



wwPDB EM Validation Summary Report ⓘ

Sep 3, 2024 – 02:52 PM JST

PDB ID : 7VZ3
EMDB ID : EMD-32219
Title : Cryo-EM structure of Depo32, a Klebsiella phage depolymerase targets the K2 serotype K. pneumoniae
Authors : Cai, R.; Ren, Z.; Zhao, R.; Wang, X.; Guo, Z.; Du, R.; Han, W.; Ru, H.; Gu, J.
Deposited on : 2021-11-15
Resolution : 2.46 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.dev112
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) : 2.38.2

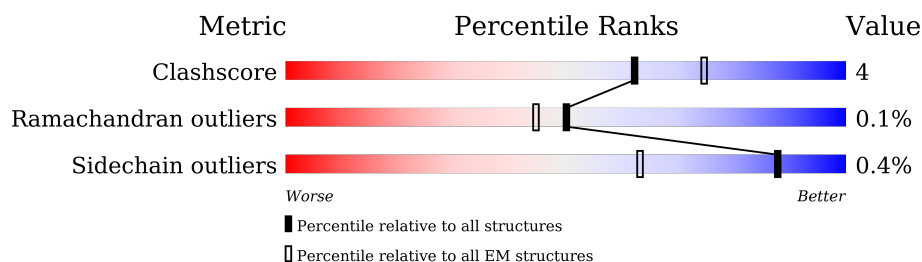
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 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	928	<div> <div>55%</div> <div>73% 7% 19%</div> </div>
1	B	928	<div> <div>58%</div> <div>72% 9% 19%</div> </div>
1	C	928	<div> <div>56%</div> <div>75% 6% 19%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17415 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 Depolymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	751	Total	C	N	O	S	0	0
			5798	3658	982	1136	22		
1	B	754	Total	C	N	O	S	0	0
			5819	3669	986	1142	22		
1	C	751	Total	C	N	O	S	0	0
			5798	3658	982	1136	22		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A3S7W7I3
A	-19	GLY	-	expression tag	UNP A0A3S7W7I3
A	-18	SER	-	expression tag	UNP A0A3S7W7I3
A	-17	SER	-	expression tag	UNP A0A3S7W7I3
A	-16	HIS	-	expression tag	UNP A0A3S7W7I3
A	-15	HIS	-	expression tag	UNP A0A3S7W7I3
A	-14	HIS	-	expression tag	UNP A0A3S7W7I3
A	-13	HIS	-	expression tag	UNP A0A3S7W7I3
A	-12	HIS	-	expression tag	UNP A0A3S7W7I3
A	-11	HIS	-	expression tag	UNP A0A3S7W7I3
A	-10	SER	-	expression tag	UNP A0A3S7W7I3
A	-9	SER	-	expression tag	UNP A0A3S7W7I3
A	-8	GLY	-	expression tag	UNP A0A3S7W7I3
A	-7	LEU	-	expression tag	UNP A0A3S7W7I3
A	-6	VAL	-	expression tag	UNP A0A3S7W7I3
A	-5	PRO	-	expression tag	UNP A0A3S7W7I3
A	-4	ARG	-	expression tag	UNP A0A3S7W7I3
A	-3	GLY	-	expression tag	UNP A0A3S7W7I3
A	-2	SER	-	expression tag	UNP A0A3S7W7I3
A	-1	HIS	-	expression tag	UNP A0A3S7W7I3
A	0	MET	-	expression tag	UNP A0A3S7W7I3
B	-20	MET	-	initiating methionine	UNP A0A3S7W7I3
B	-19	GLY	-	expression tag	UNP A0A3S7W7I3
B	-18	SER	-	expression tag	UNP A0A3S7W7I3

