



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 01:29 pm BST

PDB ID : 9G9L / pdb_00009g9l
EMDB ID : EMD-51156
Title : DNA-PK + Polymerase lambda
Authors : Chaplin, A.K.; Amin, H.; Zahid, S.; Hardwick, S.W.
Deposited on : 2024-07-25
Resolution : 4.63 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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

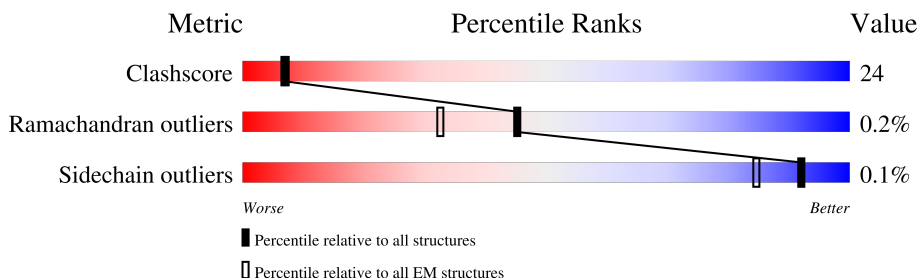
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 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	4128	
2	B	609	
3	C	732	
4	F	575	
5	M	204	
6	D	24	
7	E	23	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39800 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	3688	Total	C	N	O	S	0	0
			29010	18609	4895	5318	188		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	488	Total	C	N	O	S	0	0
			3825	2453	645	709	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	647	Total	C	N	O	S	0	0
			5093	3248	849	970	26		

- Molecule 4 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	98	Total	C	N	O	S	0	0
			755	482	141	129	3		

- Molecule 5 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	23	Total	C	N	O	S	0	0
			155	99	25	30	1		

- Molecule 6 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	24	Total	C	N	O	P	0	0
			488	238	89	138	23		

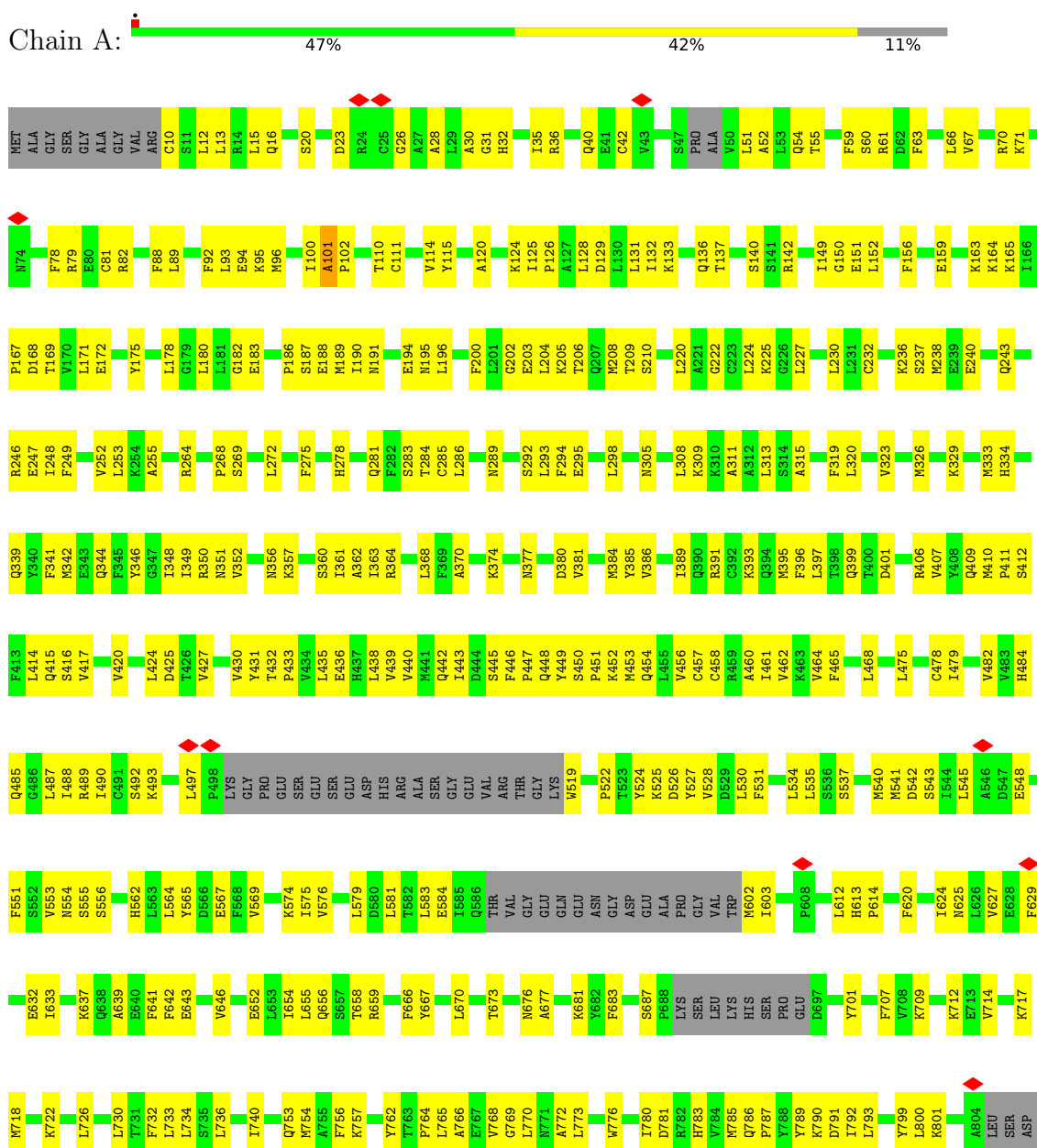
- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	23	Total	C	N	O	P	0	0
			474	230	79	142	23		

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: DNA-dependent protein kinase catalytic subunit

