



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 5NUG / pdb_00005nug
EMDB ID : EMD-3698
Title : Motor domains from human cytoplasmic dynein-1 in the phi-particle conformation
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on : 2017-04-30
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
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 : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

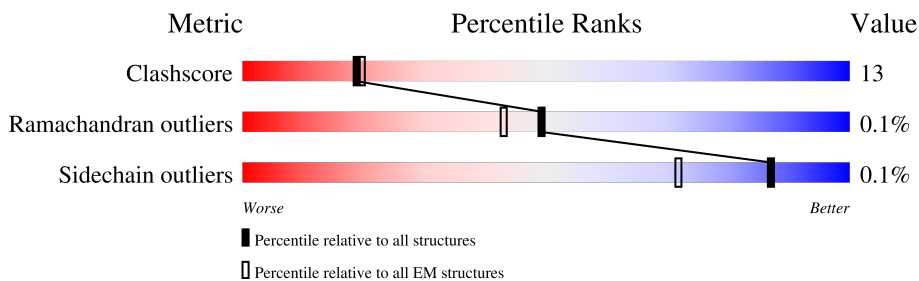
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	
1	B	4646	

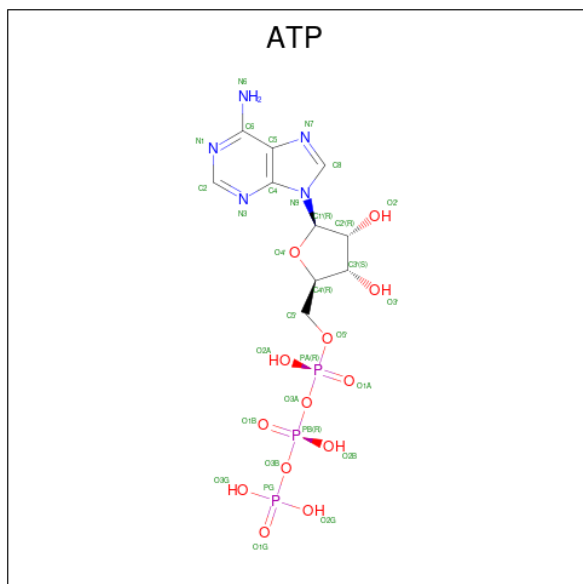
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	4801	-	-	X	-
2	ADP	B	4801	-	-	X	-

Continued from previous page...

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

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



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	



L2521	M2461	L2341	T2281	M2221	L2161	G2101	M2041	A1981	H1921	M1861	P1801
T2522	L2462	M2342	H2282	M2222	S2162	N2102	T2042	L1982	Q1922	A1862	P1802
T2523	H2463	F2343	V2283	V2223	D2163	V2103	K2043	R1983	L1923	N1863	L1803
V2524	Q2464	E2344	L2284	G2224	V2164	K2104	P2044	E1984	G1924	A1864	R1804
L2525	A2465	V2345	R2285	P2225	F2165	E2106	D2045	H1985	R1925	K1865	R1805
L2526	C2466	Q2346	K2286	P2226	P2166	E2106	R2046	S1986	F1926	F1866	R1806
P2527	R2467	D2347	L2287	G2227	G2167	R2107	Q2047	M1987	V1927	N1867	K1807
T2528	N2468	L2348	L2288	S2228	V2168	T2108	L2048	PRO	L1928	Y1868	L1808
A2529	V2469	K2349	D2289	G2229	Q2169	Q2109	I2049	ASN	L1929	Y1869	E1809
P2530	A2470	R2350	S2290	K2230	Q2170	Q2110	A2050	TVR	F1930	F1870	H1810
M2531	Q2471	A2351	V2291	S2231	H2171	I2111	Q2051	LYS	M1931	E1871	L1811
L2532	Y2472	T2352	R2292	M2232	R2172	K2112	V2052	THR	C1932	Y1872	I1812
P2533	N2473	L2353	G2293	A2233	G2173	R2113	M2053	SER	D1933	L1873	T1813
L2534	A2474	A2354	E2294	V2234	E2174	E2114	L2054	ALA	E1934	G1874	E1814
T2535	N2475	T2355	L2295	A2235	M2175	LYS	Y2055	I1997	T1935	V1875	L1815
D2536	H2476	V2356	Q2296	V2236	T2176	GLU	S2056	TYR	F1936	Q1876	V1816
V2537	D2477	S2357	K2297	L2237	A2177	ARG	Q2057	ASP	D1937	D1877	H1817
E2538	P2478	R2358	R2298	L2238	L2178	GLY	G2058	GLY	F1938	K1878	Q1818
V2539	F2479	C2359	Q2299	K2239	R2179	GLU	F2059	E2000	Q1939	L1879	R1819
S2540	P2480	G2360	V2300	A2240	E2180	ALA	R2060	L2001	A1940	V1880	D1820
L2541	M2481	M2361	I2301	L2241	E2181	ASP	T2061	L2002	M1941	Q1881	V1821
S2542	Q2482	V2362	F2302	E2242	L2182	GLU	A2062	N2003	G1942	T1882	T1822
G2543	L2483	K2363	F2303	A2243	K2183	GLY	E2063	K2004	R1943	P1883	R1823
E2544	E2484	F2364	D2304	L2244	K2184	GLU	V2064	V2006	I1944	L1884	S1824
M2545	Q2485	S2365	G2305	E2245	V2185	TLE	L2065	K2007	F1945	T1885	L1825
S2546	L2486	R2366	D2306	G2246	C2186	E2129	A2066	V2008	V1946	D1886	I1826
P2547	T2487	D2367	V2307	V2247	Q2187	N2130	N2067	S2009	G1947	R1887	K1827
W2548	R2488	V2368	D2308	E2248	E2188	L2131	K2068	P2010	L1948	C1888	S1828
Q2549	Y2489	L2369	P2309	G2249	M2189	L2132	I2069	D2011	C1949	Y1889	K1829
A2550	Q2490	S2370	E2310	V2250	L2190	E2133	V2070	M2012	Q1950	L1890	I1830
K2551	Q2491	T2371	W2311	A2251	L2191	Q2134	P2071	A2013	V1951	T1891	D1831
V2552	R2492	D2372	E2312	H2252	T2192	E2135	F2072	T2014	G1952	M1892	N1832
P2553	Y2493	M2373	E2313	L2253	Y2193	L2136	T2073	F2015	A1953	T1893	A1833
Q2554	L2494	L2374	N2314	I2254	Q2194	L2137	K2074	T2016	W1954	Q1894	K1834
L2555	V2495	F2375	L2315	D2255	D2195	L2138	L2075	T2017	G1955	A1895	S1835
E2556	Y2496	M2376	N2316	P2256	Q2196	Q2139	C2076	M2018	C1956	F1896	F1836
A2557	A2497	R2377	S2317	K2257	E2197	S2140	D2077	N2019	F1957	E1897	E1837
T2558	I2498	F2378	L2318	A2258	E2198	V2141	E2078	P2020	D1958	A1898	W1838
V2559	L2499	L2379	L2319	I2259	V2199	C2142	Q2079	G2021	E1959	R1899	L1839
H2560	W2500	A2380	D2320	S2260	G2200	E2143	L2080	Y2022	F1960	L1900	S1840
S2501	Q2442	R2381	D2321	K2261	G2201	T2144	S2081	A2023	N1961	G1901	Q1841
L2502	L2443	L2382	N2322	D2262	W2202	W2145	S2082	G2024	R1962	G1902	M1842
S2503	H2444	R2383	K2323	H2263	W2203	V2146	Q2083	R2025	L1963	S1903	R1843
Q2504	T2446	S2384	L2324	L2264	V2204	P2147	S2084	S2026	E1964	P1904	F1844
D2505	M2447	I2385	L2325	Y2265	E2205	K2148	H2085	N2027	E1965	F1905	Y1845
S2506	D2448	T2386	T2326	G2266	K2206	L2149	Y2086	L2028	R1966	G1906	F1846
R2507	L2449	L2387	L2327	T2267	V2207	V2150	D2087	P2029	M1967	P1907	D1847
L2508	T2450	D2388	L2328	L2268	Q2208	A2151	F2088	D2030	L1968	A1908	P1848
M2509	R2451	E2389	P2329	D2269	Q2209	E2152	G2089	N2031	S1969	G1909	K1849
Q2510	L2452	GLY	M2330	G2266	L2210	D2153	R2091	L2032	A1970	T1910	Q1850
T2511	R2453	ASP	Q2330	T2267	Y2211	T2154	A2092	K2033	G1911	G1911	T1851
A2512	C2454	GLU	E2331	T2272	Q2212	P2155	L2093	K2034	S1972	K1912	D1852
L2513	L2455	ALA	R2332	E2274	I2213	L2156	L2093	L2035	Q1973	T1913	V1853
E2514	G2456	GLN	S2334	E2274	T2214	L2157	K2094	F2036	Q1974	E1914	L1854
Q2515	S2457	ARG	L2335	W2275	Q2215	F2158	S2095	R2037	V1975	S1915	Q1855
E2516	L2458	ARG	P2336	T2276	I2216	S2159	V2096	L2038	Q1976	V1916	Q1856
L2517	F2459	LYS	P2337	D2277	N2217	L2160	L2097	L2039	C1977	K1917	L1857
I2518	S2460	GLY	N2338	G2278	H2218		V2098	A2040	I1978	A1918	S1858
R2519			V2339	L2279	G2219		S2099		Q1979	L1919	T1859
L2520			R2340	F2280	L2220		A2100		E1980	G1920	Q1860

