



# wwPDB EM Validation Summary Report ⓘ

Apr 13, 2026 – 04:30 pm BST

PDB ID : 9SKZ / pdb\_00009skz  
EMDB ID : EMD-54980  
Title : Cryo-EM structure of H. neapolitanus CsoSCA C283A/C284A inactive mutant, dimer, state 2  
Authors : Gaullier, G.; Vogiatzi, N.; Blikstad, C.  
Deposited on : 2025-09-02  
Resolution : 2.22 Å(reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

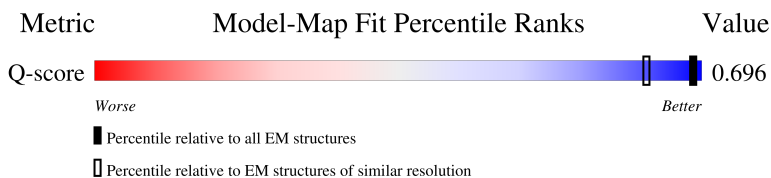
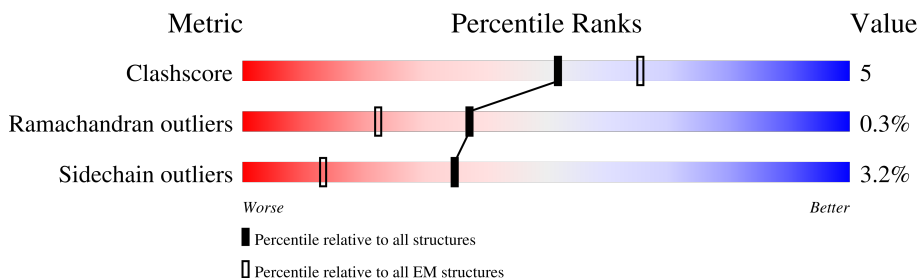
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.22 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	3277 ( 1.73 - 2.72 )

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  $\geq 3$ , 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	919	 44% 6% 49%
1	B	919	 43% 7% 49%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14647 atoms, of which 7032 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 Maltose/maltodextrin-binding periplasmic protein, Carboxysome shell carbonic anhydrase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	467	Total	C	H	N	O	S	0	0
			7184	2307	3516	655	697	9		
1	B	467	Total	C	H	N	O	S	0	0
			7184	2307	3516	655	697	9		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-404	MET	-	initiating methionine	UNP P0AEX9
A	-403	TRP	-	expression tag	UNP P0AEX9
A	-402	SER	-	expression tag	UNP P0AEX9
A	-401	HIS	-	expression tag	UNP P0AEX9
A	-400	PRO	-	expression tag	UNP P0AEX9
A	-399	GLN	-	expression tag	UNP P0AEX9
A	-398	PHE	-	expression tag	UNP P0AEX9
A	-397	GLU	-	expression tag	UNP P0AEX9
A	-396	LYS	-	expression tag	UNP P0AEX9
A	-395	GLY	-	expression tag	UNP P0AEX9
A	-394	SER	-	expression tag	UNP P0AEX9
A	-393	SER	-	expression tag	UNP P0AEX9
A	-392	MET	-	expression tag	UNP P0AEX9
A	-25	ASN	-	linker	UNP P0AEX9
A	-24	SER	-	linker	UNP P0AEX9
A	-23	SER	-	linker	UNP P0AEX9
A	-22	SER	-	linker	UNP P0AEX9
A	-21	ASN	-	linker	UNP P0AEX9
A	-20	ASN	-	linker	UNP P0AEX9
A	-19	ASN	-	linker	UNP P0AEX9
A	-18	ASN	-	linker	UNP P0AEX9
A	-17	ASN	-	linker	UNP P0AEX9
A	-16	ASN	-	linker	UNP P0AEX9
A	-15	ASN	-	linker	UNP P0AEX9
A	-14	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	ASN	-	linker	UNP P0AEX9
A	-12	ASN	-	linker	UNP P0AEX9
A	-11	LEU	-	linker	UNP P0AEX9
A	-10	GLY	-	linker	UNP P0AEX9
A	-9	ILE	-	linker	UNP P0AEX9
A	-8	GLU	-	linker	UNP P0AEX9
A	-7	GLU	-	linker	UNP P0AEX9
A	-6	ASN	-	linker	UNP P0AEX9
A	-5	LEU	-	linker	UNP P0AEX9
A	-4	TYR	-	linker	UNP P0AEX9
A	-3	PHE	-	linker	UNP P0AEX9
A	-2	GLN	-	linker	UNP P0AEX9
A	-1	SER	-	linker	UNP P0AEX9
A	0	ASN	-	linker	UNP P0AEX9
A	1	ALA	-	linker	UNP P0AEX9
A	283	ALA	CYS	engineered mutation	UNP O85042
A	284	ALA	CYS	engineered mutation	UNP O85042
B	-404	MET	-	initiating methionine	UNP P0AEX9
B	-403	TRP	-	expression tag	UNP P0AEX9
B	-402	SER	-	expression tag	UNP P0AEX9
B	-401	HIS	-	expression tag	UNP P0AEX9
B	-400	PRO	-	expression tag	UNP P0AEX9
B	-399	GLN	-	expression tag	UNP P0AEX9
B	-398	PHE	-	expression tag	UNP P0AEX9
B	-397	GLU	-	expression tag	UNP P0AEX9
B	-396	LYS	-	expression tag	UNP P0AEX9
B	-395	GLY	-	expression tag	UNP P0AEX9
B	-394	SER	-	expression tag	UNP P0AEX9
B	-393	SER	-	expression tag	UNP P0AEX9
B	-392	MET	-	expression tag	UNP P0AEX9
B	-25	ASN	-	linker	UNP P0AEX9
B	-24	SER	-	linker	UNP P0AEX9
B	-23	SER	-	linker	UNP P0AEX9
B	-22	SER	-	linker	UNP P0AEX9
B	-21	ASN	-	linker	UNP P0AEX9
B	-20	ASN	-	linker	UNP P0AEX9
B	-19	ASN	-	linker	UNP P0AEX9
B	-18	ASN	-	linker	UNP P0AEX9
B	-17	ASN	-	linker	UNP P0AEX9
B	-16	ASN	-	linker	UNP P0AEX9
B	-15	ASN	-	linker	UNP P0AEX9
B	-14	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	ASN	-	linker	UNP P0AEX9
B	-12	ASN	-	linker	UNP P0AEX9
B	-11	LEU	-	linker	UNP P0AEX9
B	-10	GLY	-	linker	UNP P0AEX9
B	-9	ILE	-	linker	UNP P0AEX9
B	-8	GLU	-	linker	UNP P0AEX9
B	-7	GLU	-	linker	UNP P0AEX9
B	-6	ASN	-	linker	UNP P0AEX9
B	-5	LEU	-	linker	UNP P0AEX9
B	-4	TYR	-	linker	UNP P0AEX9
B	-3	PHE	-	linker	UNP P0AEX9
B	-2	GLN	-	linker	UNP P0AEX9
B	-1	SER	-	linker	UNP P0AEX9
B	0	ASN	-	linker	UNP P0AEX9
B	1	ALA	-	linker	UNP P0AEX9
B	283	ALA	CYS	engineered mutation	UNP O85042
B	284	ALA	CYS	engineered mutation	UNP O85042

