



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:16 PM UTC

PDB ID : 6ZHE / pdb_00006zhe
EMDB ID : EMD-11219
Title : Cryo-EM structure of DNA-PK dimer
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-23
Resolution : 7.24 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

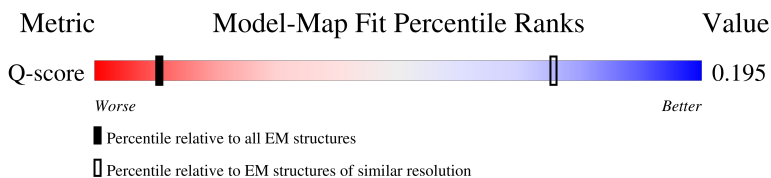
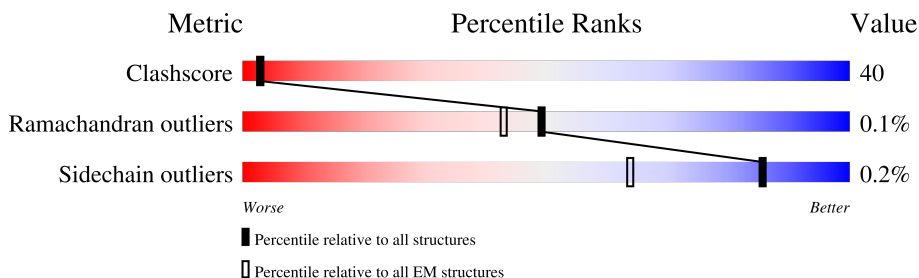
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.24 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	402 (6.74 - 7.70)

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	4156	
1	F	4156	
2	B	609	
2	G	609	

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Mol	Chain	Length	Quality of chain
3	C	732	43%53%
3	H	732	43%52%
4	J	25	20%72%8%
5	I	27	26%74%
6	D	26	8%92%
7	E	28	18%82%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 78785 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,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3768	Total	C	N	O	S	0	0
			29018	18632	4914	5293	179		
1	F	3731	Total	C	N	O	S	0	0
			29012	18636	4896	5295	185		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	489	Total	C	N	O	S	0	0
			3789	2430	640	704	15		
2	G	489	Total	C	N	O	S	0	0
			3797	2434	640	708	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	705	Total	C	N	O	S	0	0
			5490	3502	927	1037	24		
3	H	700	Total	C	N	O	S	0	0
			5517	3522	929	1041	25		

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

- Molecule 5 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	27	Total	C	N	O	P	0	0
			552	265	102	158	27		

- Molecule 6 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	26	Total 528	C 253	N 89	O 160	P 26	0	0

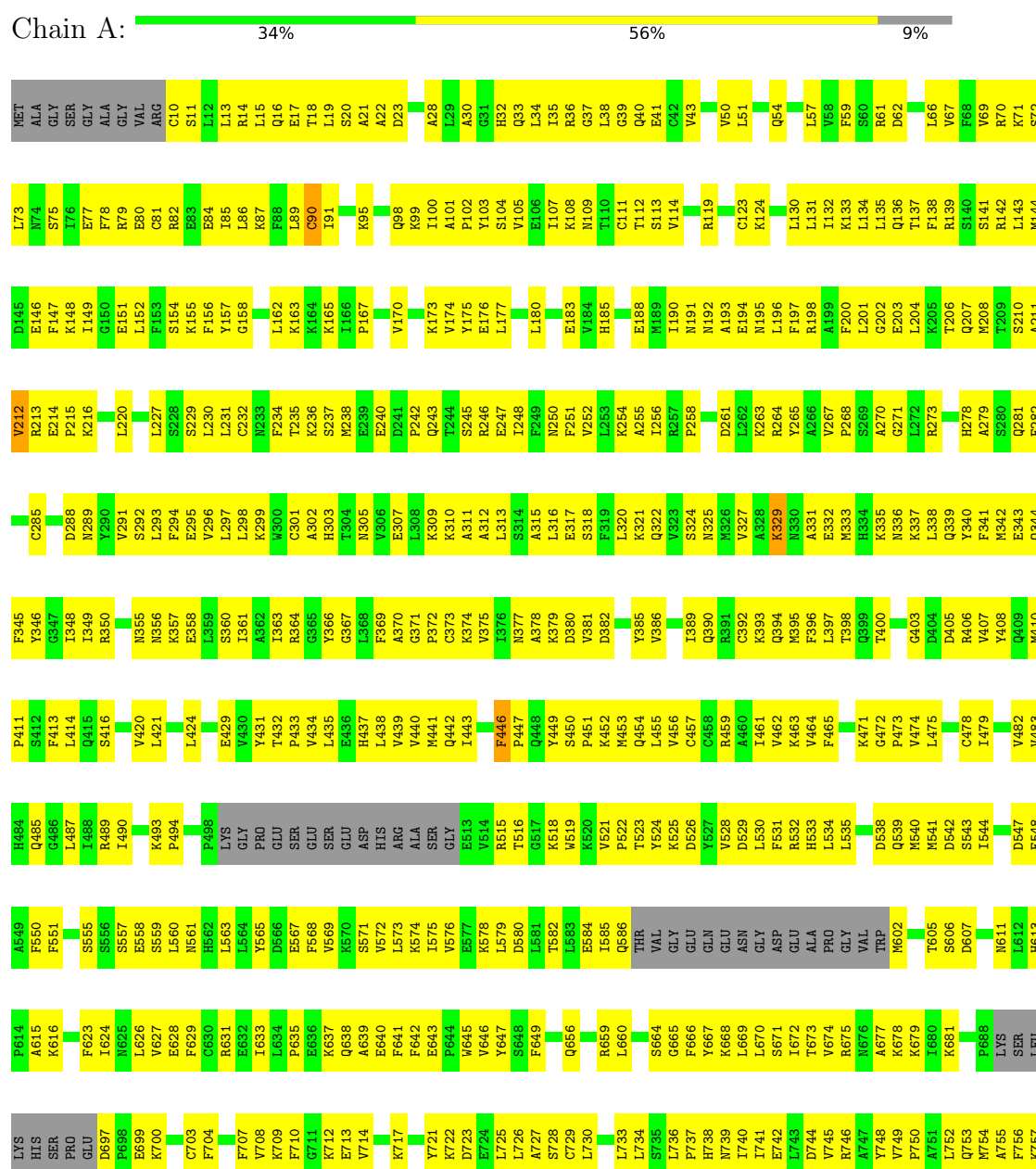
- Molecule 7 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	28	Total 573	C 275	N 107	O 163	P 28	0	0