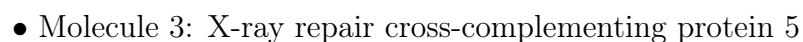


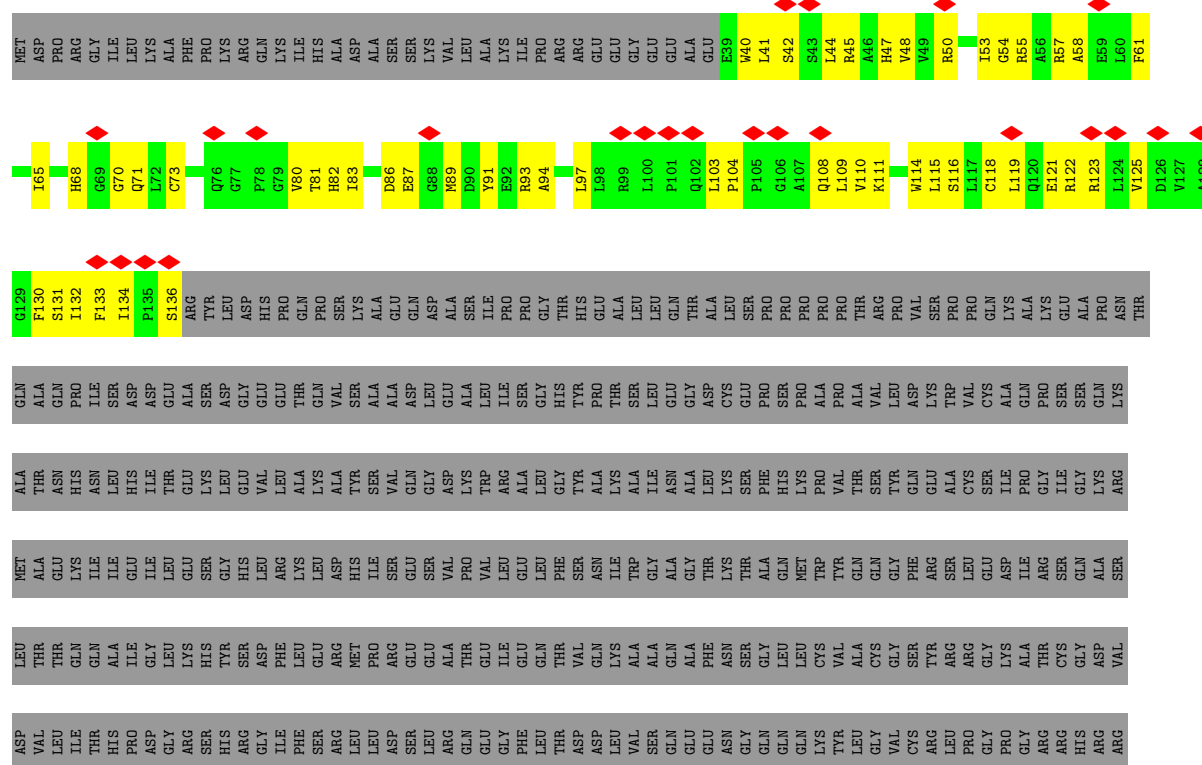




L4117	R4049	E3976	A3899	K3825	E3747	N3679	E3582	A3504	E3428	E3350	K3256	I3103
G4118	K4050	T3977	L3900	A3826	H3748	L3680	L3583	L3505	E3429	I3351	K3257	Q3104
R4119	G4053	G3978	R3901	A3827	P3749	E3681	W3588	L3506	ASN	E3352	L3258	I3107
T4120	L4054	L3979	F3904	Y3828	F3750	E3682	S3589	D3509	ALA	E3353	L3259	Q3108
W4121	N4055	K3980	H3908	D3831	L3751	P3685	S3590	Q3510	SER	A3356	K3260	R3111
E4122	P4056	Y3981	H3908	P3832	G3755	V3686	N3591	A3511	VAL	R3357	E3261	K3112
G4123	A4057	K3984	I3911	R3833	L3758	M3687	D3591	Q3515	ILE	R3358	L3262	Q3113
W4124	V4058	V3985	C3912	A3834	R3759	S3688	V3592	K3518	ASP	I3359	L3266	Y3114
E4125	I4059	H3986	I3913	E3838	R3759	F3689	A3594	Q3518	SER	L3360	S3266	I3193
P4126	A3987	L3988	C3912	F3690	G3762	K3691	E3595	V3518	ALA	E3361	K3272	S3115
W4127	L3989	R3989	I3917	V3692	K3763	K3691	K3598	I3521	GLU	L3439	L3273	L3197
N4128	E3841	E3765	E3841	V3692	V3764	V3692	T3599	T3522			L3274	I3117
	W3842	E3765	W3842	L3695	E3765	L3695	K3608	D3523	Y3442		S3275	PRO
	L3843	E3766	L3843	R3696	R3766	R3696	M3609	N3524	P3443		V3277	LEU
	T3844	E3766	T3844	N3697	Q3769	N3697	K3612	Y3525	Y3446		Y3277	GLU
	K3845	Q3769	K3845	E3698	V3770	E3698	M3613	P3526	V3447		Y3280	ASP
	N3926	N3771	N3926	L3699	N3771	L3699	K3613	A3528	E3448		R3287	ASN
	N3927	N3772	N3927	E3700	N3772	E3700	K3621	I3529	K3449		Q3291	SER
	F3928	G3848	F3928	L3701	N3772	L3701	A3622	V3530	M3450		Q3291	MET
	V4004	G3848	V4004	P3702	L3775	P3702	F3623	P3531	K3380		Q3291	ASN
	V4005	G3848	V4005	Q3703	L3775	Q3703	G3624	P3532	H3384		Q3291	VAL
	V4006	G3848	V4006	G3706	L3786	G3706	L3625	F3533	L3385		Q3291	GLN
	V4007	G3848	V4007	G3707	Q3787	G3707	G3626	Y3537	E3386		Q3291	ASP
	V4008	G3848	V4008	R3708	R3788	R3708	G3626	Y3537	E3387		Q3291	GLY
	V4009	G3848	V4009	Y3791	R3789	Y3791	G3626	Y3537	V3297		Q3291	ASP
	V4010	G3848	V4010	Y3791	R3790	Y3791	G3626	Y3537	L3298		Q3291	PRO
	V4011	G3848	V4011	Y3791	R3791	Y3791	G3626	Y3537	A3388		Q3291	SER
	V4012	G3848	V4012	Y3791	R3791	Y3791	G3626	Y3537	A3392		Q3291	ARG
	V4013	G3848	V4013	Y3791	R3791	Y3791	G3626	Y3537	E3393		Q3291	GLU
	V4014	G3848	V4014	Y3791	R3791	Y3791	G3626	Y3537	E3394		Q3291	MET
	V4015	G3848	V4015	Y3791	R3791	Y3791	G3626	Y3537	E3395		Q3291	VAL
	V4016	G3848	V4016	Y3791	R3791	Y3791	G3626	Y3537	A3396		Q3291	GLN
	V4017	G3848	V4017	Y3791	R3791	Y3791	G3626	Y3537	GLN		Q3291	GLU
	V4018	G3848	V4018	Y3791	R3791	Y3791	G3626	Y3537	PRO		Q3291	GLU
	V4019	G3848	V4019	Y3791	R3791	Y3791	G3626	Y3537	TRP		Q3291	GLU
	V4020	G3848	V4020	Y3791	R3791	Y3791	G3626	Y3537	SER		Q3291	GLU
	V4021	G3848	V4021	Y3791	R3791	Y3791	G3626	Y3537	CYS		Q3291	GLU
	V4022	G3848	V4022	Y3791	R3791	Y3791	G3626	Y3537	GLY		Q3291	GLU
	V4023	G3848	V4023	Y3791	R3791	Y3791	G3626	Y3537	PRO		Q3291	GLU
	V4024	G3848	V4024	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4025	G3848	V4025	Y3791	R3791	Y3791	G3626	Y3537	PRO		Q3291	GLU
	V4026	G3848	V4026	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4027	G3848	V4027	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4028	G3848	V4028	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4029	G3848	V4029	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
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	V4049	G3848	V4049	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4050	G3848	V4050	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4051	G3848	V4051	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4052	G3848	V4052	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
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	V4055	G3848	V4055	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4056	G3848	V4056	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4057	G3848	V4057	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4058	G3848	V4058	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4059	G3848	V4059	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4060	G3848	V4060	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4061	G3848	V4061	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
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	V4080	G3848	V4080	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
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	V4091	G3848	V4091	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4092	G3848	V4092	Y3791	R3791	Y3791	G3626	Y3537	A3406		Q3291	GLU
	V4093	G3848	V4093									

Chain B:



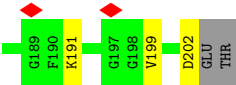


LEU	ASP	ILE	ILE	VAL	PRO	TYR	SER	GLU	PHE	ALA	CYS	ALA	LEU	LEU	TYR	THR	GLY	SER	ALA	HIS	PHE	ASN	ARG	SER	MET	ARG	ALA	LEU	ALA	LYS	THR	LYS	GLY	MET	SER	LEU	SER	GLU	HIS	ALA	LEU	SER	THR	ALA	VAL	VAL	ARG	ASN	THR	HIS	GLY	CYS	LYS	VAL	GLY	PRO	GLY
ARG	VAL	LEU	THR	PRO	PRO	GLU	LYS	ASP	VAL	PHE	ARG	LEU	LEU	GLY	LEU	PRO	TYR	ARG	GLU	PRO	ALA	ALA	GLU	ASP	TRP																																

