



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:06 AM UTC

PDB ID : 7K19 / pdb_00007k19
EMDB ID : EMD-22622
Title : CryoEM structure of DNA-PK catalytic subunit complexed with DNA (Complex I)
Authors : Chen, X.; Gellert, M.; Yang, W.
Deposited on : 2020-09-07
Resolution : 4.30 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

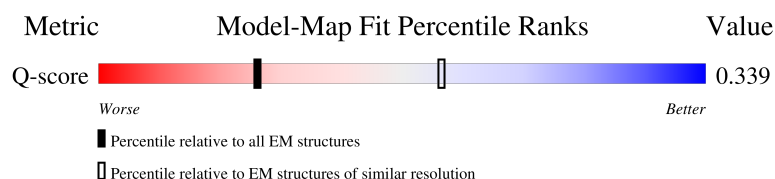
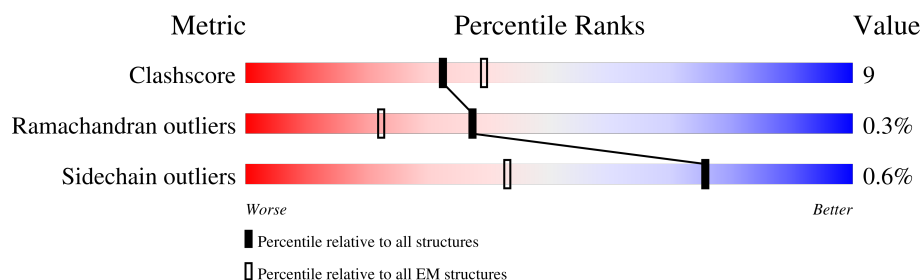
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	4128	
2	D	24	
2	F	24	
3	G	16	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29158 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3569	Total	C	N	O	S	0	0
			28180	18091	4776	5128	185		

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	24	Total	C	N	O	P	0	0
			484	233	82	146	23		
2	F	8	Total	C	N	O	P	0	0
			164	78	30	48	8		

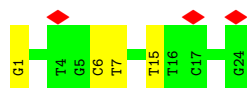
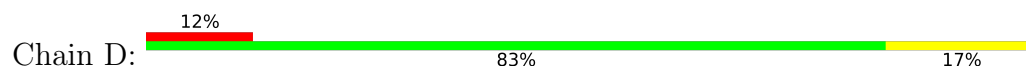
- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	16	Total	C	N	O	P	0	0
			330	157	68	90	15		

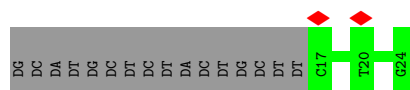
L2545	Y2546	S2547	P2548	S2567	MET	SER	PRO	ASP	TYR	PRO	ASN	PRO	MET	PHE	GLU	HIS	PRO	PRO	LEU	SER	GLU	CYS	GLU	PHE	GLN	GLU	TYR	THR	ILE	ASP	SER	ASP	TRP	ARG	PHE	ARG	SER	THR	VAL	LEU	THR	PRO	PHE	VAL	GLU	THR	GLN	ALA	SER	GLN	GLY	GLY	THR	LEU	GLN	THR	ARG	THR	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
D2428	Q2432	C2435	K2441	M2442	L2446	K2447	P2448	V2458	V2459	E2460	H2464	P2465	S2466	T2467	C2469	R2470	E2471	N2475	L2476	L2477	I2480	Y2484	E2488	T2491	D2492	N2493	V2494	S2495	Q2496	E2497	K2500	I2507	H2527	E2528	T2529	R2530	L2531	R2538	L2539	L2540	A2541	L2542																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L2237	I2238	L2241	Y2253	R2254	F2257	E2258	S2261	D2264	P2265	N2266	G2278	A2282	L2285	P2290	G2293	L2294	Q2295	V2315	A2319	L2323	L2327	V2330	L2341	L2344	F2383	F2384	L2385	C2403	R2404	L2415	K2418	F2420	M2424	R2425																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					</