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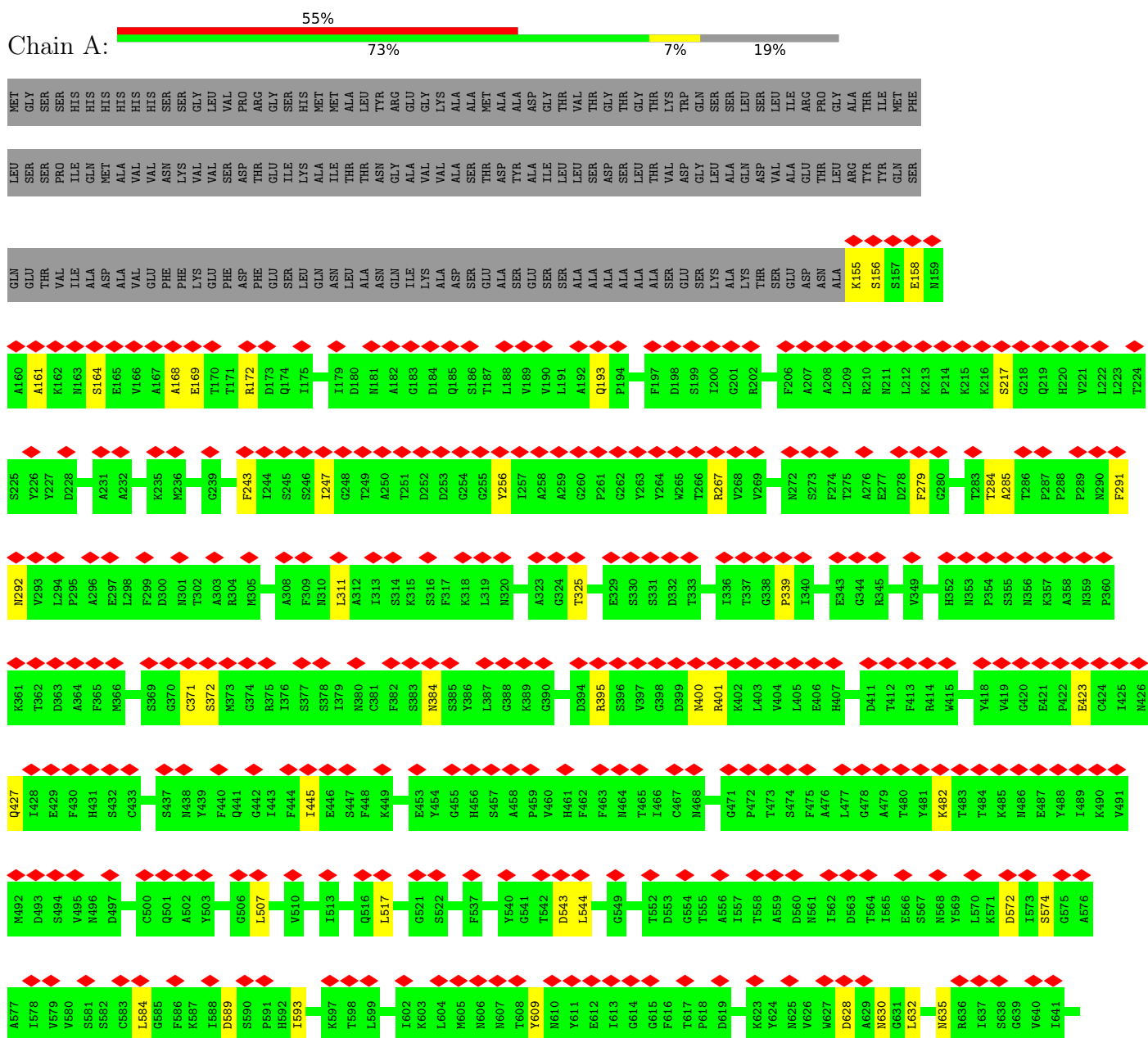
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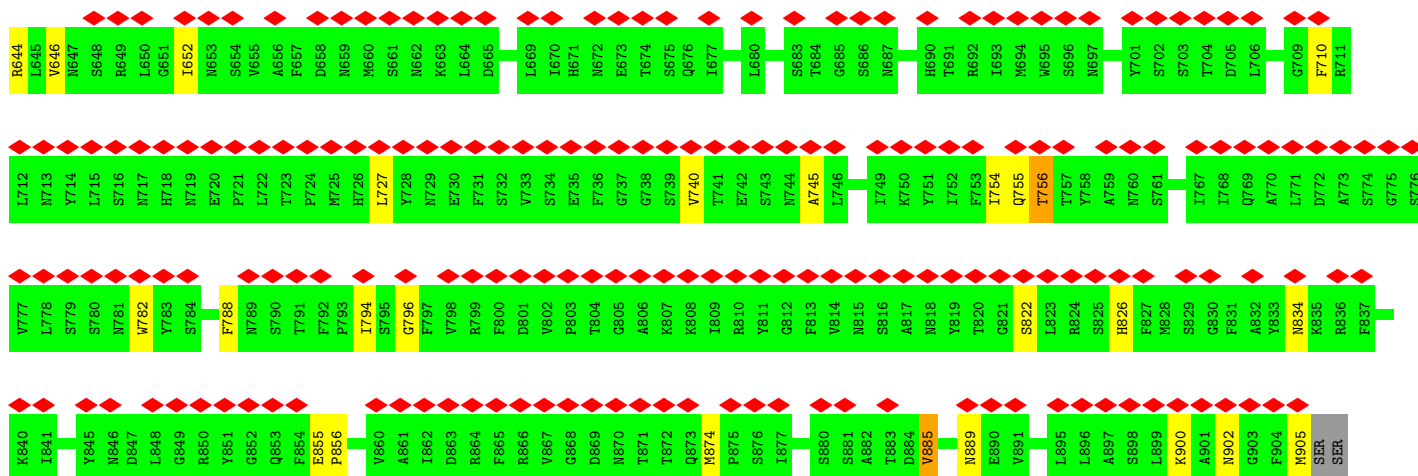
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP A0A3S7W7I3
B	-16	HIS	-	expression tag	UNP A0A3S7W7I3
B	-15	HIS	-	expression tag	UNP A0A3S7W7I3
B	-14	HIS	-	expression tag	UNP A0A3S7W7I3
B	-13	HIS	-	expression tag	UNP A0A3S7W7I3
B	-12	HIS	-	expression tag	UNP A0A3S7W7I3
B	-11	HIS	-	expression tag	UNP A0A3S7W7I3
B	-10	SER	-	expression tag	UNP A0A3S7W7I3
B	-9	SER	-	expression tag	UNP A0A3S7W7I3
B	-8	GLY	-	expression tag	UNP A0A3S7W7I3
B	-7	LEU	-	expression tag	UNP A0A3S7W7I3
B	-6	VAL	-	expression tag	UNP A0A3S7W7I3
B	-5	PRO	-	expression tag	UNP A0A3S7W7I3
B	-4	ARG	-	expression tag	UNP A0A3S7W7I3
B	-3	GLY	-	expression tag	UNP A0A3S7W7I3
B	-2	SER	-	expression tag	UNP A0A3S7W7I3
B	-1	HIS	-	expression tag	UNP A0A3S7W7I3
B	0	MET	-	expression tag	UNP A0A3S7W7I3
C	-20	MET	-	initiating methionine	UNP A0A3S7W7I3
C	-19	GLY	-	expression tag	UNP A0A3S7W7I3
C	-18	SER	-	expression tag	UNP A0A3S7W7I3
C	-17	SER	-	expression tag	UNP A0A3S7W7I3
C	-16	HIS	-	expression tag	UNP A0A3S7W7I3
C	-15	HIS	-	expression tag	UNP A0A3S7W7I3
C	-14	HIS	-	expression tag	UNP A0A3S7W7I3
C	-13	HIS	-	expression tag	UNP A0A3S7W7I3
C	-12	HIS	-	expression tag	UNP A0A3S7W7I3
C	-11	HIS	-	expression tag	UNP A0A3S7W7I3
C	-10	SER	-	expression tag	UNP A0A3S7W7I3
C	-9	SER	-	expression tag	UNP A0A3S7W7I3
C	-8	GLY	-	expression tag	UNP A0A3S7W7I3
C	-7	LEU	-	expression tag	UNP A0A3S7W7I3
C	-6	VAL	-	expression tag	UNP A0A3S7W7I3
C	-5	PRO	-	expression tag	UNP A0A3S7W7I3
C	-4	ARG	-	expression tag	UNP A0A3S7W7I3
C	-3	GLY	-	expression tag	UNP A0A3S7W7I3
C	-2	SER	-	expression tag	UNP A0A3S7W7I3
C	-1	HIS	-	expression tag	UNP A0A3S7W7I3
C	0	MET	-	expression tag	UNP A0A3S7W7I3

3 Residue-property plots

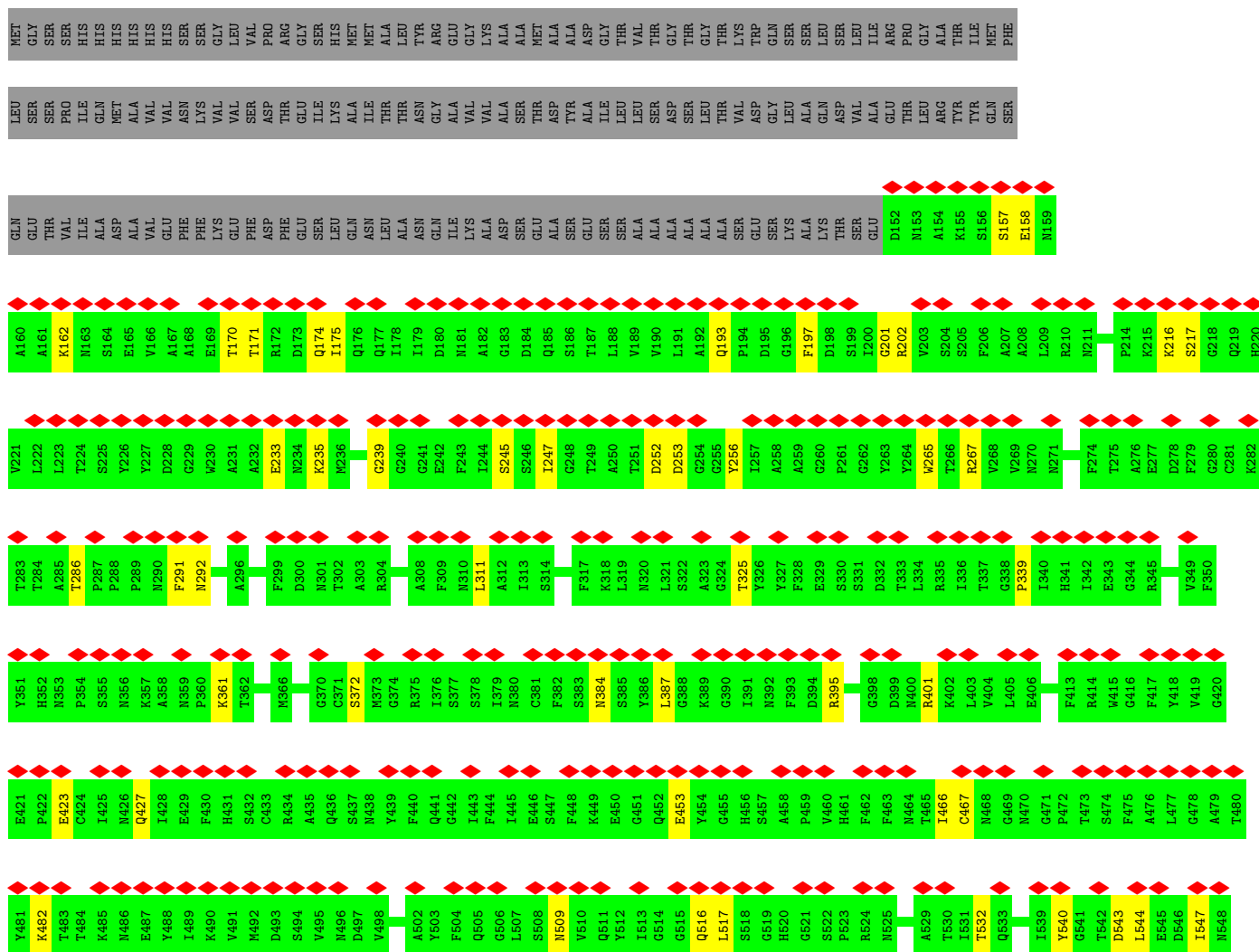
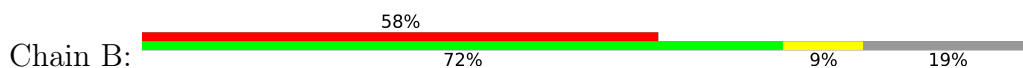
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