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,DNA-PKcs







F3768	F3769	V3770	M3771	N3772	L3775	A3780	C3781	R3784	R3785	L3786	Q3787	L3788	R3789	T3790	S3791	S3792	V3793	V3794	P3795	M3796	T3797	S3798	R3799	L3800	G3801	L3802	L3803	E3804	W3805	R3806	E3807	N3808	R3809	V3810	T3811	L3812	K3813	L3814	L3815	L3816	L3817	N3818	T3819	S3820	S3821	Q3822	E3823	E3824	K3825	Y3828	L3829	S3830	D3831	P3832	R3833
Q3704	V3705	D3706	G3707	R3708	G3709	K3710	P3711	L3712	P3713	V3717	R3718	A3720	G3721	F3722	D3723	E3724	R3725	V3726	T3727	V3728	N3729	A3730	S3731	L3732	R3733	R3734	P3735	K3736	R3737	L3738	K3739	S3740	R3741	G3742	H3743	E3745	R3746	P3749	F3750	L3751	V3752	K3753	G3754	G3755	E3756	D3757	L3758	Q3762	R3763	V3764	E3765	Q3766	L3767		
F3632	I3633	Q3634	T3635	F3636	G3637	K3638	E3639	K3642	K3643	F3644	G3645	K3646	K3650	L3651	L3652	R3653	M3654	F3659	V3660	T3663	M3664	M3665	L3666	L3667	K3668	K3669	M3670	N3671	K3672	S3673	S3674	P3675	P3676	L3680	K3681	E3682	C3683	W3686	D3689	F3690	K3691	V3692	E3693	L3695	L3696	Q3762	R3763	V3764	E3765	Q3766	L3767				
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Q3704	V3705	D3706	G3707	R3708	G3709	K3710	P3711	L3712	P3713	V3717	R3718	A3720	G3721	F3722	D3723	E3724	R3725	V3726	T3727	V3728	N3729	A3730	S3731	L3732	R3733	R3734	P3735	K3736	R3737	L3738	K3739	S3740	R3741	G3742	H3743	E3745	R3746	P3749	F3750	L3751	V3752	K3753	G3754	G3755	E3756	D3757	L3758	Q3762	R3763	V3764	E3765	Q3766	L3767		
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S728	C729	L730	L731	T732	L736	F737	H738	E739	L740	I741	D744	V745	L746	A747	Y748	V749	L752	Q753	A754	A755	F756	G759	Y762	T763	R764	L765	A766	E767	V768	N771	A772	E775	W776	S777	L780	D781	R782	H783	V784	M785	Q786	Y789	K790	D791	W792	T793	L794	C795	L796	D797																								
K801	T802	S803	A804	LEU	SER	ASP	GLU	THR	LYS	ASN	TRP	GLU	VAL	SER	ALA	LEU	ARG	ALA	GLN	GLY	F826	N827	K828	W829	V830	L831	K832	H833	K836	L840	S847	L848	E849	E850	R851	R852	I853	V855	W856	Q857	M858	L859	G860	S861	D862	G863	G864	Q865	L866	N867																								
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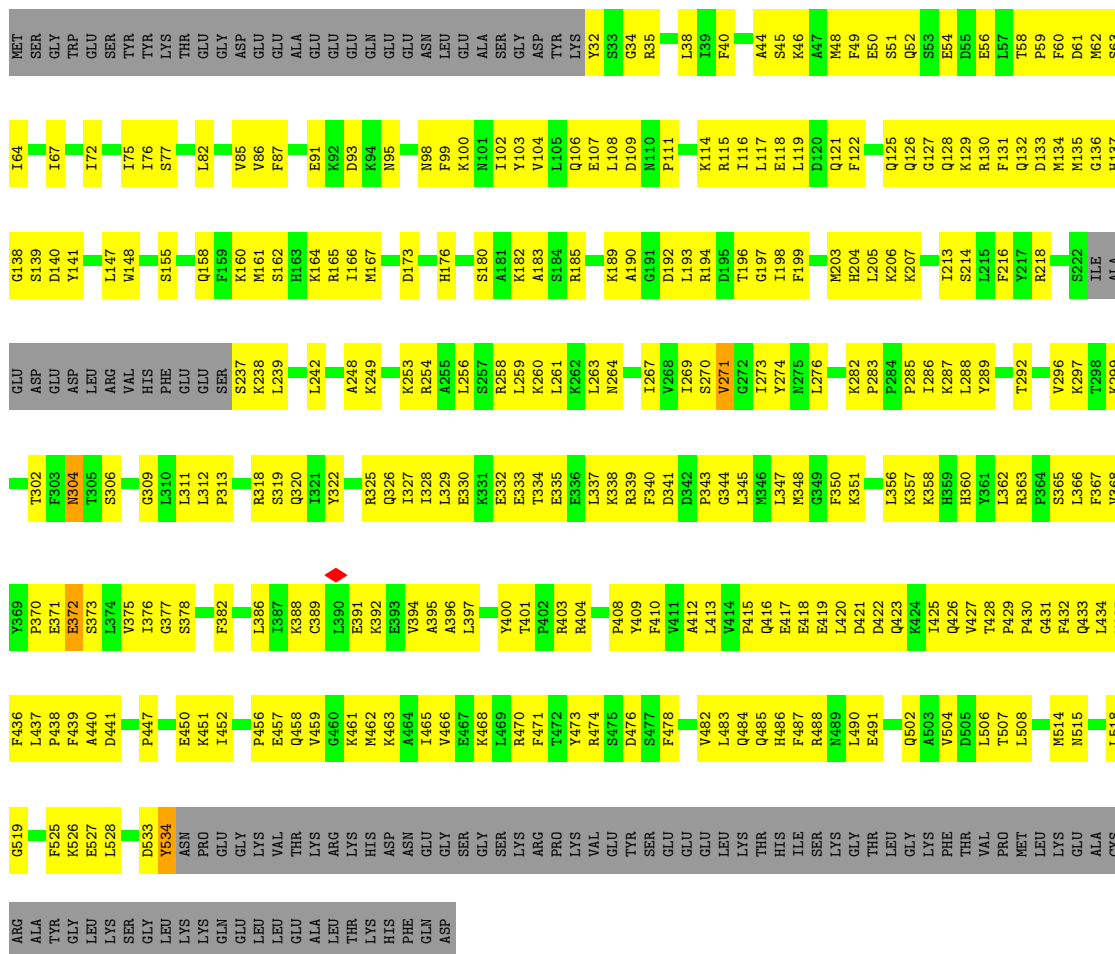
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TRP	E2564		P2373	P2309	C2245	K2102	K2102	E1979	C1904	L1836	E1769	L1702
PRO	T2565	L2438	L2374	R2311	W2245	M2103	M2104	N1980	I1905	R1837	Q1771	T1703
VAL	K2503	L2439	A2375	R2312	C2248	E2180	H2105	L1981	T1906	E1838	Q1771	
GLY	D2504	V2440	D2376	V2312	L2249	G2181	R2106	I1982	E1907	F1839	L1707	
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ARG	D2571	P2444	M2380	V2316	P2252	M2185	SER	K1986	L1911	L1712	E1776	
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THR	P2573	L2446	V2382	L2418	R2254	V2187	GLY	TVR	K1913	D1846		
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SER	THR	E2471	M2408	V2345	M2281	L2147	ASP	GLU	Y1940	D1878	V1740	
THR	PRO	Q2472	T2409	A2346	A2282	A2147	PRO	ALA		M1879	D1809	
ASP	ASP	M2473	E2410	K2347	N2283	L2148	THR	ALA	M1946	M1880	P1810	
PRO	PHE	L2474	L2411	Q2348	N2284	L2149	VAL	ASN	C1947	Y1881	R1811	
LEU	VAL	M2475	Y2412	L2349	D2285	L2151	HIS	GLY	A1948	S1882	L1812	
VAL	VAL	L2476	F2413	K2350	L2285	N2152	ASP	ASP	I1949	R1883	S1813	
ASP	THR	L2477	Q2414	Q2351	P2287	T2153	ASP	SER	S1950	L1884	F1814	
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SER	SER	T2480	K2418		P2290	E2156	LEU	PRO		D1887	S1818	
PRO	GLN	H2481	F2420	E2357	Q2291	F2157	LEU	SER	L1959	F1888	F1819	
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SER	THR	M2483		K2359	I2294	P2159	GLU	MET	F1961	A1891	D1821	
ASP	LEU	Y2484		F2360	L2294	Y2160	D2085	SER		A1892	R1822	
SER	GLN	R2485	M2424	F2361	Q2295	A2161	D2086	SER	F1967	K1892	S1823	
SER	LEU		R2425	S2296	S2296	K2162	R2090	LEU	S1968	E1893	L1824	
LEU	ARG		H2426	V2362	S2297	H2163	H2091	SER	E1969	S1894	L1758	
PHE	THR		R2427	C2363	E2298	N2234	C2093	TVR	K1970	T1895	L1825	
ALA	GLN		D2428		Y2299	P2167	M2094	LEU	P1971	L1896	T1826	
HIS	GLU		D2429	K2366	F2300	L2168		ALA	E1972	N1897	L1828	
LYS	GLY		E2430	V2367		L2169		ASP	Q1898	Q1898	M1829	
ARG	SER		R2431	T2368	L2303	Q2170	L2097	SER	N1974	F1899	H1830	
SER	LEU		Q2432	K2369	V2304	L2171	T2098	THR		F1900	V1765	

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L3680	A3616	G3548	R3467	SER	K3235	K3235	M3173	Q3108	Y3043	A2967	R2891	L2816	LEU
K3681	L3617	H3550	L3468	TRP	K3241	K3241	D3174	D3174	G3046	A2968	L2892	L2817	GLN
E3682	G3618	N3551	I3471	SER	K3319	K3239	P3175	M3112	R3047	A2969	L2893	E2819	ARG
C3683	D3619	K3552	K3552	CYS	I3320	K3241	N3177	N3113	K3048	K2970	E2894	M2820	ALA
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P3685	L3625	F3554	F3476	PRO	A3322	D3244	W3179	G3116	K3050	L2976	L2898	D2822	LEU
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S3688	A3627	A3556	E3478	GLY	R3324	A3246	D3181	S3117	L3052	Q2979	L2897	K2824	SER
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K3691	R3630	S3559	I3487	Y3413	N3327	R3247	I3183	D3119	G3054	Q2981	L2897	T2825	GLY
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G3693	K3632	Q3564	S3488	F3419	Y3334	N3251	N3185	L3121	G3056	Q2982	L2897	T2825	PHE
F3694	L3633	G3565	S3489	G3420	Y3334	F3252	R3186	H3122	L3121	Q2983	L2897	T2825	ALA
L3695	D3634	G3566	F3490	F3421	R3335	S3253	C3187	Q3123	L3122	Q2983	L2897	T2825	LYS
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D3706	D3641	N3580	W3507	ASP	E3352	L3262	K3196	Q3133	A3068	E2995	L2897	T2825	GLU
G3707	K3642	L3583	W3507	ASP	E3353	H3263	K3196	Q3133	A3068	E2995	L2897	T2825	VAL
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L3710	G3645	H3501	F3502	SER	R3355	S3265	LEU	T3136	L3073	P2852	L2897	T2825	LYS
L3711	G3646	K3502	M3502	VAL	A3356	S3266	VAL	E3137	Q3074	P2853	L2897	T2825	VAL
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H3715	K3650	F3585	V3514	GLN	G3364	W3272	MET	S3143	L3078	A3006	L2897	T2825	ALA
V3716	L3651	K3586	Q3515	GLN	S3365	L3273	ASN	F3144	E3079	A3006	L2897	T2825	ALA
R3717	L3652	K3586	H3516	VAL	S3366	V3274	VAL	L3145	H3081	Y2930	L2897	T2825	GLY
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F3722	S3657	D3591	E3520	V3447	I3374	Q3278	GLY	G3149	L3088	E3012	L2897	T2825	ARG
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R3725	N3660	A3594	P3525	M3450	Q3379	L3283	SER	S3152	Y3090	P2873	L2897	T2825	ARG
T3726	L3662	E3595	Q3527	L3451	Q3379	L3283	ASP	Q3154	L3092	E2946	L2897	T2825	PHE
V3728	T3663	L3596	A3528	K3452	F3382	R3287	MET	P3155	Q3093	L3027	L2897	T2825	MET
M3729	N3664	V3601	I3529	A3453	F3382	R3288	GLU	P3156	B3094	N3028	L2897	T2825	ARG
A3730	L3665	N3602	V3530	L3454	L3385	R3289	VAL	L3157	D3095	L2947	L2897	T2825	ASP
R3733	L3666	K3603	P3532	K3455	L3385	R3289	GLN	Q3096	V3096	K3029	L2897	T2825	GLN
R3734	L3667	K3604	F3532	L3456	A3388	E3295	GLU	D3097	V3096	W3031	L2897	T2825	GLN
P3735	L3668	N3605	F3533	N3457	V3389	E3295	GLN	L3161	R3098	L3034	L2897	T2825	LYS
R3736	L3669	L3606	L3534	S3458	Q3390	L3298	GLN	W3164	A3099	P3034	L2897	T2825	LYS
R3737	N3670	E3607	L3535	K3459	A3391	T3299	GLU	W3164	K3100	F3035	L2897	T2825	SER
R3738	N3671	K3608	Y3540	N3460	A3392	V3300	GLU	W3164	K3100	F3035	L2897	T2825	SER
I3739	K3672	M3609	Y3540	A3481	E3393	L3301	D3226	R3167	Y3102	Q3037	L2897	T2825	LEU
E3740	K3675	Y3610	D3544	R3462	E3394	K3302	I3227	I3168	I3103	Q3038	L2897	T2825	MET
R3741	P3676	L3612	T3545	K3464	E3395	T3303	S3228	P3169	Q3104	T3039	L2897	T2825	TYR
R3741	P3676	L3612	T3545	K3464	A3396	V3304	I3231	D3170	N3105	Y3040	L2897	T2825	ARG

