



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:00 AM UTC

PDB ID : 6V9W / pdb_00006v9w
EMDB ID : EMD-21128
Title : Structure of TRPA1 (ligand-free) with bound calcium, LMNG
Authors : Zhao, J.; Lin King, J.V.; Paulsen, C.E.; Cheng, Y.; Julius, D.
Deposited on : 2019-12-16
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

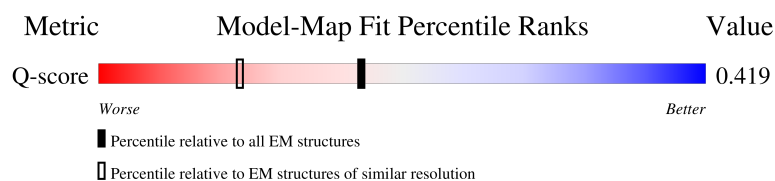
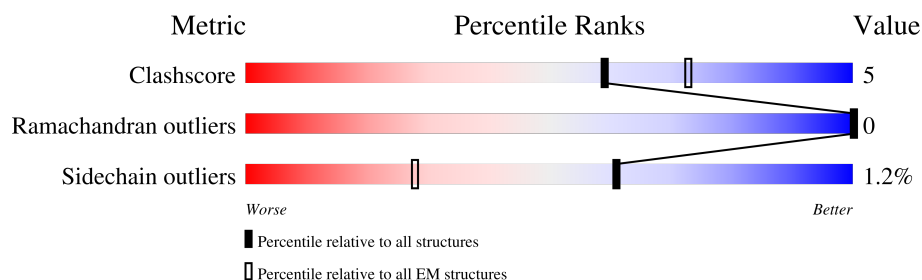
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1119	
1	B	1119	
1	C	1119	
1	D	1119	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18812 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily A member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		
1	B	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		
1	D	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		
1	C	597	Total	C	N	O	S	0	0
			4702	3088	781	799	34		

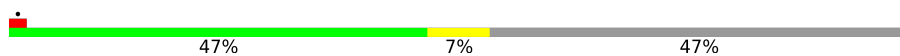
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	966	ASP	GLU	engineered mutation	UNP O75762
B	966	ASP	GLU	engineered mutation	UNP O75762
D	966	ASP	GLU	engineered mutation	UNP O75762
C	966	ASP	GLU	engineered mutation	UNP O75762

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

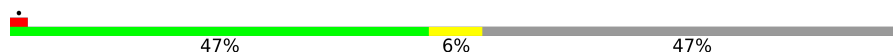
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	

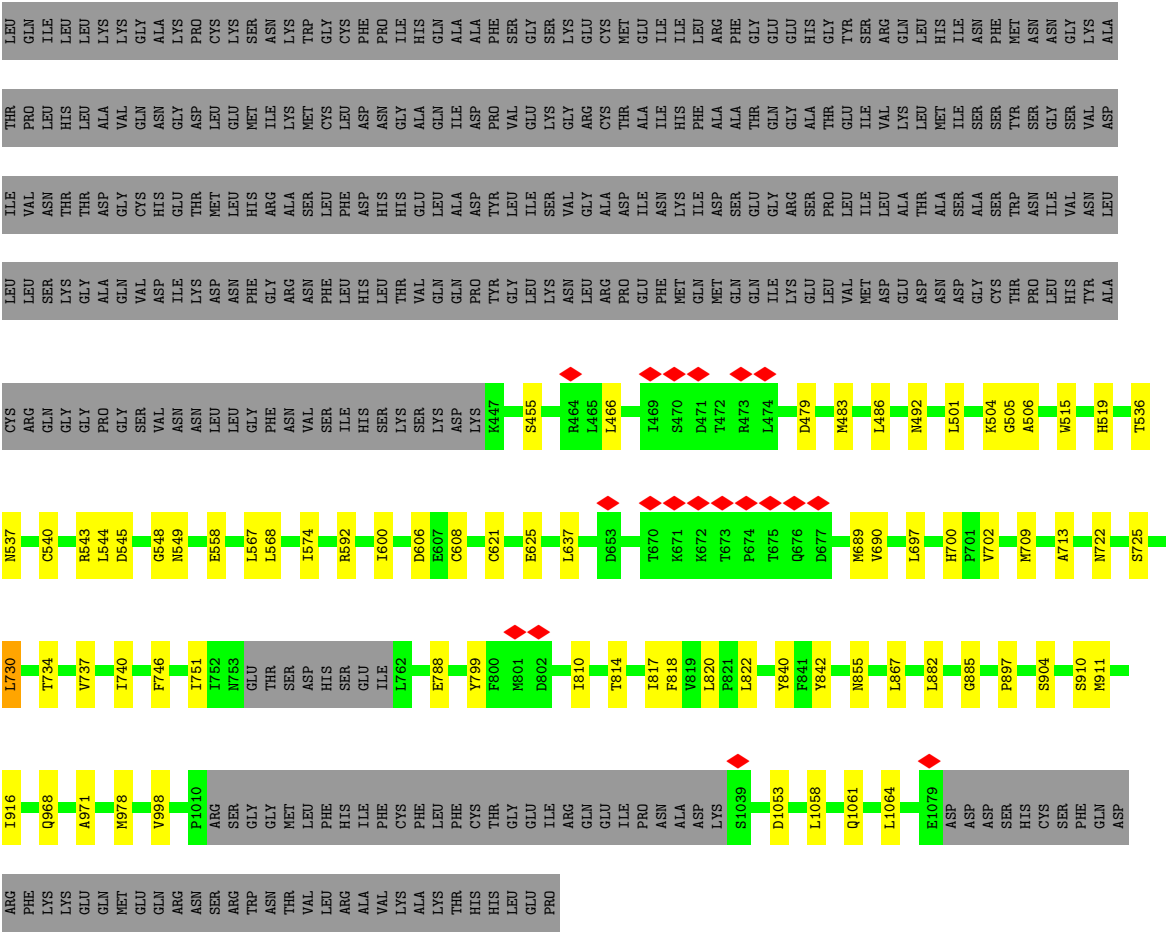
Chain B:



SER	HIS	H700	A883	T516	CYS	LEU	VAL	ILE	THR	LEU	GLN	GLY	ASP	MET	LYS
CYS	P701	H702	P702	H519	GLN	SER	ASN	ASN	PRO	LEU	ASN	ALA	MET	ASP	THR
SER	S910	P702	P702	H519	ARG	LEU	THR	THR	HIS	THR	LEU	PRO	THR	PHE	THR
PHE	E324	W711	L712	T536	GLY	GLY	THR	THR	ALA	VAL	LYS	LEU	PHE	PHE	ARG
ASN	R928	A713	A713	N537	PRO	ALA	ASP	GLY	VAL	VAL	GLY	ARG	LEU	LEU	ARG
ASP	Q968	F716	F716	K539	SER	VAL	CYS	CYS	GLN	HIS	GLY	ASN	HIS	HIS	MET
PHE	Q968	F716	F716	K539	VAL	ASP	GLU	HIS	ASN	GLY	ASN	PHE	TYR	ARG	THR
LYS	A971	N722	N722	C540	ASN	ILE	THR	THR	ASP	ASP	PRO	MET	ALA	ALA	PRO
GLU	A971	N722	N722	C540	ASN	LYS	MET	MET	LEU	LEU	CYS	MET	ALA	ALA	GLY
GLN	R978	S725	S725	R543	LEU	ASN	LEU	LEU	GLU	GLU	LYS	ALA	GLU	GLU	GLU
MET	V998	L730	L730	L544	GLY	PHE	HIS	HIS	MET	MET	SER	PRO	GLY	GLY	LYS
GLN	P1010	T734	T734	E546	ASN	VAL	ALA	ALA	LEU	LEU	ASN	ILE	ILE	ILE	PRO
ASN	ARG	T734	T734	E546	VAL	SER	LEU	LEU	CYS	CYS	GLY	VAL	LEU	LEU	GLY
SER	SER	V737	V737	G548	ILE	SER	PHE	PHE	LEU	LEU	GLY	VAL	MET	MET	GLY
ARG	GLY	V737	V737	G548	ILE	ILE	ASN	ASN	LEU	LEU	GLY	VAL	MET	MET	GLY
TRP	GLY	I740	I740	E558	SER	SER	HIS	HIS	ASP	ASP	PHE	GLN	GLU	GLU	VAL
THR	MET	I740	I740	E558	LYS	LYS	THR	THR	ASN	ASN	PRO	GLY	LYS	LYS	VAL
VAL	PHE	F746	F746	L567	SER	VAL	GLU	GLU	ALA	ALA	GLN	ASN	THR	THR	GLU
LEU	HIS	I751	I751	I574	LYS	GLN	LEU	LEU	ILE	ILE	ALA	GLU	ARG	ASP	ASP
ALA	ILE	I752	I752	R592	ASP	PRO	ASP	ASP	ASN	ASN	ALA	VAL	SER	ASP	PRO
ARG	PHE	N753	N753	R592	LYS	TYR	TYR	TYR	LEU	LEU	PHE	MET	SER	SER	ASN
VAL	CYS	GLU	GLU	R592	GLY	LEU	LEU	LEU	GLY	GLY	ASN	LEU	LEU	LEU	VAL
LYS	PHE	THR	THR	V595	LYS	LYS	ILE	ILE	GLU	GLU	SER	VAL	GLU	GLU	THR
ALA	LEU	SER	SER	V595	SER	LYS	SER	ASN	LYS	LYS	LEU	LEU	VAL	VAL	ASP
LYS	PHE	ASP	ASP	T598	ASN	ASN	VAL	VAL	ASN	GLY	LYS	LEU	LEU	LEU	GLU
THR	CYS	HIS	HIS	T598	LEU	LEU	GLY	GLY	ARG	ARG	GLY	GLU	HIS	HIS	PHE
HIS	THR	SER	SER	I599	ARG	ARG	ALA	ALA	CYS	CYS	GLY	GLY	GLU	GLY	LYS
GLU	GLY	GLU	GLU	I600	PRO	PRO	ALA	ALA	MET	MET	MET	ARG	MET	MET	GLU
LEU	GLU	ILE	ILE	D606	GLU	GLU	ILE	ILE	ALA	ALA	ILE	ILE	ASP	ASP	SER
GLU	ILE	L762	L762	E697	PHE	PHE	ASN	ASN	ILE	ILE	ILE	ILE	ASP	ASP	LEU
ARG	ARG	L776	L776	G608	MET	MET	LYS	LYS	HIS	HIS	ILE	ASP	TYR	TYR	LYS
GLN	GLU	L776	L776	G608	GLN	GLN	ILE	ILE	PHE	PHE	VAL	VAL	GLY	GLY	VAL
ILE	ILE	M801	M801	C621	MET	GLN	ILE	ILE	ALA	ALA	ARG	ASN	THR	THR	PHE
PRO	PRO	D802	D802	E625	GLN	GLN	GLU	GLU	THR	THR	GLY	GLU	PRO	PRO	GLY
ASN	ASN	L810	L810	L637	ILE	ILE	GLY	GLY	GLN	GLN	GLY	GLY	LEU	LEU	SER
ASP	ASP	I810	I810	L637	LYS	LYS	ARG	SER	ALA	ALA	HIS	ASN	CYS	CYS	ALA
GLN	GLN	T814	T814	S645	GLU	GLU	ARG	ALA	GLU	GLU	GLY	GLY	ALA	ALA	TYR
ILE	ILE	S1039	S1039	S645	GLN	LEU	PRO	PRO	THR	THR	TYR	GLY	VAL	VAL	GLY
PRO	PRO	D1053	D1053	D653	LYS	ASP	ILE	ILE	ILE	ILE	SER	THR	GLU	GLU	GLN
ASN	ASN	F818	F818	P674	GLY	MET	LEU	LEU	VAL	VAL	ARG	ALA	LYS	LYS	GLN
ASN	ASN	L820	L820	K671	ASP	ASP	THR	THR	GLY	GLY	GLN	VAL	ASN	ASN	ASN
GLU	GLU	Y840	Y840	K672	ASN	ASN	ASN	ASN	ASN	ASN	LEU	VAL	GLN	PHE	PHE
GLU	GLU	Y842	Y842	P674	CYS	CYS	THR	THR	GLY	GLY	ASN	THR	VAL	VAL	LYS
GLU	GLU	N855	N855	T675	PRO	PRO	ASN	ASN	THR	THR	ASN	MET	LYS	LYS	LEU
GLU	GLU	T1077	T1077	Q676	THR	THR	ILE	ILE	SER	SER	ASN	THR	VAL	VAL	LEU
GLU	GLU	E1079	E1079	Q677	ASN	ASN	GLY	GLY	GLY	GLY	ASN	ASN	PHE	PHE	LEU
GLU	GLU	L880	L880	D677	LEU	LEU	VAL	VAL	GLY	GLY	ASN	ASN	LEU	LEU	LYS
GLU	GLU	L881	L881	M689	HIS	HIS	ILE	ILE	ASN	ASN	GLY	GLY	LEU	LEU	LYS
GLU	GLU	L882	L882	V690	TYR	TYR	ASN	ASN	VAL	VAL	LYS	GLU	SER	SER	ASP
GLU	GLU	L897	L897	V690	ALA	ALA	LEU	LEU	ASP	ASP	ALA	ALA	ARG	ARG	CYS
GLU	GLU	L897	L897	V690	ALA	ALA	LEU	LEU	ASP	ASP	ALA	ALA	ARG	ARG	CYS

