



wwPDB EM Validation Summary Report ⓘ

Apr 6, 2026 – 03:29 AM UTC

PDB ID : 9K4A / pdb_00009k4a
EMDB ID : EMD-62051
Title : Cryo-EM structure of depolymerase S2-4 from Klebsiella phage K64-1
Authors : Zhao, R.; Du, T.; Ren, Z.; Gu, J.; Ru, H.
Deposited on : 2024-10-21
Resolution : 2.24 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

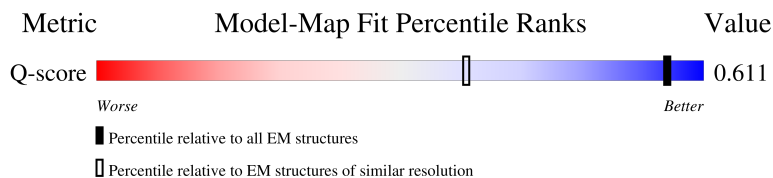
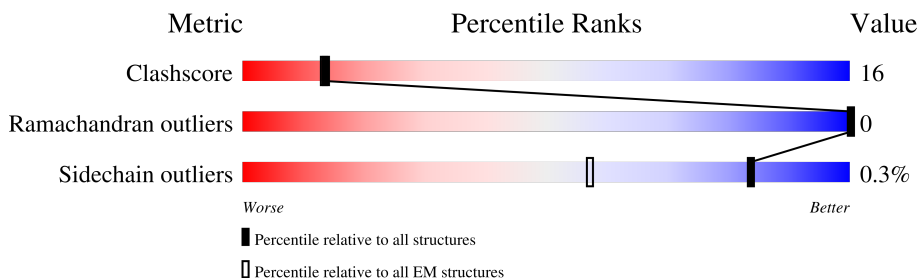
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 2.24 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	3381 (1.75 - 2.74)

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	922	 49% 23% 28%
1	B	922	 48% 25% 28%
1	C	922	 50% 23% 28%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15447 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, capsule K1-specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	668	Total	C	N	O	S	0	0
			5149	3220	858	1046	25		
1	B	668	Total	C	N	O	S	0	0
			5149	3220	858	1046	25		
1	C	668	Total	C	N	O	S	0	0
			5149	3220	858	1046	25		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP A0A0A8J8T2
A	-32	GLY	-	expression tag	UNP A0A0A8J8T2
A	-31	SER	-	expression tag	UNP A0A0A8J8T2
A	-30	SER	-	expression tag	UNP A0A0A8J8T2
A	-29	HIS	-	expression tag	UNP A0A0A8J8T2
A	-28	HIS	-	expression tag	UNP A0A0A8J8T2
A	-27	HIS	-	expression tag	UNP A0A0A8J8T2
A	-26	HIS	-	expression tag	UNP A0A0A8J8T2
A	-25	HIS	-	expression tag	UNP A0A0A8J8T2
A	-24	HIS	-	expression tag	UNP A0A0A8J8T2
A	-23	SER	-	expression tag	UNP A0A0A8J8T2
A	-22	SER	-	expression tag	UNP A0A0A8J8T2
A	-21	GLY	-	expression tag	UNP A0A0A8J8T2
A	-20	LEU	-	expression tag	UNP A0A0A8J8T2
A	-19	VAL	-	expression tag	UNP A0A0A8J8T2
A	-18	PRO	-	expression tag	UNP A0A0A8J8T2
A	-17	ARG	-	expression tag	UNP A0A0A8J8T2
A	-16	GLY	-	expression tag	UNP A0A0A8J8T2
A	-15	SER	-	expression tag	UNP A0A0A8J8T2
A	-14	HIS	-	expression tag	UNP A0A0A8J8T2
A	-13	MET	-	expression tag	UNP A0A0A8J8T2
A	-12	ALA	-	expression tag	UNP A0A0A8J8T2
A	-11	SER	-	expression tag	UNP A0A0A8J8T2
A	-10	MET	-	expression tag	UNP A0A0A8J8T2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	THR	-	expression tag	UNP A0A0A8J8T2
A	-8	GLY	-	expression tag	UNP A0A0A8J8T2
A	-7	GLY	-	expression tag	UNP A0A0A8J8T2
A	-6	GLN	-	expression tag	UNP A0A0A8J8T2
A	-5	GLN	-	expression tag	UNP A0A0A8J8T2
A	-4	MET	-	expression tag	UNP A0A0A8J8T2
A	-3	GLY	-	expression tag	UNP A0A0A8J8T2
A	-2	ARG	-	expression tag	UNP A0A0A8J8T2
A	-1	GLY	-	expression tag	UNP A0A0A8J8T2
A	0	SER	-	expression tag	UNP A0A0A8J8T2
B	-33	MET	-	initiating methionine	UNP A0A0A8J8T2
B	-32	GLY	-	expression tag	UNP A0A0A8J8T2
B	-31	SER	-	expression tag	UNP A0A0A8J8T2
B	-30	SER	-	expression tag	UNP A0A0A8J8T2
B	-29	HIS	-	expression tag	UNP A0A0A8J8T2
B	-28	HIS	-	expression tag	UNP A0A0A8J8T2
B	-27	HIS	-	expression tag	UNP A0A0A8J8T2
B	-26	HIS	-	expression tag	UNP A0A0A8J8T2
B	-25	HIS	-	expression tag	UNP A0A0A8J8T2
B	-24	HIS	-	expression tag	UNP A0A0A8J8T2
B	-23	SER	-	expression tag	UNP A0A0A8J8T2
B	-22	SER	-	expression tag	UNP A0A0A8J8T2
B	-21	GLY	-	expression tag	UNP A0A0A8J8T2
B	-20	LEU	-	expression tag	UNP A0A0A8J8T2
B	-19	VAL	-	expression tag	UNP A0A0A8J8T2
B	-18	PRO	-	expression tag	UNP A0A0A8J8T2
B	-17	ARG	-	expression tag	UNP A0A0A8J8T2
B	-16	GLY	-	expression tag	UNP A0A0A8J8T2
B	-15	SER	-	expression tag	UNP A0A0A8J8T2
B	-14	HIS	-	expression tag	UNP A0A0A8J8T2
B	-13	MET	-	expression tag	UNP A0A0A8J8T2
B	-12	ALA	-	expression tag	UNP A0A0A8J8T2
B	-11	SER	-	expression tag	UNP A0A0A8J8T2
B	-10	MET	-	expression tag	UNP A0A0A8J8T2
B	-9	THR	-	expression tag	UNP A0A0A8J8T2
B	-8	GLY	-	expression tag	UNP A0A0A8J8T2
B	-7	GLY	-	expression tag	UNP A0A0A8J8T2
B	-6	GLN	-	expression tag	UNP A0A0A8J8T2
B	-5	GLN	-	expression tag	UNP A0A0A8J8T2
B	-4	MET	-	expression tag	UNP A0A0A8J8T2
B	-3	GLY	-	expression tag	UNP A0A0A8J8T2
B	-2	ARG	-	expression tag	UNP A0A0A8J8T2

Continued on next page...