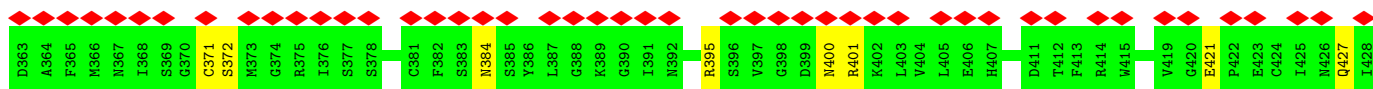
• Molecule 1: Depolymerase





• Molecule 1: Depolymerase





K840	A843	N846	D847	L848	G849	R850	Y851	G852	Q853	F854	E855	P856	F857	Y858	S859	V860	A861	I862	D863	R864	F865	D869	N870	T871	T872	Q873	K874	P875	S876	L877	P878	A879	S880	S881	A882	T883	D884	G887	V888	N889	L892	N893	S894	L895	L896	A897	S898	L899	K900	A901	N902	N905	SER				
S774	G775	S776	V777	L778	S779	S780	N781	W782	Y783	S784	P785	Q786	S787	F788	N789	S790	T791	F792	P793	F797	W798	D801	V802	P803	T804	G805	A806	K807	K808	I809	R810	N815	S816	A817	N818	Y819	T820	G821	S822	L823	R824	S825	H826	F827	N828	S829	G830	F831	A832	Y833	N834	K835	R836	F837	F838	L839	
L712	N713	Y714	L715	S716	N717	H718	N719	E720	P721	L722	T723	P724	M725	H726	L727	Y728	N729	E730	F731	S732	E735	F736	G737	G738	S739	V740	T741	E742	S743	N744	A745	L746	D747	E748	I749	K750	Y751	I752	F753	I754	Q755	Y758	A759	N760	S761	G762	D763	G764	R765	F766	I767	I768	Q769	A770	L771	D772	A773
N647	S648	R649	L650	G651	I652	N653	S654	V655	A656	F657	D658	N659	N662	K663	L664	D665	V666	S667	S668	L669	I670	H671	N672	E673	Q676	I677	I678	G679	L680	T681	P682	S683	T684	G685	S686	N687	V688	P689	H690	T691	R692	I693	M694	W695	S696	N697	G698	A699	M700	Y701	D705	L706	N707	N708	G709		
Y569	L570	K571	D572	I573	S574	G575	A576	A577	I578	S581	S582	C583	L584	D589	H592	I593	F594	K595	L599	S600	L604	M605	N606	N607	T608	Y609	E612	I613	G614	G615	F616	D619	E620	A621	L622	N625	V626	W627	N630	G631	I637	V640	I641	H642	P643	R644	L645	V646									
D493	S494	V495	M496	D497	V498	G499	C500	Q501	A502	Y503	F504	Q505	G506	L507	S508	N509	Y512	I513	G514	G515	Q516	L517	S518	G519	H520	G521	S522	P523	R524	N525	T526	S527	L528	A529	T532	Q533	F537	Y540	I547	N548	G549	T552	D553	G554	T555	T558	I559	A559	D560	N561	I562	N568					
E429	F430	H431	S432	C433	R434	A435	Q436	S437	M438	Y439	F440	Q441	G442	E446	S447	F448	K449	E450	G451	Q452	E453	Y454	G455	H456	S457	A458	P459	V460	F461	F462	M464	T465	I466	C467	N470	T473	S474	F475	A476	L477	G478	A479	T480	Y481	K482	T483	T484	K485	M486	E487	Y488	I489	K490	V491	M492		

SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	462388	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0139	Depositor
Map size (Å)	278.272, 278.272, 278.272	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	0.45	0/5936	0.63	0/8059
1	B	0.44	0/5957	0.61	0/8088
1	C	0.45	0/5936	0.62	0/8059
All	All	0.44	0/17829	0.62	0/24206

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	5798	0	5549	53	0
1	B	5819	0	5564	58	0
1	C	5798	0	5549	38	0
All	All	17415	0	16662	138	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 4.

The worst 5 of 138 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:B:197:PHE:CE1	1:B:202:ARG:NH2	2.43	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:THR:HG22	1:A:788:PHE:CG	2.14	0.83
1:C:874:MET:HG2	1:C:902:ASN:HD22	1.50	0.76
1:A:395:ARG:NH2	1:A:423:GLU:O	2.22	0.71
1:A:371:CYS:H	1:A:400:ASN:HD22	1.37	0.71

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	749/928 (81%)	710 (95%)	38 (5%)	1 (0%)	48	61
1	B	752/928 (81%)	714 (95%)	37 (5%)	1 (0%)	48	61
1	C	749/928 (81%)	702 (94%)	46 (6%)	1 (0%)	48	61
All	All	2250/2784 (81%)	2126 (94%)	121 (5%)	3 (0%)	50	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	885	VAL
1	A	885	VAL
1	C	884	ASP

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	633/774 (82%)	631 (100%)	2 (0%)	91	95
1	B	635/774 (82%)	631 (99%)	4 (1%)	84	91
1	C	633/774 (82%)	631 (100%)	2 (0%)	91	95
All	All	1901/2322 (82%)	1893 (100%)	8 (0%)	88	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	782	TRP
1	C	216	LYS
1	B	605	MET
1	B	598	THR
1	B	782	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	292	ASN
1	C	873	GLN
1	C	163	ASN
1	C	672	ASN
1	B	755	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 ⓘ

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.

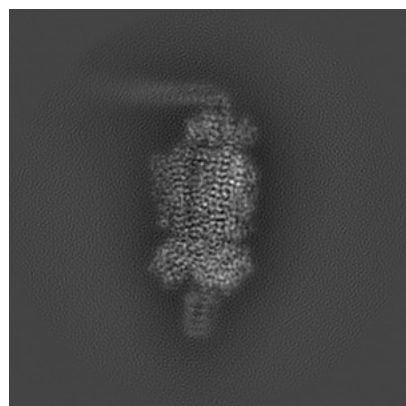
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32219. These allow visual inspection of the internal detail of the map and identification of artifacts.

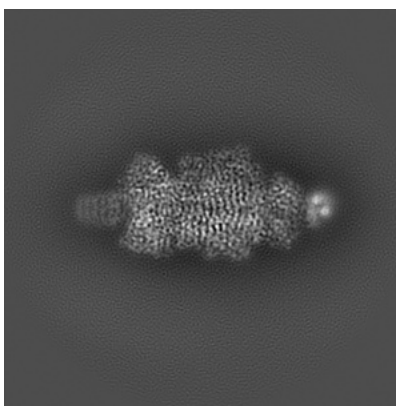
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

