



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 04:49 pm GMT

PDB ID : 5NUG
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)

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<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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

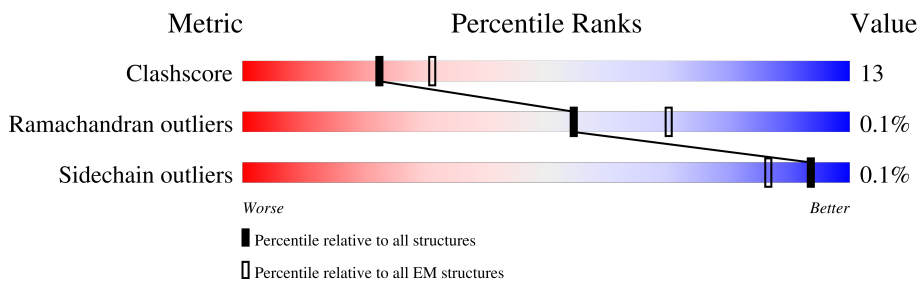
1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	-

2 Entry composition [i](#)

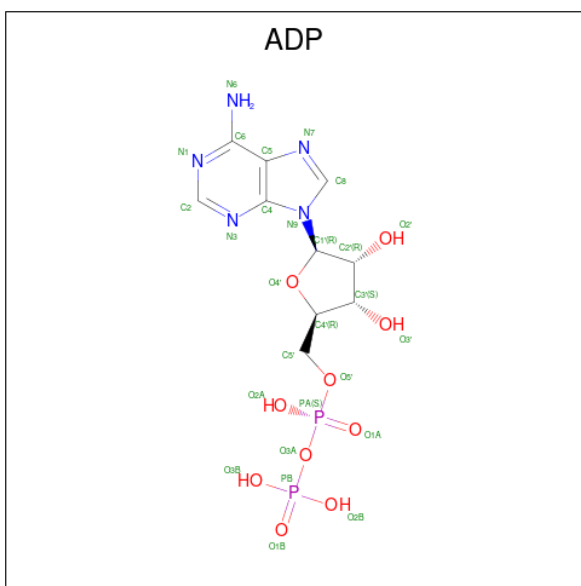
There are 4 unique types of molecules in this entry. The entry contains 46232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		
1	B	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



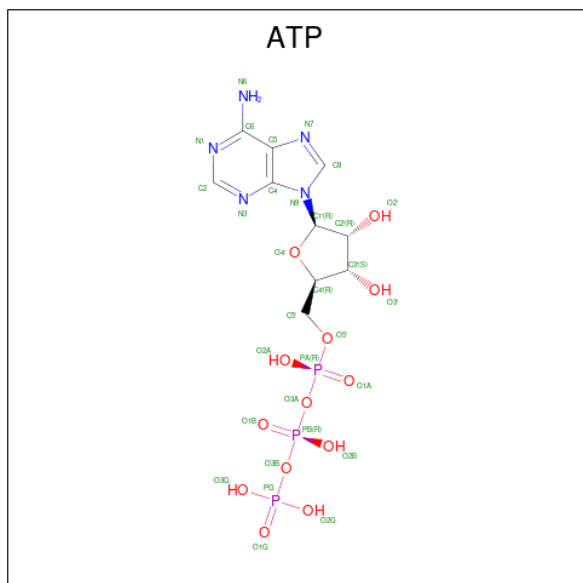
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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 (three-letter code: MG) (formula: Mg).

