Full wwPDB EM Validation Report ⓘ

Mar 26, 2024 – 01:56 am GMT

PDB ID	:	8R0G
EMDB ID	:	EMD-18792
Title	:	Capsid structure of Giardiavirus (GLV) CAT strain
Authors	:	Wang, H.; Gianluca, M.; Munke, A.; Hassan, M.M.; Lalle, M.; Okamoto, K.
Deposited on	:	2023-10-31
Resolution	:	2.60 Å(reported)
Based on initial model	:	6S2C

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:

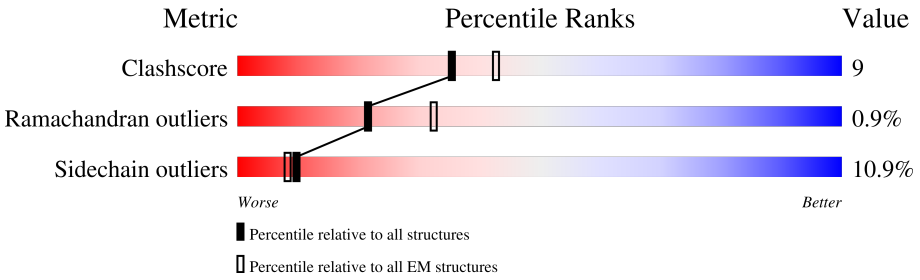
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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	929	67% 22% • 8%
1	B	929	66% 22% • 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13445 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	855	Total	C	N	O	S	0	0
			6732	4320	1124	1260	28		
1	B	853	Total	C	N	O	S	0	0
			6713	4305	1124	1256	28		

There are 12 discrepancies between the modelled and reference sequences:

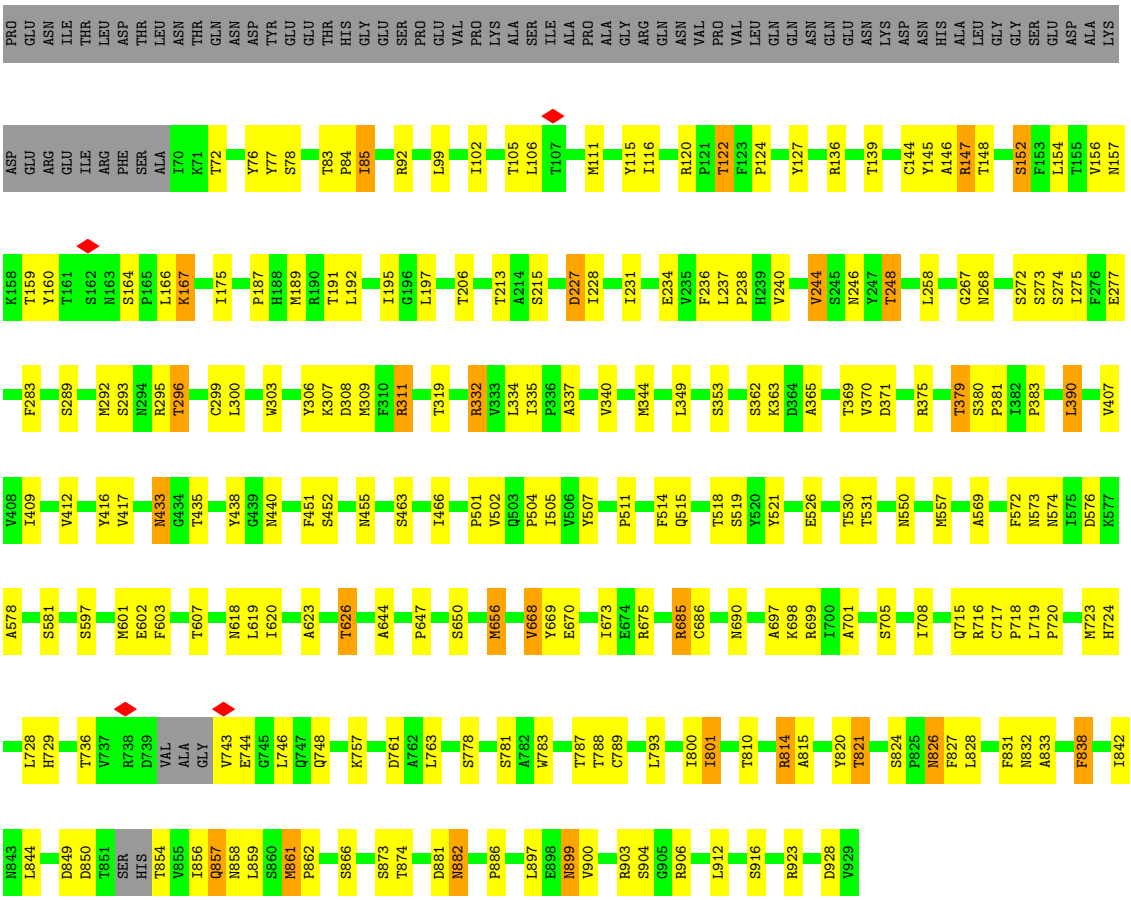
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	SER	ASN	conflict	UNP A0A8F6AGH5
A	202	GLN	LEU	conflict	UNP A0A8F6AGH5
A	203	ASN	ALA	conflict	UNP A0A8F6AGH5
A	204	LEU	THR	conflict	UNP A0A8F6AGH5
A	205	ALA	SER	conflict	UNP A0A8F6AGH5
A	206	THR	GLN	conflict	UNP A0A8F6AGH5
B	201	SER	ASN	conflict	UNP A0A8F6AGH5
B	202	GLN	LEU	conflict	UNP A0A8F6AGH5
B	203	ASN	ALA	conflict	UNP A0A8F6AGH5
B	204	LEU	THR	conflict	UNP A0A8F6AGH5
B	205	ALA	SER	conflict	UNP A0A8F6AGH5
B	206	THR	GLN	conflict	UNP A0A8F6AGH5

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.

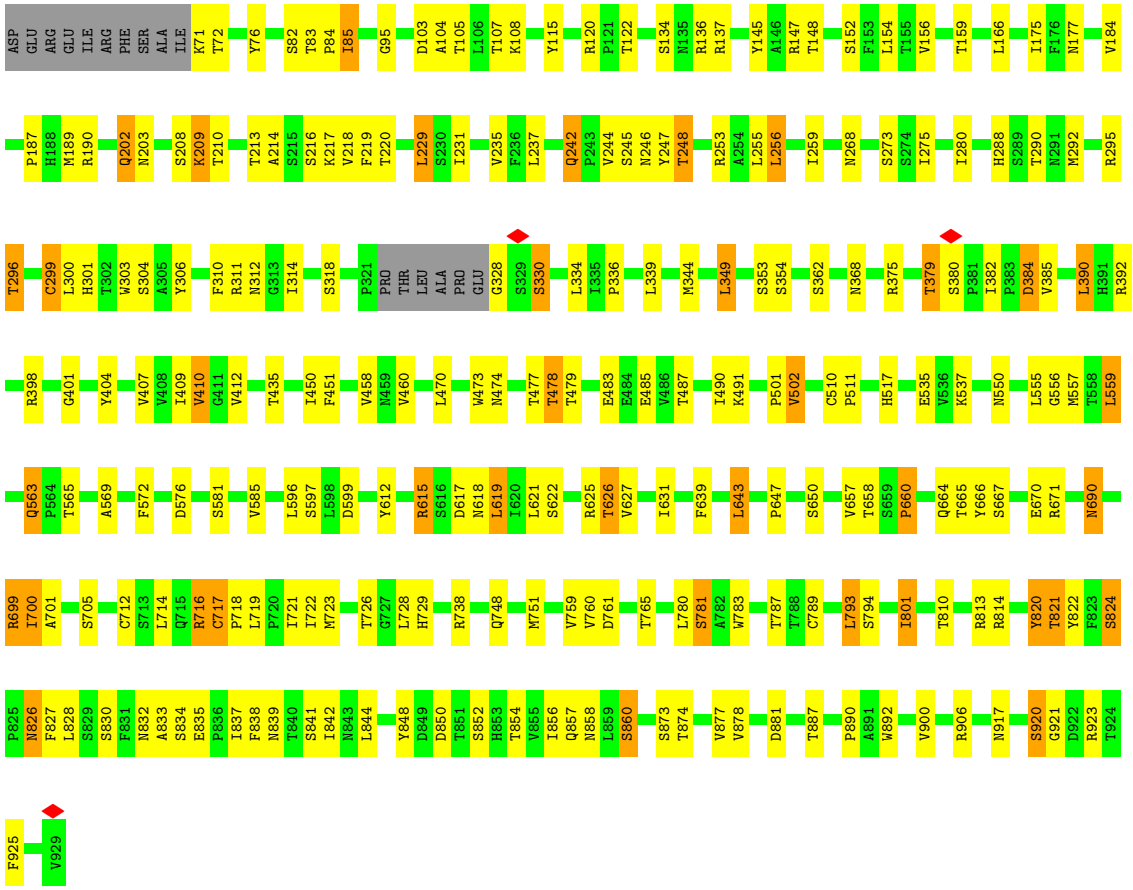
- Molecule 1: Capsid protein

Chain A:



- Molecule 1: Capsid protein

Chain B:


