



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:31 PM UTC

PDB ID : 8UQ6 / pdb_00008uq6
EMDB ID : EMD-42462
Title : Human Plasminogen bound to streptococcal surface enolase
Authors : Tjia-Fleck, S.; Readnour, B.M.; Castellino, F.J.
Deposited on : 2023-10-23
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

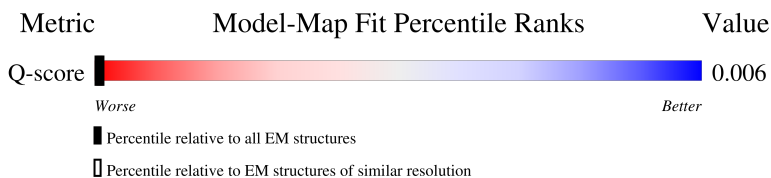
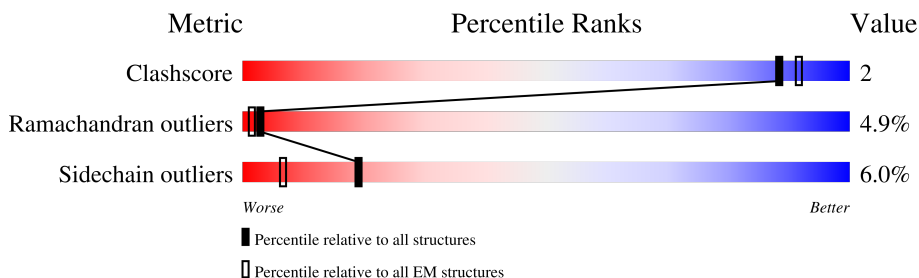
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	791	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11700 atoms, of which 5689 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.

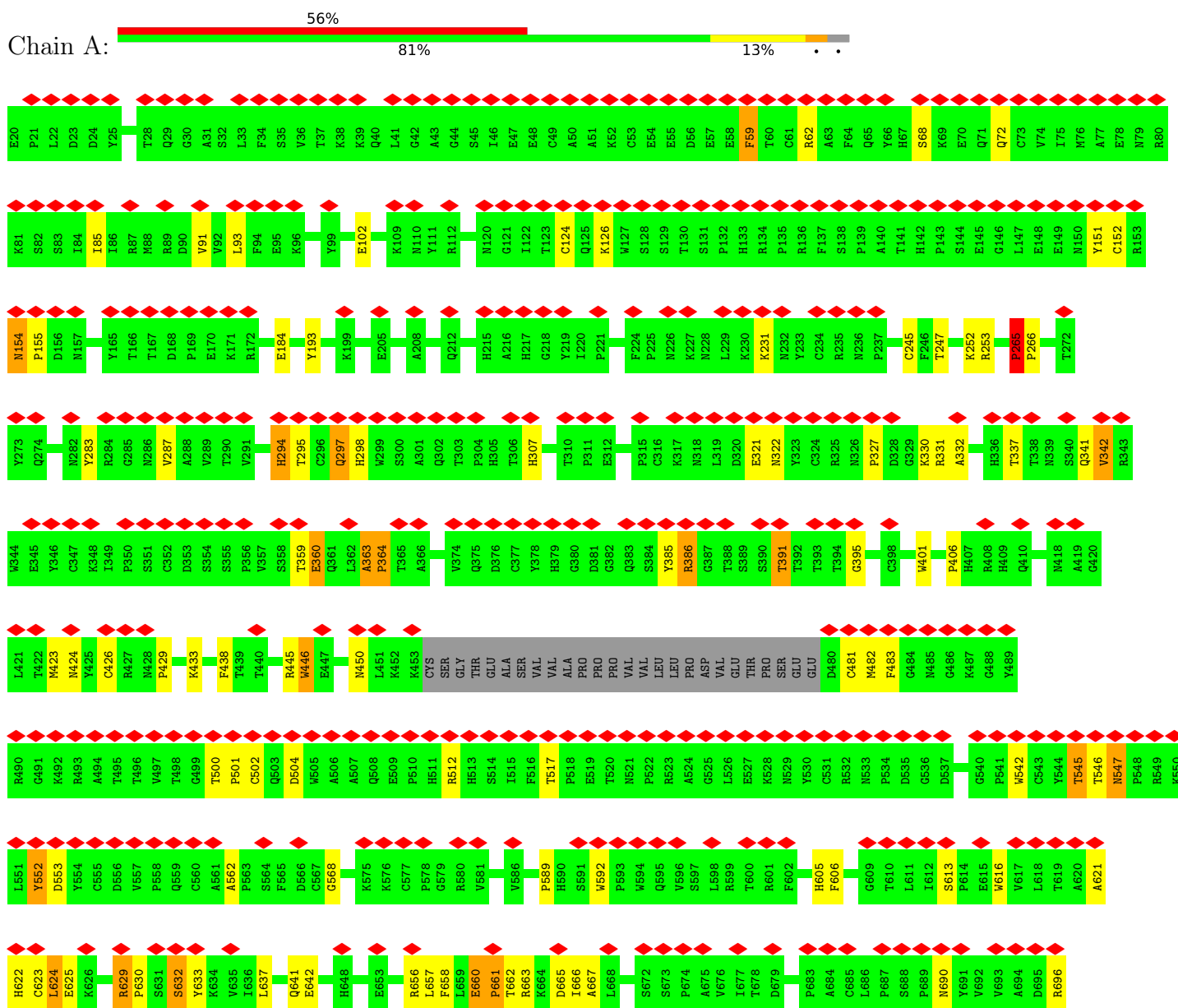
- Molecule 1 is a protein called Plasminogen.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	765	11700	3734	5689	1073	1147	57	0	0

