



wwPDB EM Validation Summary Report ⓘ

Oct 26, 2024 – 03:40 PM EDT

PDB ID : 6U5Z
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.dev113
MolProbity : 4.02b-467
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) : 2.39

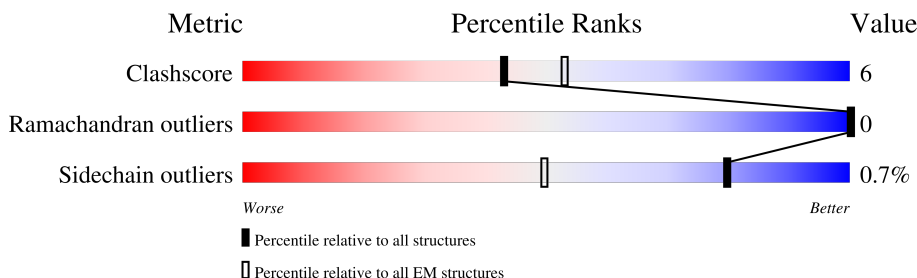
1 Overall quality at a glance

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)
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	784	<div> <div>39%</div> <div>56%</div> <div>11%</div> <div>33%</div> </div>
1	B	784	<div> <div>9%</div> <div>56%</div> <div>11%</div> <div>33%</div> </div>
1	C	784	<div> <div>•</div> <div>56%</div> <div>11%</div> <div>33%</div> </div>
1	D	784	<div> <div>•</div> <div>56%</div> <div>11%</div> <div>33%</div> </div>
1	E	784	<div> <div>11%</div> <div>55%</div> <div>12%</div> <div>33%</div> </div>
1	F	784	<div> <div>57%</div> <div>56%</div> <div>11%</div> <div>33%</div> </div>

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.

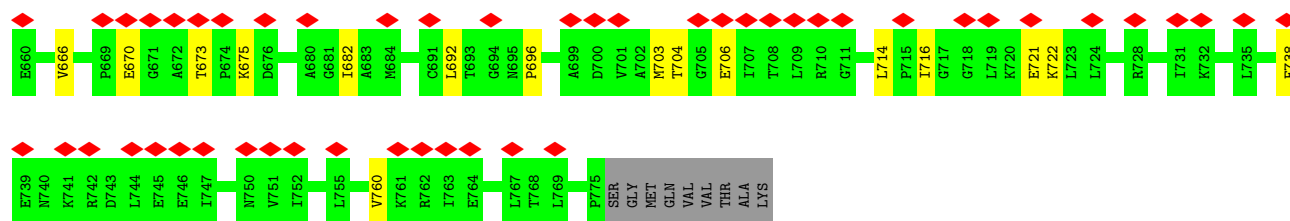
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lon protease.

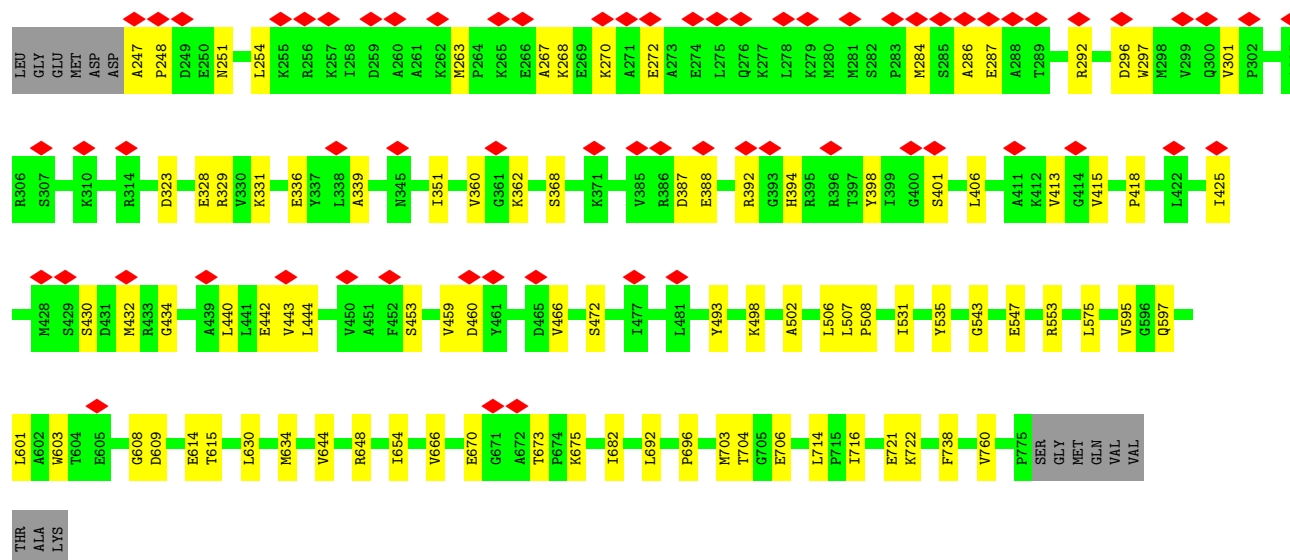
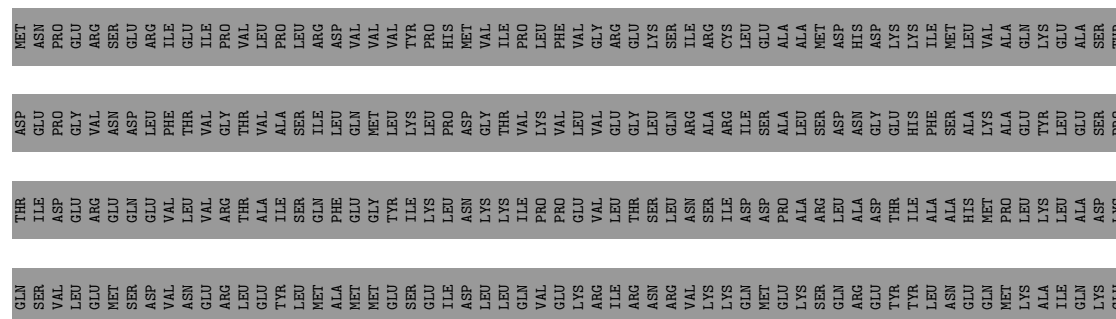
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	B	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	C	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	D	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21		
1	E	529	Total	C	N	O	S	0	0
			4101	2577	730	773	21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

