



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 01:59 AM UTC

PDB ID : 6U5Z / pdb_00006u5z
EMDB ID : EMD-20659
Title : Cryo-EM structure of E. coli LonA S679A
Authors : Botos, I.; Lountos, G.T.; Weimin, W.; Wlodawer, A.
Deposited on : 2019-08-28
Resolution : 3.50 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:

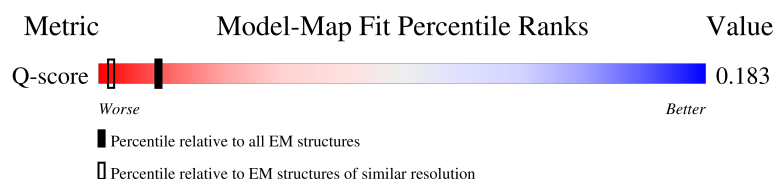
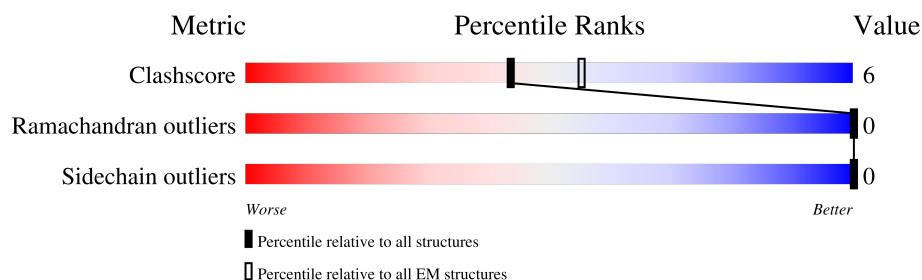
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.50 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.



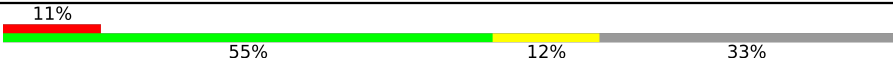
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	784	
1	B	784	
1	C	784	
1	D	784	

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Mol	Chain	Length	Quality of chain
1	E	784	 11% 55% 12% 33%
1	F	784	 57% 56% 11% 33%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24606 atoms, of which 0 are hydrogens and 0 are deuteriums.

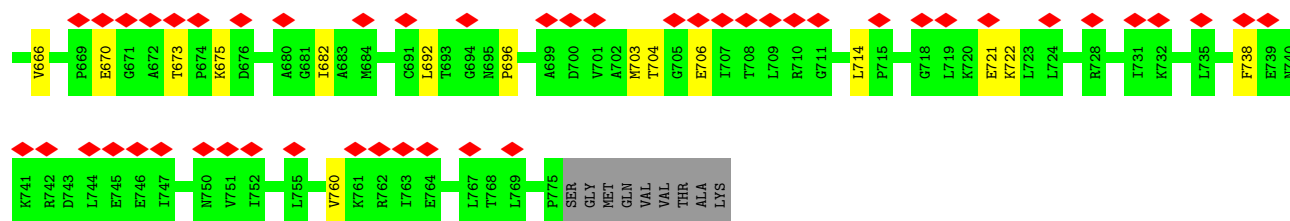
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lon protease.

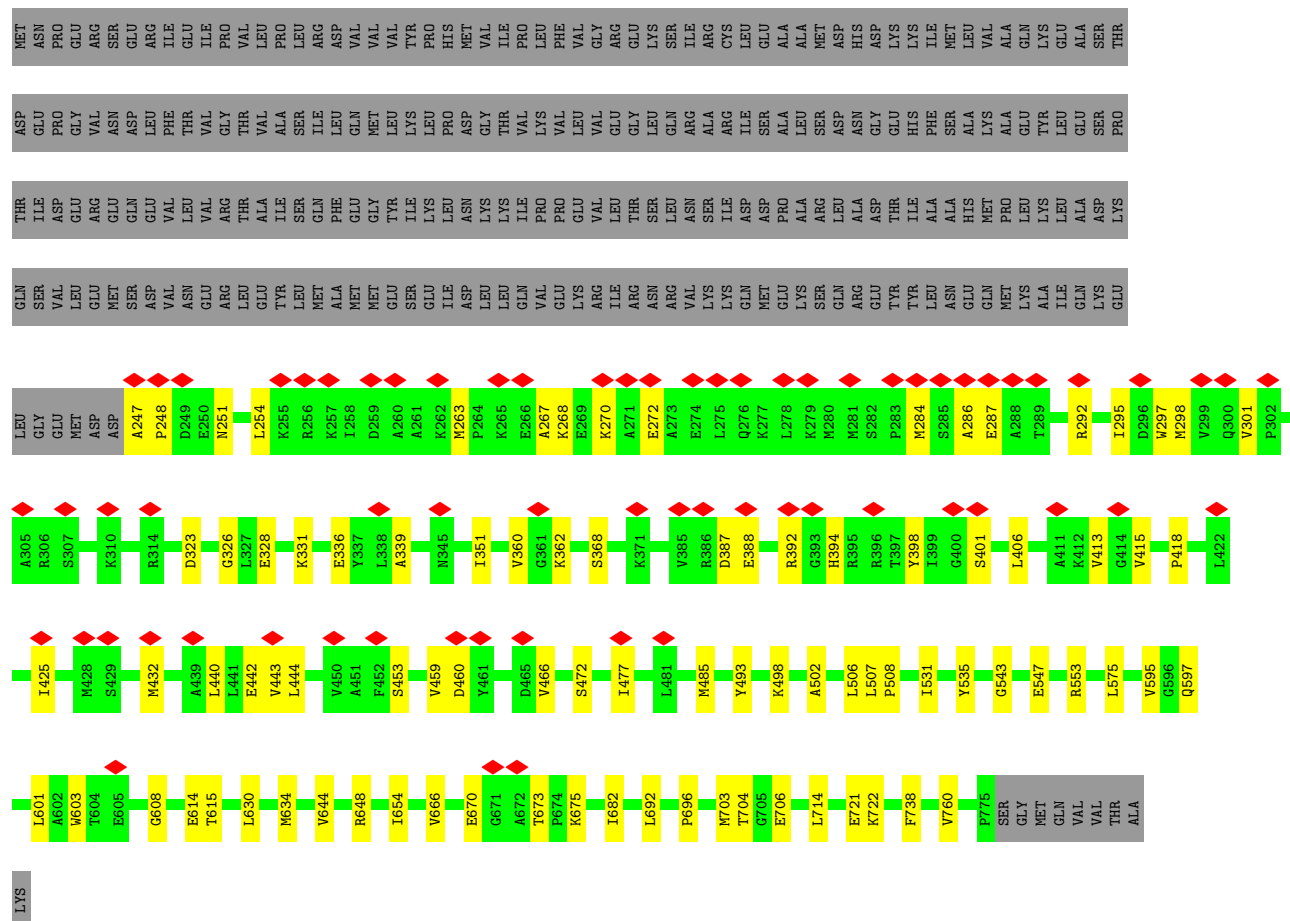
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	B	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	C	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	D	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	E	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	F	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		