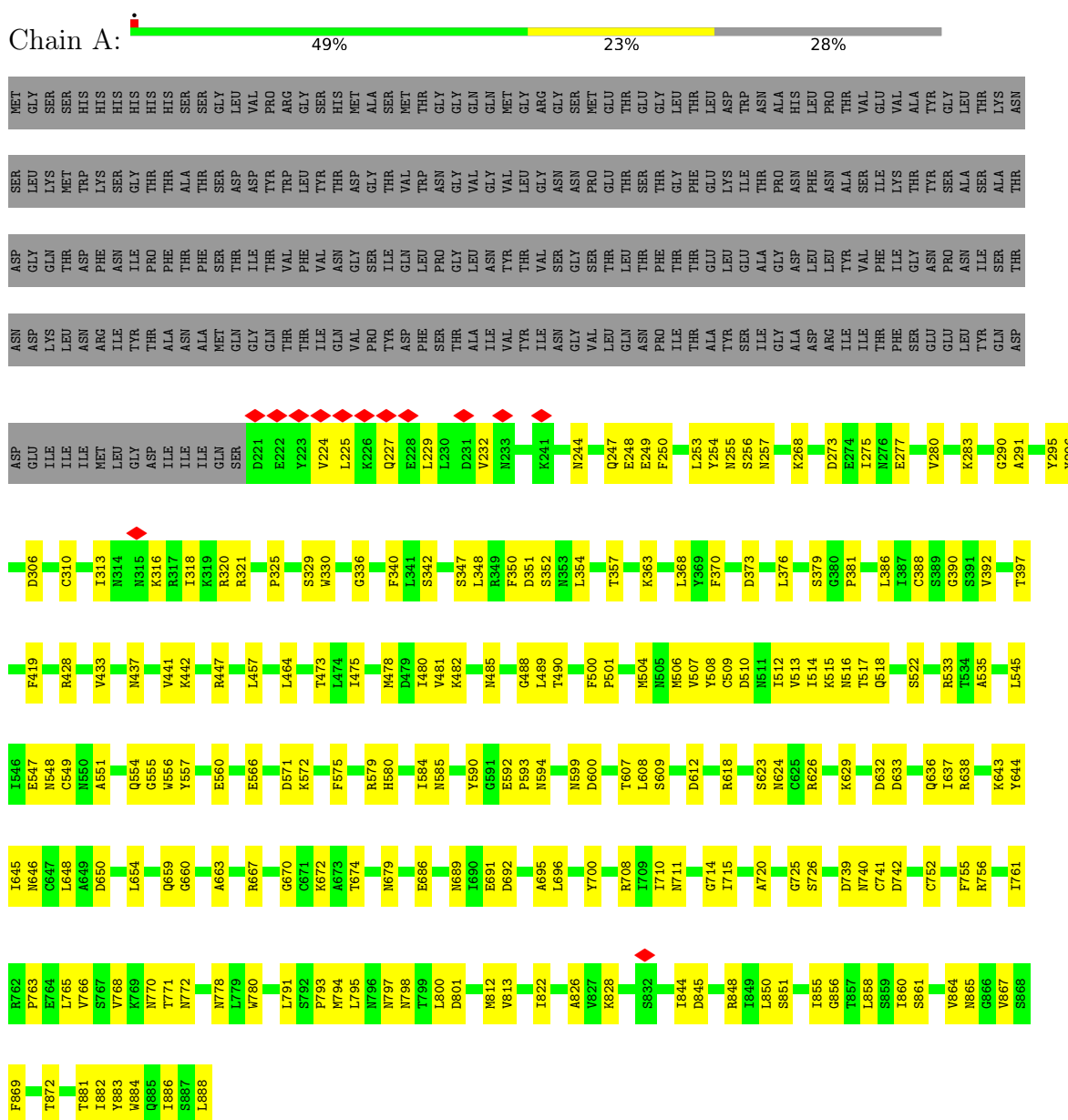
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A0A8J8T2
B	0	SER	-	expression tag	UNP A0A0A8J8T2
C	-33	MET	-	initiating methionine	UNP A0A0A8J8T2
C	-32	GLY	-	expression tag	UNP A0A0A8J8T2
C	-31	SER	-	expression tag	UNP A0A0A8J8T2
C	-30	SER	-	expression tag	UNP A0A0A8J8T2
C	-29	HIS	-	expression tag	UNP A0A0A8J8T2
C	-28	HIS	-	expression tag	UNP A0A0A8J8T2
C	-27	HIS	-	expression tag	UNP A0A0A8J8T2
C	-26	HIS	-	expression tag	UNP A0A0A8J8T2
C	-25	HIS	-	expression tag	UNP A0A0A8J8T2
C	-24	HIS	-	expression tag	UNP A0A0A8J8T2
C	-23	SER	-	expression tag	UNP A0A0A8J8T2
C	-22	SER	-	expression tag	UNP A0A0A8J8T2
C	-21	GLY	-	expression tag	UNP A0A0A8J8T2
C	-20	LEU	-	expression tag	UNP A0A0A8J8T2
C	-19	VAL	-	expression tag	UNP A0A0A8J8T2
C	-18	PRO	-	expression tag	UNP A0A0A8J8T2
C	-17	ARG	-	expression tag	UNP A0A0A8J8T2
C	-16	GLY	-	expression tag	UNP A0A0A8J8T2
C	-15	SER	-	expression tag	UNP A0A0A8J8T2
C	-14	HIS	-	expression tag	UNP A0A0A8J8T2
C	-13	MET	-	expression tag	UNP A0A0A8J8T2
C	-12	ALA	-	expression tag	UNP A0A0A8J8T2
C	-11	SER	-	expression tag	UNP A0A0A8J8T2
C	-10	MET	-	expression tag	UNP A0A0A8J8T2
C	-9	THR	-	expression tag	UNP A0A0A8J8T2
C	-8	GLY	-	expression tag	UNP A0A0A8J8T2
C	-7	GLY	-	expression tag	UNP A0A0A8J8T2
C	-6	GLN	-	expression tag	UNP A0A0A8J8T2
C	-5	GLN	-	expression tag	UNP A0A0A8J8T2
C	-4	MET	-	expression tag	UNP A0A0A8J8T2
C	-3	GLY	-	expression tag	UNP A0A0A8J8T2
C	-2	ARG	-	expression tag	UNP A0A0A8J8T2
C	-1	GLY	-	expression tag	UNP A0A0A8J8T2
C	0	SER	-	expression tag	UNP A0A0A8J8T2

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, capsule K1-specific



Chain B:



N796	Y702	D612	M504	F419	T303	ASP	ASN	ASP	SER
N797	A703	R618	M505	S420	D306	ILE	ASP	GLY	LEU
N798	M704	R618	M506	V421	D306	ILE	LYS	LYS	LYS
T799			V507	G422	C310	ILE	ASN	THR	MET
L800	R708	S623	V508	D423		ILE	ASP	TRP	LYS
D801	T709	M624	G509			MET	ARG	PHE	THR
	I710		M511	I427	K316	LEU	ILE	ASN	SER
S810	M711	D632	M511		R317	GLY	TYR	ILE	GLY
L815	G714	D633	F512	M437	I318	ASP	THR	PRO	THR
	I715		F513		K319	ILE	ALA	PHE	THR
K828	D716	Q636	M516	V441	R320	ILE	ASN	THR	ALA
		I637	T517			ILE	ALA	PHE	THR
D845	A720	R638	Q518	M446	P325	GLN	MET	SER	SER
				R447	A326	SER	GLN	THR	ASP
R848		Y644	S522	Q448	L327	ILE	GLY	THR	ASP
G725	S726	I645	S522	I449	S328	THR	GLN	TYR	ASP
T849		M646	T450	T450	S329	VAL	THR	VAL	TRP
L850	P730	G647	K525	K451	W330	THR	THR	PHE	LEU
		L648	R533	I452		Y224	ILE	VAL	LEU
T855		A649			G336		ASN	GLN	THR
G856	D739	R650	R537	Q456		L225	VAL	GLY	THR
T857	M740	Y651	K537	L457	F340	K226	PRO	ASP	MET
L858	G741		I538			Q227	TYR	ILE	SER
	D742	L654		K461	S347	E228	ASP	GLN	VAL
			R542		L348	L229	PHE	LEU	TRP
S861	S746	Q659	M548	L464	R349	Y230	SER	PRO	ASN
T872		G660		Y465	F350		THR	GLY	GLY
				D466	D351	L230	ALA	VAL	GLN
D878	Q749	A663	A551	F467		M233	ILE	ASN	GLN
T750	T750	T664			T357	A234	VAL	TYR	MET
R751	C752	M665	W556	T473			TYR	THR	GLY
L753	T666	R667	Y557	L474	N365	Y237	ILE	VAL	ARG
Y754			I475	I475	T366	I238	ASN	GLY	GLY
R755	F754	R67	E560	S476	N367	M239	GLY	ASN	SER
G885	R755	G670	F561	K477	L368	T240	VAL	SER	PRO
R756		C671	L562	M478	Y369	K241	LEU	THR	GLU
		K672		D479	F370		GLN	LEU	THR
S789			E566	I480			ASN	SER	GLU
G760	T761	M675		V481	D373	M244	PRO	PHE	GLY
L761			D571	K482		S245	ILE	THR	GLY
R763		R678	K572	M483	P378	I246	THR	THR	PHE
M764		M679		V484	S379	Q247	ALA	GLU	GLU
L765	V766	G680	F575	M485	G380	E248	TYR	LYS	ASP
		S682	D576	I486	P381	E249	SER	ILE	TRP
K769		L683	R579	D487	L386	L253	ILE	ALA	THR
L683		W684	H580	I489	F387	Y254	GLY	PRO	ALA
T770		W685		T490	C388	ASP	ALA	ASN	LYS
T771			I584	F491	S389	M257	ASP	PHE	THR
M772			W586		G390		ARG	ASN	PRO
M773	A774	D692	W586	I494		D273	ILE	TYR	ALA
			E691	M495	T397		ILE	VAL	THR
W780		D692	N594	Y496	T398	V280	THR	PHE	GLU
				T497	T399	C281	PHE	ILE	VAL
Y781			M599	T498	L400	G282	SER	GLY	VAL
		A695	D600	L499		K283	GLU	THR	ALA
L791		M697		F500	N412		ASN	PRO	TYR
S792			L608	P501		G290	LEU	GLY	GLY
T793						A291	ASN	ALA	THR
M794		Y700	S609	T502	D415		TYR	ILE	SER
L795		T723		S523			GLN	THR	LYS
							ASN	SER	THR