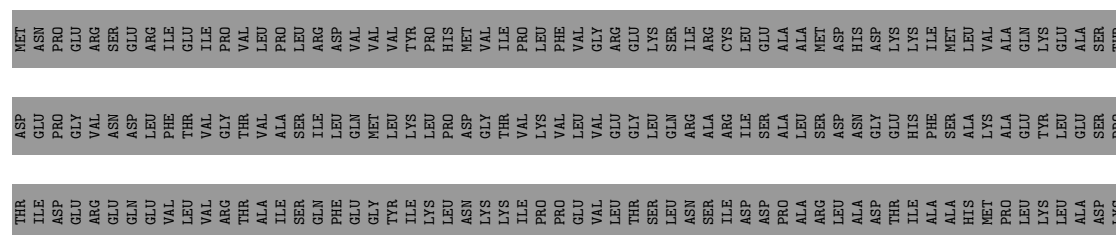
Chain	Residue	Modelled	Actual	Comment	Reference
A	679	ALA	SER	engineered mutation	UNP C3TLS2
B	679	ALA	SER	engineered mutation	UNP C3TLS2
C	679	ALA	SER	engineered mutation	UNP C3TLS2
D	679	ALA	SER	engineered mutation	UNP C3TLS2
E	679	ALA	SER	engineered mutation	UNP C3TLS2
F	679	ALA	SER	engineered mutation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