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

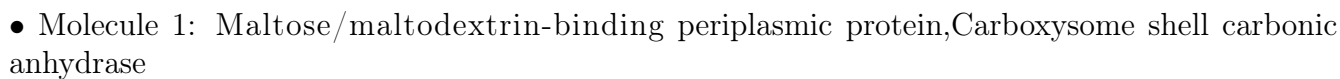
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	135	Total	O	0
			135	135	
3	B	142	Total	O	0
			142	142	



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Carboxysome shell carbonic anhydrase



Q500	S287	S148	SER	VAL	ILE	GLU	GLY	ALA	ILE	PRO	PHE	ALA	ILE	PRO	MET
A514	I288	E149	SER	SER	ASN	GLY	TRP	PHE	ALA	GLN	TYR	GLN	VAL	GLN	TRP
	L293	K150	VAL	VAL	ALA	ALA	TRP	TYR	GLU	ALA	GLU	ALA	ALA	ALA	HIS
	S309	D151	LYS	LYS	GLY	VAL	SER	ASN	LEU	THR	ASN	LEU	THR	THR	GLN
	N321	H166	ARG	ARG	GLN	ASN	ASN	GLY	GLY	ASP	GLY	GLY	ASP	GLY	PHE
	R337	I170	ASP	ASP	THR	ASP	THR	TYR	ILE	LYS	TYR	TYR	PRO	GLY	LYS
	H341	K179	ILE	ILE	ASP	PRO	SER	ILE	ASN	LYS	ILE	ASN	ILE	ASP	SER
	S350	L182	GLU	GLU	GLY	LEU	GLY	VAL	LYS	LEU	ASP	ASP	ILE	ILE	SER
	D351	T191	ALA	ALA	LYS	VAL	TYR	GLY	VAL	ASN	GLY	PRO	THR	PHE	ILE
	G352	A192	ASN	ASN	ALA	LEU	VAL	VAL	ASP	GLY	ASP	HIS	ASP	GLY	GLY
	H353	F193	PRO	PRO	GLN	LYS	THR	THR	ASN	THR	ASN	PRO	PRO	ARG	LYS
	N357	T194	ALA	ALA	ASN	TYR	ASN	GLY	GLY	PRO	GLY	GLY	THR	VAL	VAL
	N375	Y195	ASP	ASP	SER	GLU	SER	THR	THR	ASP	LYS	ILE	GLY	ILE	TRP
	N375	Y199	ARG	ARG	SER	GLU	SER	PHE	GLU	THR	ALA	GLU	LEU	TYR	TRP
	D380	A200	HIS	HIS	ASN	GLY	ASN	GLY	GLY	ALA	GLY	ALA	LEU	ALA	GLY
	Y381	G201	PRO	PRO	ASN	LEU	ASN	ASN	LEU	GLY	GLY	GLY	LEU	ALA	TYR
	N384	S202	ALA	ALA	ASN	ASN	ASN	THR	LEU	VAL	ASP	LYS	ALA	ALA	ASN
	R385	M203	CYS	CYS	ASN	ASP	PRO	PHE	LEU	LYS	GLY	LYS	THR	GLY	GLY
	R389	F204	ILE	ILE	ASN	PRO	SER	VAL	ASN	ALA	ASN	ALA	PRO	ALA	GLY
	Y390	D209	THR	THR	ASN	ARG	ASN	VAL	VAL	ASP	VAL	LYS	LEU	LEU	GLY
	D394	R222	GLU	GLU	ASN	ILE	PRO	ASN	ASN	PRO	ASP	LYS	ALA	ALA	TYR
	H397	E223	ARG	ARG	ASN	ALA	PHE	LEU	ILE	GLY	LEU	GLY	ILE	GLY	ASN
	A398	G224	GLY	GLY	ASN	THR	GLY	GLY	THR	VAL	LYS	LYS	THR	LEU	ASN
	E399	V225	ILE	ILE	ASN	MET	VAL	ASN	ALA	ASN	ASN	ALA	PRO	ALA	GLY
	F408	T228	GLY	GLY	ASN	ASN	SER	GLY	LYS	LEU	HIS	LYS	ASP	VAL	VAL
	D409	A229	ASN	ASN	GLY	ASN	ALA	ALA	LYS	ALA	MET	LYS	ALA	GLY	GLY
	E410	D230	GLY	GLY	GLN	GLN	GLY	ASN	ILE	ILE	ASN	GLN	PHE	PHE	LYS
	Y411	K237	LEU	LEU	TYR	GLY	ASN	ASP	THR	THR	MET	LYS	ASP	PHE	PHE
	R421	V240	PHE	PHE	GLN	ILE	ALA	ASP	ALA	ALA	PHE	LYS	LEU	LYS	LYS
	L422	S246	GLN	GLN	SER	MET	PRO	TYR	ASN	PRO	TYR	ASN	TYR	THR	THR
	A429	H250	ALA	ALA	THR	THR	LEU	THR	GLY	GLY	GLY	GLY	ASP	VAL	VAL
	R446	S258	ASN	ASN	ARG	SER	GLY	PHE	ALA	ALA	PHE	ALA	VAL	VAL	VAL
	R457	L264	ASN	ASN	THR	SER	LEU	THR	GLY	GLY	THR	THR	ARG	ARG	HIS
	T469	A267	LYS	LYS	GLN	TYR	THR	GLY	TYR	GLY	GLY	ASN	PRO	PRO	ASP
	R475	L268	ARG	ARG	ALA	VAL	THR	THR	ALA	THR	THR	GLY	GLY	LYS	LYS
	I476	T269	ALA	ALA	ARG	VAL	THR	THR	TYR	LEU	THR	ALA	ILE	ILE	GLY
	R483	E276	PRO	PRO	ALA	THR	ARG	LEU	THR	LEU	THR	ALA	ASP	GLY	GLY
			PHE	PHE	GLY	VAL	ALA	THR	ALA	THR	ILE	ASN	TYR	LYS	PRO

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	525107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	68.973	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.642	Depositor
Minimum map value	-0.391	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.83	1/3744 (0.0%)	1.32	19/5080 (0.4%)
1	B	0.85	0/3744	1.31	23/5080 (0.5%)
All	All	0.84	1/7488 (0.0%)	1.32	42/10160 (0.4%)

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	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	ARG	NE-CZ	-5.26	1.27	1.33

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	ARG	NE-CZ-NH1	-9.37	112.13	121.50
1	A	88	LEU	CA-C-N	-9.28	109.68	122.57
1	A	88	LEU	C-N-CA	-9.28	109.68	122.57
1	B	88	LEU	CA-C-N	-8.27	111.07	122.57
1	B	88	LEU	C-N-CA	-8.27	111.07	122.57

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	GLY	Peptide
1	A	457	ARG	Sidechain
1	A	496	ARG	Sidechain
1	A	72	ARG	Sidechain
1	B	50	ARG	Sidechain

## 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	3668	3516	3601	37	0
1	B	3668	3516	3601	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	135	0	0	6	0
3	B	142	0	0	5	0
All	All	7615	7032	7202	79	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 5.