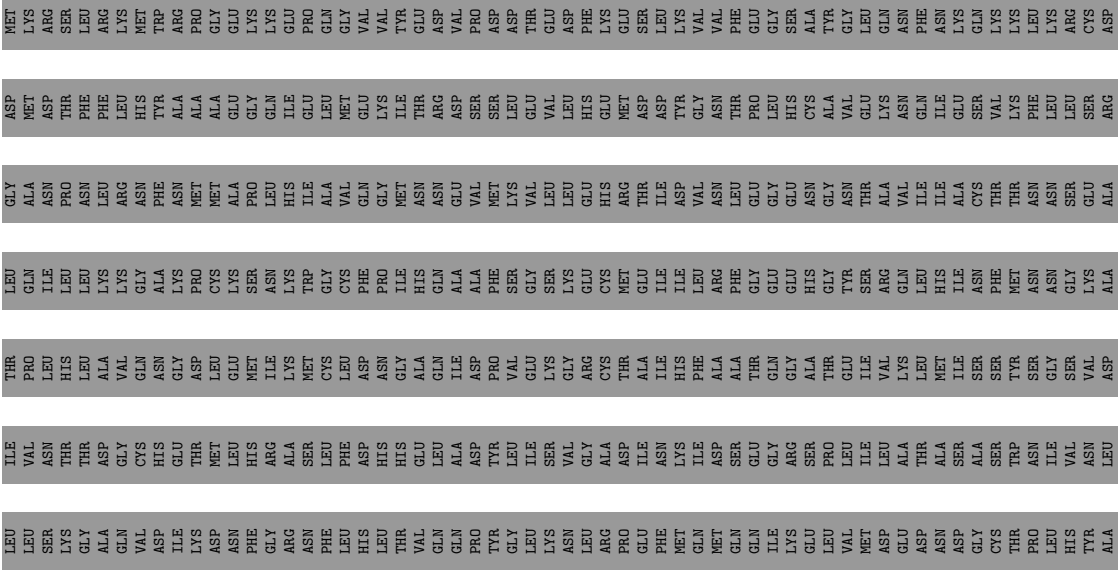
Chain D:

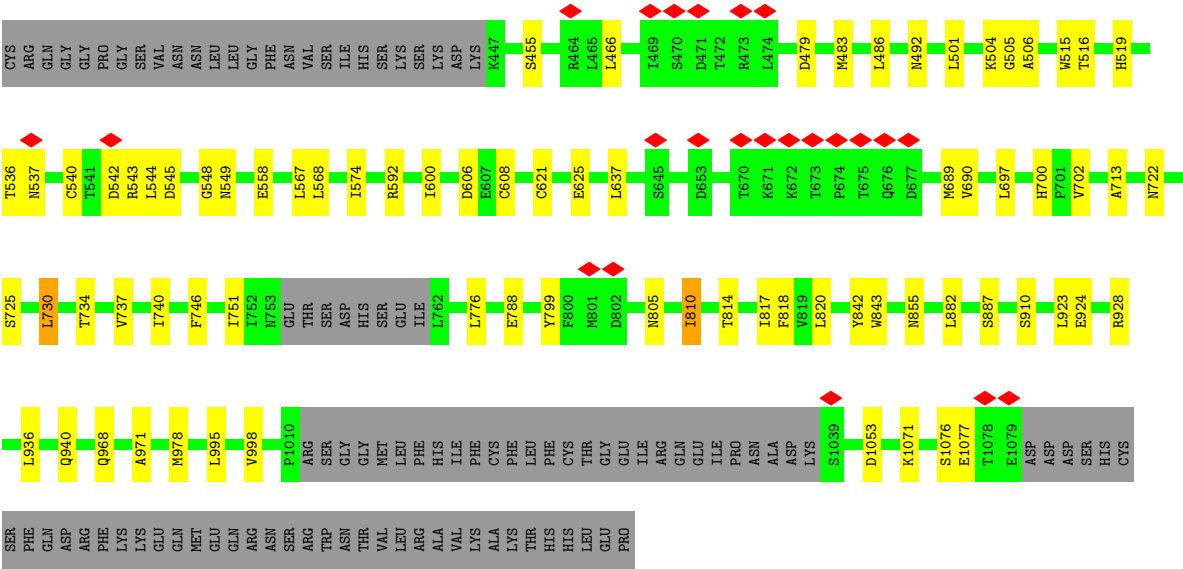
[illegible]



● Molecule 1: Transient receptor potential cation channel subfamily A member 1

Chain C: 47% 7% 47%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	130595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	33.166	Depositor
Minimum map value	-14.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.8	Depositor
Map size (Å)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/4810	0.54	0/6527
1	B	0.38	0/4810	0.54	0/6527
1	C	0.38	0/4810	0.54	0/6527
1	D	0.38	0/4810	0.54	0/6527
All	All	0.38	0/19240	0.54	0/26108