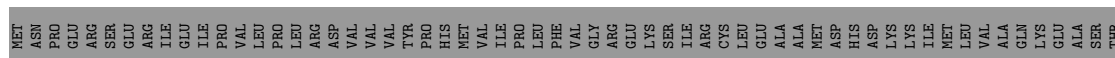


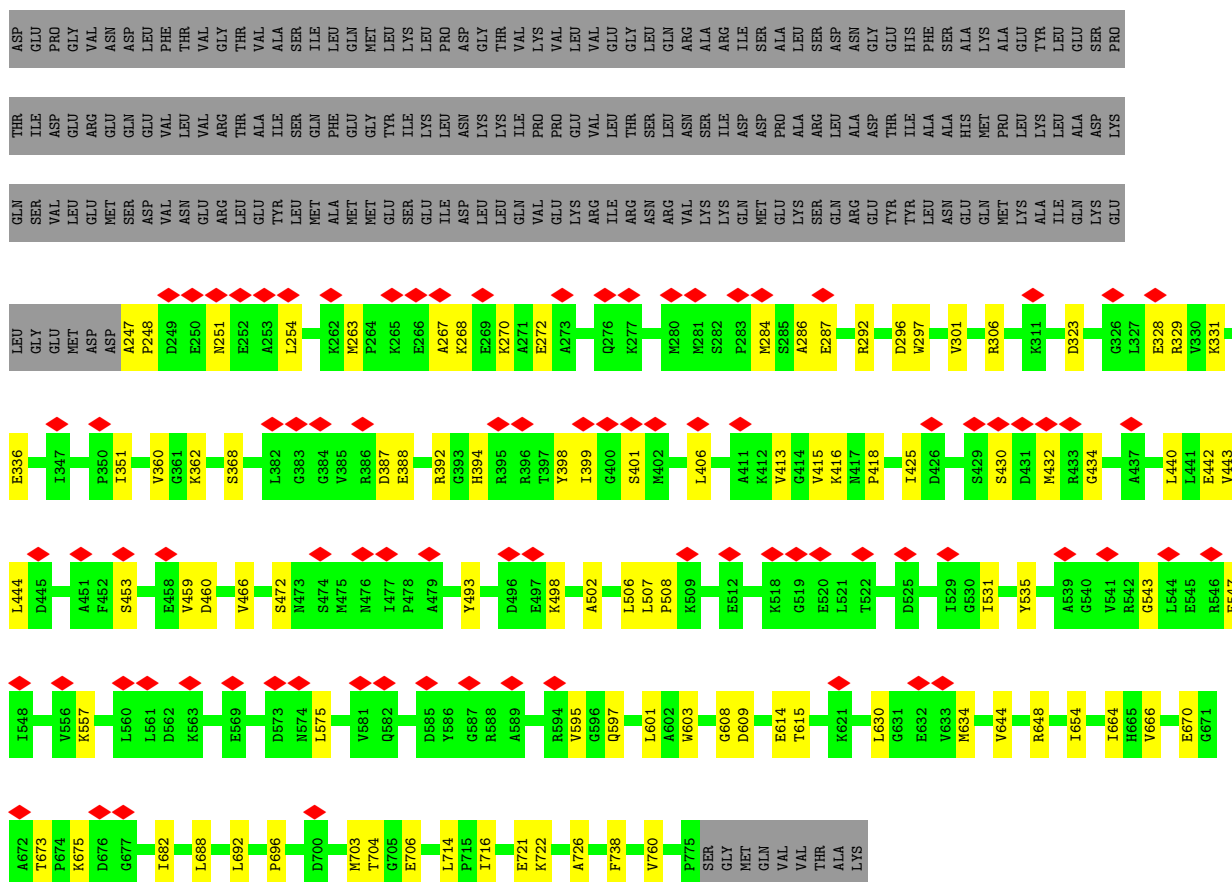
• Molecule 1: Lon protease



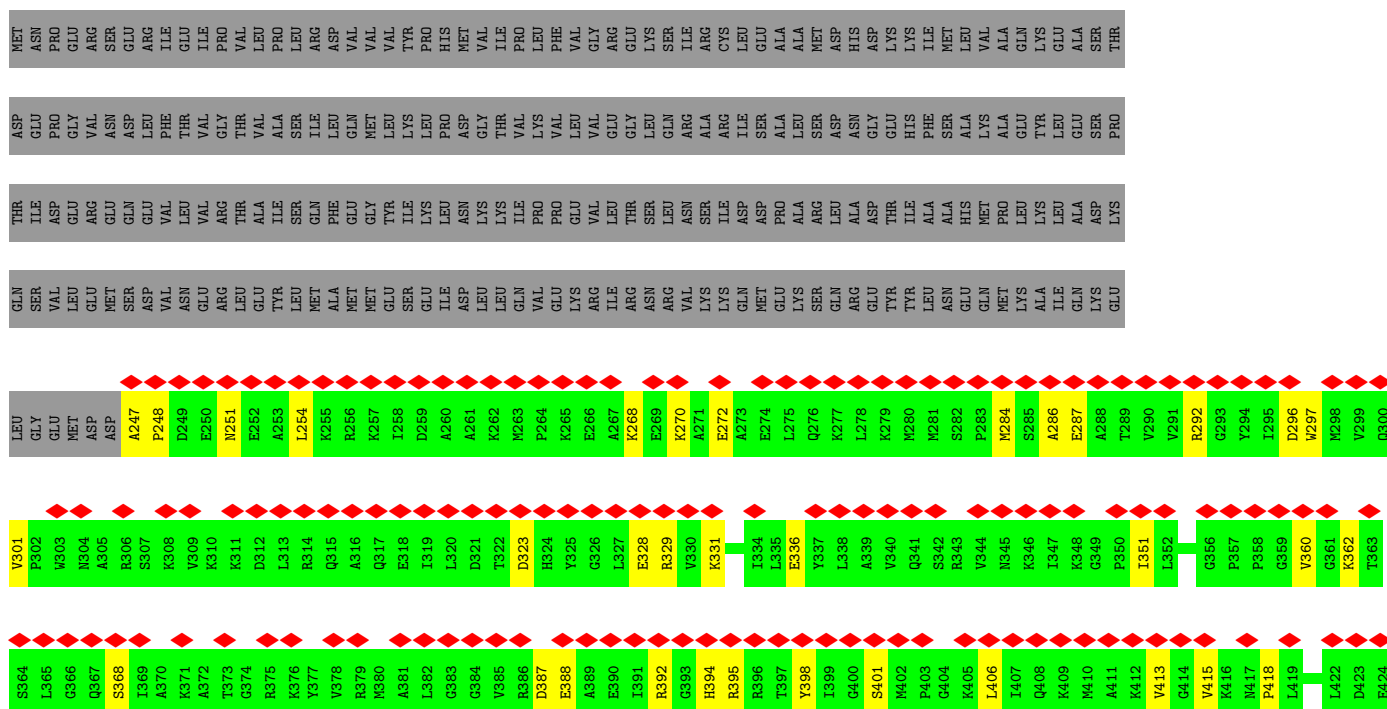
• Molecule 1: Lon protease







- Molecule 1: Lon protease



L735	V668	E605	E545	M485	I425
P669	P669	V606	R546	E486	D426
F738	B670	G607	E547	E487	K427
E739	G671	G608	I548	I488	M428
N740	A672	D609	S549	R489	S429
K741	T673	L610	K550	L490	S430
R742	P674	L611	L551	S491	D431
D743	K675	T612	C552	G492	M432
L744	D676	L613	R553	Y493	R433
E745	G677	E614	X554	T494	G434
E746	P678	T615	A555	E495	D435
L747	A679	A616	V556	D496	P436
P748	C617	C617	K557	E497	A437
D749	G681	V618	Q558	K498	S438
N750	L682	G620	L559	L499	A439
V751	A683	G620	L560	N500	L440
L755	M684	K621	L561	I501	L441
D756	C685	G622	D562	A502	E442
L757	T686	K623	K563	R503	V443
L758	A687	L624	S564	K504	L444
P759	L688	T625	L565	H505	D445
V760	L692	T627	X566	L506	P446
K761	T693	G628	H567	L507	E447
R762	G694	S629	I568	P508	Q448
L763	P696	L630	E569	K509	M449
E764	A699	G631	I570	Q510	V450
D765	D700	E632	N571	I511	A451
V766	V766	V633	G572	E512	F452
L767	V701	M634	D573	R513	S453
T768	A702	Q635	N574	N514	D454
L769	M703	E636	L575	A515	H455
L770	T704	S637	H576	L516	Y456
L771	G705	E637	D577	K517	L457
Q772	E706	E706	Y578	K518	E458
N773	I707	A641	L579	G519	Y459
E774	Q712	L642	G580	E520	D460
P775	V713	T643	V581	L521	Y461
SER	L714	G644	Q582	T522	D462
GLY	P715	R648	R583	V523	L463
MET	L716	A649	F584	D524	S464
GLN	V716	E650	D585	D525	D465
VAL	L717	V650	Y586	S526	V466
VAL	G717	K651	G587	A527	M467
THR	L720	L652	R588	I528	F468
ALA	E721	G653	A589	L529	V469
LYS	K722	L654	E589	G530	A470
L723	L723	N655	D590	I531	T471
L724	L724	P656	N591	E532	S472
A725	A725	D657	E592	I532	N473
A726	A726	F658	N593	R533	S474
H727	H727	Y659	R594	Y534	M475
R728	R728	E660	V595	E535	N476
G729	G729	K661	G596	T536	I477
G730	G730	R662	Q597	R537	P478
I731	I731	D663	Y596	E538	A479
K732	K732	I664	T599	A539	P480
T733	T733	H665	G600	G540	L481
V734	V734	V666	L601	E540	L482
		H667	A602	V541	D483
			W603	R542	R484
			T604	L544	

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 (\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 (\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	0.24	0/4161	0.42	0/5614
1	B	0.24	0/4161	0.42	0/5614
1	C	0.24	0/4161	0.42	0/5614
1	D	0.24	0/4161	0.42	0/5614
1	E	0.24	0/4161	0.42	0/5614
1	F	0.24	0/4161	0.42	0/5614
All	All	0.24	0/24966	0.42	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	54	0
1	B	4101	0	4229	55	0
1	C	4101	0	4229	55	0
1	D	4101	0	4229	52	0
1	E	4101	0	4229	58	0
1	F	4101	0	4229	54	0
All	All	24606	0	25374	318	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 318 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%)	439 (99%)	3 (1%)	81	89
1	B	442/670 (66%)	439 (99%)	3 (1%)	81	89
1	C	442/670 (66%)	439 (99%)	3 (1%)	81	89
1	D	442/670 (66%)	439 (99%)	3 (1%)	81	89
1	E	442/670 (66%)	439 (99%)	3 (1%)	81	89
1	F	442/670 (66%)	439 (99%)	3 (1%)	81	89
All	All	2652/4020 (66%)	2634 (99%)	18 (1%)	80	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	609	ASP
1	F	609	ASP
1	F	329	ARG
1	C	609	ASP
1	E	329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	510	GLN
1	E	510	GLN
1	F	510	GLN
1	B	510	GLN
1	A	510	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 [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.

