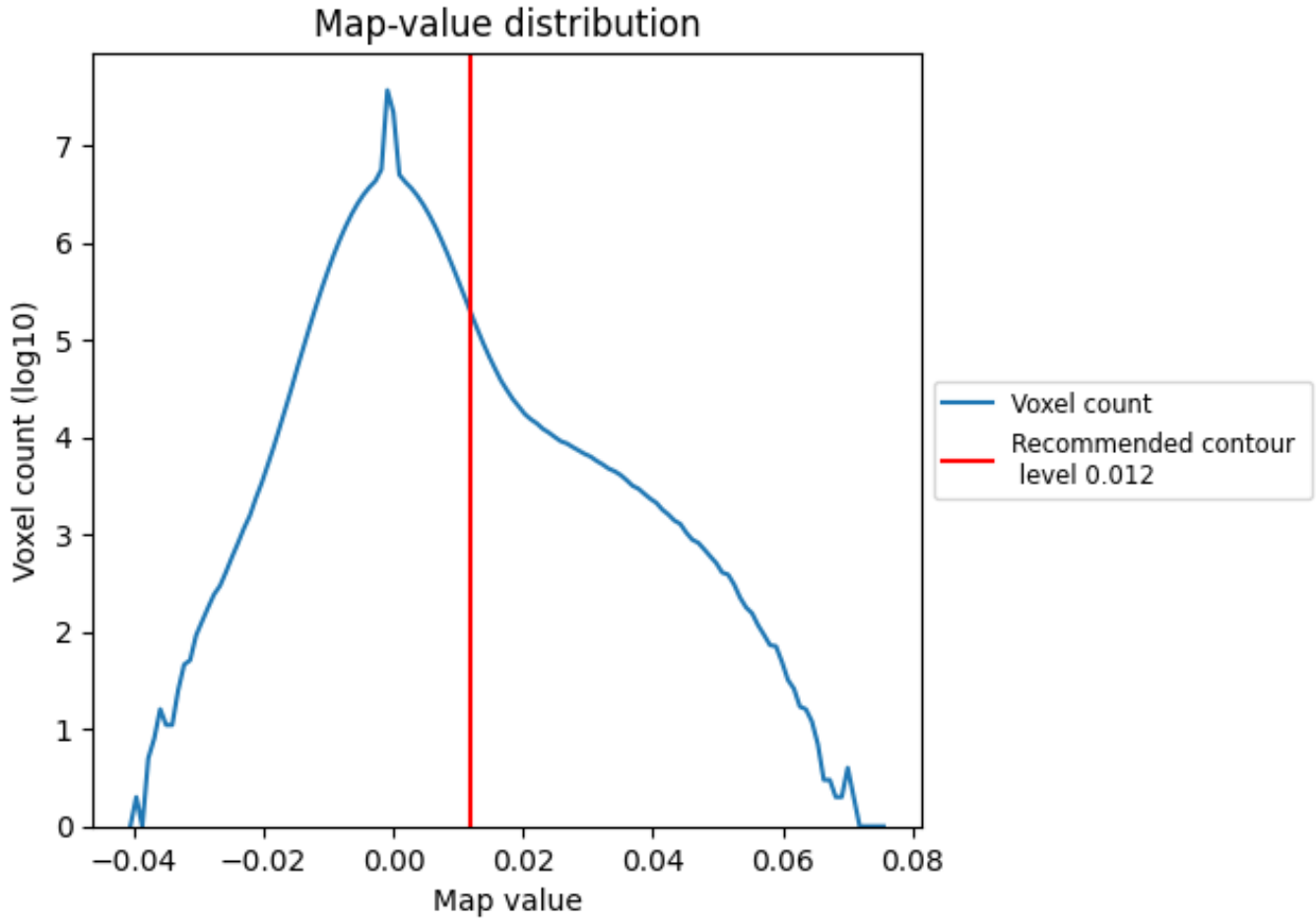
6.6 Mask visualisation (i)

