



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 12:37 AM UTC

PDB ID : 8BHV / pdb_00008bhv
EMDB ID : EMD-16070
Title : DNA-PK XLF mediated dimer bound to PAXX
Authors : Hardwick, S.W.; Chaplin, A.K.
Deposited on : 2022-11-01
Resolution : 4.51 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

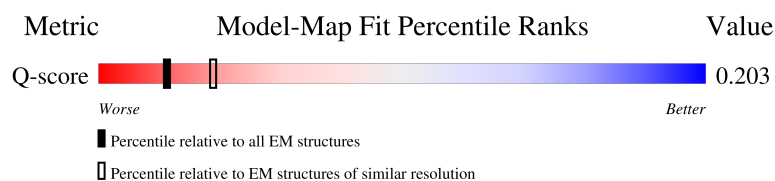
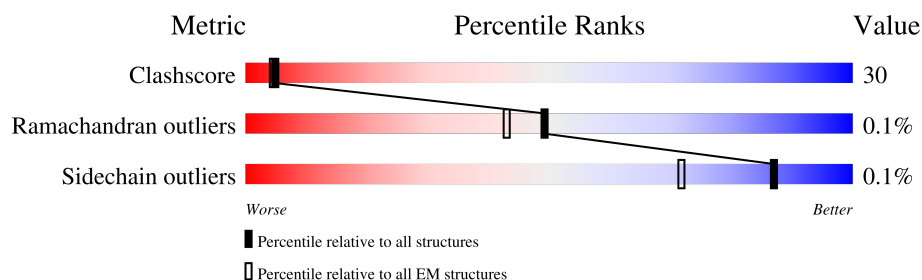
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.51 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	2518 (4.01 - 5.01)

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	
1	F	4128	
2	K	336	
2	L	336	

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Mol	Chain	Length	Quality of chain
2	N	336	
2	O	336	
3	M	911	
3	P	911	
4	Q	299	
4	R	299	
5	a	609	
5	h	609	
6	b	732	
6	j	732	
7	c	204	
7	i	204	
8	D	27	
9	E	28	
10	I	24	
11	J	24	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 91357 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	3549	Total	C	N	O	S	0	0
			28250	18146	4783	5134	187		
1	F	3543	Total	C	N	O	S	0	0
			28263	18162	4780	5132	189		

- Molecule 2 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
2	L	195	Total	C	N	O	S	0	0
			1589	1009	271	302	7		
2	N	201	Total	C	N	O	S	0	0
			1625	1030	278	310	7		
2	O	194	Total	C	N	O	S	0	0
			1589	1009	271	302	7		

- Molecule 3 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	258	Total	C	N	O	S	0	0
			2085	1327	349	396	13		
3	P	246	Total	C	N	O	S	0	0
			1983	1261	339	371	12		

- Molecule 4 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	218	Total	C	N	O	S	0	0
			1745	1119	294	319	13		
4	R	225	Total	C	N	O	S	0	0
			1796	1150	301	330	15		

- Molecule 5 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	505	Total	C	N	O	S	0	0
			4038	2583	691	747	17		
5	h	505	Total	C	N	O	S	0	0
			4026	2578	681	750	17		

- Molecule 6 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	650	Total	C	N	O	S	0	0
			5214	3328	876	985	25		
6	j	636	Total	C	N	O	S	0	0
			5082	3252	854	951	25		

- Molecule 7 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	23	Total	C	N	O	S	0	0
			165	105	27	32	1		
7	i	23	Total	C	N	O	S	0	0
			162	102	27	32	1		

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	27	Total	C	N	O	P	0	0
			556	268	95	166	27		

- Molecule 9 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	28	Total	C	N	O	P	0	0
			576	277	107	164	28		

- Molecule 10 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	24	Total	C	N	O	P	0	0
			494	238	92	140	24		

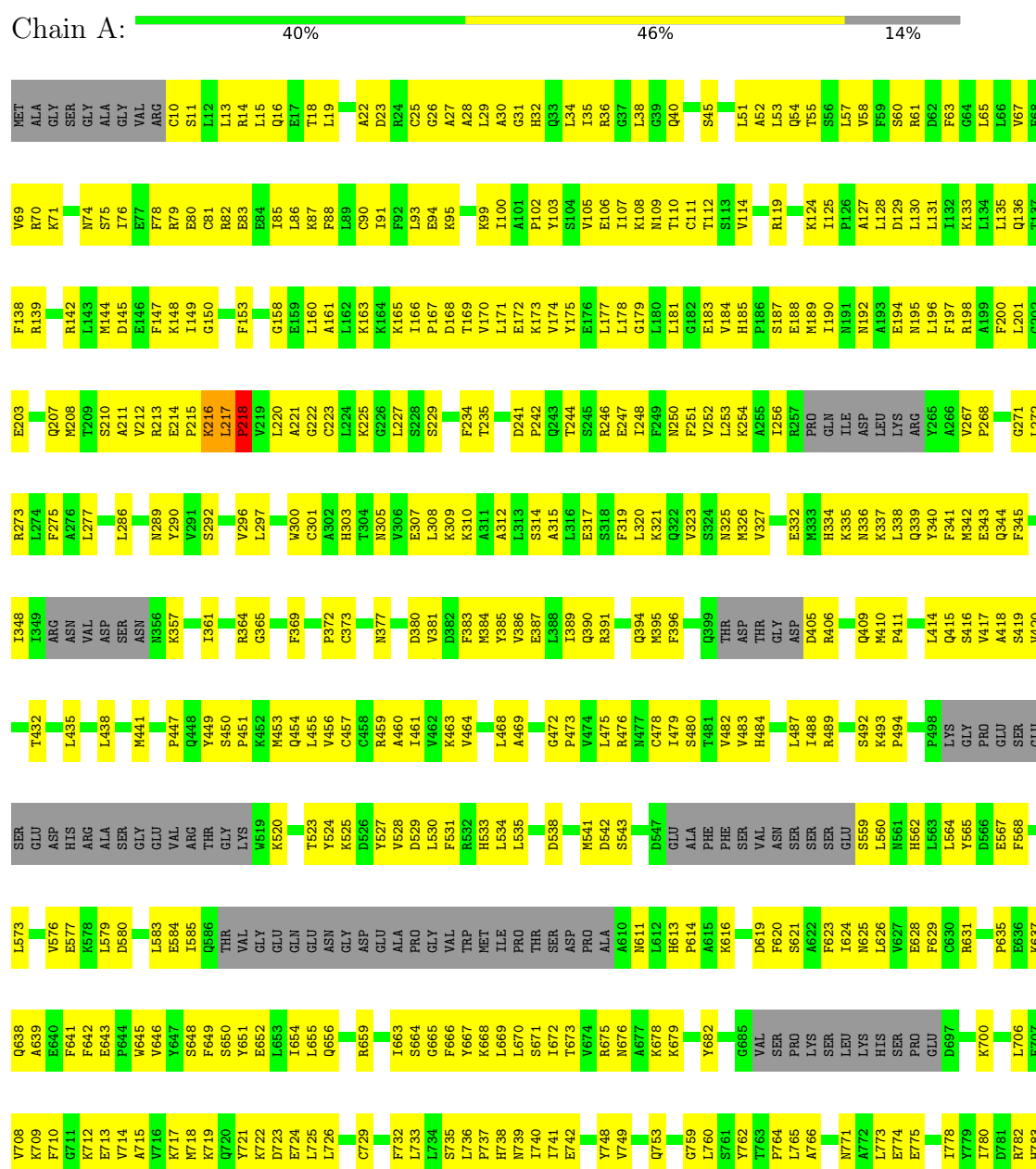
- Molecule 11 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	24	Total 491	C 239	N 79	O 149	P 24	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.

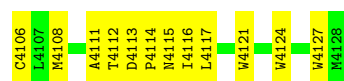
- Molecule 1: DNA-dependent protein kinase catalytic subunit