Chain C:

[illegible]

ASP	GLU	ILE	ILE	ILE	MET	LEU	GLY	ASP	ILE	ILE	ILE	GLN	SER	D221	E222	Y223	V224	L225	K226	Q227	E228	L229	L230	D231	V232	N233	S236	Y237	L238	N239	T240	K241	N244	S245	I246	Q247	E248	E249	F250	L253	Y254	N255	S256	N257	E277	V280	N286	G290	A291	Y296										
														T303	V304	E305	D306	F311	K316	R317	R320	R321	W330	G336	L341	S342	T343	G344	N345	V346	R349	F350	L354	T355	L356	I362	K363	N367	F370	N371	V374	F375	L376	P381	G385	L386	I387	C388	S389	G390	T397	V404	E430	K431	L432	V433				
														N437	V441	K442	L445	M446	R447	I462	F467	L474	V481	V484	N485	I486	D487	G488	L489	T490	F491	N492	N493	P501	M504	N505	M506	V507	Y508	I512	K515	N516	T517	Q518	L519	S522	R533	T534	A535	L545	I546	E547	N548	C549	H550	A551	Y552	H553		
														Q554	G555	W556	Y557	E566	D571	K572	C573	F574	F575	R579	H580	I584	N585	Y590	G591	E592	P593	N594	N599	D600	C601	L608	S609	D612	T613	H614	D615	I616	G617	R618	S623	N624	D632	D633	Q636	I637	R638	K643	Y644	I645	N646	C647	L648	A649	D650	L654
														G660	A663	R667	G670	C671	K672	A673	T674	N675	L683	N689	I690	E691	D692	A695	L696	T697	L700	M704	R708	I709	I710	N711	G714	I715	D716	A720	G725	P730	D739	N740	C741	D742	Q749	T750	R751	C752	L753	Y754	F755	S759	G760	I761				
														P763	V766	S767	V768	R769	N770	N771	N772	W780	Y781	L791	S792	P793	N794	L795	N796	N797	N798	T799	L800	D801	S810	G811	A826	W827	K828	L829	V841	R848	I849	L850	I855	G856	T857	L858	S861	N862	I863	T872	S880	T881	I882	Q885	I886	S887	L888	
														T303	V304	E305	D306	F311	K316	R317	R320	R321	W330	G336	L341	S342	T343	G344	N345	V346	R349	F350	L354	T355	L356	I362	K363	N367	F370	N371	V374	F375	L376	P381	G385	L386	I387	C388	S389	G390	T397	V404	E430	K431	L432	V433				
														N437	V441	K442	L445	M446	R447	I462	F467	L474	V481	V484	N485	I486	D487	G488	L489	T490	F491	N492	N493	P501	M504	N505	M506	V507	Y508	I512	K515	N516	T517	Q518	L519	S522	R533	T534	A535	L545	I546	E547	N548	C549	H550	A551	Y552	H553		
														Q554	G555	W556	Y557	E566	D571	K572	C573	F574	F575	R579	H580	I584	N585	Y590	G591	E592	P593	N594	N599	D600	C601	L608	S609	D612	T613	H614	D615	I616	G617	R618	S623	N624	D632	D633	Q636	I637	R638	K643	Y644	I645	N646	C647	L648	A649	D650	L654
														G660	A663	R667	G670	C671	K672	A673	T674	N675	L683	N689	I690	E691	D692	A695	L696	T697	L700	M704	R708	I709	I710	N711	G714	I715	D716	A720	G725	P730	D739	N740	C741	D742	Q749	T750	R751	C752	L753	Y754	F755	S759	G760	I761				
P763	V766	S767	V768	R769	N770	N771	N772	W780	Y781	L791	S792	P793	N794	L795	N796	N797	N798	T799	L800	D801	S810	G811	A826	W827	K828	L829	V841	R848	I849	L850	I855	G856	T857	L858	S861	N862	I863	T872	S880	T881	I882	Q885	I886	S887	L888															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4015926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.984	Depositor
Minimum map value	-1.935	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.51	0/5235	0.78	0/7109
1	B	0.49	0/5235	0.79	2/7109 (0.0%)
1	C	0.50	0/5235	0.76	0/7109
All	All	0.50	0/15705	0.78	2/21327 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	585	ASN	N-CA-C	6.65	119.31	110.53
1	B	503	THR	N-CA-C	5.28	116.84	111.14

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	5149	0	5016	171	0
1	B	5149	0	5016	180	0
1	C	5149	0	5016	161	0
All	All	15447	0	15048	484	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 16.

The worst 5 of 484 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:O	1:A:579:ARG:HB3	1.65	0.96
1:C:556:TRP:O	1:C:579:ARG:HB3	1.69	0.93
1:B:556:TRP:O	1:B:579:ARG:HB3	1.70	0.91
1:A:851:SER:HB3	1:A:855:ILE:HD11	1.56	0.88
1:B:501:PRO:O	1:B:533:ARG:HA	1.74	0.86

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	666/922 (72%)	641 (96%)	25 (4%)	0	100	100
1	B	666/922 (72%)	638 (96%)	28 (4%)	0	100	100
1	C	666/922 (72%)	643 (96%)	23 (4%)	0	100	100
All	All	1998/2766 (72%)	1922 (96%)	76 (4%)	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	588/804 (73%)	588 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	588/804 (73%)	584 (99%)	4 (1%)	76	81
1	C	588/804 (73%)	587 (100%)	1 (0%)	87	92
All	All	1764/2412 (73%)	1759 (100%)	5 (0%)	84	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	498	THR
1	B	503	THR
1	B	509	CYS
1	B	726	SER
1	C	552	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	699	GLN
1	C	689	ASN
1	C	371	ASN
1	C	619	ASN
1	C	823	ASN

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.

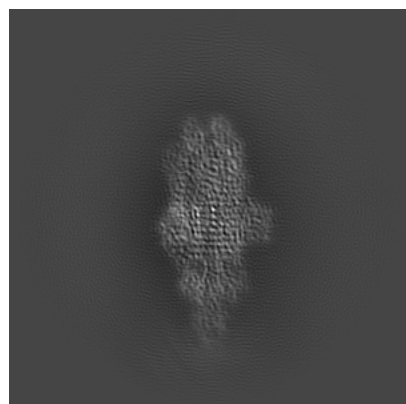
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62051. These allow visual inspection of the internal detail of the map and identification of artifacts.