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

W1741	G1681	L1561	I1501	ALA	VAL	TRP	ARG	GLU	ALA	ASN	GLU	LEU	ARG	PHE
I1742	E1622	P1562	M1502	SER	ALA	GLU	PHE	ASN	LEU	ALA	ASN	LEU	LEU	ASN
D1743	E1623	P1563	S1503	TYR	GLU	GLU	THR	GLN	LEU	LEU	LEU	ARG	THR	PHE
K1744	R1624	E1564	V1504	PHE	LEU	LEU	THR	PRO	GLU	THR	THR	MET	THR	GLN
Y1745	S1625	T1565	S1505	VAL	GLN	GLN	PRO	PRO	ILE	GLN	ASN	GLN	ASN	LYS
F1686	F1626	Q1566	A1506	GLN	ASP	ASP	VAL	TRP	SER	ASP	VAL	GLU	VAL	VAL
A1747	P1627	R1567	M1507	ARG	LEU	LEU	THR	GLY	LYS	ASP	ASP	VAL	VAL	GLU
Q1748	R1628	F1568	K1508	LEU	LEU	LEU	ARG	LEU	GLY	GLY	LEU	VAL	ILE	LEU
L1749	F1629	S1569	L1509	LEU	GLY	GLY	ASN	TYR	ASN	LEU	VAL	GLY	ASN	ILE
V1750	Y1630	S1570	S1510	GLY	TRP	TRP	PRO	ASN	LEU	PRO	PRO	VAL	ARG	GLU
V1751	F1631	I1571	P1511	MET	SER	SER	GLU	ILE	GLU	GLU	ARG	VAL	GLU	GLU
L1752	V1632	S1572	Y1512	ILE	GLU	GLU	GLU	LYS	LEU	GLU	LEU	ASP	LEU	GLU
S1753	G1633	T1573	Y1513	ILE	LEU	LEU	ALA	GLY	HIS	GLY	GLY	ASP	LEU	LYS
A1754	E1634	E1574	K1514	ASN	SER	SER	LEU	TRP	LEU	ALA	ASP	TRP	GLY	GLN
Q1755	D1635	F1575	V1515	MET	LYS	VAL	GLN	VAL	THR	THR	SER	GLY	CYS	ALA
I1756	E1636	F1576	F1516	LEU	VAL	VAL	ALA	GLY	ASP	ALA	ALA	LEU	ARG	LEU
A1757	D1636	L1576	F1516	VAL	TRP	TRP	LEU	ALA	THR	VAL	VAL	ARG	TYR	GLU
W1758	L1637	A1577	E1517	ILE	GLU	GLU	THR	PHE	ALA	MET	VAL	VAL	GLY	ALA
W1759	E1638	L1578	E1518	LEU	LEU	LEU	ILE	ASN	GLY	GLY	PHE	LEU	GLY	LYS
E1760	G1639	M1579	D1519	GLY	GLN	GLN	LYS	ASN	TRP	ASP	THR	THR	THR	ARG
M1761	I1640	K1580	A1520	ILE	ASP	ASP	ASP	ASN	GLY	GLY	GLY	GLY	GLY	TRP
W1762	I1641	K1581	L1521	LEU	TRP	TRP	ILE	ASP	TRP	TRP	ASP	THR	THR	TRP
E1763	G1642	V1582	S1522	LEU	GLU	GLU	LYS	TRP	PHE	THR	ASP	VAL	VAL	ALA
T1764	M1643	S1583	W1523	LEU	GLN	GLN	GLY	ASP	TRP	GLN	GLY	GLN	GLN	TYR
A1765	S1644	K1584	E1524	ASP	TRP	TRP	LYS	ALA	ALA	LYS	VAL	VAL	VAL	LYS
W1766	R1645	S1585	D1525	HIS	VAL	VAL	ASP	ILE	THR	LYS	VAL	VAL	VAL	LYS
W1767	M1646	P1586	K1526	TRP	VAL	VAL	ASP	TRP	THR	ASP	VAL	VAL	VAL	TRP
S1768	V1647	L1587	L1527	GLN	VAL	VAL	GLU	ARG	GLN	TRP	TRP	TRP	TRP	GLN
MET	A1648	V1588	M1528	LEU	GLN	GLN	GLY	GLN	LEU	TRP	LEU	LEU	LEU	LEU
GLY	K1649	M1589	R1529	MET	ARG	ARG	CYS	ASN	ASN	TYR	PRO	ARG	ARG	ASN
GLY	L1650	D1590	L1530	LYS	LYS	LYS	ALA	LYS	ASN	GLN	VAL	VAL	VAL	ASN
GLY	Q1651	V1591	M1531	ARG	LEU	LEU	LYS	LEU	LEU	LEU	ILE	ILE	ILE	ASN
ASP	K1652	L1592	A1532	HIS	ARG	ARG	LYS	GLN	GLN	GLN	LYS	LYS	LYS	TRP
A1775	H1653	M1593	L1533	VAL	LEU	LEU	ASP	ASN	ASN	ASN	GLY	GLN	GLN	ALA
A1776	F1654	I1594	F1534	VAL	VAL	VAL	LEU	ASN	VAL	TRP	VAL	VAL	VAL	GLY
P1777	K1655	Q1595	D1535	VAL	VAL	VAL	ASP	VAL	VAL	ASP	VAL	VAL	VAL	ASP
L1778	K1656	G1596	V1536	VAL	VAL	VAL	ALA	ALA	ALA	VAL	LYS	LYS	LYS	VAL
H1779	M1657	V1597	W1537	GLY	GLU	GLU	LEU	LEU	LEU	LEU	THR	THR	THR	GLY
S1780	F1658	Q1598	I1538	THR	LEU	LEU	GLN	GLN	GLN	GLY	GLY	GLY	GLY	ARG
V1781	A1659	R1599	D1539	GLY	LEU	LEU	LEU	LEU	LEU	SER	SER	SER	SER	ASN
L1782	G1660	S1600	V1540	GLN	ASP	ASP	ASP	GLN	GLN	ASP	ASP	ASP	ASP	ASN
S1783	V1661	L1601	Q1541	LEU	TRP	TRP	ILE	ILE	ILE	TRP	TRP	TRP	TRP	TRP
M1784	S1662	E1602	R1542	THR	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
W1785	G1663	R1603	R1543	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
E1786	E1664	L1604	W1544	ASP	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
W1787	L1665	A1605	V1545	VAL	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
L1788	E1666	D1606	L1546	VAL	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
M1789	M1667	L1607	L1547	GLY	LEU	LEU	SER	SER	SER	SER	SER	SER	SER	SER
M1790	E1668	L1608	L1547	GLY	LEU	LEU	SER	SER	SER	SER	SER	SER	SER	SER
V1791	D1669	G1609	G1548	GLN	PHE	PHE	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY
L1792	M1670	K1610	G1549	THR	ALA	ALA	ALA	ALA	ALA	VAL	VAL	VAL	VAL	VAL
A1793	S1671	I1611	I1550	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D1794	V1672	Q1612	F1551	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
S1795	L1673	K1613	G1553	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
V1796	D1734	A1614	S1554	ASP	ALA	ALA	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
M1797	P1735	L1615	A1555	VAL	ARG	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
M1798	N1736	G1616	D1556	VAL	LEU	LEU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
E1799	T1737	E1617	I1557	ASP	LEU	LEU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
Q1800	Y1738	V1618	K1496	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
	H1739	L1619	H1559	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR
	E1680	E1620	H1560	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN

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										
M1861	A1862	N1863	A1864	K1865	F1866	N1867	Y1868	G1869	F1870	E1871	Y1872	L1873	G1874	V1875	Q1876	D1877	K1878	L1879	V1880	Q1881	T1882	P1883	L1884	T1885	D1886	R1887	C1888	Y1889	L1890	T1891	M1892	T1893	Q1894	A1895	G1896	F1897	D1898	A1899	R1899	F1900	M1901	G1902	S1903	P1904	F1905	G1906	P1907	A1908	G1909	T1910	G1911	L1912	T1913	Y1914	S1915	V1916	K1917	A1918	L1919	G1920									
H1921	Q1922	L1923	G1924	R1925	F1926	V1927	L1928	V1929	F1930	M1931	C1932	D1933	E1934	T1935	F1936	D1937	F1938	Q1939	A1940	M1941	G1942	L1943	I1944	F1945	V1946	G1947	L1948	C1949	Y1950	V1951	Q1952	A1953	W1954	G1955	C1956	D1957	L1958	E1959	F1960	M1961	L1962	L1963	E1964	E1965	L1966	M1967	L1968	S1969	A1970	V1971	S1972	Q1973	Q1974	V1975	Q1976	C1977	L1978	Q1979	E1980										
A1981	L1982	R1983	E1984	H1985	S1986	N1987	PRO	ASN	TVR	ASP	LYS	THR	SER	ALA	F1996	I1997	T1998	C1999	E2000	L2001	L2002	N2003	K2004	Q2005	V2006	K2007	V2008	S2009	P2010	D2011	M2012	A2013	T2014	F2015	T2016	A1955	G1955	C1956	D1957	N2019	P2020	G2021	G2022	Y2022	A2023	G2024	R2025	S2026	N2027	L2028	P2029	D2030	N2031	L2032	K2033	K2034	L2035	F2036	R2037	S2038	L2039	A2040							
M2041	T2042	K2043	P2044	D2045	R2046	Q2047	L2048	I2049	A2050	Q2051	V2052	M2053	L2054	Y2055	S2056	Q2057	G2058	F2059	R2060	L2061	A2062	E2063	V2064	L2065	A2066	N2067	K2068	I2069	V2070	P2071	F2072	F2073	K2074	L2075	C2076	D2077	E2078	Q2079	L2080	S2081	S2082	Q2083	S2084	H2085	Y2086	D2087	F2088	G2089	L2090	R2091	A2092	L2093	K2094	S2095	V2096	L2097	S2098	S2099	A2100										
G2101	N2102	V2103	K2104	R2105	E2106	R2107	T2108	Q2109	K2110	T2111	K2112	L2113	E2114	LYS	GLU	GLU	ARG	GLY	ALA	VAL	ASP	GLU	GLU	ILE	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	T2136	L2137	L2138	L2139	S2140	V2141	C2142	E2143	M2144	W2145	V2146	P2147	K2148	L2149	V2150	A2151	E2152	D2153	T2154	L2155	L2156	L2157	F2158	S2159	L2160												
L2161	S2162	D2163	V2164	P2165	F2166	G2167	V2168	Q2169	Y2170	H2171	R2172	G2173	E2174	M2175	T2176	A2177	L2178	R2179	E2180	L2181	L2182	K2183	K2184	V2185	C2186	Q2187	E2188	M2189	Y2190	L2191	T2192	Y2193	G2194	D2195	G2196	E2197	E2198	V2199	G2200	G2201	M2202	W2203	V2204	E2205	S2206	K2207	V2208	V2209	L2210	Y2211	Q2212	L2213	L2214	Q2215	I2216	N2217	H2218	G2219	L2220										
M2221	V2223	G2224	P2225	S2226	G2227	S2228	G2229	K2230	S2231	M2232	A2233	W2234	R2235	V2236	L2237	L2238	K2239	A2240	L2241	E2242	R2243	L2244	E2245	G2246	V2247	E2248	G2249	V2250	A2251	H2252	L2253	I2254	D2255	P2256	K2257	A2258	L2259	S2260	G2261	D2262	H2263	L2264	Y2265	G2266	T2267	L2268	D2269	M2270	N2271	T2272	L2273	E2274	W2275	T2276	D2277	G2278	L2279	F2280											
T2281	H2282	V2283	L2284	K2285	R2286	L2287	L2288	D2289	S2290	V2291	R2292	G2293	E2294	L2295	Q2296	S2297	R2298	Q2299	V2300	I2301	V2302	F2303	F2304	D2305	G2306	V2307	D2308	P2309	E2310	M2311	V2312	E2313	N2314	L2315	N2316	S2317	V2318	L2319	D2320	D2321	N2322	K2323	L2324	L2325	L2326	L2327	P2328	N2329	G2330	E2331	R2332	L2333	S2334	L2335	P2336	R2337	N2338	V2339	R2340										
I2341	M2342	F2343	E2344	V2345	Q2346	D2347	L2348	K2349	Y2350	A2351	T2352	L2353	A2354	T2355	V2356	S2357	R2358	C2359	G2360	M2361	V2362	K2363	F2364	S2365	S2366	D2367	V2368	L2369	S2370	T2371	D2372	M2373	I2374	F2375	N2376	M2377	F2378	L2379	A2380	D2381	L2382	R2383	S2384	L2385	T2386	L2387	D2388	E2389	GLY	GLU	ASP	GLU	ALA	ARG	ARG	ARG	LYS	GLY											
L2391	L2392	L2393	L2394	L2395	L2396	L2397	L2398	L2399	L2400	L2401	L2402	L2403	L2404	L2405	L2406	L2407	L2408	L2409	L2410	L2411	L2412	L2413	L2414	L2415	L2416	L2417	L2418	L2419	L2420	L2421	L2422	L2423	L2424	L2425	L2426	L2427	L2428	L2429	L2430	L2431	L2432	L2433	L2434	L2435	L2436	L2437	E2438	H2439	A2440	F2441	Q2442	L2443	E2444	H2445	L2446	M2447	D2448	L2449	T2450	R2451	L2452	R2453	C2454	L2455	G2456	S2457	L2458	F2459	S2460
M2461	L2462	H2463	Q2464	A2465	C2466	R2467	N2468	V2469	A2470	Q2471	Y2472	N2473	A2474	N2475	H2476	P2477	D2478	F2479	P2480	M2481	Q2482	G2483	E2484	W2485	L2486	E2487	R2488	V2489	I2490	Q2491	R2492	Y2493	L2494	V2495	Y2496	A2497	I2498	L2499	V2500	S2501	L2502	S2503	G2504	D2505	D2506	S2507	L2508	S2509	M2510	R2511	A2512	E2513	L2514	G2515	E2516	Y2517	I2518	R2519	L2520										
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L2581	L2582	L2583	L2584	L2585	L2586	L2587	L2588	L2589	L2590	L2591	L2592	L2593	L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	L2638	L2639	L2640	
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K3241	K3242	M3243	V3244	K3245	D3246	Q3247	Q3248	E3249	A3250	E3251	K3252	K3253	LYS	VAL	LEU	ALA	GLY	ILE	CYS	LEU	LEU	HIS	GLY	GLN	SER	THR	THR	ASP	TRP	LYS	ASP	GLN	ILE	ARG	SER	ILE	VAL	VAL	PRO	ILE	VAL	ASN	PHE	ILE	PRO	THR	ILE	VAL	ASN	PHE	SER	ILE	ALA	ALA	GLU	GLU	ILE	SER		