H4068	M3932	V3794	I3662	Q3577	A3441	MET	Q3123	D2980	S2856	HIS	GLU
A4071	I3938	P3795	K3672	P3581	P3346	GLU	S3124	G2984	L2871	LYS	GLY
F4074	D3941	T3797	D3673	F3584	L3348	VAL	R3125	E2985	D2872	ARG	SER
R4075	Q3951	S3798	P3676	F3585	L3445	GLU	L3129	P2986	A2875	GLY	LEU
D4076	P3954	R3799	G3678	K3586	V3446	GLN	T3136	K2991	Q2885	ARG	ALA
V4077	P3954	L3800	N3677	N3587	N3450	GLU	Q3139	D2992	P2887	LEU	TRP
R4082	E3957	T3803	C3683	W3588	R3462	GLU	E3140	E2995	Q2886	ALA	ALA
N4088	L3958	E3804	L3463	N3589	L3463	GLU	K3147	L2999	P2887	VAL	ALA
I4089	P3960	N3809	F3465	D3591	K3464	GLN	N3150	L3011	I2890	GLY	GLY
Q4092	F3961	V3810	P3466	R3593	P3466	SER	N3162	L3011	R2899	LYS	ILE
E4101	R3962	M3820	R3467	A3594	R3467	GLY	N3163	L3011	R2899	VAL	ARG
T4102	L3963	K3825	L3468	T3599	L3468	SER	K3248	Y3013	R2899	GLY	ALA
Q4103	R3965	N3830	L3470	P3600	Q3470	SER	K3164	A3017	LEU	PRO	THR
D4109	S3982	S3830	I3471	N3601	I3471	GLU	N3165	P3024	ALA	PHE	GLN
P4114	H3986	E3838	I3472	N3602	I3472	R3380	K3166	P3025	GLY	GLY	GLN
E4125	A3987	N3846	R3473	N3602	R3473	R3381	R3167	P3026	LEU	LYS	HIS
M4128	L3988	M3846	Y3475	M3609	Y3475	F3382	D3170	L3027	PRO	LYS	ASP
	R3992	K3849	P3476	M3609	P3476	F3382	K3172	N3028	ARG	LYS	THR
	V4004	H3850	D3706	L3617	D3706	A3391	K3172	ASP	VAL	GLY	LEU
D4012	M3858	H3850	G3707	G3618	L3480	ALA	P3175	W3031	ARG	PRO	THR
K4019	Y3859	D3851	R3708	D3619	M3483	GLU	M3176	G3043	ARG	GLN	GLN
K4022	K3860	D3851	G3709	P3620	K3489	GLU	N3177	VAL	VAL	ASP	ALA
K4023	V3868	P3711	K3710	F3620	S3497	GLN	I3178	S3047	ALA	GLY	ASP
S4026	R3872	D3723	K3711	G3624	S3497	PRO	K3179	K3048	ARG	GLY	GLY
W4027	R3873	E3724	G3624	L3625	M3502	PRO	D3180	L3049	LEU	ARG	ARG
I4028	R3874	R3725	L3625	F3628	L3505	TRP	D3181	Q3054	PRO	LYS	SER
Q4029	S3875	V3728	F3628	R3629	R3506	SER	N3185	L3061	D2919	LYS	PHE
R4030	S3876	M3729	R3629	R3630	Q3510	CYS	F3189	R2022	R2022	GLY	ASP
I4031	K3877	A3730	K3630	K3631	G3261	GLY	K3192	E2925	E2925	ALA	LEU
N4032	V3878	L3732	F3632	F3633	R3282	PRO	T3198	R2031	R2031	GLY	THR
V4033	L3882	R3741	T3635	F3636	L3283	ASP	PRO	D2937	D2937	ILE	ASP
K4036	R3885	R3746	F3640	F3641	R3287	LEU	LEU	Y3090	Y3090	GLN	THR
N4037	V3888	L3751	D3641	K3642	Q3291	GLU	ASP	L3091	L3091	ILE	ASP
R4041	V3888	V3752	K3642	H3643	G3292	ASN	ASN	L3092	L3092	ARG	LEU
C4045	L3898	K3753	H3643	G3644	Q3296	SER	MET	D3094	D3094	ARG	VAL
L4051	S3914	G3754	T3547	D3544	K3296	ASN	ASN	V3096	V3096	ARG	HIS
H3915	H3915	M3771	G3645	G3646	N3310	VAL	VAL	S2955	S2955	ARG	THR
W3916	W3916	K3647	G3646	G3647	N3311	ASP	ASP	A2956	A2956	PHE	SER
L3917	L3917	K3650	K3647	K3647	V3312	ASP	GLN	L2957	L2957	MET	PRO
L3918	L3918	L3651	N3551	N3551	S3313	ASP	GLY	R2862	R2862	ASP	SER
V3930	V3930	M3654	R3557	R3557	S3314	ASP	ASP	Q2971	Q2971	GLN	ASP
A3931	A3931	K3655	Q3564	Q3564	L3329	GLY	GLY	Y2972	Y2972	LYS	SER
		L3656	F3659	F3659	T3332	PRO	PRO	D2973	D2973	LEU	LEU
					T3333	SER	ASP	N2877	N2877	SER	PHE
					Q3440	LEU	ARG	T2846	T2846	LEU	ALA

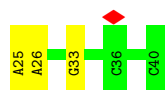
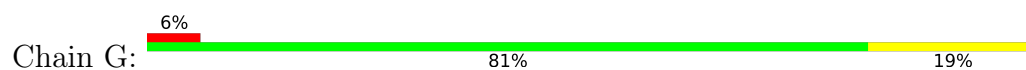
- Molecule 2: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3')



- Molecule 2: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3')



- Molecule 3: DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*AP*TP*GP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62117	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 ($e^-/\text{\AA}^2$)	45	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	0.059	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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	0.29	0/28742	0.65	20/38884 (0.1%)
2	D	0.30	0/540	0.58	0/831
2	F	0.28	0/183	0.49	0/280
3	G	0.31	0/372	0.58	0/573
All	All	0.29	0/29837	0.65	20/40568 (0.0%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3311	ASN	N-CA-C	-22.78	82.19	112.03
1	A	1469	PRO	N-CA-C	-11.82	88.12	112.47
1	A	4033	VAL	N-CA-C	-7.62	105.88	113.20
1	A	1019	ASP	CA-C-N	7.41	129.10	119.84
1	A	1019	ASP	C-N-CA	7.41	129.10	119.84

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	28180	0	28380	493	0
2	D	484	0	274	3	0
2	F	164	0	91	0	0
3	G	330	0	180	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29158	0	28925	495	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 9.

