



wwPDB EM Validation Summary Report ⓘ

May 13, 2025 – 04:14 AM EDT

PDB ID : 8ET2 / pdb_00008et2
EMDB ID : EMD-28584
Title : CryoEM structure of the GSDMB pore
Authors : Wang, C.; Ruan, J.
Deposited on : 2022-10-15
Resolution : 4.96 Å(reported)

This is a wwPDB EM Validation Summary 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

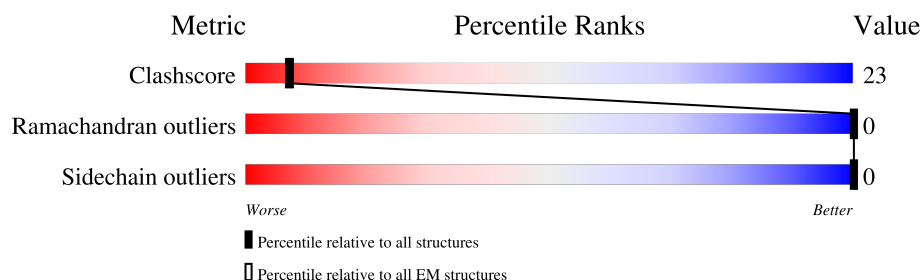
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.96 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.



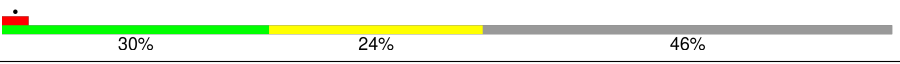

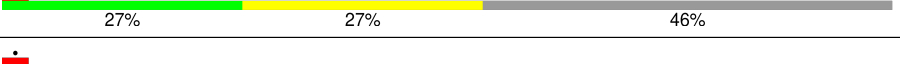
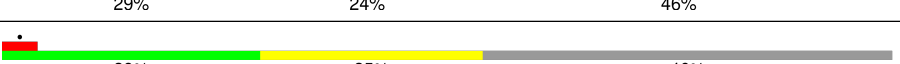
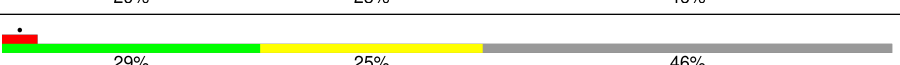
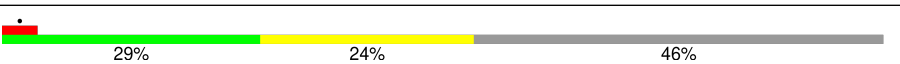
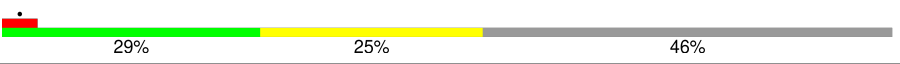
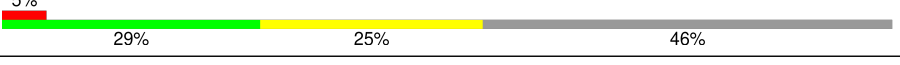
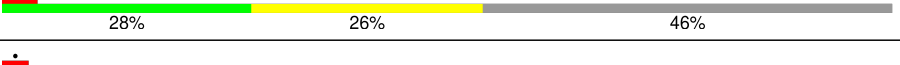



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	411	
1	B	411	
1	C	411	
1	D	411	
1	E	411	
1	F	411	
1	G	411	
1	H	411	

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Mol	Chain	Length	Quality of chain
1	I	411	
1	J	411	
1	K	411	
1	L	411	
1	M	411	
1	N	411	
1	O	411	
1	P	411	
1	Q	411	
1	R	411	
1	S	411	
1	T	411	
1	U	411	
1	V	411	
1	W	411	
1	X	411	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 43584 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 Isoform 1 of Gasdermin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	B	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	C	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	D	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	E	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	F	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	G	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	H	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	I	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	J	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	K	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	L	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	M	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	N	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	O	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	P	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	Q	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		

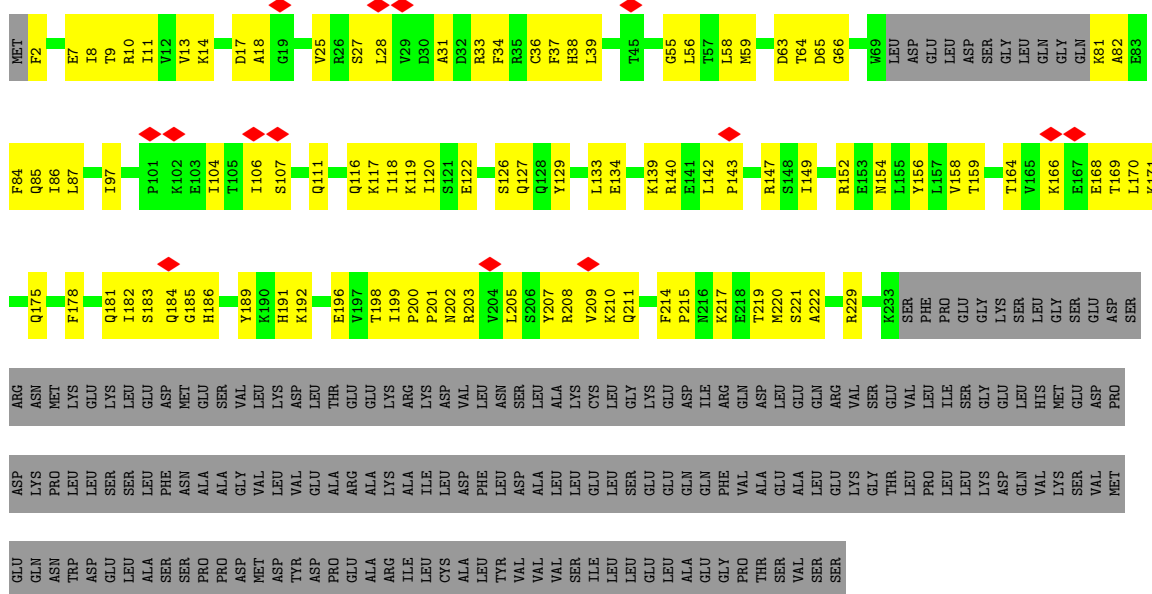
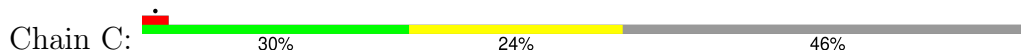
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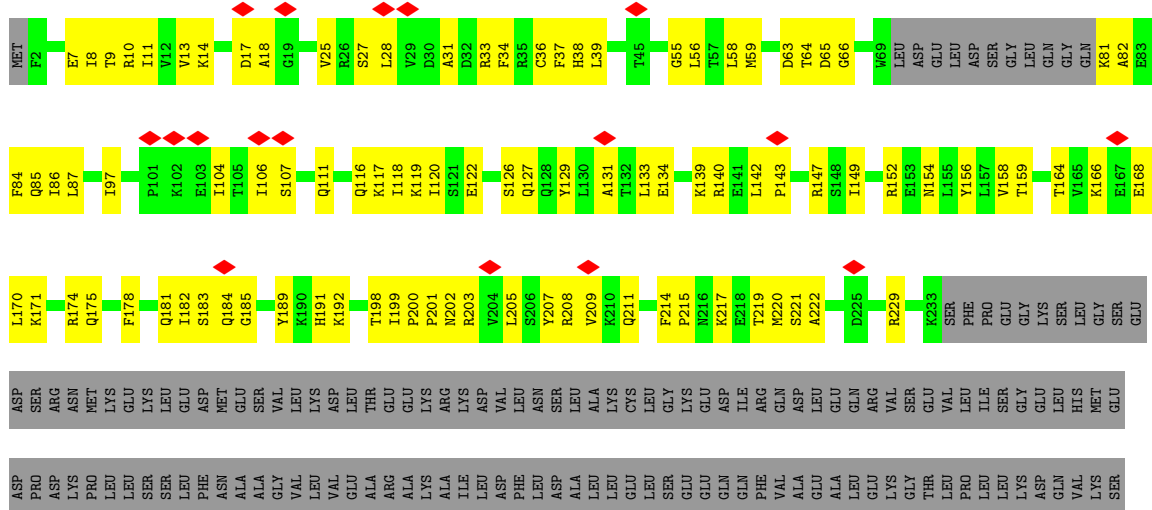
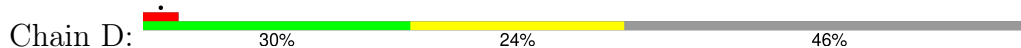
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	S	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	T	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	U	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	V	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	W	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		
1	X	221	Total	C	N	O	S	0	0
			1816	1153	323	334	6		

[illegible]

- Molecule 1: Isoform 1 of Gasdermin-B

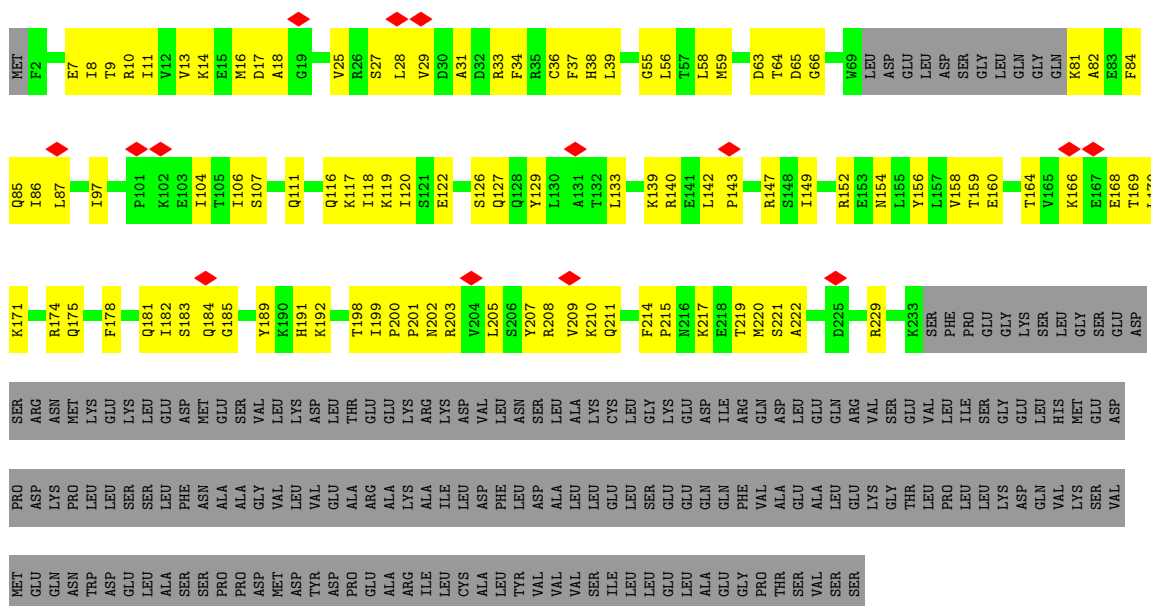
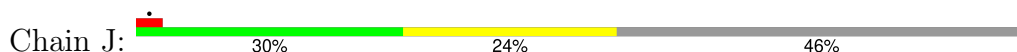


