



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:07 AM UTC

PDB ID : 8CMT / pdb_00008cmt
EMDB ID : EMD-16745
Title : Structure of the plasma coagulation Factor XIII A2B2 heterotetrameric complex.
Authors : Singh, S.; Ugurlar, D.; Hagelueken, G.; Geyer, M.; Biswas, A.
Deposited on : 2023-02-21
Resolution : 3.04 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.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

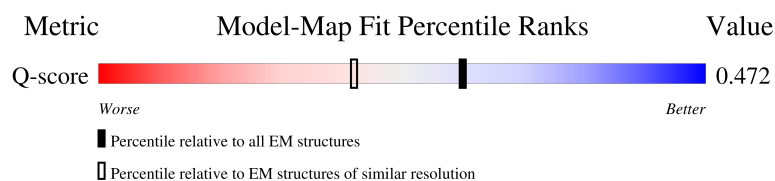
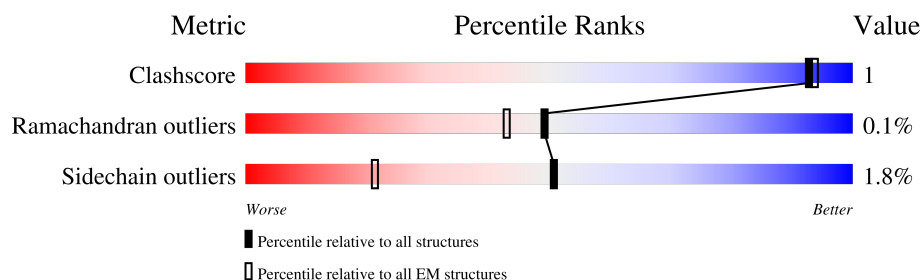
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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	13952 (2.54 - 3.54)

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	732	94%
1	B	732	95%
2	C	661	42%
2	D	661	43%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16518 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 Coagulation factor XIII A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	722	Total	C	N	O	S	0	0
			5791	3670	1001	1093	27		
1	B	722	Total	C	N	O	S	0	0
			5791	3670	1001	1093	27		

- Molecule 2 is a protein called Coagulation factor XIII B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	307	Total	C	N	O	S	0	0
			2468	1561	408	477	22		
2	D	307	Total	C	N	O	S	0	0
			2468	1561	408	477	22		

[illegible]

- Molecule 2: Coagulation factor XIII B chain



Residue	Position	Score	Conservation	Annotations
SER	1	0.85	High	
LEU	2	0.75	Medium	
GLN	3	0.65	Low	
GLU	4	0.55	Low	
PRO	5	0.45	Low	
LEU	6	0.35	Low	
THR	7	0.25	Low	
GLY	8	0.15	Low	
ASP	9	0.05	Low	
ASN	10	0.00	Low	
ARG	11	0.00	Low	
PRO	12	0.00	Low	
HIS	13	0.00	Low	
LEU	14	0.00	Low	
SER	15	0.00	Low	
HIS	16	0.00	Low	
GLY	17	0.00	Low	
GLU	18	0.00	Low	
TYR	19	0.00	Low	
ASP	20	0.00	Low	
GLY	21	0.00	Low	
ASP	22	0.00	Low	
GLY	23	0.00	Low	
ASP	24	0.00	Low	
GLY	25	0.00	Low	
ASP	26	0.00	Low	
GLY	27	0.00	Low	
ASP	28	0.00	Low	
GLY	29	0.00	Low	
ASP	30	0.00	Low	
GLY	31	0.00	Low	
ASP	32	0.00	Low	
GLY	33	0.00	Low	
ASP	34	0.00	Low	
GLY	35	0.00	Low	
ASP	36	0.00	Low	
GLY	37	0.00	Low	
ASP	38	0.00	Low	
GLY	39	0.00	Low	
ASP	40	0.00	Low	
GLY	41	0.00	Low	
ASP	42	0.00	Low	
GLY	43	0.00	Low	
ASP	44	0.00	Low	
GLY	45	0.00	Low	
ASP	46	0.00	Low	
GLY	47	0.00	Low	
ASP	48	0.00	Low	
GLY	49	0.00	Low	
ASP	50	0.00	Low	
GLY	51	0.00	Low	
ASP	52	0.00	Low	
GLY	53	0.00	Low	
ASP	54	0.00	Low	
GLY	55	0.00	Low	
ASP	56	0.00	Low	
GLY	57	0.00	Low	
ASP	58	0.00	Low	
GLY	59	0.00	Low	
ASP	60	0.00	Low	
GLY	61	0.00	Low	
ASP	62	0.00	Low	
GLY	63	0.00	Low	
ASP	64	0.00	Low	
GLY	65	0.00	Low	
ASP	66	0.00	Low	
GLY	67	0.00	Low	
ASP	68	0.00	Low	
GLY	69	0.00	Low	
ASP	70	0.00	Low	
GLY	71	0.00	Low	
ASP	72	0.00	Low	
GLY	73	0.00	Low	
ASP	74	0.00	Low	
GLY	75	0.00	Low	
ASP	76	0.00	Low	
GLY	77	0.00	Low	
ASP	78	0.00	Low	
GLY	79	0.00	Low	
ASP	80	0.00	Low	
GLY	81	0.00	Low	
ASP	82	0.00	Low	
GLY	83	0.00	Low	
ASP	84	0.00	Low	
GLY	85	0.00	Low	
ASP	86	0.00	Low	
GLY	87	0.00	Low	
ASP	88	0.00	Low	
GLY	89	0.00	Low	
ASP	90	0.00	Low	
GLY	91	0.00	Low	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20436	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.369	Depositor
Minimum map value	-0.176	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0344	Depositor
Map size ($\text{\AA}$)	356.864, 356.864, 356.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.697, 0.697, 0.697	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	0.72	0/5928	1.23	12/8045 (0.1%)
1	B	0.72	0/5928	1.24	14/8045 (0.2%)
2	C	0.80	0/2539	1.23	1/3437 (0.0%)
2	D	0.82	0/2539	1.26	2/3437 (0.1%)
All	All	0.75	0/16934	1.24	29/22964 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
2	C	0	4
2	D	0	5
All	All	0	14

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	612	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	A	612	ARG	NE-CZ-NH2	6.36	124.93	119.20
2	C	24	PRO	CA-N-CD	-6.36	103.09	112.00
1	B	91	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	372	ASN	CA-CB-CG	6.02	118.62	112.60
2	D	226	PRO	CA-N-CD	-5.91	103.72	112.00
1	B	618	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	159	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	A	59	ASP	CA-C-N	5.57	128.06	120.54
1	A	59	ASP	C-N-CA	5.57	128.06	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	GLU	CB-CA-C	5.55	119.49	109.45
1	B	159	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	B	405	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	91	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	A	202	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	D	134	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	B	372	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	59	ASP	CA-C-N	5.36	127.72	120.38
1	B	59	ASP	C-N-CA	5.36	127.72	120.38
1	B	108	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	311	ARG	CA-C-N	5.14	130.96	121.70
1	B	311	ARG	C-N-CA	5.14	130.96	121.70
1	B	682	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	B	334	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	A	52	HIS	CB-CG-CD2	-5.07	124.62	131.20
1	B	52	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	A	334	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	311	ARG	CA-C-N	5.00	130.71	121.70
1	A	311	ARG	C-N-CA	5.00	130.71	121.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	TYR	Sidechain
1	B	284	TYR	Sidechain
1	B	405	ASP	Mainchain
1	B	547	ARG	Sidechain
1	B	97	ARG	Sidechain
2	C	147	ARG	Sidechain
2	C	270	ARG	Sidechain
2	C	271	ARG	Sidechain
2	C	273	ARG	Sidechain
2	D	246	TYR	Sidechain
2	D	270	ARG	Sidechain
2	D	271	ARG	Sidechain
2	D	273	ARG	Sidechain
2	D	40	TYR	Sidechain

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	5791	0	5655	16	0
1	B	5791	0	5655	7	0
2	C	2468	0	2324	11	0
2	D	2468	0	2322	11	0
All	All	16518	0	15956	45	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 1.