The worst 5 of 495 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:1687:HIS:CE1	1:A:1688:LEU:HD12	1.75	1.22
1:A:1687:HIS:CE1	1:A:1688:LEU:CD1	2.33	1.11
1:A:1687:HIS:ND1	1:A:1688:LEU:HD12	1.73	1.02
1:A:3647:GLY:O	1:A:3651:LEU:HB2	1.70	0.92
1:A:2467:THR:O	1:A:2471:GLU:HB2	1.77	0.84

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	3527/4128 (85%)	3067 (87%)	449 (13%)	11 (0%)	36	71

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1020	PRO
1	A	399	GLN
1	A	1992	VAL
1	A	2183	HIS
1	A	2467	THR

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	3094/3671 (84%)	3074 (99%)	20 (1%)	78 80

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2944	THR
1	A	3601	VAL
1	A	4033	VAL
1	A	3918	LEU
1	A	870	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2481	HIS
1	A	3944	HIS
1	A	3093	GLN
1	A	3924	HIS
1	A	3660	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

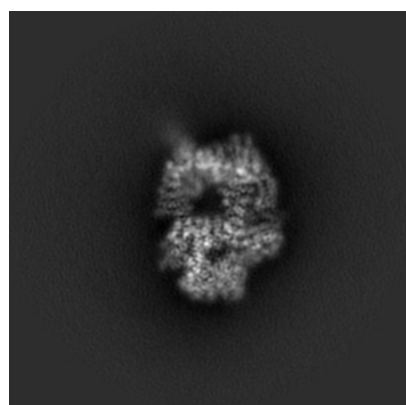
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22622. These allow visual inspection of the internal detail of the map and identification of artifacts.

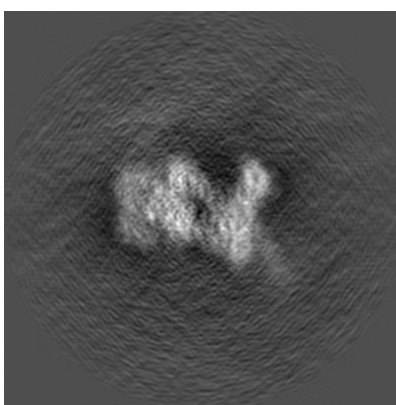
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

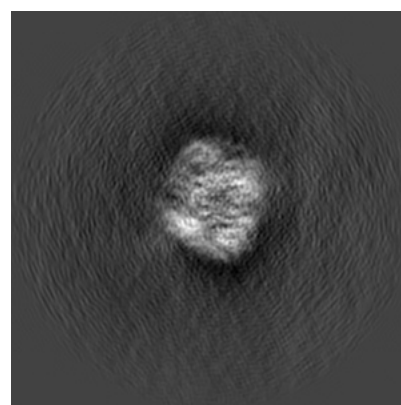
6.1.1 Primary map



X



Y

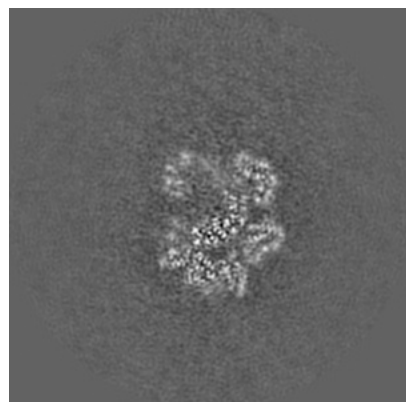


Z

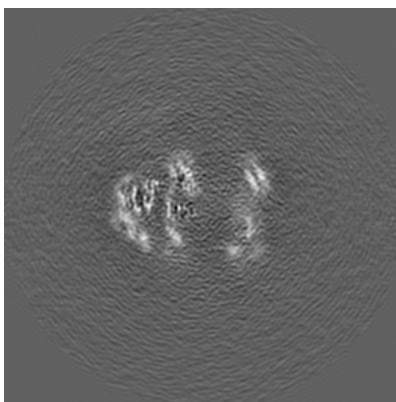
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