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: Plasminogen





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1024556	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	181.10399, 181.10399, 181.10399	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.539, 0.539, 0.539	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	0.99	1/6184 (0.0%)	1.60	56/8408 (0.7%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	630	PRO	CA-C	5.05	1.59	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	TYR	N-CA-C	8.45	125.33	107.67
1	A	59	PHE	CA-CB-CG	8.33	122.13	113.80
1	A	332	ALA	N-CA-C	8.18	115.58	108.22
1	A	545	THR	N-CA-C	7.12	119.52	110.33
1	A	759	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	265	PRO	CA-N-CD	-6.71	102.10	111.50
1	A	450	ASN	N-CA-C	6.70	125.06	110.80
1	A	386	ARG	N-CA-C	6.61	124.88	110.80
1	A	85	ILE	CA-C-N	6.58	132.03	122.69
1	A	85	ILE	C-N-CA	6.58	132.03	122.69
1	A	68	SER	N-CA-C	6.43	119.11	111.71
1	A	297	GLN	N-CA-C	6.29	118.69	107.80
1	A	126	LYS	N-CA-C	6.15	120.08	110.17
1	A	298	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	294	HIS	CA-CB-CG	5.87	119.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	THR	N-CA-C	5.85	118.75	109.50
1	A	483	PHE	CA-CB-CG	5.85	119.65	113.80
1	A	660	GLU	CA-C-N	5.85	127.15	119.84
1	A	660	GLU	C-N-CA	5.85	127.15	119.84
1	A	330	LYS	CA-C-N	5.83	132.68	121.54
1	A	330	LYS	C-N-CA	5.83	132.68	121.54
1	A	332	ALA	CA-C-N	5.83	125.74	119.85
1	A	332	ALA	C-N-CA	5.83	125.74	119.85
1	A	605	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	A	661	PRO	CA-C-N	5.72	128.98	120.17
1	A	661	PRO	C-N-CA	5.72	128.98	120.17
1	A	622	HIS	CA-C-N	5.70	132.43	121.54
1	A	622	HIS	C-N-CA	5.70	132.43	121.54
1	A	481	CYS	CA-C-N	5.70	128.93	120.90
1	A	481	CYS	C-N-CA	5.70	128.93	120.90
1	A	295	THR	CA-CB-CG2	5.62	120.06	110.50
1	A	154	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	391	THR	N-CA-C	5.55	117.68	110.53
1	A	700	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	720	GLN	OE1-CD-NE2	-5.34	117.25	122.60
1	A	252	LYS	CA-C-N	5.31	131.69	121.54
1	A	252	LYS	C-N-CA	5.31	131.69	121.54
1	A	547	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	779	SER	CA-C-N	5.23	131.53	121.54
1	A	779	SER	C-N-CA	5.23	131.53	121.54
1	A	265	PRO	CA-C-N	5.22	125.75	120.38
1	A	265	PRO	C-N-CA	5.22	125.75	120.38
1	A	360	GLU	CA-C-N	5.20	131.47	121.54
1	A	360	GLU	C-N-CA	5.20	131.47	121.54
1	A	126	LYS	CA-C-N	5.18	127.54	120.54
1	A	126	LYS	C-N-CA	5.18	127.54	120.54
1	A	72	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	629	ARG	CA-C-N	5.11	126.23	119.84
1	A	629	ARG	C-N-CA	5.11	126.23	119.84
1	A	606	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	704	TRP	CA-CB-CG	5.08	123.25	113.60
1	A	641	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	151	TYR	CA-C-N	5.04	128.02	120.87
1	A	151	TYR	C-N-CA	5.04	128.02	120.87
1	A	385	TYR	CA-C-N	5.03	131.15	121.54
1	A	385	TYR	C-N-CA	5.03	131.15	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	TYR	Sidechain
1	A	445	ARG	Sidechain
1	A	552	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	6011	5689	5725	22	0
All	All	6011	5689	5725	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (22) 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:613:SER:HG	1:A:616:TRP:CD1	2.12	0.67
1:A:621:ALA:HB3	1:A:665:ASP:HA	1.81	0.61
1:A:613:SER:HG	1:A:616:TRP:CG	2.19	0.60
1:A:363:ALA:H	1:A:364:PRO:CD	2.20	0.55
1:A:502:CYS:HA	1:A:546:THR:HB	1.92	0.50
1:A:363:ALA:H	1:A:364:PRO:HD3	1.78	0.48
1:A:545:THR:HG21	1:A:553:ASP:HB2	1.97	0.47
1:A:592:TRP:CE3	1:A:702:THR:HG22	2.50	0.46
1:A:433:LYS:HE3	1:A:446:TRP:CZ3	2.51	0.46
1:A:500:THR:HB	1:A:501:PRO:CD	2.46	0.45
1:A:542:TRP:CD2	1:A:552:TYR:CD2	3.05	0.45
1:A:545:THR:HG21	1:A:553:ASP:CB	2.47	0.45
1:A:502:CYS:HA	1:A:546:THR:H	1.82	0.44
1:A:423:MET:HG2	1:A:424:ASN:H	1.83	0.42
1:A:621:ALA:HB2	1:A:667:ALA:HB2	2.01	0.42
1:A:660:GLU:C	1:A:662:THR:H	2.27	0.41
1:A:776:GLY:HA2	1:A:796:VAL:HG23	2.02	0.41
1:A:502:CYS:SG	1:A:545:THR:HA	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLN:HE22	1:A:307:HIS:CE1	2.38	0.41
1:A:616:TRP:CE3	1:A:807:MET:HE3	2.56	0.41
1:A:624:LEU:HD21	1:A:633:TYR:CD2	2.57	0.40
1:A:613:SER:HB3	1:A:616:TRP:CD2	2.56	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	761/791 (96%)	545 (72%)	179 (24%)	37 (5%)	1	16

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	PRO
1	A	331	ARG
1	A	363	ALA
1	A	406	PRO
1	A	624	LEU
1	A	657	LEU
1	A	661	PRO
1	A	780	TRP
1	A	266	PRO
1	A	321	GLU
1	A	364	PRO
1	A	386	ARG
1	A	395	GLY
1	A	429	PRO
1	A	568	GLY
1	A	642	GLU
1	A	102	GLU

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Mol	Chain	Res	Type
1	A	124	CYS
1	A	231	LYS
1	A	245	CYS
1	A	632	SER
1	A	696	ARG
1	A	93	LEU
1	A	360	GLU
1	A	623	CYS
1	A	690	ASN
1	A	253	ARG
1	A	327	PRO
1	A	342	VAL
1	A	666	ILE
1	A	708	GLN
1	A	770	ASP
1	A	562	ALA
1	A	629	ARG
1	A	589	PRO
1	A	155	PRO
1	A	783	GLY

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	671/694 (97%)	631 (94%)	40 (6%)	17	45

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	62	ARG
1	A	91	VAL
1	A	152	CYS
1	A	154	ASN
1	A	184	GLU

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Mol	Chain	Res	Type
1	A	193	TYR
1	A	247	THR
1	A	265	PRO
1	A	287	VAL
1	A	294	HIS
1	A	322	ASN
1	A	337	THR
1	A	341	GLN
1	A	342	VAL
1	A	391	THR
1	A	401	TRP
1	A	426	CYS
1	A	438	PHE
1	A	446	TRP
1	A	482	MET
1	A	504	ASP
1	A	512	ARG
1	A	517	THR
1	A	547	ASN
1	A	625	GLU
1	A	632	SER
1	A	637	LEU
1	A	656	ARG
1	A	658	PHE
1	A	663	ARG
1	A	698	GLU
1	A	701	ILE
1	A	704	TRP
1	A	736	ASN
1	A	759	ASP
1	A	773	ILE
1	A	782	LEU
1	A	794	VAL
1	A	810	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	40	GLN
1	A	67	HIS
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	133	HIS
1	A	142	HIS
1	A	297	GLN
1	A	302	GLN
1	A	326	ASN
1	A	336	HIS
1	A	341	GLN
1	A	409	HIS
1	A	595	GLN
1	A	641	GLN
1	A	720	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.