The worst 5 of 79 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:399:GLU:OE2	3:A:2101:HOH:O	1.99	0.80
1:B:399:GLU:OE2	3:B:2101:HOH:O	2.00	0.79
1:A:173:CYS:HB2	1:A:201:GLY:O	1.86	0.76
1:B:422:LEU:C	1:B:422:LEU:HD23	2.17	0.69
1:B:209:ASP:OD2	1:B:237:LYS:NZ	2.25	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	465/919 (51%)	448 (96%)	16 (3%)	1 (0%)	43	50
1	B	465/919 (51%)	450 (97%)	13 (3%)	2 (0%)	30	33
All	All	930/1838 (51%)	898 (97%)	29 (3%)	3 (0%)	37	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	SER
1	B	258	SER
1	B	411	VAL

### 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	388/759 (51%)	378 (97%)	10 (3%)	40	53
1	B	388/759 (51%)	373 (96%)	15 (4%)	28	37
All	All	776/1518 (51%)	751 (97%)	25 (3%)	35	45

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	191	THR
1	B	225	VAL
1	B	475	ARG

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Mol	Chain	Res	Type
1	B	209	ASP
1	B	287	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	HIS
1	B	421	HIS
1	B	212	GLN
1	B	461	ASN
1	B	341	HIS

### 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](#)

Of 2 ligands modelled in this entry, 2 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.

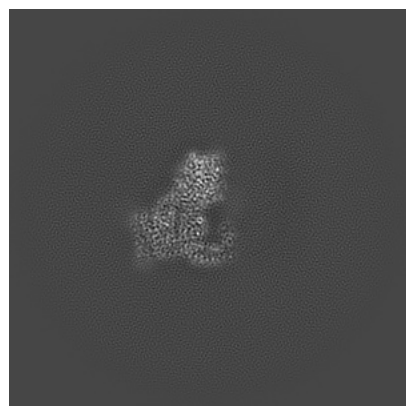
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54980. These allow visual inspection of the internal detail of the map and identification of artifacts.

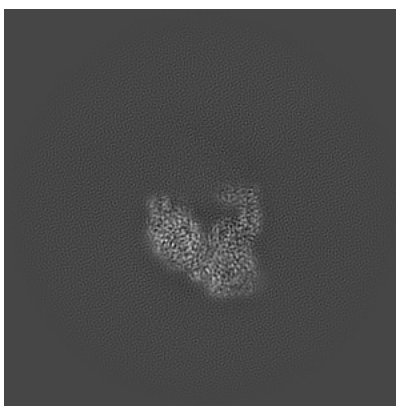
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

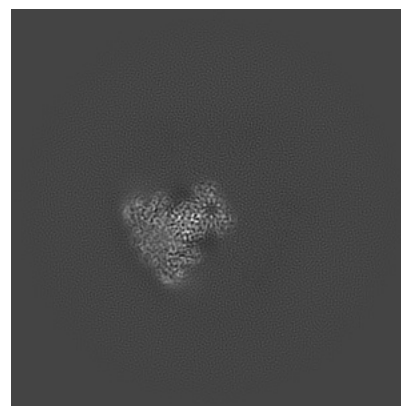
#### 6.1.1 Primary map



X

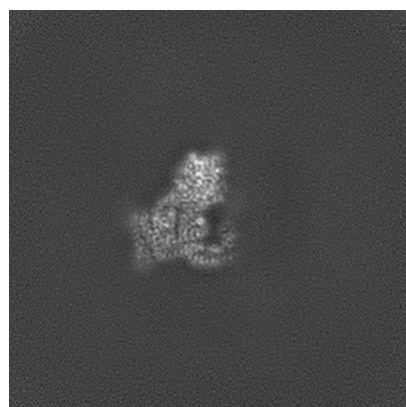


Y

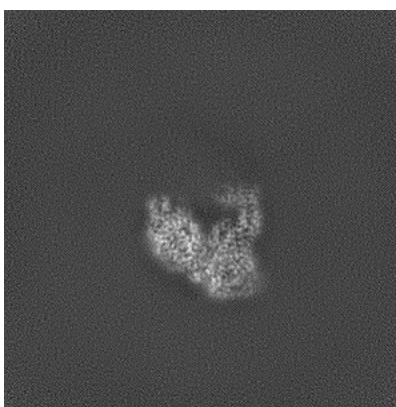


Z

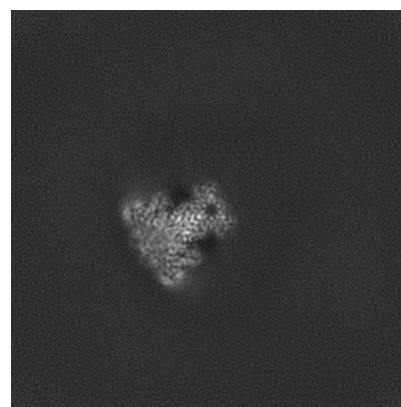
#### 6.1.2 Raw map



X



Y

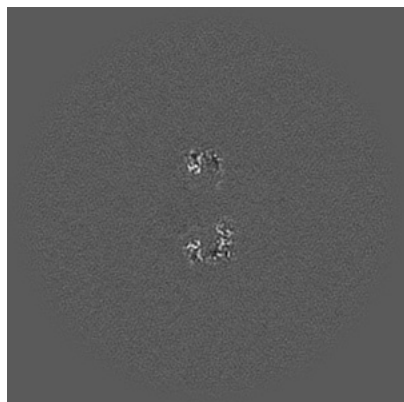


Z

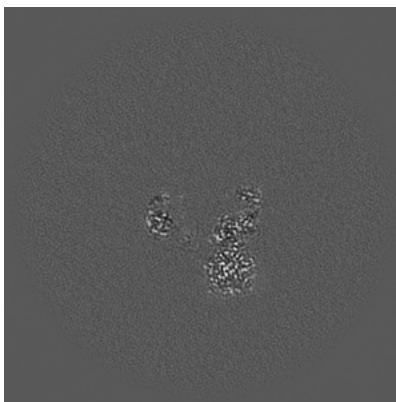
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

