



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 11:37 PM UTC

PDB ID : 9HEY / pdb_00009hey
EMDB ID : EMD-52101
Title : CryoEM structure of mouse Panx1-R75A, narrow conformation
Authors : Gaullier, G.; Zhang, Q.; Mim, C.; Dahl, G.
Deposited on : 2024-11-14
Resolution : 3.52 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:

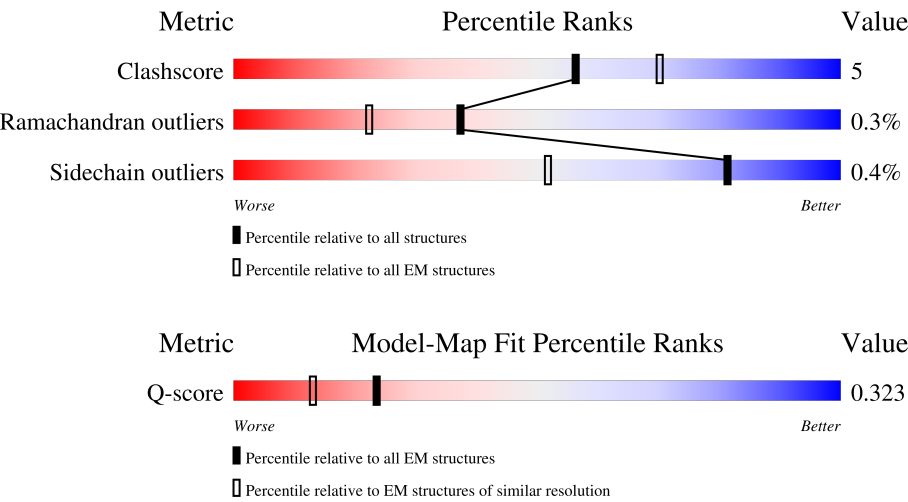
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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	13017 (3.02 - 4.02)

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	444	
1	B	444	
1	C	444	
1	D	444	

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Mol	Chain	Length	Quality of chain
1	E	444	
1	F	444	
1	G	444	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17038 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 Pannexin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	302	Total	C	N	O	S	0	0
			2434	1625	372	424	13		
1	B	302	Total	C	N	O	S	0	0
			2434	1625	372	424	13		
1	C	302	Total	C	N	O	S	0	0
			2434	1625	372	424	13		
1	D	302	Total	C	N	O	S	0	0
			2434	1625	372	424	13		
1	E	302	Total	C	N	O	S	0	0
			2434	1625	372	424	13		
1	F	302	Total	C	N	O	S	0	0
			2434	1625	372	424	13		
1	G	302	Total	C	N	O	S	0	0
			2434	1625	372	424	13		

There are 133 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	ALA	ARG	engineered mutation	UNP Q9JIP4
A	427	GLY	-	expression tag	UNP Q9JIP4
A	428	SER	-	expression tag	UNP Q9JIP4
A	429	ALA	-	expression tag	UNP Q9JIP4
A	430	ALA	-	expression tag	UNP Q9JIP4
A	431	ALA	-	expression tag	UNP Q9JIP4
A	432	GLU	-	expression tag	UNP Q9JIP4
A	433	ASN	-	expression tag	UNP Q9JIP4
A	434	LEU	-	expression tag	UNP Q9JIP4
A	435	TYR	-	expression tag	UNP Q9JIP4
A	436	PHE	-	expression tag	UNP Q9JIP4
A	437	GLN	-	expression tag	UNP Q9JIP4
A	438	GLY	-	expression tag	UNP Q9JIP4
A	439	HIS	-	expression tag	UNP Q9JIP4
A	440	HIS	-	expression tag	UNP Q9JIP4
A	441	HIS	-	expression tag	UNP Q9JIP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	442	HIS	-	expression tag	UNP Q9JIP4
A	443	HIS	-	expression tag	UNP Q9JIP4
A	444	HIS	-	expression tag	UNP Q9JIP4
B	75	ALA	ARG	engineered mutation	UNP Q9JIP4
B	427	GLY	-	expression tag	UNP Q9JIP4
B	428	SER	-	expression tag	UNP Q9JIP4
B	429	ALA	-	expression tag	UNP Q9JIP4
B	430	ALA	-	expression tag	UNP Q9JIP4
B	431	ALA	-	expression tag	UNP Q9JIP4
B	432	GLU	-	expression tag	UNP Q9JIP4
B	433	ASN	-	expression tag	UNP Q9JIP4
B	434	LEU	-	expression tag	UNP Q9JIP4
B	435	TYR	-	expression tag	UNP Q9JIP4
B	436	PHE	-	expression tag	UNP Q9JIP4
B	437	GLN	-	expression tag	UNP Q9JIP4
B	438	GLY	-	expression tag	UNP Q9JIP4
B	439	HIS	-	expression tag	UNP Q9JIP4
B	440	HIS	-	expression tag	UNP Q9JIP4
B	441	HIS	-	expression tag	UNP Q9JIP4
B	442	HIS	-	expression tag	UNP Q9JIP4
B	443	HIS	-	expression tag	UNP Q9JIP4
B	444	HIS	-	expression tag	UNP Q9JIP4
C	75	ALA	ARG	engineered mutation	UNP Q9JIP4
C	427	GLY	-	expression tag	UNP Q9JIP4
C	428	SER	-	expression tag	UNP Q9JIP4
C	429	ALA	-	expression tag	UNP Q9JIP4
C	430	ALA	-	expression tag	UNP Q9JIP4
C	431	ALA	-	expression tag	UNP Q9JIP4
C	432	GLU	-	expression tag	UNP Q9JIP4
C	433	ASN	-	expression tag	UNP Q9JIP4
C	434	LEU	-	expression tag	UNP Q9JIP4
C	435	TYR	-	expression tag	UNP Q9JIP4
C	436	PHE	-	expression tag	UNP Q9JIP4
C	437	GLN	-	expression tag	UNP Q9JIP4
C	438	GLY	-	expression tag	UNP Q9JIP4
C	439	HIS	-	expression tag	UNP Q9JIP4
C	440	HIS	-	expression tag	UNP Q9JIP4
C	441	HIS	-	expression tag	UNP Q9JIP4
C	442	HIS	-	expression tag	UNP Q9JIP4
C	443	HIS	-	expression tag	UNP Q9JIP4
C	444	HIS	-	expression tag	UNP Q9JIP4
D	75	ALA	ARG	engineered mutation	UNP Q9JIP4

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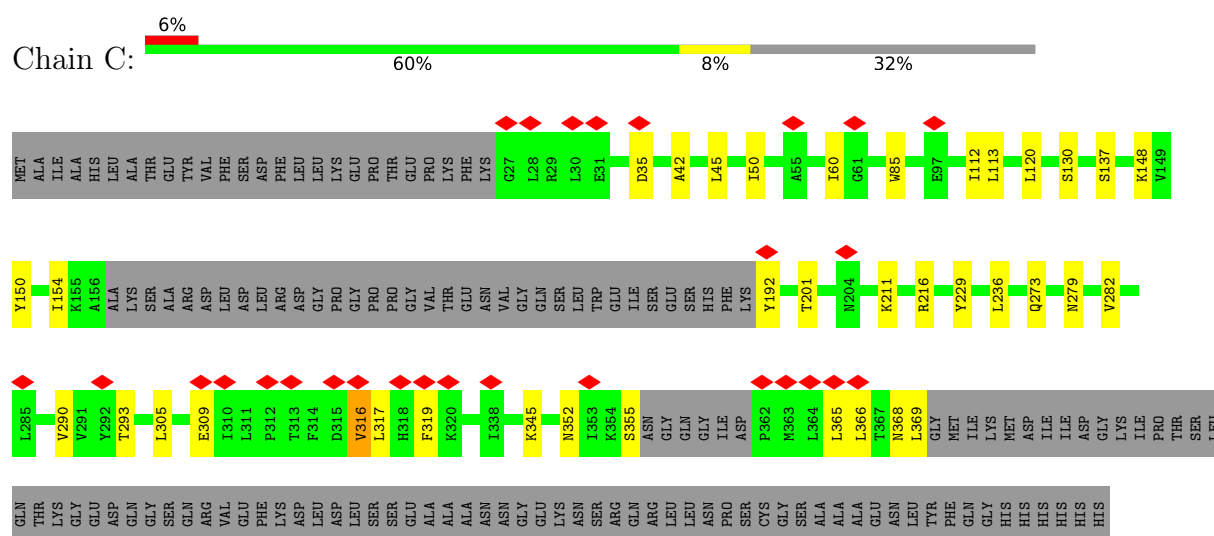
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Chain	Residue	Modelled	Actual	Comment	Reference
D	427	GLY	-	expression tag	UNP Q9JIP4
D	428	SER	-	expression tag	UNP Q9JIP4
D	429	ALA	-	expression tag	UNP Q9JIP4
D	430	ALA	-	expression tag	UNP Q9JIP4
D	431	ALA	-	expression tag	UNP Q9JIP4
D	432	GLU	-	expression tag	UNP Q9JIP4
D	433	ASN	-	expression tag	UNP Q9JIP4
D	434	LEU	-	expression tag	UNP Q9JIP4
D	435	TYR	-	expression tag	UNP Q9JIP4
D	436	PHE	-	expression tag	UNP Q9JIP4
D	437	GLN	-	expression tag	UNP Q9JIP4
D	438	GLY	-	expression tag	UNP Q9JIP4
D	439	HIS	-	expression tag	UNP Q9JIP4
D	440	HIS	-	expression tag	UNP Q9JIP4
D	441	HIS	-	expression tag	UNP Q9JIP4
D	442	HIS	-	expression tag	UNP Q9JIP4
D	443	HIS	-	expression tag	UNP Q9JIP4
D	444	HIS	-	expression tag	UNP Q9JIP4
E	75	ALA	ARG	engineered mutation	UNP Q9JIP4
E	427	GLY	-	expression tag	UNP Q9JIP4
E	428	SER	-	expression tag	UNP Q9JIP4
E	429	ALA	-	expression tag	UNP Q9JIP4
E	430	ALA	-	expression tag	UNP Q9JIP4
E	431	ALA	-	expression tag	UNP Q9JIP4
E	432	GLU	-	expression tag	UNP Q9JIP4
E	433	ASN	-	expression tag	UNP Q9JIP4
E	434	LEU	-	expression tag	UNP Q9JIP4
E	435	TYR	-	expression tag	UNP Q9JIP4
E	436	PHE	-	expression tag	UNP Q9JIP4
E	437	GLN	-	expression tag	UNP Q9JIP4
E	438	GLY	-	expression tag	UNP Q9JIP4
E	439	HIS	-	expression tag	UNP Q9JIP4
E	440	HIS	-	expression tag	UNP Q9JIP4
E	441	HIS	-	expression tag	UNP Q9JIP4
E	442	HIS	-	expression tag	UNP Q9JIP4
E	443	HIS	-	expression tag	UNP Q9JIP4
E	444	HIS	-	expression tag	UNP Q9JIP4
F	75	ALA	ARG	engineered mutation	UNP Q9JIP4
F	427	GLY	-	expression tag	UNP Q9JIP4
F	428	SER	-	expression tag	UNP Q9JIP4
F	429	ALA	-	expression tag	UNP Q9JIP4
F	430	ALA	-	expression tag	UNP Q9JIP4