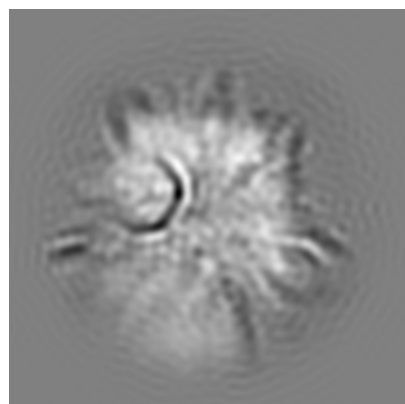
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42462. These allow visual inspection of the internal detail of the map and identification of artifacts.

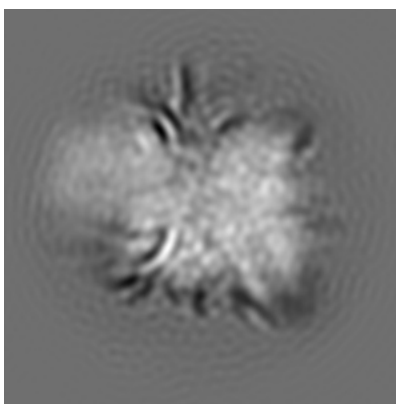
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

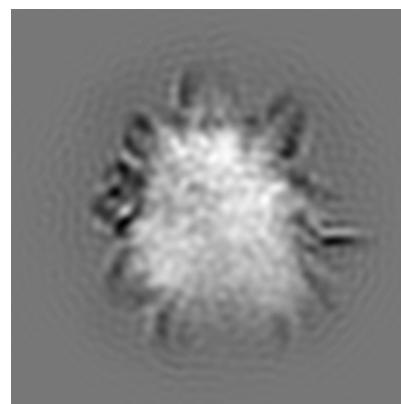
6.1.1 Primary map



X

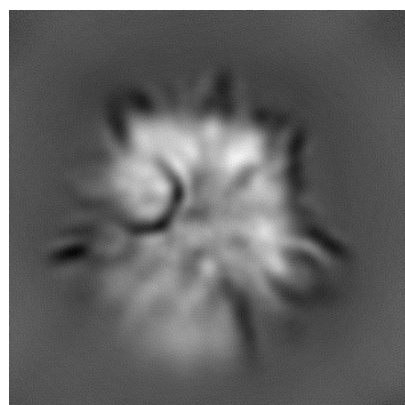


Y

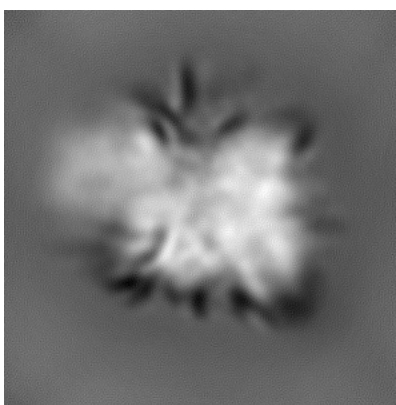


Z

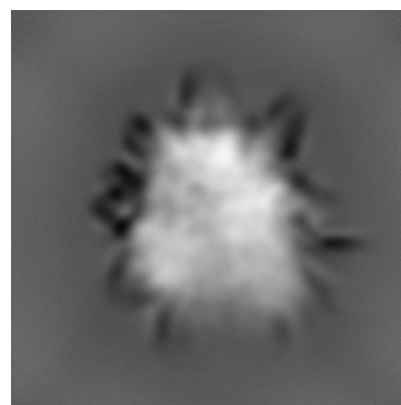
6.1.2 Raw map



X



Y

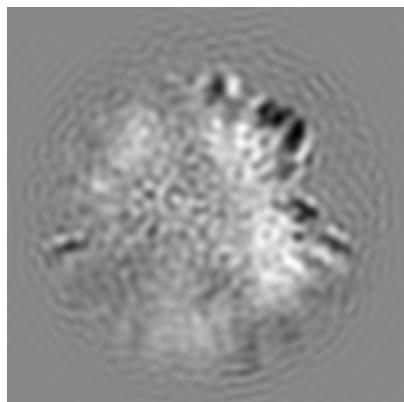


Z

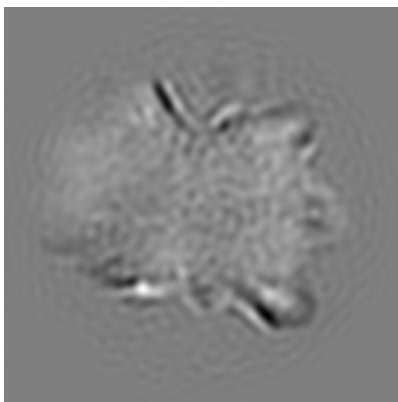
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