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4702	0	4733	48	0
1	B	4702	0	4733	45	0
1	C	4702	0	4733	47	0
1	D	4702	0	4733	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	18812	0	18932	175	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 (175) 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:D:600:ILE:HD11	1:D:637:LEU:HD13	1.75	0.69
1:C:740:ILE:HD12	1:C:751:ILE:HD11	1.75	0.69
1:B:740:ILE:HD12	1:B:751:ILE:HD11	1.75	0.69
1:C:600:ILE:HD11	1:C:637:LEU:HD13	1.75	0.68
1:D:740:ILE:HD12	1:D:751:ILE:HD11	1.75	0.67
1:B:600:ILE:HD11	1:B:637:LEU:HD13	1.75	0.66
1:A:740:ILE:HD12	1:A:751:ILE:HD11	1.75	0.66
1:A:600:ILE:HD11	1:A:637:LEU:HD13	1.75	0.66
1:D:545:ASP:OD1	1:D:549:ASN:N	2.35	0.60
1:D:466:LEU:HD23	1:D:504:LYS:HD2	1.84	0.59
1:C:606:ASP:N	1:C:606:ASP:OD1	2.35	0.59
1:C:466:LEU:HD23	1:C:504:LYS:HD2	1.84	0.59
1:C:817:ILE:HA	1:C:820:LEU:HB2	1.84	0.59
1:B:466:LEU:HD23	1:B:504:LYS:HD2	1.84	0.59
1:A:466:LEU:HD23	1:A:504:LYS:HD2	1.84	0.58
1:B:545:ASP:OD1	1:B:549:ASN:N	2.35	0.58
1:B:817:ILE:HA	1:B:820:LEU:HB2	1.84	0.58
1:A:817:ILE:HA	1:A:820:LEU:HB2	1.84	0.58
1:D:817:ILE:HA	1:D:820:LEU:HB2	1.84	0.57
1:B:730:LEU:HD12	1:B:842:TYR:HB3	1.86	0.57
1:C:730:LEU:HD12	1:C:842:TYR:HB3	1.86	0.57
1:B:606:ASP:OD1	1:B:606:ASP:N	2.35	0.57
1:A:730:LEU:HD12	1:A:842:TYR:HB3	1.86	0.57
1:A:545:ASP:OD1	1:A:549:ASN:N	2.35	0.56
1:A:606:ASP:N	1:A:606:ASP:OD1	2.35	0.56
1:C:689:MET:HE2	1:C:697:LEU:HB3	1.87	0.56
1:B:689:MET:HE2	1:B:697:LEU:HB3	1.87	0.56
1:D:689:MET:HE2	1:D:697:LEU:HB3	1.87	0.56
1:B:1077:GLU:HG2	1:C:1071:LYS:HG2	1.86	0.56
1:D:730:LEU:HD12	1:D:842:TYR:HB3	1.86	0.56
1:C:545:ASP:OD1	1:C:549:ASN:N	2.35	0.56
1:A:689:MET:HE2	1:A:697:LEU:HB3	1.87	0.56
1:D:486:LEU:HD22	1:D:506:ALA:HB3	1.88	0.55
1:B:486:LEU:HD22	1:B:506:ALA:HB3	1.89	0.55
1:C:486:LEU:HD22	1:C:506:ALA:HB3	1.89	0.55
1:A:486:LEU:HD22	1:A:506:ALA:HB3	1.89	0.55
1:A:479:ASP:OD1	1:A:483:MET:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ASP:OD1	1:B:483:MET:N	2.36	0.55
1:B:501:LEU:O	1:B:505:GLY:N	2.39	0.54
1:D:713:ALA:HB1	1:D:998:VAL:HG22	1.90	0.54
1:B:713:ALA:HB1	1:B:998:VAL:HG22	1.90	0.54
1:B:968:GLN:HA	1:B:971:ALA:HB2	1.91	0.53
1:A:713:ALA:HB1	1:A:998:VAL:HG22	1.90	0.53
1:A:968:GLN:HA	1:A:971:ALA:HB2	1.91	0.53
1:C:713:ALA:HB1	1:C:998:VAL:HG22	1.90	0.53
1:D:479:ASP:OD1	1:D:483:MET:N	2.36	0.52
1:C:455:SER:O	1:C:492:ASN:ND2	2.42	0.52
1:A:501:LEU:O	1:A:505:GLY:N	2.39	0.52
1:D:968:GLN:HA	1:D:971:ALA:HB2	1.91	0.52
1:C:542:ASP:OD1	1:C:542:ASP:N	2.40	0.52
1:C:968:GLN:HA	1:C:971:ALA:HB2	1.91	0.52
1:D:501:LEU:O	1:D:505:GLY:N	2.39	0.52
1:B:455:SER:O	1:B:492:ASN:ND2	2.42	0.52
1:A:455:SER:O	1:A:492:ASN:ND2	2.42	0.51
1:B:536:THR:OG1	1:B:537:ASN:N	2.43	0.51
1:D:455:SER:O	1:D:492:ASN:ND2	2.42	0.51
1:C:501:LEU:O	1:C:505:GLY:N	2.39	0.51
1:C:479:ASP:OD1	1:C:483:MET:N	2.36	0.51
1:B:700:HIS:HD2	1:B:702:VAL:HG12	1.76	0.50
1:D:700:HIS:HD2	1:D:702:VAL:HG12	1.76	0.50
1:D:840:TYR:HB2	1:C:887:SER:HB3	1.91	0.50
1:C:700:HIS:HD2	1:C:702:VAL:HG12	1.76	0.50
1:D:574:ILE:HD13	1:D:608:CYS:HB3	1.94	0.50
1:A:700:HIS:HD2	1:A:702:VAL:HG12	1.76	0.50
1:D:606:ASP:OD1	1:D:606:ASP:N	2.36	0.50
1:B:574:ILE:HD13	1:B:608:CYS:HB3	1.94	0.50
1:C:544:LEU:HD23	1:C:548:GLY:HA2	1.94	0.49
1:B:883:ALA:HB2	1:C:843:TRP:HB2	1.93	0.49
1:D:544:LEU:HD23	1:D:548:GLY:HA2	1.94	0.49
1:A:855:ASN:OD1	1:A:855:ASN:N	2.46	0.49
1:C:574:ILE:HD13	1:C:608:CYS:HB3	1.94	0.49
1:A:574:ILE:HD13	1:A:608:CYS:HB3	1.94	0.48
1:C:855:ASN:OD1	1:C:855:ASN:N	2.46	0.48
1:B:558:GLU:HA	1:B:592:ARG:HH21	1.79	0.48
1:C:536:THR:OG1	1:C:537:ASN:N	2.43	0.48
1:A:544:LEU:HD23	1:A:548:GLY:HA2	1.94	0.48
1:B:544:LEU:HD23	1:B:548:GLY:HA2	1.94	0.48
1:D:536:THR:OG1	1:D:537:ASN:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:PHE:HB3	1:D:751:ILE:HD13	1.96	0.48
1:A:558:GLU:HA	1:A:592:ARG:HH21	1.79	0.47
1:A:746:PHE:HB3	1:A:751:ILE:HD13	1.96	0.47
1:D:537:ASN:N	1:D:537:ASN:OD1	2.47	0.47
1:D:855:ASN:OD1	1:D:855:ASN:N	2.46	0.47
1:B:746:PHE:HB3	1:B:751:ILE:HD13	1.96	0.47
1:D:558:GLU:HA	1:D:592:ARG:HH21	1.79	0.47
1:D:515:TRP:HA	1:D:519:HIS:HD2	1.80	0.47
1:C:746:PHE:HB3	1:C:751:ILE:HD13	1.96	0.47
1:A:537:ASN:N	1:A:537:ASN:OD1	2.47	0.47
1:B:515:TRP:HA	1:B:519:HIS:HD2	1.80	0.47
1:C:537:ASN:N	1:C:537:ASN:OD1	2.47	0.47
1:C:558:GLU:HA	1:C:592:ARG:HH21	1.79	0.47
1:A:515:TRP:HA	1:A:519:HIS:HD2	1.80	0.47
1:A:1061:GLN:HE22	1:D:1061:GLN:HG2	1.80	0.46
1:D:540:CYS:HA	1:D:543:ARG:HG3	1.98	0.46
1:B:722:ASN:O	1:B:725:SER:OG	2.33	0.46
1:C:515:TRP:HA	1:C:519:HIS:HD2	1.80	0.46
1:C:722:ASN:O	1:C:725:SER:OG	2.33	0.46
1:B:537:ASN:N	1:B:537:ASN:OD1	2.47	0.46
1:A:540:CYS:HA	1:A:543:ARG:HG3	1.98	0.46
1:D:788:GLU:OE1	1:D:799:TYR:OH	2.32	0.46
1:B:700:HIS:CD2	1:B:702:VAL:HG12	2.51	0.45
1:A:722:ASN:O	1:A:725:SER:OG	2.33	0.45
1:B:540:CYS:HA	1:B:543:ARG:HG3	1.98	0.45
1:D:814:THR:O	1:D:818:PHE:N	2.50	0.45
1:C:814:THR:O	1:C:818:PHE:N	2.50	0.45
1:A:700:HIS:CD2	1:A:702:VAL:HG12	2.51	0.45
1:C:700:HIS:CD2	1:C:702:VAL:HG12	2.51	0.45
1:A:1077:GLU:HG2	1:B:1071:LYS:HG2	1.99	0.45
1:B:814:THR:O	1:B:818:PHE:N	2.50	0.45
1:B:810:ILE:HD12	1:B:810:ILE:HA	1.83	0.45
1:D:700:HIS:CD2	1:D:702:VAL:HG12	2.51	0.45
1:C:540:CYS:HA	1:C:543:ARG:HG3	1.98	0.45
1:A:542:ASP:OD1	1:A:542:ASP:N	2.40	0.44
1:C:776:LEU:HD12	1:C:776:LEU:HA	1.86	0.44
1:A:887:SER:HB3	1:B:840:TYR:HB2	1.99	0.43
1:A:533:ILE:HD12	1:A:533:ILE:HA	1.87	0.43
1:D:621:CYS:N	1:D:625:GLU:OE2	2.52	0.43
1:A:814:THR:O	1:A:818:PHE:N	2.50	0.43
1:B:711:TRP:O	1:B:716:PHE:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:CYS:N	1:C:625:GLU:OE2	2.52	0.43
1:A:1076:SER:OG	1:A:1077:GLU:OE2	2.32	0.43
1:C:810:ILE:HD12	1:C:810:ILE:HA	1.83	0.43
1:B:1067:LEU:HD12	1:B:1067:LEU:HA	1.89	0.43
1:C:1076:SER:OG	1:C:1077:GLU:OE2	2.32	0.43
1:B:595:VAL:O	1:B:598:THR:OG1	2.33	0.43
1:B:1053:ASP:N	1:B:1053:ASP:OD1	2.51	0.43
1:C:799:TYR:O	1:C:805:ASN:ND2	2.47	0.43
1:A:822:LEU:HD23	1:A:822:LEU:HA	1.92	0.42
1:A:1065:ILE:HD13	1:A:1065:ILE:HA	1.87	0.42
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.51	0.42
1:A:1064:LEU:HD12	1:A:1064:LEU:HA	1.88	0.42
1:B:855:ASN:OD1	1:B:855:ASN:N	2.46	0.42
1:C:936:LEU:HD23	1:C:936:LEU:HA	1.88	0.42
1:A:536:THR:OG1	1:A:537:ASN:N	2.43	0.42
1:D:1053:ASP:OD1	1:D:1053:ASP:N	2.51	0.42
1:C:568:LEU:HD23	1:C:568:LEU:HA	1.89	0.42
1:A:486:LEU:HD12	1:A:486:LEU:HA	1.90	0.42
1:A:844:MET:HE3	1:A:844:MET:HB3	1.93	0.42
1:A:568:LEU:HD23	1:A:568:LEU:HA	1.89	0.42
1:B:567:LEU:HD23	1:B:567:LEU:HA	1.79	0.42
1:D:885:GLY:O	1:D:904:SER:OG	2.36	0.42
1:B:880:LEU:HD23	1:B:880:LEU:HA	1.90	0.41
1:D:567:LEU:HA	1:D:567:LEU:HD23	1.79	0.41
1:D:568:LEU:HD23	1:D:568:LEU:HA	1.89	0.41
1:C:1053:ASP:N	1:C:1053:ASP:OD1	2.51	0.41
1:A:741:LYS:HA	1:A:742:PRO:HD3	1.88	0.41
1:A:936:LEU:O	1:A:940:GLN:N	2.50	0.41
1:D:822:LEU:HD23	1:D:822:LEU:HA	1.92	0.41
1:A:799:TYR:O	1:A:805:ASN:ND2	2.47	0.41
1:A:1069:ILE:HD11	1:B:1068:ILE:HG13	2.03	0.41
1:B:496:LYS:O	1:B:500:LEU:N	2.53	0.41
1:D:722:ASN:O	1:D:725:SER:OG	2.33	0.41
1:A:885:GLY:O	1:A:904:SER:OG	2.36	0.41
1:C:788:GLU:OE1	1:C:799:TYR:OH	2.32	0.41
1:A:788:GLU:OE1	1:A:799:TYR:OH	2.32	0.41
1:A:911:MET:HG2	1:A:916:ILE:HG13	2.03	0.41
1:B:621:CYS:N	1:B:625:GLU:OE2	2.52	0.41
1:B:776:LEU:HA	1:B:776:LEU:HD12	1.86	0.41
1:D:1064:LEU:HD12	1:D:1064:LEU:HA	1.88	0.41
1:C:734:THR:HA	1:C:737:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:MET:HE3	1:D:709:MET:HB3	1.96	0.41
1:D:1058:LEU:HD12	1:D:1058:LEU:HA	1.90	0.40
1:B:924:GLU:O	1:B:928:ARG:NE	2.54	0.40
1:D:867:LEU:HD12	1:D:867:LEU:HA	1.93	0.40
1:C:924:GLU:O	1:C:928:ARG:NE	2.54	0.40
1:C:936:LEU:O	1:C:940:GLN:N	2.50	0.40
1:B:516:THR:H	1:B:519:HIS:CD2	2.40	0.40
1:C:567:LEU:HD23	1:C:567:LEU:HA	1.79	0.40
1:A:810:ILE:HA	1:A:810:ILE:HD12	1.83	0.40
1:D:734:THR:HA	1:D:737:VAL:HG12	2.03	0.40
1:D:897:PRO:HA	1:C:923:LEU:HD21	2.02	0.40
1:C:516:THR:H	1:C:519:HIS:CD2	2.40	0.40
1:B:734:THR:HA	1:B:737:VAL:HG12	2.03	0.40
1:D:911:MET:HG2	1:D:916:ILE:HG13	2.03	0.40
1:C:995:LEU:HD13	1:C:995:LEU:HA	1.93	0.40