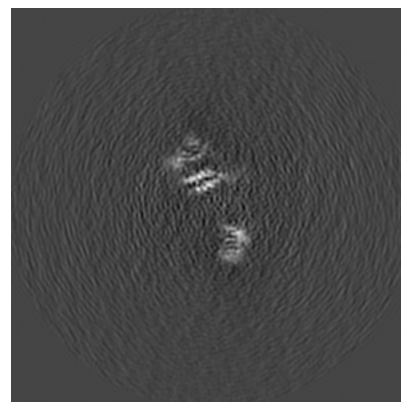
6.2.1 Primary map



X Index: 176



Y Index: 176

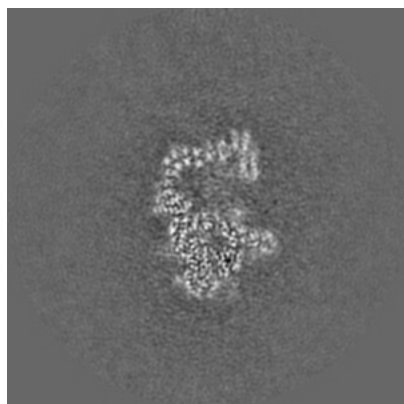


Z Index: 176

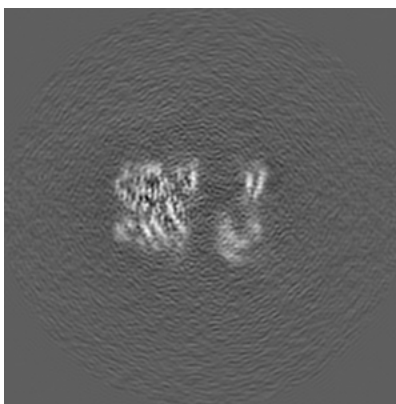
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

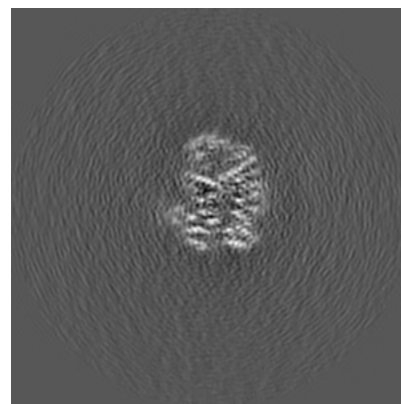
6.3.1 Primary map



X Index: 193



Y Index: 166

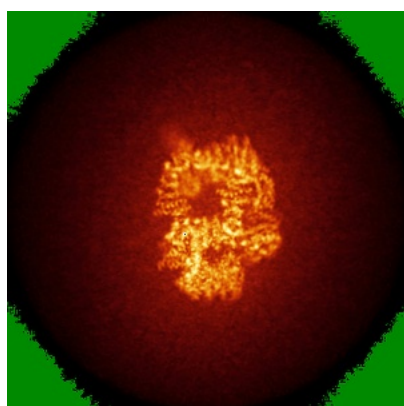


Z Index: 155

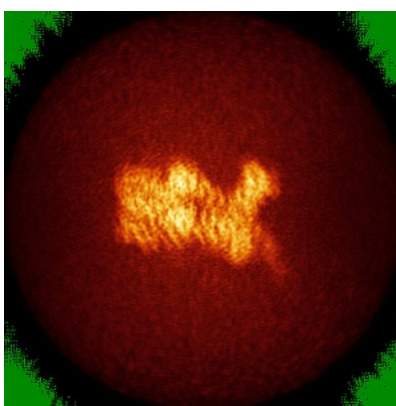
The images above show the largest variance slices of the map in three orthogonal directions.