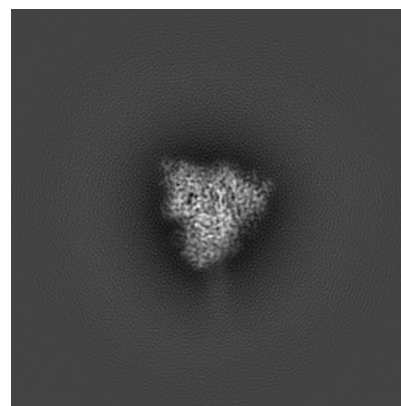
6.1.1 Primary map



X

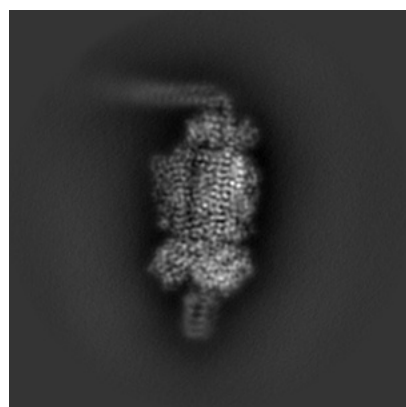


Y

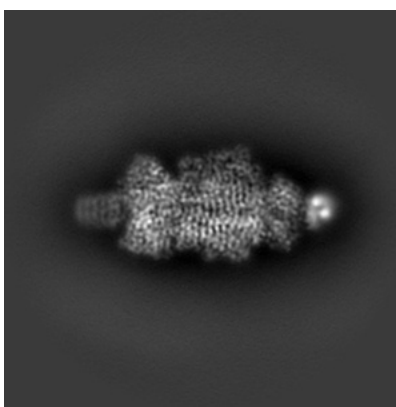


Z

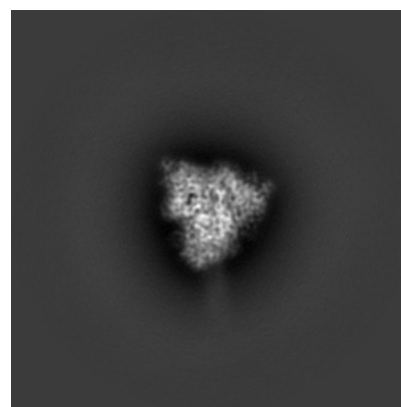
6.1.2 Raw map



X



Y

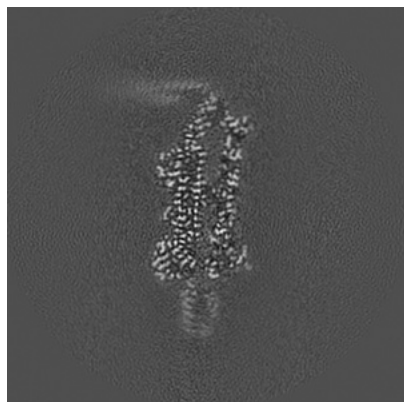


Z

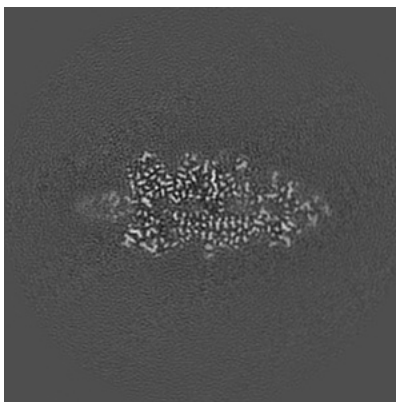
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

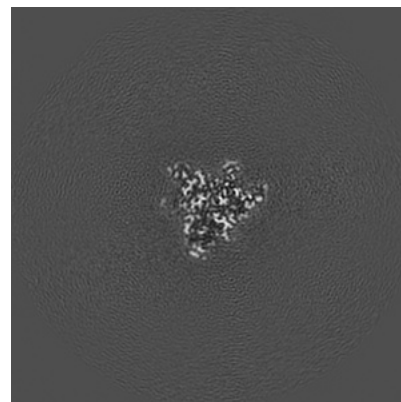
6.2.1 Primary map



X Index: 128

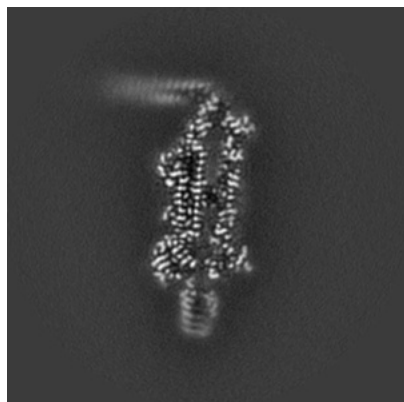


Y Index: 128

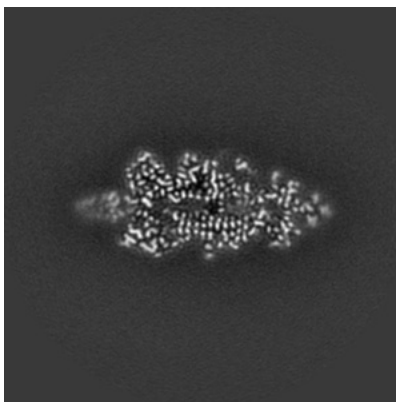


Z Index: 128

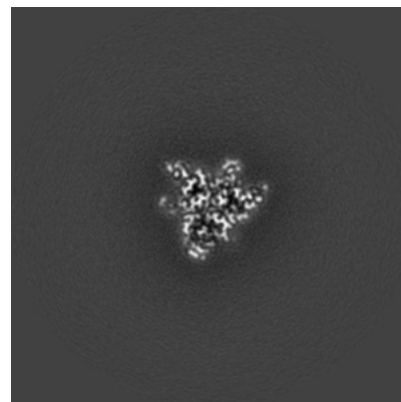
6.2.2 Raw map



X Index: 128



Y Index: 128

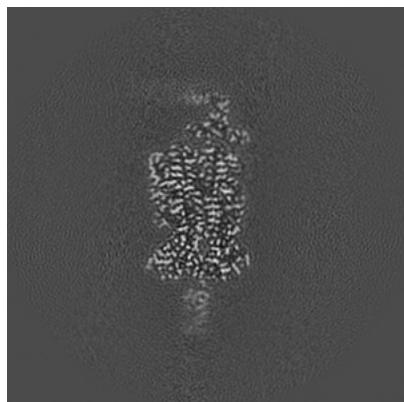


Z Index: 128

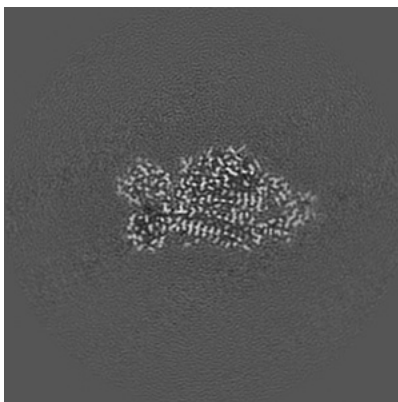
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