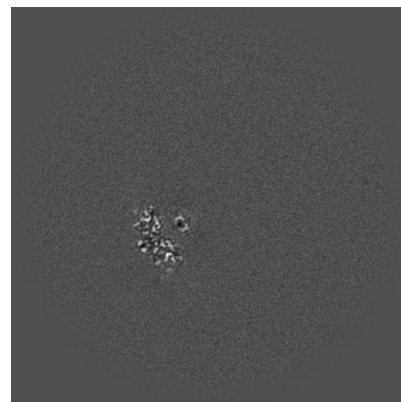
### 6.2.1 Primary map



X Index: 240

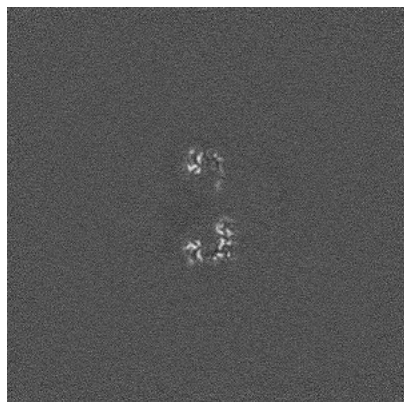


Y Index: 240

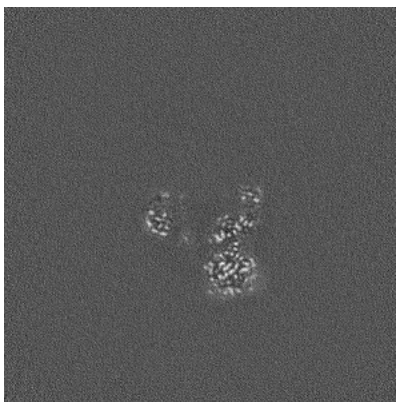


Z Index: 240

### 6.2.2 Raw map



X Index: 240



Y Index: 240



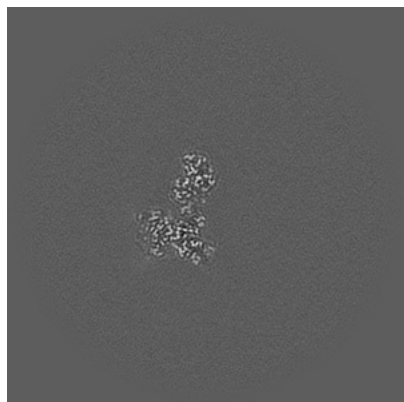
Z Index: 240

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

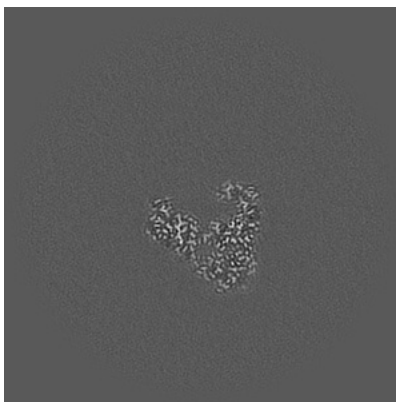


## 6.3 Largest variance slices [i](#)

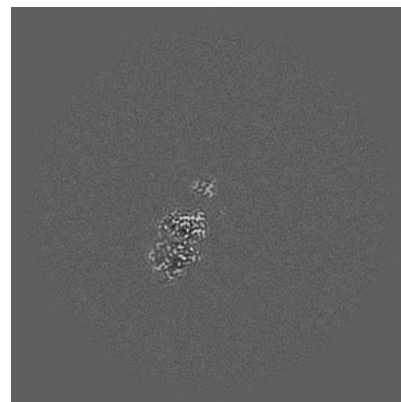
### 6.3.1 Primary map



X Index: 209

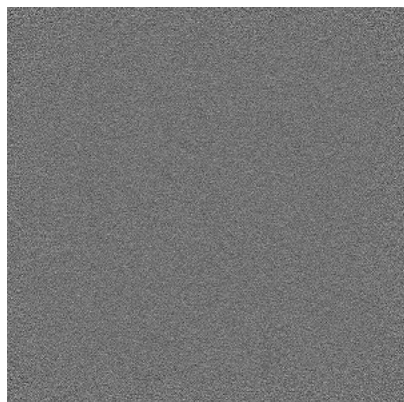


Y Index: 226

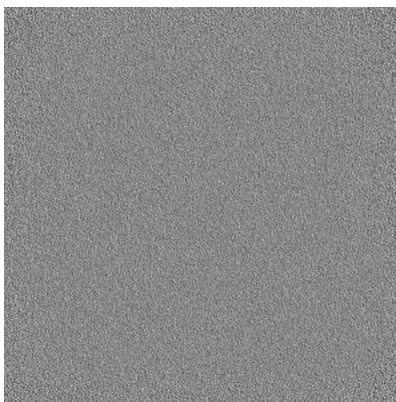


Z Index: 210

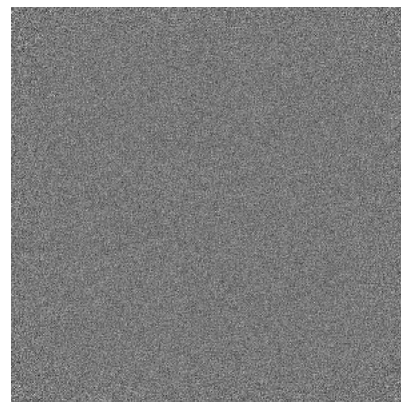
### 6.3.2 Raw map



X Index: 0



Y Index: 0



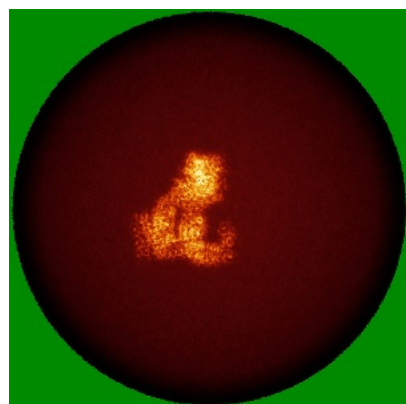
Z Index: 0

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

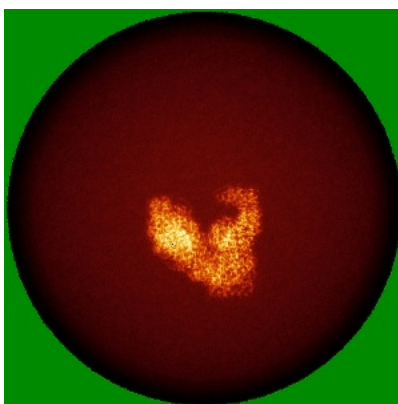


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

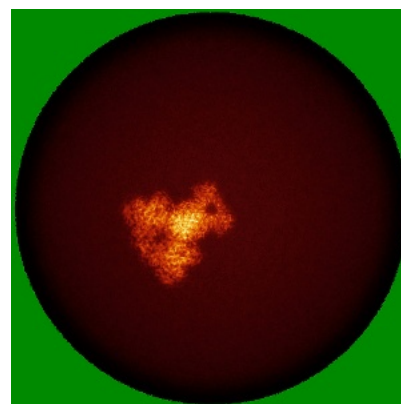
### 6.4.1 Primary map



X

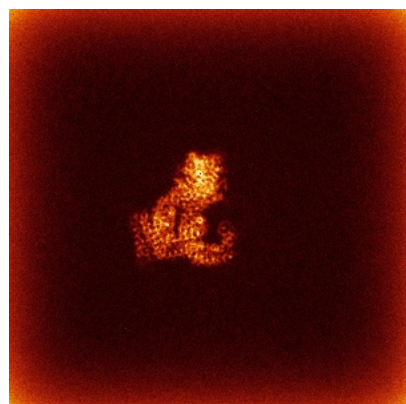


Y

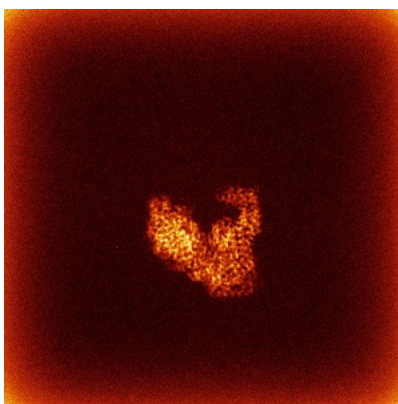


Z

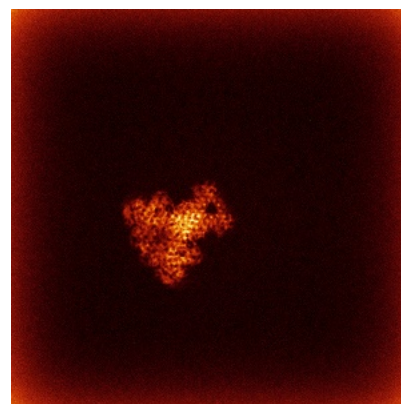
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



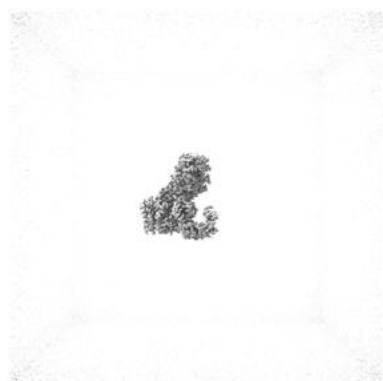
Y



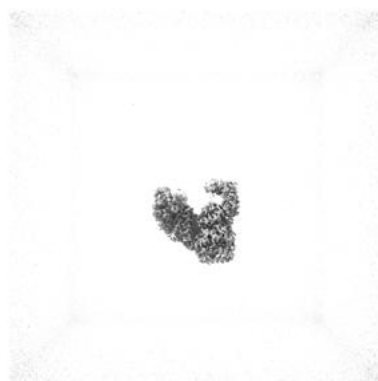
Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