There are 6 discrepancies between the modelled and reference sequences:

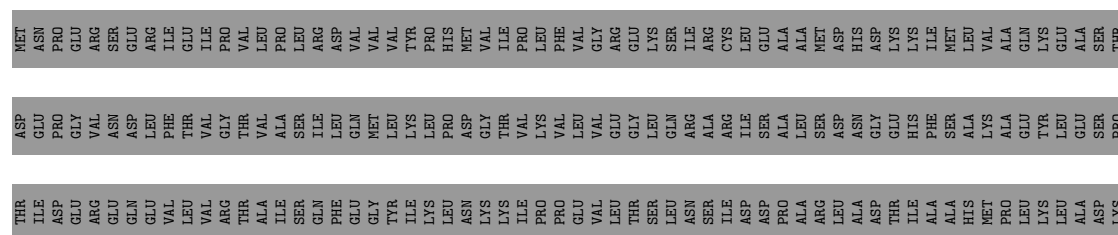
Chain	Residue	Modelled	Actual	Comment	Reference
A	679	ALA	SER	engineered mutation	UNP C3TLS2
B	679	ALA	SER	engineered mutation	UNP C3TLS2
C	679	ALA	SER	engineered mutation	UNP C3TLS2
D	679	ALA	SER	engineered mutation	UNP C3TLS2
E	679	ALA	SER	engineered mutation	UNP C3TLS2
F	679	ALA	SER	engineered mutation	UNP C3TLS2