● Molecule 5: Protein PAXX



MET	ASP	PRO	LEU	SER	PRO	PRO	LEU	CYS	THR	GLU	LEU	PRO	PRO	GLY	PRO	GLU	ARG	PRO	PHE	VAL	CYS	TYR	CYS	GLU	GLY	GLU	GLY	GLY	ASP	GLY	ASP	THR	VAL	THR	ASP	ALA	ALA	GLU	LEU	TRP	SER	THR	CYS	PRO	THR	PRO	ASP	SER	LEU	ALA	ALA	PRO	LEU
LYS	ALA	ARG	PHE	GLY	LEU	SER	ALA	ALA	GLU	THR	ILE	PRO	THR	PRO	PHE	ARG	ALA	ALA	CYS	GLU	GLN	TYR	ALA	VAL	ALA	LEU	THR	GLN	GLY	ASP	ARG	ALA	SER	PRO	ASP	LEU	ALA	PHE	PRO	ASP	LEU	SER	LYS	VAL	PHE	GLY	PRO	GLY	VAL	ARG	ALA	PRO	ARG
LEU	ARG	ALA	LEU	THR	LEU	GLY	LEU	ALA	LYS	ARG	VAL	TRP	SER	LEU	GLU	ARG	LEU	ALA	ALA	ALA	GLU	GLU	THR	ALA	VAL	SER	PRO	ARG	LYS	PRO	ARG	ALA	PRO	ASP	PRO	PRO	ASP	PRO	GLN	ARG	GLY	GLY	PRO	GLY	PRO	GLY	VAL	ARG	ARG	ALA	PRO	ARG	C180



● Molecule 6: DNA



T20	A21	A24	A25	A26	C27	T28	A29	A30	A31	A32	A33	C34	T35	A36	T37	T38	A39	T40	T41	A42	T43
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● Molecule 7: DNA



A15	A16	T17	A18	A19	T20	A21	G22	T23	T24	T25	T26	T27	A28	G29	T30	T31	T32	A33	T34	T35	A36	G37
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12656	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 ($e^-/\text{\AA}^2$)	51.96	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.640	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	417.28, 417.28, 417.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	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	0.18	0/29602	0.46	2/40074 (0.0%)
2	B	0.24	0/3900	0.49	2/5268 (0.0%)
3	C	0.15	0/5185	0.39	0/6998
4	F	0.27	0/771	0.50	0/1046
5	M	0.09	0/159	0.34	0/216
6	D	0.23	0/548	0.49	0/843
7	E	0.24	0/530	0.49	0/817
All	All	0.19	0/40695	0.46	4/55262 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	PRO	N-CA-CB	6.58	110.57	103.33
1	A	2297	SER	N-CA-C	-5.35	107.77	114.56
2	B	281	LEU	CA-C-N	5.24	130.90	120.94
2	B	281	LEU	C-N-CA	5.24	130.90	120.94

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	29010	0	28916	1364	0
2	B	3825	0	3813	248	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5093	0	5039	247	0
4	F	755	0	767	54	0
5	M	155	0	135	3	0
6	D	488	0	275	39	0
7	E	474	0	266	29	0
All	All	39800	0	39211	1882	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 24.

The worst 5 of 1882 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)
2:B:420:LEU:HA	2:B:426:GLN:CA	1.78	1.12
2:B:420:LEU:CA	2:B:426:GLN:HA	1.79	1.11
1:A:3226:ASP:N	1:A:3229:SER:HG	1.69	0.89
1:A:3868:VAL:HG12	1:A:3872:ARG:HE	1.38	0.88
2:B:407:PRO:HG2	3:C:486:ARG:HD2	1.54	0.88

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	3652/4128 (88%)	3389 (93%)	258 (7%)	5 (0%)	48	83
2	B	484/609 (80%)	434 (90%)	44 (9%)	6 (1%)	11	44
3	C	639/732 (87%)	586 (92%)	52 (8%)	1 (0%)	44	78
4	F	96/575 (17%)	91 (95%)	5 (5%)	0	100	100
5	M	21/204 (10%)	21 (100%)	0	0	100	100
All	All	4892/6248 (78%)	4521 (92%)	359 (7%)	12 (0%)	45	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	426	GLN
2	B	418	GLU
2	B	420	LEU
2	B	425	ILE
2	B	429	PRO

5.3.2 Protein sidechains ⓘ

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	3158/3671 (86%)	3157 (100%)	1 (0%)	100	100
2	B	414/548 (76%)	412 (100%)	2 (0%)	86	89
3	C	559/649 (86%)	559 (100%)	0	100	100
4	F	78/480 (16%)	78 (100%)	0	100	100
5	M	15/160 (9%)	15 (100%)	0	100	100
All	All	4224/5508 (77%)	4221 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	855	VAL
2	B	421	ASP
2	B	423	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	68	GLN
2	B	458	GLN
3	C	359	ASN
1	A	1941	HIS
1	A	1771	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

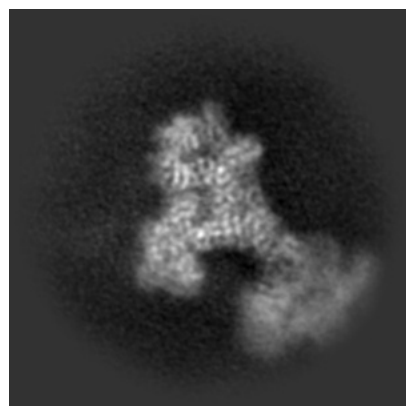
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51156. These allow visual inspection of the internal detail of the map and identification of artifacts.

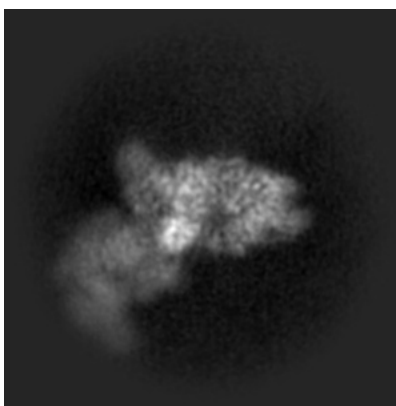
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