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

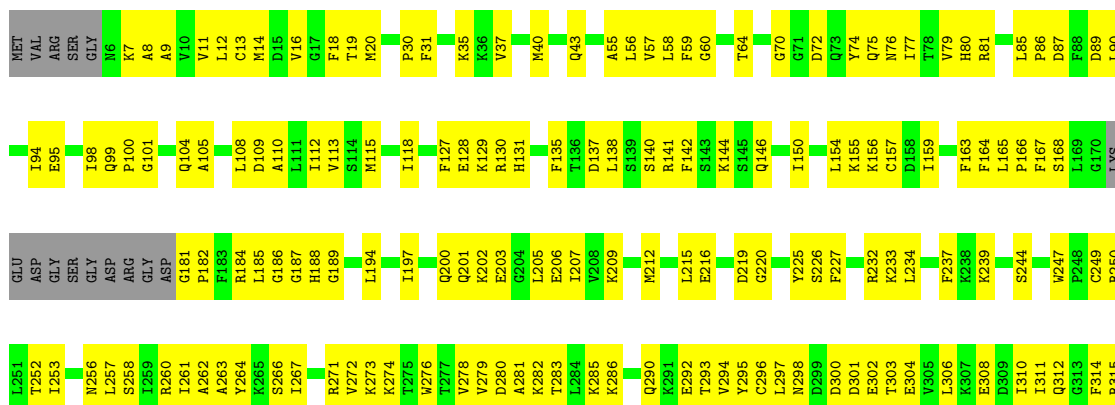
• Molecule 2: X-ray repair cross-complementing protein 6

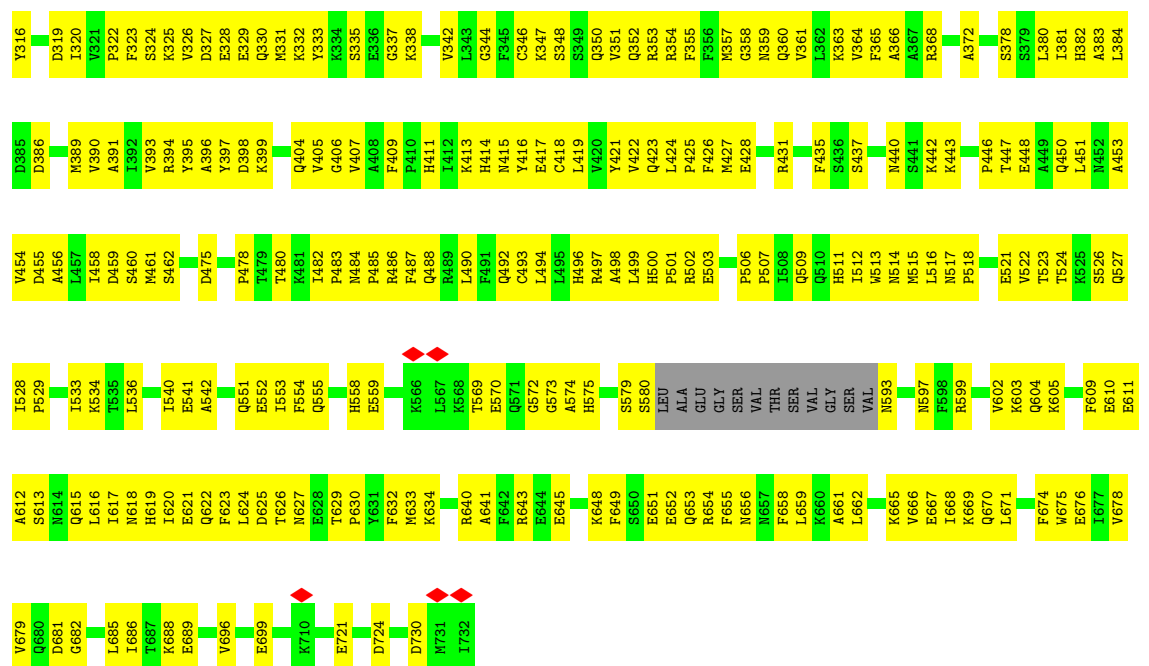
Chain G: 35% 45% 20%



• Molecule 3: X-ray repair cross-complementing protein 5

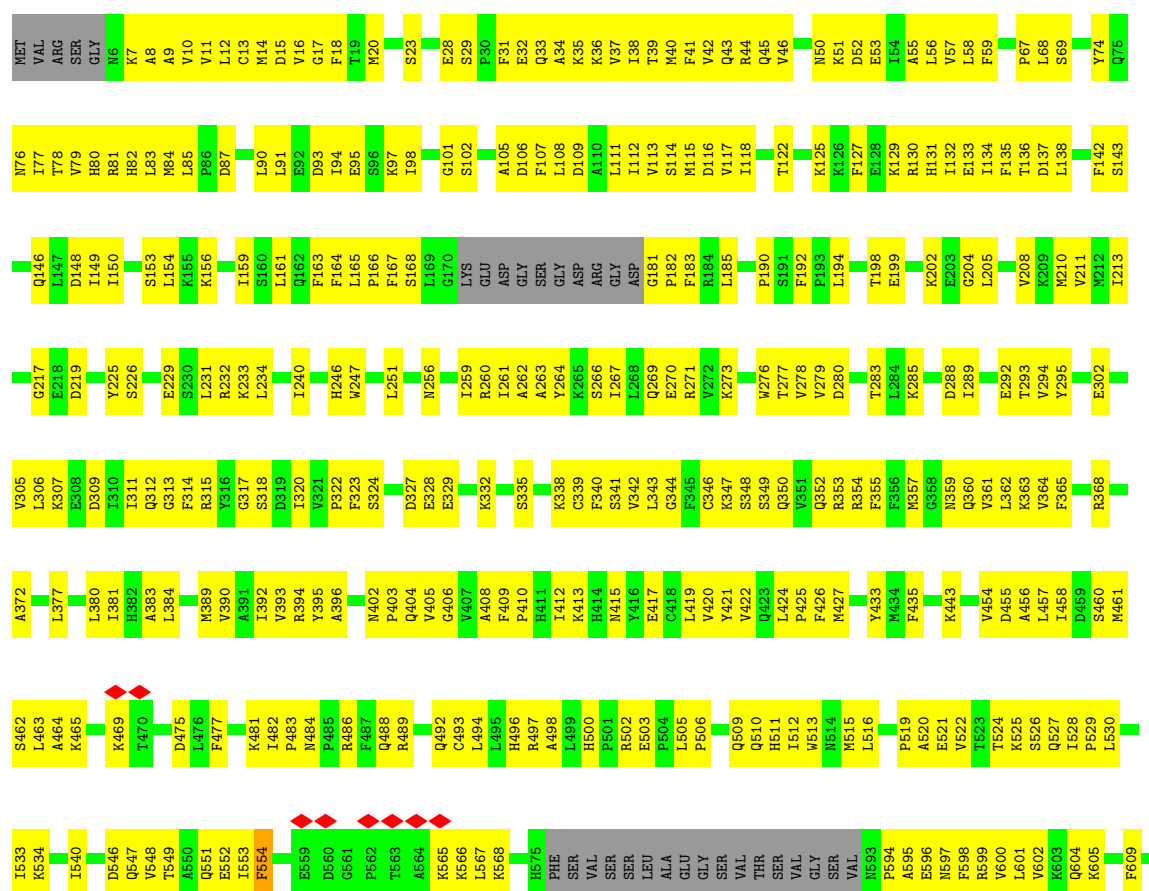
Chain C: 43% 53%

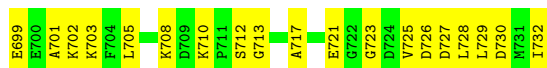
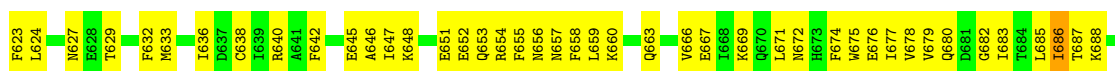




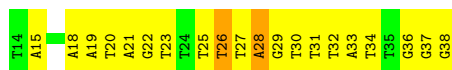
• Molecule 3: X-ray repair cross-complementing protein 5

Chain H: 43% 52% .