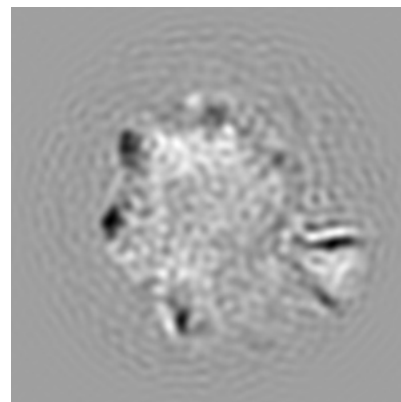
6.2.1 Primary map



X Index: 168

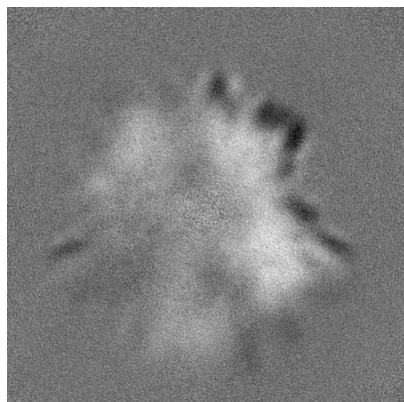


Y Index: 168

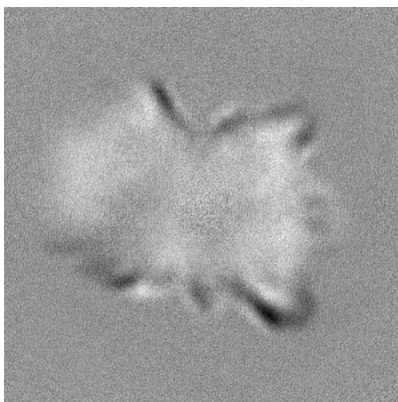


Z Index: 168

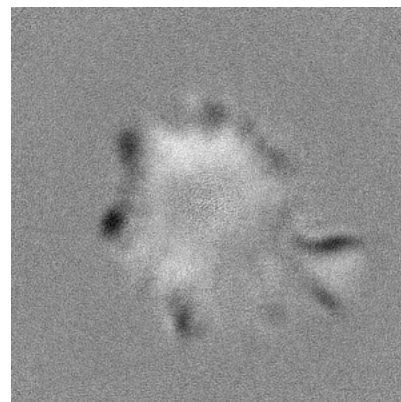
6.2.2 Raw map



X Index: 168



Y Index: 168

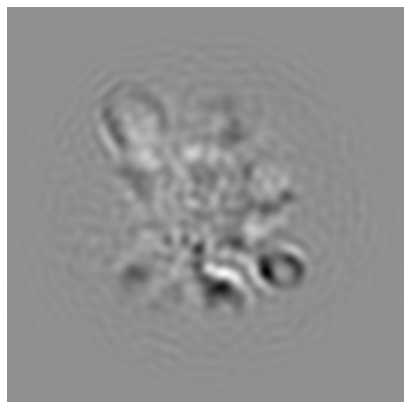


Z Index: 168

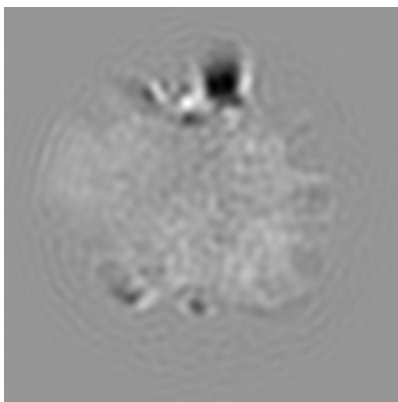
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

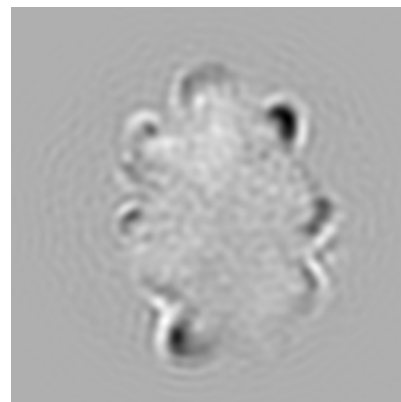
6.3.1 Primary map



X Index: 103

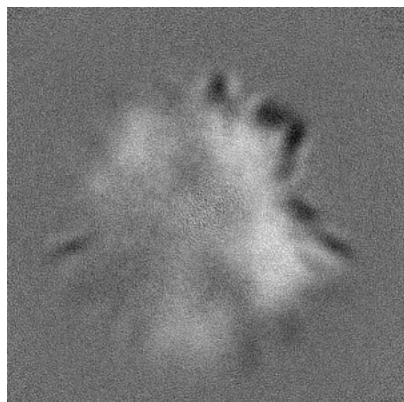


Y Index: 141

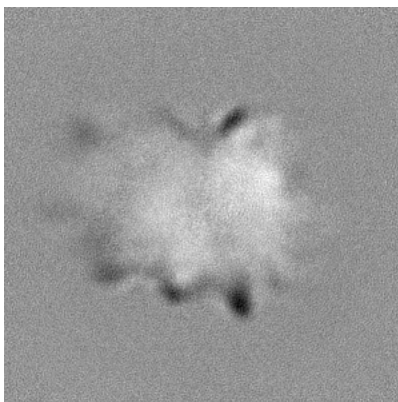


Z Index: 132

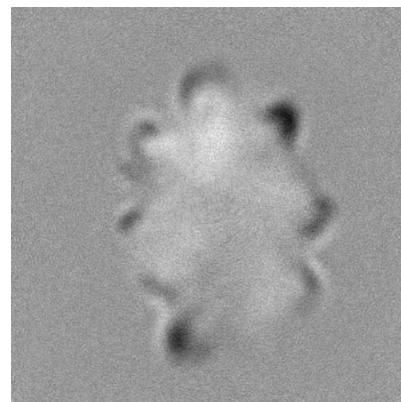
6.3.2 Raw map



X Index: 169



Y Index: 199

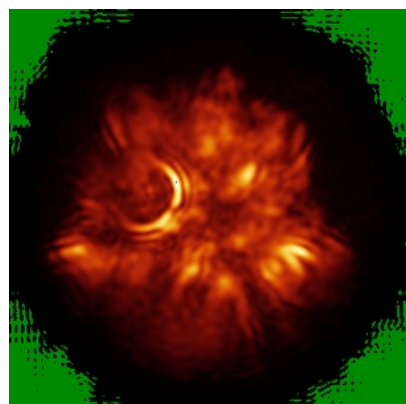


Z Index: 131

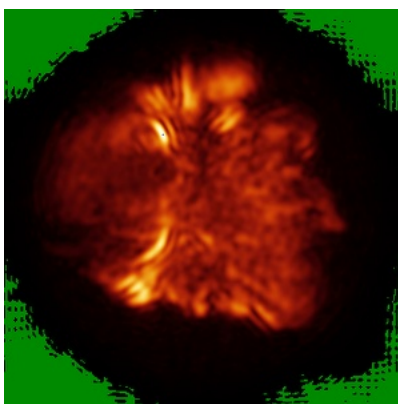
The images above show the largest variance slices of the map in three orthogonal directions.