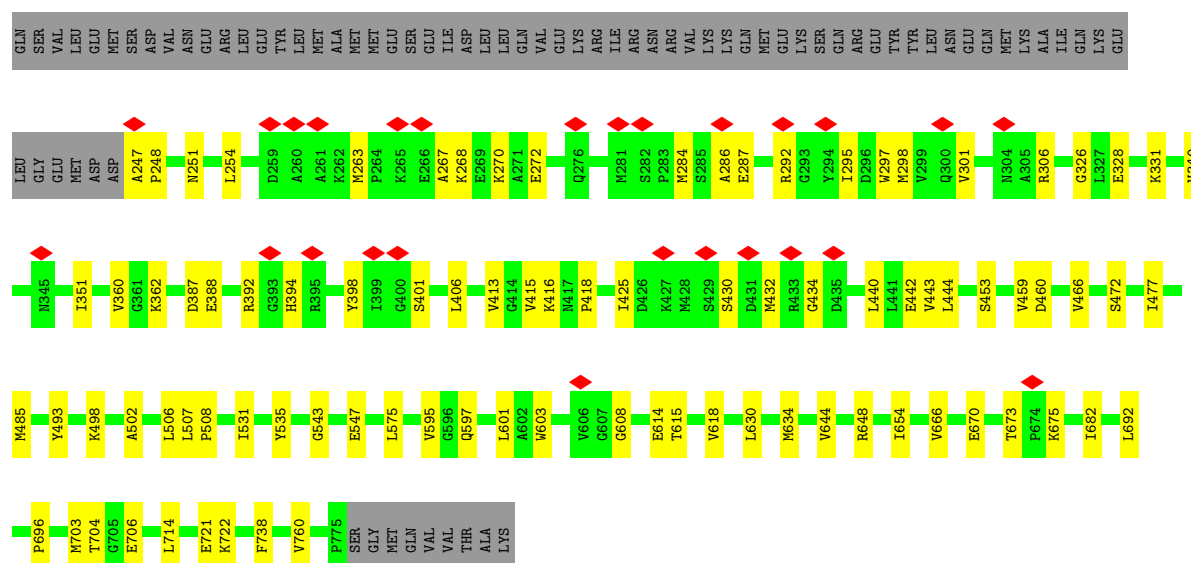


• Molecule 1: Lon protease

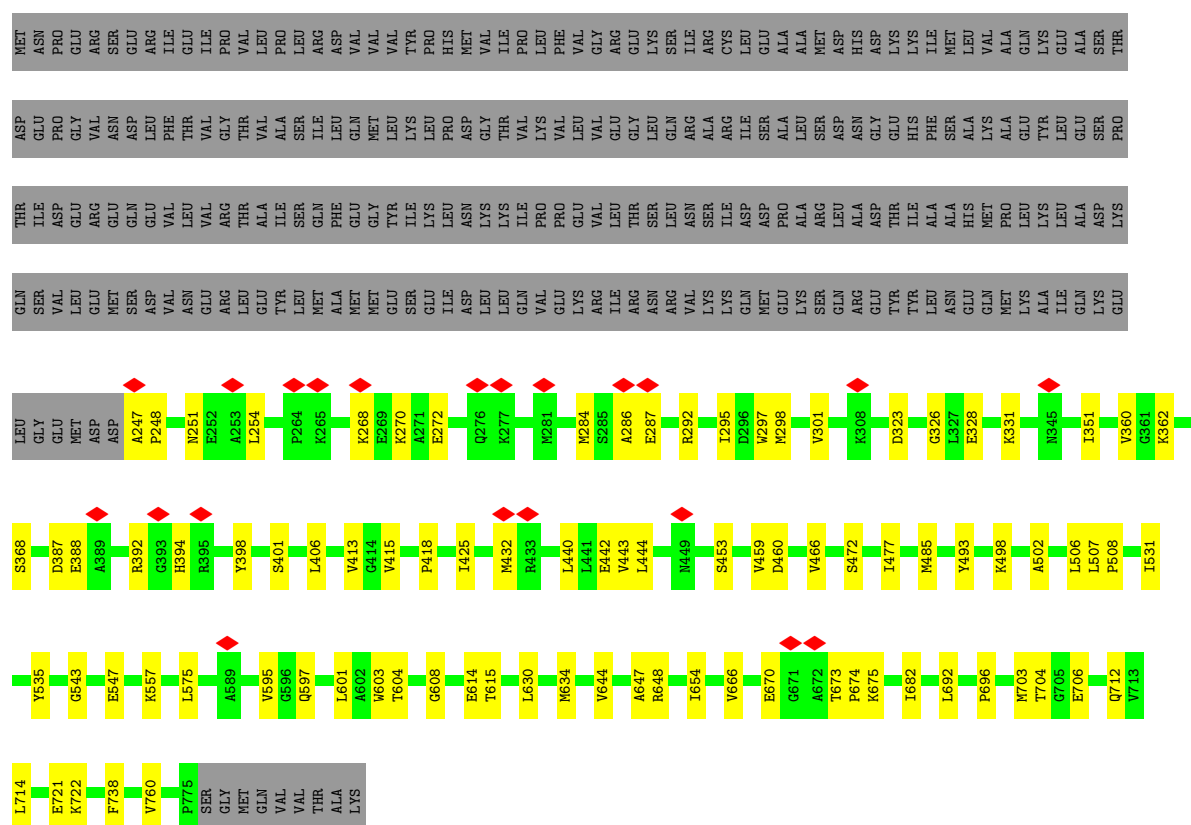


• Molecule 1: Lon protease

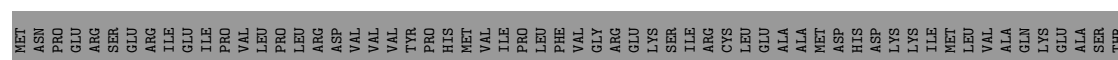


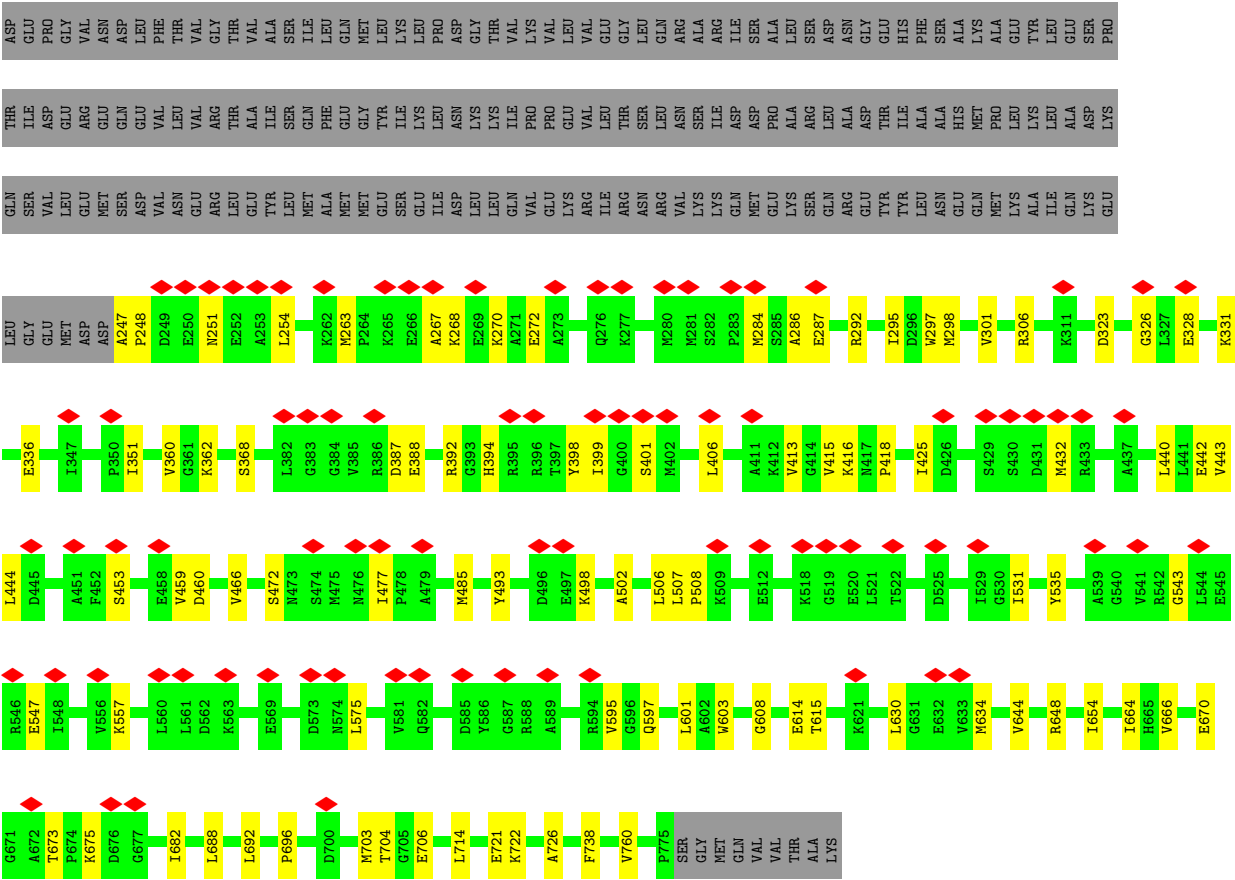


• Molecule 1: Lon protease

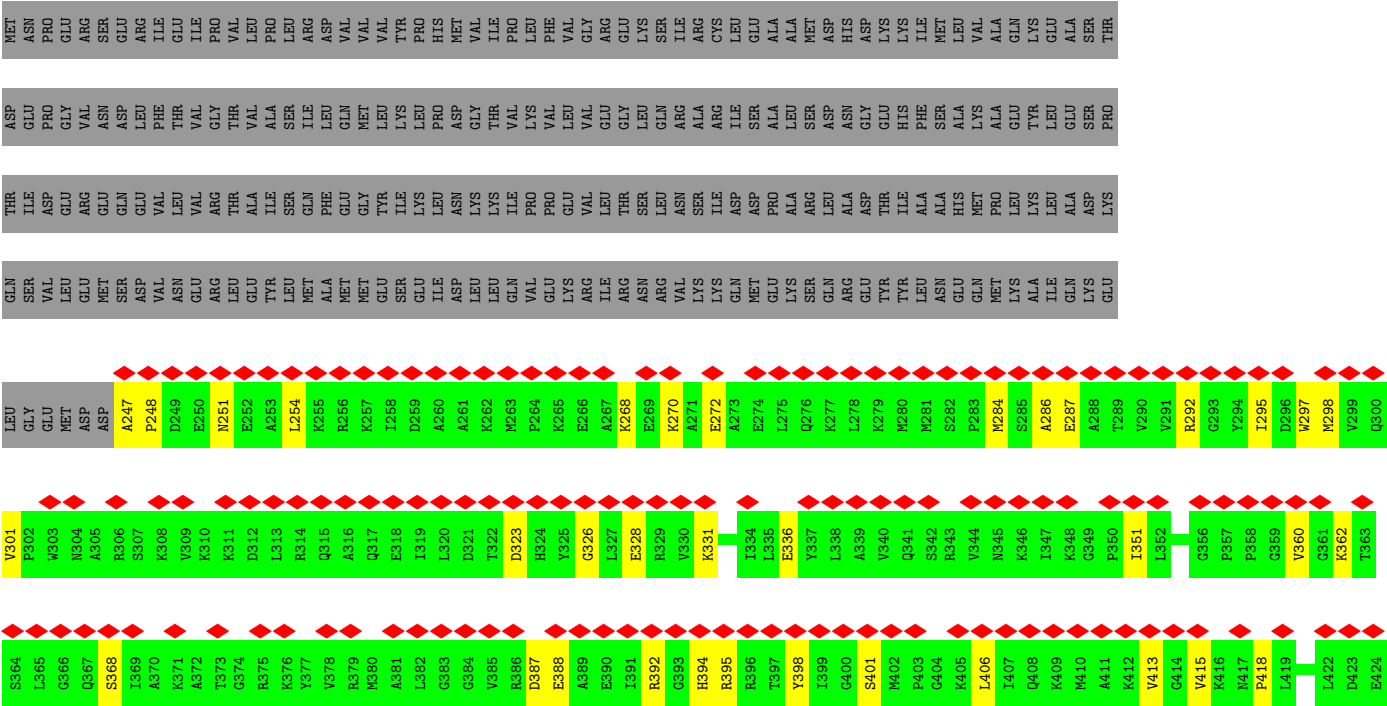


• Molecule 1: Lon protease





● Molecule 1: Lon protease



L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	SER	GLY	MET	GLN	VAL	VAL	THR	ALA	LYS																	
V668	P669	E670	G671	A672	T673	R674	K675	D676	G677	P678	A679	A680	P681	T682	A683	M684	C685	T686	A687	L688	L689	L690	L691	L692	T693	G694	H695	P696	A697	D698	T699	T700	A701	M702	T703	T704	G705	E706	I707	H708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	A725	A726	H727	R728	G729	G730	I731	K732	T733	V734
E605	V606	G607	G608	D609	L610	L611	T612	I613	E614	T615	A616	C617	V618	P619	G620	K621	G622	K623	L624	T625	Y626	T627	G628	S629	L630	G631	E632	V633	M634	Q635	E636	S637	I638	A641	L642	T643	V644	R648	A649	E650	K651	L652	G653	I654	M655	P656	D657	F658	H659	E660	K661	R662	D663	I664	H665	V666	H667									
E545	R546	E547	I548	S549	K550	L551	C552	R553	K554	A555	V556	K557	Q558	L559	L560	L561	D562	K563	S564	L565	K566	H567	I568	E569	I570	N571	G572	D573	N574	L575	H576	D577	Y578	L579	G580	V581	Q582	R583	F584	D585	Y586	G587	R588	A589	D590	N591	E592	N593	N594	V595	G596	Q597	V598	T599	L601	A602	W603	T604								
M485	E486	V487	I488	R489	L490	S491	G492	Y493	T494	E495	D496	E497	K498	L499	N500	I501	A502	K503	R504	H505	L506	L507	P508	K509	Q510	I511	E512	R513	N514	A515	L516	K517	K518	G519	E520	L521	T522	V523	D524	D525	S526	A527	I528	I529	G530	I531	I532	S533	Y534	Y535	T536	R537	E538	A539	G540	V541	R542	G543	L544							
I425	D426	K427	M428	S429	S430	D431	M432	R433	G434	D435	P436	A437	S438	A439	L440	L441	E442	V443	L444	D445	P446	E447	Q448	N449	V450	A451	F452	S453	D454	H455	Y456	L457	E458	V459	D460	Y461	D462	L463	S464	D465	V466	M467	F468	V469	A470	T471	S472	N473	S474	M475	N476	I477	P478	A479	P480	L481	L482	D483	R484							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	274765	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0048	Depositor
