



## Full wwPDB EM Validation Report ⓘ

Apr 13, 2026 – 04:37 pm BST

PDB ID : 9SKR / pdb\_00009skr  
EMDB ID : EMD-54972  
Title : Cryo-EM structure of H. neapolitanus CsoSCA in oxidizing conditions, hexamer  
Authors : Gaullier, G.; Vogiatzi, N.; Blikstad, C.  
Deposited on : 2025-09-02  
Resolution : 2.13 Å(reported)  
Based on initial model : .

This is a Full wwPDB EM Validation 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

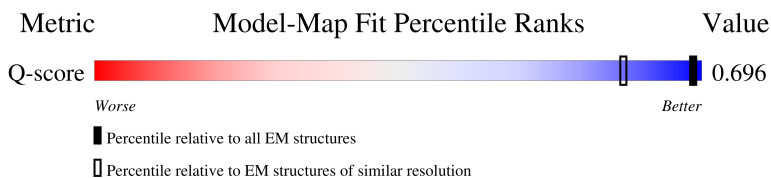
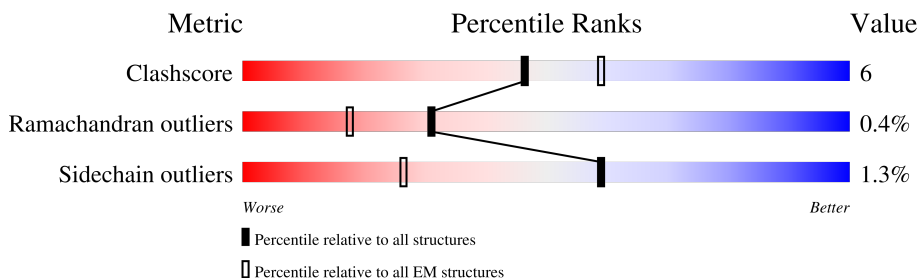
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

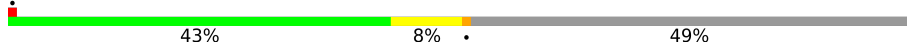
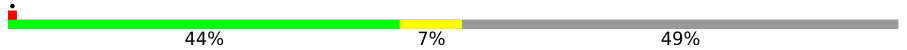
The reported resolution of this entry is 2.13 Å.

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	2439 ( 1.64 - 2.63 )

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	
1	B	919	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14731 atoms, of which 7028 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	3514	655	697	11		
1	B	467	Total	C	H	N	O	S	0	0
			7184	2307	3514	655	697	11		

There are 80 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
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
B	-13	ASN	-	linker	UNP P0AEX9
B	-12	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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 1	Zn 1	0
2	B	1	Total 1	Zn 1	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	171	Total 171	O 171	0
3	B	190	Total 190	O 190	0





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	486613	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 ( $e^-/\text{\AA}^2$ )	64.757	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	0.563	Depositor
Minimum map value	-0.363	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.05	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	0.79	1/3746 (0.0%)	1.26	14/5082 (0.3%)
1	B	0.80	2/3746 (0.1%)	1.27	17/5082 (0.3%)
All	All	0.79	3/7492 (0.0%)	1.27	31/10164 (0.3%)

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
1	B	0	3
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	SER	CA-CB	-8.15	1.41	1.53
1	B	403	SER	CA-CB	-8.06	1.41	1.53
1	B	328	THR	C-O	7.82	1.34	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	ARG	CD-NE-CZ	7.38	134.74	124.40
1	B	496	ARG	N-CA-CB	-7.20	98.24	111.13
1	A	496	ARG	N-CA-CB	-7.18	98.28	111.13
1	B	496	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	A	496	ARG	NE-CZ-NH1	-6.72	114.78	121.50
1	A	116	ASN	CA-CB-CG	6.52	119.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASN	CA-CB-CG	6.22	118.82	112.60
1	B	73	PHE	N-CA-CB	6.19	119.29	110.13
1	A	73	PHE	N-CA-CB	6.13	119.20	110.13
1	A	77	ILE	O-C-N	-5.97	116.60	120.42
1	A	424	THR	OG1-CB-CG2	-5.90	97.50	109.30
1	B	496	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	B	424	THR	OG1-CB-CG2	-5.89	97.53	109.30
1	A	496	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	296	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	77	ILE	O-C-N	-5.62	116.82	120.42
1	B	446	ARG	CG-CD-NE	-5.54	99.81	112.00
1	A	97	GLN	CB-CA-C	-5.47	102.25	110.90
1	A	500	GLN	N-CA-CB	-5.47	101.34	111.52
1	A	469	THR	CA-CB-OG1	-5.47	101.40	109.60
1	B	500	GLN	N-CA-CB	-5.44	101.40	111.52
1	B	482	GLU	CB-CA-C	5.43	119.49	110.90
1	A	81	GLN	N-CA-C	-5.38	105.45	112.23
1	B	446	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	69	VAL	N-CA-C	-5.37	105.15	111.00
1	B	469	THR	CA-CB-OG1	-5.27	101.69	109.60
1	B	69	VAL	N-CA-C	-5.26	105.27	111.00
1	A	77	ILE	CA-C-O	5.21	122.18	118.69
1	B	397	HIS	CA-CB-CG	-5.18	108.62	113.80
1	B	77	ILE	CA-C-O	5.14	122.14	118.69
1	A	397	HIS	CA-CB-CG	-5.10	108.70	113.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	TRP	Mainchain
1	A	317	ARG	Sidechain
1	A	496	ARG	Sidechain
1	B	117	TRP	Mainchain
1	B	317	ARG	Sidechain
1	B	496	ARG	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	3670	3514	3601	49	0
1	B	3670	3514	3601	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	171	0	0	8	0
3	B	190	0	0	7	0
All	All	7703	7028	7202	88	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.

