



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2024 – 11:16 PM JST

PDB ID : 7YVS
EMDB ID : EMD-34137
Title : Complex structure of Clostridioides difficile binary toxin unfolded CDTa-bound CDTb-pore (short).
Authors : Yamada, T.; Kawamoto, A.; Yoshida, T.; Sato, Y.; Kato, T.; Tsuge, H.
Deposited on : 2022-08-19
Resolution : 2.80 Å(reported)
Based on initial model : 7VNJ

This is a wwPDB EM Validation Summary 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:

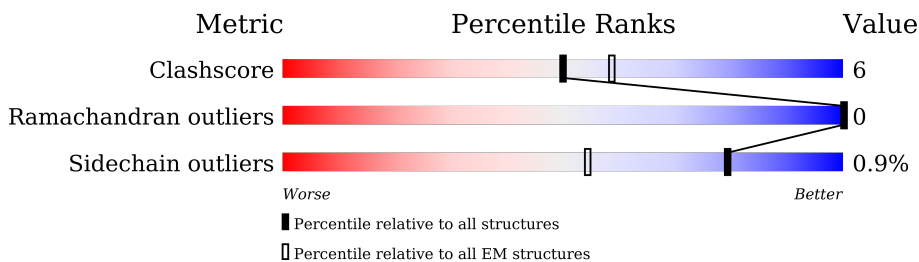
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 2.80 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 $\leq 5\%$. 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	675	
1	B	675	
1	C	675	
1	D	675	
1	E	675	
1	F	675	
1	G	675	
2	H	428	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 30593 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 ADP-ribosylating binary toxin binding subunit CdtB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	494	3935	2458	640	831	6	11	0
1	B	494	3935	2458	640	831	6	11	0
1	C	494	3867	2418	627	816	6	1	0
1	D	497	3898	2438	631	823	6	1	0
1	E	494	3935	2458	640	831	6	11	0
1	F	494	3867	2418	627	816	6	1	0
1	G	494	3935	2458	640	831	6	21	0

- Molecule 2 is a protein called ADP-ribosylating binary toxin enzymatic subunit CdtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	395	3200	2038	534	623	5	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	414	GLU	-	expression tag	UNP Q9KH42
H	415	ASN	-	expression tag	UNP Q9KH42
H	416	LEU	-	expression tag	UNP Q9KH42
H	417	TYR	-	expression tag	UNP Q9KH42
H	418	PHE	-	expression tag	UNP Q9KH42
H	419	GLN	-	expression tag	UNP Q9KH42
H	420	GLY	-	expression tag	UNP Q9KH42
H	421	LEU	-	expression tag	UNP Q9KH42
H	422	GLU	-	expression tag	UNP Q9KH42

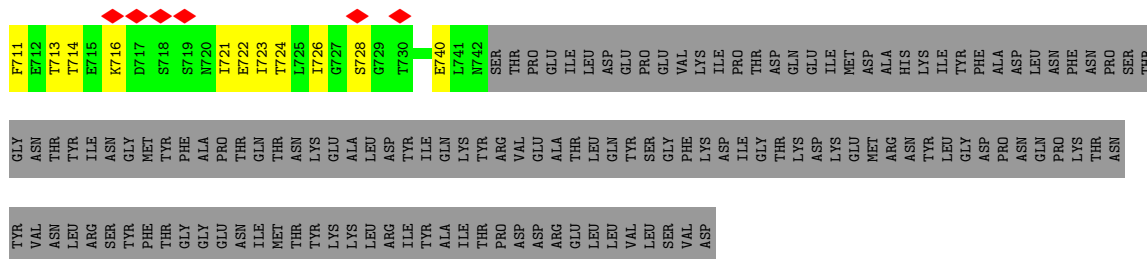
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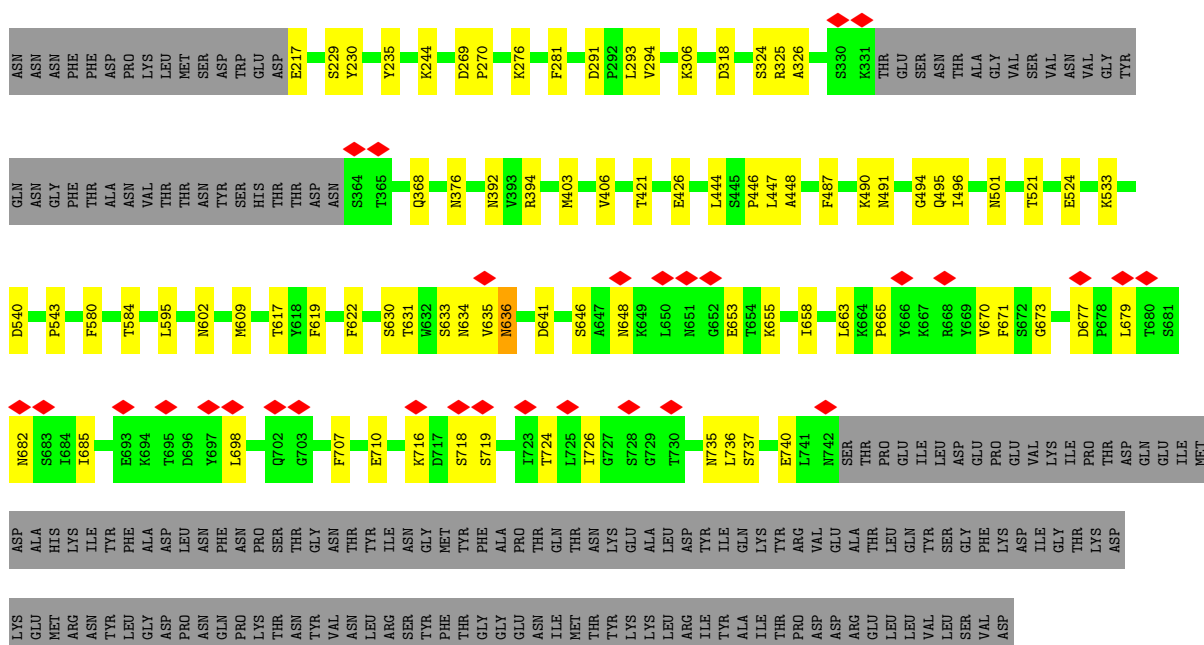
Chain	Residue	Modelled	Actual	Comment	Reference
H	423	HIS	-	expression tag	UNP Q9KH42
H	424	HIS	-	expression tag	UNP Q9KH42
H	425	HIS	-	expression tag	UNP Q9KH42
H	426	HIS	-	expression tag	UNP Q9KH42
H	427	HIS	-	expression tag	UNP Q9KH42
H	428	HIS	-	expression tag	UNP Q9KH42

