



Full wwPDB EM Validation Report ⓘ

Apr 24, 2025 – 01:03 PM EDT

PDB ID : 9BMD / pdb_00009bmd
EMDB ID : EMD-44696
Title : Motor domain from full-length human dynein-1 bound to microtubules in 5mM AMPPNP condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.90 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

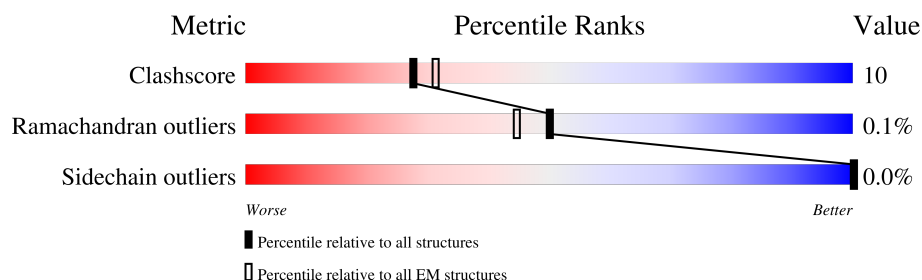
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	<div> <div>21%</div> <div>49%</div> <div>16%</div> <div>35%</div> </div>

2 Entry composition [i](#)

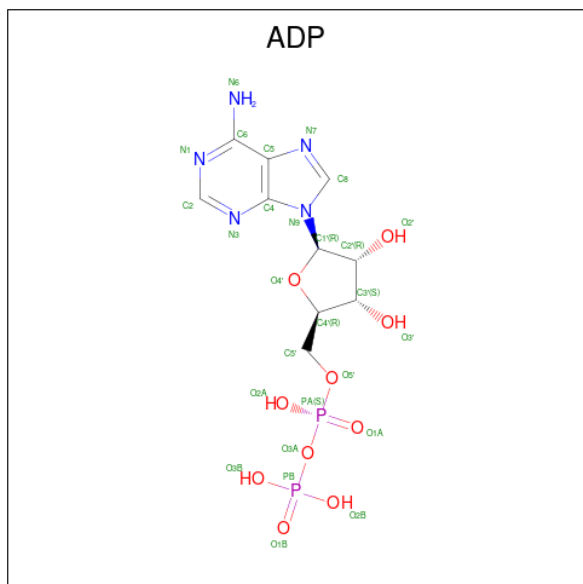
There are 5 unique types of molecules in this entry. The entry contains 24603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
1	A	3038	24479	15591	4228	4538	122	1	0

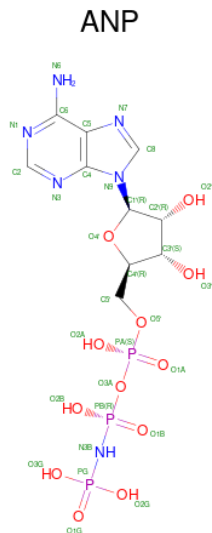
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0
4	A	1	Total 31	C 10	N 6	O 12	P 3	0

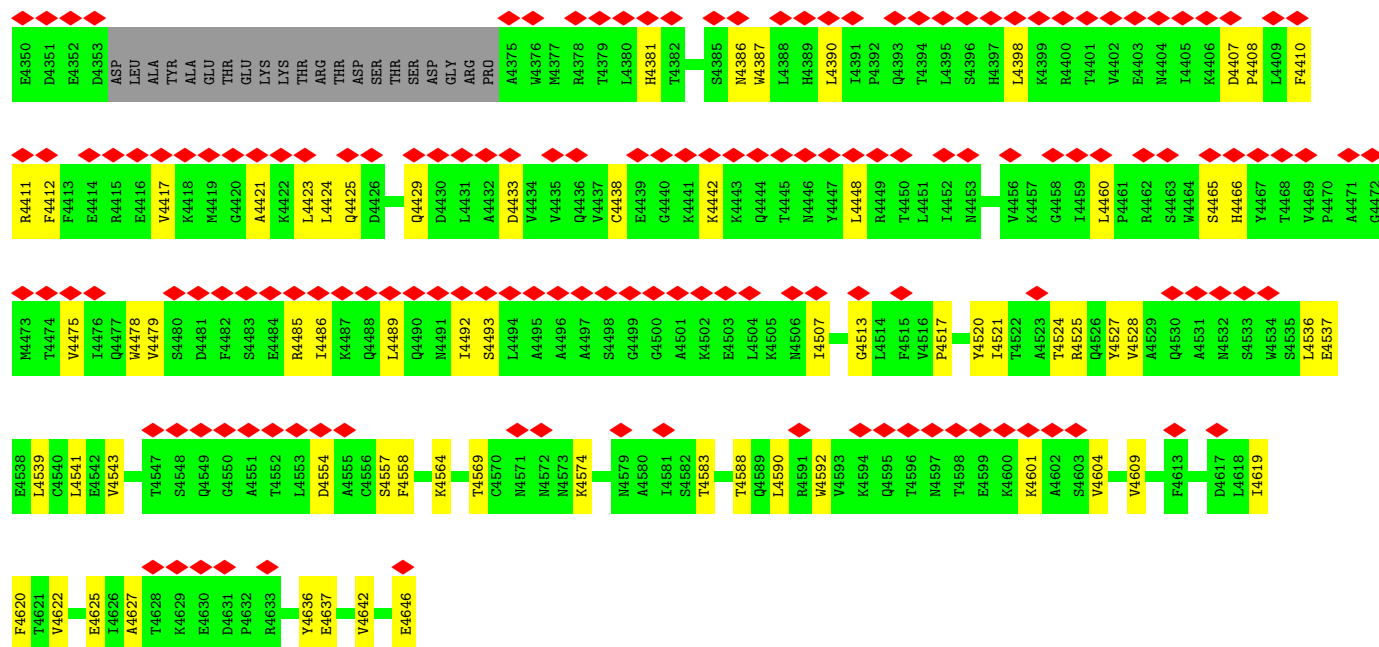
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total 4	Mg 4	0

P1988	T1889	D1734	V1632	F1516	K1441	A1381	VAL	TRP	ARG	GLU	ALA	THR	LEU	ASN	PHE
N1989		P1735	D1633	E1517	N1442	S1382	ALA	GLU	PHE	PHE	LEU	GLN	LEU	LYS	ASN
Y1990	Y1888	N1736	G1634	E1518			GLU	GLU	PHE	THR	GLU	THR	ARG	LEU	PHE
D1991	E1871	T1737	D1635	E1524	A1444	E1384	GLU	LYS	PRO	LYS	GLN	GLN	GLN	MET	GLY
K1992	K1871	Y1738	D1636	E1524	I1445	F1385	LEU	VAL	PRO	VAL	ILE	ASN	ASN	GLY	LYS
T1993	Y1872		L1638	D1535	V1446	V1386		THR	THR	THR	SER	SER	ARG	VAL	VAL
S1994	L1873	V1750	E1639	V1540	K1447	Q1387		GLY	TRP	GLY	LEU	LEU	LYS	GLU	GLU
A1995	Q1876	V1751			D1448	R1388		ASN	TYR	ARG	GLY	GLN	ALA	ASP	ASP
P1996	D1877	Q1755	N1643	V1545	V1449	L1389		LEU	ILE	ILE	GLN	GLN	VAL	VAL	GLY
E2000	K1878		S1644	Y1546	L1450	L1390		PRO	ASN	ASP	GLY	LEU	ALA	ALA	GLY
M2003	T1882	A1765	N1646	E1548	L1451	K1391		GLU	ILE	ASN	GLY	LEU	ALA	LEU	GLY
N2012	A1898	L1766	K1649	T1552	Q1454	Y1393		ALA	GLY	LYS	THR	ASP	LYS	ARG	GLY
T2019	R1899	S1767		G1553	E1455	M1394		GLN	GLY	VAL	VAL	ASP	VAL	VAL	GLY
G2020	T1910	S1768	K1656	S1554	E1456	K1395		ALA	PHE	LYS	GLY	GLY	VAL	GLY	GLY
G2021	G1911	M1769	V1661	S1555	A1458	I1396		ILE	ASN	THR	ASN	SER	ALA	THR	GLY
TYR	K1912	G1770	N1667	D1556	E1460	N1397		GLY	ASP	GLY	ASP	THR	VAL	VAL	GLN
ALA	H1921	G1772	E1668	T1557	E1461	M1398		GLY	ILE	ILE	ILE	SER	VAL	SER	GLN
GLY	R1925	G1773	D1669	K1558	F1462	L1399		VAL	ARG	ARG	VAL	VAL	VAL	GLY	LEU
ARG	F1926	D1774	V1672	H1559	K1464	V1400		VAL	LYS	THR	ILE	ALA	VAL	GLY	THR
S2026	V1927	A1775		L1561	Q1465	I1401		ARG	LYS	THR	VAL	VAL	VAL	GLY	LEU
M2027	N1931	A1776	I1676	E1564	T1466	E1402		GLY	ASP	PHE	THR	GLY	THR	GLN	GLY
D2030	C1932	L1792			R1467	L1403		LYS	LEU	SER	ILE	LYS	VAL	LYS	ALA
K2043	D1933	A1793	R1679	Q1569	E1468	K1404		ASP	ALA	ASP	ILE	VAL	VAL	VAL	GLY
P2044	E1934	D1794	E1680	S1570	V1469	S1405		ARG	ASP	GLN	GLN	GLN	GLN	LEU	ASP
L2048	D1937	S1795	K1687	I1571	T1472	A1407		GLY	GLY	VAL	VAL	SER	SER	LEU	GLY
L2049	F1938	E1799	T1688	E1574	E1474	L1408		CYS	ALA	LYS	LYS	VAL	VAL	GLN	GLY
V2052	Q1939	H1810	E1694	F1575	D1476	K1409		LYS	LYS	GLN	GLN	GLN	GLN	GLY	ASP
M2053	G1947	E1814	I1698	K1584	N1479	R1411		ALA	LYS	LYS	ILE	LYS	LYS	ASP	ASP
R2060	V1951	L1815		S1585	Y1480	H1412		GLY	LYS	LYS	ILE	LYS	LYS	ASP	ASP
T2061	G1952	W1816	Y1701		Q1481	W1413		ALA	LYS	LYS	ILE	LYS	LYS	ASP	ASP
L2065	A1953	L1825	L1702	D1590	N1482	K1414		ALA	GLY	GLY	ILE	GLN	GLN	ASP	ASP
K2068	W1954	L1825	V1705		C1483	Q1415		THR	THR	THR	ASP	VAL	VAL	ILE	ILE
P2071	N1961	R1829	E1708	M1593	R1485	M1417		ASP	ALA	ARG	ALA	LEU	LEU	VAL	VAL
F2072	R1962	I1830		I1594	R1488	K1418		THR	VAL	VAL	THR	GLY	GLY	GLY	GLY
L2075	E1964	D1831	Y1713	Q1595		R1419		GLY	GLY	GLY	THR	LEU	LEU	THR	THR
G2076	E1965	E1837	K1715	R1602	D1491	H1421		LEU	SER	SER	ARG	ASN	ASN	GLY	GLY
D2077	R1966	W1838	V1721	R1603	D1492	N1422		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
E2078	Q1974	R1843	V1724	L1604	H1500	N1423		ASP	ASP	ASP	THR	LEU	LEU	ASP	ASP
Q2079	I1978	D1847	E1725	L1607	A1506	W1424		GLY	VAL	VAL	THR	GLY	GLY	GLY	GLY
S2081	R1983	P1848	G1728	L1608	M1507	V1425		GLY	GLY	GLY	THR	ARG	ARG	LEU	LEU
S2082	E1984	K1729		L1619	K1508	N1426		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
Q2083	H1985	Q1850	A1730	E1620	L1509	S1427		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
F2088	S1986	T1851	T1731	R1621	S1510	E1428		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
G2089	N1987	D1852	S1732	R1628	Y1512	L1429		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
L2090		Q1855	I1733		K1513	T1430		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
		Q1856			K1514	L1431		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
					V1515	Q1433		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
						I1434		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
						W1435		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
						D1436		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
						Y1437		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
						D1438		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
						L1439		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY
						Q1440		GLY	GLY	GLY	THR	GLY	GLY	GLY	GLY