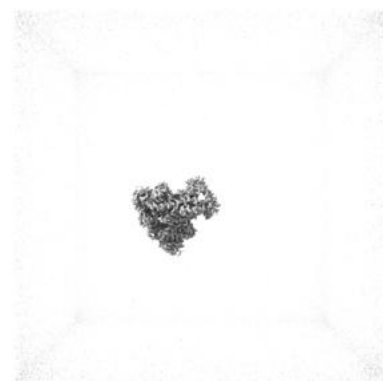
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

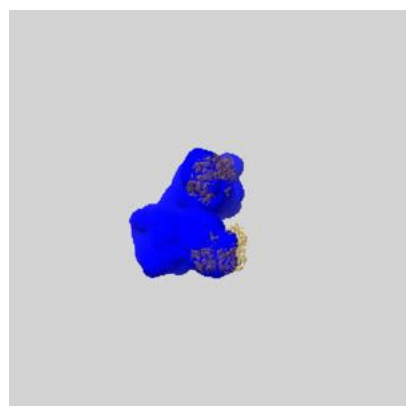
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

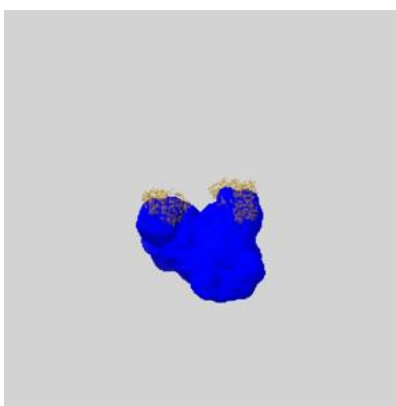
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

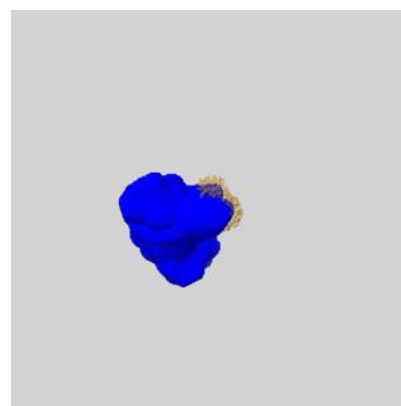
### 6.6.1 emd\_54980\_msk\_1.map [i](#)



X

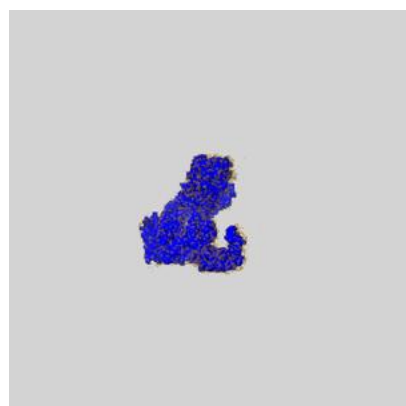


Y

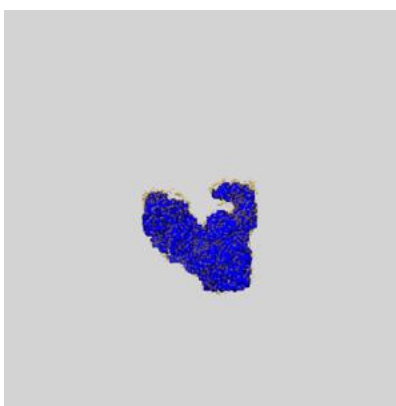


Z

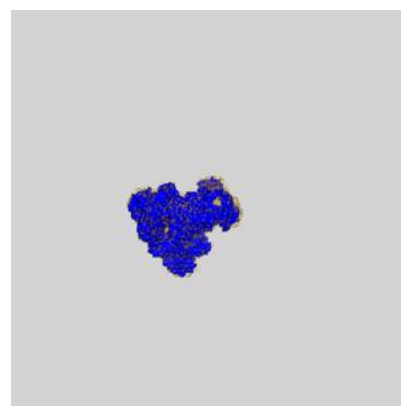
### 6.6.2 emd\_54980\_msk\_2.map [i](#)



