



Full wwPDB EM Validation Report ⓘ

Apr 13, 2026 – 04:30 pm BST

PDB ID : 9SKV / pdb_00009skv
EMDB ID : EMD-54976
Title : Cryo-EM structure of H. neapolitanus CsoSCA in reducing conditions, dimer, major state, inactive conformation
Authors : Gaullier, G.; Vogiatzi, N.; Blikstad, C.
Deposited on : 2025-09-02
Resolution : 2.12 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

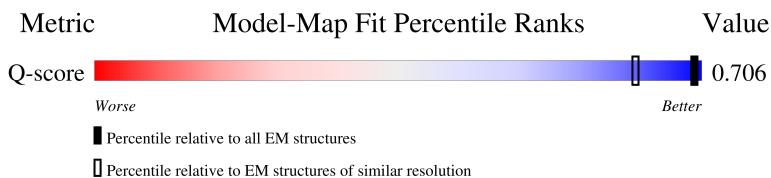
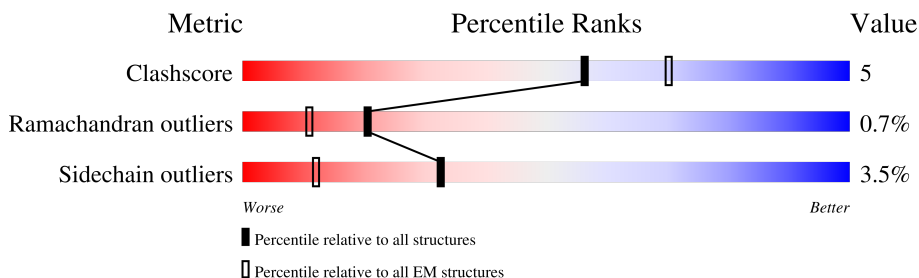
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.12 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	2398 (1.64 - 2.62)

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	919	
1	B	919	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15016 atoms, of which 7154 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	475	Total	C	H	N	O	S	0	0
			7308	2345	3577	666	708	12		
1	B	475	Total	C	H	N	O	S	0	0
			7308	2345	3577	666	708	12		

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

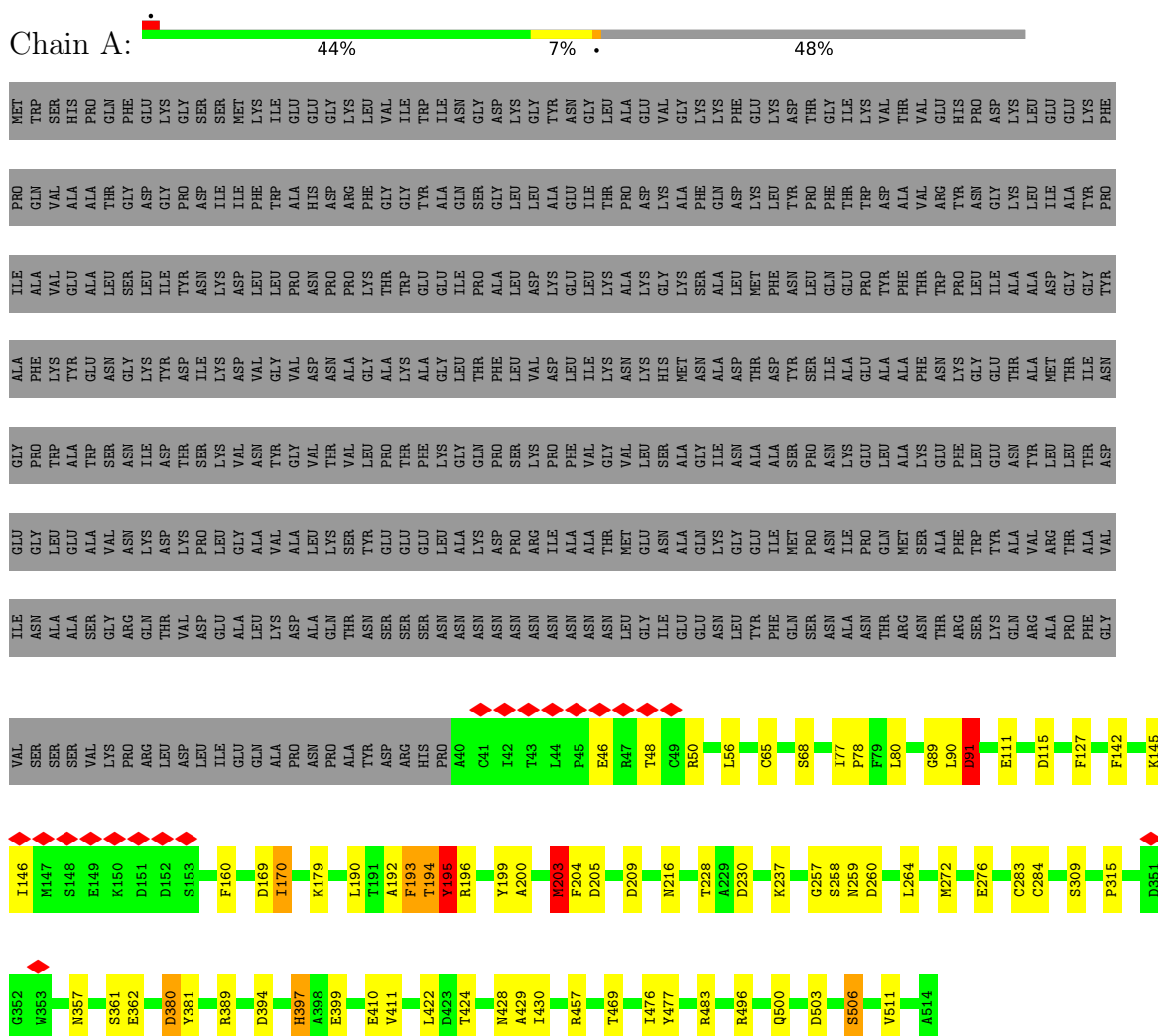
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	180	Total 180	O 180	0
3	B	218	Total 218	O 218	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