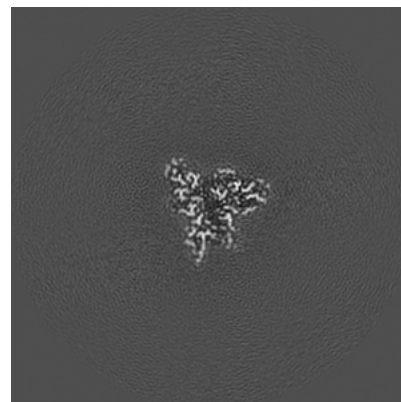
6.3.1 Primary map



X Index: 121

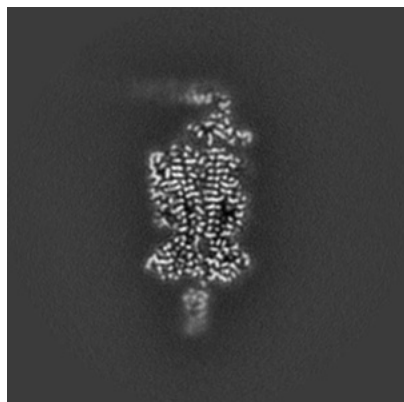


Y Index: 139

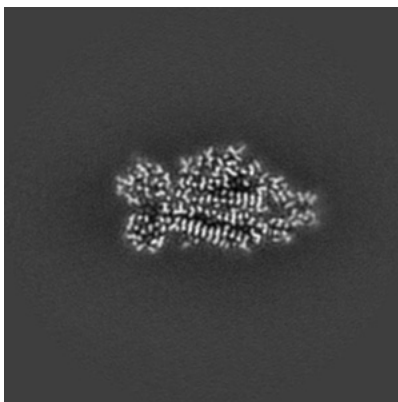


Z Index: 136

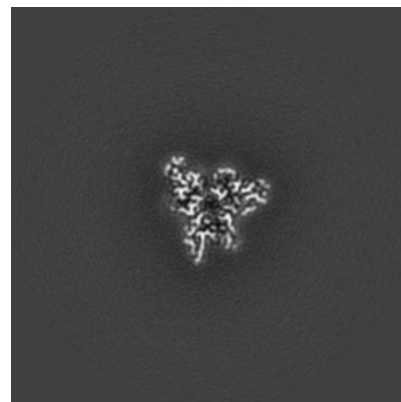
6.3.2 Raw map



X Index: 120



Y Index: 139

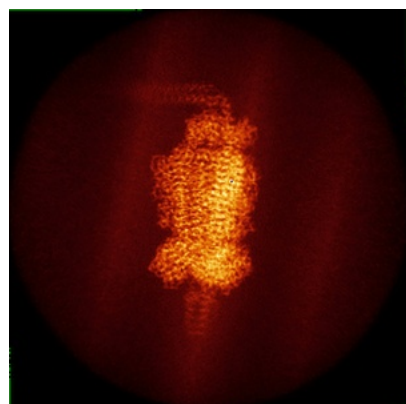


Z Index: 136

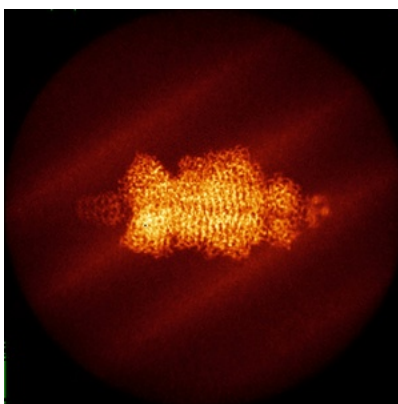
The images above show the largest variance slices of the map in three orthogonal directions.

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

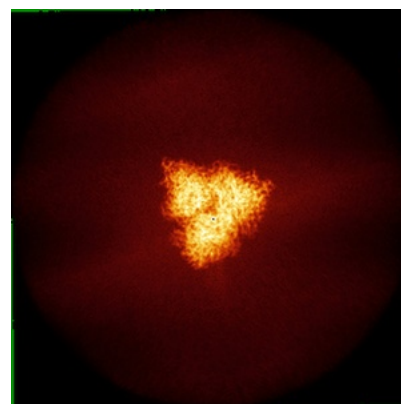
6.4.1 Primary map



X

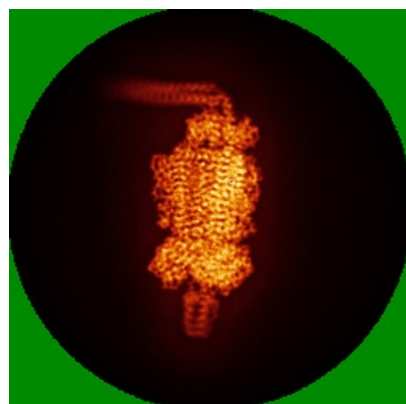


Y

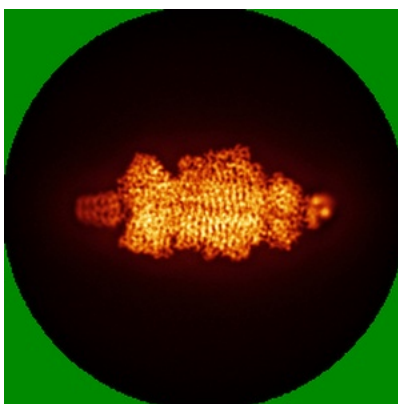


Z

6.4.2 Raw map



X



Y

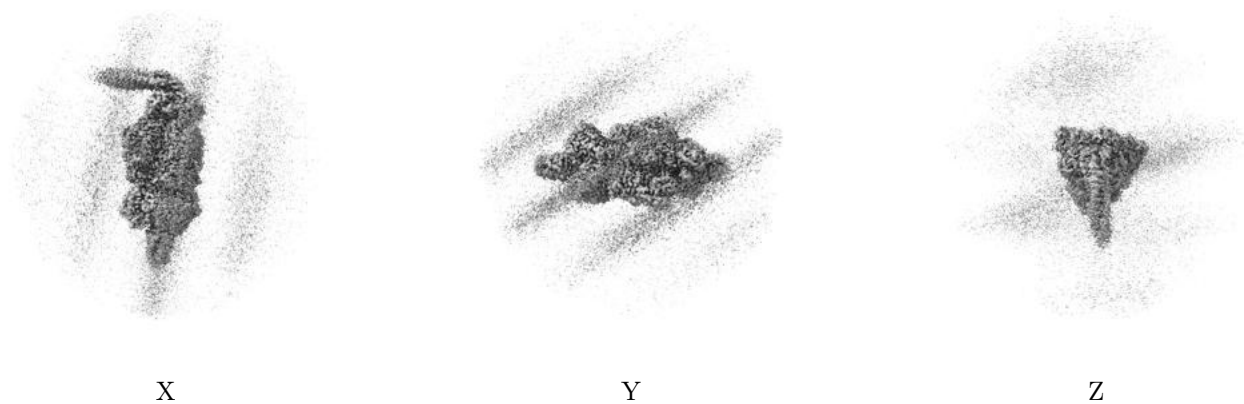


Z

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.

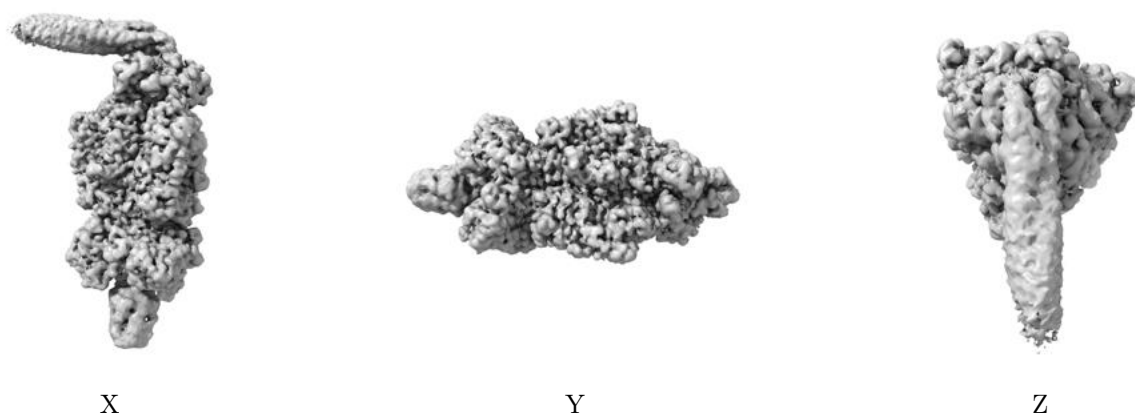
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0139. 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.

