



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:55 PM UTC

PDB ID : 8R0G / pdb_00008r0g
EMDB ID : EMD-18792
Title : Capsid structure of Giardavirus (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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

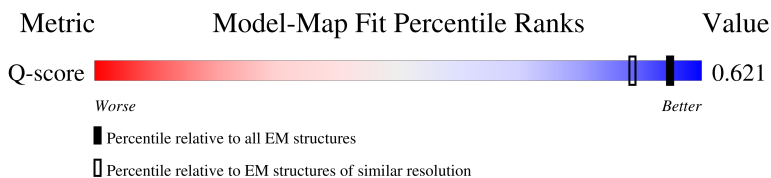
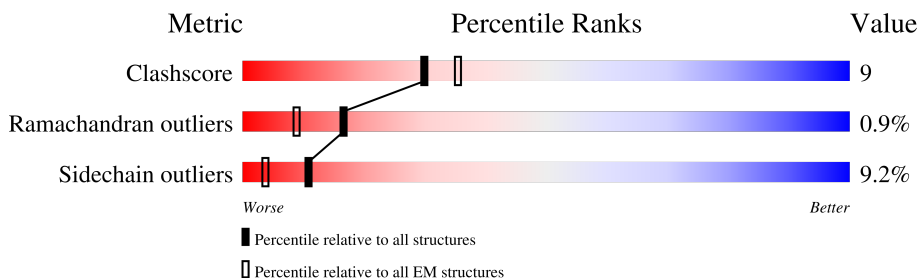
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	929	 67% 23% • 8%
1	B	929	 67% 21% • 8%

2 Entry composition

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

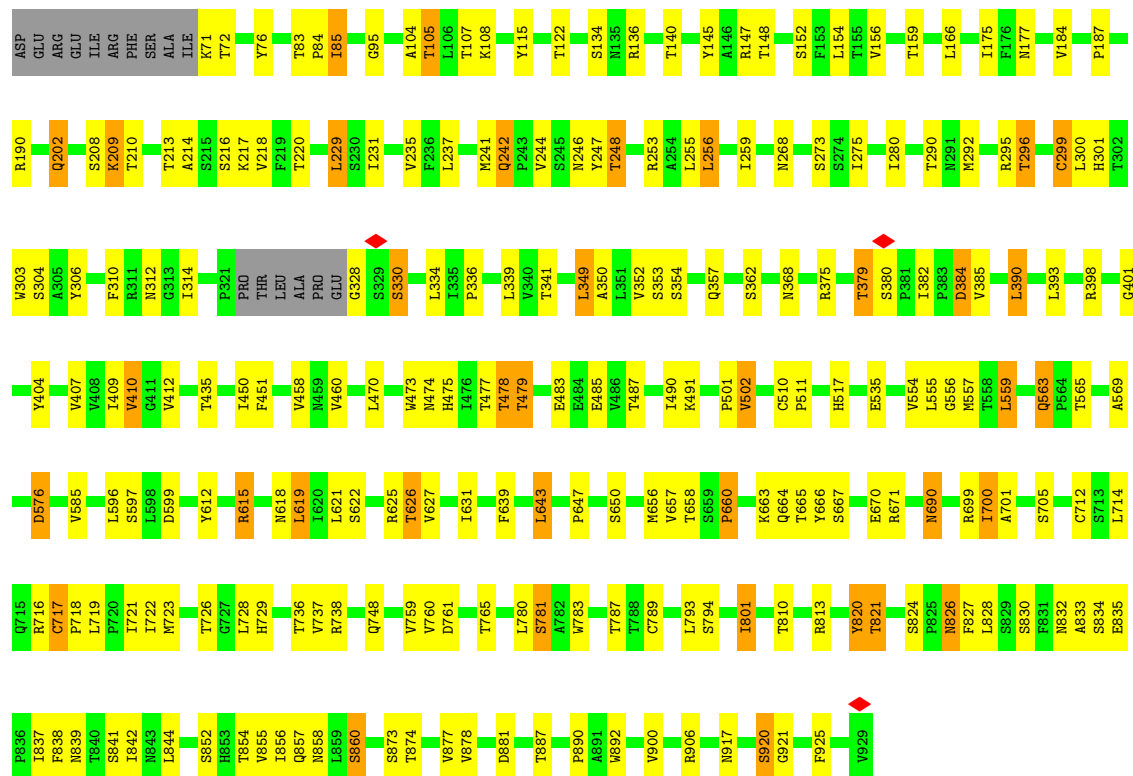
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



• Molecule 1: Capsid protein





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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	0.12	0/6918	0.33	0/9453
1	B	0.29	3/6899 (0.0%)	0.42	5/9426 (0.1%)
All	All	0.22	3/13817 (0.0%)	0.38	5/18879 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	660	PRO	CG-CD	-11.53	1.11	1.50
1	B	208	SER	CA-C	-7.62	1.43	1.52
1	B	660	PRO	N-CD	6.02	1.56	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	660	PRO	N-CD-CG	-13.39	83.11	103.20
1	B	660	PRO	CA-N-CD	-12.45	94.58	112.00
1	B	208	SER	N-CA-C	-7.65	95.79	108.34
1	B	660	PRO	CA-CB-CG	-7.28	90.66	104.50
1	B	660	PRO	N-CA-CB	-5.60	97.37	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	124	0
1	B	6713	0	6560	119	0
All	All	13445	0	13144	241	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 (241) 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:A:111:MET:HE3	1:A:111:MET:HA	1.83	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:B:576:ASP:OD1	1:B:576:ASP:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:881:ASP:O	1:A:882:ASN:HB2	2.01	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
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:241:MET:HE3	1:B:241:MET:HA	1.88	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:582:MET:HE3	1:B:341:THR:HG22	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:B:824:SER:HG	1:B:827:PHE:H	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:HIS:O	1:B:479:THR:OG1	2.27	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
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:225:THR:OG1	1:A:227:ASP:OD1	2.25	0.49
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:478:THR:O	1:A:608:THR:OG1	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:A:789:CYS:HB2	1:A:800:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:787:THR:O	1:B:820:TYR:OH	2.22	0.47
1:B:622:SER:O	1:B:626:THR:HG23	2.15	0.47
1:A:825:PRO:O	1:A:829:SER:OG	2.29	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
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:111:MET:HE2	1:A:115:TYR:CE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:223:LEU:HD22	1:A:601:MET:HE2	2.01	0.43
1:A:350:ALA:C	1:A:352:VAL:H	2.26	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: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:A:554:VAL:HA	1:A:557:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:350:ALA:C	1:B:352:VAL:H	2.29	0.41
1:B:656:MET:HE1	1:B:663:LYS:HG2	2.02	0.41
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:418:TRP:CD1	1:A:421:GLN:H	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	14	30
1	B	849/929 (91%)	805 (95%)	37 (4%)	7 (1%)	16	34
All	All	1698/1858 (91%)	1602 (94%)	81 (5%)	15 (1%)	16	30