ASP GLU ARG GLU ILE ARG PHE SER ALA ILE K71 T72 Y76 S82 T83 P84 I85 G95 D103 A104 T105 L106 T107 K108 Y115 R120 P121 T122 S134 N135 R136 R137 Y145 A146 R147 T148 S152 F153 L154 T155 V156 T159 L166 I175 F176 N177 V184
P187 H188 M189 R190 Q202 N203 S208 K209 T210 T213 A214 S215 S216 K217 V218 F219 T220 L229 S230 I231 V235 F236 L237 Q242 P243 V244 S245 N246 Y247 T248 R253 A254 L255 L256 I259 N268 S273 S274 I275 I280 H288 S289 T290 N291 M292 R295
T296 C299 L300 H301 T302 W303 S304 A305 Y306 F310 R311 N312 G313 I314 S318 P321 PRO THR LEU ALA PRO GLU G328 S329 S330 L334 I335 P336 L339 M344 L349 S353 S354 S362 N368 R375 T379 S380 P381 I382 P383 D384 V385 L390 H391 R392
R398 G401 Y404 V407 V408 I409 V410 G411 V412 T435 I450 F451 V458 N459 V460 L470 W473 N474 T477 T478 T479 E483 E484 E485 V486 T487 I490 K491 P501 V502 C510 P511 H517 E535 V536 K537 N550 L555 G556 M557 T558 L559
Q563 P564 T565 A569 F572 D576 S581 V585 L596 S597 L598 D599 Y612 R615 S616 D617 N618 L619 I620 L621 S622 R625 T626 V627 I631 F639 L643 P647 S650 V657 T658 S659 P660 Q664 T665 Y666 S667 E670 R671 N690
R699 I700 A701 S705 C712 S713 L714 Q715 R716 C717 P718 L719 P720 I721 I722 M723 T726 G727 L728 H729 R738 Q748 M751 V759 V760 D761 T765 L780 S781 A782 W783 T787 T788 C789 L793 S794 I801 T810 R813 R814 Y820 T821 Y822 F823 S824
P825 N826 F827 L828 S829 S830 F831 N832 A833 S834 E835 P836 I837 F838 N839 T840 S841 I842 N843 L844 Y848 D849 D850 T851 S852 H853 T854 V855 I856 Q857 N858 L859 S860 S873 T874 V877 V878 D881 T887 P890 A891 W892 V900 R906 N917 S920 G921 D922 R923 T924
F925 V929

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5804	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.947	Depositor
Minimum map value	-1.352	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	678.39996, 678.39996, 678.39996	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.25	0/6918	0.49	0/9453
1	B	0.33	2/6899 (0.0%)	0.55	4/9426 (0.0%)
All	All	0.29	2/13817 (0.0%)	0.52	4/18879 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	660	PRO	CG-CD	-11.85	1.11	1.50
1	B	660	PRO	N-CD	5.95	1.56	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	660	PRO	N-CD-CG	-13.39	83.11	103.20
1	B	660	PRO	CA-N-CD	-12.09	94.58	111.50
1	B	660	PRO	CA-CB-CG	-7.02	90.66	104.00
1	B	208	SER	N-CA-C	-5.63	95.79	111.00