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	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
1	B	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
1	C	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
1	D	591/1119 (53%)	563 (95%)	28 (5%)	0	100	100
All	All	2364/4476 (53%)	2252 (95%)	112 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	496/995 (50%)	490 (99%)	6 (1%)	63	78
1	B	496/995 (50%)	490 (99%)	6 (1%)	63	78
1	C	496/995 (50%)	490 (99%)	6 (1%)	63	78
1	D	496/995 (50%)	490 (99%)	6 (1%)	63	78
All	All	1984/3980 (50%)	1960 (99%)	24 (1%)	61	78

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	VAL
1	A	730	LEU
1	A	810	ILE
1	A	882	LEU
1	A	910	SER
1	A	978	MET
1	B	690	VAL
1	B	730	LEU
1	B	810	ILE
1	B	882	LEU
1	B	910	SER
1	B	978	MET
1	D	690	VAL
1	D	730	LEU
1	D	810	ILE
1	D	882	LEU
1	D	910	SER
1	D	978	MET
1	C	690	VAL
1	C	730	LEU
1	C	810	ILE
1	C	882	LEU
1	C	910	SER
1	C	978	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	467	GLN
1	A	476	ASN
1	A	519	HIS
1	A	520	HIS
1	A	528	GLN
1	A	580	GLN
1	A	619	ASN
1	A	692	ASN
1	A	700	HIS
1	A	907	GLN
1	A	929	ASN
1	A	1061	GLN
1	B	467	GLN
1	B	476	ASN
1	B	519	HIS
1	B	520	HIS
1	B	528	GLN
1	B	580	GLN
1	B	619	ASN
1	B	644	HIS
1	B	692	ASN
1	B	700	HIS
1	B	893	ASN
1	B	907	GLN
1	B	929	ASN
1	D	467	GLN
1	D	476	ASN
1	D	512	HIS
1	D	519	HIS
1	D	520	HIS
1	D	528	GLN
1	D	549	ASN
1	D	580	GLN
1	D	619	ASN
1	D	692	ASN
1	D	700	HIS
1	D	766	ASN
1	D	893	ASN
1	D	907	GLN
1	D	929	ASN
1	C	467	GLN

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Mol	Chain	Res	Type
1	C	476	ASN
1	C	519	HIS
1	C	520	HIS
1	C	528	GLN
1	C	549	ASN
1	C	580	GLN
1	C	619	ASN
1	C	692	ASN
1	C	700	HIS
1	C	907	GLN
1	C	929	ASN
1	C	1061	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

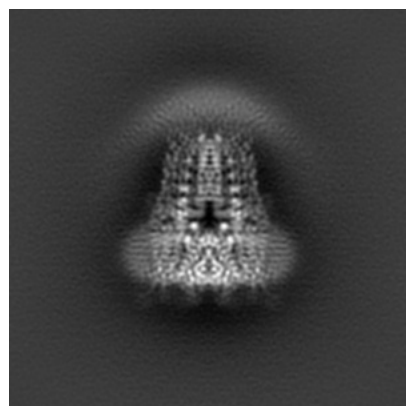
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21128. These allow visual inspection of the internal detail of the map and identification of artifacts.

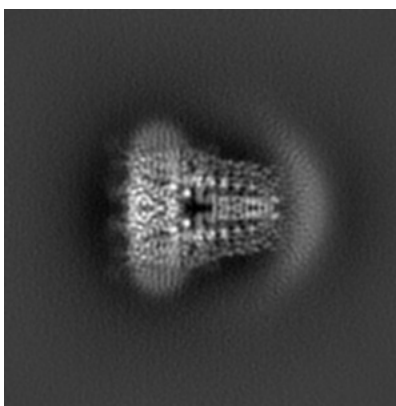
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

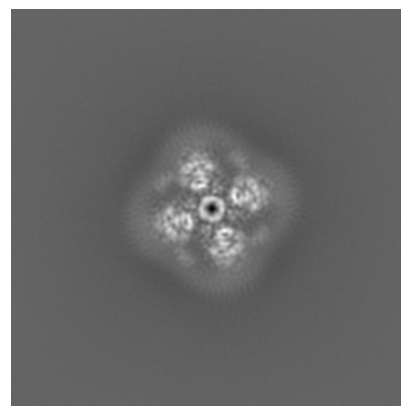
6.1.1 Primary map



X

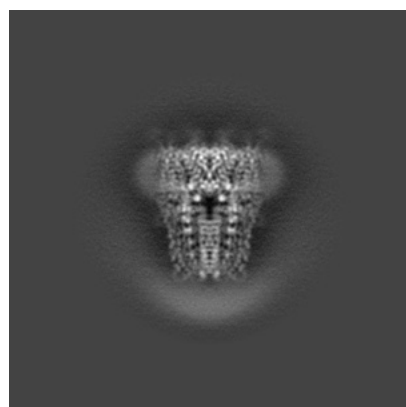


Y

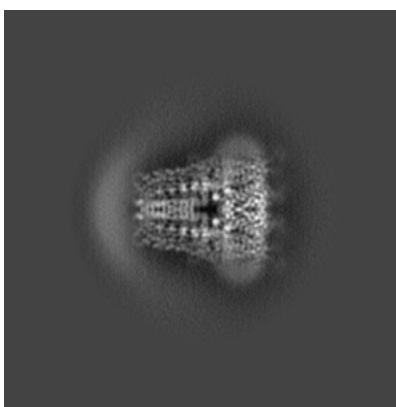


Z

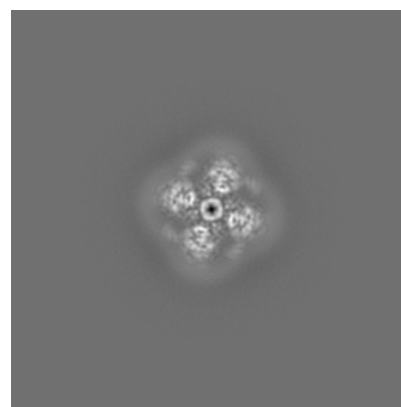
6.1.2 Raw map



X



Y

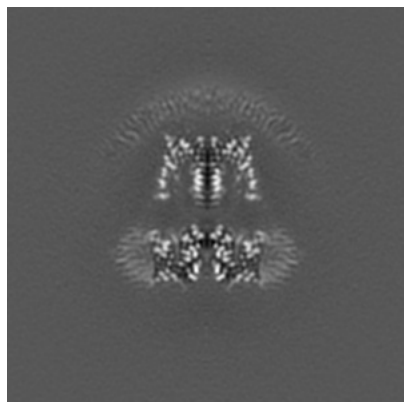


Z

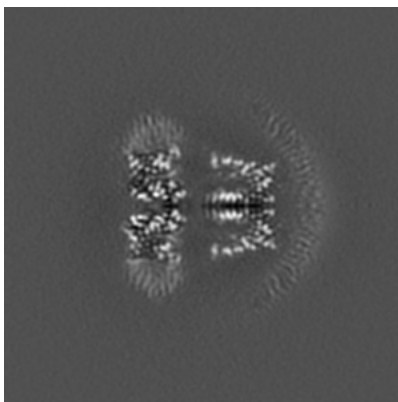
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