All (88) 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:169:ASP:OD1	3:A:2101:HOH:O	1.96	0.83
1:B:183:PRO:O	3:B:2101:HOH:O	1.94	0.83
1:A:183:PRO:O	3:A:2102:HOH:O	2.03	0.76
1:B:478:ASN:OD1	3:B:2102:HOH:O	2.03	0.75
1:B:66:GLU:OE1	1:B:381:TYR:OH	2.05	0.73
1:A:66:GLU:OE1	1:A:381:TYR:OH	2.05	0.73
1:B:253:CYS:SG	3:B:2273:HOH:O	2.50	0.69
1:A:253:CYS:SG	3:A:2261:HOH:O	2.52	0.67
1:A:384:ASN:C	1:A:384:ASN:OD1	2.40	0.63
1:B:422:LEU:C	1:B:422:LEU:HD12	2.25	0.62
1:B:120:GLY:O	3:B:2103:HOH:O	2.16	0.60
1:A:422:LEU:HD12	1:A:422:LEU:C	2.27	0.59
1:A:404:VAL:CG2	1:A:454:ILE:HG12	2.33	0.59
1:B:404:VAL:CG2	1:B:454:ILE:HG12	2.33	0.58
1:B:86:ILE:O	1:B:121:HIS:HE1	1.87	0.58
1:A:86:ILE:O	1:A:121:HIS:HE1	1.88	0.57
1:B:384:ASN:OD1	1:B:384:ASN:C	2.48	0.56
1:A:283:CYS:SG	1:A:284:CYS:SG	3.02	0.55
1:B:307:PRO:O	1:B:360:ALA:HB2	2.09	0.53
1:B:477:TYR:CE1	1:B:481:LYS:HD2	2.45	0.52
1:B:380:ASP:O	1:B:383:VAL:N	2.42	0.52
1:A:386:HIS:ND1	1:A:391:PRO:HD3	2.25	0.51
1:A:497:LEU:HD12	1:A:497:LEU:N	2.26	0.51
1:B:364:MET:O	1:B:368:ILE:HG13	2.11	0.51
1:B:497:LEU:HD12	1:B:497:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:THR:C	3:B:2153:HOH:O	2.54	0.50
1:A:380:ASP:O	1:A:383:VAL:N	2.44	0.50
1:B:380:ASP:O	1:B:381:TYR:C	2.54	0.50
1:B:80:LEU:HD11	1:B:127:PHE:HB2	1.94	0.50
1:A:364:MET:O	1:A:368:ILE:HG13	2.11	0.50
1:B:474:ARG:CZ	1:B:514:ALA:OXT	2.59	0.50
1:A:380:ASP:O	1:A:381:TYR:C	2.55	0.50
1:A:80:LEU:HD11	1:A:127:PHE:HB2	1.95	0.49
1:B:275:ARG:NH1	3:B:2122:HOH:O	2.45	0.49
1:B:86:ILE:O	1:B:121:HIS:CE1	2.66	0.49
1:A:197:LYS:HE3	3:A:2101:HOH:O	2.13	0.48
1:A:474:ARG:CZ	1:A:514:ALA:OXT	2.60	0.48
1:A:297:THR:C	3:A:2143:HOH:O	2.56	0.48
1:B:404:VAL:HG21	1:B:454:ILE:HG12	1.95	0.48
1:A:307:PRO:O	1:A:360:ALA:HB2	2.14	0.47
1:B:54:THR:OG1	1:B:380:ASP:OD2	2.33	0.47
1:A:404:VAL:HG21	1:A:454:ILE:HG12	1.95	0.47
1:A:54:THR:OG1	1:A:380:ASP:OD2	2.31	0.47
1:A:86:ILE:O	1:A:121:HIS:CE1	2.68	0.47
1:A:97:GLN:HA	1:A:97:GLN:OE1	2.15	0.46
1:B:386:HIS:ND1	1:B:391:PRO:HD3	2.30	0.46
1:A:87:PRO:O	3:A:2103:HOH:O	2.20	0.46
1:A:477:TYR:CE1	1:A:481:LYS:HD2	2.51	0.46
1:A:309:SER:OG	1:A:357:ASN:O	2.28	0.46
1:A:429:ALA:HB1	1:A:483:ARG:CZ	2.45	0.46
1:B:92:TYR:OH	1:B:116:ASN:ND2	2.46	0.46
1:B:429:ALA:HB1	1:B:483:ARG:CZ	2.46	0.45
1:B:477:TYR:CZ	1:B:481:LYS:HD2	2.50	0.45
1:B:275:ARG:CZ	3:B:2122:HOH:O	2.65	0.45
1:A:436:ILE:O	1:A:440:THR:OG1	2.30	0.45
1:A:72:ARG:HH21	1:A:72:ARG:HD3	1.59	0.45
1:B:264:LEU:HD23	1:B:264:LEU:O	2.17	0.44
1:A:175:ASP:OD2	1:A:397:HIS:HE1	1.99	0.44
1:B:97:GLN:OE1	1:B:97:GLN:HA	2.18	0.44
1:B:430:ILE:HD12	1:B:430:ILE:HA	1.91	0.44
1:B:175:ASP:OD2	1:B:397:HIS:HE1	1.99	0.44
1:A:264:LEU:HD23	1:A:264:LEU:O	2.18	0.44
1:A:70:LYS:NZ	3:A:2129:HOH:O	2.50	0.43
1:A:243:PHE:CE2	1:A:296:ASP:HB2	2.53	0.43
1:B:230:ASP:OD1	1:B:230:ASP:N	2.50	0.43
1:A:496:ARG:C	1:A:497:LEU:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ARG:HH21	1:B:72:ARG:HD3	1.60	0.43
1:A:257:GLY:O	1:A:258:SER:CB	2.67	0.43
1:A:467:GLU:O	1:A:471:VAL:HG23	2.19	0.42
1:B:283:CYS:SG	1:B:284:CYS:SG	3.02	0.42
1:A:60:GLU:OE2	1:A:64:ARG:NE	2.46	0.42
1:A:497:LEU:N	1:A:497:LEU:CD1	2.82	0.42
1:B:274:PHE:CD2	1:B:288:ILE:CD1	3.02	0.42
1:B:497:LEU:N	1:B:497:LEU:CD1	2.82	0.42
1:A:257:GLY:O	1:A:258:SER:HB2	2.20	0.42
1:A:175:ASP:OD2	1:A:397:HIS:CE1	2.73	0.42
1:B:496:ARG:C	1:B:497:LEU:HD12	2.44	0.42
1:A:230:ASP:OD1	1:A:230:ASP:N	2.51	0.42
1:A:92:TYR:OH	1:A:116:ASN:ND2	2.49	0.41
1:A:477:TYR:CZ	1:A:481:LYS:HD2	2.54	0.41
1:A:60:GLU:CD	1:A:64:ARG:HE	2.26	0.41
1:A:197:LYS:CE	3:A:2101:HOH:O	2.69	0.41
1:A:274:PHE:CD2	1:A:288:ILE:CD1	3.03	0.41
1:B:175:ASP:OD2	1:B:397:HIS:CE1	2.74	0.41
1:A:335:GLU:OE1	1:A:335:GLU:N	2.54	0.41
1:A:399:GLU:HA	1:A:415:ASN:O	2.21	0.41
1:A:430:ILE:HD12	1:A:430:ILE:HA	1.92	0.41
1:B:399:GLU:HA	1:B:415:ASN:O	2.22	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	465/919 (51%)	435 (94%)	27 (6%)	3 (1%)	21	15
1	B	465/919 (51%)	435 (94%)	29 (6%)	1 (0%)	43	42
All	All	930/1838 (51%)	870 (94%)	56 (6%)	4 (0%)	31	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	SER
1	A	117	TRP
1	B	117	TRP
1	A	258	SER

### 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	390/761 (51%)	386 (99%)	4 (1%)	68	74
1	B	390/761 (51%)	384 (98%)	6 (2%)	57	63
All	All	780/1522 (51%)	770 (99%)	10 (1%)	59	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	179	LYS
1	A	209	ASP
1	A	395	ILE
1	B	90	LEU
1	B	94	THR
1	B	179	LYS
1	B	190	LEU
1	B	383	VAL
1	B	395	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	121	HIS
1	A	250	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	341	HIS
1	A	348	ASN
1	B	101	GLN
1	B	121	HIS
1	B	250	HIS
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.

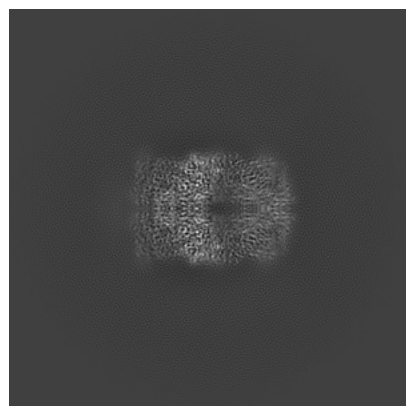
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54972. These allow visual inspection of the internal detail of the map and identification of artifacts.

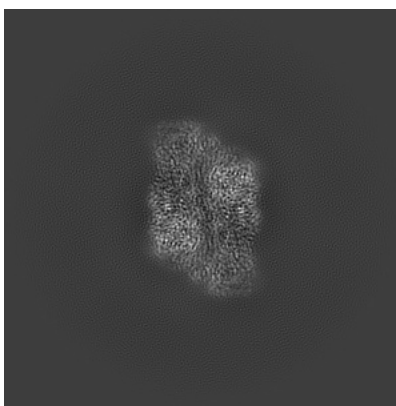
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