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	6732	0	6584	114	0
1	B	6713	0	6560	115	0
All	All	13445	0	13144	228	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 9.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:HG23	1:A:84:PRO:HD3	1.58	0.85
1:B:296:THR:HG21	1:B:353:SER:HB3	1.66	0.76
1:A:85:ILE:HD11	1:B:925:PHE:HB3	1.68	0.76
1:A:296:THR:HG21	1:A:353:SER:HB3	1.66	0.75
1:A:76:TYR:O	1:A:92:ARG:NH2	2.26	0.69
1:A:656:MET:HB2	1:A:697:ALA:HB3	1.76	0.68
1:B:104:ALA:O	1:B:107:THR:OG1	2.11	0.67
1:B:253:ARG:NH2	1:B:353:SER:O	2.28	0.67
1:A:167:LYS:HD2	1:A:383:PRO:HG2	1.76	0.66
1:A:370:VAL:HG23	1:A:380:SER:HA	1.78	0.66
1:B:789:CYS:O	1:B:858:ASN:ND2	2.28	0.66
1:A:349:LEU:HD12	1:A:451:PHE:HE2	1.62	0.65
1:B:722:ILE:O	1:B:726:THR:OG1	2.15	0.65
1:A:308:ASP:OD1	1:A:311:ARG:NH1	2.30	0.64
1:A:861:MET:HG3	1:A:862:PRO:HD2	1.80	0.64
1:A:334:LEU:HB2	1:A:597:SER:HB2	1.79	0.64
1:A:289:SER:OG	1:A:576:ASP:OD2	2.15	0.64
1:A:365:ALA:O	1:A:369:THR:OG1	2.15	0.63
1:B:187:PRO:HB2	1:B:244:VAL:HB	1.80	0.62
1:B:650:SER:O	1:B:666:TYR:OH	2.17	0.62
1:A:793:LEU:HA	1:A:856:ILE:HD11	1.81	0.61
1:B:115:TYR:HB3	1:B:280:ILE:HD13	1.81	0.61
1:B:148:THR:HG21	1:B:717:CYS:HB3	1.83	0.60
1:A:147:ARG:NH2	1:A:833:ALA:O	2.34	0.60
1:A:906:ARG:HG3	1:A:906:ARG:HH11	1.66	0.60
1:A:283:PHE:HB3	1:A:363:LYS:HD3	1.83	0.60
1:A:838:PHE:HA	1:A:842:ILE:HG13	1.84	0.59
1:B:290:THR:HG23	1:B:295:ARG:HH12	1.67	0.59
1:B:242:GLN:O	1:B:242:GLN:NE2	2.34	0.59
1:B:328:GLY:HA3	1:B:404:TYR:HB3	1.82	0.59
1:A:881:ASP:O	1:A:882:ASN:HB2	2.01	0.59
1:B:576:ASP:OD1	1:B:576:ASP:N	2.34	0.59
1:B:793:LEU:HD12	1:B:856:ILE:HG12	1.84	0.59
1:A:92:ARG:NH1	1:A:724:HIS:O	2.36	0.59
1:A:227:ASP:OD1	1:A:227:ASP:N	2.31	0.58
1:A:293:SER:OG	1:A:295:ARG:NH1	2.36	0.58
1:B:156:VAL:HG12	1:B:166:LEU:HD12	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:SER:HB2	1:B:390:LEU:HB3	1.85	0.58
1:B:268:ASN:ND2	1:B:275:ILE:O	2.35	0.58
1:B:502:VAL:HG13	1:B:556:GLY:HA3	1.85	0.57
1:A:602:GLU:O	1:A:602:GLU:HG3	2.04	0.57
1:A:511:PRO:HD3	1:A:801:ILE:HD12	1.86	0.57
1:A:576:ASP:OD1	1:A:576:ASP:N	2.39	0.56
1:B:719:LEU:O	1:B:723:MET:HG2	2.06	0.56
1:B:700:ILE:HG22	1:B:701:ALA:H	1.71	0.56
1:B:330:SER:HB3	1:B:404:TYR:HB2	1.88	0.56
1:B:748:GLN:NE2	1:B:761:ASP:OD1	2.36	0.56
1:A:192:LEU:HD12	1:A:197:LEU:HD23	1.88	0.56
1:A:647:PRO:O	1:A:650:SER:OG	2.24	0.56
1:B:122:THR:HG23	1:B:145:TYR:HB3	1.87	0.55
1:A:746:LEU:HD21	1:A:886:PRO:HD2	1.87	0.55
1:B:517:HIS:HA	1:B:813:ARG:HH21	1.70	0.55
1:B:177:ASN:HA	1:B:398:ARG:HB3	1.88	0.55
1:A:145:TYR:HE1	1:A:903:ARG:HG2	1.70	0.54
1:A:746:LEU:HD22	1:A:763:LEU:HB3	1.89	0.54
1:A:102:ILE:HD12	1:A:102:ILE:O	2.07	0.54
1:B:828:LEU:HD12	1:B:856:ILE:HG22	1.89	0.54
1:A:824:SER:HB3	1:A:827:PHE:H	1.73	0.54
1:A:686:CYS:O	1:A:690:ASN:ND2	2.40	0.54
1:B:148:THR:HG23	1:B:721:ILE:HD12	1.89	0.54
1:B:382:ILE:HB	1:B:385:VAL:HB	1.89	0.54
1:B:821:THR:H	1:B:860:SER:HB2	1.71	0.53
1:B:470:LEU:HD23	1:B:619:LEU:HD23	1.90	0.53
1:B:255:LEU:HD13	1:B:626:THR:HG21	1.91	0.53
1:A:167:LYS:HG2	1:A:531:THR:HB	1.90	0.53
1:A:371:ASP:HB3	1:A:379:THR:HG23	1.91	0.53
1:A:175:ILE:HD11	1:A:569:ALA:HB2	1.89	0.53
1:B:175:ILE:HD11	1:B:569:ALA:HB2	1.89	0.53
1:A:148:THR:HG21	1:A:717:CYS:HA	1.91	0.53
1:B:334:LEU:HB2	1:B:597:SER:HB2	1.91	0.52
1:B:490:ILE:HG23	1:B:626:THR:HG22	1.91	0.52
1:A:148:THR:CG2	1:A:718:PRO:HD3	2.40	0.52
1:B:299:CYS:HB3	1:B:301:HIS:CE1	2.45	0.52
1:B:738:ARG:O	1:B:738:ARG:HG3	2.09	0.52
1:A:148:THR:HG21	1:A:718:PRO:HD3	1.90	0.52
1:A:160:TYR:OH	1:A:164:SER:OG	2.27	0.52
1:B:890:PRO:HB3	1:B:892:TRP:CE2	2.44	0.51
1:B:664:GLN:O	1:B:667:SER:OG	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ASN:O	1:B:478:THR:OG1	2.20	0.51
1:A:832:ASN:ND2	1:A:844:LEU:O	2.43	0.51
1:B:148:THR:HG22	1:B:718:PRO:HD2	1.91	0.51
1:B:690:ASN:N	1:B:690:ASN:OD1	2.44	0.51
1:A:515:GLN:HG3	1:A:521:TYR:CZ	2.46	0.51
1:A:187:PRO:HA	1:A:246:ASN:HB2	1.94	0.50
1:B:780:LEU:O	1:B:783:TRP:HB3	2.11	0.50
1:A:670:GLU:OE1	1:A:685:ARG:NH2	2.45	0.50
1:B:300:LEU:HD23	1:B:407:VAL:HB	1.94	0.50
1:A:826:ASN:OD1	1:A:826:ASN:N	2.45	0.49
1:B:105:THR:HA	1:B:108:LYS:HE2	1.93	0.49
1:A:156:VAL:HG12	1:A:166:LEU:HD12	1.94	0.49
1:B:136:ARG:H	1:B:136:ARG:HD3	1.77	0.49
1:B:354:SER:HB3	1:B:401:GLY:H	1.78	0.49
1:A:240:VAL:HG22	1:A:603:PHE:CZ	2.47	0.49
1:A:106:LEU:HD22	1:A:620:ILE:HG23	1.95	0.49
1:B:202:GLN:HG2	1:B:229:LEU:HD12	1.94	0.49
1:A:789:CYS:O	1:A:858:ASN:ND2	2.45	0.49
1:A:787:THR:O	1:A:820:TYR:OH	2.13	0.49
1:B:670:GLU:OE1	1:B:671:ARG:NH2	2.39	0.49
1:B:555:LEU:HD12	1:B:700:ILE:HD11	1.94	0.48
1:A:268:ASN:ND2	1:A:275:ILE:O	2.44	0.48
1:B:699:ARG:O	1:B:699:ARG:HD3	2.13	0.48
1:B:134:SER:HB2	1:B:136:ARG:HD3	1.95	0.48
1:B:563:GLN:NE2	1:B:585:VAL:O	2.47	0.48
1:A:452:SER:HA	1:A:455:ASN:ND2	2.27	0.48
1:A:501:PRO:HA	1:A:557:MET:HG3	1.95	0.48
1:B:85:ILE:HD11	1:B:639:PHE:HE2	1.79	0.48
1:B:824:SER:HG	1:B:827:PHE:H	1.58	0.48
1:A:789:CYS:HB2	1:A:800:ILE:HB	1.96	0.48
1:A:335:ILE:HG13	1:A:340:VAL:HG22	1.96	0.47
1:B:832:ASN:ND2	1:B:844:LEU:O	2.46	0.47
1:A:236:PHE:O	1:A:240:VAL:HG23	2.14	0.47
1:B:487:THR:O	1:B:491:LYS:HG3	2.14	0.47
1:B:622:SER:O	1:B:626:THR:HG23	2.15	0.47
1:A:670:GLU:HB2	1:A:685:ARG:HH21	1.80	0.47
1:B:303:TRP:HB2	1:B:410:VAL:HA	1.96	0.47
1:B:310:PHE:CD2	1:B:314:ILE:HG22	2.49	0.47
1:A:433:ASN:OD1	1:A:433:ASN:N	2.48	0.47
1:A:923:ARG:HD2	1:A:923:ARG:HA	1.61	0.47
1:B:738:ARG:HH11	1:B:887:THR:HG23	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:TRP:O	1:B:477:THR:OG1	2.25	0.46
1:A:644:ALA:HB1	1:A:668:VAL:HB	1.98	0.46
1:A:111:MET:O	1:A:115:TYR:HD1	1.99	0.46
1:A:231:ILE:HG12	1:A:303:TRP:CZ2	2.50	0.46
1:B:247:TYR:HE1	1:B:596:LEU:HD12	1.80	0.46
1:A:246:ASN:OD1	1:A:248:THR:HG23	2.16	0.46
1:A:375:ARG:HH11	1:A:375:ARG:HG3	1.80	0.46
1:A:438:TYR:CZ	1:A:440:ASN:HB2	2.51	0.46
1:B:213:THR:OG1	1:B:214:ALA:N	2.49	0.46
1:A:187:PRO:HB2	1:A:244:VAL:HG22	1.98	0.46
1:A:748:GLN:NE2	1:A:761:ASP:OD1	2.49	0.46
1:B:828:LEU:HD13	1:B:857:GLN:HB2	1.96	0.46
1:B:246:ASN:OD1	1:B:248:THR:HG23	2.16	0.45
1:B:837:ILE:O	1:B:842:ILE:HG13	2.17	0.45
1:A:154:LEU:HD11	1:A:369:THR:HG21	1.97	0.45
1:B:190:ARG:NH2	1:B:599:ASP:OD1	2.49	0.45
1:A:127:TYR:CE2	1:A:857:GLN:HG3	2.52	0.45
1:A:231:ILE:HG12	1:A:303:TRP:CE2	2.52	0.45
1:A:718:PRO:HB2	1:A:720:PRO:HD2	1.99	0.45
1:B:147:ARG:NH2	1:B:833:ALA:O	2.34	0.45
1:B:247:TYR:OH	1:B:599:ASP:OD2	2.23	0.45
1:B:295:ARG:HE	1:B:295:ARG:HB2	1.41	0.45
1:B:881:ASP:OD1	1:B:881:ASP:N	2.49	0.45
1:A:337:ALA:HB2	1:A:412:VAL:HG23	1.99	0.45
1:A:511:PRO:HG2	1:A:514:PHE:HD2	1.82	0.45
1:B:83:THR:HB	1:B:84:PRO:HD3	1.98	0.45
1:B:379:THR:OG1	1:B:380:SER:N	2.49	0.45
1:A:77:TYR:CE2	1:A:899:ASN:HB3	2.53	0.44
1:A:240:VAL:HG22	1:A:603:PHE:HZ	1.82	0.44
1:B:336:PRO:HG2	1:B:339:LEU:HD13	1.99	0.44
1:A:375:ARG:NH2	1:A:849:ASP:OD2	2.47	0.44
1:B:501:PRO:HA	1:B:557:MET:HG2	1.99	0.44
1:A:715:GLN:HB3	1:A:821:THR:HG21	1.98	0.44
1:B:458:VAL:HG12	1:B:460:VAL:HG22	1.99	0.44
1:A:743:VAL:HG13	1:A:744:GLU:HG2	1.98	0.44
1:A:349:LEU:HD12	1:A:451:PHE:CE2	2.47	0.44
1:B:510:CYS:SG	1:B:511:PRO:HD2	2.58	0.44
1:A:300:LEU:HD23	1:A:407:VAL:HB	2.00	0.43
1:A:814:ARG:H	1:A:814:ARG:HG2	1.46	0.43
1:B:801:ILE:HD12	1:B:801:ILE:HA	1.75	0.43
1:A:504:PRO:HA	1:A:526:GLU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.85	0.43
1:A:573:ASN:HB3	1:A:574:ASN:H	1.60	0.43
1:B:259:ILE:HD13	1:B:627:VAL:HG23	1.99	0.43
1:B:643:LEU:HD12	1:B:643:LEU:HA	1.84	0.43
1:A:719:LEU:O	1:A:723:MET:HG3	2.19	0.43
1:B:621:LEU:O	1:B:625:ARG:HG3	2.19	0.43
1:A:152:SER:HB2	1:A:390:LEU:HD22	2.00	0.43
1:A:380:SER:HB2	1:A:381:PRO:HD3	2.00	0.43
1:B:712:CYS:SG	1:B:821:THR:HG22	2.59	0.43
1:B:148:THR:CG2	1:B:718:PRO:HD2	2.49	0.43
1:B:821:THR:HG23	1:B:860:SER:HB2	1.99	0.43
1:B:787:THR:O	1:B:820:TYR:OH	2.22	0.43
1:A:146:ALA:HA	1:A:831:PHE:CD2	2.54	0.43
1:A:157:ASN:OD1	1:A:160:TYR:HB2	2.19	0.43
1:A:505:ILE:HD12	1:A:708:ILE:HG21	1.99	0.43
1:B:759:VAL:HG23	1:B:760:VAL:HG23	2.01	0.43
1:B:76:TYR:OH	1:B:95:GLY:HA3	2.19	0.42
1:A:267:GLY:O	1:A:277:GLU:N	2.51	0.42
1:A:507:TYR:HB2	1:A:708:ILE:HG23	2.02	0.42
1:A:319:THR:HB	1:A:332:ARG:HG2	2.01	0.42
1:B:615:ARG:HB3	1:B:621:LEU:HB3	2.02	0.42
1:A:783:TRP:CD1	1:A:862:PRO:HB2	2.53	0.42
1:A:136:ARG:HA	1:A:912:LEU:HD23	2.00	0.42
1:A:507:TYR:HB2	1:A:708:ILE:HG12	2.02	0.42
1:A:623:ALA:HA	1:A:626:THR:HG23	2.01	0.42
1:A:729:HIS:O	1:A:781:SER:OG	2.24	0.42
1:B:231:ILE:O	1:B:235:VAL:HG23	2.19	0.42
1:B:765:THR:HG22	1:B:877:VAL:HB	2.02	0.42
1:A:719:LEU:N	1:A:720:PRO:HD2	2.35	0.42
1:A:306:TYR:O	1:A:309:MET:HG2	2.20	0.42
1:A:122:THR:HA	1:A:147:ARG:HG2	2.02	0.41
1:B:671:ARG:H	1:B:671:ARG:HG2	1.72	0.41
1:A:850:ASP:OD1	1:A:850:ASP:N	2.53	0.41
1:A:859:LEU:HD22	1:A:897:LEU:HD21	2.01	0.41
1:B:559:LEU:O	1:B:716:ARG:NH1	2.52	0.41
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.87	0.41
1:A:237:LEU:N	1:A:238:PRO:HD2	2.36	0.41
1:A:597:SER:O	1:A:601:MET:HG3	2.20	0.41
1:B:751:MET:HE2	1:B:814:ARG:HD2	2.02	0.41
1:B:920:SER:HB3	1:B:921:GLY:H	1.72	0.41
1:B:248:THR:HG22	1:B:485:GLU:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:MET:HB3	1:A:578:ALA:HB2	2.01	0.41
1:B:292:MET:SD	1:B:576:ASP:HB2	2.61	0.41
1:B:483:GLU:HG2	1:B:612:TYR:CE1	2.56	0.41
1:A:828:LEU:HD13	1:A:857:GLN:HB3	2.02	0.41
1:B:306:TYR:CD2	1:B:314:ILE:HG21	2.56	0.41
1:B:384:ASP:OD1	1:B:384:ASP:N	2.54	0.41
1:B:647:PRO:HD3	1:B:665:THR:HG21	2.02	0.41
1:A:518:THR:HG22	1:A:815:ALA:O	2.20	0.41
1:B:216:SER:O	1:B:220:THR:HG23	2.21	0.41
1:A:409:ILE:HD13	1:A:416:TYR:CE2	2.56	0.41
1:A:669:TYR:CZ	1:A:673:ILE:HD11	2.56	0.41
1:B:292:MET:O	1:B:398:ARG:NH1	2.54	0.41
1:B:349:LEU:HD23	1:B:451:PHE:CZ	2.56	0.41
1:B:375:ARG:N	1:B:535:GLU:OE1	2.31	0.41
1:B:729:HIS:O	1:B:781:SER:HB3	2.20	0.41
1:B:835:GLU:HG3	1:B:906:ARG:HD3	2.02	0.41
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.92	0.41
1:A:124:PRO:HA	1:A:144:CYS:O	2.21	0.41
1:A:258:LEU:HD22	1:A:619:LEU:HG	2.03	0.41
1:B:639:PHE:CE1	1:B:728:LEU:HD11	2.57	0.41
1:A:228:ILE:HA	1:A:231:ILE:HD12	2.02	0.40
1:B:104:ALA:HB1	1:B:618:ASN:HD22	1.86	0.40
1:B:627:VAL:O	1:B:631:ILE:HG13	2.21	0.40
1:B:826:ASN:OD1	1:B:826:ASN:N	2.53	0.40
1:B:71:LYS:HE3	1:B:71:LYS:HB3	1.85	0.40
1:B:154:LEU:HD12	1:B:275:ILE:HG21	2.04	0.40
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.88	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	849/929 (91%)	797 (94%)	44 (5%)	8 (1%)	17 35
1	B	849/929 (91%)	805 (95%)	37 (4%)	7 (1%)	19 39
All	All	1698/1858 (91%)	1602 (94%)	81 (5%)	15 (1%)	21 35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	A	701	ALA
1	B	619	LEU
1	A	882	ASN
1	B	209	LYS
1	B	700	ILE
1	A	699	ARG
1	B	210	THR
1	A	417	VAL
1	A	857	GLN
1	A	900	VAL
1	B	409	ILE
1	B	820	TYR
1	A	861	MET
1	B	660	PRO