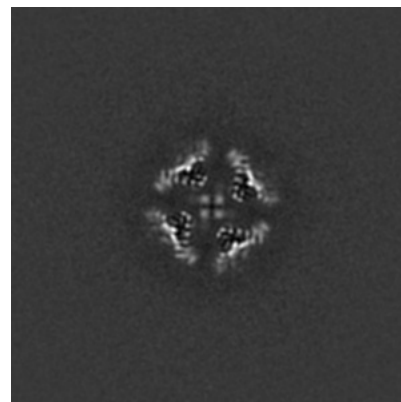
6.2.1 Primary map



X Index: 128

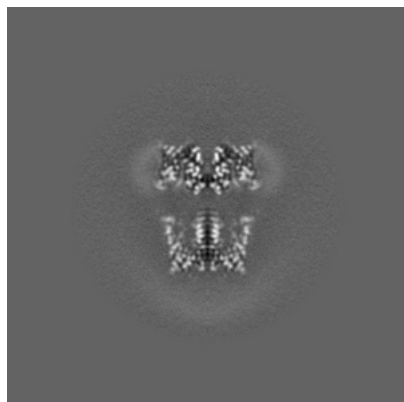


Y Index: 128

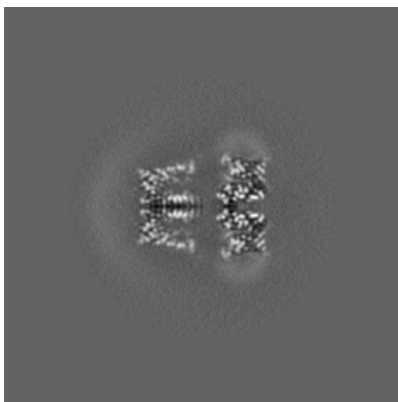


Z Index: 128

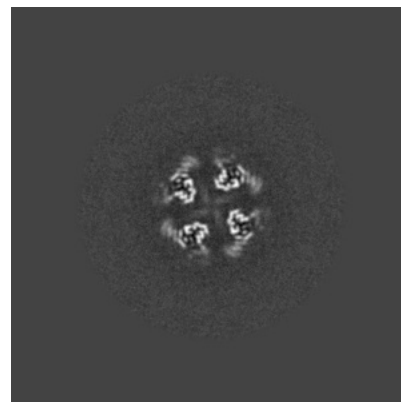
6.2.2 Raw map



X Index: 170



Y Index: 170

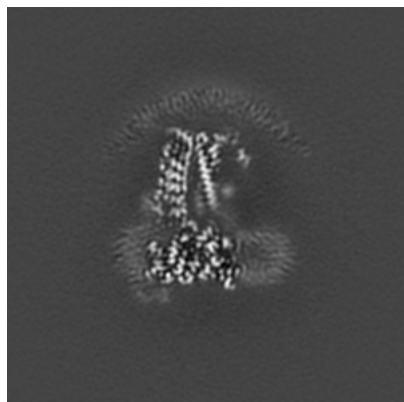


Z Index: 170

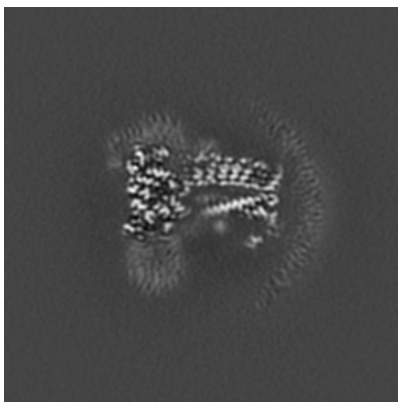
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

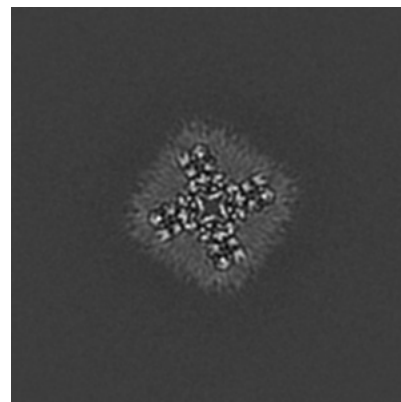
6.3.1 Primary map



X Index: 134

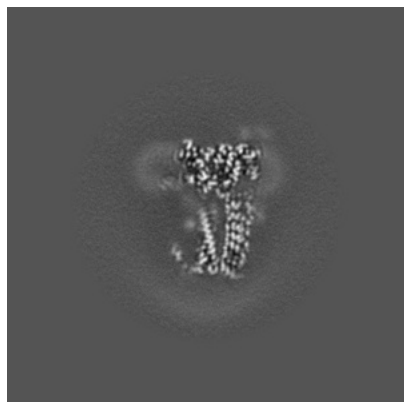


Y Index: 134

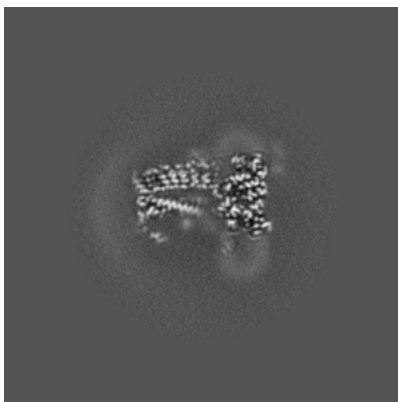


Z Index: 86

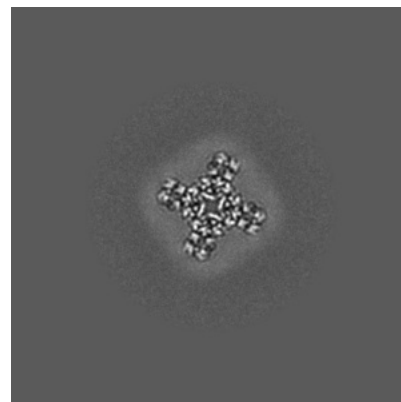
6.3.2 Raw map



X Index: 177



Y Index: 163

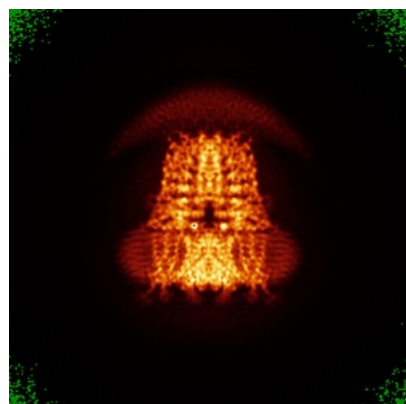


Z Index: 214

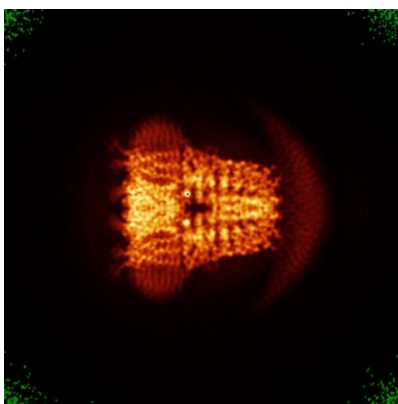
The images above show the largest variance slices of the map in three orthogonal directions.

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

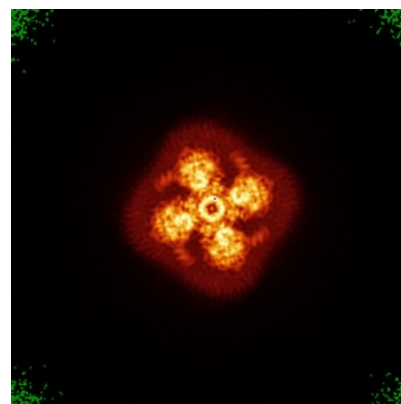
6.4.1 Primary map



X

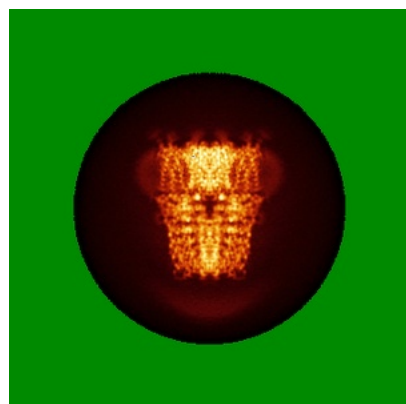


Y

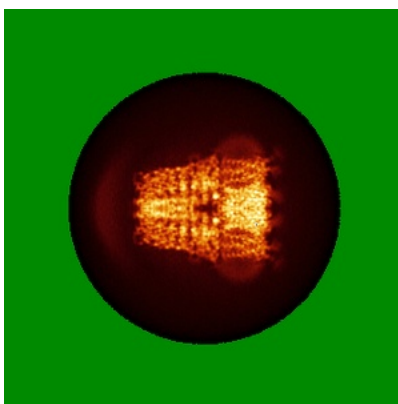


Z

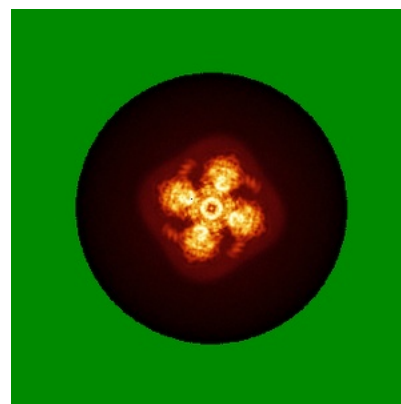
6.4.2 Raw map



X



Y

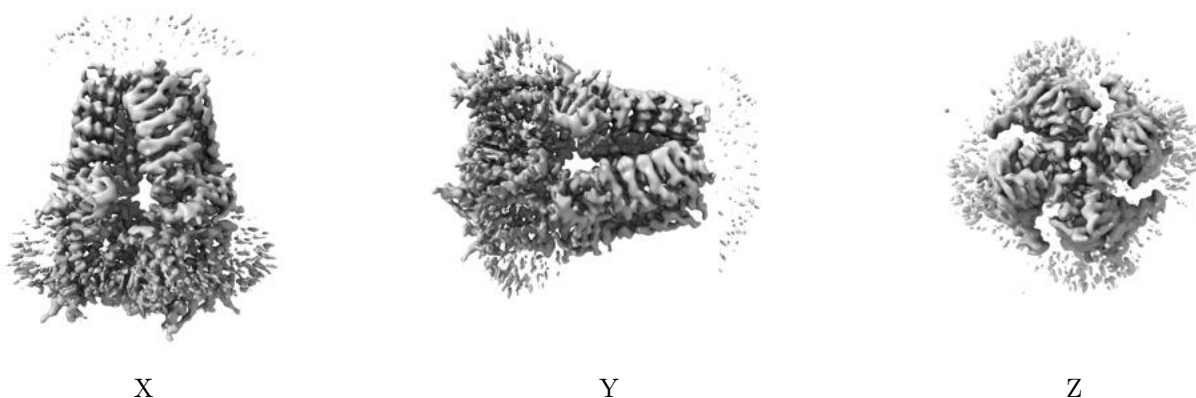


Z

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.