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

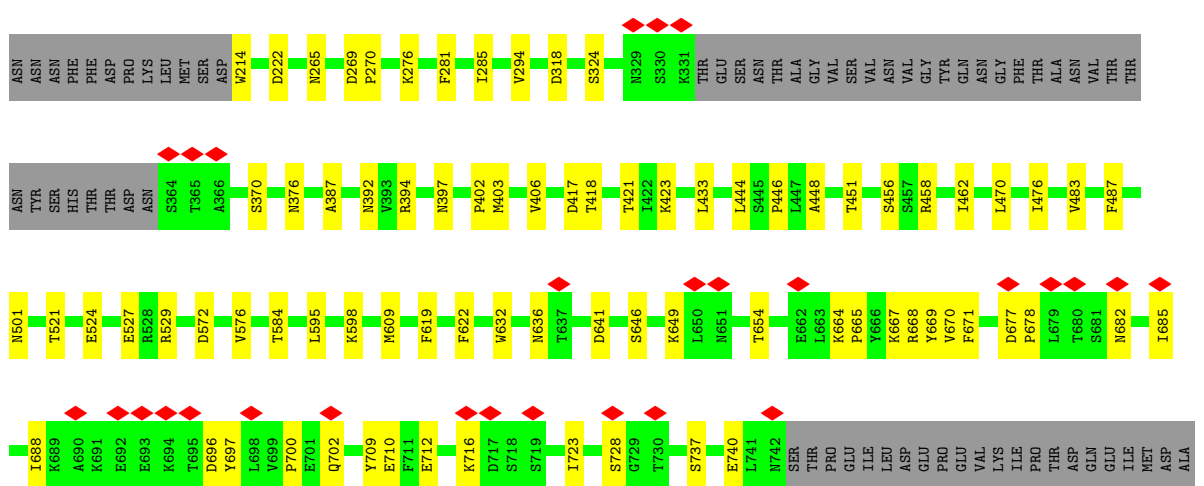
Mol	Chain	Residues	Atoms	AltConf
3	A	3	Total Ca 3 3	0
3	B	3	Total Ca 3 3	0
3	C	3	Total Ca 3 3	0
3	D	3	Total Ca 3 3	0
3	E	3	Total Ca 3 3	0
3	F	3	Total Ca 3 3	0
3	G	3	Total Ca 3 3	0



● Molecule 1: ADP-ribosylating binary toxin binding subunit CdtB



● Molecule 1: ADP-ribosylating binary toxin binding subunit CdtB



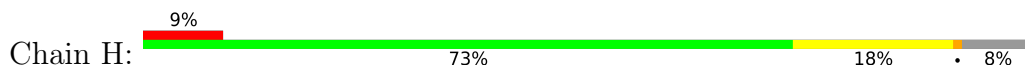
GLY	ASP	ASN	ASP	PRO	ASP	PRO	ASN	GLN	PHE	THR	ASN	ASP	PRO	THR	LYS	ASN	VAL	LEU	ASN	ARG	ASP	THR	THR	THR	THR	GLY	GLY	GLU	GLY	ASN	ASN	ILE	ILE	ARG	ARG	ILE	TYR	ALA	ILE	THR	PRO	PRO	ASP	ASP	ARG	GLU	GLU	LEU	LEU	VAL	LEU	SER	SER	VAL	ASP
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● Molecule 1: ADP-ribosylating binary toxin binding subunit CdtB



ASN	ASN	ASN	PHE	THR	ASN	PHE	ALA	VAL	VAL	THR	THR	ASN	TYR	SER	ASP	TRP	GLU	ASP	E217	D218	E231	S259	D269	P270	K276	F281	D282	K283	L293	V294	M304	L308	T317	S324	K329	S330	K331	THR	GLU	SER	ASN	THR	ALA	GLY	VAL	SER	VAL	ASN	VAL	GLY	TYR	GLN	ASN																														
ASN	GLY	THR	ALA	VAL	THR	THR	ASN	HIS	THR	THR	ASP	S364	T365	A366	S370	T377	S380	A387	N392	V393	R394	D417	L444	S445	P446	L447	A448	I462	L470	L478	K490	M491	S492	S493	G494	Q495	S516	L545	K559	K560	D561	D568	D572	V576	F580	T584	L595	N602	N610	F619	F622	D623	D624	W632	N636	T637	T638	D641	S646	A647	N648	K649	L650	N651	G652	E653	T654	K655	I656	K657	L658	P659	M660	S661	E662	Y666	V670	D677	P678	L679	T680	S681	GLU
D561	D568	D572	V576	F580	T584	L595	N602	N610	F619	F622	D623	D624	W632	N636	T637	T638	D641	S646	A647	N648	K649	L650	N651	G652	E653	T654	K655	I656	K657	L658	P659	M660	S661	E662	Y666	V670	D677	P678	L679	T680	S681	GLU																																									
N682	S683	K687	E692	E693	K694	T695	D696	Y697	L698	V699	E701	Q702	Y709	E710	I714	E715	K716	D717	S718	S719	N720	E722	I723	I724	L725	I726	G727	S728	G729	I730	I731	S737	N742	SER	THR	PRO	GLU	ILE	LEU	ASP	PRO	GLU	VAL	GLY	ILE	LYS	PRO	GLN	GLU																																		
ILE	MET	ASP	ALA	HIS	LYS	ILE	TYR	PHE	ALA	ASP	ASN	PHE	ASN	PRO	THR	THR	GLY	ASN	THR	TYR	PHE	THR	GLY	GLY	ALA	PRO	THR	GLN	THR	THR	ASN	TYR	LYS	GLU	ALA	LEU	ASP	TYR	ILE	GLN	LEU	LEU	LEU	VAL	SER	SER	VAL	ASP	ILE	THR																																	
LYS	ASP	LYS	GLU	ARG	ASN	TYR	LEU	GLY	LYS	ASP	PRO	ASN	GLN	PRO	ASN	VAL	ASN	LEU	ARG	LEU	ARG	GLY	GLU	GLU	ASN	ILE	ASN	THR	THR	THR	THR	TYR	LYS	LYS	LYS	LEU	ARG	ILE	TYR	VAL	ASP	GLU	GLU	LEU	LEU	VAL	SER	SER	VAL	ASP																																	

● Molecule 2: ADP-ribosylating binary toxin enzymatic subunit CdtA



ALA	PRO	ILE	GLU	ARG	PRO	GLU	ASP	PHE	LEU	LYS	ASP	LYS	GLU	LYS	ALA	LYS	LYS	GLU	W19	E20	R21	K22	E23	A24	E25	R26	I27	E28	Q29	K30	R33	E40	D45	E48	I49	S50	R51	Y52	S53	Q54	T55	R56	M57	E70	D86	E109	E113	L116	F117	K118
F122	I126	D134	Y142	H157	L158	M166	T172	N173	M174	N175	S176	I179	R192	I193	V194	K198	H199	K202	Q29	V207	D215	N233	K234	L235	T236	P237	N238	E239	V243	N244	D245	Y246	M247	R248	G249	N255	N256	Y257	L258	I259	S260	N261	G262	P263	V264					
N265	N266	P267	N268	P269	E270	L271	D272	S273	K274	I275	I278	E279	N280	R284	I287	R295	T305	S308	D312	N318	F322	W326	L331	I337	S338	T339	F349	R352	L356	R357	I358	T359	I360	L369	S370	A371	I372	I373	P373	G374	Y375	A376	G377	E378						
F389	D395	T401	V407	P413	GLU	ASN	LEU	TYR	PHE	GLN	GLY	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS																													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100912	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 ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.510	Depositor
Minimum map value	-0.716	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.195	Depositor
Map size (\AA)	380.16, 380.16, 380.16	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.88, 0.88, 0.88	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.29	0/4001	0.49	0/5423
1	B	0.29	0/4001	0.49	0/5423
1	C	0.29	0/3933	0.49	0/5332
1	D	0.30	0/3966	0.50	0/5378
1	E	0.29	0/4001	0.49	0/5423
1	F	0.29	0/3933	0.49	0/5332
1	G	0.29	0/4001	0.49	0/5423
2	H	0.30	0/3269	0.48	0/4414
All	All	0.29	0/31105	0.49	0/42148

There are no bond length outliers.