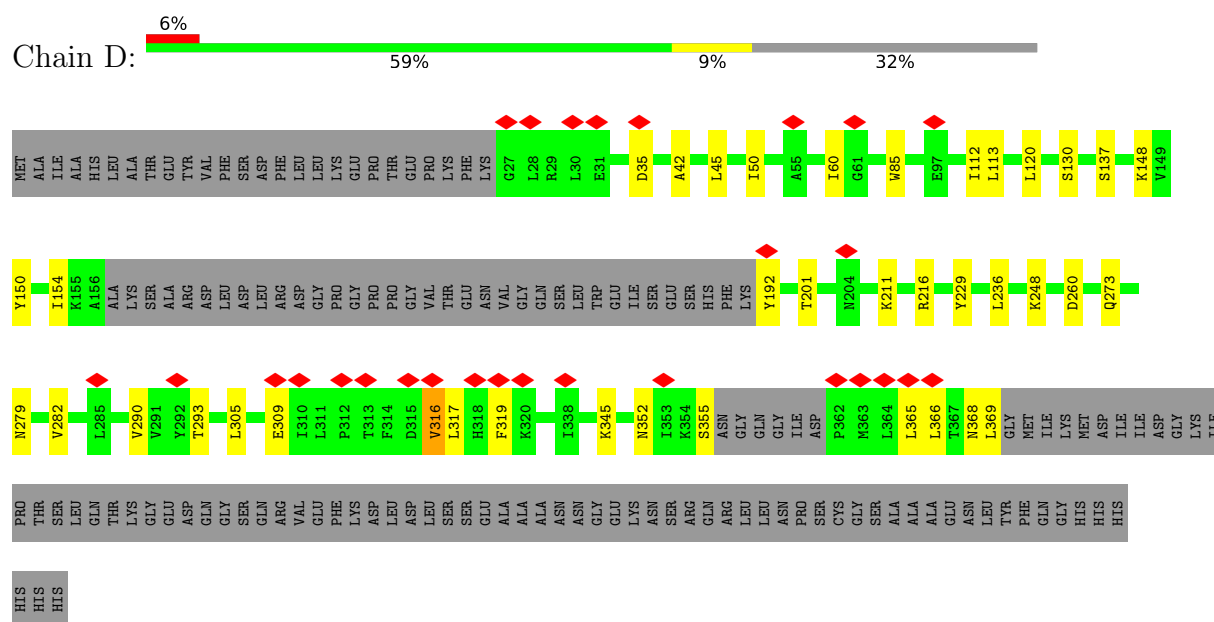
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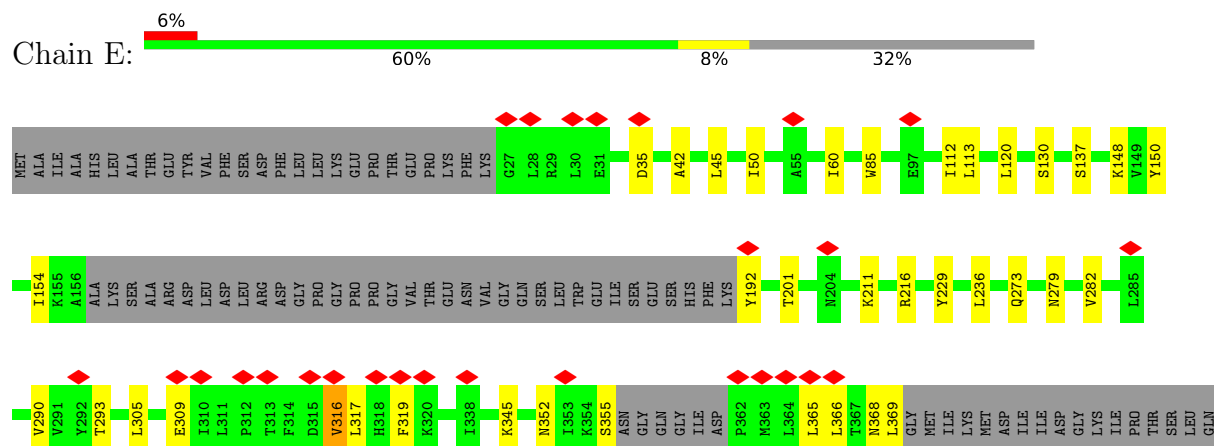
Chain	Residue	Modelled	Actual	Comment	Reference
F	431	ALA	-	expression tag	UNP Q9JIP4
F	432	GLU	-	expression tag	UNP Q9JIP4
F	433	ASN	-	expression tag	UNP Q9JIP4
F	434	LEU	-	expression tag	UNP Q9JIP4
F	435	TYR	-	expression tag	UNP Q9JIP4
F	436	PHE	-	expression tag	UNP Q9JIP4
F	437	GLN	-	expression tag	UNP Q9JIP4
F	438	GLY	-	expression tag	UNP Q9JIP4
F	439	HIS	-	expression tag	UNP Q9JIP4
F	440	HIS	-	expression tag	UNP Q9JIP4
F	441	HIS	-	expression tag	UNP Q9JIP4
F	442	HIS	-	expression tag	UNP Q9JIP4
F	443	HIS	-	expression tag	UNP Q9JIP4
F	444	HIS	-	expression tag	UNP Q9JIP4
G	75	ALA	ARG	engineered mutation	UNP Q9JIP4
G	427	GLY	-	expression tag	UNP Q9JIP4
G	428	SER	-	expression tag	UNP Q9JIP4
G	429	ALA	-	expression tag	UNP Q9JIP4
G	430	ALA	-	expression tag	UNP Q9JIP4
G	431	ALA	-	expression tag	UNP Q9JIP4
G	432	GLU	-	expression tag	UNP Q9JIP4
G	433	ASN	-	expression tag	UNP Q9JIP4
G	434	LEU	-	expression tag	UNP Q9JIP4
G	435	TYR	-	expression tag	UNP Q9JIP4
G	436	PHE	-	expression tag	UNP Q9JIP4
G	437	GLN	-	expression tag	UNP Q9JIP4
G	438	GLY	-	expression tag	UNP Q9JIP4
G	439	HIS	-	expression tag	UNP Q9JIP4
G	440	HIS	-	expression tag	UNP Q9JIP4
G	441	HIS	-	expression tag	UNP Q9JIP4
G	442	HIS	-	expression tag	UNP Q9JIP4
G	443	HIS	-	expression tag	UNP Q9JIP4
G	444	HIS	-	expression tag	UNP Q9JIP4



- Molecule 1: Pannexin-1



- Molecule 1: Pannexin-1



THR	LYS	GLY	GLU	ASP	GLN	GLY	SER	GLN	ARG	VAL	PHE	GLU	LYS	ASP	PHE	LEU	ASP	SER	LEU	LYS	SER	GLU	ALA	ALA	ALA	ASN	ASN	GLY	LYS	ASN	ARG	GLN	ARG	LEU	LEU	ASN	PRO	SER	CYS	GLY	SER	ALA	ALA	ALA	GLU	ASN	LEU	TYR	PHE	GLN	GLY	HIS	HIS	HIS	HIS
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● Molecule 1: Pannexin-1



LYS	GLY	GLU	ASP	GLN	SER	GLN	ARG	VAL	GLU	PHE	LYS	ASP	LEU	ASP	LEU	ASP	GLY	PRO	GLY	PRO	GLY	VAL	THR	GLU	ASN	GLY	GLU	LYS	ASN	ARG	GLN	ARG	LEU	LEU	ASN	PRO	SER	CYS	GLY	SER	ALA	ALA	ALA	GLU	ASN	LEU	TYR	PHE	GLN	GLY	HIS	HIS	HIS	HIS	HIS
V290	V291	T292	T293	L305	E309	I310	L311	P312	T313	F314	D315	V316	L317	H318	F319	K320	I338	K345	N352	I353	K354	S355	ASN	GLY	GLN	GLY	ILE	SER	GLU	ASP	P362	M363	L364	L365	L366	T367	N368	L369	GLY	MET	ILE	LYS	MET	ASP	ILE	ILE	ASP	GLY	LYS	ILE	PRO	SER	LEU	GLN	THR
Y150	I154	K155	A156	ALA	LYS	SER	ALA	ARG	ASP	LEU	ASP	LEU	ARG	ASP	GLY	PRO	GLY	PRO	PRO	GLY	VAL	THR	GLU	ASN	VAL	GLY	GLN	SER	GLU	SER	HIS	PHE	LYS	Y192	M204	K211	R216	Y229	L236	Q273	N279	V282	L285												
MET	ALA	ILE	ALA	HIS	LEU	ALA	THR	GLU	TYR	VAL	PHE	SER	ASP	PHE	LEU	LEU	LYS	PRO	THR	GLU	PRO	LYS	PHE	LYS	G27	L28	R29	L30	E31	D35	A42	L45	I50	A55	I60	G61	W85	E97	I112	L113	L120	S130	S137	K148	V149										

● Molecule 1: Pannexin-1



HIS	HIS	THR	SER	LEU	GLN	THR	LYS	GLY	GLU	ASP	GLN	SER	GLN	ARG	VAL	GLU	PHE	LYS	ASP	LEU	ASP	LEU	THR	GLY	ALA	ALA	ASN	ASN	GLY	GLY	LYS	ASN	ARG	GLN	ARG	LEU	LEU	ASN	PRO	SER	CYS	GLY	SER	ALA	ALA	GLU	ASN	LEU	TYR	PHE	GLN	GLY	HIS	HIS	HIS	HIS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
		V282		L285			V290	V291	V292	T293	L305		E309	I310	L311	P312	T313	F314	D315	V316	L317	H318	F319	K320	I338		K345	N352	I353	K354	S355	ASN	GLY	GLN	ARG	LEU	LEU	ASN	PRO	SER	P362	M363	L364	L365	L366	T367	N368	L369	GLY	MET	ILE	LYS	MET	ASP	ILE	ILE	ASP	GLY	LYS	ILE	PRO																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
			I154	K155	A156	ALA	LYS	SER	ALA	ARG	ASP	LEU	ARG	ASP	GLY	PRO	GLY	PRO	PRO	GLY	VAL	THR	GLU	ASN	VAL	GLY	GLN	SER	GLU	SER	HIS	PHE	LYS	Y192		T201		N204		K211		R216		Y229		L236		K248		D260		Q273		N279																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	28395	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	237.59999, 237.59999, 237.59999	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/2492	0.42	0/3380
1	B	0.26	0/2492	0.42	0/3380
1	C	0.26	0/2492	0.42	0/3380
1	D	0.26	0/2492	0.42	0/3380
1	E	0.26	0/2492	0.42	0/3380
1	F	0.26	0/2492	0.42	0/3380
1	G	0.26	0/2492	0.42	0/3380
All	All	0.26	0/17444	0.42	0/23660