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

7 Map analysis

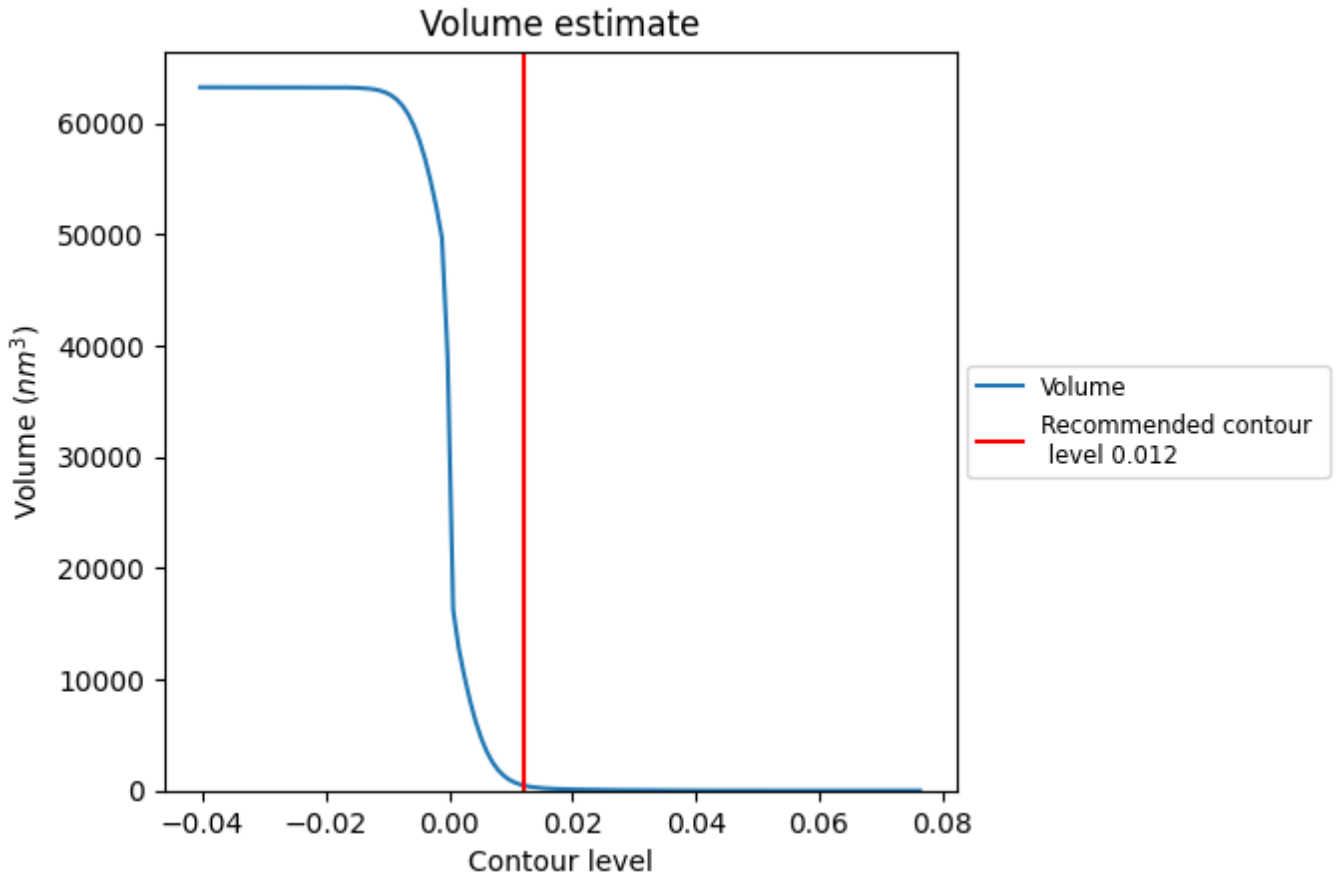
This section contains the results of statistical analysis of the map.

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.