All (45) 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:652:GLU:HG2	1:A:691:GLN:HG2	1.41	1.01
1:A:652:GLU:OE2	1:A:691:GLN:NE2	1.95	0.97
2:D:246:TYR:HB2	2:D:271:ARG:HB3	1.46	0.95
2:D:245:TYR:HA	2:D:269:GLY:HA2	1.50	0.93
1:A:539:THR:HG22	1:A:585:LYS:HG2	1.59	0.82
2:D:121:GLY:O	2:D:149:GLU:N	2.22	0.69
1:A:342:ALA:HB2	1:A:461:ILE:HD12	1.78	0.66
2:C:149:GLU:HA	2:C:199:THR:O	1.99	0.62
2:D:123:LYS:HG2	2:D:149:GLU:HB2	1.81	0.62
1:A:544:SER:O	1:A:581:LEU:N	2.30	0.60
1:A:652:GLU:CD	1:A:691:GLN:HE21	2.09	0.60
1:A:539:THR:HG22	1:A:585:LYS:HE2	1.85	0.58
1:B:93:TYR:CE2	1:B:95:PRO:HG3	2.39	0.57
1:B:566:LYS:HE3	1:B:600:LEU:HD21	1.87	0.56
1:B:94:ASP:O	1:B:97:ARG:N	2.34	0.56
2:D:246:TYR:HB2	2:D:271:ARG:CB	2.29	0.55
2:D:246:TYR:CB	2:D:271:ARG:HB3	2.31	0.53
1:B:405:ASP:O	1:B:406:GLY:C	2.52	0.51
1:A:584:LYS:HG3	1:A:585:LYS:N	2.27	0.50
2:D:122:TYR:CD2	2:D:148:LYS:HA	2.48	0.49
2:D:271:ARG:HG3	2:D:273:ARG:NH1	2.28	0.48
1:A:583:PHE:CZ	1:A:585:LYS:HD2	2.48	0.48
2:C:123:LYS:HG2	2:C:149:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ARG:HB2	1:A:580:PRO:HD3	1.95	0.47
1:A:542:ASN:O	1:A:581:LEU:HA	2.15	0.47
1:B:405:ASP:O	1:B:408:TYR:HD2	1.97	0.47
2:C:150:HIS:HB3	2:C:153:CYS:HA	1.97	0.46
1:B:566:LYS:HB2	1:B:566:LYS:HE2	1.34	0.46
2:C:294:HIS:CD2	2:C:318:ASP:H	2.34	0.46
2:D:123:LYS:HG2	2:D:149:GLU:CB	2.46	0.45
2:C:245:TYR:O	2:C:246:TYR:HD1	1.99	0.45
1:A:566:LYS:HE3	1:A:566:LYS:HB2	1.47	0.44
2:D:248:SER:HB2	2:D:268:GLU:OE2	2.18	0.44
1:A:584:LYS:HE3	1:A:584:LYS:HB2	1.29	0.44
1:A:539:THR:CG2	1:A:585:LYS:HE2	2.48	0.43
2:C:248:SER:N	2:C:266:VAL:O	2.47	0.43
1:A:601:GLU:OE1	1:A:716:ARG:HD2	2.19	0.43
2:C:147:ARG:H	2:C:147:ARG:HG2	1.52	0.43
2:D:123:LYS:CG	2:D:149:GLU:HB2	2.49	0.42
1:A:580:PRO:O	1:A:581:LEU:C	2.63	0.42
2:C:148:LYS:HB3	2:C:148:LYS:HE3	1.42	0.42
2:C:247:LEU:HG	2:C:265:PRO:HB2	2.01	0.42
2:C:122:TYR:HB3	2:C:147:ARG:O	2.19	0.41
1:B:405:ASP:O	1:B:406:GLY:O	2.38	0.41
2:C:184:TYR:CZ	2:C:210:LYS:HE3	2.55	0.41

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	720/732 (98%)	696 (97%)	24 (3%)	0	100	100
1	B	720/732 (98%)	695 (96%)	23 (3%)	2 (0%)	36	67
2	C	305/661 (46%)	290 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	305/661 (46%)	294 (96%)	10 (3%)	1 (0%)	36	67
All	All	2050/2786 (74%)	1975 (96%)	72 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	226	PRO
1	B	406	GLY
1	B	271	ASP

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	636/645 (99%)	626 (98%)	10 (2%)	55	76
1	B	636/645 (99%)	631 (99%)	5 (1%)	73	83
2	C	275/594 (46%)	267 (97%)	8 (3%)	37	67
2	D	275/594 (46%)	265 (96%)	10 (4%)	31	62
All	All	1822/2478 (74%)	1789 (98%)	33 (2%)	51	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	GLU
1	A	388	VAL
1	A	422	HIS
1	A	516	ARG
1	A	566	LYS
1	A	581	LEU
1	A	583	PHE
1	A	584	LYS
1	A	585	LYS
1	A	591	GLN
1	B	97	ARG

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Mol	Chain	Res	Type
1	B	270	LYS
1	B	341	SER
1	B	405	ASP
1	B	566	LYS
2	C	24	PRO
2	C	54	LYS
2	C	55	LEU
2	C	110	ILE
2	C	147	ARG
2	C	148	LYS
2	C	151	GLU
2	C	272	ASN
2	D	43	LYS
2	D	101	ILE
2	D	149	GLU
2	D	150	HIS
2	D	151	GLU
2	D	226	PRO
2	D	244	ASN
2	D	254	GLN
2	D	271	ARG
2	D	272	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	323	ASN
1	A	348	ASN
1	A	422	HIS
1	A	460	HIS
1	A	543	ASN
1	A	602	GLN
1	A	606	HIS
1	A	623	GLN
1	A	663	ASN
1	A	667	HIS
1	A	691	GLN
1	A	725	GLN
1	B	282	ASN
1	B	348	ASN
1	B	422	HIS

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Mol	Chain	Res	Type
1	B	518	ASN
1	B	543	ASN
1	B	667	HIS
1	B	727	GLN
2	C	29	HIS
2	C	37	GLN
2	C	167	GLN
2	D	29	HIS
2	D	73	GLN
2	D	221	ASN
2	D	238	GLN
2	D	272	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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.