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	748/810 (92%)	676 (90%)	72 (10%)	8 16
1	B	745/810 (92%)	655 (88%)	90 (12%)	5 9
All	All	1493/1620 (92%)	1331 (89%)	162 (11%)	10 11

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	78	SER
1	A	85	ILE
1	A	105	THR
1	A	116	ILE
1	A	120	ARG
1	A	122	THR
1	A	139	THR
1	A	152	SER
1	A	159	THR
1	A	167	LYS
1	A	189	MET
1	A	191	THR
1	A	195	ILE
1	A	206	THR
1	A	213	THR
1	A	215	SER
1	A	227	ASP
1	A	234	GLU
1	A	244	VAL
1	A	248	THR
1	A	272	SER
1	A	273	SER
1	A	274	SER
1	A	296	THR
1	A	299	CYS
1	A	307	LYS
1	A	311	ARG
1	A	332	ARG
1	A	344	MET
1	A	362	SER
1	A	379	THR
1	A	390	LEU
1	A	433	ASN
1	A	435	THR
1	A	463	SER
1	A	466	ILE
1	A	502	VAL
1	A	519	SER
1	A	530	THR
1	A	550	ASN
1	A	572	PHE
1	A	581	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	607	THR
1	A	618	ASN
1	A	626	THR
1	A	656	MET
1	A	668	VAL
1	A	675	ARG
1	A	685	ARG
1	A	698	LYS
1	A	705	SER
1	A	716	ARG
1	A	728	LEU
1	A	736	THR
1	A	757	LYS
1	A	778	SER
1	A	788	THR
1	A	801	ILE
1	A	810	THR
1	A	814	ARG
1	A	821	THR
1	A	826	ASN
1	A	838	PHE
1	A	854	THR
1	A	866	SER
1	A	873	SER
1	A	874	THR
1	A	899	ASN
1	A	904	SER
1	A	916	SER
1	A	928	ASP
1	B	72	THR
1	B	82	SER
1	B	85	ILE
1	B	103	ASP
1	B	120	ARG
1	B	137	ARG
1	B	152	SER
1	B	159	THR
1	B	184	VAL
1	B	189	MET
1	B	202	GLN
1	B	203	ASN
1	B	209	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	217	LYS
1	B	218	VAL
1	B	219	PHE
1	B	229	LEU
1	B	237	LEU
1	B	242	GLN
1	B	245	SER
1	B	248	THR
1	B	256	LEU
1	B	273	SER
1	B	288	HIS
1	B	296	THR
1	B	299	CYS
1	B	304	SER
1	B	311	ARG
1	B	312	ASN
1	B	318	SER
1	B	330	SER
1	B	344	MET
1	B	349	LEU
1	B	368	ASN
1	B	379	THR
1	B	384	ASP
1	B	390	LEU
1	B	392	ARG
1	B	410	VAL
1	B	412	VAL
1	B	435	THR
1	B	450	ILE
1	B	478	THR
1	B	479	THR
1	B	502	VAL
1	B	537	LYS
1	B	550	ASN
1	B	559	LEU
1	B	563	GLN
1	B	565	THR
1	B	572	PHE
1	B	581	SER
1	B	615	ARG
1	B	617	ASP
1	B	626	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	643	LEU
1	B	657	VAL
1	B	658	THR
1	B	690	ASN
1	B	699	ARG
1	B	705	SER
1	B	714	LEU
1	B	716	ARG
1	B	717	CYS
1	B	781	SER
1	B	793	LEU
1	B	794	SER
1	B	801	ILE
1	B	810	THR
1	B	821	THR
1	B	822	TYR
1	B	824	SER
1	B	826	ASN
1	B	830	SER
1	B	834	SER
1	B	838	PHE
1	B	839	ASN
1	B	841	SER
1	B	848	TYR
1	B	850	ASP
1	B	852	SER
1	B	854	THR
1	B	860	SER
1	B	873	SER
1	B	874	THR
1	B	878	VAL
1	B	900	VAL
1	B	917	ASN
1	B	920	SER
1	B	923	ARG

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.

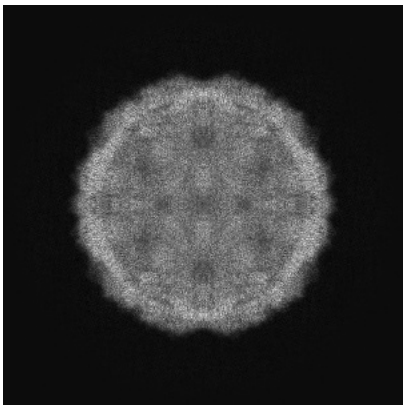
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18792. These allow visual inspection of the internal detail of the map and identification of artifacts.

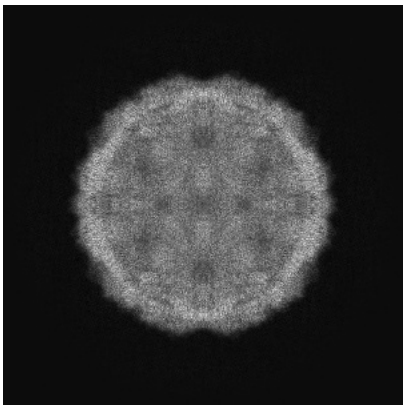
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