There are no bond angle outliers.

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	3935	0	3835	43	0
1	B	3935	0	3835	42	0
1	C	3867	0	3766	53	0
1	D	3898	0	3786	56	0
1	E	3935	0	3835	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3867	0	3766	47	0
1	G	3935	0	3833	49	0
2	H	3200	0	3179	59	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
All	All	30593	0	29835	364	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 6.

The worst 5 of 364 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:TRP:HE3	2:H:21:ARG:NH2	1.54	1.04
2:H:19:TRP:HZ2	2:H:142:TYR:HH	1.08	1.02
2:H:19:TRP:HE3	2:H:21:ARG:HH21	0.89	0.85
2:H:19:TRP:CE3	2:H:21:ARG:NH2	2.42	0.84
1:G:670:VAL:HG22	1:G:710:GLU:HG2	1.63	0.80

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	500/675 (74%)	470 (94%)	30 (6%)	0	100	100
1	B	500/675 (74%)	481 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	490/675 (73%)	462 (94%)	28 (6%)	0	100	100
1	D	493/675 (73%)	468 (95%)	25 (5%)	0	100	100
1	E	500/675 (74%)	474 (95%)	26 (5%)	0	100	100
1	F	490/675 (73%)	470 (96%)	20 (4%)	0	100	100
1	G	500/675 (74%)	472 (94%)	28 (6%)	0	100	100
2	H	393/428 (92%)	382 (97%)	11 (3%)	0	100	100
All	All	3866/5153 (75%)	3679 (95%)	187 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/601 (74%)	440 (99%)	6 (1%)	69	91
1	B	446/601 (74%)	445 (100%)	1 (0%)	93	98
1	C	438/601 (73%)	436 (100%)	2 (0%)	88	96
1	D	441/601 (73%)	440 (100%)	1 (0%)	93	98
1	E	446/601 (74%)	435 (98%)	11 (2%)	47	80
1	F	438/601 (73%)	435 (99%)	3 (1%)	84	95
1	G	446/601 (74%)	441 (99%)	5 (1%)	73	92
2	H	355/385 (92%)	344 (97%)	11 (3%)	40	74
All	All	3456/4592 (75%)	3416 (99%)	40 (1%)	79	92

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	493[B]	SER
2	H	57	ASN
2	H	21	ARG
2	H	26	ARG

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Mol	Chain	Res	Type
2	H	174	ASN

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](#)

Of 21 ligands modelled in this entry, 21 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

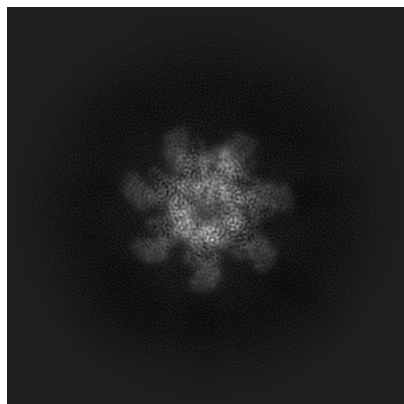
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34137. These allow visual inspection of the internal detail of the map and identification of artifacts.

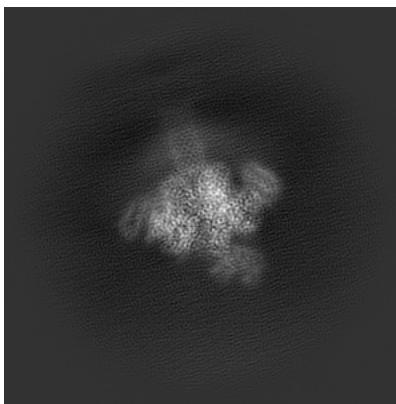
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

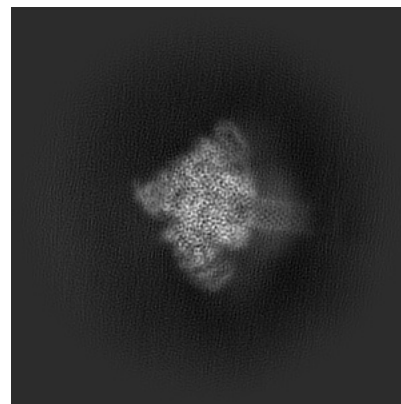
6.1.1 Primary map



X

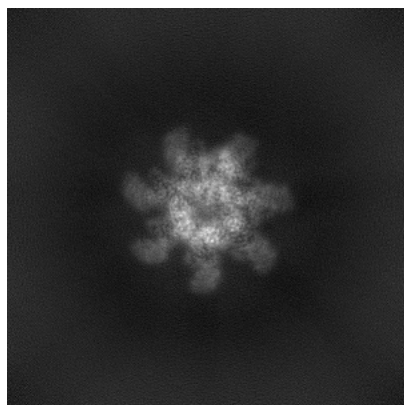


Y

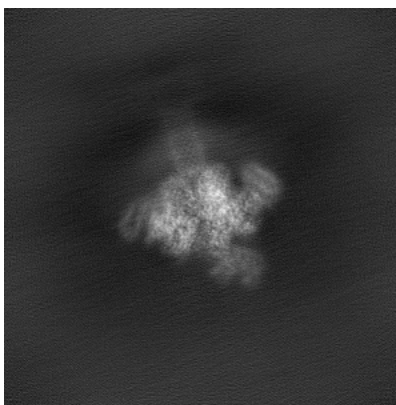


Z

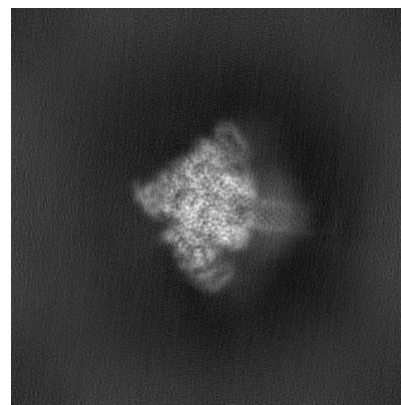
6.1.2 Raw map



X



Y

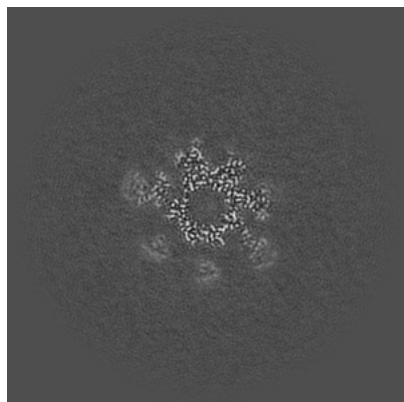


Z

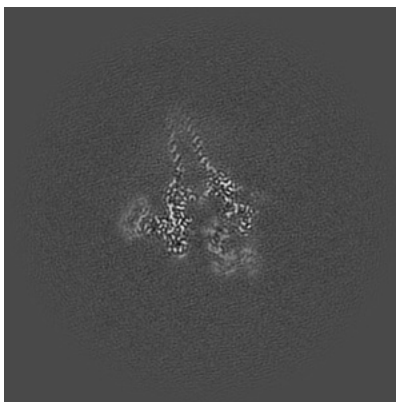
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