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

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Mol	Chain	Res	Type
1	B	660	PRO

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	748/810 (92%)	684 (91%)	64 (9%)	10	22
1	B	745/810 (92%)	672 (90%)	73 (10%)	7	17
All	All	1493/1620 (92%)	1356 (91%)	137 (9%)	11	19

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	78	SER
1	A	85	ILE
1	A	105	THR
1	A	116	ILE
1	A	122	THR
1	A	139	THR
1	A	152	SER
1	A	159	THR
1	A	191	THR
1	A	195	ILE
1	A	206	THR
1	A	210	THR
1	A	213	THR
1	A	215	SER
1	A	217	LYS
1	A	227	ASP
1	A	234	GLU
1	A	244	VAL
1	A	248	THR
1	A	272	SER
1	A	273	SER

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Mol	Chain	Res	Type
1	A	274	SER
1	A	296	THR
1	A	299	CYS
1	A	307	LYS
1	A	334	LEU
1	A	362	SER
1	A	367	ILE
1	A	379	THR
1	A	390	LEU
1	A	412	VAL
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	557	MET
1	A	581	SER
1	A	607	THR
1	A	614	ILE
1	A	620	ILE
1	A	626	THR
1	A	668	VAL
1	A	705	SER
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	840	THR
1	A	854	THR
1	A	866	SER
1	A	874	THR
1	A	904	SER
1	A	928	ASP

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Mol	Chain	Res	Type
1	B	72	THR
1	B	85	ILE
1	B	105	THR
1	B	140	THR
1	B	152	SER
1	B	159	THR
1	B	184	VAL
1	B	202	GLN
1	B	209	LYS
1	B	217	LYS
1	B	218	VAL
1	B	229	LEU
1	B	237	LEU
1	B	242	GLN
1	B	248	THR
1	B	256	LEU
1	B	273	SER
1	B	296	THR
1	B	299	CYS
1	B	304	SER
1	B	312	ASN
1	B	330	SER
1	B	349	LEU
1	B	357	GLN
1	B	368	ASN
1	B	379	THR
1	B	384	ASP
1	B	390	LEU
1	B	393	LEU
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	554	VAL
1	B	559	LEU
1	B	563	GLN
1	B	565	THR
1	B	576	ASP
1	B	615	ARG

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Mol	Chain	Res	Type
1	B	626	THR
1	B	643	LEU
1	B	657	VAL
1	B	658	THR
1	B	690	ASN
1	B	705	SER
1	B	714	LEU
1	B	717	CYS
1	B	736	THR
1	B	737	VAL
1	B	781	SER
1	B	794	SER
1	B	801	ILE
1	B	810	THR
1	B	821	THR
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	852	SER
1	B	854	THR
1	B	855	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
1	A	260	HIS
1	A	455	ASN
1	A	570	GLN
1	A	587	ASN
1	A	748	GLN
1	A	755	GLN

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Mol	Chain	Res	Type
1	A	882	ASN
1	B	203	ASN
1	B	291	ASN
1	B	440	ASN
1	B	574	ASN
1	B	587	ASN
1	B	591	GLN
1	B	618	ASN
1	B	628	ASN
1	B	711	HIS
1	B	732	GLN
1	B	863	GLN

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 oligosaccharides 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.

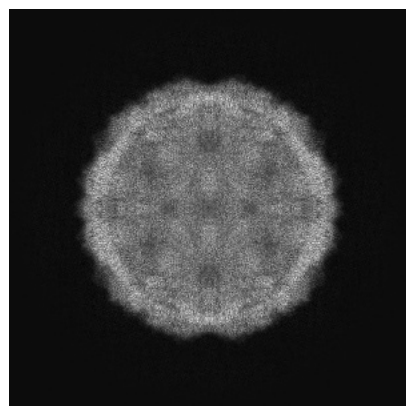
6 Map visualisation [i](#)

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

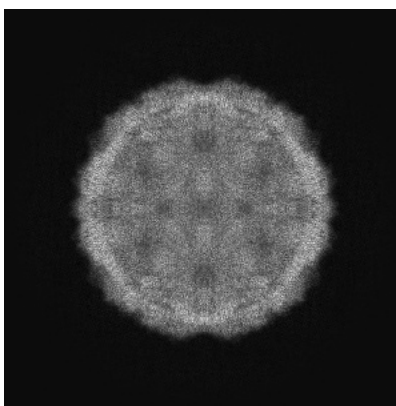
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