M3126	P3127	V3128	D3131	K3132	L3133	F3134	K3135	F3136	P3137	R3140	E3141	K3142	L3143	V3144	V3148	N3158	A3159	K3160	K3163	K3164	G3165	K3166	K3167	T3168	T3172	D3178	H3188	K3191	S3192	E3193	L3194	E3195	E3196	M3199	H3200	L3201	N3202	V3203	G3204	L3205	K3206	K3207	I3208	K3209	E3210	K3212	V3215	V3216	D3212	D3213	Q3214						
S3046	H3047	E3048	E3049	K3052	V3053	Q3057	R3060	N3061	F3066	T3067	M3068	N3069	P3070	SER	SER	GLU	GLY	LEU	LVS	ASP	ARG	M3008	N3009	L3012	A3013	N3014	G3015	E3016	V3017	P3018	G3019	L3020	F3021	E3022	G3023	D3024	E3025	Y3026	A3027	L3028	L3029	M3030	T3031	Q3032	C3033	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	N3043	L3044	D3045
K2898	V2899	F2900	Y2901	E2902	E2903	E2904	L2905	D2906	V2907	V2910	E2914	V2915	H2918	V2919	L2920	R2921	I2922	D2923	R2924	L2925	F2926	R2927	Q2928	F2929	Q2930	L2933	L2934	L2935	I2936	Q2937	V2938	K2943	L2946	S2947	R2948	F2949	V2950	L2956	I2961	K2962	V2963	H2964	R2965	K2966	Y2967	T2968	G2969	E2970	D2971	F2972	D2973						
E2808	R2811	E2814	T2815	L2816	R2823	E2828	A2829	E2836	D2840	E2841	R2844	V2845	T2846	D2847	E2848	D2851	A2854	L2855	H2857	F2858	N2859	L2860	L2861	D2862	R2863	E2864	K2865	A2866	M2867	R2868	R2869	L2872	L2877	S2878	K2879	D2880	V2884	D2885	Q2886	E2887	L2888	L2889	K2894	A2895													
K2694	T2695	S2696	D2697	V2701	F2708	C2712	N2713	P2714	L2723	R2726	F2727	L2728	V2731	P2732	V2733	V2734	V2735	D2737	T2747	T2750	R2757	L2758	T2759	P2760	R2763	E2767	E2775	F2776	T2777	T2778	E2782	D2787	E2788	R2797	E2798	R2801	W2802																				
E2808	R2811	E2814	T2815	L2816	R2823	E2828	A2829	E2836	D2840	E2841	R2844	V2845	T2846	D2847	E2848	D2851	A2854	L2855	H2857	F2858	N2859	L2860	L2861	D2862	R2863	E2864	K2865	A2866	M2867	R2868	R2869	L2872	L2877	S2878	K2879	D2880	V2884	D2885	Q2886	E2887	L2888	L2889	K2894	A2895													
K2898	V2899	F2900	Y2901	E2902	E2903	E2904	L2905	D2906	V2907	V2910	E2914	V2915	H2918	V2919	L2920	R2921	I2922	D2923	R2924	L2925	F2926	R2927	Q2928	F2929	Q2930	L2933	L2934	L2935	I2936	Q2937	V2938	K2943	L2946	S2947	R2948	F2949	V2950	L2956	I2961	K2962	V2963	H2964	R2965	K2966	Y2967	T2968	G2969	E2970	D2971	F2972	D2973						
E2974	D2975	R2982	K2986	K2989	M2994	D2995	E2996	S2997	N2998	V2999	L3000	D3001	S3002	G3003	F3004	L3005	E3006	R3007	M3008	N3009	L3012	A3013	N3014	G3015	E3016	V3017	P3018	G3019	L3020	F3021	E3022	G3023	D3024	E3025	Y3026	A3027	L3028	L3029	M3030	T3031	Q3032	C3033	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	N3043	L3044	D3045			
S3046	H3047	E3048	E3049	K3052	V3053	Q3057	R3060	N3061	F3066	T3067	M3068	N3069	P3070	SER	SER	GLU	GLY	LEU	LVS	ASP	ARG	M3008	N3009	L3012	A3013	N3014	G3015	E3016	V3017	P3018	G3019	L3020	F3021	E3022	G3023	D3024	E3025	Y3026	A3027	L3028	L3029	M3030	T3031	Q3032	C3033	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	N3043	L3044	D3045
K3126	F3127	V3128	D3131	K3132	L3133	F3134	K3135	F3136	P3137	R3140	E3141	K3142	L3143	V3144	V3148	N3158	A3159	K3160	K3163	K3164	G3165	K3166	K3167	T3168	T3172	D3178	H3188	K3191	S3192	E3193	L3194	E3195	E3196	M3199	H3200	L3201	N3202	V3203	G3204	L3205	K3206	K3207	I3208	K3209	E3210	K3212	V3215	V3216	D3212	D3213	Q3214						
D2163	V2168	Q2169	Y2170	H2171	R2172	G2173	E2174	M2175	R2179	K2180	E2181	E2188	L2191	T2192	D2195	G2196	E2197	M2202	Q2203	V2204	E2206	R2207	L2208	Q2209	L2210	Y2211	Q2212	L2213	T2214	Q2215	I2216	N2217	H2218	G2219	L2220	V2223	G2227	K2230	S2231	M2232	A2233	W2234	R2235	V2236	E2242	R2243	L2244	E2245									
E2248	S2260	K2261	D2262	T2267	L2268	D2269	P2270	N2271	T2272	R2273	E2274	W2275	T2276	D2277	G2278	T2281	H2282	R2285	T2288	D2289	S2290	V2291	R2292	Q2293	E2294	L2295	Q2296	K2297	D2306	P2309	E2313	N2314	L2319	D2320	D2321	N2322	K2323	L2324	L2325	T2326	L2327	P2328	N2329	Q2330	E2331	R2332	L2333	S2334	L2335								
R2340	T2341	Q2346	D2347	L2348	A2351	T2352	L2353	S2357	R2358	C2359	Q2360	H2361	D2367	T2371	D2372	M2373	T2374	L2382	T2385	P2386	L2387	D2388	E2389	Q2390	E2391	D2392	E2393	A2394	Q2395	R2396	R2397	K2398	K2399	G2400	K2401	E2402	D2403	E2404	G2405	E2406	E2407	A2408	A2409	S2410	P2411	M2412	L2413	Q2414	T2415	Q2416							
R2417	D2418	A2419	A2420	T2428	S2429	N2430	V2433	T2434	L2437	E2438	H2439	A2440	F2441	Q2442	L2443	E2444	H2445	R2446	M2447	D2448	L2449	T2450	R2451	R2453	C2454	S2460	A2465	C2466	R2467	N2468	Q2471	Y2472	N2473	A2474	N2475	H2476	P2477	D2478	F2479	P2480	M2481	Q2482	L2483	E2484	E2487	R2488	Y2493	L2494	V2495								
T2498	L2499	L2502	Q2503	Q2504	D2505	S2506	R2507	L2508	R2509	W2510	R2511	E2512	E2513	L2514	Q2515	E2516	T2517	L2518	R2519	R2520	M2521	T2522	T2523	V2524	P2527	T2528	A2529	P2530	N2531	T2532	F2533	L2534	T2535	T2541	S2542	Q2543	E2544	V2545	K2551	Q2554	T2555	E2556	V2557	E2558	T2559	K2560	S2561	A2564	P2565	D2566	T2571						
T2574	H2577	L2581	E2587	H2588	K2589	P2590	L2591	V2592	L2593	G2598	E2605	L2612	P2613	D2614	M2615	E2616	L2620	E2629	K2633	T2634	F2635	D2636	H2637	R2642	R2643	T2644	P2645	N2646	G2647	V2648	L2655	G2656	K2657	F2662	C2663	D2664	E2665	I2666	N2667	L2668	M2671	D2672	K2673	Y2674	Q2675												
R2694	T2695	S2696	D2697	V2701	F2708	C2712	N2713	P2714	L2723	R2726	F2727	L2728	V2731	P2732	V2733	V2734	V2735	D2737	T2747	T2750	R2757	L2758	T2759	P2760	R2763	E2767	E2775	F2776	T2777	T2778	E2782	D2787	E2788	R2797	E2798	R2801	W2802																				
E2808	R2811	E2814	T2815	L2816	R2823	E2828	A2829	E2836	D2840	E2841	R2844	V2845	T2846	D2847	E2848	D2851	A2854	L2855	H2857	F2858	N2859	L2860	L2861	D2862	R2863	E2864	K2865	A2866	M2867	R2868	R2869	L2872	L2877	S2878	K2879	D2880	V2884	D2885	Q2886	E2887	L2888	L2889	K2894	A2895													
K2898	V2899	F2900	Y2901	E2902	E2903	E2904	L2905	D2906	V2907	V2910	E2914	V2915	H2918	V2919	L2920	R2921	I2922	D2923	R2924	L2925	F2926	R2927	Q2928	F2929	Q2930	L2933	L2934	L2935	I2936	Q2937	V2938	K2943	L2946	S2947	R2948	F2949	V2950	L2956	I2961	K2962	V2963	H2964	R2965	K2966	Y2967	T2968	G2969	E2970	D2971	F2972	D2973						
E2974	D2975	R2982	K2986	K2989	M2994	D2995	E2996	S2997	N2998	V2999	L3000	D3001	S3002	G3003	F3004	L3005	E3006	R3007	M3008	N3009	L3012	A3013	N3014	G3015	E3016	V3017	P3018	G3019	L3020	F3021	E3022	G3023	D3024	E3025	Y3026	A3027	L3028	L3029	M3030	T3031	Q3032	C3033	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	N3043	L3044	D3045			
S3046	H3047	E3048	E3049	K3052	V3053	Q3057	R3060	N3061	F3066	T3067	M3068	N3069	P3070	SER	SER	GLU	GLY	LEU	LVS	ASP	ARG	M3008	N3009	L3012	A3013	N3014	G3015	E3016	V3017	P3018	G3019	L3020	F3021	E3022	G3023	D3024	E3025	Y3026	A3027	L3028	L3029	M3030	T3031	Q3032	C3033	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	N3043	L3044	D3045
K3126	F3127	V3128	D3131	K3132	L3133	F3134	K3135	F3136	P3137	R3140	E3141	K3142	L3143	V3144	V3148	N3158	A3159	K3160	K3163	K3164	G3165	K3166	K3167	T3168	T3172	D3178	H3188	K3191	S3192	E3193	L3194	E3195	E3196	M3199	H3200	L3201	N3202	V3203	G3204	L3205	K3206	K3207	I3208	K3209	E3210	K3212	V3215	V3216	D3212	D3213	Q3214						
L2093	K2094	L2097	V2103	K2104	E2105	R2106	E2107	T2108	Q2109	K2110	T2111	K2112	R2113	E2114	K2115	E2116	E2117	R2118	Q2119	E2120	A2121	D2122	D2123	E2124	Q2125	E2126	T2127	A2128	E2129	N2130	E2135	T2136	T2137	Q2138	S2140	V2141	K2148	L2149	V2150	A2151	E2152	D2153	T2154	F2155	L2156	L2157	L2160	L2161	S2162								
D2163	V2168	Q2169	Y2170	H2171	R2172	G2173	E2174	M2175	R2179	K2180	E2181	E2188	L2191	T2192	D2195	G2196	E2197	M2202	Q2203	V2204	E2206	R2207	L2208	Q2209	L2210	Y2211	Q2212	L2213	T2214	Q2215	I2216	N2217	H2218	G2219	L2220	V2223	G2227	K2230	S2231	M2232	A2233	W2234	R2235	V2236	E2242	R2243	L2244	E2245									
E2248	S2260	K2261	D2262	T2267	L2268	D2269	P2270	N2271	T2272	R2273	E2274	W2275	T2276	D2277	G2278	T2281	H2282	R2285	T2288	D2289	S2290	V2291	R2292	Q2293	E2294	L2295	Q2296	K2297	D2306	P2309	E2313	N2314	L2319	D2320	D2321	N2322	K2323	L2324	L2325	T2326	L2327	P2328	N2329	Q2330	E2331	R2332	L2333	S2334	L2335								
R2340	T2341	Q2346	D2347	L2348	A2351	T2352	L2353	S2357	R2358	C2359	Q2360	H2361	D2367	T2371	D2372	M2373	T2374	L2382	T2385	P2386	L2387	D2388	E2389	Q2390	E2391	D2392	E2393	A2394	Q2395	R2396	R2397	K2398	K2399	G2400	K2401	E2402	D2403	E2404	G2405	E2406	E2407	A2408	A2409	S2410	P2411	M2412	L2413	Q2414	T2415	Q2416							
R2417	D2418	A2419	A2420	T2428	S2429	N2430	V2433	T2434	L2437	E2438	H2439	A2440	F2441	Q2442	L2443	E2444	H2445	R2446	M2447	D2448	L2449	T2450	R2451	R2453	C2454	S2460	A2465	C2466	R2467																												





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241362	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.441	Depositor
Minimum map value	-0.841	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: ATP, MG, ADP, ANP

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	0.27	0/25000	0.48	1/33870 (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	2581	LEU	CA-CB-CG	5.30	127.50	115.30

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	24479	0	24538	468	0
2	A	27	0	12	2	0
3	A	31	0	12	2	0
4	A	62	0	26	3	0
5	A	4	0	0	0	0
All	All	24603	0	24588	468	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 10.

