



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:56 PM UTC

PDB ID : 9BN6 / pdb_00009bn6
EMDB ID : EMD-44723
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATPVi condition, class2
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
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

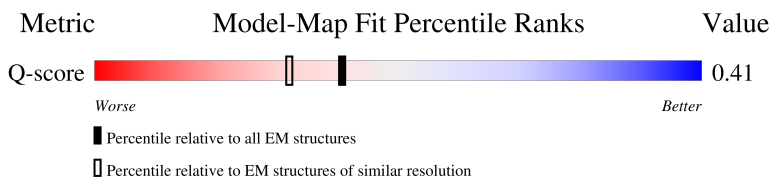
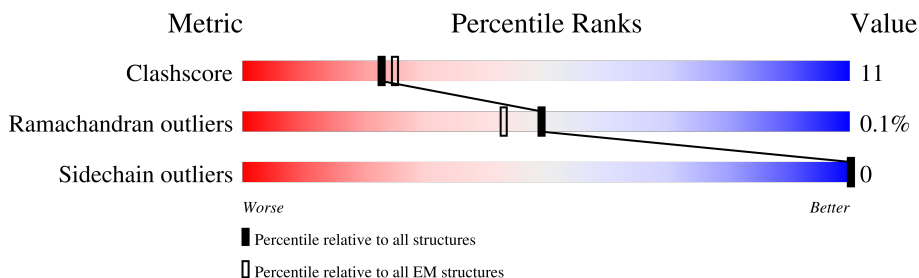
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

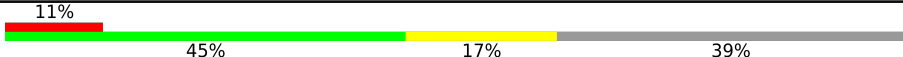
The reported resolution of this entry is 3.40 Å.

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	4646	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23078 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	2855	Total	C	N	O	S	0	0
			22962	14643	3963	4241	115		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	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: $C_{10}H_{16}N_5O_{13}P_3$)

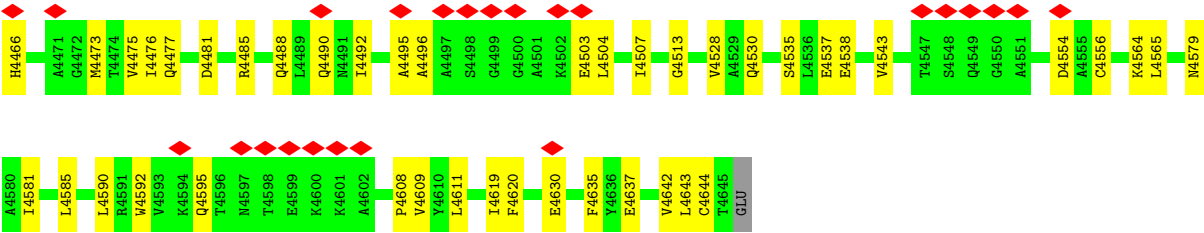
The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (a purine ring system with an amino group at N6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is linked to a chain of three phosphate groups (O=P(O)(OH)-O-P(O)(OH)-O-P(O)(OH)-OH) via a triphosphate tail. The structure is labeled with atom names (N1, N3, N7, N9, C2, C4, C6, C8, C10, C12, C14, C16, C18, C20, C22, C24, C26, C28, C30, C32, C34, C36, C38, C40, C42, C44, C46, C48, C50, C52, C54, C56, C58, C60, C62, C64, C66, C68, C70, C72, C74, C76, C78, C80, C82, C84, C86, C88, C90, C92, C94, C96, C98, C100, C102, C104, C106, C108, C110, C112, C114, C116, C118, C120, C122, C124, C126, C128, C130, C132, C134, C136, C138, C140, C142, C144, C146, C148, C150, C152, C154, C156, C158, C160, C162, C164, C166, C168, C170, C172, C174, C176, C178, C180, C182, C184, C186, C188, C190, C192, C194, C196, C198, C200, C202, C204, C206, C208, C210, C212, C214, C216, C218, C220, C222, C224, C226, C228, C230, C232, C234, C236, C238, C240, C242, C244, C246, C248, C250, C252, C254, C256, C258, C260, C262, C264, C266, C268, C270, C272, C274, C276, C278, C280, C282, C284, C286, C288, C290, C292, C294, C296, C298, C300, C302, C304, C306, C308, C310, C312, C314, C316, C318, C320, C322, C324, C326, C328, C330, C332, C334, C336, C338, C340, C342, C344, C346, C348, C350, C352, C354, C356, C358, C360, C362, C364, C366, C368, C370, C372, C374, C376, C378, C380, C382, C384, C386, C388, C390, C392, C394, C396, C398, C400, C402, C404, C406, C408, C410, C412, C414, C416, C418, C420, C422, C424, C426, C428, C430, C432, C434, C436, C438, C440, C442, C444, C446, C448, C450, C452, C454, C456, C458, C460, C462, C464, C466, C468, C470, C472, C474, C476, C478, C480, C482, C484, C486, C488, C490, C492, C494, C496, C498, C500, C502, C504, C506, C508, C510, C512, C514, C516, C518, C520, C522, C524, C526, C528, C530, C532, C534, C536, C538, C540, C542, C544, C546, C548, C550, C552, C554, C556, C558, C560, C562, C564, C566, C568, C570, C572, C574, C576, C578, C580, C582, C584, C586, C588, C590, C592, C594, C596, C598, C600, C602, C604, C606, C608, C610, C612, C614, C616, C618, C620, C622, C624, C626, C628, C630, C632, C634, C636, C638, C640, C642, C644, C646, C648, C650, C652, C654, C656, C658, C660, C662, C664, C666, C668, C670, C672, C674, C676, C678, C680, C682, C684, C686, C688, C690, C692, C694, C696, C698, C700, C702, C704, C706, C708, C710, C712, C714, C716, C718, C720, C722, C724, C726, C728, C730, C732, C734, C736, C738, C740, C742, C744, C746, C748, C750, C752, C754, C756, C758, C760, C762, C764, C766, C768, C770, C772, C774, C776, C778, C780, C782, C784, C786, C788, C790, C792, C794, C796, C798, C800, C802, C804, C806, C808, C810, C812, C814, C816, C818, C820, C822, C824, C826, C828, C830, C832, C834, C836, C838, C840, C842, C844, C846, C848, C850, C852, C854, C856, C858, C860, C862, C864, C866, C868, C870, C872, C874, C876, C878, C880, C882, C884, C886, C888, C890, C892, C894, C896, C898, C900, C902, C904, C906, C908, C910, C912, C914, C916, C918, C920, C922, C924, C926, C928, C930, C932, C934, C936, C938, C940, C942, C944, C946, C948, C950, C952, C954, C956, C958, C960, C962, C964, C966, C968, C970, C972, C974, C976, C978, C980, C982, C984, C986, C988, C990, C992, C994, C996, C998, C1000, C1002, C1004, C1006, C1008, C1010, C1012, C1014, C1016, C1018, C1020, C1022, C1024, C1026, C1028, C1030, C1032, C1034, C1036, C1038, C1040, C1042, C1044, C1046, C1048, C1050, C1052, C1054, C1056, C1058, C1060, C1062, C1064, C1066, C1068, C1070, C1072, C1074, C1076, C1078, C1080, C1082, C1084, C1086, C1088, C1090, C1092, C1094, C1096, C1098, C1100, C1102, C1104, C1106, C1108, C1110, C1112, C1114, C1116, C1118, C1120, C1122, C1124, C1126, C1128, C1130, C1132, C1134, C1136, C1138, C1140, C1142, C1144, C1146, C1148, C1150, C1152, C1154, C1156, C1158, C1160, C1162, C1164, C1166, C1168, C1170, C1172, C1174, C1176, C1178, C1180, C1182, C1184, C1186, C1188, C1190, C1192, C1194, C1196, C1198, C1200, C1202, C1204, C1206, C1208, C1210, C1212, C1214, C1216, C1218, C1220, C1222, C1224, C1226, C1228, C1230, C1232, C1234, C1236, C1238, C1240, C1242, C1244, C1246, C1248, C1250, C1252, C1254, C1256, C1258, C1260, C1262, C1264, C1266, C1268, C1270, C1272, C1274, C1276, C1278, C1280, C1282, C1284, C1286, C1288, C1290, C1292, C1294, C1296, C1298, C1300, C1302, C1304, C1306, C1308, C1310, C1312, C1314, C1316, C1318, C1320, C1322, C1324, C1326, C1328, C1330, C1332, C1334, C1336, C1338, C1340, C1342, C1344, C1346, C1348, C1350, C1352, C1354, C1356, C1358, C1360, C1362, C1364, C1366, C1368, C1370, C1372, C1374, C1376, C1378, C1380, C1382, C1384, C1386, C1388, C1390, C1392, C1394, C1396, C1398, C1400, C1402, C1404, C1406, C1408, C1410, C1412, C1414, C1416, C1418, C1420, C1422, C1424, C1426, C1428, C1430, C1432, C1434, C1436, C1438, C1440, C1442, C1444, C1446, C1448, C1450, C1452, C1454, C1456, C1458, C1460, C1462, C1464, C1466, C1468, C1470, C1472, C1474, C1476, C1478, C1480, C1482, C1484, C1486, C1488, C1490, C1492, C1494, C1496, C14

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



SER	G3166	R3167	T3168	M3169	R3174	E3189	K3190	E3193	L3194	N3087	R3088	C3089	V3090	Q3196	M3199	H3200	L3201	N3202	V3203	G3204	L3205	R3206	K3207	T3208	K3209	E3210	T3211	V3212	Q3213	Q3214	V3215	E3216	L3217	R3219	R3220	ASP	LEU	ARG	ILE	LYS	SER	GLN	LEU	GLU	LEU	GLU	VAL	LYS	ASN	ALA	ALA	ASP	LYS	LEU		
N2998	D3001	S3002	G3003	F3004	L3005	E3006	R3007	M3008	N3009	T3010	L3011	L3012	A3013	N3014	V3017	L3020	F3021	E3022	G3023	D3024	T3028	L3029	M3030	T3031	C3032	G3033	K3034	E3035	G3036	A3037	Q3038	K3039	E3040	G3041	L3042	M3043	L3044	D3045	S3046	H3047	E3048	E3049	W3053	F3054	T3055	L3059	R3060	F3066	T3067	F3070	SER					
GLU	GLY	LEU	LYS	ASP	ARG	ALA	ALA	THR	S3082	L3085	F3086	N3087	R3088	C3089	V3090	Q3196	M3199	H3200	L3201	N3202	V3203	G3204	L3205	R3206	K3207	T3208	K3209	E3210	T3211	V3212	Q3213	Q3214	V3215	E3216	L3217	R3219	R3220	ASP	LEU	ARG	ILE	LYS	SER	GLN	LEU	GLU	LEU	GLU	VAL	LYS	ASN	ALA	ALA	ASP	LYS	LEU
D2906	L2909	F2912	N2913	E2914	V2915	L2916	D2917	H2918	V2919	L2920	R2921	L2922	I2925	F2926	R2927	Q2928	P2929	Q2930	G2931	H2932	L2933	L2934	L2935	M2954	S2957	Q2960	L2961	K2962	V2963	L2964	R2965	T2966	E2970	D2971	F2972	D2973	E2974	D2975	L2976	R2977	C2985	K2986	N2987	L2990	L2993	M2994	D2995									
Q2834	D2835	R2836	L2837	V2838	E2839	D2840	E2841	R2842	R2843	W2845	T2846	D2847	E2848	N2849	T2850	D2851	T2852	L2855	K2856	H2857	F2858	P2859	N2860	L2861	D2862	R2863	E2864	K2865	A2866	N2867	S2868	R2869	F2870	L2871	W2875	S2878	K2879	D2880	D2885	Q2886	E2887	E2888	L2889	R2890	L2897	L2898	K2899	Y2901	E2902	E2903	E2904	L2905				
M2755	L2756	R2757	L2758	L2759	L2762	R2763	E2767	A2772	M2773	V2774	E2775	F2776	Y2777	T2778	M2779	R2783	F2784	T2785	Q2786	D2787	T2788	Y2792	L2793	R2794	S2795	P2796	R2797	E2798	M2799	T2800	R2801	W2802	V2803	R2804	E2808	R2811	P2812	L2813	E2814	L2815	P2817	V2818	E2819	G2820	L2821	L2822	R2823	L2824	E2828							
T2644	P2645	N2646	L2650	K2657	W2658	L2661	C2662	D2664	E2665	L2668	P2669	D2670	M2671	D2672	K2673	Y2674	Q2677	T2680	S2681	F2682	M2686	L2703	E2704	R2705	P2708	V2709	P2714	K2721	H2725	L2728	R2729	H2730	V2731	P2741	A2742	S2743	L2744	T2745	Q2746	L2747	F2751	N2752														
T2535	D2536	E2537	E2538	E2544	V2545	S2546	P2547	W2548	Q2554	L2555	E2558	V2561	V2562	A2563	A2564	P2565	D2566	R2576	H2577	L2580	S2581	V2582	L2583	W2584	P2590	L2591	V2592	L2593	P2596	S2599	Q2600	V2601	T2602	M2603	L2605	D2614	M2615	E2616	N2621	F2622	S2623	T2626	L2627	F2628	Y2641											
H2439	A2440	F2441	Q2442	L2443	E2444	H2445	L2446	M2447	D2448	L2449	L2452	R2453	C2454	M2461	A2465	R2473	F2479	M2481	Q2485	R2492	Y2493	L2494	V2495	W2500	S2501	L2502	S2503	L2508	K2509	M2510	R2511	L2514	T2518	L2521	T2522	V2524	P2525	L2526	T2527	T2528	A2529	P2530	N2531	I2534												
P2328	R2332	L2333	P2336	P2337	N2338	V2339	M2342	A2351	T2352	R2358	E2366	L2369	M2373	L2374	N2377	L2382	R2383	D2389	GLY	GLU	ASP	GLU	ALA	GLN	ARG	ARG	LYS	GLY	LYS	GLU	ASP	GLU	GLY	GLU	ALA	S2410	L2413	P2525	L2526	P2527	A2420	Q2424														
Y2211	Q2212	L2213	L2220	M2221	M2222	Q2227	S2231	W2234	L2237	L2238	E2248	Q2249	K2257	S2260	L2264	Y2265	N2271	T2272	W2275	L2284	R2285	L2288	D2289	R2292	V2291	Q2293	E2294	L2295	Q2296	K2297	W2300	V2307	D2308	P2309	F2310	W2311	D2320	L2324	L2325	T2326	L2327															
G2101	N2102	R2105	R2113	E2114	LYS	GLU	ARG	GLY	GLU	ALA	VAL	ASP	GLU	GLY	GLY	I2127	P2132	E2135	L2149	E2152	L2157	L2180	D2183	R2179	E2180	E2181	L2182	K2183	K2184	V2185	C2186	Q2187	E2188	M2189	Y2190	L2191	T2192	D2195	W2203	V2204	E2205	K2206	V2207	L2208	Q2209	L2210										
T1998	C1999	E2000	L2001	L2002	N2003	V2006	K2007	L2016	T2017	M2018	N2019	PRO	GLY	TYR	ALA	GLY	ARG	SER	ASN	L2028	L2035	F2036	R2037	S2038	L2039	M2041	T2042	L2048	L2049	V2052	S2056	F2059	R2060	E2063	A2066	N2067	K2068	L2069	V2070	P2071	K2074	L2075	C2076	Q2079	F2088											





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72335	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.597	Depositor
Minimum map value	-1.141	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	411.48, 411.48, 411.48	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.143, 1.143, 1.143	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	0.13	0/23454	0.34	1/31791 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2867	MET	N-CA-C	-6.05	107.72	114.62

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	22962	0	23030	517	0
2	A	54	0	24	2	0
3	A	62	0	24	5	0
All	All	23078	0	23078	517	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 11.