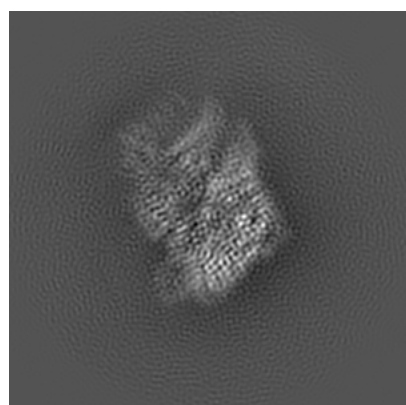
6 Map visualisation [i](#)

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.

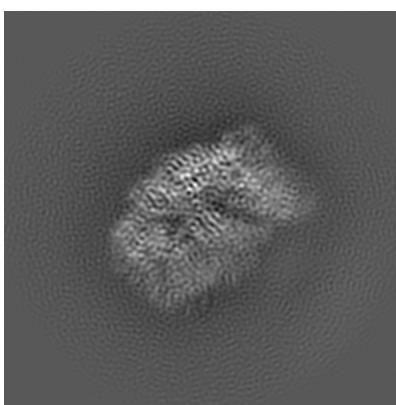
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

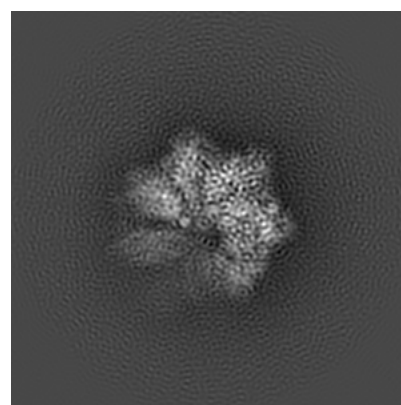
6.1.1 Primary map



X



Y

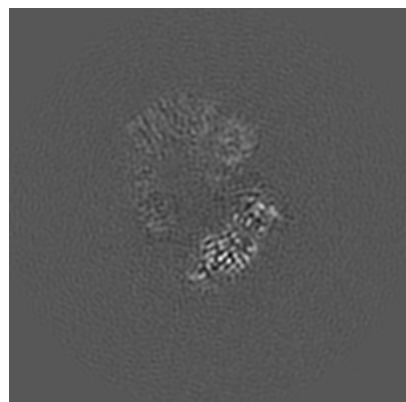


Z

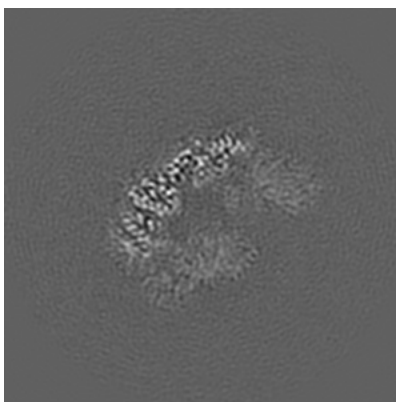
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

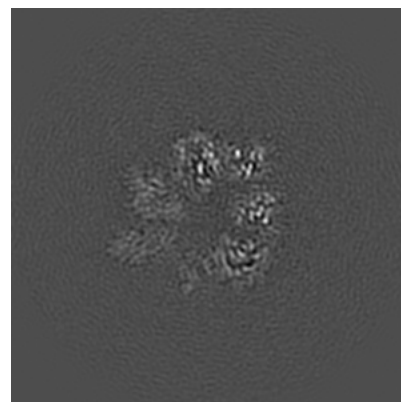
6.2.1 Primary map



X Index: 160



Y Index: 160

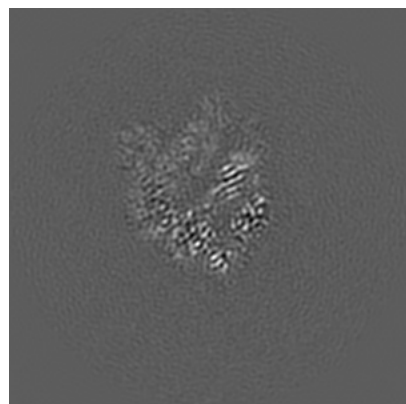


Z Index: 160

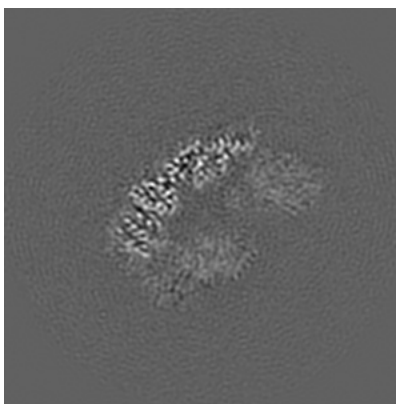
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

