



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:45 PM UTC

PDB ID : 9E0Y / pdb_00009e0y
EMDB ID : EMD-47377
Title : Cryo-EM structure of human cytoplasmic dynein-1 in the presence of ATP
Authors : Nguyen, K.H.V.; Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-10-20
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

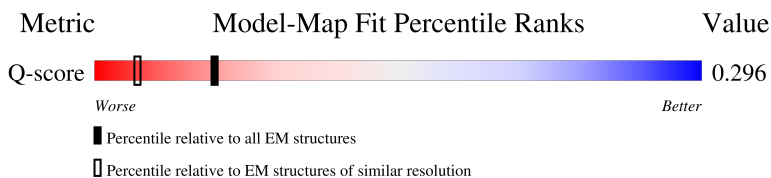
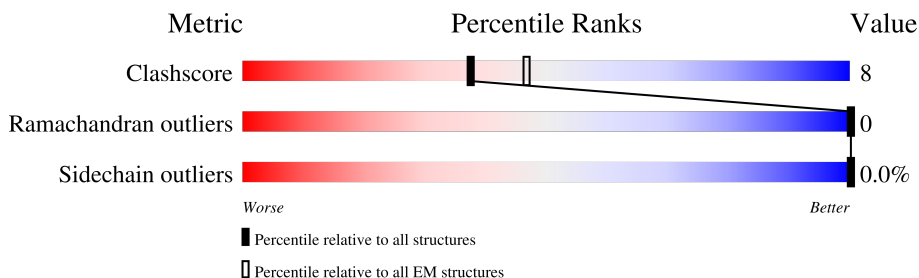
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	4843	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22201 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2753	Total	C	N	O	S	0	0
			22085	14040	3818	4115	112		

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-196	GLY	-	expression tag	UNP Q14204
A	-195	ASP	-	expression tag	UNP Q14204
A	-194	TYR	-	expression tag	UNP Q14204
A	-193	ASP	-	expression tag	UNP Q14204
A	-192	ILE	-	expression tag	UNP Q14204
A	-191	PRO	-	expression tag	UNP Q14204
A	-190	THR	-	expression tag	UNP Q14204
A	-189	THR	-	expression tag	UNP Q14204
A	-188	GLU	-	expression tag	UNP Q14204
A	-187	ASN	-	expression tag	UNP Q14204
A	-186	LEU	-	expression tag	UNP Q14204
A	-185	TYR	-	expression tag	UNP Q14204
A	-184	PHE	-	expression tag	UNP Q14204
A	-183	GLN	-	expression tag	UNP Q14204
A	-182	GLY	-	expression tag	UNP Q14204
A	-181	ASP	-	expression tag	UNP Q14204
A	-180	LYS	-	expression tag	UNP Q14204
A	-179	ASP	-	expression tag	UNP Q14204
A	-178	CYS	-	expression tag	UNP Q14204
A	-177	GLU	-	expression tag	UNP Q14204
A	-176	MET	-	expression tag	UNP Q14204
A	-175	LYS	-	expression tag	UNP Q14204
A	-174	ARG	-	expression tag	UNP Q14204
A	-173	THR	-	expression tag	UNP Q14204
A	-172	THR	-	expression tag	UNP Q14204
A	-171	LEU	-	expression tag	UNP Q14204
A	-170	ASP	-	expression tag	UNP Q14204
A	-169	SER	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-168	PRO	-	expression tag	UNP Q14204
A	-167	LEU	-	expression tag	UNP Q14204
A	-166	GLY	-	expression tag	UNP Q14204
A	-165	LYS	-	expression tag	UNP Q14204
A	-164	LEU	-	expression tag	UNP Q14204
A	-163	GLU	-	expression tag	UNP Q14204
A	-162	LEU	-	expression tag	UNP Q14204
A	-161	SER	-	expression tag	UNP Q14204
A	-160	GLY	-	expression tag	UNP Q14204
A	-159	CYS	-	expression tag	UNP Q14204
A	-158	GLU	-	expression tag	UNP Q14204
A	-157	GLN	-	expression tag	UNP Q14204
A	-156	GLY	-	expression tag	UNP Q14204
A	-155	LEU	-	expression tag	UNP Q14204
A	-154	HIS	-	expression tag	UNP Q14204
A	-153	ARG	-	expression tag	UNP Q14204
A	-152	ILE	-	expression tag	UNP Q14204
A	-151	ILE	-	expression tag	UNP Q14204
A	-150	PHE	-	expression tag	UNP Q14204
A	-149	LEU	-	expression tag	UNP Q14204
A	-148	GLY	-	expression tag	UNP Q14204
A	-147	LYS	-	expression tag	UNP Q14204
A	-146	GLY	-	expression tag	UNP Q14204
A	-145	THR	-	expression tag	UNP Q14204
A	-144	SER	-	expression tag	UNP Q14204
A	-143	ALA	-	expression tag	UNP Q14204
A	-142	ALA	-	expression tag	UNP Q14204
A	-141	ASP	-	expression tag	UNP Q14204
A	-140	ALA	-	expression tag	UNP Q14204
A	-139	VAL	-	expression tag	UNP Q14204
A	-138	GLU	-	expression tag	UNP Q14204
A	-137	VAL	-	expression tag	UNP Q14204
A	-136	PRO	-	expression tag	UNP Q14204
A	-135	ALA	-	expression tag	UNP Q14204
A	-134	PRO	-	expression tag	UNP Q14204
A	-133	ALA	-	expression tag	UNP Q14204
A	-132	ALA	-	expression tag	UNP Q14204
A	-131	VAL	-	expression tag	UNP Q14204
A	-130	LEU	-	expression tag	UNP Q14204
A	-129	GLY	-	expression tag	UNP Q14204
A	-128	GLY	-	expression tag	UNP Q14204
A	-127	PRO	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-126	GLU	-	expression tag	UNP Q14204
A	-125	PRO	-	expression tag	UNP Q14204
A	-124	LEU	-	expression tag	UNP Q14204
A	-123	MET	-	expression tag	UNP Q14204
A	-122	GLN	-	expression tag	UNP Q14204
A	-121	ALA	-	expression tag	UNP Q14204
A	-120	THR	-	expression tag	UNP Q14204
A	-119	ALA	-	expression tag	UNP Q14204
A	-118	TRP	-	expression tag	UNP Q14204
A	-117	LEU	-	expression tag	UNP Q14204
A	-116	ASN	-	expression tag	UNP Q14204
A	-115	ALA	-	expression tag	UNP Q14204
A	-114	TYR	-	expression tag	UNP Q14204
A	-113	PHE	-	expression tag	UNP Q14204
A	-112	HIS	-	expression tag	UNP Q14204
A	-111	GLN	-	expression tag	UNP Q14204
A	-110	PRO	-	expression tag	UNP Q14204
A	-109	GLU	-	expression tag	UNP Q14204
A	-108	ALA	-	expression tag	UNP Q14204
A	-107	ILE	-	expression tag	UNP Q14204
A	-106	GLU	-	expression tag	UNP Q14204
A	-105	GLU	-	expression tag	UNP Q14204
A	-104	PHE	-	expression tag	UNP Q14204
A	-103	PRO	-	expression tag	UNP Q14204
A	-102	VAL	-	expression tag	UNP Q14204
A	-101	PRO	-	expression tag	UNP Q14204
A	-100	ALA	-	expression tag	UNP Q14204
A	-99	LEU	-	expression tag	UNP Q14204
A	-98	HIS	-	expression tag	UNP Q14204
A	-97	HIS	-	expression tag	UNP Q14204
A	-96	PRO	-	expression tag	UNP Q14204
A	-95	VAL	-	expression tag	UNP Q14204
A	-94	PHE	-	expression tag	UNP Q14204
A	-93	GLN	-	expression tag	UNP Q14204
A	-92	GLN	-	expression tag	UNP Q14204
A	-91	GLU	-	expression tag	UNP Q14204
A	-90	SER	-	expression tag	UNP Q14204
A	-89	PHE	-	expression tag	UNP Q14204
A	-88	THR	-	expression tag	UNP Q14204
A	-87	ARG	-	expression tag	UNP Q14204
A	-86	GLN	-	expression tag	UNP Q14204
A	-85	VAL	-	expression tag	UNP Q14204

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-84	LEU	-	expression tag	UNP Q14204
A	-83	TRP	-	expression tag	UNP Q14204
A	-82	LYS	-	expression tag	UNP Q14204
A	-81	LEU	-	expression tag	UNP Q14204
A	-80	LEU	-	expression tag	UNP Q14204
A	-79	LYS	-	expression tag	UNP Q14204
A	-78	VAL	-	expression tag	UNP Q14204
A	-77	VAL	-	expression tag	UNP Q14204
A	-76	LYS	-	expression tag	UNP Q14204
A	-75	PHE	-	expression tag	UNP Q14204
A	-74	GLY	-	expression tag	UNP Q14204
A	-73	GLU	-	expression tag	UNP Q14204
A	-72	VAL	-	expression tag	UNP Q14204
A	-71	ILE	-	expression tag	UNP Q14204
A	-70	SER	-	expression tag	UNP Q14204
A	-69	TYR	-	expression tag	UNP Q14204
A	-68	SER	-	expression tag	UNP Q14204
A	-67	HIS	-	expression tag	UNP Q14204
A	-66	LEU	-	expression tag	UNP Q14204
A	-65	ALA	-	expression tag	UNP Q14204
A	-64	ALA	-	expression tag	UNP Q14204
A	-63	LEU	-	expression tag	UNP Q14204
A	-62	ALA	-	expression tag	UNP Q14204
A	-61	GLY	-	expression tag	UNP Q14204
A	-60	ASN	-	expression tag	UNP Q14204
A	-59	PRO	-	expression tag	UNP Q14204
A	-58	ALA	-	expression tag	UNP Q14204
A	-57	ALA	-	expression tag	UNP Q14204
A	-56	THR	-	expression tag	UNP Q14204
A	-55	ALA	-	expression tag	UNP Q14204
A	-54	ALA	-	expression tag	UNP Q14204
A	-53	VAL	-	expression tag	UNP Q14204
A	-52	LYS	-	expression tag	UNP Q14204
A	-51	THR	-	expression tag	UNP Q14204
A	-50	ALA	-	expression tag	UNP Q14204
A	-49	LEU	-	expression tag	UNP Q14204
A	-48	SER	-	expression tag	UNP Q14204
A	-47	GLY	-	expression tag	UNP Q14204
A	-46	ASN	-	expression tag	UNP Q14204
A	-45	PRO	-	expression tag	UNP Q14204
A	-44	VAL	-	expression tag	UNP Q14204
A	-43	PRO	-	expression tag	UNP Q14204

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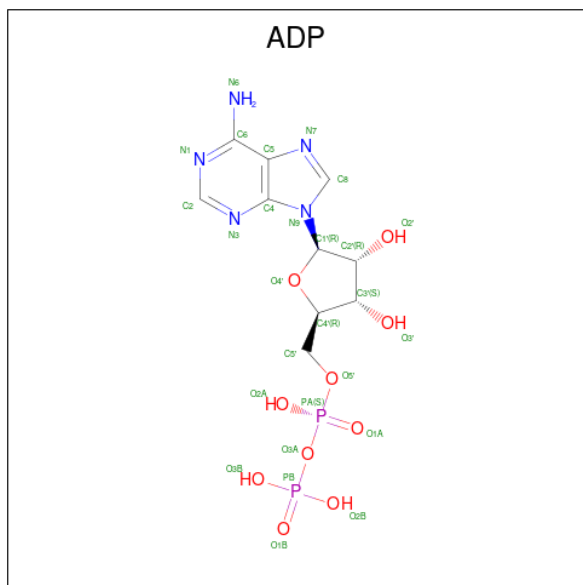
Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	ILE	-	expression tag	UNP Q14204
A	-41	LEU	-	expression tag	UNP Q14204
A	-40	ILE	-	expression tag	UNP Q14204
A	-39	PRO	-	expression tag	UNP Q14204
A	-38	CYS	-	expression tag	UNP Q14204
A	-37	HIS	-	expression tag	UNP Q14204
A	-36	ARG	-	expression tag	UNP Q14204
A	-35	VAL	-	expression tag	UNP Q14204
A	-34	VAL	-	expression tag	UNP Q14204
A	-33	GLN	-	expression tag	UNP Q14204
A	-32	GLY	-	expression tag	UNP Q14204
A	-31	ASP	-	expression tag	UNP Q14204
A	-30	LEU	-	expression tag	UNP Q14204
A	-29	ASP	-	expression tag	UNP Q14204
A	-28	VAL	-	expression tag	UNP Q14204
A	-27	GLY	-	expression tag	UNP Q14204
A	-26	GLY	-	expression tag	UNP Q14204
A	-25	TYR	-	expression tag	UNP Q14204
A	-24	GLU	-	expression tag	UNP Q14204
A	-23	GLY	-	expression tag	UNP Q14204
A	-22	GLY	-	expression tag	UNP Q14204
A	-21	LEU	-	expression tag	UNP Q14204
A	-20	ALA	-	expression tag	UNP Q14204
A	-19	VAL	-	expression tag	UNP Q14204
A	-18	LYS	-	expression tag	UNP Q14204
A	-17	GLU	-	expression tag	UNP Q14204
A	-16	TRP	-	expression tag	UNP Q14204
A	-15	LEU	-	expression tag	UNP Q14204
A	-14	LEU	-	expression tag	UNP Q14204
A	-13	ALA	-	expression tag	UNP Q14204
A	-12	HIS	-	expression tag	UNP Q14204
A	-11	GLU	-	expression tag	UNP Q14204
A	-10	GLY	-	expression tag	UNP Q14204
A	-9	HIS	-	expression tag	UNP Q14204
A	-8	ARG	-	expression tag	UNP Q14204
A	-7	LEU	-	expression tag	UNP Q14204
A	-6	GLY	-	expression tag	UNP Q14204
A	-5	LYS	-	expression tag	UNP Q14204
A	-4	PRO	-	expression tag	UNP Q14204
A	-3	GLY	-	expression tag	UNP Q14204
A	-2	LEU	-	expression tag	UNP Q14204
A	-1	GLY	-	expression tag	UNP Q14204