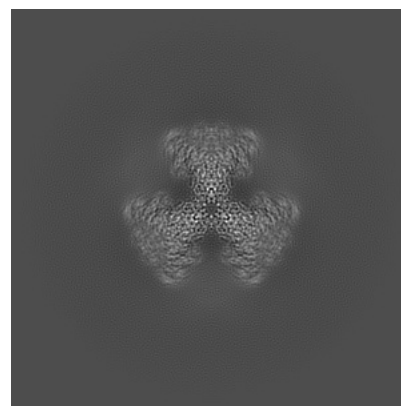
#### 6.1.1 Primary map



X

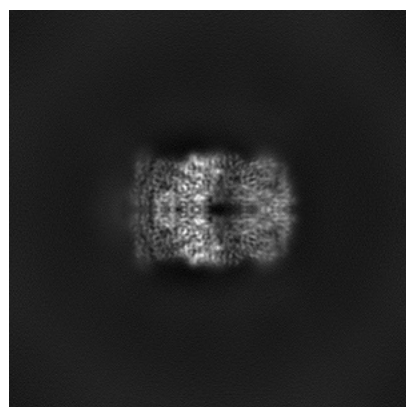


Y

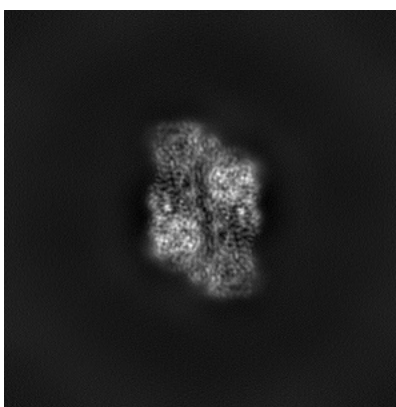


Z

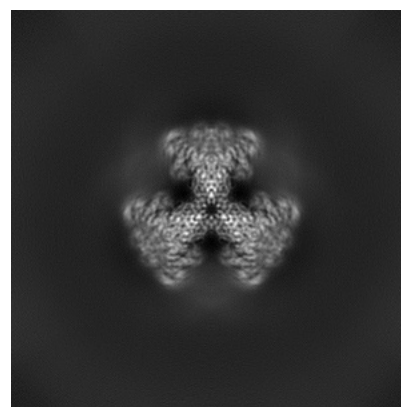
#### 6.1.2 Raw map



X



Y



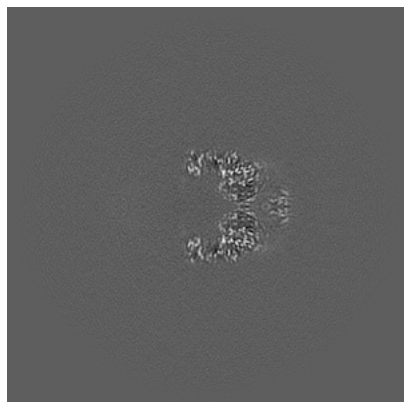
Z

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

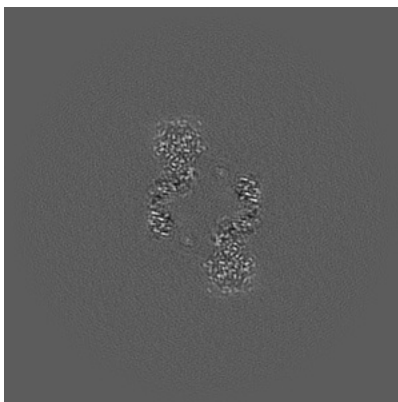


## 6.2 Central slices [i](#)

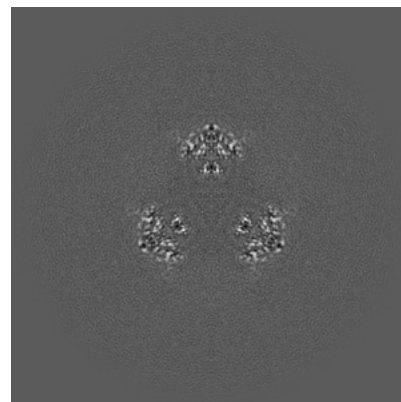
### 6.2.1 Primary map



X Index: 240

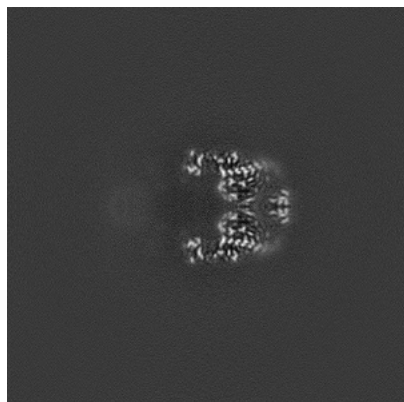


Y Index: 240

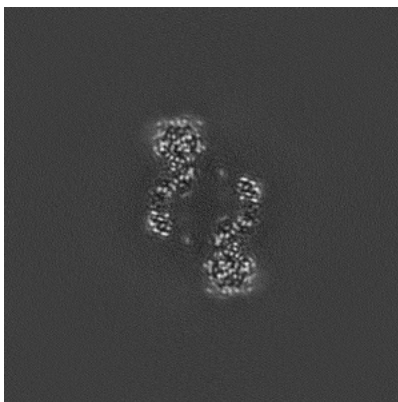


Z Index: 240

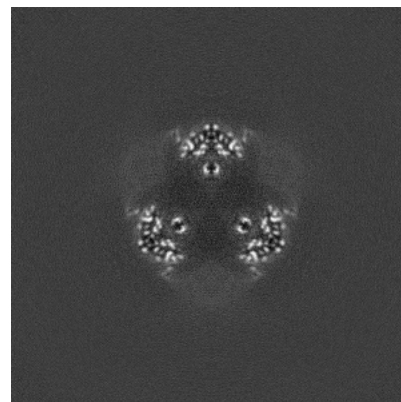
### 6.2.2 Raw map



X Index: 240



Y Index: 240

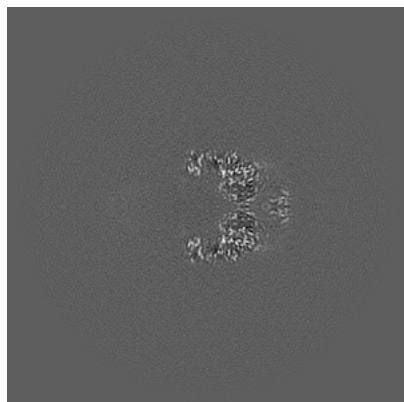


Z Index: 240

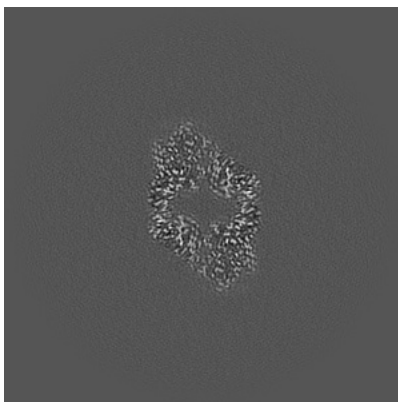
The images above show central slices of the map in three orthogonal directions.