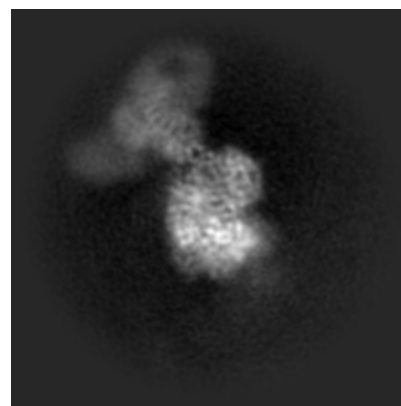
6.1.1 Primary map



X

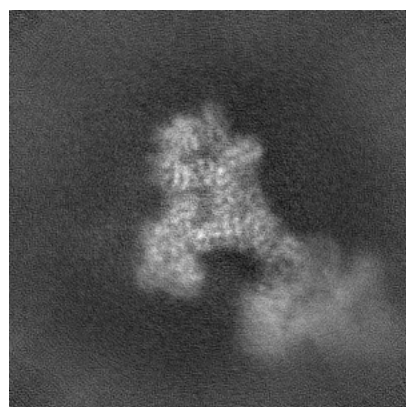


Y

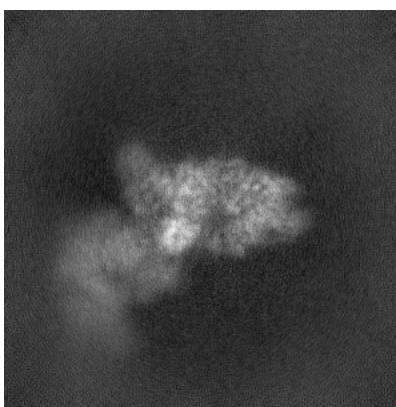


Z

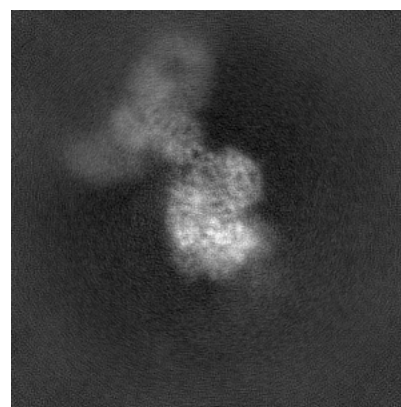
6.1.2 Raw map



X



Y

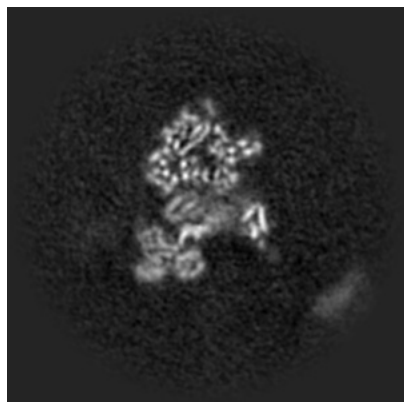


Z

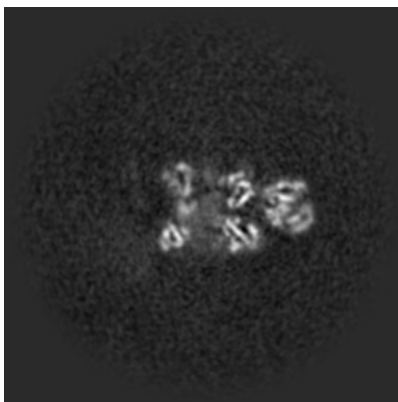
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

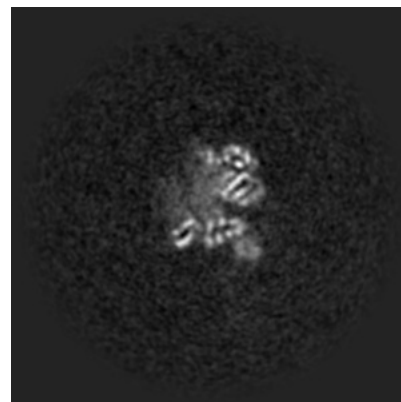
6.2.1 Primary map



X Index: 160

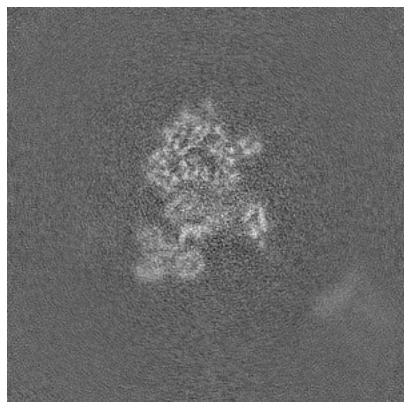


Y Index: 160

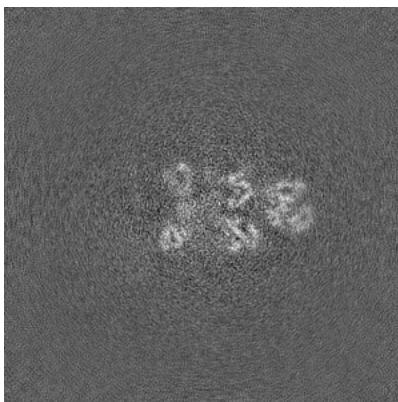


Z Index: 160

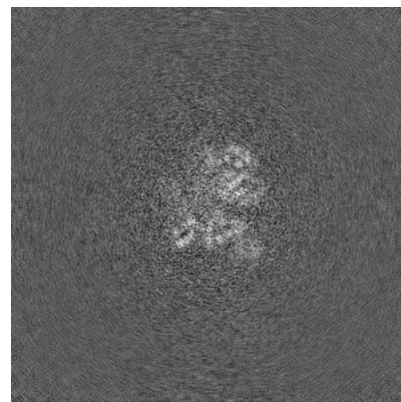
6.2.2 Raw map



X Index: 160



Y Index: 160

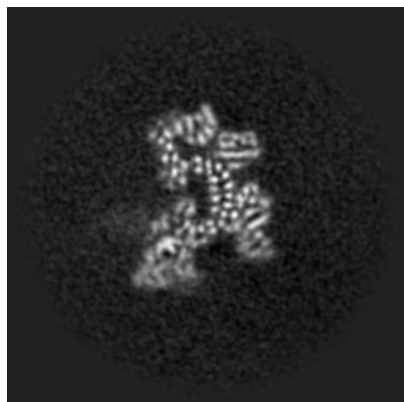


Z Index: 160

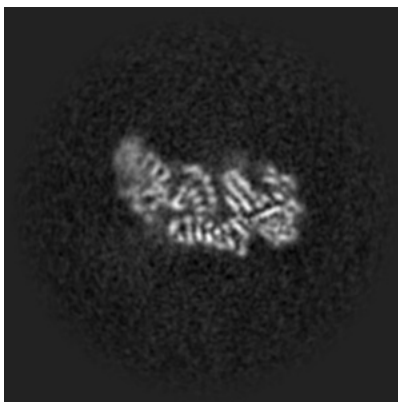
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