All (468) 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:2598:GLY:H	4:A:4703:ANP:HNB1	1.23	0.82
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.64	0.80
1:A:2581:LEU:HD21	1:A:2605:LEU:HD23	1.68	0.75
1:A:1397:ASN:O	1:A:1401:ILE:HD12	1.91	0.70
1:A:2506:SER:HB3	1:A:2510:MET:HB2	1.71	0.70
1:A:4079:GLN:HA	1:A:4082:LYS:HE3	1.73	0.69
1:A:1898:ALA:O	1:A:1983:ARG:NH1	2.26	0.68
1:A:3194:LEU:HD13	1:A:3500:MET:HE2	1.74	0.68
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.75	0.68
1:A:3691:ASP:OD1	1:A:3695:ARG:NH1	2.28	0.68
1:A:3110:THR:HG22	1:A:3113:MET:HE1	1.77	0.67
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.28	0.67
1:A:3474:ARG:HE	1:A:3764:ASP:HB3	1.59	0.66
1:A:4408:PRO:HA	1:A:4411:ARG:HE	1.59	0.66
1:A:4541:LEU:HD11	1:A:4590:LEU:HB3	1.77	0.66
1:A:2148:LYS:HG2	1:A:2361:MET:HB3	1.78	0.65
1:A:1462:PHE:HB2	1:A:3628:ARG:HD2	1.79	0.65
1:A:2925:ILE:HG21	1:A:2933:LEU:HB2	1.78	0.65
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.78	0.65
1:A:4276:ARG:NH2	1:A:4279:ASP:OD2	2.30	0.65
1:A:2925:ILE:HG13	1:A:2933:LEU:HD13	1.79	0.64
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.80	0.64
1:A:3820:GLN:HE21	1:A:4345:LYS:HG2	1.62	0.64
1:A:1571:ILE:HG23	1:A:1604:LEU:HD22	1.80	0.63
1:A:2382:LEU:HD23	1:A:2420:ALA:HB2	1.80	0.63
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.80	0.63
1:A:2320:ASP:OD1	1:A:2321:ASP:N	2.31	0.62
1:A:1688:THR:OG1	1:A:1708:GLU:OE2	2.16	0.62
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.32	0.62
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.82	0.62
1:A:3113:MET:HB3	1:A:3115:LEU:HG	1.82	0.62
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.33	0.61
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.33	0.61
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.82	0.61
1:A:2453:ARG:NH1	1:A:2505:ASP:OD2	2.33	0.61
1:A:2889:LEU:HD13	1:A:2920:LEU:HD11	1.82	0.60
1:A:2138:ILE:HG13	1:A:2161:LEU:HD21	1.82	0.60
1:A:2385:ILE:O	1:A:2416:GLN:NE2	2.32	0.60
1:A:3749:LEU:HD11	1:A:3770:LEU:HG	1.83	0.60
1:A:4564:LYS:HG3	1:A:4646:GLU:HB2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2290:SER:HB2	1:A:2295:LEU:HD23	1.85	0.59
1:A:4176:ARG:NH2	1:A:4224:ASP:OD1	2.30	0.59
1:A:2728:LEU:HA	1:A:2731:VAL:HG22	1.84	0.59
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	1.85	0.59
1:A:2230:LYS:NZ	1:A:2345:VAL:O	2.35	0.59
1:A:2433:VAL:HG22	1:A:2498:ILE:HD11	1.85	0.58
1:A:2605:LEU:HD13	1:A:2662:PHE:HE1	1.67	0.58
1:A:3553:LEU:HB2	1:A:3578:ILE:HD13	1.85	0.58
1:A:4071:ILE:HG13	1:A:4099:VAL:HG12	1.84	0.58
1:A:1419:ARG:HD2	1:A:1445:ILE:HG23	1.86	0.58
1:A:3211:THR:HG21	1:A:3753:LEU:HD11	1.86	0.58
1:A:3488:ARG:HA	1:A:3491:LYS:HE2	1.85	0.57
1:A:2386:PRO:HG3	1:A:2413:LEU:HD22	1.85	0.57
1:A:3624:GLU:HG2	1:A:3664:LEU:HD23	1.87	0.57
1:A:2593:LEU:HD23	1:A:2734:VAL:HB	1.86	0.57
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.69	0.57
1:A:3008:MET:HG2	1:A:3066:PHE:HZ	1.69	0.57
1:A:3886:LEU:HD11	1:A:4346:MET:HG3	1.86	0.57
1:A:2914:GLU:O	1:A:2918:HIS:ND1	2.28	0.57
1:A:4300:ILE:HG13	1:A:4301:ARG:HD3	1.85	0.57
1:A:2447:MET:HG3	1:A:2733:VAL:HG11	1.86	0.57
1:A:4193:ARG:NH2	1:A:4637:GLU:O	2.25	0.57
1:A:1961:ASN:ND2	1:A:2019:ASN:O	2.37	0.57
1:A:2968:THR:HG22	1:A:2970:GLU:H	1.70	0.57
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.86	0.56
1:A:2324:LEU:HD21	1:A:2332:ARG:HG2	1.87	0.56
1:A:3620:ARG:NH2	1:A:3642:ASP:OD2	2.39	0.56
1:A:3661:LEU:HD12	1:A:3668:ASP:HB3	1.86	0.56
1:A:4068:SER:HA	1:A:4095:MET:HB3	1.87	0.56
1:A:2396:ARG:NH1	1:A:2406:GLU:OE2	2.39	0.56
1:A:4386:ASN:O	1:A:4390:LEU:HG	2.05	0.56
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.33	0.56
1:A:4175:GLU:OE1	1:A:4175:GLU:N	2.38	0.56
1:A:2472:TYR:CD1	1:A:2541:ILE:HG21	2.40	0.56
1:A:4088:VAL:HG23	1:A:4118:PRO:HA	1.88	0.56
1:A:1374:PRO:HD2	1:A:1377:LEU:HD12	1.88	0.55
1:A:2188:GLU:OE1	1:A:2243:ARG:NH1	2.39	0.55
1:A:2694:ARG:HG3	1:A:2701:VAL:HG21	1.87	0.55
1:A:3931:GLN:O	1:A:3935:VAL:HG23	2.06	0.55
1:A:3889:ARG:HH12	1:A:3909:LEU:HD11	1.71	0.55
1:A:3879:ASP:OD1	1:A:4342:LYS:NZ	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2511:ARG:HD3	1:A:2535:ILE:HD13	1.87	0.55
1:A:4424:LEU:HD13	1:A:4486:ILE:HG13	1.89	0.55
1:A:1510:SER:HB2	1:A:3629:PHE:HB3	1.87	0.55
1:A:1925:ARG:HG2	1:A:1954:TRP:CD1	2.42	0.55
1:A:1545:VAL:O	1:A:1548:GLU:HG3	2.06	0.55
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.07	0.55
1:A:4527:TYR:CD2	1:A:4558:PHE:HZ	2.25	0.55
1:A:2075:LEU:HD11	1:A:4536:LEU:HD22	1.88	0.54
1:A:2965:ARG:HG3	1:A:2966:LYS:HD2	1.89	0.54
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.89	0.54
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.87	0.54
1:A:2192:THR:HB	1:A:2373:MET:HG2	1.89	0.54
1:A:2075:LEU:HD11	1:A:4536:LEU:CD2	2.38	0.54
1:A:2081:SER:O	1:A:2083:GLN:HG2	2.08	0.54
1:A:3716:VAL:HG23	1:A:3836:TYR:OH	2.06	0.54
1:A:4271:ARG:NH1	1:A:4284:LEU:O	2.38	0.54
1:A:2374:ILE:HD13	1:A:2452:LEU:HD21	1.89	0.54
1:A:2851:ASP:OD1	1:A:2867:MET:HG2	2.08	0.54
1:A:2557:VAL:O	1:A:2757:ARG:NH2	2.39	0.54
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.90	0.54
1:A:2718:PRO:HG2	1:A:3082:SER:HA	1.90	0.54
1:A:3551:GLU:HG3	1:A:3559:ARG:NH1	2.23	0.54
1:A:1765:ALA:O	1:A:1769:MET:HG3	2.08	0.53
1:A:4525:ARG:HE	1:A:4539:LEU:HB2	1.73	0.53
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	1.89	0.53
1:A:2309:PRO:HB3	1:A:2352:THR:HG23	1.90	0.53
1:A:2437:LEU:HD21	1:A:2451:ARG:HG3	1.89	0.53
1:A:2823:ARG:HH12	1:A:2868:SER:H	1.56	0.53
1:A:3499:GLN:O	1:A:3503:ILE:HG13	2.08	0.53
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	1.90	0.53
1:A:2591:LEU:HA	1:A:2732:PRO:HD2	1.91	0.53
1:A:2910:VAL:HG22	1:A:3108:GLU:HG2	1.90	0.53
1:A:3088:ARG:NH1	4:A:4703:ANP:O1G	2.42	0.53
1:A:3644:VAL:HG22	1:A:3664:LEU:HD12	1.91	0.53
1:A:3659:ARG:HG3	1:A:3661:LEU:HD21	1.90	0.53
1:A:2218:HIS:HA	1:A:2340:ARG:HD3	1.90	0.53
1:A:1632:VAL:HG12	1:A:1656:LYS:HD2	1.90	0.53
1:A:2104:LYS:HA	1:A:2136:ILE:HD13	1.89	0.53
1:A:2154:ILE:N	1:A:2155:PRO:HD2	2.24	0.53
1:A:2248:GLU:HG2	1:A:2297:LYS:NZ	2.23	0.53
1:A:2936:ILE:HG23	1:A:3093:TRP:HE3	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3891:LYS:HD2	1:A:4013:LEU:HD23	1.91	0.53
1:A:1755:GLN:HG3	1:A:1814:GLU:OE2	2.09	0.52
1:A:3194:LEU:HD11	1:A:3499:GLN:HB2	1.89	0.52
1:A:2060:ARG:HG3	1:A:2061:THR:HG23	1.92	0.52
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.91	0.52
1:A:3872:ALA:HA	1:A:3875:MET:HE2	1.91	0.52
1:A:2156:LEU:O	1:A:2160:LEU:HG	2.09	0.52
1:A:2488:ARG:HH21	1:A:2543:GLY:H	1.57	0.52
1:A:3835:ILE:HG12	1:A:3870:ARG:HG3	1.91	0.52
1:A:2080:LEU:HD12	1:A:2088:PHE:CZ	2.44	0.52
1:A:3593:SER:O	1:A:3682:ARG:NH2	2.43	0.52
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.49	0.52
1:A:2797:ARG:NH1	4:A:4703:ANP:O1G	2.36	0.52
1:A:3581:LYS:NZ	1:A:3582:ARG:HH11	2.06	0.51
1:A:3762:ASP:OD1	1:A:3763:ASP:N	2.43	0.51
1:A:4574:LYS:HE2	1:A:4625:GLU:HG2	1.91	0.51
1:A:1360:ARG:NH2	1:A:2899:VAL:HG22	2.26	0.51
1:A:1825:LEU:HA	1:A:1830:ILE:HD13	1.92	0.51
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.75	0.51
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.92	0.51
1:A:1420:LEU:HD13	1:A:1437:VAL:HG11	1.93	0.51
1:A:4520:TYR:O	1:A:4524:THR:HG23	2.10	0.51
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.91	0.51
1:A:3581:LYS:HZ2	1:A:3582:ARG:HH11	1.59	0.51
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.44	0.51
1:A:2775:GLU:OE1	1:A:2857:HIS:NE2	2.40	0.51
1:A:4465:SER:OG	1:A:4478:TRP:NE1	2.41	0.51
1:A:1513:TYR:CZ	1:A:1517:GLU:HG2	2.45	0.51
1:A:2072:PHE:HE2	1:A:2141:VAL:HG11	1.75	0.51
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.92	0.51
1:A:3561:ARG:NH1	1:A:3603:GLU:OE1	2.44	0.51
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.26	0.50
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.93	0.50
1:A:3679:LEU:HD12	1:A:3696:VAL:HG11	1.93	0.50
1:A:3143:ILE:HD13	1:A:3541:ILE:HD13	1.93	0.50
1:A:4071:ILE:HD11	1:A:4096:LEU:HD22	1.93	0.50
1:A:2666:ILE:HB	1:A:2712:CYS:SG	2.52	0.50
1:A:3044:LEU:HD22	1:A:3049:GLU:HG2	1.93	0.50
1:A:2808:GLU:OE1	1:A:2811:ARG:NH2	2.43	0.50
1:A:4342:LYS:O	1:A:4346:MET:HG2	2.12	0.50
1:A:3133:LEU:HD21	1:A:3137:PRO:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3024:ASP:O	1:A:3028:THR:HG23	2.12	0.50
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.93	0.50
1:A:1425:VAL:HB	1:A:1428:GLU:HB2	1.94	0.50
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.46	0.50
1:A:3191:ARG:O	1:A:3195:GLU:HG3	2.12	0.50
1:A:4045:SER:HB3	1:A:4049:TYR:HB3	1.93	0.50
1:A:4398:LEU:HD21	1:A:4493:SER:HA	1.93	0.50
1:A:4099:VAL:HG21	1:A:4126:LEU:HB3	1.94	0.50
1:A:4442:LYS:HE2	1:A:4448:LEU:HD11	1.94	0.50
1:A:4601:LYS:HB2	1:A:4604:VAL:HG23	1.93	0.50
1:A:1339:VAL:HG11	1:A:1370:LEU:HD21	1.94	0.49
1:A:2179:ARG:HD3	1:A:2208:LEU:HD11	1.94	0.49
1:A:2434:THR:O	1:A:2438:GLU:HG2	2.12	0.49
1:A:1964:GLU:OE2	1:A:1966:ARG:NH1	2.45	0.49
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.45	0.49
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.93	0.49
1:A:3127:PRO:HG3	1:A:3538:GLN:HB3	1.94	0.49
1:A:4465:SER:HG	1:A:4478:TRP:HE1	1.57	0.49
1:A:3551:GLU:HG3	1:A:3559:ARG:HH12	1.77	0.49
1:A:2495:VAL:HG21	1:A:2524:VAL:HG11	1.95	0.49
1:A:1751:VAL:HG11	1:A:1878:LYS:HD2	1.94	0.49
1:A:2527:PRO:HD3	1:A:2545:TRP:CE2	2.48	0.49
1:A:3591:ASP:OD2	1:A:3596:ALA:HB3	2.12	0.49
1:A:2209:GLN:O	1:A:2212:GLN:HG2	2.13	0.49
1:A:4288:VAL:HG21	1:A:4294:ILE:HG13	1.94	0.49
1:A:3597:THR:O	1:A:3601:MET:HG2	2.13	0.49
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.94	0.49
1:A:3767:ILE:HA	1:A:3770:LEU:HD13	1.94	0.49
1:A:2446:ILE:HG23	1:A:2447:MET:HG2	1.95	0.48
1:A:2844:ARG:O	1:A:2848:GLU:HG3	2.13	0.48
1:A:2918:HIS:O	1:A:2922:ILE:HG13	2.13	0.48
1:A:3194:LEU:HD22	1:A:3500:MET:HE3	1.94	0.48
1:A:4069:ILE:HD13	1:A:4079:GLN:HG2	1.95	0.48
1:A:1540:VAL:HG13	1:A:1608:LEU:HD12	1.94	0.48
1:A:3888:ALA:O	1:A:4012:ASN:ND2	2.46	0.48
1:A:1332:VAL:HB	1:A:1377:LEU:HD22	1.94	0.48
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.94	0.48
1:A:2872:LEU:HD13	1:A:2889:LEU:HD12	1.95	0.48
1:A:2223:VAL:HG11	1:A:2348:LEU:HG	1.94	0.48
1:A:2248:GLU:HG2	1:A:2297:LYS:HZ2	1.76	0.48
1:A:2472:TYR:HB2	1:A:2541:ILE:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.94	0.48
1:A:1816:VAL:HG11	1:A:2052:VAL:HG22	1.93	0.48
1:A:2053:MET:SD	1:A:2094:LYS:HG2	2.54	0.48
1:A:2094:LYS:NZ	2:A:4701:ADP:O2'	2.32	0.48
1:A:1556:ASP:O	1:A:1560:LEU:HG	2.13	0.48
1:A:2232:MET:HG3	3:A:4702:ATP:C8	2.48	0.48
1:A:2499:LEU:O	1:A:2503:SER:OG	2.25	0.48
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.94	0.48
1:A:3193:GLU:O	1:A:3196:GLU:HG3	2.13	0.48
1:A:2415:ILE:HD11	1:A:2473:ASN:HD22	1.79	0.48
1:A:3659:ARG:HG3	1:A:3661:LEU:CD2	2.44	0.48
1:A:2760:PRO:HB3	1:A:2763:ARG:HH21	1.79	0.48
1:A:3575:GLU:O	1:A:3579:MET:HG3	2.14	0.48
1:A:4081:ASP:OD1	1:A:4082:LYS:N	2.47	0.48
1:A:2534:ILE:HD12	1:A:2534:ILE:H	1.79	0.47
1:A:2465:ALA:HB2	1:A:2493:TYR:CD1	2.49	0.47
1:A:2484:GLU:O	1:A:2488:ARG:HG3	2.14	0.47
1:A:2965:ARG:HE	1:A:2966:LYS:HD2	1.78	0.47
1:A:3591:ASP:O	1:A:3682:ARG:HA	2.15	0.47
1:A:1628:ARG:NH2	1:A:1871:GLU:OE1	2.47	0.47
1:A:2956:LEU:HG	1:A:2989:LYS:HB3	1.97	0.47
1:A:3488:ARG:HH12	1:A:3773:LEU:HB3	1.79	0.47
1:A:3935:VAL:HG22	1:A:3996:PHE:HE1	1.79	0.47
1:A:4302:ARG:O	1:A:4306:VAL:HG23	2.14	0.47
1:A:4178:ARG:NH2	1:A:4299:GLY:O	2.46	0.47
1:A:3766:ILE:O	1:A:3769:THR:HG22	2.14	0.47
1:A:4044:CYS:HB3	1:A:4130:ILE:HG12	1.96	0.47
1:A:2268:LEU:HB3	1:A:2275:TRP:HE3	1.79	0.47