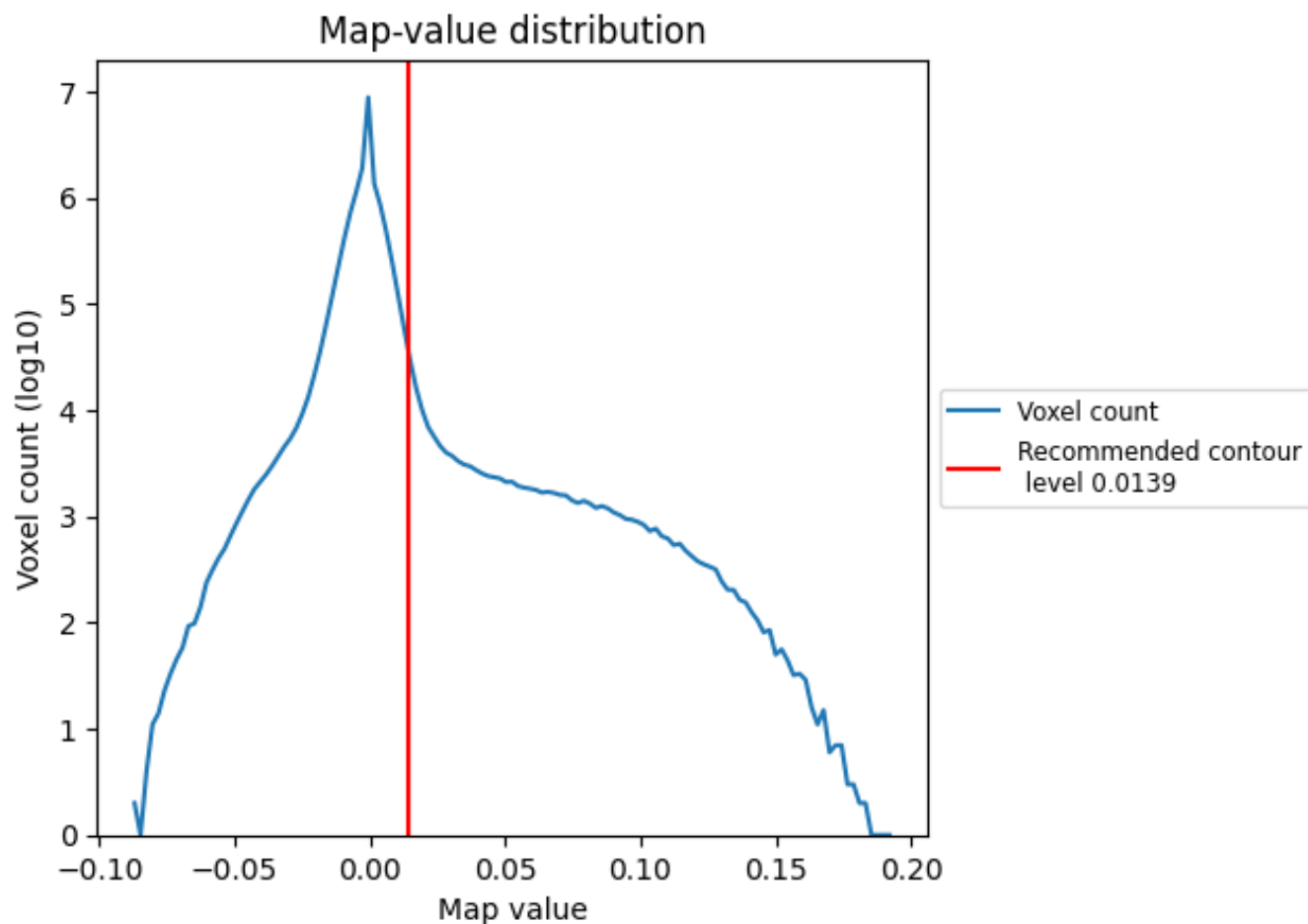
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

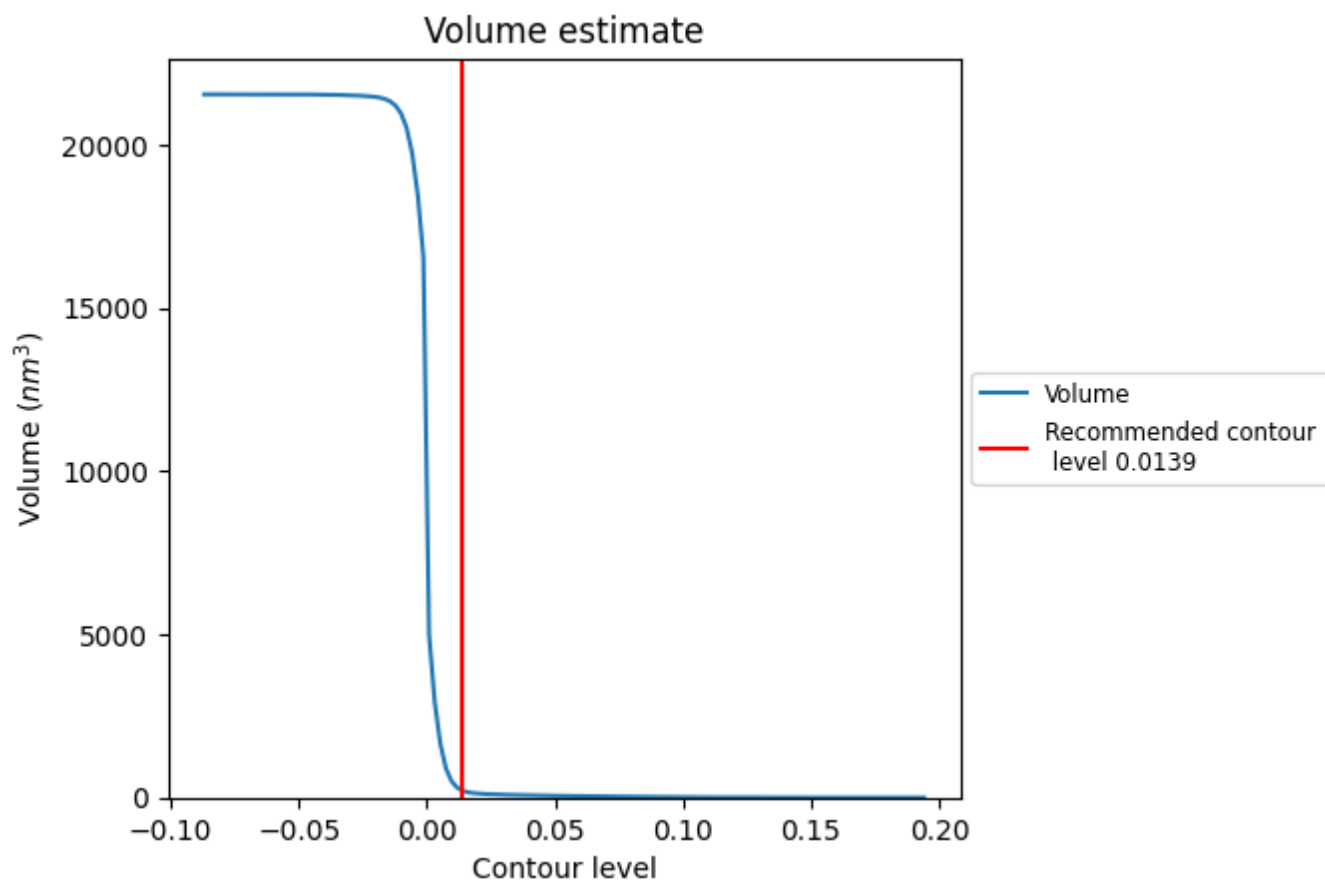
This section contains the results of statistical analysis of the map.

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.