Map size ($\text{\AA}$)	271.36, 271.36, 271.36	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84799993, 0.84799993, 0.84799993	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	0.11	0/4161	0.33	0/5614
1	B	0.12	0/4161	0.33	0/5614
1	C	0.11	0/4161	0.33	0/5614
1	D	0.12	0/4161	0.33	0/5614
1	E	0.11	0/4161	0.33	0/5614
1	F	0.12	0/4161	0.33	0/5614
All	All	0.12	0/24966	0.33	0/33684

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	4101	0	4229	55	0
1	B	4101	0	4229	55	0
1	C	4101	0	4229	56	0
1	D	4101	0	4229	54	0
1	E	4101	0	4229	59	0
1	F	4101	0	4229	55	0
All	All	24606	0	25374	324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 324 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:E:557:LYS:HD3	1:F:336:GLU:HG2	1.61	0.81
1:A:670:GLU:O	1:A:673:THR:HG23	1.83	0.79
1:E:670:GLU:O	1:E:673:THR:HG23	1.83	0.78
1:F:670:GLU:O	1:F:673:THR:HG23	1.83	0.78
1:B:670:GLU:O	1:B:673:THR:HG23	1.83	0.78

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	527/784 (67%)	502 (95%)	25 (5%)	0	100	100
1	B	527/784 (67%)	502 (95%)	25 (5%)	0	100	100
1	C	527/784 (67%)	502 (95%)	25 (5%)	0	100	100
1	D	527/784 (67%)	502 (95%)	25 (5%)	0	100	100
1	E	527/784 (67%)	502 (95%)	25 (5%)	0	100	100
1	F	527/784 (67%)	502 (95%)	25 (5%)	0	100	100
All	All	3162/4704 (67%)	3012 (95%)	150 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/670 (66%)	442 (100%)	0	100	100
1	B	442/670 (66%)	442 (100%)	0	100	100
1	C	442/670 (66%)	442 (100%)	0	100	100
1	D	442/670 (66%)	442 (100%)	0	100	100
1	E	442/670 (66%)	442 (100%)	0	100	100
1	F	442/670 (66%)	442 (100%)	0	100	100
All	All	2652/4020 (66%)	2652 (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 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	510	GLN
1	E	510	GLN
1	F	510	GLN
1	E	712	GLN
1	C	510	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

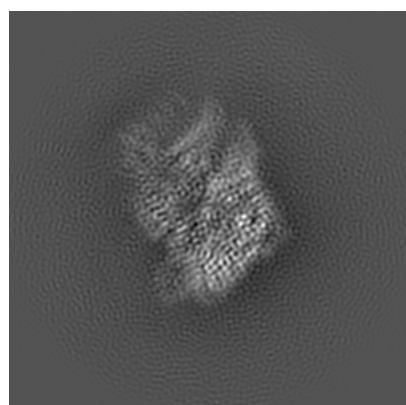
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20659. These allow visual inspection of the internal detail of the map and identification of artifacts.

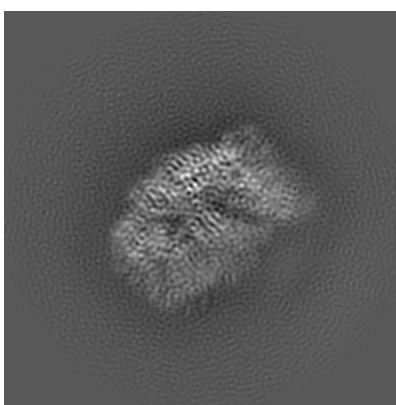
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

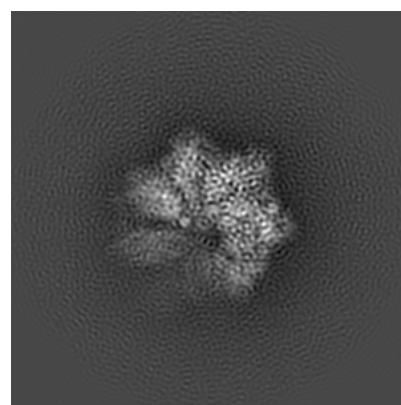
6.1.1 Primary map



X



Y

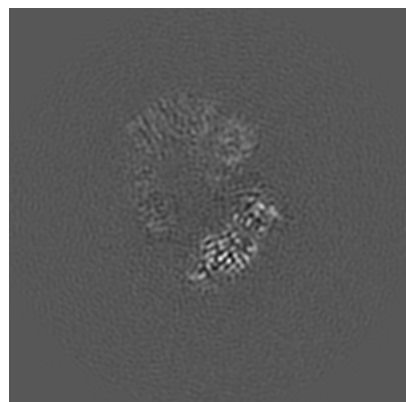


Z

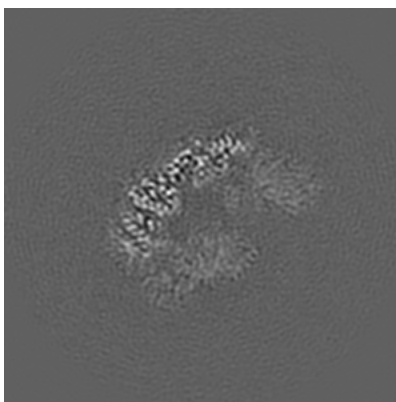
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