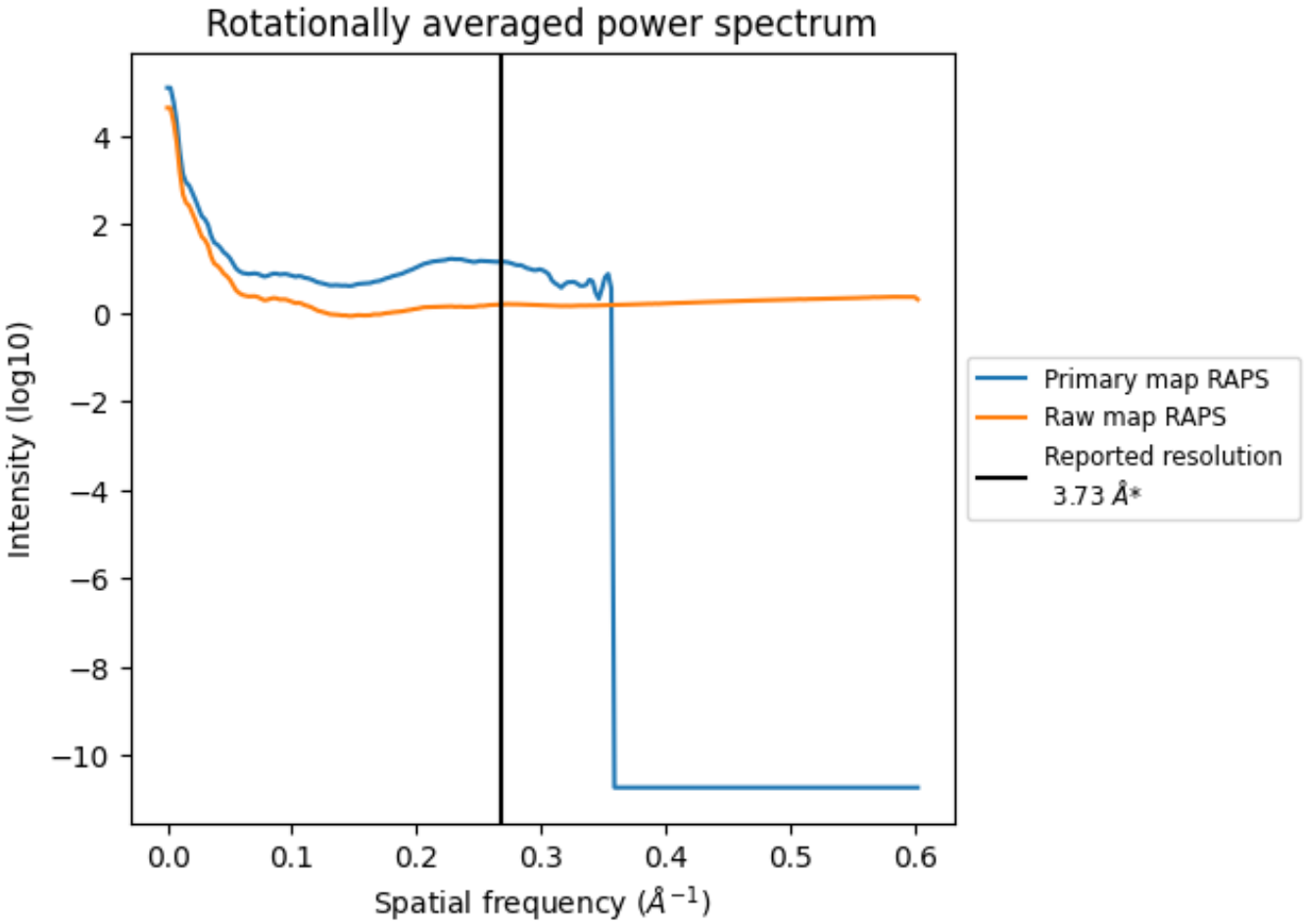
7.2 Volume estimate



The volume at the recommended contour level is 480 nm^3; this corresponds to an approximate mass of 434 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)