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



R399	D169	K179	L190	T191	A192	F193	T194	Y195	A196	K197	A198	Y199	A200	G201	F204	E207	R468	T469	R475	K481	R496	D503	S506	E510	V511	A514																								
VAL	SER	SER	VAL	LYS	PRO	ARG	LEU	ASP	LEU	ILE	GLU	ALA	LYS	ALA	PRO	ASN	PRO	ALA	TYR	ASP	ARG	HIS	PRO	A40	C41	I42	T43	I44	P45	E46	R47	T48	C49	R50	E60	R64	I77	L90	T94	F127	F142	I146	M147	S148	E149	K150	D151	S152	S153	F160
ILE	ASN	ALA	SER	GLY	ARG	GLN	THR	THR	ASP	GLU	ALA	LEU	ASP	ALA	GLN	THR	ASN	SER	SER	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	GLY	ILE	GLU	LEU	GLY	ILE	GLN	GLY	TYR	PHE	GLN	ASN	ASN	ASN	THR	ARG	THR	THR	ARG	ALA	PRO	PHE	GLY
GLU	LEU	GLU	ALA	VAL	ASN	LYS	ASP	PRO	LEU	GLY	VAL	VAL	VAL	ALA	LEU	LYS	SER	TYR	GLU	GLU	GLU	PHE	LYS	LEU	ALA	ALA	VAL	THR	MET	GLU	ASN	ARG	ILE	ASN	GLN	MET	GLN	MET	SER	ALA	GLU	PHE	TYR	VAL	ARG	THR	ALA	VAL		
PRO	TRP	ALA	TRP	SER	ASN	ILE	ASP	THR	SER	LYS	VAL	ASN	ASP	GLY	VAL	THR	VAL	LEU	PRO	THR	PHE	LYS	GLY	PRO	PHE	GLY	LEU	ASP	SER	ALA	ALA	SER	THR	ASN	TYR	THR	ASP	GLY	THR	ASP	GLY	THR	LEU	GLY	ASP	GLY	THR	PRO		
MET	TRP	SER	HIS	PRO	GLN	PHE	LYS	SER	SER	GLY	VAL	THR	THR	ASP	ASN	GLY	THR	ASN	PRO	ASP	ARG	GLY	ASN	GLY	VAL	THR	TRP	ILE	GLY	LEU	GLY	THR	GLY	ASN	ASP	THR	THR	VAL	THR	VAL	GLU	GLY	THR	LEU	GLY	THR	PRO			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	543321	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	0.551	Depositor
Minimum map value	-0.328	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	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	0.81	0/3808	1.30	21/5167 (0.4%)
1	B	0.79	0/3808	1.29	18/5167 (0.3%)
All	All	0.80	0/7616	1.29	39/10334 (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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	ARG	CD-NE-CZ	12.97	142.55	124.40
1	A	496	ARG	NE-CZ-NH1	-10.36	111.14	121.50
1	B	496	ARG	CD-NE-CZ	10.09	138.53	124.40
1	A	496	ARG	NE-CZ-NH2	9.72	127.95	119.20
1	A	195	TYR	N-CA-CB	-9.17	97.30	111.05
1	B	496	ARG	NE-CZ-NH2	8.98	127.28	119.20
1	B	475	ARG	CB-CA-C	-8.78	97.03	110.90
1	B	496	ARG	N-CA-CB	-8.76	96.10	110.81
1	B	195	TYR	N-CA-CB	-8.21	98.73	111.05
1	A	496	ARG	N-CA-CB	-8.18	96.48	111.13
1	B	412	GLN	N-CA-CB	-7.95	98.80	110.49
1	B	496	ARG	NE-CZ-NH1	-7.04	114.46	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	TYR	CB-CA-C	6.93	123.26	110.24
1	A	194	THR	CA-CB-OG1	-6.65	99.63	109.60
1	B	193	PHE	CB-CA-C	-6.59	100.67	110.62
1	A	190	LEU	N-CA-CB	6.40	119.53	110.12
1	A	496	ARG	CB-CG-CD	-6.22	96.99	111.30
1	B	475	ARG	N-CA-CB	6.13	118.96	110.07
1	B	195	TYR	CB-CA-C	5.92	121.38	110.24
1	B	280	ASN	CB-CA-C	-5.66	98.47	110.31
1	A	91	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	424	THR	OG1-CB-CG2	-5.60	98.09	109.30
1	A	193	PHE	N-CA-CB	-5.59	102.19	110.90
1	A	205	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	446	ARG	CB-CA-C	-5.54	101.20	110.56
1	A	397	HIS	CA-CB-CG	-5.50	108.30	113.80
1	A	469	THR	CA-CB-OG1	-5.43	101.45	109.60
1	B	193	PHE	N-CA-C	5.40	117.64	108.02
1	A	276	GLU	CB-CA-C	-5.39	102.18	110.81
1	A	496	ARG	CG-CD-NE	-5.38	100.17	112.00
1	B	439	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	469	THR	CA-CB-OG1	-5.32	101.62	109.60
1	B	197	LYS	CB-CA-C	-5.30	99.83	109.38
1	A	115	ASP	CB-CA-C	-5.27	102.89	111.06
1	B	179	LYS	CB-CG-CD	5.20	123.26	111.30
1	A	315	PRO	CB-CA-C	-5.19	102.33	111.21
1	A	179	LYS	CB-CG-CD	5.08	122.98	111.30
1	B	317	ARG	CA-CB-CG	-5.07	103.97	114.10
1	A	193	PHE	N-CA-C	5.04	116.51	107.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	ARG	Sidechain
1	B	201	GLY	Peptide
1	B	337	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	3731	3577	3666	37	0
1	B	3731	3577	3666	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	180	0	0	8	0
3	B	218	0	0	7	0
All	All	7862	7154	7332	72	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.

All (72) 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:B:169:ASP:OD2	3:B:2101:HOH:O	1.92	0.88
1:B:399:GLU:OE2	3:B:2102:HOH:O	1.92	0.85
1:A:399:GLU:OE2	3:A:2101:HOH:O	1.94	0.84
1:A:169:ASP:OD2	3:A:2102:HOH:O	2.04	0.74
1:A:170:ILE:HD11	1:A:193:PHE:CE1	2.28	0.69
1:A:260:ASP:OD1	3:A:2103:HOH:O	2.12	0.67
1:B:283:CYS:SG	1:B:284:CYS:SG	2.90	0.67
1:A:394:ASP:OD2	3:A:2104:HOH:O	2.14	0.65
1:B:195:TYR:O	1:B:196:ARG:HG3	2.02	0.60
1:B:146:ILE:HG23	3:B:2105:HOH:O	2.02	0.59
1:A:264:LEU:C	1:A:264:LEU:HD23	2.27	0.59
1:B:283:CYS:HG	1:B:284:CYS:HG	1.30	0.59
1:A:194:THR:OG1	1:A:195:TYR:N	2.37	0.57
1:A:309:SER:OG	1:A:357:ASN:O	2.17	0.56
1:B:142:PHE:HB2	1:B:410:GLU:HB3	1.89	0.55
1:A:91:ASP:N	1:A:91:ASP:OD1	2.40	0.53
1:A:195:TYR:O	1:A:196:ARG:HG3	2.07	0.53
1:A:228:THR:OG1	1:A:230:ASP:OD1	2.18	0.52
1:A:65:CYS:SG	1:A:145:LYS:NZ	2.79	0.52
1:B:190:LEU:HD23	1:B:196:ARG:HD2	1.90	0.52
1:A:142:PHE:HB2	1:A:410:GLU:HB3	1.92	0.51
1:B:194:THR:HG21	1:B:216:ASN:HD21	1.75	0.51
1:B:207:GLU:HA	1:B:207:GLU:OE1	2.12	0.50
1:B:394:ASP:OD2	3:B:2103:HOH:O	2.19	0.50
1:B:142:PHE:HB3	3:B:2105:HOH:O	2.12	0.50
1:A:209:ASP:OD2	1:A:237:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HD3	1:A:56:LEU:CD2	2.41	0.50
1:B:209:ASP:OD2	1:B:237:LYS:NZ	2.44	0.49
1:B:194:THR:HG21	1:B:216:ASN:ND2	2.27	0.49
1:A:422:LEU:HD12	1:A:422:LEU:C	2.37	0.48
1:B:503:ASP:O	1:B:506:SER:OG	2.29	0.47
1:A:142:PHE:CD2	1:A:410:GLU:O	2.68	0.47
1:B:77:ILE:HD11	1:B:127:PHE:HE1	1.79	0.47
1:A:77:ILE:HB	1:A:78:PRO:HD3	1.97	0.47
1:B:195:TYR:O	1:B:196:ARG:CG	2.63	0.47
1:A:503:ASP:O	1:A:506:SER:OG	2.32	0.46
1:A:203:MET:CE	3:A:2262:HOH:O	2.63	0.46
1:A:199:TYR:CD2	1:A:204:PHE:HA	2.51	0.46
1:B:307:PRO:HG2	1:B:364:MET:HG2	1.97	0.46
1:B:421:HIS:CE1	3:B:2206:HOH:O	2.69	0.46
1:B:60:GLU:OE1	1:B:64:ARG:NE	2.45	0.46
1:B:77:ILE:HD11	1:B:127:PHE:CE1	2.51	0.46
1:A:194:THR:HG21	1:A:216:ASN:ND2	2.31	0.45
1:A:397:HIS:ND1	3:A:2101:HOH:O	2.14	0.45
1:B:142:PHE:CD2	1:B:410:GLU:O	2.70	0.45
1:B:228:THR:OG1	1:B:230:ASP:OD1	2.34	0.45
1:A:283:CYS:SG	1:A:284:CYS:SG	2.95	0.44
1:A:195:TYR:O	1:A:196:ARG:CG	2.65	0.44
1:A:264:LEU:HD23	1:A:264:LEU:O	2.17	0.44
1:A:380:ASP:O	1:A:381:TYR:C	2.58	0.44
1:B:307:PRO:O	1:B:360:ALA:HB2	2.17	0.44
1:B:193:PHE:HB3	1:B:195:TYR:O	2.18	0.44
1:A:429:ALA:HB1	1:A:483:ARG:CZ	2.48	0.43
1:A:80:LEU:HD11	1:A:127:PHE:HB2	1.99	0.43
1:B:380:ASP:O	1:B:381:TYR:C	2.60	0.43
1:A:428:ASN:ND2	3:A:2119:HOH:O	2.50	0.43
1:B:419:TYR:CE2	1:B:421:HIS:HB2	2.54	0.43
1:B:160:PHE:CE2	1:B:192:ALA:HB1	2.53	0.43
1:A:170:ILE:HD11	1:A:193:PHE:HE1	1.82	0.42
1:A:476:ILE:O	1:A:477:TYR:C	2.61	0.42
1:B:190:LEU:HD23	1:B:196:ARG:CD	2.49	0.42
1:A:160:PHE:CE2	1:A:192:ALA:HB1	2.55	0.42
1:B:169:ASP:OD1	3:B:2104:HOH:O	2.21	0.41
1:B:193:PHE:O	1:B:196:ARG:NH2	2.53	0.41
1:A:230:ASP:OD1	1:A:230:ASP:N	2.53	0.41
1:B:199:TYR:CD2	1:B:204:PHE:HA	2.56	0.41
1:B:240:VAL:HA	1:B:293:ILE:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PHE:CB	1:B:410:GLU:HB3	2.51	0.40
1:B:422:LEU:C	1:B:422:LEU:HD12	2.46	0.40
1:A:257:GLY:O	1:A:259:ASN:N	2.54	0.40
1:A:457:ARG:HA	1:A:500:GLN:O	2.21	0.40
1:A:203:MET:HE3	3:A:2262:HOH:O	2.21	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	473/919 (52%)	453 (96%)	16 (3%)	4 (1%)	16	12
1	B	473/919 (52%)	452 (96%)	18 (4%)	3 (1%)	21	18
All	All	946/1838 (52%)	905 (96%)	34 (4%)	7 (1%)	20	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	SER
1	B	200	ALA
1	A	203	MET
1	B	196	ARG
1	B	361	SER
1	A	200	ALA
1	A	89	GLY