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

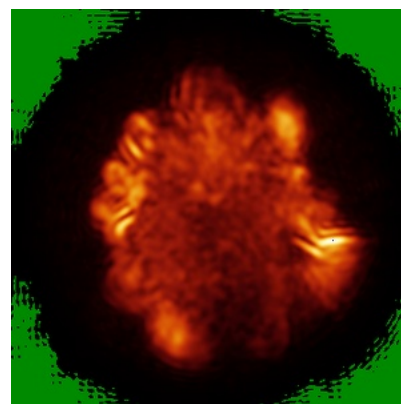
6.4.1 Primary map



X

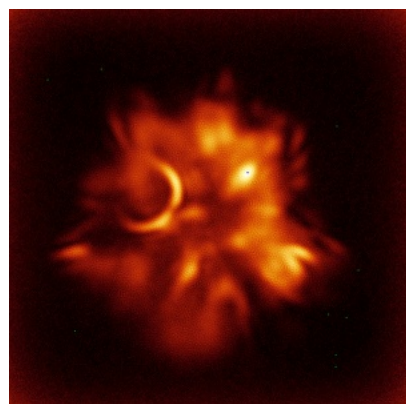


Y

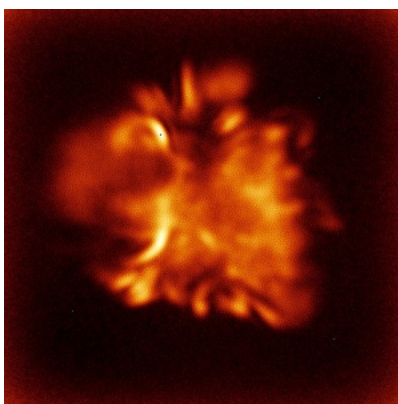


Z

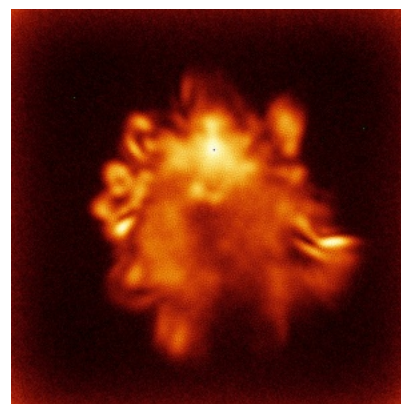
6.4.2 Raw map



X



Y

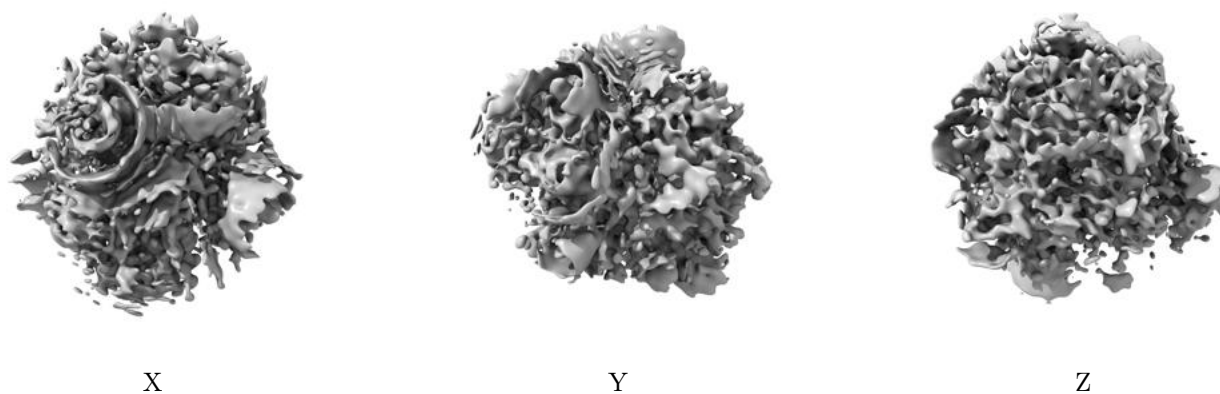


Z

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.

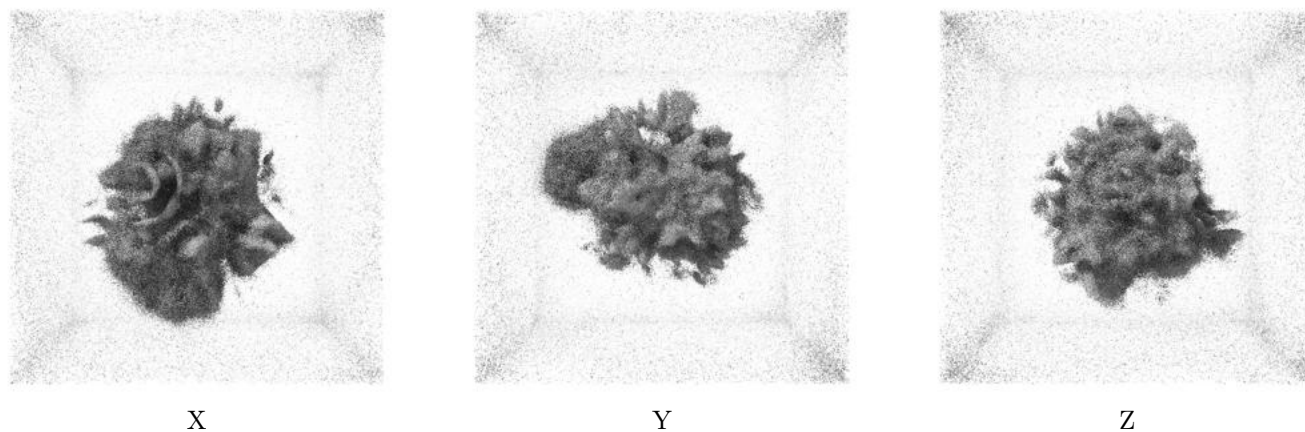
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

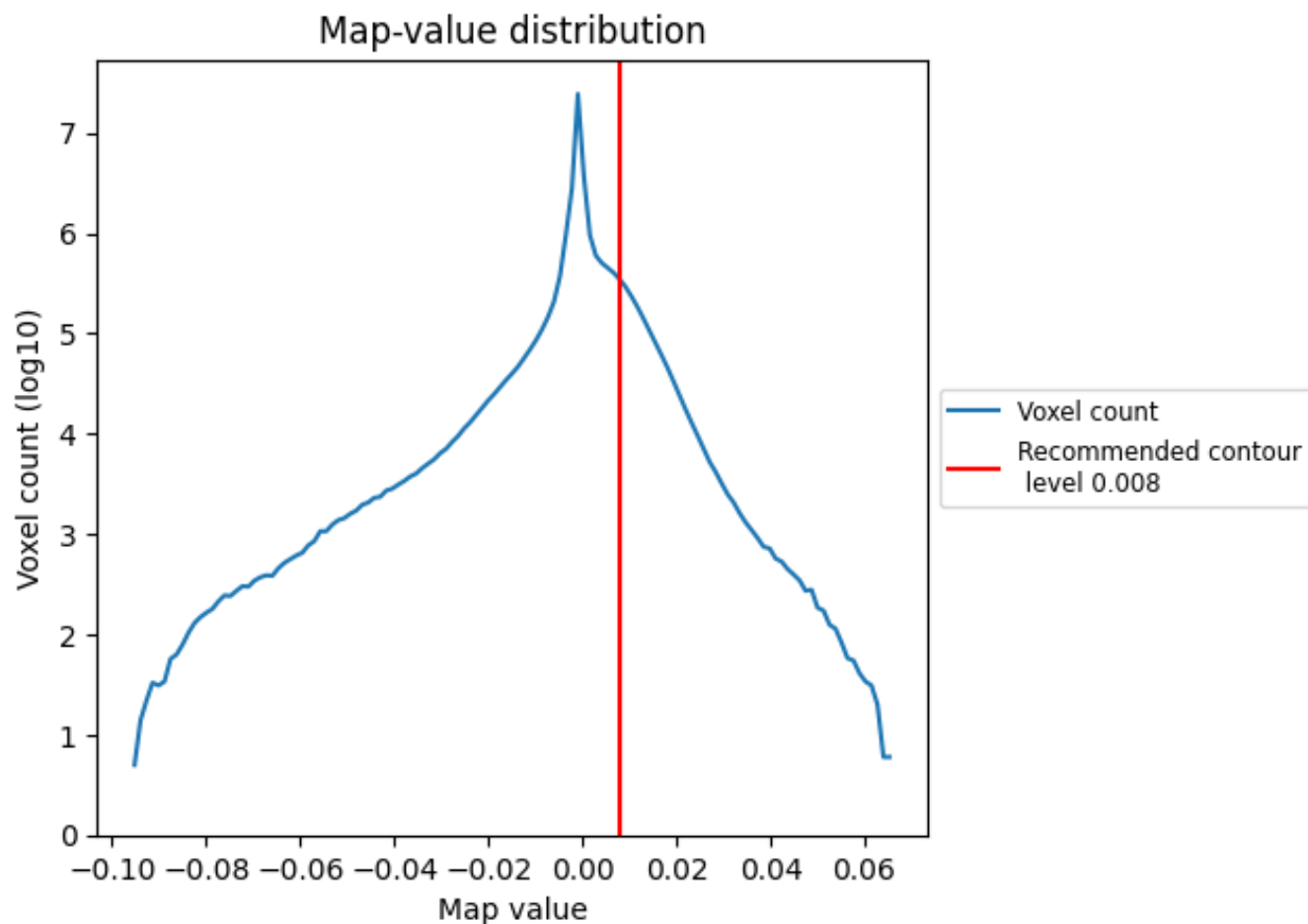
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