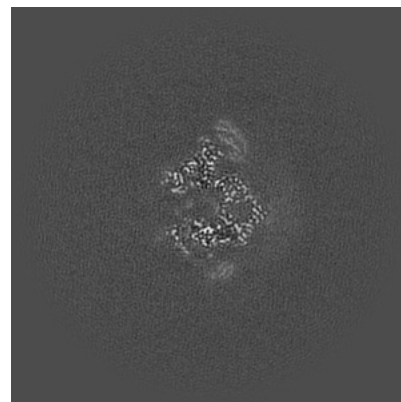
6.2.1 Primary map



X Index: 216

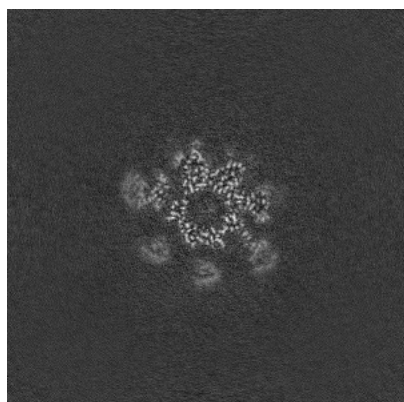


Y Index: 216

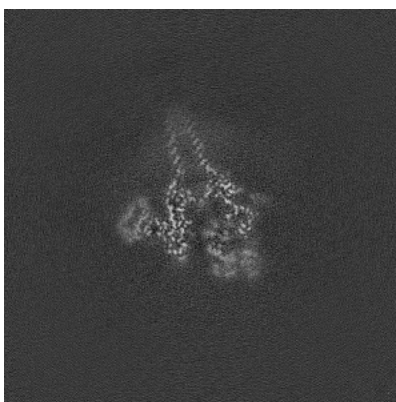


Z Index: 216

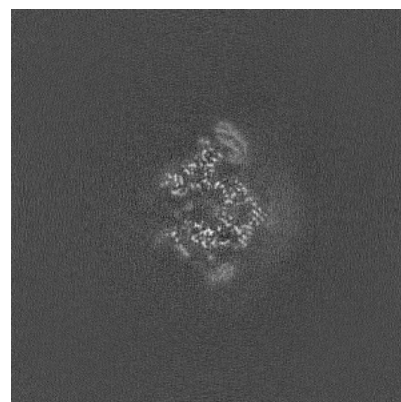
6.2.2 Raw map



X Index: 216



Y Index: 216

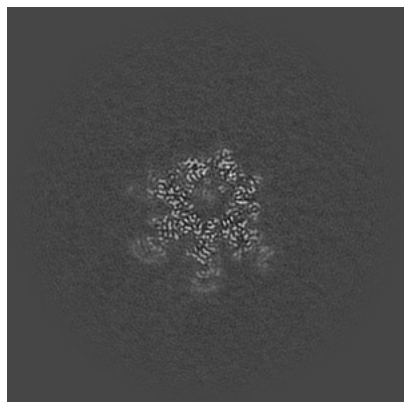


Z Index: 216

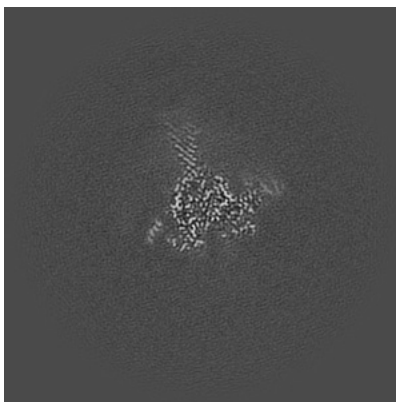
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

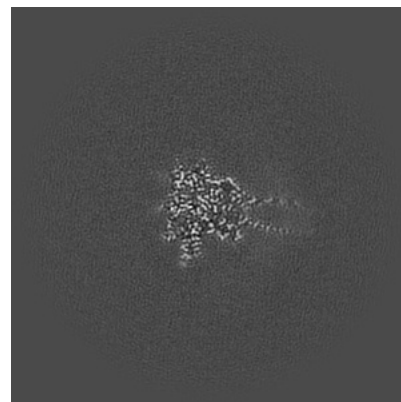
6.3.1 Primary map



X Index: 199

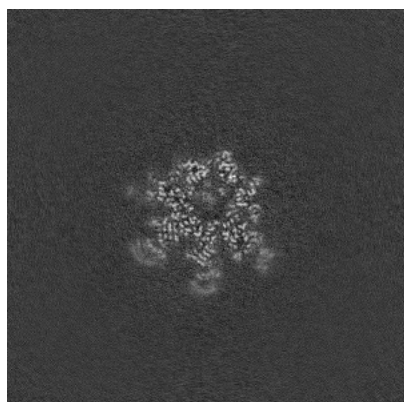


Y Index: 194

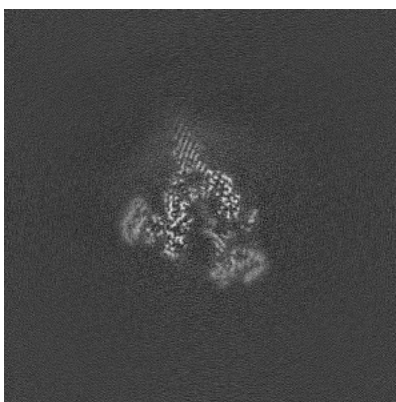


Z Index: 192

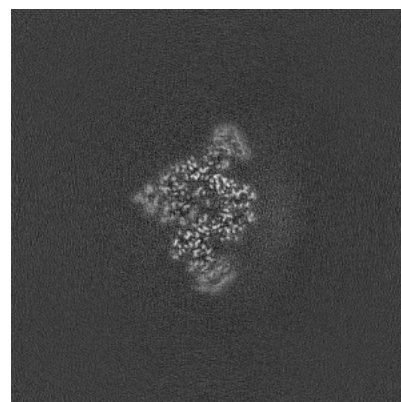
6.3.2 Raw map



X Index: 199



Y Index: 222

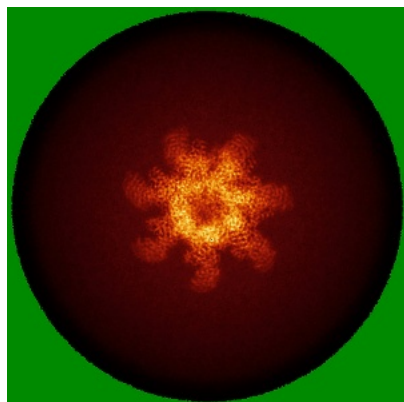


Z Index: 231

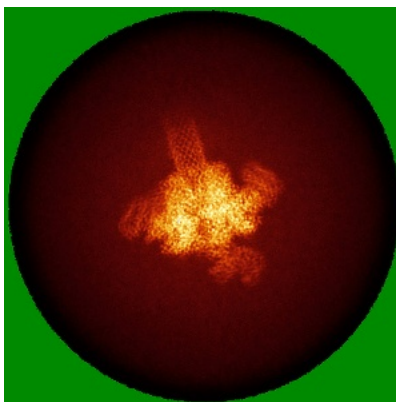
The images above show the largest variance slices of the map in three orthogonal directions.