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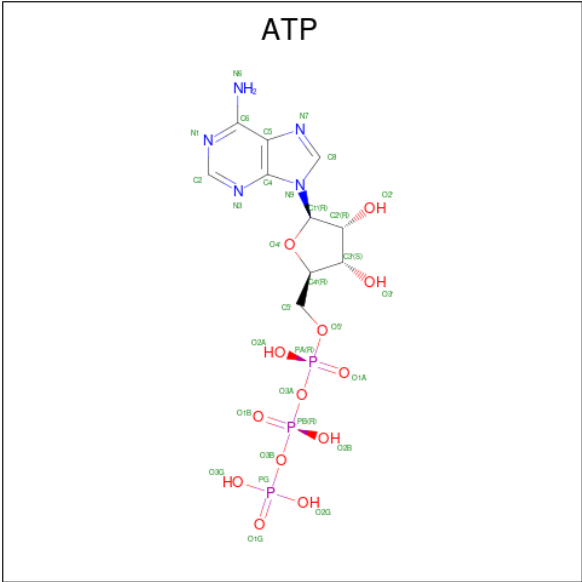
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q14204
A	1	SER	-	expression tag	UNP Q14204

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

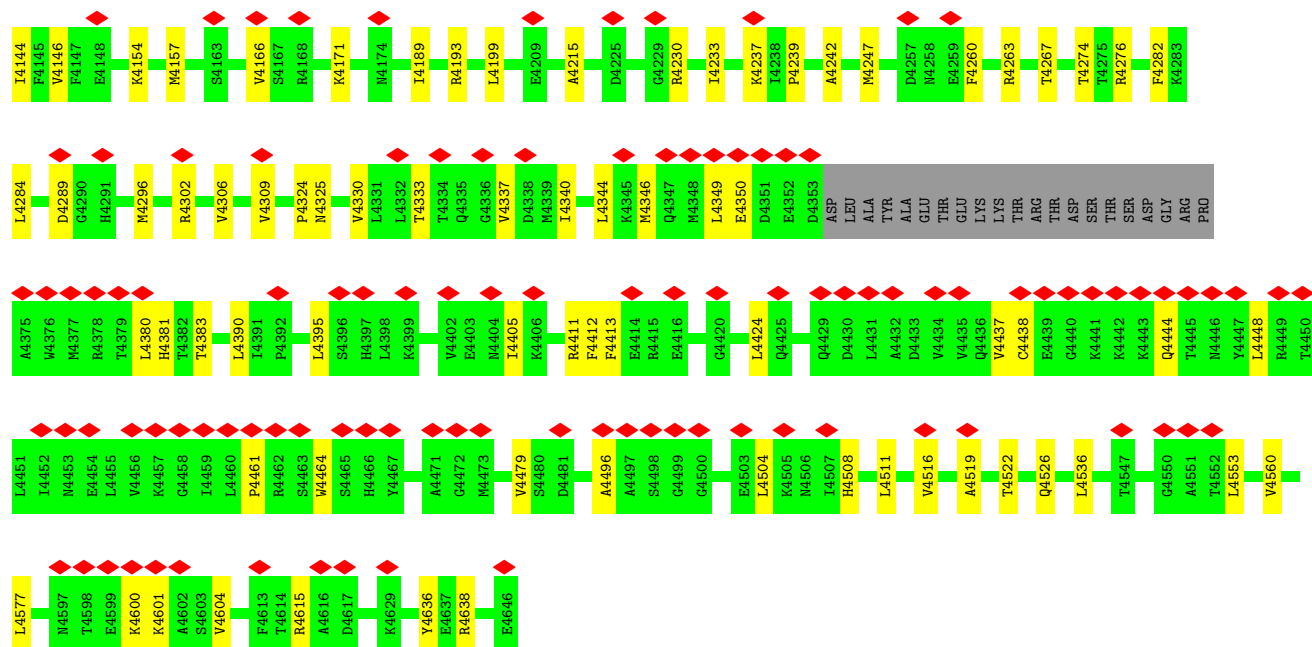


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	



V3065	F3066	T3067	K3068	N3069	F3070	S3071	S3072	E3073	G3074	K3076	D3077	K3078	A3079	A3080	T3081	S3082	F3083	A3084	L3085	C3088	V3089	E3090	N3091	N3092	F3093	G3094	G3095	D3096	D3124	Y3125	K3126	F3127	V3128	K3132	L3133	F3134	E3141	A3142	I3143	V3144	N3145	S3146	H3151	Q3152	T3153	L3154	H3155	Q3156	T3055	S3056	I3059	R3060	N3061	L3062	H3063	V3064
F2926	R2927	Q2928	P2929	Q2930	G2931	H2932	L2933	L2934	L2935	L2936	G2937	V2938	L2946	F2949	V2950	A2951	N2954	G2955	L2956	V2957	V2958	Y2959	Q2960	L2961	K2962	V2963	H2964	R2965	K2966	Y2967	T2968	G2969	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	T2978	R2981	R2982	C2985	K2986	N2987	E2988	K2989	F2992	L2993	H2994	E2996				
S2997	N2998	V2999	L3000	D3001	S3002	G3003	F3004	R3007	M3008	N3009	T3010	L3011	L3012	A3013	N3014	G3015	E3016	F3017	P3018	G3019	L3020	F3021	E3022	G3023	D3024	A3027	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	M3043	L3044	D3045	S3046	H3047	E3048	E3049	L3050	Y3051	K3052	M3053	F3054	T3055	S3056	I3059	R3060	N3061	L3062	H3063	V3064	
E2841	R2844	D2851	A2854	L2855	K2856	H2857	F2858	P2859	M2860	I2861	D2862	R2863	E2864	K2865	A2866	L2872	Y2873	S2874	M2875	D2876	L2877	K2878	L2879	L2880	P2883	E2887	E2888	L2889	D2890	Y2892	K2893	A2894	A2895	R2896	L2897	K2898	Y2901	E2902	E2903	E2904	L2905	D2906	V2910	L2911	F2912	N2913	E2914	V2915	L2925							
V2709	L2723	R2726	F2727	L2728	R2729	P2732	V2736	S2743	L2744	Q2745	L2747	Y2748	G2749	T2750	N2751	R2752	R2753	A2754	K2755	L2756	R2757	L2758	L2759	L2762	R2763	T2770	V2774	R2783	D2787	G2805	A2809	L2810	R2811	P2812	L2813	E2814	T2815	L2816	P2817	R2823	L2824	V2838	E2839	D2840												
V2618	G2619	L2620	N2621	F2622	S2623	S2624	A2625	T2626	T2627	P2628	E2629	L2630	L2631	L2632	K2633	D2636	H2637	R2642	R2643	T2644	P2645	L2655	G2656	V2660	L2661	F2662	C2663	D2664	E2665	L2666	D2670	M2671	D2672	K2673	Y2674	G2675	T2676	Q2677	R2678	V2679	L2680	S2681	F2682	L2683	R2684	T2695	S2696	D2697	E2704	Q2707	F2708					
Q2504	D2505	K2509	M2510	R2511	A2512	E2513	L2514	I2518	R2519	R2520	L2521	T2522	T2528	A2529	P2530	N2531	V2539	W2548	P2553	H2560	K2561	P2565	P2570	L2571	L2572	R2576	L2580	T2583	W2584	L2585	A2586	L2591	K2601	T2602	M2603	T2604	L2605	L2609	R2610	A2611	L2612	P2613	V2617													
R2397	R2398	K2399	G2400	K2401	E2402	D2403	E2404	G2405	E2406	E2407	A2408	A2409	S2410	P2411	W2412	Q2413	L2414	L2415	Q2416	R2417	A2420	T2421	L2422	F2427	T2428	S2429	W2430	L2437	H2445	L2449	T2450	R2451	L2452	R2453	S2457	L2458	F2459	Y2472	D2478	Y2493	L2494	L2499	S2503													
W2311	V2312	E2313	N2314	L2315	N2316	D2320	D2321	N2322	K2323	L2324	L2325	T2326	L2327	P2328	N2329	Q2330	E2331	R2332	L2333	S2334	L2335	V2339	R2340	L2341	M2342	F2343	E2344	V2345	L2348	A2351	T2352	L2353	A2354	S2357	R2358	C2359	F2375	R2381	L2382	I2385	P2386	L2387	G2390	E2391	D2392	E2393	A2394	Q2395	R2396							
L2220	H2221	N2222	V2223	K2230	W2234	R2235	L2241	L2244	E2248	A2251	T2254	A2258	D2262	H2263	T2267	L2268	D2269	P2270	N2271	T2272	R2273	E2274	W2275	T2276	D2277	T2281	H2282	V2283	L2284	R2285	K2286	L2287	I2288	D2289	R2292	G2293	E2294	K2297	R2298	Q2299	W2300	D2306	V2307	D2308												
K2074	L2075	C2076	D2077	S2084	H2085	Y2086	D2087	L2090	L2093	K2094	L2097	E2106	R2107	T2108	Q2109	K2110	K2115	E2116	E2117	R2118	Q2119	E2120	A2121	V2122	D2123	E2124	G2125	E2126	T2127	A2128	E2129	P2132	E2135	W2141	T2154	P2155	L2156	L2161	L2178	E2181	D2195	G2196	E2197	Q2215												
N1987	P1988	N1989	Y1990	D1991	K1992	T1993	S1994	A1995	P1996	I1997	T1998	C1999	E2000	L2001	L2002	N2003	K2004	Q2005	V2006	K2007	V2008	I2016	G2021	TYR	ALA	GLY	ARG	S2026	D2030	K2034	L2035	L2039	A2040	M2041	T2042	K2043	P2044	D2045	R2046	Q2047	L2048	I2049	V2052	S2056	R2060	E2063	V2070	P2071								
L1879	V1880	Q1881	Y1889	L1890	T1891	L1896	E1897	A1898	R1899	F1905	A1908	K1912	A1918	Q1922	L1923	G1924	R1925	E1934	T1935	Q1939	G1942	R1943	V1946	G1947	L1948	C1949	A1953	E1964	E1965	R1966	W1967	L1968	S1969	S1972	Q1973	Q1974	V1975	I1978	Q1979	E1980	H1985	S1986														





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	610	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.506	Depositor
Minimum map value	-0.279	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	329.12, 329.12, 329.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP

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	0/22554	0.42	1/30568 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	4004	MET	CB-CG-SD	-5.03	97.62	112.70

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	22085	0	22082	334	0
2	A	54	0	24	0	0
3	A	62	0	24	0	0
All	All	22201	0	22130	334	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 8.