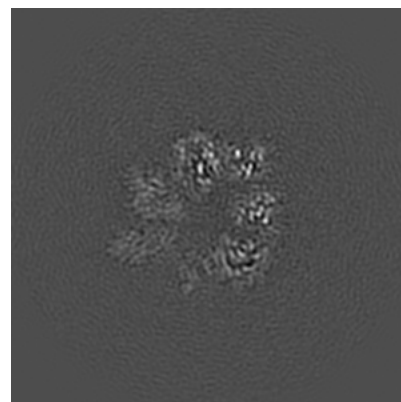
6.2.1 Primary map



X Index: 160



Y Index: 160

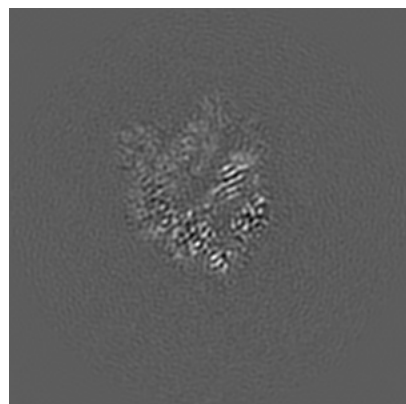


Z Index: 160

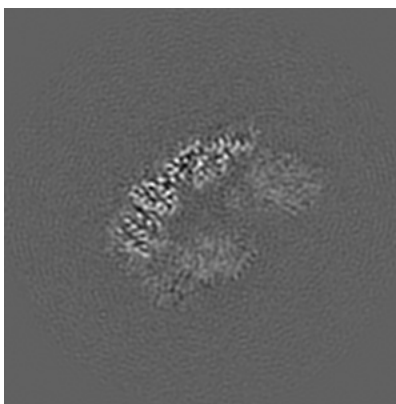
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

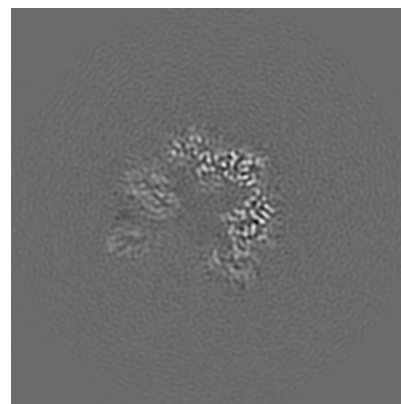
6.3.1 Primary map



X Index: 184



Y Index: 159

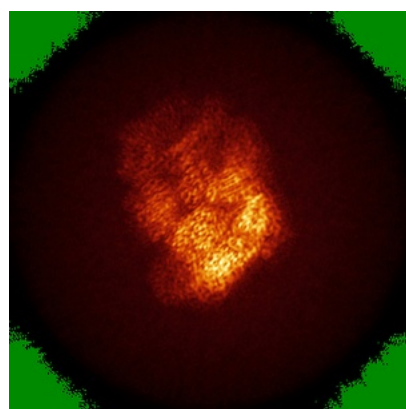


Z Index: 147

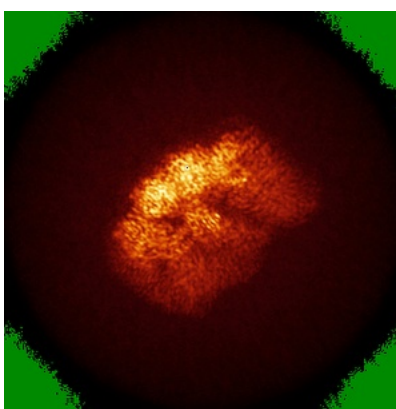
The images above show the largest variance slices of the map in three orthogonal directions.

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

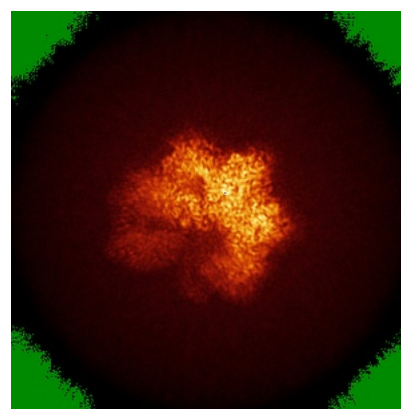
6.4.1 Primary map



X



Y

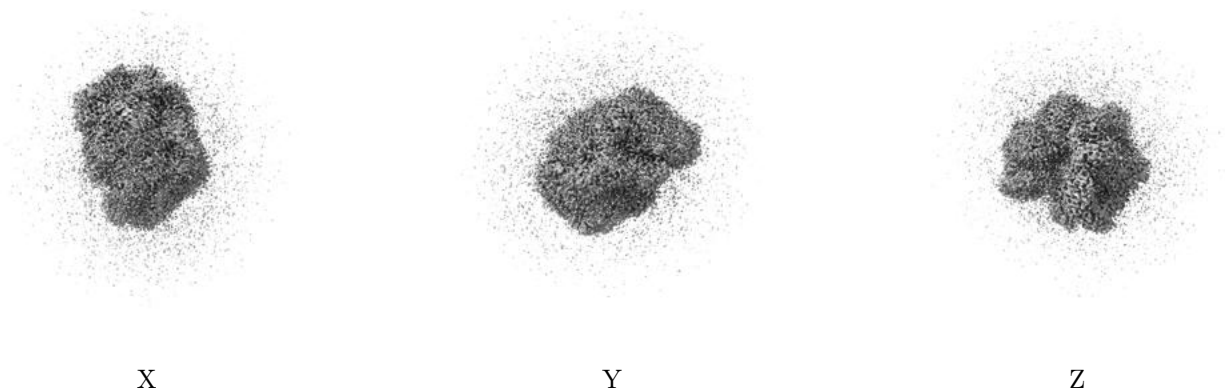


Z

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 0.0048. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