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

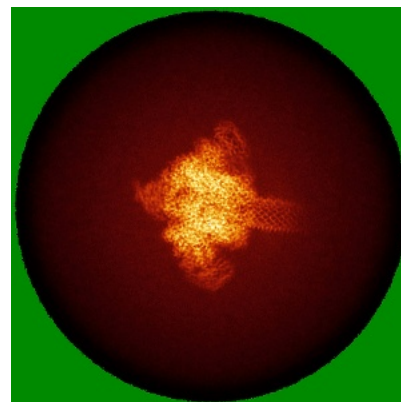
6.4.1 Primary map



X

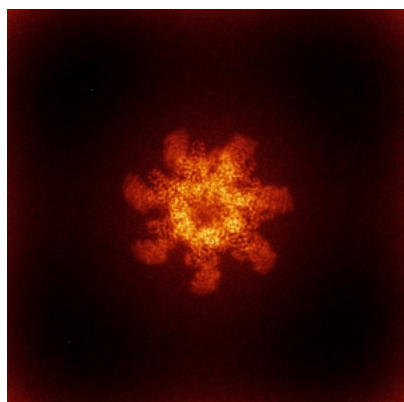


Y

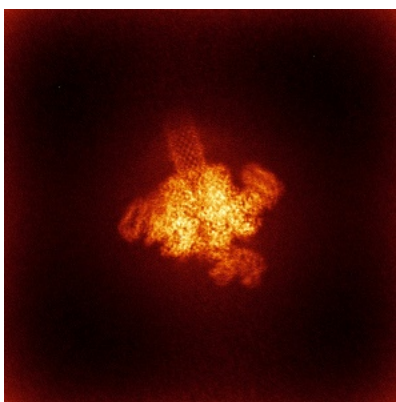


Z

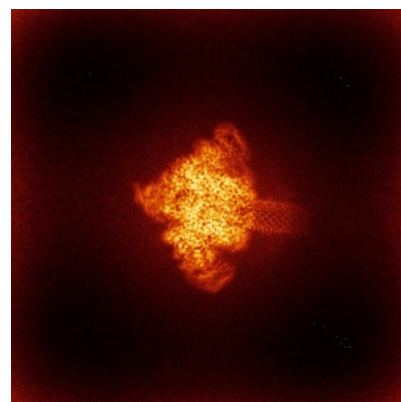
6.4.2 Raw map



X



Y

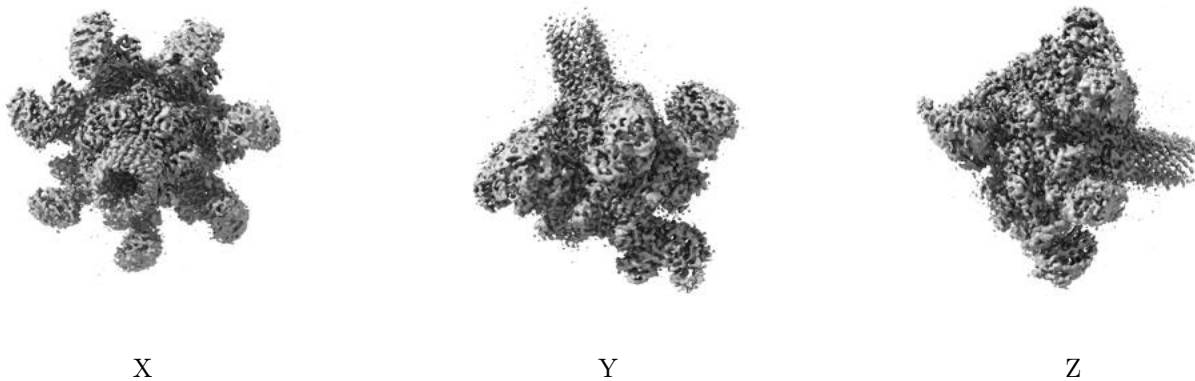


Z

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.

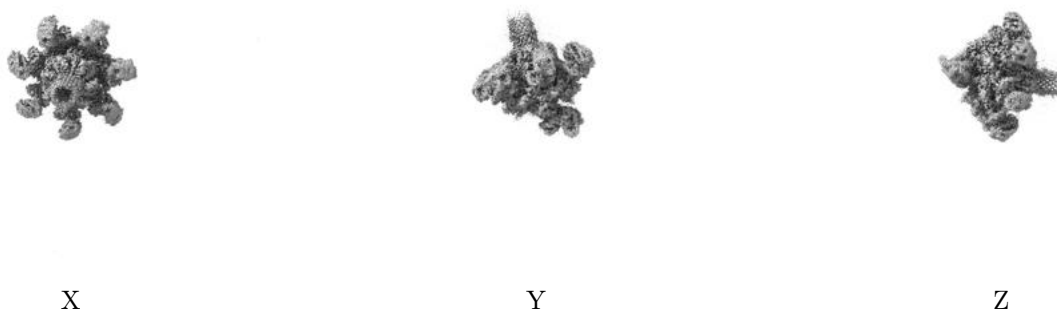
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.195. 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.

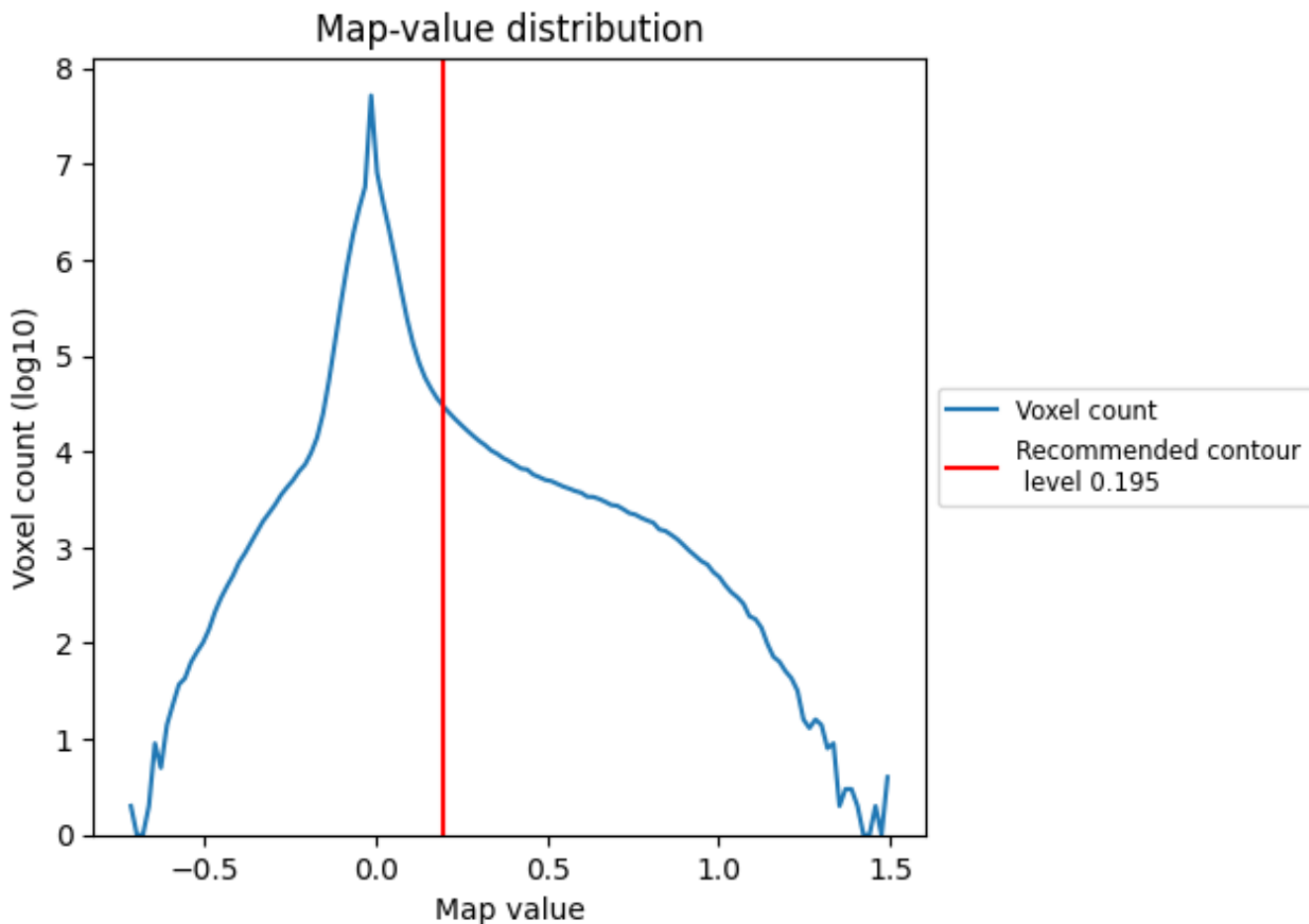
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