- Molecule 1: Isoform 1 of Gasdermin-B

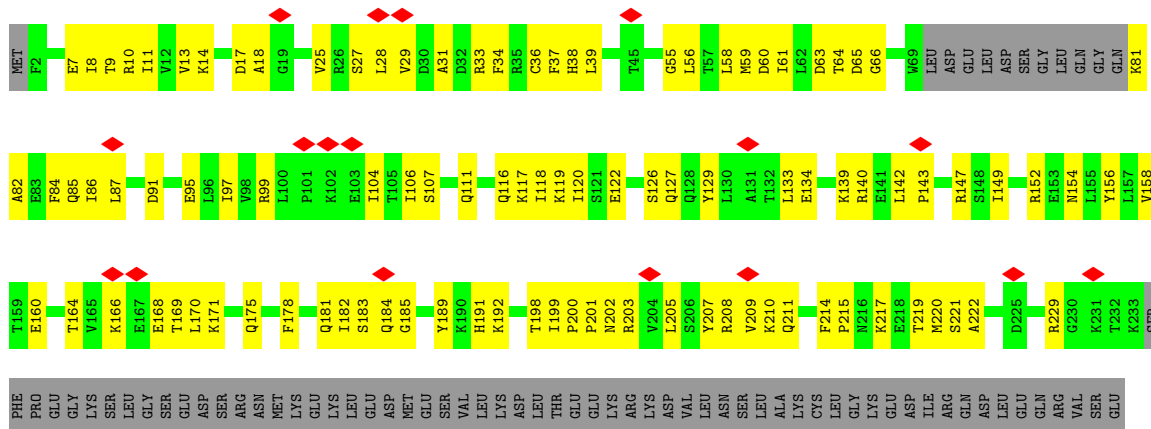
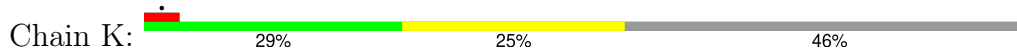