1:A:2371:THR:HG22	1:A:2451:ARG:HD2	1.97	0.47
1:A:2454:CYS:HB3	1:A:2502:LEU:HD23	1.97	0.47
1:A:3724:VAL:HG13	1:A:3794:VAL:HG12	1.96	0.47
1:A:3909:LEU:HB3	1:A:4344:LEU:HD21	1.97	0.47
1:A:1403:LEU:HD23	1:A:1450:LEU:HD11	1.96	0.47
1:A:1667:ASN:HB2	1:A:1672:VAL:HB	1.97	0.47
1:A:3194:LEU:HB3	1:A:3500:MET:HE3	1.97	0.47
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.97	0.47
1:A:3915:VAL:HG21	1:A:4390:LEU:HD22	1.97	0.47
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.48	0.46
1:A:4543:VAL:HG21	1:A:4622:VAL:HG12	1.96	0.46
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.97	0.46
1:A:1701:TRP:O	1:A:1705:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1847:ASP:OD1	1:A:1849:LYS:HG2	2.15	0.46
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.80	0.46
1:A:2884:VAL:HG13	1:A:2889:LEU:HD11	1.98	0.46
1:A:3044:LEU:HD13	1:A:3049:GLU:HG3	1.97	0.46
1:A:2135:GLU:HA	1:A:2138:ILE:HG22	1.97	0.46
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.31	0.46
1:A:2726:ARG:NH1	3:A:4702:ATP:O3G	2.48	0.46
1:A:3178:ASP:OD1	1:A:3584:ASN:HB2	2.15	0.46
1:A:2227:GLY:HA3	1:A:2452:LEU:HD12	1.97	0.46
1:A:2924:ARG:O	1:A:2928:GLN:HG2	2.16	0.46
1:A:3099:THR:HG23	1:A:3148:VAL:HG11	1.98	0.46
1:A:2453:ARG:HD3	1:A:2728:LEU:O	2.16	0.46
1:A:3196:GLU:HA	1:A:3199:MET:HG3	1.97	0.46
1:A:4267:THR:HG21	1:A:4636:TYR:HD2	1.79	0.46
1:A:1769:MET:SD	1:A:1775:ALA:HA	2.56	0.46
1:A:3123:PRO:HG2	1:A:3126:MET:HG3	1.96	0.46
1:A:1469:VAL:HG11	1:A:1500:HIS:CE1	2.50	0.46
1:A:2936:ILE:HA	1:A:3068:MET:O	2.16	0.46
1:A:2191:LEU:HD12	1:A:2236:VAL:HG21	1.98	0.46
1:A:2934:LEU:HD23	1:A:3091:LEU:CD2	2.46	0.46
1:A:4554:ASP:H	1:A:4557:SER:HB2	1.81	0.46
1:A:1456:GLU:HG2	1:A:1512:TYR:HB3	1.97	0.45
1:A:2080:LEU:HD22	1:A:2153:ASP:HB3	1.97	0.45
1:A:4214:SER:HB2	1:A:4251:ILE:HG23	1.98	0.45
1:A:2135:GLU:HG2	1:A:2168:VAL:HG13	1.97	0.45
1:A:2323:LYS:HB3	1:A:2335:LEU:HB3	1.98	0.45
1:A:2935:LEU:HD23	1:A:3092:ASN:HB3	1.99	0.45
1:A:4094:VAL:HB	1:A:4124:LEU:HD12	1.98	0.45
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.98	0.45
1:A:4429:GLN:NE2	1:A:4433:ASP:OD1	2.48	0.45
1:A:1599:ARG:HG3	1:A:1599:ARG:HH11	1.81	0.45
1:A:2093:LEU:O	1:A:2097:LEU:HG	2.17	0.45
1:A:2643:ARG:HE	1:A:2648:VAL:HG22	1.80	0.45
1:A:2996:GLU:HA	1:A:2999:VAL:HB	1.99	0.45
1:A:4407:ASP:HB3	1:A:4410:PHE:HB3	1.99	0.45
1:A:1619:LEU:HD22	1:A:1637:LEU:HD23	1.97	0.45
1:A:2065:LEU:HD21	1:A:2134:GLN:HG2	1.99	0.45
1:A:3568:PRO:HG2	1:A:3573:CYS:SG	2.56	0.45
1:A:1721:VAL:O	1:A:1725:GLU:HG3	2.17	0.45
1:A:1850:GLN:HB2	1:A:1856:GLN:HG2	1.97	0.45
1:A:2560:HIS:O	1:A:2561:LYS:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1459:LEU:HD22	1:A:1507:MET:HG3	1.99	0.45
1:A:2072:PHE:CE2	1:A:2141:VAL:HG11	2.52	0.45
1:A:3801:TYR:HD1	1:A:3856:LEU:HD13	1.80	0.45
1:A:1635:GLU:HG2	1:A:1636:ASP:N	2.32	0.45
1:A:1687:LYS:HG3	1:A:1715:LYS:HD2	1.97	0.45
1:A:2798:GLU:HG3	1:A:2801:ARG:HH21	1.81	0.45
1:A:3692:LEU:O	1:A:3696:VAL:HG22	2.16	0.45
1:A:3821:ILE:HD12	1:A:4342:LYS:HG2	1.97	0.45
1:A:1408:LEU:HD12	1:A:1408:LEU:HA	1.87	0.45
1:A:1793:ALA:HA	1:A:1796:VAL:HG12	1.98	0.45
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.27	0.45
1:A:1468:GLU:O	1:A:1472:THR:HG22	2.17	0.44
1:A:2202:MET:O	1:A:2205:GLU:HG2	2.18	0.44
1:A:2905:LEU:HD23	1:A:2948:ARG:HH22	1.82	0.44
1:A:2346:GLN:HB2	1:A:2726:ARG:HD2	1.97	0.44
1:A:2778:THR:O	1:A:2782:GLU:HG3	2.17	0.44
1:A:3057:GLN:O	1:A:3061:ASN:HB2	2.16	0.44
1:A:4423:LEU:HD13	1:A:4466:HIS:ND1	2.32	0.44
1:A:2211:TYR:O	1:A:2214:THR:OG1	2.29	0.44
1:A:3708:LEU:HD13	1:A:3829:LEU:HD11	1.99	0.44
1:A:3878:GLN:HG3	1:A:3879:ASP:OD1	2.17	0.44
1:A:2134:GLN:HE21	1:A:2168:VAL:HG21	1.82	0.44
1:A:2671:MET:HB3	1:A:2675:GLY:HA2	1.99	0.44
1:A:1561:LEU:HB3	1:A:1564:GLU:HB2	2.00	0.44
1:A:2049:ILE:HD13	1:A:2090:LEU:HD21	2.00	0.44
1:A:2204:VAL:O	1:A:2207:VAL:HG12	2.18	0.44
1:A:3724:VAL:HG21	1:A:3797:VAL:HG21	1.98	0.44
1:A:4093:TRP:CD1	1:A:4123:ARG:HB2	2.53	0.44
1:A:4191:GLN:O	1:A:4194:LEU:HB2	2.18	0.44
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.51	0.44
1:A:4517:PRO:O	1:A:4521:ILE:HG12	2.17	0.44
1:A:1409:LYS:O	1:A:1413:TRP:HD1	2.01	0.44
1:A:2938:VAL:O	1:A:2943:LYS:NZ	2.51	0.44
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.52	0.44
1:A:4324:PRO:HB2	1:A:4326:ASN:OD1	2.18	0.44
1:A:1646:ASN:ND2	1:A:1649:LYS:HE2	2.33	0.44
1:A:2915:VAL:HG13	1:A:2946:LEU:HD21	2.00	0.44
1:A:3972:TYR:OH	1:A:3976:GLU:OE1	2.30	0.44
1:A:1457:MET:HE2	1:A:1461:GLU:OE2	2.18	0.44
1:A:1911:GLY:N	2:A:4701:ADP:O1B	2.47	0.44
1:A:1974:GLN:O	1:A:1978:ILE:HG13	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3643:PRO:O	1:A:3646:ASN:ND2	2.50	0.44
1:A:3922:PRO:HD2	1:A:3936:VAL:HG21	1.99	0.43
1:A:2620:LEU:HD11	1:A:2634:THR:HG21	2.00	0.43
1:A:2828:GLU:OE1	1:A:2924:ARG:NH1	2.50	0.43
1:A:2923:ASP:OD1	1:A:2927:ARG:NH2	2.50	0.43
1:A:2288:ILE:HD12	1:A:2333:LEU:HD22	2.00	0.43
1:A:2309:PRO:HB3	1:A:2352:THR:CG2	2.49	0.43
1:A:2884:VAL:HG11	1:A:2889:LEU:HD21	1.99	0.43
1:A:2219:GLY:HA2	1:A:2341:ILE:O	2.19	0.43
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.58	0.43
1:A:4330:VAL:O	1:A:4333:THR:HG22	2.18	0.43
1:A:4492:ILE:HD12	1:A:4507:ILE:HD13	2.01	0.43
1:A:1350:PRO:O	1:A:1354:VAL:HG23	2.18	0.43
1:A:2468:ASN:HA	1:A:2471:GLN:HG2	1.99	0.43
1:A:4209:GLU:O	1:A:4213:ARG:HG3	2.19	0.43
1:A:2467:ARG:NH1	1:A:2587:GLU:OE2	2.51	0.43
1:A:2895:ALA:O	1:A:2899:VAL:HG23	2.19	0.43
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.52	0.43
1:A:2905:LEU:HD23	1:A:2948:ARG:NH2	2.32	0.43
1:A:2936:ILE:HG23	1:A:3093:TRP:CE3	2.54	0.43
1:A:3648:VAL:HA	1:A:3662:ILE:HD11	2.01	0.43
1:A:1547:LEU:HD22	1:A:1608:LEU:HD22	2.00	0.43
1:A:2483:ILE:O	1:A:2487:GLU:HG3	2.19	0.43
1:A:3818:LEU:HA	1:A:4346:MET:HE1	2.00	0.43
1:A:4100:HIS:CD2	1:A:4129:GLU:HG2	2.54	0.43
1:A:1741:TRP:CH2	1:A:1750:VAL:HG13	2.54	0.43
1:A:2460:SER:OG	1:A:2589:LYS:HD2	2.18	0.43
1:A:4096:LEU:HD13	1:A:4105:TRP:HH2	1.84	0.43
1:A:4489:LEU:O	1:A:4492:ILE:HG22	2.19	0.43
1:A:2413:LEU:HG	1:A:2417:ARG:HE	1.84	0.43
1:A:1370:LEU:HD11	1:A:1390:LEU:HD12	2.01	0.42
1:A:1927:VAL:HG22	1:A:1954:TRP:HB2	2.02	0.42
1:A:3576:ASN:ND2	1:A:3700:ASN:O	2.50	0.42
1:A:4097:LYS:HA	1:A:4127:THR:OG1	2.18	0.42
1:A:2982:ARG:HA	1:A:2986:LYS:HD2	2.00	0.42
1:A:4087:ALA:HB1	1:A:4092:ARG:O	2.18	0.42
1:A:2514:LEU:O	1:A:2518:ILE:HG12	2.19	0.42
1:A:3194:LEU:HD13	1:A:3500:MET:CE	2.44	0.42
1:A:4087:ALA:O	1:A:4091:GLY:N	2.51	0.42
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	2.00	0.42
1:A:4421:ALA:O	1:A:4425:GLN:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.19	0.42
1:A:2668:LEU:HD23	1:A:2668:LEU:HA	1.88	0.42
1:A:2559:THR:HG22	1:A:2757:ARG:HB3	2.02	0.42
1:A:1408:LEU:O	1:A:1412:HIS:HB2	2.19	0.42
1:A:1952:GLY:HA2	1:A:2012:MET:HB3	2.01	0.42
1:A:2925:ILE:HD11	1:A:3090:VAL:HG11	2.01	0.42
1:A:1356:PRO:CB	1:A:1401:ILE:HG13	2.49	0.42
1:A:1411:ARG:O	1:A:1415:GLN:HG3	2.19	0.42
1:A:1838:TRP:CZ2	1:A:1843:ARG:HG2	2.55	0.42
1:A:1481:GLN:N	1:A:2271:ASN:O	2.51	0.42
1:A:2278:GLY:N	1:A:2281:THR:OG1	2.53	0.42
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	2.02	0.42
1:A:3620:ARG:O	1:A:3624:GLU:HG3	2.20	0.42
1:A:1454:GLN:NE2	1:A:3671:LEU:O	2.41	0.42
1:A:1910:THR:HG22	1:A:2044:PRO:HD3	2.02	0.42
1:A:2994:MET:HE3	1:A:2998:ASN:ND2	2.35	0.42
1:A:3605:LYS:HE3	1:A:3605:LYS:HB2	1.86	0.42
1:A:3787:THR:O	1:A:3791:MET:HG3	2.19	0.42
1:A:3944:PHE:CE1	1:A:3974:TRP:HB3	2.55	0.42
1:A:4460:LEU:HD21	1:A:4465:SER:OG	2.20	0.42
1:A:2449:LEU:HA	1:A:2449:LEU:HD12	1.79	0.42
1:A:2863:ARG:CZ	1:A:2867:MET:HB2	2.50	0.42
1:A:3140:ARG:O	1:A:3144:VAL:HG23	2.20	0.42
1:A:1414:LYS:O	1:A:1417:MET:HB3	2.20	0.41
1:A:1511:PRO:O	1:A:1514:LYS:NZ	2.37	0.41
1:A:1873:LEU:HD13	1:A:1921:HIS:HB3	2.01	0.41
1:A:2068:LYS:HG2	1:A:4537:GLU:OE2	2.20	0.41
1:A:2440:ALA:HB2	1:A:2502:LEU:HB3	2.02	0.41
1:A:3767:ILE:O	1:A:3771:GLU:HG2	2.19	0.41
1:A:1417:MET:HE1	1:A:1423:ASN:HA	2.03	0.41
1:A:2571:THR:H	1:A:2574:THR:HB	1.85	0.41
1:A:2836:ARG:NH1	1:A:3091:LEU:HD12	2.35	0.41
1:A:3740:LEU:O	1:A:3743:ARG:HG2	2.20	0.41
1:A:3927:LEU:HD11	1:A:3957:PHE:HE2	1.85	0.41
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.55	0.41
1:A:2214:THR:HG22	1:A:2220:LEU:HD21	2.03	0.41
1:A:2593:LEU:HD12	1:A:2605:LEU:HG	2.03	0.41
1:A:3123:PRO:HB3	1:A:3540:ASN:OD1	2.20	0.41
1:A:3739:GLN:HB3	1:A:3743:ARG:HH21	1.85	0.41
1:A:2175:MET:O	1:A:2179:ARG:HG2	2.21	0.41
1:A:2529:ALA:HB1	1:A:2532:ILE:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2802:TRP:CZ2	1:A:2829:ALA:HB2	2.56	0.41
1:A:4028:THR:HA	1:A:4058:LEU:HD11	2.01	0.41
1:A:1425:VAL:O	1:A:1429:LEU:N	2.53	0.41
1:A:1990:TYR:HE2	1:A:1995:ALA:HA	1.85	0.41
1:A:4239:PRO:HB2	1:A:4242:ALA:HB3	2.03	0.41
1:A:1484:CYS:HB3	1:A:1576:LEU:HD22	2.03	0.41
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.86	0.41
1:A:1878:LYS:HE3	1:A:1878:LYS:HB3	1.84	0.41
1:A:2115:LYS:HE2	1:A:2127:ILE:HD11	2.02	0.41
1:A:2668:LEU:HD21	1:A:2720:ARG:HH11	1.85	0.41
1:A:3158:ASN:OD1	1:A:3168:THR:HB	2.21	0.41
1:A:1464:LYS:HB2	1:A:1464:LYS:HE3	1.78	0.41
1:A:2077:ASP:OD2	1:A:2088:PHE:HB2	2.21	0.41
1:A:2103:VAL:O	1:A:2106:GLU:HG2	2.21	0.41
1:A:3966:PRO:HD2	1:A:4000:ARG:HG3	2.03	0.41
1:A:4543:VAL:HG13	1:A:4588:THR:HG23	2.02	0.41
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	2.02	0.41
1:A:1397:ASN:O	1:A:1400:VAL:HB	2.20	0.41
1:A:1987:ASN:OD1	1:A:1987:ASN:N	2.54	0.41
1:A:2231:SER:HA	1:A:2234:TRP:NE1	2.36	0.41
1:A:2673:LYS:NZ	1:A:2674:TYR:OH	2.53	0.41
1:A:3013:ALA:HB2	1:A:3088:ARG:NE	2.36	0.41
1:A:3103:TYR:OH	1:A:3141:GLU:HG2	2.20	0.41
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.54	0.41
1:A:3523:GLN:HG2	1:A:3706:SER:CB	2.50	0.41
1:A:4248:ALA:O	1:A:4253:GLY:HA3	2.21	0.41
1:A:4387:TRP:NE1	1:A:4479:VAL:HG21	2.35	0.41
1:A:4485:ARG:HG2	1:A:4513:GLY:HA2	2.03	0.41
1:A:1698:ILE:O	1:A:1702:LEU:HB2	2.20	0.41
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.21	0.41
1:A:3007:ARG:HH21	1:A:3020:LEU:HD13	1.85	0.41
1:A:3033:CYS:HG	1:A:3053:TRP:HE3	1.67	0.41
1:A:3645:LEU:HG	1:A:3649:LEU:HG	2.02	0.41
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.84	0.41
1:A:2577:HIS:CD2	1:A:2736:VAL:HG22	2.56	0.40
1:A:2590:PRO:HA	1:A:2708:PHE:O	2.21	0.40
1:A:2667:ASN:HB3	1:A:2720:ARG:HB3	2.02	0.40
1:A:2854:ALA:O	1:A:2858:PHE:HB2	2.21	0.40
1:A:2920:LEU:HD23	1:A:2920:LEU:HA	1.86	0.40
1:A:3508:LEU:HD22	1:A:3536:LEU:HD11	2.02	0.40
1:A:1461:GLU:O	1:A:1465:GLN:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2445:HIS:CD2	1:A:2449:LEU:HD22	2.56	0.40
1:A:4528:VAL:HG21	1:A:4592:TRP:HB2	2.03	0.40
1:A:1354:VAL:HG21	1:A:1431:LEU:HB2	2.03	0.40
1:A:1360:ARG:HH11	1:A:1394:MET:HE2	1.87	0.40
1:A:1417:MET:CE	1:A:1423:ASN:HA	2.51	0.40
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.52	0.40
1:A:1876:GLN:HG2	1:A:1921:HIS:CD2	2.57	0.40
1:A:1899:ARG:HD3	1:A:1899:ARG:HA	1.86	0.40
1:A:1912:LYS:HE3	1:A:1912:LYS:HB2	1.84	0.40
1:A:3548:ALA:HB1	1:A:3551:GLU:OE1	2.22	0.40
1:A:3756:VAL:HG12	1:A:3760:ILE:HD13	2.03	0.40
1:A:4307:GLN:O	1:A:4311:LEU:HG	2.21	0.40
1:A:1359:LEU:HD11	1:A:1435:TRP:CZ2	2.57	0.40
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.86	0.40
1:A:1713:LEU:HD23	1:A:1713:LEU:HA	1.92	0.40
1:A:3012:LEU:HD11	1:A:3066:PHE:HE2	1.87	0.40
1:A:3143:ILE:HG23	1:A:3508:LEU:HD12	2.04	0.40
1:A:4569:THR:HG22	1:A:4583:THR:HG21	2.04	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	3029/4646 (65%)	2974 (98%)	53 (2%)	2 (0%)	48 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4292	LYS
1	A	4130	ILE