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	2434	0	2525	35	0
1	B	2434	0	2525	37	0
1	C	2434	0	2525	36	0
1	D	2434	0	2525	35	0
1	E	2434	0	2525	36	0
1	F	2434	0	2525	31	0
1	G	2434	0	2525	33	0
All	All	17038	0	17675	170	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 (170) 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:365:LEU:HD21	1:G:192:TYR:CD2	2.30	0.66
1:B:192:TYR:CD2	1:C:365:LEU:HD21	2.31	0.66
1:A:365:LEU:HD21	1:G:192:TYR:CE2	2.32	0.65
1:C:192:TYR:CD2	1:D:365:LEU:HD21	2.33	0.64
1:E:192:TYR:CD2	1:F:365:LEU:HD21	2.32	0.64
1:D:85:TRP:NE1	1:E:60:ILE:HD13	2.13	0.64
1:A:192:TYR:CD2	1:B:365:LEU:HD21	2.33	0.64
1:E:192:TYR:CE2	1:F:365:LEU:HD21	2.32	0.64
1:C:192:TYR:CE2	1:D:365:LEU:HD21	2.33	0.64
1:F:85:TRP:NE1	1:G:60:ILE:HD13	2.13	0.64
1:D:192:TYR:CD2	1:E:365:LEU:HD21	2.32	0.64
1:B:192:TYR:CE2	1:C:365:LEU:HD21	2.33	0.63
1:A:192:TYR:CE2	1:B:365:LEU:HD21	2.34	0.63
1:C:85:TRP:NE1	1:D:60:ILE:HD13	2.14	0.63
1:F:192:TYR:CD2	1:G:365:LEU:HD21	2.34	0.62
1:A:85:TRP:NE1	1:B:60:ILE:HD13	2.14	0.62
1:B:42:ALA:HB1	1:B:120:LEU:HD13	1.82	0.62
1:C:42:ALA:HB1	1:C:120:LEU:HD13	1.82	0.62
1:B:85:TRP:NE1	1:C:60:ILE:HD13	2.14	0.62
1:A:42:ALA:HB1	1:A:120:LEU:HD13	1.82	0.61
1:D:42:ALA:HB1	1:D:120:LEU:HD13	1.82	0.61
1:D:192:TYR:CE2	1:E:365:LEU:HD21	2.35	0.61
1:G:42:ALA:HB1	1:G:120:LEU:HD13	1.82	0.61
1:E:85:TRP:NE1	1:F:60:ILE:HD13	2.16	0.61
1:F:192:TYR:CE2	1:G:365:LEU:HD21	2.36	0.61
1:A:60:ILE:HD13	1:G:85:TRP:NE1	2.14	0.61
1:F:42:ALA:HB1	1:F:120:LEU:HD13	1.82	0.61
1:E:42:ALA:HB1	1:E:120:LEU:HD13	1.82	0.60
1:F:236:LEU:O	1:F:273:GLN:NE2	2.37	0.55
1:D:137:SER:HB2	1:E:345:LYS:HE2	1.88	0.55
1:A:345:LYS:HE2	1:G:137:SER:HB2	1.87	0.55
1:E:236:LEU:O	1:E:273:GLN:NE2	2.37	0.55
1:D:236:LEU:O	1:D:273:GLN:NE2	2.37	0.55
1:C:236:LEU:O	1:C:273:GLN:NE2	2.37	0.55
1:F:137:SER:HB2	1:G:345:LYS:HE2	1.89	0.54
1:B:236:LEU:O	1:B:273:GLN:NE2	2.37	0.54
1:C:137:SER:HB2	1:D:345:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:SER:HB2	1:F:345:LYS:HE2	1.90	0.54
1:B:137:SER:HB2	1:C:345:LYS:HE2	1.89	0.53
1:A:137:SER:HB2	1:B:345:LYS:HE2	1.89	0.53
1:A:305:LEU:H	1:A:305:LEU:HD12	1.75	0.52
1:C:305:LEU:HD12	1:C:305:LEU:H	1.75	0.52
1:B:305:LEU:H	1:B:305:LEU:HD12	1.75	0.52
1:F:305:LEU:H	1:F:305:LEU:HD12	1.75	0.52
1:G:305:LEU:HD12	1:G:305:LEU:H	1.75	0.52
1:D:305:LEU:HD12	1:D:305:LEU:H	1.75	0.52
1:A:236:LEU:O	1:A:273:GLN:NE2	2.37	0.51
1:A:365:LEU:CD2	1:G:192:TYR:CD2	2.93	0.51
1:E:305:LEU:H	1:E:305:LEU:HD12	1.75	0.51
1:B:192:TYR:CD2	1:C:365:LEU:CD2	2.95	0.50
1:E:112:ILE:HG21	1:E:229:TYR:CZ	2.46	0.50
1:B:112:ILE:HG21	1:B:229:TYR:CZ	2.46	0.50
1:D:112:ILE:HG21	1:D:229:TYR:CZ	2.46	0.50
1:C:112:ILE:HG21	1:C:229:TYR:CZ	2.46	0.50
1:C:192:TYR:HD1	1:D:368:ASN:HD22	1.59	0.50
1:A:112:ILE:HG21	1:A:229:TYR:CZ	2.46	0.50
1:C:192:TYR:CD2	1:D:365:LEU:CD2	2.95	0.50
1:F:112:ILE:HG21	1:F:229:TYR:CZ	2.46	0.50
1:G:112:ILE:HG21	1:G:229:TYR:CZ	2.46	0.49
1:D:352:ASN:O	1:D:355:SER:OG	2.26	0.49
1:A:192:TYR:CD2	1:B:365:LEU:CD2	2.96	0.49
1:B:248:LYS:NZ	1:B:260:ASP:OD1	2.37	0.49
1:E:192:TYR:CD2	1:F:365:LEU:CD2	2.94	0.49
1:E:192:TYR:HD1	1:F:368:ASN:HD22	1.59	0.48
1:G:236:LEU:O	1:G:273:GLN:NE2	2.37	0.48
1:D:148:LYS:NZ	1:E:369:LEU:C	2.72	0.48
1:E:150:TYR:CE2	1:E:154:ILE:HD11	2.49	0.48
1:A:150:TYR:CE2	1:A:154:ILE:HD11	2.49	0.48
1:G:130:SER:O	1:G:211:LYS:NZ	2.47	0.47
1:B:150:TYR:CE2	1:B:154:ILE:HD11	2.49	0.47
1:C:290:VAL:O	1:C:293:THR:OG1	2.31	0.47
1:D:192:TYR:CD2	1:E:365:LEU:CD2	2.97	0.47
1:D:150:TYR:CE2	1:D:154:ILE:HD11	2.49	0.47
1:F:148:LYS:NZ	1:G:369:LEU:C	2.72	0.47
1:F:150:TYR:CE2	1:F:154:ILE:HD11	2.49	0.47
1:G:150:TYR:CE2	1:G:154:ILE:HD11	2.49	0.47
1:A:130:SER:O	1:A:211:LYS:NZ	2.47	0.47
1:A:192:TYR:HD1	1:B:368:ASN:HD22	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:ASN:O	1:E:355:SER:OG	2.26	0.47
1:A:369:LEU:C	1:G:148:LYS:NZ	2.73	0.47
1:C:150:TYR:CE2	1:C:154:ILE:HD11	2.49	0.47
1:E:290:VAL:O	1:E:293:THR:OG1	2.31	0.47
1:F:290:VAL:O	1:F:293:THR:OG1	2.31	0.47
1:C:352:ASN:O	1:C:355:SER:OG	2.26	0.47
1:A:368:ASN:HD22	1:G:192:TYR:HD1	1.63	0.46
1:B:352:ASN:O	1:B:355:SER:OG	2.26	0.46
1:D:290:VAL:O	1:D:293:THR:OG1	2.31	0.46
1:D:35:ASP:OD1	1:D:216:ARG:NH1	2.50	0.45
1:B:130:SER:O	1:B:211:LYS:NZ	2.47	0.45
1:B:192:TYR:HD1	1:C:368:ASN:HD22	1.63	0.45
1:A:35:ASP:OD1	1:A:216:ARG:NH1	2.50	0.45
1:C:130:SER:O	1:C:211:LYS:NZ	2.47	0.45
1:E:35:ASP:OD1	1:E:216:ARG:NH1	2.50	0.45
1:F:192:TYR:CD2	1:G:365:LEU:CD2	2.98	0.45
1:F:192:TYR:HD1	1:G:368:ASN:HD22	1.64	0.45
1:B:35:ASP:OD1	1:B:216:ARG:NH1	2.50	0.45
1:C:35:ASP:OD1	1:C:216:ARG:NH1	2.50	0.45
1:D:130:SER:O	1:D:211:LYS:NZ	2.48	0.45
1:F:35:ASP:OD1	1:F:216:ARG:NH1	2.50	0.45
1:D:248:LYS:NZ	1:D:260:ASP:OD1	2.37	0.45
1:D:148:LYS:HZ3	1:E:369:LEU:C	2.24	0.44
1:B:148:LYS:NZ	1:C:369:LEU:C	2.74	0.44
1:D:192:TYR:HD1	1:E:368:ASN:HD22	1.64	0.44
1:G:45:LEU:HD22	1:G:282:VAL:HG11	1.99	0.44
1:A:148:LYS:NZ	1:B:369:LEU:C	2.75	0.44
1:A:45:LEU:HD22	1:A:282:VAL:HG11	1.99	0.44
1:D:45:LEU:HD22	1:D:282:VAL:HG11	1.99	0.44
1:E:130:SER:O	1:E:211:LYS:NZ	2.47	0.44
1:G:35:ASP:OD1	1:G:216:ARG:NH1	2.50	0.44
1:E:45:LEU:HD22	1:E:282:VAL:HG11	1.99	0.44
1:C:45:LEU:HD22	1:C:282:VAL:HG11	1.99	0.43
1:F:45:LEU:HD22	1:F:282:VAL:HG11	1.99	0.43
1:G:352:ASN:O	1:G:355:SER:OG	2.26	0.43
1:E:201:THR:HG21	1:F:352:ASN:CG	2.44	0.43
1:A:352:ASN:CG	1:G:201:THR:HG21	2.44	0.43
1:B:45:LEU:HD22	1:B:282:VAL:HG11	1.99	0.43
1:E:148:LYS:NZ	1:F:369:LEU:C	2.77	0.43
1:F:130:SER:O	1:F:211:LYS:NZ	2.47	0.43
1:A:365:LEU:HD23	1:G:192:TYR:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:TYR:HD1	1:D:368:ASN:ND2	2.16	0.42
1:C:148:LYS:NZ	1:D:369:LEU:C	2.76	0.42
1:E:309:GLU:HG3	1:E:316:VAL:HA	2.01	0.42
1:A:201:THR:HG21	1:B:352:ASN:CG	2.45	0.42
1:F:309:GLU:HG3	1:F:316:VAL:HA	2.01	0.42
1:A:192:TYR:HD1	1:B:368:ASN:ND2	2.17	0.42
1:A:352:ASN:OD1	1:G:201:THR:HG21	2.19	0.42
1:C:201:THR:HG21	1:D:352:ASN:CG	2.44	0.42
1:D:317:LEU:HA	1:D:319:PHE:CZ	2.55	0.42
1:E:317:LEU:HA	1:E:319:PHE:CZ	2.55	0.42
1:G:317:LEU:HA	1:G:319:PHE:CZ	2.55	0.42
1:D:309:GLU:HG3	1:D:316:VAL:HA	2.01	0.42
1:B:290:VAL:O	1:B:293:THR:OG1	2.31	0.41
1:C:317:LEU:HA	1:C:319:PHE:CZ	2.55	0.41
1:B:201:THR:HG21	1:C:352:ASN:OD1	2.20	0.41
1:B:309:GLU:HG3	1:B:316:VAL:HA	2.01	0.41
1:F:50:ILE:HD11	1:F:113:LEU:HB2	2.03	0.41
1:F:317:LEU:HA	1:F:319:PHE:CZ	2.55	0.41
1:A:50:ILE:HD11	1:A:113:LEU:HB2	2.03	0.41
1:A:317:LEU:HA	1:A:319:PHE:CZ	2.55	0.41
1:D:85:TRP:HE1	1:E:60:ILE:HD13	1.84	0.41
1:E:192:TYR:HD1	1:F:368:ASN:ND2	2.16	0.41
1:G:50:ILE:HD11	1:G:113:LEU:HB2	2.03	0.41
1:G:309:GLU:HG3	1:G:316:VAL:HA	2.01	0.41
1:B:201:THR:HG21	1:C:352:ASN:CG	2.45	0.41
1:C:309:GLU:HG3	1:C:316:VAL:HA	2.01	0.41
1:A:290:VAL:O	1:A:293:THR:OG1	2.31	0.41
1:B:50:ILE:HD11	1:B:113:LEU:HB2	2.03	0.41
1:G:248:LYS:NZ	1:G:260:ASP:OD1	2.37	0.41
1:E:50:ILE:HD11	1:E:113:LEU:HB2	2.03	0.41
1:B:317:LEU:HA	1:B:319:PHE:CZ	2.55	0.41
1:D:201:THR:HG21	1:E:352:ASN:OD1	2.21	0.41
1:C:201:THR:HG21	1:D:352:ASN:OD1	2.21	0.41
1:A:309:GLU:HG3	1:A:316:VAL:HA	2.01	0.41
1:B:85:TRP:HE1	1:C:60:ILE:HD13	1.85	0.41
1:B:192:TYR:CG	1:C:365:LEU:HD23	2.56	0.41
1:E:201:THR:HG21	1:F:352:ASN:OD1	2.21	0.41
1:G:290:VAL:O	1:G:293:THR:OG1	2.31	0.41
1:B:148:LYS:HZ3	1:C:369:LEU:C	2.29	0.40
1:B:366:LEU:HA	1:B:369:LEU:HG	2.04	0.40
1:C:50:ILE:HD11	1:C:113:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ILE:HD11	1:D:113:LEU:HB2	2.03	0.40
1:E:192:TYR:CG	1:F:365:LEU:HD23	2.56	0.40
1:A:365:LEU:HD23	1:G:192:TYR:CD1	2.56	0.40
1:D:366:LEU:HA	1:D:369:LEU:HG	2.04	0.40
1:E:85:TRP:HE1	1:F:60:ILE:HD13	1.86	0.40
1:A:201:THR:HG21	1:B:352:ASN:OD1	2.21	0.40
1:C:366:LEU:HA	1:C:369:LEU:HG	2.04	0.40
1:E:366:LEU:HA	1:E:369:LEU:HG	2.04	0.40
1:A:366:LEU:HA	1:A:369:LEU:HG	2.04	0.40
1:A:368:ASN:ND2	1:G:192:TYR:HD1	2.19	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	296/444 (67%)	282 (95%)	13 (4%)	1 (0%)	36	66
1	B	296/444 (67%)	282 (95%)	13 (4%)	1 (0%)	36	66
1	C	296/444 (67%)	282 (95%)	13 (4%)	1 (0%)	36	66
1	D	296/444 (67%)	282 (95%)	13 (4%)	1 (0%)	36	66
1	E	296/444 (67%)	282 (95%)	13 (4%)	1 (0%)	36	66
1	F	296/444 (67%)	282 (95%)	13 (4%)	1 (0%)	36	66
1	G	296/444 (67%)	282 (95%)	13 (4%)	1 (0%)	36	66
All	All	2072/3108 (67%)	1974 (95%)	91 (4%)	7 (0%)	37	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	316	VAL