All (334) 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:3600:ILE:O	1:A:3604:TYR:HB2	1.81	0.79
1:A:4437:VAL:HG21	1:A:4444:GLN:HG3	1.65	0.77
1:A:2854:ALA:O	1:A:2858:PHE:HB2	1.85	0.76
1:A:1623:ARG:HH21	1:A:1946:VAL:HG12	1.51	0.74
1:A:3208:ILE:HD13	1:A:3751:GLN:HB2	1.76	0.68
1:A:4004:MET:HA	1:A:4007:MET:HG3	1.76	0.68
1:A:1690:VAL:HG21	1:A:1705:VAL:HA	1.76	0.67
1:A:2601:LYS:HB3	1:A:2736:VAL:HG21	1.76	0.67
1:A:1879:LEU:HB3	1:A:1918:ALA:HB2	1.75	0.67
1:A:2503:SER:HB3	1:A:2514:LEU:HD23	1.76	0.67
1:A:1899:ARG:HG2	1:A:1985:HIS:HB2	1.76	0.66
1:A:2323:LYS:HD2	1:A:2335:LEU:HB3	1.78	0.66
1:A:3818:LEU:HA	1:A:4346:MET:HE1	1.77	0.66
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.77	0.65
1:A:2992:PHE:HB3	1:A:3064:VAL:HG22	1.79	0.65
1:A:2890:ARG:HB3	1:A:2894:LYS:HZ3	1.62	0.64
1:A:1978:ILE:HD11	1:A:2001:LEU:HD21	1.79	0.64
1:A:3214:GLN:HB3	1:A:3757:LYS:H	1.62	0.64
1:A:3878:GLN:HE22	1:A:4002:LEU:HD21	1.64	0.63
1:A:3983:ILE:HD13	1:A:4012:ASN:HB3	1.79	0.63
1:A:1880:VAL:HG11	1:A:2052:VAL:HG11	1.81	0.63
1:A:2956:LEU:HD21	1:A:2989:LYS:HE2	1.80	0.63
1:A:3888:ALA:HB1	1:A:4012:ASN:HD21	1.64	0.62
1:A:3874:GLY:HA2	1:A:4146:VAL:H	1.65	0.62
1:A:2999:VAL:HG11	1:A:3078:ARG:HH11	1.65	0.61
1:A:1654:PHE:HA	1:A:1657:MET:HB3	1.82	0.61
1:A:1975:VAL:HG21	1:A:2016:ILE:HD11	1.82	0.61
1:A:3745:LEU:HB2	1:A:3773:LEU:HD21	1.83	0.61
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.83	0.60
1:A:4461:PRO:HD2	1:A:4464:TRP:HD1	1.67	0.60
1:A:1724:VAL:HA	1:A:1727:PHE:HB2	1.84	0.60
1:A:2220:LEU:HA	1:A:2359:CYS:HB3	1.84	0.60
1:A:2472:TYR:HE2	1:A:2481:MET:HB3	1.67	0.59
1:A:2248:GLU:HB3	1:A:2297:LYS:HG3	1.83	0.59
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.84	0.59
1:A:3128:VAL:HA	1:A:3145:ASN:HD21	1.68	0.58
1:A:3661:LEU:HD21	1:A:3675:PHE:H	1.67	0.58
1:A:2085:HIS:HB3	1:A:2348:LEU:HD21	1.85	0.58
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.86	0.57
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.85	0.57
1:A:2628:PRO:HG2	1:A:2682:PHE:CD2	2.38	0.57
1:A:3190:LYS:HD3	1:A:3503:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2294:GLU:HG2	1:A:2299:GLN:HE21	1.68	0.57
1:A:2316:ASN:O	1:A:2320:ASP:HB2	2.05	0.57
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	1.85	0.57
1:A:2518:ILE:O	1:A:2522:THR:HB	2.05	0.56
1:A:2548:TRP:CE2	1:A:2576:ARG:HG2	2.40	0.56
1:A:2757:ARG:HA	1:A:2763:ARG:HH12	1.70	0.56
1:A:2071:PRO:O	1:A:2075:LEU:HB2	2.05	0.56
1:A:2548:TRP:HB2	1:A:2572:LEU:HD12	1.86	0.56
1:A:3909:LEU:HD21	1:A:4344:LEU:HA	1.87	0.56
1:A:3944:PHE:HB3	1:A:3947:LEU:HB2	1.86	0.56
1:A:1979:GLN:HB3	1:A:2035:LEU:HD13	1.88	0.56
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.88	0.56
1:A:4282:PHE:HB3	1:A:4296:MET:HE1	1.88	0.56
1:A:2503:SER:HB2	1:A:2511:ARG:HA	1.87	0.56
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.88	0.56
1:A:2751:PHE:O	1:A:2755:MET:HB2	2.05	0.56
1:A:2872:LEU:HD22	1:A:2889:LEU:HD22	1.87	0.56
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.88	0.55
1:A:2890:ARG:HA	1:A:2893:VAL:HG12	1.87	0.55
1:A:3556:ALA:HB3	1:A:3737:GLU:H	1.72	0.55
1:A:3012:LEU:HD22	1:A:3088:ARG:HB3	1.88	0.55
1:A:3873:ARG:HE	1:A:4030:ILE:HD13	1.70	0.55
1:A:1640:ILE:HG12	1:A:1650:LEU:HG	1.89	0.55
1:A:2841:GLU:HG2	1:A:2844:ARG:HH21	1.72	0.55
1:A:2281:THR:HG22	1:A:2325:LEU:HD21	1.89	0.55
1:A:3947:LEU:HA	1:A:3950:LYS:HD2	1.89	0.54
1:A:1830:ILE:HD12	1:A:1837:GLU:HB3	1.88	0.54
1:A:3009:ASN:HD21	1:A:3085:LEU:HG	1.71	0.54
1:A:4107:MET:HE1	1:A:4137:ASN:HD21	1.73	0.54
1:A:3649:LEU:HD21	1:A:3696:VAL:HB	1.88	0.53
1:A:2933:LEU:HB3	1:A:3065:VAL:HG12	1.90	0.53
1:A:4230:ARG:HE	1:A:4233:ILE:HG22	1.73	0.53
1:A:4516:VAL:HG22	1:A:4519:ALA:H	1.74	0.53
1:A:1881:GLN:HG2	1:A:1889:TYR:HE2	1.73	0.53
1:A:2759:ILE:HD12	1:A:2762:LEU:HD13	1.89	0.53
1:A:3471:LYS:HG2	1:A:3761:LEU:HD13	1.89	0.53
1:A:2938:VAL:HA	1:A:3070:PRO:HD3	1.91	0.53
1:A:3519:TYR:HB2	1:A:3698:PHE:HB2	1.91	0.53
1:A:1832:ASN:HB3	1:A:1835:SER:HB2	1.90	0.53
1:A:2222:MET:HE1	1:A:2342:MET:HB3	1.90	0.53
1:A:2876:TRP:CG	1:A:2892:TYR:HH	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1658:PHE:HB2	1:A:1661:VAL:HB	1.91	0.53
1:A:3704:THR:HG22	1:A:3705:ARG:H	1.74	0.53
1:A:3967:GLU:HB3	1:A:4004:MET:HE2	1.90	0.53
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.90	0.53
1:A:2609:LEU:HB3	1:A:2617:VAL:HG21	1.91	0.53
1:A:2262:ASP:HB2	1:A:2267:THR:HB	1.90	0.52
1:A:2450:THR:HG22	1:A:2453:ARG:H	1.75	0.52
1:A:2823:ARG:HE	1:A:2883:PRO:HB3	1.74	0.52
1:A:3597:THR:HA	1:A:3634:LEU:HD23	1.90	0.52
1:A:1766:LEU:HD23	1:A:1833:ALA:HA	1.92	0.52
1:A:4284:LEU:HG	1:A:4296:MET:HG3	1.90	0.52
1:A:2452:LEU:HD22	1:A:2729:ARG:HG2	1.92	0.52
1:A:2386:PRO:HA	1:A:2413:LEU:HD11	1.92	0.52
1:A:4306:VAL:HA	1:A:4309:VAL:HG22	1.92	0.52
1:A:3556:ALA:HA	1:A:3559:ARG:HB2	1.91	0.52
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.75	0.52
1:A:3938:LEU:HD21	1:A:3995:ALA:HB2	1.92	0.52
1:A:3200:HIS:HE1	1:A:3747:LYS:HB2	1.73	0.52
1:A:4215:ALA:HB1	1:A:4247:MET:HE1	1.91	0.51
1:A:4337:VAL:HA	1:A:4340:ILE:HD12	1.92	0.51
1:A:3757:LYS:HD3	1:A:3759:ARG:HE	1.75	0.51
1:A:4092:ARG:HE	1:A:4094:VAL:HG22	1.76	0.51
1:A:3126:MET:HG3	1:A:3128:VAL:HG23	1.92	0.51
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.92	0.51
1:A:1830:ILE:HD11	1:A:1835:SER:HB3	1.92	0.51
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.92	0.51
1:A:1964:GLU:O	1:A:1968:LEU:HB3	2.11	0.51
1:A:2930:GLN:HB3	1:A:3059:ILE:HG12	1.92	0.51
1:A:3909:LEU:HD11	1:A:4344:LEU:HB2	1.92	0.51
1:A:1964:GLU:O	1:A:1968:LEU:CB	2.59	0.51
1:A:3935:VAL:O	1:A:3939:SER:HB3	2.11	0.51
1:A:2553:PRO:HB2	1:A:2570:PRO:HG2	1.92	0.51
1:A:3986:ALA:HA	1:A:3989:ARG:HE	1.75	0.51
1:A:4413:PHE:HD2	1:A:4504:LEU:HD13	1.76	0.51
1:A:3575:GLU:HA	1:A:3578:ILE:HD12	1.93	0.50
1:A:4289:ASP:HA	1:A:4325:ASN:HD21	1.76	0.50
1:A:3522:GLN:HG2	1:A:3572:LEU:HD13	1.93	0.50
1:A:4324:PRO:HD3	1:A:4638:ARG:HD3	1.94	0.50
1:A:2583:THR:HG22	1:A:2584:TRP:CD1	2.46	0.50
1:A:3590:ILE:HA	1:A:3681:THR:HG22	1.92	0.50
1:A:3942:PRO:HA	1:A:3945:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3010:THR:HG23	1:A:3017:VAL:HG22	1.93	0.50
1:A:2223:VAL:HG11	1:A:2348:LEU:HD23	1.93	0.50
1:A:2999:VAL:HA	1:A:3004:PHE:HZ	1.77	0.50
1:A:2413:LEU:HD23	1:A:2417:ARG:HH21	1.76	0.50
1:A:2591:LEU:HB3	1:A:2709:VAL:HG23	1.93	0.50
1:A:2410:SER:HB2	1:A:2413:LEU:HD13	1.93	0.49
1:A:2132:PRO:HB2	1:A:2135:GLU:HB2	1.94	0.49
1:A:1698:ILE:HA	1:A:1701:TRP:CD1	2.46	0.49
1:A:3499:GLN:O	1:A:3503:ILE:HB	2.12	0.49
1:A:4010:SER:HB3	1:A:4015:GLU:HG3	1.95	0.49
1:A:2972:PHE:HE2	1:A:3007:ARG:HH11	1.61	0.49
1:A:3511:ALA:HA	1:A:3514:ILE:HD12	1.94	0.49
1:A:3954:ASP:HB3	1:A:3957:PHE:HB2	1.93	0.49
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.93	0.49
1:A:4233:ILE:HB	1:A:4237:LYS:HD2	1.93	0.49
1:A:2427:PHE:HE2	1:A:2459:PHE:HE1	1.60	0.49
1:A:2453:ARG:HH21	1:A:2728:LEU:HD22	1.77	0.49
1:A:4071:ILE:HD12	1:A:4099:VAL:HG12	1.94	0.49
1:A:1623:ARG:HH22	1:A:1947:GLY:HA2	1.77	0.48
1:A:1850:GLN:HB2	1:A:1856:GLN:HG2	1.95	0.48
1:A:1979:GLN:HG3	1:A:2035:LEU:HD22	1.94	0.48
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.94	0.48
1:A:2678:ARG:O	1:A:2682:PHE:HD2	1.97	0.48
1:A:2156:LEU:HD21	1:A:4405:ILE:HG13	1.96	0.48
1:A:3151:HIS:CE1	1:A:3176:TYR:HB2	2.48	0.48
1:A:4274:THR:HG23	1:A:4276:ARG:H	1.78	0.48
1:A:1843:ARG:H	1:A:1861:MET:HE1	1.79	0.48
1:A:3169:MET:HG3	1:A:3698:PHE:HE2	1.78	0.48
1:A:3812:TYR:HA	1:A:3815:MET:HG2	1.96	0.48
1:A:3598:GLU:O	1:A:3602:ASN:HB2	2.14	0.48
1:A:2993:ILE:HD11	1:A:3067:THR:HG23	1.94	0.48
1:A:4199:LEU:HD12	1:A:4615:ARG:HH22	1.78	0.48
1:A:1812:ILE:HD13	1:A:2056:SER:HA	1.96	0.47
1:A:2684:ARG:HG3	1:A:2726:ARG:HG3	1.95	0.47
1:A:3009:ASN:HB3	1:A:3088:ARG:HH21	1.79	0.47
1:A:2284:LEU:HA	1:A:2287:ILE:HG22	1.97	0.47
1:A:3590:ILE:HG23	1:A:3700:ASN:HA	1.97	0.47
1:A:3881:ILE:HG12	1:A:4006:HIS:CE1	2.49	0.47
1:A:4395:LEU:HB2	1:A:4424:LEU:HD13	1.96	0.47
1:A:2287:ILE:HD13	1:A:2339:VAL:HG22	1.96	0.47
1:A:1638:LEU:HD12	1:A:1641:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:ARG:HG3	1:A:2090:LEU:HD13	1.95	0.47
1:A:2752:ASN:HA	1:A:2755:MET:HB3	1.96	0.47
1:A:3743:ARG:HA	1:A:3746:GLU:HB3	1.97	0.47
1:A:4349:LEU:HD23	1:A:4350:GLU:HB2	1.96	0.47
1:A:3875:MET:HB2	1:A:3880:HIS:CD2	2.50	0.47
1:A:2492:ARG:HB3	1:A:2539:VAL:HG12	1.96	0.47
1:A:4260:PHE:HD1	1:A:4263:ARG:HH22	1.64	0.47
1:A:2893:VAL:HG13	1:A:2911:LEU:HD12	1.95	0.46
1:A:3661:LEU:HD22	1:A:3672:SER:HB3	1.95	0.46
1:A:3861:LYS:HZ3	1:A:3891:LYS:HE3	1.79	0.46
1:A:3888:ALA:HB1	1:A:4012:ASN:ND2	2.30	0.46
1:A:3749:LEU:HG	1:A:3773:LEU:HD22	1.96	0.46
1:A:4330:VAL:HA	1:A:4333:THR:HG22	1.97	0.46
1:A:3831:PHE:O	1:A:3835:ILE:HG12	2.16	0.46
1:A:2277:ASP:HB3	1:A:2282:HIS:HB2	1.96	0.46
1:A:3496:PHE:HD1	1:A:3500:MET:HE1	1.81	0.46
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.98	0.46
1:A:2890:ARG:HB3	1:A:2894:LYS:NZ	2.30	0.46
1:A:2897:LEU:HD23	1:A:2911:LEU:HD22	1.96	0.46
1:A:2387:LEU:HB2	1:A:2416:GLN:HE22	1.79	0.46
1:A:2605:LEU:O	1:A:2609:LEU:HB2	2.16	0.46
1:A:3190:LYS:HE2	1:A:3190:LYS:HB2	1.79	0.46
1:A:3970:VAL:HG11	1:A:3989:ARG:HG2	1.98	0.46
1:A:2680:ILE:HG12	1:A:2723:LEU:HD22	1.98	0.46
1:A:4412:PHE:HE1	1:A:4516:VAL:HG13	1.80	0.46
1:A:1825:LEU:HD22	1:A:1830:ILE:HG21	1.98	0.45
1:A:2415:ILE:HD12	1:A:2486:LEU:HD21	1.98	0.45
1:A:3154:LEU:HD23	1:A:3171:ILE:HG12	1.98	0.45
1:A:4600:LYS:HE2	1:A:4604:VAL:HG11	1.98	0.45
1:A:2156:LEU:HD13	1:A:4411:ARG:HD3	1.97	0.45
1:A:2241:LEU:HB3	1:A:2298:ARG:HH22	1.81	0.45
1:A:2393:GLU:HA	1:A:2396:ARG:HB2	1.98	0.45
1:A:3893:LYS:HG2	1:A:3900:THR:HB	1.97	0.45
1:A:2049:ILE:HD13	1:A:2090:LEU:HD21	1.98	0.45
1:A:4157:MET:HE2	1:A:4157:MET:HB3	1.73	0.45
1:A:2628:PRO:HD3	1:A:2679:VAL:HG22	1.99	0.45
1:A:2972:PHE:HE2	1:A:3007:ARG:HD2	1.81	0.45
1:A:4444:GLN:HG2	1:A:4448:LEU:HD13	1.98	0.45
1:A:2754:ALA:HA	1:A:2757:ARG:HE	1.81	0.45
1:A:4390:LEU:HD11	1:A:4479:VAL:HG12	1.99	0.45
1:A:1697:LYS:HD2	1:A:1697:LYS:HA	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1738:TYR:CZ	1:A:1742:ILE:HD11	2.51	0.45
1:A:3169:MET:HE1	1:A:3519:TYR:CZ	2.51	0.45
1:A:1628:ARG:HD3	1:A:1657:MET:HE1	1.97	0.45
1:A:4230:ARG:HH21	1:A:4237:LYS:HD3	1.82	0.45
1:A:1796:VAL:HA	1:A:1805:ARG:HH22	1.82	0.44
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	2.00	0.44
1:A:2932:HIS:CE1	1:A:3064:VAL:HB	2.52	0.44
1:A:1866:PHE:HZ	1:A:1896:LEU:HB3	1.82	0.44
1:A:3017:VAL:HB	1:A:3020:LEU:HG	1.99	0.44
1:A:4003:ALA:HA	1:A:4006:HIS:HD2	1.82	0.44
1:A:2445:HIS:CD2	1:A:2449:LEU:HD13	2.53	0.44
1:A:3993:ILE:HG13	1:A:4004:MET:HE1	1.99	0.44
1:A:4070:ALA:HA	1:A:4097:LYS:HB2	1.99	0.44
1:A:1630:TYR:HE2	1:A:1946:VAL:HB	1.82	0.44
1:A:3824:LEU:HA	1:A:4139:LEU:HD13	1.99	0.44
1:A:4042:LEU:HB3	1:A:4144:ILE:HA	2.00	0.44
1:A:3596:ALA:HA	1:A:3599:PHE:HD2	1.83	0.44
1:A:4380:LEU:HA	1:A:4383:THR:HG22	2.00	0.44
1:A:3715:GLU:HG3	1:A:3718:LYS:HE3	2.00	0.44
1:A:2628:PRO:HG2	1:A:2682:PHE:CG	2.53	0.44
1:A:2745:THR:HG22	1:A:2774:VAL:HG21	2.00	0.43
1:A:1912:LYS:HG2	1:A:2041:MET:HG3	2.01	0.43
1:A:2981:ARG:O	1:A:2985:CYS:HB2	2.18	0.43
1:A:4093:TRP:HB3	1:A:4125:PHE:HE2	1.83	0.43
1:A:1948:LEU:HD23	1:A:1953:ALA:HB3	2.00	0.43
1:A:2409:ALA:HB3	1:A:2413:LEU:HD22	2.00	0.43
1:A:2743:SER:O	1:A:2747:ILE:HG22	2.19	0.43
1:A:2307:VAL:HG11	1:A:2351:ALA:HB2	2.00	0.43
1:A:2375:PHE:HB3	1:A:2427:PHE:HB3	2.01	0.43
1:A:4511:LEU:HD12	1:A:4560:VAL:HG11	2.01	0.43
1:A:2307:VAL:HB	1:A:2345:VAL:HG11	2.00	0.43
1:A:2308:ASP:HB3	1:A:2311:TRP:NE1	2.34	0.43
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	2.00	0.43
1:A:4522:THR:O	1:A:4526:GLN:HG3	2.19	0.43
1:A:2241:LEU:HB3	1:A:2298:ARG:NH2	2.33	0.43
1:A:2381:ARG:O	1:A:2385:ILE:HB	2.18	0.43
1:A:3134:PRO:HD2	1:A:3141:GLU:HG2	2.00	0.43
1:A:3187:PHE:HA	1:A:3190:LYS:HG2	2.01	0.43
1:A:3485:GLU:HB3	1:A:3489:TRP:CZ3	2.53	0.43
1:A:3908:PHE:HD1	1:A:3991:LEU:HD23	1.84	0.43
1:A:2910:VAL:HG12	1:A:2912:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2972:PHE:CE2	1:A:3007:ARG:HD2	2.54	0.42
1:A:2230:LYS:NZ	1:A:2726:ARG:HH22	2.17	0.42
1:A:2660:VAL:HG22	1:A:2707:GLN:HB2	2.02	0.42
1:A:2824:ILE:HA	1:A:2873:TYR:HE2	1.83	0.42
1:A:3052:LYS:HE2	1:A:3052:LYS:HB2	1.85	0.42
1:A:3493:SER:HA	1:A:3496:PHE:CE2	2.53	0.42
1:A:4042:LEU:HD23	1:A:4144:ILE:HG23	2.01	0.42
1:A:2046:ARG:HD2	1:A:2070:VAL:HG13	2.00	0.42
1:A:2565:PRO:HG2	1:A:2603:MET:HE1	1.99	0.42
1:A:3069:ASN:HD21	1:A:3691:ASP:HB2	1.83	0.42
1:A:1792:LEU:O	1:A:1796:VAL:HB	2.19	0.42
1:A:4171:LYS:HD2	1:A:4171:LYS:HA	1.78	0.42
1:A:2254:ILE:HD11	1:A:2283:VAL:HG21	2.01	0.42
1:A:3009:ASN:HB3	1:A:3088:ARG:NH2	2.34	0.42
1:A:3195:GLU:HA	1:A:3198:GLN:HB2	2.01	0.42
1:A:3513:PHE:CD2	1:A:3549:ARG:HG2	2.55	0.42
1:A:4095:MET:HA	1:A:4125:PHE:HB2	2.02	0.42
1:A:4508:HIS:HE1	1:A:4553:LEU:HD11	1.84	0.42
1:A:1949:CYS:HB3	1:A:2008:VAL:HA	2.00	0.42
1:A:3586:TYR:HB2	1:A:3649:LEU:HD12	2.02	0.42
1:A:3908:PHE:CD1	1:A:3991:LEU:HD23	2.55	0.42
1:A:2937:GLY:HA3	1:A:3094:PHE:HB3	2.00	0.42
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	2.02	0.42
1:A:3043:MET:HE3	1:A:3043:MET:HB3	1.96	0.42
1:A:3904:GLU:HA	1:A:3941:LEU:HD13	2.01	0.42
1:A:1972:SER:HA	1:A:1975:VAL:HG12	2.02	0.42
1:A:2548:TRP:CD2	1:A:2576:ARG:HG2	2.55	0.42
1:A:2978:THR:HG22	1:A:2981:ARG:HE	1.85	0.42
1:A:2618:VAL:HB	1:A:2661:LEU:HD23	2.02	0.41
1:A:1899:ARG:HD3	1:A:1986:SER:HA	2.02	0.41
1:A:2982:ARG:HA	1:A:2982:ARG:HD3	1.88	0.41
1:A:3205:LEU:O	1:A:3208:ILE:HG22	2.20	0.41
1:A:4166:VAL:HG23	1:A:4302:ARG:HD2	2.02	0.41
1:A:2154:ILE:HG13	1:A:2155:PRO:HD3	2.03	0.41
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	2.01	0.41
1:A:4577:LEU:HD22	1:A:4638:ARG:CZ	2.50	0.41
1:A:2311:TRP:HZ3	1:A:2343:PHE:HE2	1.67	0.41
1:A:2978:THR:HA	1:A:2981:ARG:HE	1.85	0.41
1:A:3561:ARG:HH21	1:A:3603:GLU:HG2	1.84	0.41
1:A:4040:PRO:HD3	1:A:4113:LEU:HD21	2.01	0.41
1:A:1733:ILE:HD13	1:A:1733:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2300:TRP:CD1	1:A:2340:ARG:HB2	2.55	0.41
1:A:2499:LEU:HD23	1:A:2499:LEU:HA	1.87	0.41
1:A:2680:ILE:HD12	1:A:2680:ILE:HA	1.83	0.41
1:A:3171:ILE:HD12	1:A:3171:ILE:HA	1.96	0.41
1:A:3993:ILE:HD13	1:A:3993:ILE:HA	1.95	0.41
1:A:4601:LYS:HB2	1:A:4604:VAL:HG23	2.01	0.41
1:A:1872:TYR:CZ	1:A:1874:GLY:HA2	2.56	0.41
1:A:1891:THR:HG21	1:A:2039:LEU:HD12	2.02	0.41
1:A:2561:LYS:HD2	1:A:2561:LYS:HA	1.74	0.41
1:A:3196:GLU:HB2	1:A:3199:MET:HE2	2.03	0.41
1:A:3209:LYS:HD3	1:A:3209:LYS:HA	1.76	0.41
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.01	0.41
1:A:1819:ARG:HG2	1:A:1823:ARG:NE	2.36	0.41
1:A:2178:LEU:HD12	1:A:2178:LEU:HA	1.92	0.41
1:A:2393:GLU:HG3	1:A:2396:ARG:HH11	1.85	0.41
1:A:2915:VAL:HG23	1:A:2946:LEU:HD11	2.03	0.41
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	2.03	0.41
1:A:3143:ILE:HD13	1:A:3143:ILE:HA	1.95	0.41
1:A:3927:LEU:HD21	1:A:3957:PHE:HE2	1.86	0.41
1:A:4003:ALA:O	1:A:4006:HIS:HB2	2.21	0.41
1:A:4023:GLN:HG2	1:A:4024:PRO:HD2	2.02	0.41
1:A:1881:GLN:HG3	1:A:1922:GLN:HE22	1.84	0.41
1:A:2838:VAL:HA	1:A:3093:TRP:CD1	2.56	0.41
1:A:1717:LEU:HD13	1:A:1749:LEU:HD22	2.01	0.41
1:A:2234:TRP:HE1	1:A:2342:MET:HE3	1.85	0.41
1:A:3570:ASP:OD1	1:A:3573:CYS:HB2	2.21	0.41
1:A:3873:ARG:HB2	1:A:4143:ARG:HH12	1.86	0.41
1:A:3208:ILE:HD12	1:A:3208:ILE:HA	1.91	0.41
1:A:3873:ARG:HA	1:A:3873:ARG:HD3	1.84	0.41
1:A:4536:LEU:HD23	1:A:4536:LEU:HA	1.90	0.41
1:A:2422:ILE:HD13	1:A:2422:ILE:HA	1.92	0.40
1:A:3646:ASN:O	1:A:3650:ASN:HB2	2.21	0.40
1:A:2993:ILE:HD13	1:A:3065:VAL:HG23	2.02	0.40
1:A:3713:LEU:HA	1:A:3716:VAL:HG12	2.03	0.40
1:A:4154:LYS:HE2	1:A:4154:LYS:HB2	1.89	0.40
1:A:4189:ILE:O	1:A:4193:ARG:HB2	2.21	0.40
1:A:4405:ILE:HD12	1:A:4405:ILE:HA	1.91	0.40
1:A:1899:ARG:HB2	1:A:1986:SER:HB3	2.03	0.40
1:A:3220:ARG:HA	1:A:3220:ARG:HD2	1.91	0.40
1:A:3811:ILE:HD12	1:A:3887:LEU:HD22	2.02	0.40
1:A:4004:MET:HE2	1:A:4004:MET:HB3	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1925:ARG:HD3	1:A:1925:ARG:HA	1.81	0.40
1:A:2580:LEU:HD23	1:A:2580:LEU:HA	1.85	0.40
1:A:2896:ARG:HD3	1:A:2949:PHE:HZ	1.85	0.40
1:A:2090:LEU:HD12	1:A:2093:LEU:HB3	2.03	0.40
1:A:2510:MET:HA	1:A:2513:GLU:HG2	2.02	0.40