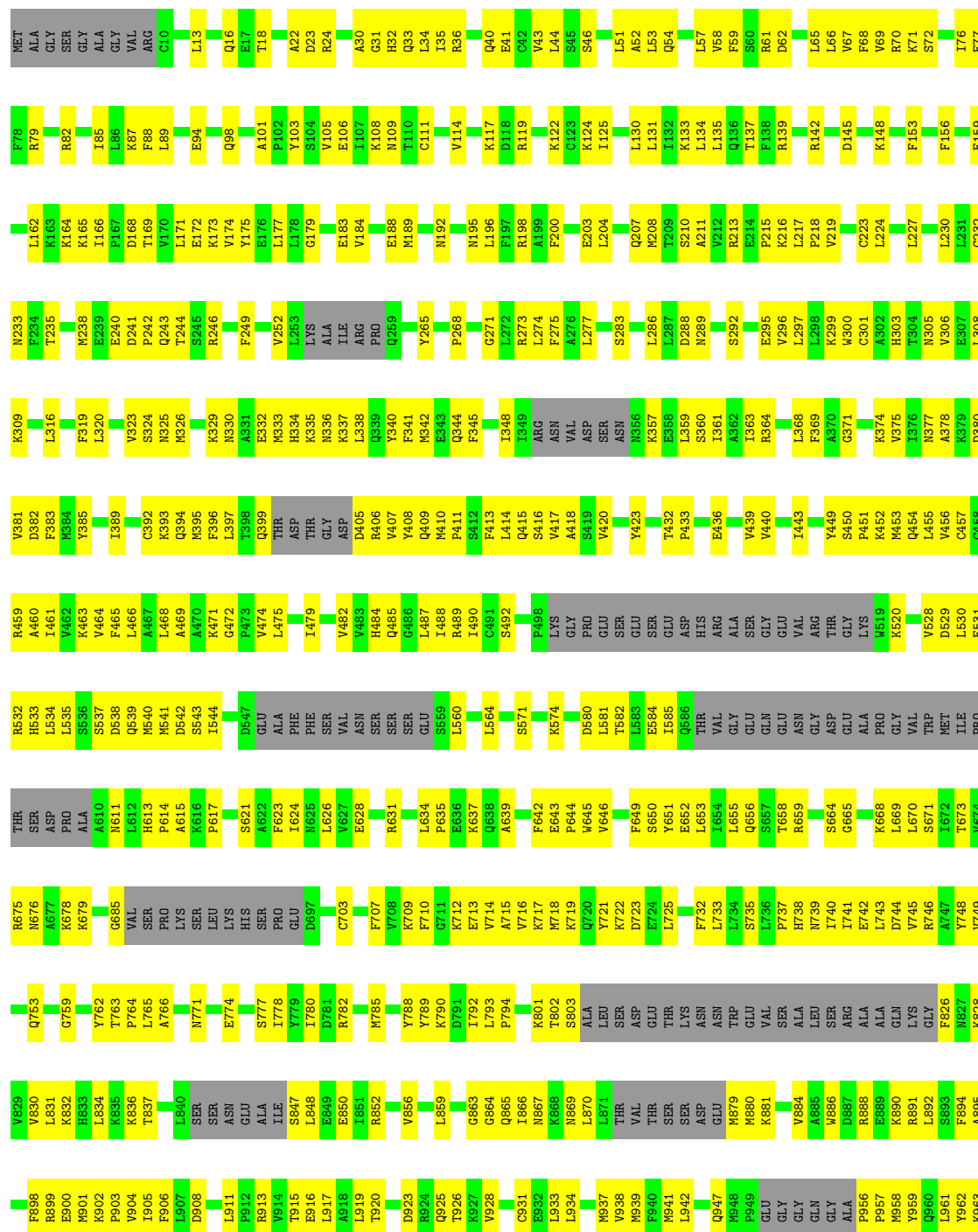






● Molecule 1: DNA-dependent protein kinase catalytic subunit

Chain F: 40% 46% 14%

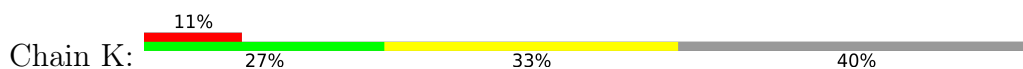




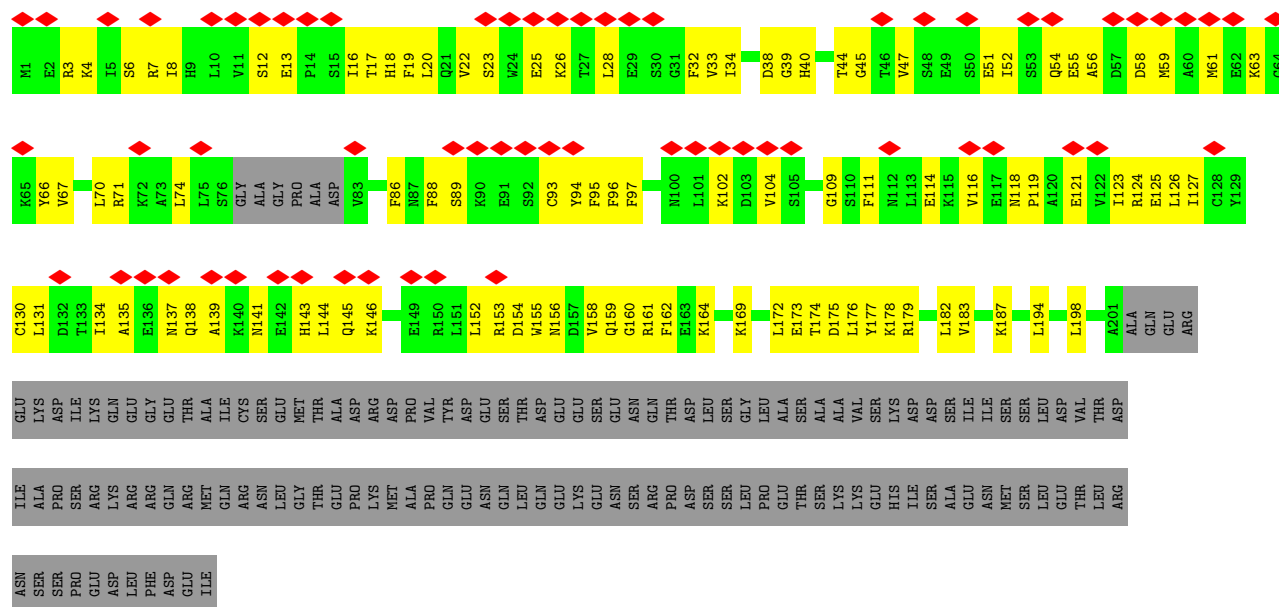
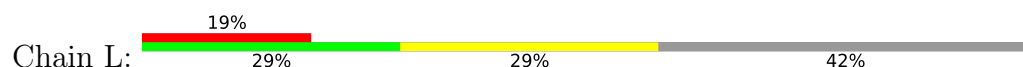
I3065	T2987	GLY	A749	GLY	K2549	N2475	E2406	N2335	P2265	L2194	PRO	SER
E2988	E2988	LYS	E2750	SER	I2550	L2476	G2407	I2336		S2195	R2120	GLN
A2989	K2829	SER	R2763	LEU	E2551	L2477	M2408		K2268	W2196	R2123	ASP
E2990	N2830	GLU	R2763	SER	E2552	K2478		E2339	D2269		P2123	PRO
K2991	ARG	ARG	E2754	ALA	H2553	K2479	L2411		D2270	L2199	S2124	ARG
	Q2834	LEU	K2765	ALA	L2555	N2480	F2413	C2342	S2271	A2200	W2125	PRO
F2993	F2840	GLN	E2756	TRP	L2555	L2480	F2413		V2272	T2201	M2126	ALA
E2994		ARG		PRO	S2556		Q2414	A2346	G2273	P2202		THR
E2995	F2840	ARG	L2757	ALA	L2557		L2415	F2347	L2274	P2206	H2130	GLY
	F2843	ALA	E2759	ALA		K2485	K2416		Q2275		L2133	ARG
L2999	E2760	LEU	L2761	GLY	F2561	D2486	S2417	L2348	Q2276		L2133	PHE
D3000	L2926	GLN		ILE		PRO	K2418	K2350	L2277	E2209	G2134	ARG
C3001	L2761	SER		GLU	E2564	GLU	D2419	Q2351	G2278		N2135	ARG
		VAL	V2769	ARG	K2565	SER	F2420	H2352	I2279	R2214		ARG
L3004	F2850	GLY		ALA	T2566	GLU		Q2353	V2280		L2140	GLU
L3088	F2851	PRO	R2773	THR	S2567	T2491	M2424	Q2354		F2218		GLN
L3089	F2854	ASP	S2774	GLN	N2568	D2492		N2355	N2283	L2219	R2143	ARG
Y3090	Y2775	PHE	K2776	GLN	S2569	N2493	R2427	M2356	M2220	M2220		ASP
D3094	R2776	GLY	R2776	GLN	P2570	D2494	D2428	E2357	K2221	K2221	L2149	PRO
D3095	G2777	LYS	D2777	HIS	D2571		D2429	D2358	V2222	V2222	V2150	THR
V3096	G2778	LYS		ASP	Y2572	E2497	E2430	D2359	H2223	H2223	L2151	VAL
D3097	D2779	ARG	D2779	PHE	N2573	F2498	R2431	F2360	F2224	F2224	N2152	HIS
R3098	D2860	LEU	L2780	THR	N2574	F2499	Q2432	T2361	C2292	C2292	T2153	ASP
A3099	L2861	GLY	P2781	GLY	P2575	K2500	K2433	C2363	G2293	P2226	E2154	ASP
K3100	S2862	LEU	D2782	THR	M2576		V2434	V2362	I2294	K2227	E2155	VAL
	C2863	PRO	L2783	GLN	F2577	K2503	C2435	L2364	Q2295	R2228	V2156	LEU
I3103	Q2864	GLY	Q2784	THR	E2578		L2436	N2365	S2296	A2229	F2157	GLU
Q3104	Q2865	ASP	L2785	ALA	H2579	L2507	D2437	K2366	S2297	V2230	R2158	LEU
N3105	A2866	GLU	H2787	ASP	P2580	L2507	L2437	K2367	E2298	F2231	P2159	GLU
		VAL		GLY	L2581	L2510	L2439	T2368	Y2299	F2231	Y2160	MET
I3107		ASP		ARG	S2582	L2511	Y2440	F2300	P2300	H2233	A2161	ASP
Q3108	L2869	ASN	L2791	ASN	E2583		K2441	P2372	Q2301	N2234	K2162	GLU
S3109	L2871	LYS	T2792	SER	C2584	Q2518	M2442		L2334	W2236	H2163	LEU
F3110	P2793	VAL	L2794	PHE	E2585		M2443	D2376	N2305	E2236	W2164	ASN
Q3111	G2879	GLY	L2795	ASP	F2586	R2522	L2446	K2377	N2306	I2237	L2165	
N3112	C2880	GLY	Q2796	TRP		F2524	K2447	N2379	M2307	I2238	S2166	
N3113	A2796	ALA	V2797	LEU	Y2589	F2524	L2446	N2380	S2308		P2167	
Y3114	V2797	ALA		THR	T2590	W2525	E2450	A2381	S2308	L2241	L2168	
	Q2885			GLY	I2591	S2526	L2451	V2382	F2309	V2242	L2169	
I3117	V2888	SER	R2800	SER	T2603	H2527	R2452	F2383	R2310	E2243	Q2170	
D3118	R2801	THR	D2801	THR	PRO	T2529	R2455		R2311	C2244	L2171	
V3119	R2891	ASP	L2804	ASP	NET	R2530	L2455	L2386	Y2312	W2245	A2172	
L3120	L2892	PRO	A2805	PRO	PHE	L2531	K2456	P2387	K2313	D2247	W2176	
L3121	L2893	LEU	K2806	LEU	VAL	P2532	P2457	K2388	E2314	C2248	H2103	
H3122	E2894	VAL	Q2807	VAL	GLU	S2533	V2458	F2389	V2315	L2249	W2104	
Q3123	E2895	ASP	L2728	ASP	THR	H2534			Y2316	S2250	H2105	
S3124	L2897	HIS	R2730	HIS	GLN	T2535	F2461	G2391	A2317	I2251	R2106	
R3125		THR	F2809	THR	ALA	L2536		V2392	A2320	P2252	G2181	
L3126	L2901	SER	S2810	SER	SER	D2537	H2464	L2393	E2321	Y2253	L2182	
L3127	PRO	PRO	S2811	PRO	GLN	R2538	F2465	K2394		R2294	H2183	
K3128	ALA	ALA	L2812	ALA	GLY	R2539	S2466	T2395	L2325	L2255	Y2184	PRO
L3129	GLU	THR	F2813	THR	THR	L2540	T2467	L2396	I2326	I2256	M2185	PRO
Q3130	LEU	ASP	L2817	ASP	LEU	K2541	T2468	C2397	L2327	F2257	V2186	GLN
S3131	PRO	SER	K2818	SER	GLN	L2542	C2469	L2398	R2328	K2258	V2187	GLY
	ALA	LEU	E2819	LEU	THR	W2543	R2470	E2399	Y2329	E2259	I2188	GLY
L3135	LYS	LEU	M2820	LEU	ARG	S2544	E2471	V2400	V2330	F2260	I2189	GLU
	LYS	PHE		PHE	THR		Q2472					ASP
I3138	VAL	THR	K2824	THR	GLN	S2547	M2473	R2404	R2333	K2263	T2192	SER
Q3139	ARG	GLU	T2825	GLU			Y2474	V2405	K2334	D2264	I2193	VAL
E3140	ARG											