D4081	K4082	A4083	T4084	N4085	T4086	A4087	V4088	K4089	S4090	G4091	R4092	W4093	V4094	M4095	L4096	K4097	N4098	V4099	H4100	L4101	A4102	P4103	G4104	W4105	L4106	M4107	Q4108	L4109	E4110	K4111	K4112	L4113	H4114	S4115	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	T4127	M4128	E4129	L4130	M4131	P4132	K4133	V4134	P4135	V4136	M4137	L4138	L4139	R4140		
M4021	F4022	Q4023	P4024	L4025	D4026	L4027	T4028	H4029	L4030	V4031	G4032	T4033	F4034	V4035	K4036	P4037	N4038	T4039	P4040	V4041	L4042	M4043	C4044	S4045	V4046	P4047	G4048	V4049	D4050	A4051	S4052	H4053	H4054	V4055	E4056	D4057	A4058	A4059	A4060	E4061	Q4062	M4063	T4064	Q4065	L4066	T4067	S4068	I4069	A4070	I4071	G4072	S4073	A4074	E4075	G4076	F4077	M4078	S4079	A4080		
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Y3841	E3842	N3843	P3844	L3845	L3846	LYS	GLY	V3849	T3850	D3851	H3852	T3853	Q3854	R3855	L3856	S3857	I3858	I3859	S3860	K3861	D3862	F3864	Q3865	V3866	A3867	F3868	R3869	R3870	V3871	A3872	R3873	G3874	M3875	L3876	H3877	Q3878	H3879	H3880	I3881	T3882	F3883	A3884	M3885	L3886	L3887	A3888	R3889	I3890	K3891	L3892	K3893	G3894	L3895	G3897	E3898	T3899					
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I3541	Q3542	F3543	R3544	K3545	D3546	I3547	A3548	R3549	T3550	E3551	Y3552	L3553	S3554	N3555	A3556	D3557	R3558	R3559	L3560	R3561	Y3562	Q3563	A3564	S3565	S3566	L3567	P3568	A3569	D3570	D3571	L3572	C3573	T3574	E3575	A3576	A3577	I3578	M3579	L3580	K3581	R3582	F3583	N3584	R3585	Y3586	P3587	L3588	I3589	I3590	D3591	P3592	S3593	G3594	Q3595	A3596	L3597	F3598	I3599	L3600		
S3481	L3482	S3483	A3484	E3485	R3486	E3487	R3488	W3489	E3490	T3491	T3492	S3493	E3494	T3495	F3496	K3497	N3498	Q3499	N3500	S3501	R3502	L3503	A3504	G3505	D3506	C3507	L3508	L3509	S3510	A3511	A3512	F3513	L3514	A3515	Y3516	A3517	G3518	Y3519	F3520	D3521	Q3522	Q3523	N3524	R3525	R3526	N3527	L3528	F3529	T3530	T3531	W3532	S3533	H3534	H3535	L3536	Q3537	A3538	I3539	N3540		
ASP	ALA	ILE	ARG	LYS	GLY	MET	LYS	LYS	ASN	TYR	MET	SER	ASN	PRO	SER	TYR	TYR	GLY	ILE	VAL	ASN	ARG	ALA	SER	LEU	ALA	CYS	GLY	PRO	MET	VAL	LYS	TRP	ALA	ILE	ALA	GLN	ASN	TYR	ALA	ASP	MET	LEU	LYS	ARG	VAL	GLY	PRO	LEU	ARG	ASN	GLY	LEU	GLN	LYS	LEU	GLY				
ASP	ASP	LYS	ASP	ASN	GLN	GLN	LYS	LYS	ALA	TYR	GLY	VAL	GLU	Q3435	M3436	I3437	R3438	D3439	L3440	E3441	A3442	S3443	SER	LEU	ALA	ALA	CYS	GLY	PRO	MET	VAL	LYS	TRP	Y3451	A3452	V3453	L3454	I3455	S3456	A3457	A3458	Q3459	A3460	I3461	K3462	A3463	D3464	L3465	A3466	A3467	A3470	K3471	N3472	N3473	R3474	S3475	T3476	A3477	L3478	L3479	K3480

LYS	ASN	GLU	ALA	TRP	VAL	TRP	GLU	THR	ARG	GLU	ASN	PHE	LEU	LEU	ALA	GLU	ASP	ASN	ASN	GLU	THR	VAL	THR	GLN	LEU	GLY	THR	ASP	LEU	
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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
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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
L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220
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