LYS	K3241	N3181	I3121	N3061	D3001	A2941	Y2881	S2761	V2701	L2581
GLN	K3242	H3182	V3122	L3062	S3002	G2942	T2882	L2762	K2702	Y2582
HIS	M3243	Y3183	P3123	H3063	G3003	K2943	P2883	R2763	L2703	T2583
LEU	V3244	A3184	D3124	V3064	F3004	T2944	V2884	T2764	E2704	W2584
GLU	K3245	N3185	Y3125	V3065	L3005	T2945	Q2885	Y2765	L2705	L2585
VAL	D3246	L3186	M3126	F3066	E3006	L2946	Q2886	A2766	K2706	A2586
ARG	Q3247	F3187	M3127	T3067	R3007	S2947	E2887	E2767	Q2707	E2587
SER	K3248	H3188	V3128	M3068	N3008	R2948	E2888	P2768	P2708	H2588
MET	E3249	K3189	V3129	N3069	M3009	R2949	E2889	V2649	V2709	K2589
ASN	K3250	K3190	Y3130	P3070	T3010	V2950	R2890	K2710	G2710	P2590
PRO	E3251	R3191	D3131	S3071	L3011	A2951	D2891	A2711	A2711	L2591
ALA	K3252	S3192	K3132	S3072	L3012	W2952	Y2892	C2712	C2712	V2592
ALA	K3253	E3193	L3133	E3073	A3013	M2953	Y2893	A2772	N2713	L2593
VAL	L3254	L3194	P3134	G3074	N3014	N2954	K2894	W2774	P2714	C2594
LYS	VAL	E3195	Q3135	G3075	G3015	G2955	A2895	E2775	P2715	G2595
VAL	MET	E3196	P3136	K3076	E3016	L2956	R2896	F2776	T2716	P2596
MET	SER	E3197	D3077	D3077	V3017	S2957	L2897	Y2777	D2717	P2597
GLN	GLU	Q3198	S3137	R3078	P3018	V2958	K2898	T2778	P2718	G2598
ILE	GLU	M3199	H3139	A3079	G3019	Y2959	V2899	M2779	G2719	S2599
GLN	GLN	H3200	R3140	A3080	L3020	Q2960	F2900	S2780	R2720	G2600
GLU	GLN	L3201	E3141	T3081	F3021	I2961	Y2901	E2841	K2721	L2601
LEU	LEU	N3202	A3142	S3082	E3022	K2962	E2902	Q2782	P2722	T2602
LEU	GLY	V3203	I3143	F3083	G3023	V2963	E2903	R2783	L2723	C2603
GLY	GLY	G3204	V3144	A3084	D3024	H2964	E2904	F2784	S2724	T2604
SER	GLN	L3205	M3145	L3085	E3025	R2965	L2905	T2785	H2725	L2605
THR	GLN	R3206	S3146	F3086	Y3026	K2966	D2906	Q2786	R2726	P2606
ASP	VAL	K3207	C3147	N3087	A3027	Y2967	V2907	D2787	F2727	S2607
ILE	ASP	I3208	V3148	R3088	T3028	T2968	P2908	L2788	L2728	A2608
ALA	ASP	K3209	F3149	C3089	L3029	G2969	L2909	Q2789	R2729	L2609
GLN	LYS	E3210	V3150	V3090	M3030	E2970	V2910	P2790	K2730	R2610
GLN	ARG	T3211	H3151	L3091	T3031	D2971	L2911	H2791	V2731	A2611
SER	MET	V3212	K3152	N3092	Q3032	F2972	F2912	T2792	P2732	L2612
ILE	VAL	D3213	T3153	W3093	C3033	D2973	M2913	L2793	V2733	P2613
ILE	GLU	Q3214	L3154	F3094	K3034	E2974	E2914	Y2794	V2734	D2614
ARG	GLU	V3215	H3155	G3095	E3035	D2975	V2915	S2795	Y2735	M2615
ASP	LEU	V3216	Q3156	D3096	G3036	L2976	L2916	P2796	V2736	E2616
ASN	ASP	E3217	A3157	W3097	A3037	D2977	D2917	R2797	Q2677	V2617
PHE	PHE	L3218	S3158	S3098	Q3038	T2978	H2918	E2798	R2678	W2618
ILE	ILE	R3219	A3159	T3099	K3039	V2979	V2919	M2799	P2739	G2619
THR	PRO	R3220	R3160	E3100	E3040	L2980	L2920	T2800	Q2740	L2620
ILE	VAL	D3221	L3161	A3101	G3041	R2981	R2921	K2801	P2741	M2621
ASN	VAL	L3222	A3162	L3102	L3042	R2982	T2922	W2802	A2742	S2622
ILE	ILE	R3223	K3163	Y3103	M3043	S2983	D2923	V2803	S2743	S2623
GLU	GLU	T3224	R3164	Q3104	L3044	G2984	R2924	R2804	L2744	R2624
ALA	ASN	K3225	G3165	V3105	D3045	C2985	L2925	G2805	T2745	A2625
VAL	ALA	S3226	G3166	G3106	S3046	K2986	F2926	T2806	Q2746	Q2626
VAL	VAL	Q3227	R3167	K3107	H3047	N2987	R2927	F2807	L2747	M2627
LYS	LYS	E3228	T3168	E3108	E3048	Q2988	Q2928	E2808	V2748	P2628
SER	SER	L3229	M3169	F3109	E3049	K2989	P2929	A2809	Q2749	E2629
ILE	ILE	E3230	A3170	T3110	L3050	T2990	Q2930	L2810	T2750	L2630
LYS	LYS	V3231	I3171	S3111	Y3051	A2991	Q2931	R2811	P2751	L2631
ILE	ILE	K3232	T3172	K3112	K3052	F2992	H2932	P2812	N2752	L2632
ILE	ILE	N3233	P3173	D3113	W3053	I2993	L2933	L2813	R2753	K2633
ILE	ILE	A3234	R3174	M3114	F3054	M2994	E2874	E2814	A2754	T2634
ILE	ILE	A3235	H3175	L3115	T3055	D2995	N2875	T2815	M2755	P2635
ILE	ILE	A3236	Y3176	E3116	S3056	E2996	W2876	L2816	L2756	D2636
ILE	ILE	N3237	L3177	K3117	Q3057	S2997	L2877	P2817	R2757	H2637
ILE	ILE	D3238	D3178	P3118	V3058	T2998	L2878	V2818	L2758	Q2638
ILE	ILE	K3239	F3179	N3119	I3059	V2999	K2879	E2819	I2759	C2639
ILE	ILE	L3240	I3180	Y3120	R3060	L3000	G2940	G2820	P2760	E2640





L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560
L1561	L1562	L1563	L1564	L1565	L1566	L1567	L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620
L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680
L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740
L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800
L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860
L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880	L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920
L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980
L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040
L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100
L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160
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L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280

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F3004	T2944	V2884	I2824	T2764	E2704	T2644	W2584	V2524	Q2464	GLY	E2344	L2284
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N3008	R2948	E2888	E2828	P2768	F2708	V2648	H2588	T2528	N2468	L2348	K2348	I2288
N3009	F2949	R2889	A2829	L2769	V2709	V2649	K2589	A2529	V2469	P2411	Y2350	I2289
T3010	V2950	R2890	L2830	T2770	G2710	L2650	P2590	P2530	A2470	M2412	S2290	S2290
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L3012	V2952	V2892	L2832	M2772	G2712	P2652	V2592	I2532	Y2472	Q2414	T2352	R2292
A3013	M2953	V2893	F2833	M2773	N2713	V2653	L2593	P2533	M2473	I2415	L2353	G2293
N3014	K2954	K2894	Q2834	V2774	P2714	Q2654	C2594	I2534	A2474	R2417	A2354	E2294
G3015	G2955	A2895	D2835	E2775	P2715	L2655	Q2595	I2535	M2475	D2418	T2355	L2295
E3016	L2956	R2896	R2836	F2776	T2716	G2656	P2596	D2536	H2476	R2297	V2356	Q2296
V3017	S2957	L2897	L2837	Y2777	D2717	K2657	P2597	Y2537	P2477	A2419	S2357	K2297
P3018	V2958	K2898	V2838	T2778	P2718	W2658	G2598	E2538	D2478	A2420	R2358	R2298
G3019	V2959	V2899	E2839	M2779	G2719	L2659	S2599	V2539	F2479	T2421	C2359	Q2299
L3020	Q2960	F2900	D2840	S2780	R2720	V2660	G2600	S2540	P2480	I2422	G2360	W2300
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E3022	K2962	E2902	E2842	E2782	P2722	F2662	T2602	S2542	Q2482	Q2424	V2362	V2302
G3023	V2963	E2903	R2843	R2783	L2723	C2663	K2603	G2543	I2483	P2425	W2363	F2303
D3024	H2964	E2904	R2844	F2784	S2724	D2664	T2604	E2544	E2484	Y2426	F2364	D2304
R2965	R2965	L2905	W2845	T2785	H2725	E2665	L2605	W2545	Q2485	P2427	G2365	G2305
E3026	K2966	V2906	T2846	Q2786	R2726	I2666	F2606	S2546	L2486	T2428	E2366	D2306
A3027	Y2967	V2907	D2847	D2787	F2727	N2667	S2607	P2547	E2487	S2429	D2367	V2307
T3028	T2968	P2908	T2848	T2788	L2728	L2668	A2608	W2548	R2488	N2430	D2368	D2308
L3029	G2969	V2909	N2849	Q2789	R2729	P2669	L2609	Q2549	Y2489	L2432	L2369	P2309
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D2971	L2911	L2911	D2851	H2791	V2731	M2671	A2611	K2551	Q2491	V2433	T2371	E2311
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G2973	M2913	M2913	V2853	I2793	V2733	K2673	P2613	P2553	Y2493	M2373	M2373	E2313
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D2975	V2915	V2915	L2855	G2795	Y2735	G2675	M2615	I2555	V2495	F2375	F2375	L2315
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A3037	R2917	R2917	H2857	P2797	D2737	Q2677	V2617	V2557	A2497	S2377	S2377	S2317
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K3039	V2979	V2919	P2859	M2799	P2739	V2679	G2619	T2559	L2499	L2379	L2379	L2319
E3040	L2980	L2920	N2860	T2800	G2740	I2680	L2620	H2560	W2500	A2380	A2380	D2320
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L3045	C2985	L2925	A2865	G2805	T2745	Q2685	A2625	P2565	D2505	I2385	I2385	L2325
S3046	K2986	F2926	K2866	T2806	Q2746	M2686	T2626	D2566	S2506	M2447	M2447	T2326
H3047	R2987	R2927	M2867	T2807	I2747	V2687	T2627	V2567	R2507	L2387	L2387	L2327
E3048	E2988	Q2928	S2868	E2808	V2748	E2688	P2628	V2568	L2508	P2388	P2388	P2328
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Y3051	A2991	Q2931	I2871	R2811	T2751	G2691	L2631	P2571	M2510	GLY	GLY	Q2330
K3052	F2992	H2932	L2872	P2812	N2752	F2692	F2632	T2572	R2511	ASP	ASP	E2331
W3053	I2993	L2933	Y2873	R2813	R2753	Y2693	K2633	D2573	A2512	GLU	GLU	R2332
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D2995	D2995	L2935	N2875	T2815	M2755	T2695	F2635	G2515	G2455	ARG	ARG	L2335
E2996	E2996	L2936	W2876	L2816	L2756	S2696	D2636	R2516	E2516	ARG	ARG	P2336
S2997	S2997	Q2937	L2877	R2817	L2757	D2697	D2637	H2577	Y2517	LYS	LYS	P2337
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V2999	V2999	S2939	K2879	E2819	I2759	T2699	C2639	A2579	S2460			V2339
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T3781	R3782	K3783	V3784	E3785	F3786	T3787	D3788	S3789	V3790	M3791	Q3792	E3793	V3794	E3795	T3796	V3797	S3798	Q3799	Q3800	Y3801	L3802	P3803	L3804	S3805	T3806	A3807	C3808	S3809	S3810	I3811	F3812	F3813	T3814	M3815	E3816	S3817	L3818	K3819	Q3820	I3821	H3822	F3823	L3824	Y3825	Q3826	Y3827	S3828	L3829	Q3830	F3831	F3832	L3833	L3834	I3835	Y3836	H3837	N3838	V3839	L3840	
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N3181	H3182	Y3183	A3184	N3185	L3186	F3187	H3188	E3189	K3190	R3191	S3192	E3193	L3194	E3195	E3196	Q3197	Q3198	Q3199	H3200	L3201	N3202	V3203	G3204	L3205	R3206	K3207	I3208	R3209	E3210	T3211	V3212	D3213	Q3214	V3215	E3216	E3217	L3218	R3219	K3220	D3221	L3222	R3223	I3224	K3225	S3226	Q3227	E3228	L3229	E3230	V3231	K3232	N3233	A3234	A3235	A3236	N3237	D3238	K3239	L3240	
I3121	V3122	P3123	D3124	Y3125	M3126	P3127	V3128	V3129	V3130	D3131	K3132	L3133	P3134	Q3135	P3136	P3137	S3138	H3139	R3140	E3141	A3142	I3143	V3144	N3145	S3146	C3147	V3148	F3149	V3150	H3151	Q3152	T3153	L3154	H3155	Q3156	A3157	N3158	A3159	R3160	L3161	A3162	K3163	R3164	G3165	G3166	R3167	T3168	M3169	A3170	I3171	T3172	P3173	D3174	H3175	Y3176	L3177	F3178	F3179	I3180	
R3061	L3062	R3063	V3064	V3065	F3066	T3067	K3068	R3069	P3070	S3071	S3072	E3073	G3074	L3075	K3076	D3077	R3078	A3079	A3080	T3081	S3082	P3083	A3084	L3085	F3086	R3087	R3088	C3089	V3090	L3091	N3092	W3093	F3094	G3095	D3096	W3097	S3098	T3099	E3100	A3101	L3102	F3103	D3104	V3105	G3106	K3107	E3108	F3109	T3110	S3111	K3112	H3113	L3114	L3115	E3116	K3117	N3118	N3119	V3120	