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Mol	Chain	Res	Type
1	G	316	VAL
1	A	316	VAL
1	B	316	VAL
1	C	316	VAL
1	D	316	VAL
1	E	316	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/395 (70%)	276 (100%)	1 (0%)	84	82
1	B	277/395 (70%)	276 (100%)	1 (0%)	84	82
1	C	277/395 (70%)	276 (100%)	1 (0%)	84	82
1	D	277/395 (70%)	276 (100%)	1 (0%)	84	82
1	E	277/395 (70%)	276 (100%)	1 (0%)	84	82
1	F	277/395 (70%)	276 (100%)	1 (0%)	84	82
1	G	277/395 (70%)	276 (100%)	1 (0%)	84	82
All	All	1939/2765 (70%)	1932 (100%)	7 (0%)	81	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	B	279	ASN
1	C	279	ASN
1	D	279	ASN
1	E	279	ASN
1	F	279	ASN
1	G	279	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	HIS
1	A	331	ASN
1	B	318	HIS
1	B	331	ASN
1	B	368	ASN
1	C	318	HIS
1	C	331	ASN
1	C	368	ASN
1	D	318	HIS
1	D	331	ASN
1	D	368	ASN
1	E	318	HIS
1	E	331	ASN
1	E	368	ASN
1	F	318	HIS
1	F	331	ASN
1	F	368	ASN
1	G	318	HIS
1	G	331	ASN
1	G	368	ASN

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 ⓘ

There are no ligands in this entry.

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.

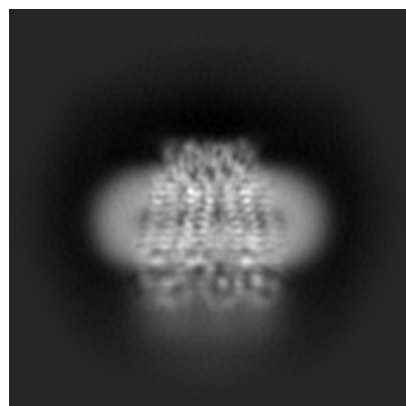
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52101. These allow visual inspection of the internal detail of the map and identification of artifacts.

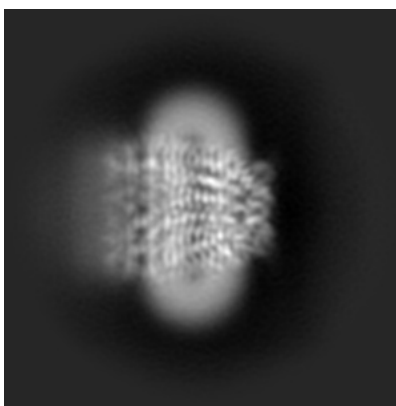
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

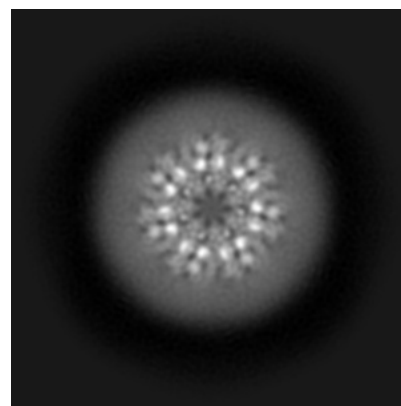
6.1.1 Primary map



X

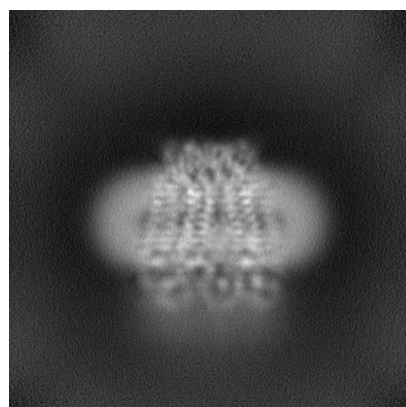


Y

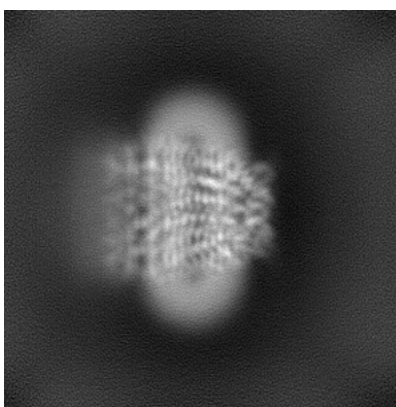


Z

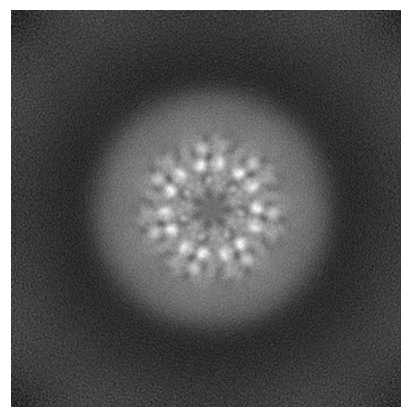
6.1.2 Raw map



X



Y

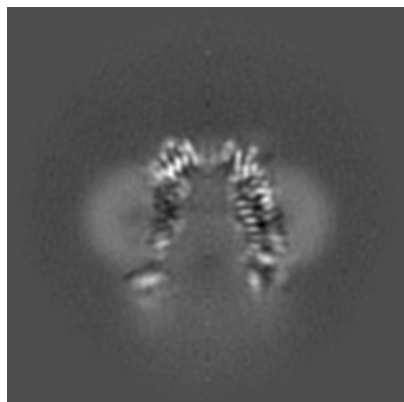


Z

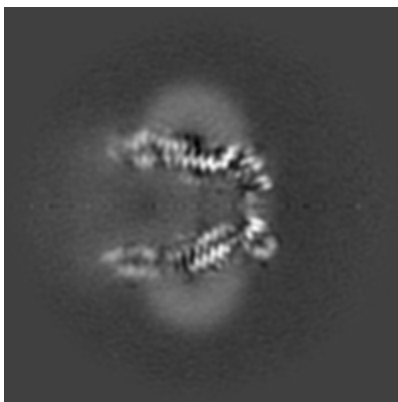
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