All (517) 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:4377:MET:HE3	1:A:4438:CYS:HA	1.54	0.89
1:A:4037:PRO:HG2	1:A:4117:GLN:HE21	1.40	0.87
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.18	0.86
1:A:2929:PRO:HB3	1:A:3060:ARG:HA	1.61	0.83
1:A:1938:PHE:HB2	1:A:1967:MET:HE1	1.62	0.80
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.64	0.79
1:A:2930:GLN:HE21	1:A:3059:ILE:HA	1.45	0.79
1:A:3040:GLU:OE2	1:A:3053:TRP:NE1	2.18	0.75
1:A:2925:ILE:HG13	1:A:2933:LEU:HD13	1.68	0.75
1:A:2621:ASN:HA	1:A:2664:ASP:HB2	1.68	0.75
1:A:2836:ARG:HG2	1:A:3091:LEU:HB2	1.69	0.74
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.69	0.73
1:A:4288:VAL:HG21	1:A:4294:ILE:HG12	1.70	0.73
1:A:2605:LEU:HD23	1:A:2662:PHE:HE1	1.53	0.72
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.21	0.72
1:A:3203:VAL:HA	1:A:3206:ARG:HE	1.56	0.71
1:A:2308:ASP:OD1	1:A:2311:TRP:NE1	2.24	0.71
1:A:3585:ARG:HB2	1:A:3697:THR:HG23	1.73	0.70
1:A:4396:SER:HB2	1:A:4398:LEU:HD23	1.73	0.70
1:A:2745:THR:HG22	1:A:2774:VAL:HG21	1.73	0.69
1:A:3588:LEU:HD11	1:A:3638:VAL:HG21	1.75	0.69
1:A:4038:ASN:ND2	1:A:4117:GLN:OE1	2.26	0.69
1:A:2222:MET:HE1	1:A:2234:TRP:HB3	1.74	0.68
1:A:1748:GLN:NE2	1:A:1868:TYR:OH	2.25	0.68
1:A:3843:ASN:HD22	1:A:3846:LEU:HG	1.59	0.68
1:A:1623:ARG:NH2	1:A:1632:VAL:O	2.28	0.67
1:A:2752:ASN:HD22	1:A:2755:MET:HE2	1.58	0.67
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.76	0.66
1:A:2977:ARG:NH1	1:A:3020:LEU:O	2.27	0.66
1:A:2671:MET:HE3	1:A:2721:LYS:HB3	1.78	0.66
1:A:2446:ILE:HG23	1:A:2447:MET:HG3	1.78	0.66
1:A:4537:GLU:O	1:A:4595:GLN:NE2	2.29	0.66
1:A:1470:TRP:HB3	1:A:1589:MET:HE1	1.78	0.66
1:A:3133:LEU:HB3	1:A:3134:PRO:HD3	1.78	0.65
1:A:2823:ARG:HA	1:A:2866:ALA:HB1	1.78	0.65
1:A:2163:ASP:OD1	1:A:4530:GLN:NE2	2.29	0.65
1:A:2265:TYR:OH	1:A:2311:TRP:O	2.14	0.65
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.76	0.65
1:A:1959:GLU:OE2	1:A:1962:ARG:NH1	2.30	0.65
1:A:1698:ILE:HD13	1:A:1701:TRP:HE1	1.61	0.64
1:A:3764:ASP:HA	1:A:3767:ILE:HB	1.79	0.64
1:A:1747:ALA:HB2	1:A:1807:LYS:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3035:GLU:OE1	1:A:3038:GLN:NE2	2.31	0.64
1:A:4074:ALA:HA	1:A:4077:PHE:HD2	1.62	0.64
1:A:3190:LYS:HB3	1:A:3503:ILE:HD11	1.78	0.64
1:A:3521:ASP:HB2	1:A:3704:THR:HG21	1.79	0.64
1:A:3881:ILE:O	1:A:3885:MET:HG2	1.97	0.64
1:A:2960:GLN:O	1:A:2962:LYS:NZ	2.30	0.63
1:A:4454:GLU:HG2	1:A:4461:PRO:HA	1.79	0.63
1:A:2804:ARG:HH22	1:A:2929:PRO:HB2	1.63	0.63
1:A:3519:TYR:HA	1:A:3700:ASN:HB2	1.81	0.63
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.81	0.63
1:A:4395:LEU:HA	1:A:4490:GLN:HE22	1.63	0.63
1:A:2590:PRO:HB2	1:A:2731:VAL:HG12	1.81	0.63
1:A:2326:THR:HG22	1:A:2332:ARG:HG2	1.79	0.62
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.32	0.62
1:A:3035:GLU:HB3	1:A:3039:LYS:NZ	2.14	0.62
1:A:1463:LEU:HD22	1:A:1467:ARG:HH21	1.65	0.62
1:A:3158:ASN:ND2	1:A:3169:MET:O	2.32	0.62
1:A:3818:LEU:HA	1:A:4346:MET:HE1	1.81	0.62
1:A:1825:LEU:HD21	1:A:1837:GLU:HB2	1.81	0.62
1:A:2865:LYS:HD2	1:A:2869:ARG:HA	1.81	0.62
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.33	0.62
1:A:4097:LYS:HA	1:A:4127:THR:HB	1.82	0.61
1:A:4161:PHE:O	1:A:4302:ARG:NH2	2.34	0.61
1:A:4169:ILE:HG21	1:A:4302:ARG:HD2	1.82	0.61
1:A:2596:PRO:O	1:A:2601:LYS:NZ	2.34	0.61
1:A:3898:GLU:OE2	1:A:3981:THR:OG1	2.16	0.61
1:A:1786:GLU:OE2	1:A:1823:ARG:NH2	2.34	0.61
1:A:2686:MET:HG2	1:A:2703:LEU:HD11	1.82	0.61
1:A:2960:GLN:HB3	1:A:2993:ILE:HG13	1.83	0.61
1:A:3584:ASN:O	1:A:3651:ARG:NH2	2.34	0.60
1:A:3708:LEU:HD11	1:A:3829:LEU:HD11	1.82	0.60
1:A:2205:GLU:O	1:A:2209:GLN:HG3	2.02	0.60
1:A:3208:ILE:O	1:A:3212:VAL:HG23	2.02	0.60
1:A:3921:THR:OG1	1:A:3923:ARG:NH1	2.34	0.59
1:A:2785:THR:OG1	1:A:2787:ASP:OD1	2.20	0.59
1:A:2845:TRP:O	1:A:2849:ASN:ND2	2.35	0.59
1:A:3627:LEU:HD11	1:A:3671:LEU:HD12	1.84	0.59
1:A:3989:ARG:HB3	1:A:4004:MET:HE2	1.84	0.59
1:A:2291:VAL:HG12	1:A:2292:ARG:HG2	1.84	0.59
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.84	0.59
1:A:4399:LYS:HE2	1:A:4413:PHE:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1914:GLU:HG3	2:A:4701:ADP:H3'	1.85	0.59
1:A:2581:LEU:HD21	1:A:2593:LEU:HD21	1.84	0.59
1:A:1531:MET:HE2	1:A:1531:MET:HA	1.85	0.58
1:A:3009:ASN:O	1:A:3088:ARG:NH1	2.35	0.58
1:A:4565:LEU:HB2	1:A:4585:LEU:HD11	1.85	0.58
1:A:1912:LYS:HA	1:A:2041:MET:HE1	1.86	0.58
1:A:4381:HIS:HB2	1:A:4438:CYS:HB3	1.86	0.58
1:A:1882:THR:HG22	1:A:2048:LEU:HD23	1.84	0.58
1:A:2063:GLU:OE2	1:A:2067:ASN:ND2	2.37	0.58
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.86	0.58
1:A:2822:ILE:HG13	1:A:2861:ILE:HG12	1.85	0.58
1:A:4611:LEU:HD12	1:A:4644:CYS:HB2	1.84	0.58
1:A:1866:PHE:HE2	1:A:1893:THR:HG22	1.67	0.58
1:A:1497:VAL:HG11	1:A:1531:MET:HE3	1.86	0.57
1:A:2324:LEU:HD21	1:A:2332:ARG:HD3	1.85	0.57
1:A:1544:TRP:HE1	1:A:1572:SER:HA	1.69	0.57
1:A:3638:VAL:HG11	1:A:3679:LEU:HB3	1.86	0.57
1:A:4128:MET:HE3	1:A:4134:VAL:HG21	1.87	0.57
1:A:3488:ARG:HH21	1:A:3742:LEU:HG	1.68	0.57
1:A:3751:GLN:HA	1:A:3754:ASN:ND2	2.19	0.57
1:A:2783:ARG:HG2	1:A:2784:PHE:H	1.70	0.56
1:A:3836:TYR:HA	1:A:3839:VAL:HG12	1.86	0.56
1:A:2102:ASN:OD1	1:A:2105:ARG:NH2	2.35	0.56
1:A:2179:ARG:NH1	1:A:2195:ASP:OD1	2.38	0.56
1:A:2969:GLY:HA2	1:A:3004:PHE:HE1	1.70	0.56
1:A:4609:VAL:HG22	1:A:4642:VAL:HB	1.88	0.56
1:A:1665:ILE:N	1:A:1675:GLY:O	2.38	0.56
1:A:2581:LEU:HD13	1:A:2591:LEU:HD11	1.87	0.56
1:A:1792:LEU:HD21	1:A:1811:LEU:HB3	1.88	0.56
1:A:2890:ARG:NH2	1:A:2913:ASN:OD1	2.39	0.56
1:A:2503:SER:HB2	1:A:2514:LEU:HD22	1.88	0.56
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.88	0.56
1:A:3034:LYS:HB2	1:A:3044:LEU:HD22	1.86	0.56
1:A:3168:THR:C	1:A:3169:MET:HE2	2.30	0.56
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.87	0.56
1:A:3724:VAL:O	1:A:3728:ARG:HG2	2.06	0.56
1:A:4071:ILE:HG21	1:A:4099:VAL:HA	1.88	0.56
1:A:1582:VAL:HG23	1:A:1591:VAL:HG11	1.88	0.55
1:A:4042:LEU:HD21	1:A:4138:LEU:HG	1.88	0.55
1:A:4211:ASP:OD1	1:A:4255:ARG:NH2	2.39	0.55
1:A:4110:GLU:OE2	1:A:4114:HIS:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4206:GLU:O	1:A:4255:ARG:NH1	2.40	0.55
1:A:3031:THR:HG23	1:A:3034:LYS:HE2	1.88	0.55
1:A:1734:ASP:HB2	1:A:1737:THR:HG22	1.87	0.55
1:A:2623:SER:N	1:A:2626:THR:OG1	2.40	0.55
1:A:2935:LEU:N	1:A:3066:PHE:O	2.35	0.55
1:A:3738:PHE:O	1:A:3741:ARG:HD3	2.07	0.55
1:A:4038:ASN:HD21	1:A:4116:LEU:HD13	1.71	0.55
1:A:1987:ASN:HB2	1:A:1990:TYR:HB3	1.89	0.54
1:A:2320:ASP:OD2	1:A:2358:ARG:NH1	2.40	0.54
1:A:2500:TRP:CZ2	1:A:2576:ARG:HD2	2.43	0.54
1:A:2889:LEU:HD21	1:A:2920:LEU:HD21	1.89	0.54
1:A:2260:SER:O	1:A:2264:LEU:N	2.40	0.54
1:A:4445:THR:HG22	1:A:4448:LEU:HD23	1.88	0.54
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.89	0.54
1:A:3087:ASN:O	1:A:3088:ARG:HG2	2.08	0.54
1:A:3620:ARG:HE	1:A:3644:VAL:HG21	1.72	0.54
1:A:1487:ILE:O	1:A:2271:ASN:ND2	2.40	0.54
1:A:1884:LEU:HD21	1:A:2041:MET:HB3	1.89	0.54
1:A:2816:LEU:HD12	1:A:2817:PRO:HD2	1.89	0.54
1:A:1947:GLY:O	1:A:1951:VAL:HG12	2.08	0.54
1:A:2957:SER:HB2	1:A:2990:ILE:HD13	1.90	0.54
1:A:3134:PRO:HG2	1:A:3137:PRO:HA	1.90	0.54
1:A:1485:ARG:O	1:A:1486:LEU:HD23	2.08	0.53
1:A:1680:GLU:OE1	1:A:1875:VAL:N	2.42	0.53
1:A:1756:ILE:HD13	1:A:1846:PHE:HB2	1.89	0.53
1:A:2192:THR:HB	1:A:2373:MET:HG3	1.90	0.53
1:A:2808:GLU:OE2	1:A:2811:ARG:NH2	2.34	0.53
1:A:4454:GLU:HG3	1:A:4459:ILE:HG23	1.89	0.53
1:A:3012:LEU:HD11	1:A:3066:PHE:HE2	1.74	0.53
1:A:1647:VAL:HG11	1:A:1666:LEU:HD11	1.90	0.53
1:A:2834:GLN:HG2	1:A:2843:ARG:HG2	1.90	0.53
1:A:3008:MET:HG3	1:A:3066:PHE:HZ	1.74	0.53
1:A:3219:ARG:HD3	1:A:3475:SER:HB3	1.91	0.53
1:A:1511:PRO:HG2	1:A:3670:ASP:HB3	1.91	0.53
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.44	0.53
1:A:2927:ARG:HH22	1:A:2954:ASN:HB3	1.73	0.53
1:A:2492:ARG:HH11	1:A:2544:GLU:HA	1.74	0.53
1:A:2492:ARG:NH1	1:A:2544:GLU:OE1	2.39	0.53
1:A:2993:ILE:C	1:A:2994:MET:HE2	2.34	0.53
1:A:1486:LEU:HD13	1:A:2271:ASN:HB3	1.91	0.52
1:A:3488:ARG:O	1:A:3491:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4088:VAL:HB	1:A:4118:PRO:HD2	1.90	0.52
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.43	0.52
1:A:1836:PHE:O	1:A:1840:SER:N	2.39	0.52
1:A:2291:VAL:N	1:A:2294:GLU:OE1	2.42	0.52
1:A:3510:SER:O	1:A:3514:ILE:HG12	2.09	0.52
1:A:3103:TYR:OH	1:A:3141:GLU:OE2	2.28	0.52
1:A:4439:GLU:HB3	1:A:4441:LYS:NZ	2.25	0.52
1:A:4485:ARG:NH1	1:A:4513:GLY:O	2.43	0.52
1:A:1651:GLN:HA	1:A:1654:PHE:HD2	1.73	0.52
1:A:2934:LEU:HD23	1:A:3091:LEU:HG	1.91	0.52
1:A:1614:ALA:O	1:A:1617:GLU:HG3	2.10	0.52
1:A:1806:ARG:HG3	1:A:1806:ARG:HH11	1.75	0.52
1:A:1830:ILE:HG12	1:A:1837:GLU:HG3	1.91	0.52
1:A:1769:MET:SD	1:A:1777:PRO:HD2	2.49	0.52
1:A:4179:LEU:HD12	1:A:4223:LEU:HD22	1.92	0.52
1:A:2535:ILE:HD12	1:A:2535:ILE:H	1.75	0.51
1:A:2898:LYS:HA	1:A:2901:TYR:CE2	2.45	0.51
1:A:3189:GLU:O	1:A:3193:GLU:HG2	2.10	0.51
1:A:3203:VAL:HG13	1:A:3206:ARG:HH21	1.75	0.51
1:A:2605:LEU:HD21	1:A:2709:VAL:HG12	1.92	0.51
1:A:2804:ARG:NH1	1:A:2929:PRO:O	2.42	0.51
1:A:2813:LEU:HD21	1:A:2816:LEU:HD13	1.92	0.51
1:A:3751:GLN:HA	1:A:3754:ASN:HD21	1.74	0.51
1:A:4326:ASN:HD21	1:A:4581:ILE:HG23	1.75	0.51
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.92	0.51
1:A:2374:ILE:HD13	3:A:4702:ATP:C8	2.45	0.51
1:A:4069:ILE:HG23	1:A:4079:GLN:HE21	1.75	0.51
1:A:4423:LEU:HD22	1:A:4466:HIS:HB2	1.91	0.51
1:A:4287:LYS:N	1:A:4293:ASP:OD1	2.43	0.51
1:A:3488:ARG:NH2	1:A:3743:ARG:HH21	2.08	0.51
1:A:4023:GLN:HG2	1:A:4024:PRO:HD2	1.92	0.51
1:A:4564:LYS:N	1:A:4643:LEU:O	2.40	0.51
1:A:2446:ILE:HD11	1:A:2714:PRO:HG3	1.92	0.51
1:A:2443:LEU:HD12	1:A:2510:MET:SD	2.50	0.51
1:A:2448:ASP:OD1	1:A:2448:ASP:N	2.43	0.51
1:A:2777:TYR:CE1	1:A:2794:TYR:HB3	2.46	0.51
1:A:3557:ASP:OD1	1:A:3558:GLU:N	2.44	0.51
1:A:3205:LEU:HG	1:A:3489:TRP:HE3	1.76	0.51
1:A:2185:VAL:HA	1:A:2188:GLU:HG2	1.92	0.50
1:A:2525:PRO:O	1:A:2545:TRP:NE1	2.35	0.50
1:A:2673:LYS:NZ	1:A:2674:TYR:OH	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3614:PHE:HE2	1:A:3638:VAL:HG12	1.76	0.50
1:A:1724:VAL:HA	1:A:1727:PHE:CD2	2.46	0.50
1:A:3789:ILE:O	1:A:3792:GLN:HG3	2.11	0.50
1:A:1880:VAL:HG11	1:A:2049:ILE:HA	1.92	0.50
1:A:4473:MET:HG2	1:A:4477:GLN:HB2	1.92	0.50
1:A:4528:VAL:HG11	1:A:4592:TRP:HB2	1.94	0.50
1:A:2580:LEU:HB3	1:A:2584:TRP:HZ3	1.76	0.50
1:A:3850:THR:HA	1:A:3855:ARG:HD2	1.93	0.50
1:A:4456:VAL:HG23	1:A:4457:LYS:HD3	1.94	0.50
1:A:4496:ALA:HB2	1:A:4504:LEU:HD21	1.94	0.50
1:A:1691:SER:OG	1:A:1694:GLU:OE1	2.29	0.50
1:A:2132:PRO:HB2	1:A:2135:GLU:OE1	2.12	0.50
1:A:1726:ILE:O	1:A:1729:LYS:HG2	2.12	0.50
1:A:3207:LYS:HE2	1:A:3754:ASN:HB3	1.93	0.50
1:A:3551:GLU:OE1	1:A:3551:GLU:N	2.32	0.49
1:A:4172:SER:HB2	1:A:4173:PRO:HD2	1.94	0.49
1:A:1524:GLU:HA	1:A:1527:LEU:HD12	1.93	0.49
1:A:2762:LEU:HD11	1:A:2816:LEU:HB3	1.94	0.49
1:A:2796:PRO:HA	1:A:2799:MET:HE2	1.94	0.49
1:A:3035:GLU:HB3	1:A:3039:LYS:HZ1	1.76	0.49
1:A:4543:VAL:HG22	1:A:4590:LEU:HD23	1.94	0.49
1:A:1967:MET:O	1:A:1971:VAL:HG22	2.12	0.49
1:A:2677:GLN:HB2	1:A:2680:ILE:HB	1.94	0.49
1:A:2904:GLU:O	1:A:3654:ARG:NH2	2.44	0.49
1:A:2918:HIS:O	1:A:2922:ILE:HG13	2.13	0.49
1:A:1903:SER:N	1:A:2037:ARG:O	2.44	0.49
1:A:3893:LYS:NZ	1:A:3902:ASP:OD1	2.41	0.49
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.94	0.49
1:A:2285:ARG:HA	1:A:2288:ILE:HG22	1.95	0.49
1:A:2308:ASP:OD1	1:A:2308:ASP:N	2.45	0.49
1:A:2605:LEU:HD23	1:A:2662:PHE:CE1	2.42	0.49
1:A:2628:PRO:HB3	1:A:2682:PHE:CD2	2.48	0.49
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.93	0.49
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.94	0.49
1:A:1931:ASN:OD1	1:A:1932:CYS:N	2.46	0.49
1:A:3005:LEU:HD11	1:A:3085:LEU:HD22	1.94	0.48
1:A:2183:LYS:O	1:A:2187:GLN:HG2	2.13	0.48
1:A:2741:PRO:O	1:A:2745:THR:HG23	2.12	0.48
1:A:2897:LEU:HD21	1:A:2909:LEU:HB2	1.95	0.48
1:A:3035:GLU:O	1:A:3038:GLN:HG2	2.13	0.48
1:A:3113:MET:HE2	1:A:3115:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3196:GLU:O	1:A:3199:MET:HG3	2.12	0.48
1:A:3628:ARG:HB2	1:A:3669:ILE:HD11	1.95	0.48
1:A:3828:SER:HB3	1:A:4140:ARG:HG2	1.95	0.48
1:A:2580:LEU:HB3	1:A:2584:TRP:CZ3	2.47	0.48
1:A:3002:SER:O	1:A:3006:GLU:HG2	2.13	0.48
1:A:3202:ASN:O	1:A:3206:ARG:HG3	2.13	0.48
1:A:4153:VAL:O	1:A:4157:MET:HG3	2.13	0.48
1:A:2231:SER:HA	1:A:2234:TRP:CD1	2.49	0.48
1:A:2495:VAL:HG21	1:A:2524:VAL:HG21	1.95	0.48
1:A:3154:LEU:HD22	1:A:3516:TYR:CG	2.49	0.48
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.94	0.48
1:A:1680:GLU:OE1	1:A:1875:VAL:HG12	2.13	0.48
1:A:1907:PRO:HD2	1:A:2042:THR:HA	1.94	0.48