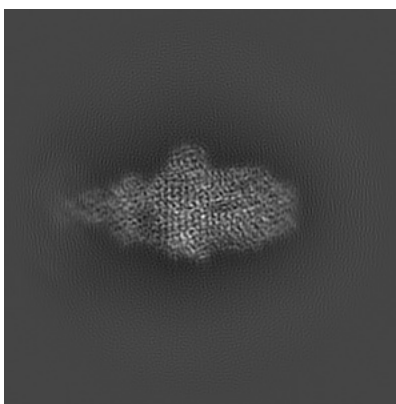
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

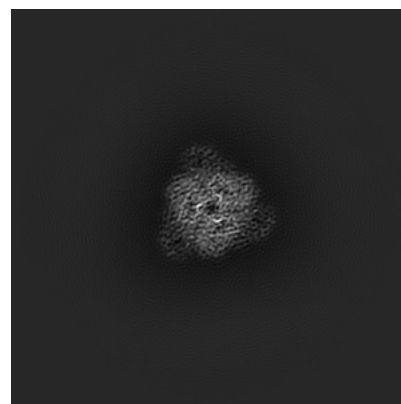
6.1.1 Primary map



X

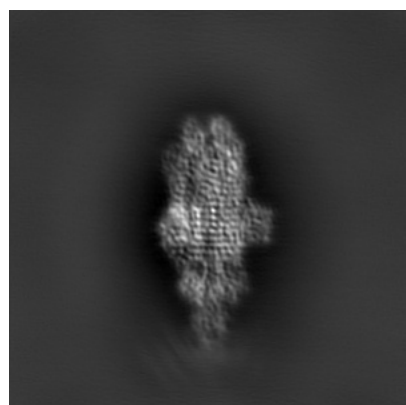


Y

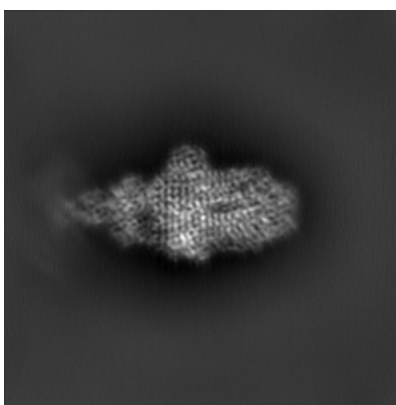


Z

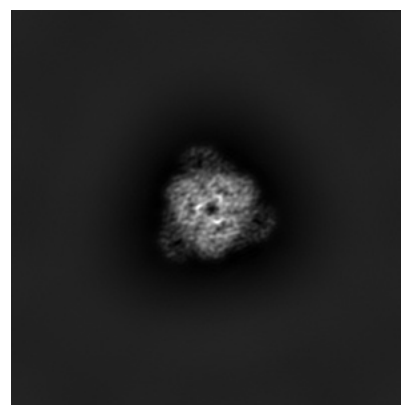
6.1.2 Raw map



X



Y

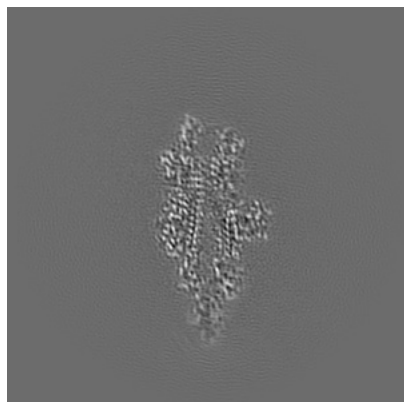


Z

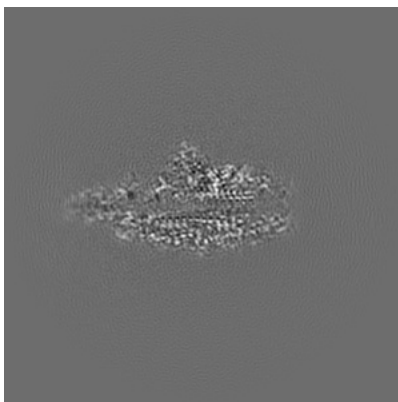
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

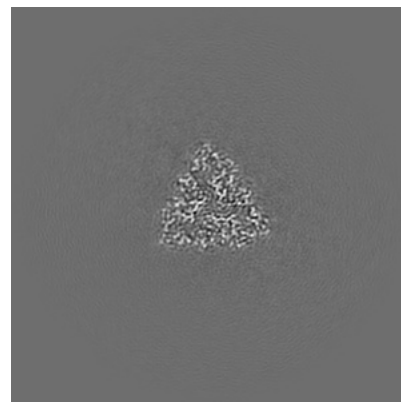
6.2.1 Primary map



X Index: 128

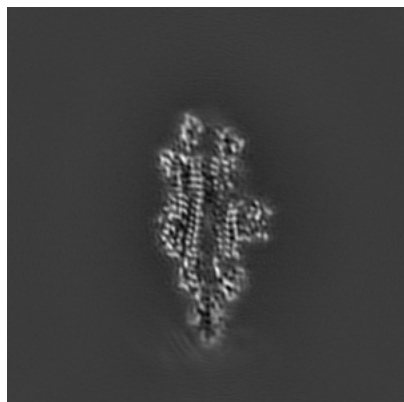


Y Index: 128

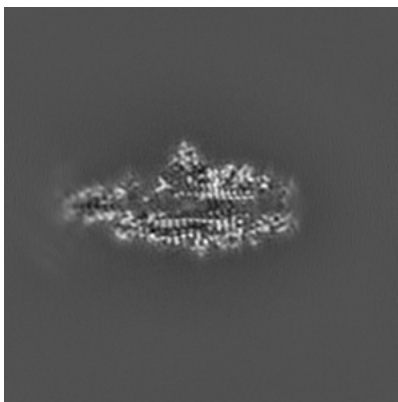


Z Index: 128

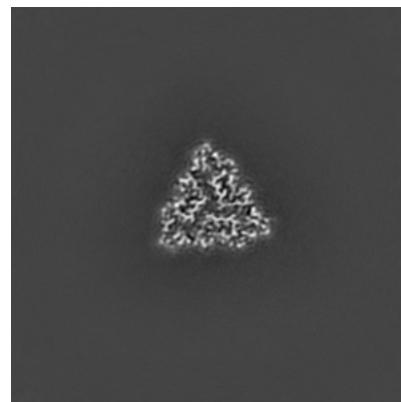
6.2.2 Raw map



X Index: 128



Y Index: 128

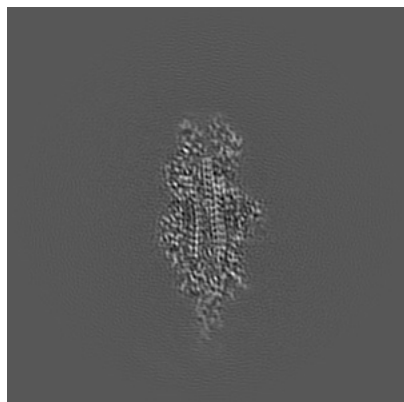


Z Index: 128

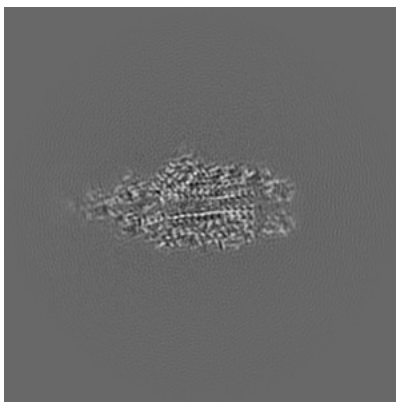
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