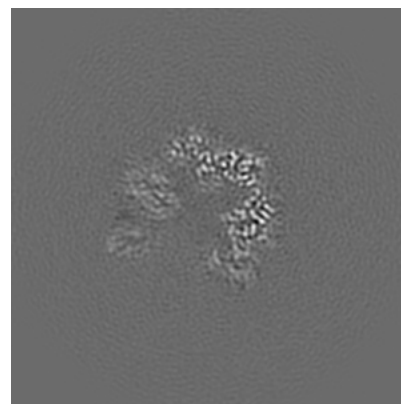
6.3.1 Primary map



X Index: 184



Y Index: 159

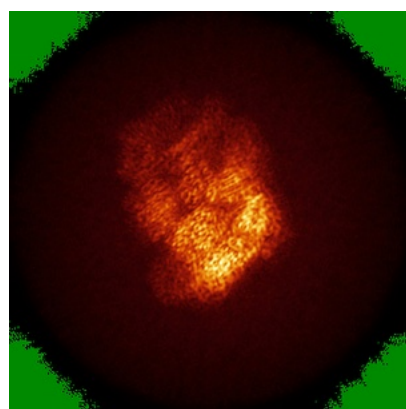


Z Index: 147

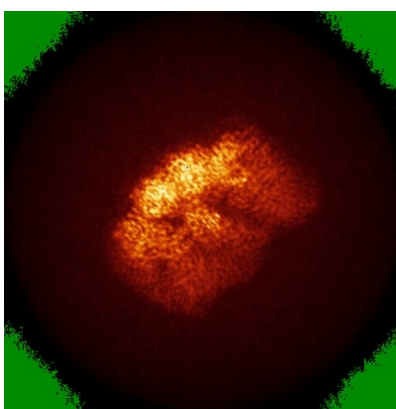
The images above show the largest variance slices of the map in three orthogonal directions.

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

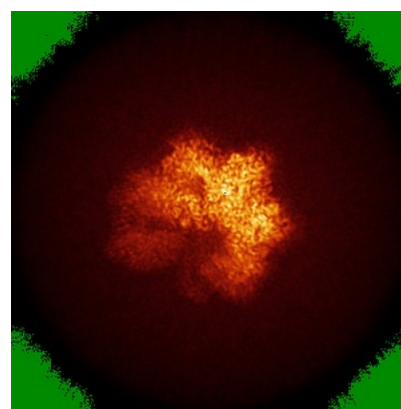
6.4.1 Primary map



X



Y

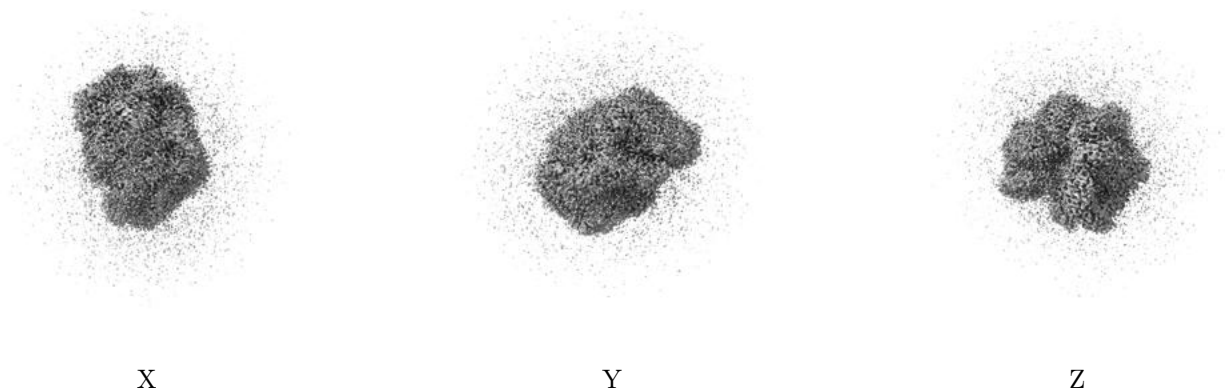


Z

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.

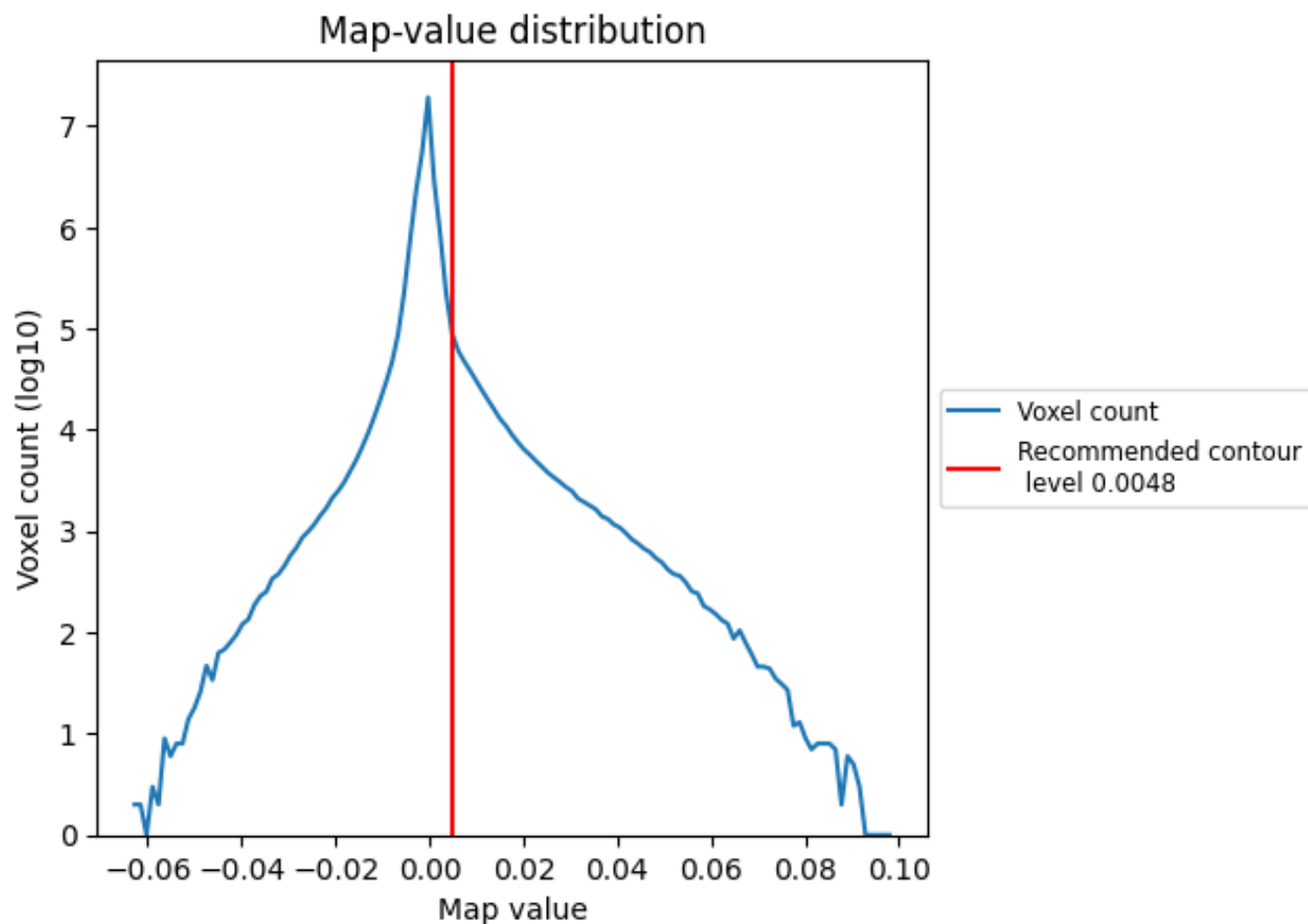
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