T4561	A4502	K4441	H4381	L4321	D4261	W4201	A4141	D4081	M4021	L3961	Y3901	E3841
G4562	E4503	K4442	T4382	G4322	Q4262	S4202	G4142	K4082	E4022	D3962	D3902	E3842
L4563	L4504	K4443	T4383	L4323	R4263	K4203	R4143	A4083	Q4023	S3963	A3903	N3843
K4564	L4505	Q4444	A4384	P4324	L4264	K4204	T4144	I4084	P4024	S3964	E3904	P3844
L4565	K4506	T4445	S4385	M4325	L4265	Y4205	F4145	M4085	L4025	S3965	F3905	N3845
Q4566	N4507	N4446	M4386	M4326	N4266	E4206	V4146	T4086	D4026	P3966	Q3906	L3846
G4567	L4507	Y4447	V4387	A4327	T4267	F4207	F4147	A4087	L4027	E3967	H3907	LYS
A4568	H4508	L4448	L4388	E4328	F4268	G4208	E4148	V4088	T4028	Q3968	F3908	V3849
A4569	V4509	R4449	H4389	E4329	L4269	E4209	P4149	K4089	H4029	T3969	L3909	T3850
C4570	C4510	T4450	L4390	V4330	E4270	S4210	P4150	S4090	I4030	V3970	R3910	D3851
N4571	L4511	L4451	T4391	L4331	R4271	D4211	P4151	G4091	V4031	P3971	G3911	H3852
M4572	G4512	I4452	P4392	L4332	L4272	L4212	G4152	R4092	G4032	Y3972	N3912	T3853
N4573	G4513	N4453	Q4393	T4333	F4273	R4213	V4153	W4093	E3913	L3973	E3913	Q3854
K4574	L4514	E4454	T4394	T4334	T4274	S4214	K4154	V4094	E4034	Y3974	I3914	R3855
L4575	V4515	L4455	L4395	Q4335	T4275	A4215	M4155	M4095	V4035	SER	V3915	L3856
S4576	V4516	V4456	S4396	G4336	R4276	C4216	A4156	L4096	K4036	GLU	L3916	L3857
L4577	P4517	K4457	H4397	V4337	S4277	D4217	M4157	K4097	P4037	T3978	S3917	S3857
S4578	E4518	Q4458	L4398	D4338	F4278	T4218	L4158	N4098	N4038	P3979	A3918	T3858
N4579	A4519	I4459	K4399	M4339	D4279	V4219	R4159	V4099	T4039	A3980	G3919	I3859
A4580	Y4520	L4460	R4400	I4340	S4280	D4220	T4160	H4100	P4040	T3981	S3920	T3860
L4581	T4521	S4341	T4401	E4341	E4281	T4221	F4161	L4100	V4041	P3982	T3921	K3861
S4582	T4522	R4462	VAL	K4342	F4282	W4222	S4162	A4102	L4042	L3983	P3922	D3862
T4583	A4523	S4463	E4403	M4343	K4283	L4223	S4163	P4103	M4043	G3984	R3923	L3863
L4584	T4524	V4464	M4404	L4344	L4284	D4224	T4164	G4104	C4044	Q3985	I3924	F3864
L4585	R4525	S4465	T4405	K4345	A4285	D4225	P4165	W4105	S4045	A3986	Q3925	Q3865
P4586	Q4526	H4466	K4406	M4346	C4286	T4226	V4166	L4106	V4046	I3987	G3926	V3866
L4587	Y4527	Y4467	D4407	Q4347	K4287	A4227	S4167	M4107	P4047	T3987	L3927	A3867
T4588	V4528	T4468	P4408	K4348	V4288	K4228	R4168	Q4108	G4048	H3988	T3928	F3868
Q4589	A4529	V4469	L4409	L4349	D4289	G4229	T4169	L4109	Y4049	R3989	V3929	N3869
L4590	Q4630	P4470	F4410	E4350	G4290	R4230	C4170	E4110	D4050	L3991	E3930	K3870
A4591	A4631	A4471	R4411	ASP	H4291	Q4231	K4171	K4111	A4051	L3992	Q3931	V3871
L4592	L4632	Q4472	F4412	GLU	K4292	M4232	S4172	L4112	S4052	A3932	A3932	A3872
W4593	S4533	F4473	F4413	ASP	D4293	L4233	P4173	L4113	G4053	T3993	E3933	R3873
K4594	W4534	T4474	E4414	LEU	I4294	S4234	M4174	H4114	H4054	Q3994	A3934	K3874
L4595	S4535	V4475	R4415	ALA	Q4295	P4235	E4175	S4115	V4055	A3995	A3935	G3875
THR	E4536	I4476	E4416	ALA	M4296	D4236	R4176	L4116	E4056	F3996	V3936	L3876
ASN	E4537	Q4477	V4417	GLU	P4297	K4237	A4177	Q4117	D4057	R3997	V3936	H3877
THR	E4538	W4478	K4418	THR	D4298	L4238	R4178	P4118	L4058	P3998	R3937	Q3878
GLU	L4539	V4479	M4419	GLU	G4299	P4239	L4179	E4119	A4059	D3999	L3938	D3879
LYS	C4540	S4480	G4420	LYS	I4300	W4240	L4179	H4119	A4059	R4000	S3939	H3880
ALA	L4541	D4481	G4420	THR	R4301	S4241	F4181	A4120	E4061	L4001	C3940	I3881
S4603	E4542	F4482	K4422	ARG	R4302	A4242	L4182	C4121	E4061	L4002	P3942	T3882
V4605	V4543	S4483	L4423	ASP	E4303	L4243	L4183	F4122	Q4062	A4003	F3942	F3883
L4607	N4544	E4484	L4424	THR	A4304	K4244	A4184	L4124	M4063	M4004	A3943	A3884
T4608	W4545	Q4425	Q4425	THR	F4305	T4245	W4185	F4125	T4064	A4005	F3944	K3885
P4608	THR	D4426	V4427	SER	V4306	L4246	F4186	L4126	I4066	H4006	D3946	L3886
L4609	THR	V4427	V4427	GLY	Q4307	M4247	H4187	T4127	T4067	F4008	L3947	L3887
V4609	SER	K4487	R4428	GLN	W4308	A4248	E4128	M4128	V4009	A3888	A3948	A3889
Y4610	GLY	Q4488	R4428	ALA	V4309	Q4249	E4189	I4129	I4069	S4010	A3949	R3889
L4611	ALA	L4489	Q4429	TRP	V4309	W4249	T4189	E4129	A4069	T4011	K3950	T3890
N4612	THR	Q4490	L4431	MET	E4310	S4250	I4190	I4130	A4070	M4012	V3951	I3890
F4613	LEU	K4491	L4431	ARG	L4311	I4251	Q4191	M4131	A4070	L4012	Q3952	K3991
L4615	ASP	I4492	A4432	THR	L4312	Y4252	E4192	P4132	G4072	L4013	A3953	K3993
A4616	ALA	D4493	D4433	ARG	P4313	G4253	R4193	K4133	S4073	E4014	A3953	G3894
L4617	C4557	V4434	V4435	D4314	D4314	G4254	L4194	V4134	A4074	G4014	D3954	T3895
L4618	F4558	V4436	V4436	T4315	T4315	R4255	L4195	P4135	E4075	E4015	E3955	C3894
L4619	A4496	Q4436	Q4436	Q4316	Q4316	V4256	Y4196	V4136	G4076	S4016	Q3956	G3895
L4620	V4560	V4437	V4437	T4317	T4317	D4257	A4197	N4137	F4077	F4017	F3957	T3895
F4620	VAL	C4438	C4438	P4318	P4318	M4258	P4198	L4138	M4078	M4018	G3958	V3897
	GLY	S4498	E4439	S4319	S4319	E4259	L4199	L4139	Q4079	S4019	G3958	E3898
	GLY	T4499	E4440	T4320	T4320	F4260	G4200	R4140	A4080	L4020	W3960	F3899
												T3900

T4621	Y4622	D4623	F4624	E4625	T4626	A4627	T4628	R4629	E4630	D4631	P4632	R4633	S4634	F4635	Y4636	E4637	R4638	C4639	Y4640	A4641	Y4642	L4643	C4644	T4645	E4646
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	233227	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 ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	106061	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.57	0/23474	1.03	33/31851 (0.1%)
1	B	0.57	0/23474	1.03	33/31851 (0.1%)
All	All	0.57	0/46948	1.03	66/63702 (0.1%)

There are no bond length outliers.

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3821	ILE	N-CA-C	16.76	126.51	110.42
1	A	3821	ILE	N-CA-C	16.76	126.51	110.42
1	A	4250	SER	N-CA-C	13.35	125.91	111.36
1	B	4250	SER	N-CA-C	13.35	125.91	111.36
1	B	3578	ILE	CB-CA-C	-8.26	101.40	111.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23003	0	22805	604	0
1	B	23003	0	22805	597	0
2	A	81	0	36	13	0
2	B	81	0	36	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	4	0
3	B	31	0	12	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	46232	0	45706	1184	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 13.

The worst 5 of 1184 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:3638:VAL:HG12	1:A:3681:THR:CG2	1.29	1.60
1:A:3815:MET:HE2	1:A:3871:VAL:CG2	1.34	1.55
1:B:3815:MET:HE2	1:B:3871:VAL:CG2	1.34	1.54
1:B:3638:VAL:HG12	1:B:3681:THR:CG2	1.29	1.54
1:B:3749:LEU:HD13	1:B:3773:LEU:CD1	1.44	1.46

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	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	48	79
1	B	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	48	79
All	All	5776/9292 (62%)	5428 (94%)	342 (6%)	6 (0%)	49	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1647	VAL
1	B	1647	VAL
1	A	1964	GLU
1	B	1964	GLU
1	A	1511	PRO

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	2472/4125 (60%)	2469 (100%)	3 (0%)	88	89
1	B	2472/4125 (60%)	2469 (100%)	3 (0%)	88	89
All	All	4944/8250 (60%)	4938 (100%)	6 (0%)	87	89

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2445	HIS
1	B	2702	LYS
1	B	2796	PRO
1	A	2702	LYS
1	A	2445	HIS

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

Mol	Chain	Res	Type
1	B	1670	ASN
1	B	1979	GLN
1	B	4062	GLN
1	B	1746	GLN
1	B	1881	GLN

5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
2	ADP	A	4804	-	28,29,29	1.41	5 (17%)	43,45,45	1.79	10 (23%)
2	ADP	A	4801	-	28,29,29	1.54	6 (21%)	43,45,45	1.95	8 (18%)
2	ADP	A	4805	-	28,29,29	1.35	4 (14%)	43,45,45	1.96	11 (25%)
2	ADP	B	4805	-	28,29,29	1.35	4 (14%)	43,45,45	1.96	11 (25%)
2	ADP	B	4801	-	28,29,29	1.54	6 (21%)	43,45,45	1.95	8 (18%)
2	ADP	B	4804	-	28,29,29	1.41	5 (17%)	43,45,45	1.79	11 (25%)
3	ATP	A	4802	4	32,33,33	1.52	6 (18%)	48,52,52	1.71	11 (22%)
3	ATP	B	4802	4	32,33,33	1.51	6 (18%)	48,52,52	1.71	11 (22%)

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	4804	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4801	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4805	-	-	3/16/32/32	0/3/3/3
2	ADP	B	4805	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	4801	-	-	3/16/32/32	0/3/3/3
2	ADP	B	4804	-	-	3/16/32/32	0/3/3/3
3	ATP	A	4802	4	-	2/22/38/38	0/3/3/3
3	ATP	B	4802	4	-	2/22/38/38	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4801	ADP	C5-C4	4.86	1.47	1.39
2	A	4801	ADP	C5-C4	4.85	1.47	1.39
3	A	4802	ATP	C5-C4	4.70	1.47	1.39
3	B	4802	ATP	C5-C4	4.65	1.47	1.39
2	A	4804	ADP	C5-C4	4.19	1.46	1.39

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4801	ADP	C5-C4-N3	-6.36	117.96	126.72
2	A	4801	ADP	C5-C4-N3	-6.36	117.97	126.72
2	A	4805	ADP	C5-C4-N3	-6.30	118.04	126.72
2	B	4805	ADP	C5-C4-N3	-6.30	118.04	126.72
2	A	4805	ADP	N3-C4-N9	5.04	135.75	127.17

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4804	ADP	PA-O3A-PB-O2B
2	A	4804	ADP	C5'-O5'-PA-O1A
2	A	4805	ADP	C5'-O5'-PA-O2A
2	A	4805	ADP	C5'-O5'-PA-O3A
2	B	4804	ADP	PA-O3A-PB-O2B

There are no ring outliers.