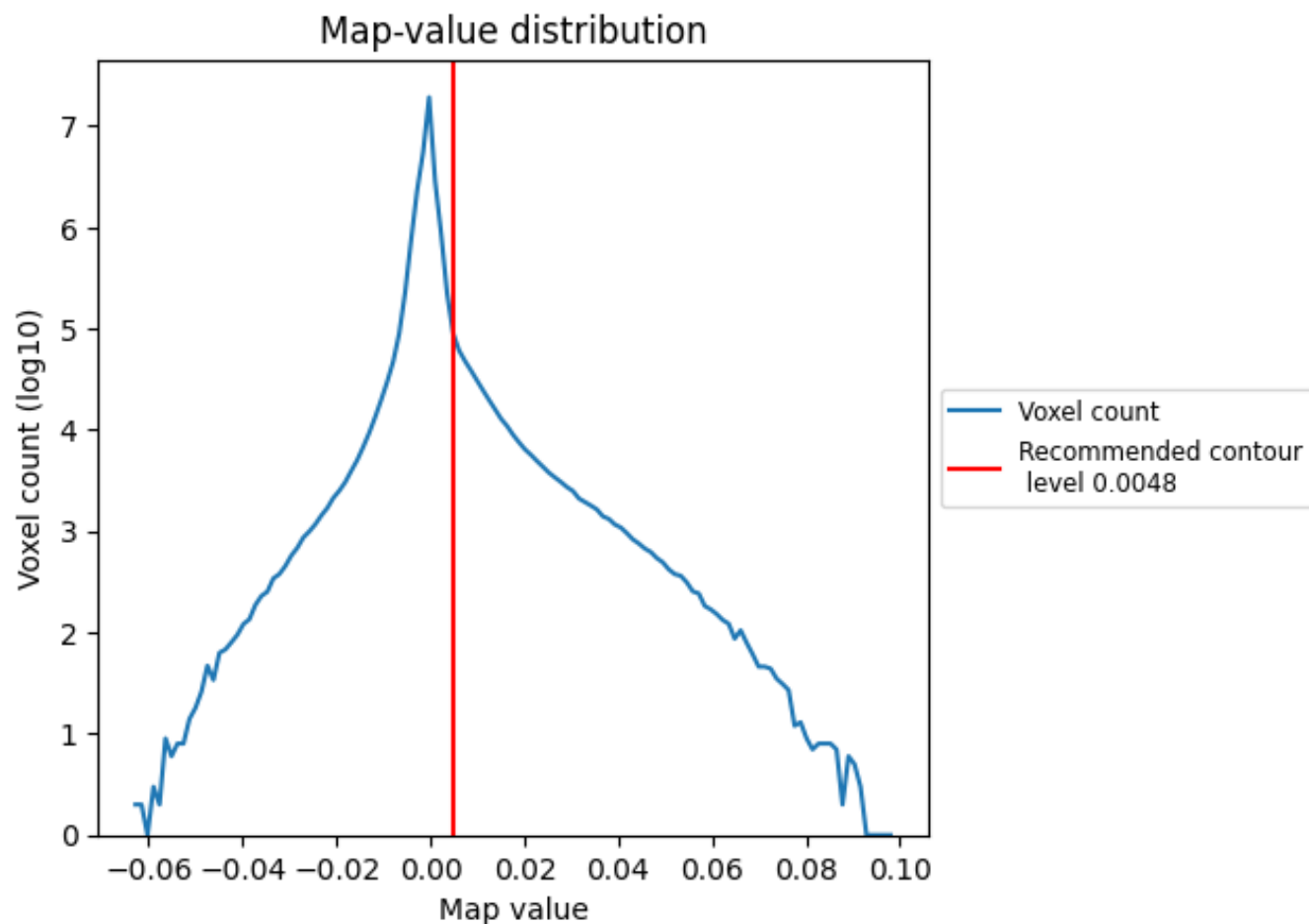
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

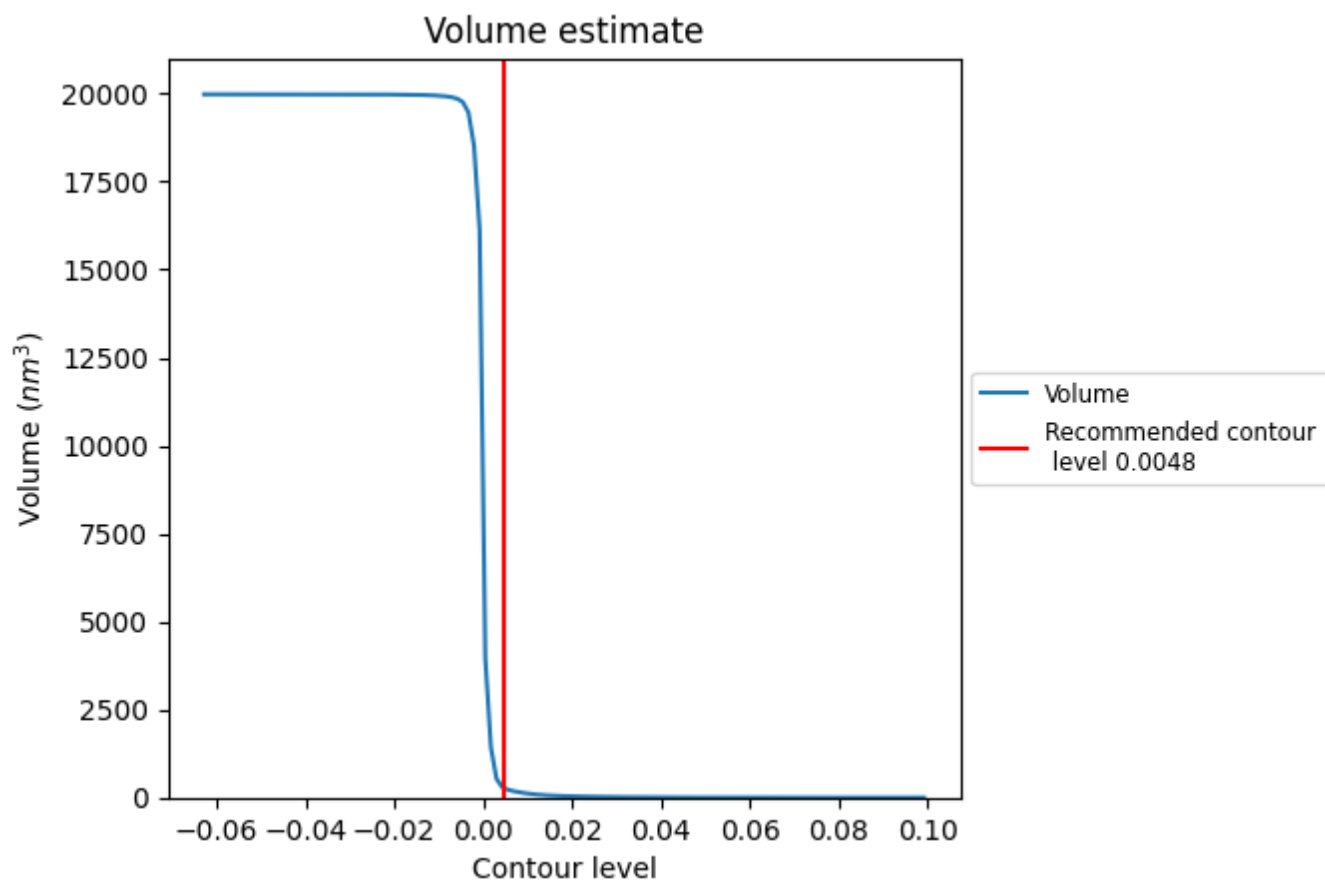
This section contains the results of statistical analysis of the map.