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

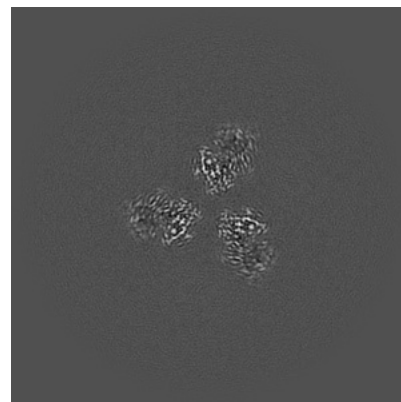
### 6.3.1 Primary map



X Index: 240

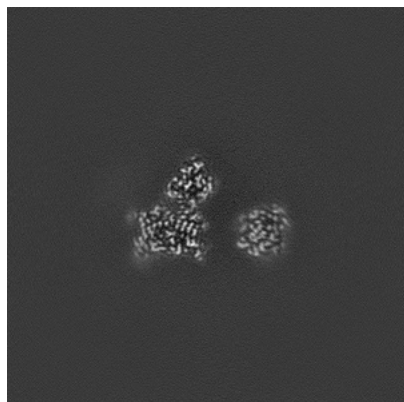


Y Index: 225

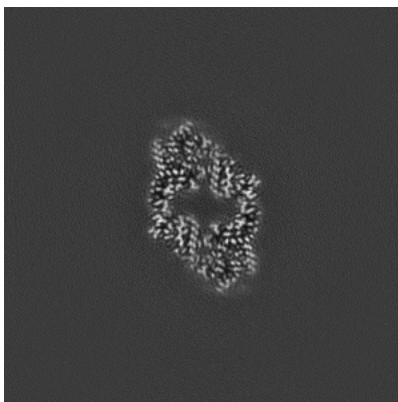


Z Index: 268

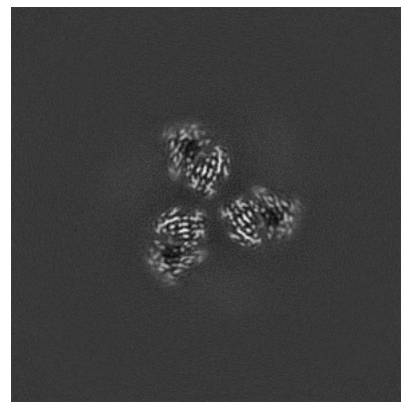
### 6.3.2 Raw map



X Index: 202



Y Index: 225

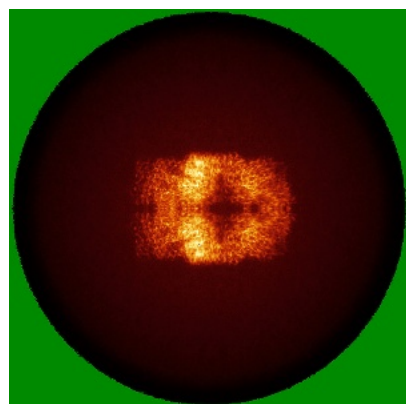


Z Index: 213

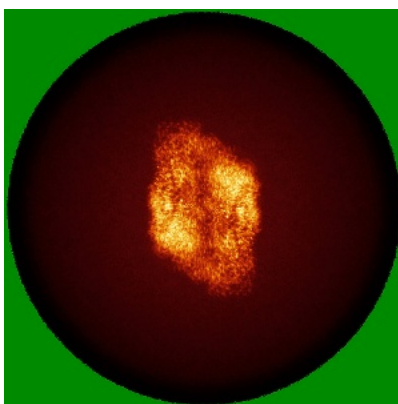
The images above show the largest variance slices of the map in three orthogonal directions.

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

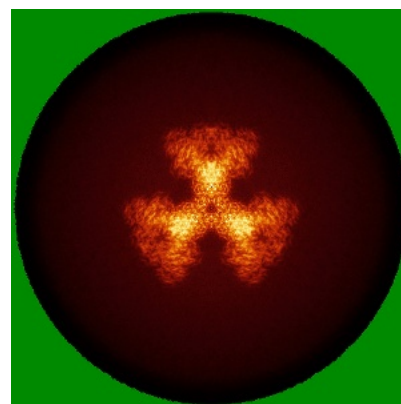
### 6.4.1 Primary map



X

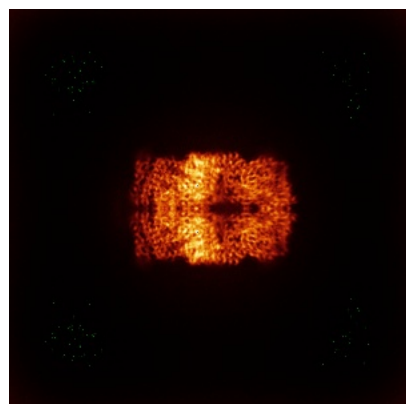


Y

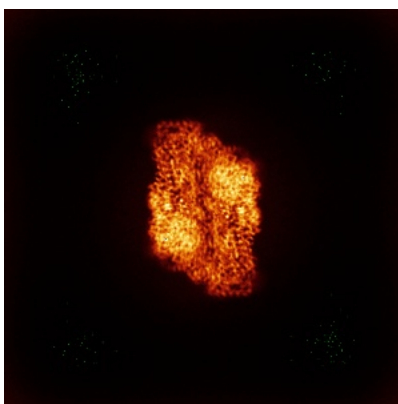


Z

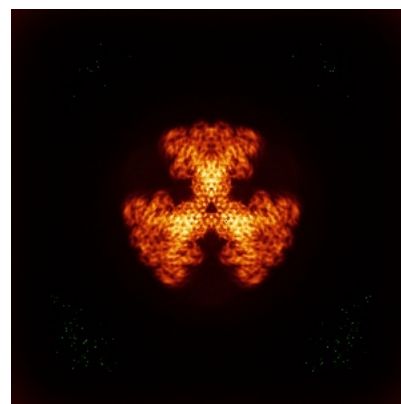
### 6.4.2 Raw map



X



Y

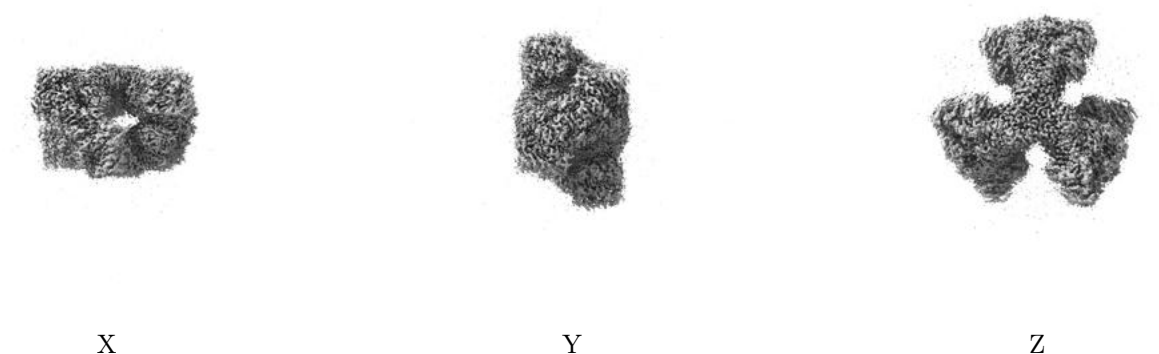


Z

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.

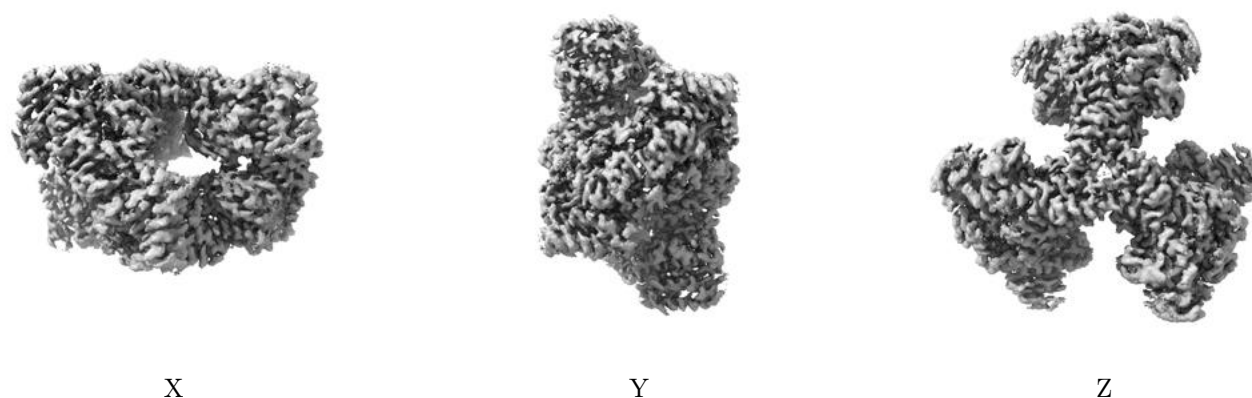
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

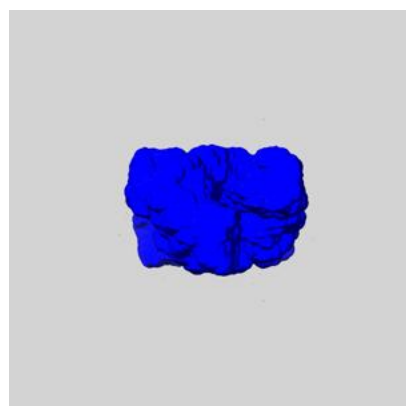
## 6.6 Mask visualisation [i](#)