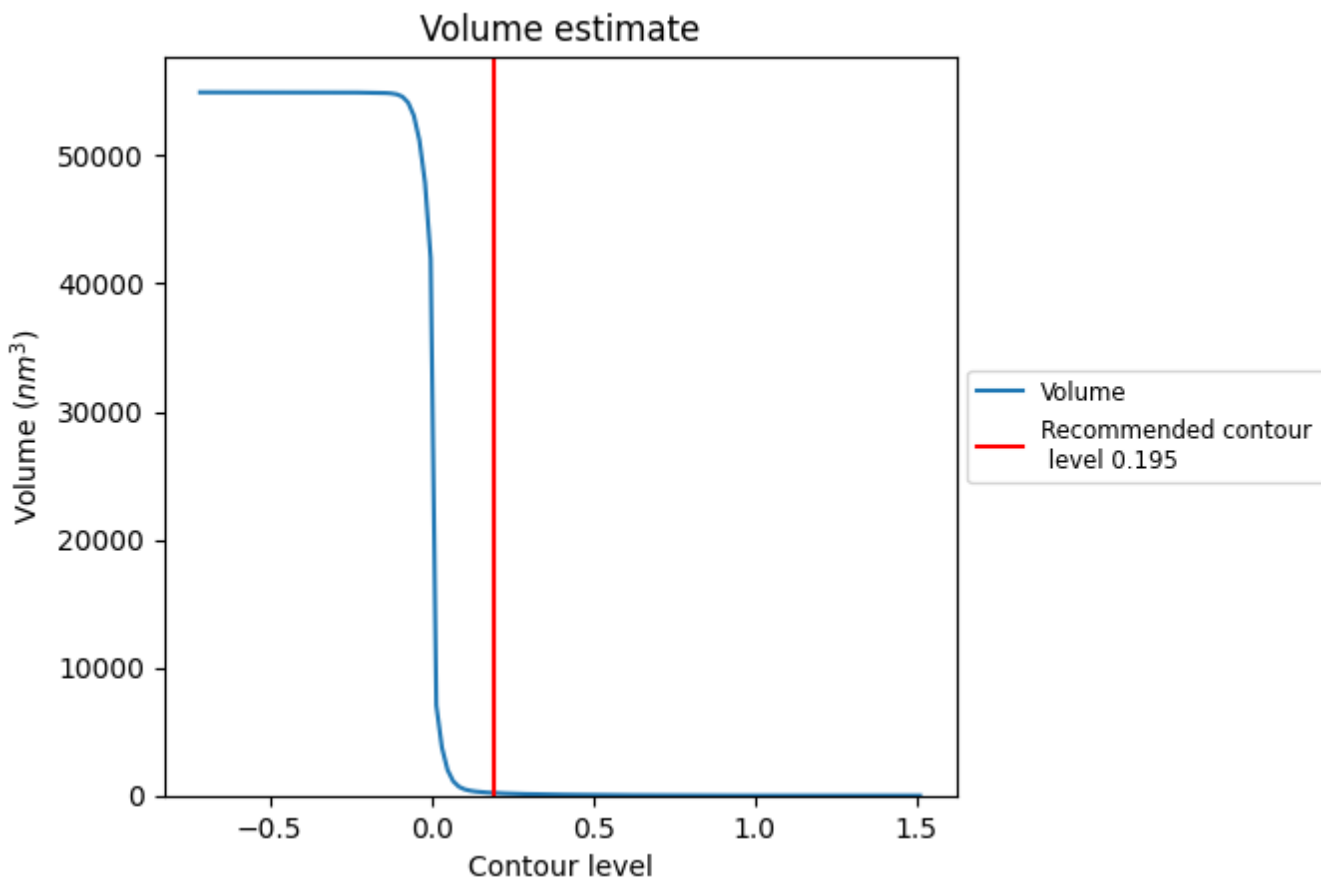
This section contains the results of statistical analysis of the map.

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.

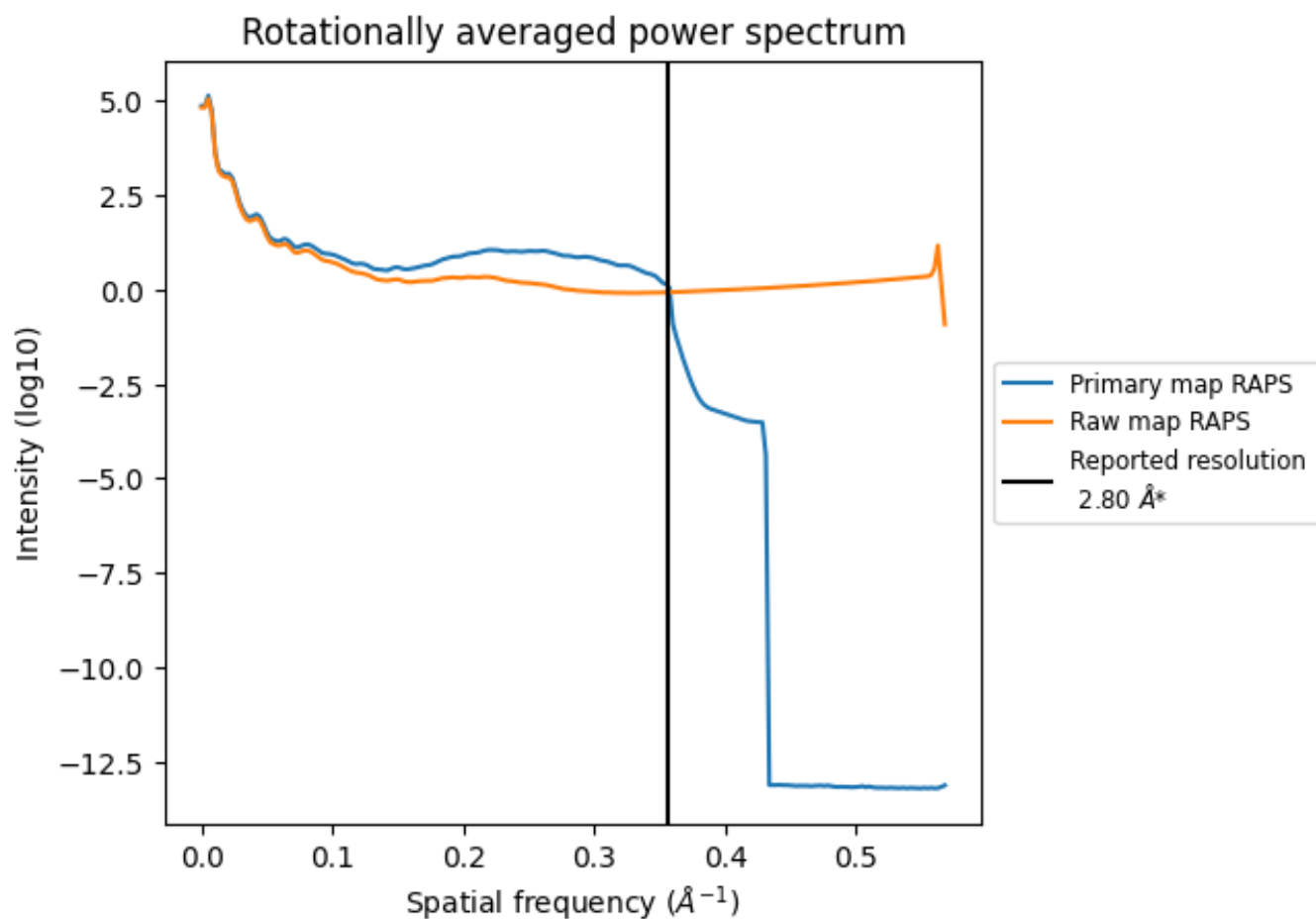
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 201 nm^3 ; this corresponds to an approximate mass of 182 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](#)