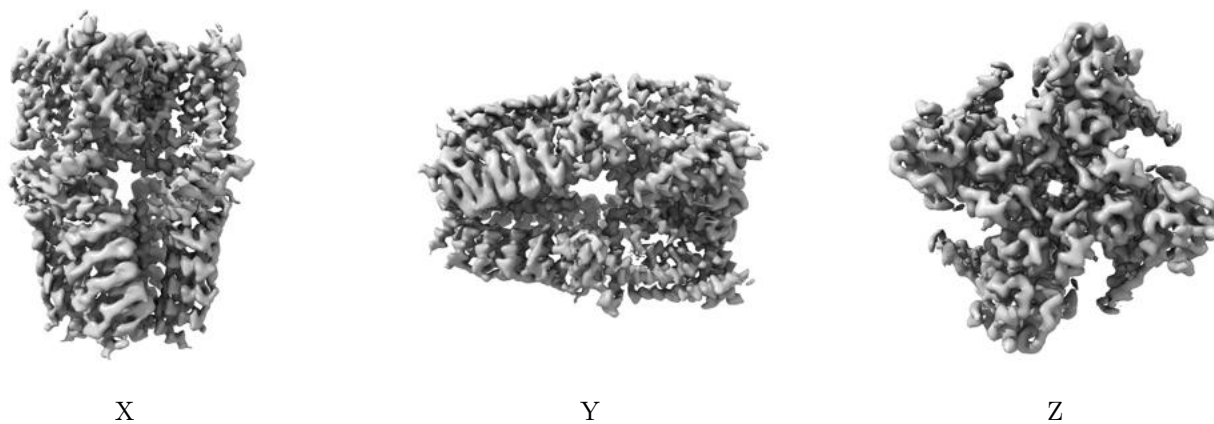
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.8. 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.

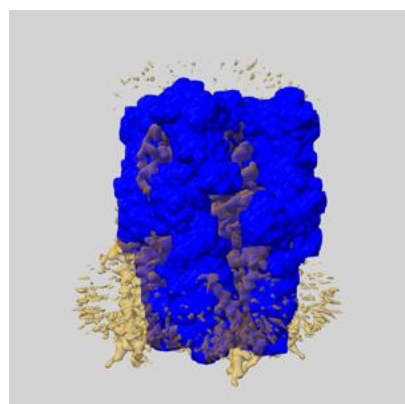
6.6 Mask visualisation [i](#)

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

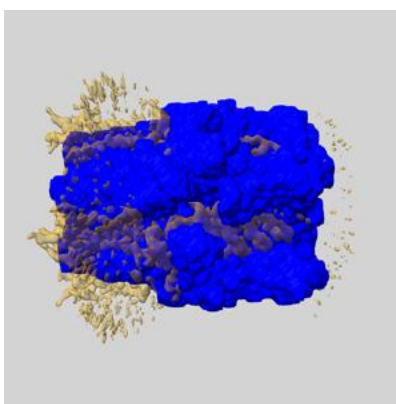
A mask typically either:

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

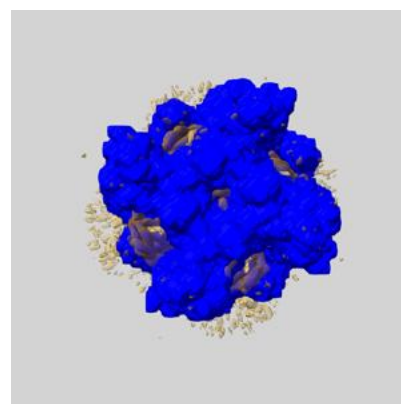
6.6.1 emd_21128_msk_1.map [i](#)