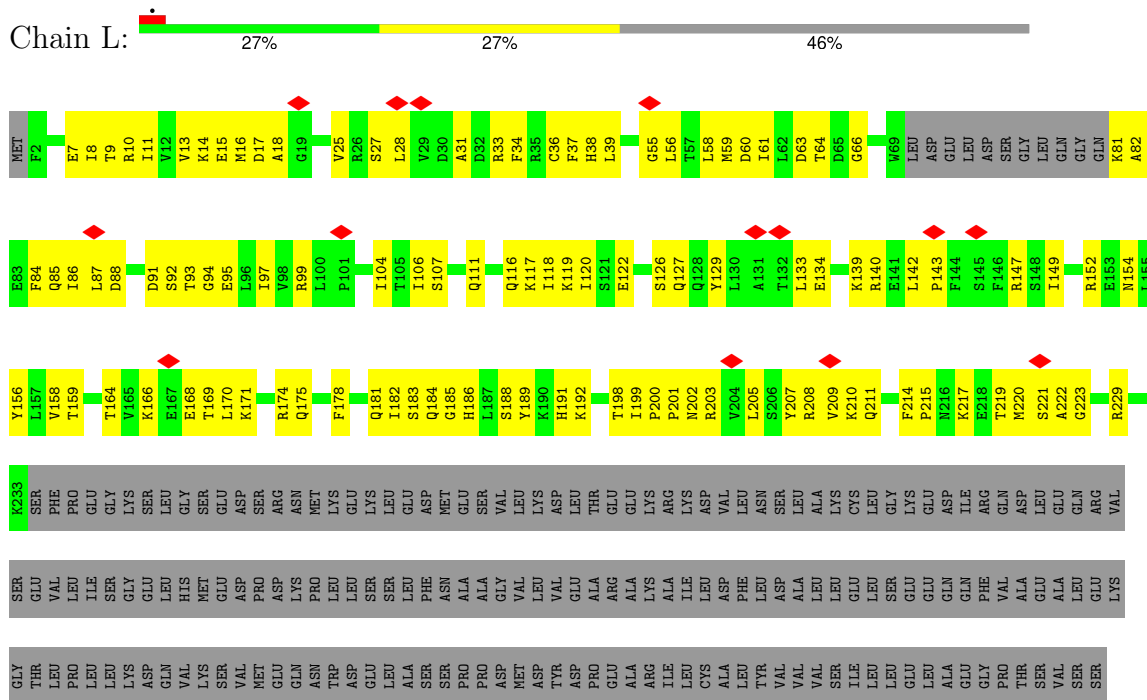
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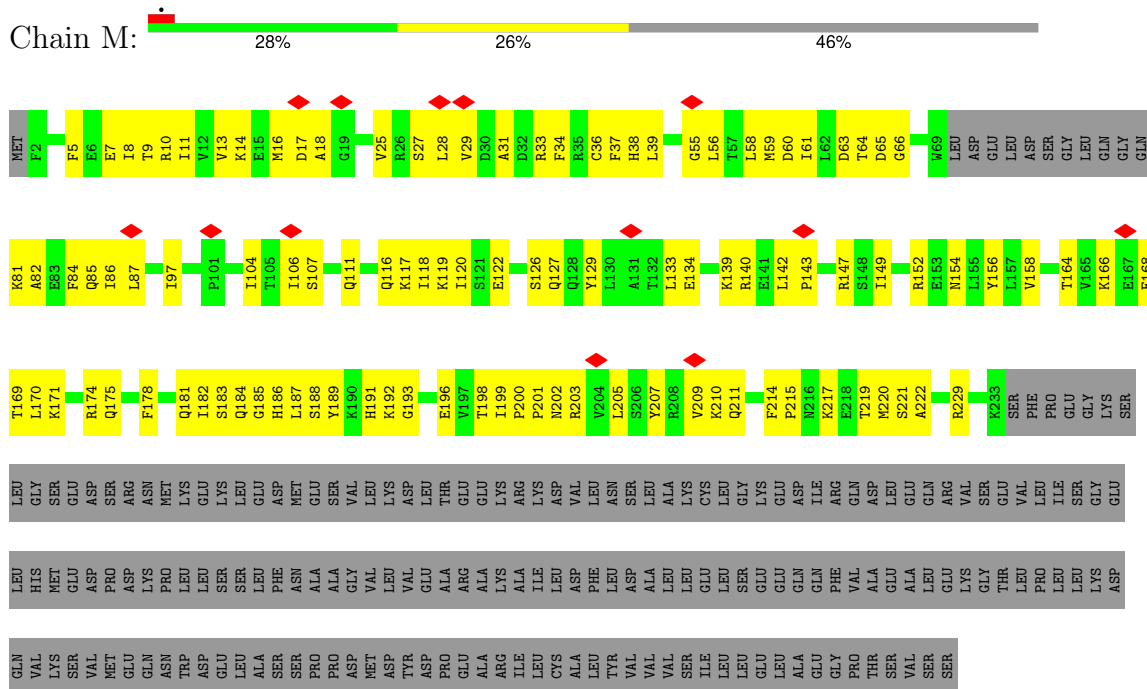
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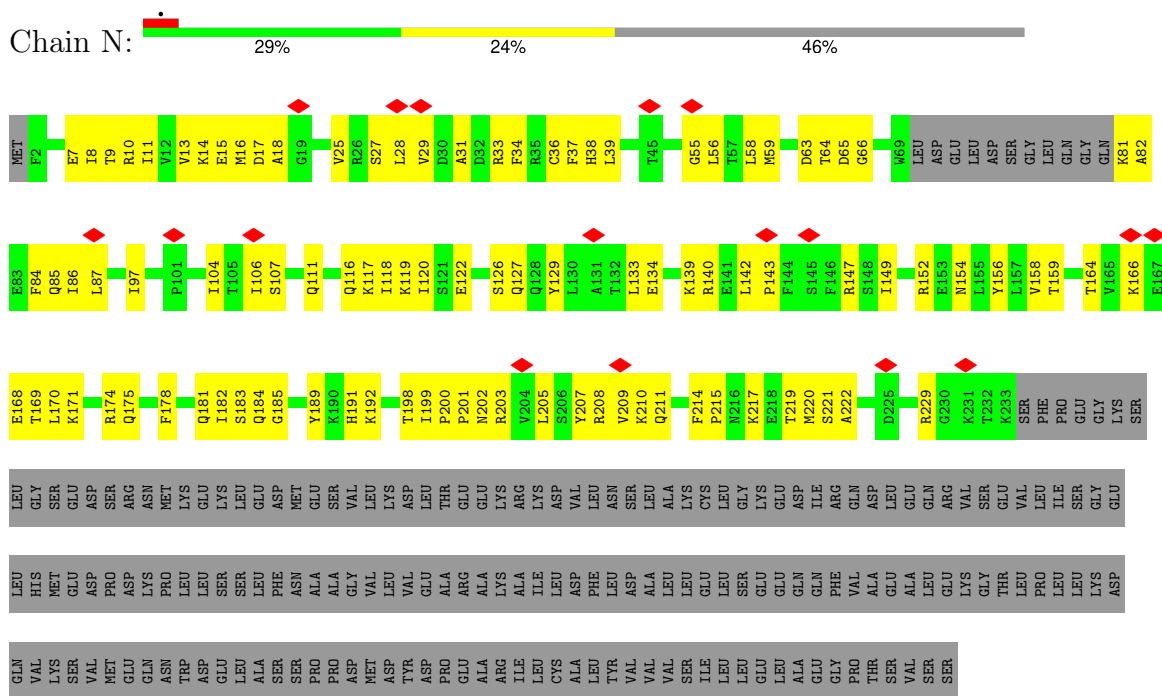
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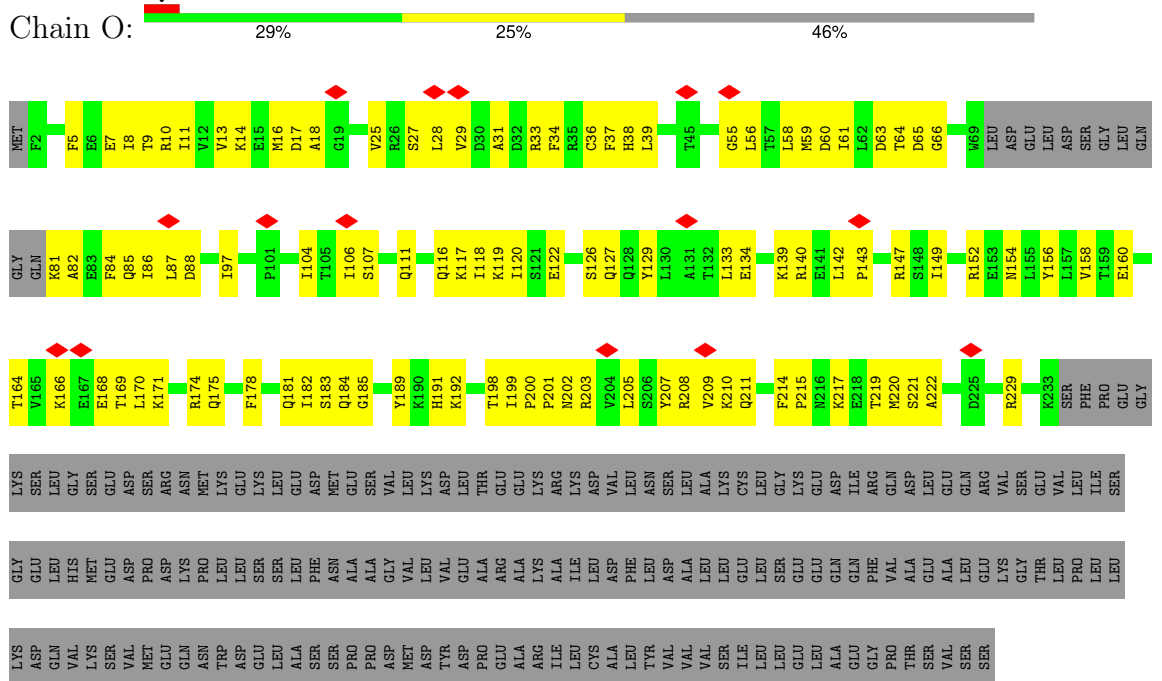
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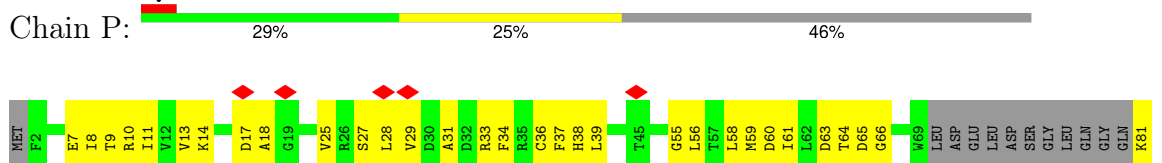
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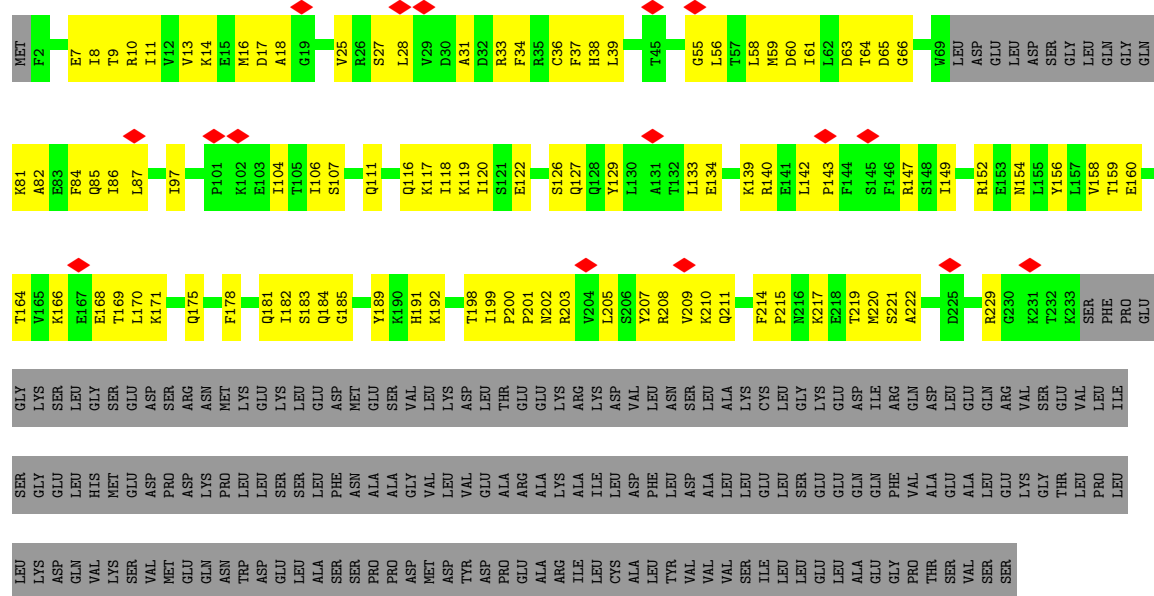
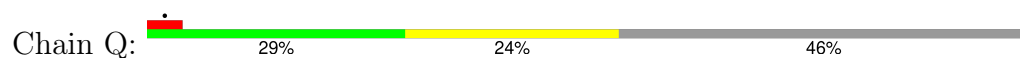
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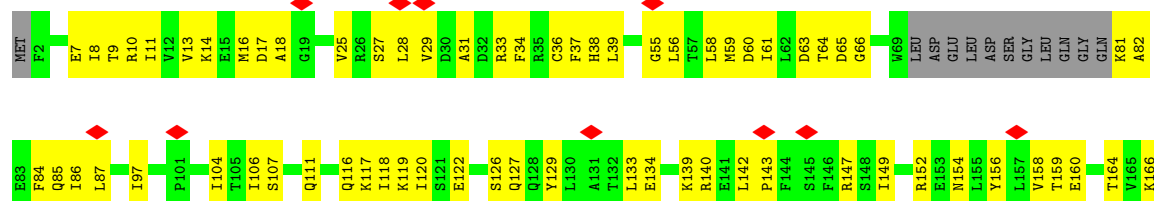
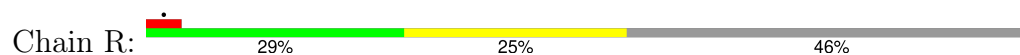
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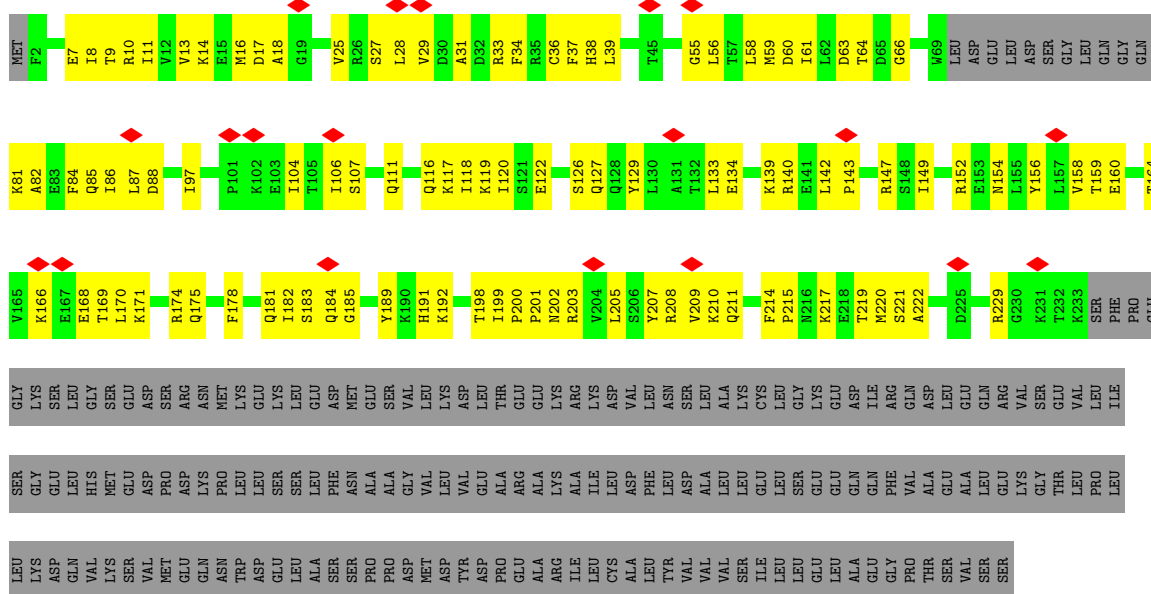
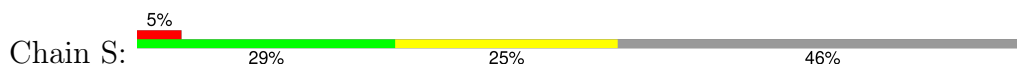
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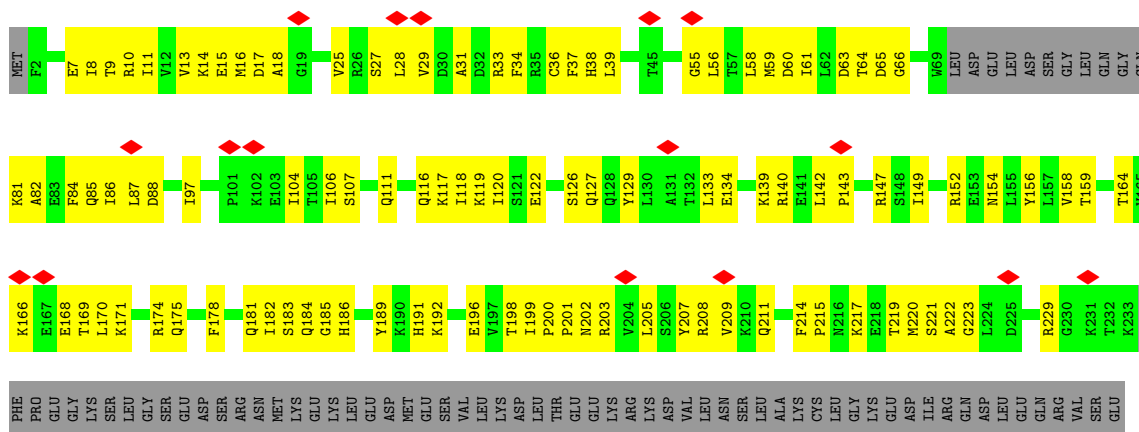
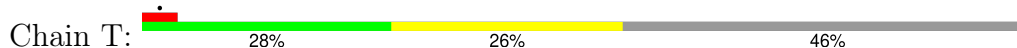
- Molecule 1: Isoform 1 of Gasdermin-B



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- Molecule 1: Isoform 1 of Gasdermin-B