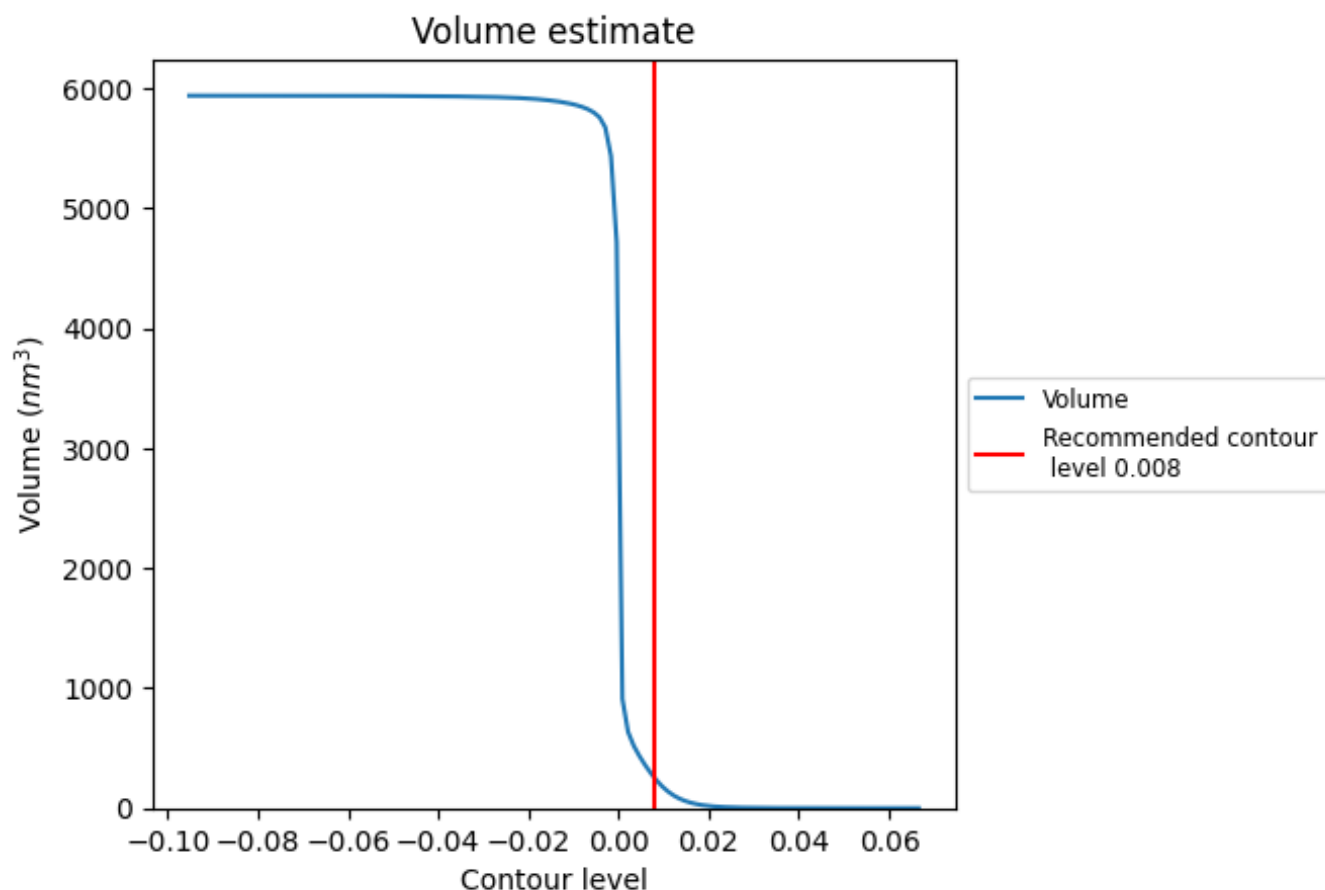
This section contains the results of statistical analysis of the map.

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.