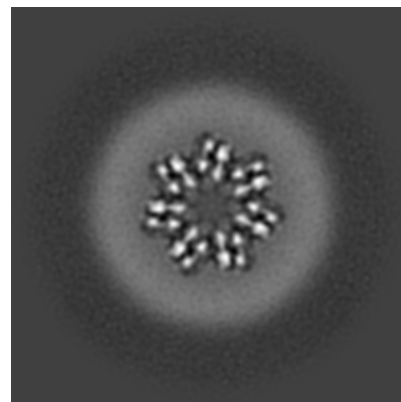
6.2.1 Primary map



X Index: 144

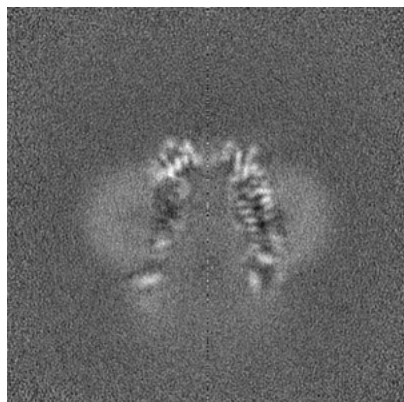


Y Index: 144

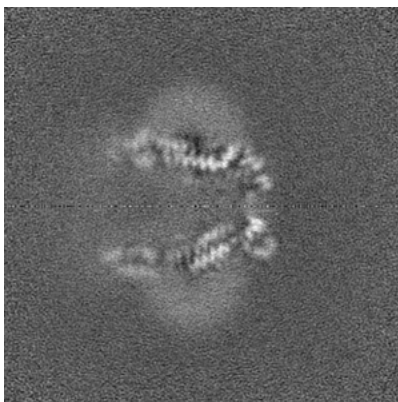


Z Index: 144

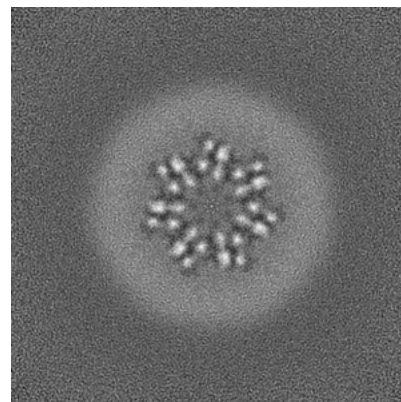
6.2.2 Raw map



X Index: 144



Y Index: 144

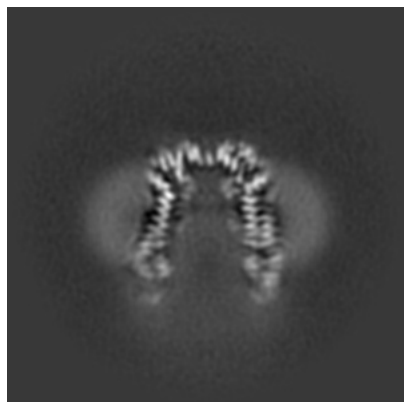


Z Index: 144

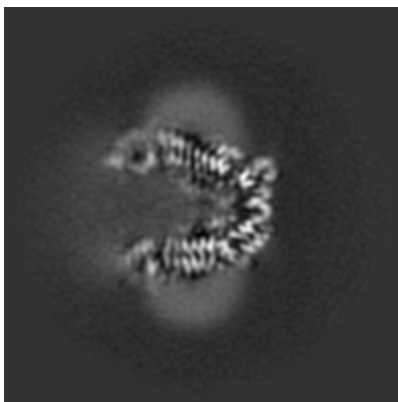
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

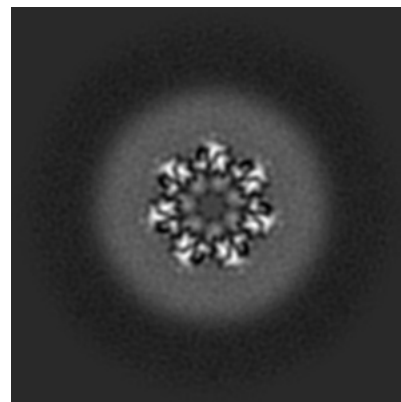
6.3.1 Primary map



X Index: 136

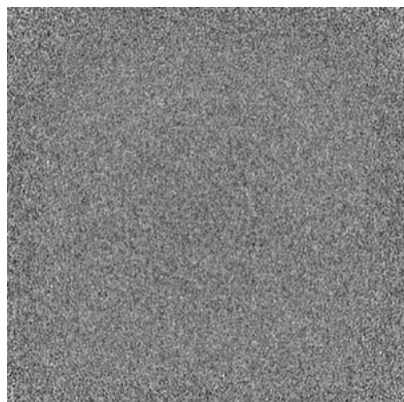


Y Index: 130

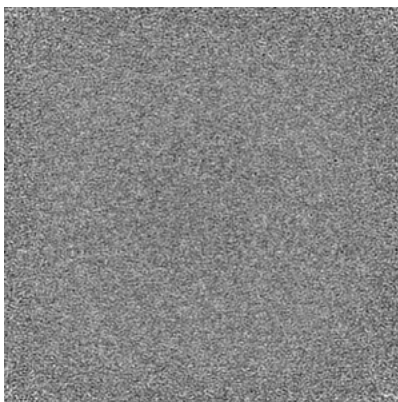


Z Index: 155

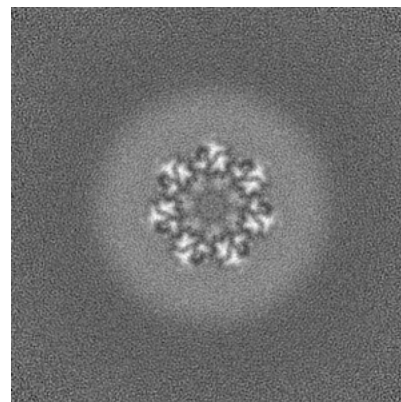
6.3.2 Raw map



X Index: 0



Y Index: 0

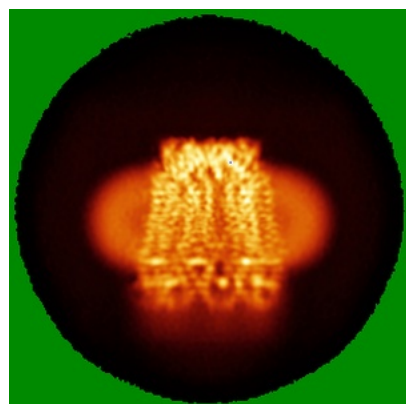


Z Index: 155

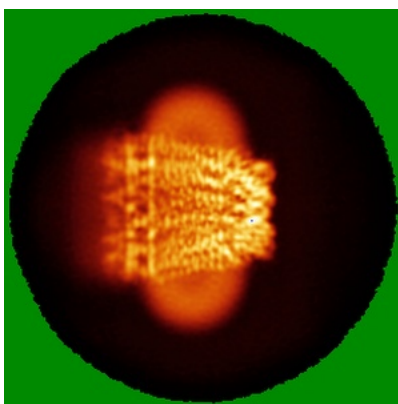
The images above show the largest variance slices of the map in three orthogonal directions.

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

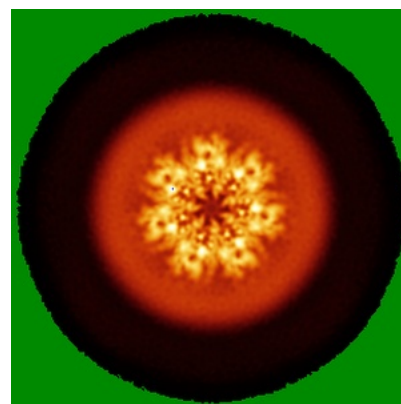
6.4.1 Primary map



X

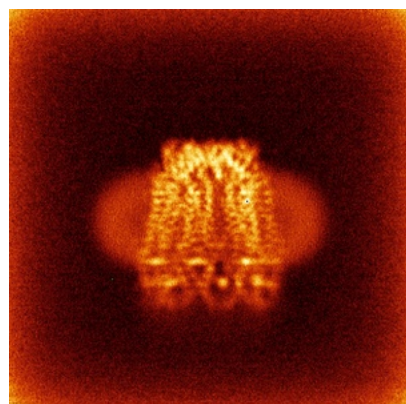


Y

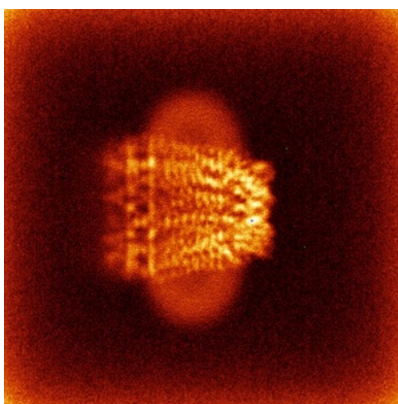


Z

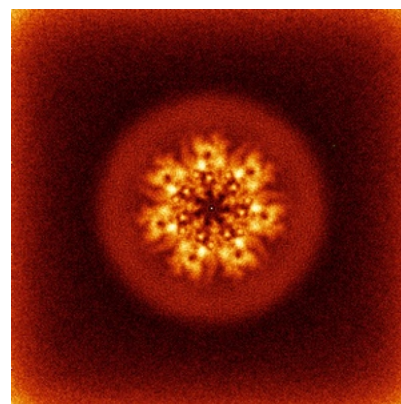
6.4.2 Raw map



X



Y

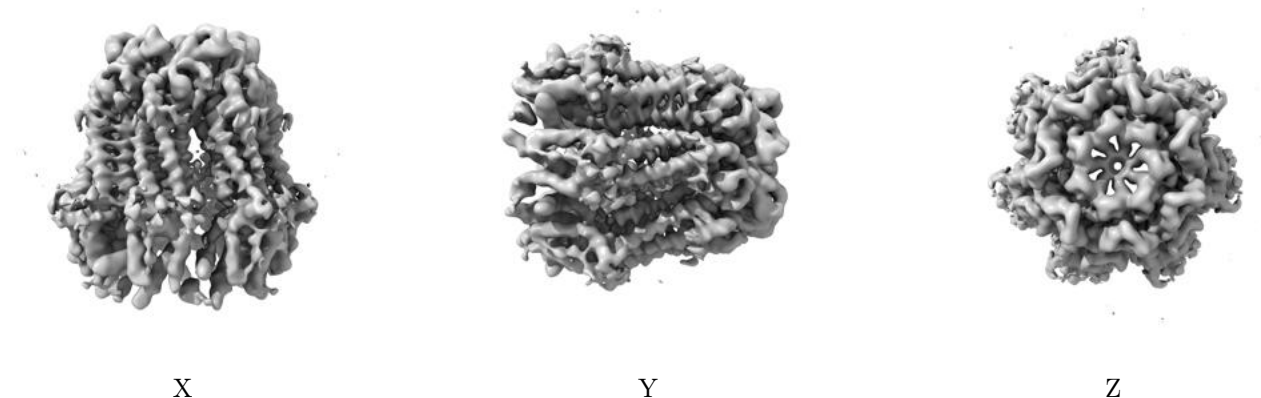


Z

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.