6 monomers are involved in 34 short contacts:

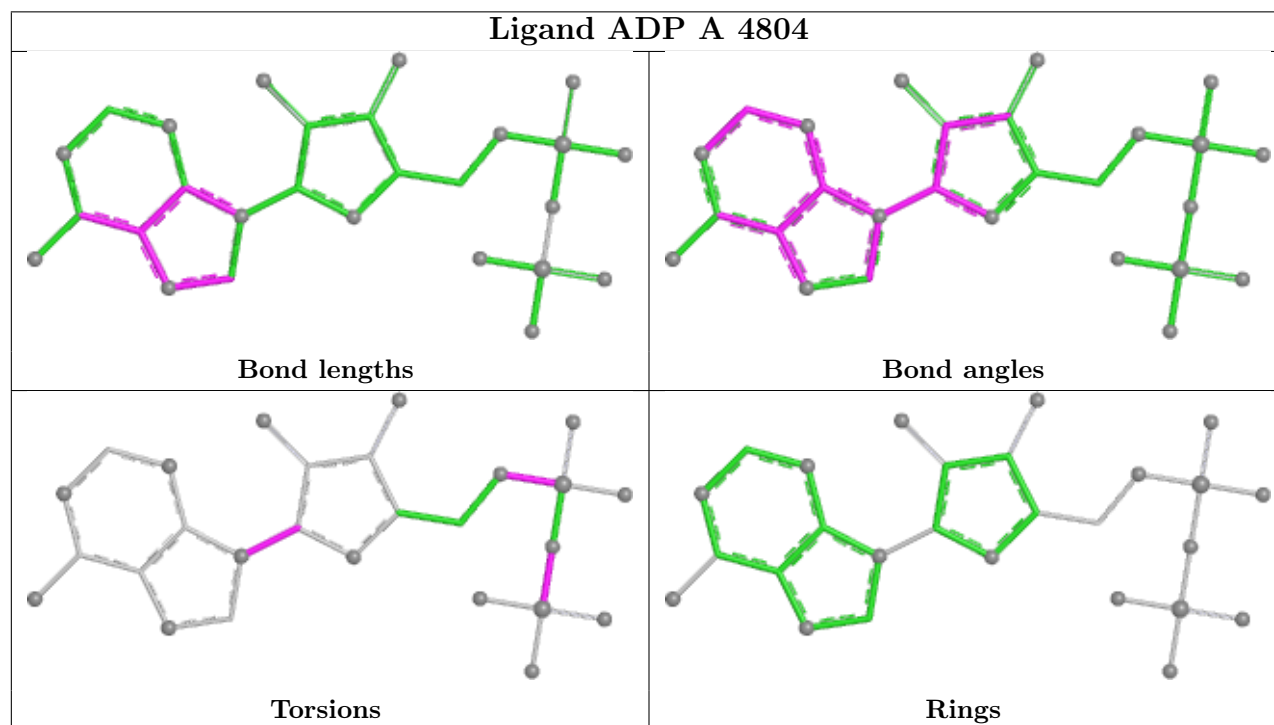
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4804	ADP	2	0
2	A	4801	ADP	11	0
2	B	4801	ADP	11	0

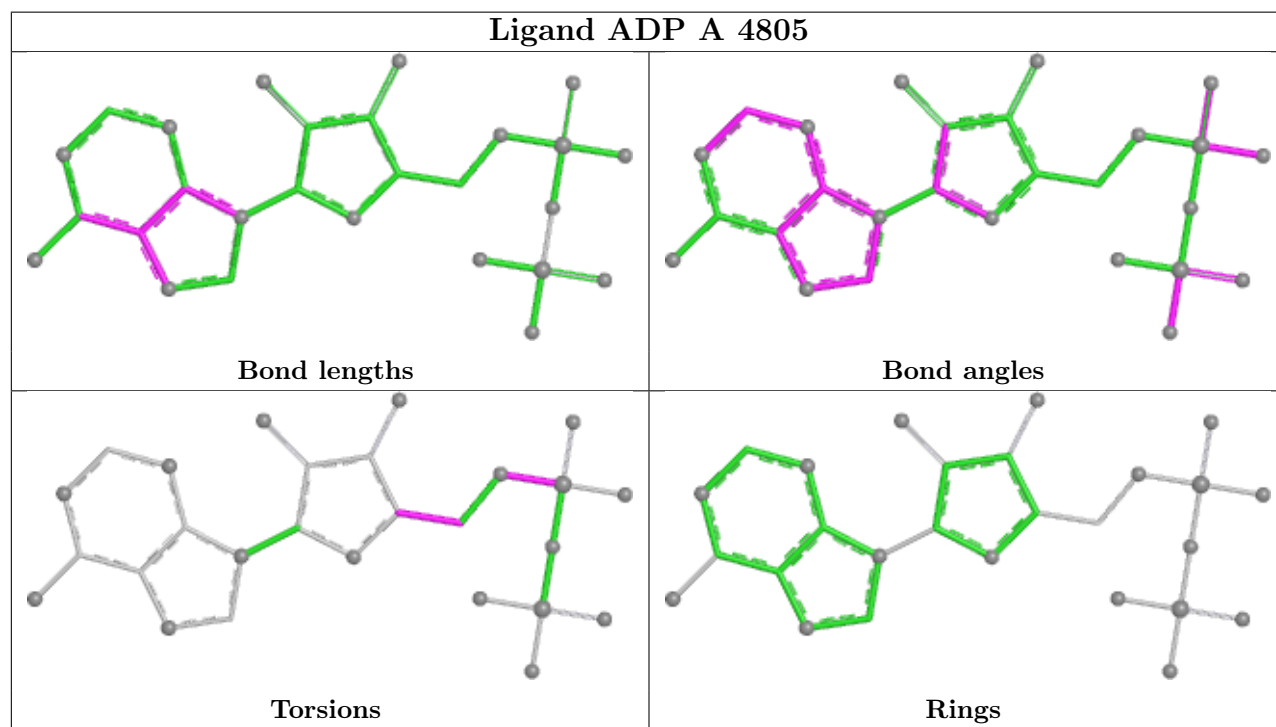
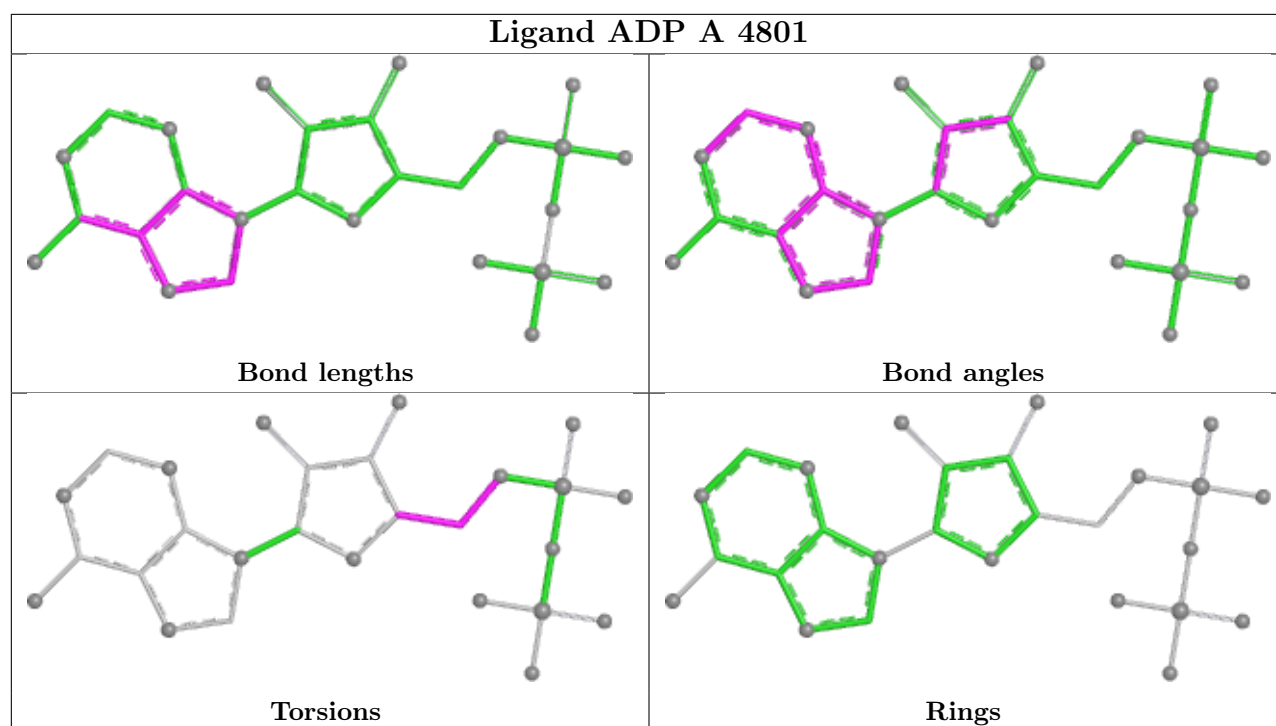
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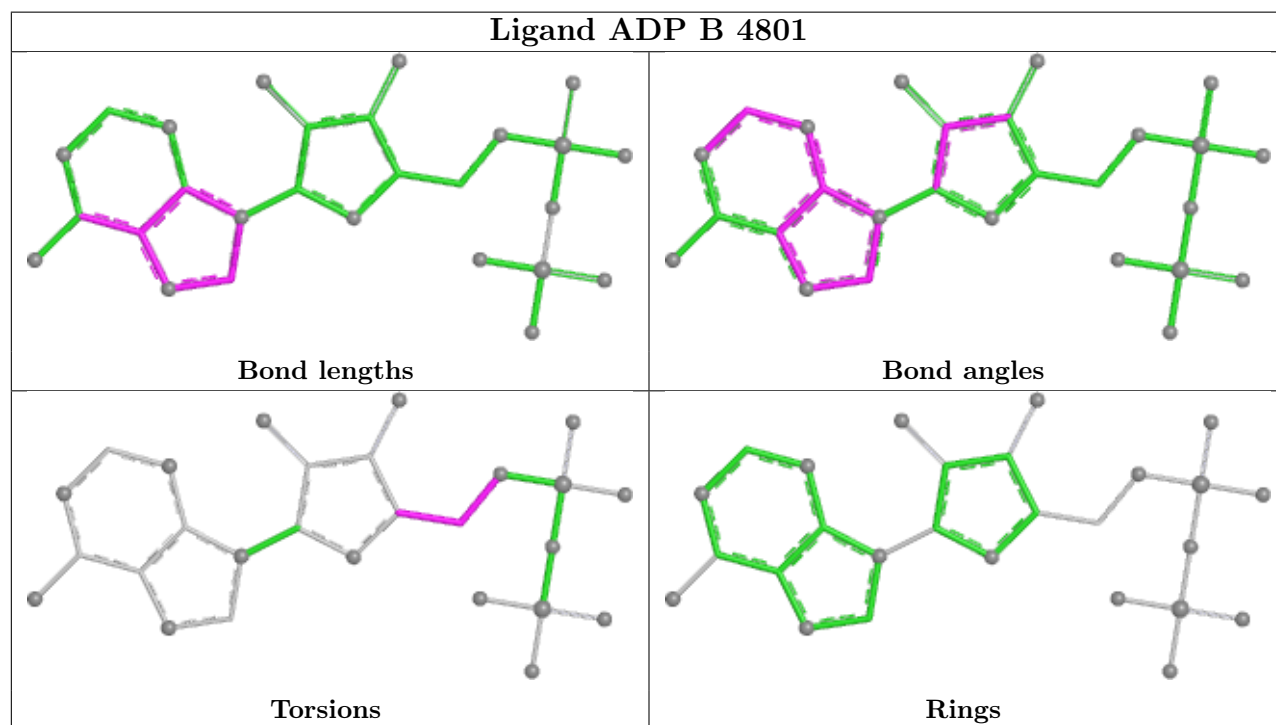
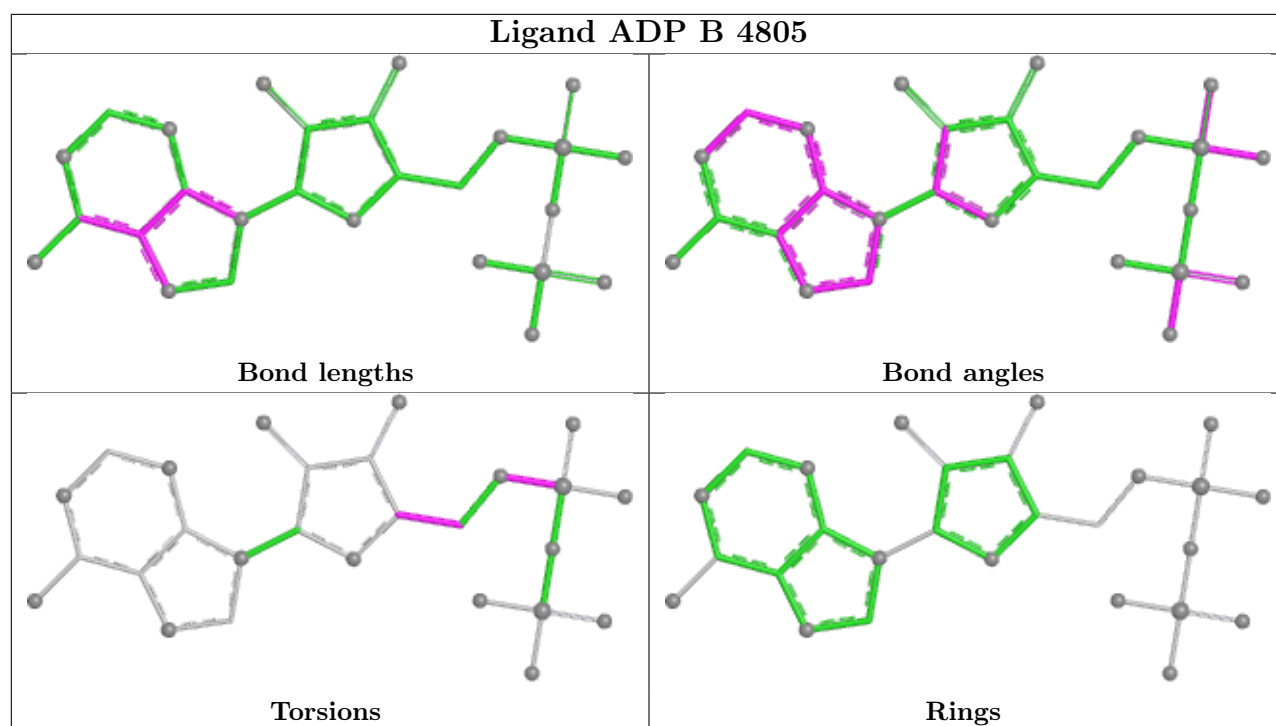
Continued from previous page...