X



Y

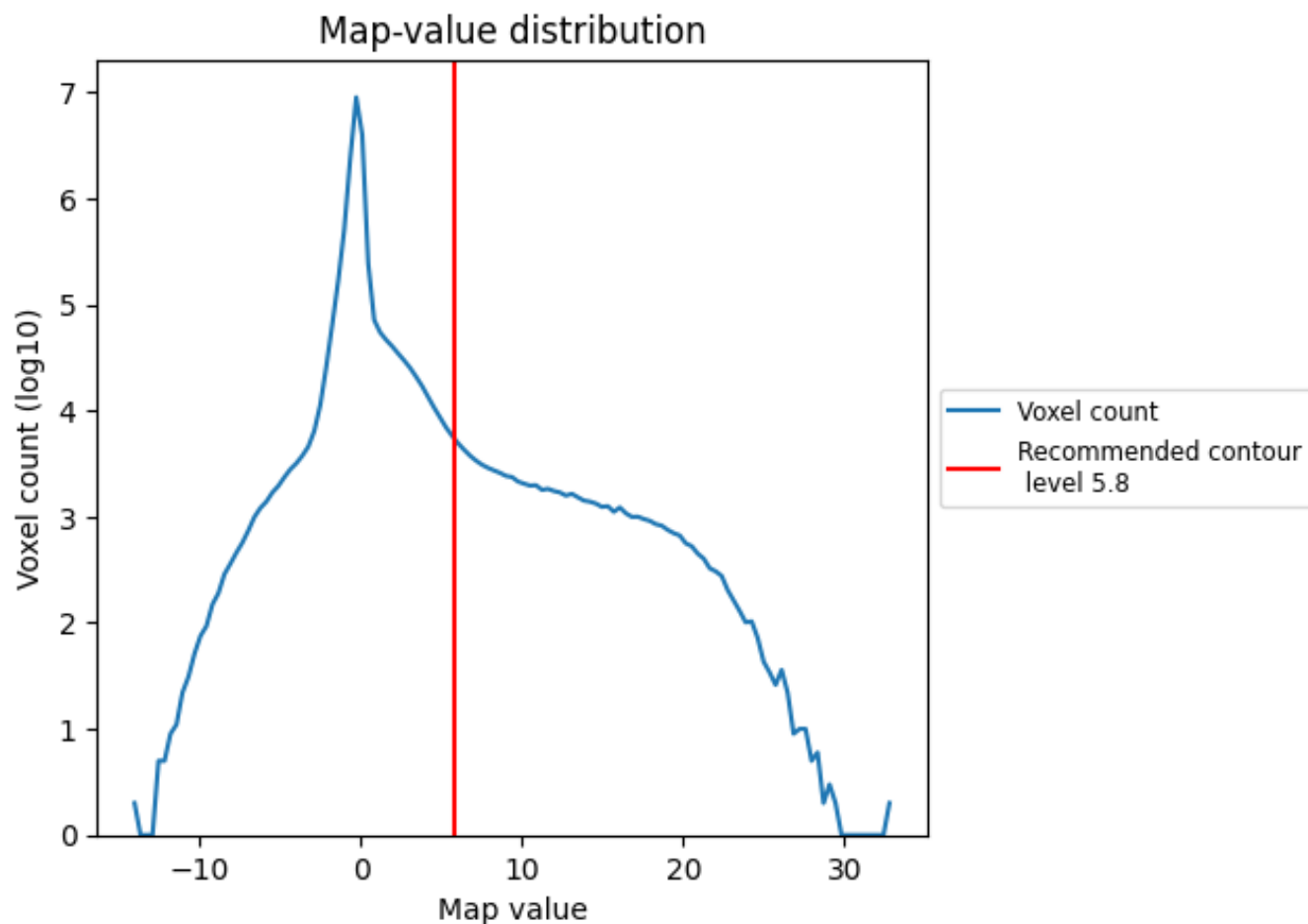


Z

7 Map analysis [i](#)

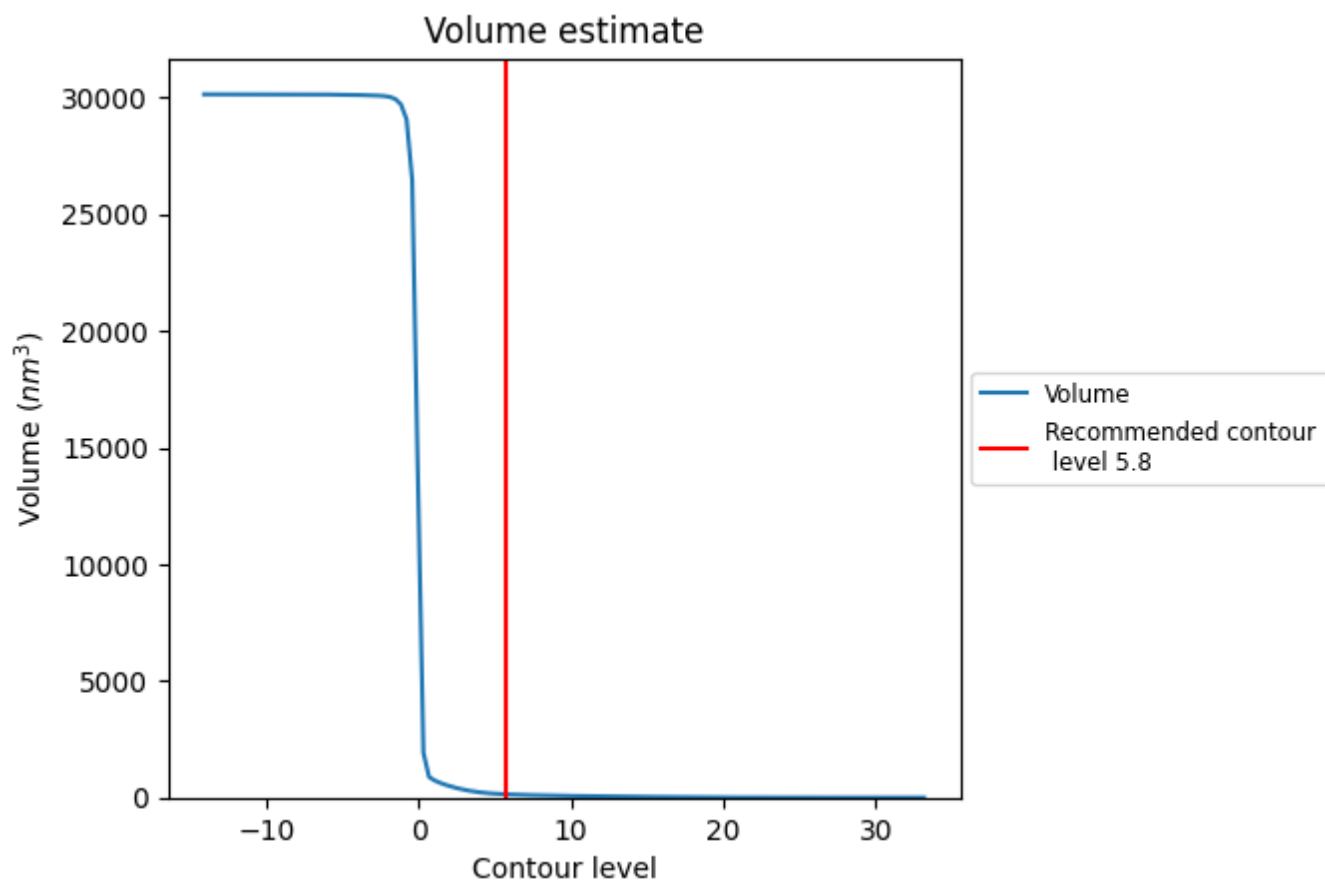
This section contains the results of statistical analysis of the map.

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.

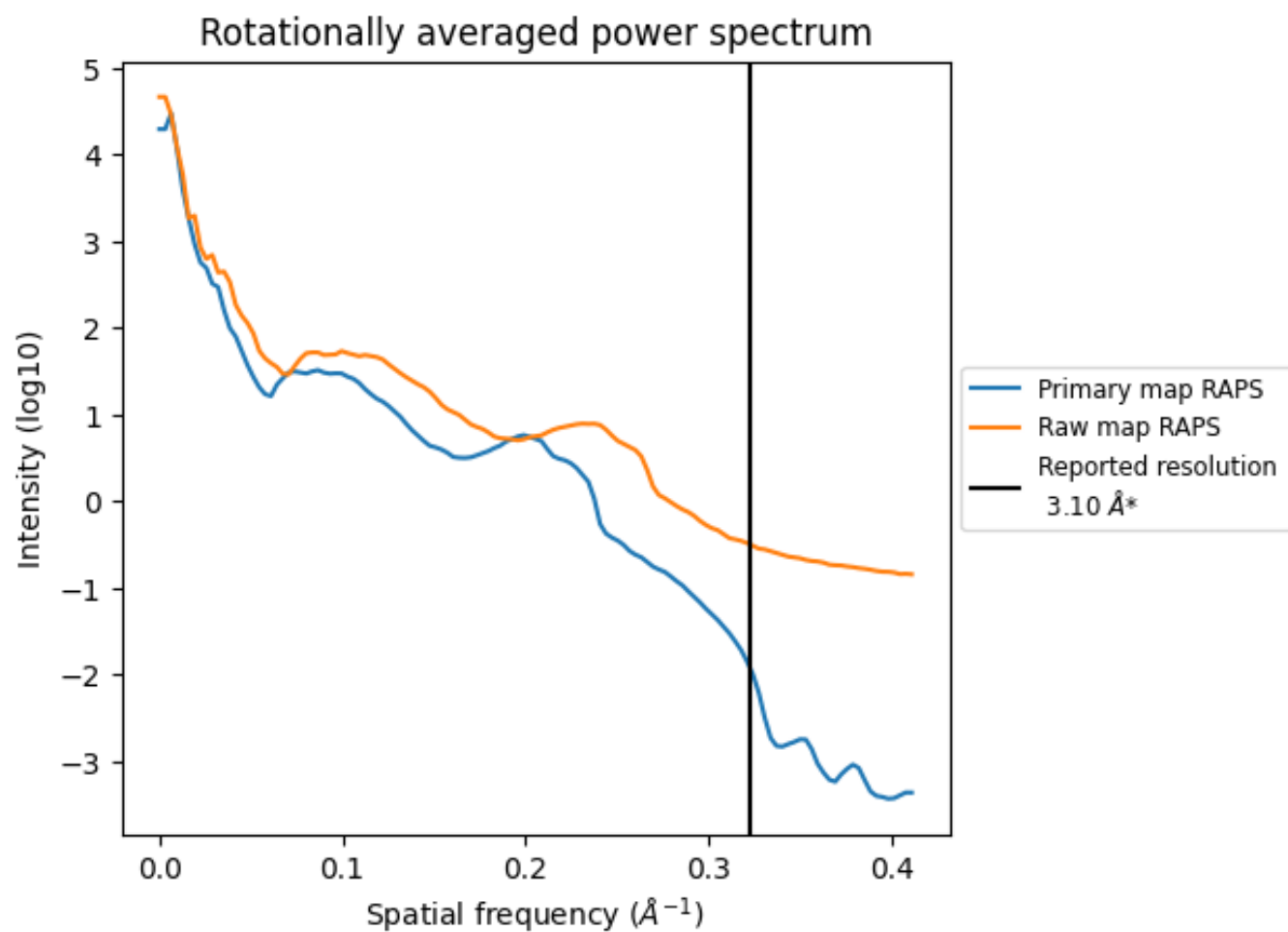
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 125 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 ⓘ