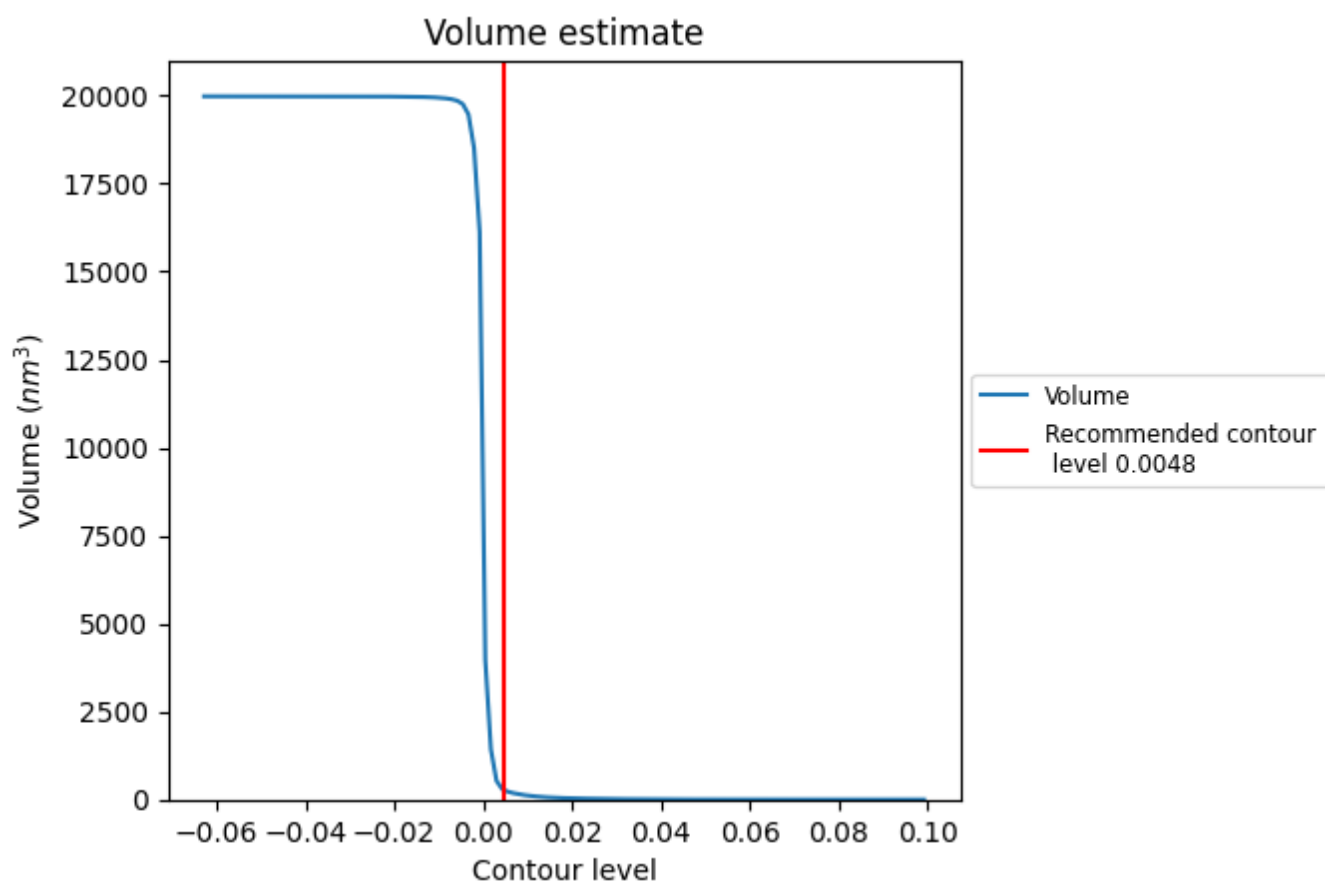
This section contains the results of statistical analysis of the map.

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.