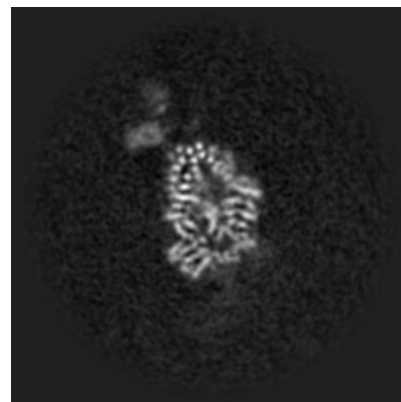
6.3.1 Primary map



X Index: 176

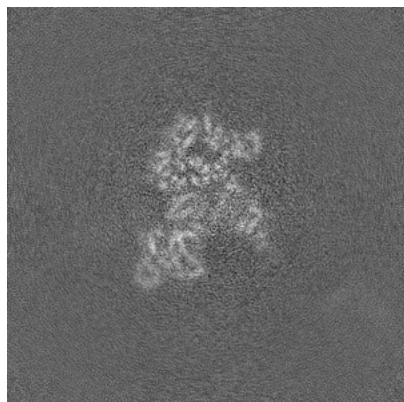


Y Index: 141

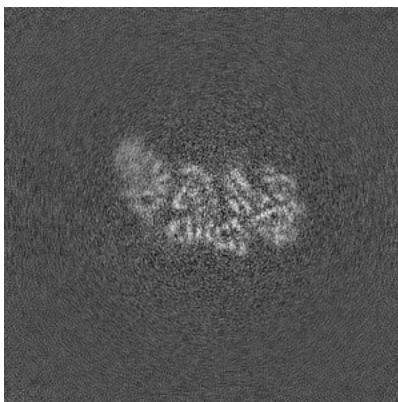


Z Index: 141

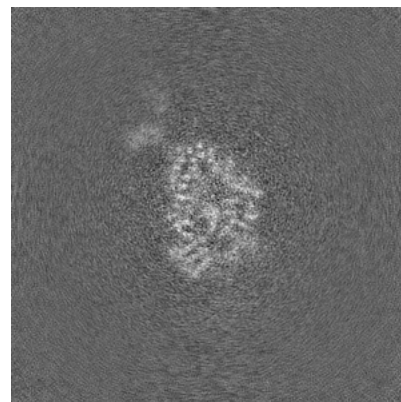
6.3.2 Raw map



X Index: 165



Y Index: 142

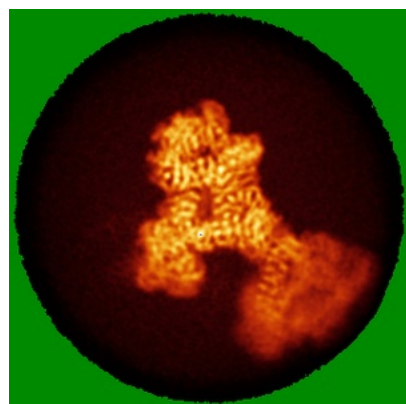


Z Index: 142

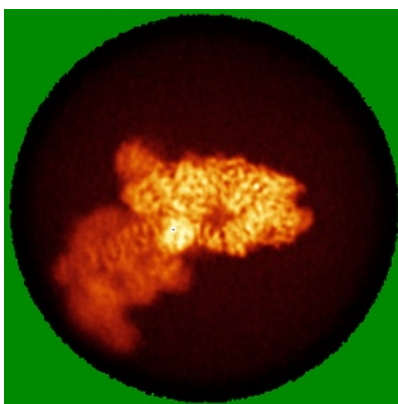
The images above show the largest variance slices of the map in three orthogonal directions.

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

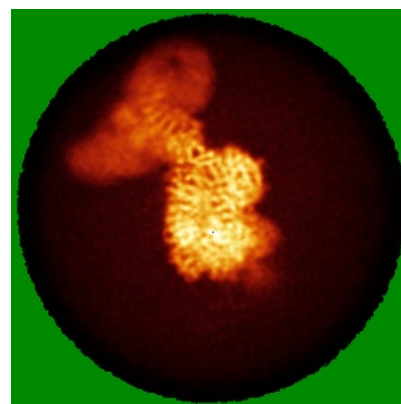
6.4.1 Primary map



X

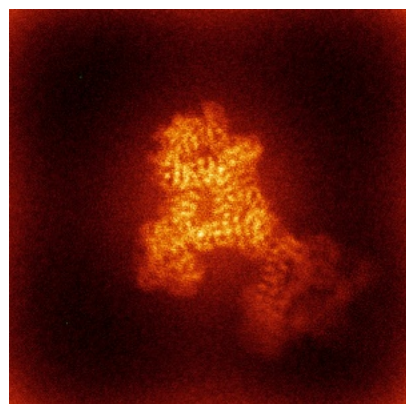


Y

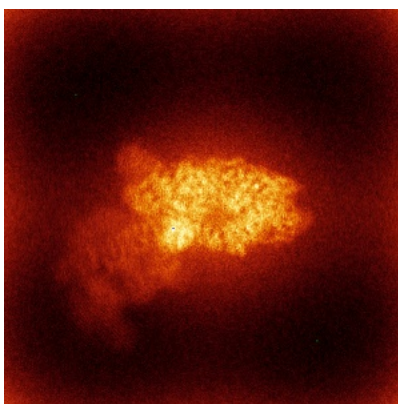


Z

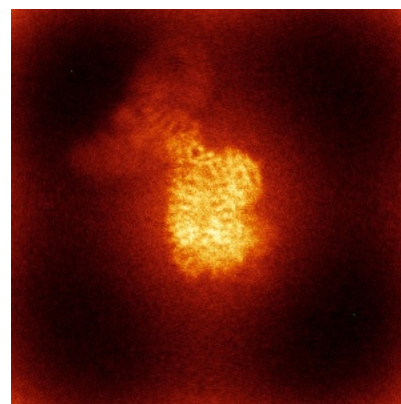
6.4.2 Raw map



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.

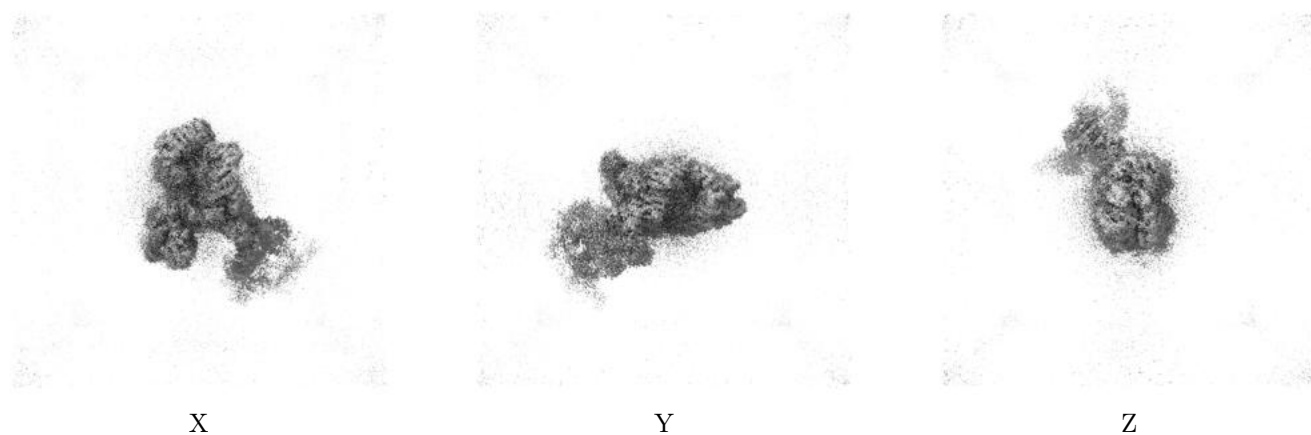
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

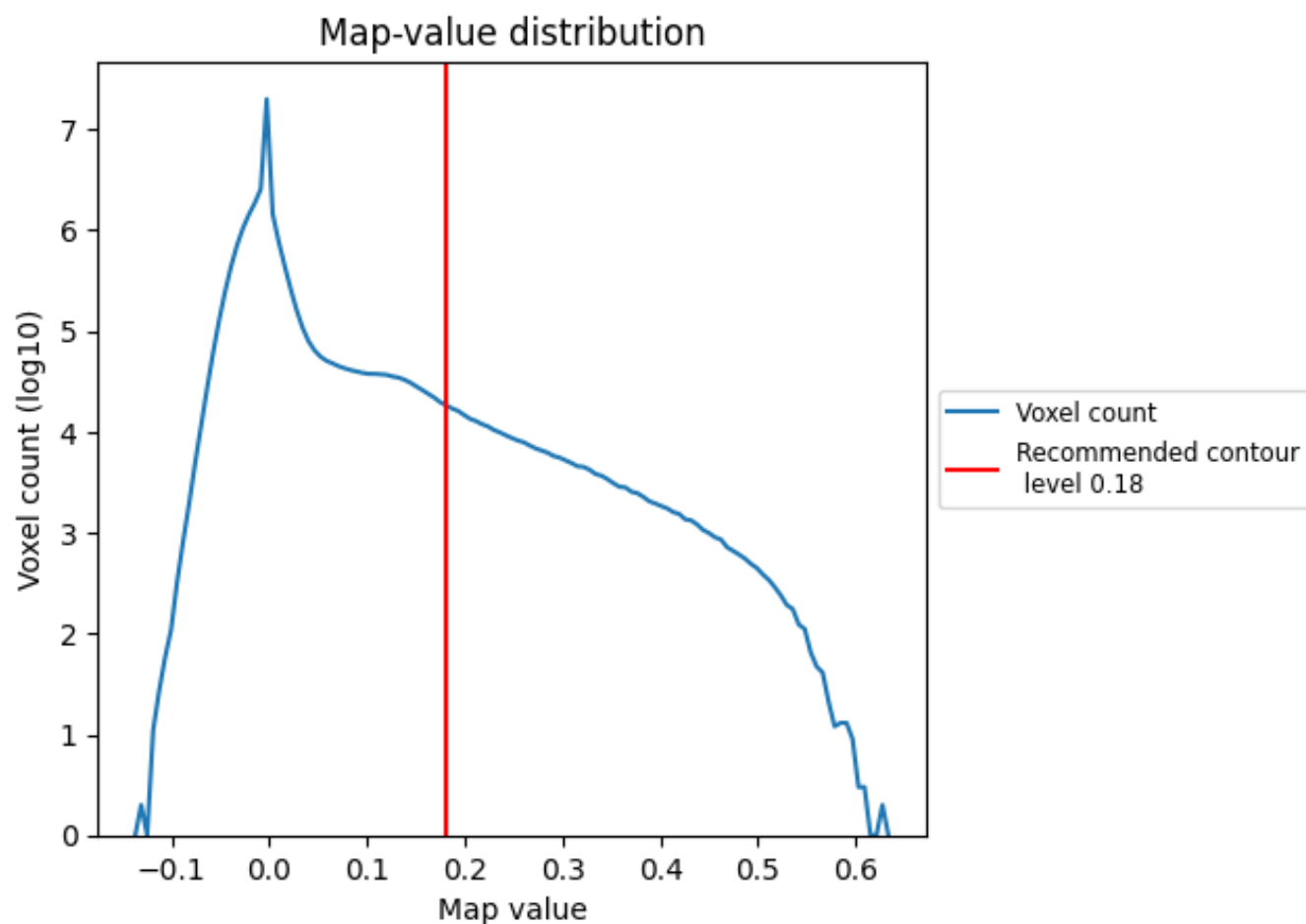
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