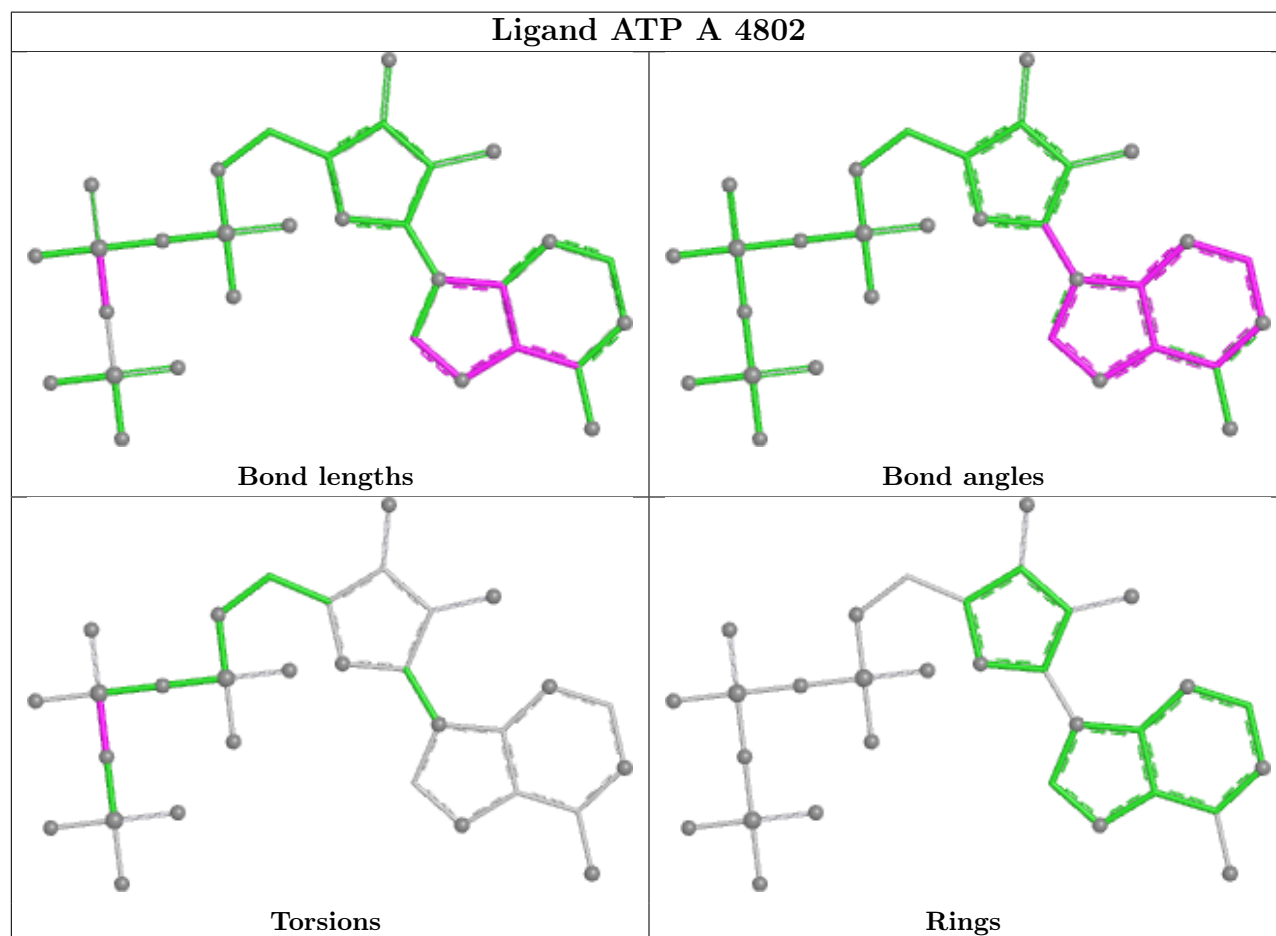
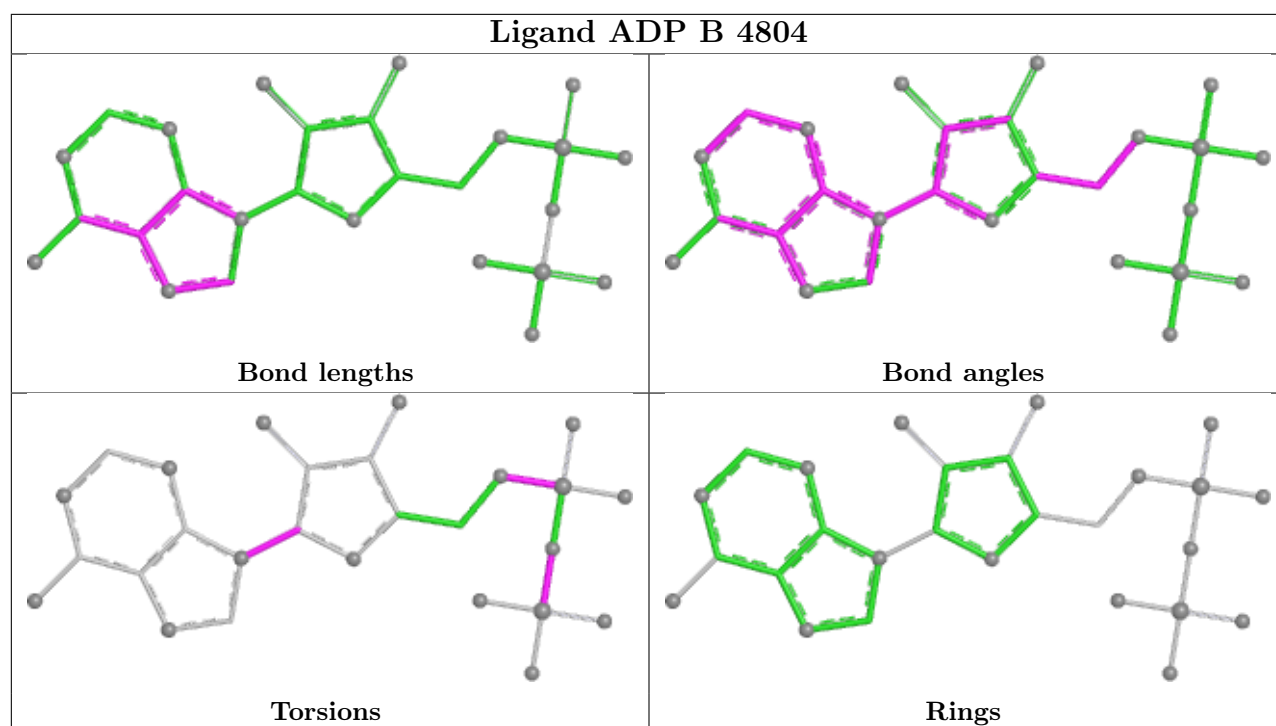
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4804	ADP	2	0
3	A	4802	ATP	4	0
3	B	4802	ATP	4	0