• Molecule 4: DNA (25-MER)



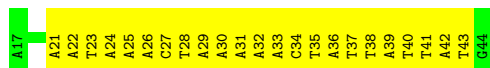
• Molecule 5: DNA (27-MER)



• Molecule 6: DNA (26-MER)



• Molecule 7: DNA (28-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10808	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 ($e^-/\text{\AA}^2$)	52.97	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	0.469	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	588.0, 588.0, 588.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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	0.28	0/29462	0.55	1/39939 (0.0%)
1	F	0.25	0/29464	0.49	1/39913 (0.0%)
2	B	0.25	0/3864	0.52	0/5226
2	G	0.22	0/3871	0.49	0/5236
3	C	0.19	0/5595	0.41	0/7557
3	H	0.19	0/5625	0.45	1/7589 (0.0%)
4	J	0.33	0/570	0.55	2/876 (0.2%)
5	I	0.31	0/620	0.39	0/953
6	D	0.38	0/591	0.47	0/908
7	E	0.33	0/644	0.39	0/990
All	All	0.26	0/80306	0.50	5/109187 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2259	LYS	CB-CG-CD	6.56	126.38	111.30
4	J	28	DA	C2'-C3'-O3'	-6.37	101.95	111.50
1	A	212	VAL	N-CA-C	-5.83	105.70	112.98
4	J	26	DT	C2'-C3'-O3'	-5.34	103.49	111.50
3	H	686	ILE	N-CA-C	-5.12	108.85	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	29018	0	28461	2444	0
1	F	29012	0	28652	2271	0
2	B	3789	0	3721	359	0
2	G	3797	0	3734	326	0
3	C	5490	0	5397	402	0
3	H	5517	0	5468	397	0
4	J	509	0	271	33	0
5	I	552	0	301	35	0
6	D	528	0	282	49	0
7	E	573	0	312	48	0
All	All	78785	0	76599	6108	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 40.

The worst 5 of 6108 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:3443:PRO:HB2	1:A:3478:GLU:CB	1.66	1.26
2:G:271:VAL:HG12	2:G:370:PRO:CA	1.72	1.20
1:A:446:PHE:H	1:A:447:PRO:CD	1.54	1.19
2:G:271:VAL:CG1	2:G:370:PRO:HA	1.72	1.17
2:G:273:ILE:CG1	2:G:368:VAL:HG22	1.75	1.13

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	3714/4156 (89%)	3263 (88%)	446 (12%)	5 (0%)	48	83
1	F	3675/4156 (88%)	3257 (89%)	416 (11%)	2 (0%)	48	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	485/609 (80%)	422 (87%)	63 (13%)	0	100	100
2	G	485/609 (80%)	428 (88%)	56 (12%)	1 (0%)	43	78
3	C	699/732 (96%)	633 (91%)	66 (9%)	0	100	100
3	H	694/732 (95%)	625 (90%)	69 (10%)	0	100	100
All	All	9752/10994 (89%)	8628 (88%)	1116 (11%)	8 (0%)	49	83

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	PHE
1	A	3487	ILE
2	G	372	GLU
1	F	2257	PHE
1	A	2333	ARG

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	3033/3671 (83%)	3027 (100%)	6 (0%)	87	87
1	F	3087/3671 (84%)	3084 (100%)	3 (0%)	88	89
2	B	400/548 (73%)	398 (100%)	2 (0%)	81	83
2	G	402/548 (73%)	399 (99%)	3 (1%)	76	81
3	C	591/649 (91%)	591 (100%)	0	100	100
3	H	601/649 (93%)	600 (100%)	1 (0%)	87	87
All	All	8114/9736 (83%)	8099 (100%)	15 (0%)	85	87

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	271	VAL
2	G	534	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	554	ASN
3	H	554	PHE
2	G	271	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	330	ASN
1	F	1477	HIS
2	G	515	ASN
1	F	477	ASN
1	F	1146	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	4128:MET	C	5009:UNK	N	96.98
1	A	4128:MET	C	5009:UNK	N	96.43
1	A	5016:UNK	C	6004:UNK	N	49.12
1	F	5016:UNK	C	6004:UNK	N	48.83

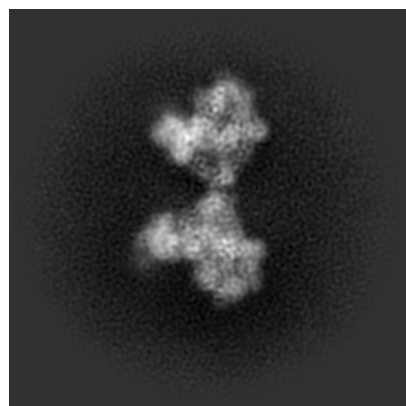
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11219. These allow visual inspection of the internal detail of the map and identification of artifacts.

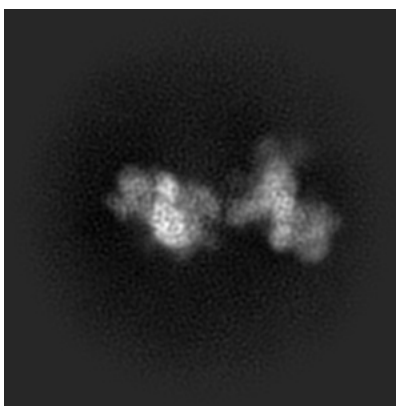
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

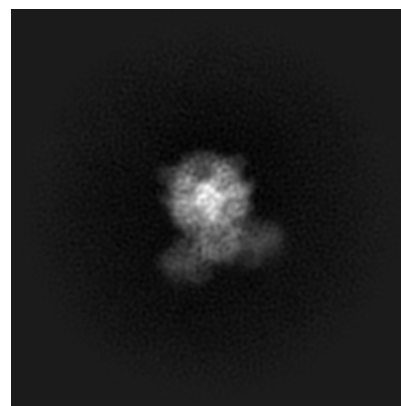
6.1.1 Primary map



X

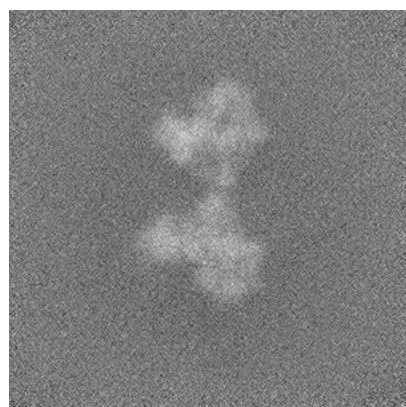


Y

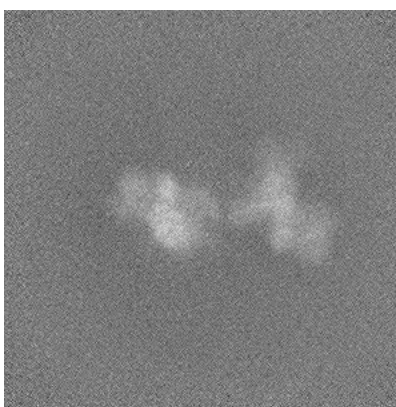


Z

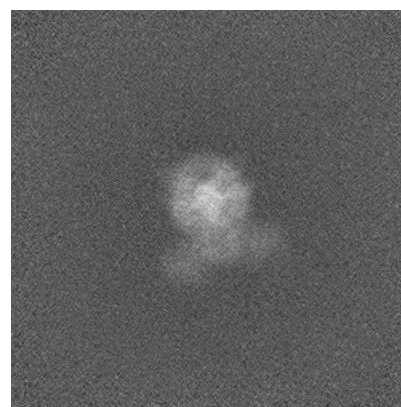
6.1.2 Raw map



X



Y

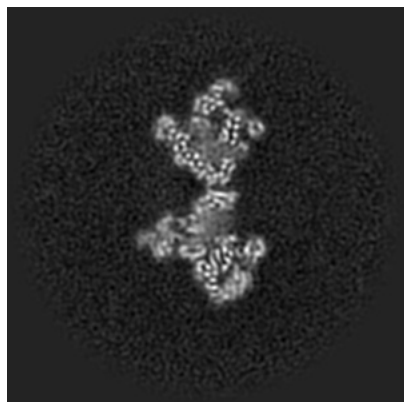


Z

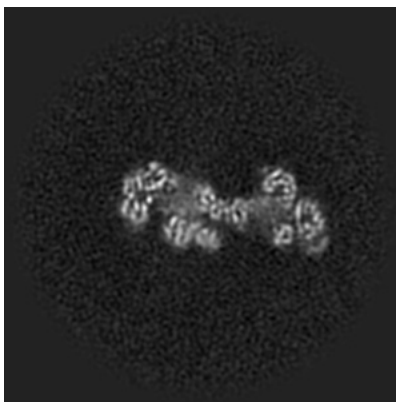
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