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

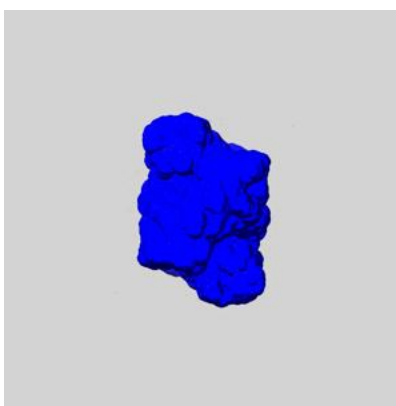
A mask typically either:

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

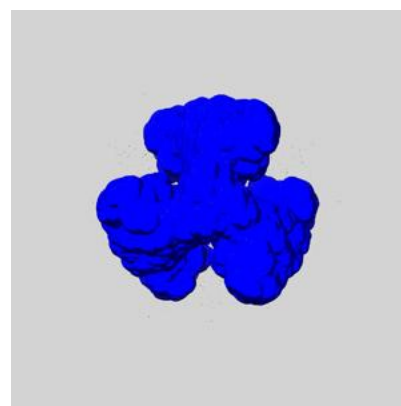
### 6.6.1 emd\_54972\_msk\_1.map [i](#)



X

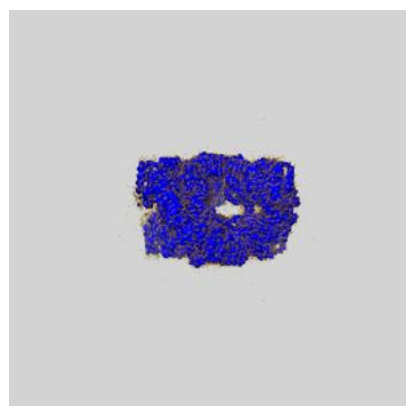


Y

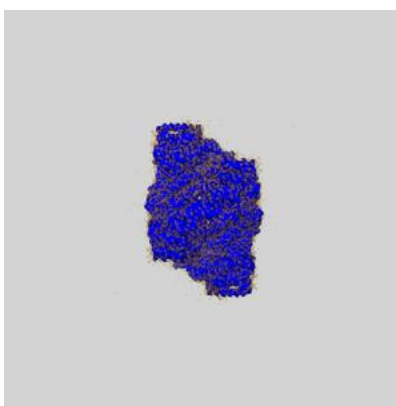


Z

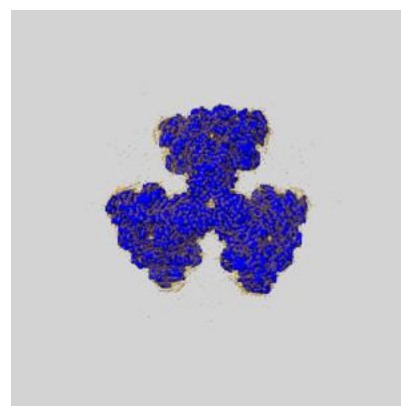
### 6.6.2 emd\_54972\_msk\_2.map [i](#)



X

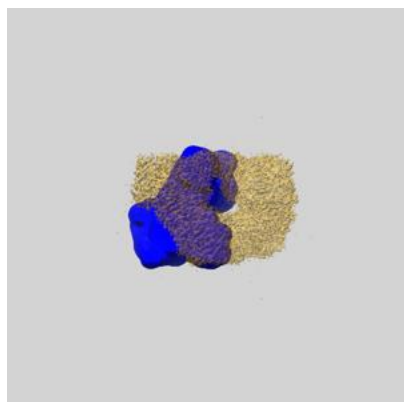


Y

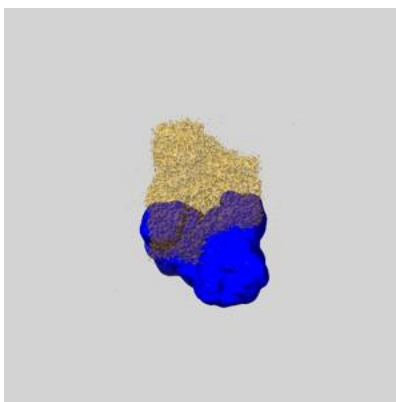


Z

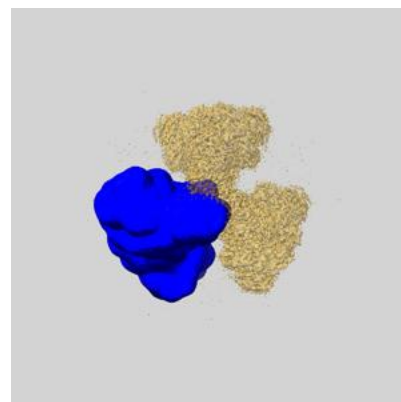
### 6.6.3 emd\_54972\_msk\_3.map [i](#)