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

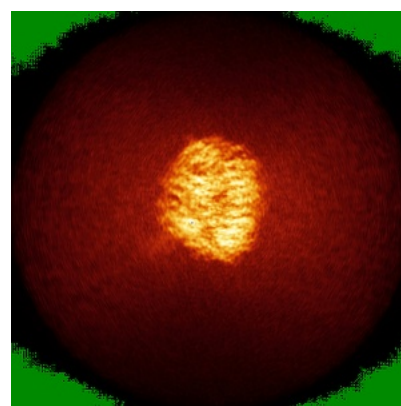
6.4.1 Primary map



X



Y

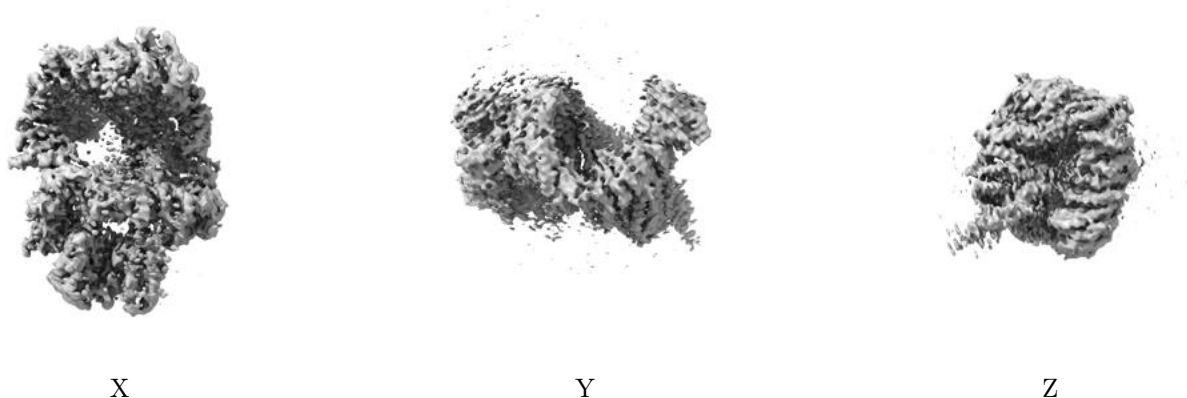


Z

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

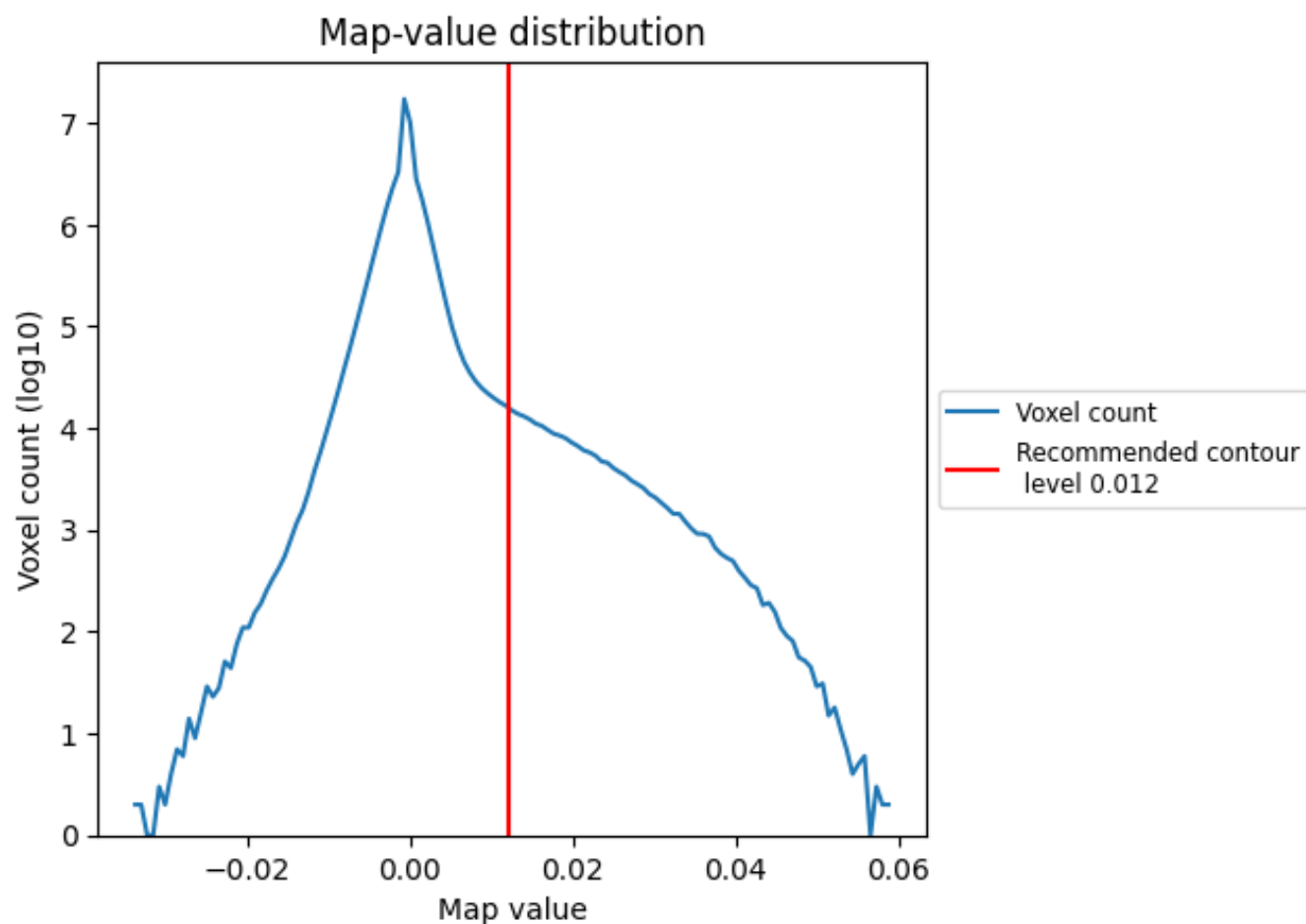
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