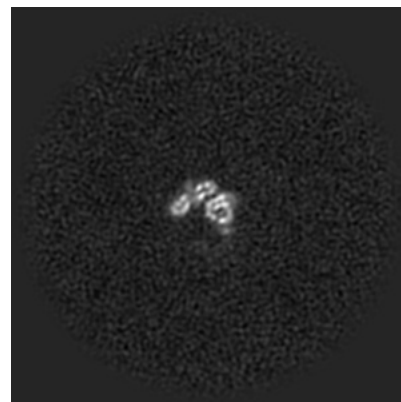
6.2.1 Primary map



X Index: 280

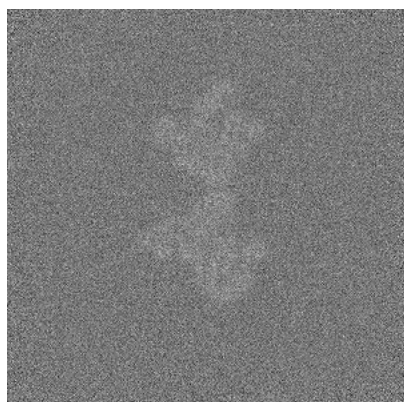


Y Index: 280

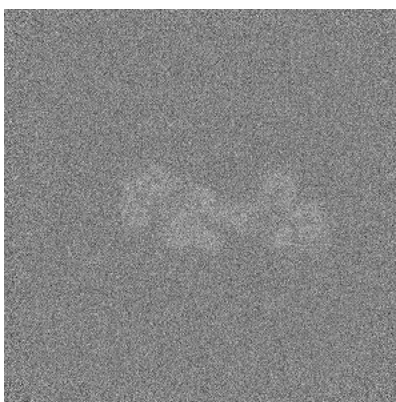


Z Index: 280

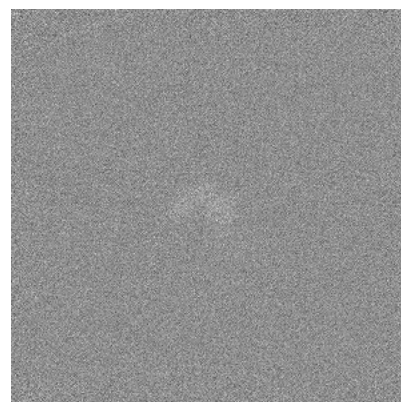
6.2.2 Raw map



X Index: 280



Y Index: 280

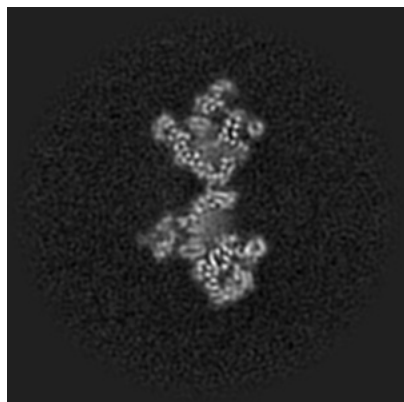


Z Index: 280

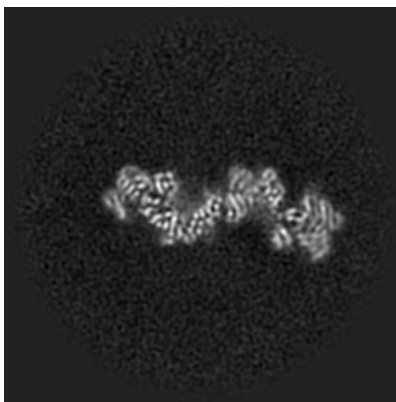
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

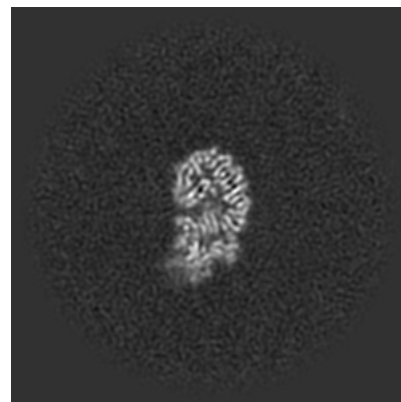
6.3.1 Primary map



X Index: 282

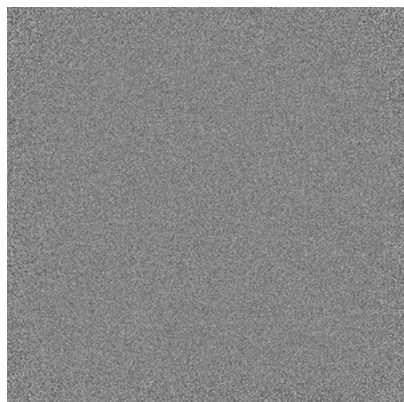


Y Index: 299

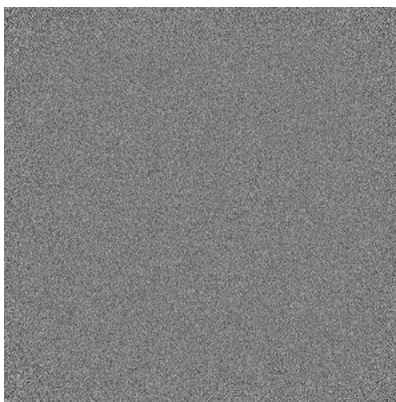


Z Index: 225

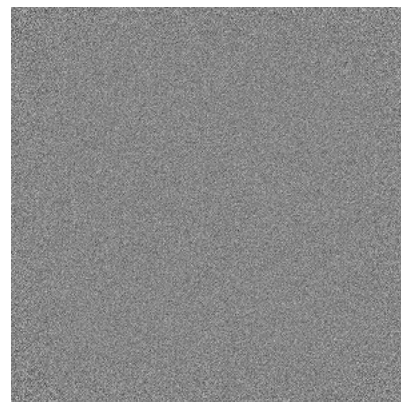
6.3.2 Raw map



X Index: 0



Y Index: 0

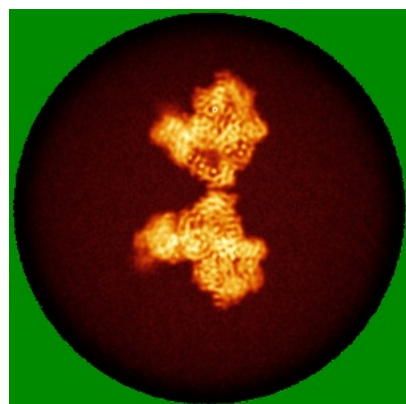


Z Index: 0

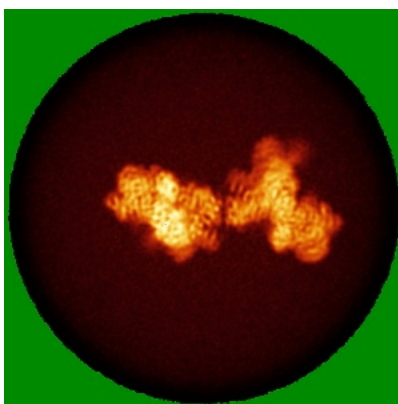
The images above show the largest variance slices of the map in three orthogonal directions.