VAL	LEU	ILE	SER	GLY	LEU	HIS	MET	GLU	ASP	PRO	PRO	GLY	ASP	LYS	PRO	LEU	SER	GLY	VAL	LEU	SER	ALA	LEU	PHE	SER	ASN	ALA	ALA	GLY	VAL	VAL	LEU	TYR	ASP	GLU	PRO	ALA	ALA	ARG	GLY	ALA	ALA	LYS	ILE	LEU	LEU	CYS	LEU	ASP	PHE	LEU	ASP	VAL	VAL	LEU	LEU	SER	ILE	LEU	SER	LEU	GLU	GLU	GLN	GLN	PHE	GLY	VAL	THR	SER	GLY	VAL	SER	LEU	LYS	THR
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• Molecule 1: Isoform 1 of Gasdermin-B

Chain U: 

GLY	THR	LEU	LEU	PRO	LEU	LEU	LEU	LYS	GLY	GLU	GLN	VAL	ASP	GLN	VAL	LYS	SER	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER	VAL	GLY	THR	SER
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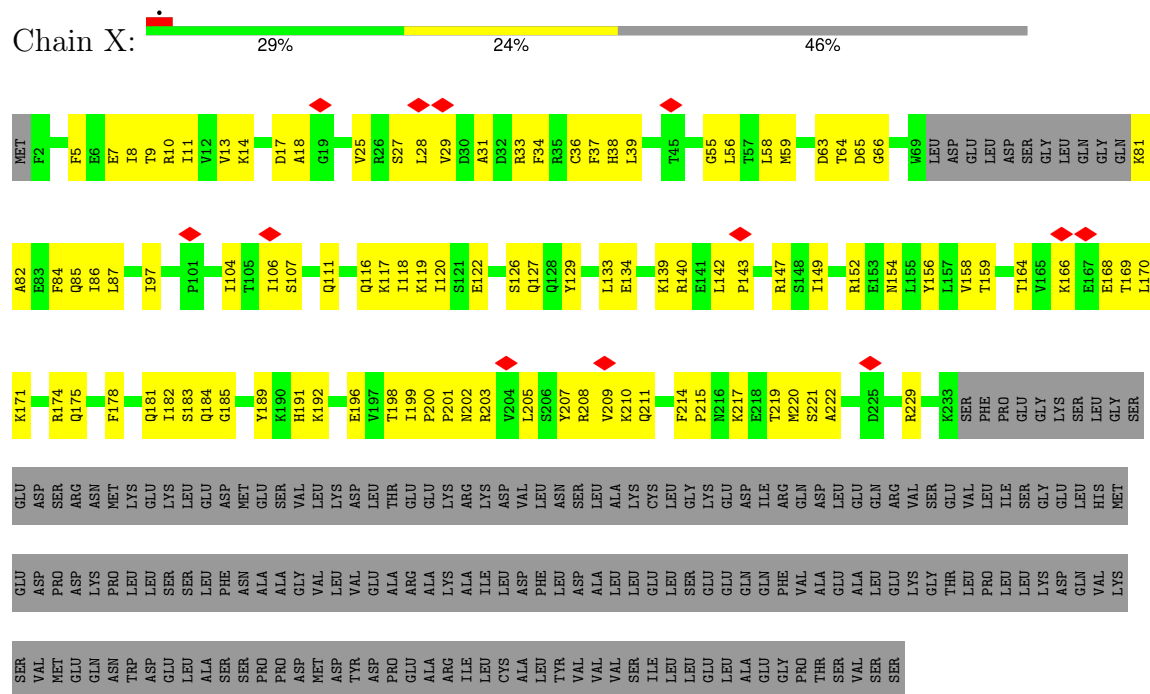
• Molecule 1: Isoform 1 of Gasdermin-B

Chain V: 

LEU	LYS	ASP	GLN	VAL	LYS	SER	GLU	VAL	MET	GLU	ASN	SER	ASP	PRO	ALA	PRO	ASP	MET	ASP	TYR	ASP	PRO	GLU	ARG	ALA	ALA	ILE	LEU	CYS	LEU	PHE	LEU	THR	VAL	VAL	VAL	SER	ILE	LEU	LEU	GLY	PRO	THR	SER	VAL	SER	SER	SER	SER							
GLY	LYS	GLU	LEU	HIS	MET	SER	GLU	ASP	PRO	SER	ASN	GLY	ASP	LYS	LEU	GLY	GLU	VAL	LEU	VAL	VAL	GLY	THR	GLU	LYS	GLU	ALA	ALA	ASP	VAL	LEU	ASN	SER	ALA	LEU	ALA	LEU	GLY	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
T169	L170	K171	R174	Q175	F178	Q181	I182	S183	Q184	G185	H186	L187	S188	Y189	K190	H191	K192	G193	E196	V197	T198	I199	P200	P201	M202	R203	V204	L205	S206	Y207	R208	V209	K210	Q211	F214	P215	K216	K217	E218	T219	M220	S221	A222	D225	R229	K233	SER	PHE	PRO	GLU						
E168	T169	K171	R174	Q175	F178	Q181	I182	S183	Q184	G185	H186	L187	S188	Y189	K190	H191	K192	G193	E196	V197	T198	I199	P200	P201	M202	R203	V204	L205	S206	Y207	R208	V209	K210	Q211	F214	P215	K216	K217	E218	T219	M220	S221	A222	D225	R229	K233	SER	PHE	PRO	GLU						
GLY	LYS	SER	GLY	SER	SER	ASN	MET	LYS	GLY	LYS	GLY	GLY	ASP	MET	GLY	SER	VAL	LYS	ASP	VAL	THR	GLU	GLY	LYS	LYS	ARG	ASP	VAL	LEU	ASN	SER	ALA	ALA	ALA	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY							
A82	E83	F84	Q85	T86	L87	D91	I97	P101	I104	T105	I106	S107	Q111	Q116	K117	I118	K119	I120	S121	E122	S126	Q127	Q128	Y129	L133	E134	K139	R140	E141	L142	P143	F144	S145	F146	R147	S148	I149	R152	E153	N154	I155	Y156	L157	V158	T164	V165	K166	E167								
MET	F2	E7	T8	T9	R10	I11	V12	K14	D17	A18	G19	V25	R26	S27	L28	V29	D30	A31	D32	R33	F34	R35	G36	F37	H38	L39	T45	G55	L56	T57	L58	M59	D60	I61	L62	D63	T64	D65	G66	W69	LEU	ASP	GLU	LEU	ASP	SER	GLY	LEU	GLN	GLY	GLY	GLN	GLY	GLY	GLN	K81

• Molecule 1: Isoform 1 of Gasdermin-B

- Molecule 1: Isoform 1 of Gasdermin-B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41799	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.058	Depositor
Minimum map value	-0.716	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	424.96, 424.96, 424.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.66, 1.66, 1.66	Depositor

5 Model quality

5.1 Standard geometry

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	0.20	0/1850	0.58	0/2484
1	B	0.20	0/1850	0.58	0/2484
1	C	0.20	0/1850	0.58	0/2484
1	D	0.20	0/1850	0.58	0/2484
1	E	0.20	0/1850	0.58	0/2484
1	F	0.20	0/1850	0.58	0/2484
1	G	0.20	0/1850	0.58	0/2484
1	H	0.20	0/1850	0.58	0/2484
1	I	0.20	0/1850	0.58	0/2484
1	J	0.20	0/1850	0.58	0/2484
1	K	0.20	0/1850	0.58	0/2484
1	L	0.20	0/1850	0.58	0/2484
1	M	0.20	0/1850	0.58	0/2484
1	N	0.20	0/1850	0.58	0/2484
1	O	0.20	0/1850	0.58	0/2484
1	P	0.20	0/1850	0.58	0/2484
1	Q	0.20	0/1850	0.58	0/2484
1	R	0.20	0/1850	0.58	0/2484
1	S	0.20	0/1850	0.58	0/2484
1	T	0.20	0/1850	0.58	0/2484
1	U	0.20	0/1850	0.58	0/2484
1	V	0.20	0/1850	0.58	0/2484
1	W	0.20	0/1850	0.58	0/2484
1	X	0.20	0/1850	0.58	0/2484
All	All	0.20	0/44400	0.58	0/59616

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 ⓘ

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	1816	0	1829	85	0
1	B	1816	0	1829	90	0
1	C	1816	0	1829	87	0
1	D	1816	0	1829	83	0
1	E	1816	0	1829	84	0
1	F	1816	0	1829	88	0
1	G	1816	0	1829	87	0
1	H	1816	0	1829	82	0
1	I	1816	0	1829	84	0
1	J	1816	0	1829	91	0
1	K	1816	0	1829	91	0
1	L	1816	0	1829	110	0
1	M	1816	0	1829	105	0
1	N	1816	0	1829	85	0
1	O	1816	0	1829	94	0
1	P	1816	0	1829	89	0
1	Q	1816	0	1829	82	0
1	R	1816	0	1829	89	0
1	S	1816	0	1829	92	0
1	T	1816	0	1829	94	0
1	U	1816	0	1829	106	0
1	V	1816	0	1829	103	0
1	W	1816	0	1829	94	0
1	X	1816	0	1829	88	0
All	All	43584	0	43896	2034	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 23.

The worst 5 of 2034 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:I:168:GLU:HA	1:I:199:ILE:O	1.67	0.95
1:O:168:GLU:HA	1:O:199:ILE:O	1.67	0.95
1:H:168:GLU:HA	1:H:199:ILE:O	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:GLU:HA	1:N:199:ILE:O	1.67	0.95
1:R:168:GLU:HA	1:R:199:ILE:O	1.67	0.95

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	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	B	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	C	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	D	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	E	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	F	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	G	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	H	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	I	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	J	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	K	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	L	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	M	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	N	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	O	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	P	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	Q	217/411 (53%)	190 (88%)	27 (12%)	0	100	100
1	R	217/411 (53%)	192 (88%)	25 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	T	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	U	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	V	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
1	W	217/411 (53%)	192 (88%)	25 (12%)	0	100	100
1	X	217/411 (53%)	191 (88%)	26 (12%)	0	100	100
All	All	5208/9864 (53%)	4597 (88%)	611 (12%)	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	202/370 (55%)	202 (100%)	0	100	100
1	B	202/370 (55%)	202 (100%)	0	100	100
1	C	202/370 (55%)	202 (100%)	0	100	100
1	D	202/370 (55%)	202 (100%)	0	100	100
1	E	202/370 (55%)	202 (100%)	0	100	100
1	F	202/370 (55%)	202 (100%)	0	100	100
1	G	202/370 (55%)	202 (100%)	0	100	100
1	H	202/370 (55%)	202 (100%)	0	100	100
1	I	202/370 (55%)	202 (100%)	0	100	100
1	J	202/370 (55%)	202 (100%)	0	100	100
1	K	202/370 (55%)	202 (100%)	0	100	100
1	L	202/370 (55%)	202 (100%)	0	100	100
1	M	202/370 (55%)	202 (100%)	0	100	100
1	N	202/370 (55%)	202 (100%)	0	100	100
1	O	202/370 (55%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	202/370 (55%)	202 (100%)	0	100	100
1	Q	202/370 (55%)	202 (100%)	0	100	100
1	R	202/370 (55%)	202 (100%)	0	100	100
1	S	202/370 (55%)	202 (100%)	0	100	100
1	T	202/370 (55%)	202 (100%)	0	100	100
1	U	202/370 (55%)	202 (100%)	0	100	100
1	V	202/370 (55%)	202 (100%)	0	100	100
1	W	202/370 (55%)	202 (100%)	0	100	100
1	X	202/370 (55%)	202 (100%)	0	100	100
All	All	4848/8880 (55%)	4848 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	186	HIS
1	P	216	ASN
1	W	51	HIS
1	M	216	ASN
1	O	181	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 [i](#)

There are no ligands in this entry.