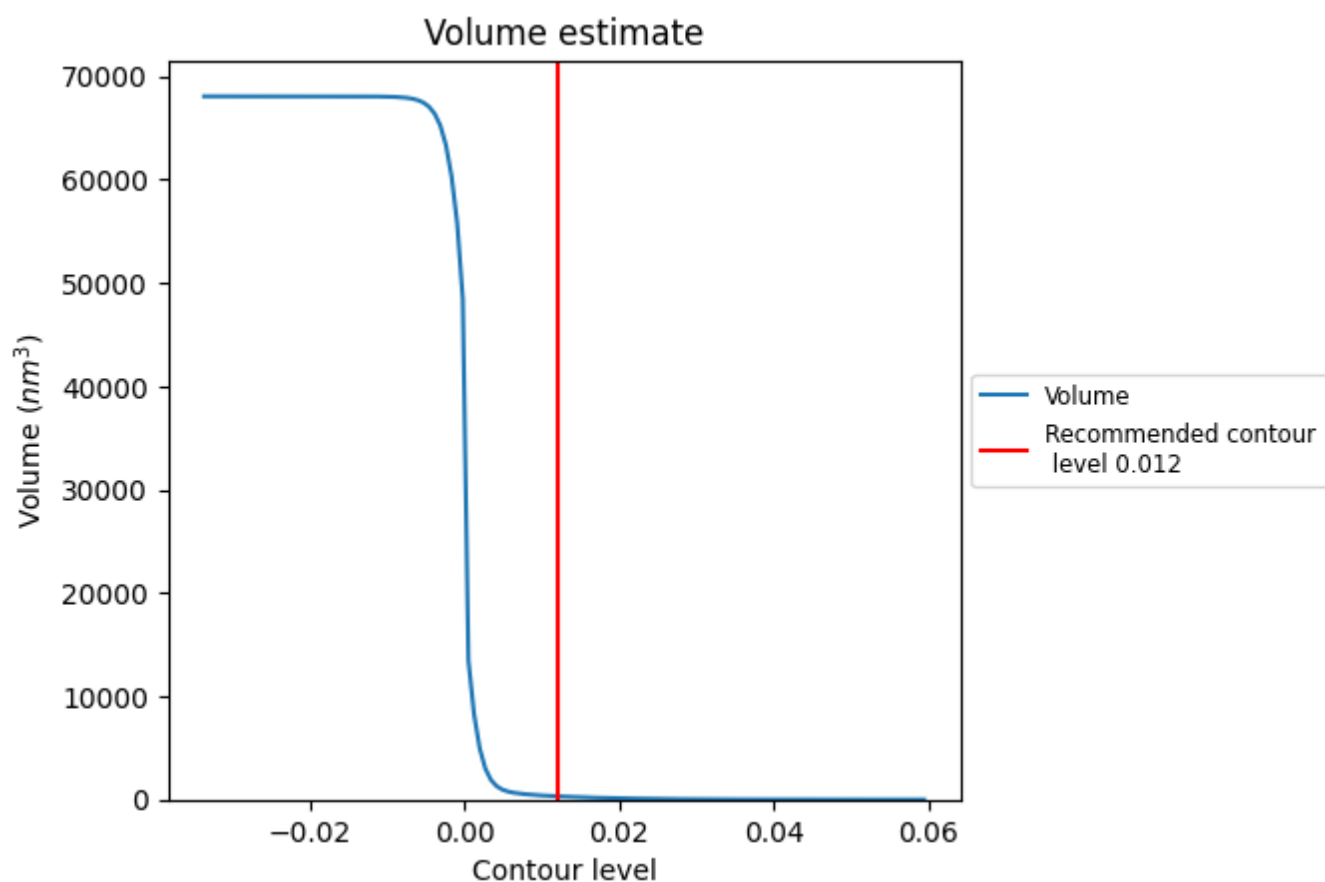
This section contains the results of statistical analysis of the map.

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.