X



Y

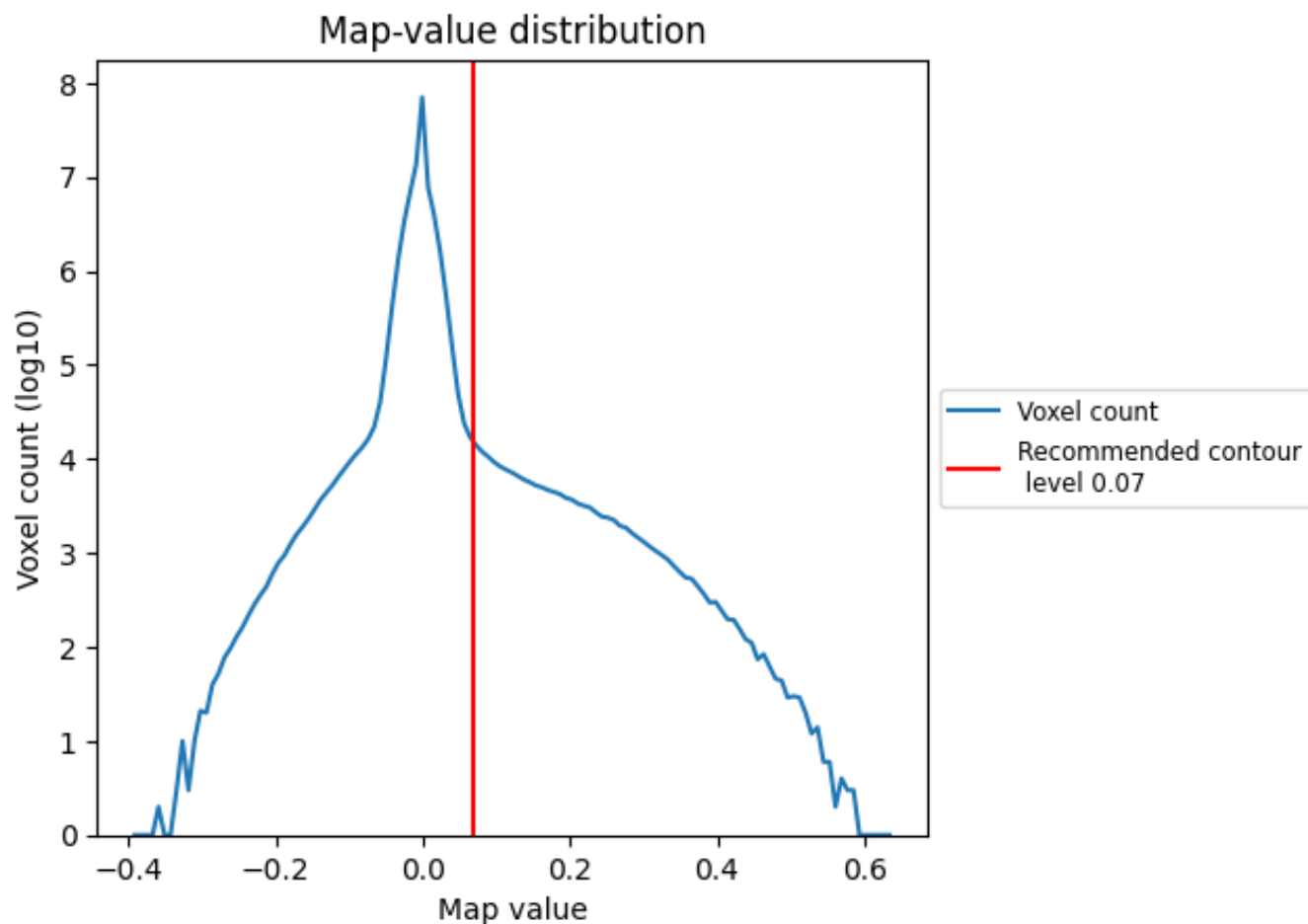


Z

## 7 Map analysis [i](#)

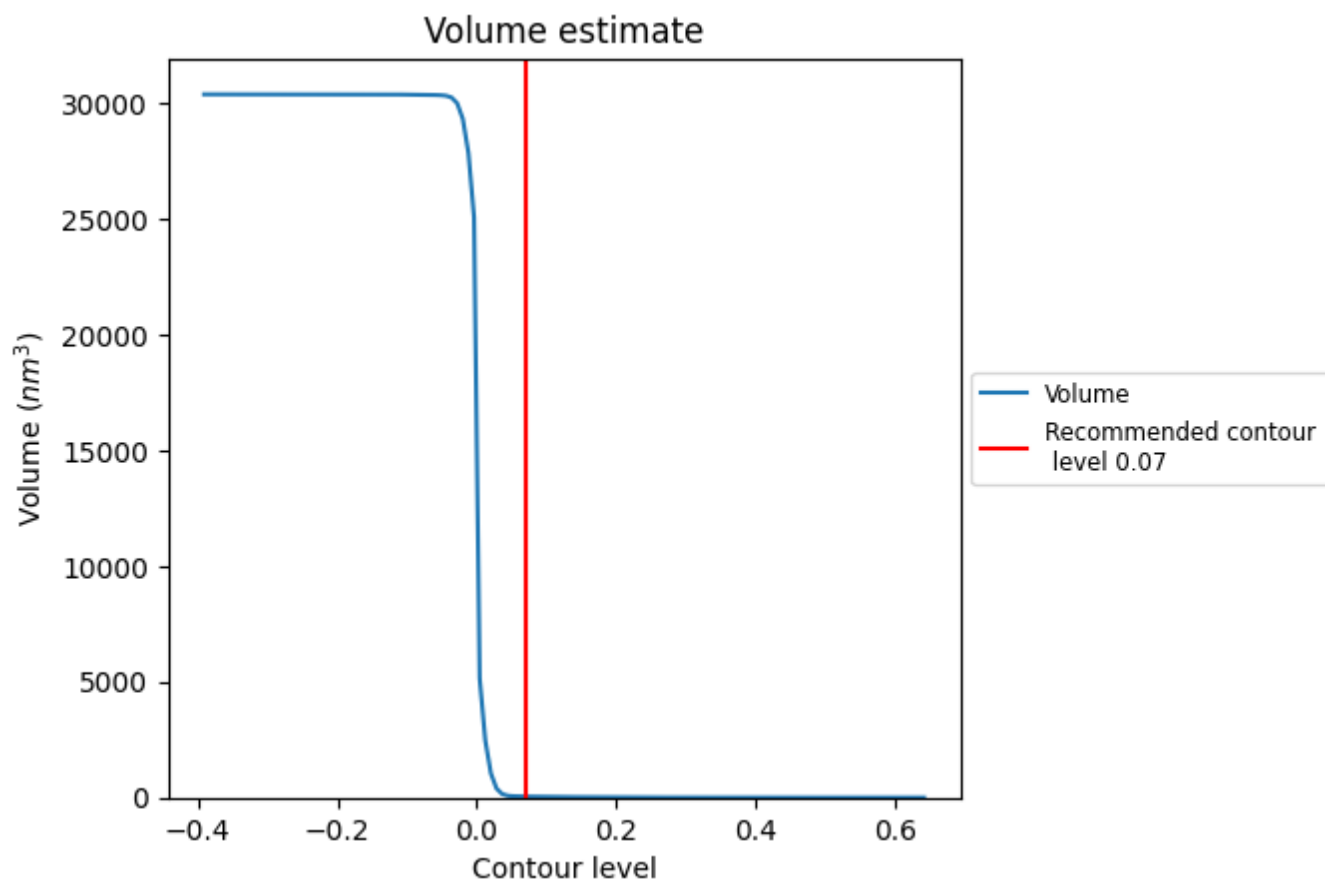
This section contains the results of statistical analysis of the map.

### 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.

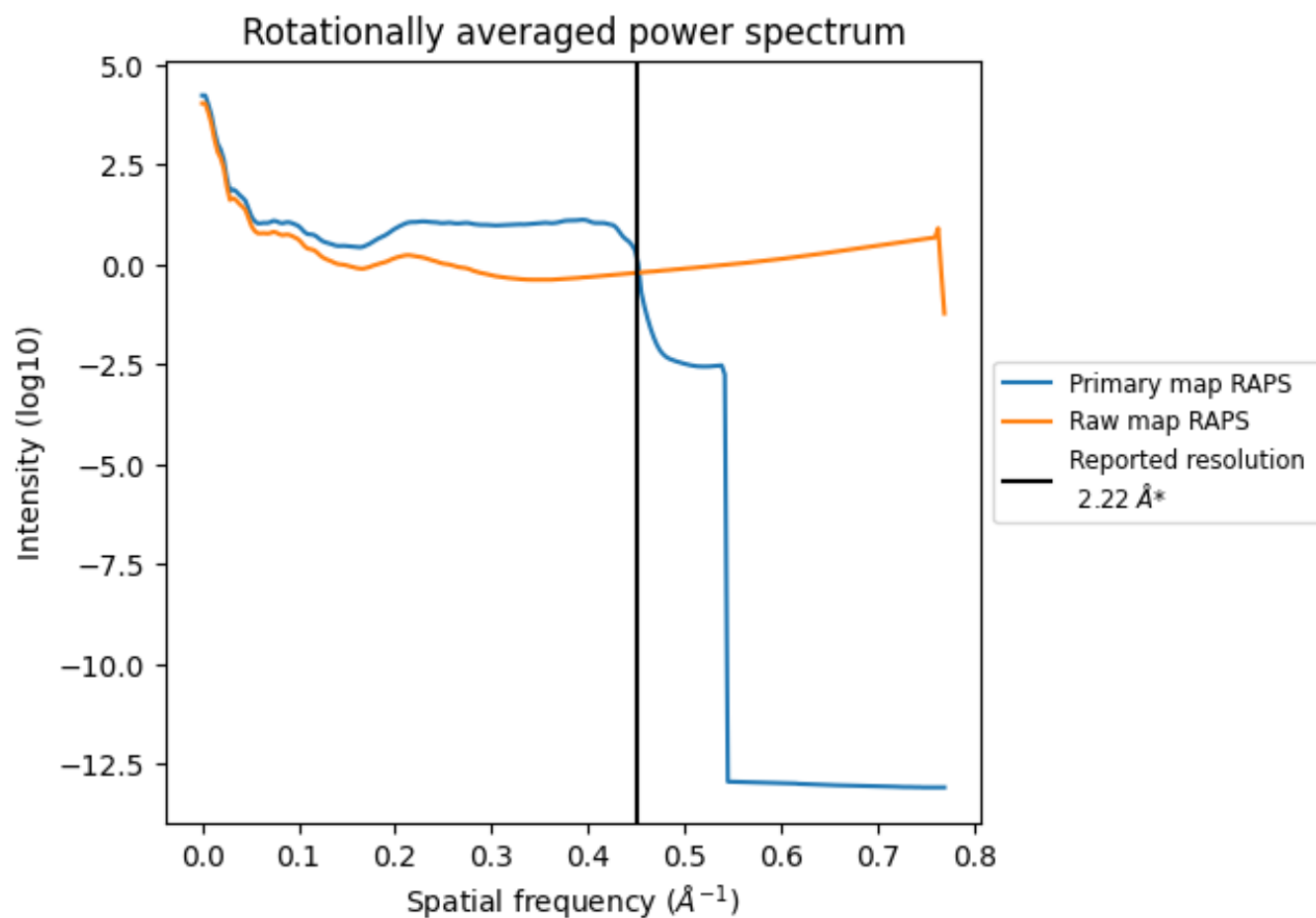
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm<sup>3</sup>; this corresponds to an approximate mass of 40 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 ⓘ