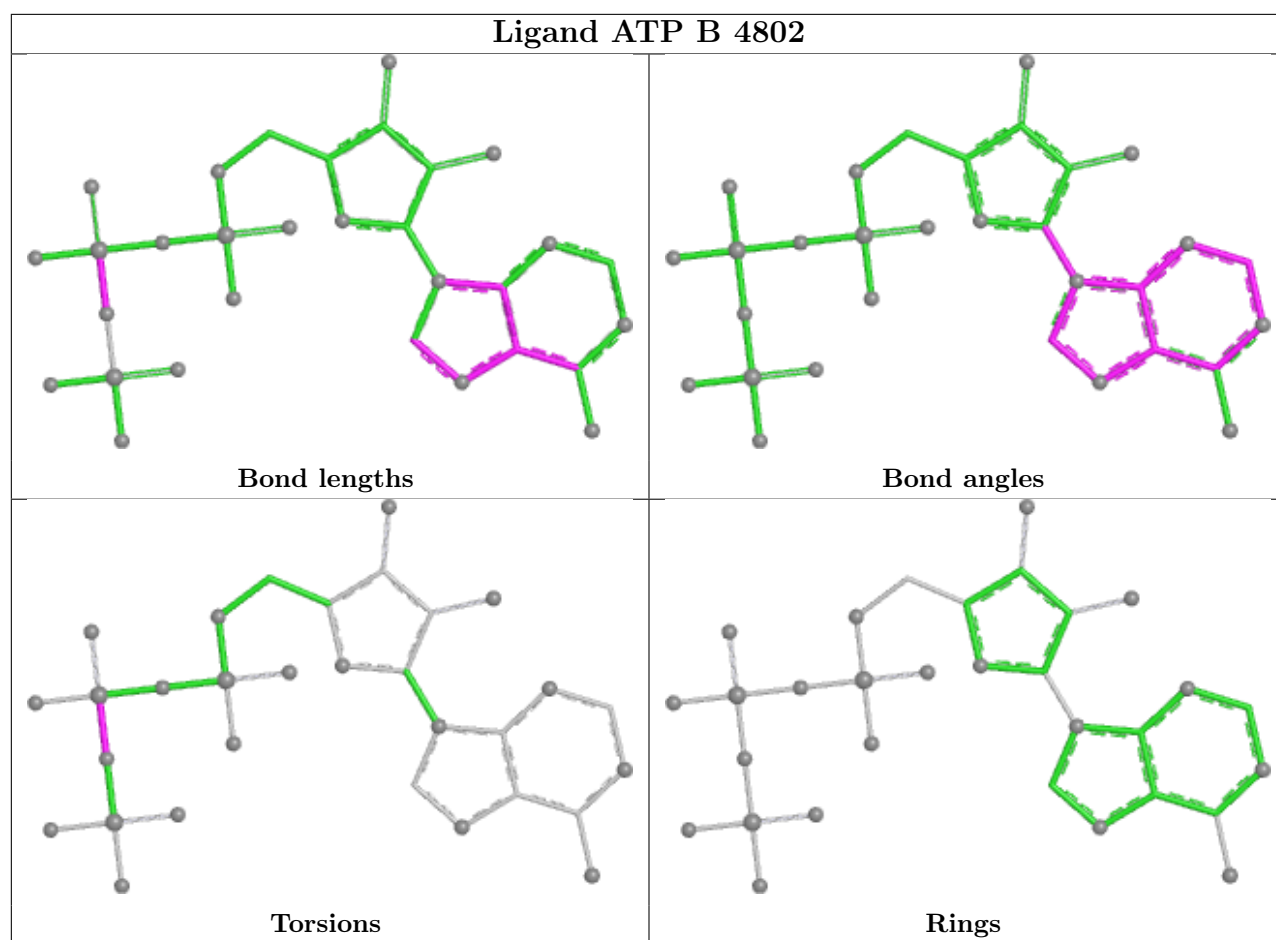
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3803:PRO	C	3804:LEU	N	2.62
1	B	3803:PRO	C	3804:LEU	N	2.62
1	A	3203:VAL	C	3204:GLY	N	2.58
1	B	3203:VAL	C	3204:GLY	N	2.58

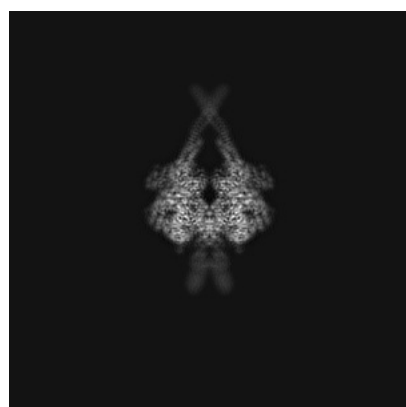
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3698. These allow visual inspection of the internal detail of the map and identification of artifacts.

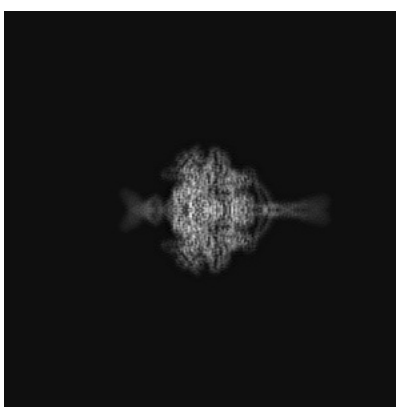
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

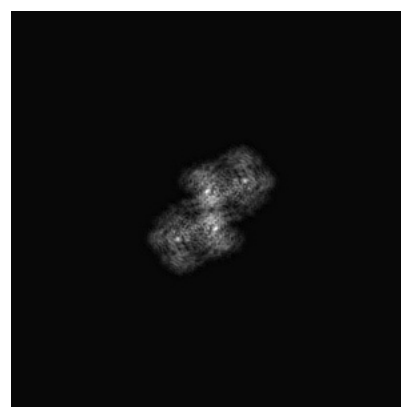
6.1.1 Primary map



X



Y

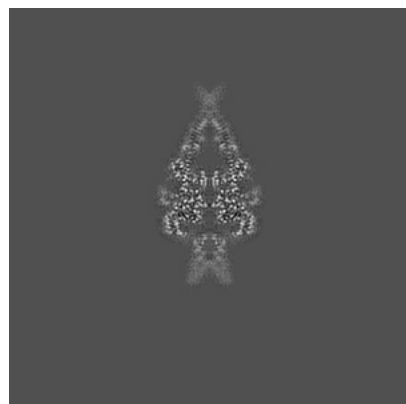


Z

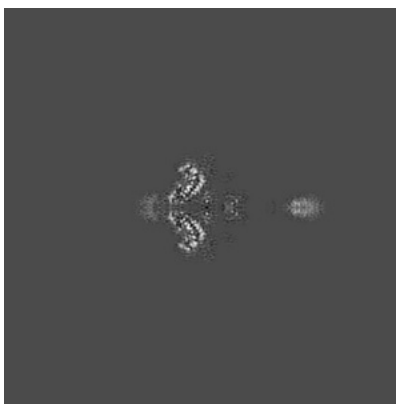
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

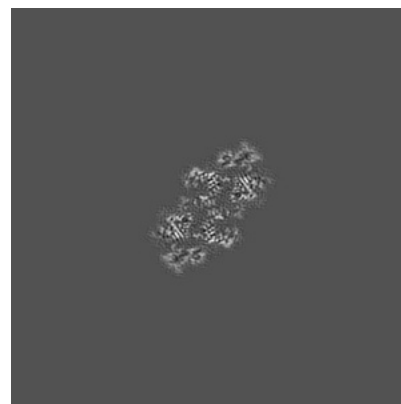
6.2.1 Primary map



X Index: 200



Y Index: 200

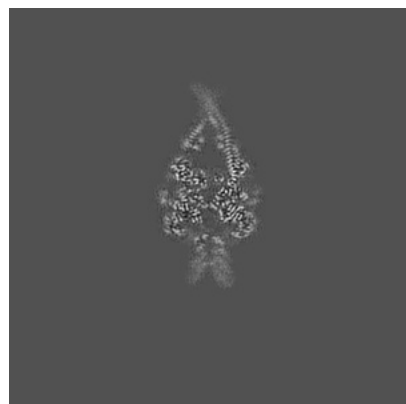


Z Index: 200

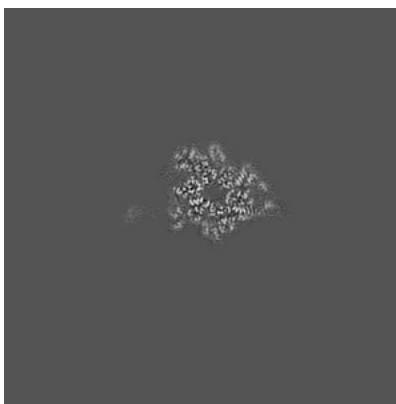
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 198



Y Index: 223

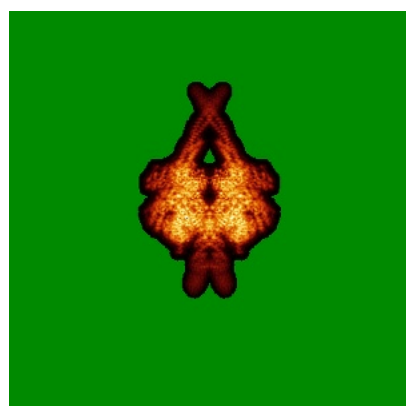


Z Index: 189

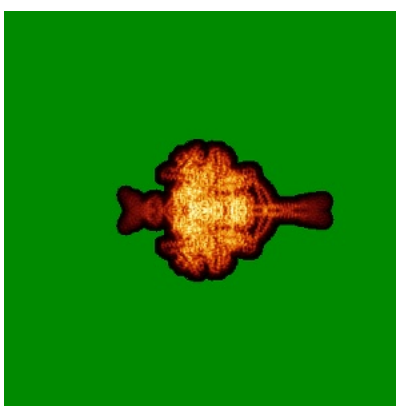
The images above show the largest variance slices of the map in three orthogonal directions.