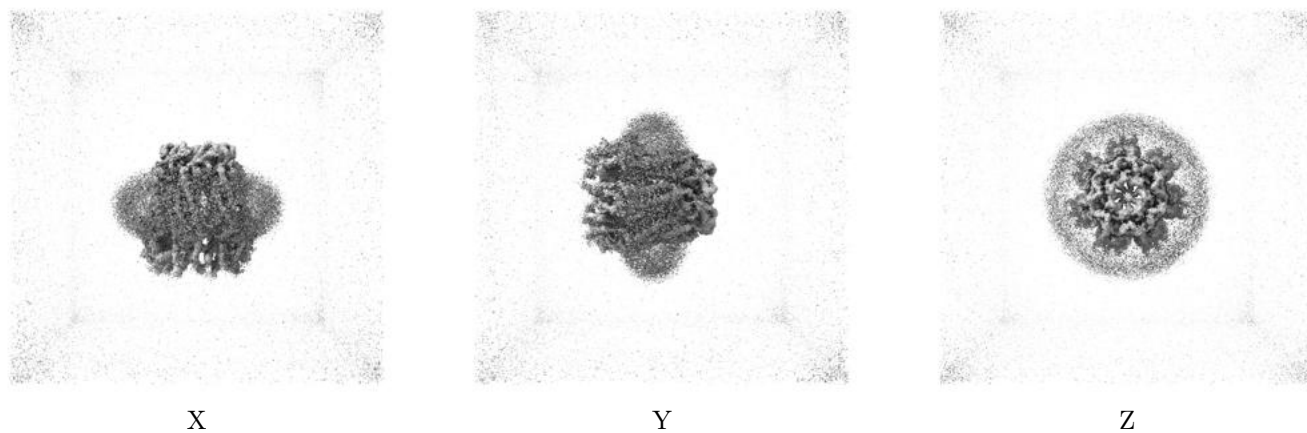
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.026. 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.

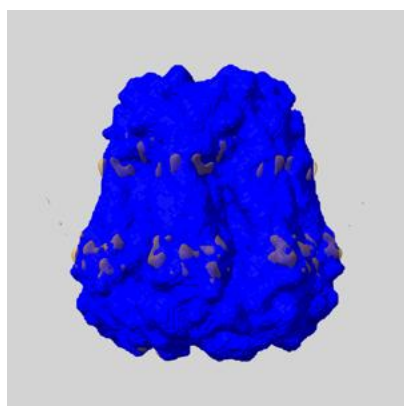
6.6 Mask visualisation [i](#)

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

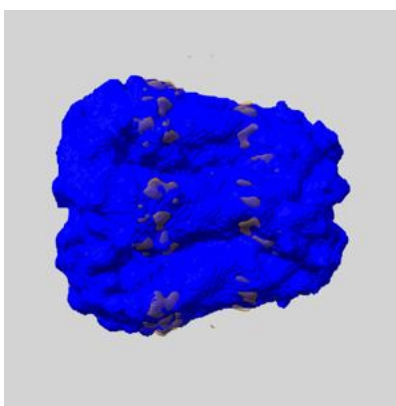
A mask typically either:

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

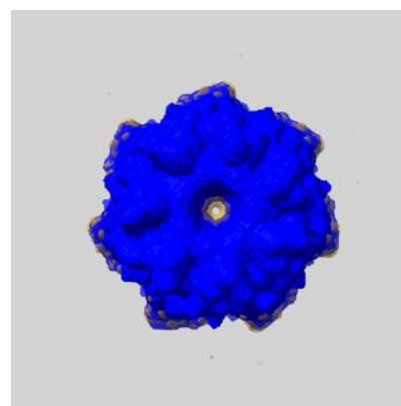
6.6.1 emd_52101_msk_2.map [i](#)



X

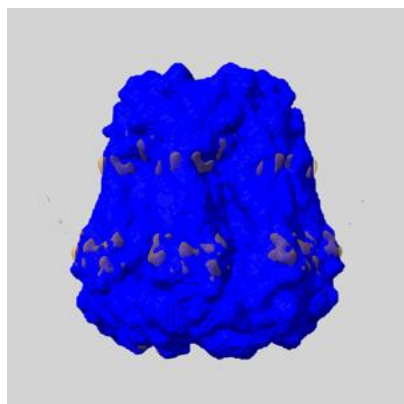


Y

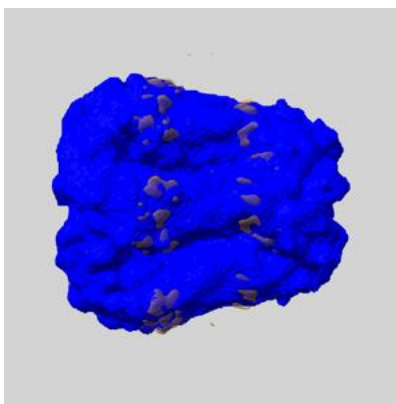


Z

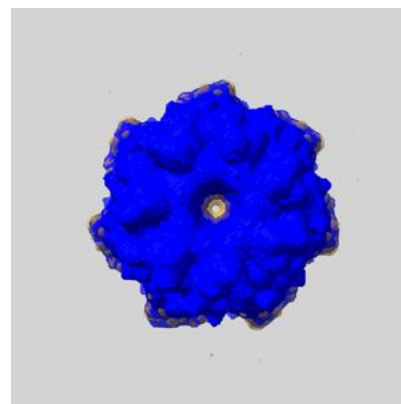
6.6.2 emd_52101_msk_1.map [i](#)