1:A:3152:GLN:HG2	1:A:3156:GLN:HE21	1.77	0.48
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.47	0.48
1:A:3826:GLN:OE1	1:A:4140:ARG:NH2	2.46	0.48
1:A:3932:ALA:O	1:A:3936:VAL:HG23	2.12	0.48
1:A:1638:LEU:HD23	1:A:1641:ILE:HD11	1.96	0.48
1:A:1958:ASP:O	1:A:2017:THR:OG1	2.31	0.48
1:A:2658:TRP:CE3	1:A:2705:ARG:HA	2.49	0.48
1:A:2837:LEU:HD13	1:A:2842:GLU:HB3	1.96	0.48
1:A:3031:THR:O	1:A:3035:GLU:HG2	2.14	0.48
1:A:1721:VAL:O	1:A:1725:GLU:HG2	2.14	0.48
1:A:3788:ASP:N	1:A:3788:ASP:OD1	2.46	0.47
1:A:2577:HIS:O	1:A:2581:LEU:HD23	2.13	0.47
1:A:3028:THR:O	1:A:3032:GLN:HG2	2.14	0.47
1:A:4303:GLU:O	1:A:4307:GLN:HG2	2.13	0.47
1:A:4395:LEU:HA	1:A:4490:GLN:NE2	2.28	0.47
1:A:1579:MET:HA	1:A:1582:VAL:HG12	1.95	0.47
1:A:2059:PHE:HE1	1:A:2101:GLY:HA2	1.79	0.47
1:A:2238:LEU:HD11	1:A:2249:GLY:HA3	1.96	0.47
1:A:2481:MET:SD	1:A:2485:GLN:HB3	2.55	0.47
1:A:2537:TYR:HA	1:A:2547:PRO:HA	1.96	0.47
1:A:4095:MET:HG2	1:A:4125:PHE:HB2	1.96	0.47
1:A:2518:ILE:O	1:A:2522:THR:HG22	2.14	0.47
1:A:3641:TYR:HE1	1:A:3645:LEU:HD23	1.80	0.47
1:A:3748:SER:HA	1:A:3751:GLN:CD	2.39	0.47
1:A:1533:LEU:HD11	1:A:1597:VAL:HG12	1.97	0.47
1:A:1892:MET:N	1:A:1892:MET:HE2	2.30	0.47
1:A:2209:GLN:O	1:A:2213:ILE:HG12	2.15	0.47
1:A:3514:ILE:HD11	1:A:3553:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4062:GLN:O	1:A:4064:THR:OG1	2.31	0.47
1:A:4169:ILE:HG13	1:A:4180:TYR:CD2	2.49	0.47
1:A:2783:ARG:HG2	1:A:2784:PHE:N	2.29	0.47
1:A:2852:THR:O	1:A:2856:LYS:HG2	2.14	0.47
1:A:3031:THR:O	1:A:3034:LYS:HG2	2.15	0.47
1:A:2203:TRP:O	1:A:2207:VAL:HG23	2.15	0.47
1:A:2441:PHE:HA	1:A:2449:LEU:HD23	1.97	0.47
1:A:3055:THR:O	1:A:3059:ILE:HG12	2.15	0.47
1:A:1647:VAL:HA	1:A:1650:LEU:HG	1.97	0.46
1:A:1803:LEU:HG	1:A:1807:LYS:HE3	1.96	0.46
1:A:3829:LEU:HG	1:A:3833:LEU:HD13	1.97	0.46
1:A:4630:GLU:HB3	1:A:4635:PHE:HE1	1.79	0.46
1:A:1501:ILE:HG12	1:A:1527:LEU:HB3	1.97	0.46
1:A:3724:VAL:HG21	1:A:3797:VAL:HG21	1.98	0.46
1:A:4176:ARG:NH1	1:A:4220:ASP:OD1	2.47	0.46
1:A:4495:ALA:HB1	1:A:4503:GLU:HB3	1.98	0.46
1:A:1903:SER:HA	1:A:2016:ILE:O	2.15	0.46
1:A:1729:LYS:HG3	1:A:1730:ALA:N	2.29	0.46
1:A:2439:HIS:O	1:A:2442:GLN:HG3	2.16	0.46
1:A:2492:ARG:NH1	1:A:2544:GLU:HA	2.31	0.46
1:A:3154:LEU:HD22	1:A:3516:TYR:CD2	2.51	0.46
1:A:4069:ILE:HD13	1:A:4079:GLN:HG3	1.97	0.46
1:A:2445:HIS:NE2	1:A:2449:LEU:HD22	2.30	0.46
1:A:1587:LEU:HB2	1:A:1590:ASP:HB2	1.97	0.46
1:A:1672:VAL:HA	1:A:1691:SER:HA	1.98	0.46
1:A:1711:VAL:O	1:A:1715:LYS:HG2	2.16	0.46
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	1.95	0.46
1:A:4117:GLN:OE1	1:A:4117:GLN:N	2.49	0.46
1:A:1981:ALA:HB2	1:A:1999:CYS:HB3	1.98	0.46
1:A:2191:LEU:HD22	3:A:4702:ATP:C5	2.50	0.46
1:A:2665:GLU:HB3	1:A:2668:LEU:HB2	1.97	0.46
1:A:3595:GLN:O	1:A:3598:GLU:HG2	2.16	0.46
1:A:4388:LEU:HD21	1:A:4431:LEU:HB3	1.97	0.46
1:A:4033:THR:O	1:A:4034:GLU:HG2	2.16	0.46
1:A:3892:LEU:HD13	1:A:3983:ILE:HG21	1.98	0.46
1:A:2935:LEU:HD12	1:A:3067:THR:HG22	1.98	0.46
1:A:4400:ARG:HH22	1:A:4405:ILE:HD11	1.81	0.46
1:A:1493:LEU:HD23	1:A:1534:PHE:CE2	2.51	0.45
1:A:2448:ASP:OD2	1:A:2725:HIS:NE2	2.49	0.45
1:A:1808:LEU:O	1:A:1812:ILE:HG13	2.16	0.45
1:A:2784:PHE:O	1:A:2792:TYR:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.49	0.45
1:A:3655:ARG:HB3	1:A:3660:VAL:HG12	1.98	0.45
1:A:4153:VAL:HG23	1:A:4316:GLN:NE2	2.31	0.45
1:A:4305:PHE:O	1:A:4309:VAL:HG23	2.16	0.45
1:A:4481:ASP:CG	1:A:4485:ARG:HE	2.25	0.45
1:A:2383:ARG:NH2	1:A:2424:GLN:OE1	2.50	0.45
1:A:3843:ASN:ND2	1:A:3862:ASP:OD2	2.46	0.45
1:A:1522:SER:HA	1:A:1525:ASP:OD2	2.16	0.45
1:A:2599:SER:OG	1:A:2601:LYS:NZ	2.48	0.45
1:A:1822:THR:O	1:A:1827:LYS:HG2	2.16	0.45
1:A:4166:VAL:HA	1:A:4169:ILE:HG22	1.98	0.45
1:A:2820:GLY:HA2	1:A:2823:ARG:HG2	1.98	0.45
1:A:3128:VAL:HB	1:A:3145:ASN:OD1	2.16	0.45
1:A:2865:LYS:HG3	1:A:2866:ALA:H	1.81	0.45
1:A:1508:LYS:HA	1:A:1508:LYS:HD2	1.70	0.44
1:A:1649:LYS:O	1:A:1652:LYS:HG2	2.17	0.44
1:A:1682:GLU:OE1	1:A:1872:TYR:OH	2.25	0.44
1:A:2300:TRP:CD2	1:A:2342:MET:HE1	2.52	0.44
1:A:1470:TRP:HH2	1:A:1497:VAL:HG22	1.82	0.44
1:A:3510:SER:HB3	1:A:3553:LEU:HD11	2.00	0.44
1:A:3748:SER:HA	1:A:3751:GLN:NE2	2.32	0.44
1:A:3768:THR:O	1:A:3771:GLU:HG2	2.17	0.44
1:A:4235:PRO:HB3	1:A:4278:PHE:CD1	2.52	0.44
1:A:1497:VAL:O	1:A:1501:ILE:HG13	2.17	0.44
1:A:2616:GLU:HG3	1:A:2657:LYS:HB3	1.99	0.44
1:A:1626:PHE:CE2	1:A:1628:ARG:HB2	2.52	0.44
1:A:1917:LYS:HE2	1:A:1929:VAL:HG21	1.99	0.44
1:A:1979:GLN:HG2	1:A:2035:LEU:HB3	2.00	0.44
1:A:2071:PRO:O	1:A:2075:LEU:HG	2.18	0.44
1:A:2798:GLU:OE2	1:A:2836:ARG:NH1	2.50	0.44
1:A:3219:ARG:NH2	1:A:3479:LEU:HD21	2.32	0.44
1:A:3721:ARG:HH22	1:A:3723:ASP:HB3	1.82	0.44
1:A:2257:LYS:HA	1:A:2257:LYS:HD2	1.76	0.44
1:A:2369:LEU:HD12	1:A:2373:MET:HE3	2.00	0.44
1:A:2511:ARG:HB3	1:A:2535:ILE:HG12	1.99	0.44
1:A:3012:LEU:HD13	1:A:3089:CYS:SG	2.57	0.44
1:A:2382:LEU:HD22	1:A:2420:ALA:HB2	2.00	0.44
1:A:4088:VAL:O	1:A:4118:PRO:HG2	2.18	0.44
1:A:4503:GLU:N	1:A:4503:GLU:OE1	2.51	0.44
1:A:3740:LEU:O	1:A:3744:GLN:HG2	2.18	0.44
1:A:4378:ARG:HA	1:A:4378:ARG:HD3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2751:PHE:HB3	1:A:2803:VAL:HG11	1.99	0.44
1:A:2759:ILE:HG23	1:A:2762:LEU:HB2	2.00	0.44
1:A:4301:ARG:NH1	1:A:4303:GLU:OE1	2.51	0.44
1:A:1736:ASN:OD1	1:A:1737:THR:N	2.51	0.44
1:A:1538:ILE:O	1:A:1542:ARG:HG2	2.18	0.43
1:A:3784:VAL:HA	1:A:3787:THR:HG23	2.00	0.43
1:A:1746:GLN:HB2	1:A:1749:LEU:HD12	2.00	0.43
1:A:1806:ARG:HG3	1:A:1806:ARG:NH1	2.34	0.43
1:A:2284:LEU:HD12	1:A:2284:LEU:HA	1.90	0.43
1:A:2787:ASP:OD1	1:A:2788:THR:N	2.51	0.43
1:A:4264:LEU:HD13	1:A:4637:GLU:HA	2.00	0.43
1:A:4460:LEU:HA	1:A:4475:VAL:HG22	1.98	0.43
1:A:1550:ILE:HD12	1:A:1638:LEU:HD13	2.00	0.43
1:A:3011:LEU:HD13	1:A:3017:VAL:HG23	2.00	0.43
1:A:3556:ALA:HB2	1:A:3737:GLU:CD	2.43	0.43
1:A:2181:GLU:HA	1:A:2184:LYS:HD2	2.00	0.43
1:A:2704:GLU:HG2	1:A:2705:ARG:HG3	1.99	0.43
1:A:2912:PHE:HE2	1:A:2914:GLU:HB2	1.84	0.43
1:A:4240:TRP:HZ2	1:A:4278:PHE:HE1	1.65	0.43
1:A:1844:PHE:HZ	1:A:1922:GLN:HE21	1.66	0.43
1:A:1998:THR:HG22	1:A:2007:LYS:HA	2.01	0.43
1:A:2227:GLY:HA2	1:A:2452:LEU:HD12	2.00	0.43
1:A:2963:VAL:HG11	1:A:2998:ASN:HA	1.99	0.43
1:A:3808:CYS:HG	1:A:3836:TYR:HE1	1.62	0.43
1:A:1463:LEU:HD21	1:A:1523:TRP:CD1	2.54	0.43
1:A:1937:ASP:OD1	1:A:1937:ASP:N	2.50	0.43
1:A:3566:SER:O	1:A:3595:GLN:NE2	2.51	0.43
1:A:2465:ALA:HB2	1:A:2493:TYR:CE1	2.54	0.43
1:A:2841:GLU:O	1:A:2844:ARG:HG2	2.19	0.43
1:A:3174:ARG:NH2	2:A:4704:ADP:H5'1	2.34	0.43
1:A:3913:GLU:HB3	1:A:4476:ILE:HD12	2.01	0.43
1:A:4093:TRP:HB3	1:A:4125:PHE:HE2	1.83	0.43
1:A:1536:VAL:HG12	1:A:1601:LEU:HG	1.99	0.43
1:A:1603:ARG:HH12	1:A:1604:LEU:HD23	1.83	0.43
1:A:1880:VAL:HG21	1:A:2052:VAL:HG21	2.01	0.43
1:A:2275:TRP:CH2	1:A:2328:PRO:HD2	2.54	0.43
1:A:2454:CYS:SG	1:A:2502:LEU:HG	2.59	0.43
1:A:2538:GLU:HB2	1:A:2548:TRP:CE2	2.53	0.43
1:A:2743:SER:O	1:A:2747:ILE:HG12	2.18	0.43
1:A:4042:LEU:HD13	1:A:4142:GLY:HA3	2.01	0.43
1:A:4282:PHE:HD2	1:A:4296:MET:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2288:ILE:HD13	1:A:2336:PRO:HD3	2.01	0.43
1:A:2452:LEU:HD23	1:A:2452:LEU:HA	1.79	0.43
1:A:4139:LEU:HB3	1:A:4144:ILE:HD11	1.99	0.43
1:A:1678:SER:OG	1:A:1679:ARG:N	2.51	0.43
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.50	0.43
1:A:2453:ARG:HH11	1:A:2728:LEU:HD11	1.84	0.42
1:A:3654:ARG:HB2	1:A:3661:LEU:HG	2.01	0.42
1:A:4400:ARG:NH2	1:A:4405:ILE:HD11	2.33	0.42
1:A:2220:LEU:O	1:A:2342:MET:HA	2.20	0.42
1:A:2972:PHE:CZ	1:A:3008:MET:HE3	2.54	0.42
1:A:3488:ARG:HG2	1:A:3491:LYS:HE3	2.00	0.42
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	2.01	0.42
1:A:4098:ASN:N	1:A:4127:THR:O	2.52	0.42
1:A:4283:LYS:HD2	1:A:4293:ASP:HB3	2.00	0.42
1:A:2670:ASP:HA	1:A:2721:LYS:HD3	2.02	0.42
1:A:2867:MET:HE2	1:A:2871:ILE:HA	2.01	0.42
1:A:3043:MET:N	1:A:3043:MET:SD	2.92	0.42
1:A:3846:LEU:HD11	1:A:3859:ILE:HG12	2.01	0.42
1:A:3872:ALA:HB1	1:A:3880:HIS:NE2	2.34	0.42
1:A:1887:ARG:HG3	1:A:2039:LEU:HD11	2.01	0.42
1:A:2369:LEU:HD12	1:A:2373:MET:CE	2.50	0.42
1:A:2603:MET:HG3	3:A:4703:ATP:H2'	2.01	0.42
1:A:2641:TYR:CE1	1:A:2650:LEU:HD13	2.54	0.42
1:A:2775:GLU:OE1	1:A:2779:MET:HE1	2.19	0.42
1:A:4260:PHE:CE2	1:A:4608:PRO:HB3	2.55	0.42
1:A:1574:GLU:HB2	1:A:1604:LEU:HD21	2.01	0.42
1:A:1905:PHE:HB3	1:A:2018:MET:HB2	2.01	0.42
1:A:2307:VAL:HG23	1:A:2351:ALA:HB2	2.02	0.42
1:A:4439:GLU:HB3	1:A:4441:LYS:HZ3	1.84	0.42
1:A:2661:LEU:HD12	1:A:2708:PHE:CE2	2.55	0.42
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.54	0.42
1:A:4226:THR:HG21	1:A:4239:PRO:HD3	2.02	0.42
1:A:4277:SER:HA	1:A:4282:PHE:CG	2.55	0.42
1:A:4375:ALA:O	1:A:4379:THR:HG23	2.20	0.42
1:A:1809:GLU:HG3	1:A:2056:SER:HB2	2.01	0.42
1:A:2373:MET:SD	3:A:4702:ATP:N6	2.93	0.42
1:A:4106:LEU:HD12	1:A:4138:LEU:HD22	2.02	0.42
1:A:1470:TRP:CH2	1:A:1497:VAL:HG22	2.54	0.42
1:A:2074:LYS:HE3	1:A:2074:LYS:HB3	1.84	0.42
1:A:3030:MET:HA	1:A:3030:MET:HE3	2.02	0.42
1:A:3492:THR:HA	1:A:3495:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1853:VAL:HG13	1:A:1854:LEU:HG	2.01	0.42
1:A:1872:TYR:CZ	1:A:1874:GLY:HA2	2.55	0.42
1:A:3475:SER:O	1:A:3479:LEU:HD23	2.20	0.42
1:A:2527:PRO:HG2	1:A:2534:ILE:HG23	2.01	0.41
1:A:2777:TYR:HE1	1:A:2794:TYR:HB3	1.83	0.41
1:A:3985:GLN:HE21	1:A:3989:ARG:HH22	1.68	0.41
1:A:4149:PRO:HA	1:A:4150:PRO:HD3	1.95	0.41
1:A:1685:MET:HE2	1:A:1685:MET:HA	2.02	0.41
1:A:3151:HIS:HA	1:A:3516:TYR:HE2	1.85	0.41
1:A:3203:VAL:HG22	1:A:3206:ARG:HH21	1.85	0.41
1:A:4157:MET:HE2	1:A:4309:VAL:HG22	2.02	0.41
1:A:4492:ILE:HG12	1:A:4507:ILE:HD12	2.02	0.41
1:A:2336:PRO:HG2	1:A:2339:VAL:HG23	2.01	0.41
1:A:2529:ALA:HB3	1:A:2537:TYR:OH	2.20	0.41
1:A:2930:GLN:NE2	1:A:3059:ILE:HA	2.22	0.41
1:A:3126:MET:N	1:A:3127:PRO:HD3	2.35	0.41
1:A:2772:ALA:HA	1:A:2857:HIS:CE1	2.55	0.41
1:A:1546:TYR:O	1:A:1550:ILE:HG12	2.20	0.41
1:A:3488:ARG:NH2	1:A:3742:LEU:HG	2.35	0.41
1:A:1464:LYS:HG3	1:A:1467:ARG:NH1	2.36	0.41
1:A:2079:GLN:HG3	1:A:2160:LEU:HD21	2.02	0.41
1:A:2191:LEU:HD22	3:A:4702:ATP:C6	2.56	0.41
1:A:2309:PRO:HG3	1:A:2352:THR:HG23	2.02	0.41
1:A:2453:ARG:HD3	1:A:2728:LEU:HG	2.02	0.41
1:A:3985:GLN:HE21	1:A:3989:ARG:NH2	2.18	0.41
1:A:1480:TYR:CD1	1:A:2272:THR:HG23	2.56	0.41
1:A:2325:LEU:N	1:A:2333:LEU:O	2.54	0.41
1:A:3005:LEU:HD12	1:A:3005:LEU:HA	1.89	0.41
1:A:3609:ILE:HB	1:A:3632:PRO:HG2	2.03	0.41
1:A:4117:GLN:HG2	1:A:4117:GLN:O	2.19	0.41
1:A:4554:ASP:C	1:A:4556:CYS:H	2.29	0.41
1:A:1829:LYS:HA	1:A:1829:LYS:HD3	1.90	0.41
1:A:2067:ASN:O	1:A:4537:GLU:HG2	2.20	0.41
1:A:2413:LEU:HD23	1:A:2413:LEU:HA	1.95	0.41
1:A:2824:ILE:O	1:A:2828:GLU:HG2	2.20	0.41
1:A:1698:ILE:HA	1:A:1701:TRP:NE1	2.36	0.41
1:A:2076:CYS:HB3	1:A:2088:PHE:CE1	2.56	0.41
1:A:2445:HIS:CD2	1:A:2449:LEU:HD22	2.56	0.41
1:A:2930:GLN:OE1	1:A:2932:HIS:NE2	2.33	0.41
1:A:3948:ILE:O	1:A:3952:GLN:HG2	2.21	0.41
1:A:4192:GLU:OE2	1:A:4195:ARG:NH2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4481:ASP:O	1:A:4485:ARG:HG3	2.21	0.41
1:A:4535:SER:HB3	1:A:4538:GLU:HG3	2.03	0.41
1:A:4619:ILE:HG22	1:A:4620:PHE:HD1	1.86	0.41
1:A:1494:PHE:CZ	1:A:1534:PHE:HB3	2.56	0.41
1:A:3941:LEU:HD23	1:A:3944:PHE:HD2	1.86	0.41
1:A:3738:PHE:HE2	1:A:3783:LYS:HD2	1.85	0.40
1:A:3791:MET:O	1:A:3795:GLU:OE1	2.40	0.40
1:A:1608:LEU:HA	1:A:1611:ILE:HG22	2.03	0.40
1:A:4030:ILE:HG21	1:A:4145:PHE:HZ	1.85	0.40
1:A:1480:TYR:HD1	1:A:2272:THR:HG23	1.86	0.40
1:A:2291:VAL:O	1:A:2292:ARG:HD2	2.20	0.40
1:A:2744:LEU:HA	1:A:2747:ILE:HG12	2.02	0.40
1:A:3769:THR:O	1:A:3773:LEU:HD23	2.22	0.40
1:A:3938:LEU:HD22	1:A:3995:ALA:HB2	2.03	0.40
1:A:1512:TYR:N	1:A:3659:ARG:HH22	2.19	0.40
1:A:1803:LEU:O	1:A:1807:LYS:HG3	2.22	0.40
1:A:3916:LEU:HD13	1:A:3936:VAL:HG12	2.04	0.40
1:A:1714:ALA:HB2	1:A:1853:VAL:HG23	2.04	0.40
1:A:2801:ARG:HH21	1:A:3088:ARG:H	1.70	0.40
1:A:2921:ARG:O	1:A:2925:ILE:HG12	2.21	0.40
1:A:2985:CYS:SG	1:A:2986:LYS:N	2.94	0.40
1:A:3611:ARG:NH1	1:A:3636:GLN:HE22	2.18	0.40
1:A:4078:ASN:O	1:A:4082:LYS:HD3	2.21	0.40
1:A:4485:ARG:HA	1:A:4488:GLN:HG2	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	2841/4646 (61%)	2759 (97%)	78 (3%)	4 (0%)	48 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	1730	ALA
1	A	2871	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2540/4125 (62%)	2540 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1541	GLN
1	A	1595	GLN
1	A	1598	GLN
1	A	1643	ASN
1	A	1695	HIS
1	A	1748	GLN
1	A	1922	GLN
1	A	1979	GLN
1	A	2005	GLN
1	A	2282	HIS
1	A	2346	GLN
1	A	2677	GLN
1	A	2689	HIS
1	A	2713	ASN
1	A	3032	GLN
1	A	3069	ASN
1	A	3104	GLN
1	A	3152	GLN
1	A	3526	GLN