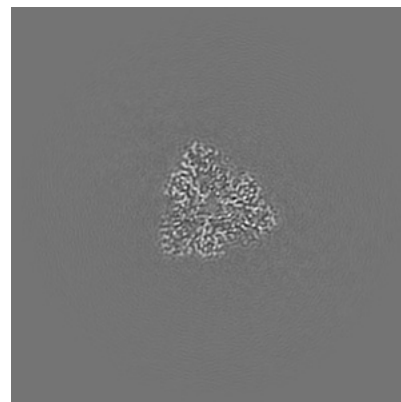
6.3.1 Primary map



X Index: 134



Y Index: 132

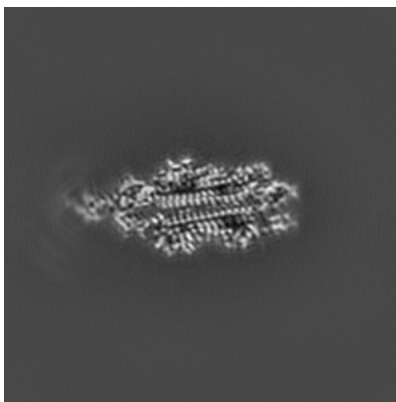


Z Index: 118

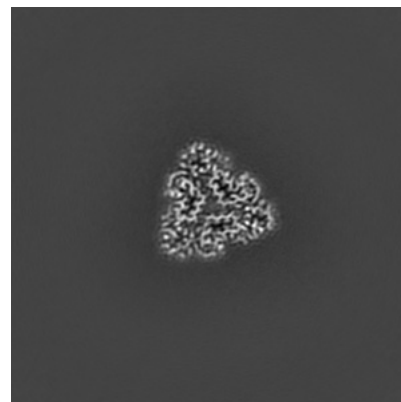
6.3.2 Raw map



X Index: 133



Y Index: 136

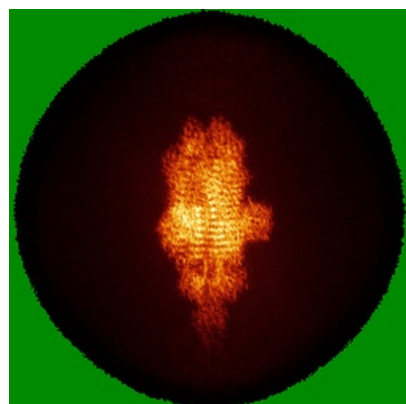


Z Index: 119

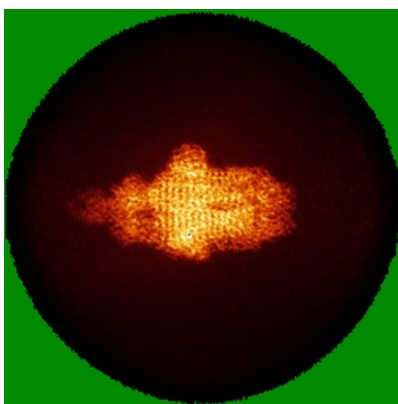
The images above show the largest variance slices of the map in three orthogonal directions.

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

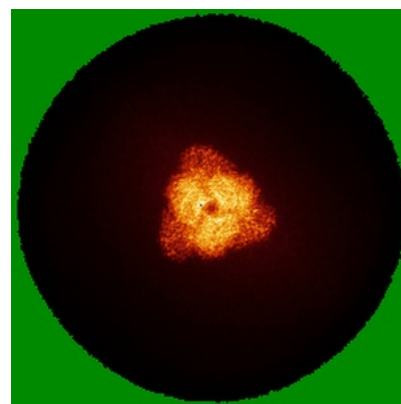
6.4.1 Primary map



X



Y

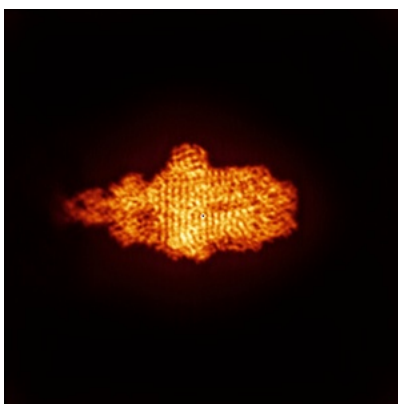


Z

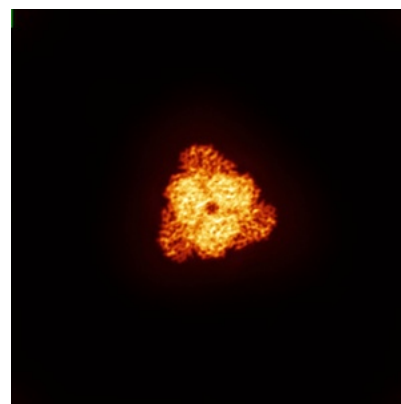
6.4.2 Raw map



X



Y

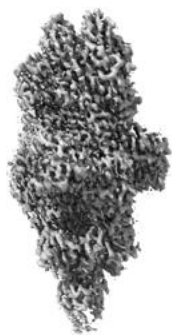


Z

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](#)

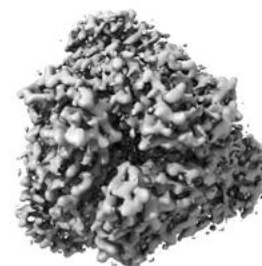
6.5.1 Primary map



X



Y



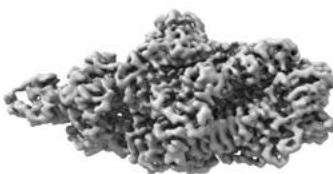
Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. 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



X



Y



Z

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.

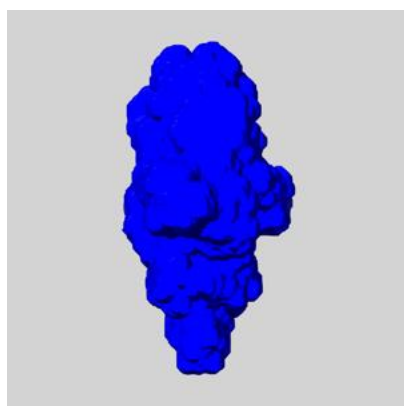
6.6 Mask visualisation [i](#)

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

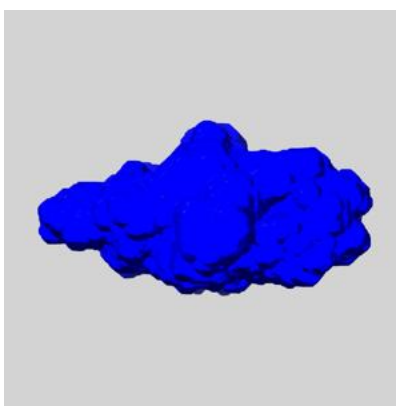
A mask typically either:

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

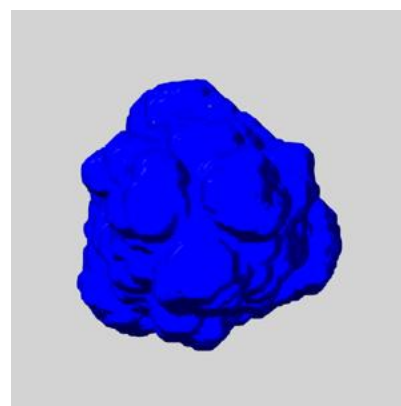
6.6.1 emd_62051_msk_1.map [i](#)