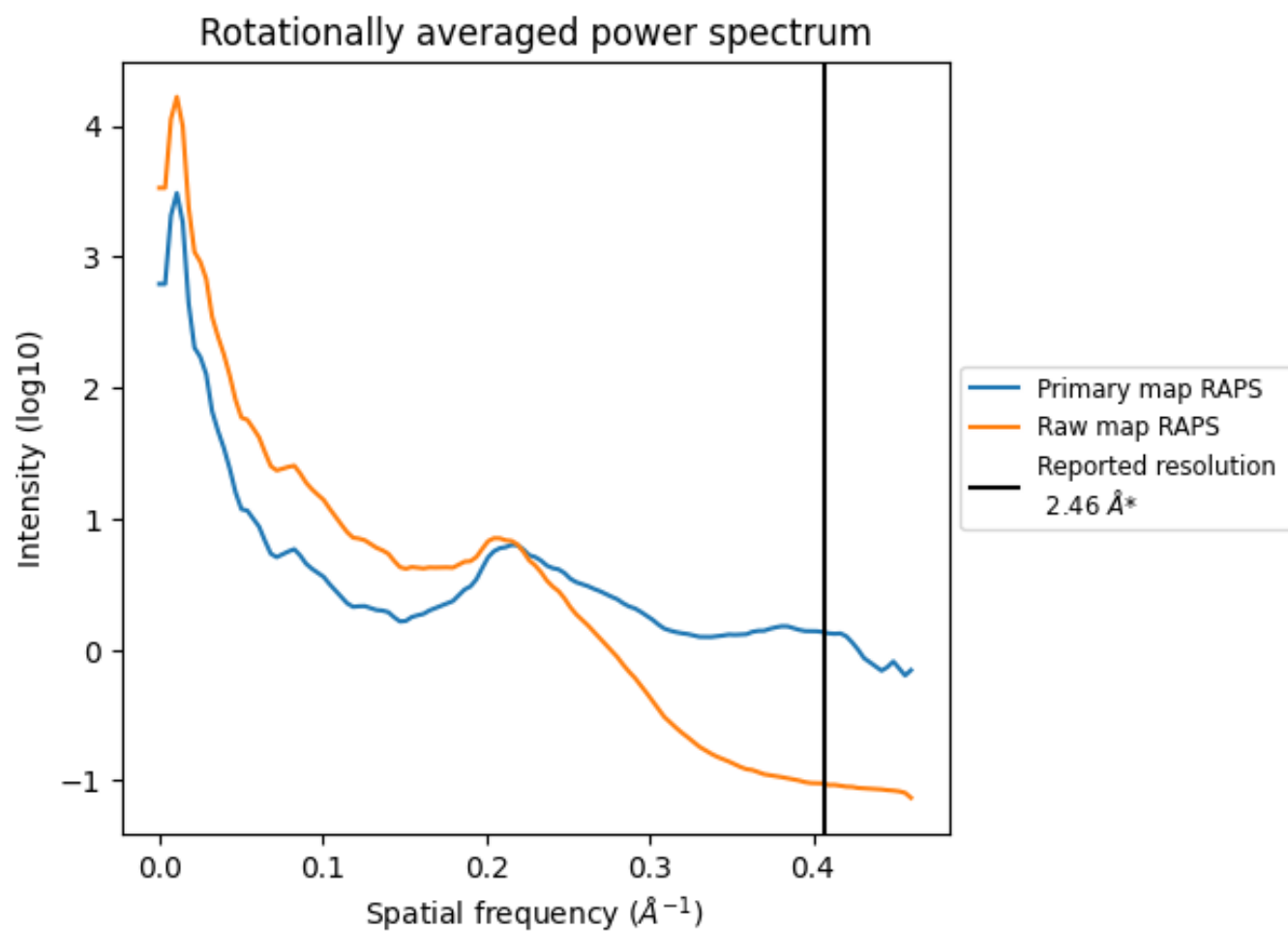
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm³; this corresponds to an approximate mass of 194 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 ⓘ

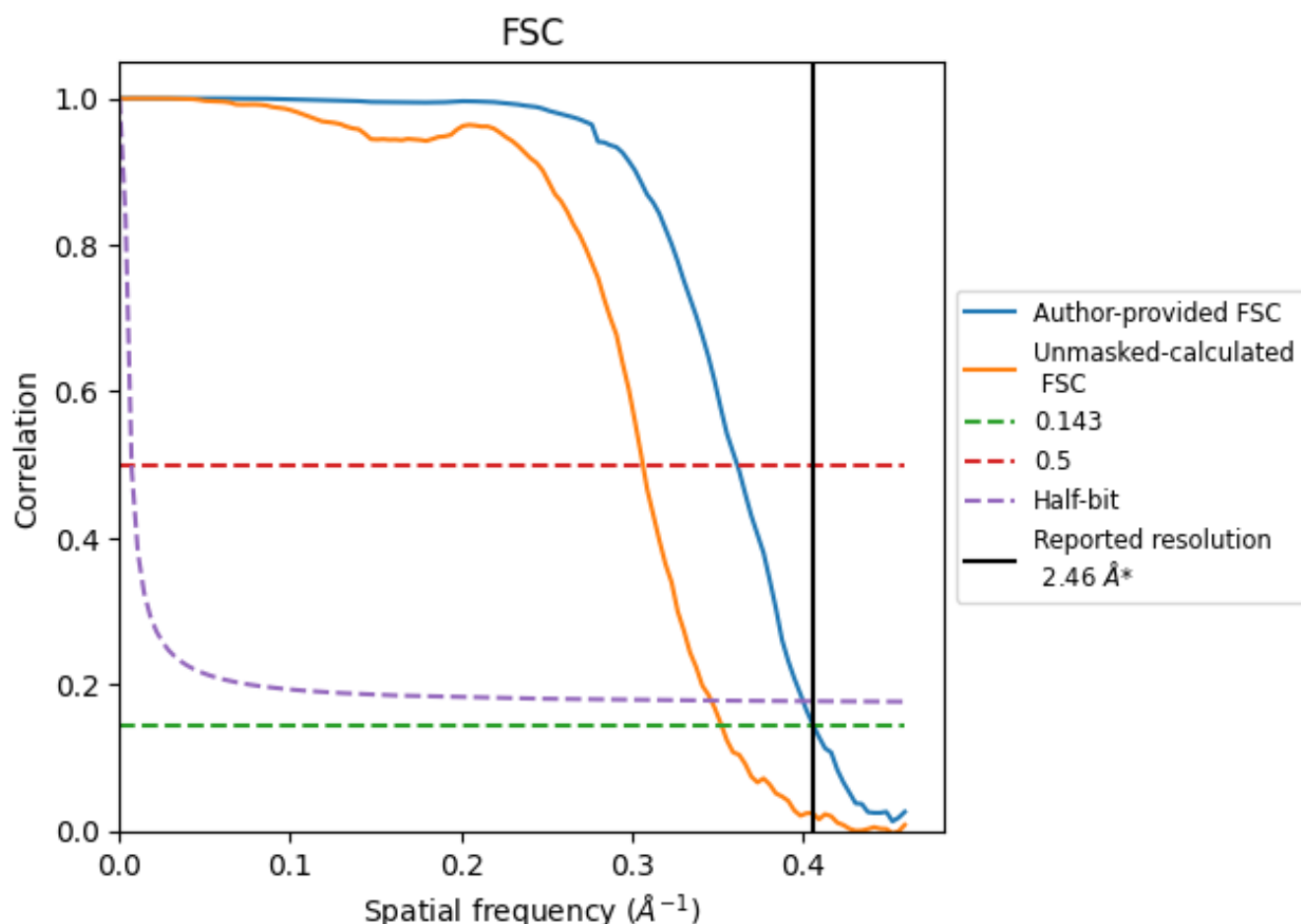


*Reported resolution corresponds to spatial frequency of 0.407 Å⁻¹

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 0.407 Å⁻¹

8.2 Resolution estimates [i](#)

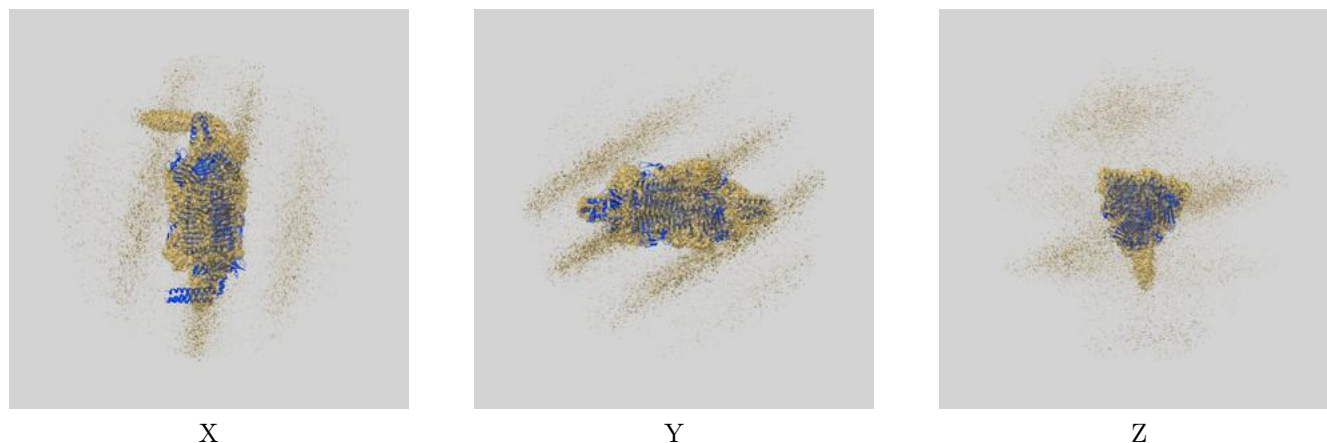
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	2.46	2.76	2.50
Unmasked-calculated*	2.84	3.26	2.89