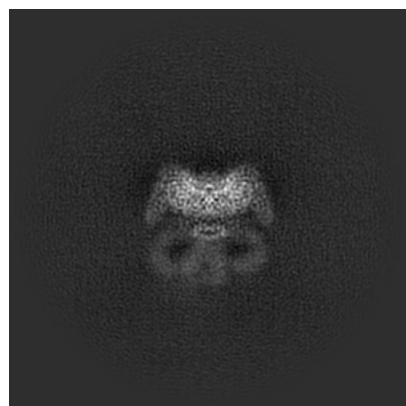
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16745. These allow visual inspection of the internal detail of the map and identification of artifacts.

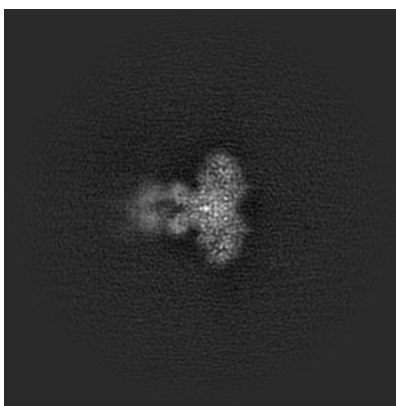
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

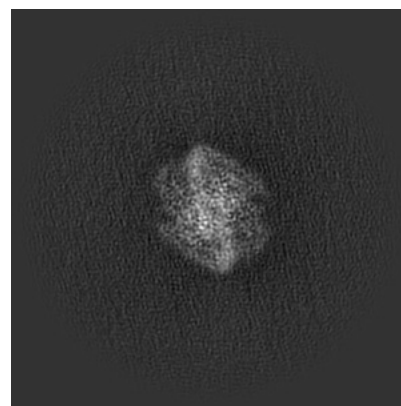
6.1.1 Primary map



X

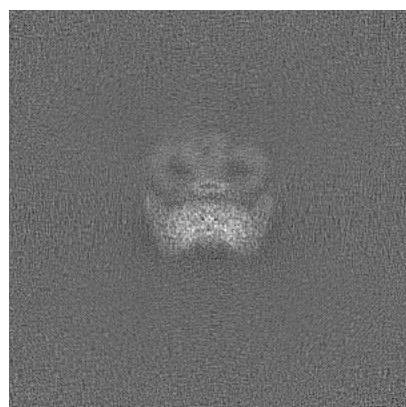


Y

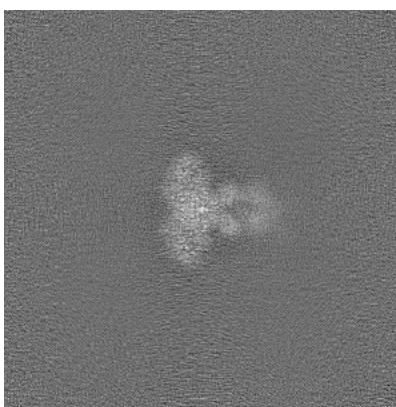


Z

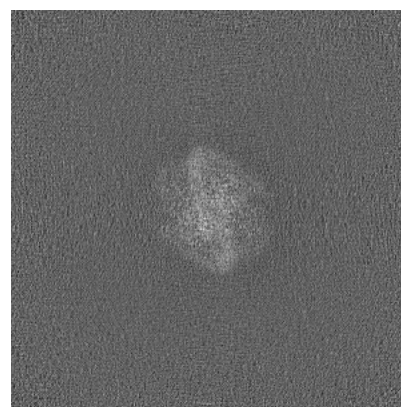
6.1.2 Raw map



X



Y

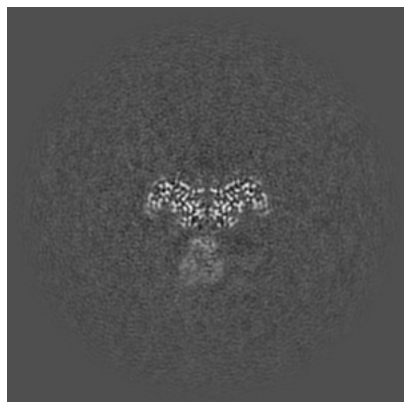


Z

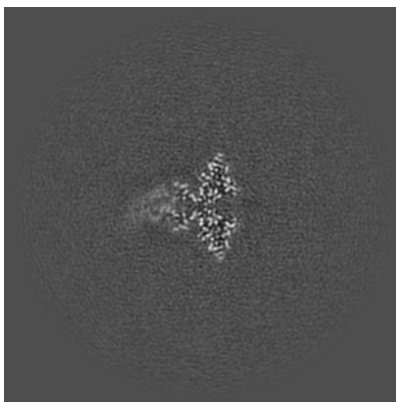
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

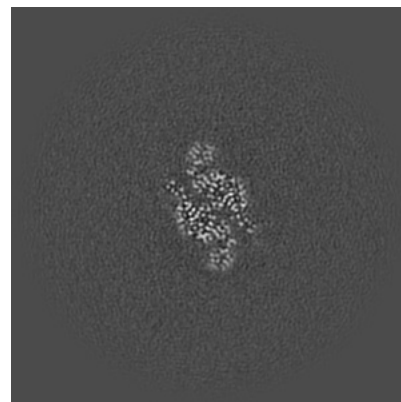
6.2.1 Primary map



X Index: 256

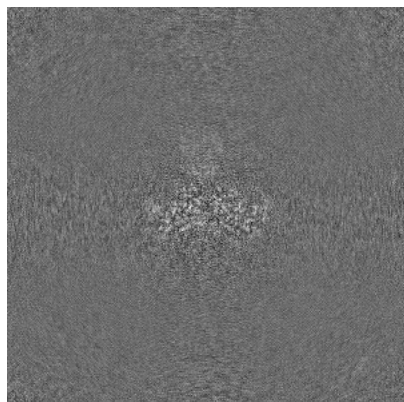


Y Index: 256

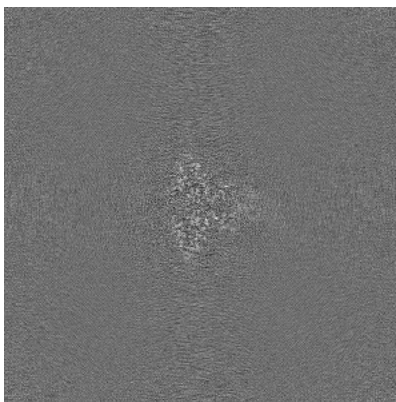


Z Index: 256

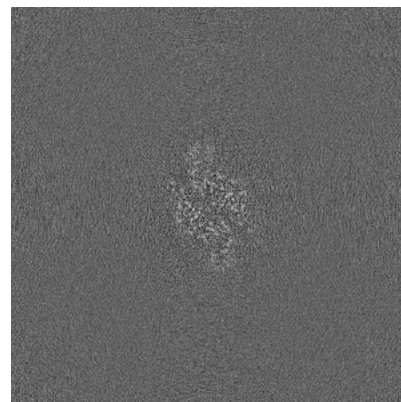
6.2.2 Raw map



X Index: 256



Y Index: 256

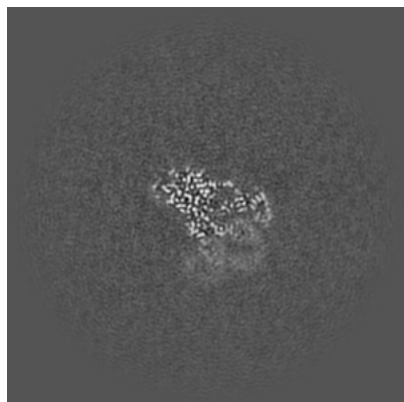


Z Index: 256

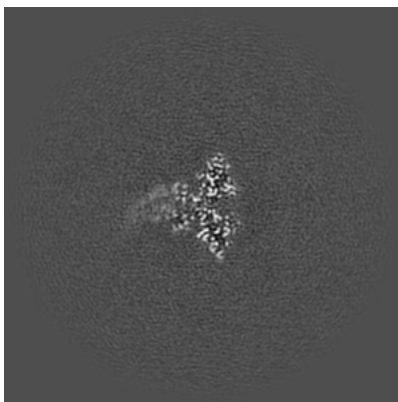
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