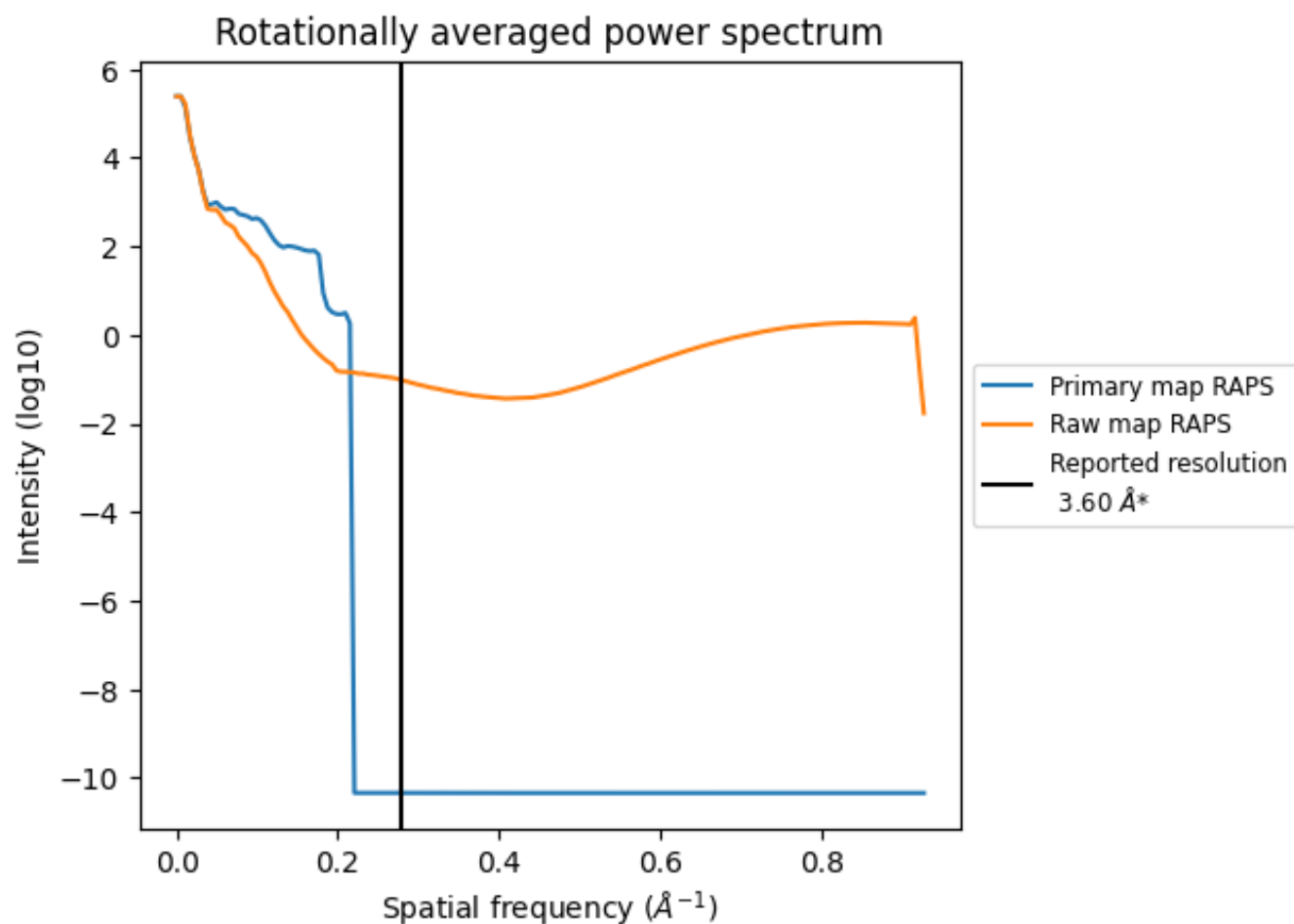
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm^3 ; this corresponds to an approximate mass of 228 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 ⓘ

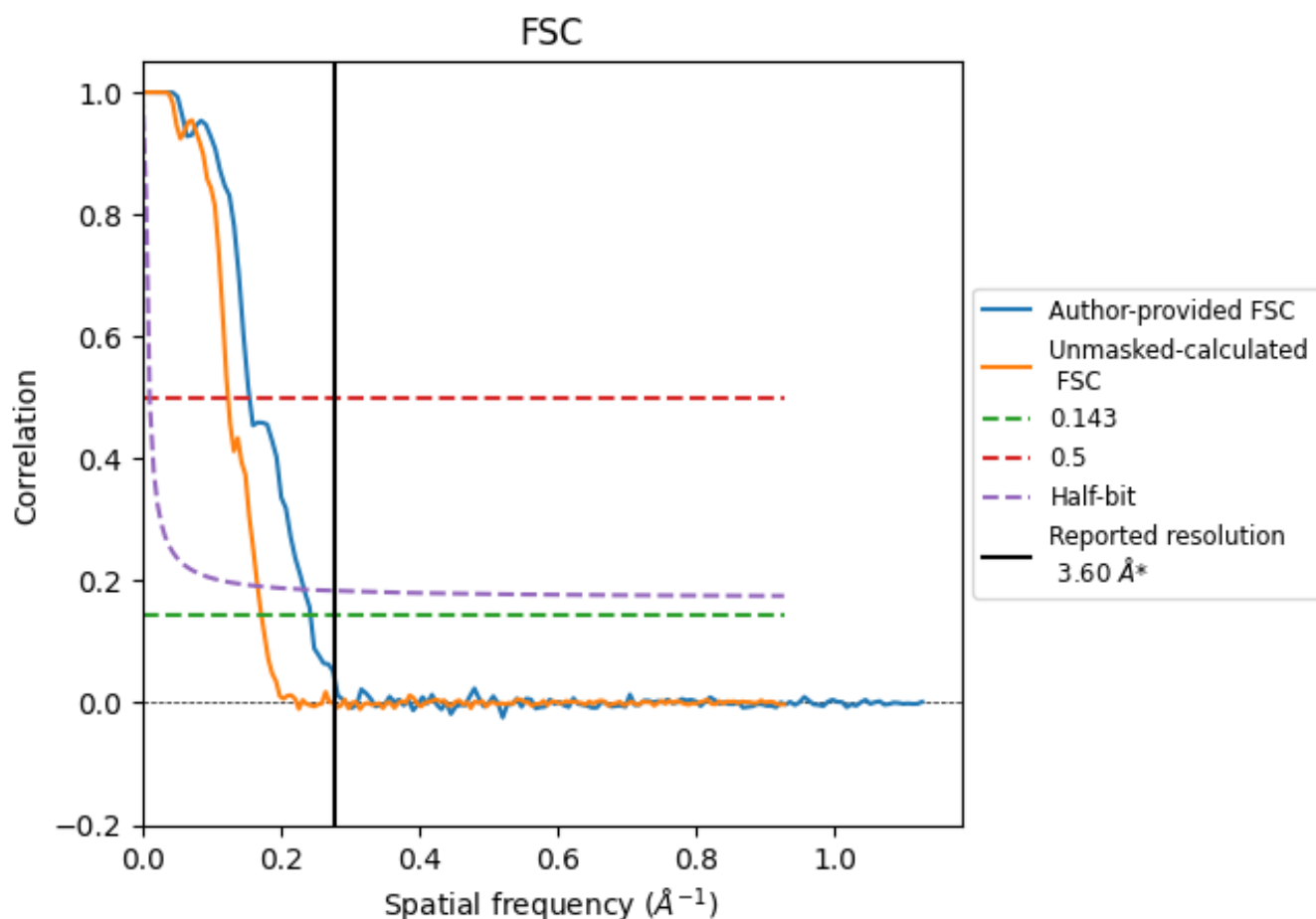


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	4.11	6.45	4.29
Unmasked-calculated*	5.81	8.06	6.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.6 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.81 differs from the reported value 3.6 by more than 10 %