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	397/761 (52%)	379 (96%)	18 (4%)	24	24
1	B	397/761 (52%)	387 (98%)	10 (2%)	42	47
All	All	794/1522 (52%)	766 (96%)	28 (4%)	32	34

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	48	THR
1	A	68	SER
1	A	90	LEU
1	A	91	ASP
1	A	111	GLU
1	A	146	ILE
1	A	170	ILE
1	A	195	TYR
1	A	203	MET
1	A	272	MET
1	A	361	SER
1	A	362	GLU
1	A	380	ASP
1	A	411	VAL
1	A	430	ILE
1	A	506	SER
1	A	511	VAL
1	B	50	ARG
1	B	90	LEU
1	B	94	THR
1	B	195	TYR
1	B	389	ARG
1	B	467	GLU
1	B	481	LYS
1	B	506	SER
1	B	510	GLU
1	B	511	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	HIS
1	B	116	ASN
1	B	216	ASN
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.

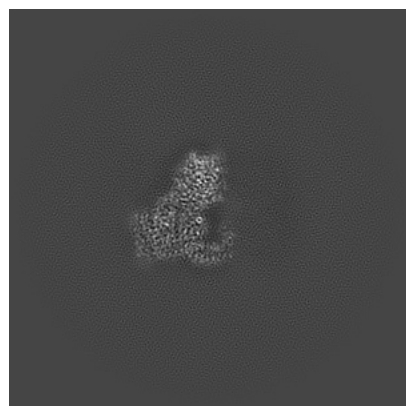
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54976. These allow visual inspection of the internal detail of the map and identification of artifacts.

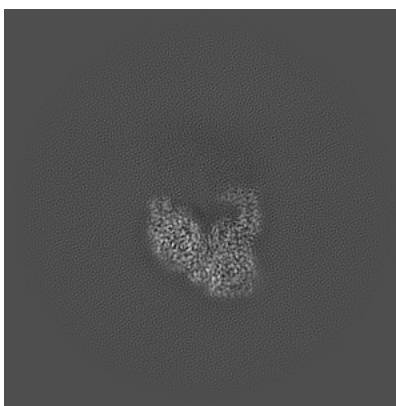
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

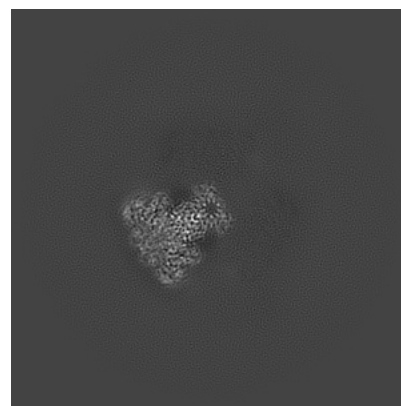
6.1.1 Primary map



X

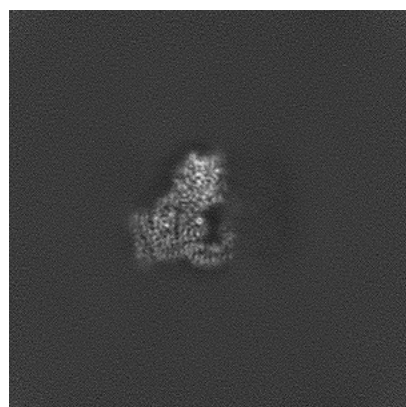


Y

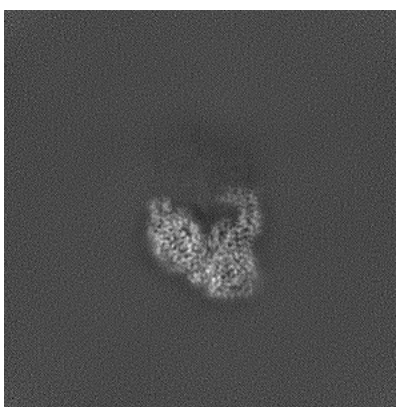


Z

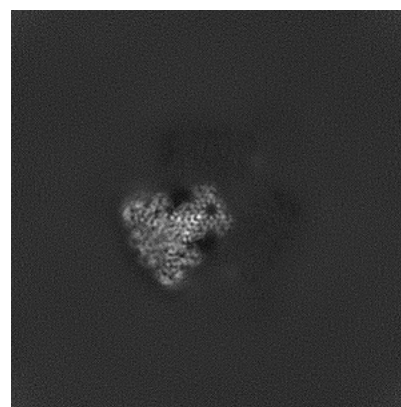
6.1.2 Raw map



X



Y

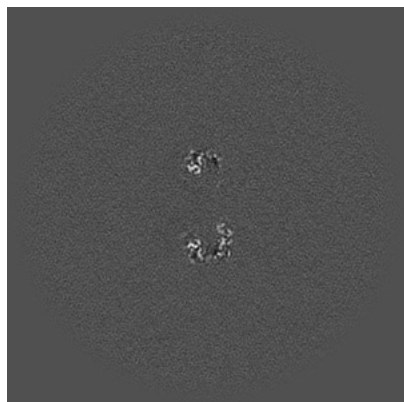


Z

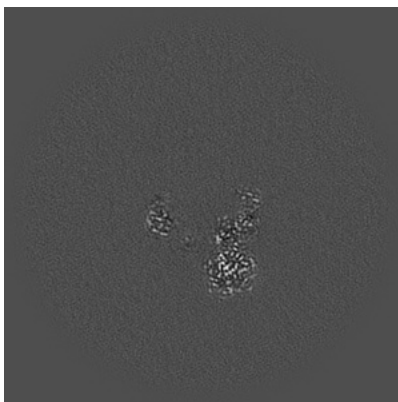
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