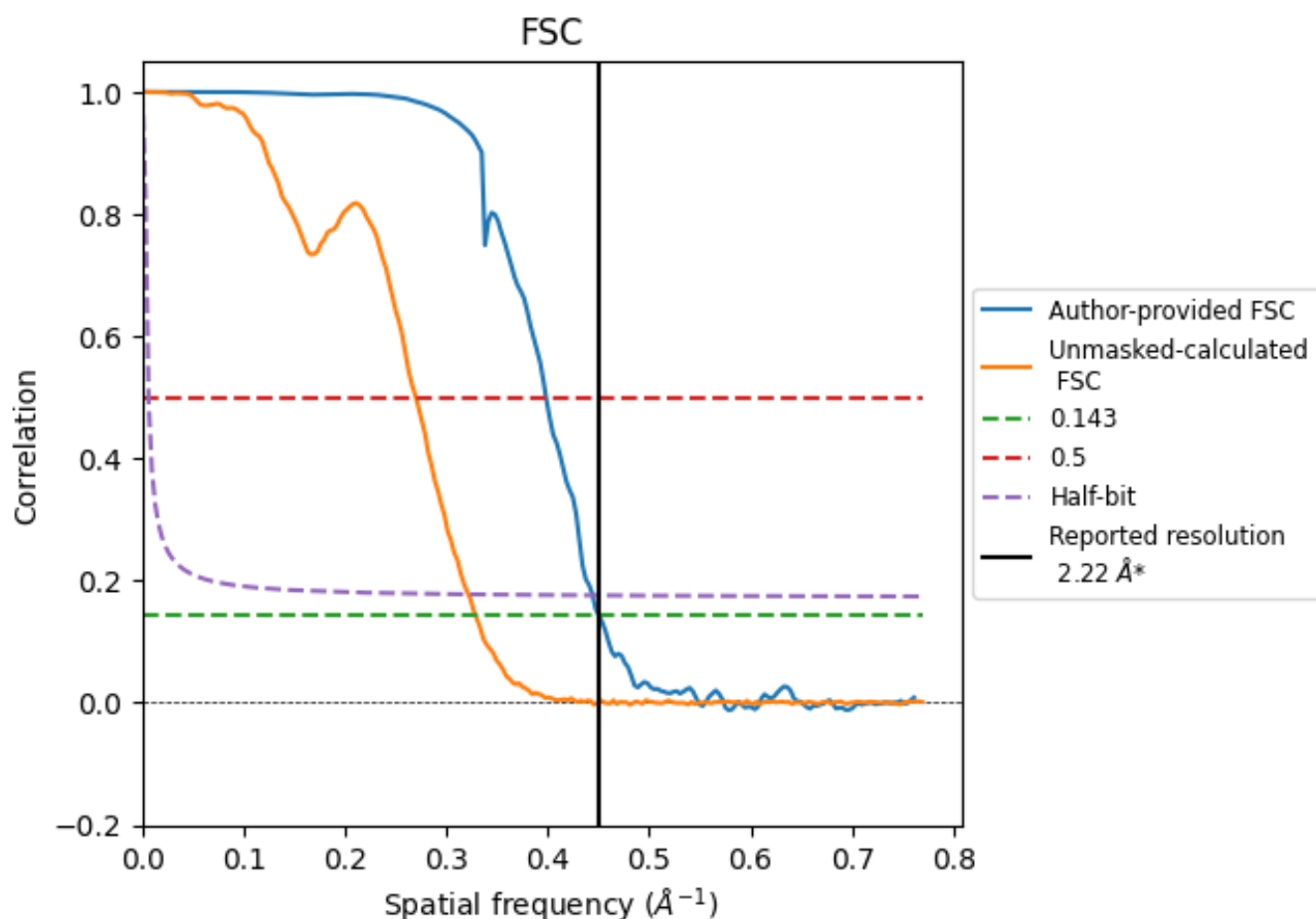


\*Reported resolution corresponds to spatial frequency of 0.450 Å<sup>-1</sup>

## 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 0.450  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.22	-	-
Author-provided FSC curve	2.22	2.51	2.25
Unmasked-calculated*	3.04	3.71	3.11

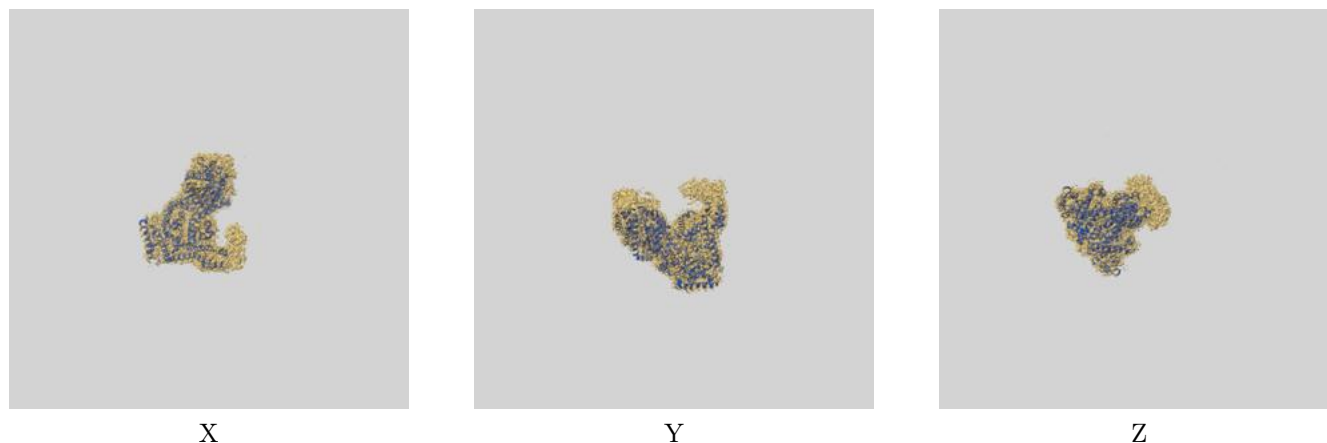
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.04 differs from the reported value 2.22 by more than 10 %