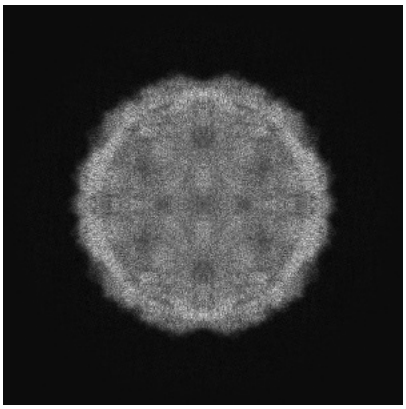
6.1.1 Primary map



X

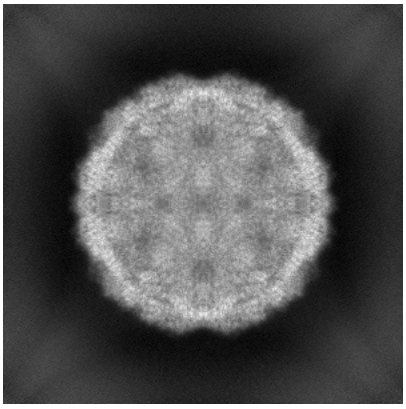


Y

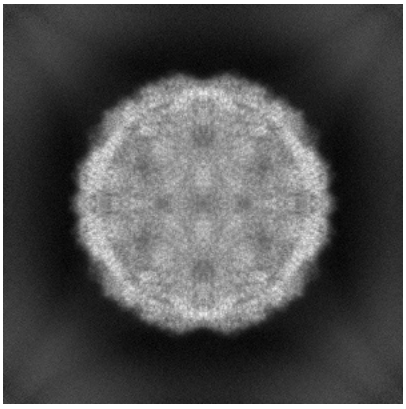


Z

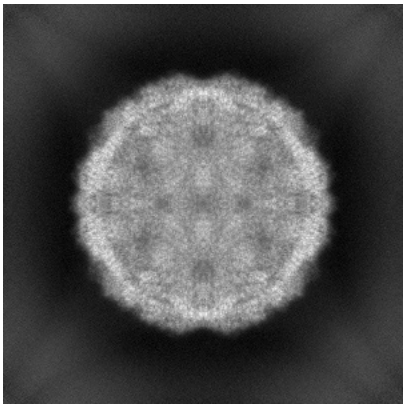
6.1.2 Raw map



X



Y

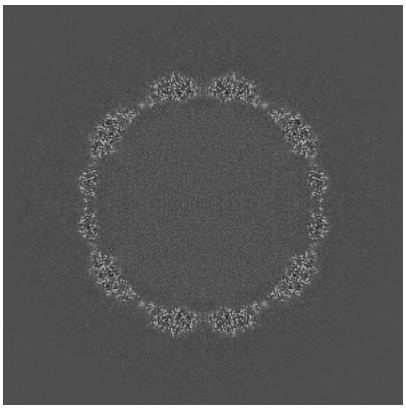


Z

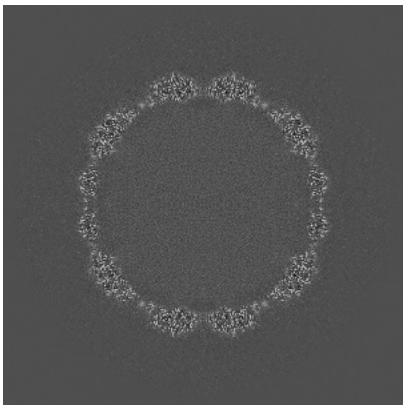
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

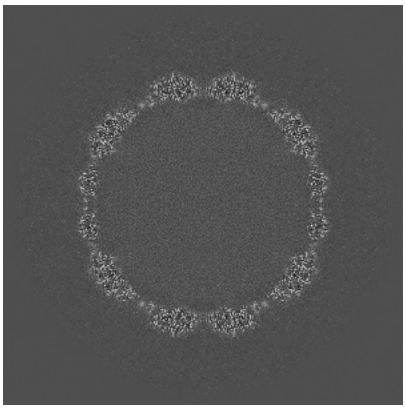
6.2.1 Primary map



X Index: 320

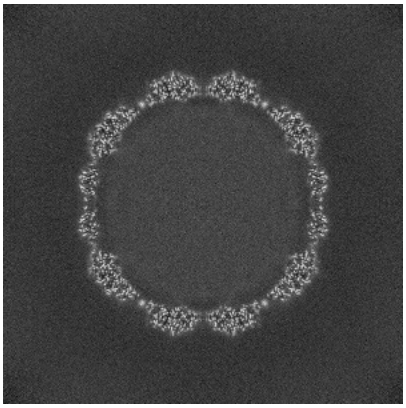


Y Index: 320

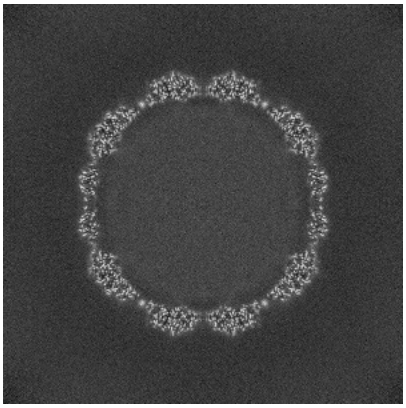


Z Index: 320

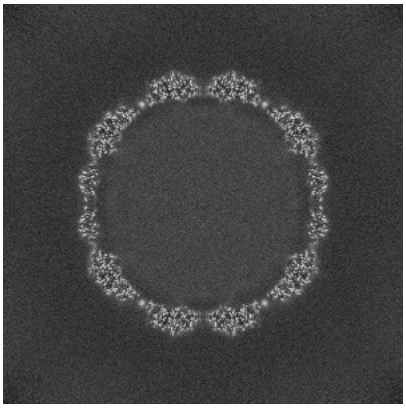
6.2.2 Raw map



X Index: 320



Y Index: 320

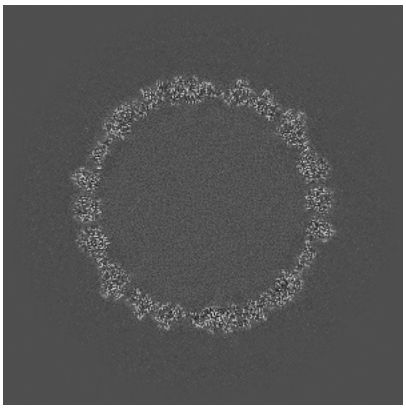


Z Index: 320

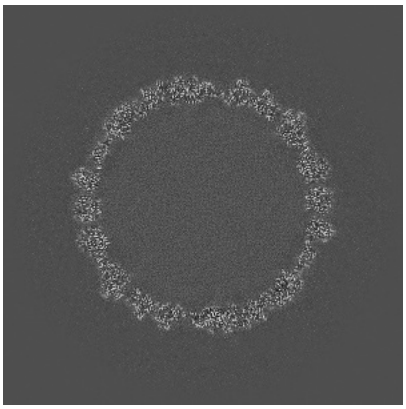
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

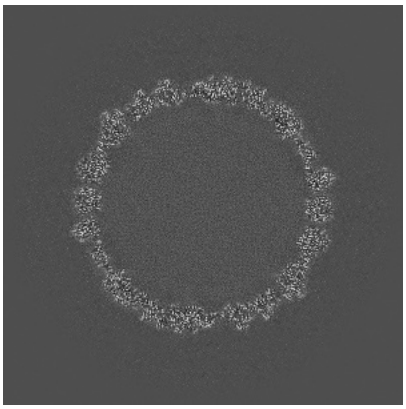
6.3.1 Primary map



X Index: 355

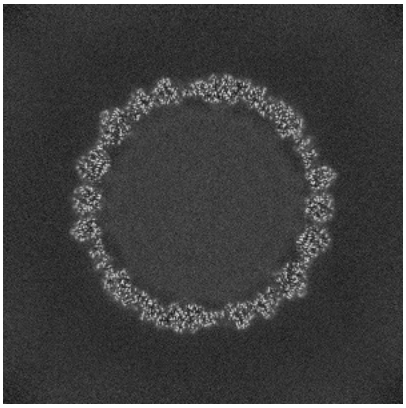


Y Index: 355

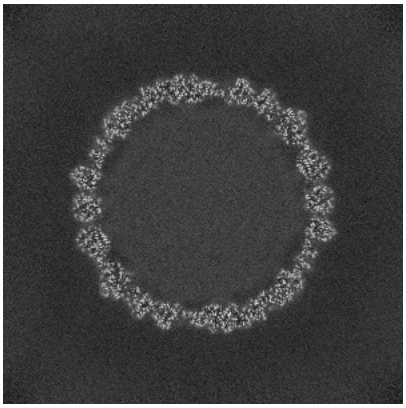


Z Index: 285

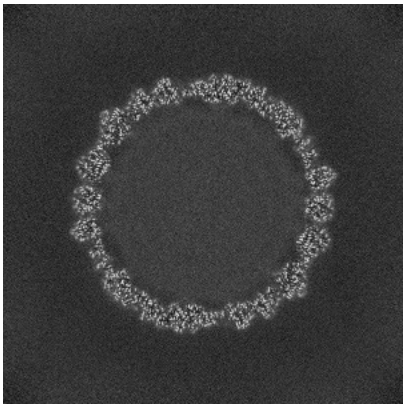
6.3.2 Raw map



X Index: 286



Y Index: 354

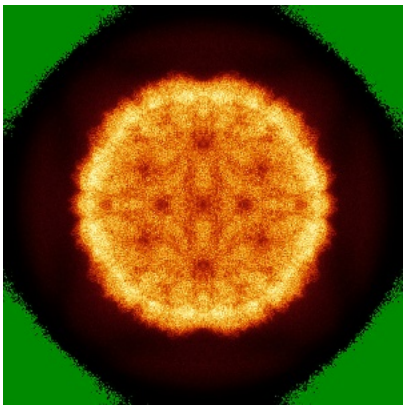


Z Index: 286

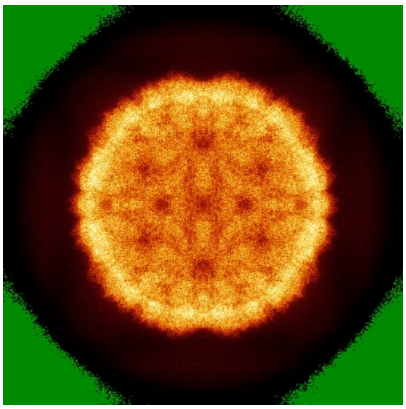
The images above show the largest variance slices of the map in three orthogonal directions.