W4124	R4041	K3975	P3879	L3806	R3737	K3870	K3588	A3513	V3447	R3380	C3281	GLN
E4125	Q4042	E3976	A3860	E3907	I3738	M3671	S3589	V3514	E3448	A3581	R3282	ASP
P4126	K4043	T3977	D3881	M3808	I3739	K3672	M3590	K3515	K3449	F3382	F3283	GLY
W4127	L4044	G3978	L3882	T3809	I3740	R3673	K3590	H3516	F3144	F3383	F3284	ASP
M4128	L3979	L3979	R3885	T3811	G3741	S3674	R3593	S3517	K3452	H3384	S3285	PRO
	L4051	M3980	R3885	T3811	R3742	K3675	L3596	V3518	K3453	L3385	C3286	SER
	A4052	Y3981	R3889	D3814	R3743	P3676	L3596	E3519	A3453	L3386	R3287	ASP
	G4053	S3982	R3889	D3814	R3743	P3676	L3596	E3520	K3454	E3387	R3288	ARG
	A4054	I3983	P3894	L3815	D3744	P3677	ALA	I3521	L3454	A3388	R3289	MET
	M4055	M3984	P3894	L3815	E3747	L3680	THR	N3524	N3459	E3389	R3290	GLU
	P4056	V3985	P3894	L3816	K3748	K3681	PRO	Y3525	A3461	E3390	G3292	VAL
	A4057	H3986	F3897	L3817	P3749	C3682	VAL		A3462	E3391	E3295	GLN
	V4058	H3986	L3898	T3819	F3750	C3683	ASN		L3463	E3392	E3295	GLU
I4059	R3992	R3992	L3898	M3820	L3751	S3684	LYS	I3529	K3464	E3393	E3295	GLN
	S3993	R3993	R3992	K3825	V3752	S3684	K3604	I3530	P3465	E3394	E3295	GLU
C4081	D3994	K3994	S3902	K3825	E3755	M3687	K3608	Y3531	P3466	E3395	T3299	ALA
E4082	P3995	K3995	K3992	Y3828	G3756	S3688	M3609	F3532	F3466	ALA	T3299	GLN
L4084	G3996	L3997	I3913	L3829	D3757	F3690	M3609	F3532	P3466	PRO	L3301	D3226
H4088	L3998	L3998	I3920	S3830	L3758	K3691	R3612	F3533	P3466	PRO	L3302	I3227
A4073	T3999	T3999	H3924	D3831	R3759	V3692	M3613	F3533	P3466	GLY	L3303	I3227
F4074	M4000	T4001	L3925	P3832	Q3760	E3693	Y3614	F3533	P3466	CYS	T3303	I3227
R4075	M4002	N3926	N3926	A3834	Q3762	F3694	L3617	SER	R3474	GLY	S3314	S3228
	D4003	F3928	F3928	P3835	R3763	L3695	G3618	PHE	Y3475	PRO	S3317	S3228
				P3836	V3764	L3695	G3618	LYS	P3476	ALA	K3318	K3235
V4078	K4007	M3929	M3929	C3837	L3767	I3701	L3625	ASP	E3477	A3407	S3319	F3236
A4081	E4008	V3930	V3930	E3838	L3767	I3701	G3626	T3545	E3478	Y3413	I3320	A3171
R4082	P4009	F4011	F4011	Y3839	F3768	Q3704	A3627	S3546	T3479	L3416	F3323	K3238
K4085	S4010	F4011	F4011	K3940	Q3768	R3705	R3629	T3547	L3482	F3419	F3323	K3238
D4086	D4012	L3938	L3938	D3841	R3771	D3706	K3630	G3548	K3483	D3421	Q3326	M3240
I4089	L4013	G3939	G3939	K3842	N3772	G3707	K3631	K3551	T3484	D3422	N3327	K3241
	PHE	D3941	D3941	L3843	G3773	G3709	L3632	E3552	E3486	Q3423	L3328	M3242
	GLY			THR	L3774	L3775	I3633	F3554	E3487	L3424	L3330	
	LYS			LYS	L3775	L3775	Q3634	S3555	S3488	L3424	L3330	
	LEU			GLY	D3778	P3713	G3647	A3596	S3489	R3425	R3335	
	GLY			LYS	S3779	E3714	GLY	K3557	V3490	R3425	R3335	
	LEU			HIS	C3780	H3715	SER	I3558	C3491	E3426	N3339	
	LYS			D3851	S3782	V3717	LEU	K3558	C3492	E3427	F3189	
	LYS			Y3855	S3782	I3718	LEU	K3561	Q3493	E3428	C3347	
	GLY			M3856	A3785	R3719	ARG	L3562	F3495	E3429	L3348	
	SER			K3856	L3786	A3720	MET	F3571	I3496	ALA	L3349	
	TRP			K3860	Q3787	G3721	LYS	S3497	S3497	SER	E3350	
	ILE			R3864	L3788	F3722	LEU	A3574	I3499	ILE	E3352	
	GLN			R3864	S3792	D3723	S3657	D3575	K3502	ASP	G3364	
	GLY			R3864	S3792	E3724	D3658	D3575	PRO	THR	L3197	
	ILE			R3864	S3792	R3725	F3659	D3575	LEU	SER	L3197	
	ASN			V3868	P3795	V3726	K3660	D3575	GLU	SER	S3266	
	VAL			T3869	M3796	V3726	K3660	D3575	LEU	SER	S3266	
	ALA			S3870	F3797	V3728	T3662	K3505	GLU	SER	R3269	
	GLU			F3871	R3799	M3729	T3663	P3581	LEU	SER	R3269	
	LYS			R3872	L3800	A3730	K3664	E3582	GLN	ASP	W3272	
	ASN			K3873	G3801		K3665	K3583	Y3441	ASN	L3273	
	W4038			R3874	L3802	R3733	L3666	L3584	Z3442	SER	V3276	
	Y4039			K3877	L3803	R3734	L3667	F3585	P3443	MET	W3276	
	P4040			K3877	E3804	P3735	L3668	K3586	A3444	ASN	V3277	
				V3878	W3805	K3736	K3669	D3587	V3446	ASP	Q3278	

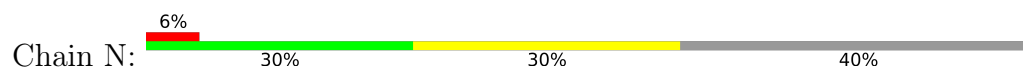
• Molecule 2: DNA repair protein XRCC4



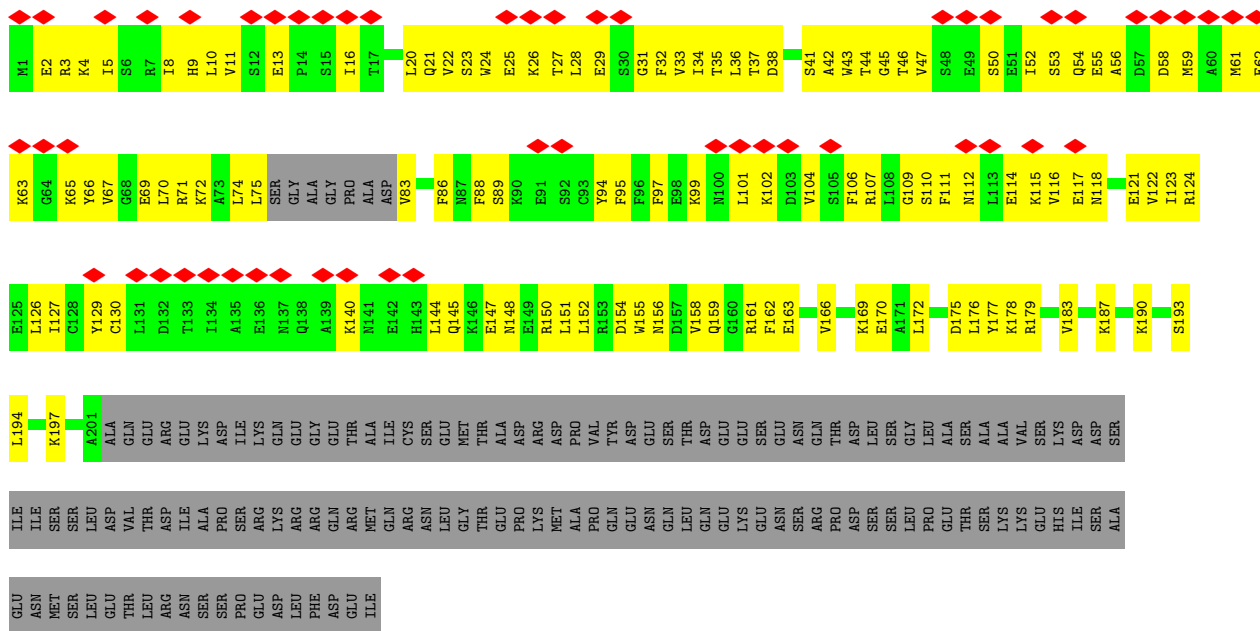
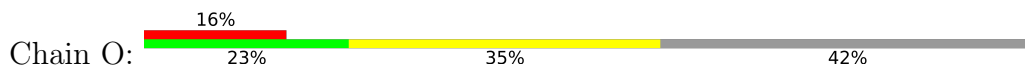
- Molecule 2: DNA repair protein XRCC4