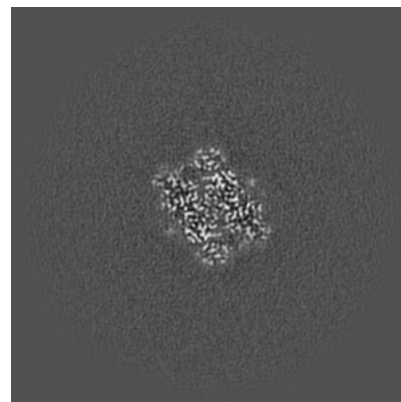
6.3.1 Primary map



X Index: 242

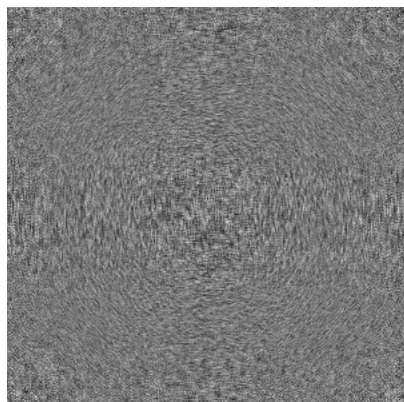


Y Index: 254

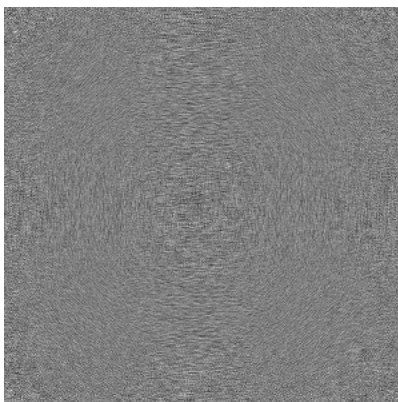


Z Index: 271

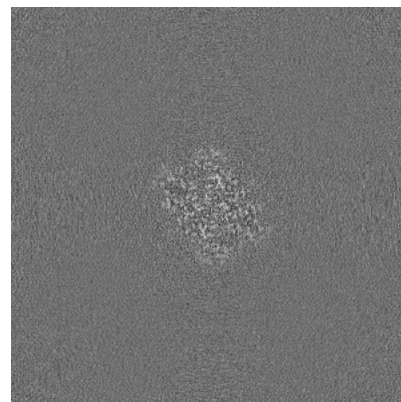
6.3.2 Raw map



X Index: 0



Y Index: 0

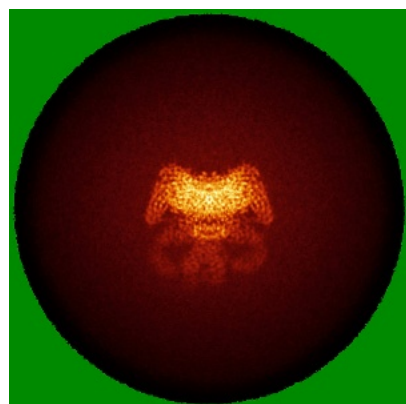


Z Index: 241

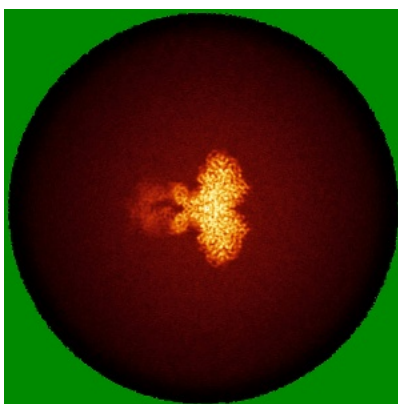
The images above show the largest variance slices of the map in three orthogonal directions.