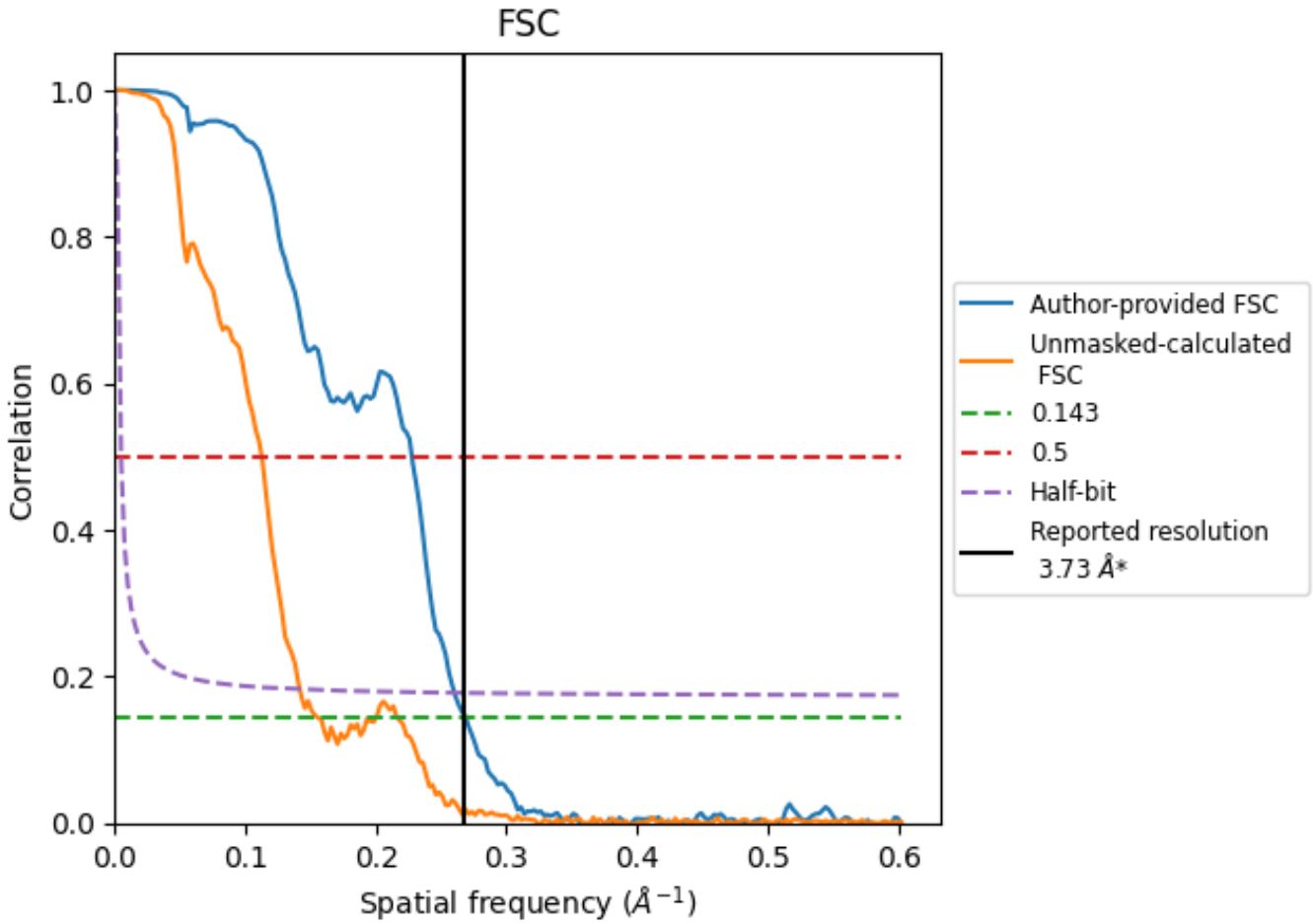


*Reported resolution corresponds to spatial frequency of 0.268 Å^{-1}

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 0.268 Å^{-1}

8.2 Resolution estimates (i)

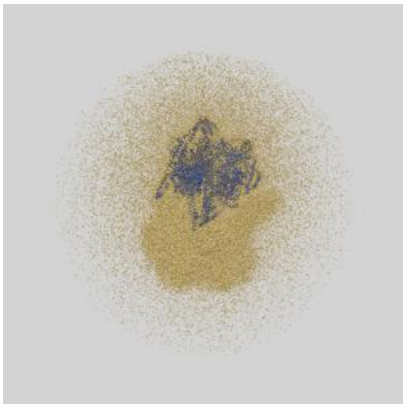
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	3.72	4.40	3.84
Unmasked-calculated*	6.42	8.88	7.06

*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 6.42 differs from the reported value 3.73 by more than 10 %

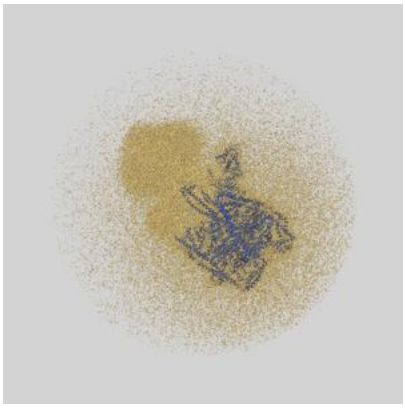
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26622 and PDB model 7UNE. Per-residue inclusion information can be found in section 3 on page 6.