D3001	A2941	Y2881	L2821	S2761	V2701	Y2641	L2581	I2521	M2461	LYS	I2341	T2281
S3002	G2942	L2882	L2822	L2762	K2702	R2642	Y2582	T2522	L2462	GLU	M2342	H2282
G3003	K2943	P2883	E2823	R2763	L2703	R2643	T2583	T2523	H2463	ASP	F2343	V2283
F3004	T2944	V2884	I2824	T2764	E2704	T2644	W2584	V2524	Q2464	GLY	E2344	L2284
L3005	L2945	D2885	W2825	A2765	R2705	P2645	A2585	L2525	A2465	GLU	Q2345	R2285
E3006	L2946	Q2886	A2826	Y2766	I2706	N2646	A2586	L2526	C2466	GLU	Q2346	R2286
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N3008	R2948	E2888	E2828	P2768	F2708	V2648	H2588	T2528	N2468	A2409	L2348	I2288
N3009	F2949	L2889	A2829	L2769	V2709	V2649	L2589	A2529	V2469	S2410	K2349	D2289
T3010	V2950	R2890	L2830	T2770	G2710	L2650	P2590	P2530	A2470	M2411	Y2350	S2290
L3011	A2951	D2891	R2831	A2771	A2711	A2651	L2591	N2531	Q2471	M2412	A2351	V2291
L3012	V2952	V2892	L2832	A2772	G2712	P2652	V2592	L2532	Y2472	L2413	T2352	R2292
A3013	M2953	V2893	F2833	M2773	N2713	V2653	L2593	P2533	M2473	I2415	L2353	G2293
N3014	N2954	K2894	Q2834	Q2774	P2714	Q2654	C2594	I2534	A2474	R2416	A2354	E2294
G3015	G2955	A2895	D2835	E2775	P2715	L2655	G2595	I2535	M2475	Q2417	T2355	L2295
E3016	L2956	R2896	R2836	F2776	T2716	G2656	P2596	D2536	H2476	D2418	V2356	Q2296
V3017	S2957	L2897	L2837	Y2777	D2717	K2657	P2597	Y2537	P2477	A2419	R2357	R2297
P3018	V2958	K2898	V2838	T2778	P2718	W2658	G2598	E2538	F2478	A2420	R2358	R2298
G3019	Y2959	V2899	E2839	M2779	G2719	L2659	S2599	V2539	F2479	A2420	C2359	Q2299
L3020	Q2960	F2900	D2840	S2780	R2720	V2660	G2600	S2540	P2480	I2422	G2360	W2300
F3021	L2961	Y2901	E2841	Q2781	K2721	L2661	T2601	I2541	M2481	M2423	M2361	I2301
E3022	K2962	E2902	E2842	E2782	P2722	F2662	R2602	S2542	Q2482	Q2424	V2362	V2302
G3023	V2963	E2903	R2843	R2783	L2723	C2663	M2603	G2543	I2483	P2425	W2363	F2303
D3024	H2964	E2904	R2844	F2784	S2724	D2664	T2604	E2544	E2484	Y2426	F2364	D2304
E3025	R2965	L2905	W2845	T2785	H2725	E2665	L2605	W2545	Q2485	F2427	S2365	G2305
S3026	K2966	D2906	R2846	Q2786	R2726	I2666	F2606	S2546	I2486	T2428	E2366	D2306
A3027	Y2967	V2907	D2847	D2787	F2727	N2667	S2607	P2547	E2487	S2429	D2367	V2307
T3028	T2968	L2908	E2848	T2788	L2728	L2668	A2608	W2548	R2488	M2430	V2368	D2308
L3029	G2969	F2909	N2849	Q2789	R2729	P2669	L2609	Q2549	Y2489	G2431	L2369	P2309
N3030	E2970	V2910	I2850	T2790	H2730	D2670	R2610	A2550	I2490	V2433	S2370	E2310
T3031	D2971	L2911	D2851	H2791	Y2731	M2671	A2611	K2551	Q2491	I2433	T2371	W2311
Q3032	F2972	M2912	T2852	Y2792	P2732	D2672	L2612	V2552	R2492	T2434	D2372	V2312
C3033	D2973	N2913	V2853	I2793	K2673	K2673	P2613	P2553	Y2493	T2435	M2373	E2313
E3035	E2974	E2914	A2854	Y2794	Y2734	Y2674	D2614	Q2554	L2494	A2436	I2374	N2314
G3036	D2975	V2915	L2855	I2795	W2675	G2675	M2615	I2555	V2495	L2437	F2375	L2315
A3037	L2976	L2916	K2856	S2796	Y2736	T2676	E2616	E2556	Y2496	E2438	N2376	N2316
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R3039	T2978	E2918	F2858	E2798	Y2738	V2678	W2618	E2558	I2498	A2440	F2378	V2318
L3040	V2979	V2919	P2859	M2799	P2739	G2679	G2619	T2559	L2499	F2441	L2379	L2319
E3041	L2980	L2920	M2860	T2800	G2740	I2680	L2620	H2560	W2500	Q2442	A2380	D2320
G3042	R2981	R2921	I2861	R2801	P2741	S2681	M2621	K2561	S2501	L2443	R2381	D2321
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R3044	G2983	D2923	R2863	V2803	S2743	I2683	S2623	A2563	S2503	H2445	R2383	K2323
D3045	C2984	R2924	E2864	R2804	L2744	R2684	S2624	A2564	G2504	I2446	S2384	L2324
S3046	C2985	L2925	A2865	G2805	T2745	Q2685	A2625	P2565	D2505	M2447	I2385	L2325
K3047	K2986	F2926	A2866	L2806	Q2746	Q2686	I2626	D2566	S2506	D2448	P2386	T2326
E3048	N2987	R2927	M2867	T2807	I2747	V2687	T2627	V2567	R2507	L2449	L2387	L2327
E3049	E2988	Q2928	S2868	E2808	Y2748	E2688	P2628	V2568	L2508	T2450	D2388	P2328
L3050	P2989	P2929	R2869	A2809	G2749	H2689	E2629	V2569	K2509	R2451	E2389	M2329
Y3051	I2990	L2930	P2870	L2810	T2750	G2690	L2630	P2570	M2510	L2452	GLY	Q2330
K3052	A2991	G2931	I2871	R2811	F2751	G2691	L2631	T2571	R2511	R2453	ASP	E2331
F3053	F2992	L2932	L2872	P2812	N2752	F2692	L2632	L2572	A2512	C2454	GLU	R2332
W3054	I2993	L2933	Y2873	L2813	R2753	Y2693	K2633	D2573	E2513	L2455	ALA	L2333
F3055	M2994	L2934	E2874	E2814	A2754	T2694	T2634	T2574	L2514	G2456	GLM	S2334
D3056	D2995	L2935	N2875	T2815	M2755	T2695	F2635	V2575	G2515	S2457	ARG	L2335
S3057	E2996	L2936	W2876	L2816	L2756	D2696	D2636	R2576	E2516	L2458	ARG	P2336
Q3057	S2997	G2937	W2877	R2817	R2757	D2697	D2637	H2577	I2517	F2459	ARG	P2337
L3058	N2998	V2938	L2878	V2818	L2758	Q2698	Y2638	E2578	T2518	S2460	LYS	N2338
S2999	V2999	S2939	K2879	E2819	I2759	T2699	C2639	A2579	R2519		GLY	V2339
R3060	L3000	G2940	D2880	G2820	P2760	W2700	E2640	L2580	R2520			R2340