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

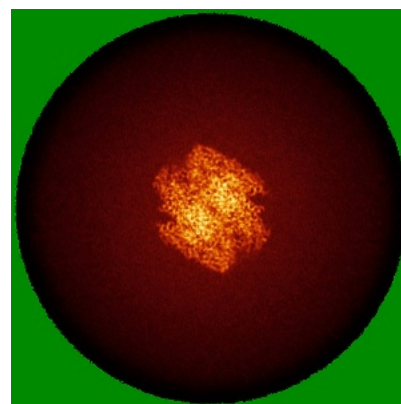
6.4.1 Primary map



X

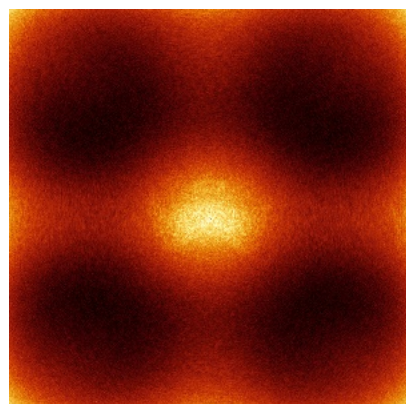


Y

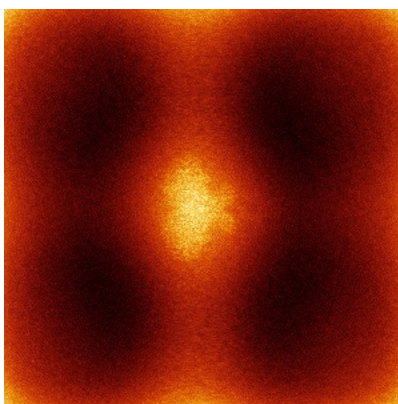


Z

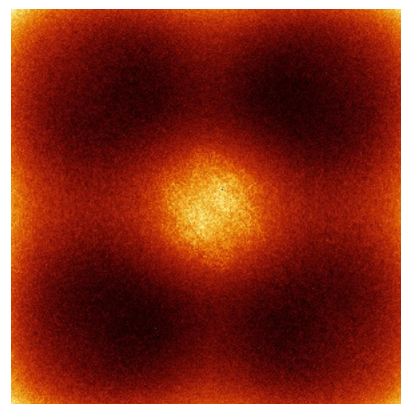
6.4.2 Raw map



X



Y

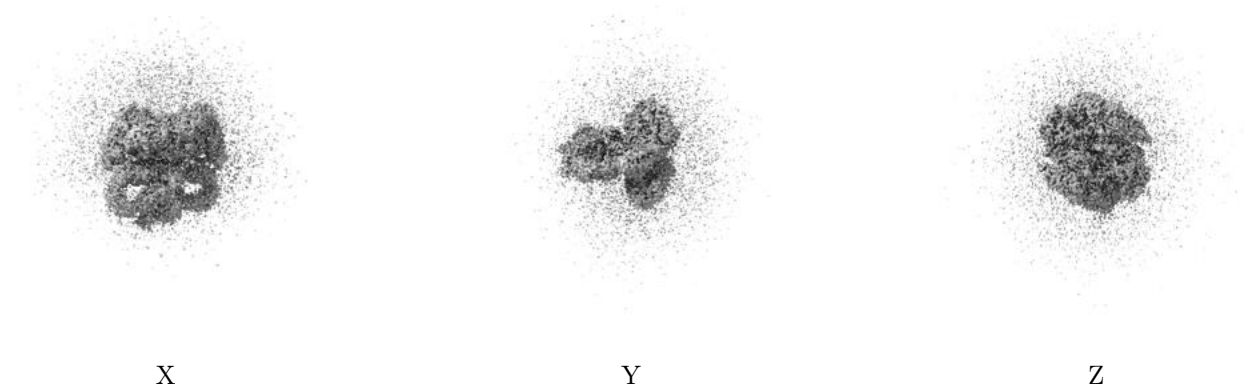


Z

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.

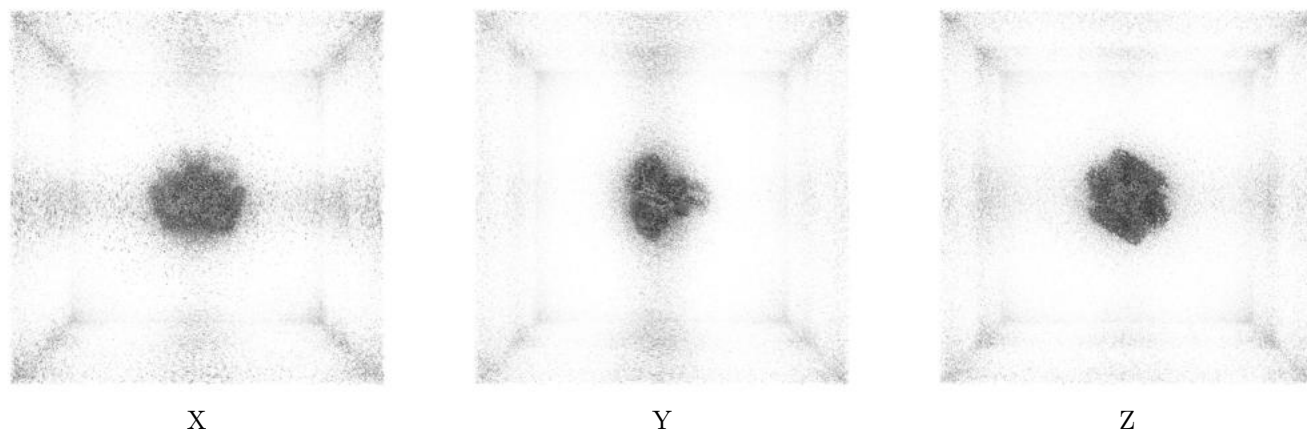
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0344. 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



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.

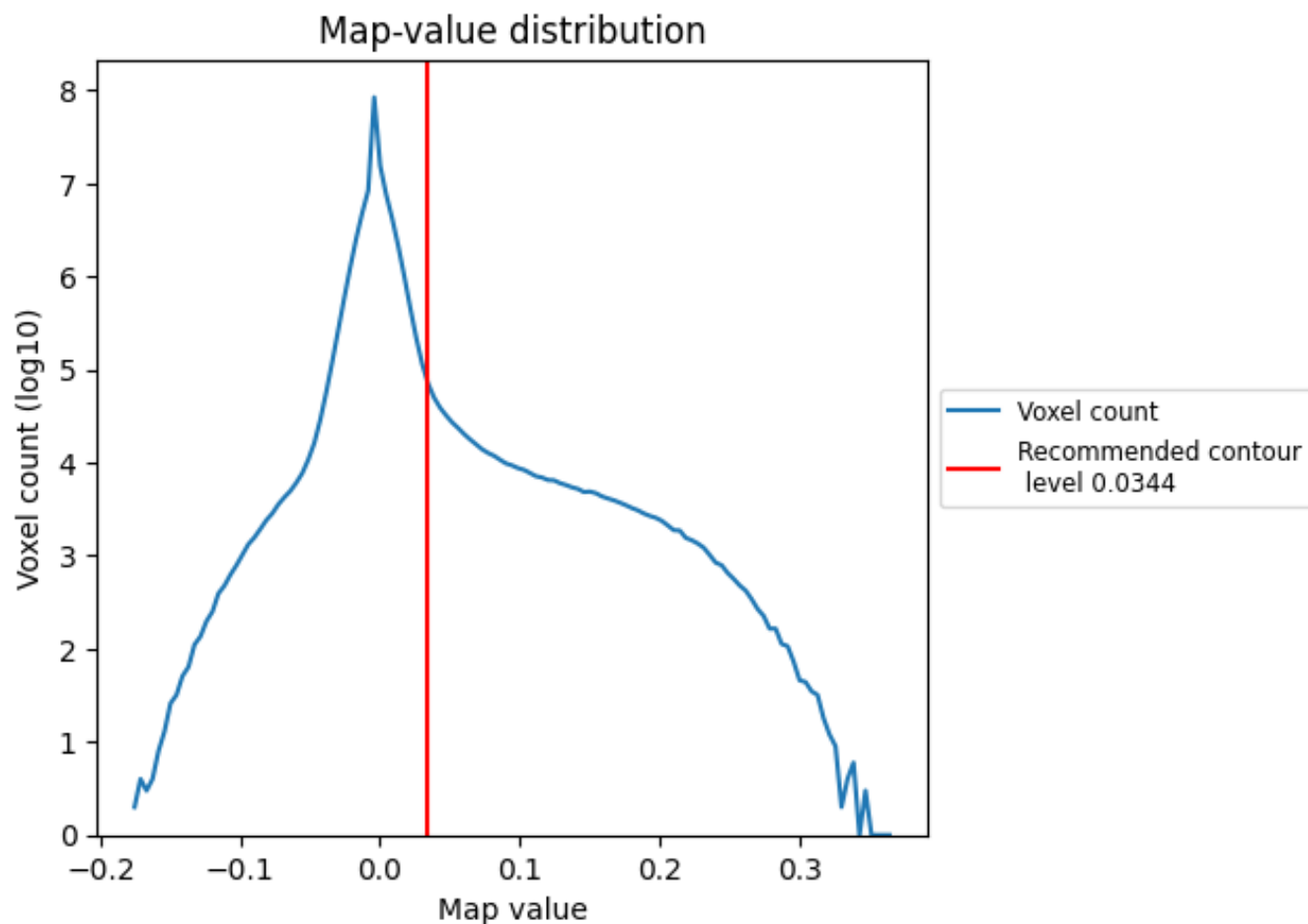
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