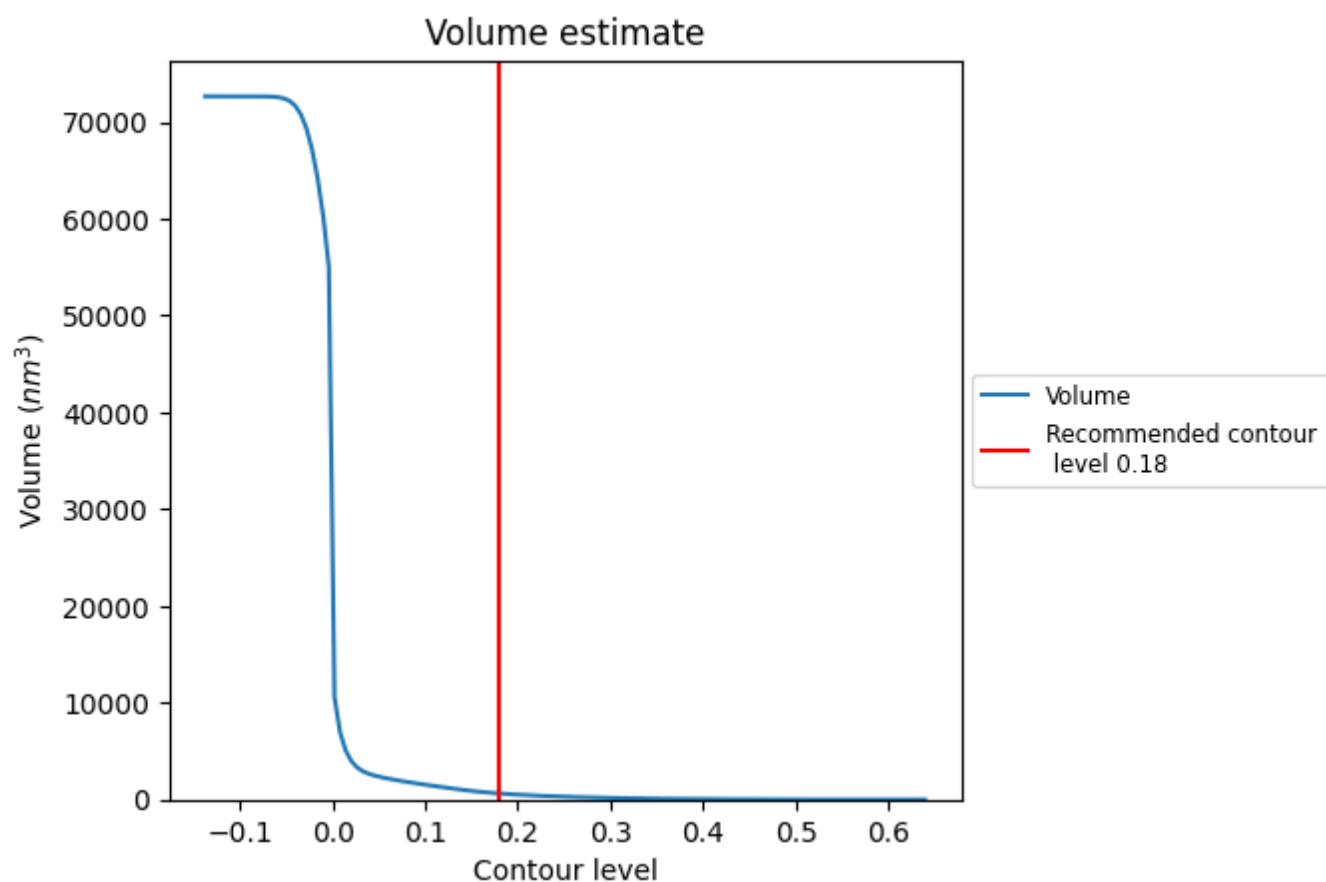
This section contains the results of statistical analysis of the map.

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.

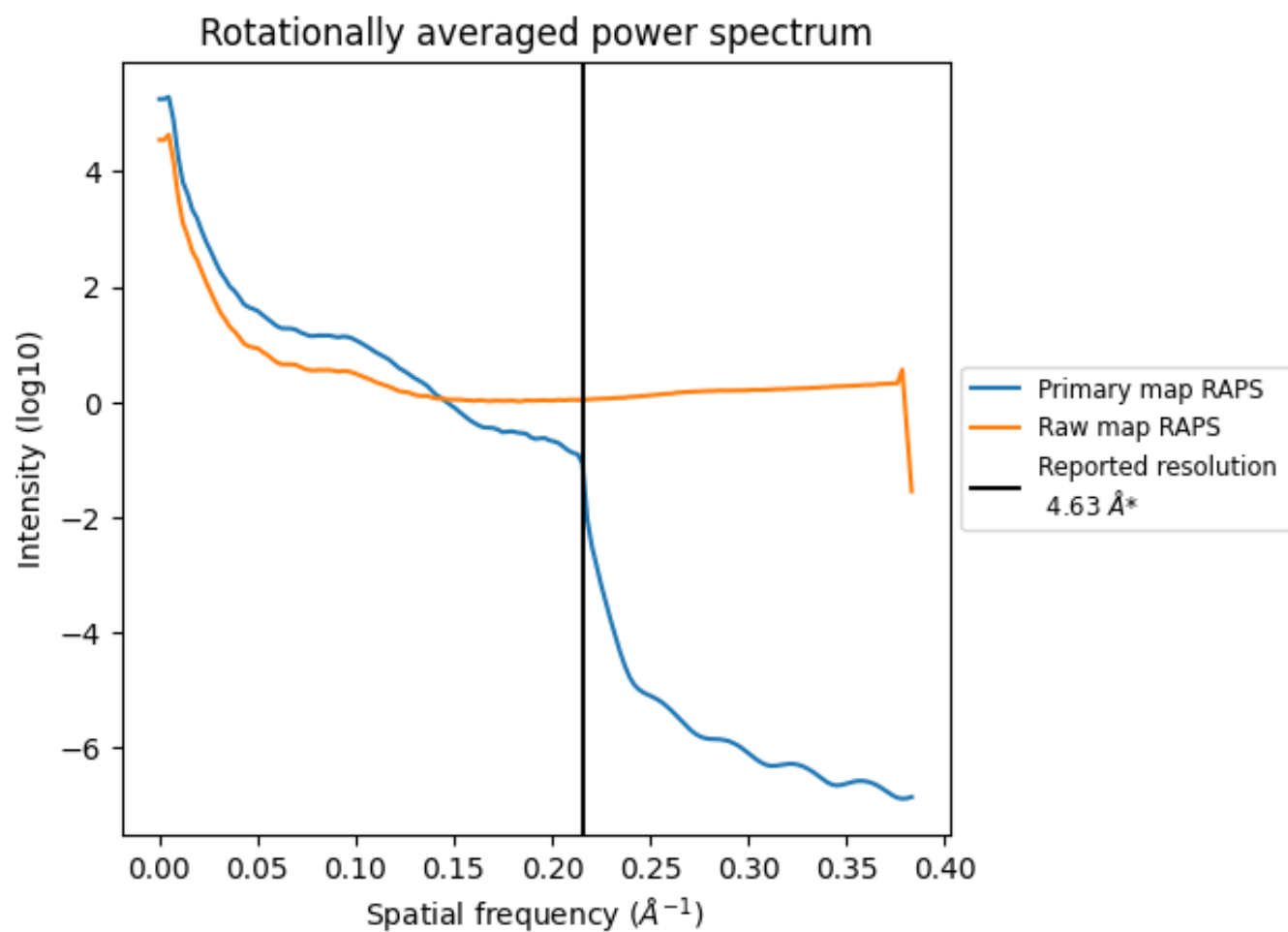
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 632 nm^3 ; this corresponds to an approximate mass of 570 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 ⓘ