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

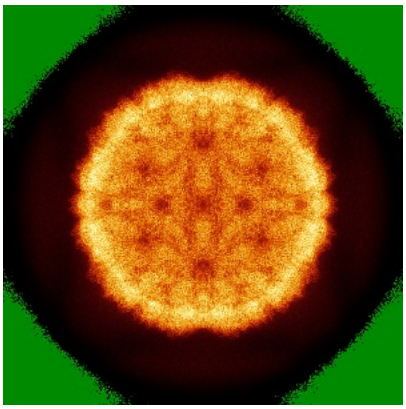
6.4.1 Primary map



X

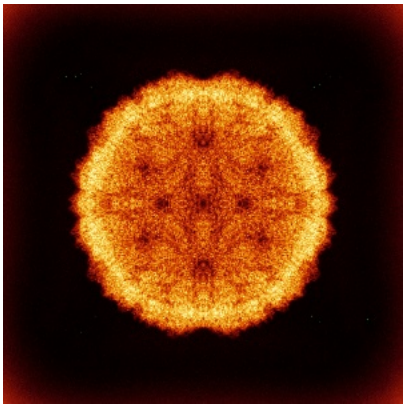


Y

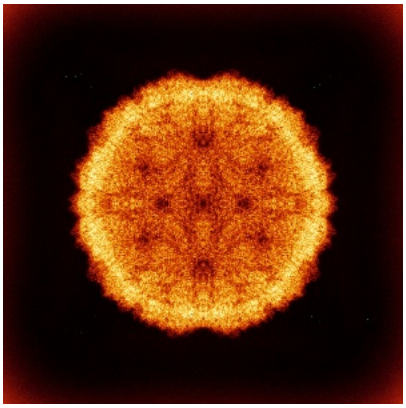


Z

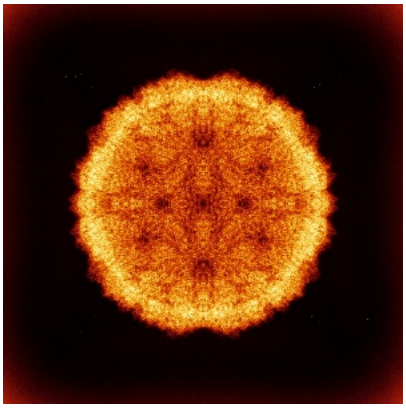
6.4.2 Raw map



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.

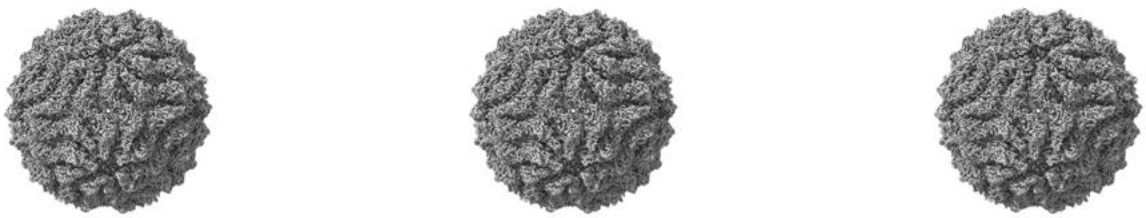
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

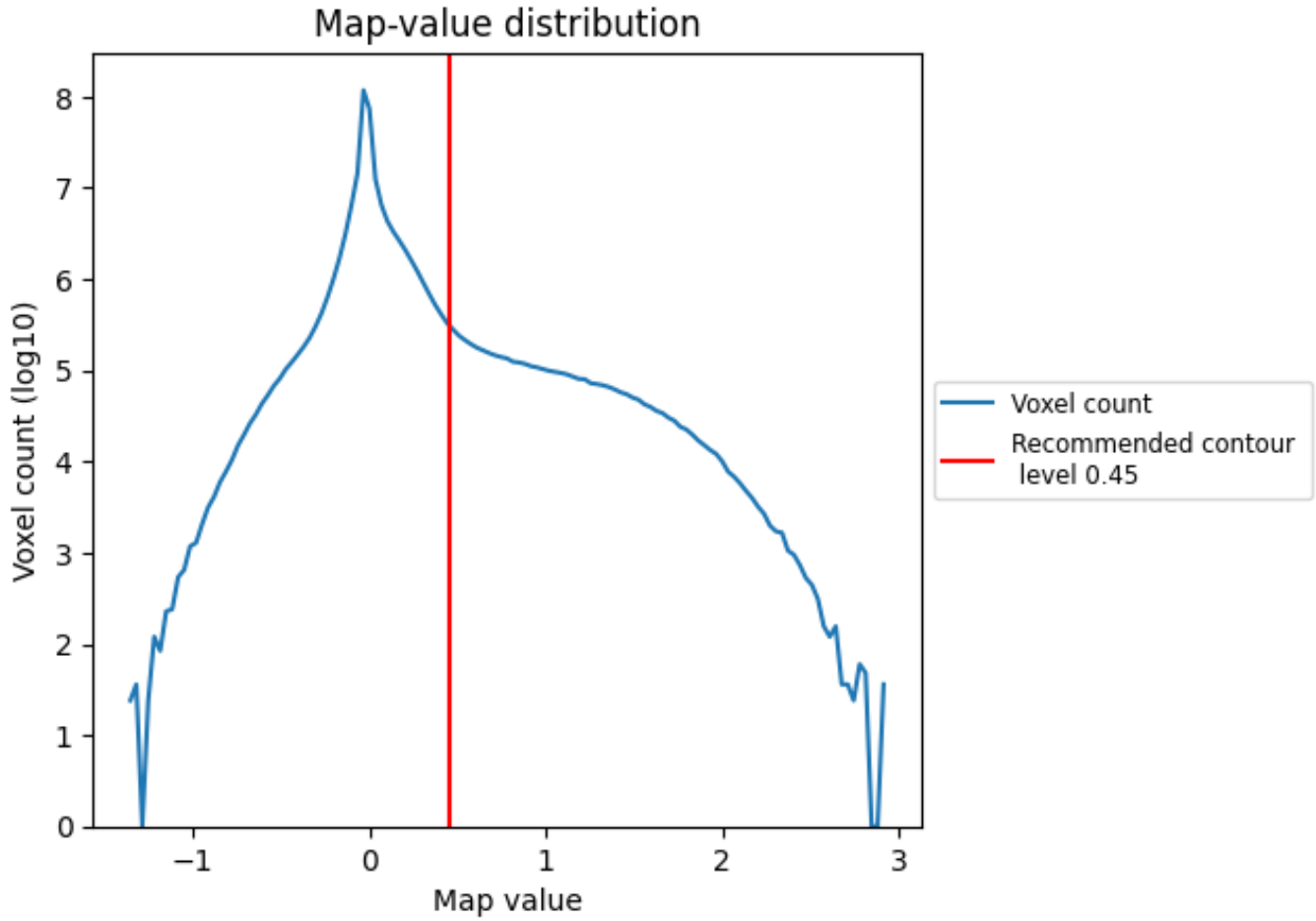
6.6 Mask visualisation (i)

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

7 Map analysis

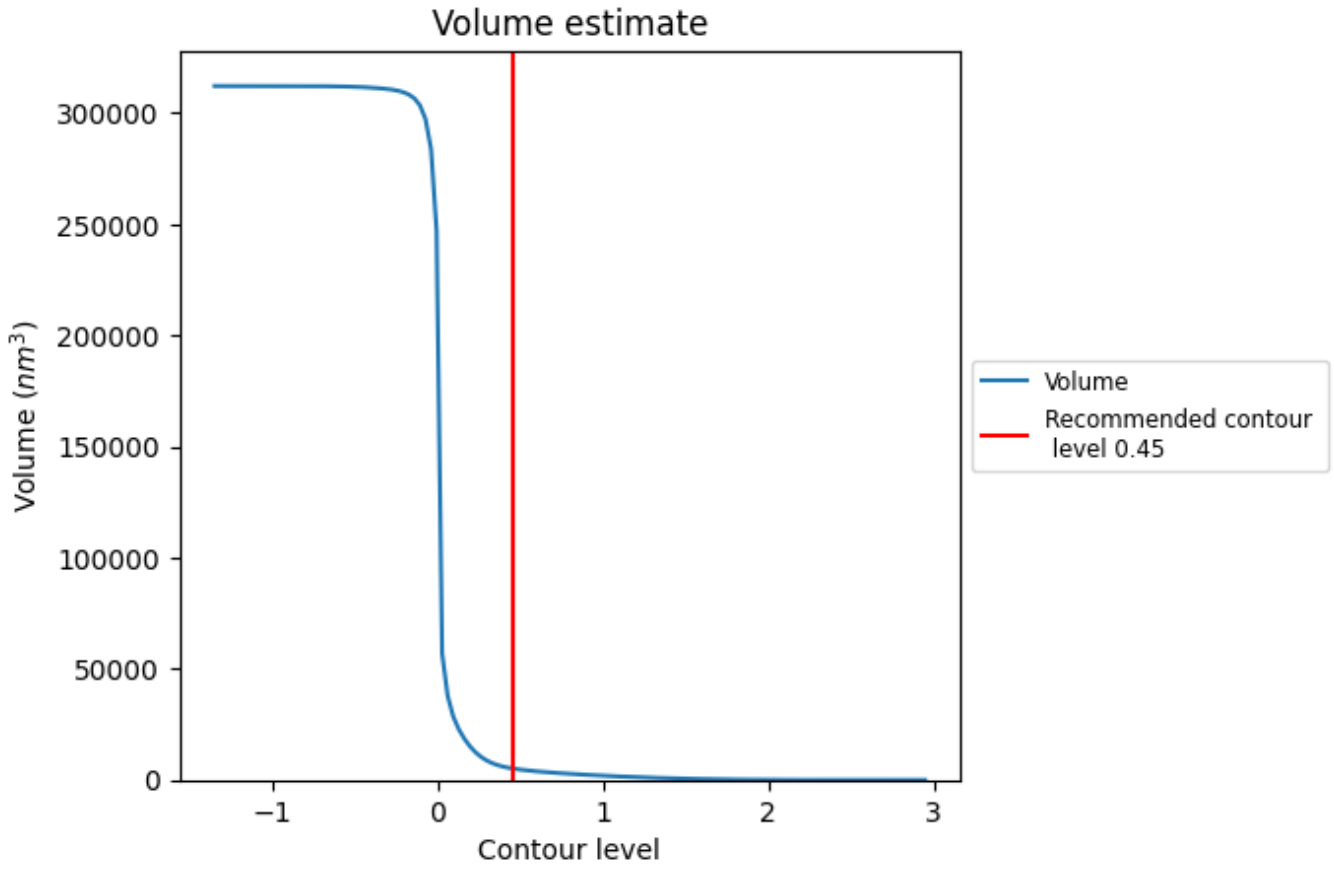
This section contains the results of statistical analysis of the map.