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	2745/4843 (57%)	2614 (95%)	131 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2440/4279 (57%)	2439 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3038	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1643	ASN
1	A	1670	ASN
1	A	1784	ASN
1	A	1876	GLN
1	A	1922	GLN
1	A	2252	HIS
1	A	2376	ASN
1	A	2439	HIS
1	A	2442	GLN
1	A	2482	GLN
1	A	2667	ASN
1	A	2932	HIS
1	A	2960	GLN
1	A	3047	HIS
1	A	3057	GLN
1	A	3200	HIS
1	A	3631	ASN
1	A	3650	ASN
1	A	3735	GLN
1	A	3878	GLN
1	A	3988	HIS
1	A	4231	GLN
1	A	4325	ASN
1	A	4335	GLN
1	A	4381	HIS
1	A	4386	ASN
1	A	4490	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	A	4702	-	32,33,33	0.42	0	48,52,52	0.39	0
2	ADP	A	4704	-	28,29,29	1.39	5 (17%)	43,45,45	1.80	10 (23%)
3	ATP	A	4703	-	32,33,33	0.36	0	48,52,52	0.60	1 (2%)
2	ADP	A	4701	-	28,29,29	1.42	4 (14%)	43,45,45	1.94	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4702	-	-	5/22/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4703	-	-	7/22/38/38	0/3/3/3
2	ADP	A	4701	-	-	5/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C5-C4	4.70	1.47	1.39
2	A	4704	ADP	C5-C4	4.61	1.47	1.39
2	A	4704	ADP	C5-C6	2.62	1.48	1.41
2	A	4701	ADP	C5-C6	2.56	1.48	1.41
2	A	4701	ADP	C5-N7	-2.55	1.34	1.39
2	A	4704	ADP	C5-N7	-2.30	1.34	1.39
2	A	4701	ADP	C8-N7	2.27	1.36	1.31
2	A	4704	ADP	C8-N7	2.25	1.36	1.31
2	A	4704	ADP	C4-N9	-2.05	1.33	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-6.85	117.28	126.72
2	A	4704	ADP	C5-C4-N3	-5.47	119.18	126.72
2	A	4701	ADP	N3-C4-N9	5.37	136.31	127.17
2	A	4704	ADP	N3-C4-N9	4.51	134.83	127.17
2	A	4701	ADP	C2-N3-C4	4.03	121.67	111.83
2	A	4704	ADP	C2-N3-C4	3.50	120.37	111.83
2	A	4701	ADP	C4-C5-N7	-3.40	106.70	110.58
2	A	4704	ADP	C4-C5-N7	-3.31	106.79	110.58
2	A	4704	ADP	N3-C2-N1	-3.22	123.72	128.58
2	A	4701	ADP	N3-C2-N1	-3.12	123.86	128.58
2	A	4704	ADP	C4-N9-C8	3.06	108.95	105.74
2	A	4701	ADP	C3'-C2'-C1'	2.54	106.28	101.46
2	A	4704	ADP	C5-N7-C8	2.47	107.34	103.45
2	A	4701	ADP	C5-N7-C8	2.45	107.29	103.45
2	A	4704	ADP	N9-C8-N7	-2.12	110.93	113.94
3	A	4703	ATP	C4-N9-C1'	2.08	131.50	126.63
2	A	4704	ADP	C2-N1-C6	2.08	122.15	118.73
2	A	4701	ADP	C4-N9-C8	2.02	107.86	105.74
2	A	4704	ADP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	PB-O3A-PA-O5'
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4703	ATP	PB-O3B-PG-O3G
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
2	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4703	ATP	C2'-C1'-N9-C4
3	A	4703	ATP	C2'-C1'-N9-C8
2	A	4701	ADP	C5'-O5'-PA-O1A
3	A	4703	ATP	O4'-C4'-C5'-O5'
3	A	4703	ATP	C3'-C4'-C5'-O5'
3	A	4703	ATP	PB-O3B-PG-O1G
3	A	4702	ATP	PB-O3B-PG-O2G
3	A	4703	ATP	PB-O3B-PG-O2G
3	A	4702	ATP	PG-O3B-PB-O2B