X



Y

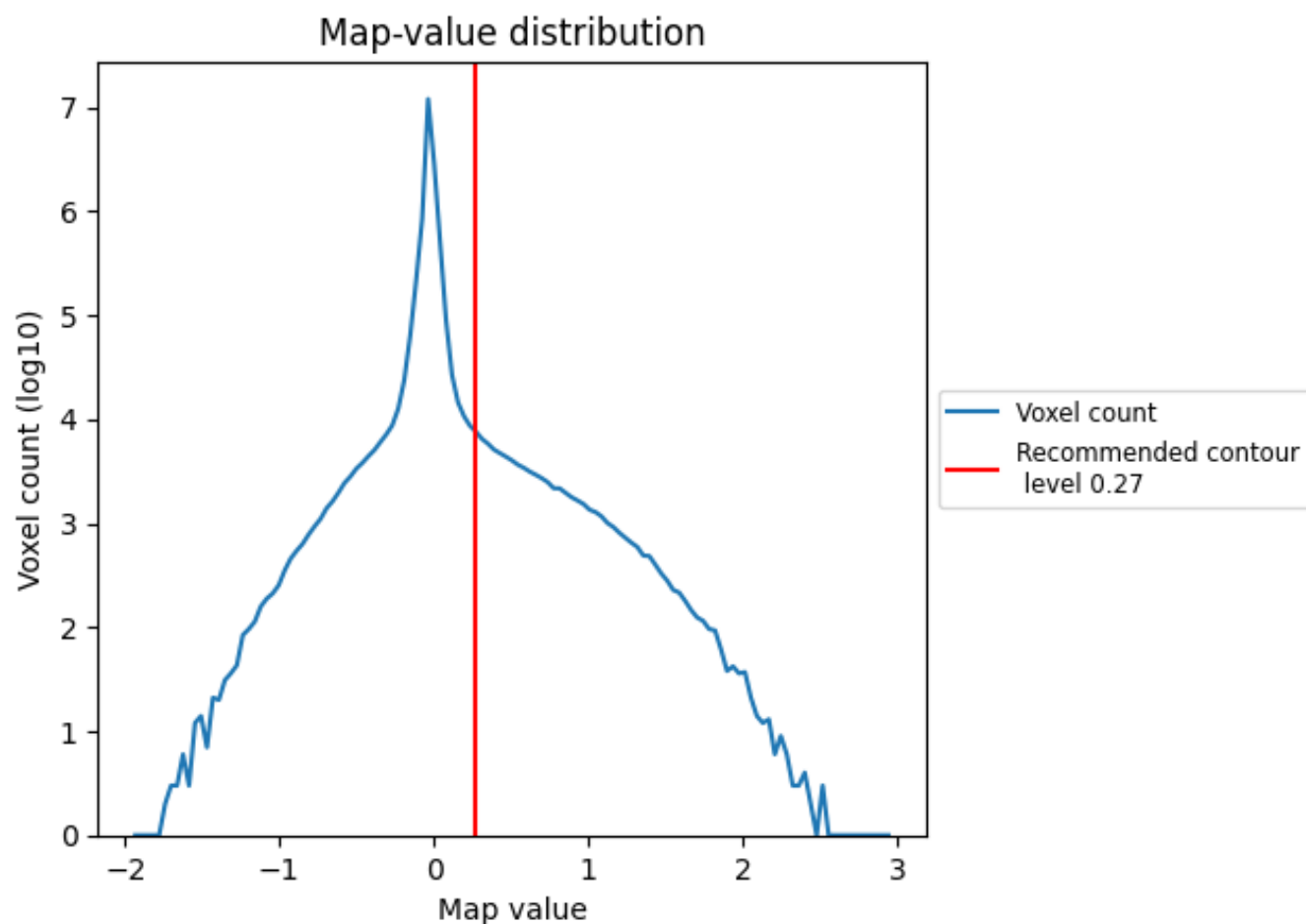


Z

7 Map analysis [i](#)

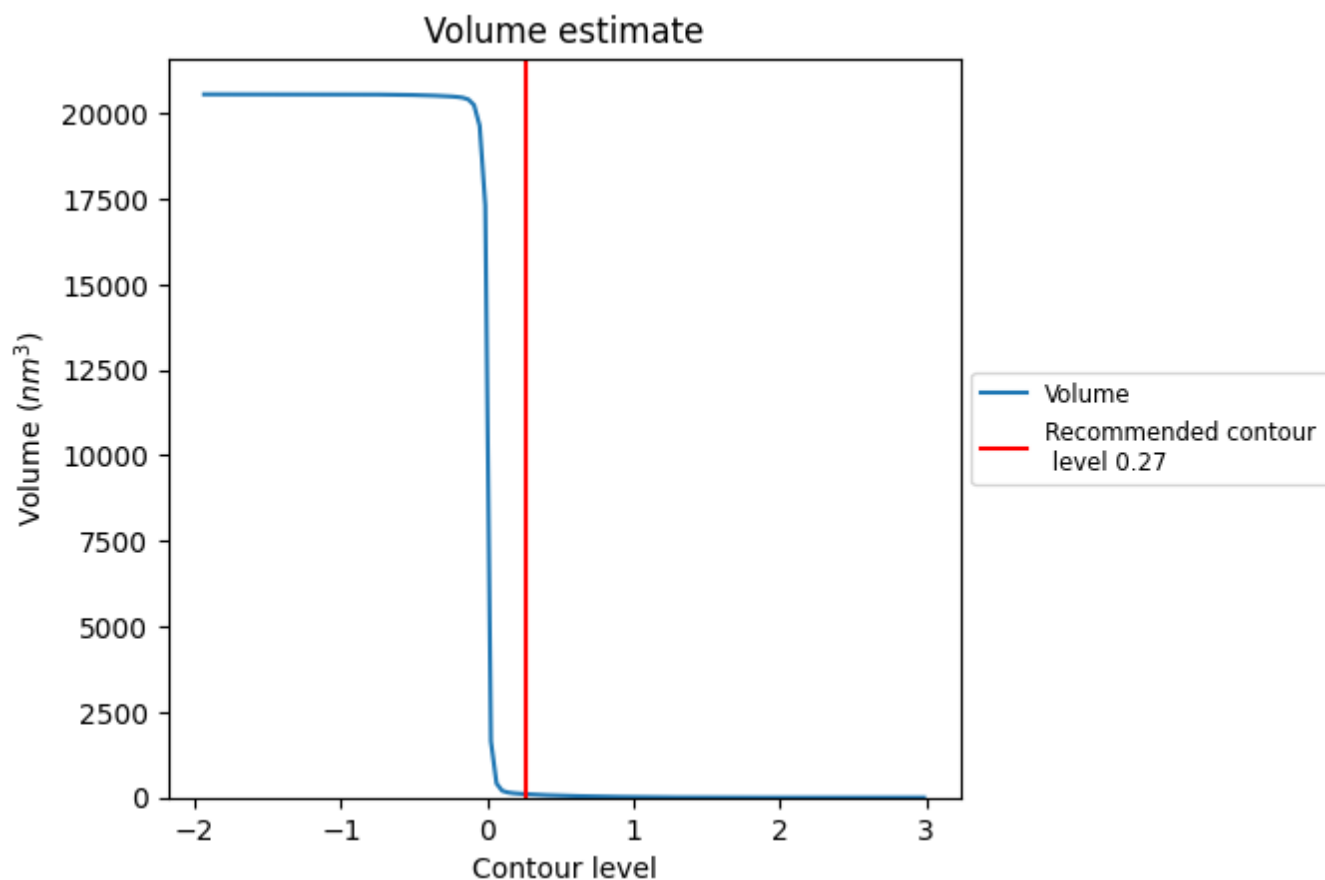
This section contains the results of statistical analysis of the map.

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.