T3781	R3061	L3121	N3181	K3241	LYS	ASP	S9481	I3541	M3601	L3661	R3721	T3781
R3782	L3062	V3122	H3182	K3242	GLN	ASP	L3482	Q3542	N3602	I3662	P3722	R3782
K3783	R3063	P3123	Y3183	M3243	HIS	ALA	S9483	F3543	E3603	T3663	D3723	K3783
V3784	V3064	D3124	A3184	V3244	LEU	ARG	A3484	R3544	Y3604	L3664	V3724	V3784
E3785	V3065	M3125	N3185	K3245	VAL	GLY	A3485	D3545	K3605	G3665	D3725	E3785
E3786	V3066	M3126	L3186	D3246	VAL	MET	R3486	D3546	K3606	D3666	E3726	E3786
T3787	T3067	P3127	F3187	Q3247	ARG	LYS	E3487	I3547	R3607	Q3667	K3727	T3787
D3788	M3068	V3128	H3188	Q3248	SER	ASN	R3488	A3548	K3608	D3668	R3728	D3788
V3789	R3069	V3129	E3189	E3249	MET	TRP	W3489	R3549	I3609	I3669	S3729	V3789
M3791	P3070	Y3130	K3190	A3250	ASN	PRO	E3490	T3550	T3609	D3670	D3730	M3791
Q3792	S3071	D3131	R3191	E3251	PRO	ALA	K3491	E3551	T3610	L3671	L3731	Q3792
E3793	S3072	K3132	S3192	K3252	ALA	SER	T3492	Y3552	T3612	S3672	L3732	E3793
V3794	E3073	L3133	E3193	K3253	VAL	TRV	S3493	L3553	S3613	S3673	K3733	V3794
E3795	G3074	P3134	L3194	VAL	LYS	ASN	M3436	M3554	F3614	S3674	L3734	E3795
T3796	L3075	Q3135	E3195	VAL	LEU	LEU	I3437	N3555	L3615	F3675	Q3735	T3796
V3797	K3076	P3136	E3196	MET	ALA	ALA	R3438	A3556	D3616	V3676	G3736	V3797
S3798	D3077	P3137	Q3197	GLN	LEU	LEU	F3496	D3557	D3617	I3677	E3737	S3798
Q3799	R3078	S3138	Q3198	GLU	SER	ASN	N3498	E3558	A3618	F3678	F3738	Q3799
Q3800	A3079	H3139	M3199	ILE	SER	ALA	Q3499	R3559	F3619	L3679	Q3739	Q3800
Y3801	A3080	R3140	H3200	GLU	CYS	SER	M3500	L3560	R3620	S3680	L3740	Y3801
P3803	T3081	E3141	L3201	LEU	LEU	LEU	S3501	W3562	K3621	T3681	R3741	P3803
L3804	F3083	A3142	N3202	LEU	LEU	ALA	A3445	Q3563	L3622	R3682	L3742	L3804
S3805	A3084	I3143	V3203	HIS	GLY	GLY	R3446	R3564	L3623	D3683	R3743	S3805
T3806	L3085	V3144	G3204	GLN	GLY	GLN	I3447	A3564	E3624	P3684	Q3744	T3806
A3807	L3086	N3145	L3205	GLN	SER	THR	Y3447	S3565	S3625	T3685	L3745	A3807
C3808	R3087	S3146	R3206	GLU	THR	THR	E3449	S3566	A3626	V3687	E3746	C3808
S3809	R3088	C3147	K3207	VAL	LYS	TRP	E3450	L3567	L3627	E3687	K3747	S3809
S3810	C3089	V3148	I3208	ALA	ALA	ALA	Y3451	P3568	R3628	F3688	S3748	S3810
I3811	V3090	F3149	R3209	ASP	GLN	ASP	A3452	A3569	F3629	P3689	L3749	I3811
Y3812	L3091	V3150	E3210	LYS	ILE	ILE	R3453	R3570	Q3630	Q3690	L3750	Y3812
F3813	N3092	H3151	T3211	GLN	ARG	ALA	L3454	D3571	N3631	R3691	Q3751	F3813
M3815	W3093	Q3152	V3212	ASN	ILE	ASN	S3455	L3572	P3632	L3692	A3752	M3815
E3816	G3095	T3153	W3213	VAL	ILE	VAL	I3456	F3573	L3633	C3693	L3753	E3816
L3817	D3096	L3154	Q3214	GLU	ARG	ASP	E3457	T3574	L3634	S3694	M3754	L3817
S3818	W3097	H3155	R3215	ASP	GLU	MET	A3458	E3575	V3635	R3695	E3755	S3818
R3819	R3099	Q3156	E3216	LEU	ASN	LEU	Q3459	N3576	Q3636	V3696	V3756	R3819
Q3820	E3100	R3158	E3217	ASP	PHE	LYS	A3460	A3577	D3637	F3697	K3757	Q3820
H3822	A3101	N3158	R3218	LYS	ASN	LYS	I3461	I3578	V3638	V3698	G3758	H3822
F3823	F3102	A3161	R3219	VAL	PRO	VAL	R3462	M3579	E3639	V3699	R3759	F3823
L3824	F3103	R3162	R3220	PRO	ALA	ALA	A3463	L3580	S3640	N3700	I3760	L3824
Q3825	Y3104	L3161	D3221	ALA	ASN	ILE	D3464	K3581	Y3641	F3701	L3761	Q3825
Y3826	V3105	A3162	L3222	ILE	ASN	PHE	L3465	R3582	D3642	T3702	T3762	Y3826
Y3827	G3106	K3163	R3223	GLU	SER	GLU	A3466	F3583	F3643	V3703	D3763	Y3827
Y3828	R3107	R3164	I3224	ALA	ALA	ALA	M3467	F3584	V3644	T3704	D3764	Y3828
S3828	E3108	G3165	S3225	ASN	GLU	GLU	V3468	R3585	L3645	R3705	T3765	S3828
Q3830	F3109	G3166	Q3227	VAL	VAL	VAL	E3469	Y3586	N3646	S3706	I3766	Q3830
F3831	T3110	R3167	Q3228	LEU	SER	SER	A3470	P3587	F3647	S3707	I3767	F3831
L3833	F3111	T3168	E3228	ILE	ILE	ILE	V3471	L3588	V3648	L3708	T3768	L3833
R3834	S3111	M3169	E3229	LYS	ASN	ASN	M3472	I3589	L3649	Q3709	T3769	R3834
R3835	K3112	A3170	E3230	ASN	ASN	ASN	N3473	I3590	N3650	S3710	L3770	R3835
Y3836	R3113	I3171	V3231	GLN	GLU	GLU	R3474	D3591	R3651	Q3711	E3771	Y3836
H3837	D3114	T3172	K3232	ASN	GLN	GLN	T3475	P3592	E3652	C3712	L3772	H3837
R3838	L3115	R3173	N3233	LYS	LYS	LYS	T3476	S3593	F3653	L3713	L3773	R3838
F3839	E3116	H3175	A3234	ASN	LEU	LEU	A3477	Q3594	R3654	N3714	K3774	F3839
L3840	R3117	Y3176	A3235	LEU	LEU	LEU	L3478	Q3595	R3655	E3715	R3775	L3840
	R3118	L3177	L3236	VAL	VAL	VAL	L3479	A3596	T3656	V3716	L3717	
	R3119	F3179	K3239	SER	SER	SER	K3480	T3597	Q3657	L3717	K3718	
	Y3120	L3180	L3240	LYS	LYS	LYS		F3599	R3659	A3719	A3719	
								I3600	V3660	E3720	E3720	