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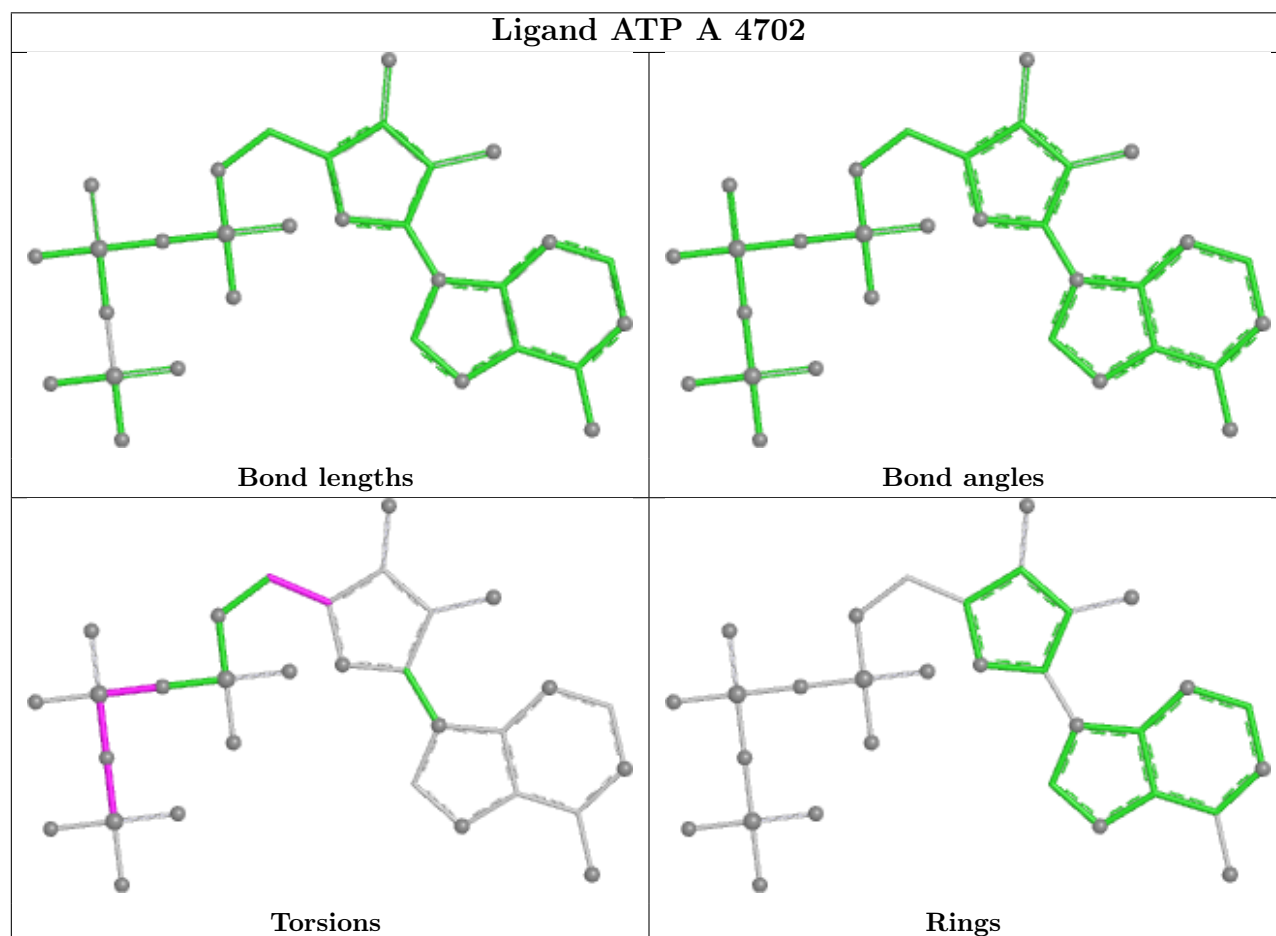
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Mol	Chain	Res	Type	Atoms
3	A	4702	ATP	PA-O3A-PB-O2B
2	A	4701	ADP	O4'-C4'-C5'-O5'

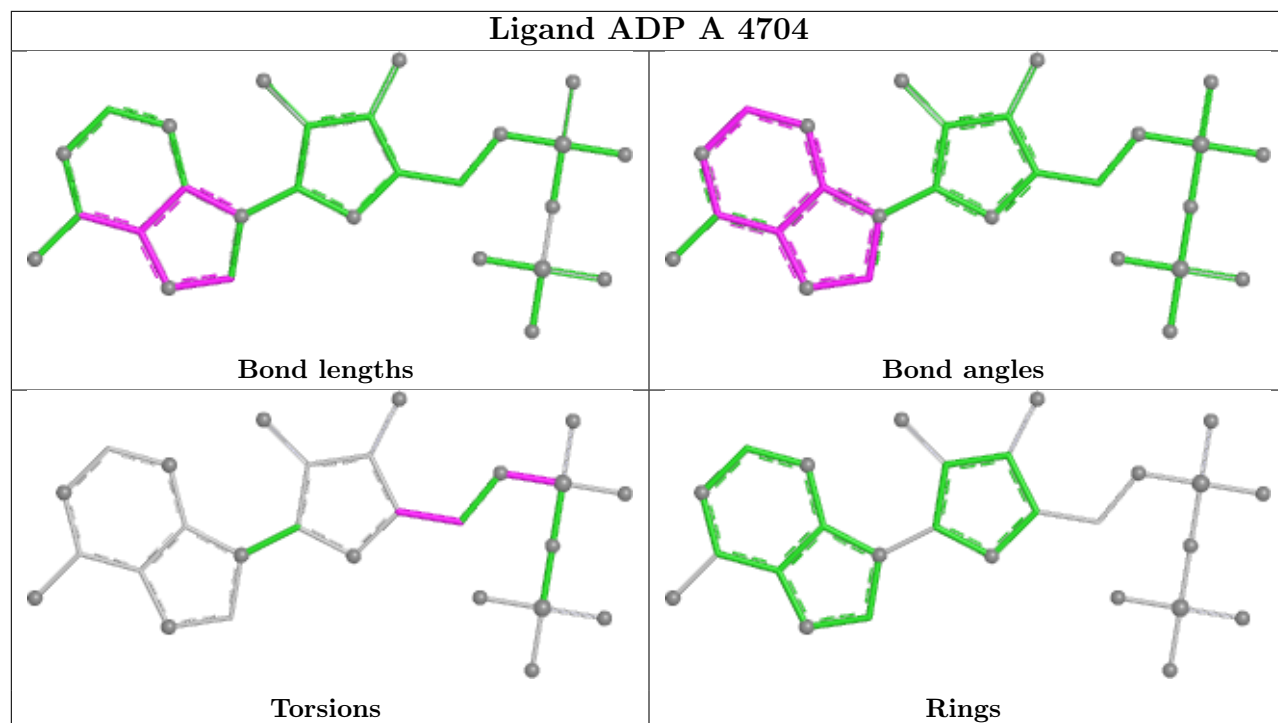
There are no ring outliers.

No monomer is involved in short contacts.

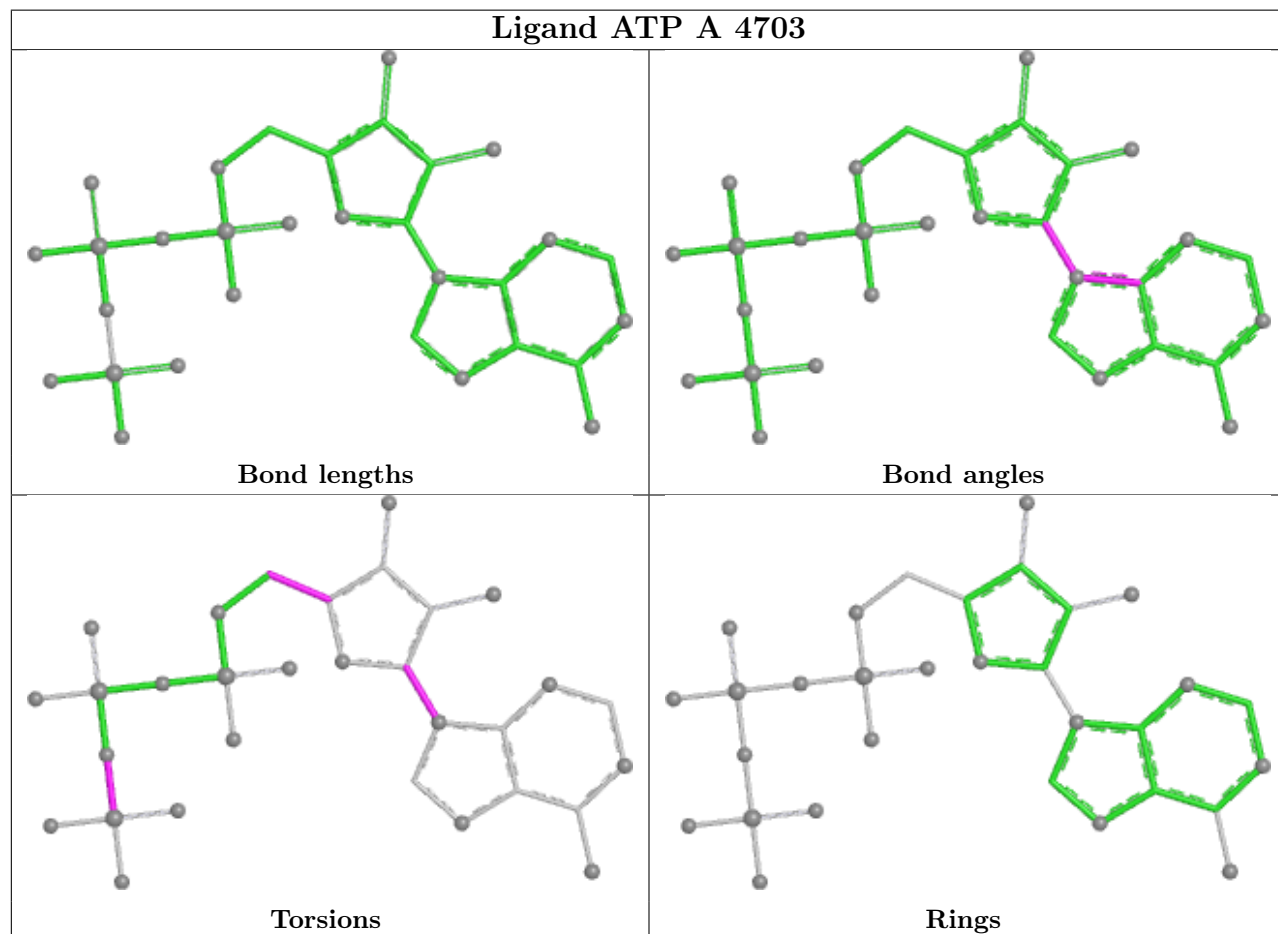
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