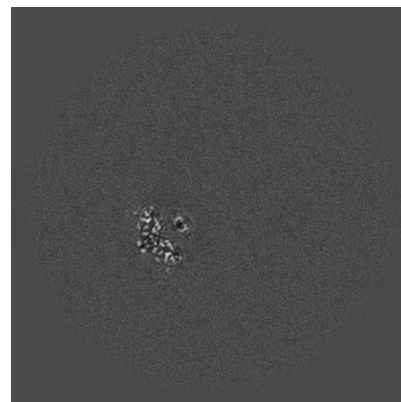
6.2.1 Primary map



X Index: 240



Y Index: 240

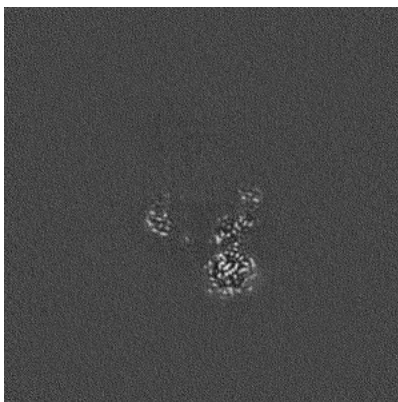


Z Index: 240

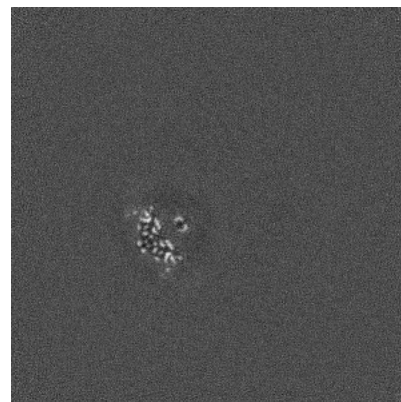
6.2.2 Raw map



X Index: 240



Y Index: 240

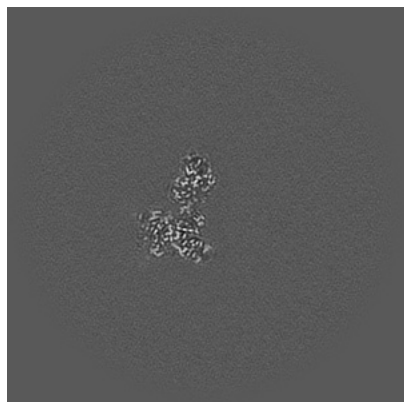


Z Index: 240

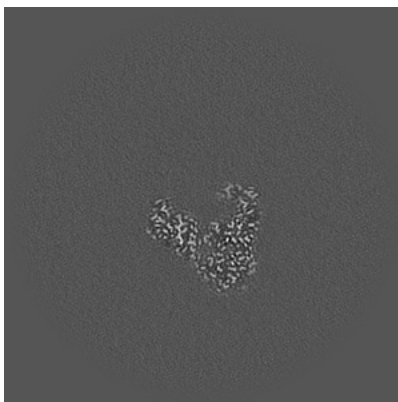
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

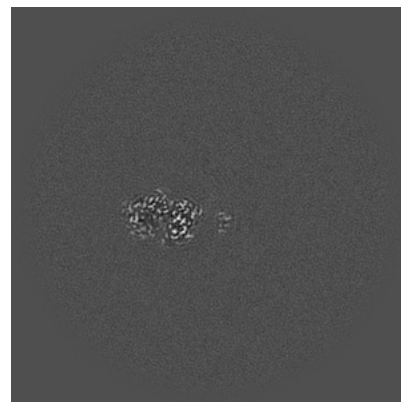
6.3.1 Primary map



X Index: 208

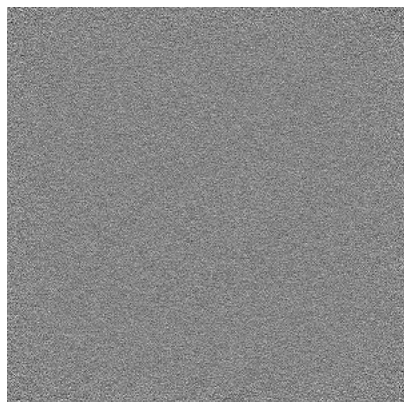


Y Index: 226

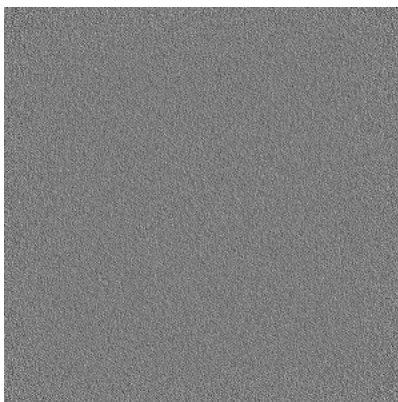


Z Index: 268

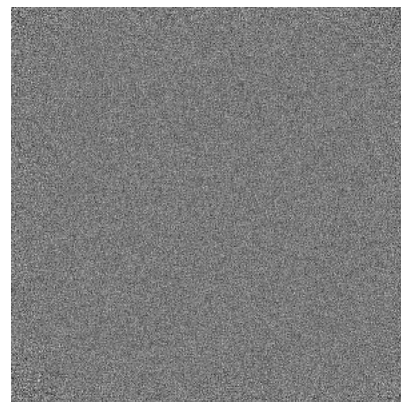
6.3.2 Raw map



X Index: 0



Y Index: 0

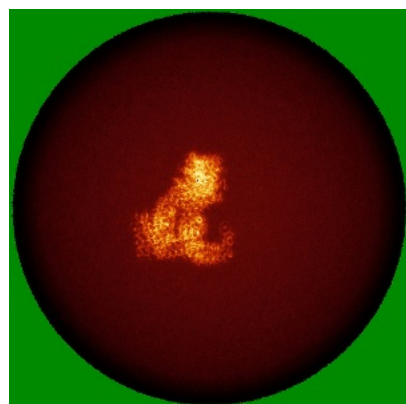


Z Index: 0

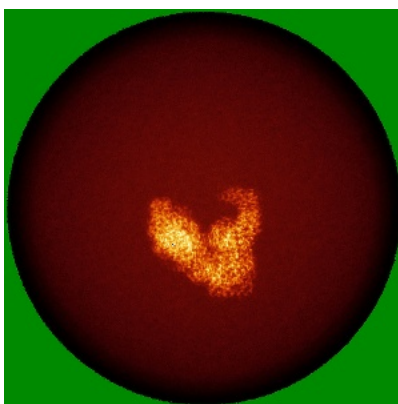
The images above show the largest variance slices of the map in three orthogonal directions.