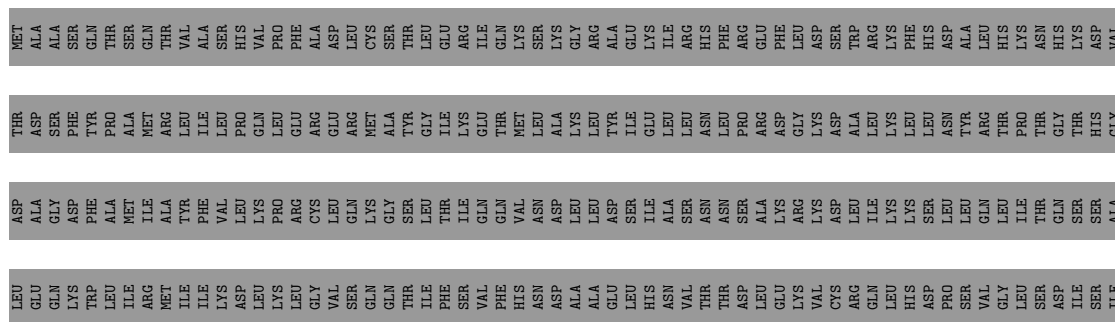
- Molecule 2: DNA repair protein XRCC4

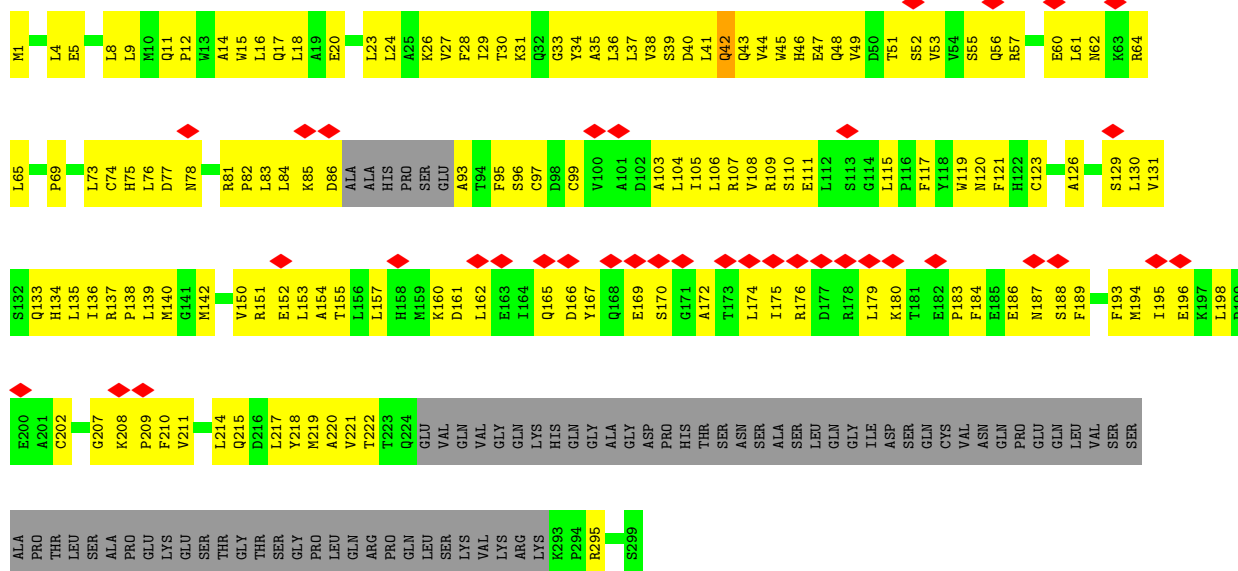


- Molecule 2: DNA repair protein XRCC4

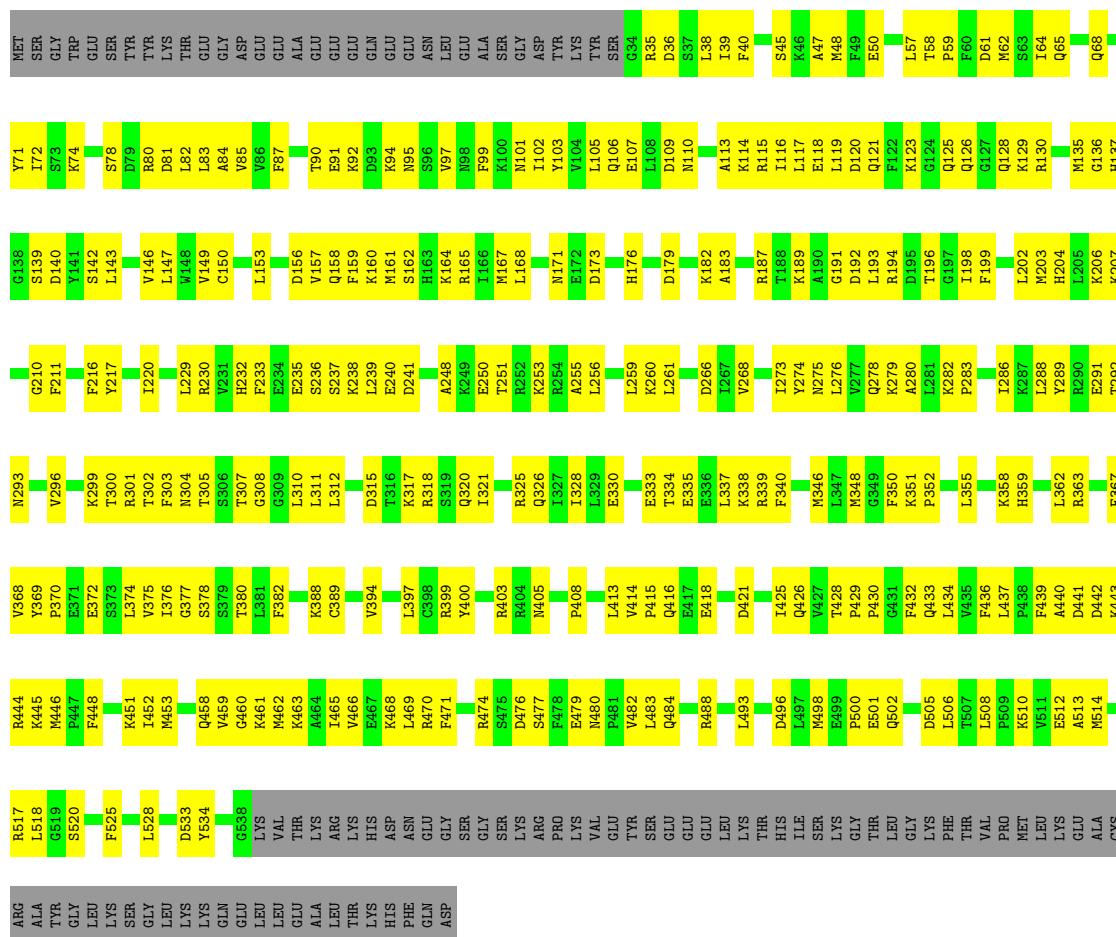


- Molecule 3: DNA ligase 4





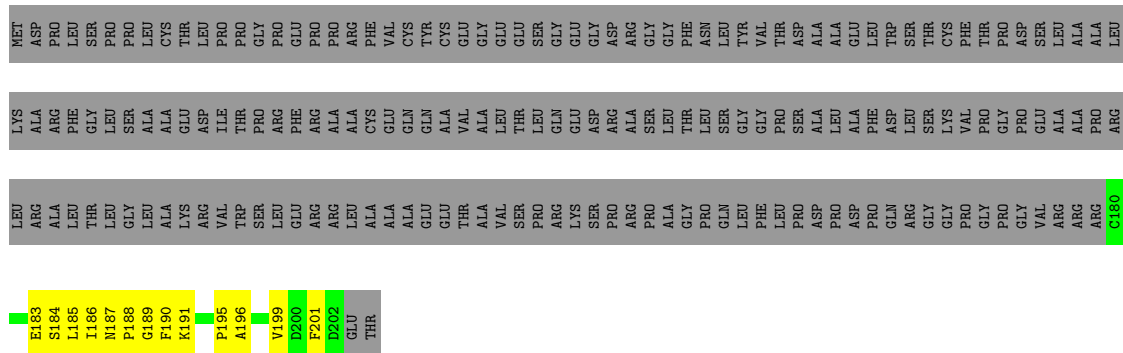
• Molecule 5: X-ray repair cross-complementing protein 6





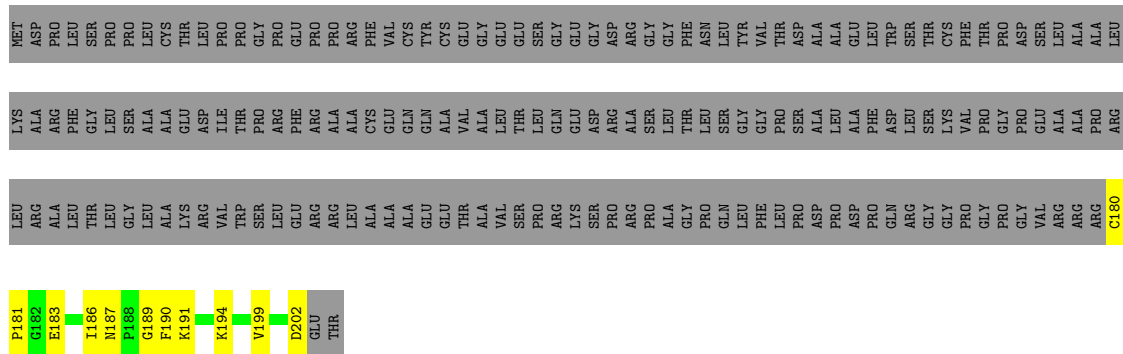
- Molecule 7: Protein PAXX

Chain c: 5% 6% 89%



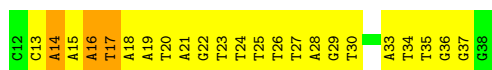
- Molecule 7: Protein PAXX

Chain i: 6% 5% 89%



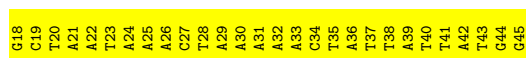
- Molecule 8: DNA (26-MER)

Chain D: 15% 74% 11%



- Molecule 9: DNA (27-MER)

Chain E: 100%



● Molecule 10: DNA (28-MER)



● Molecule 11: DNA (24-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11019	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 ($e^-/\text{\AA}^2$)	48.03	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.720	Depositor
Minimum map value	-0.164	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.168	Depositor
Map size (Å)	678.08, 678.08, 678.08	wwPDB
Map dimensions	520, 520, 520	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	0.22	0/28804	0.40	0/38906
1	F	0.22	0/28820	0.40	2/38928 (0.0%)
2	K	0.15	0/1657	0.34	0/2228
2	L	0.16	0/1616	0.35	0/2170
2	N	0.15	0/1654	0.35	0/2224
2	O	0.14	0/1616	0.35	0/2170
3	M	0.16	0/2134	0.34	1/2884 (0.0%)
3	P	0.21	0/2028	0.39	0/2737
4	Q	0.21	0/1778	0.44	0/2403
4	R	0.17	0/1831	0.43	0/2476
5	a	0.18	0/4116	0.35	0/5549
5	h	0.18	0/4105	0.35	0/5538
6	b	0.15	0/5313	0.33	0/7159
6	j	0.17	0/5178	0.36	1/6979 (0.0%)
7	c	0.14	0/169	0.26	0/226
7	i	0.15	0/166	0.27	0/222
8	D	0.38	0/622	0.66	3/959 (0.3%)
9	E	0.30	0/647	0.43	0/996
10	I	0.31	0/555	0.48	0/854
11	J	0.35	0/548	0.55	0/844
All	All	0.21	0/93357	0.39	7/126452 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	14	DA	P-O3'-C3'	-7.09	109.56	120.20
1	F	956	PRO	N-CA-CB	6.89	110.58	103.00
8	D	17	DT	P-O3'-C3'	-6.78	110.04	120.20
8	D	16	DA	P-O3'-C3'	-6.33	110.71	120.20
3	M	670	THR	N-CA-C	-5.50	108.34	114.62

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	28250	0	28465	1646	0
1	F	28263	0	28500	1660	0
2	K	1628	0	1620	125	0
2	L	1589	0	1581	101	0
2	N	1625	0	1612	124	0
2	O	1589	0	1587	124	0
3	M	2085	0	2024	151	0
3	P	1983	0	1924	137	0
4	Q	1745	0	1754	146	0
4	R	1796	0	1814	146	0
5	a	4038	0	4092	273	0
5	h	4026	0	4069	287	0
6	b	5214	0	5231	297	0
6	j	5082	0	5069	288	0
7	c	165	0	160	13	0
7	i	162	0	151	9	0
8	D	556	0	310	60	0
9	E	576	0	318	58	0
10	I	494	0	273	53	0
11	J	491	0	278	46	0
All	All	91357	0	90832	5315	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 30.