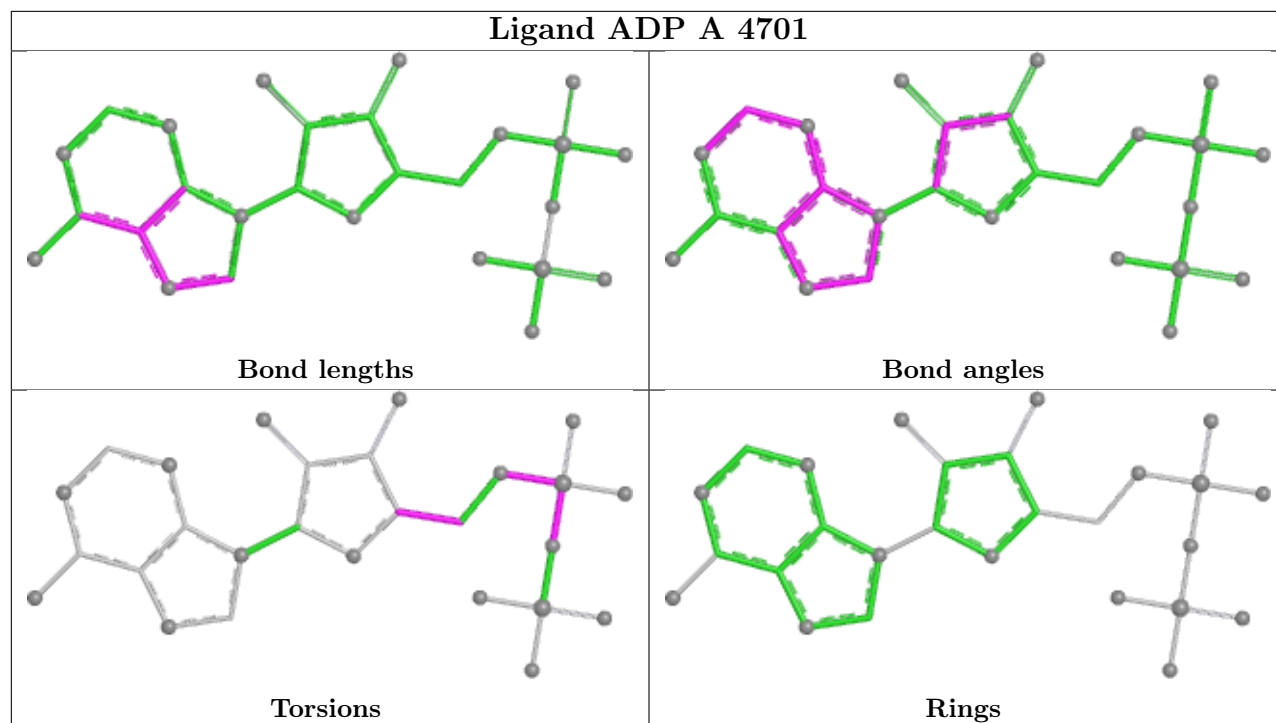


Ligand ADP A 4704



Ligand ATP A 4703





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.

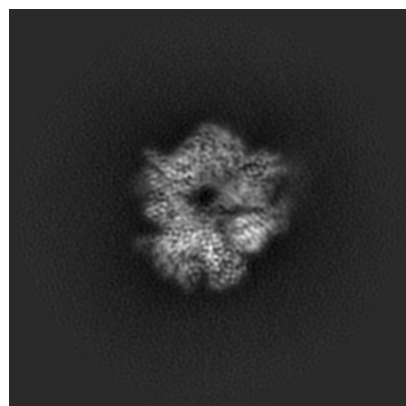
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47377. These allow visual inspection of the internal detail of the map and identification of artifacts.

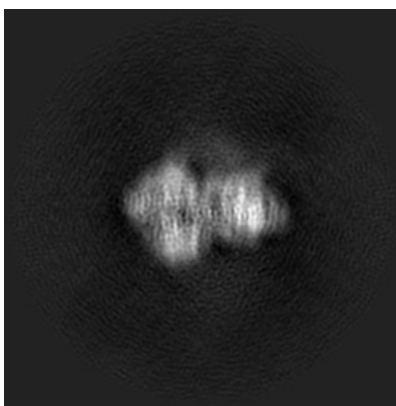
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

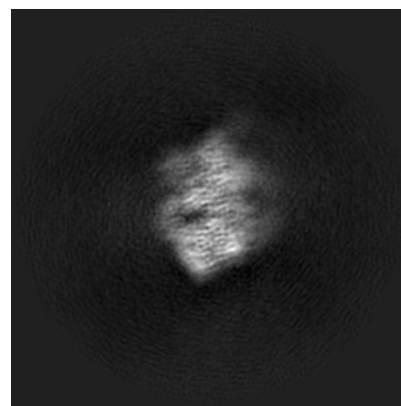
6.1.1 Primary map



X

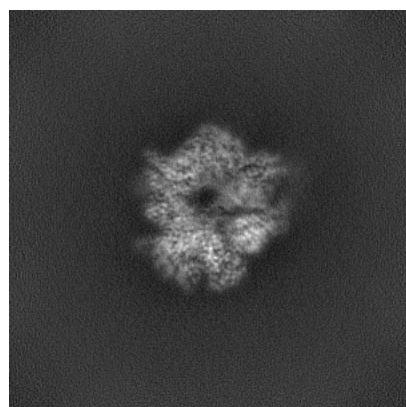


Y

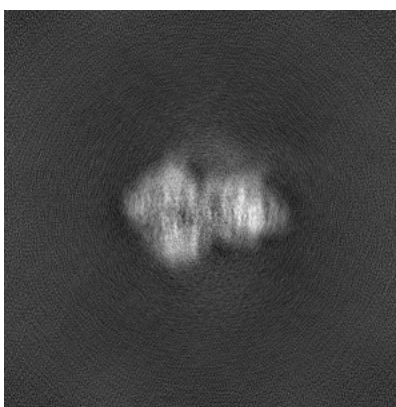


Z

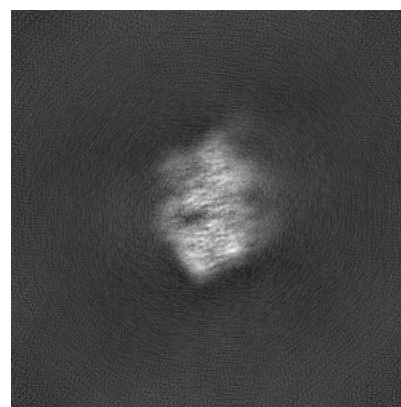
6.1.2 Raw map



X



Y

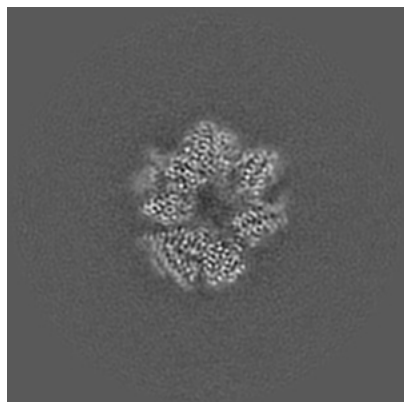


Z

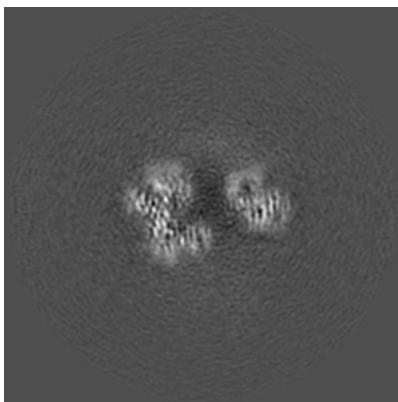
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

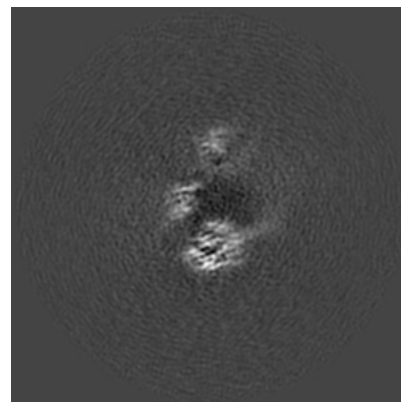
6.2.1 Primary map



X Index: 176

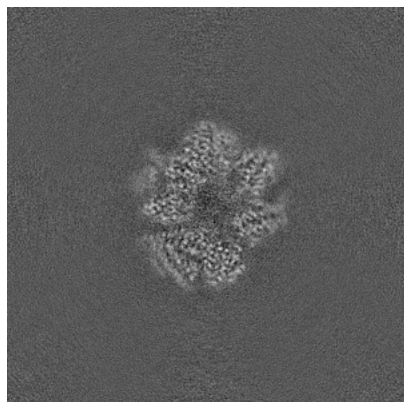


Y Index: 176

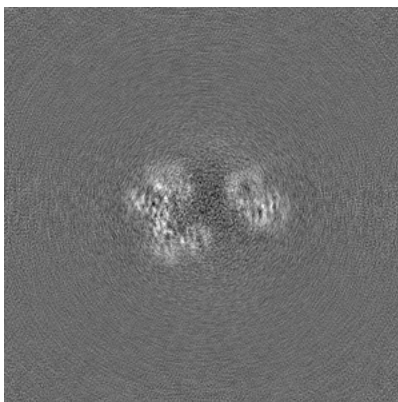


Z Index: 176

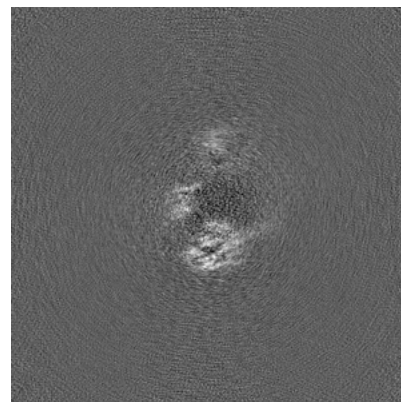
6.2.2 Raw map



X Index: 176



Y Index: 176

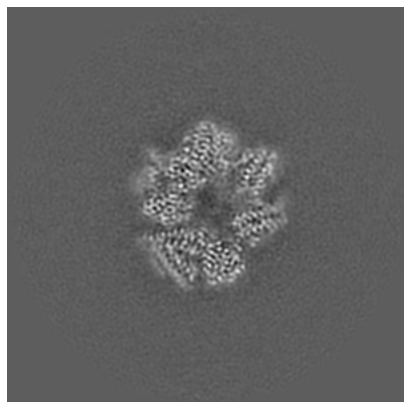


Z Index: 176

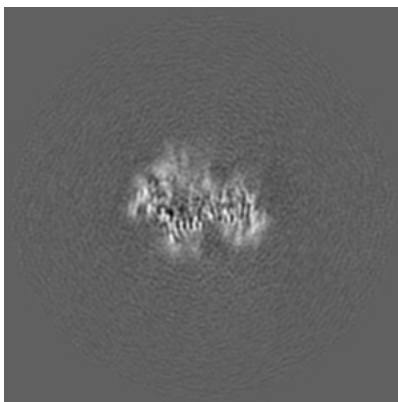
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