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.

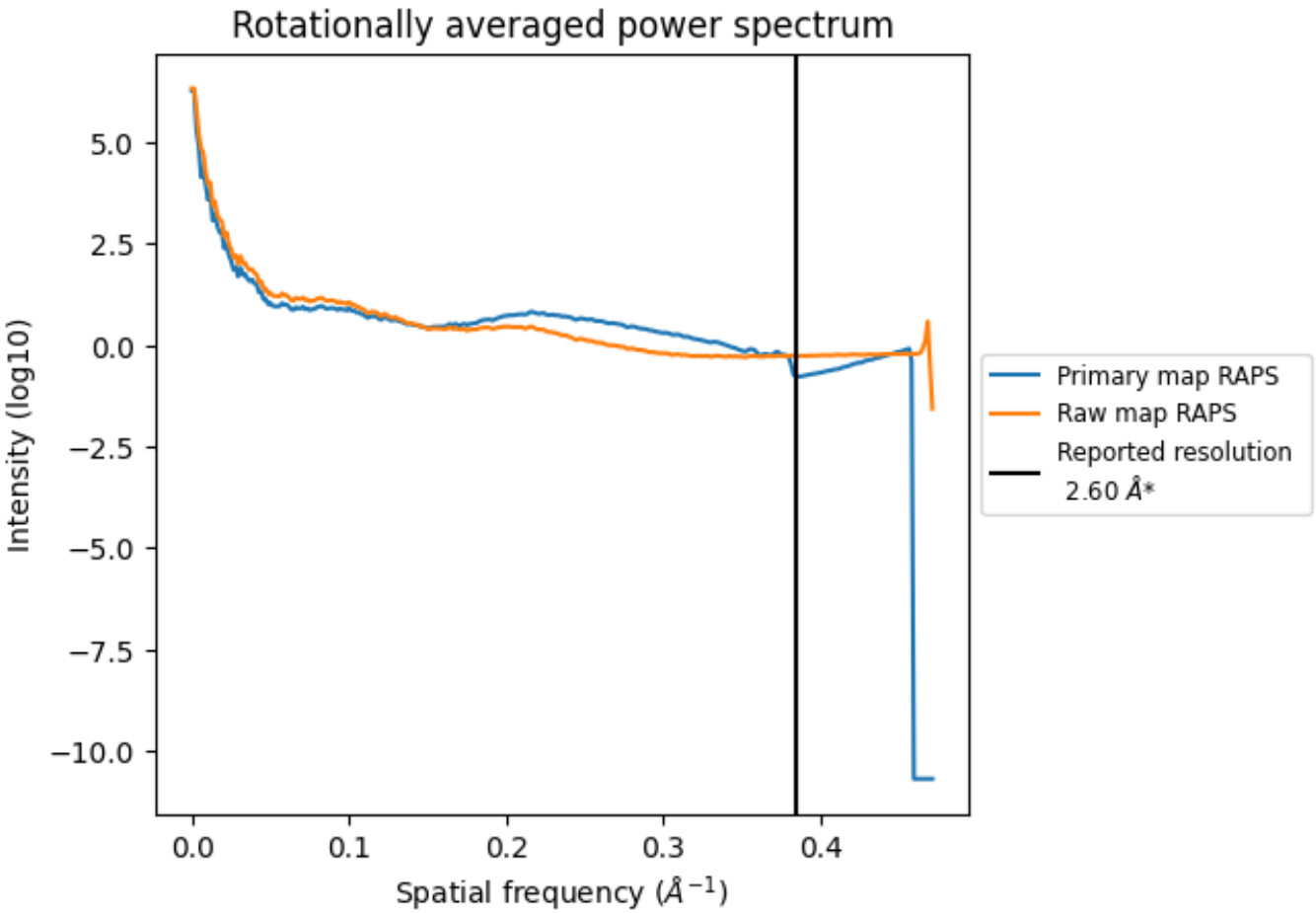
7.2 Volume estimate



The volume at the recommended contour level is 5174 nm^3; this corresponds to an approximate mass of 4674 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

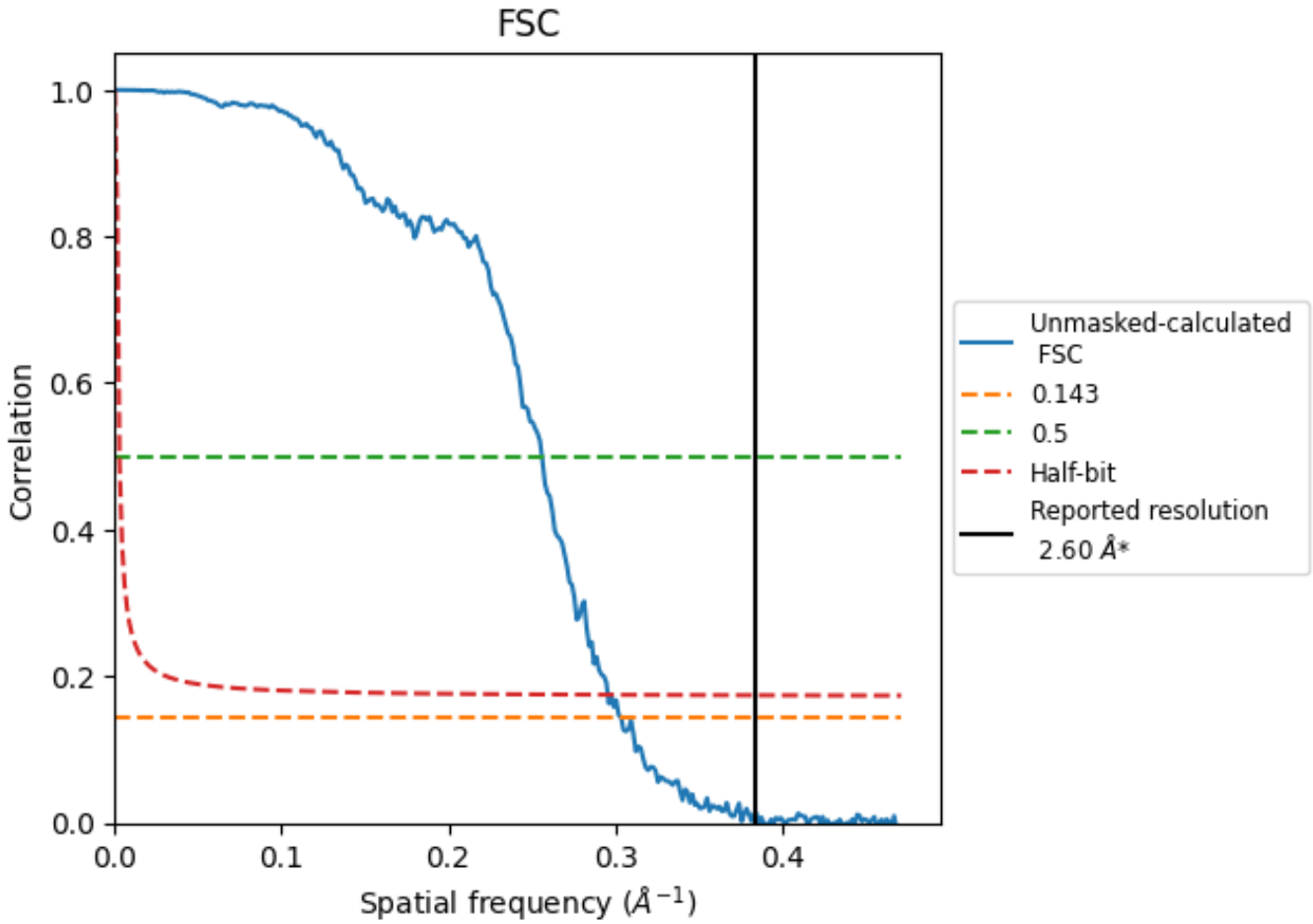


*Reported resolution corresponds to spatial frequency of 0.385 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	3.90	3.38

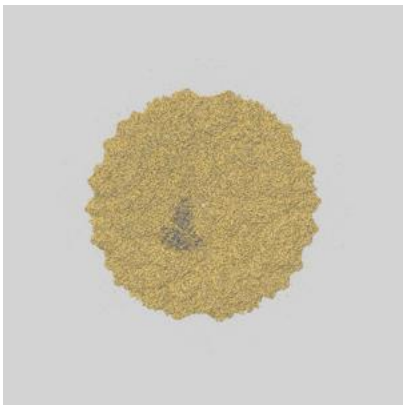
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.6 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18792 and PDB model 8R0G. Per-residue inclusion information can be found in section 3 on page 4.