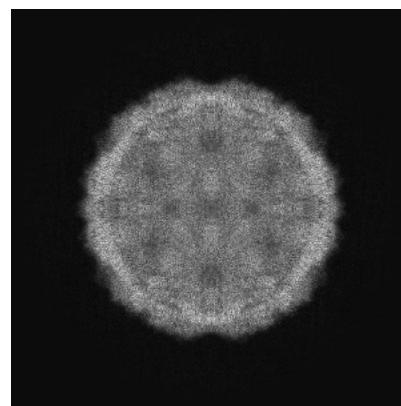
6.1.1 Primary map



X

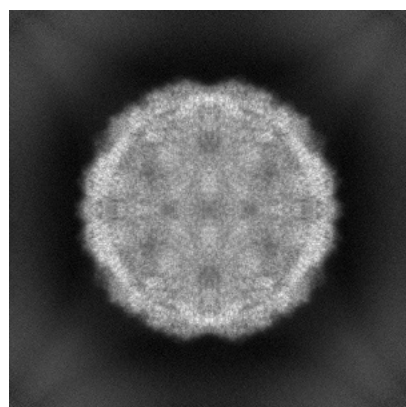


Y

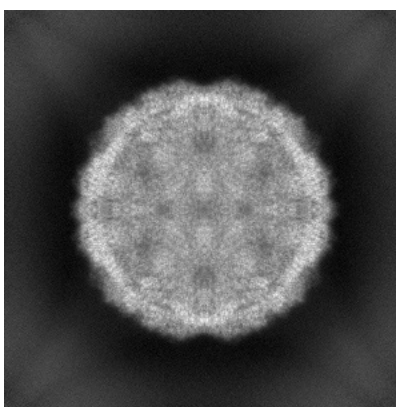


Z

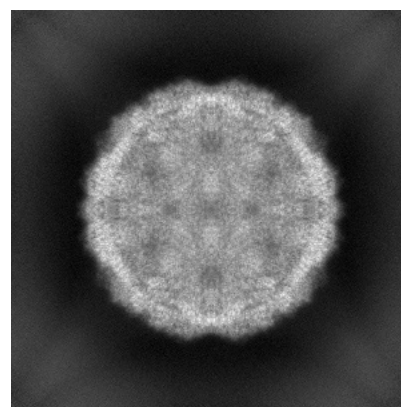
6.1.2 Raw map



X



Y

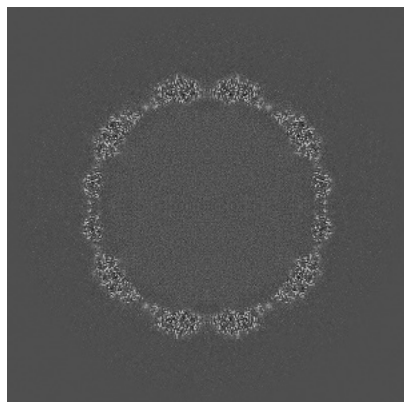


Z

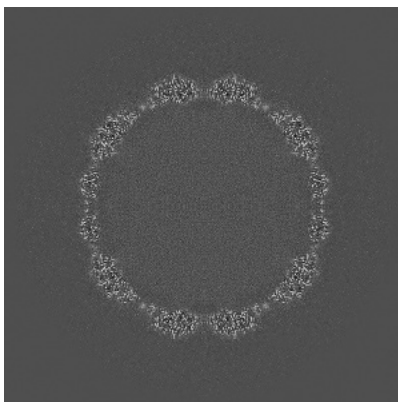
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

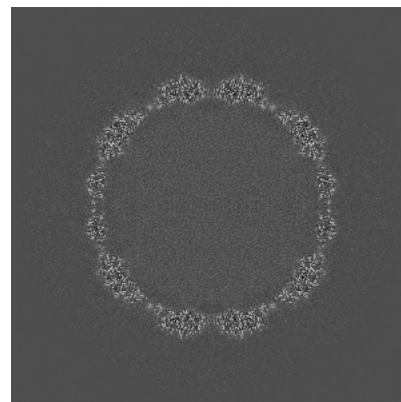
6.2.1 Primary map



X Index: 320

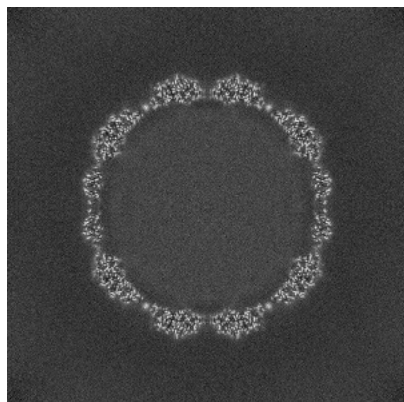


Y Index: 320

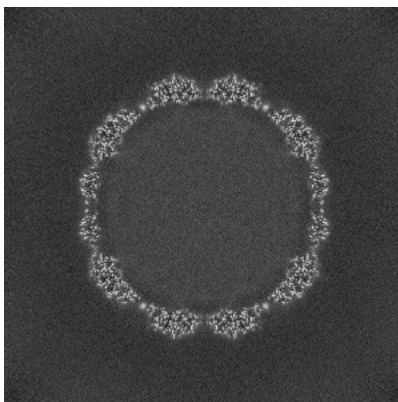


Z Index: 320

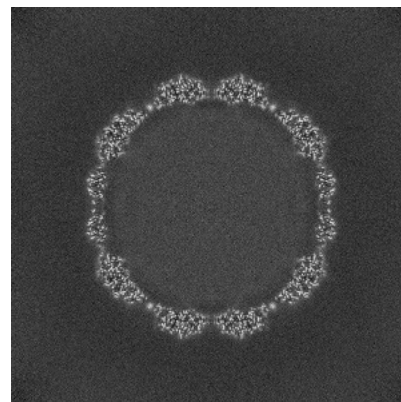
6.2.2 Raw map



X Index: 320



Y Index: 320

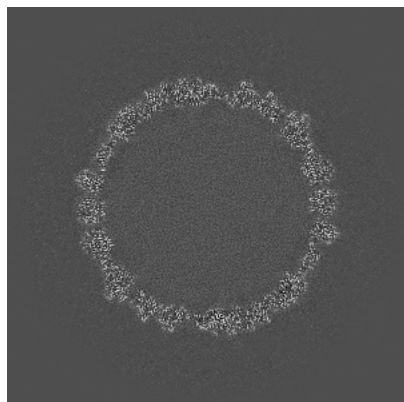


Z Index: 320

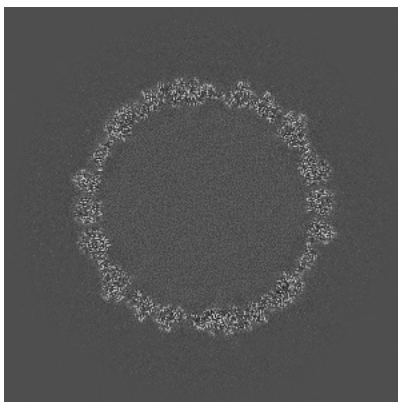
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