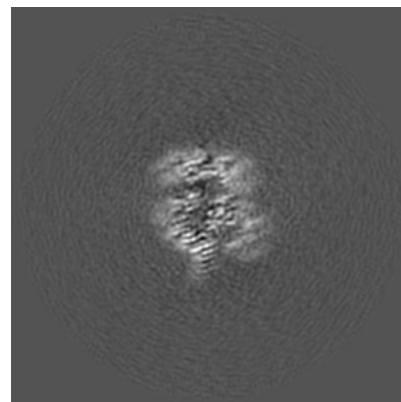
6.3.1 Primary map



X Index: 175

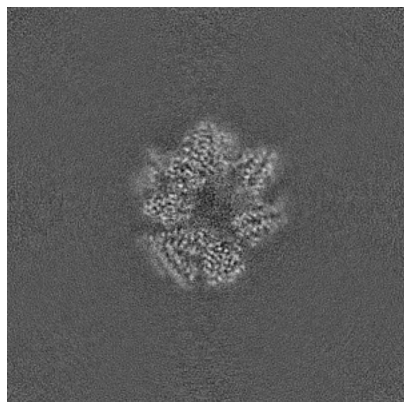


Y Index: 150

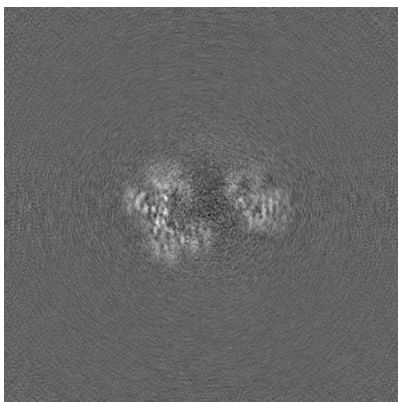


Z Index: 151

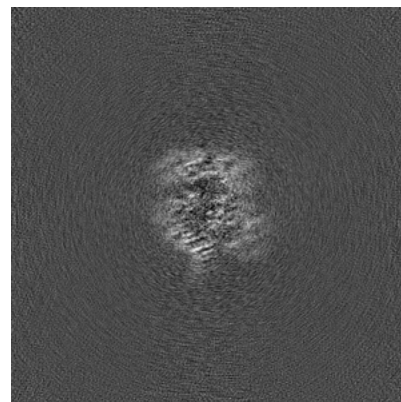
6.3.2 Raw map



X Index: 175



Y Index: 177

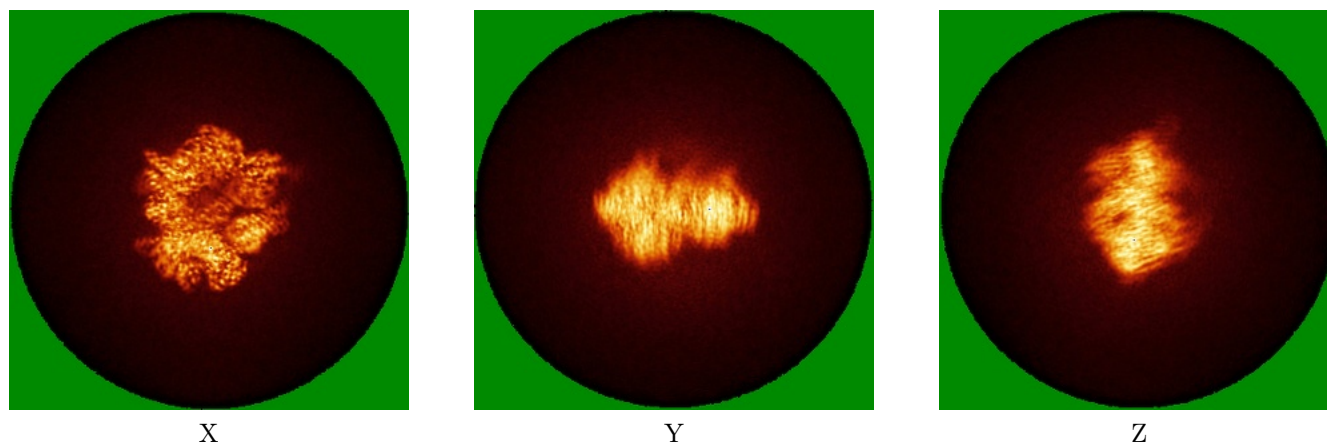


Z Index: 151

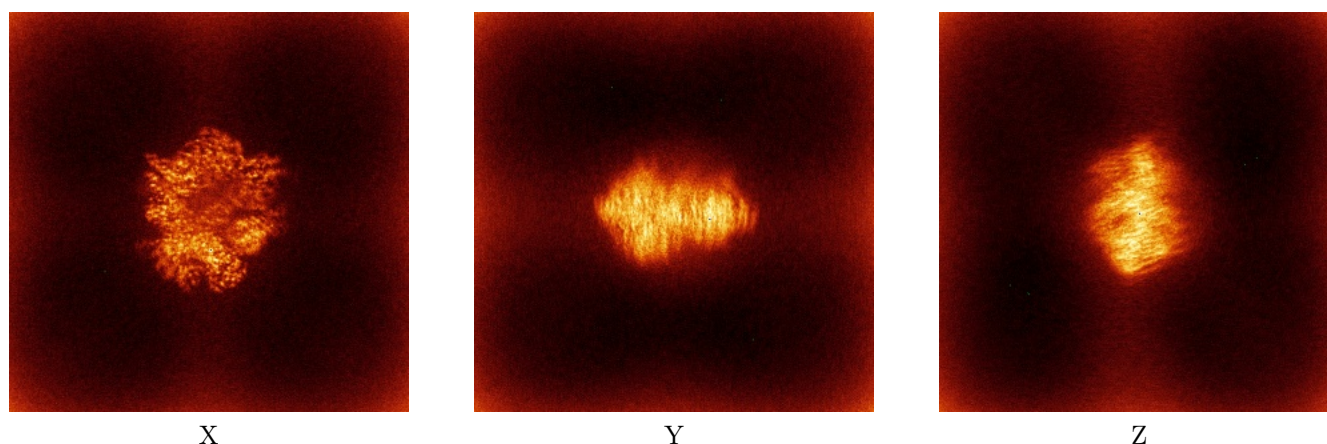
The images above show the largest variance slices of the map in three orthogonal directions.

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.

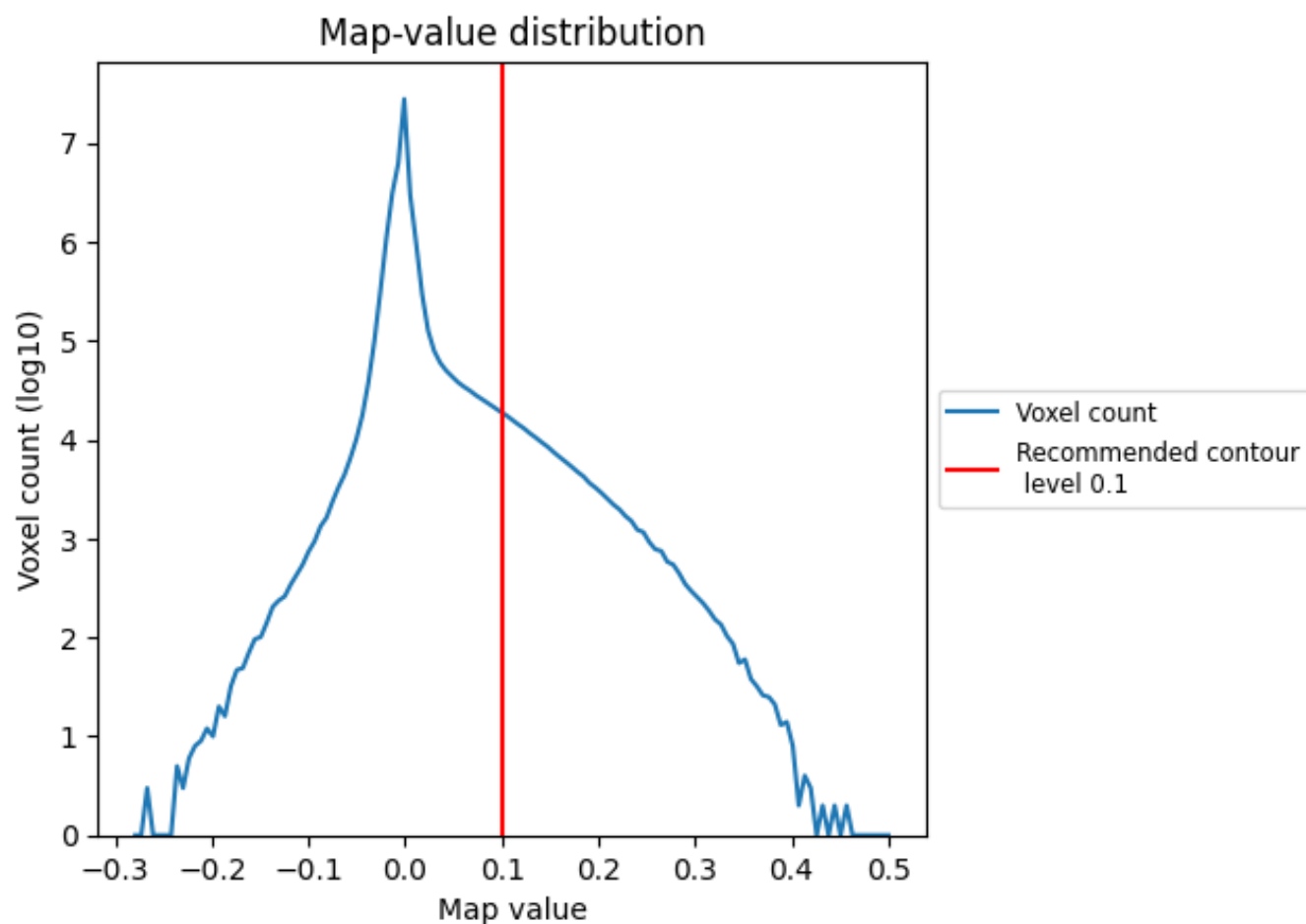
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

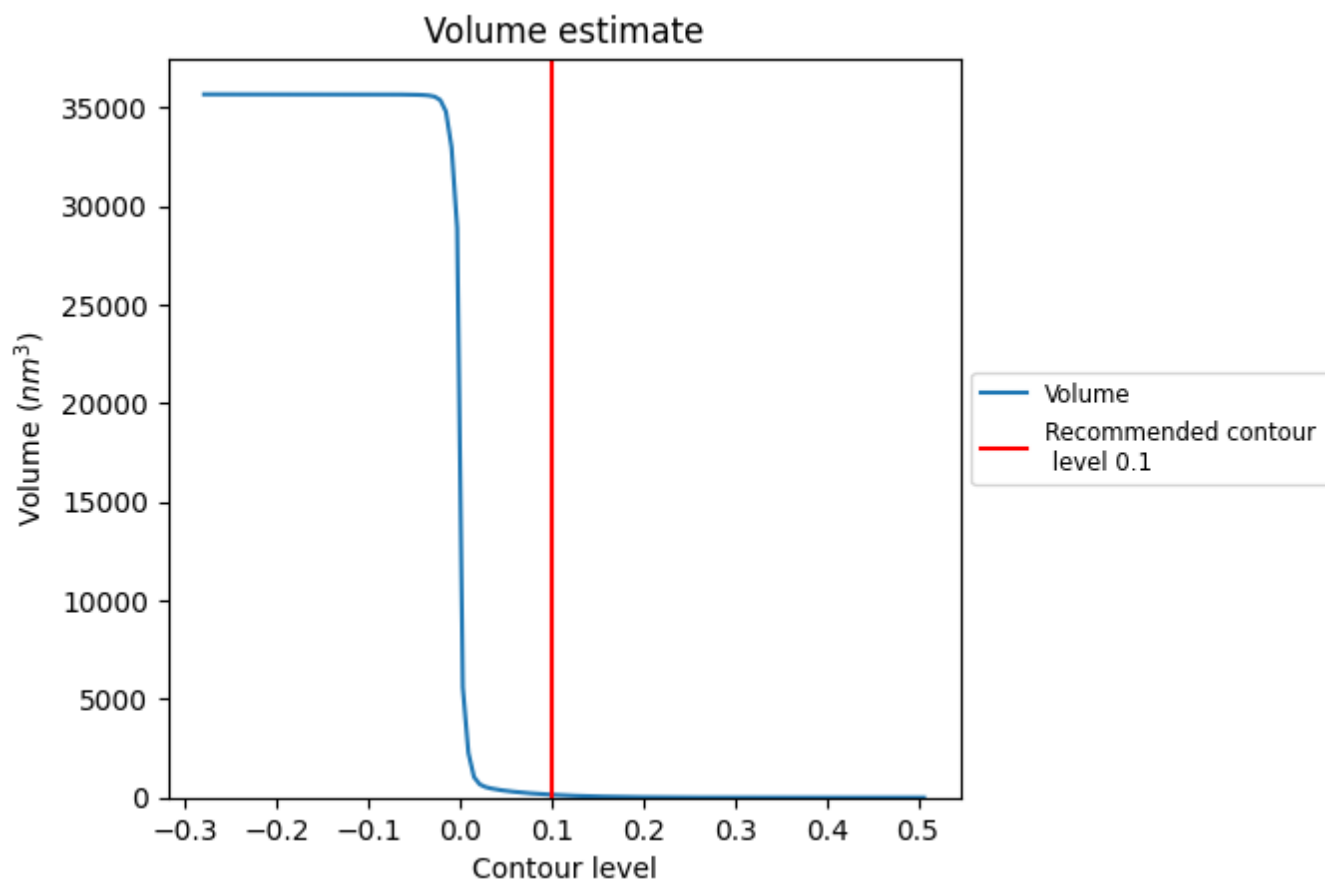
This section contains the results of statistical analysis of the map.

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.