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	2704/4125 (66%)	2703 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	4301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3820	GLN
1	A	4012	ASN
1	A	4232	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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
4	ANP	A	4703	5	29,33,33	2.49	6 (20%)	31,52,52	1.46	3 (9%)
4	ANP	A	4704	5	29,33,33	2.51	6 (20%)	31,52,52	1.50	4 (12%)
3	ATP	A	4702	5	28,33,33	0.71	0	34,52,52	0.58	1 (2%)
2	ADP	A	4701	-	24,29,29	0.88	0	29,45,45	1.22	2 (6%)

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
4	ANP	A	4703	5	-	4/14/38/38	0/3/3/3
4	ANP	A	4704	5	-	8/14/38/38	0/3/3/3
3	ATP	A	4702	5	-	3/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4704	ANP	PB-O3A	8.86	1.70	1.59
4	A	4703	ANP	PB-O3A	8.78	1.70	1.59
4	A	4703	ANP	PG-N3B	6.25	1.79	1.63
4	A	4704	ANP	PG-N3B	6.20	1.79	1.63
4	A	4704	ANP	PG-O1G	4.70	1.53	1.46
4	A	4703	ANP	PG-O1G	4.64	1.53	1.46
4	A	4704	ANP	PB-O1B	2.65	1.50	1.46
4	A	4703	ANP	PB-O1B	2.61	1.50	1.46
4	A	4703	ANP	C8-N7	-2.36	1.30	1.34
4	A	4704	ANP	C8-N7	-2.31	1.30	1.34
4	A	4703	ANP	PB-O2B	-2.23	1.50	1.56
4	A	4704	ANP	PB-O2B	-2.22	1.50	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4703	ANP	O2B-PB-O1B	4.89	120.35	109.87
4	A	4704	ANP	O2B-PB-O1B	4.81	120.17	109.87
4	A	4704	ANP	O1G-PG-N3B	-4.10	105.73	111.77
4	A	4703	ANP	O1G-PG-N3B	-3.87	106.07	111.77
2	A	4701	ADP	N3-C2-N1	-3.72	123.62	128.67
4	A	4704	ANP	O2G-PG-O3G	2.56	114.47	107.59
2	A	4701	ADP	C4-C5-N7	-2.54	106.65	109.34
4	A	4703	ANP	O2G-PG-O3G	2.47	114.23	107.59
3	A	4702	ATP	C5-C6-N6	2.30	123.81	120.31
4	A	4704	ANP	C4'-O4'-C1'	-2.05	108.05	109.92

There are no chirality outliers.

All (18) torsion outliers are listed below:

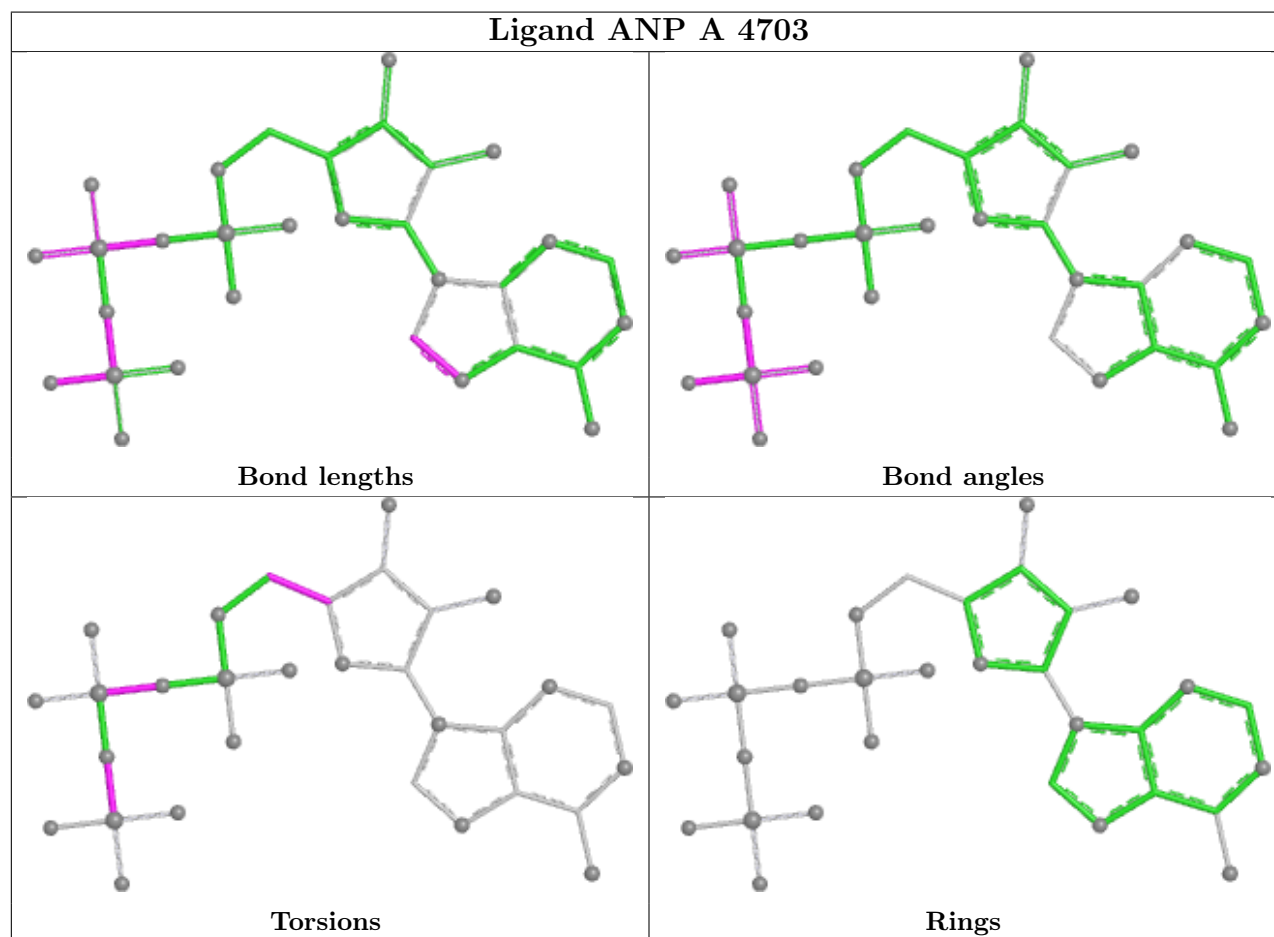
Mol	Chain	Res	Type	Atoms
4	A	4703	ANP	PB-N3B-PG-O1G
4	A	4703	ANP	PA-O3A-PB-O2B
4	A	4704	ANP	PB-N3B-PG-O1G
4	A	4704	ANP	PG-N3B-PB-O1B
4	A	4704	ANP	C5'-O5'-PA-O2A
4	A	4704	ANP	C5'-O5'-PA-O3A
4	A	4704	ANP	O4'-C4'-C5'-O5'
4	A	4704	ANP	C3'-C4'-C5'-O5'
2	A	4701	ADP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O1G
3	A	4702	ATP	PB-O3B-PG-O2G
2	A	4701	ADP	PB-O3A-PA-O2A
2	A	4701	ADP	PB-O3A-PA-O1A
4	A	4703	ANP	O4'-C4'-C5'-O5'
4	A	4704	ANP	PB-O3A-PA-O2A
4	A	4703	ANP	PA-O3A-PB-O1B
4	A	4704	ANP	PG-N3B-PB-O3A
3	A	4702	ATP	PG-O3B-PB-O2B

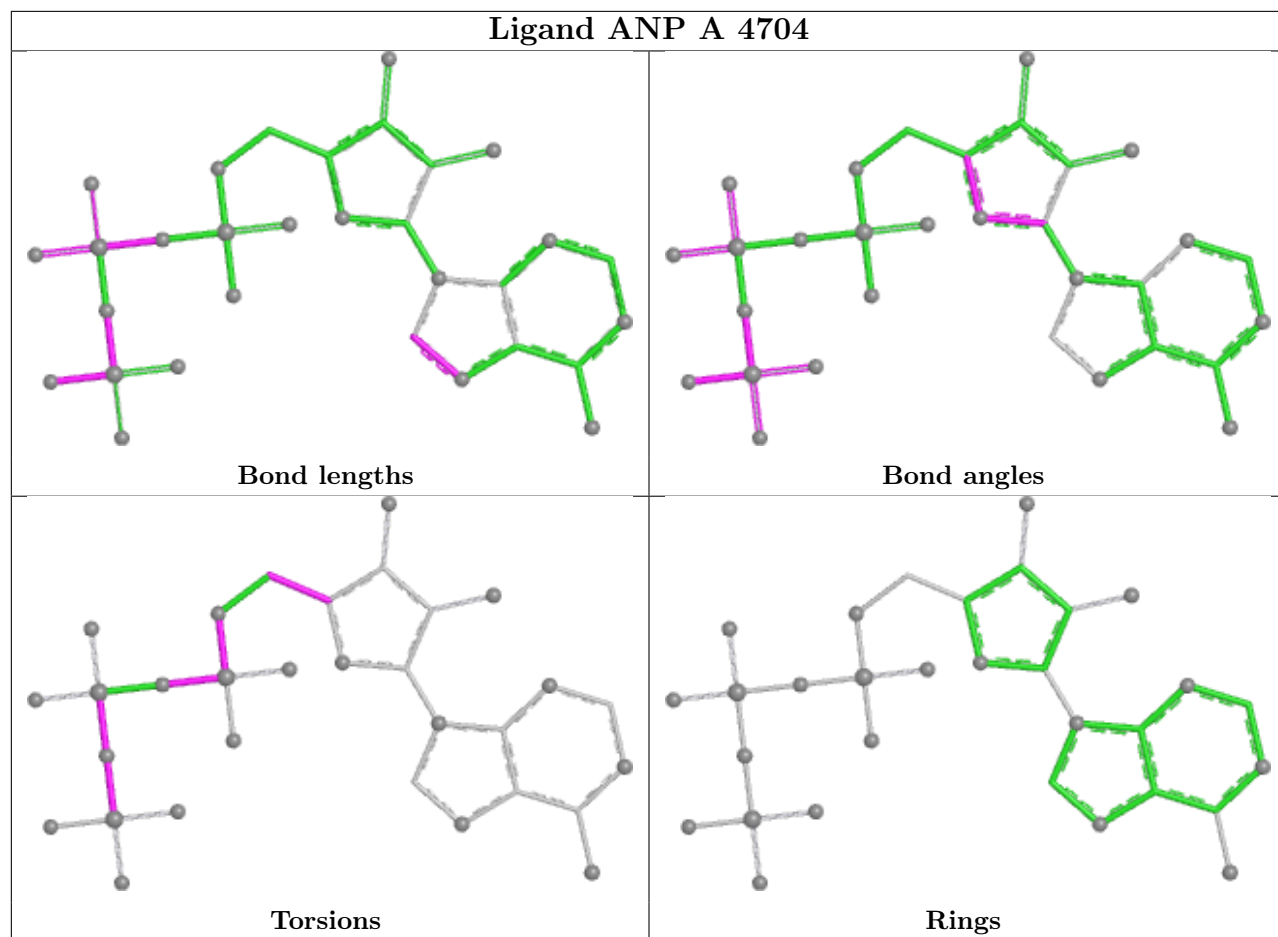
There are no ring outliers.

3 monomers are involved in 7 short contacts:

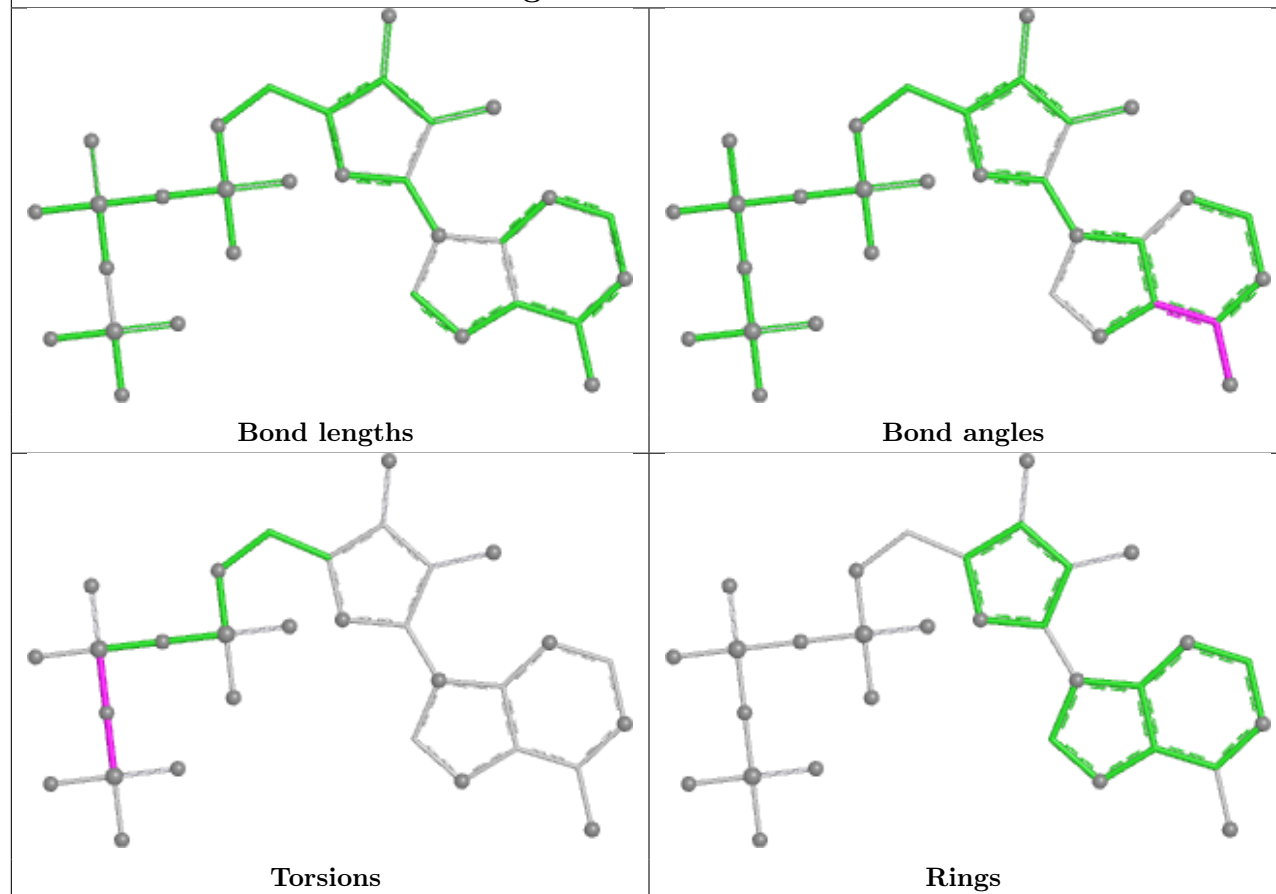
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ANP	3	0
3	A	4702	ATP	2	0
2	A	4701	ADP	2	0

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.