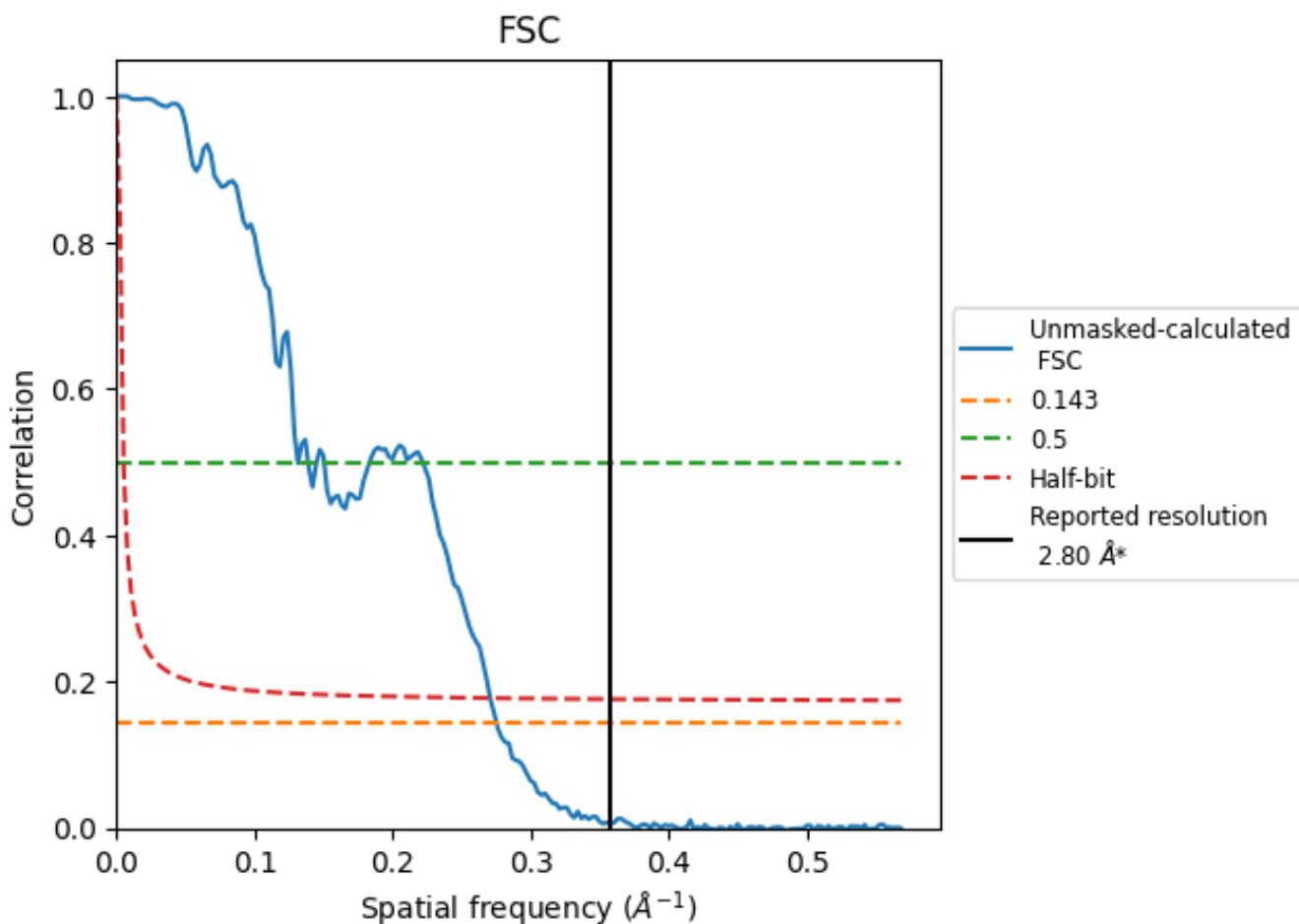


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

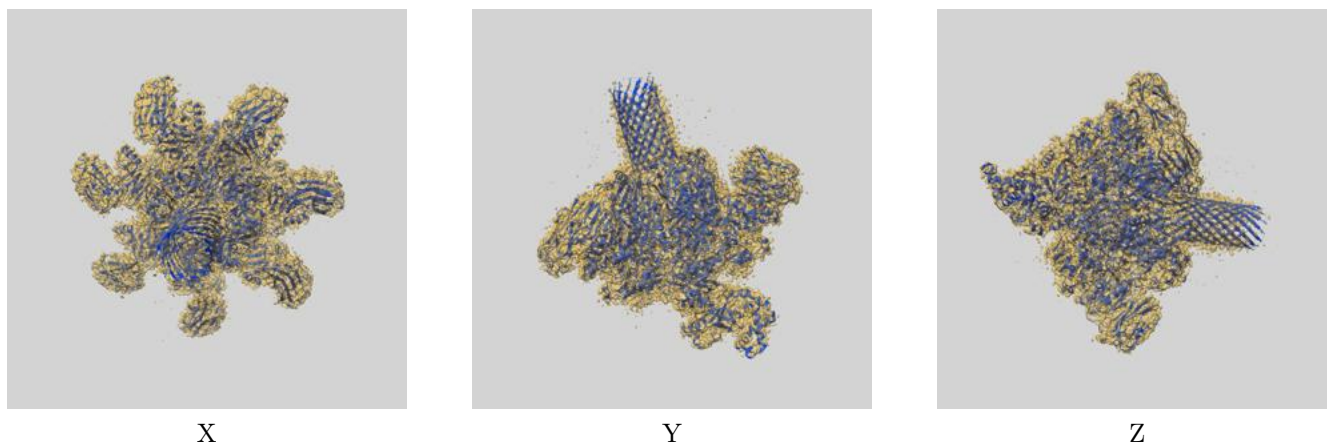
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.63	7.61	3.69

*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 3.63 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