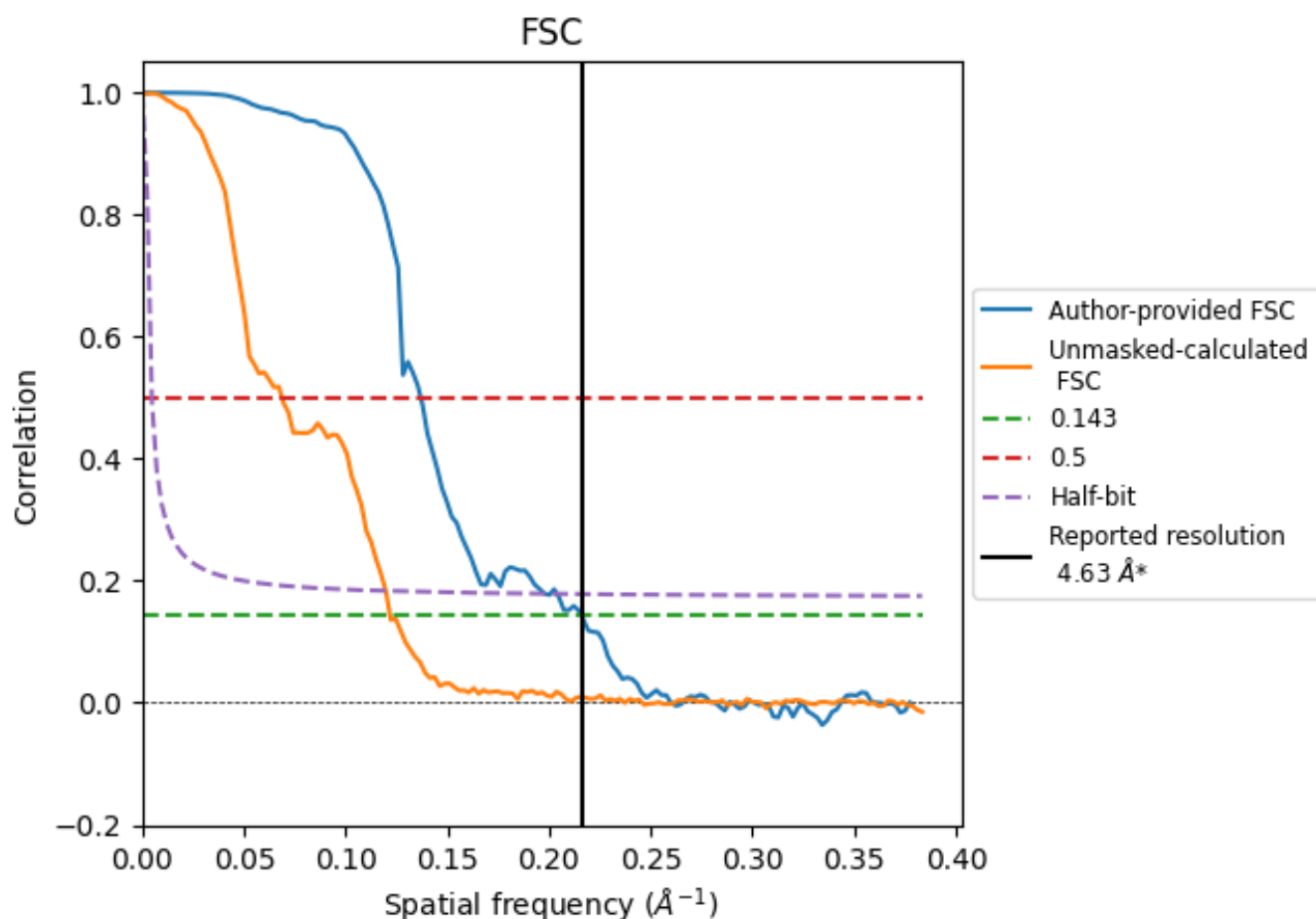


*Reported resolution corresponds to spatial frequency of 0.216 \AA^{-1}

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 0.216 \AA^{-1}

8.2 Resolution estimates [i](#)

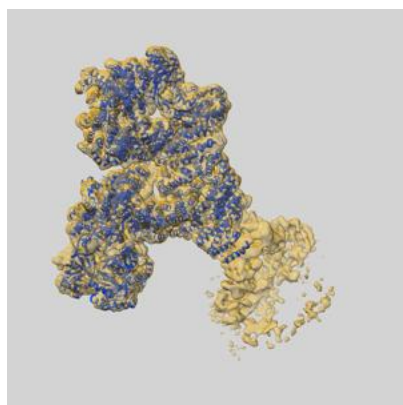
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	7.30	5.05
Unmasked-calculated*	8.20	14.56	8.35

*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 8.20 differs from the reported value 4.63 by more than 10 %

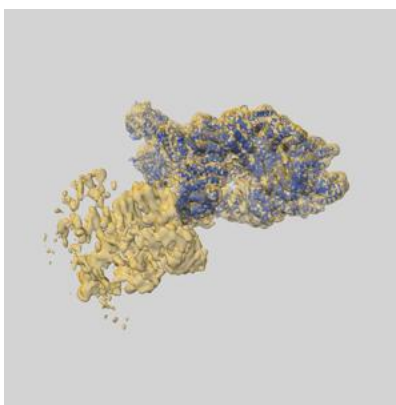
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51156 and PDB model 9G9L. Per-residue inclusion information can be found in section [3](#) on page [5](#).