X



Y

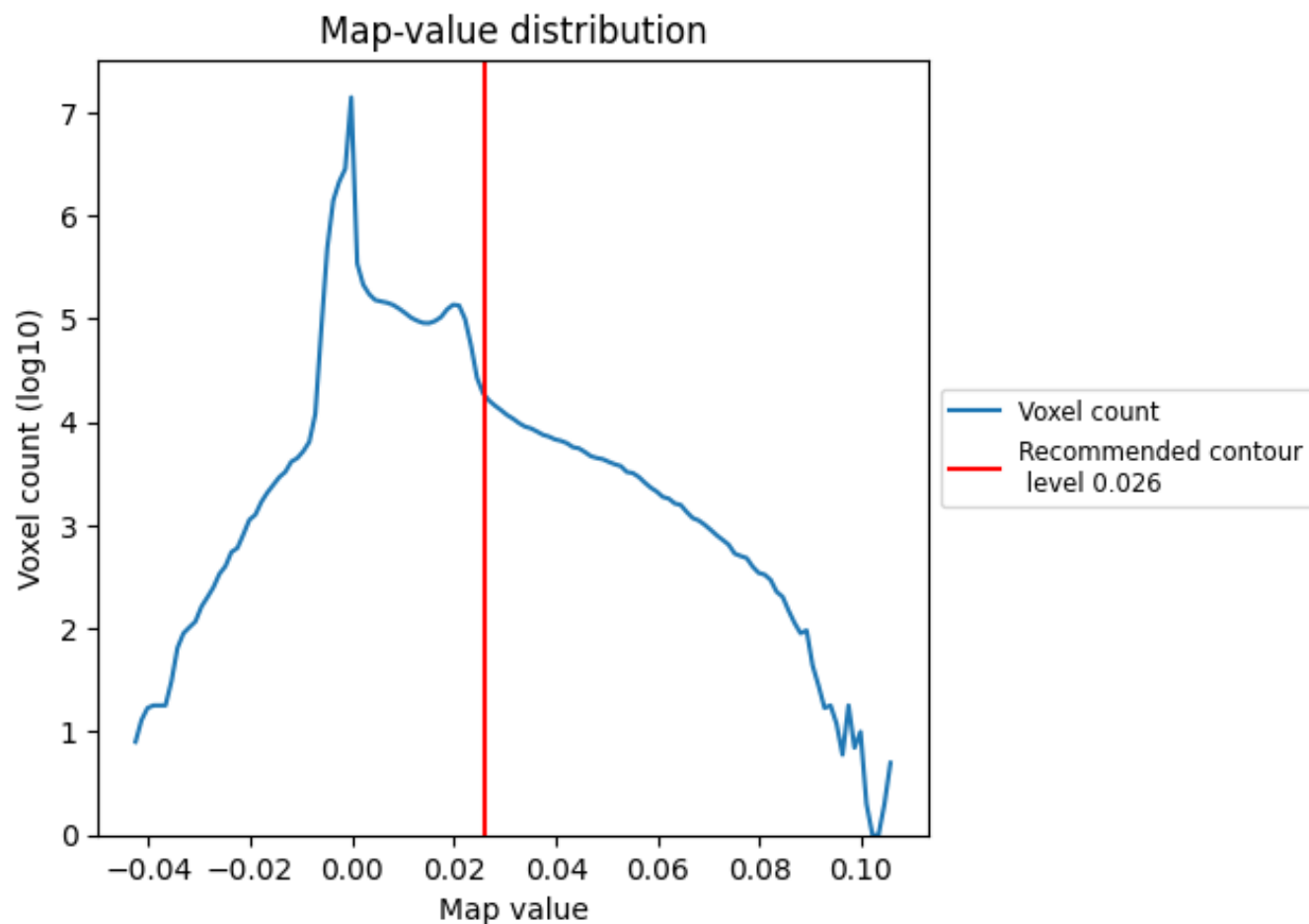


Z

7 Map analysis [i](#)

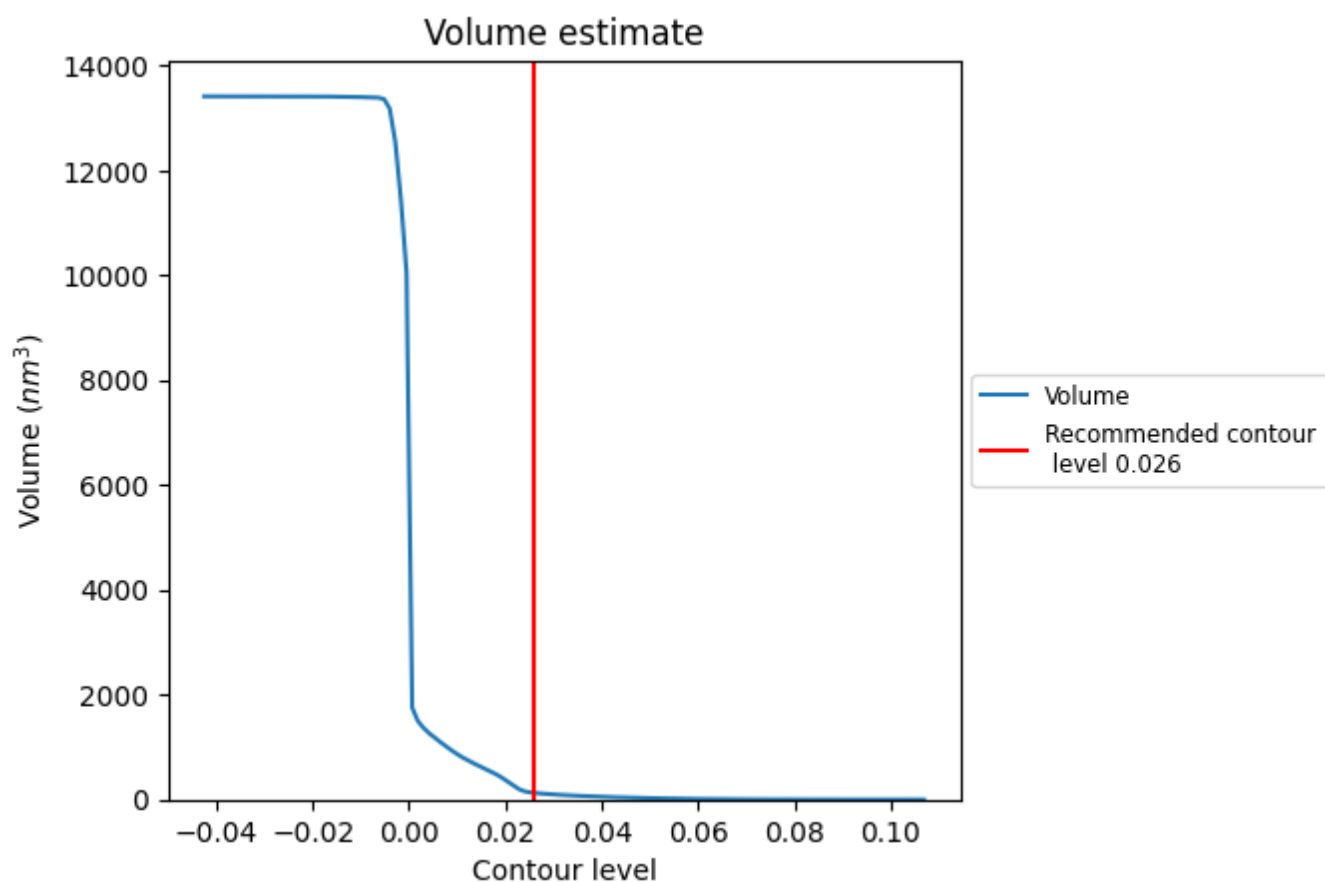
This section contains the results of statistical analysis of the map.

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.

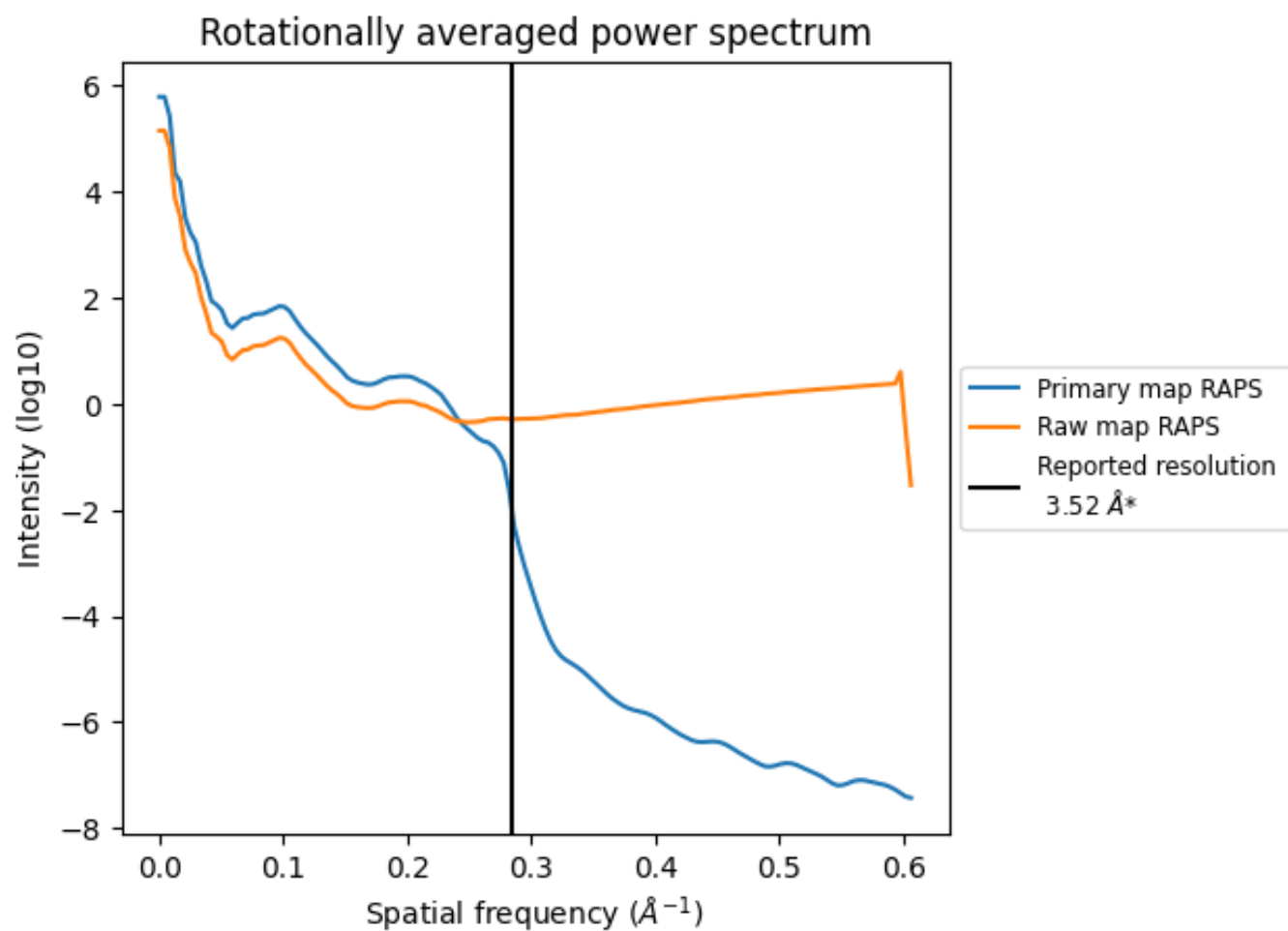
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 ⓘ

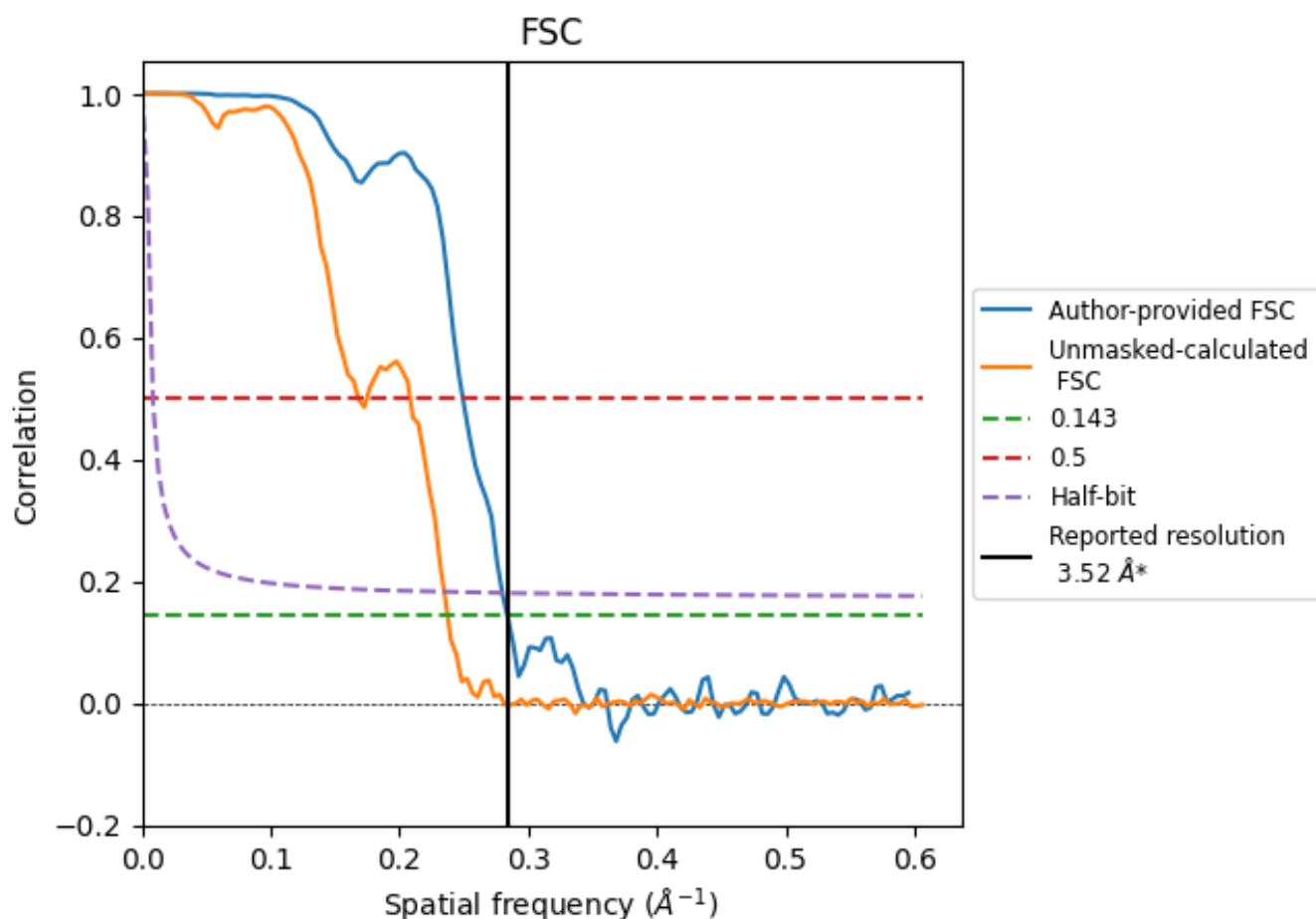


*Reported resolution corresponds to spatial frequency of 0.284 Å⁻¹

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 0.284 \AA^{-1}

8.2 Resolution estimates [i](#)

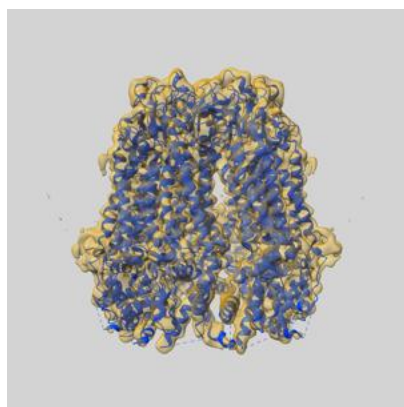
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.52	4.01	3.57
Unmasked-calculated*	4.21	5.95	4.26