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Mol	Chain	Res	Type
1	A	3667	GLN
1	A	3744	GLN
1	A	3754	ASN
1	A	3820	GLN
1	A	3843	ASN
1	A	3985	GLN
1	A	4038	ASN
1	A	4062	GLN
1	A	4079	GLN
1	A	4108	GLN
1	A	4117	GLN
1	A	4249	GLN
1	A	4386	ASN
1	A	4530	GLN
1	A	4595	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)
3	ATP	A	4702	-	32,33,33	0.29	0	48,52,52	0.28	0
2	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
3	ATP	A	4703	-	32,33,33	0.28	0	48,52,52	0.28	0

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
2	ADP	A	4701	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4702	-	-	9/22/38/38	0/3/3/3
2	ADP	A	4704	-	-	4/16/32/32	0/3/3/3
3	ATP	A	4703	-	-	3/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4704	ADP	C5-C4	4.60	1.47	1.39
2	A	4701	ADP	C5-C4	4.58	1.47	1.39
2	A	4704	ADP	C5-C6	2.70	1.48	1.41
2	A	4701	ADP	C5-C6	2.67	1.48	1.41
2	A	4704	ADP	C8-N7	2.39	1.36	1.31
2	A	4704	ADP	C5-N7	-2.35	1.34	1.39
2	A	4701	ADP	C8-N7	2.32	1.36	1.31
2	A	4701	ADP	C5-N7	-2.29	1.34	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	C5-C4-N3	-5.74	118.81	126.72
2	A	4701	ADP	C5-C4-N3	-5.72	118.84	126.72
2	A	4701	ADP	N3-C4-N9	4.51	134.83	127.17
2	A	4704	ADP	N3-C4-N9	4.51	134.83	127.17
2	A	4704	ADP	C2-N3-C4	3.68	120.83	111.83
2	A	4701	ADP	C2-N3-C4	3.64	120.73	111.83
2	A	4701	ADP	C4-C5-N7	-3.49	106.59	110.58
2	A	4704	ADP	C4-C5-N7	-3.46	106.63	110.58
2	A	4704	ADP	N3-C2-N1	-3.24	123.68	128.58
2	A	4701	ADP	N3-C2-N1	-3.19	123.75	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C4-N9-C8	2.69	108.56	105.74
2	A	4704	ADP	C4-N9-C8	2.68	108.55	105.74
2	A	4701	ADP	C5-N7-C8	2.53	107.43	103.45
2	A	4704	ADP	C5-N7-C8	2.48	107.35	103.45
2	A	4704	ADP	C6-C5-N7	2.14	136.21	132.09
2	A	4701	ADP	C6-C5-N7	2.09	136.12	132.09
2	A	4704	ADP	C3'-C2'-C1'	2.08	105.40	101.46
2	A	4701	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 7 short contacts:

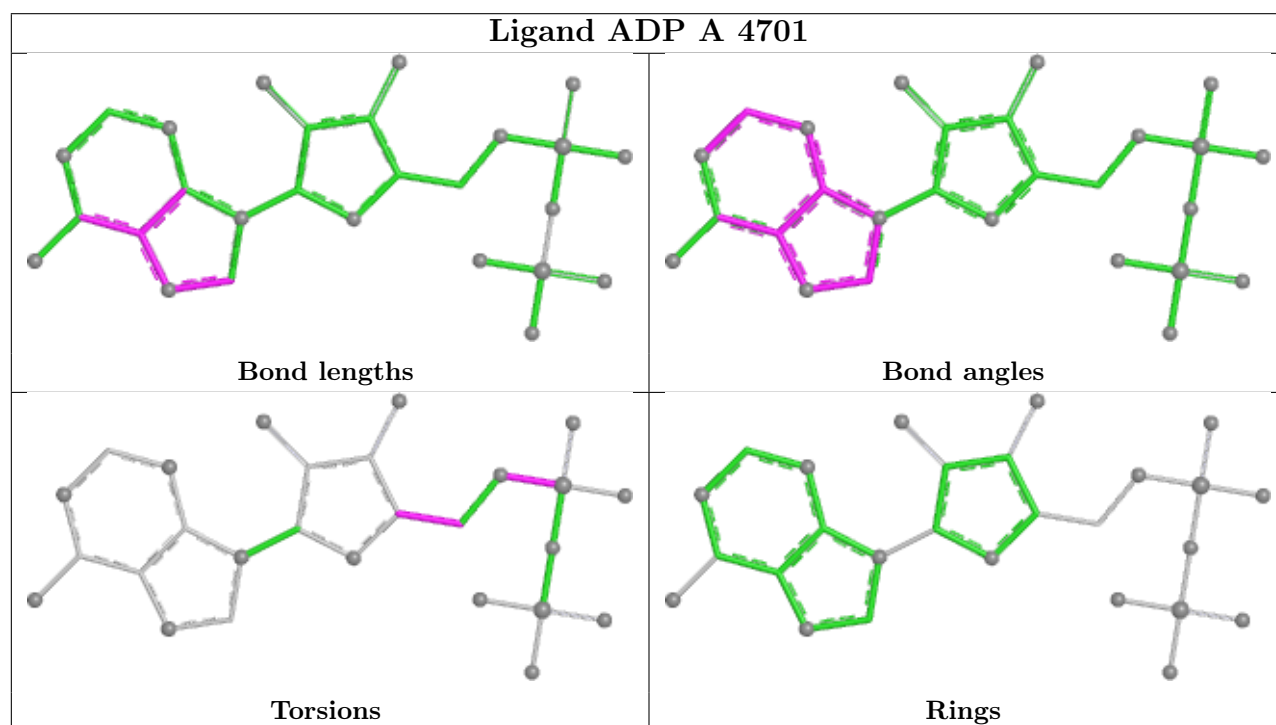
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	0
3	A	4702	ATP	4	0
2	A	4704	ADP	1	0

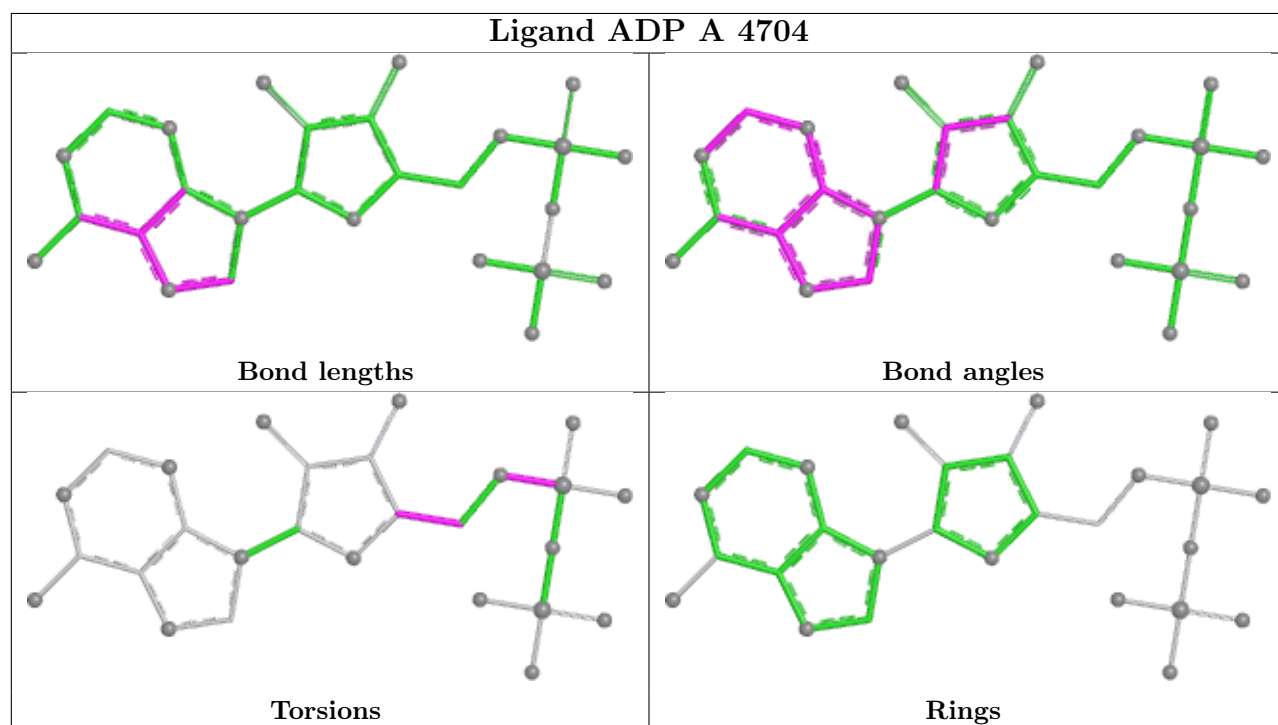
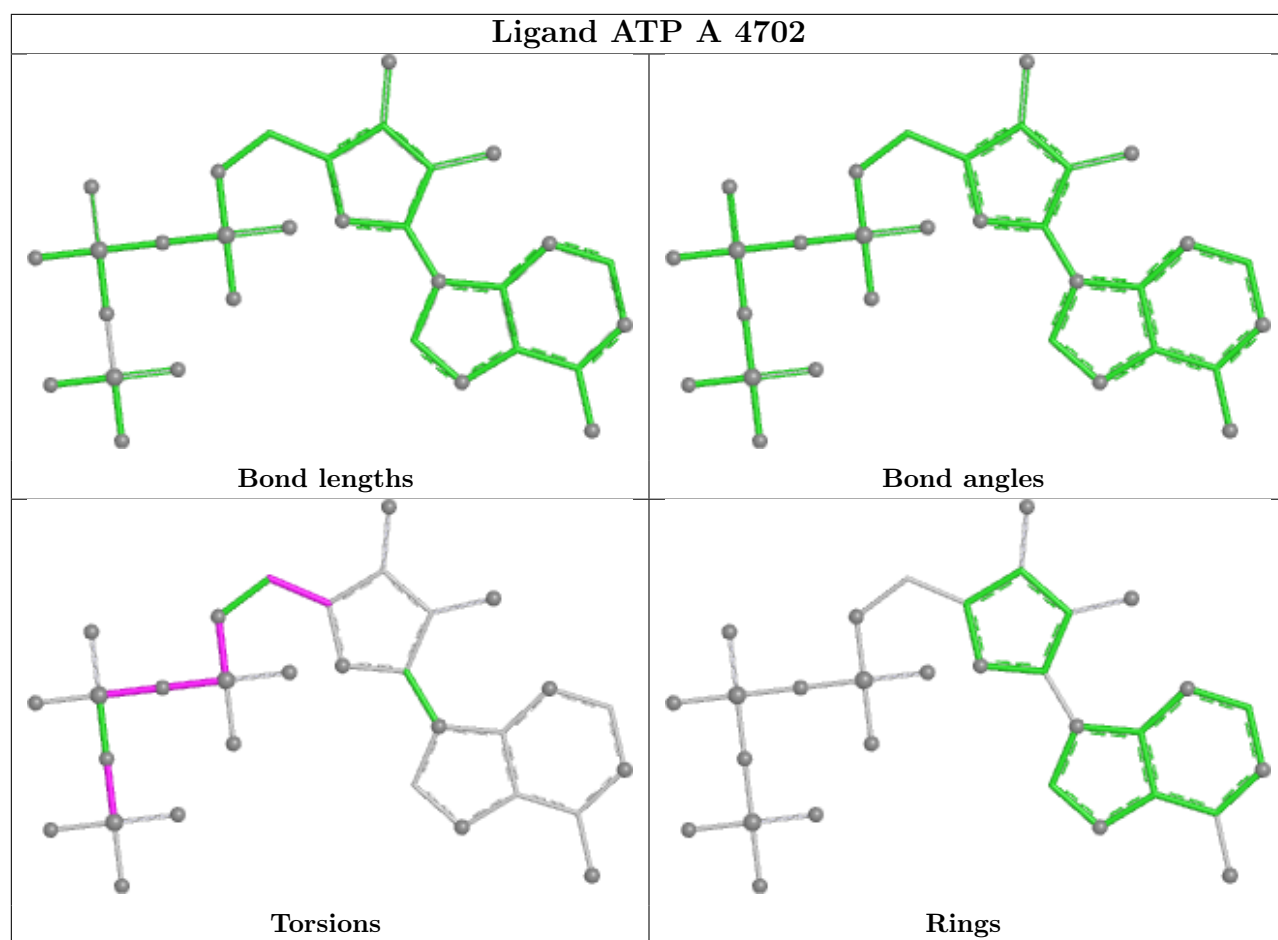
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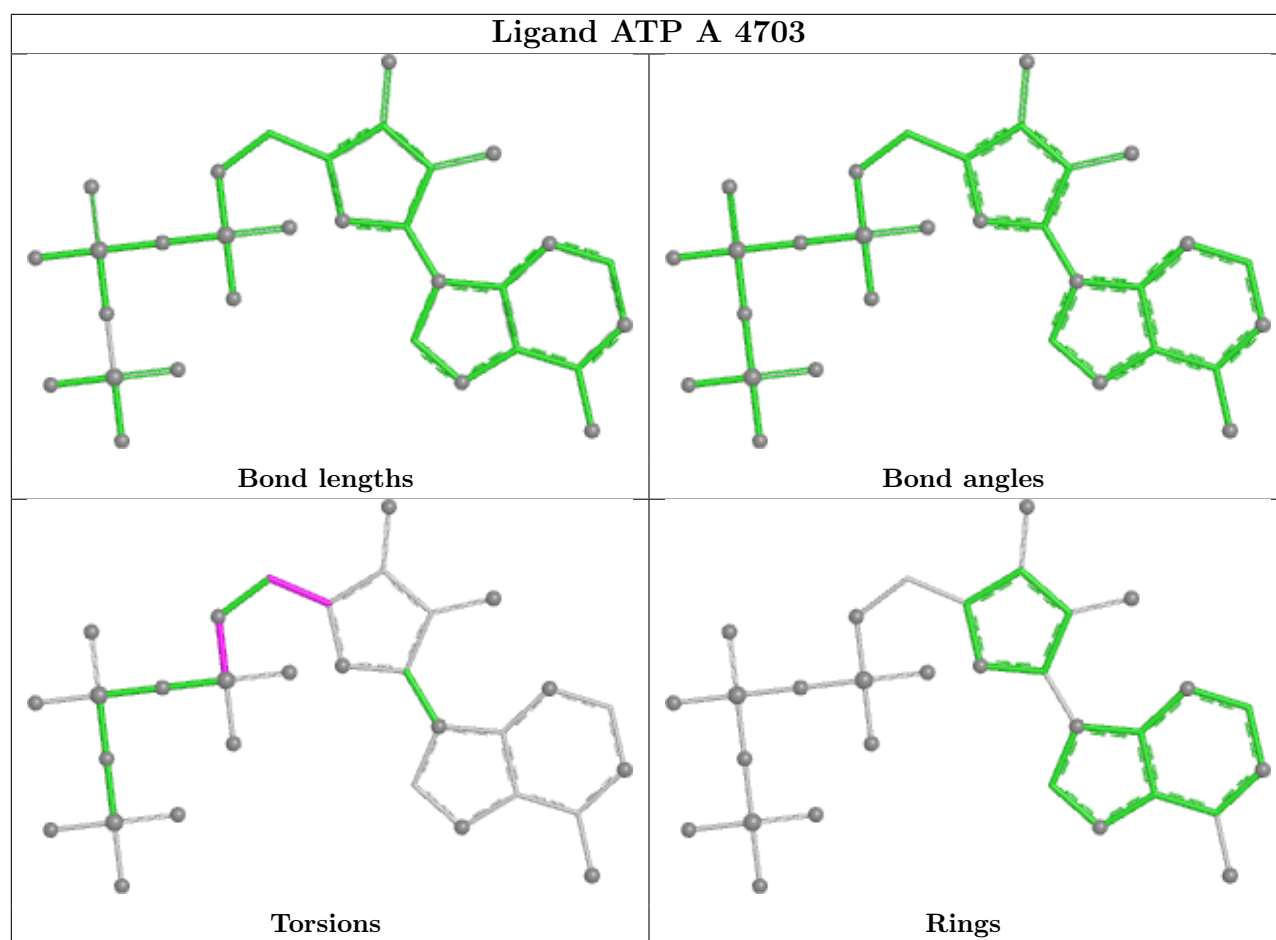
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4703	ATP	1	0