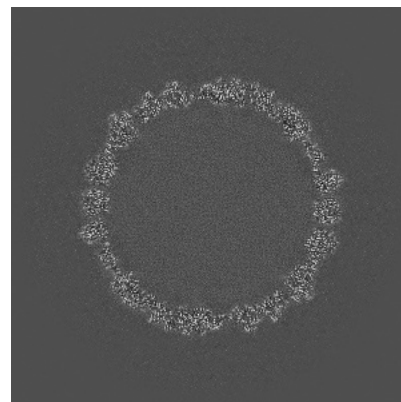
6.3.1 Primary map



X Index: 355

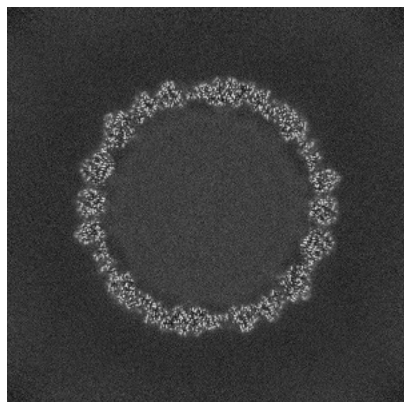


Y Index: 355

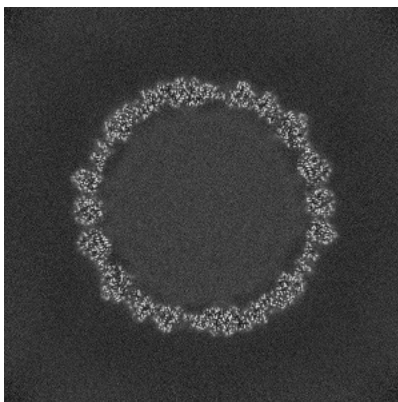


Z Index: 285

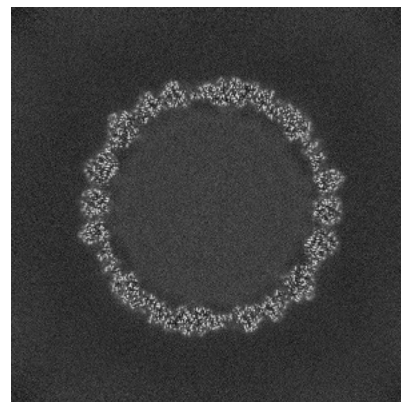
6.3.2 Raw map



X Index: 286



Y Index: 354

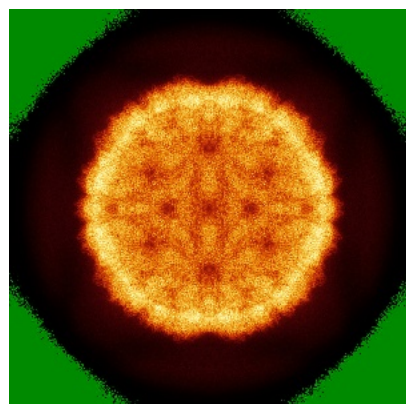


Z Index: 286

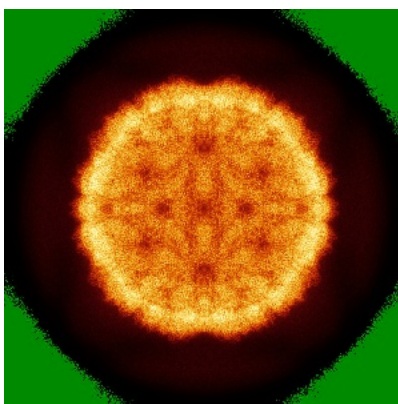
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

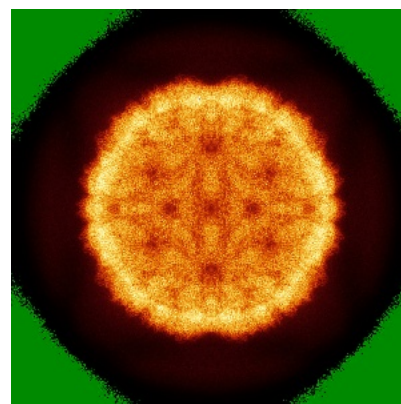
6.4.1 Primary map



X

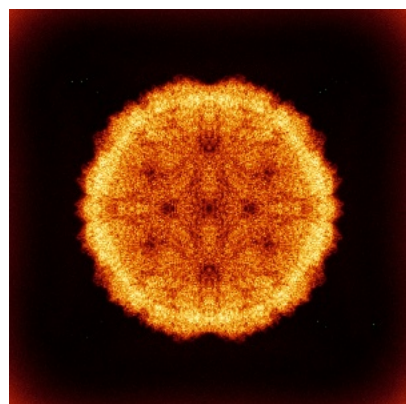


Y

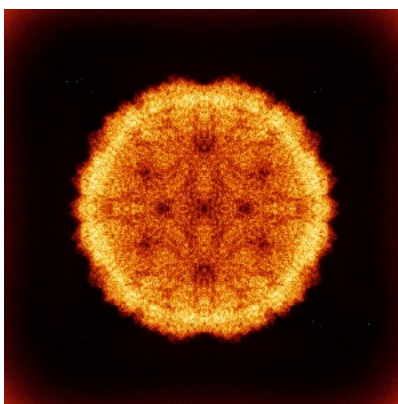


Z

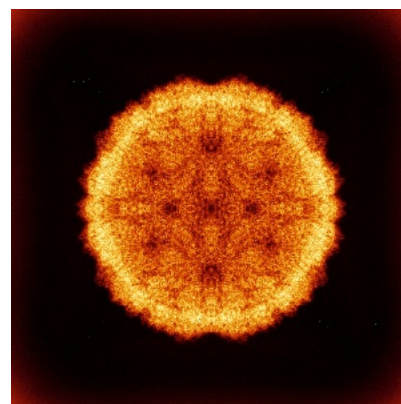
6.4.2 Raw map



X



Y

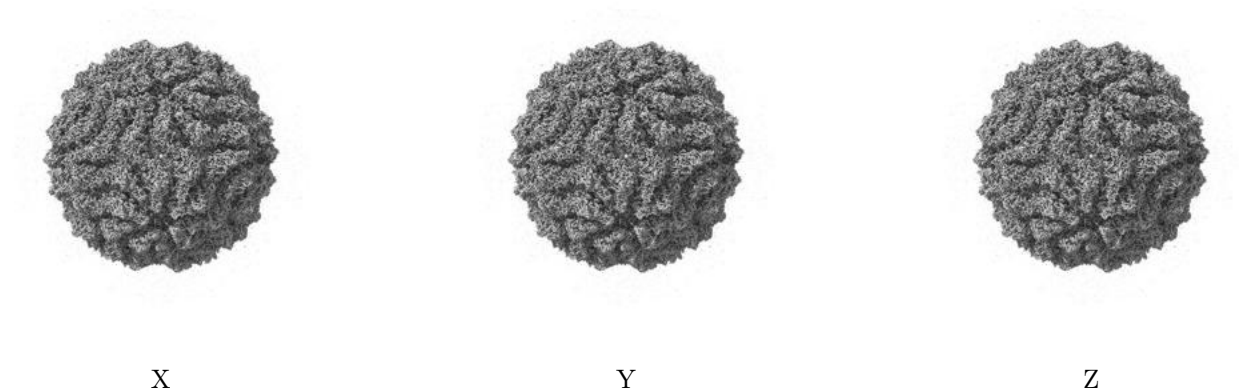


Z

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



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.