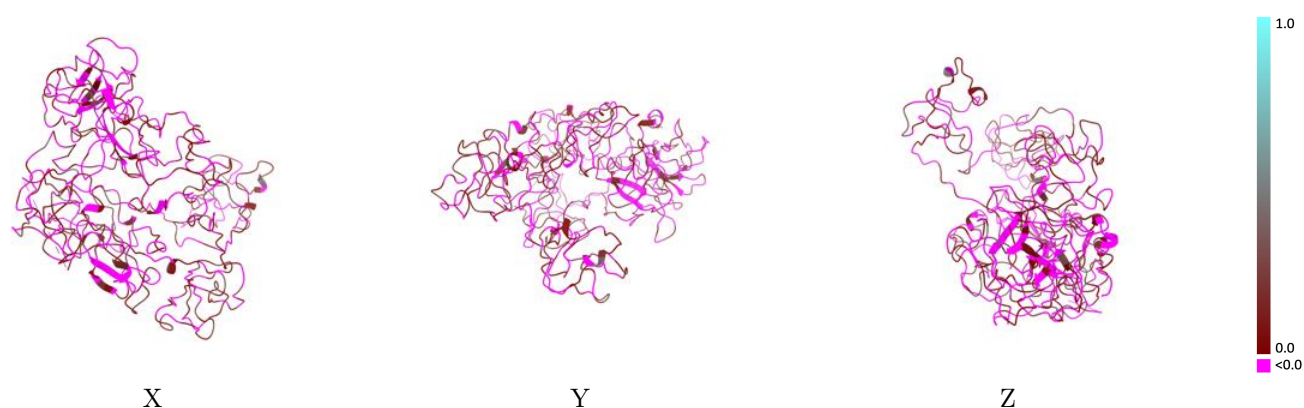
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-42462 and PDB model 8UQ6. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

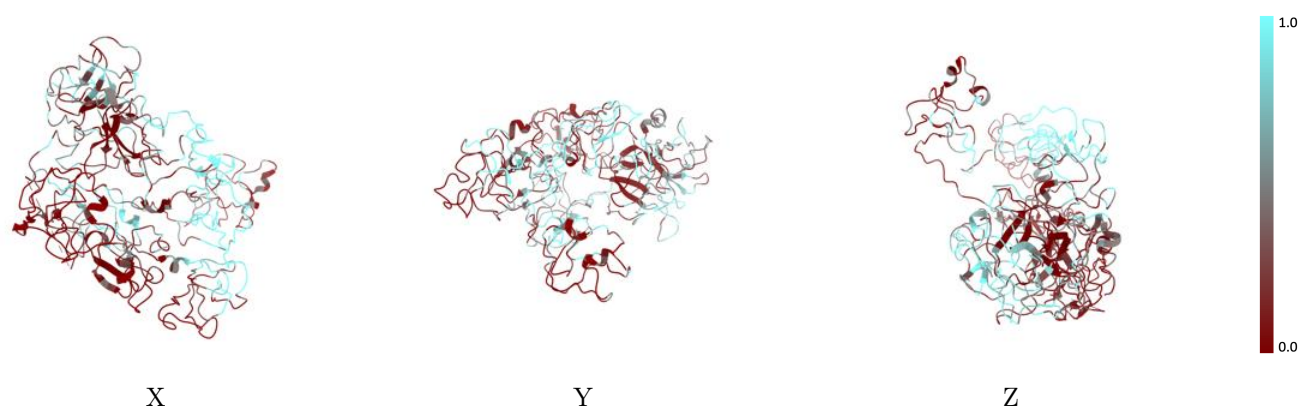
This section was not generated.

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



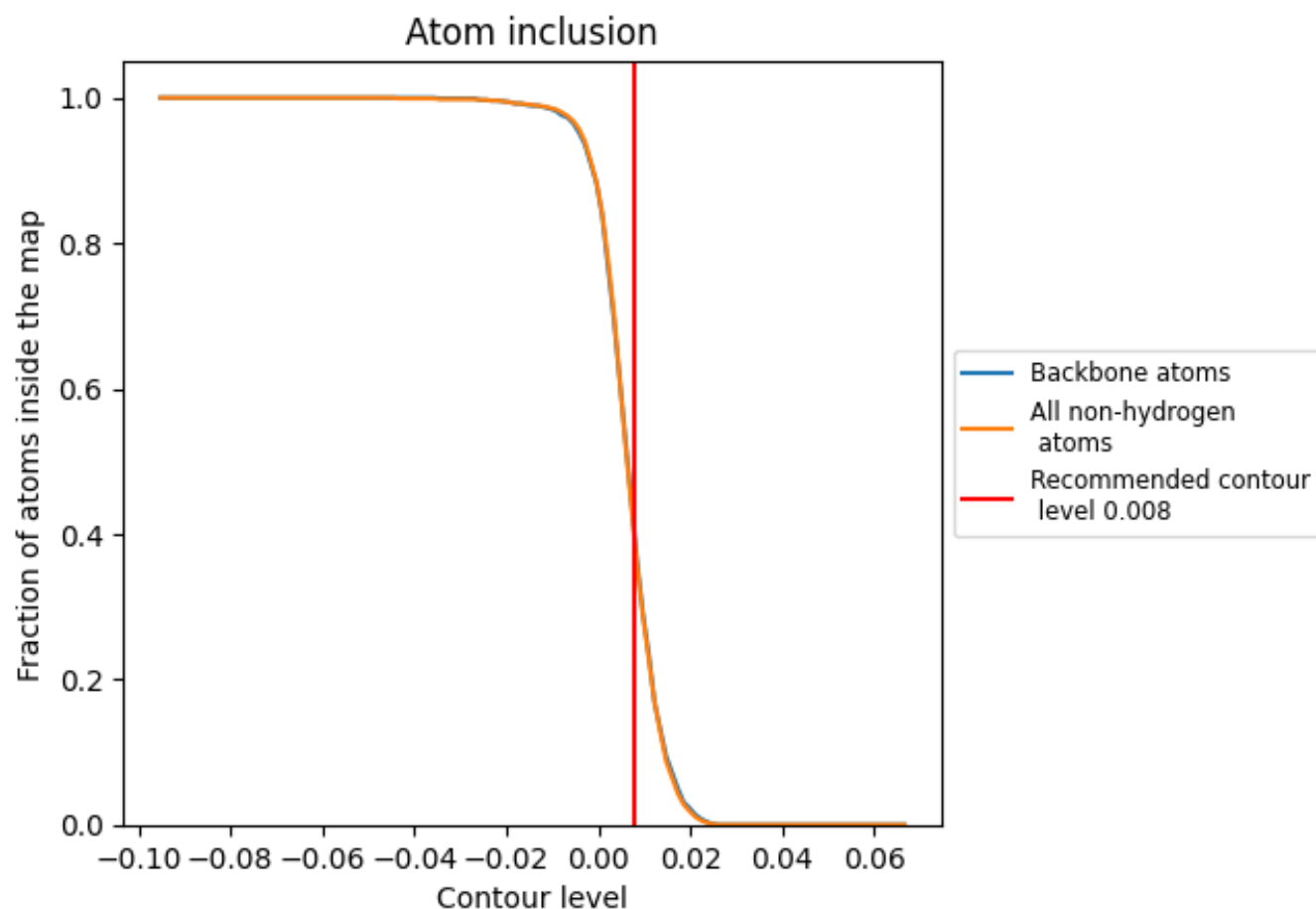
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 39% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3870	0.0060
A	0.3840	0.0060