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.

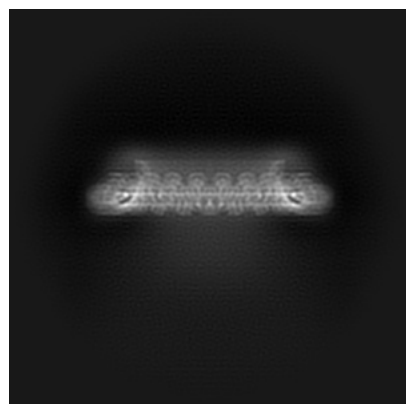
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28584. These allow visual inspection of the internal detail of the map and identification of artifacts.

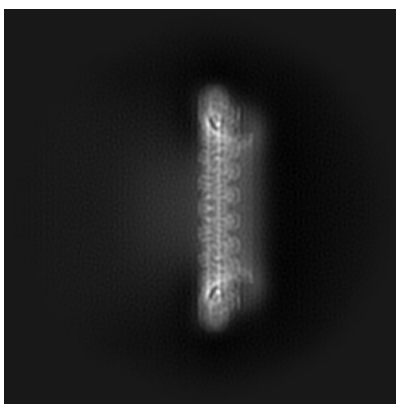
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

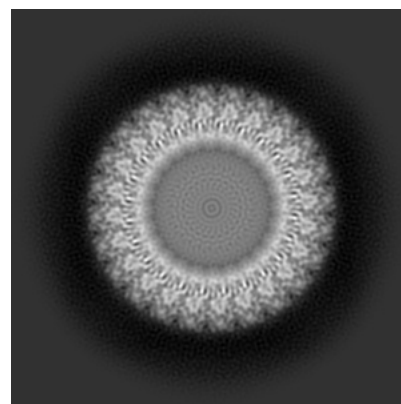
6.1.1 Primary map



X

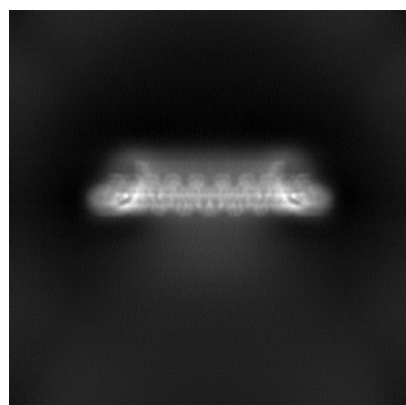


Y

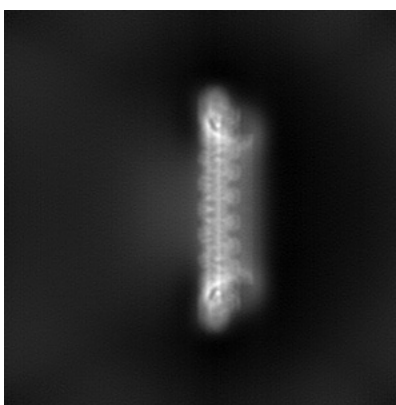


Z

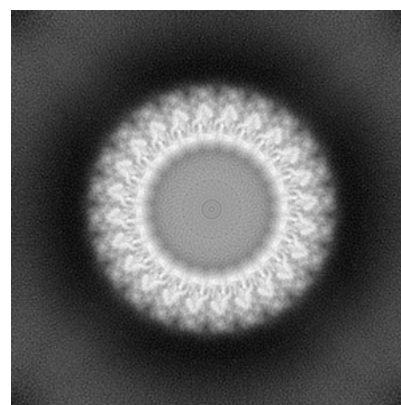
6.1.2 Raw map



X



Y

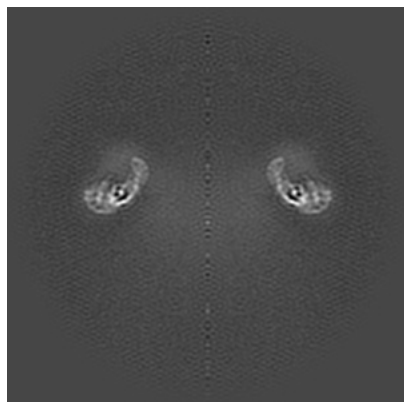


Z

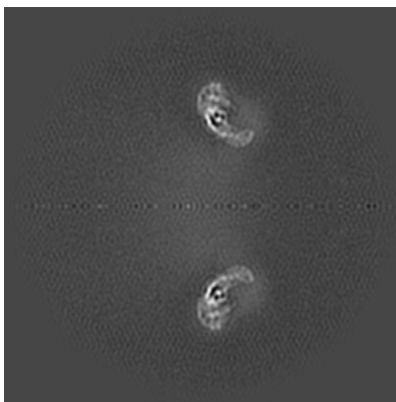
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

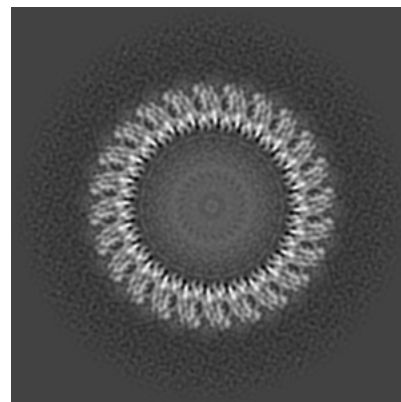
6.2.1 Primary map



X Index: 128

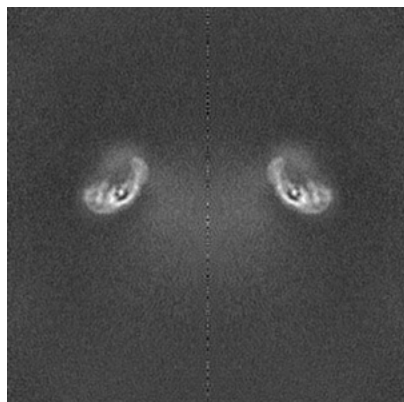


Y Index: 128

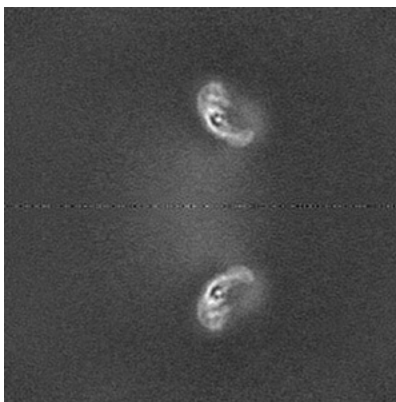


Z Index: 128

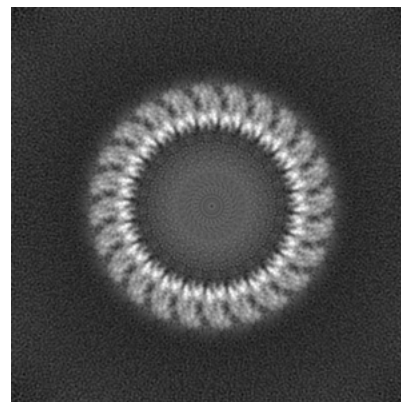
6.2.2 Raw map



X Index: 128



Y Index: 128

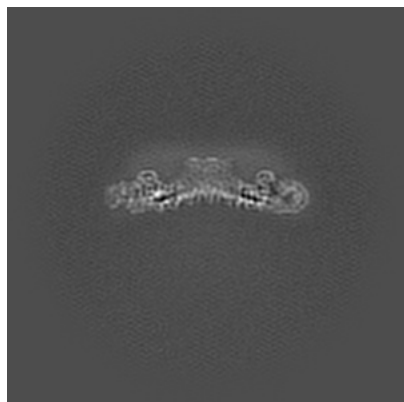


Z Index: 128

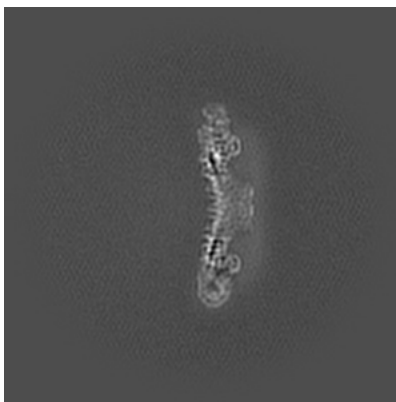
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

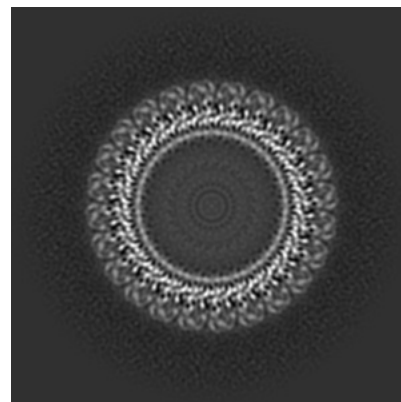
6.3.1 Primary map



X Index: 175

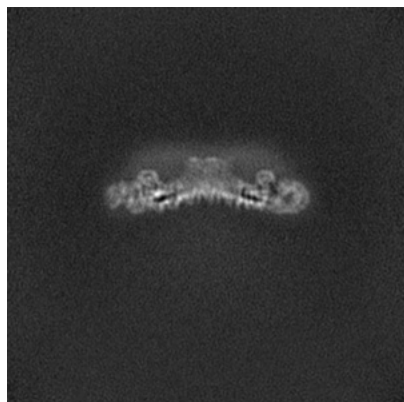


Y Index: 175



Z Index: 137

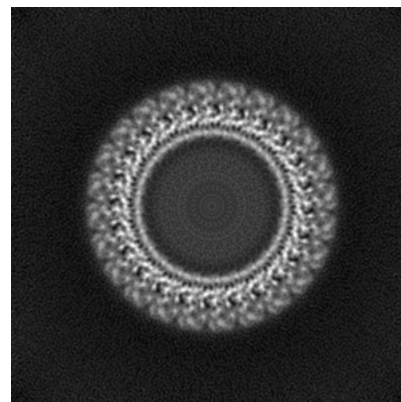
6.3.2 Raw map



X Index: 175



Y Index: 81

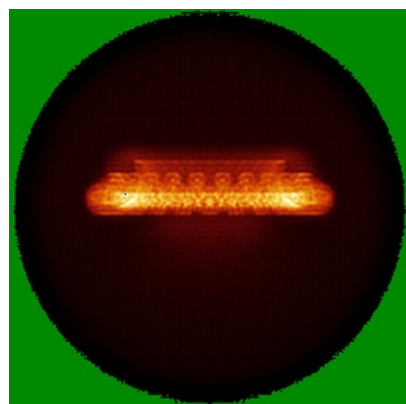


Z Index: 137

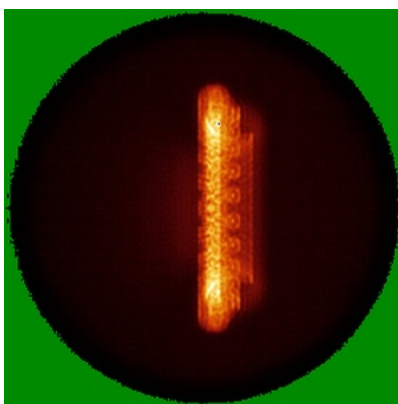
The images above show the largest variance slices of the map in three orthogonal directions.