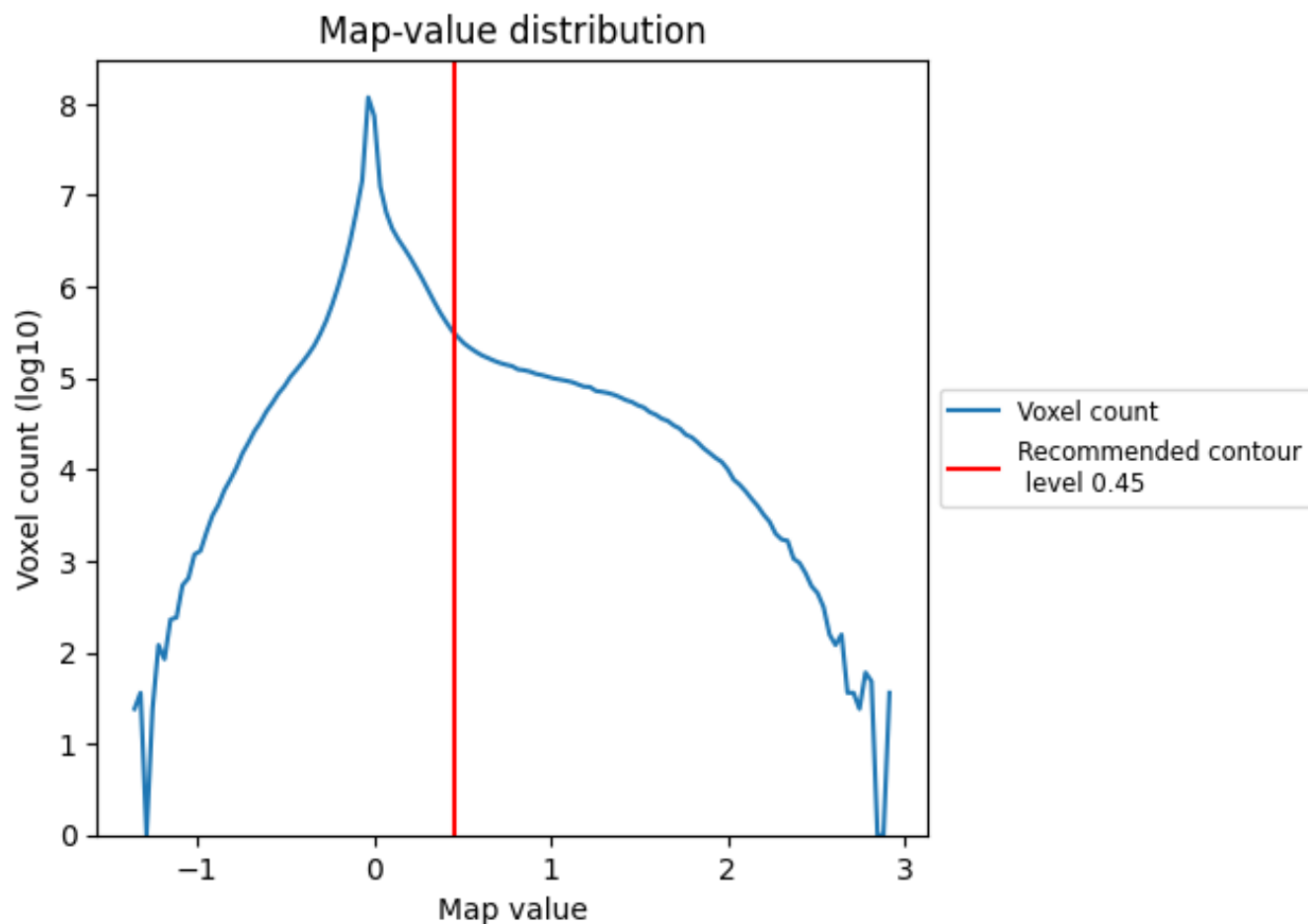
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