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.







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.

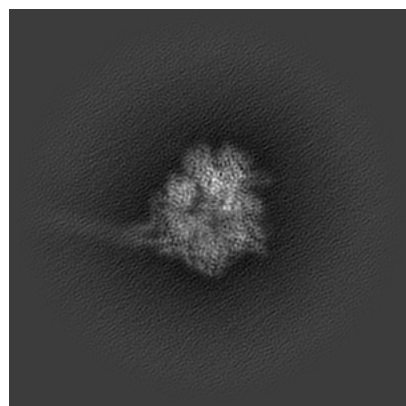
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44723. These allow visual inspection of the internal detail of the map and identification of artifacts.

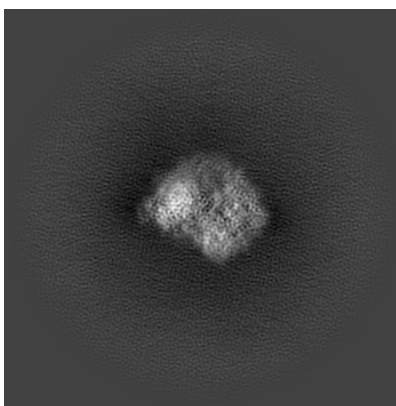
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

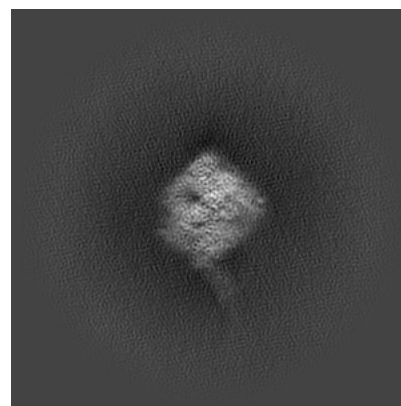
6.1.1 Primary map



X

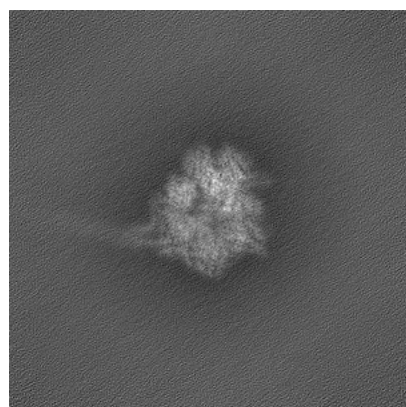


Y

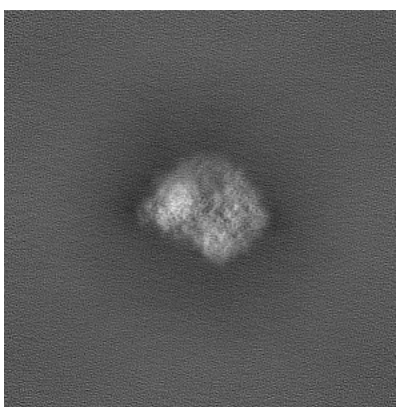


Z

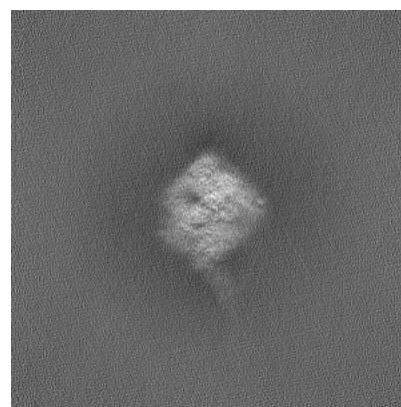
6.1.2 Raw map



X



Y

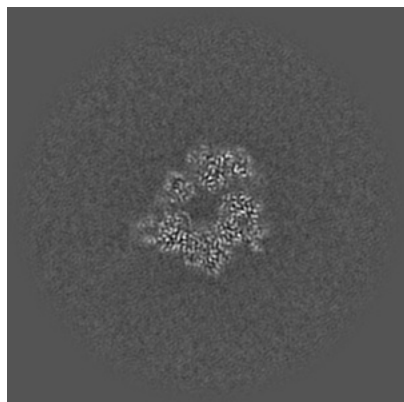


Z

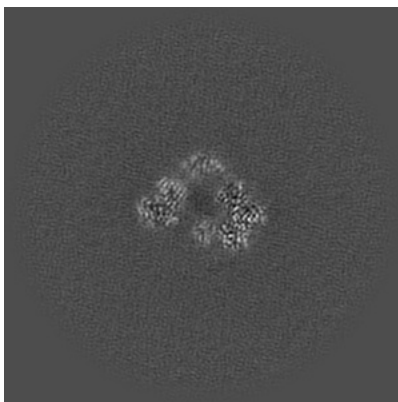
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

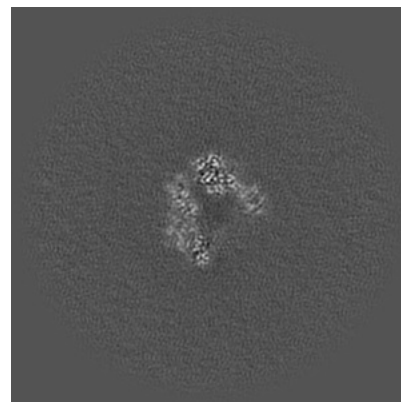
6.2.1 Primary map



X Index: 180

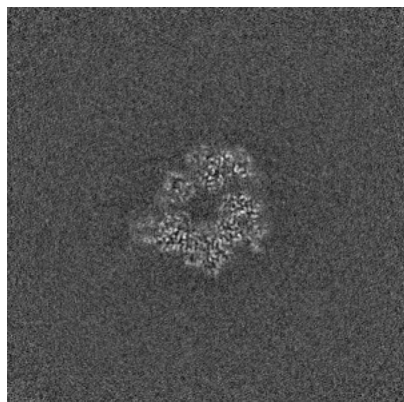


Y Index: 180

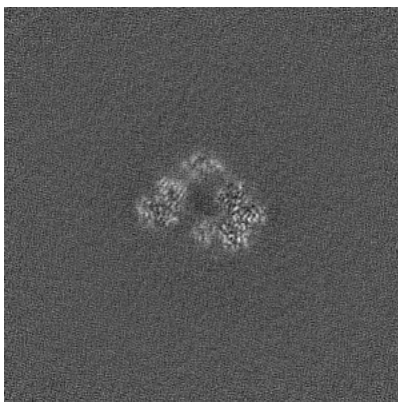


Z Index: 180

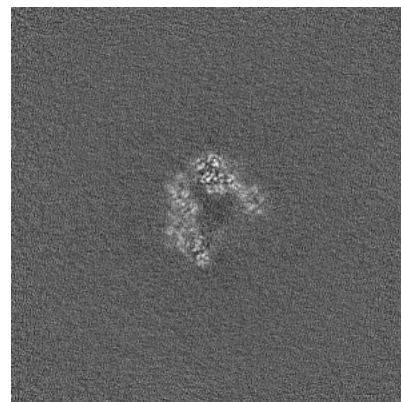
6.2.2 Raw map



X Index: 180



Y Index: 180

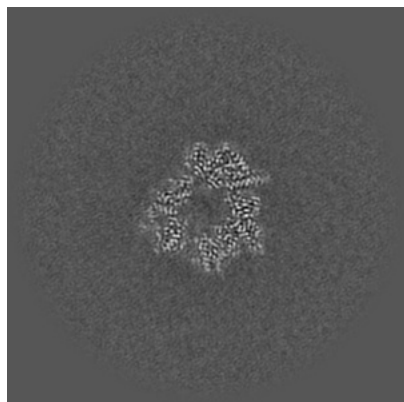


Z Index: 180

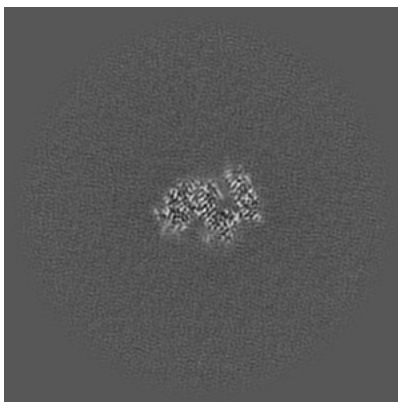
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

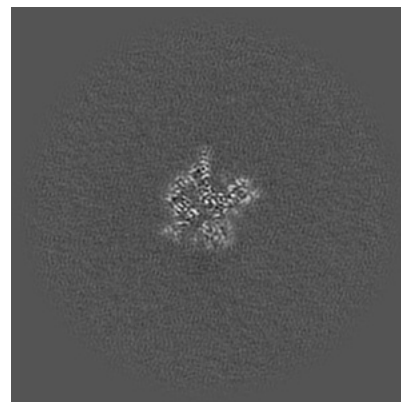
6.3.1 Primary map



X Index: 174

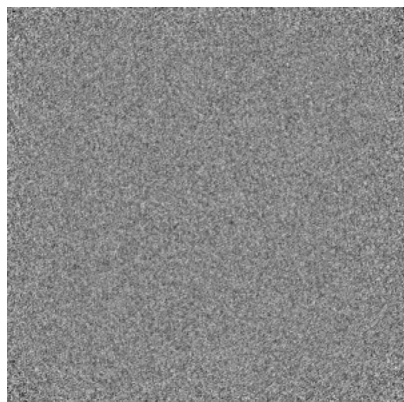


Y Index: 204

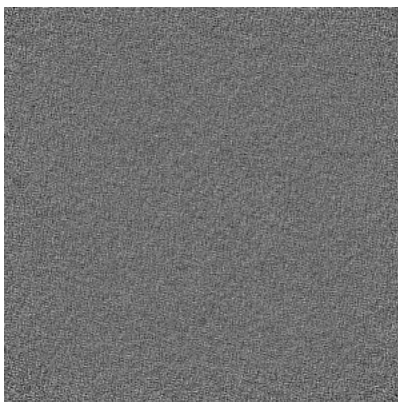


Z Index: 202

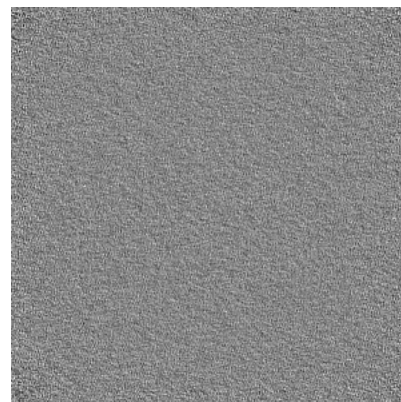
6.3.2 Raw map



X Index: 0



Y Index: 0

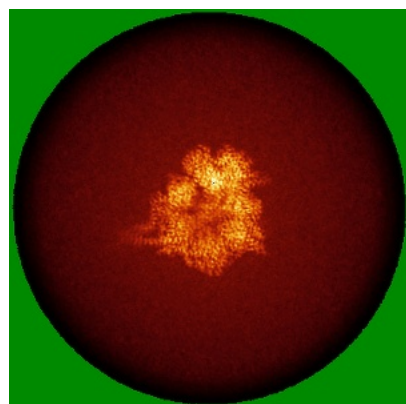


Z Index: 0

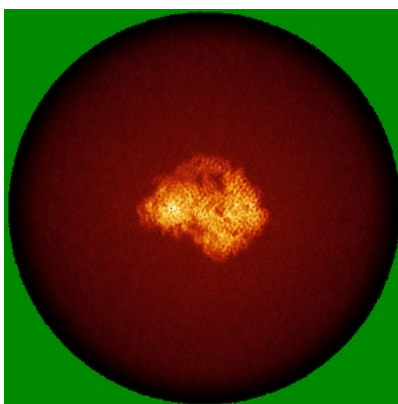
The images above show the largest variance slices of the map in three orthogonal directions.