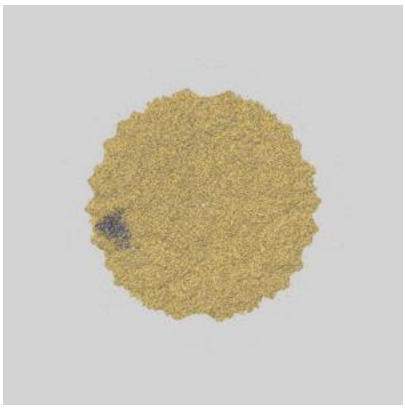
9.1 Map-model overlays

9.1.1 Map-model overlay



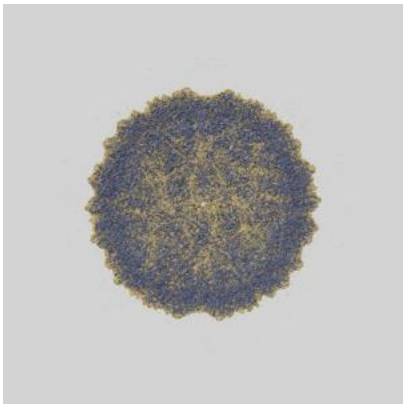
X

Y

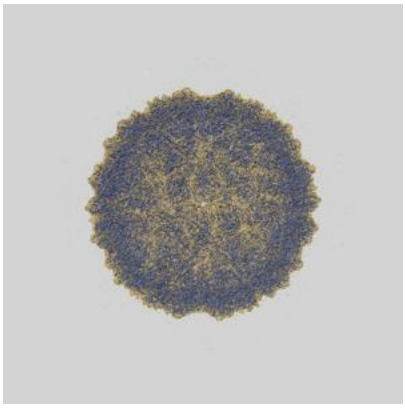


Z

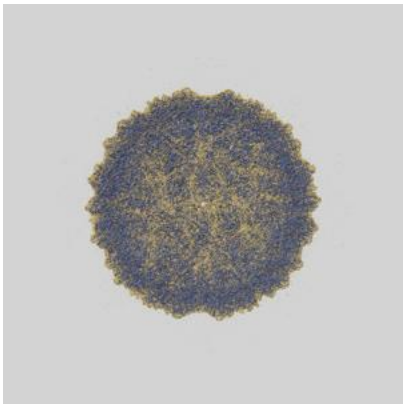
9.1.2 Map-model assembly overlay



X



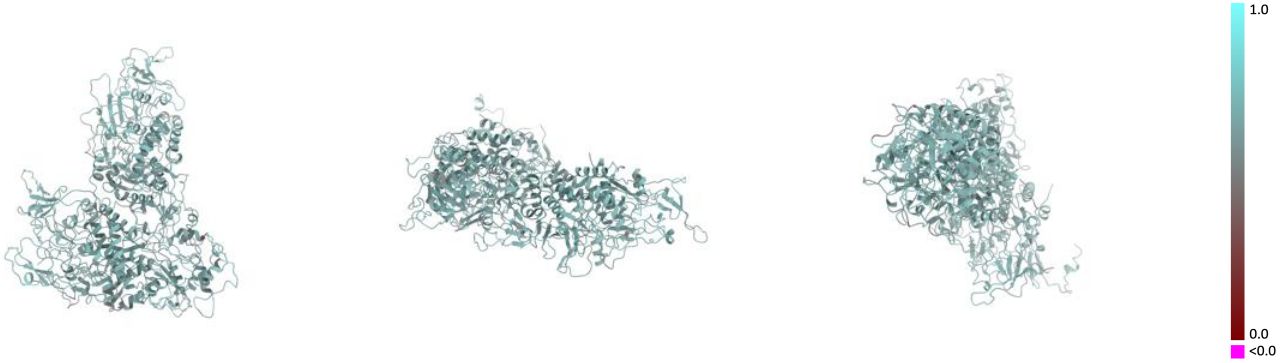
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

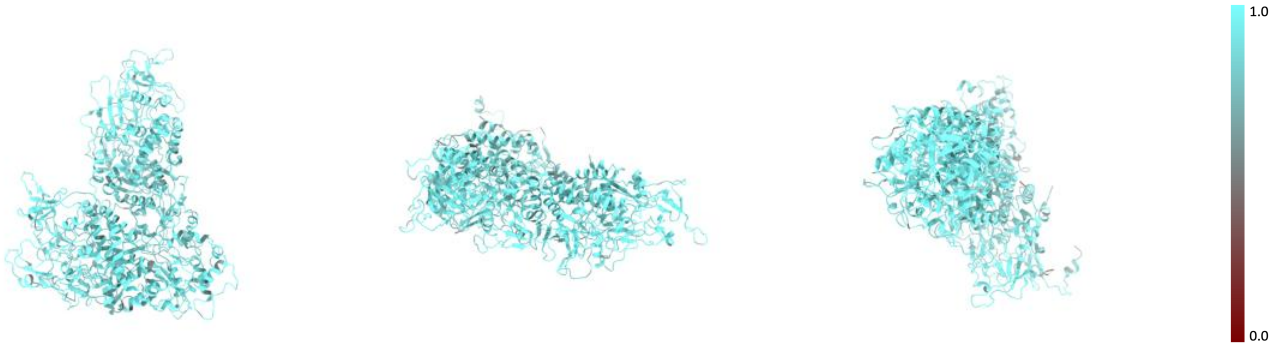
9.2 Q-score mapped to coordinate model (i)



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.

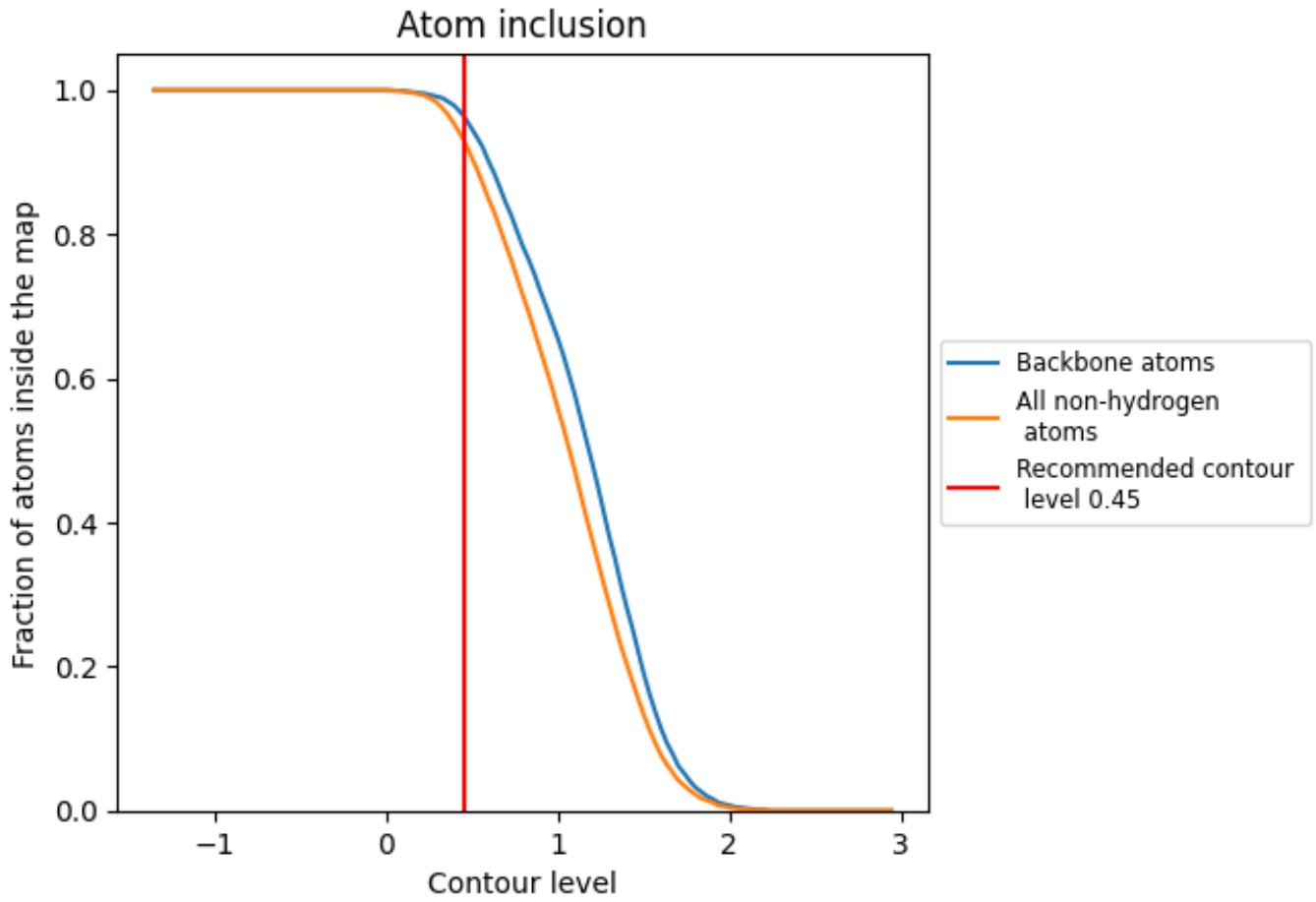
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.6210
A	0.9220	0.6170
B	0.9410	0.6250