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

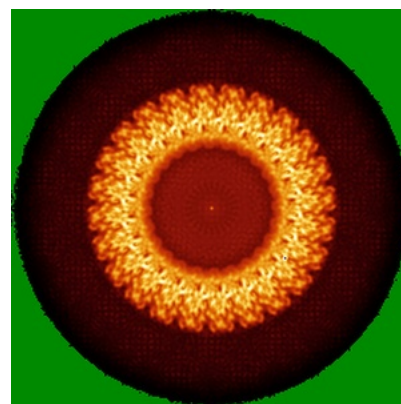
6.4.1 Primary map



X

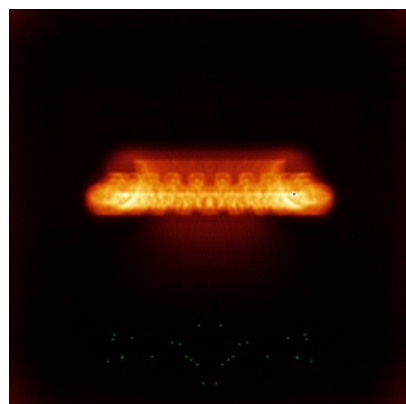


Y

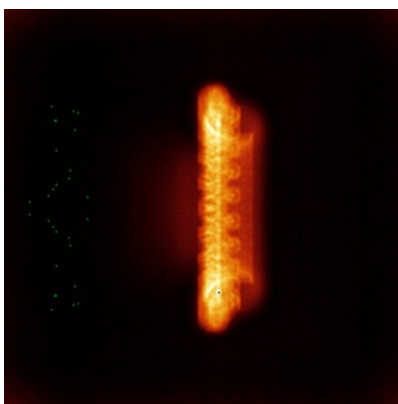


Z

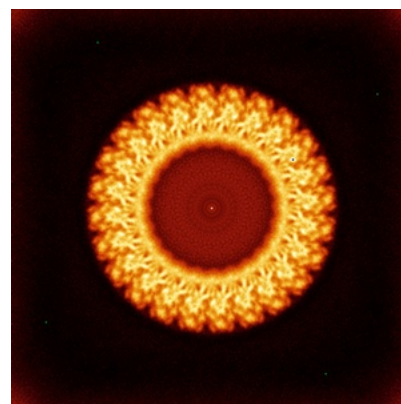
6.4.2 Raw map



X



Y

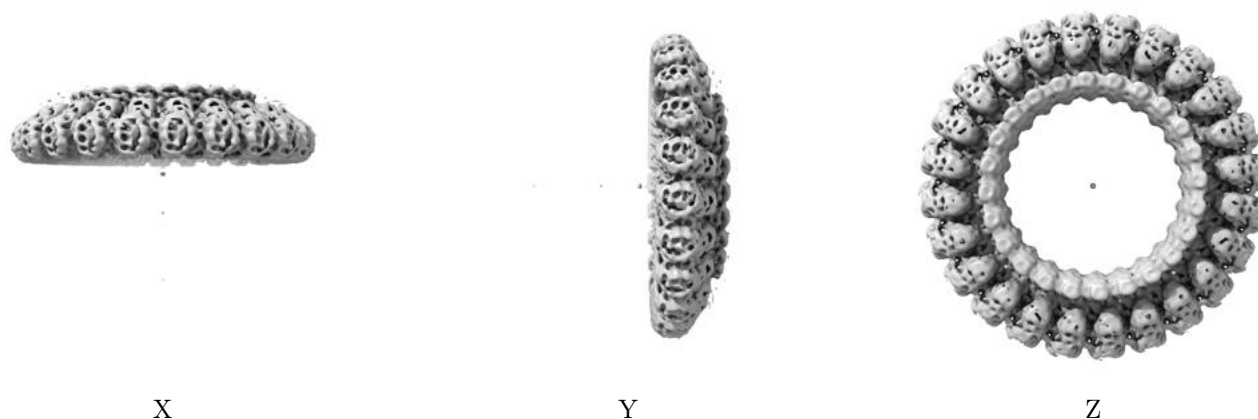


Z

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 0.15. 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

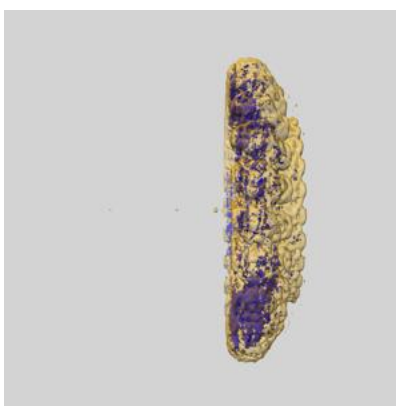
A mask typically either:

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

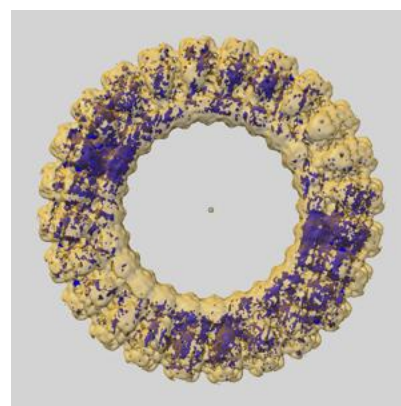
6.6.1 emd_28584_msk_1.map [i](#)