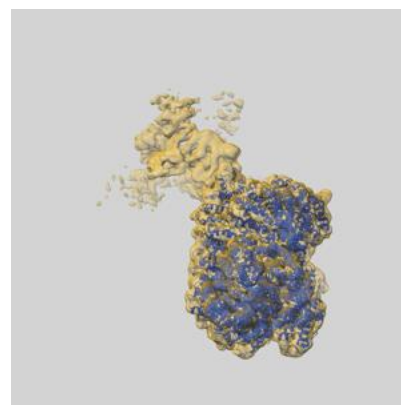
9.1 Map-model overlay [i](#)



X



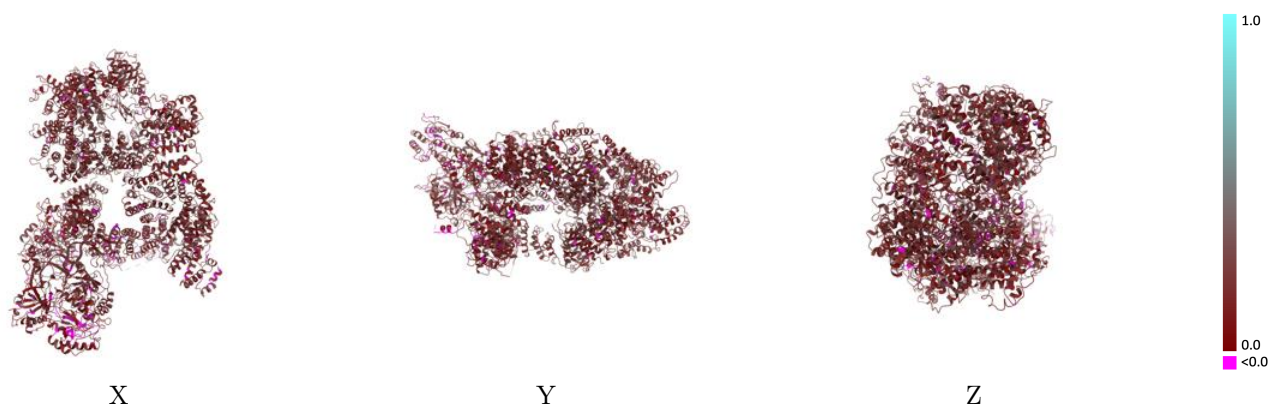
Y



Z

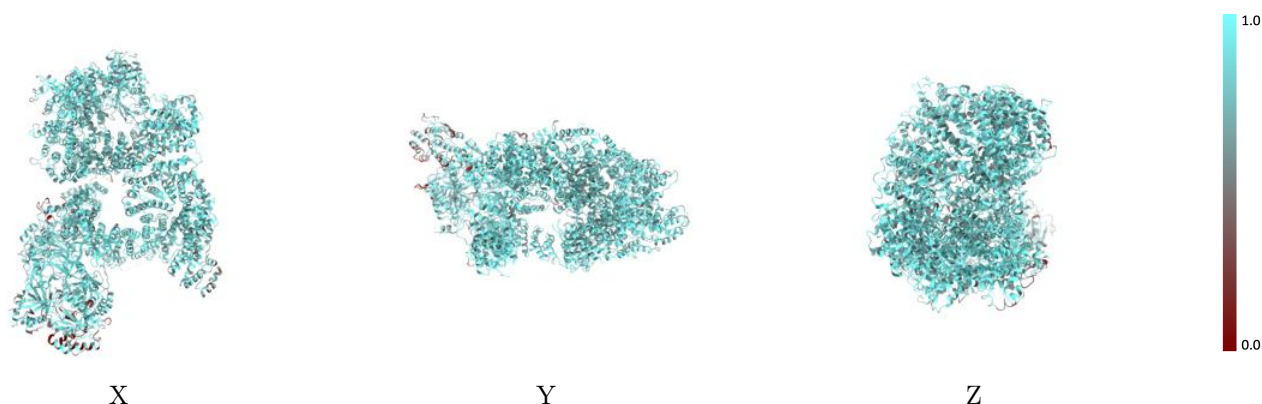
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



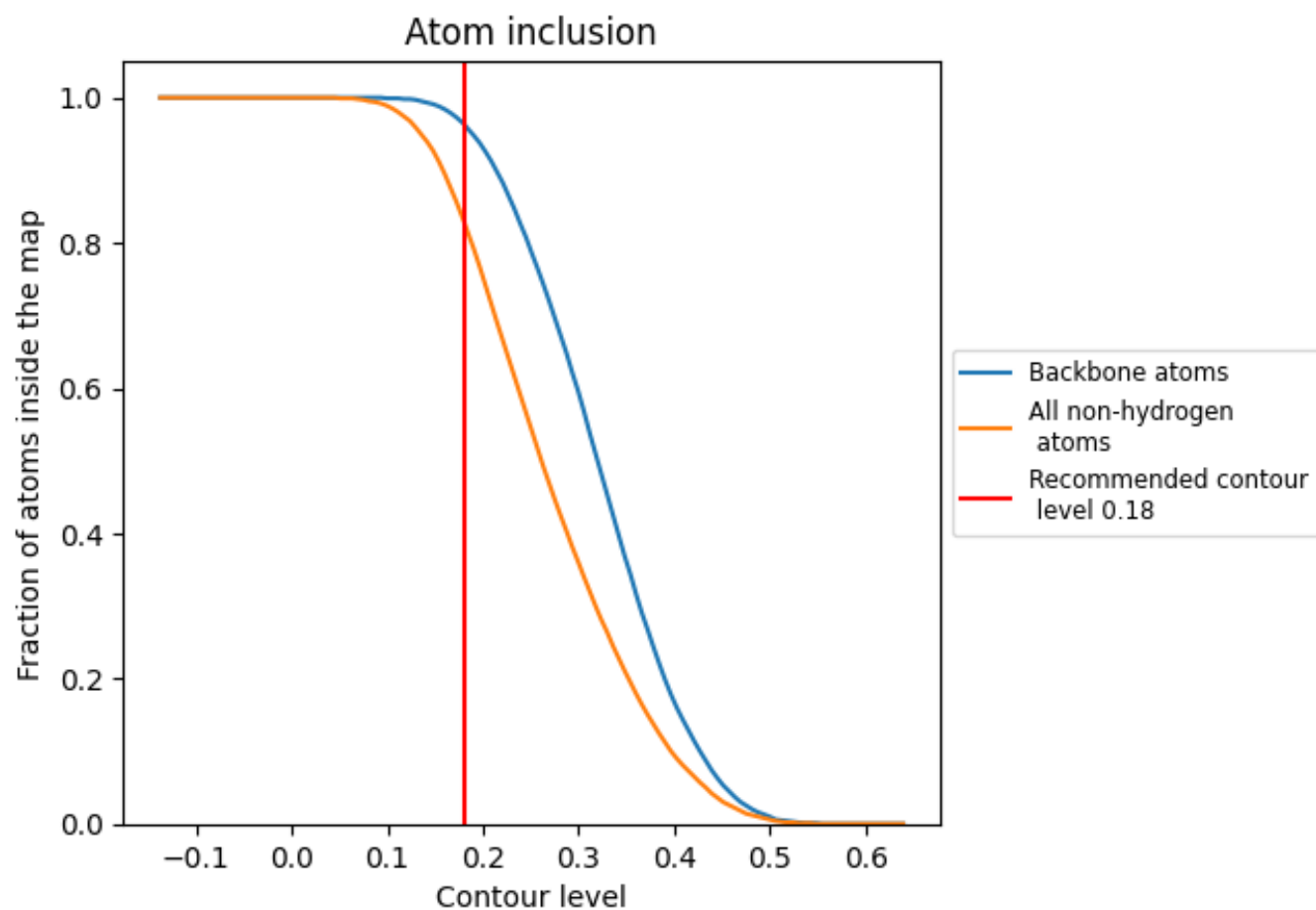
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 83% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8300</div>	<div><div></div>0.1880</div>
A	<div><div></div>0.8470</div>	<div><div></div>0.1930</div>
B	<div><div></div>0.8470</div>	<div><div></div>0.1870</div>
C	<div><div></div>0.7270</div>	<div><div></div>0.1580</div>
D	<div><div></div>0.9570</div>	<div><div></div>0.2320</div>
E	<div><div></div>0.9410</div>	<div><div></div>0.2140</div>
F	<div><div></div>0.6190</div>	<div><div></div>0.1540</div>
M	<div><div></div>0.8520</div>	<div><div></div>0.2220</div>

1.0

0.0

<0.0