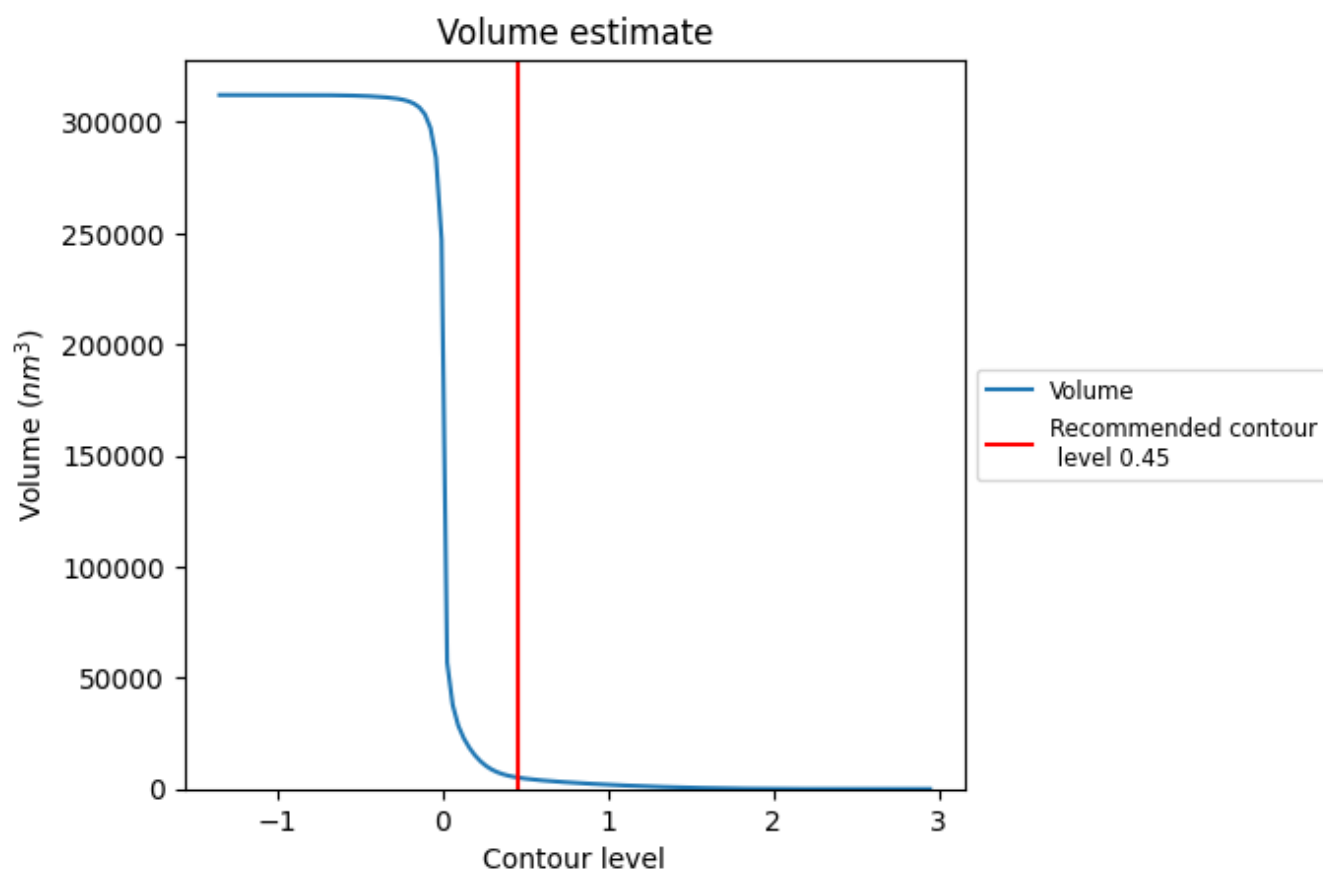
This section contains the results of statistical analysis of the map.

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.

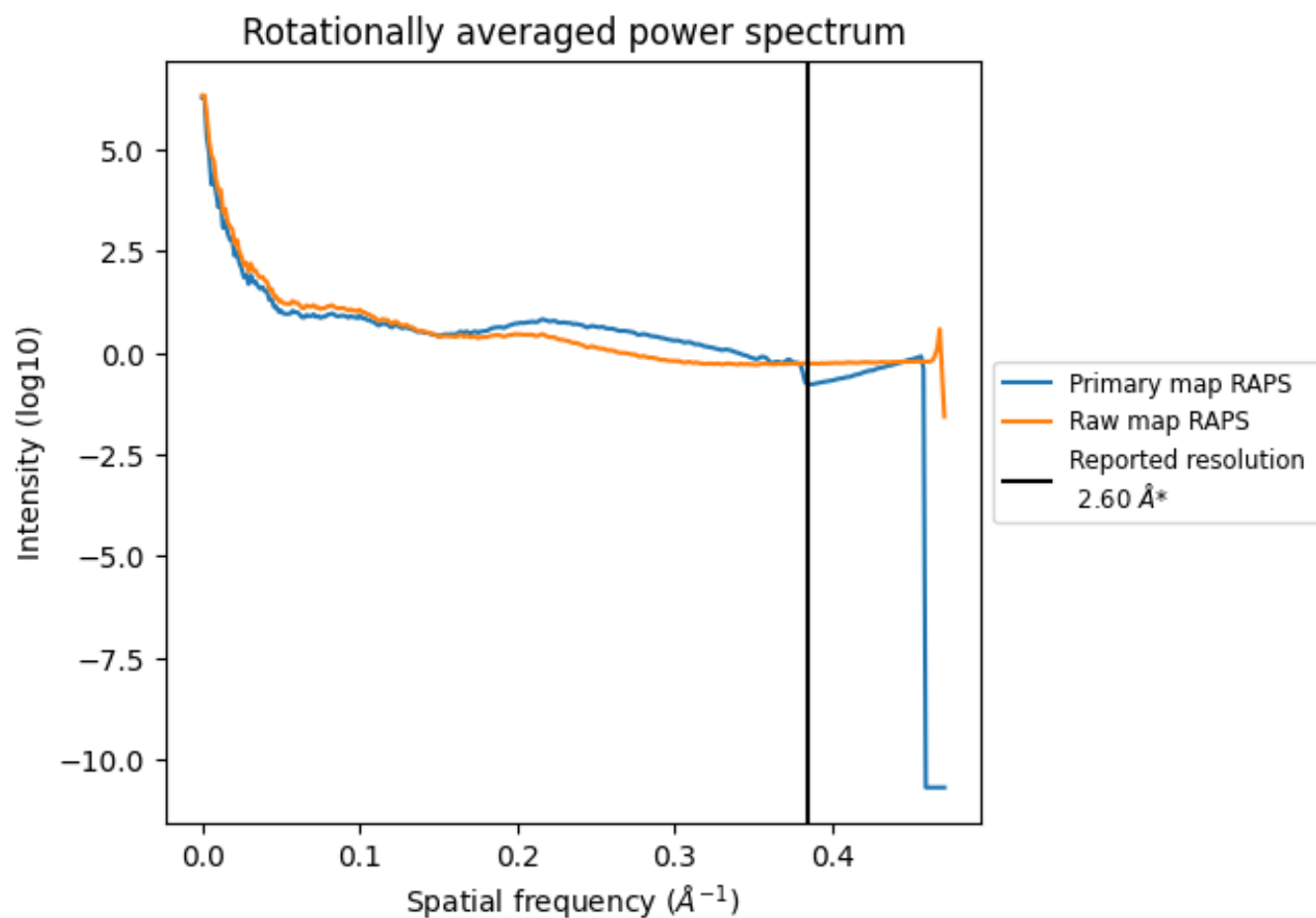
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5174 nm³; 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 ⓘ