X



Y

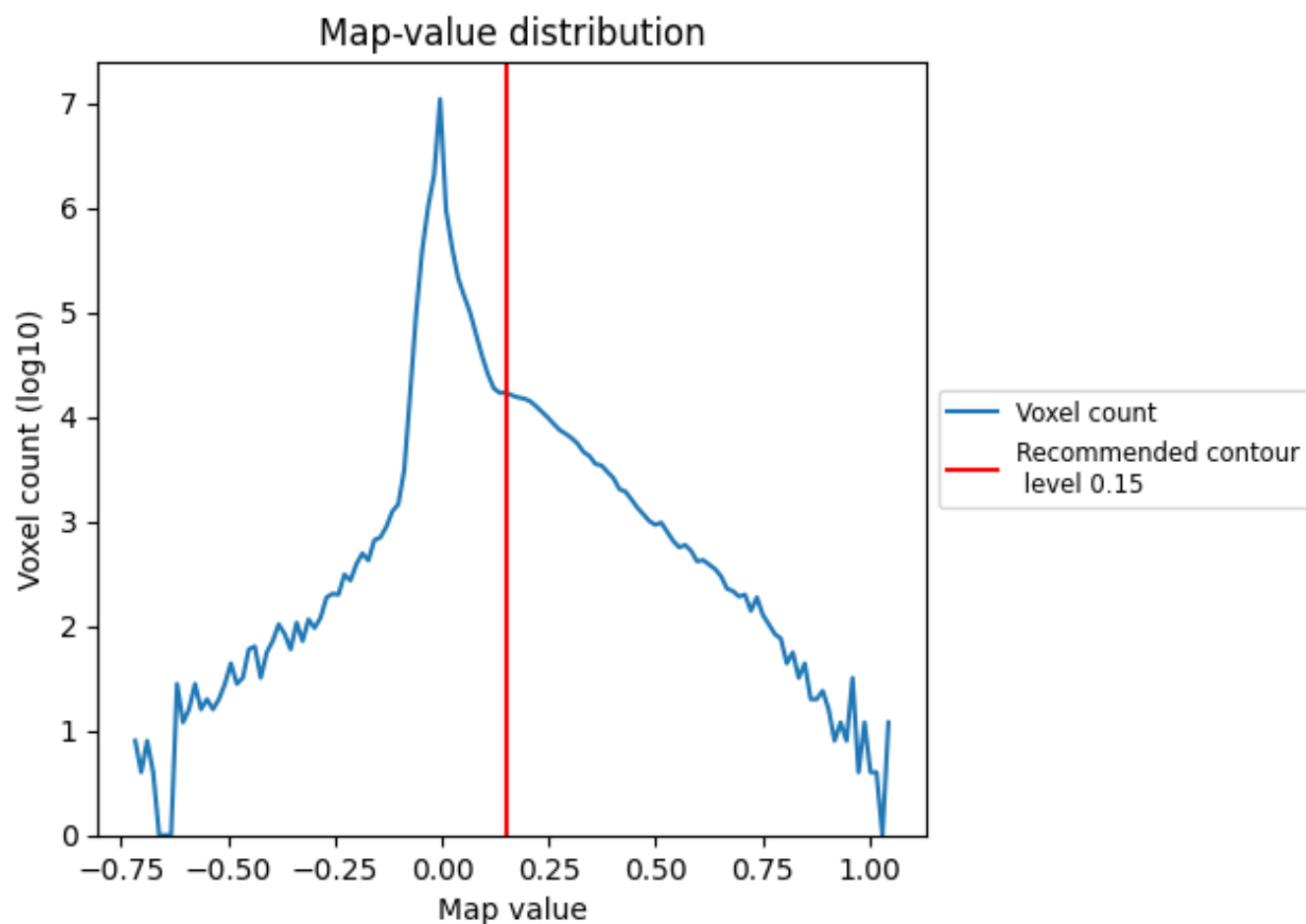


Z

7 Map analysis [i](#)

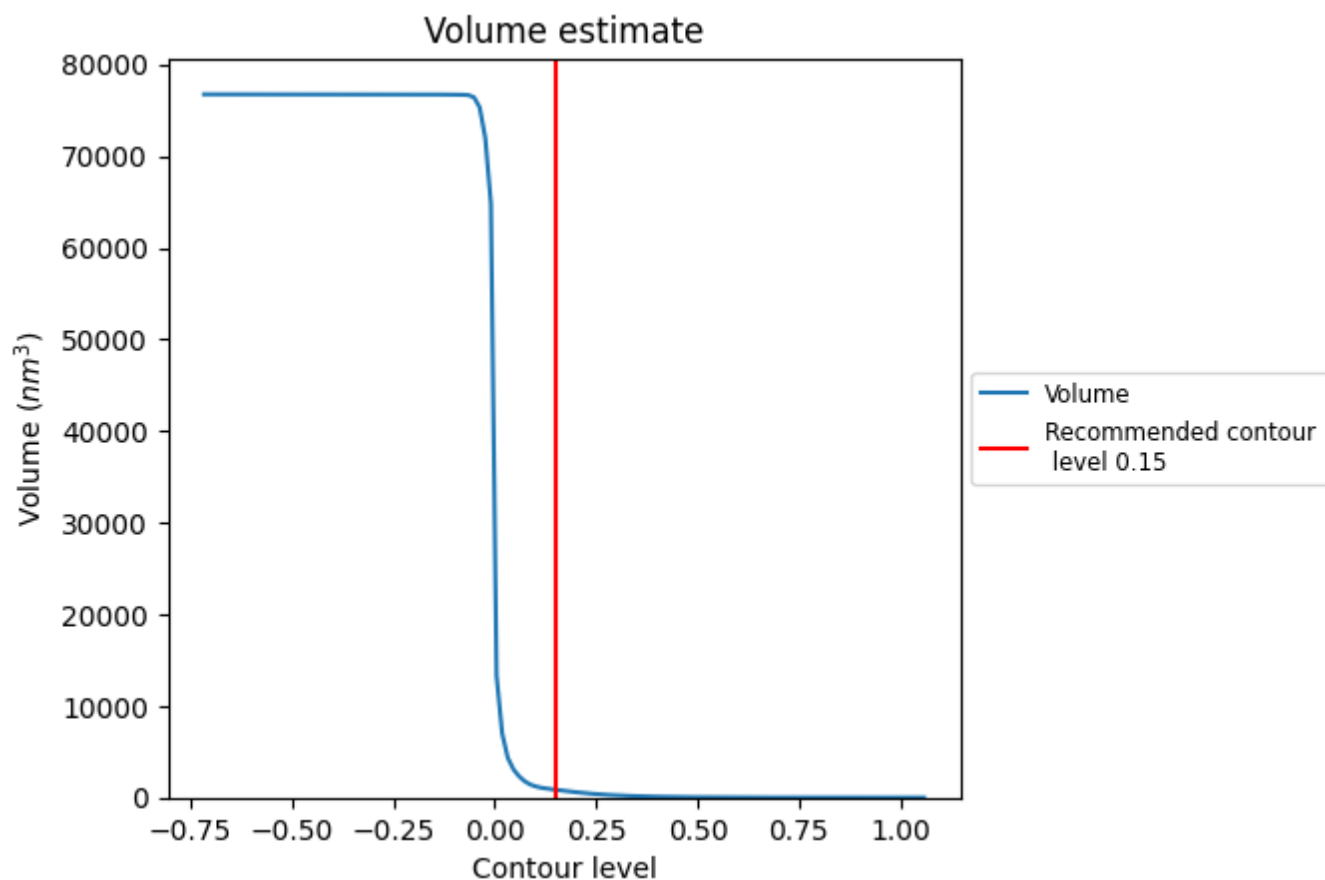
This section contains the results of statistical analysis of the map.

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.

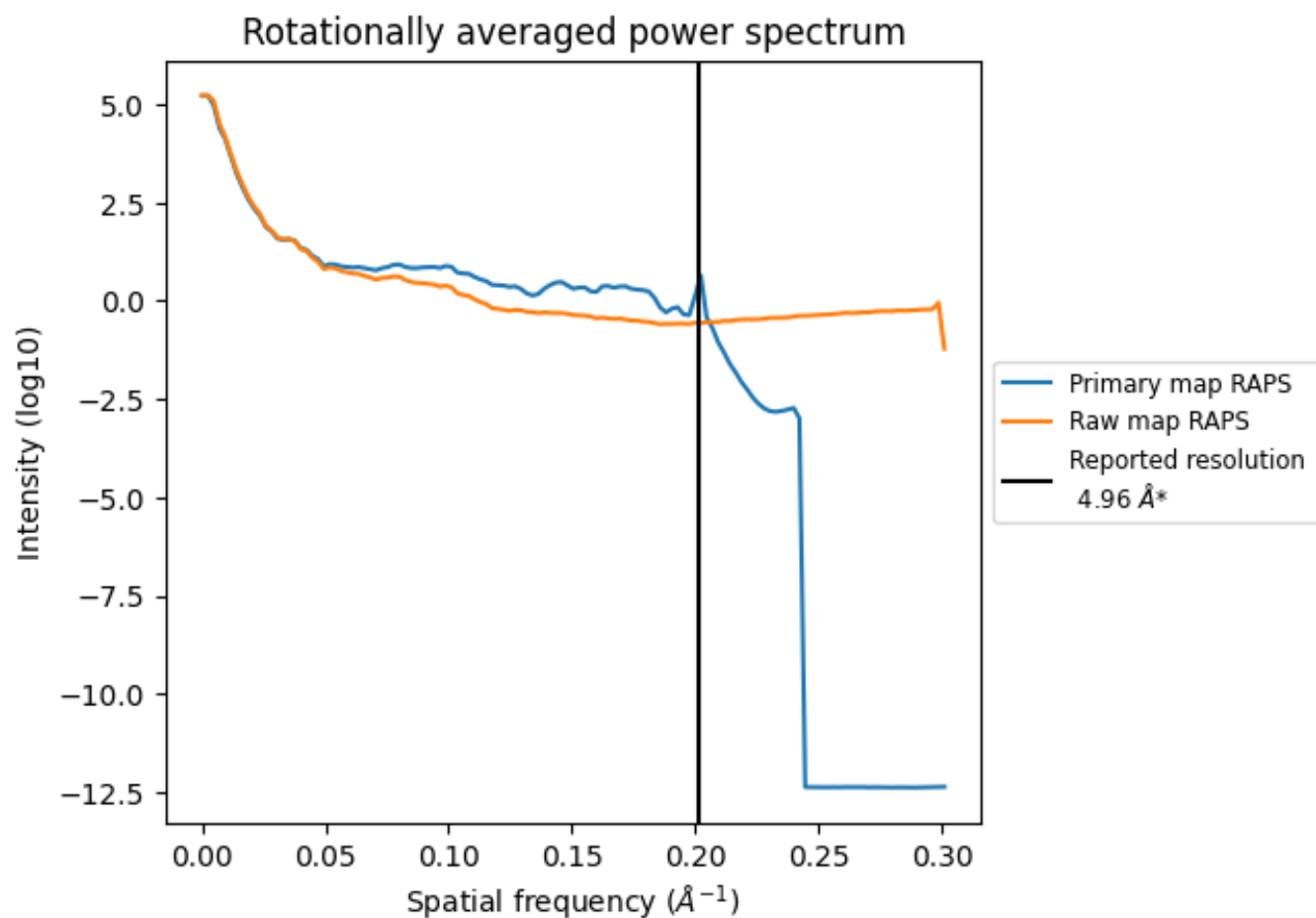
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 852 nm³; this corresponds to an approximate mass of 769 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 ⓘ