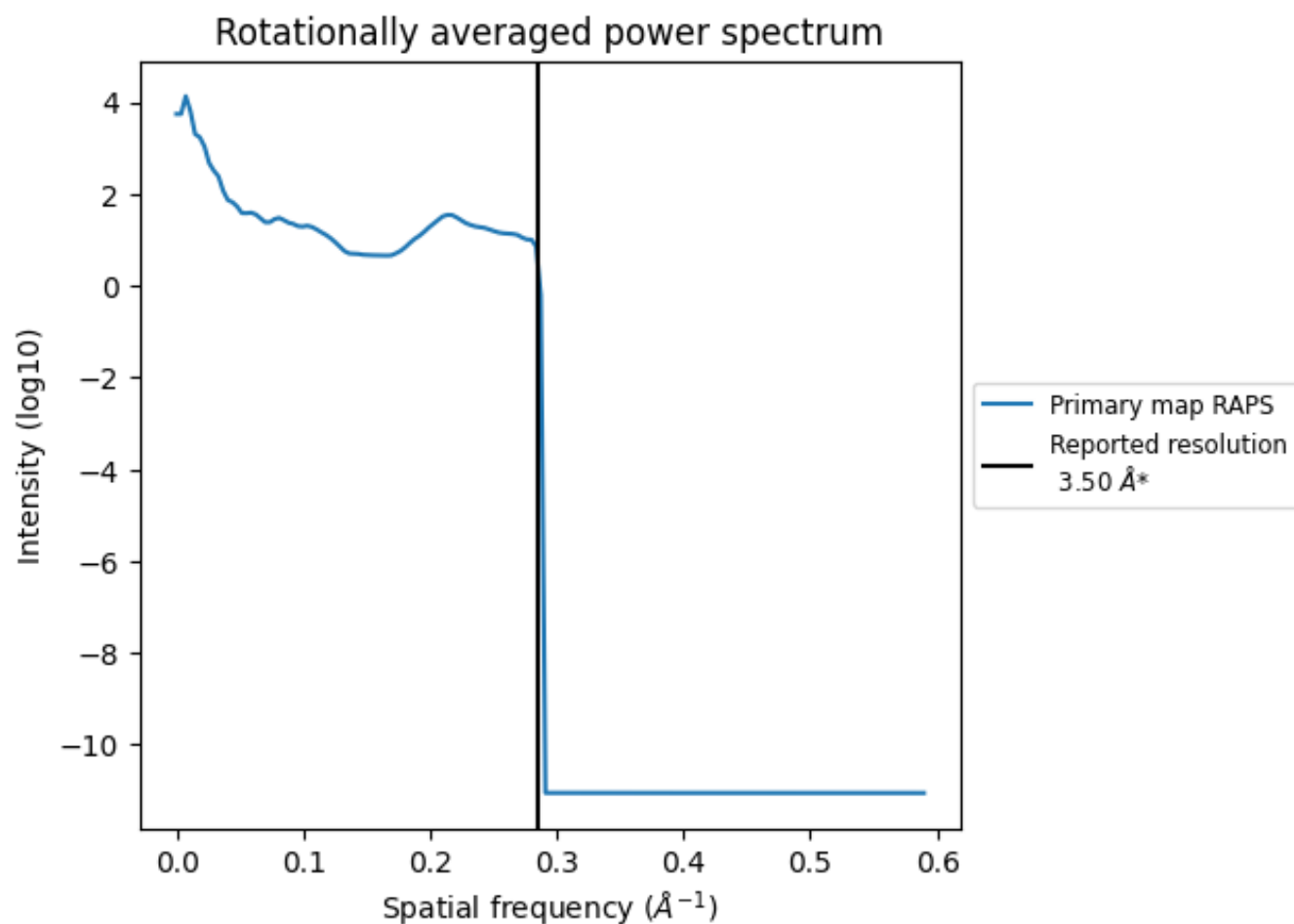
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm^3 ; 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 Å⁻¹

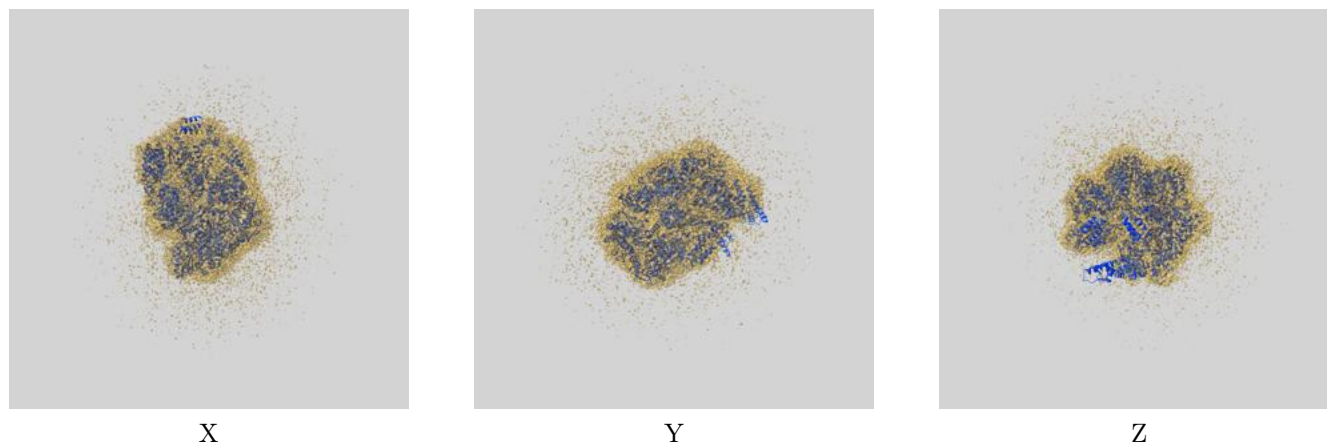
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

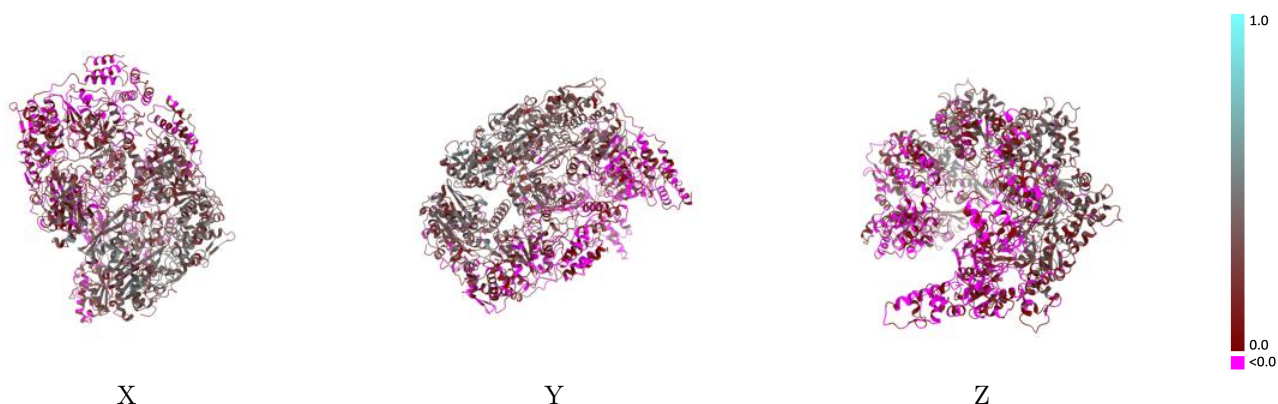
This section contains information regarding the fit between EMDB map EMD-20659 and PDB model 6U5Z. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