The worst 5 of 5315 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:F:2440:TYR:HA	1:F:2443:MET:HE3	1.42	0.97
1:F:1269:THR:O	1:F:1273:GLU:HB2	1.66	0.95
1:A:2405:VAL:HA	1:A:2408:MET:HE3	1.49	0.95
5:a:203:MET:HE1	5:a:238:LYS:H	1.32	0.93
1:F:1268:ASN:HD21	1:F:1344:PHE:HA	1.34	0.92

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	3436/4128 (83%)	3110 (90%)	321 (9%)	5 (0%)	48	83
1	F	3467/4128 (84%)	3148 (91%)	319 (9%)	0	100	100
2	K	199/336 (59%)	179 (90%)	20 (10%)	0	100	100
2	L	191/336 (57%)	182 (95%)	9 (5%)	0	100	100
2	N	199/336 (59%)	186 (94%)	13 (6%)	0	100	100
2	O	190/336 (56%)	183 (96%)	7 (4%)	0	100	100
3	M	256/911 (28%)	238 (93%)	18 (7%)	0	100	100
3	P	242/911 (27%)	218 (90%)	21 (9%)	3 (1%)	10	43
4	Q	210/299 (70%)	185 (88%)	24 (11%)	1 (0%)	24	63
4	R	219/299 (73%)	192 (88%)	26 (12%)	1 (0%)	24	63
5	a	503/609 (83%)	464 (92%)	39 (8%)	0	100	100
5	h	503/609 (83%)	471 (94%)	32 (6%)	0	100	100
6	b	640/732 (87%)	599 (94%)	41 (6%)	0	100	100
6	j	624/732 (85%)	597 (96%)	27 (4%)	0	100	100
7	c	21/204 (10%)	21 (100%)	0	0	100	100
7	i	21/204 (10%)	21 (100%)	0	0	100	100
All	All	10921/15110 (72%)	9994 (92%)	917 (8%)	10 (0%)	49	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	PRO
3	P	814	ARG
4	Q	131	VAL
1	A	216	LYS

Continued on next page...

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Mol	Chain	Res	Type
3	P	812	MET

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	3097/3671 (84%)	3095 (100%)	2 (0%)	88	88
1	F	3109/3671 (85%)	3108 (100%)	1 (0%)	100	100
2	K	180/303 (59%)	180 (100%)	0	100	100
2	L	176/303 (58%)	176 (100%)	0	100	100
2	N	178/303 (59%)	178 (100%)	0	100	100
2	O	177/303 (58%)	177 (100%)	0	100	100
3	M	232/808 (29%)	232 (100%)	0	100	100
3	P	217/808 (27%)	216 (100%)	1 (0%)	81	81
4	Q	192/262 (73%)	191 (100%)	1 (0%)	81	81
4	R	200/262 (76%)	200 (100%)	0	100	100
5	a	445/548 (81%)	445 (100%)	0	100	100
5	h	445/548 (81%)	445 (100%)	0	100	100
6	b	583/649 (90%)	583 (100%)	0	100	100
6	j	562/649 (87%)	562 (100%)	0	100	100
7	c	18/160 (11%)	18 (100%)	0	100	100
7	i	17/160 (11%)	17 (100%)	0	100	100
All	All	9828/13408 (73%)	9823 (100%)	5 (0%)	87	88

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

Mol	Chain	Res	Type
1	A	217	LEU
1	A	218	PRO
1	F	2170	GLN

Continued on next page...

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Mol	Chain	Res	Type
3	P	813	PHE
4	Q	131	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
4	R	32	GLN
5	a	137	HIS
6	b	627	ASN
1	F	753	GLN
1	F	720	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.

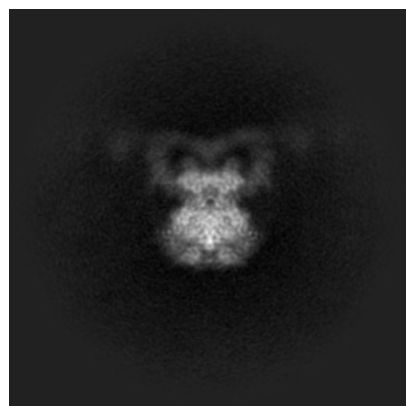
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16070. These allow visual inspection of the internal detail of the map and identification of artifacts.

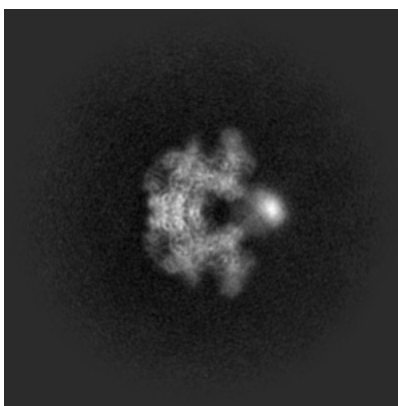
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

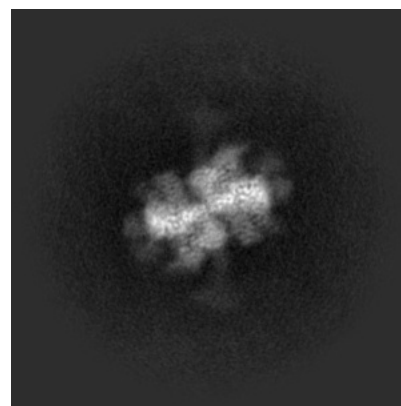
6.1.1 Primary map



X

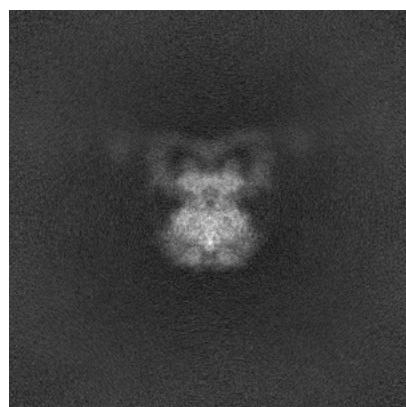


Y

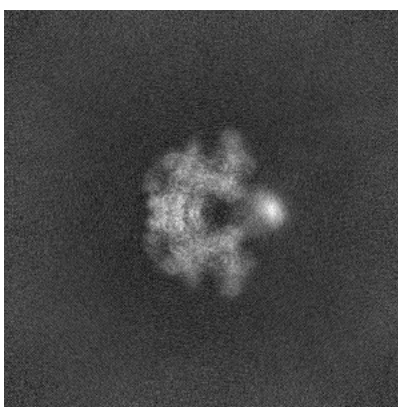


Z

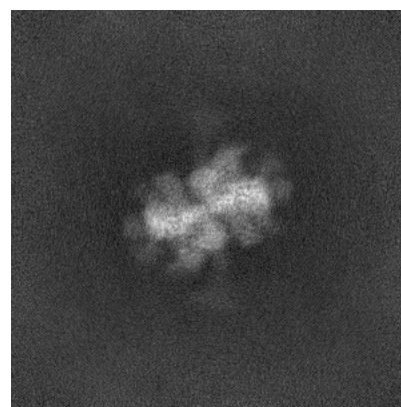
6.1.2 Raw map



X



Y

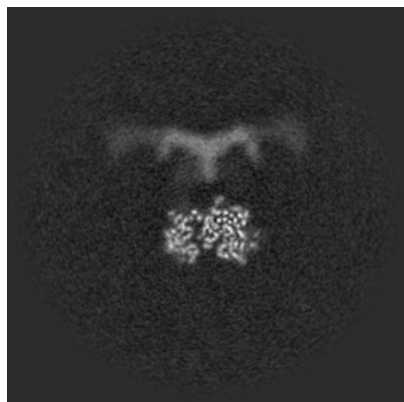


Z

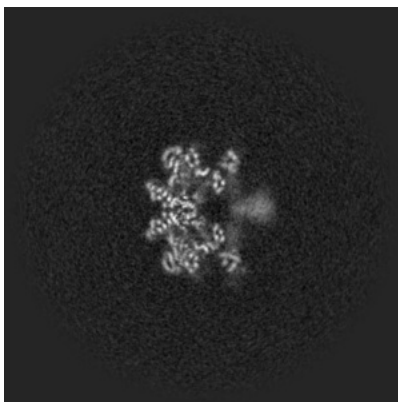
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