*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 2.84 differs from the reported value 2.46 by more than 10 %

9 Map-model fit [i](#)

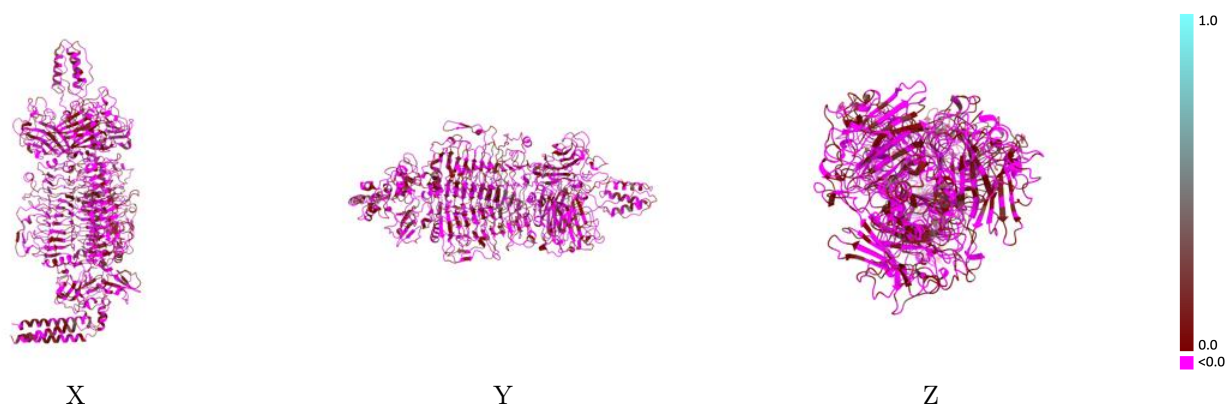
This section contains information regarding the fit between EMDB map EMD-32219 and PDB model 7VZ3. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



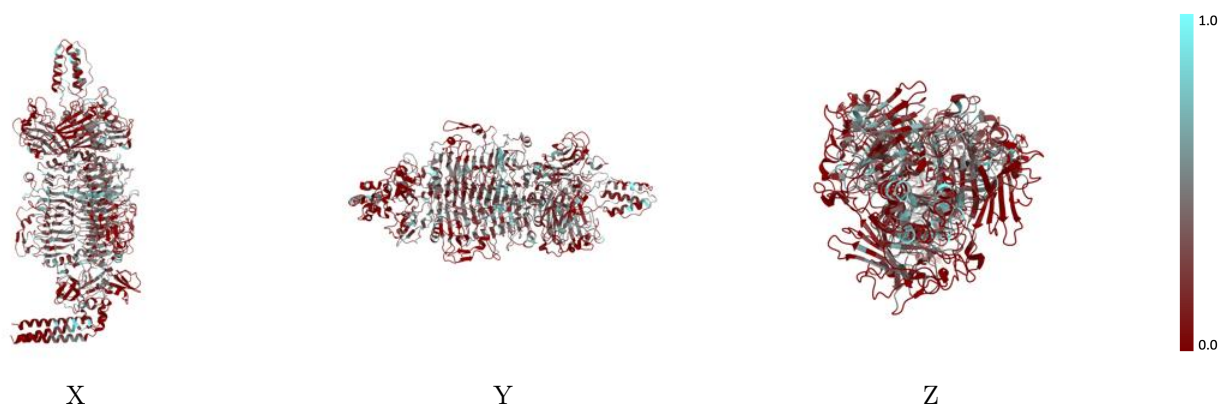
The images above show the 3D surface view of the map at the recommended contour level 0.0139 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



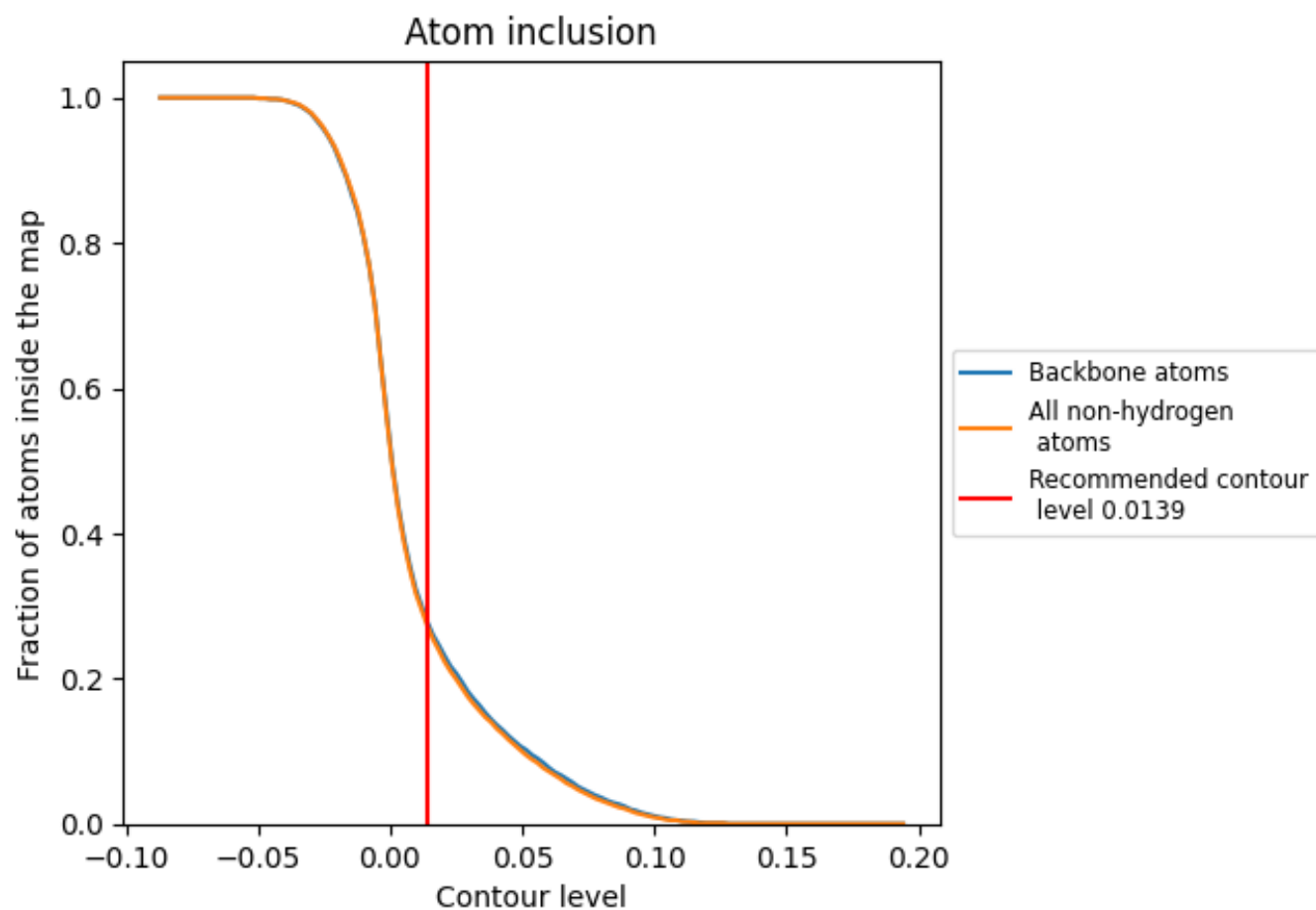
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0139).

9.4 Atom inclusion ⓘ



At the recommended contour level, 28% of all backbone atoms, 28% 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 (0.0139) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2750	<div></div> -0.0150
A	<div></div> 0.2760	<div></div> -0.0120
B	<div></div> 0.2740	<div></div> -0.0180
C	<div></div> 0.2750	<div></div> -0.0170