X



Y

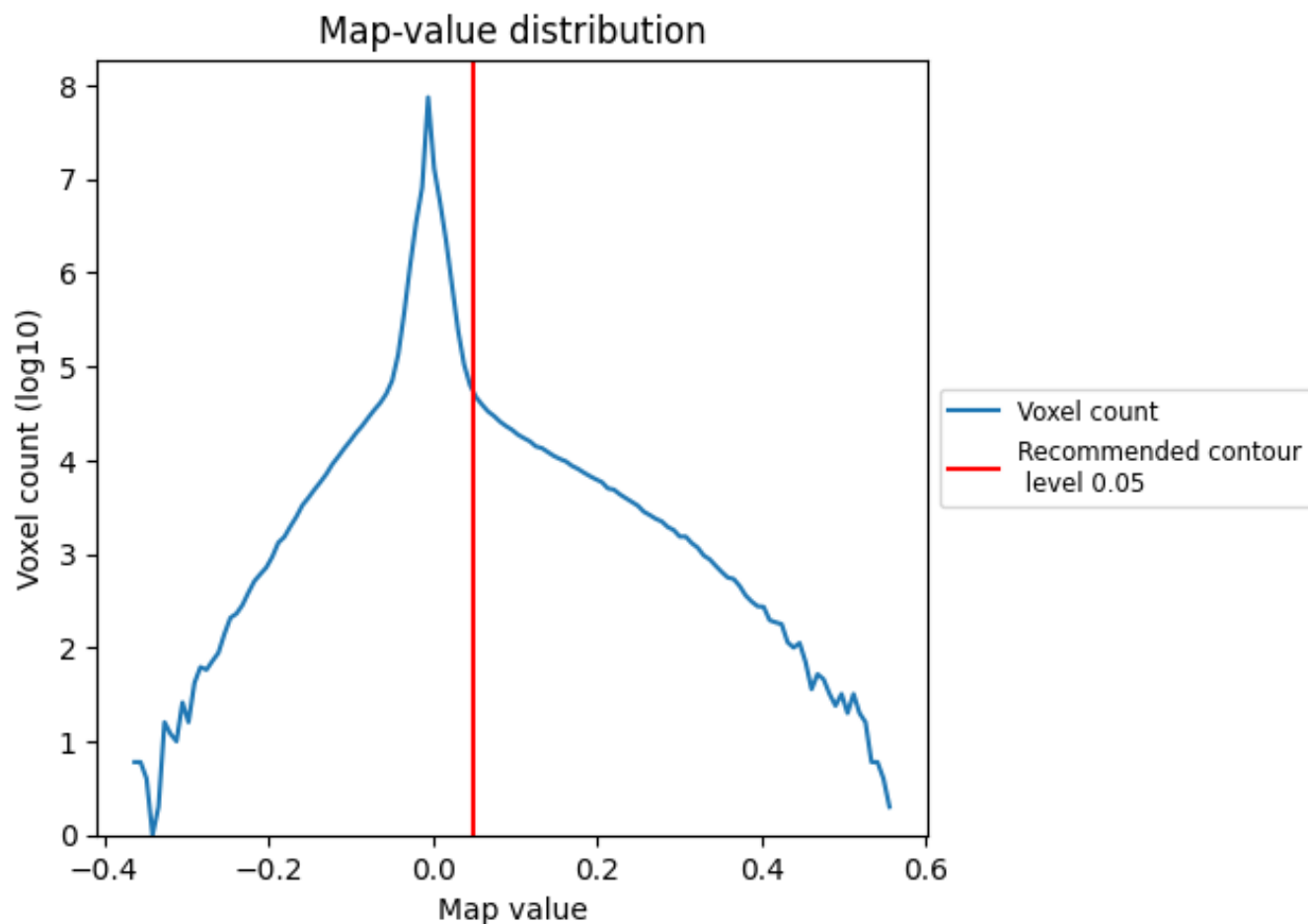


Z

## 7 Map analysis [i](#)

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

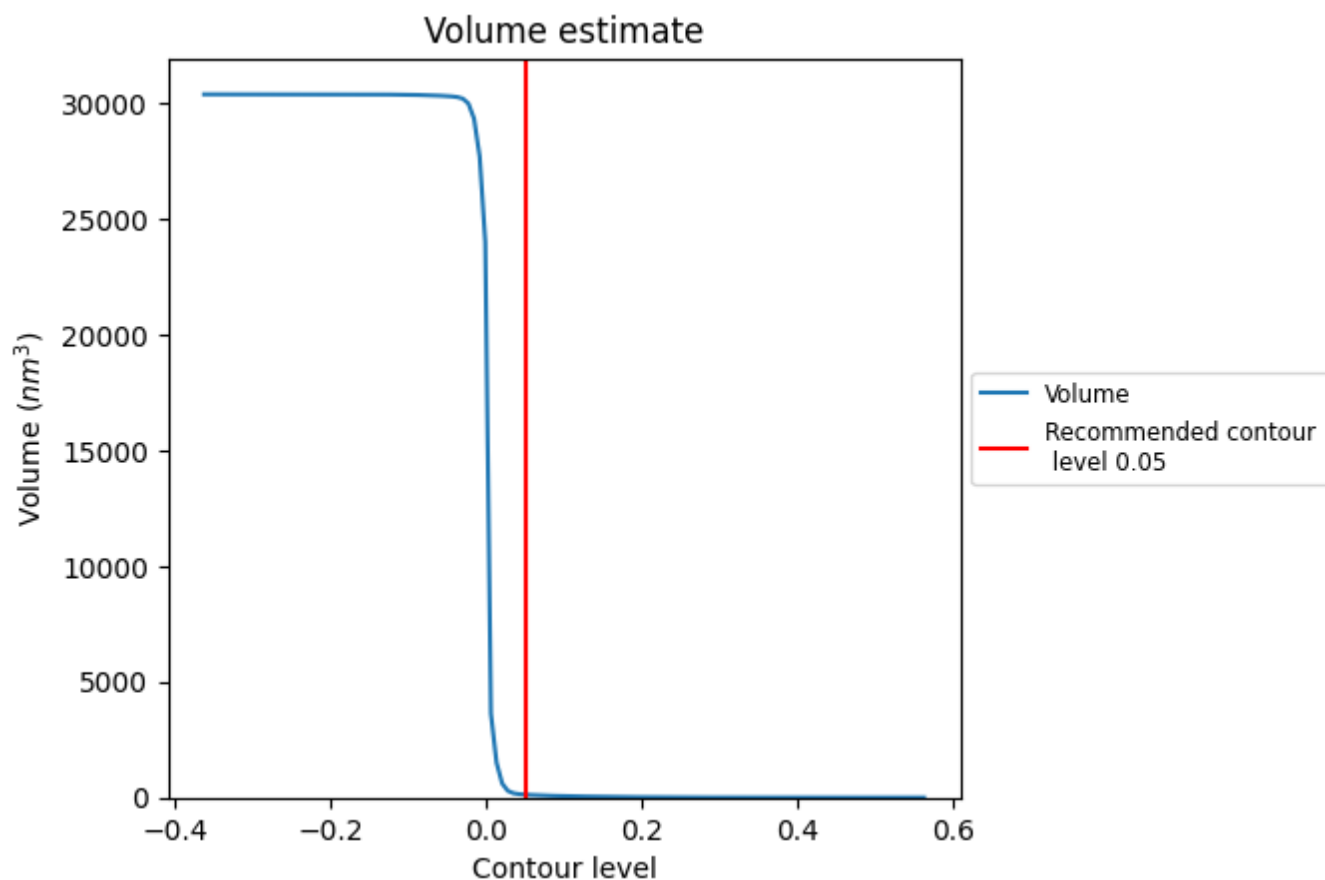
### 7.1 Map-value distribution [i](#)



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](#)

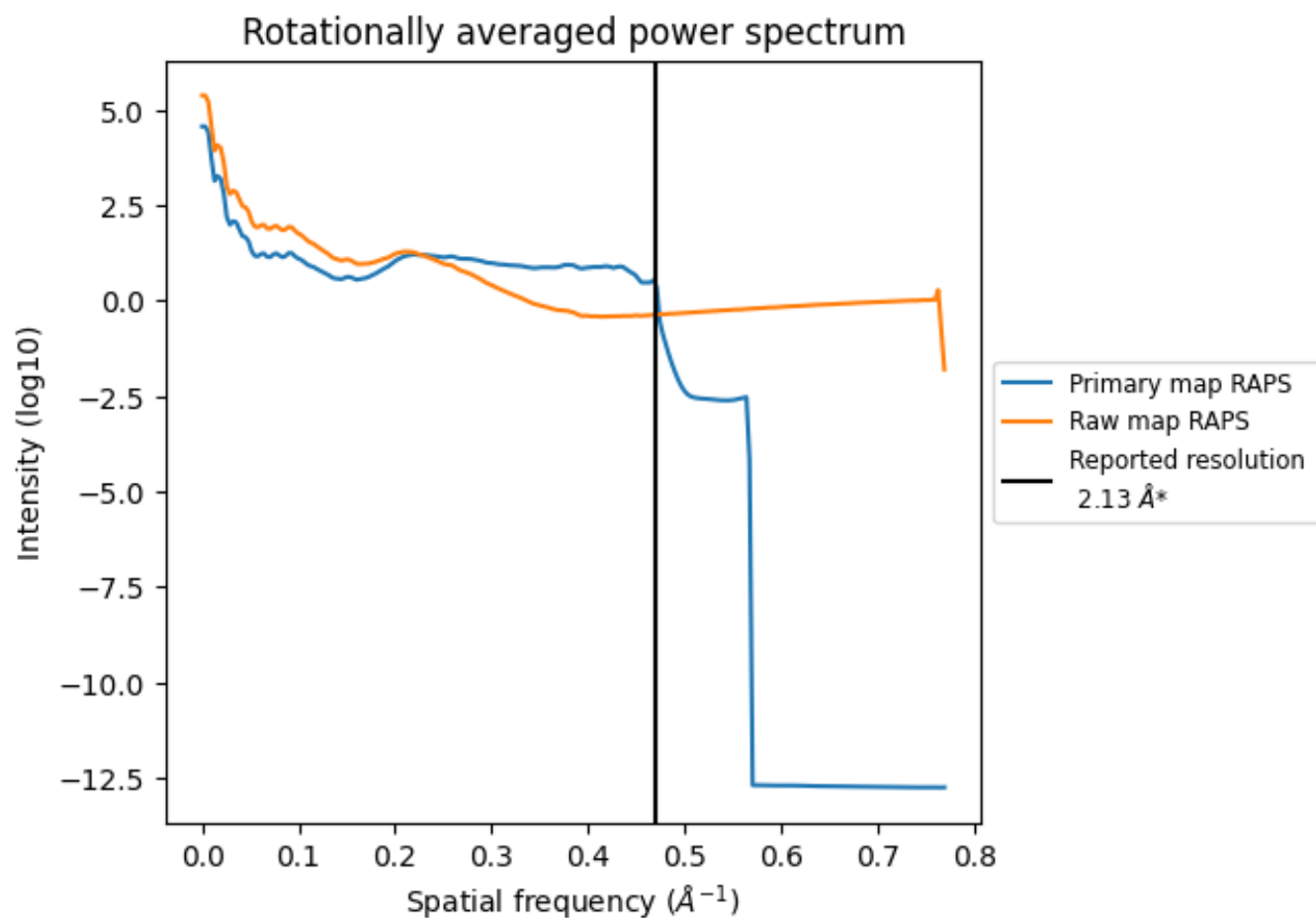


The volume at the recommended contour level is 125 nm<sup>3</sup>; this corresponds to an approximate mass of 113 kDa.