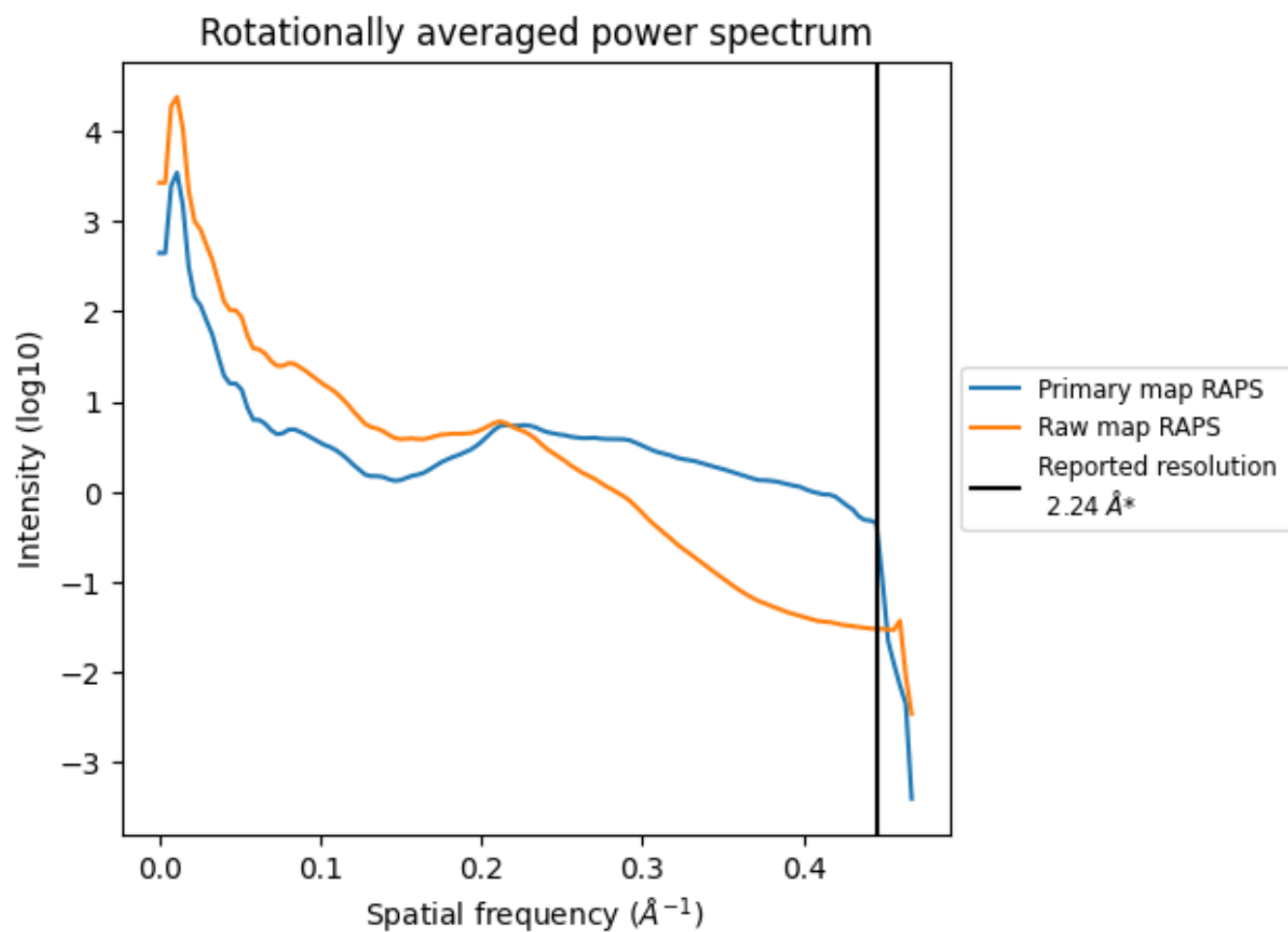
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm^3 ; this corresponds to an approximate mass of 89 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 ⓘ

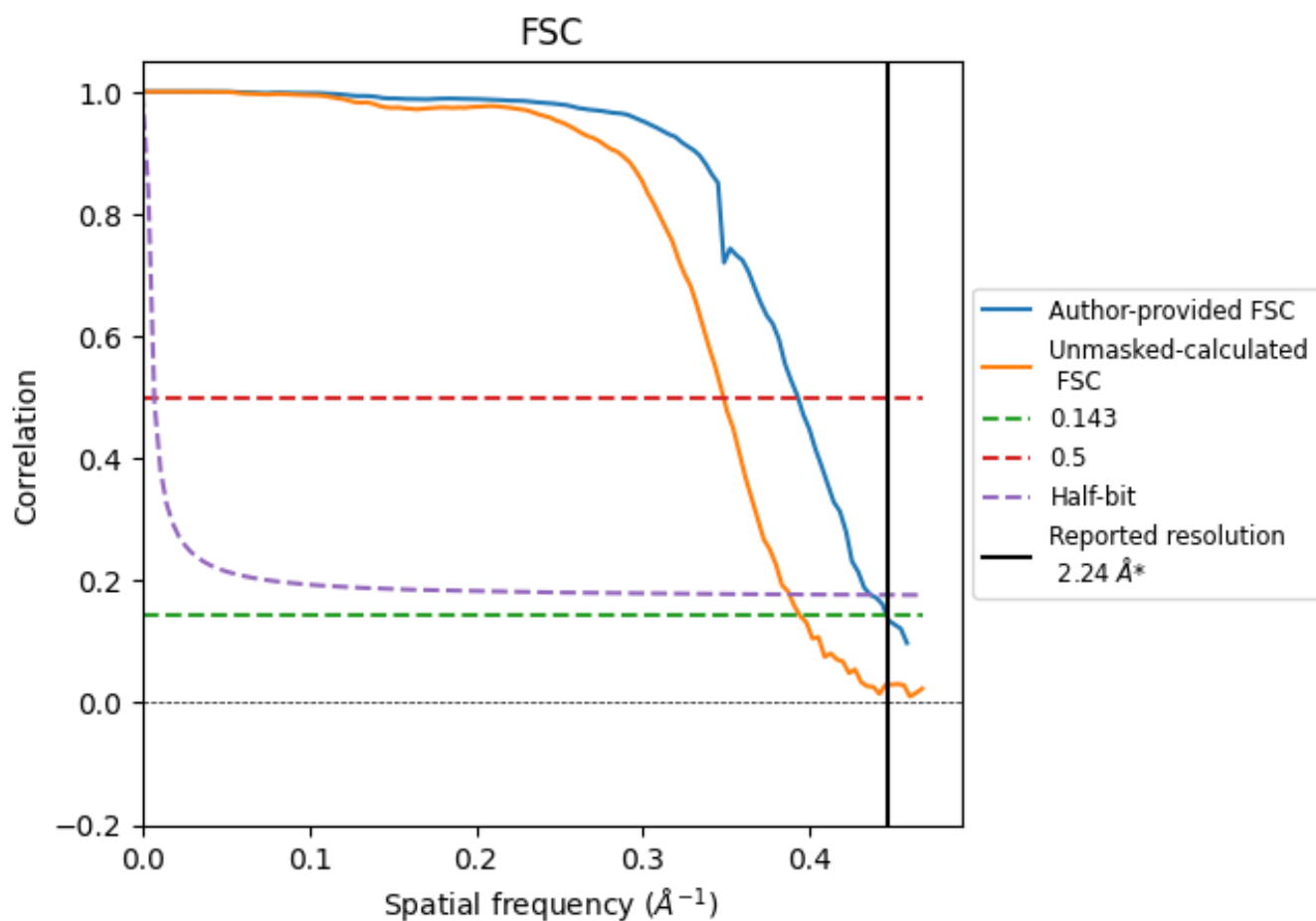


*Reported resolution corresponds to spatial frequency of 0.446 Å⁻¹

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 0.446 \AA^{-1}

8.2 Resolution estimates [i](#)

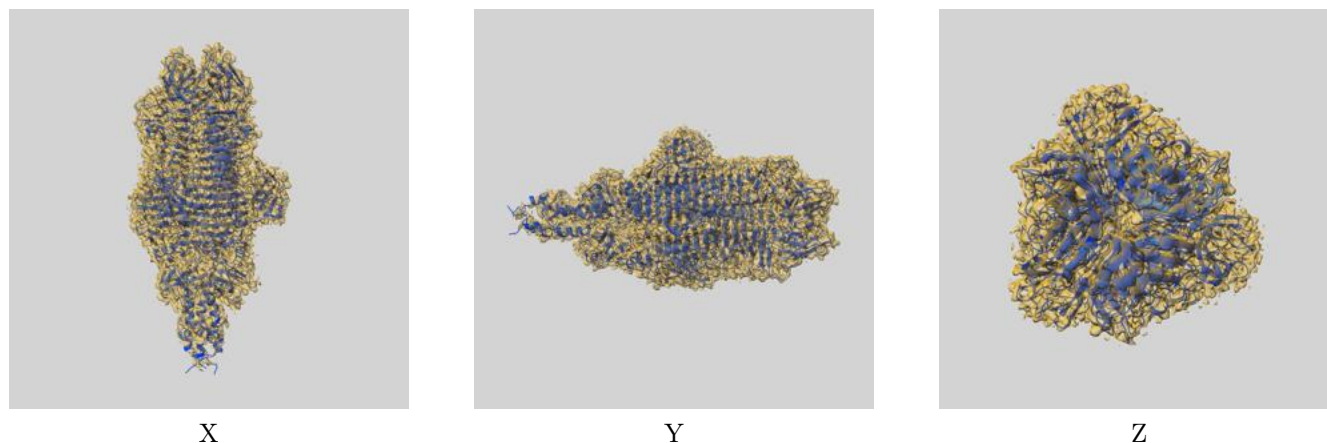
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.55	2.29
Unmasked-calculated*	2.54	2.87	2.58