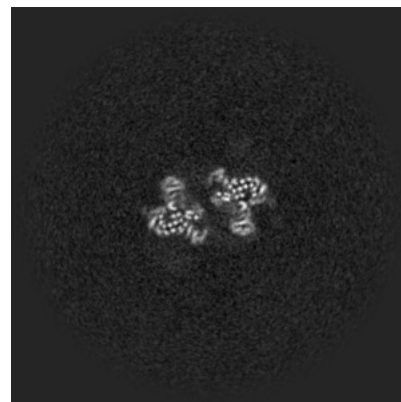
6.2.1 Primary map



X Index: 260

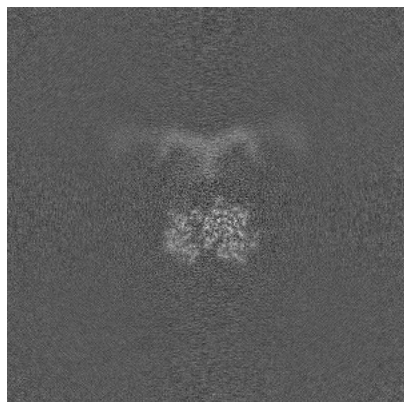


Y Index: 260

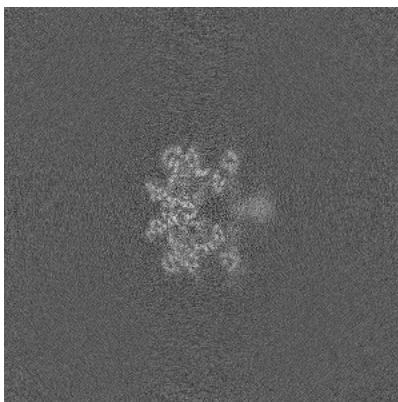


Z Index: 260

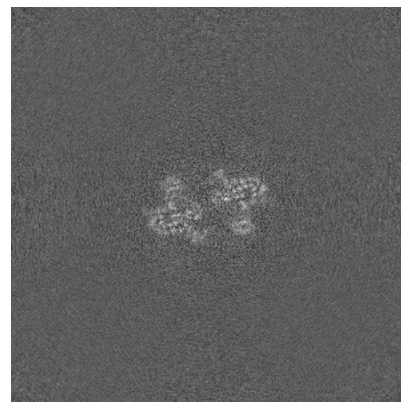
6.2.2 Raw map



X Index: 260



Y Index: 260

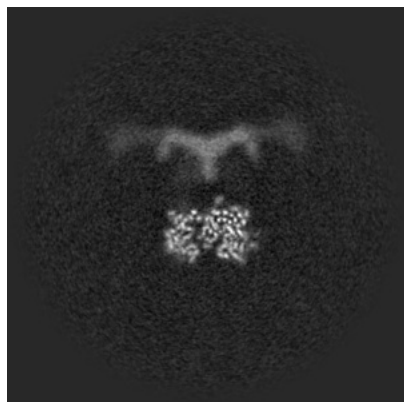


Z Index: 260

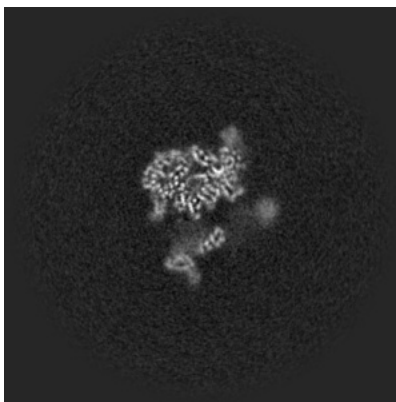
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

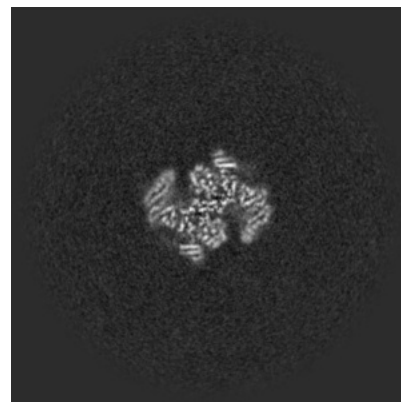
6.3.1 Primary map



X Index: 259

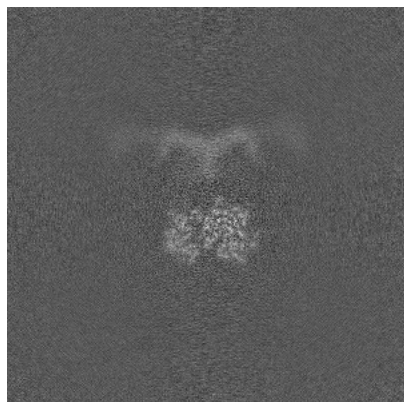


Y Index: 275

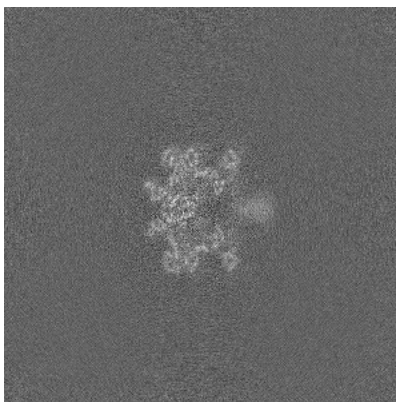


Z Index: 229

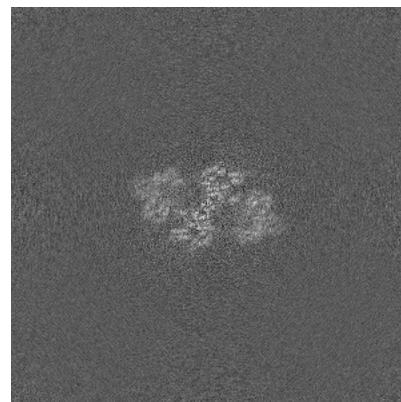
6.3.2 Raw map



X Index: 260



Y Index: 262

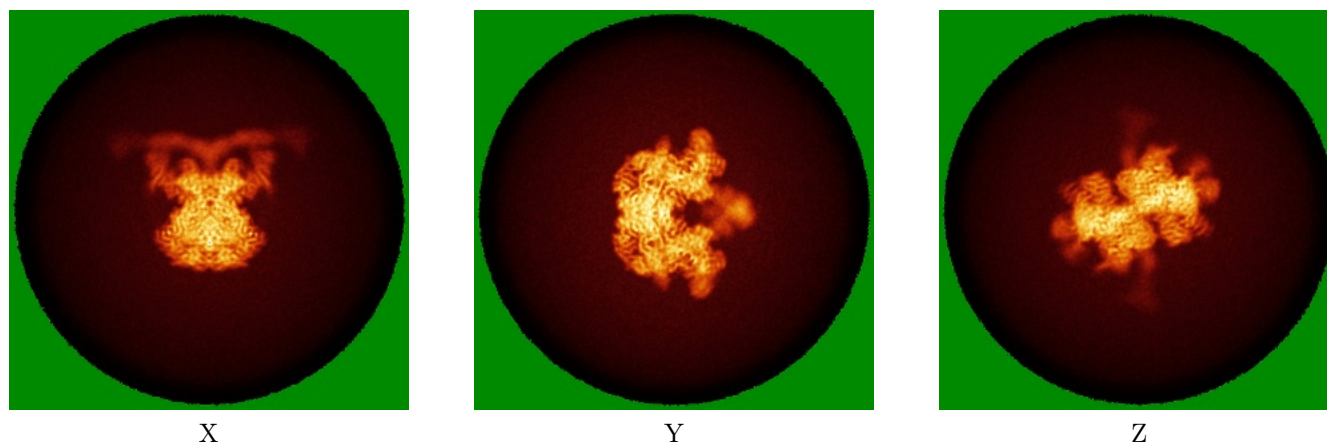


Z Index: 242

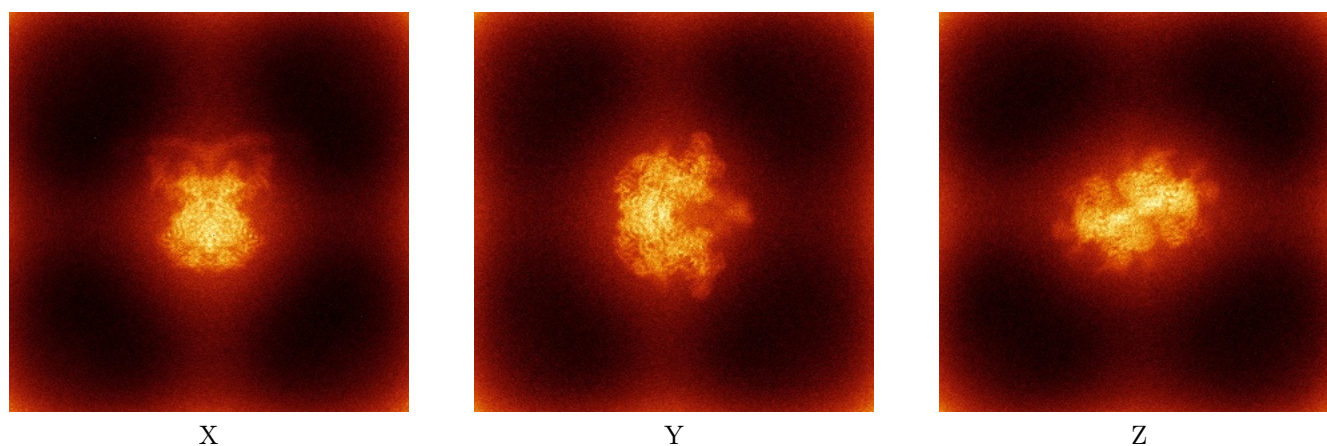
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

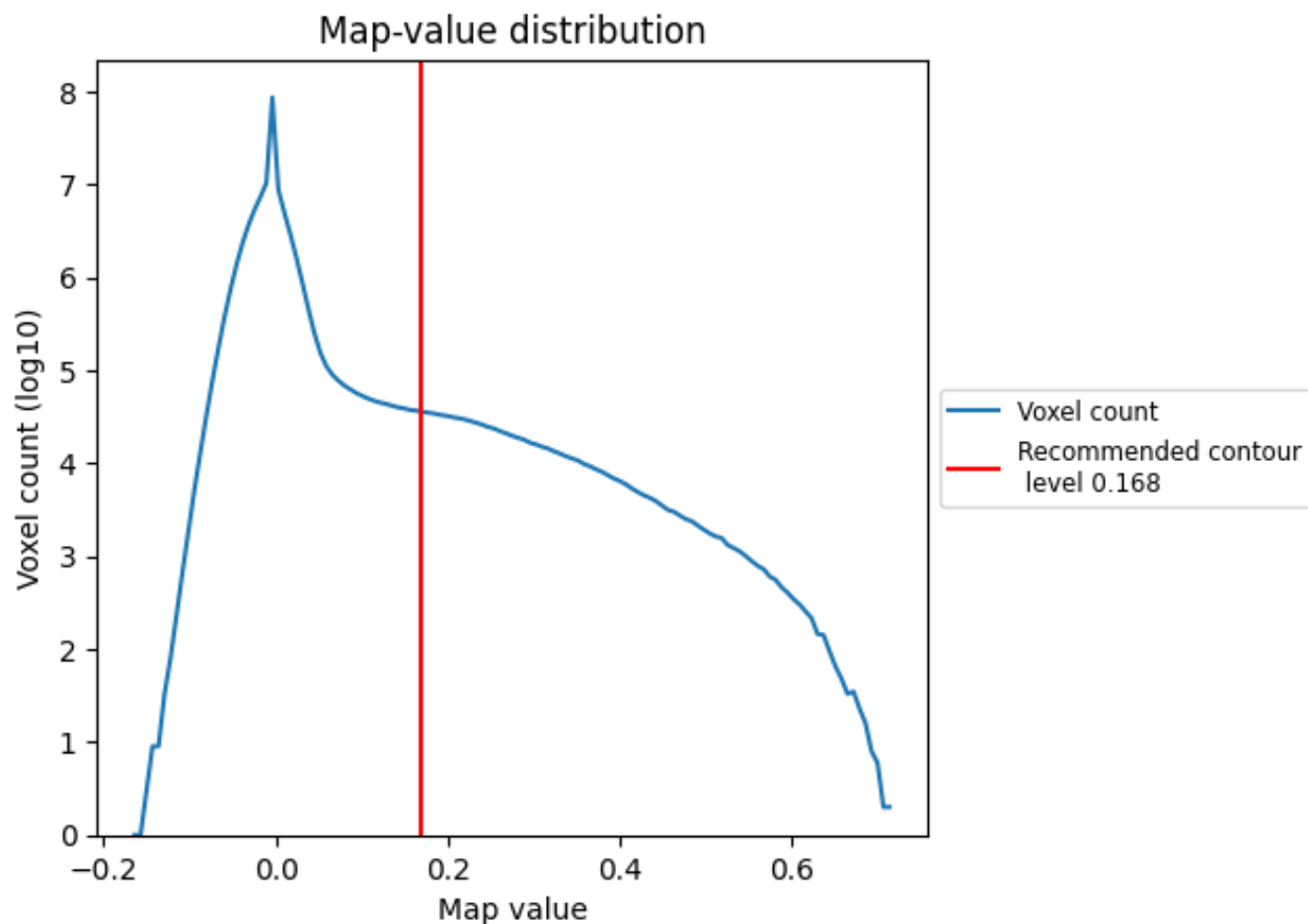
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