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 ⓘ

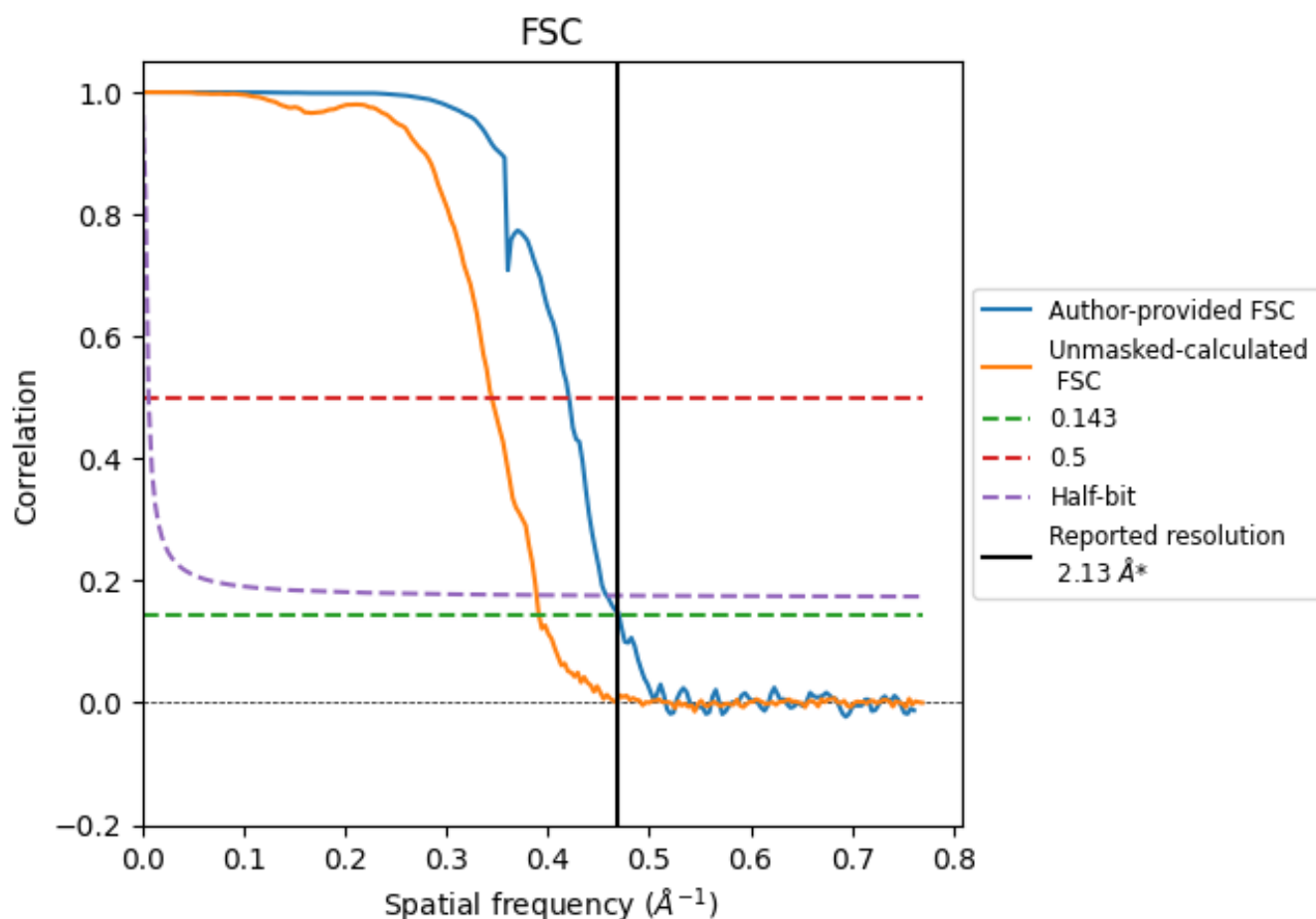


\*Reported resolution corresponds to spatial frequency of 0.469 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	2.13	2.38	2.18
Unmasked-calculated*	2.56	2.90	2.57

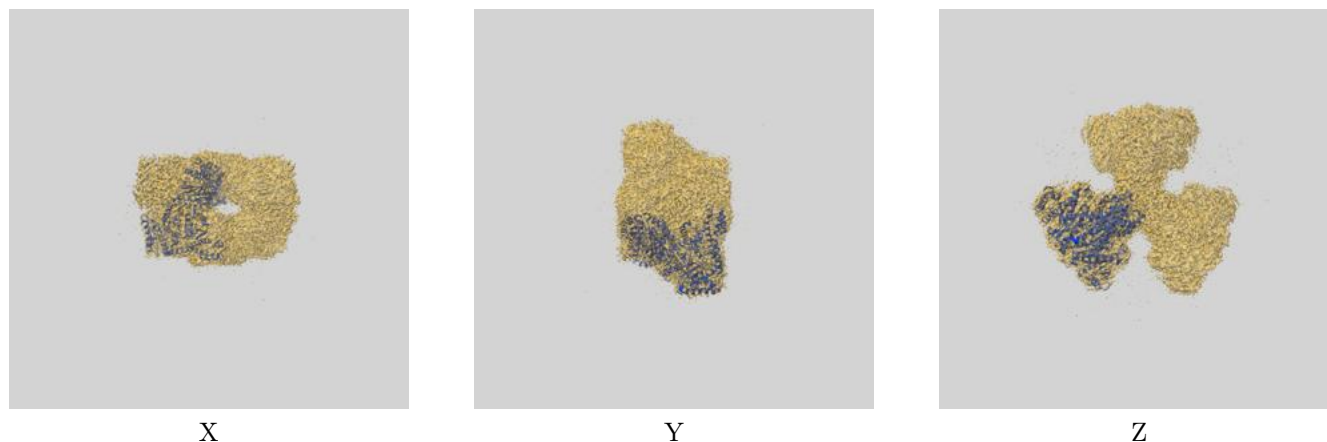
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.56 differs from the reported value 2.13 by more than 10 %

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

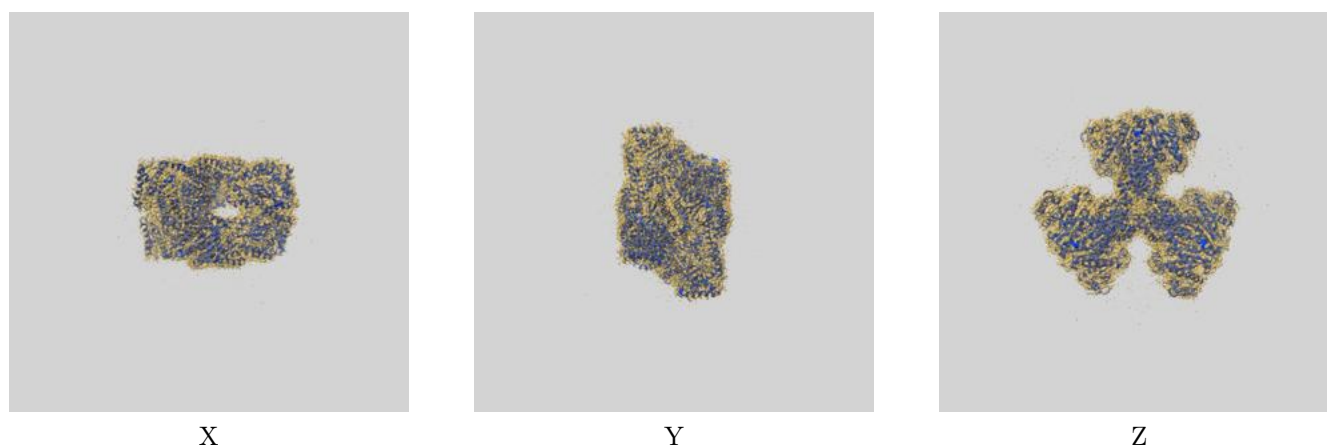
This section contains information regarding the fit between EMDB map EMD-54972 and PDB model 9SKR. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