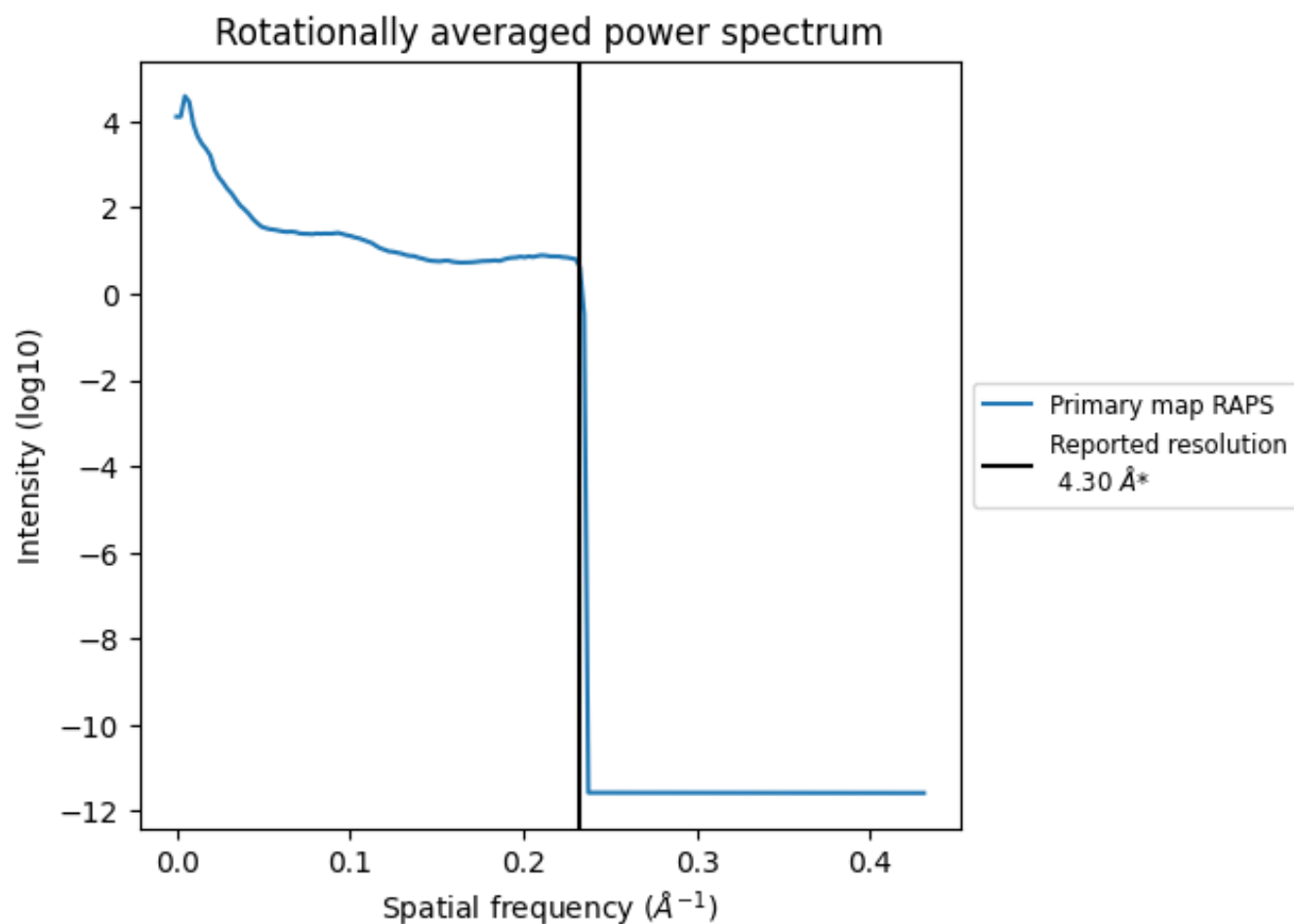
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm³; this corresponds to an approximate mass of 286 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 0.233 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

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

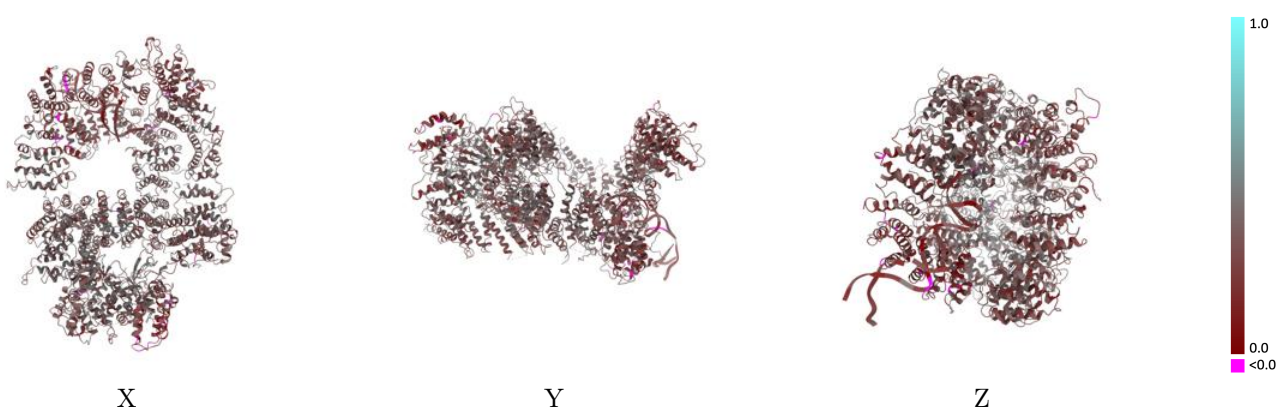
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22622 and PDB model 7K19. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