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

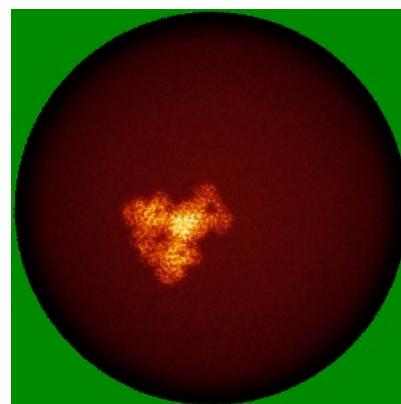
6.4.1 Primary map



X

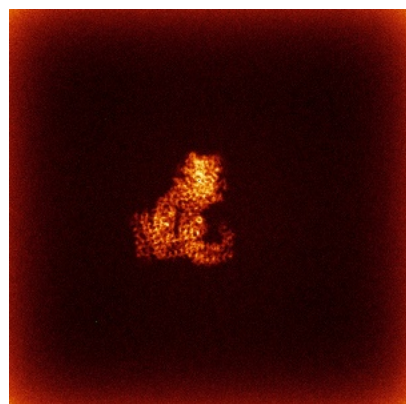


Y

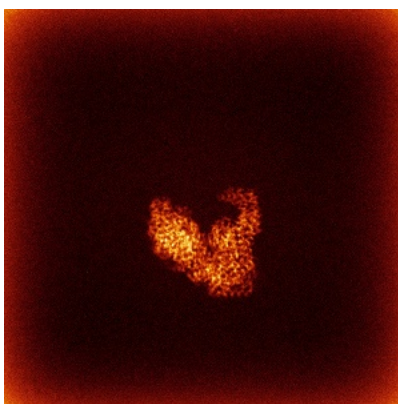


Z

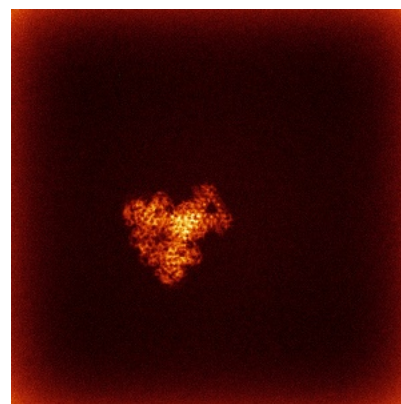
6.4.2 Raw map



X



Y

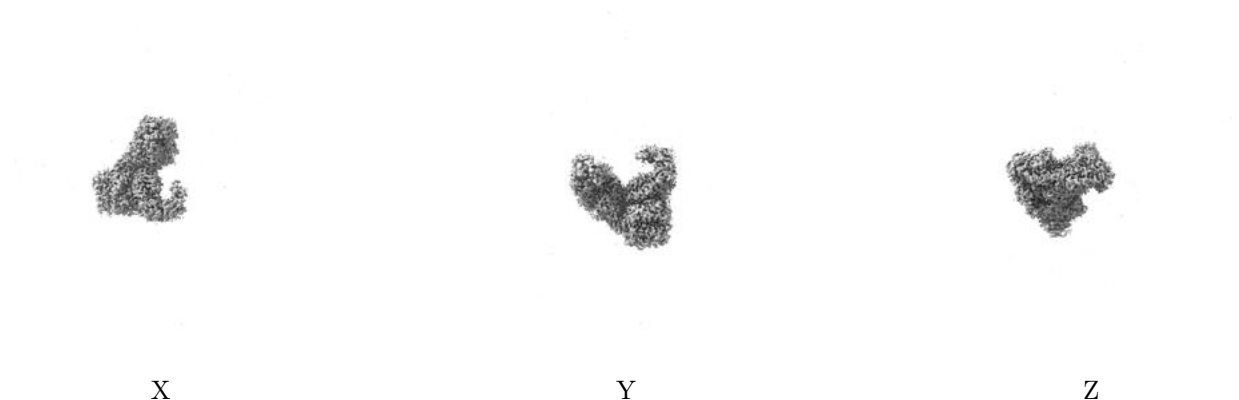


Z

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.

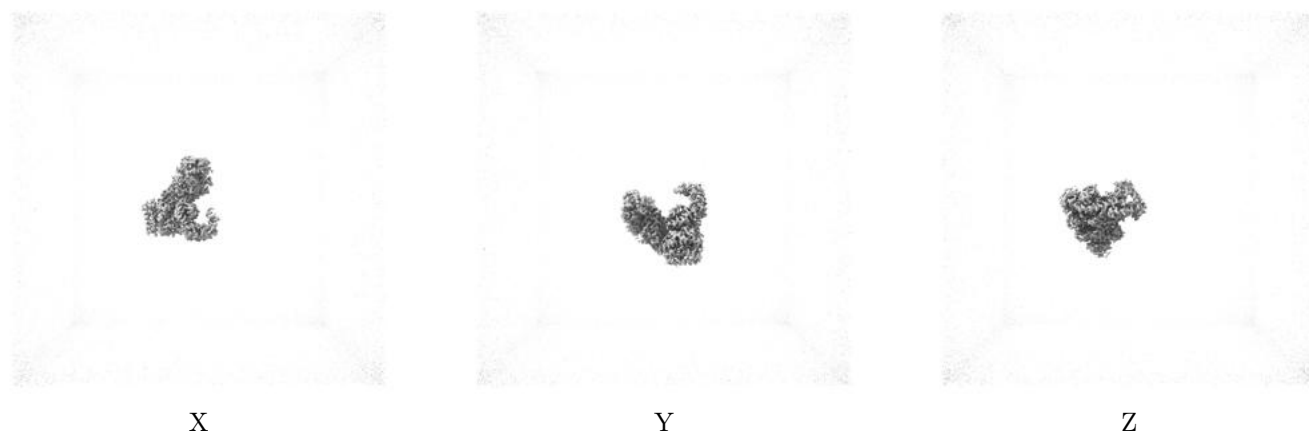
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

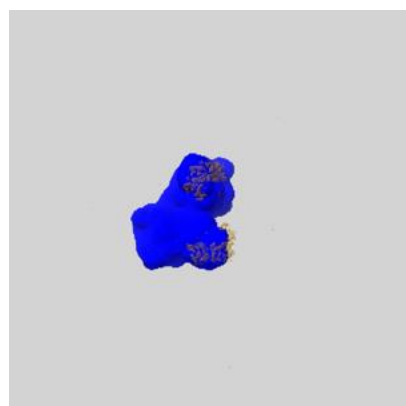
6.6 Mask visualisation [i](#)

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

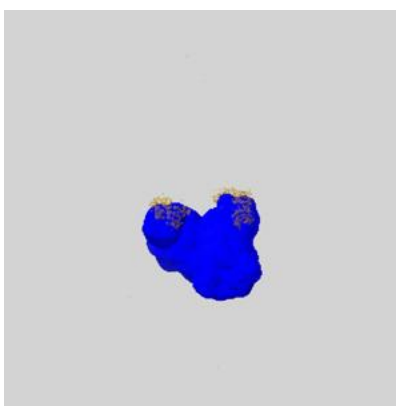
A mask typically either:

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

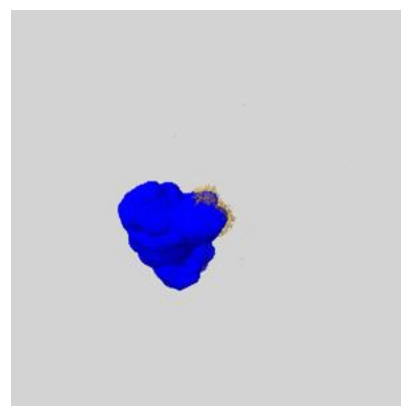
6.6.1 emd_54976_msk_1.map [i](#)



X

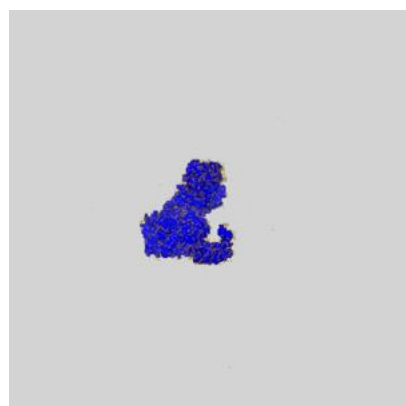


Y

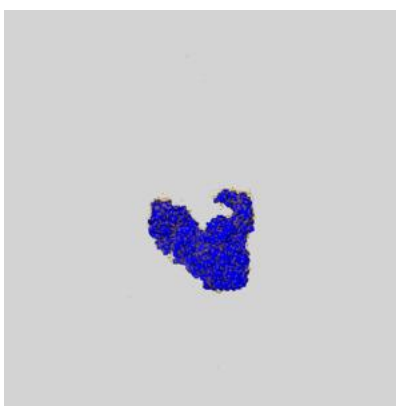


Z

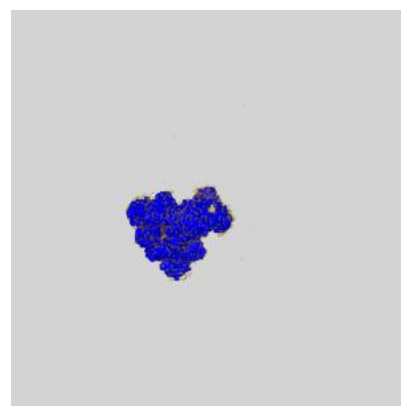
6.6.2 emd_54976_msk_2.map [i](#)