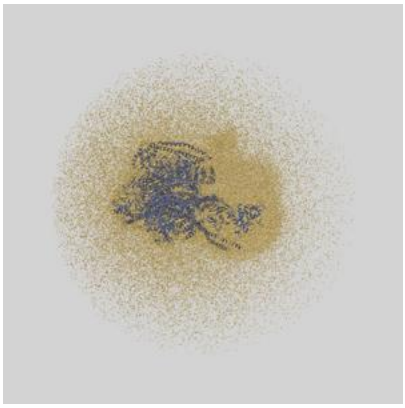
9.1 Map-model overlay



X



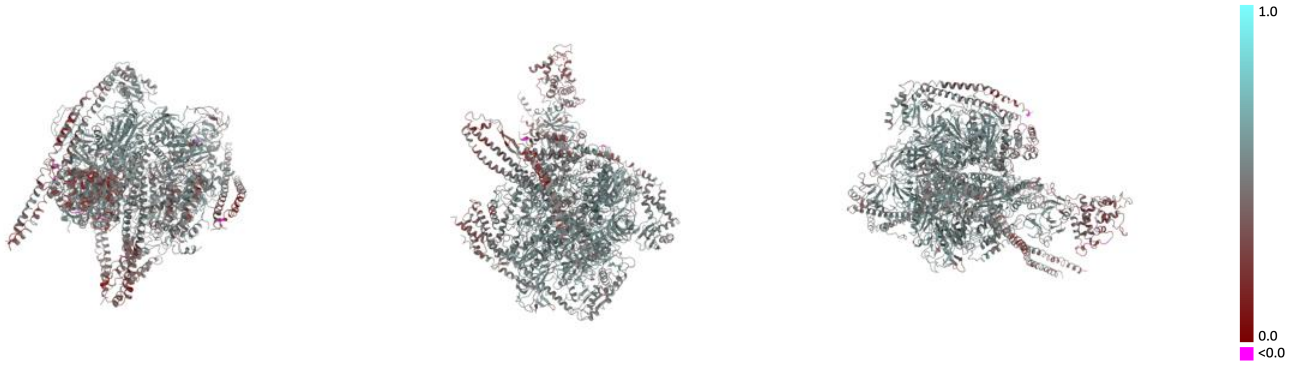
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

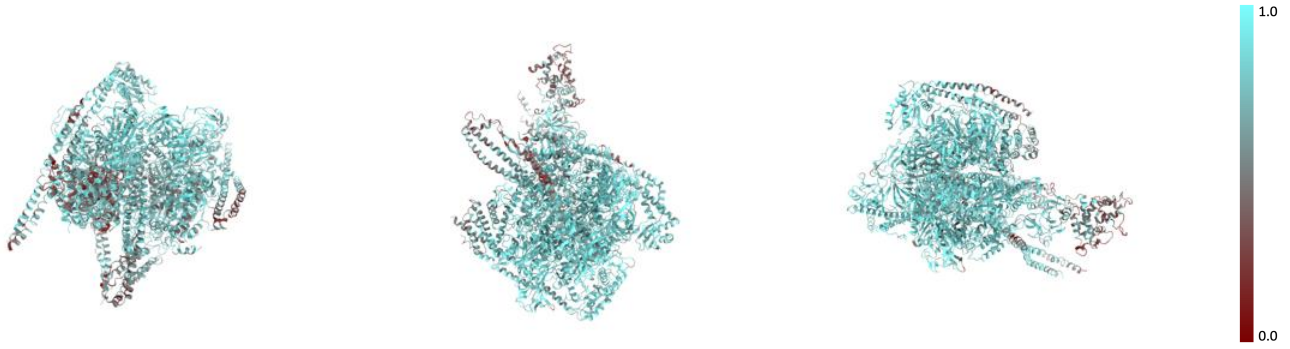
9.2 Q-score mapped to coordinate model (i)



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.