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

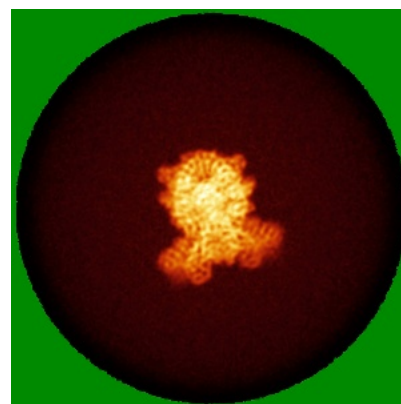
6.4.1 Primary map



X

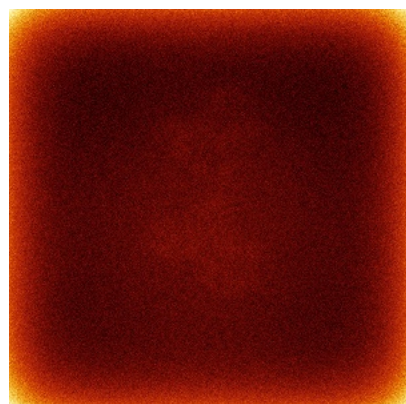


Y

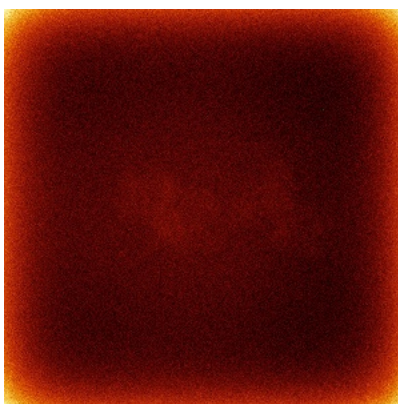


Z

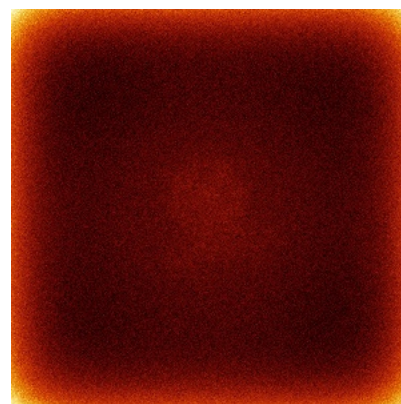
6.4.2 Raw map



X



Y

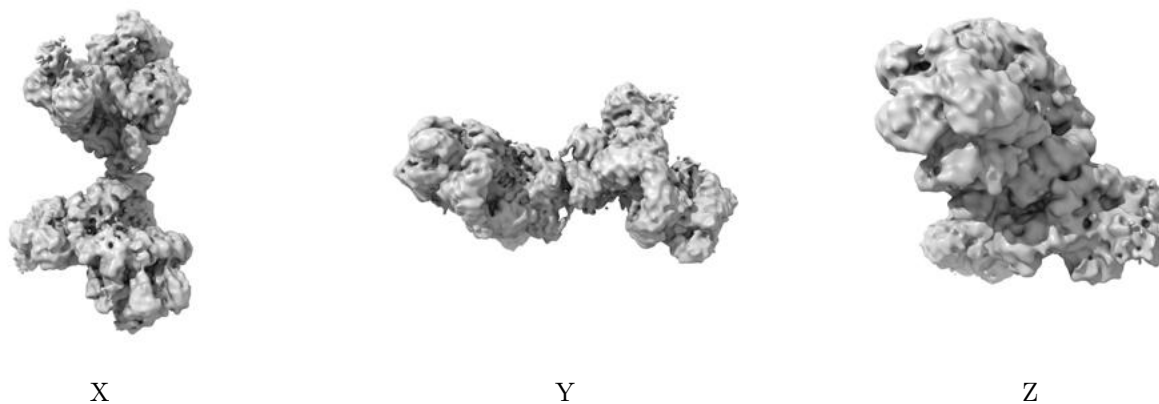


Z

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.

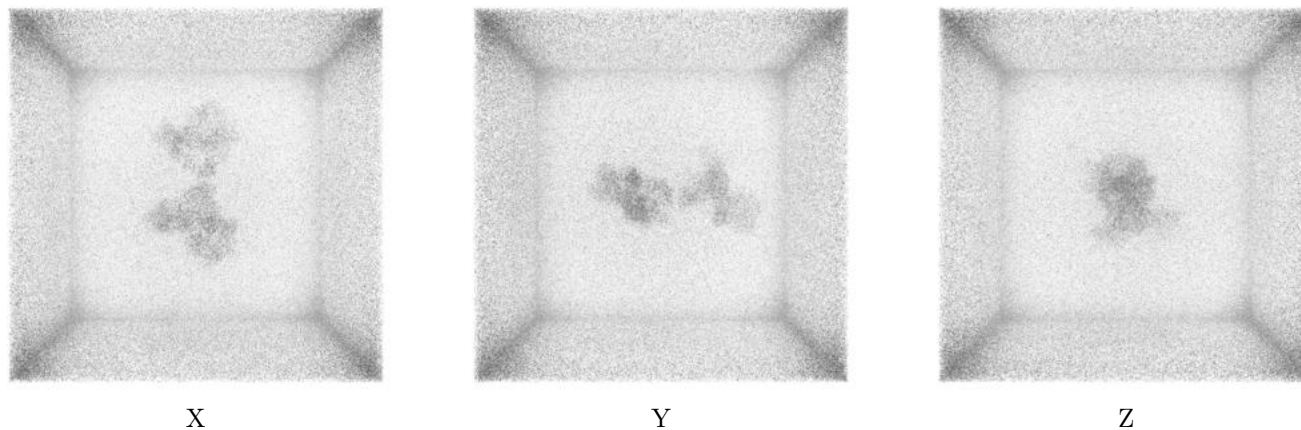
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. 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.

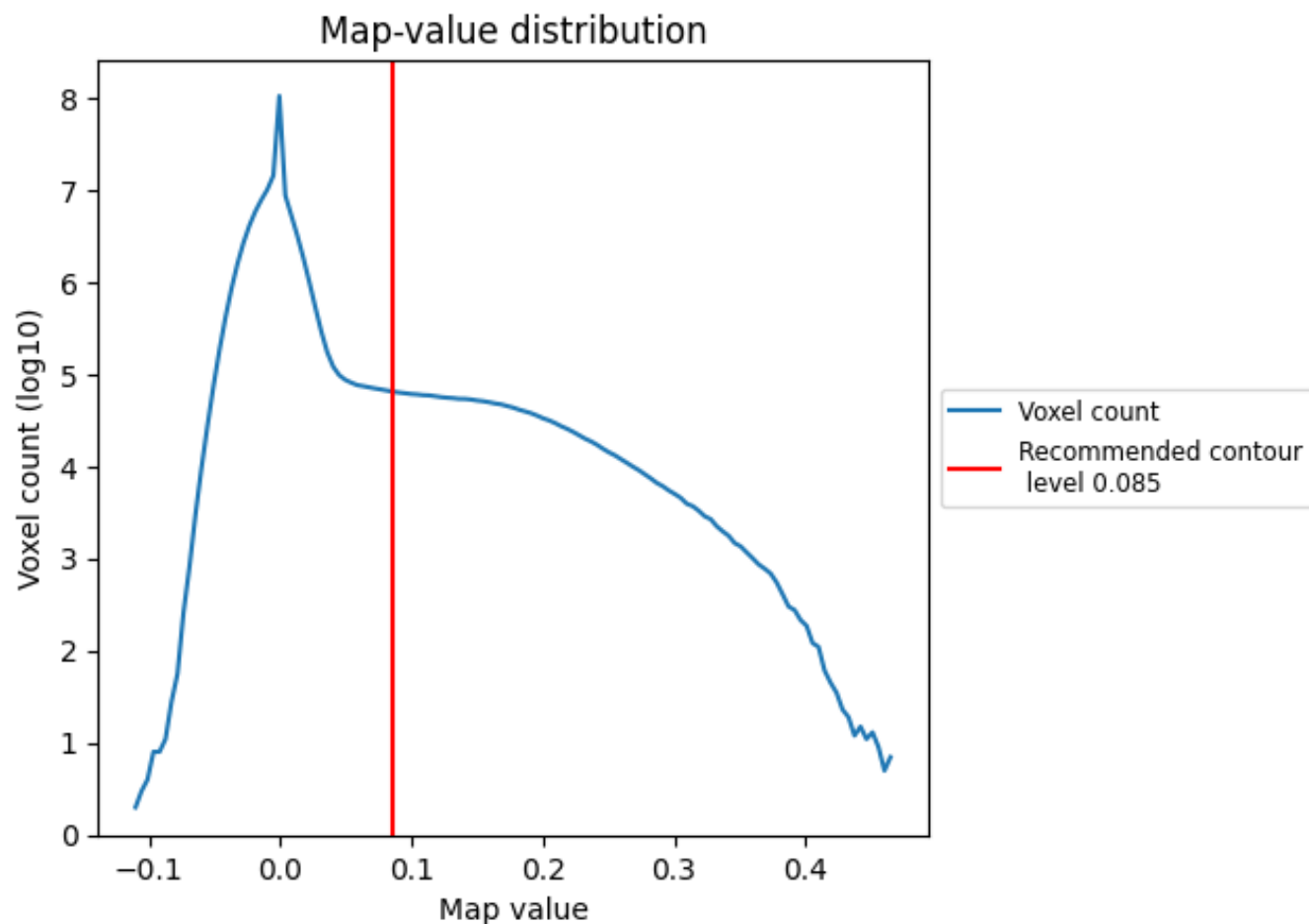
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