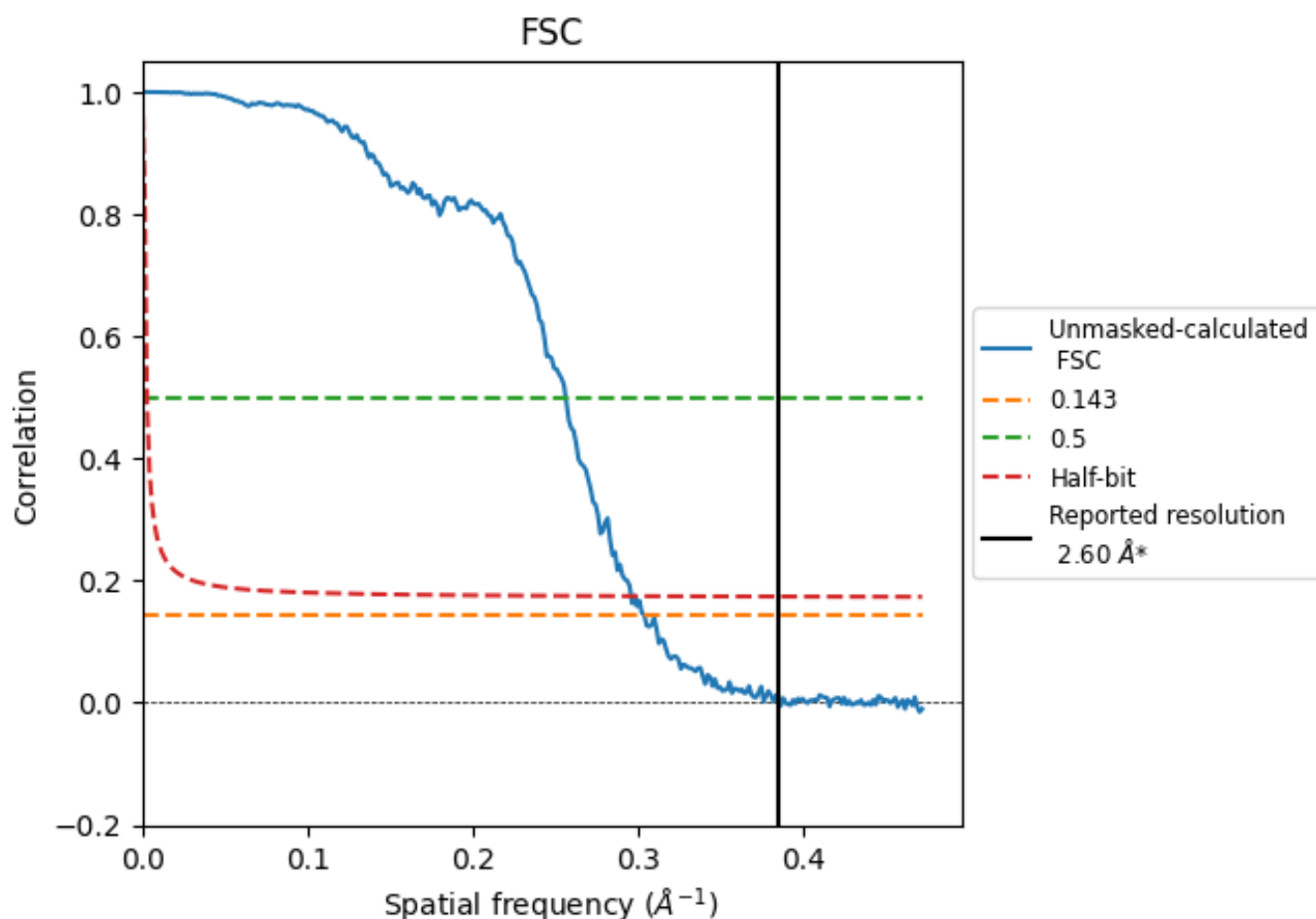


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

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

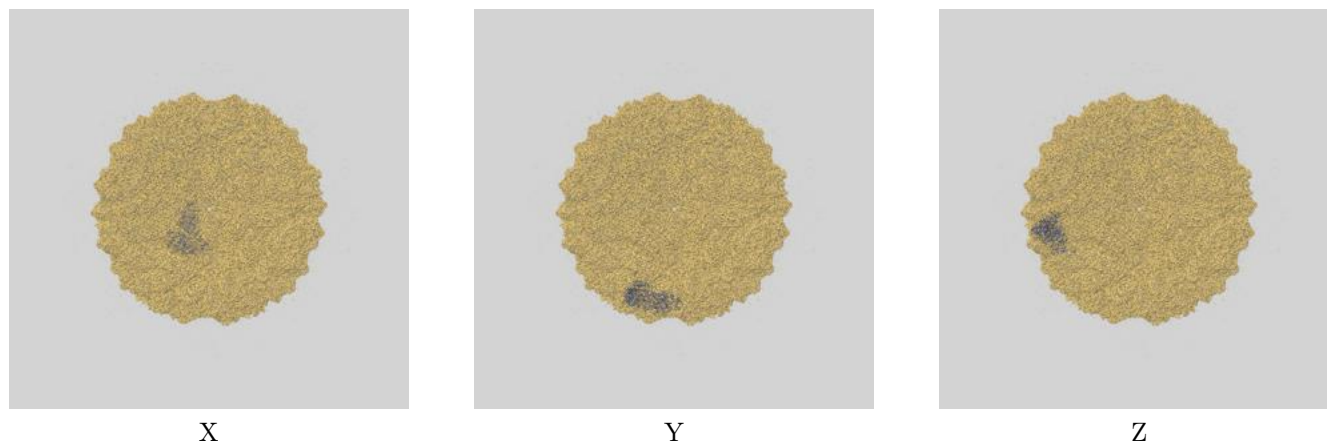
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

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](#).

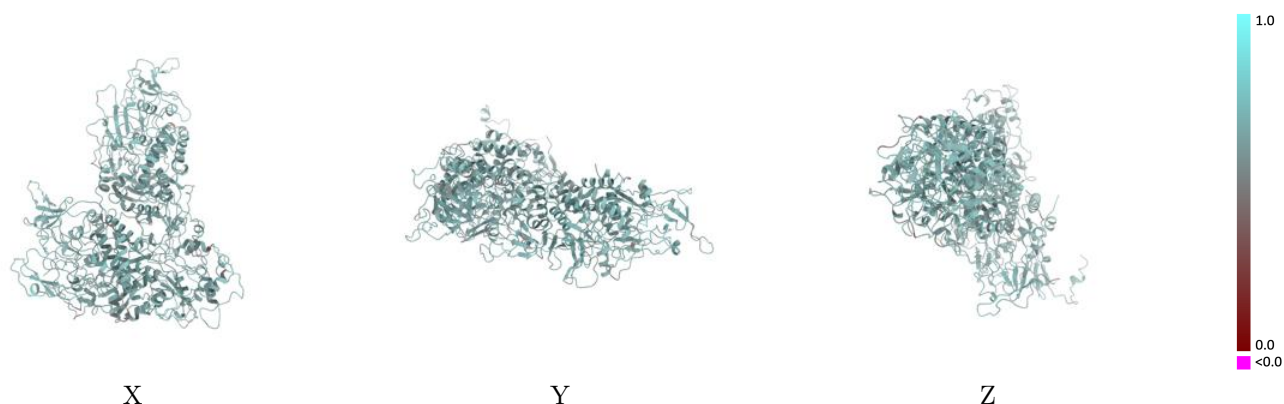
9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