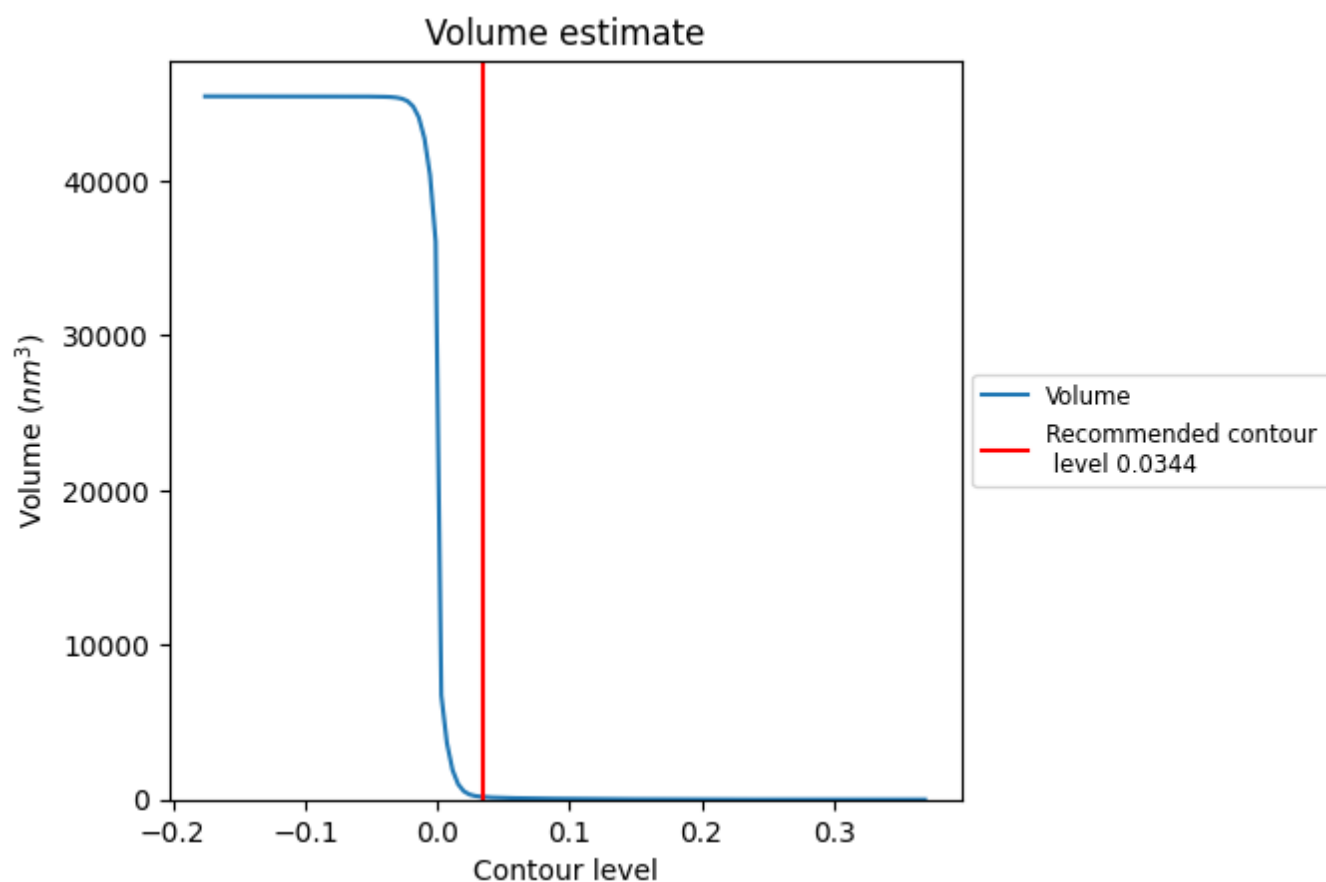
This section contains the results of statistical analysis of the map.

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.

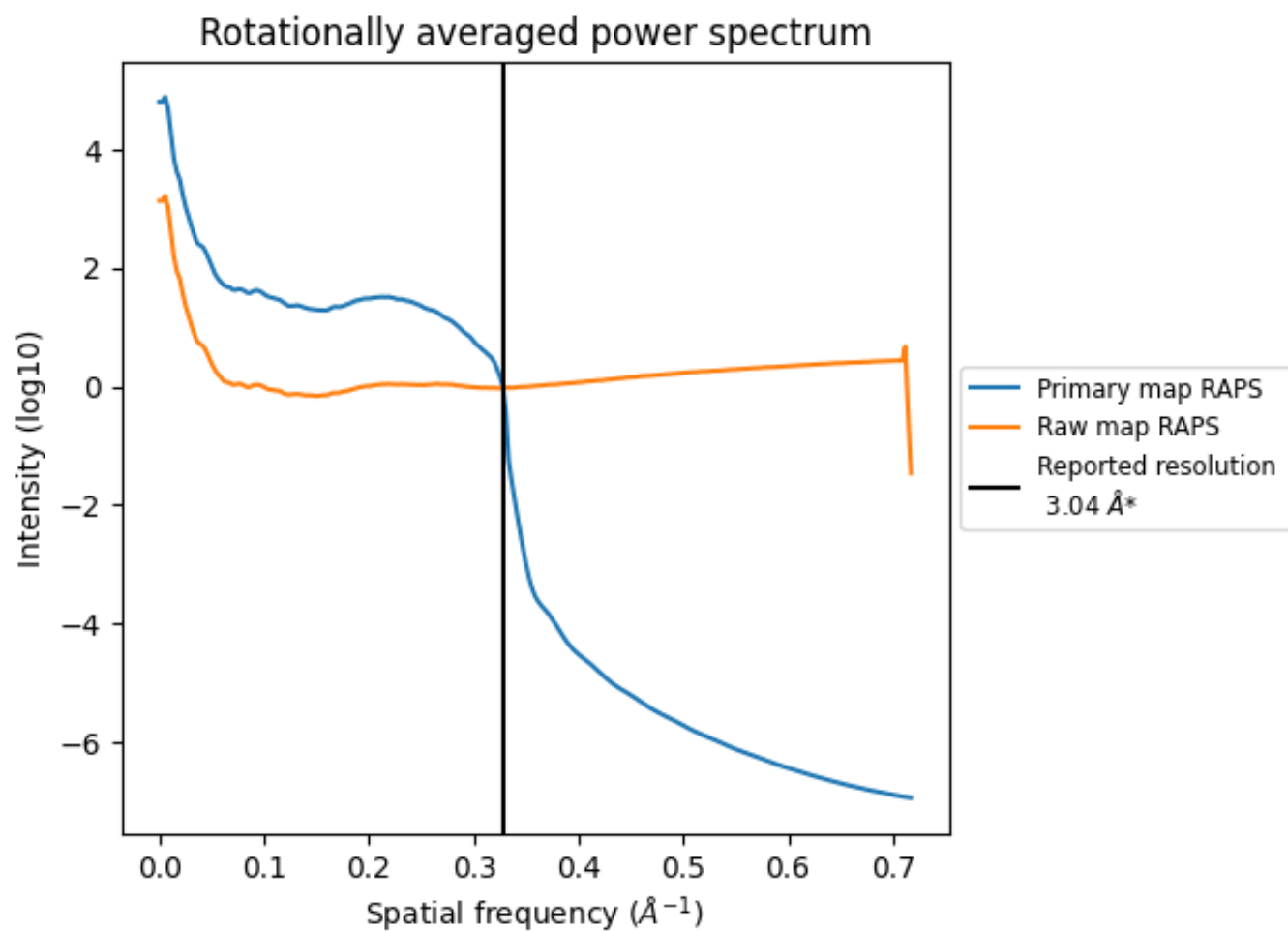
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 158 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 ⓘ