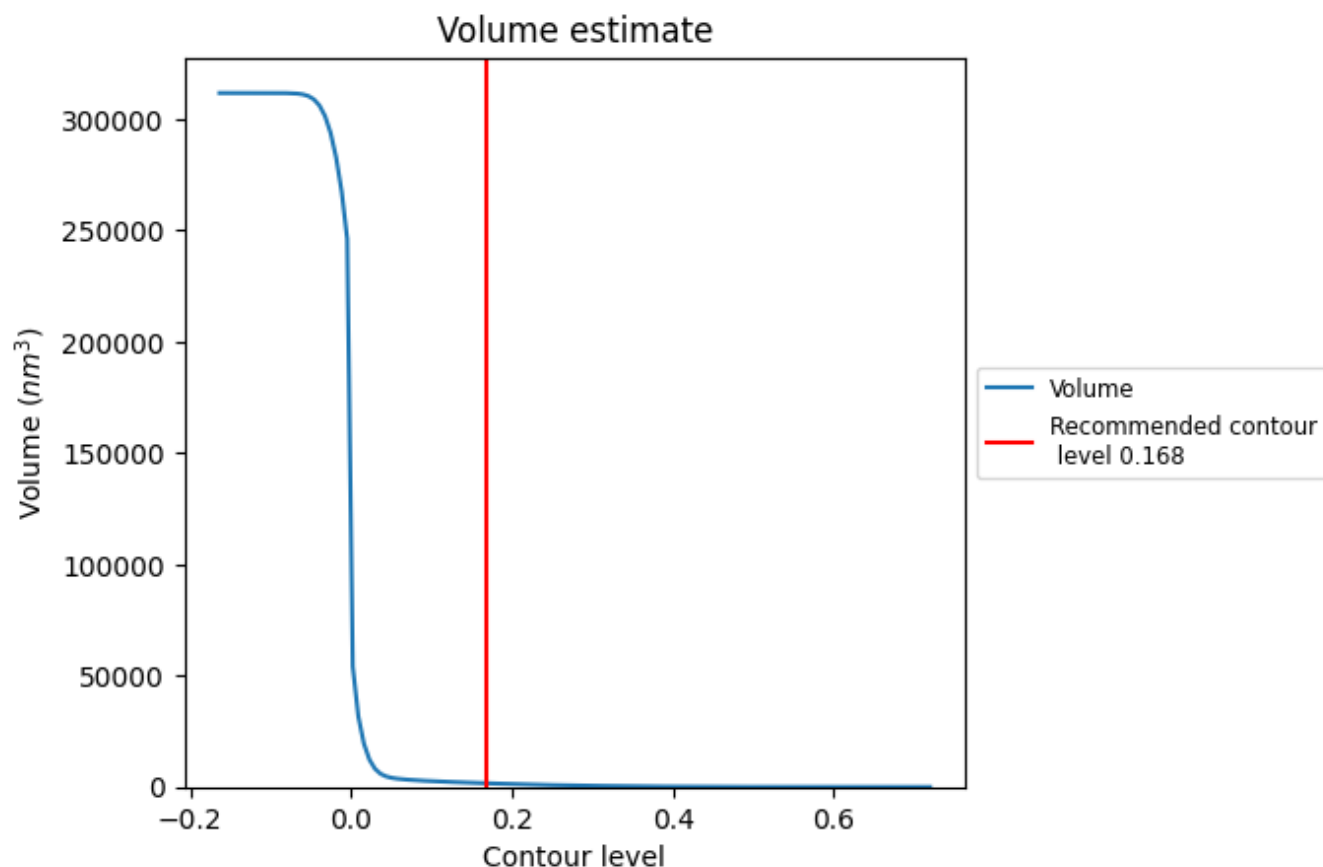
This section contains the results of statistical analysis of the map.

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.

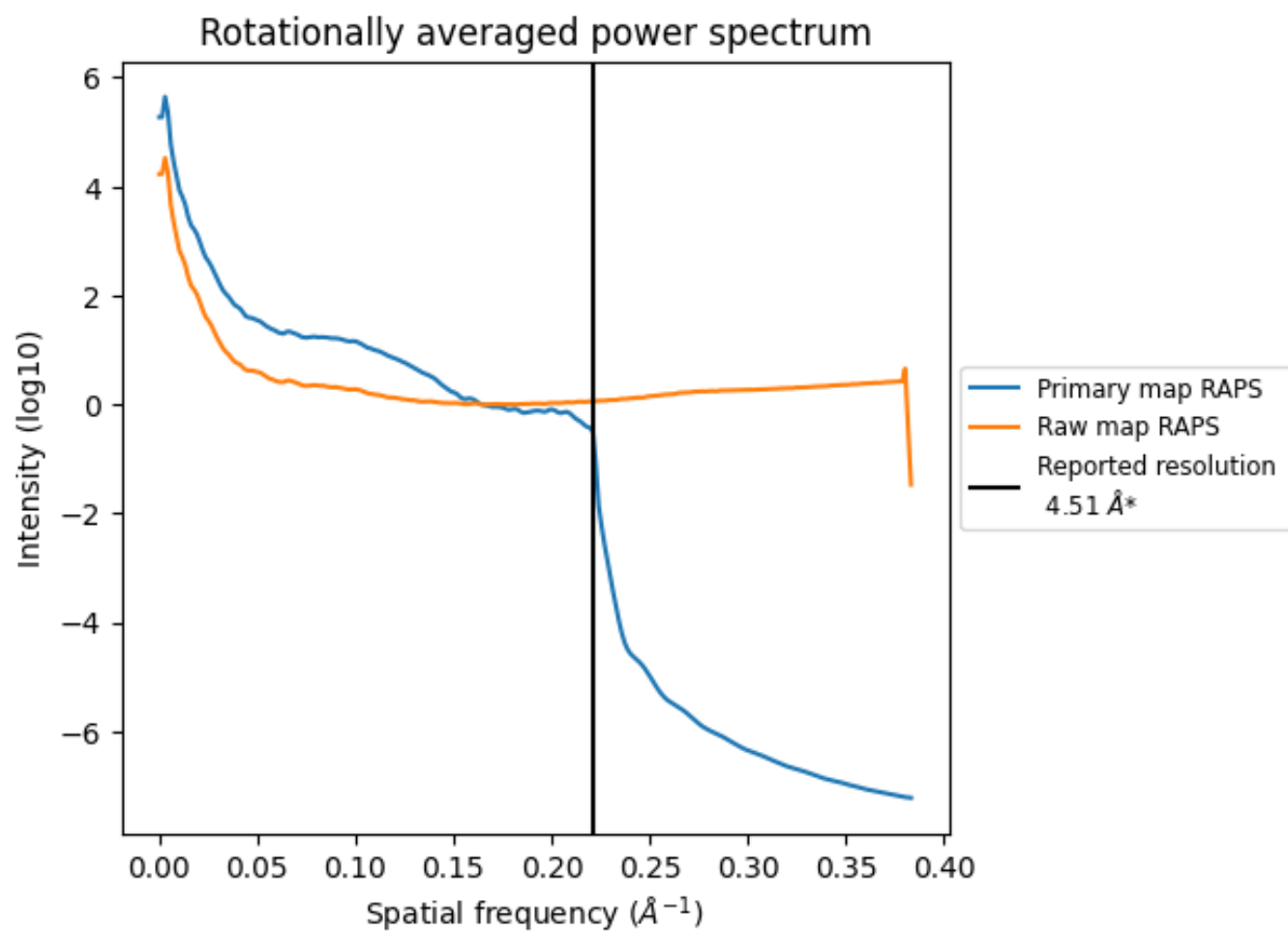
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1663 nm³; this corresponds to an approximate mass of 1502 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 [i](#)