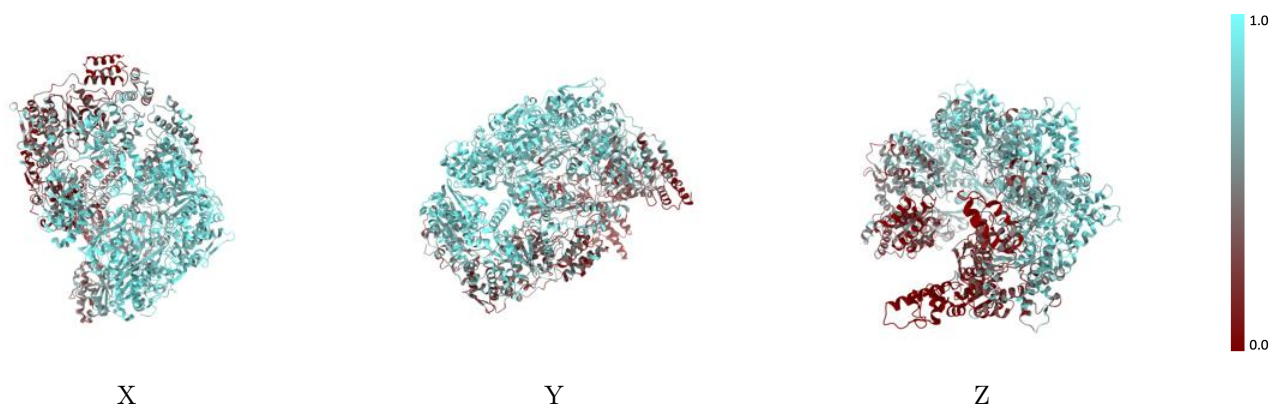
The images above show the 3D surface view of the map at the recommended contour level 0.0048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



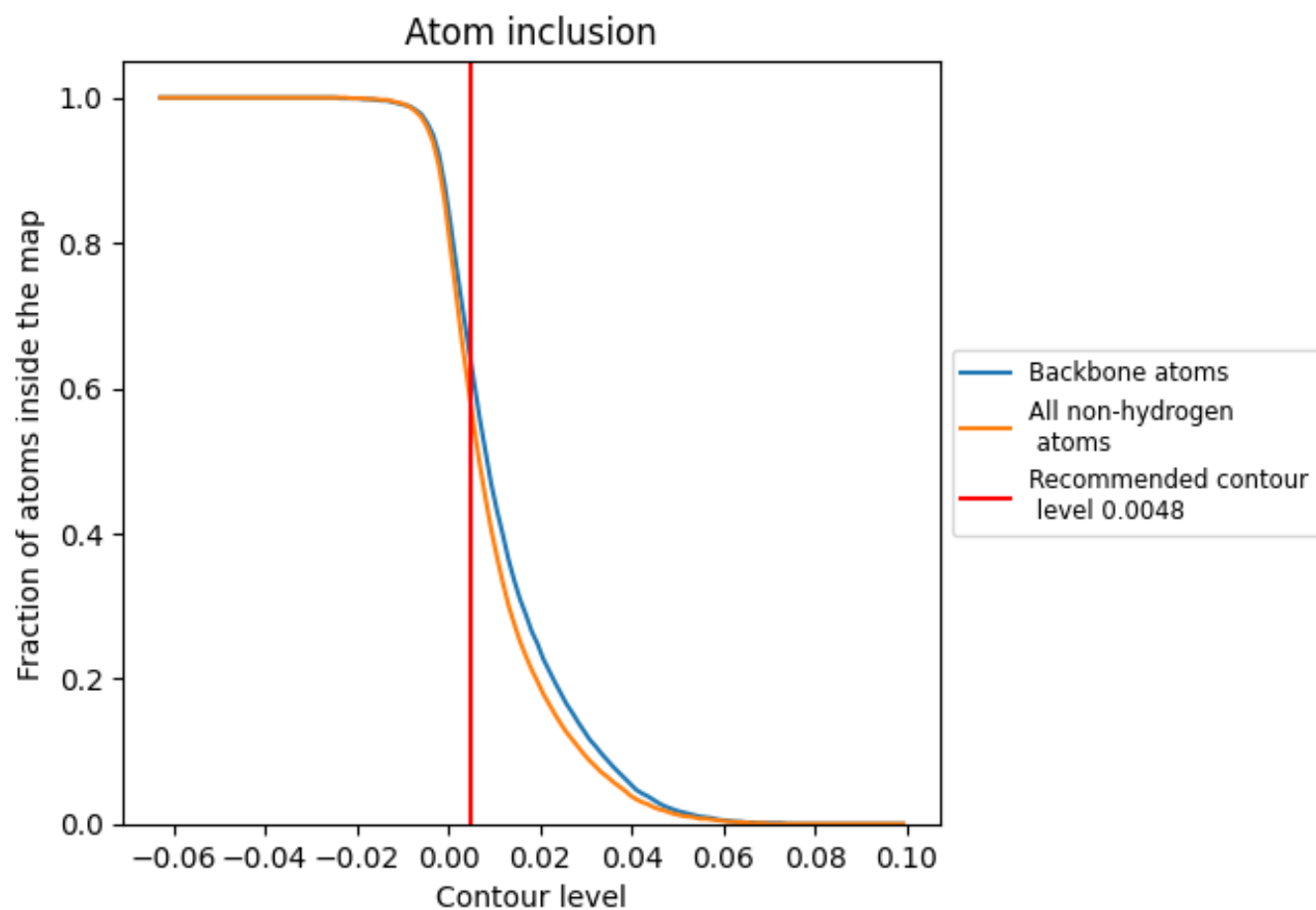
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.5830	<div></div> 0.1830
A	<div></div> 0.3620	<div></div> 0.0810
B	<div></div> 0.7300	<div></div> 0.2250
C	<div></div> 0.7890	<div></div> 0.2970
D	<div></div> 0.7920	<div></div> 0.2900
E	<div></div> 0.6470	<div></div> 0.1790
F	<div></div> 0.1780	<div></div> 0.0250