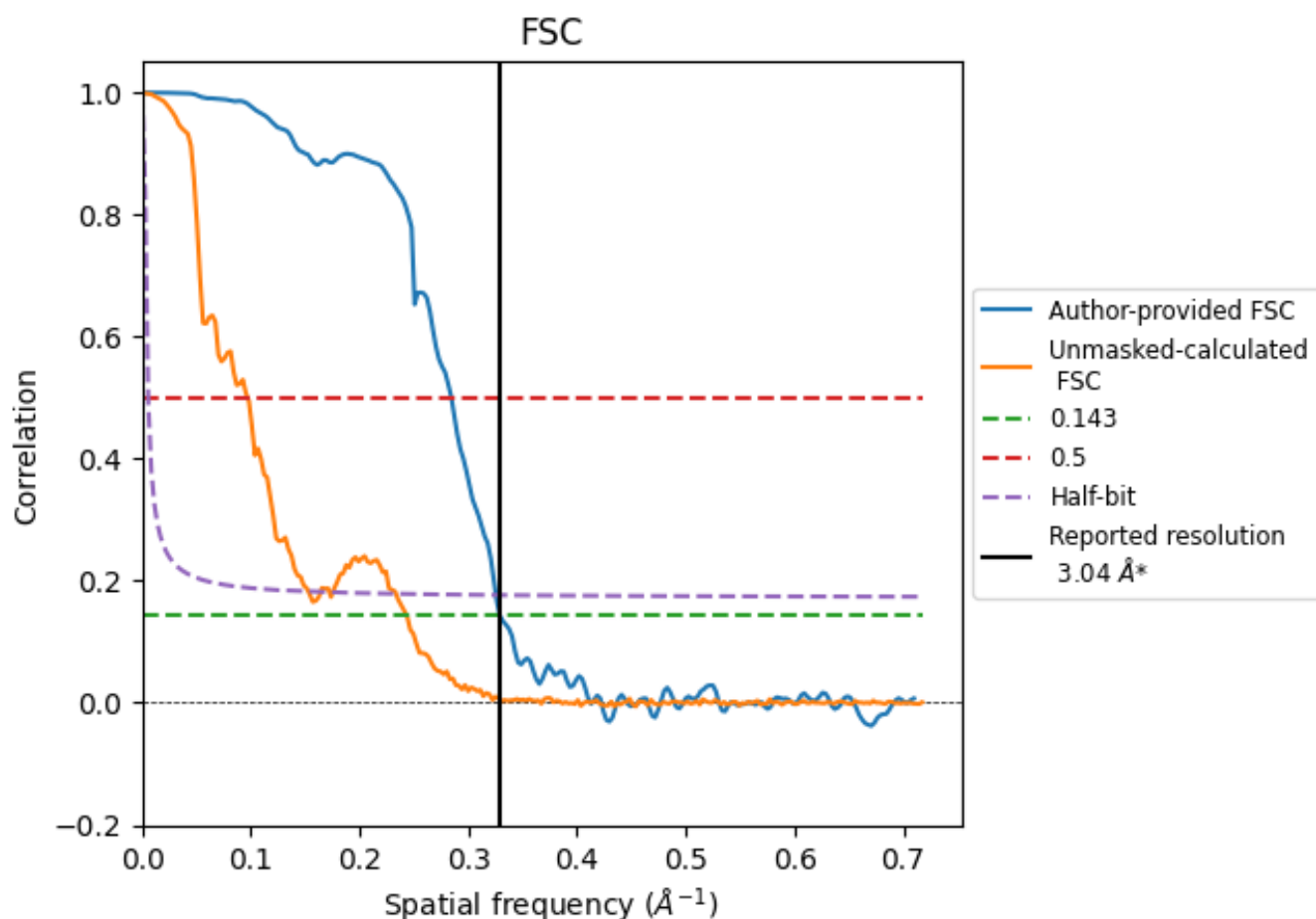


*Reported resolution corresponds to spatial frequency of 0.329 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.329 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

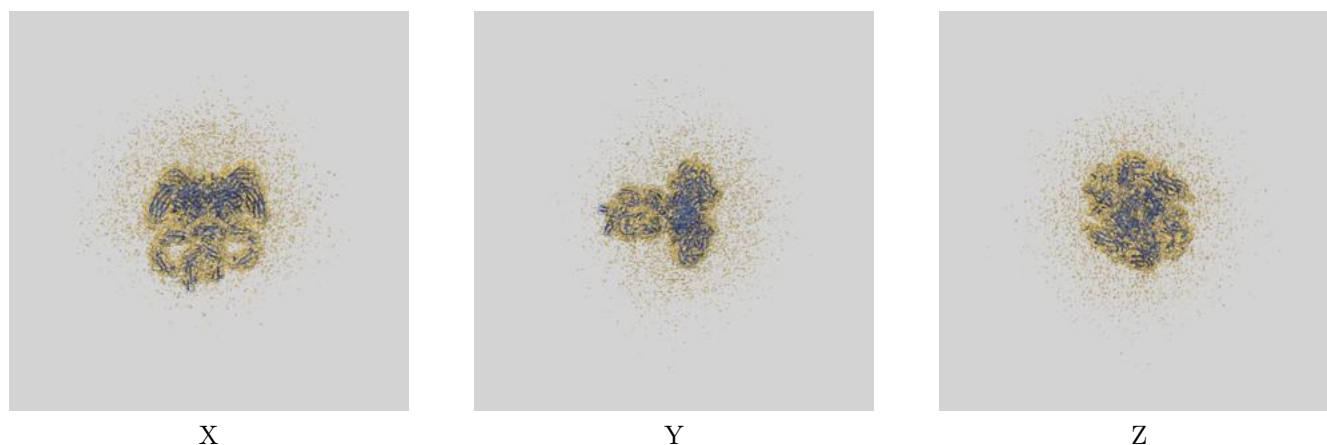
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.52	3.07
Unmasked-calculated*	4.11	10.31	6.54

*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 4.11 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