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

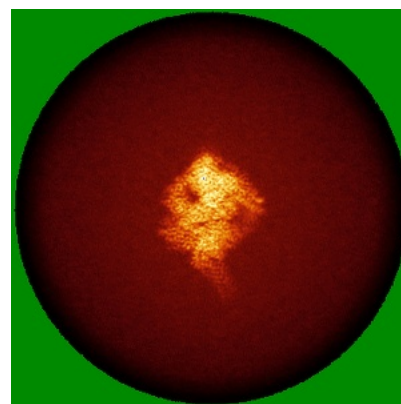
6.4.1 Primary map



X

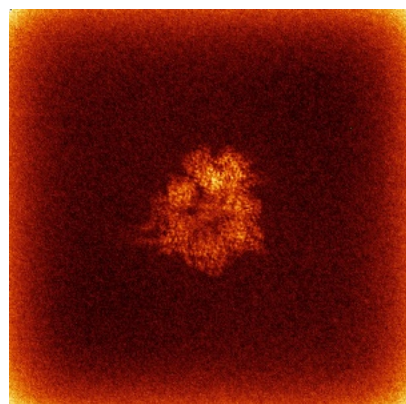


Y

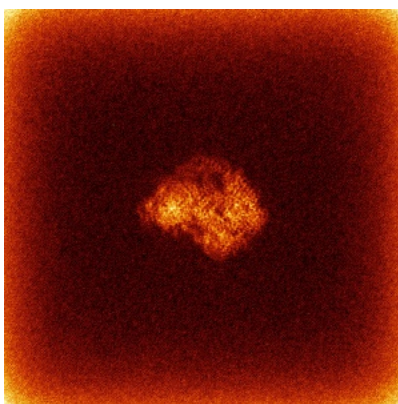


Z

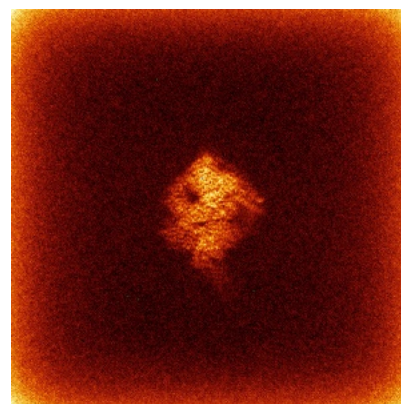
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

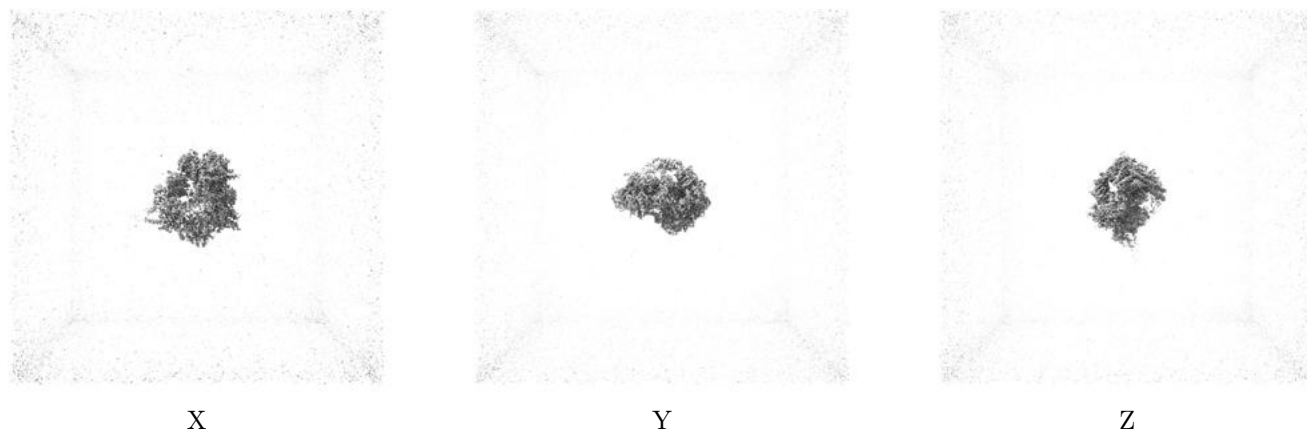
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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



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.

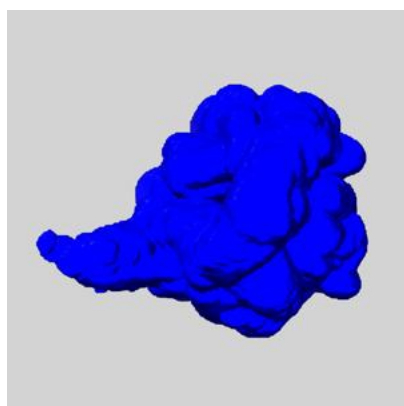
6.6 Mask visualisation [i](#)

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

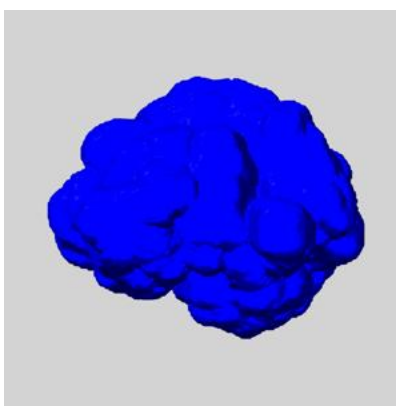
A mask typically either:

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

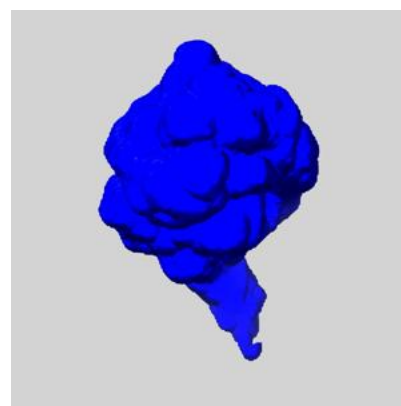
6.6.1 emd_44723_msk_1.map [i](#)



X



Y

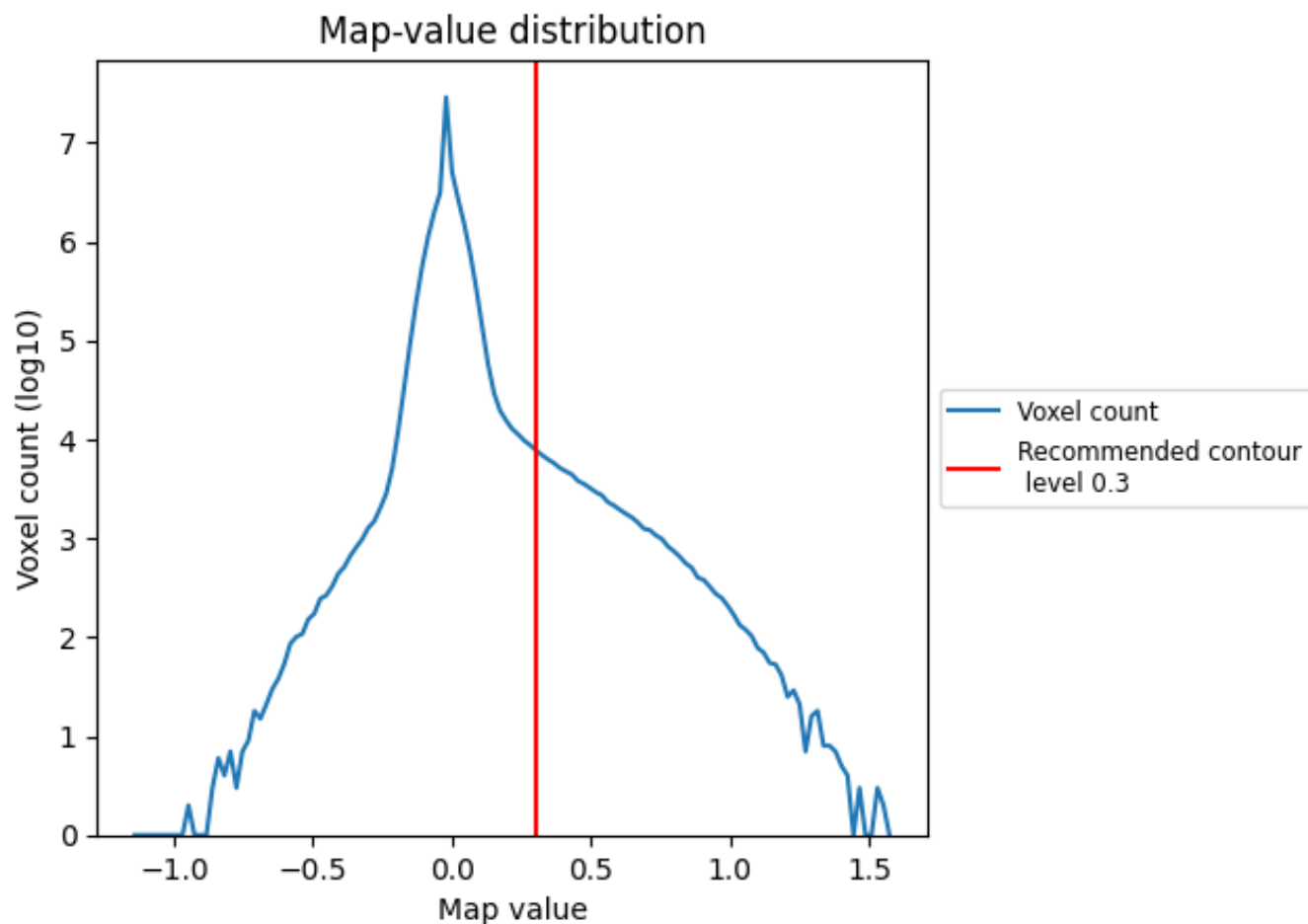


Z

7 Map analysis [i](#)

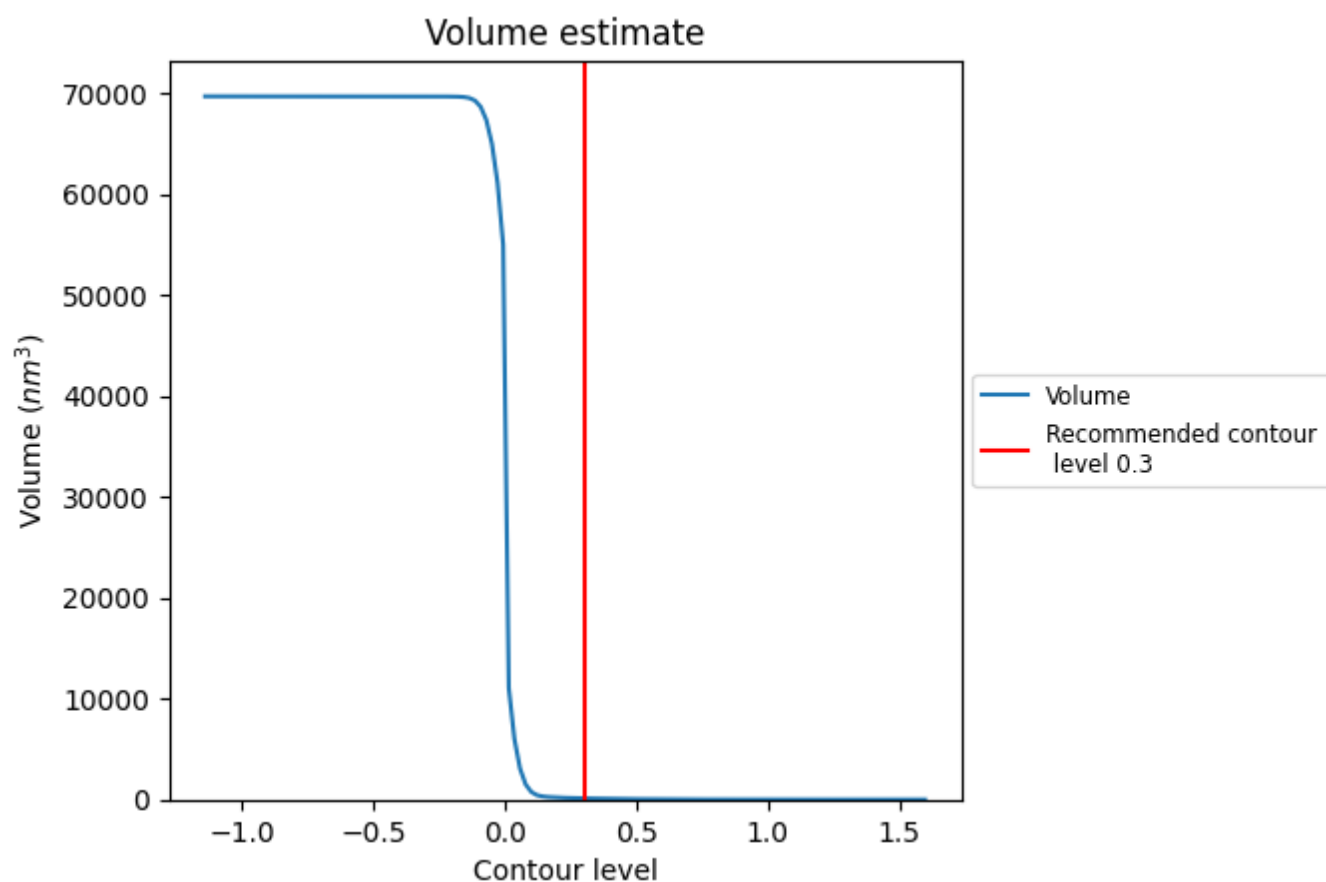
This section contains the results of statistical analysis of the map.

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.