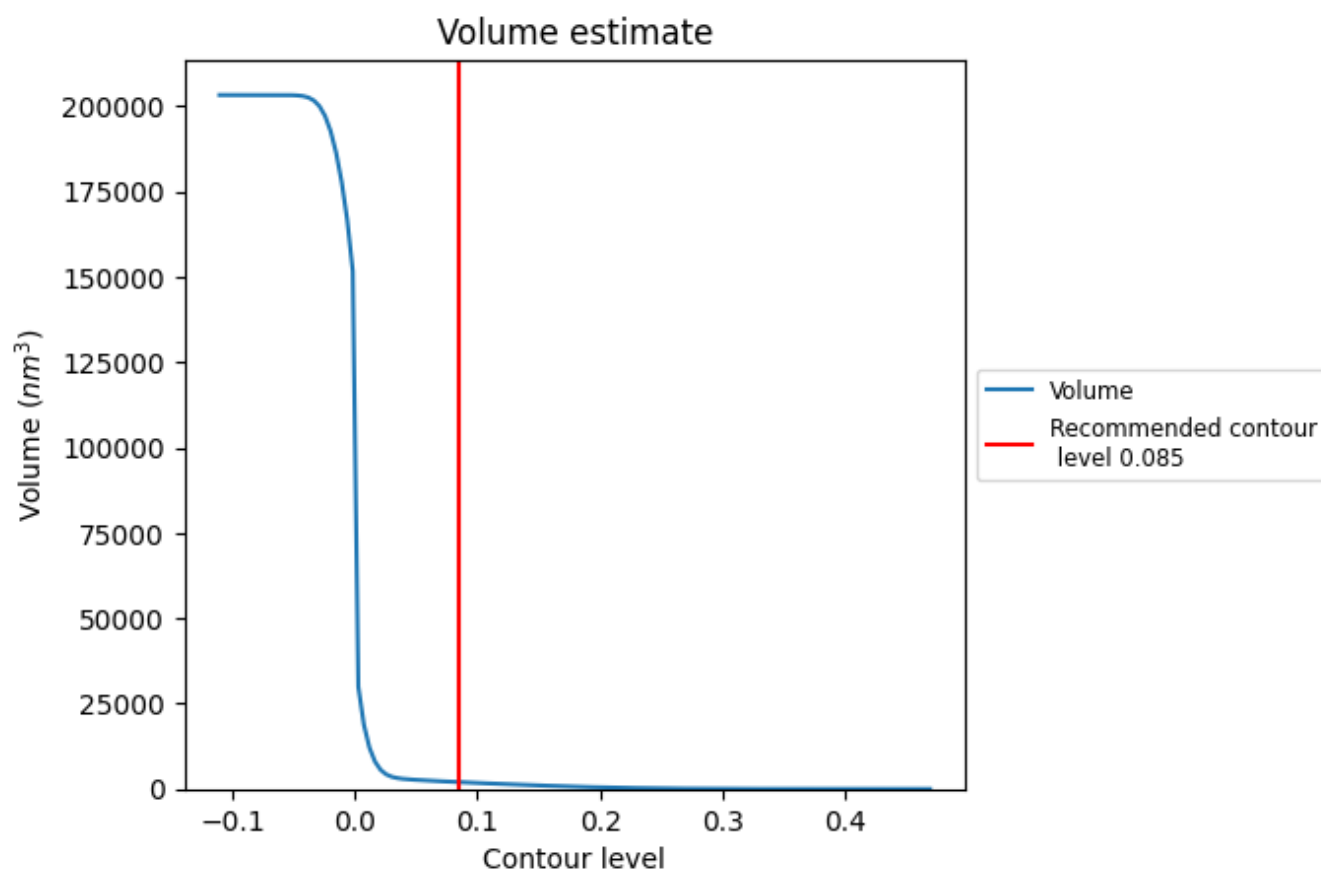
This section contains the results of statistical analysis of the map.

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.

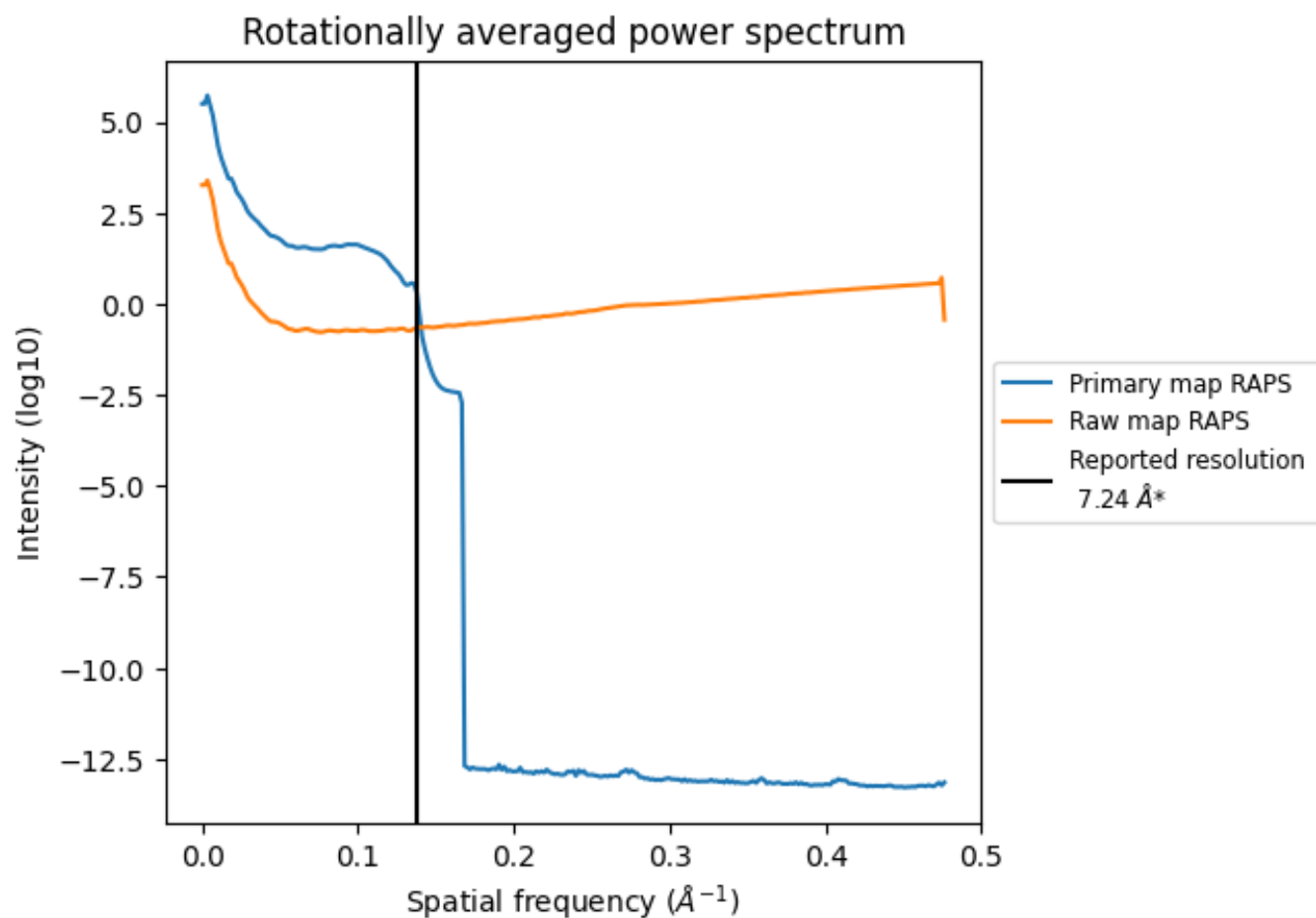
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1998 nm³; this corresponds to an approximate mass of 1805 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 ⓘ