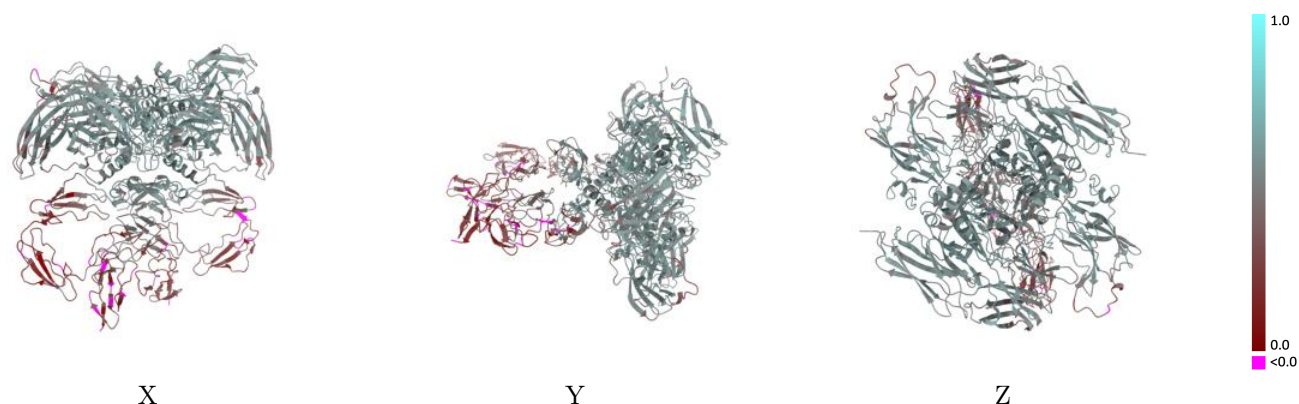
This section contains information regarding the fit between EMDB map EMD-16745 and PDB model 8CMT. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



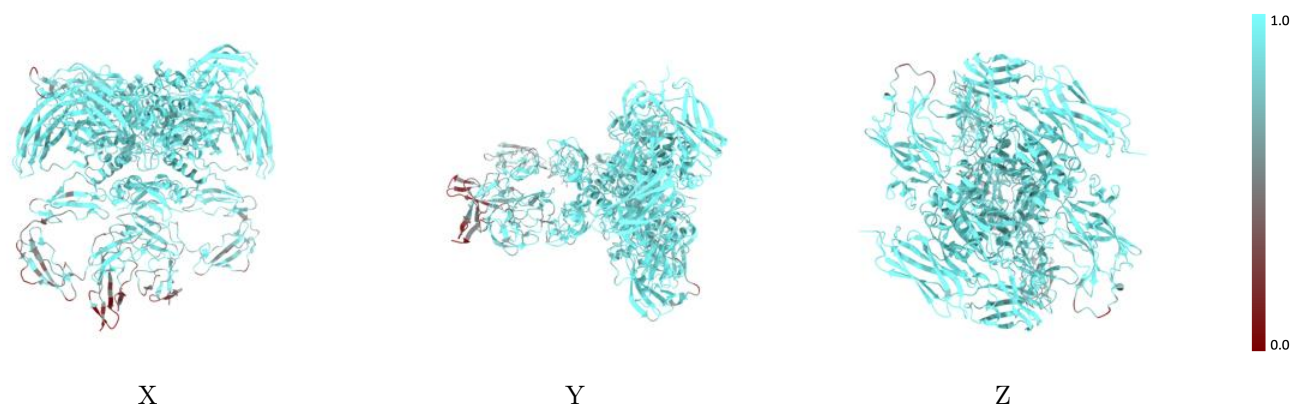
The images above show the 3D surface view of the map at the recommended contour level 0.0344 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



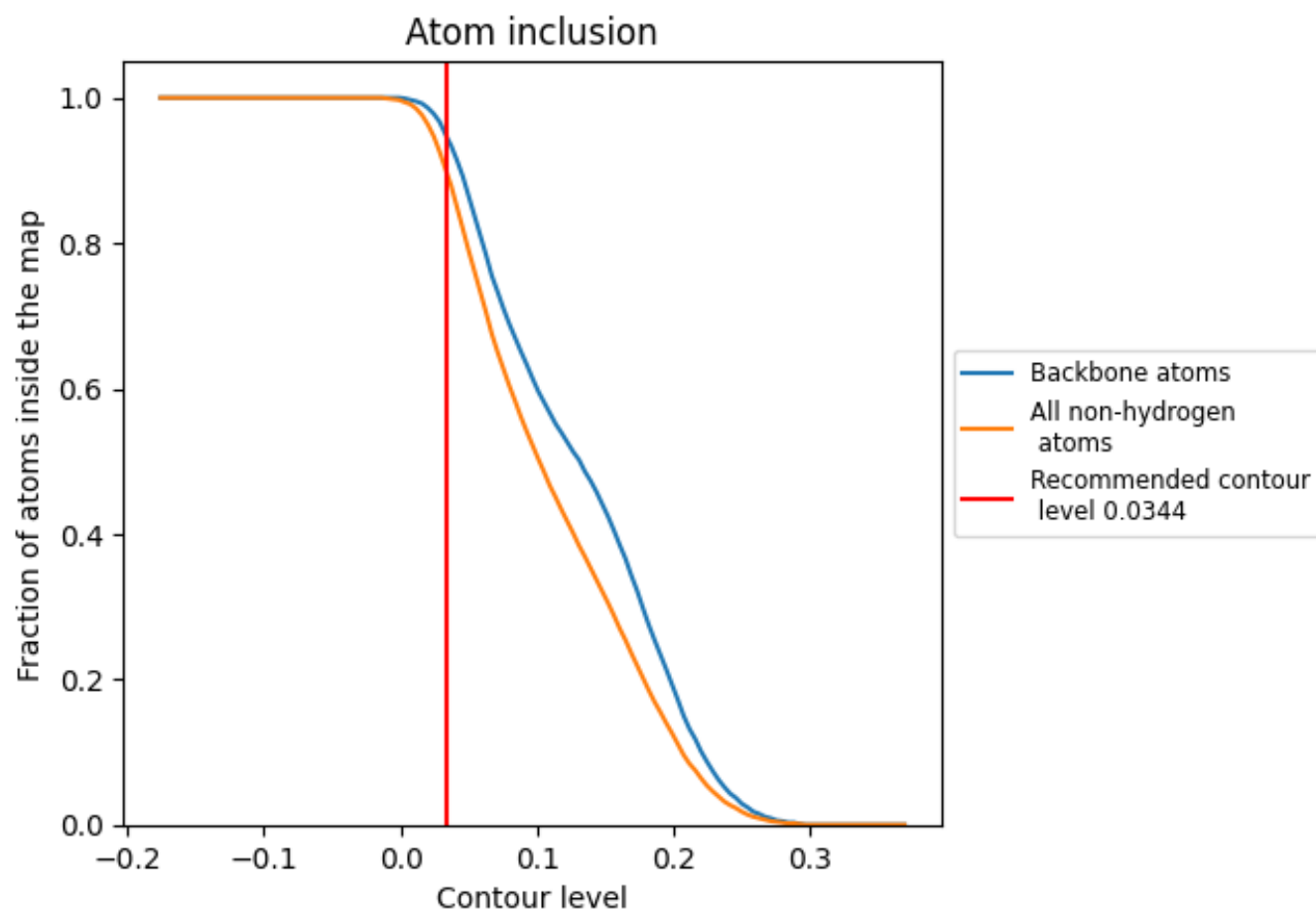
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0344).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.0344) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.4720
A	0.9500	0.5350
B	0.9480	0.5340
C	0.7780	0.3380
D	0.7540	0.3150