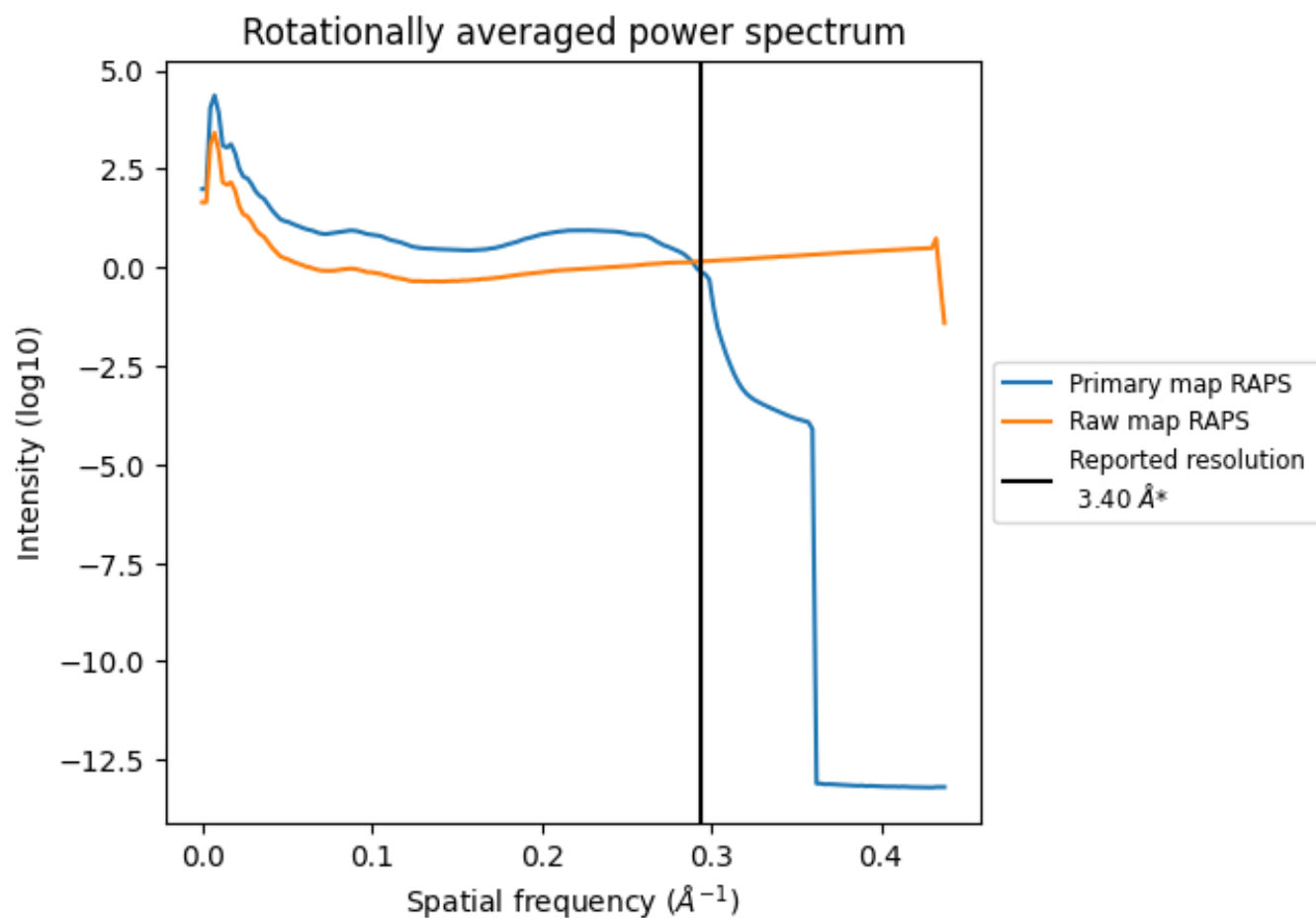
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 109 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 ⓘ

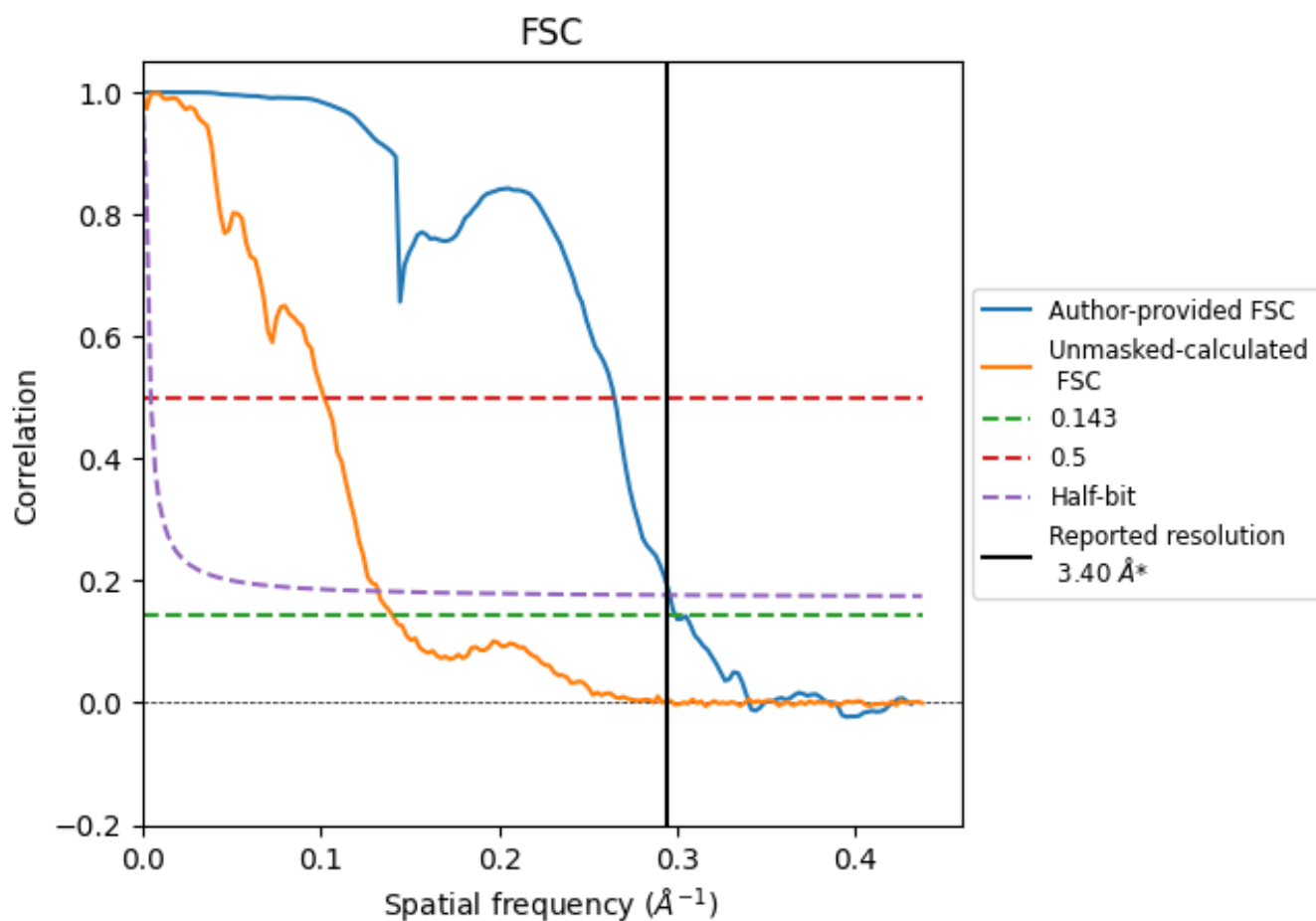


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

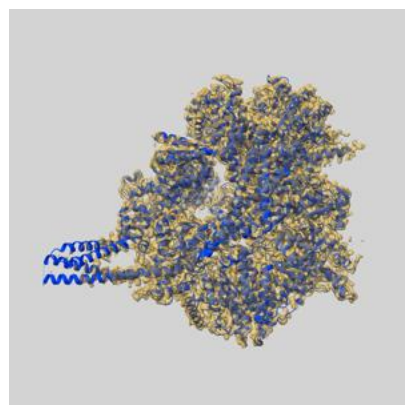
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.78	3.38
Unmasked-calculated*	7.12	9.80	7.56

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

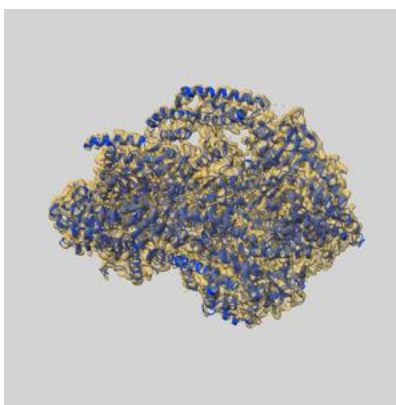
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44723 and PDB model 9BN6. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

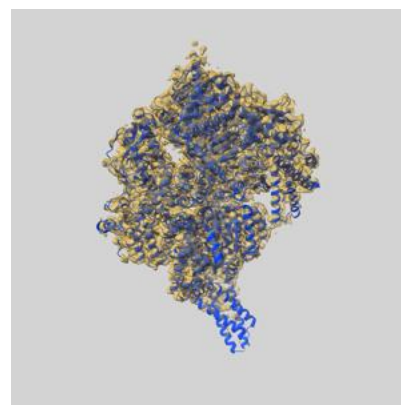
9.1 Map-model overlay [i](#)



X



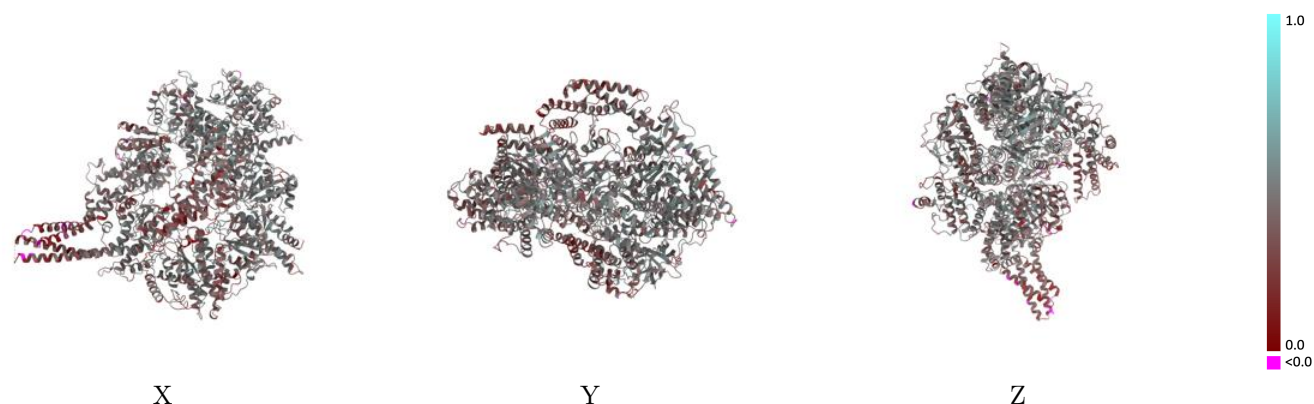
Y



Z

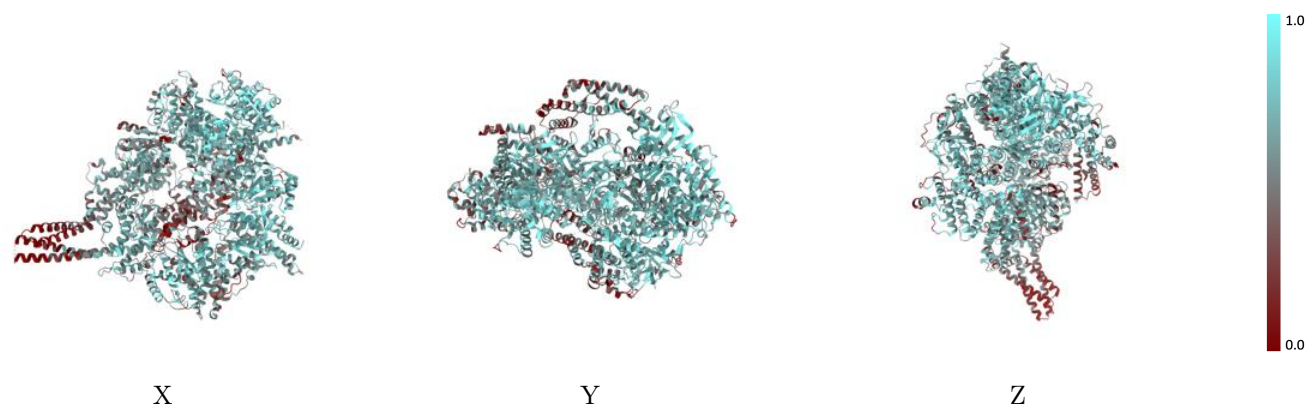
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



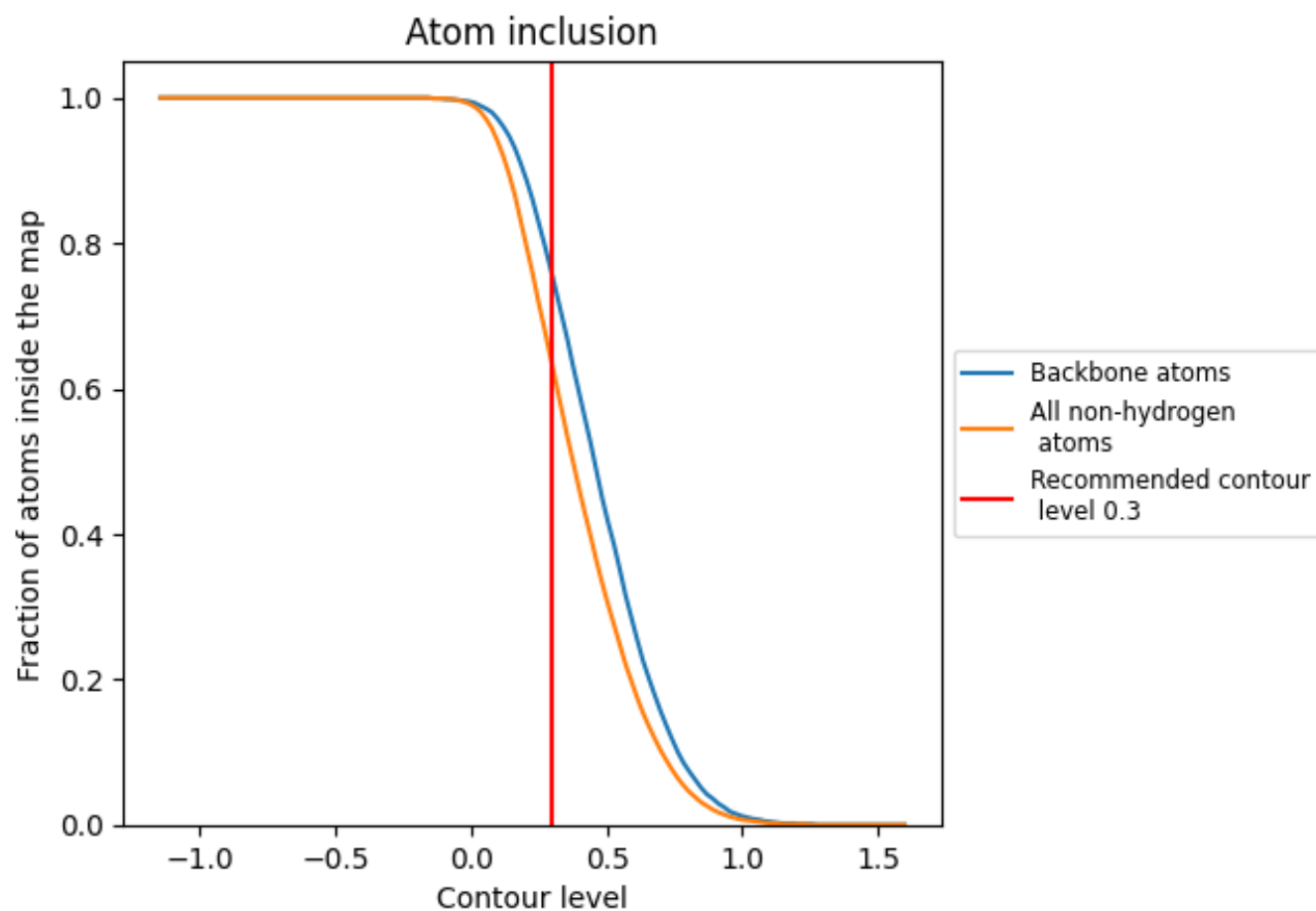
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 76% of all backbone atoms, 63% 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	0.6320	0.4100
A	0.6320	0.4100