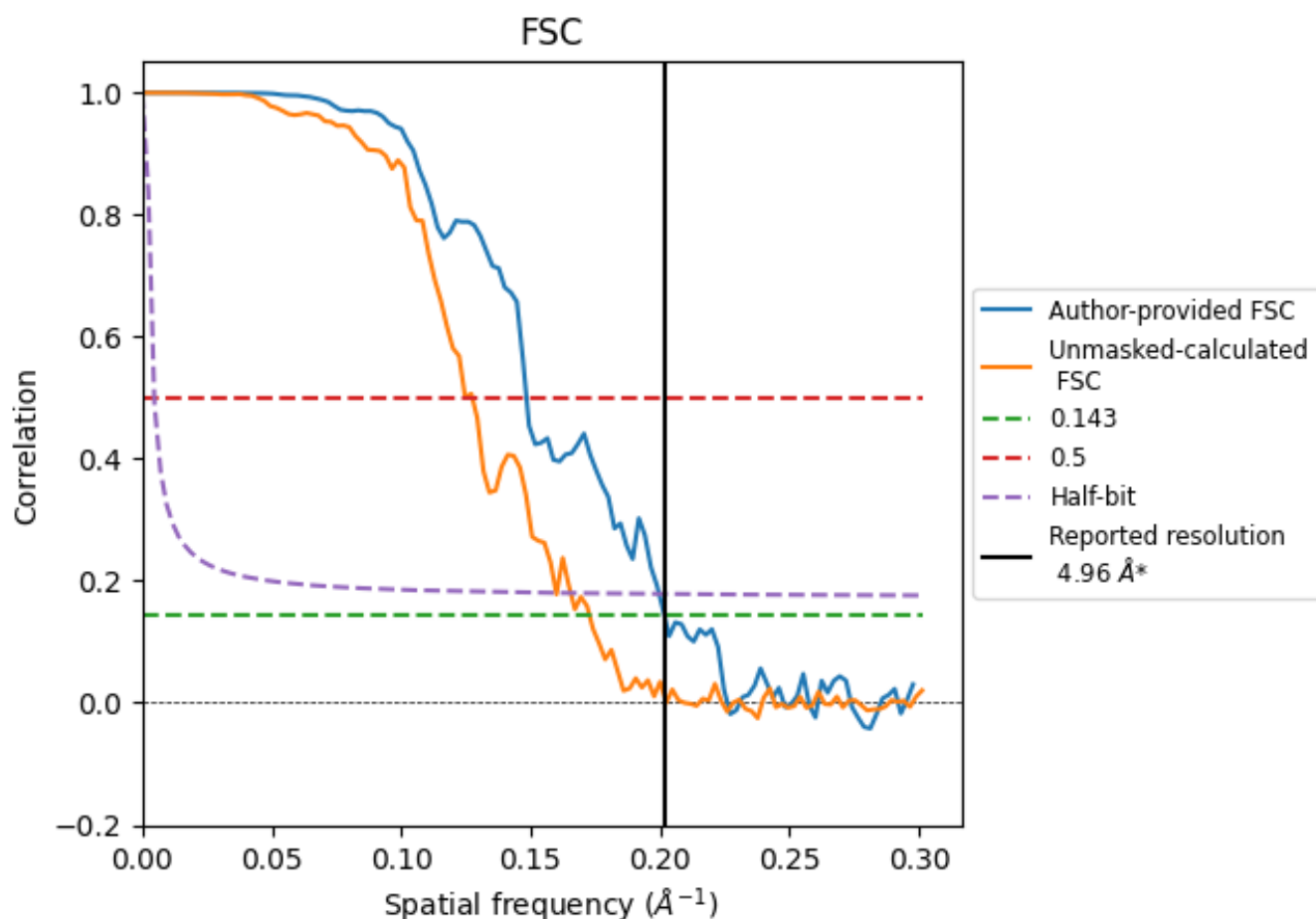


*Reported resolution corresponds to spatial frequency of 0.202 \AA^{-1}

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 0.202 \AA^{-1}

8.2 Resolution estimates [i](#)

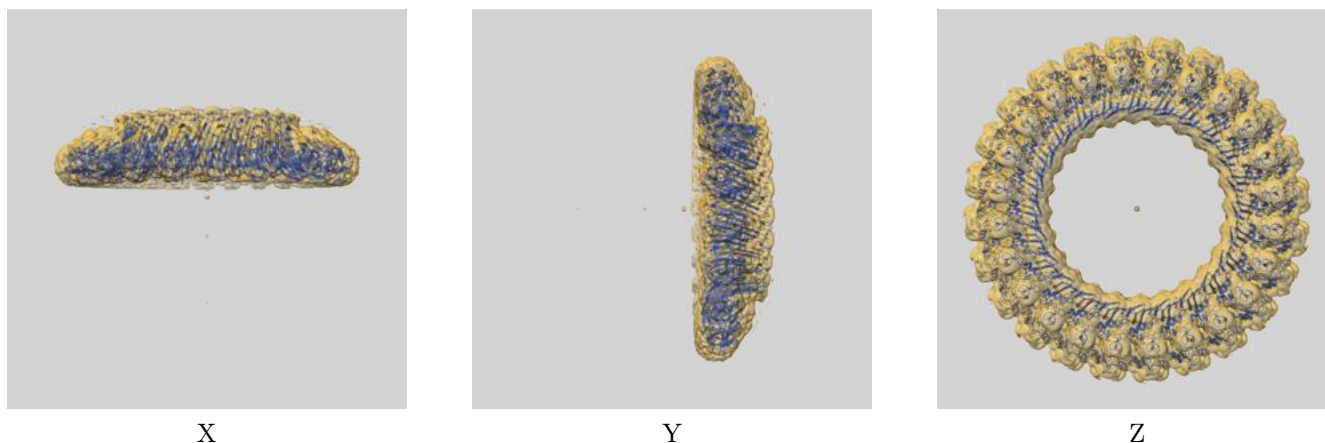
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.96	-	-
Author-provided FSC curve	4.96	6.74	5.01
Unmasked-calculated*	5.79	7.84	6.25

*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 5.79 differs from the reported value 4.96 by more than 10 %

9 Map-model fit [i](#)

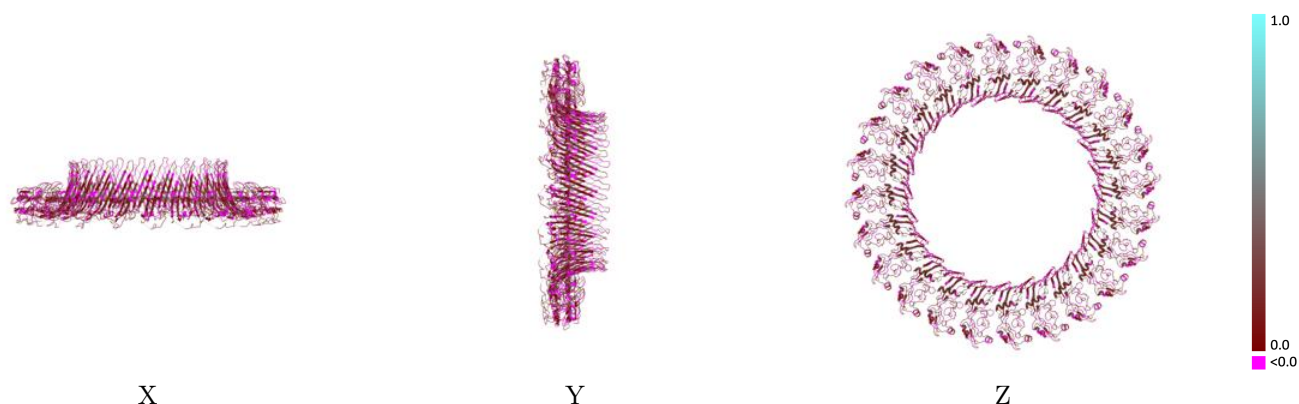
This section contains information regarding the fit between EMDB map EMD-28584 and PDB model 8ET2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



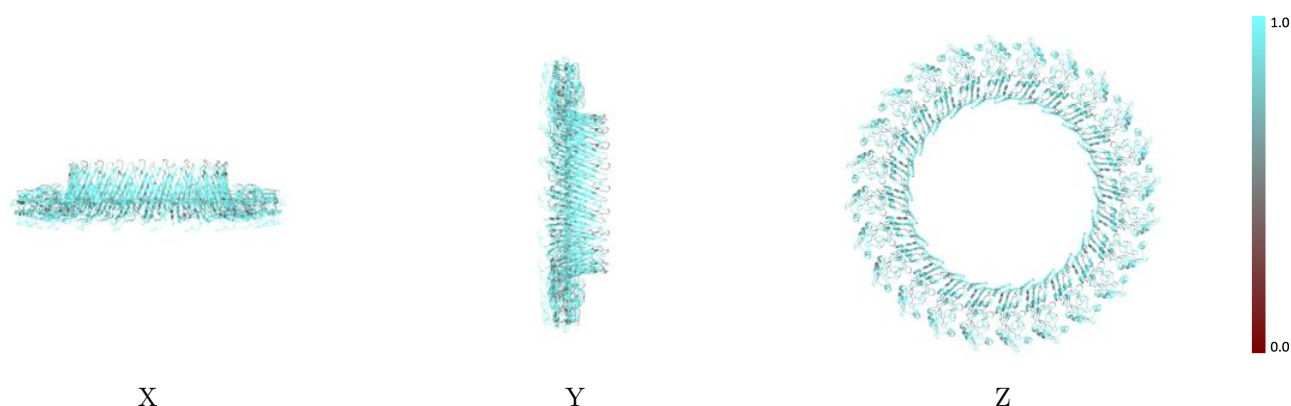
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



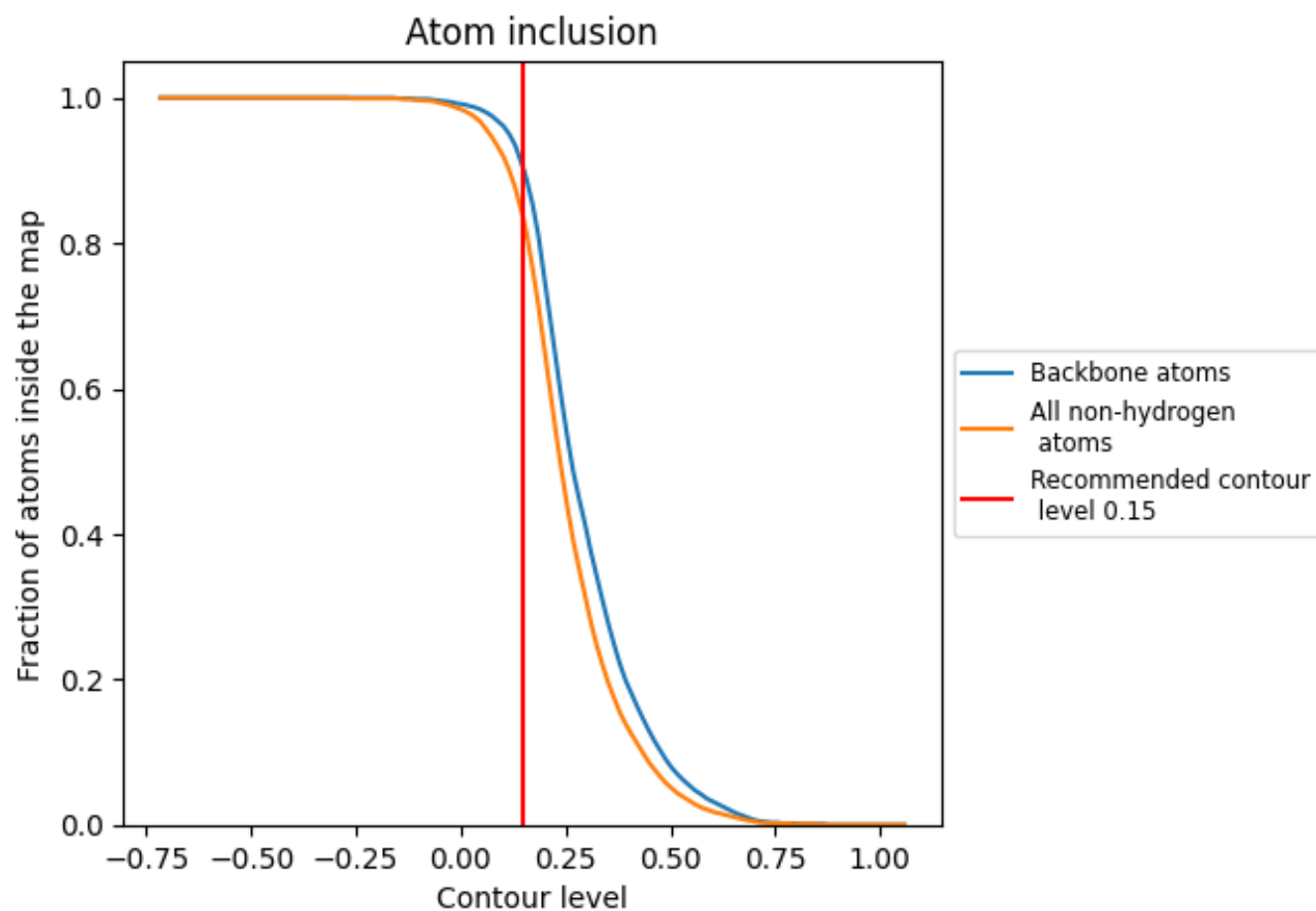
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.1180
A	 0.8380	 0.1200
B	 0.8350	 0.1170
C	 0.8360	 0.1180
D	 0.8300	 0.1170
E	 0.8350	 0.1200
F	 0.8310	 0.1200
G	 0.8300	 0.1190
H	 0.8300	 0.1210
I	 0.8340	 0.1200
J	 0.8300	 0.1210
K	 0.8280	 0.1170
L	 0.8320	 0.1210
M	 0.8360	 0.1180
N	 0.8350	 0.1190
O	 0.8360	 0.1200
P	 0.8350	 0.1160
Q	 0.8290	 0.1140
R	 0.8290	 0.1180
S	 0.8210	 0.1140
T	 0.8260	 0.1150
U	 0.8320	 0.1170
V	 0.8380	 0.1150
W	 0.8370	 0.1180
X	 0.8320	 0.1160