*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 2.54 differs from the reported value 2.24 by more than 10 %

9 Map-model fit [i](#)

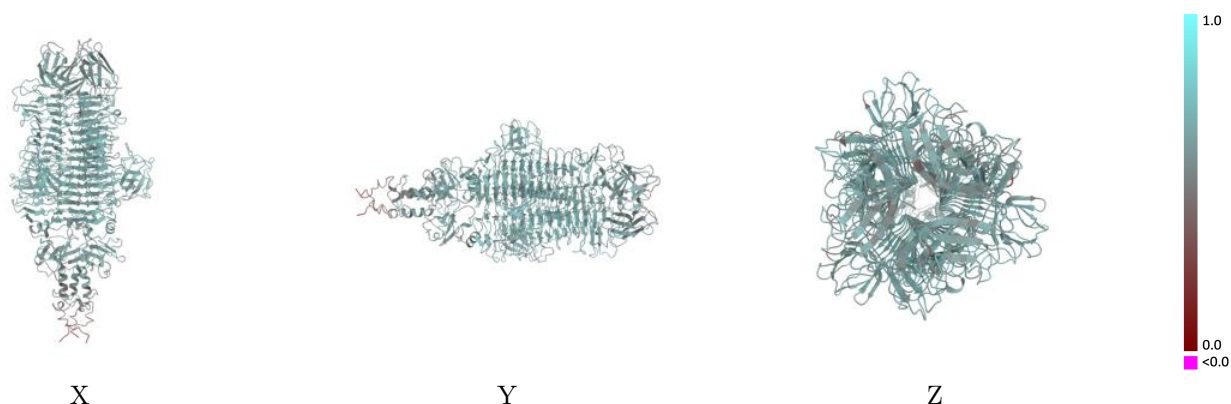
This section contains information regarding the fit between EMDB map EMD-62051 and PDB model 9K4A. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



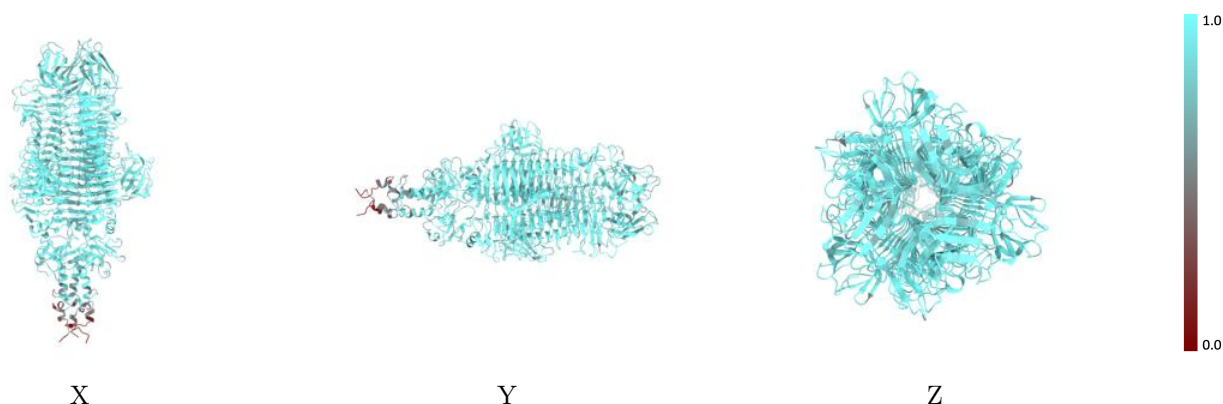
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



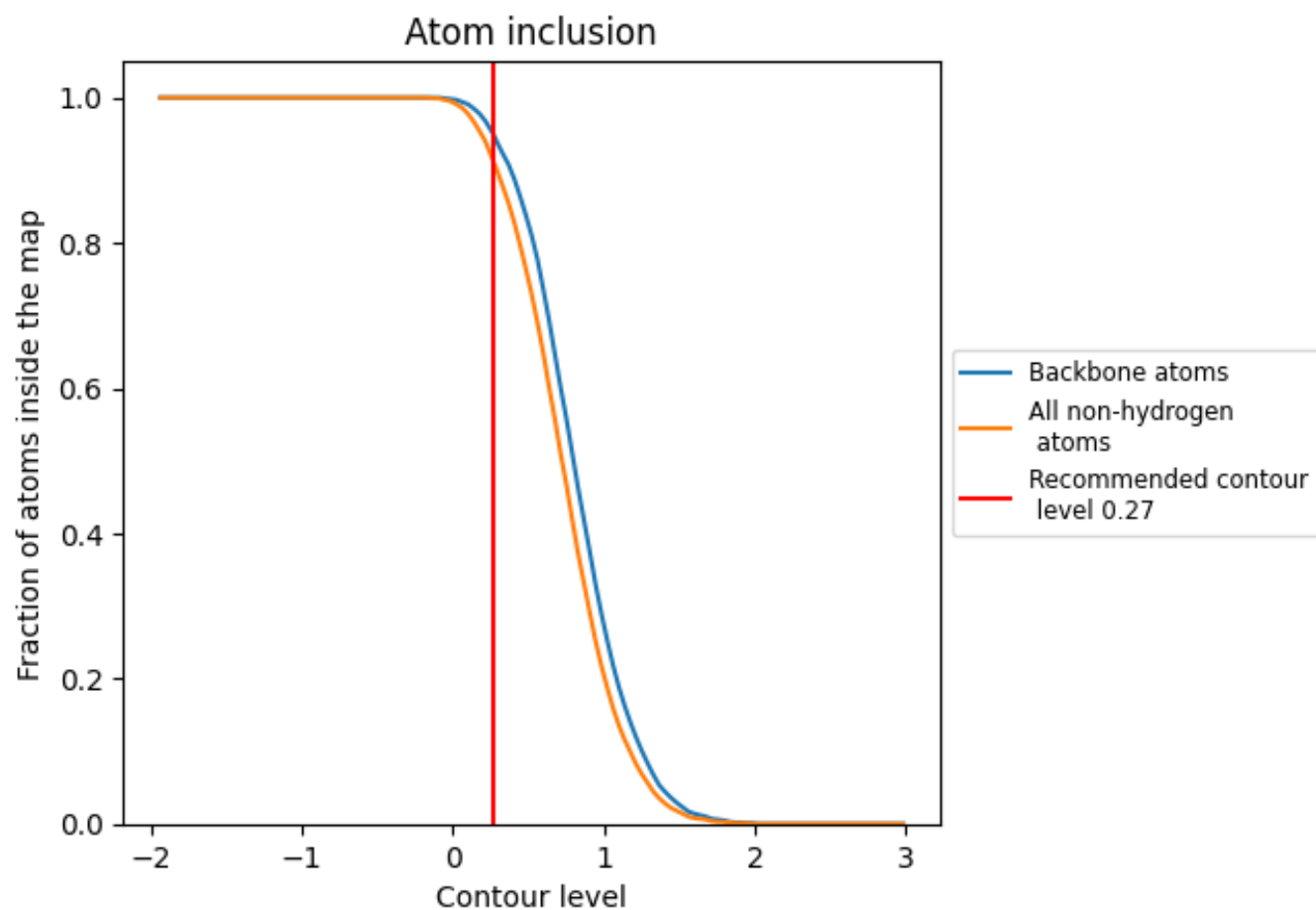
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9130	<div></div> 0.6110
A	<div></div> 0.9140	<div></div> 0.6080
B	<div></div> 0.9080	<div></div> 0.6080
C	<div></div> 0.9160	<div></div> 0.6190