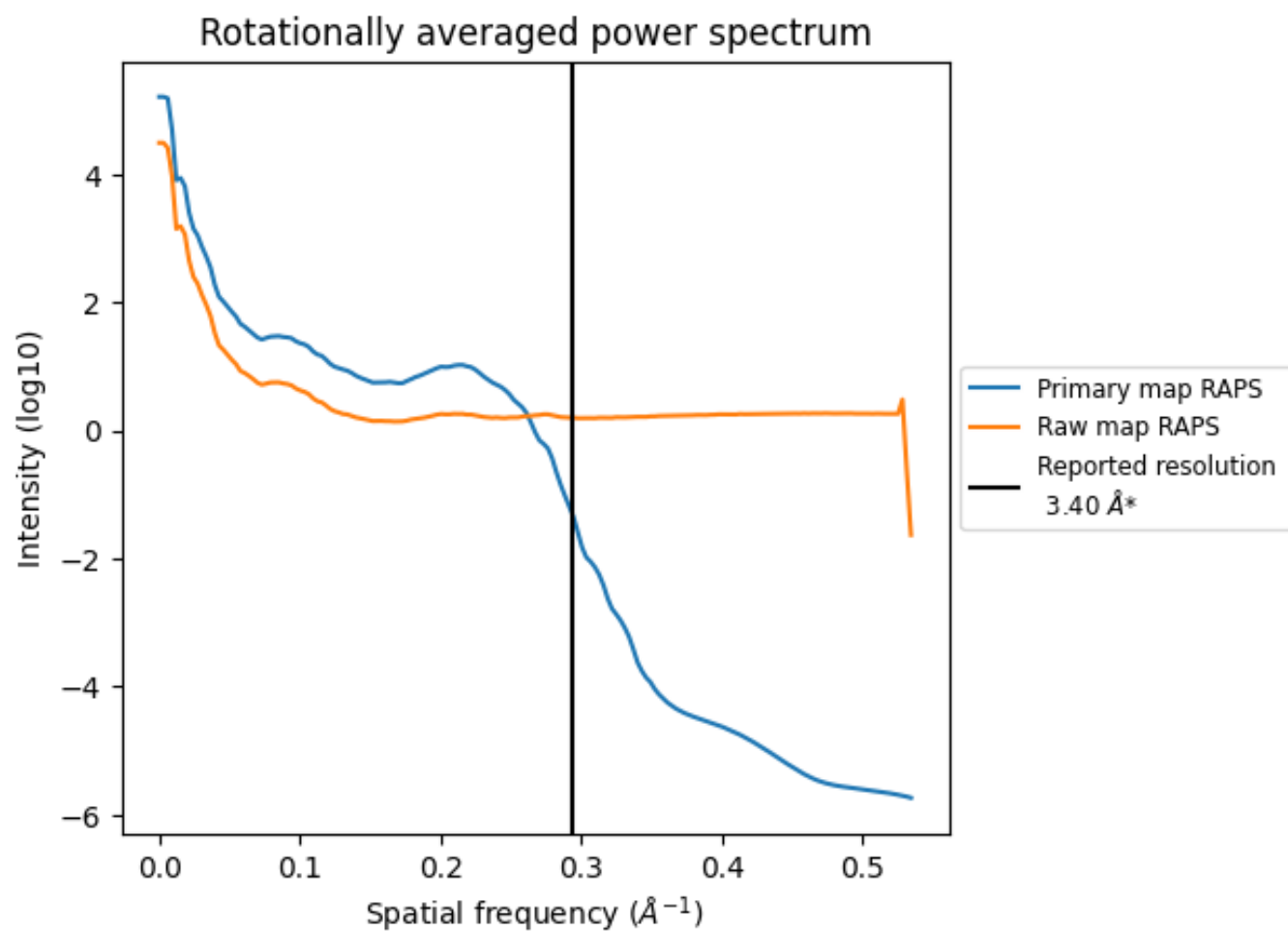
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145 nm^3 ; this corresponds to an approximate mass of 131 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 ⓘ

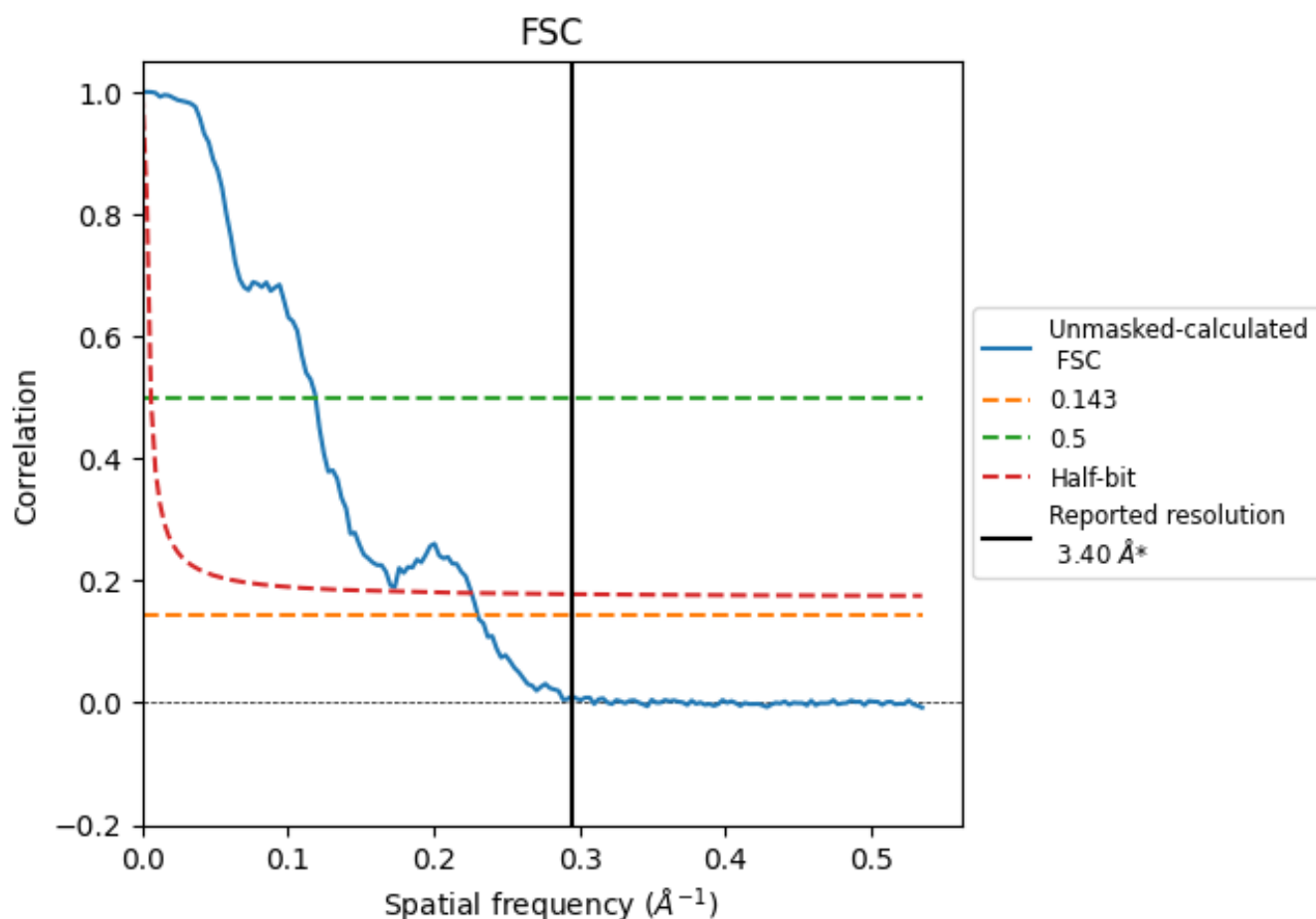


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.34	8.42	4.43

*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 4.34 differs from the reported value 3.4 by more than 10 %

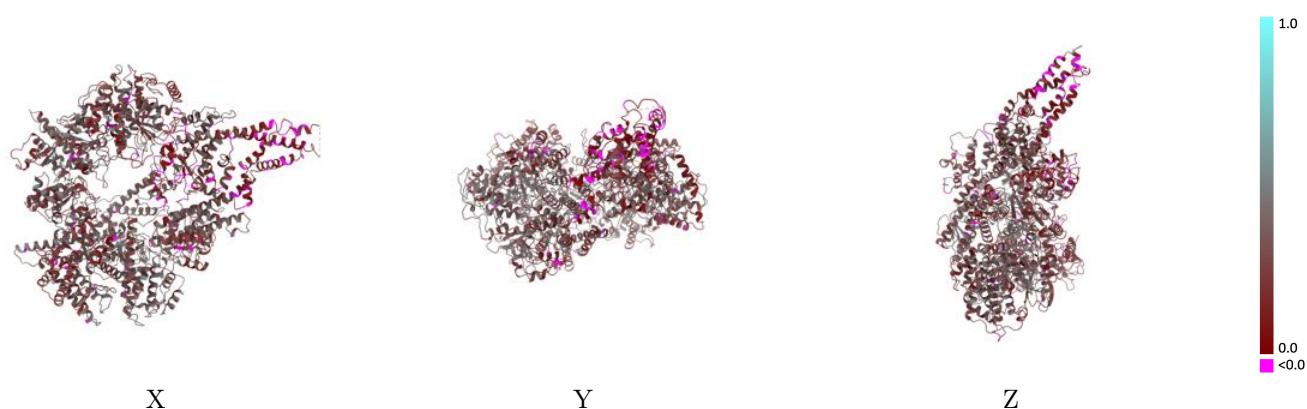
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-47377 and PDB model 9E0Y. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay ⓘ

This section was not generated.

9.2 Q-score mapped to coordinate model ⓘ

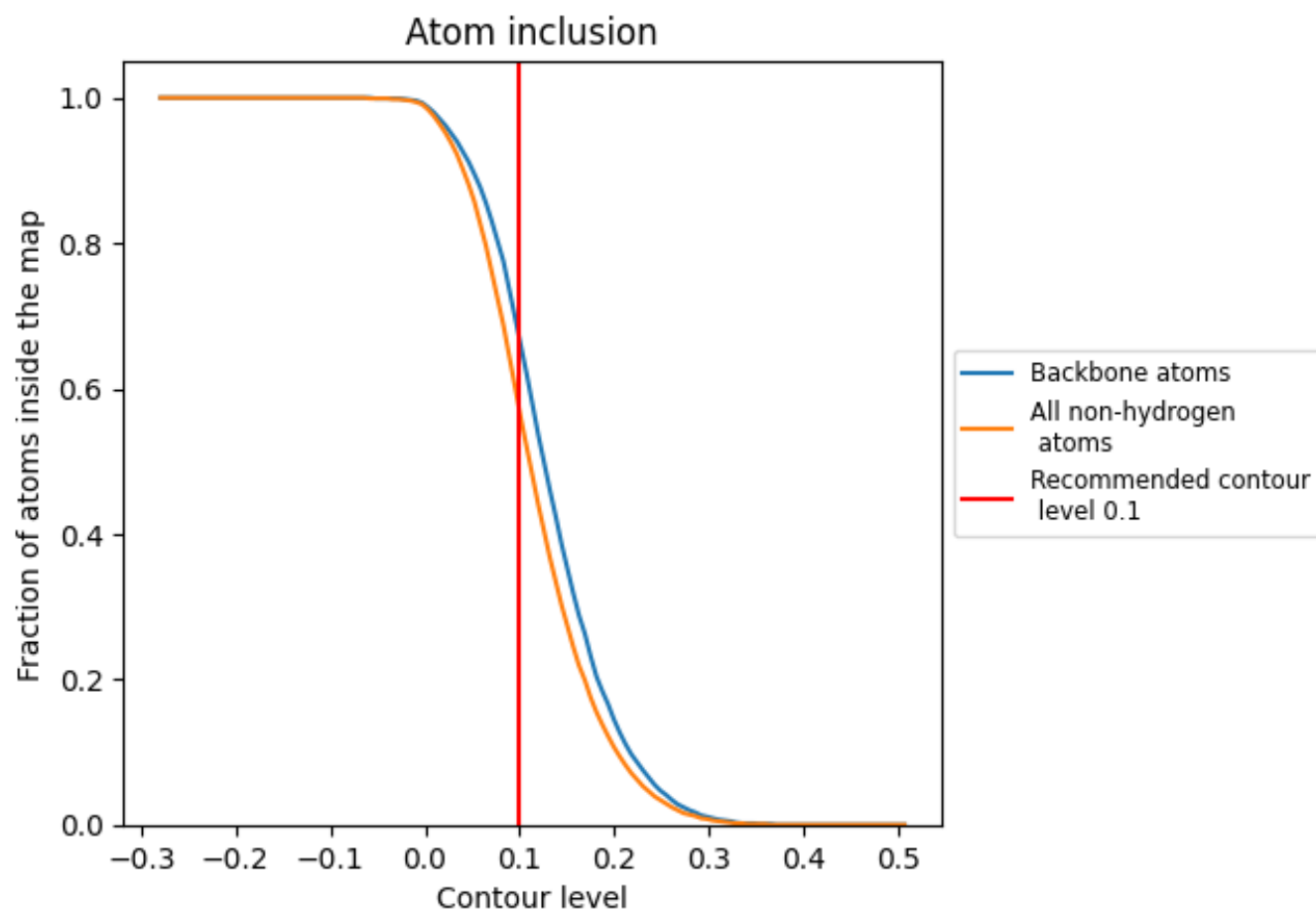


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 57% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5670	<div></div> 0.2960
A	<div></div> 0.5670	<div></div> 0.2960