T4561	T4562	T4563	T4564	T4565	T4566	T4567	T4568	T4569	T4570	T4571	T4572	T4573	T4574	T4575	T4576	T4577	T4578	T4579	T4580	T4581	T4582	T4583	T4584	T4585	T4586	T4587	T4588	T4589	T4590	T4591	T4592	T4593	T4594	T4595	THR	ASN	THR	THR	LYS	LYS	ALA	S4603	V4604	V4605	T4606	L4607	V4608	V4609	Y4610	L4611	N4612	F4613	T4614	R4615	A4616	D4617	L4618	I4619	F4620			
ALA	K4502	E4503	K4504	K4505	M4506	I4507	H4508	V4509	C4510	L4511	G4512	G4513	L4514	F4515	V4516	P4517	E4518	A4519	Y4520	I4521	T4522	A4523	T4524	R4525	Q4526	Y4527	V4528	A4529	Q4530	A4531	M4532	S4533	W4534	S4535	L4536	E4537	E4538	L4539	C4540	L4541	E4542	V4543	M4544	V4545	THR	THR	THR	GLN	GLY	ALA	ALA	THR	LEU	ASP	ALA	CYS	S4557	F4558	G4559	Y4560	GLY	GLY
K4441	K4442	K4443	Q4444	T4445	M4446	Y4447	L4448	R4449	T4450	L4451	I4452	M4453	E4454	L4455	V4456	K4457	G4458	I4459	L4460	P4461	L4462	S4463	W4464	S4465	H4466	Y4467	T4468	V4469	P4470	A4471	G4472	M4473	T4474	V4475	I4476	Q4477	K4478	M4479	S4480	D4481	F4482	S4483	E4484	R4485	L4486	K4487	Q4488	L4489	Q4490	M4491	T4492	S4493	L4494	A4495	A4496	Q4497	S4498	GLY	GLY			
H4381	T4382	T4383	A4384	S4385	M4386	W4387	L4388	H4389	L4390	I4391	P4392	Q4393	T4394	L4395	S4396	H4397	L4398	K4399	R4400	T4401	VAL	E4403	M4404	I4405	K4406	D4407	P4408	L4409	F4410	R4411	F4412	F4413	E4414	R4415	E4416	V4417	K4418	M4419	G4420	A4421	L4422	L4423	L4424	Q4425	D4426	V4427	R4428	Q4429	PRO	ALA	D4430	L4431	A4432	D4433	V4434	V4435	Q4436	V4437	C4438	E4439	G4440	
L4321	G4322	L4323	P4324	M4325	M4326	A4327	E4328	R4329	V4330	L4331	L4332	T4333	T4334	Q4335	G4336	V4337	D4338	M4339	I4340	S4341	K4342	M4343	L4344	K4345	M4346	Q4347	L4348	E4350	ASP	GLU	ASP	ASP	LEU	ALA	TWR	ALA	GLU	THR	THR	LYS	THR	ARG	THR	ASP	THR	THR	SER	ASP	GLY	GLY	ARG	ARG	PRO	ALA	TRP	MET	ARG	T4379	L4380			
D4261	Q4262	R4263	L4264	L4265	M4266	T4267	F4268	L4269	E4270	R4271	L4272	F4273	T4274	T4275	R4276	S4277	F4278	D4279	S4280	E4281	F4282	K4283	L4284	A4285	C4286	K4287	V4288	D4289	G4290	H4291	M4292	D4293	I4294	ALA	Q4295	M4296	P4297	D4298	I4299	G4299	W4300	R4301	A4302	E4303	F4304	F4305	V4306	Q4307	W4308	V4309	E4310	L4311	L4312	P4313	D4314	T4315	Q4316	T4317	P4318	S4319	W4320	
W4201	S4202	K4203	K4204	F4205	E4206	F4207	G4208	E4209	S4210	D4211	L4212	R4213	S4214	A4215	C4216	D4217	T4218	V4219	D4220	T4221	W4222	L4223	D4224	D4225	D4226	A4227	R4228	G4229	R4230	Q4231	M4232	I4233	S4234	ALA	P4235	D4236	K4237	A4238	P4239	W4240	S4241	R4242	L4243	K4244	T4245	W4246	M4247	A4248	Q4249	S4250	I4251	Y4252	G4253	G4254	R4255	R4256	D4257	M4258	E4259	F4260		
A4141	G4142	R4143	T4144	F4145	W4146	F4147	E4148	P4149	P4150	P4151	G4152	W4153	K4154	A4155	W4156	W4157	L4158	R4159	D4160	F4161	S4162	S4163	T4164	A4165	W4166	S4167	R4168	L4169	Q4170	K4171	S4172	P4173	L4174	ALA	E4175	R4176	A4177	L4178	L4179	V4180	F4181	A4182	L4183	A4184	W4185	W4186	H4187	A4188	T4189	I4190	Q4191	E4192	R4193	L4194	R4195	W4196	A4197	L4198	L4199	G4200		
D4081	K4082	A4083	I4084	N4085	T4086	A4087	V4088	K4089	S4090	G4091	R4092	W4093	W4094	M4095	L4096	K4097	M4098	V4099	H4100	L4101	A4102	P4103	G4104	W4105	L4106	M4107	Q4108	L4109	E4110	K4111	K4112	L4113	H4114	S4115	L4116	Q4117	P4118	H4119	A4120	C4121	F4122	R4123	L4124	F4125	L4126	T4127	M4128	E4129	I4130	M4131	P4132	K4133	V4134	P4135	W4136	M4137	L4138	L4139	R4140			
M4021	E4022	Q4023	P4024	L4025	M4026	L4027	T4028	H4029	L4030	G4031	G4032	T4033	E4034	V4035	K4036	P4037	M4038	T4039	P4040	W4041	L4042	M4043	C4044	S4045	W4046	P4047	G4048	Y4049	D4050	A4051	S4052	G4053	H4054	W4055	E4056	D4057	L4058	A4059	A4060	E4061	Q4062	M4063	M4064	A4065	H4066	M4067	T4068	V4069	S4070	I4069	A4071	G4072	S4073	A4074	E4075	G4076	F4077	M4078	S4079	A4080		
L3961	D3962	S3963	S3964	S3965	S3966	E3967	Q3968	S3969	V3970	P3971	Y3972	L3973	W3974	SER	GLU	T3978	P3979	A3980	T3981	P3982	S3983	Q3984	Q3985	A3986	S3987	F3988	M3989	L3990	E3991	L3992	S3993	Q3994	A3995	F3996	R3997	P3998	R4000	R4001	L4002	A4003	M4004	A4005	H4006	M4007	F4008	V4009	S4010	K3991	M4012	L4013	G4014	E4015	S4016	F4017	M4018	S4019	I4020					
Y3901	D3902	A3903	E3904	F3905	Q3906	H3907	F3908	L3909	R3910	G3911	N3912	S3913	I3914	V3915	L3916	S3917	A3918	G3919	S3920	T3921	P3922	R3923	I3924	Q3925	G3926	L3927	T3928	Y3929	E3930	Q3931	A3932	E3933	G3934	M3935	V3936	R3937	L3938	S3939	C3940	L3941	P3942	A3943	F3944	M3945	K3946	L3947	I3948	K3949	V3951	Q3952	A3953	G3954	E3955	Q3956	F3957	M3958	I3959	W3960				
Y3841	E3842	R3843	P3844	R3845	L3846	LYS	GLY	V3849	T3850	D3851	H3852	L3853	Q3854	R3855	L3856	S3857	T3858	I3859	T3860	K3861	D3862	L3863	F3864	Q3865	V3866	A3867	F3868	M3869	R3870	V3871	A3872	R3873	K3874	G3875	L3876	H3877	Q3878	D3879	H3880	I3881	T3882	F3883	A3884	M3885	L3886	L3887	A3888	R3889	I3890	K3891	L3892	K3893	G3894	T3895	VAL	G3897	E3898	F3899	T3900			