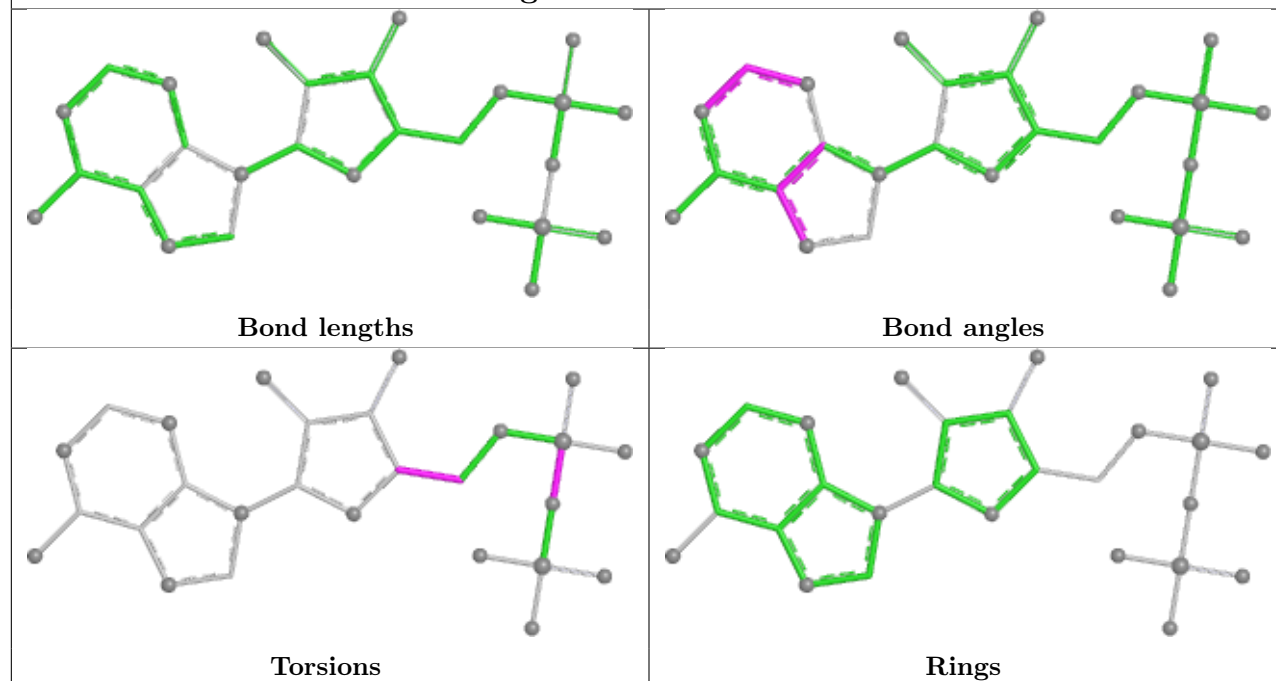




Ligand ATP A 4702



Ligand ADP A 4701



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

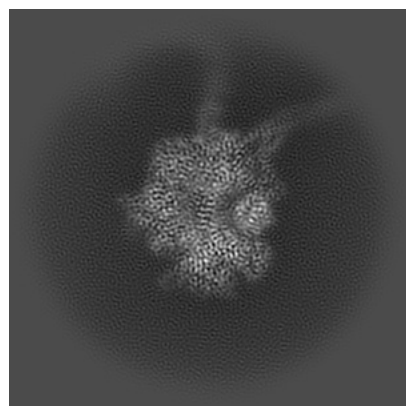
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44696. These allow visual inspection of the internal detail of the map and identification of artifacts.

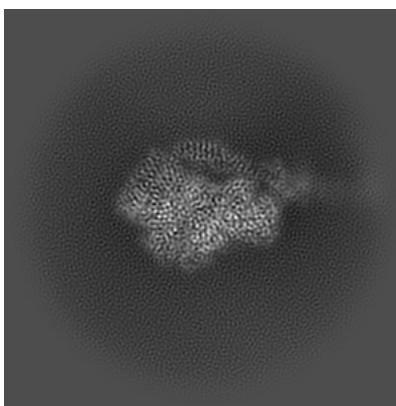
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

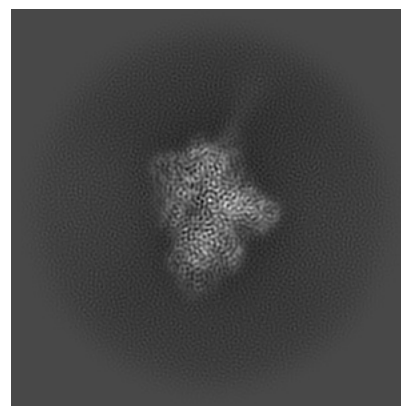
6.1.1 Primary map



X

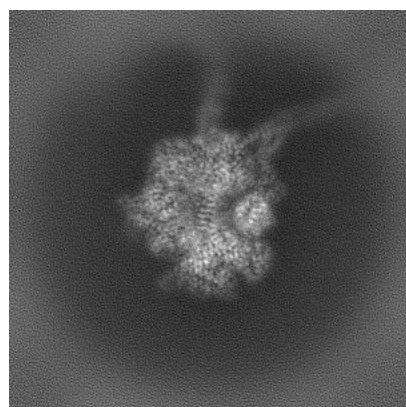


Y

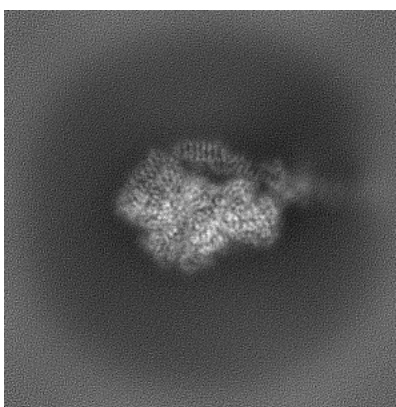


Z

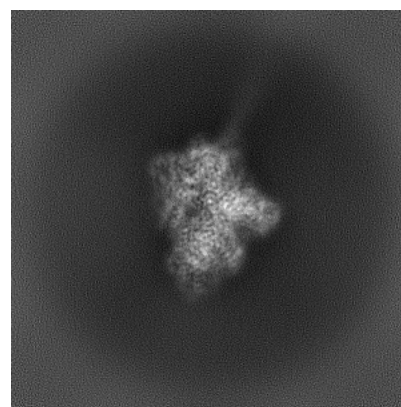
6.1.2 Raw map



X



Y

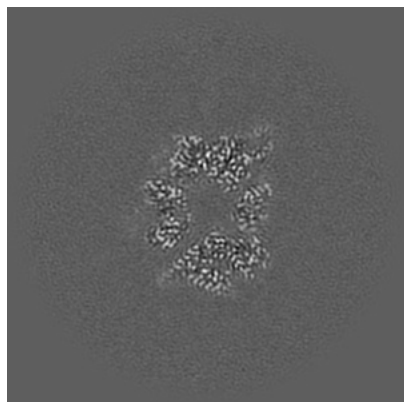


Z

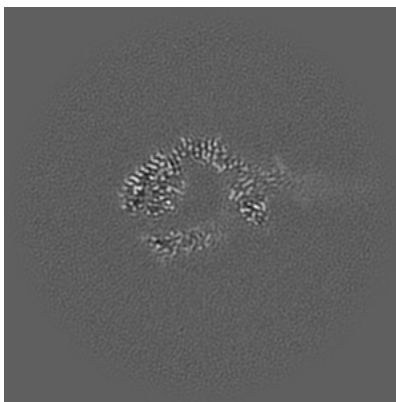
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

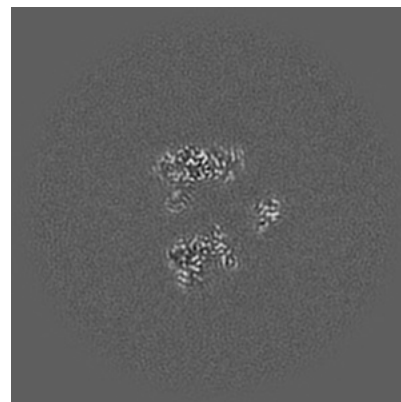
6.2.1 Primary map



X Index: 192

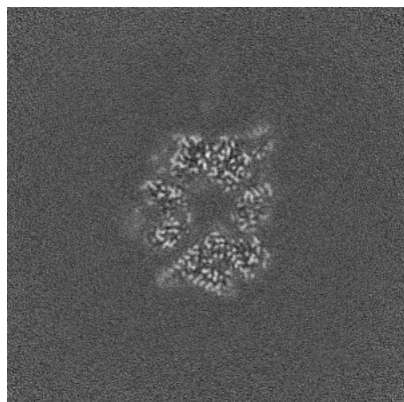


Y Index: 192

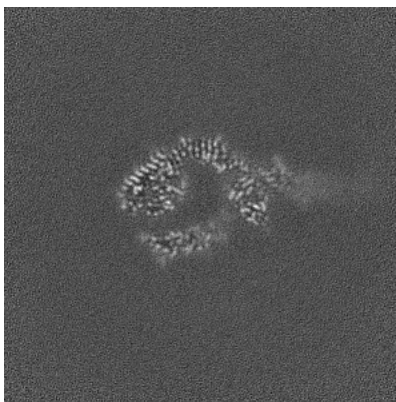


Z Index: 192

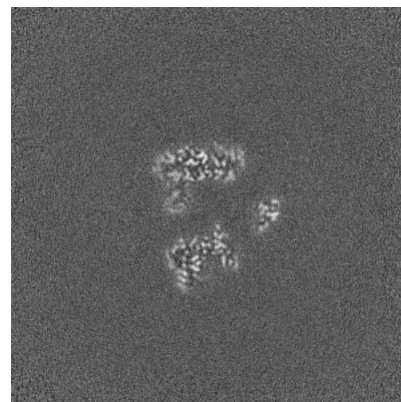
6.2.2 Raw map



X Index: 192



Y Index: 192

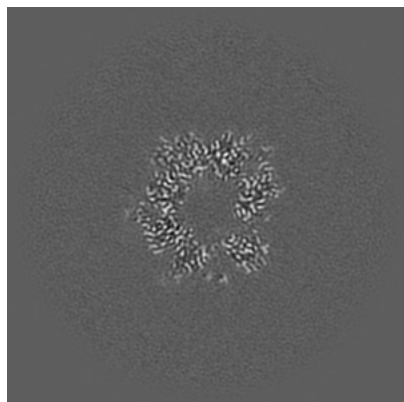


Z Index: 192

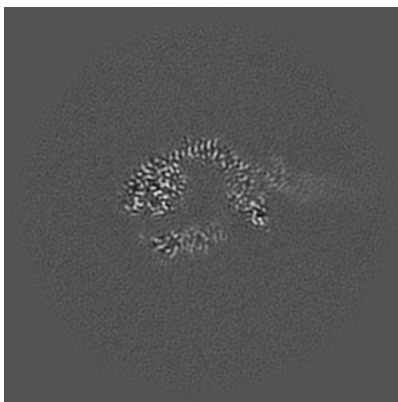
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

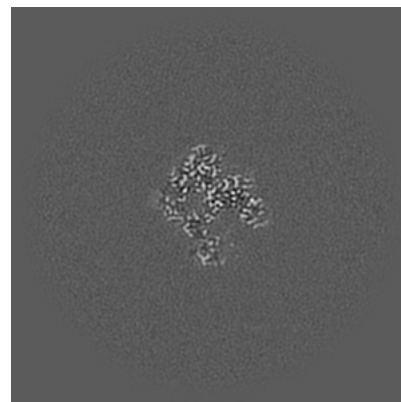
6.3.1 Primary map



X Index: 184

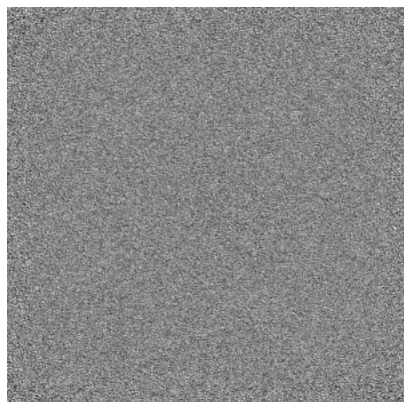


Y Index: 194

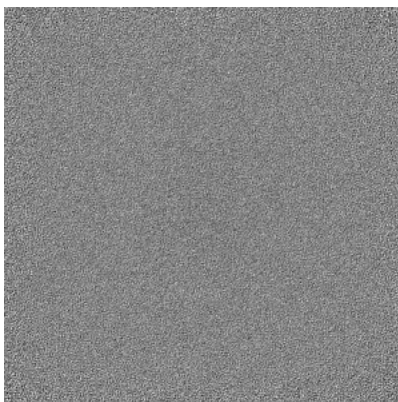


Z Index: 154

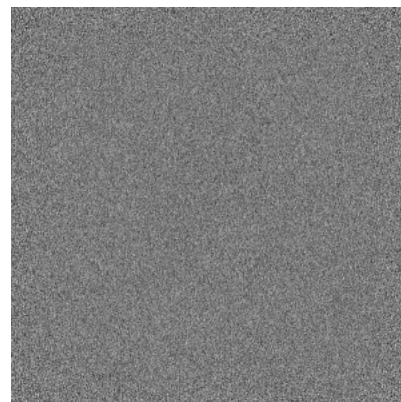
6.3.2 Raw map



X Index: 0



Y Index: 0

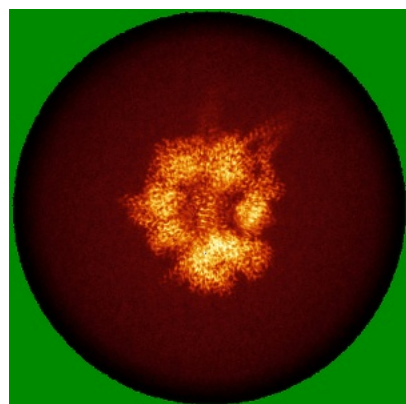


Z Index: 0

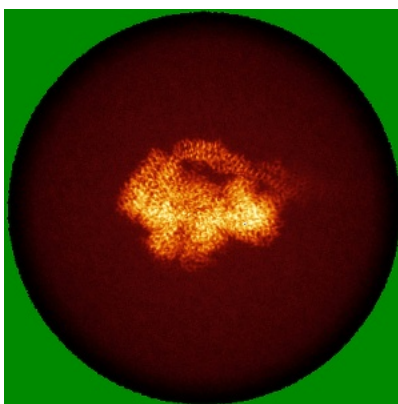
The images above show the largest variance slices of the map in three orthogonal directions.