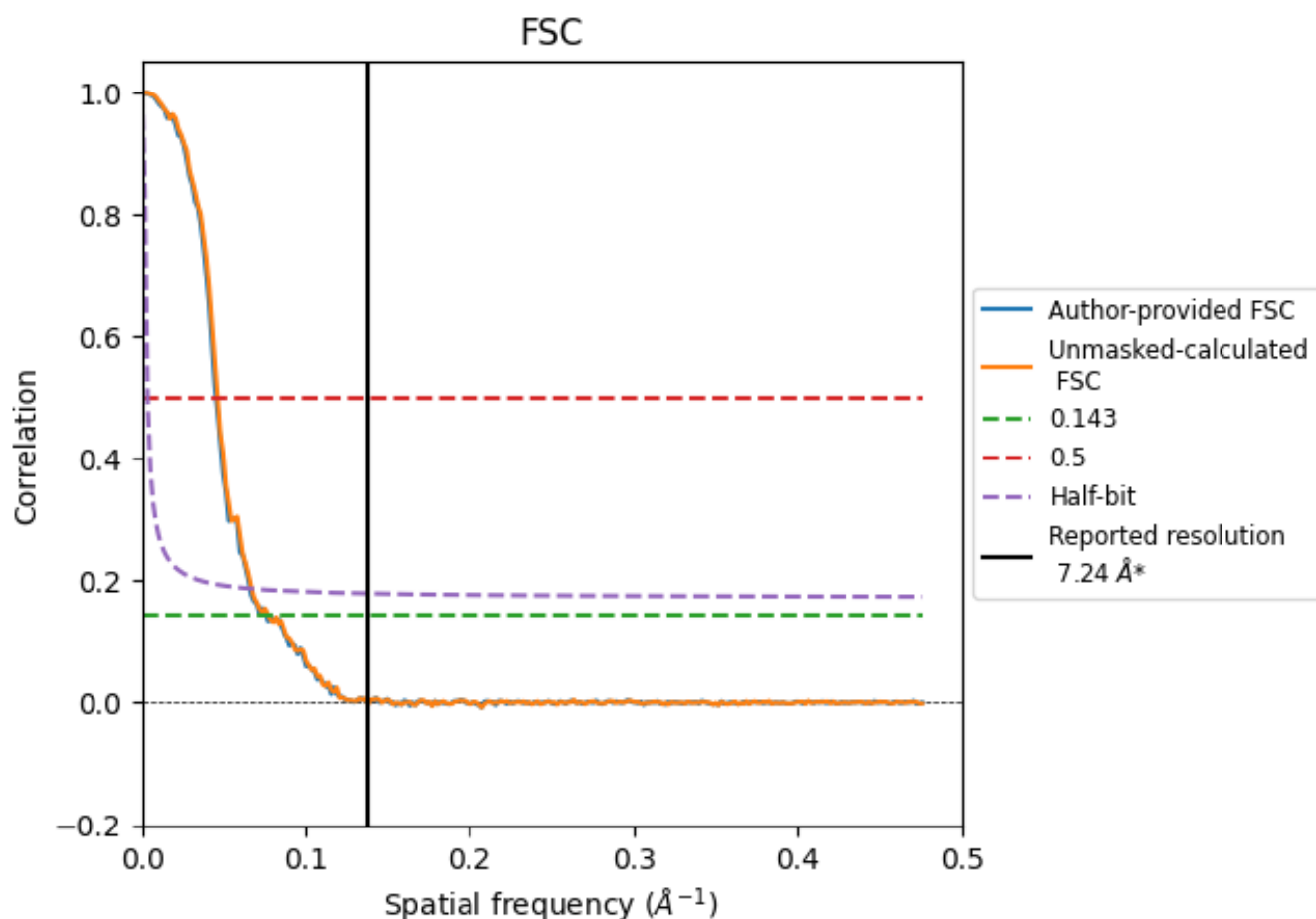


*Reported resolution corresponds to spatial frequency of 0.138 $\text{\AA}^{-1}$

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 0.138 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.24	-	-
Author-provided FSC curve	13.23	22.27	15.24
Unmasked-calculated*	13.02	21.74	14.99

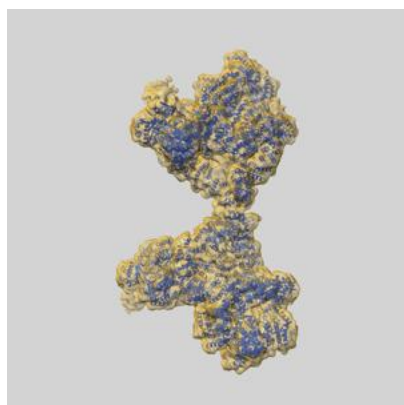
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 13.23 differs from the reported value 7.24 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.02 differs from the reported value 7.24 by more than 10 %

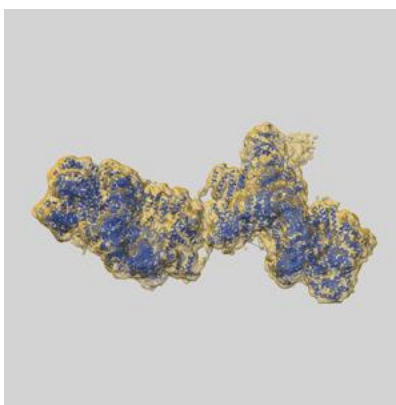
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11219 and PDB model 6ZHE. Per-residue inclusion information can be found in section 3 on page 6.

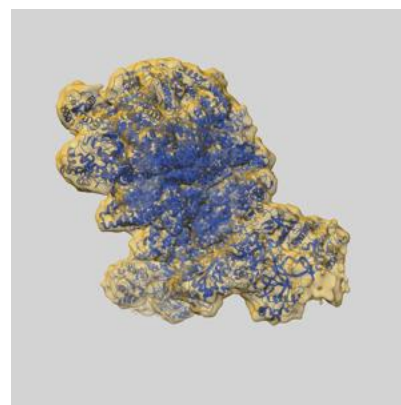
9.1 Map-model overlay [i](#)



X



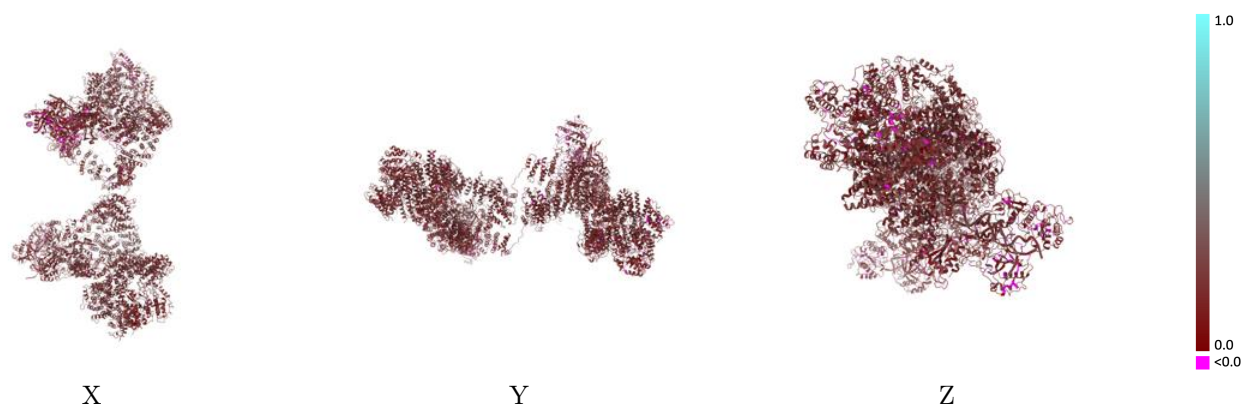
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 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](#)

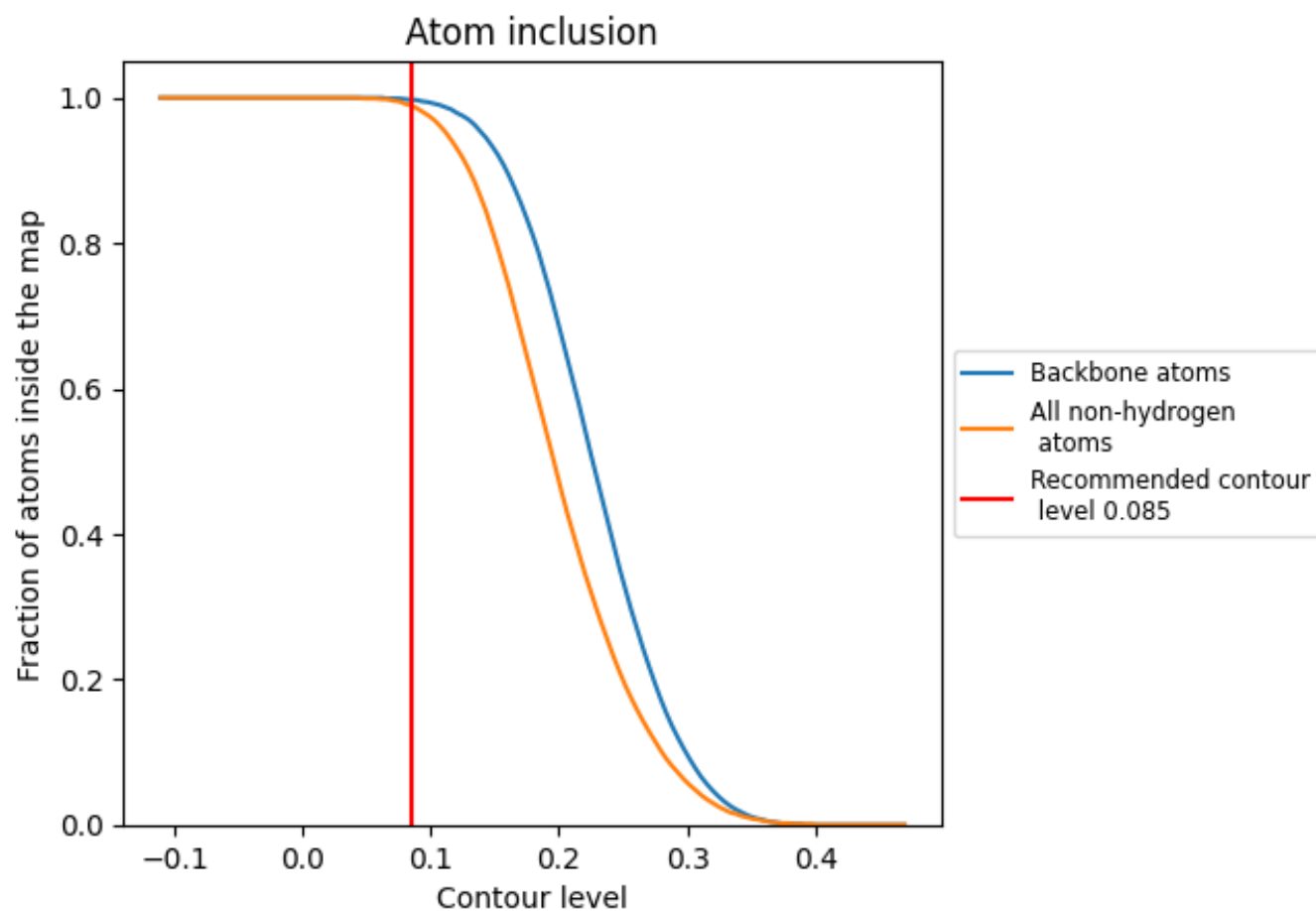


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9890	0.1950
A	0.9910	0.2070
B	0.9950	0.1870
C	0.9840	0.1740
D	1.0000	0.2510
E	1.0000	0.2500
F	0.9890	0.1970
G	0.9900	0.1600
H	0.9730	0.1600
I	1.0000	0.2540
J	1.0000	0.2430

1.0

0.0

<0.0