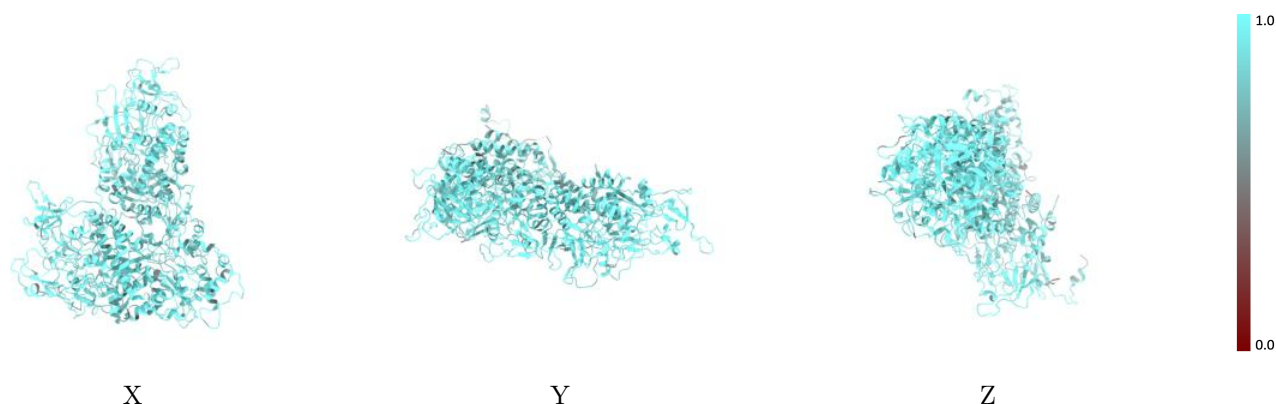
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



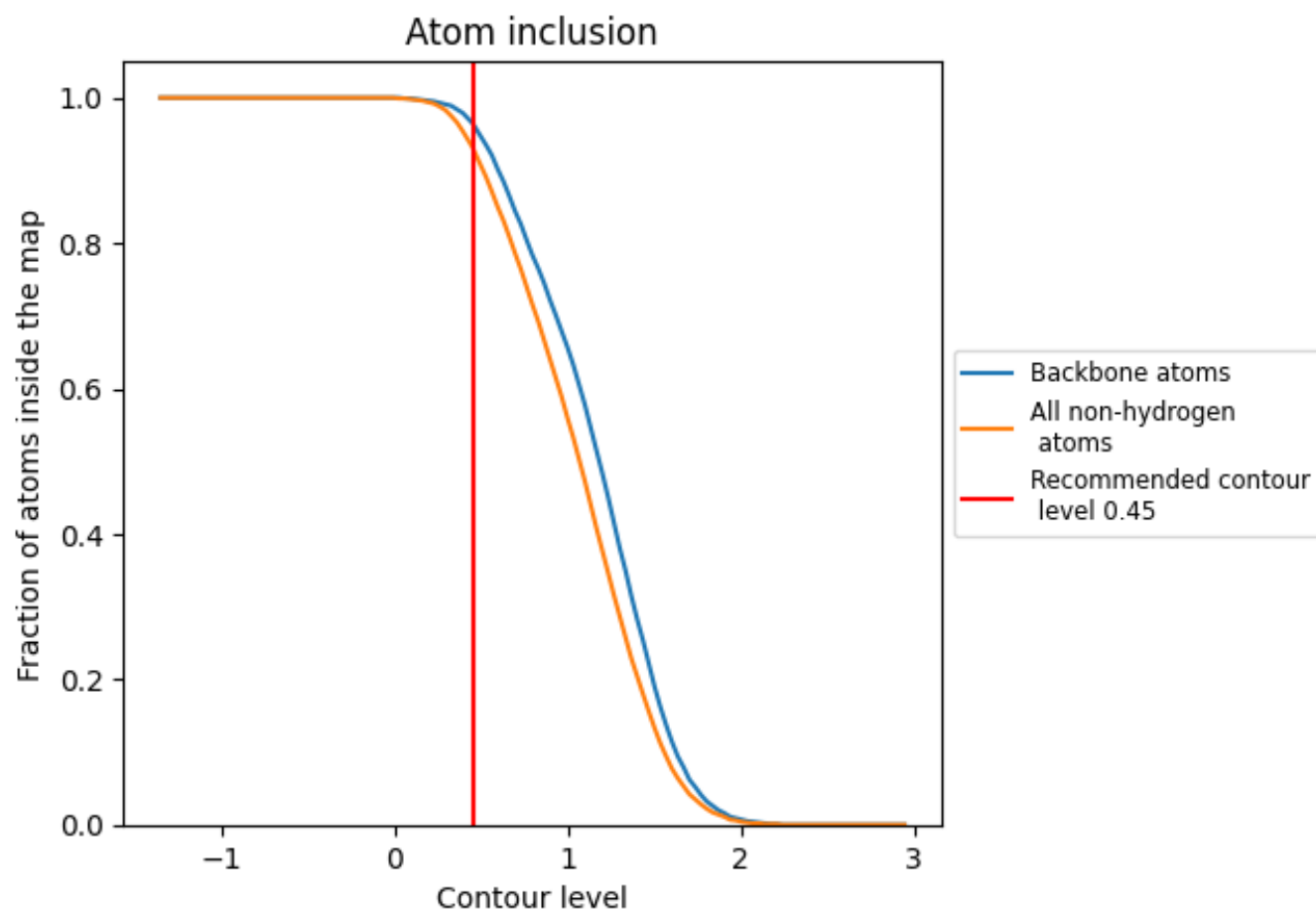
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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