## 9 Map-model fit [i](#)

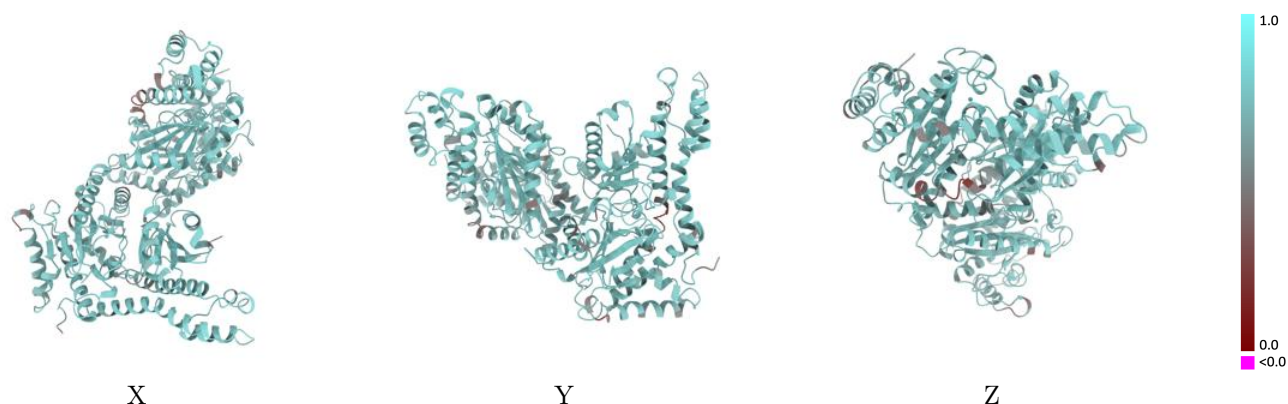
This section contains information regarding the fit between EMDB map EMD-54980 and PDB model 9SKZ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



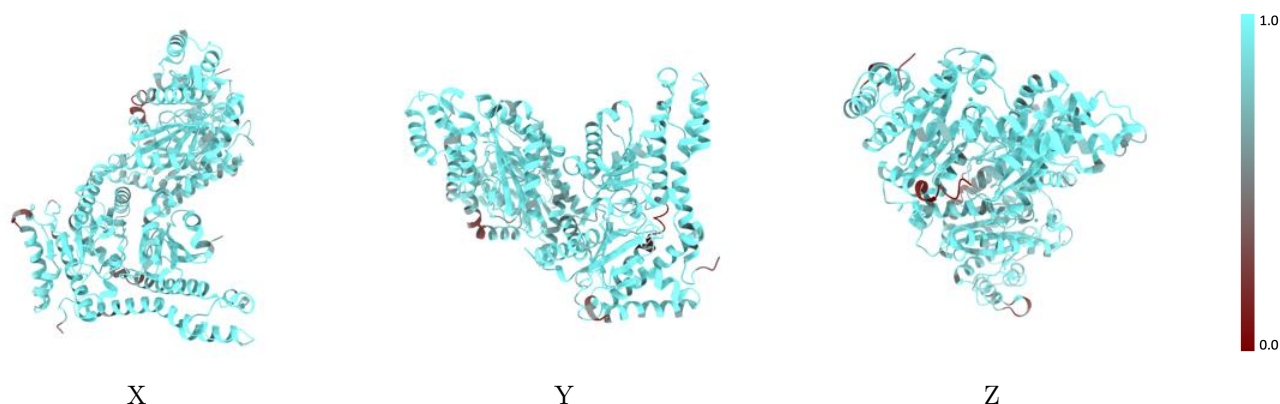
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



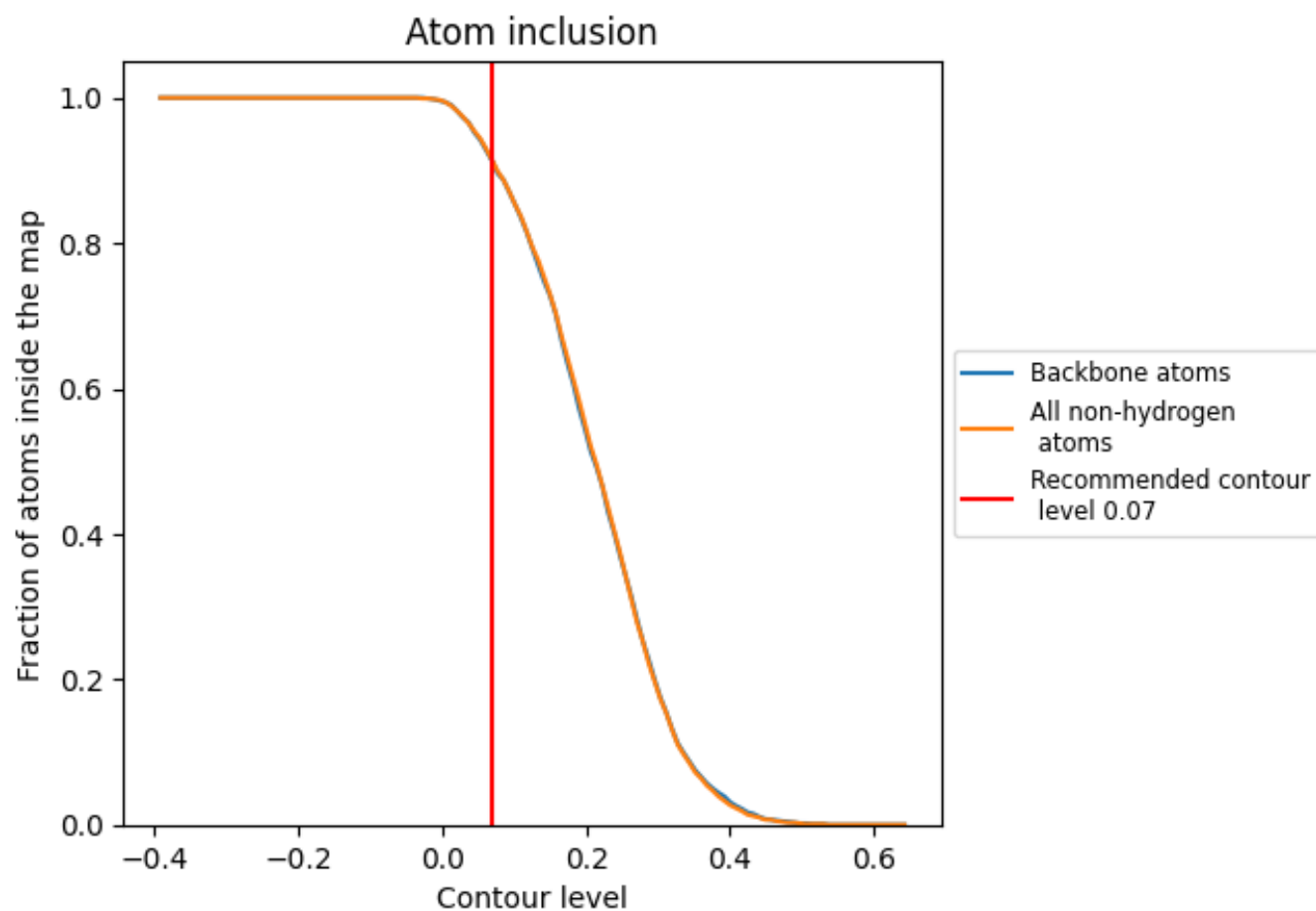
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9130	<div></div> 0.6960
A	<div></div> 0.9140	<div></div> 0.6930
B	<div></div> 0.9250	<div></div> 0.6980