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.

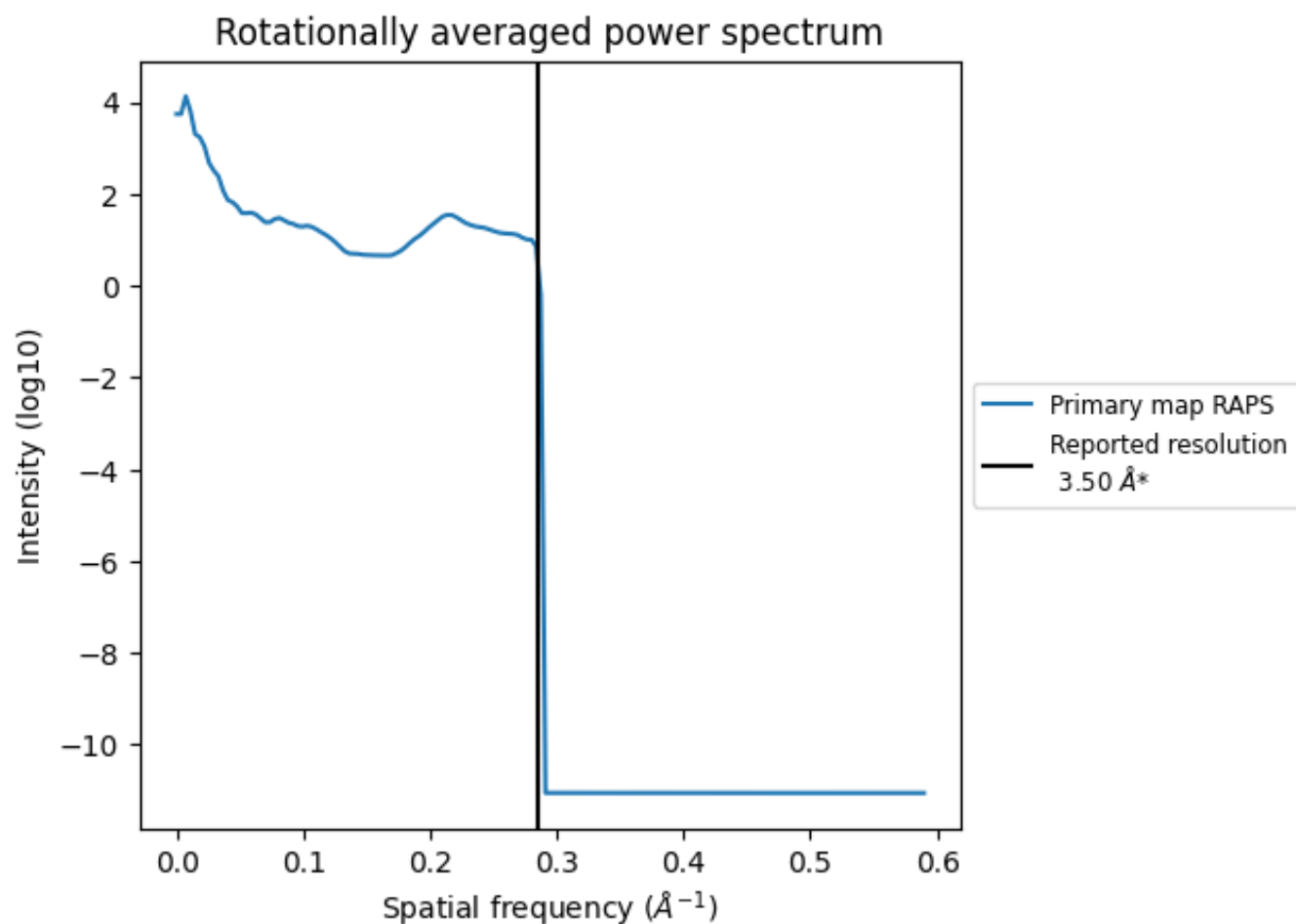
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 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 0.286 $\text{\AA}^{-1}$

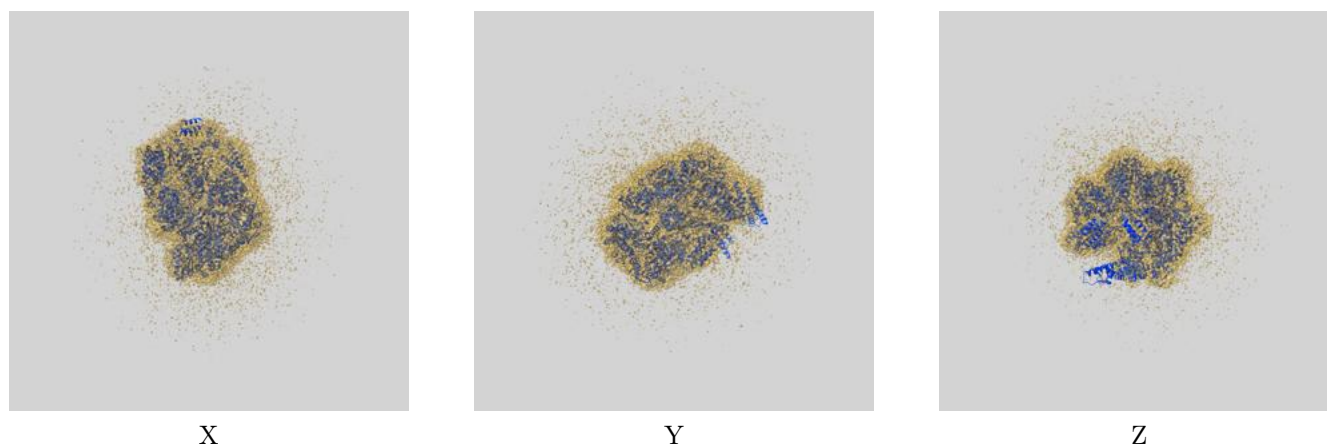
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