X



Y

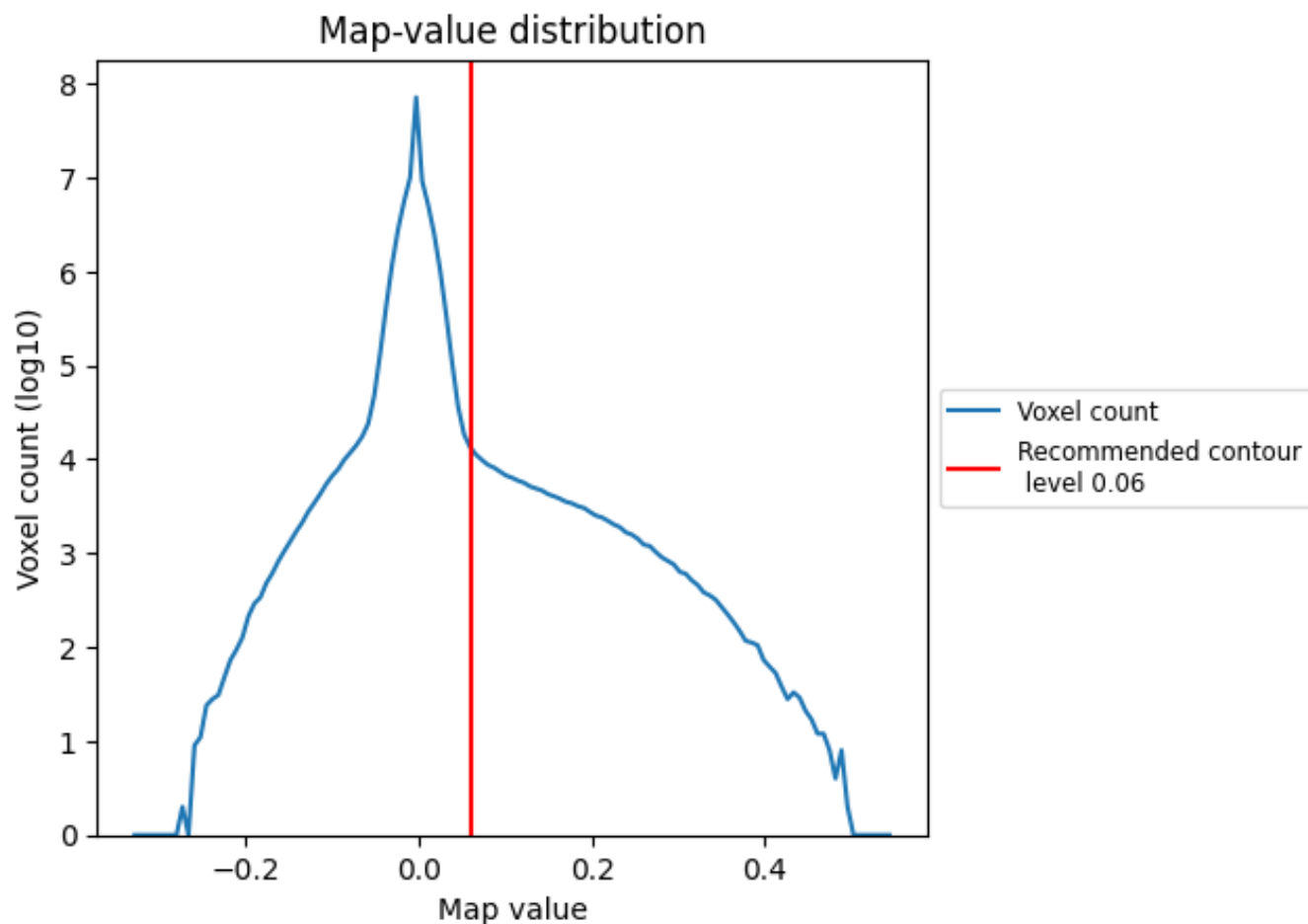


Z

7 Map analysis [i](#)

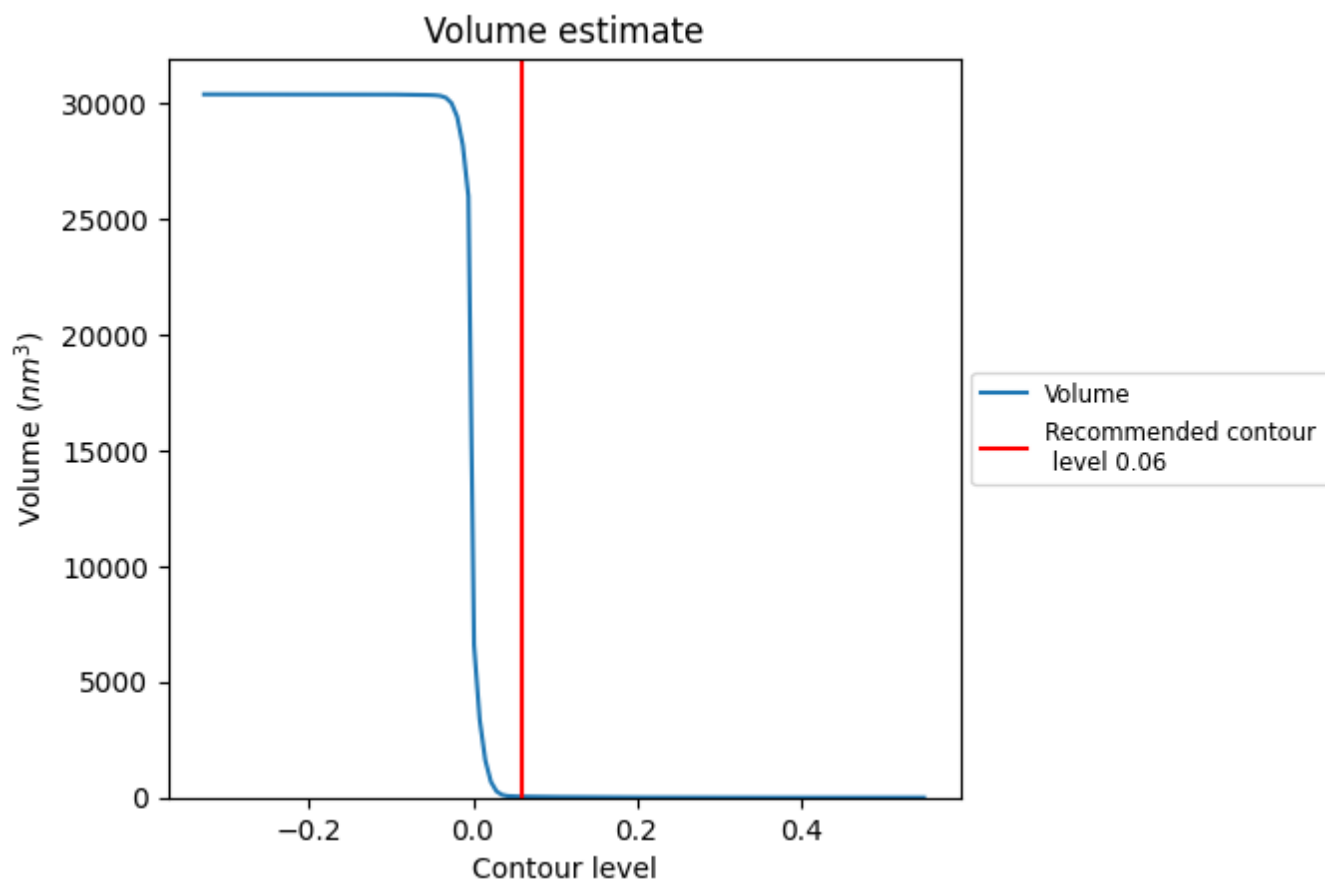
This section contains the results of statistical analysis of the map.

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.