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

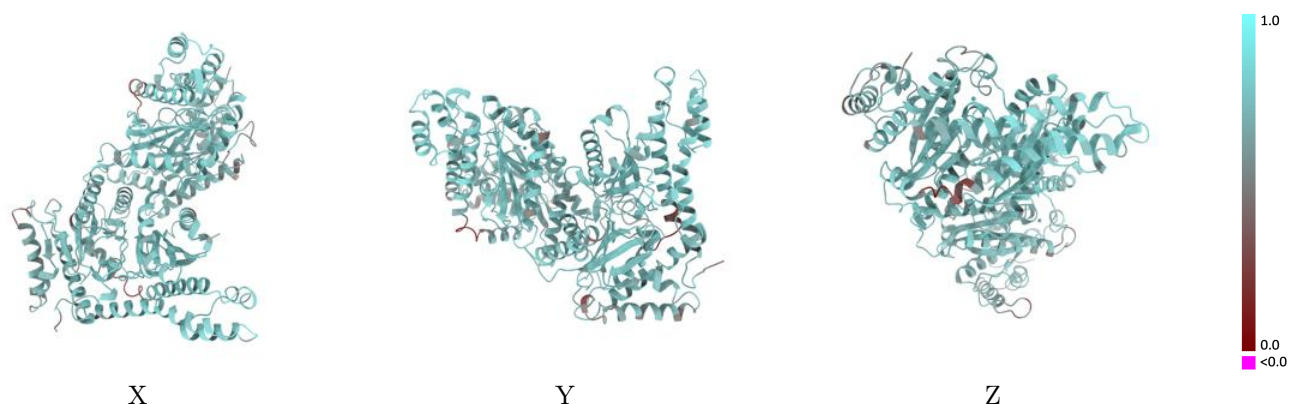


#### 9.1.2 Map-model assembly overlay [i](#)



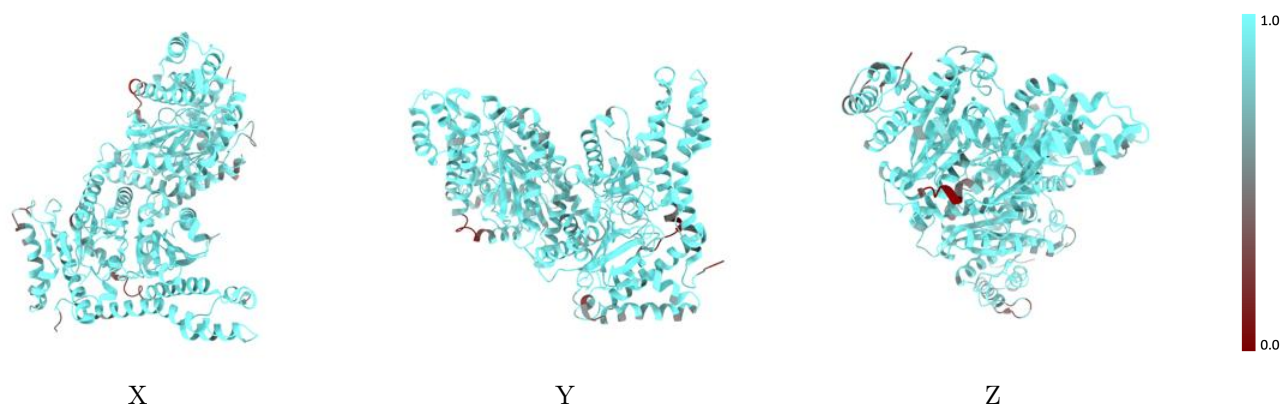
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



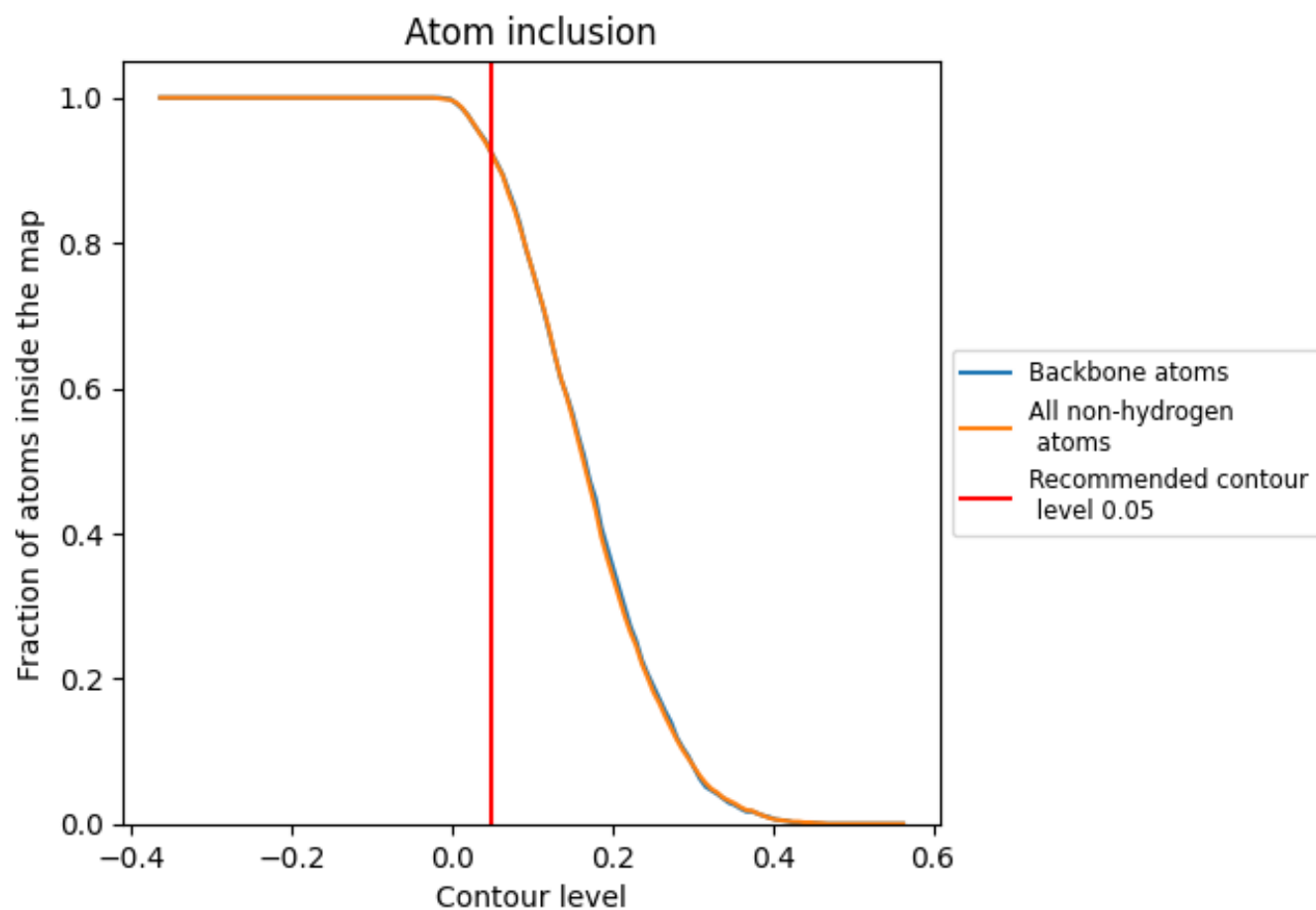
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9230	<div></div> 0.6960
A	<div></div> 0.9230	<div></div> 0.6980
B	<div></div> 0.9220	<div></div> 0.6950