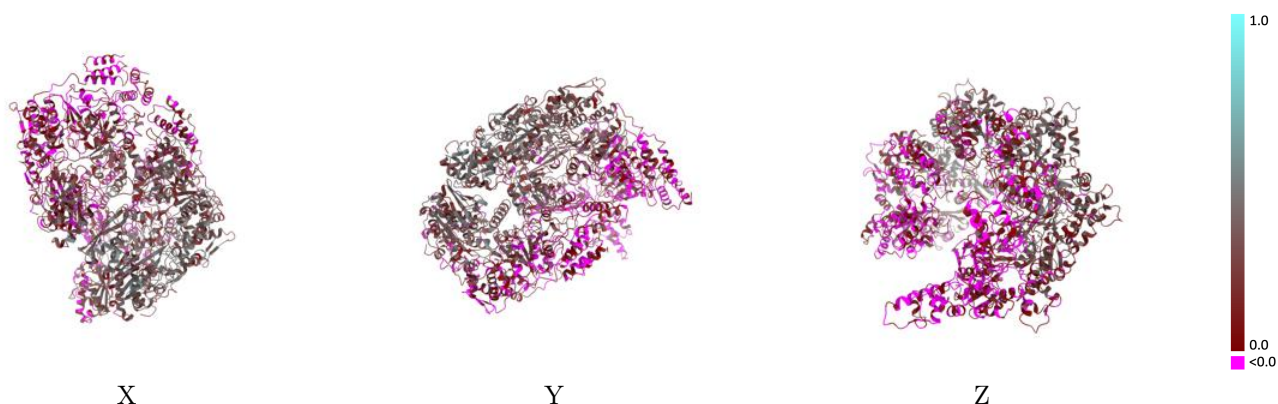
This section contains information regarding the fit between EMDB map EMD-20659 and PDB model 6U5Z. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



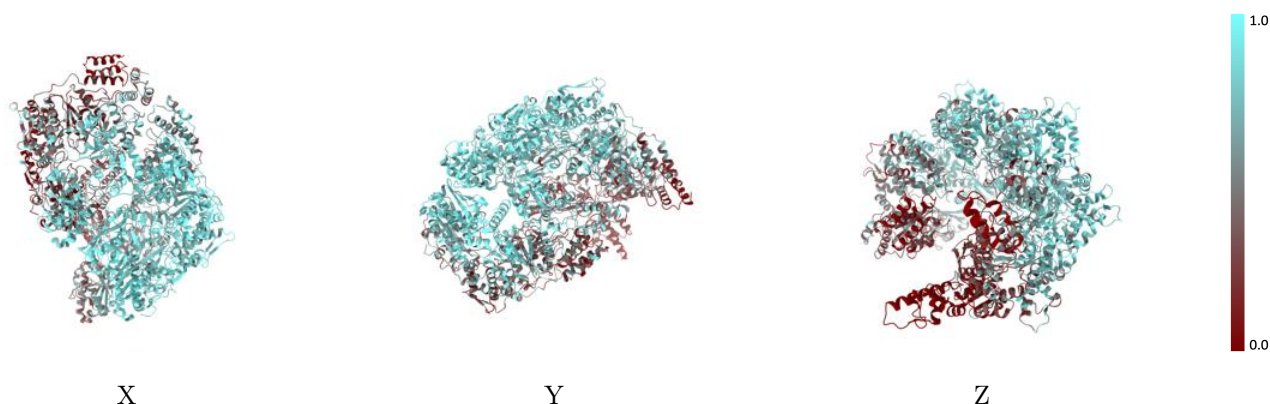
The images above show the 3D surface view of the map at the recommended contour level 0.0048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



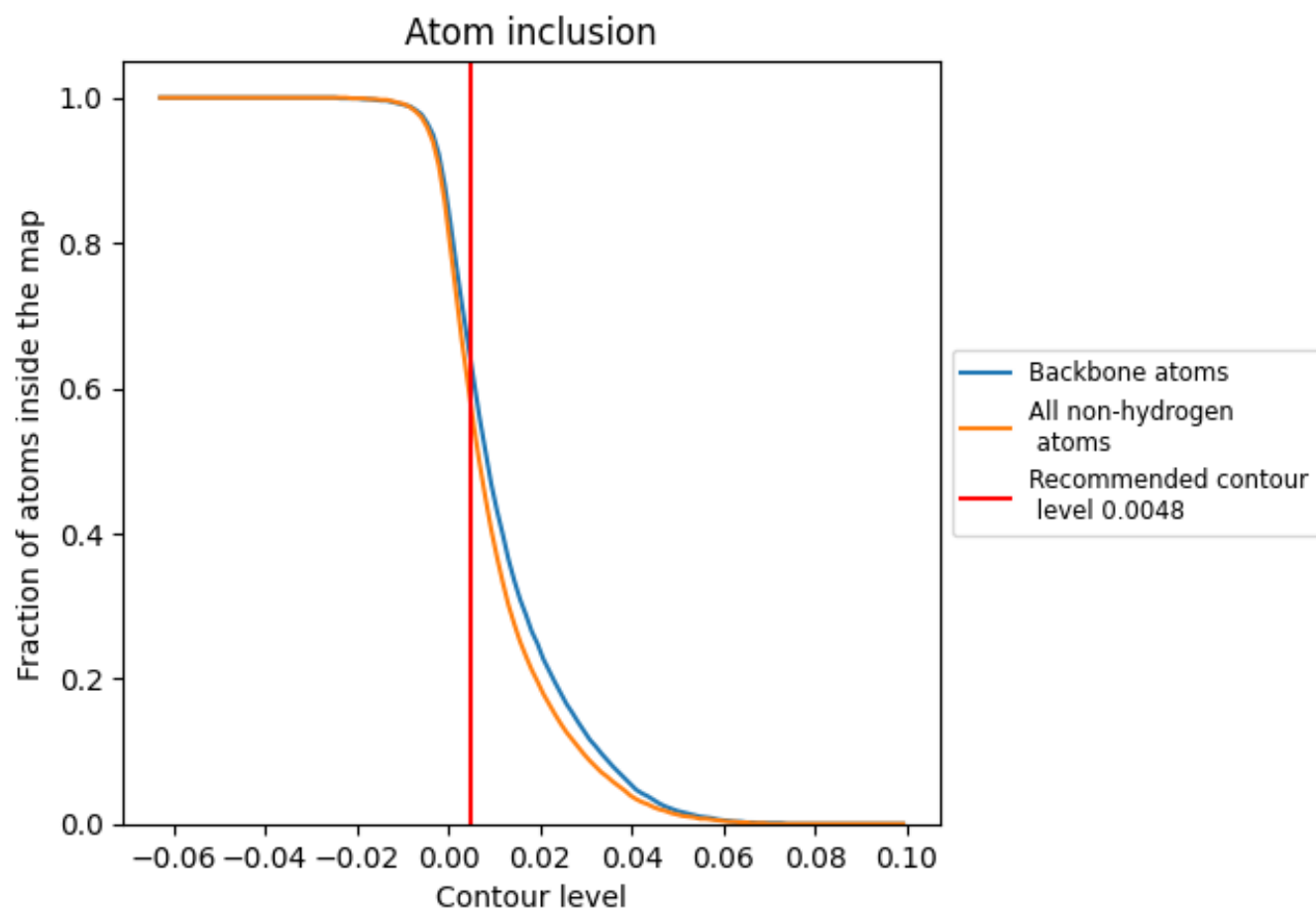
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0048).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 58% 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 (0.0048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5830	0.1830
A	0.3620	0.0810
B	0.7300	0.2250
C	0.7890	0.2970
D	0.7920	0.2900
E	0.6470	0.1790
F	0.1780	0.0250

1.0

0.0

<0.0