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

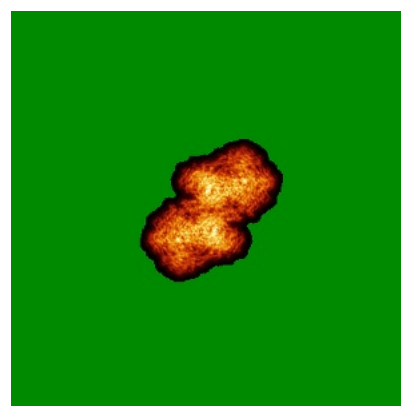
6.4.1 Primary map



X



Y

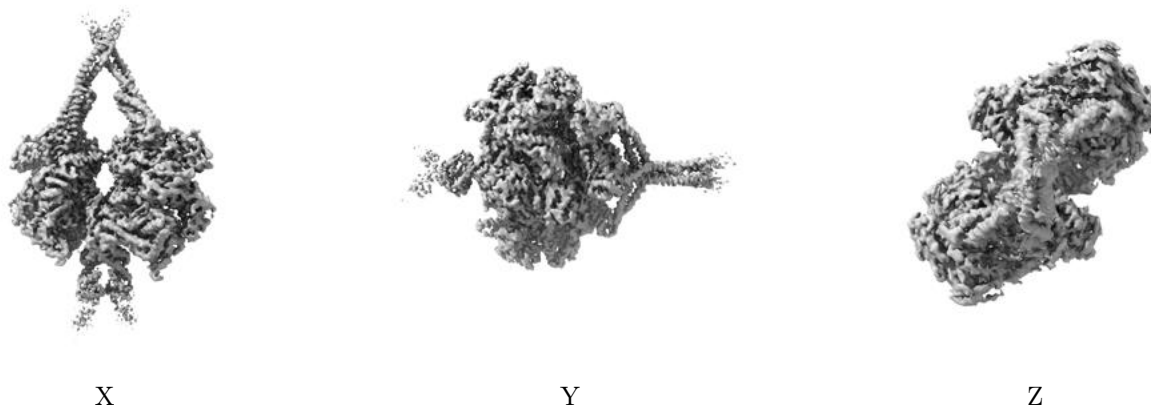


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

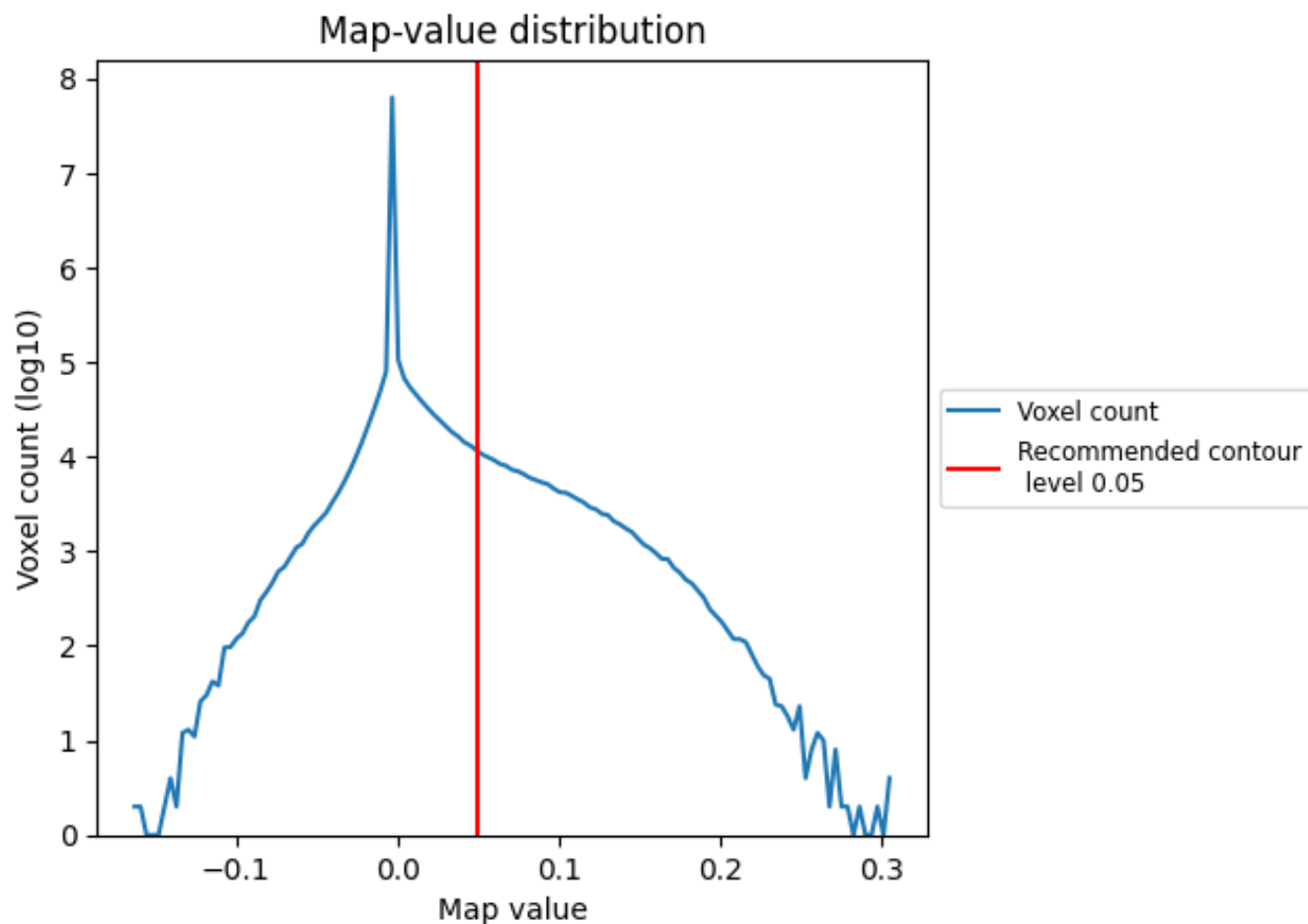
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

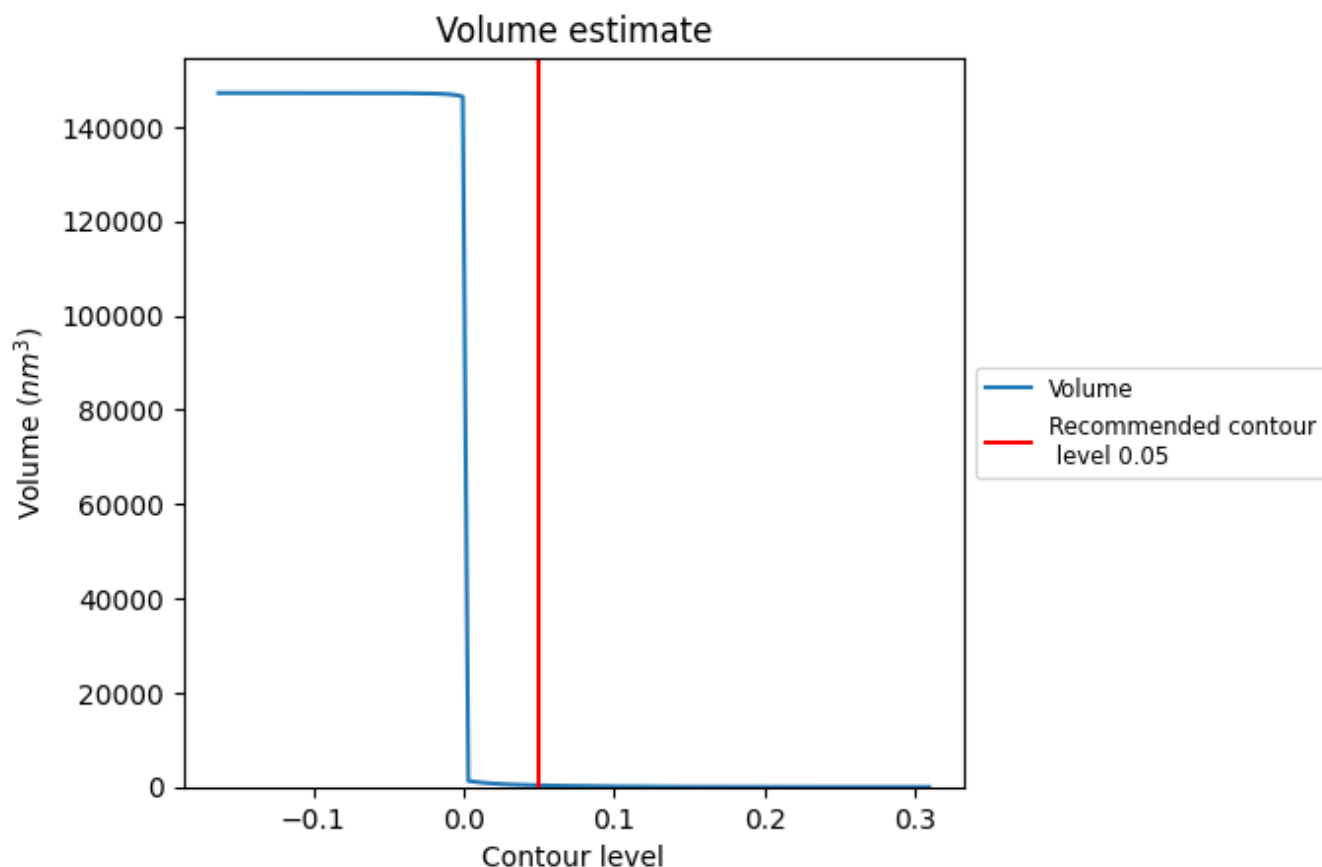
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

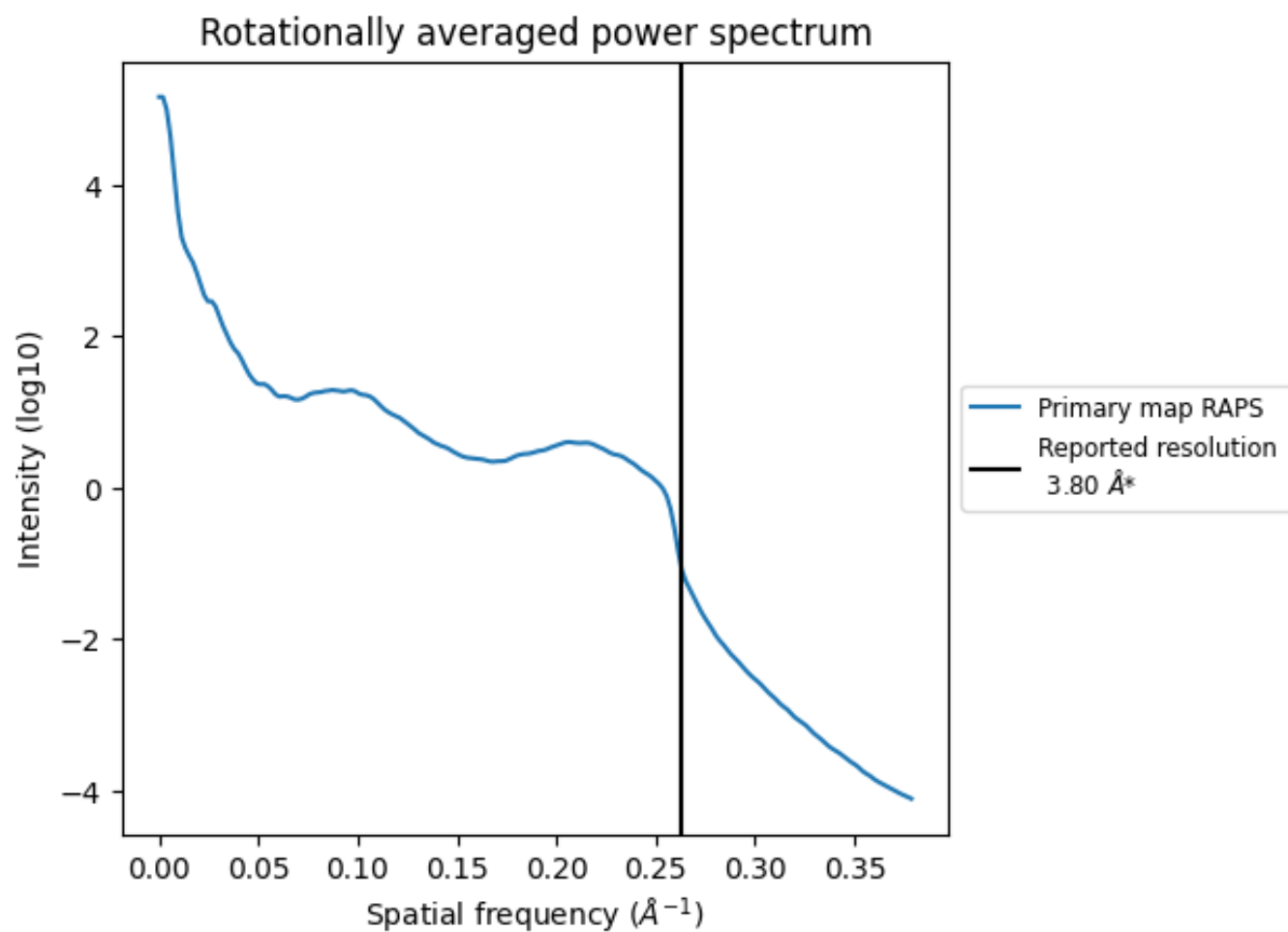
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 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 ⓘ