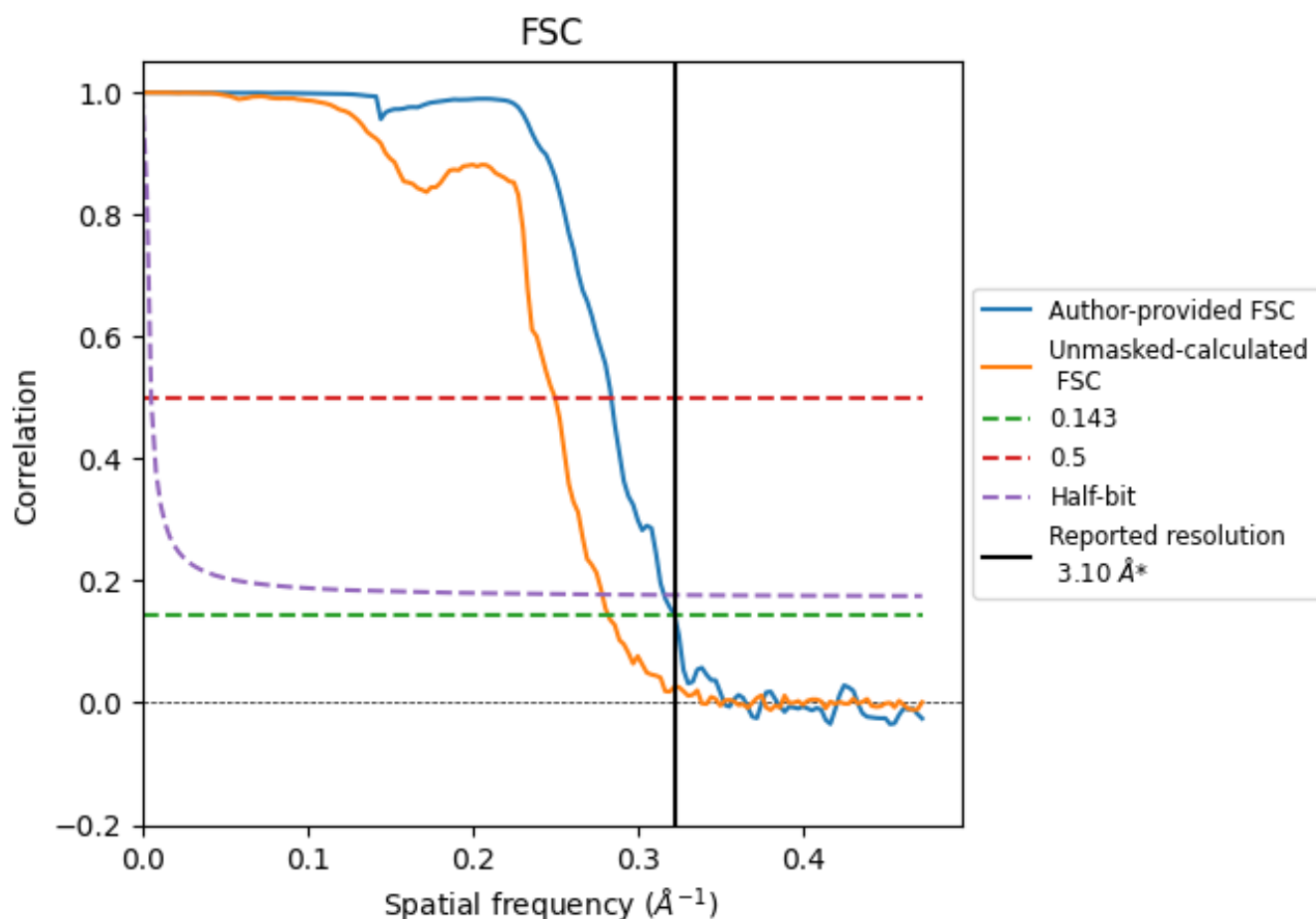


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

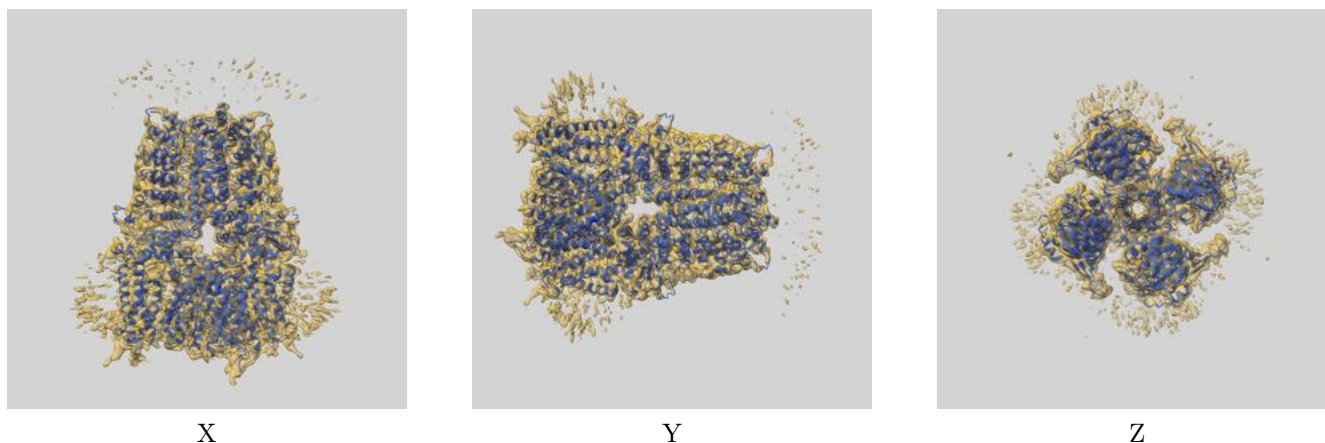
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.52	3.17
Unmasked-calculated*	3.55	4.00	3.59

*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 3.55 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

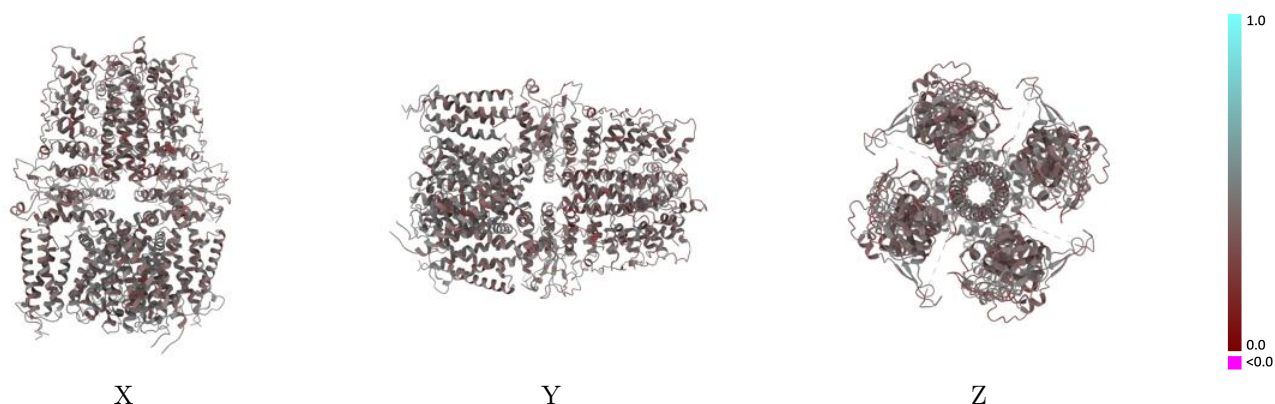
This section contains information regarding the fit between EMDB map EMD-21128 and PDB model 6V9W. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



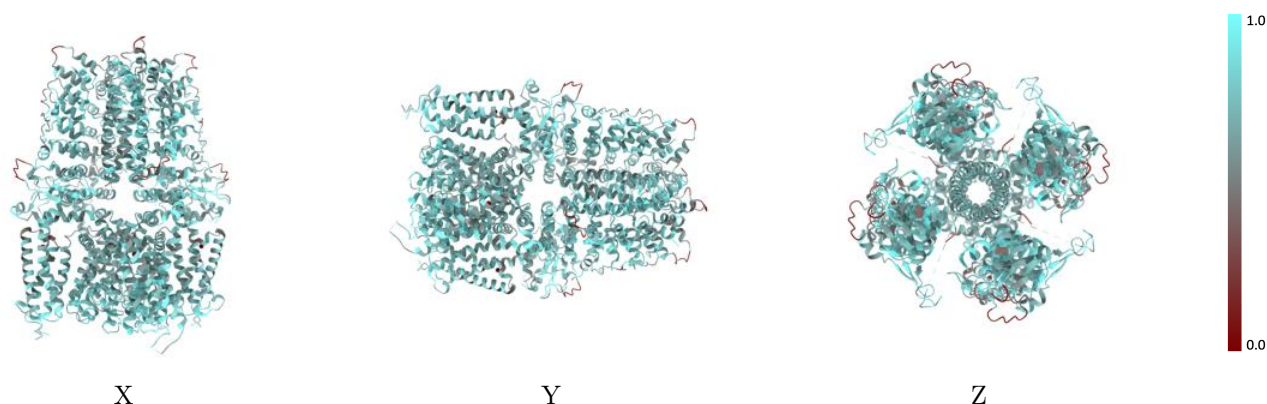
The images above show the 3D surface view of the map at the recommended contour level 5.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



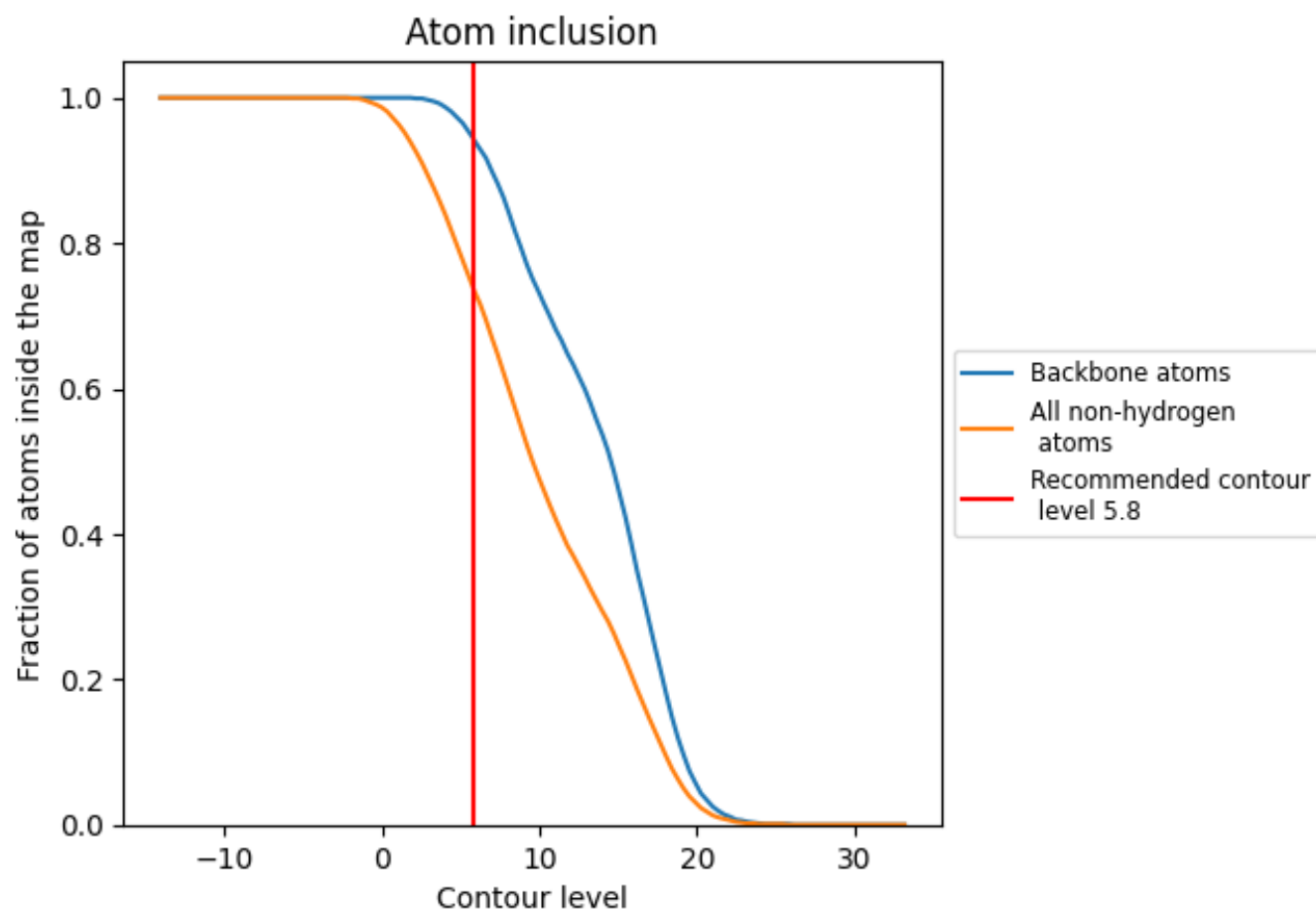
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 74% 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 (5.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.4190
A	0.7370	0.4210
B	0.7380	0.4190
C	0.7410	0.4200
D	0.7360	0.4180