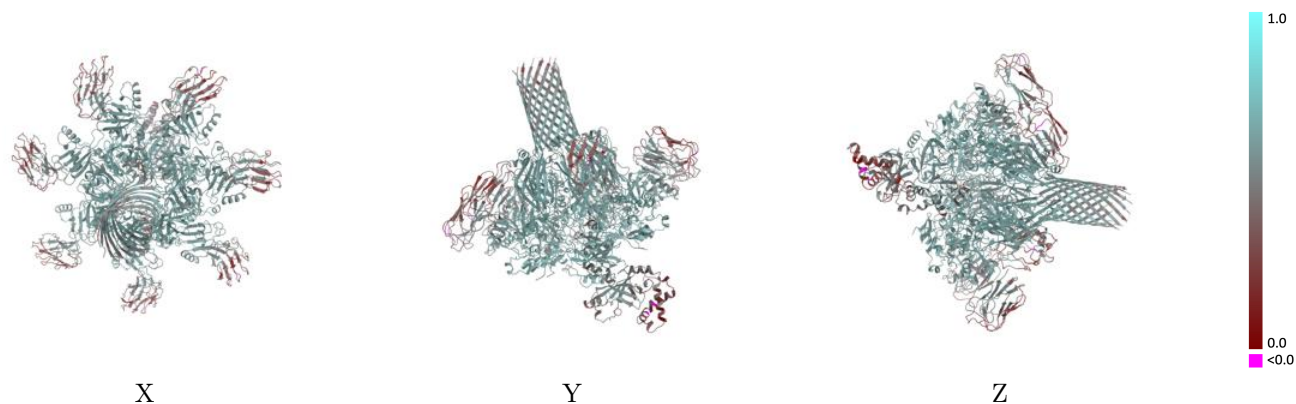
This section contains information regarding the fit between EMDB map EMD-34137 and PDB model 7YVS. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



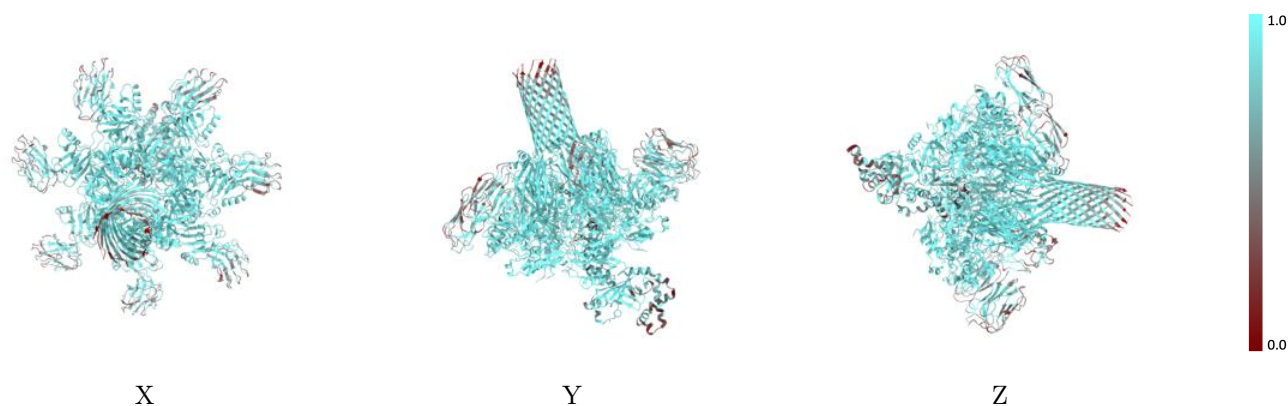
The images above show the 3D surface view of the map at the recommended contour level 0.195 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



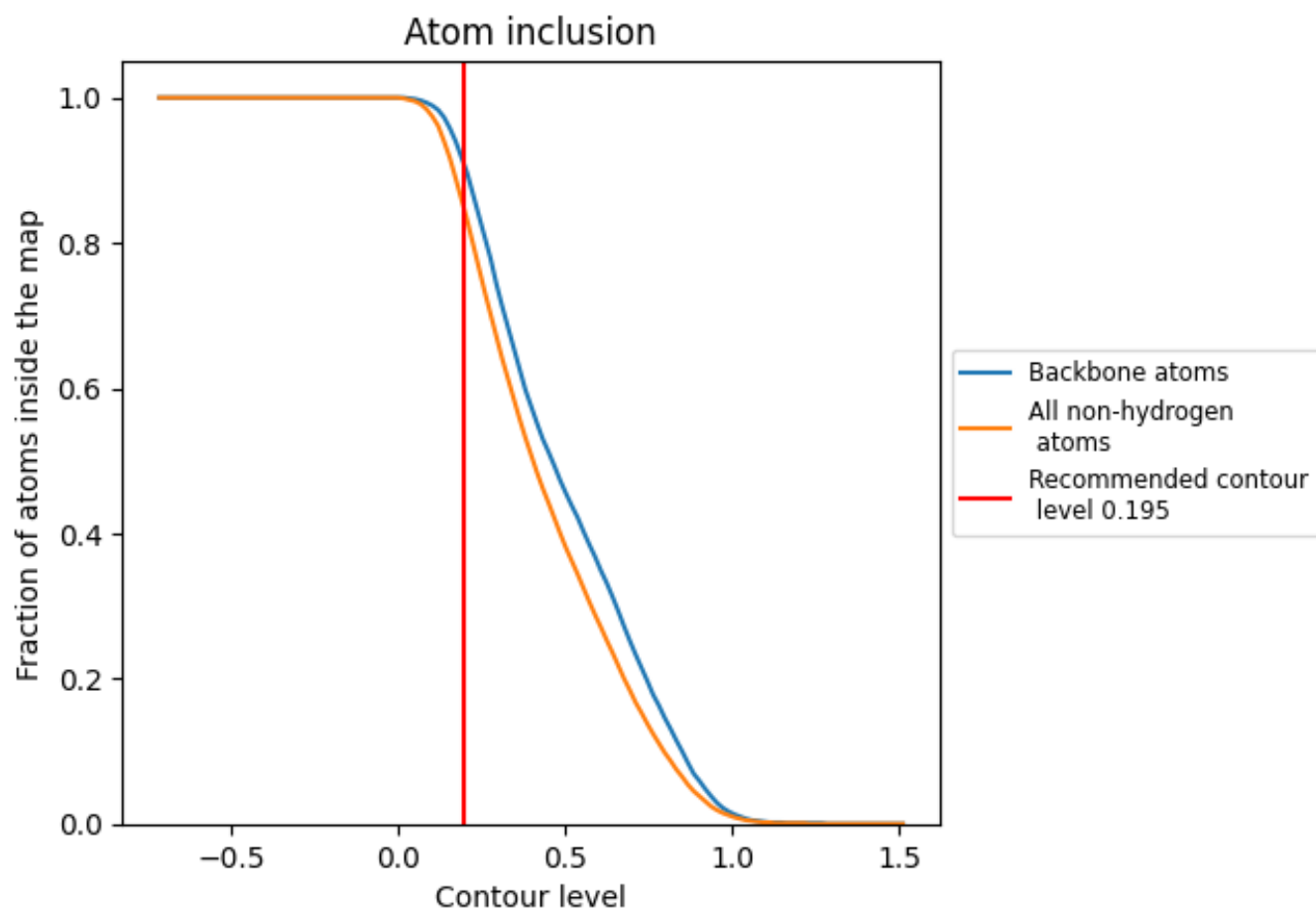
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.195).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.195) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.5490
A	 0.8450	 0.5540
B	 0.8610	 0.5590
C	 0.8600	 0.5590
D	 0.8620	 0.5600
E	 0.8560	 0.5540
F	 0.8580	 0.5540
G	 0.8550	 0.5570
H	 0.7850	 0.4860