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

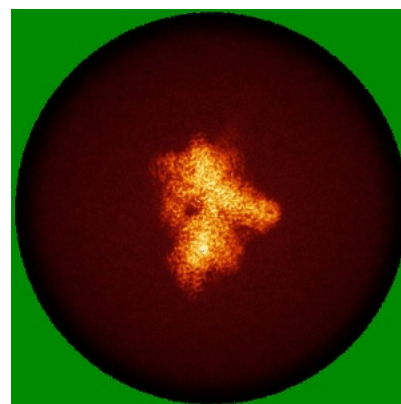
6.4.1 Primary map



X

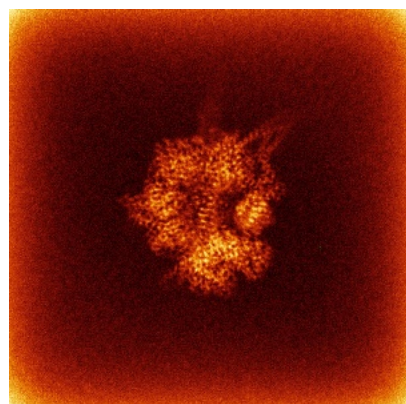


Y

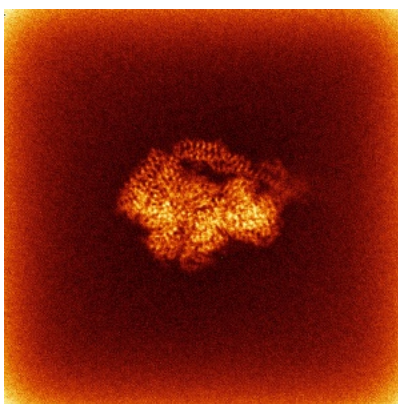


Z

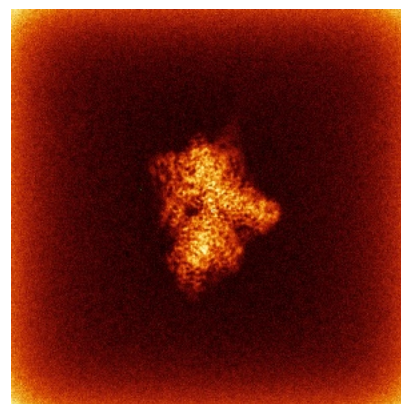
6.4.2 Raw map



X



Y

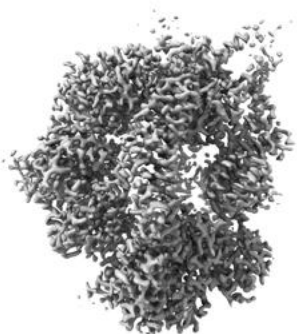


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

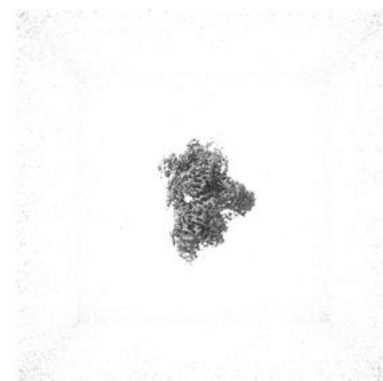
6.5.2 Raw map



X



Y



Z

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.

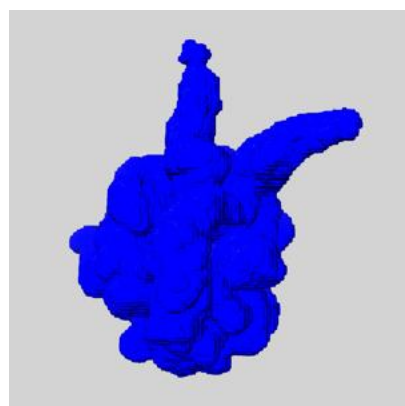
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

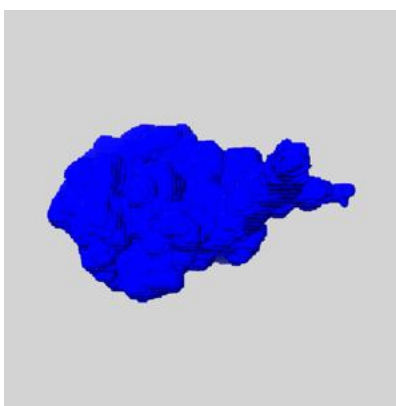
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

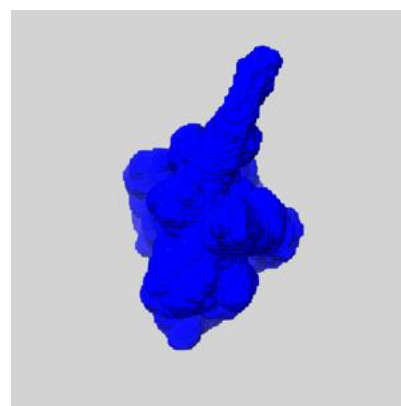
6.6.1 emd_44696_msk_1.map [i](#)



X



Y

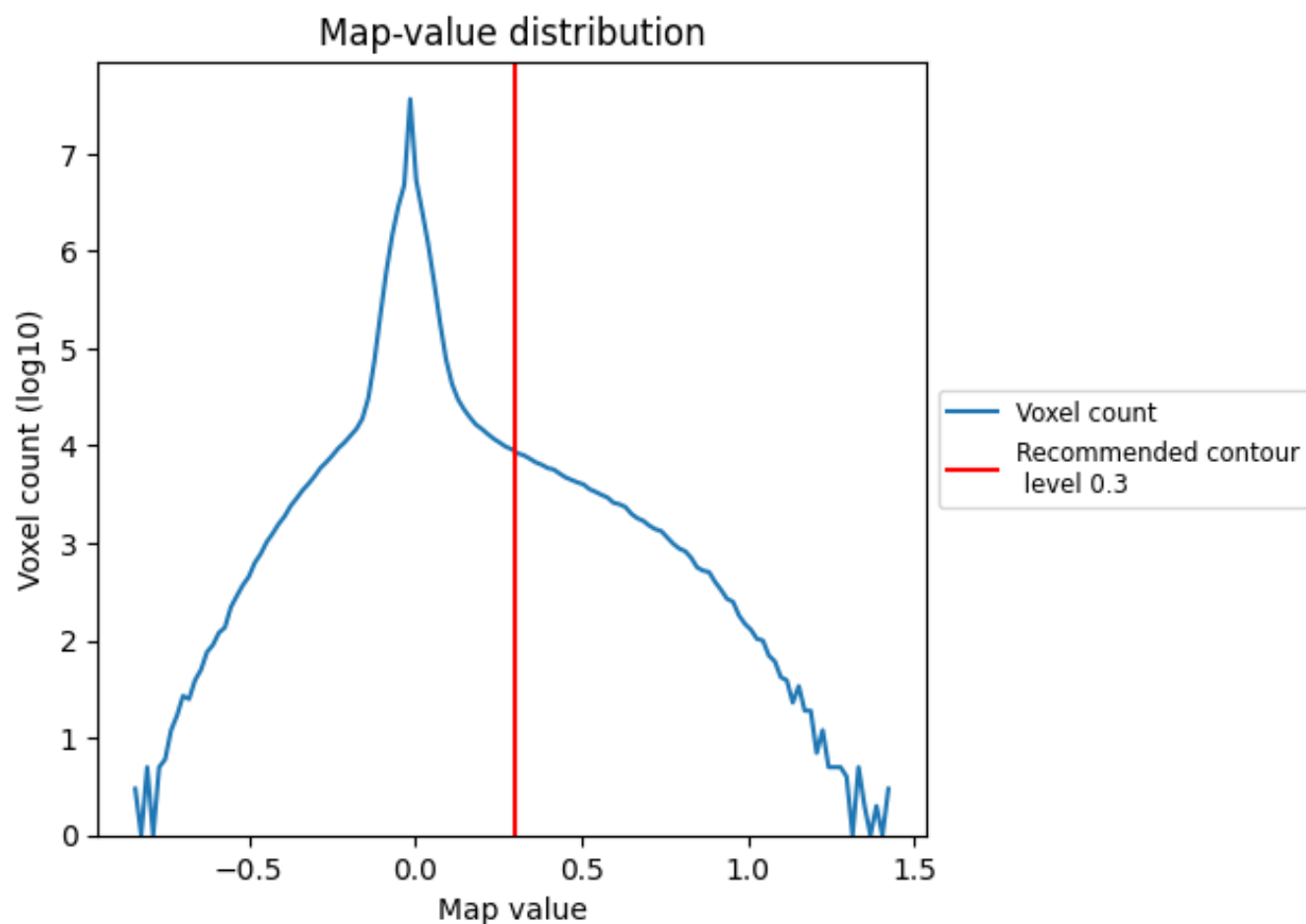


Z

7 Map analysis [i](#)

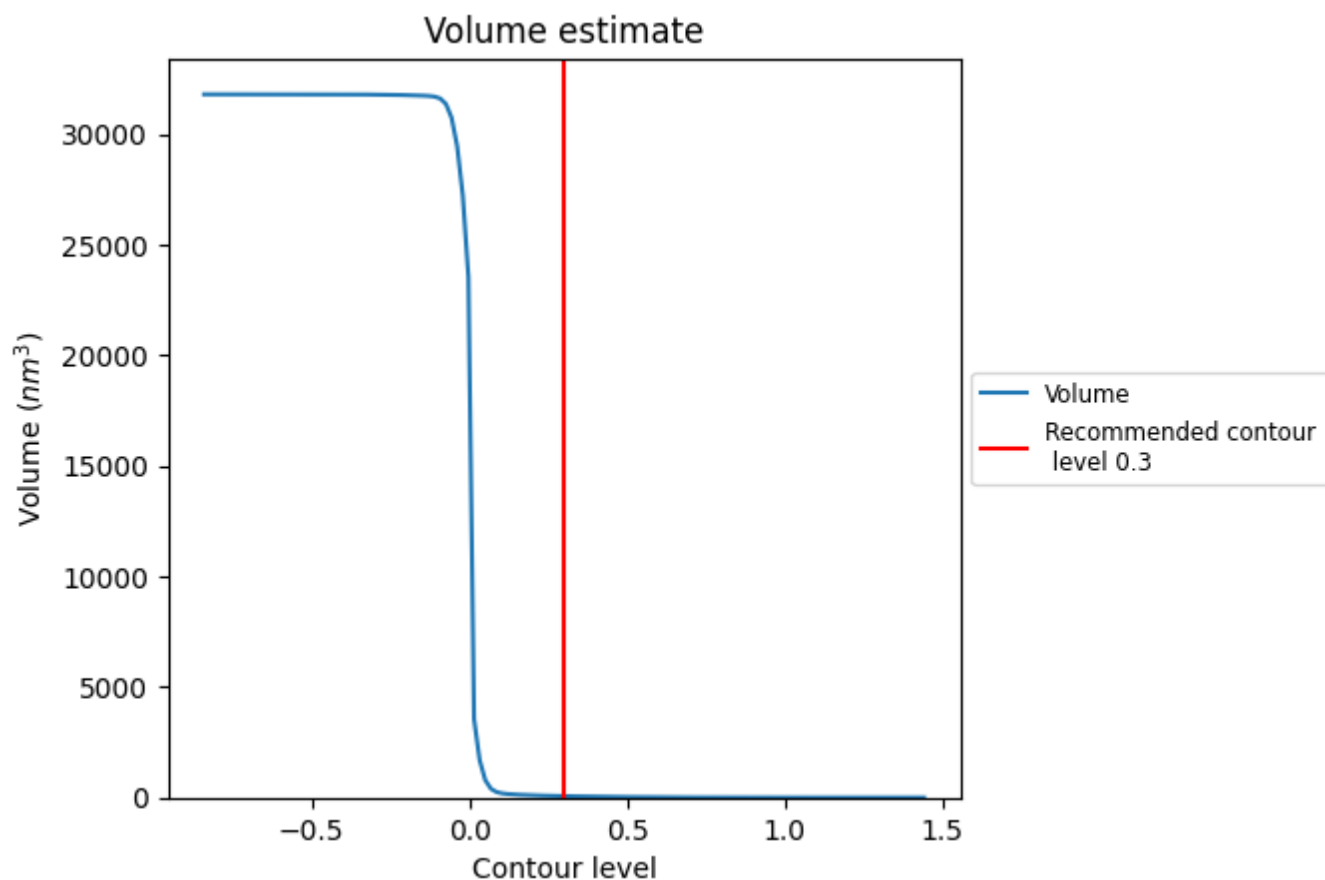
This section contains the results of statistical analysis of the map.

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.