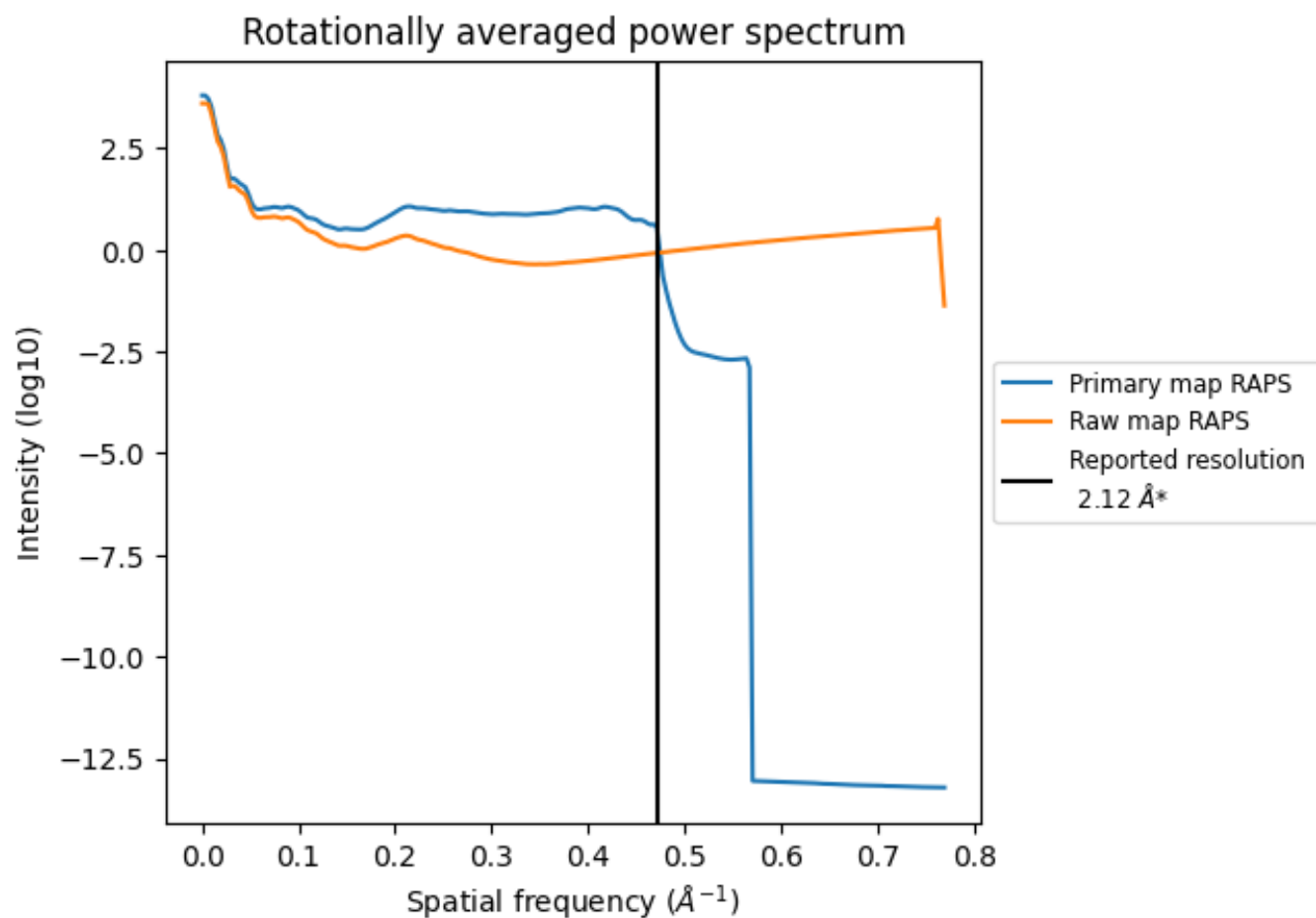
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm³; this corresponds to an approximate mass of 38 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 ⓘ

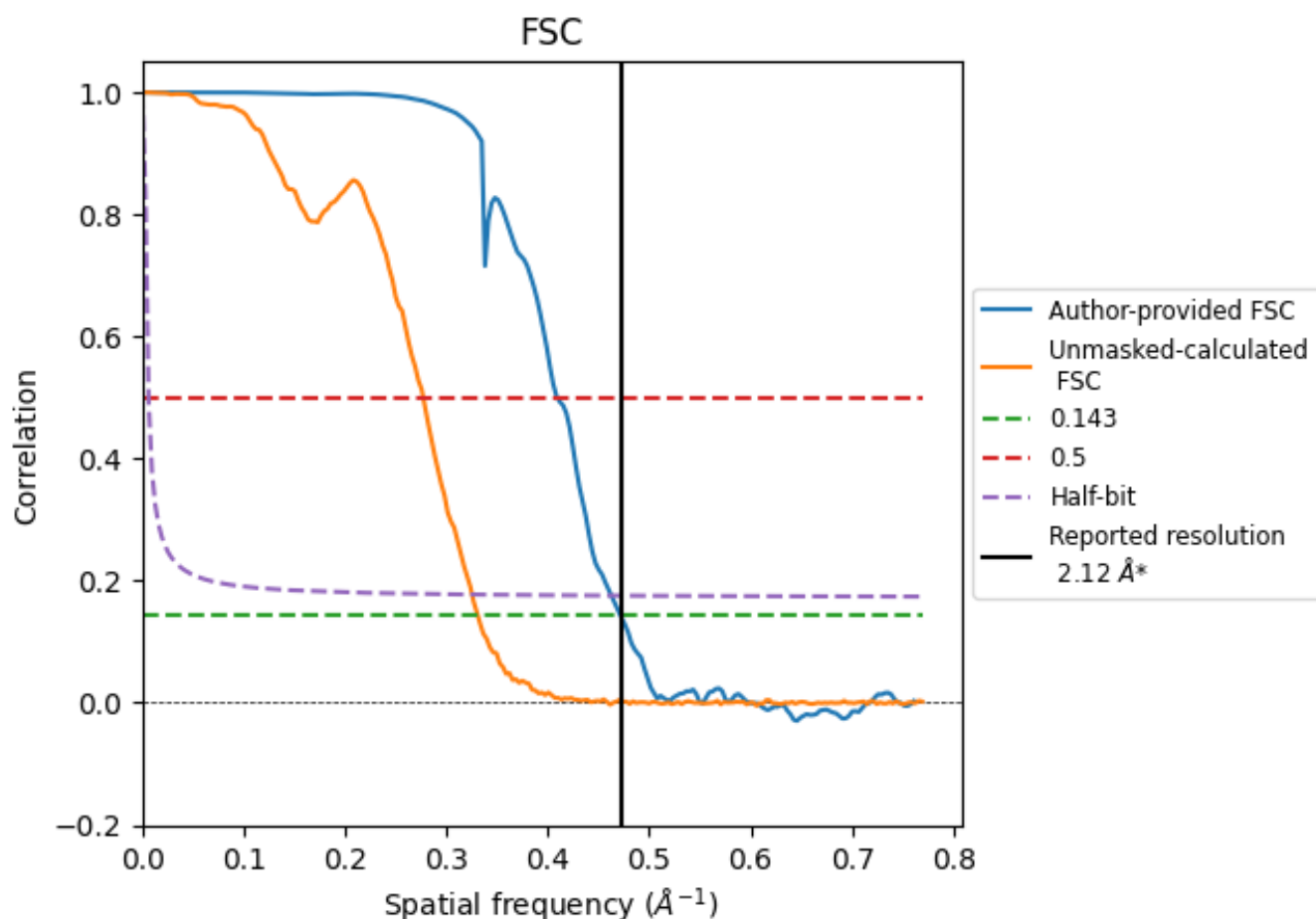


*Reported resolution corresponds to spatial frequency of 0.472 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.472 \AA^{-1}

8.2 Resolution estimates [i](#)

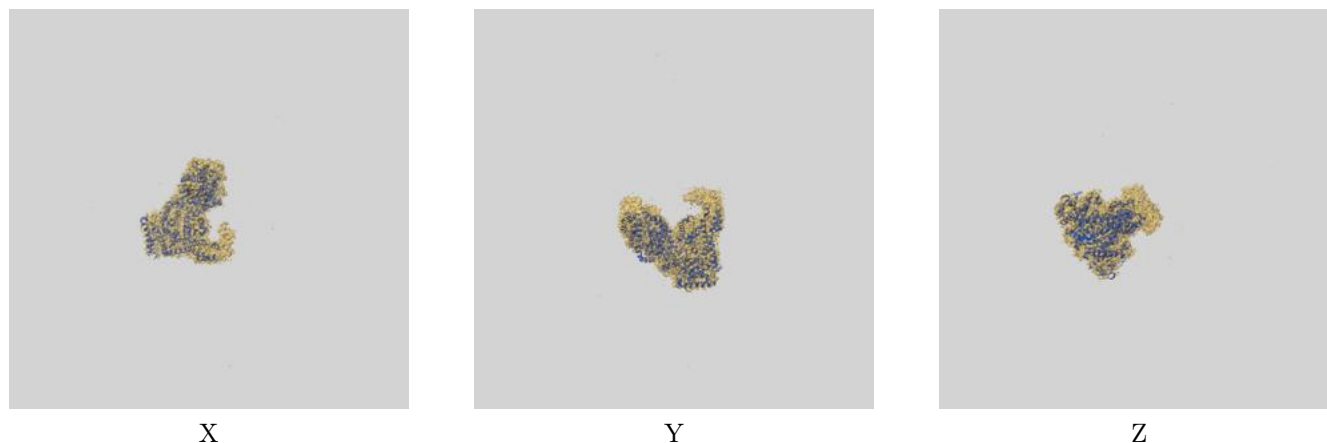
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.12	-	-
Author-provided FSC curve	2.12	2.44	2.16
Unmasked-calculated*	3.02	3.61	3.07