*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 4.21 differs from the reported value 3.52 by more than 10 %

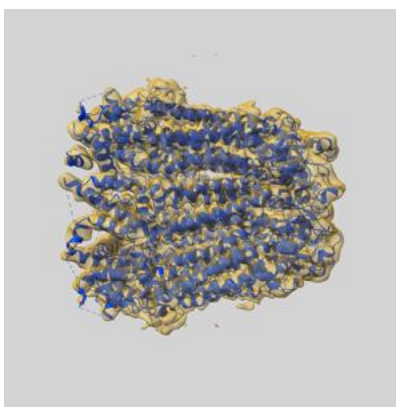
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52101 and PDB model 9HEY. Per-residue inclusion information can be found in section [3](#) on page [8](#).

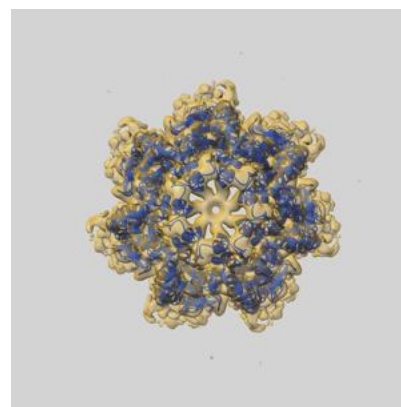
9.1 Map-model overlay [i](#)



X



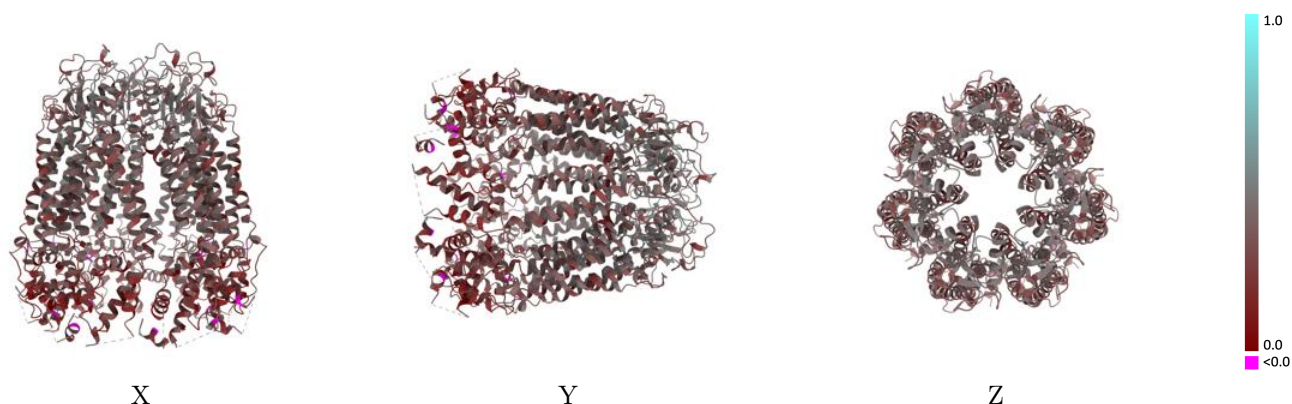
Y



Z

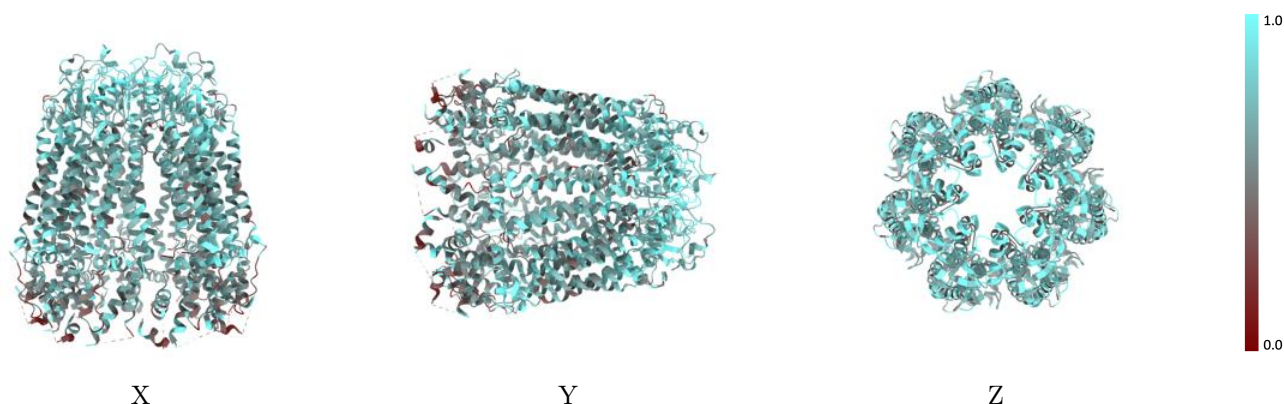
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



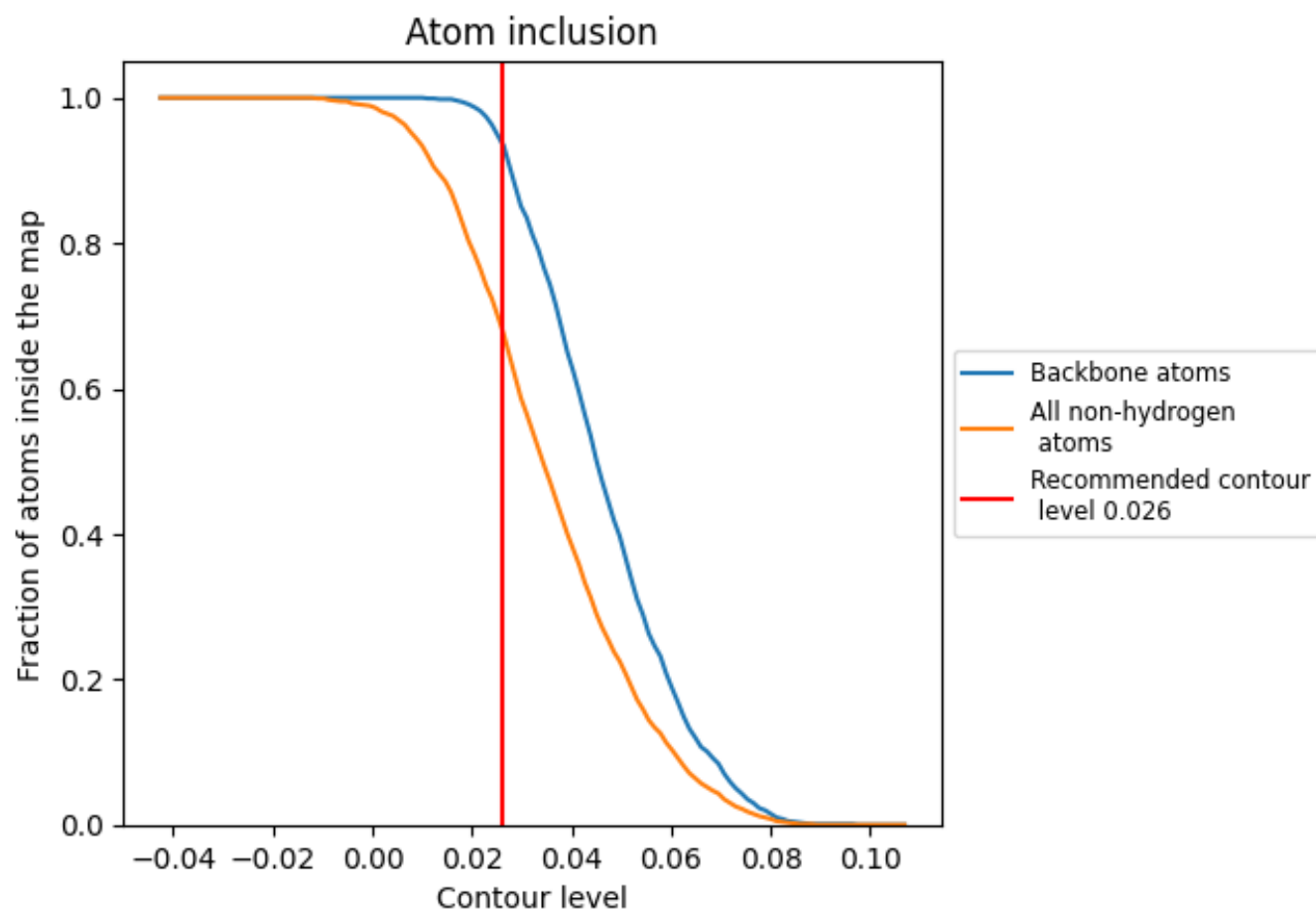
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 68% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6830	<div><div></div></div> 0.3230
A	<div><div></div></div> 0.6840	<div><div></div></div> 0.3230
B	<div><div></div></div> 0.6830	<div><div></div></div> 0.3240
C	<div><div></div></div> 0.6810	<div><div></div></div> 0.3230
D	<div><div></div></div> 0.6820	<div><div></div></div> 0.3230
E	<div><div></div></div> 0.6810	<div><div></div></div> 0.3230
F	<div><div></div></div> 0.6840	<div><div></div></div> 0.3230
G	<div><div></div></div> 0.6830	<div><div></div></div> 0.3230

1.0

0.0

<0.0