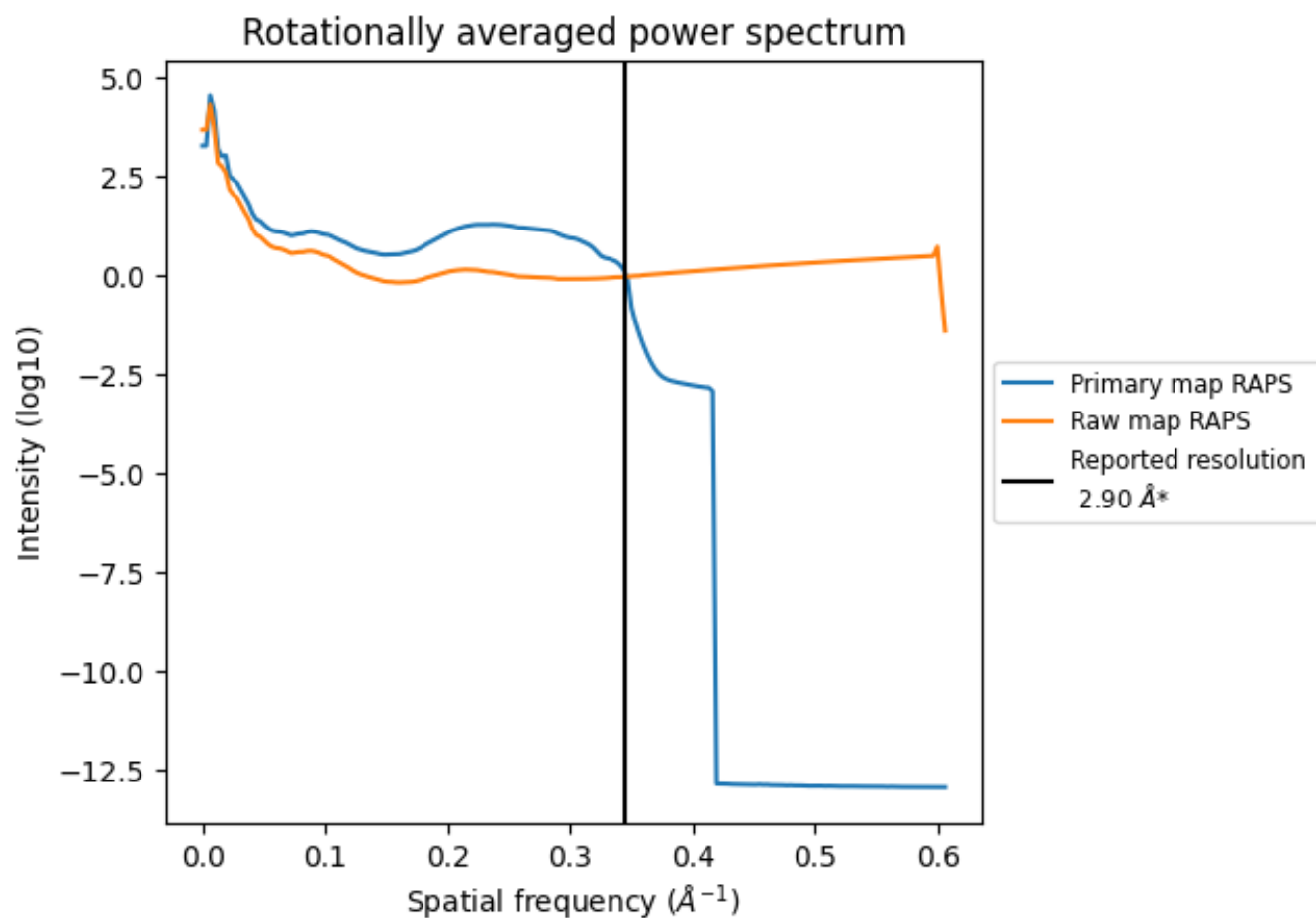
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm³; this corresponds to an approximate mass of 58 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 ⓘ

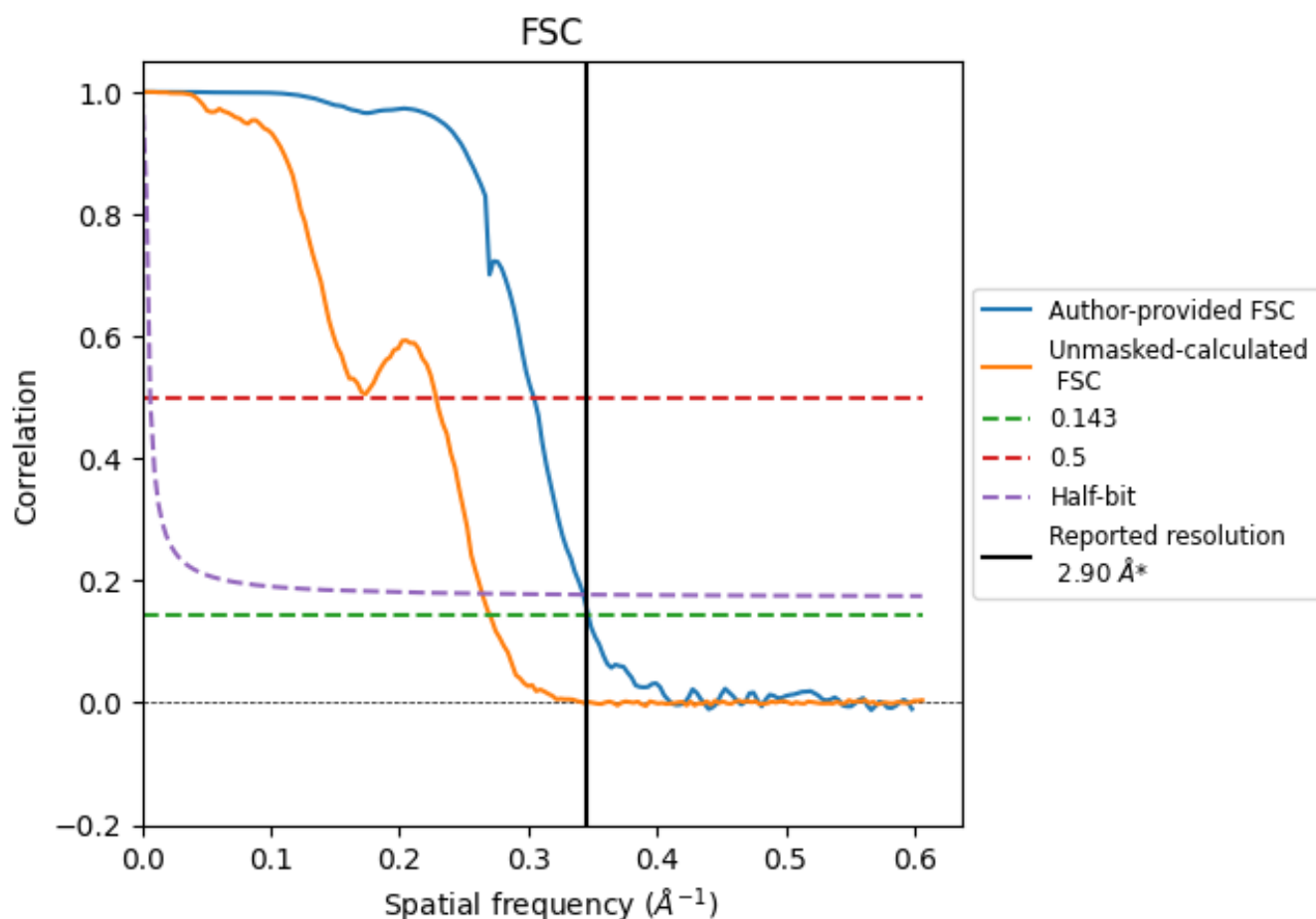


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

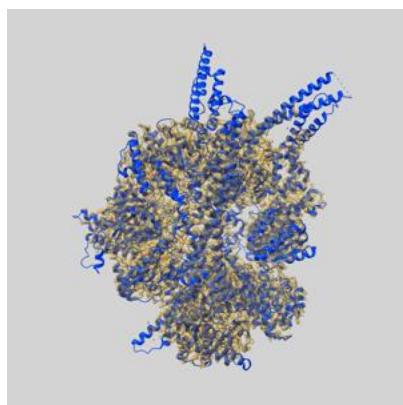
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.29	2.92
Unmasked-calculated*	3.70	4.38	3.79

*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 3.70 differs from the reported value 2.9 by more than 10 %

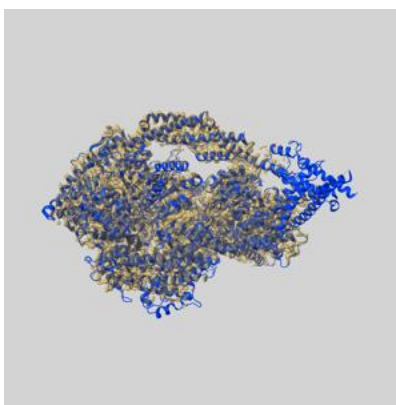
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44696 and PDB model 9BMD. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

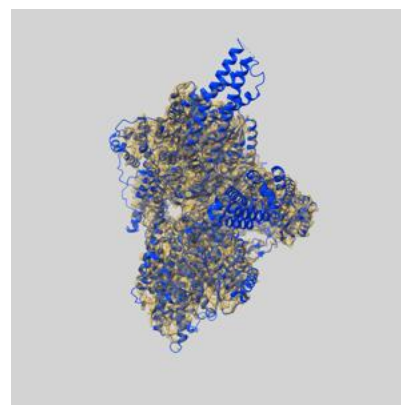
9.1 Map-model overlay [i](#)



X



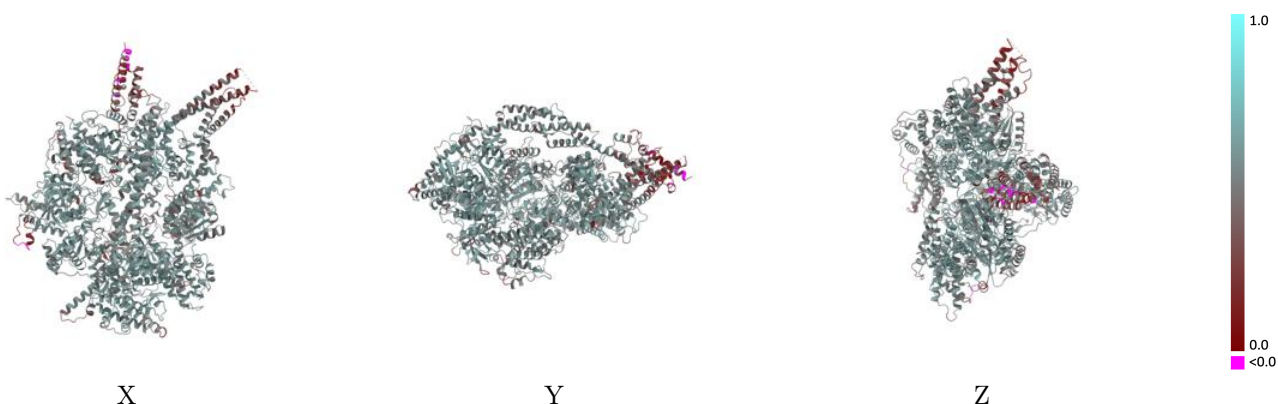
Y



Z

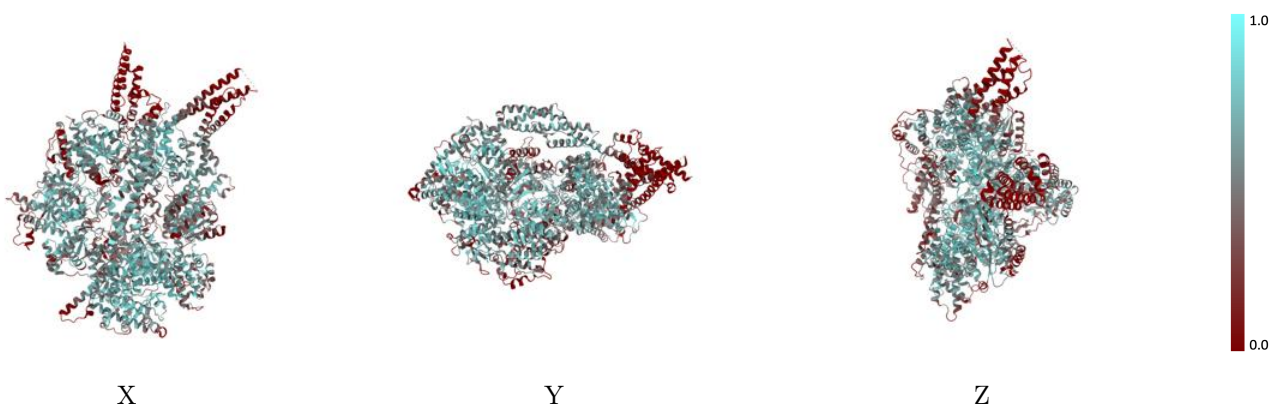
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



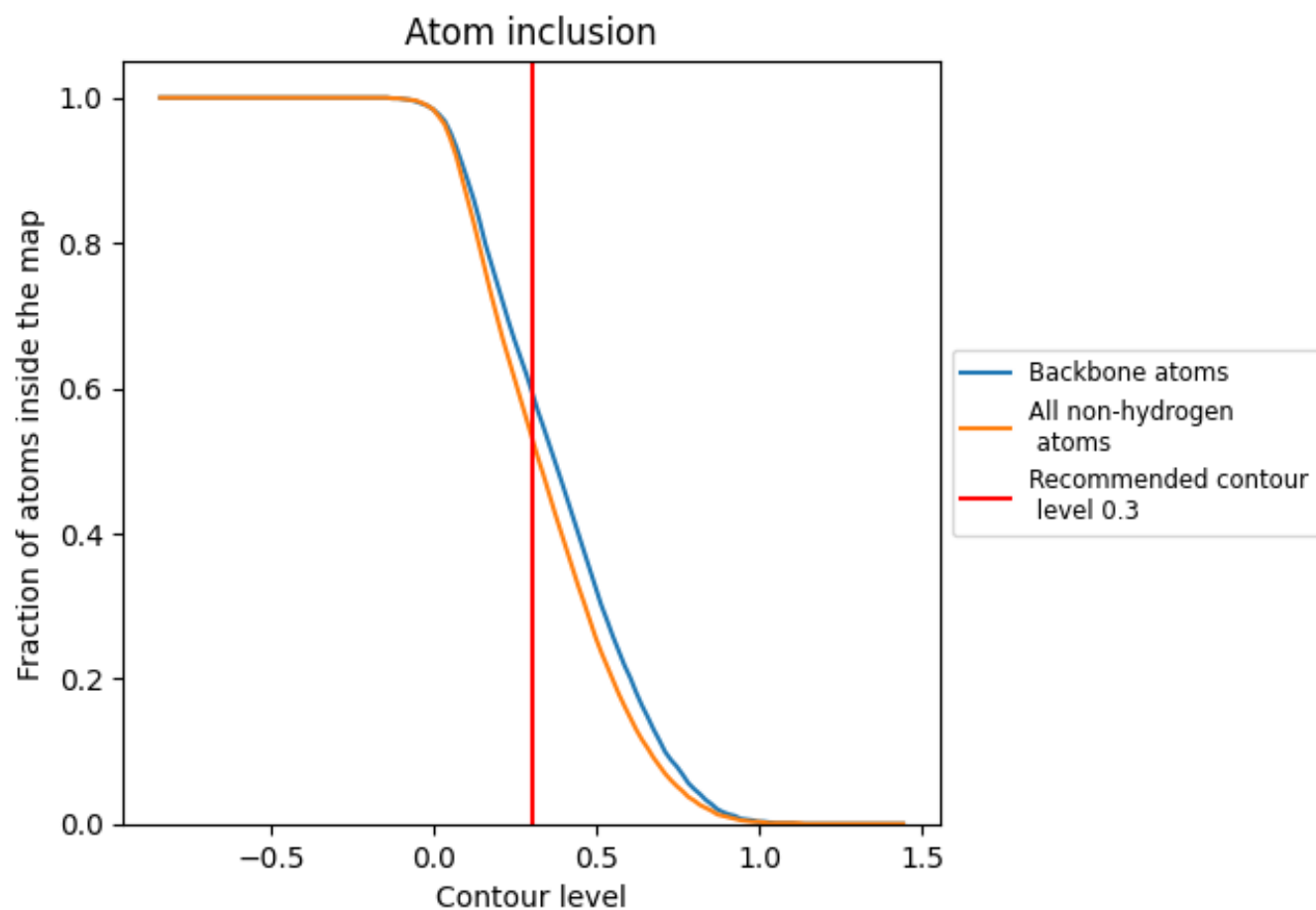
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 53% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5330	<div></div> 0.5260
A	<div></div> 0.5330	<div></div> 0.5260