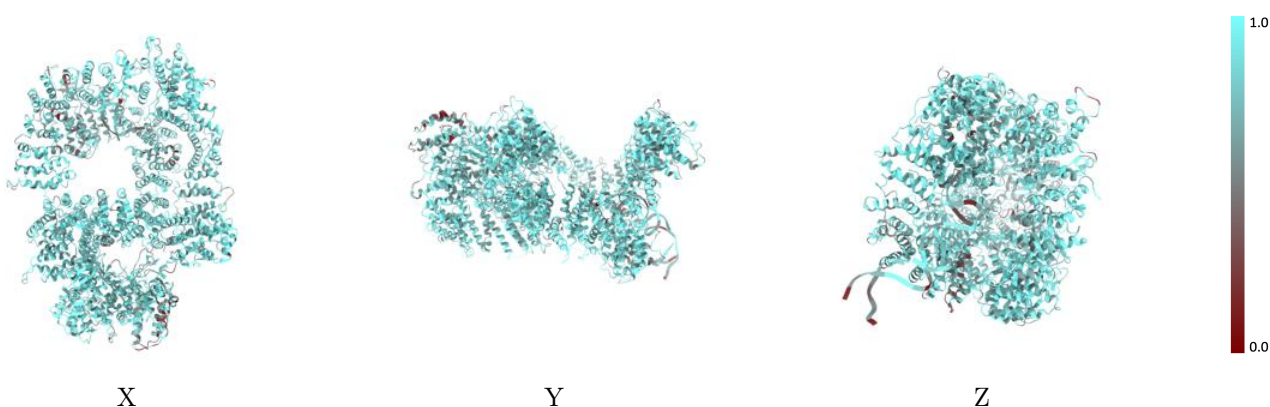
This section was not generated.

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



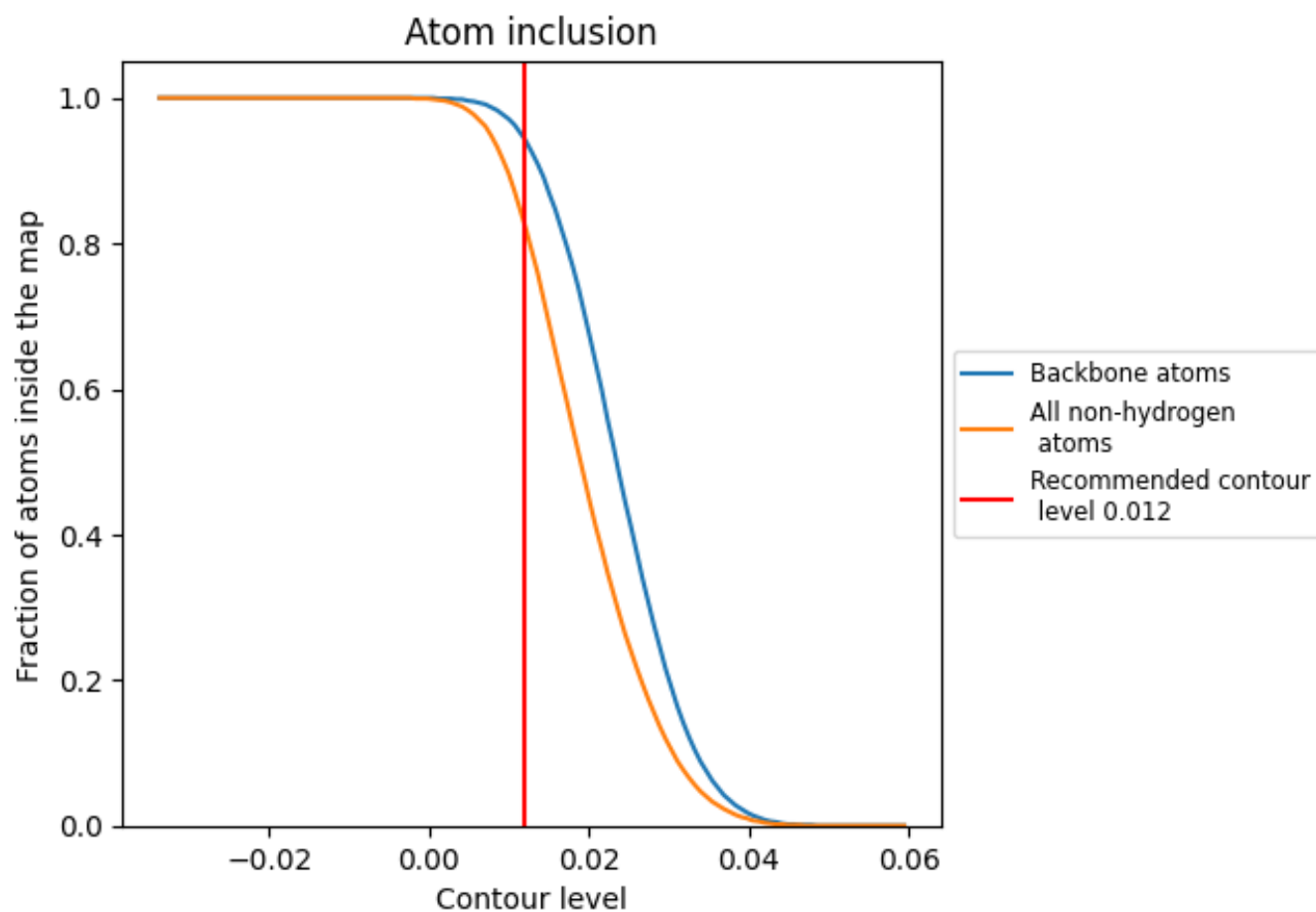
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.3390
A	0.8290	0.3430
D	0.6610	0.2000
F	0.5670	0.2560
G	0.7640	0.2420