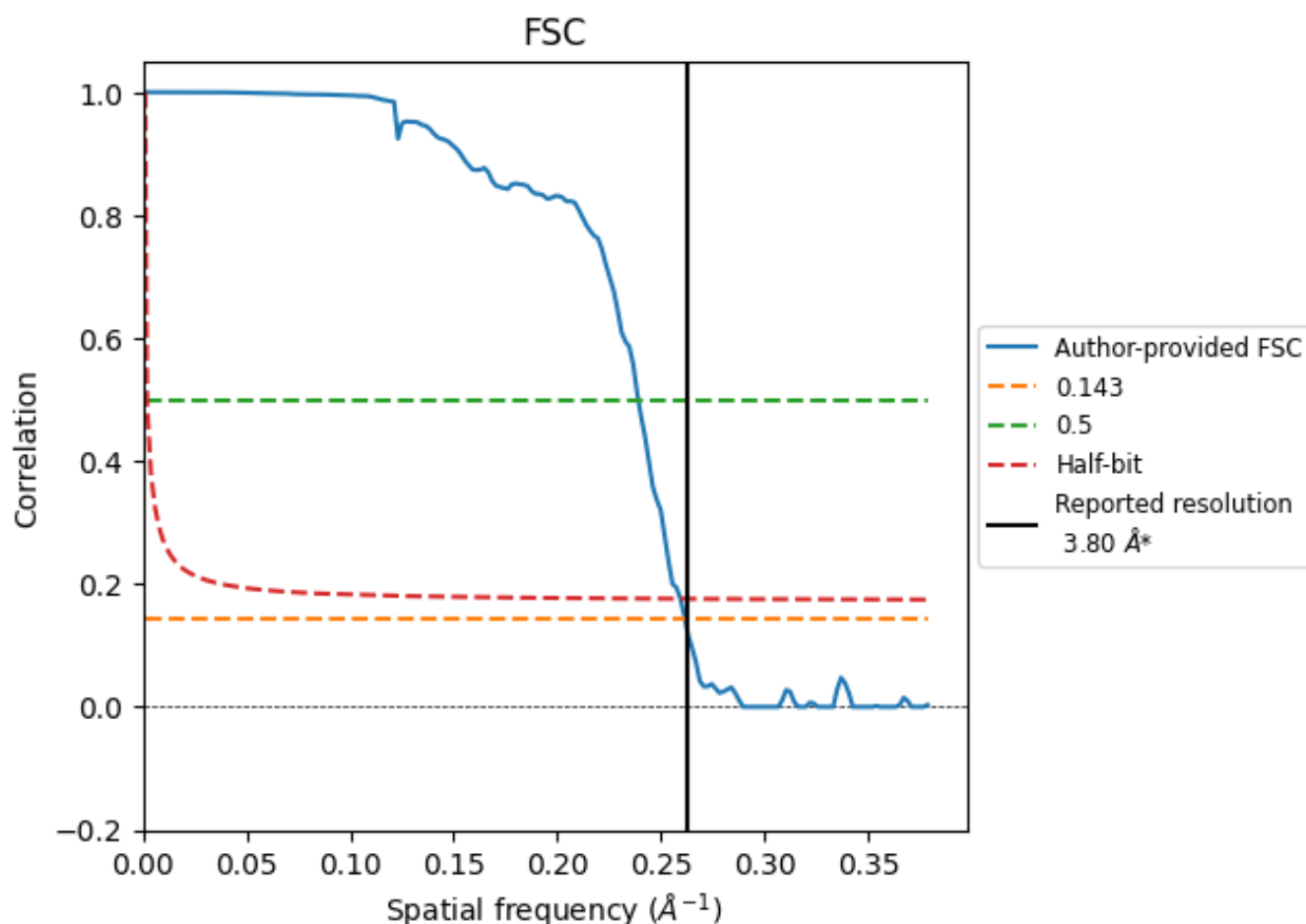


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

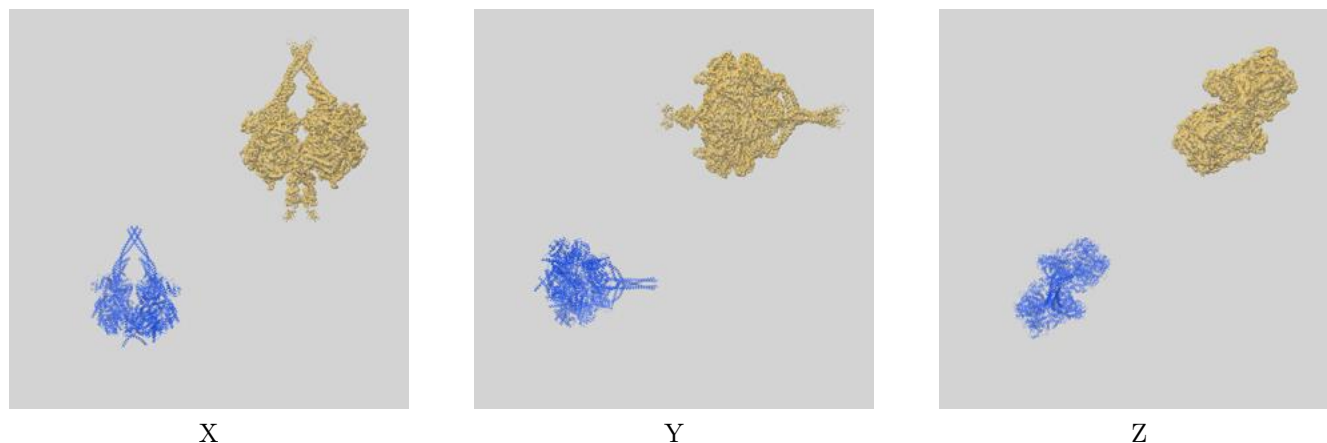
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.18	3.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

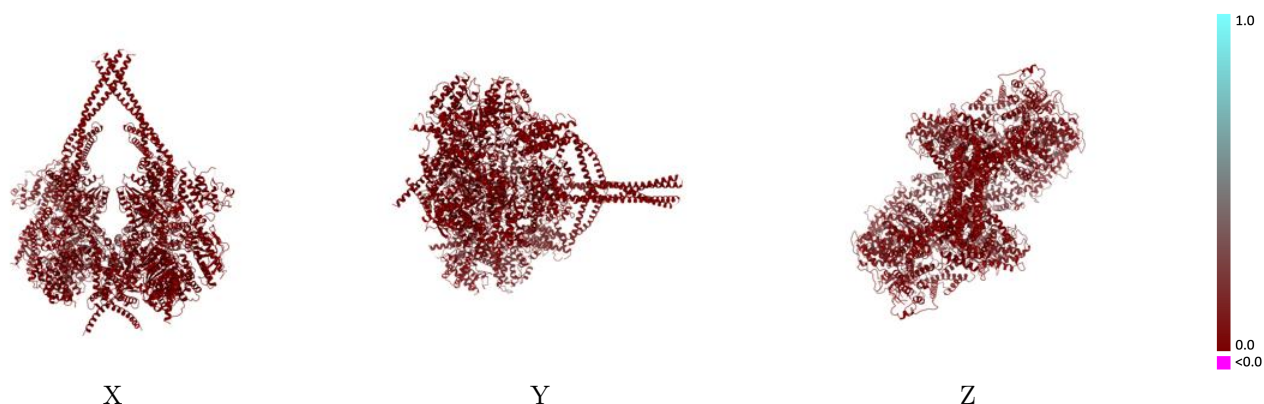
This section contains information regarding the fit between EMDB map EMD-3698 and PDB model 5NUG. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

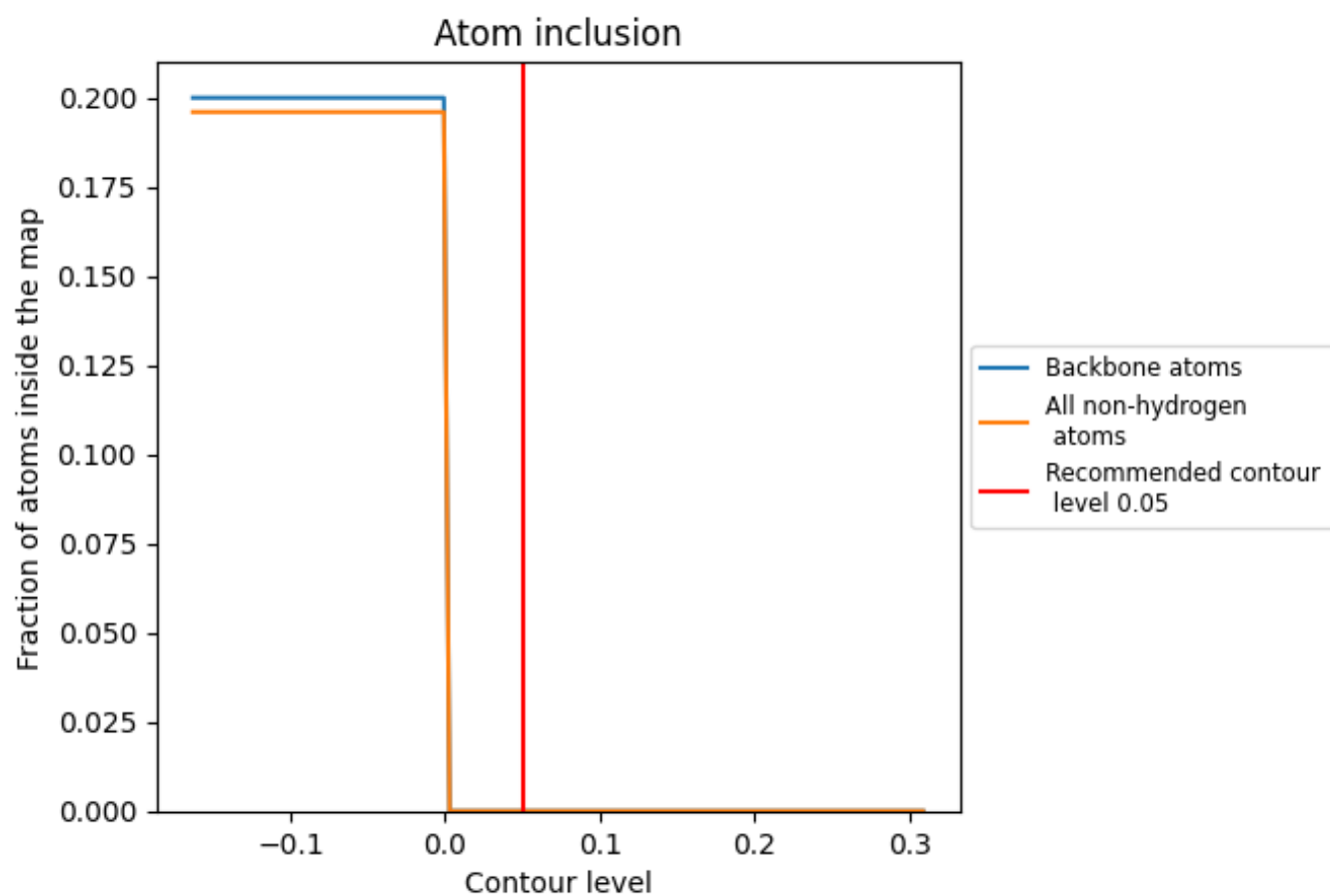


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0000
B	0.0000	0.0000