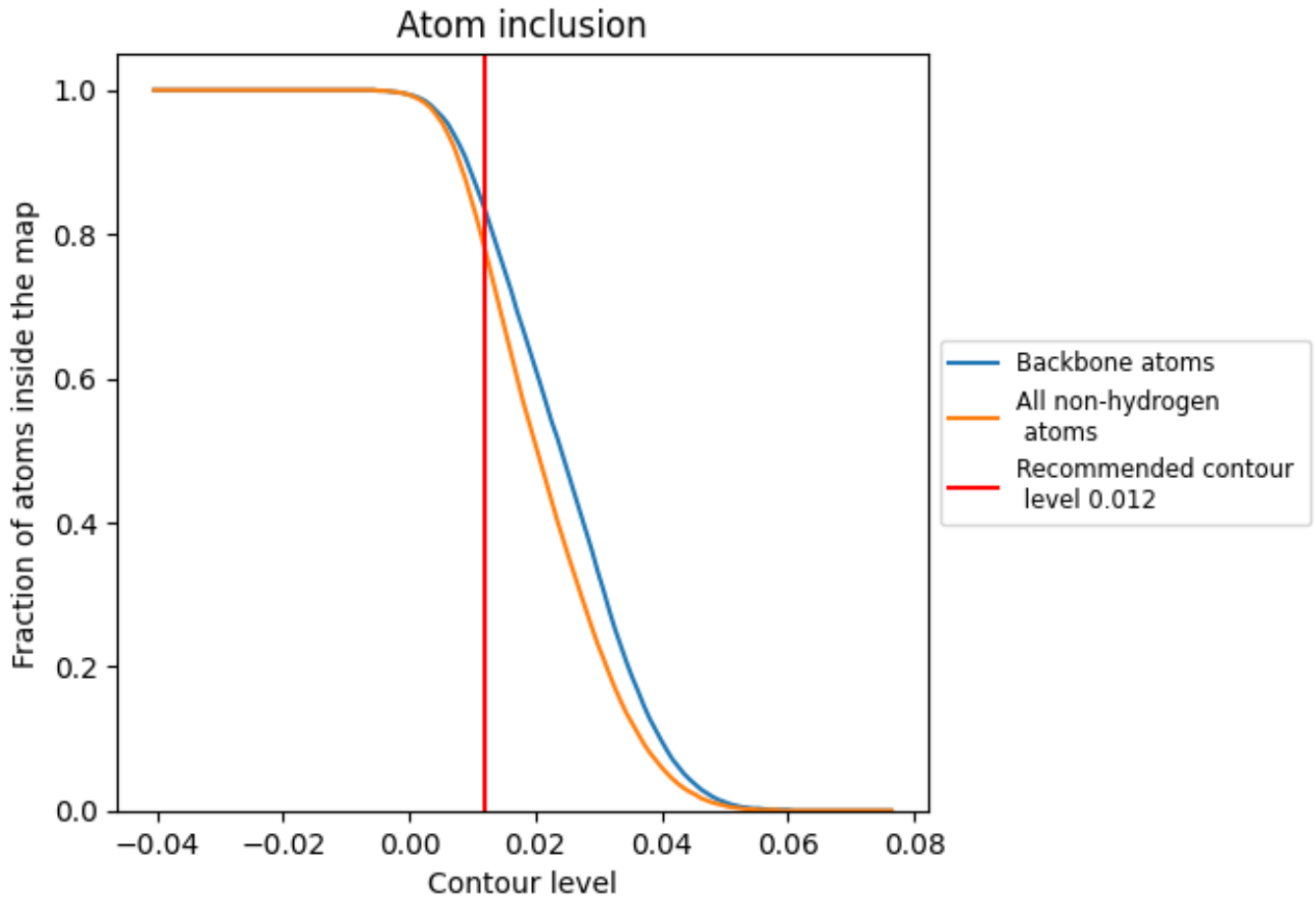
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.4960
D	0.6450	0.4310
L	0.7930	0.4980
M	0.8250	0.5240
N	0.7710	0.4870
O	0.8450	0.5420
P	0.8550	0.5470
Q	0.8560	0.5440
U	0.6030	0.4150
b	0.7540	0.4800
c	0.7910	0.4760
d	0.7420	0.4650
e	0.6690	0.3990
f	0.7480	0.4270
g	0.7110	0.4080