*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 3.02 differs from the reported value 2.12 by more than 10 %

9 Map-model fit [i](#)

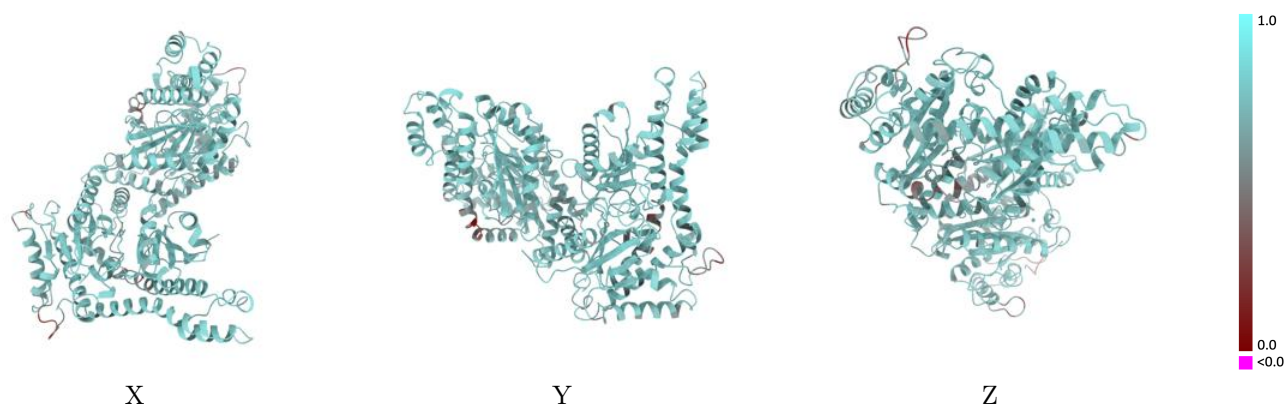
This section contains information regarding the fit between EMDB map EMD-54976 and PDB model 9SKV. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



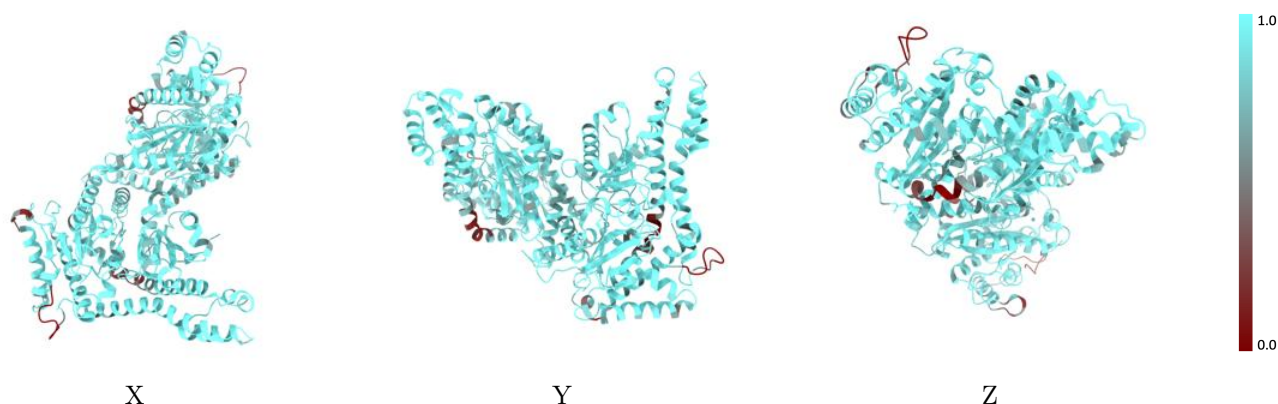
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



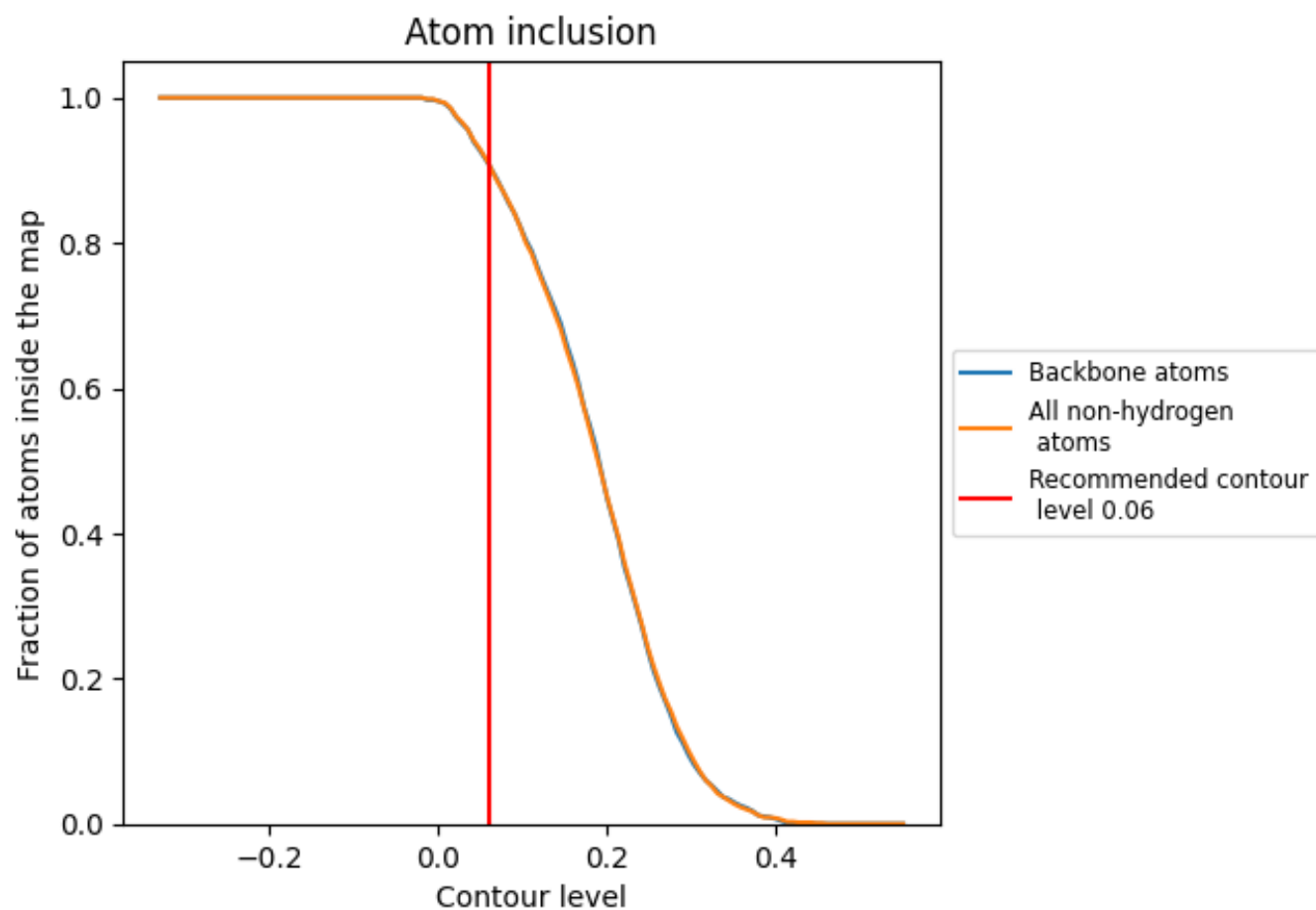
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9100	<div></div> 0.7060
A	<div></div> 0.9090	<div></div> 0.7070
B	<div></div> 0.9090	<div></div> 0.7050