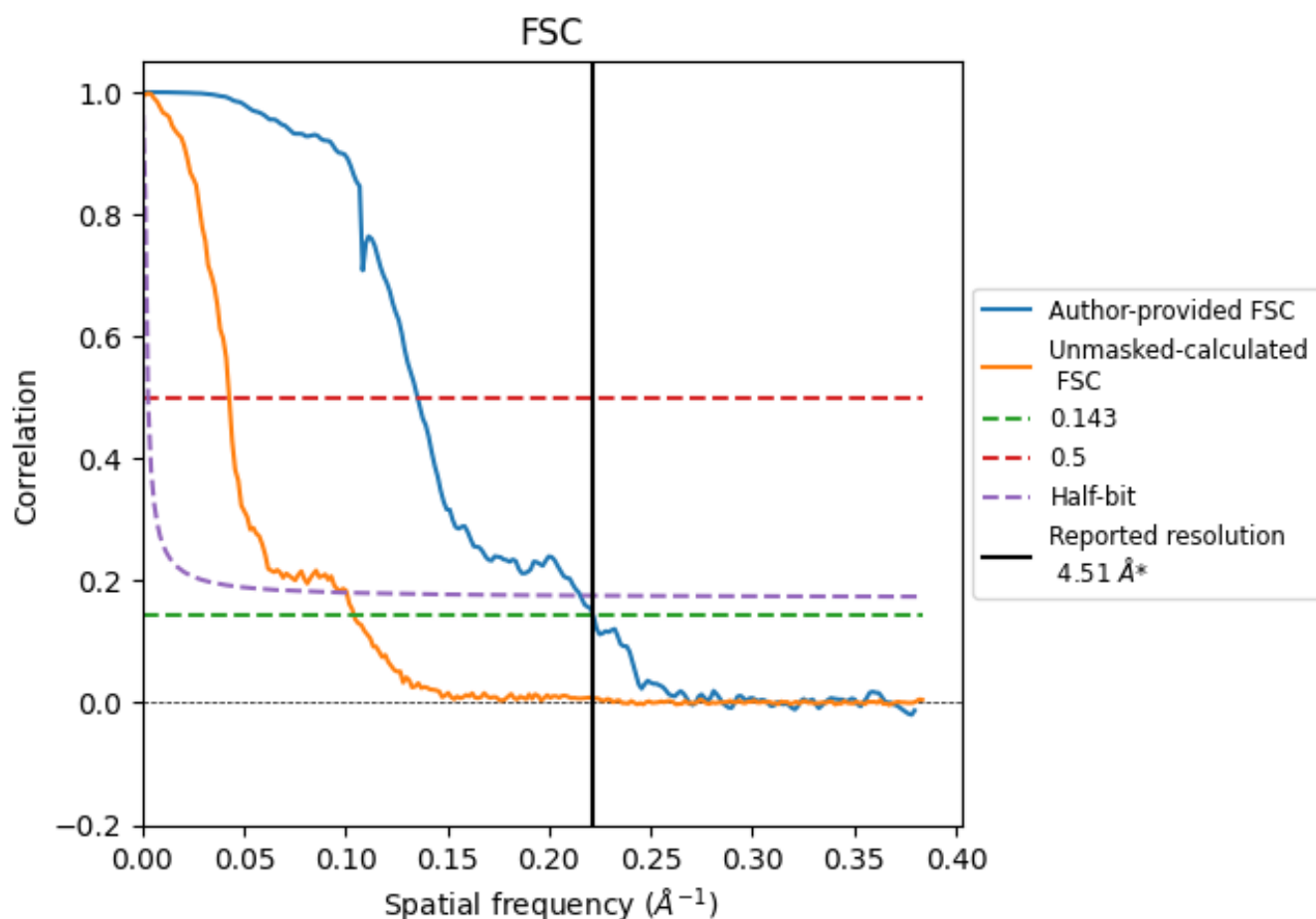


*Reported resolution corresponds to spatial frequency of 0.222 $\text{\AA}^{-1}$

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.51	-	-
Author-provided FSC curve	4.51	7.39	4.64
Unmasked-calculated*	9.60	23.42	9.95

*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 9.60 differs from the reported value 4.51 by more than 10 %

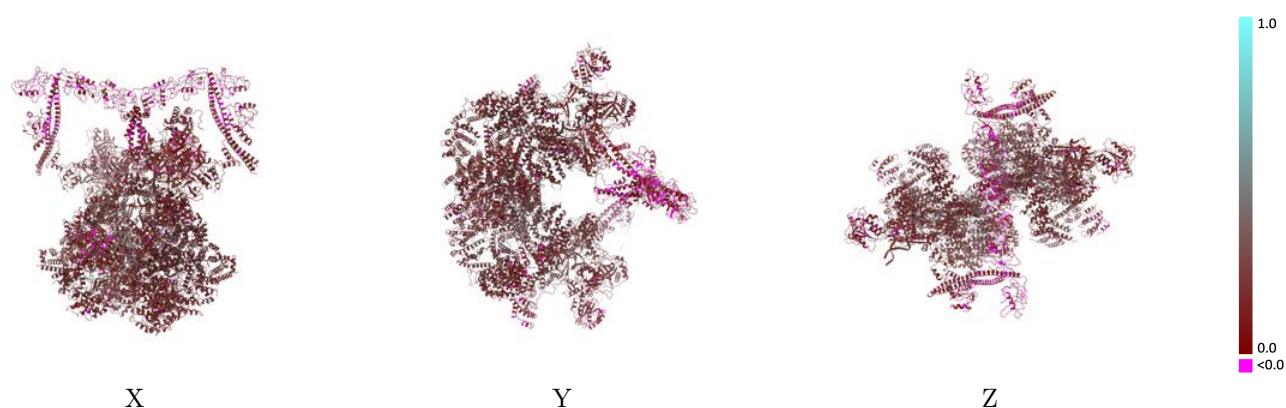
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16070 and PDB model 8BHV. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

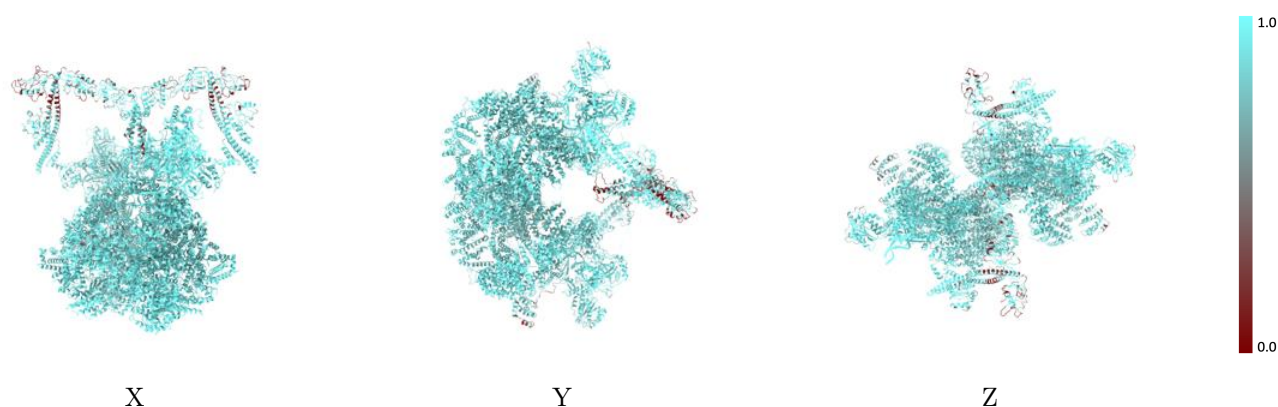
This section was not generated.

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



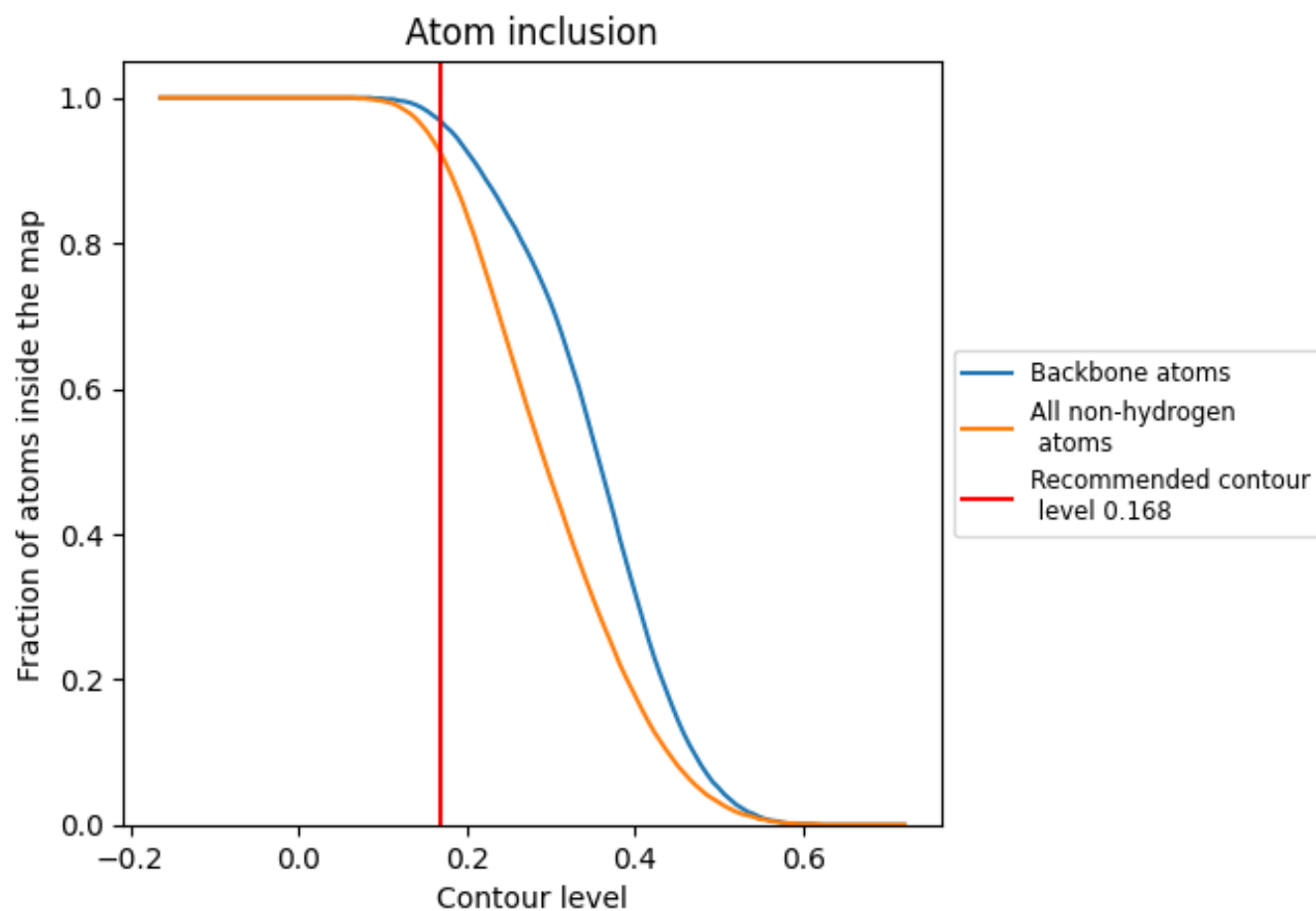
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.168).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.168) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.2030
A	 0.9500	 0.2210
D	 0.9570	 0.2520
E	 0.9790	 0.2310
F	 0.9560	 0.2290
I	 0.9720	 0.2110
J	 0.9800	 0.2680
K	 0.7510	 0.0990
L	 0.6330	 0.1040
M	 0.9080	 0.1520
N	 0.8230	 0.0990
O	 0.6800	 0.1210
P	 0.9420	 0.1500
Q	 0.8030	 0.0910
R	 0.7830	 0.0720
a	 0.9610	 0.2170
b	 0.8810	 0.1760
c	 0.9700	 0.2440
h	 0.9610	 0.2310
i	 0.9940	 0.2550
j	 0.9380	 0.1920