T4.621	Y4.622	D4.623	F4.624	E4.625	I4.626	A4.627	T4.628	R4.629	E4.630	D4.631	P4.632	R4.633	S4.634	F4.635	Y4.636	E4.637	R4.638	C4.639	Y4.640	A4.641	Y4.642	L4.643	C4.644	T4.645	E4.646
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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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/23474	0.71	4/31851 (0.0%)
1	B	0.43	0/23474	0.71	4/31851 (0.0%)
All	All	0.43	0/46948	0.71	8/63702 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3821	ILE	N-CA-C	5.74	126.51	111.00
1	B	3821	ILE	N-CA-C	5.74	126.51	111.00
1	A	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	3578	ILE	CB-CA-C	-5.10	101.40	111.60

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	23003	0	22805	587	0
1	B	23003	0	22805	582	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	1155	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 1155 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: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
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG2	1.50	1.45
1:A:3749:LEU:HD13	1:A:3773:LEU:CD1	1.44	1.43

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%)	51 83
1	B	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	51 83
All	All	5776/9292 (62%)	5428 (94%)	342 (6%)	6 (0%)	54 83

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2472/4125 (60%)	2469 (100%)	3 (0%)	93	97
1	B	2472/4125 (60%)	2469 (100%)	3 (0%)	93	97
All	All	4944/8250 (60%)	4938 (100%)	6 (0%)	93	97

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

Mol	Chain	Res	Type
1	B	2796	PRO
1	B	3825	TYR
1	B	3905	PHE
1	A	3825	TYR
1	A	2796	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2913	ASN
1	B	4393	GLN
1	B	3014	ASN
1	B	3540	ASN
1	B	4566	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 monosaccharides 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	4805	-	24,29,29	0.86	0	29,45,45	1.58	7 (24%)
2	ADP	B	4805	-	24,29,29	0.86	0	29,45,45	1.58	7 (24%)
2	ADP	B	4801	-	24,29,29	1.09	2 (8%)	29,45,45	1.61	5 (17%)
3	ATP	B	4802	4	26,33,33	0.96	1 (3%)	31,52,52	1.77	7 (22%)
3	ATP	A	4802	4	26,33,33	0.97	1 (3%)	31,52,52	1.77	7 (22%)
2	ADP	B	4804	-	24,29,29	0.94	1 (4%)	29,45,45	1.69	5 (17%)
2	ADP	A	4801	-	24,29,29	1.10	2 (8%)	29,45,45	1.61	5 (17%)
2	ADP	A	4804	-	24,29,29	0.94	1 (4%)	29,45,45	1.69	5 (17%)

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	4805	-	-	2/12/32/32	0/3/3/3
2	ADP	B	4805	-	-	2/12/32/32	0/3/3/3
2	ADP	B	4801	-	-	3/12/32/32	0/3/3/3
3	ATP	B	4802	4	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4802	4	-	1/18/38/38	0/3/3/3
2	ADP	B	4804	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4801	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4804	-	-	3/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4801	ADP	C5-C4	2.58	1.47	1.40
2	A	4801	ADP	C5-C4	2.57	1.47	1.40
2	A	4801	ADP	C2-N3	2.51	1.36	1.32
3	A	4802	ATP	C5-C4	2.47	1.47	1.40
2	B	4801	ADP	C2-N3	2.45	1.36	1.32

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4802	ATP	PA-O3A-PB	-5.44	114.16	132.83
3	B	4802	ATP	PA-O3A-PB	-5.44	114.16	132.83
2	A	4804	ADP	PA-O3A-PB	-4.51	117.35	132.83
2	B	4804	ADP	PA-O3A-PB	-4.51	117.35	132.83
2	B	4801	ADP	PA-O3A-PB	-4.15	118.57	132.83

There are no chirality outliers.

5 of 18 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:

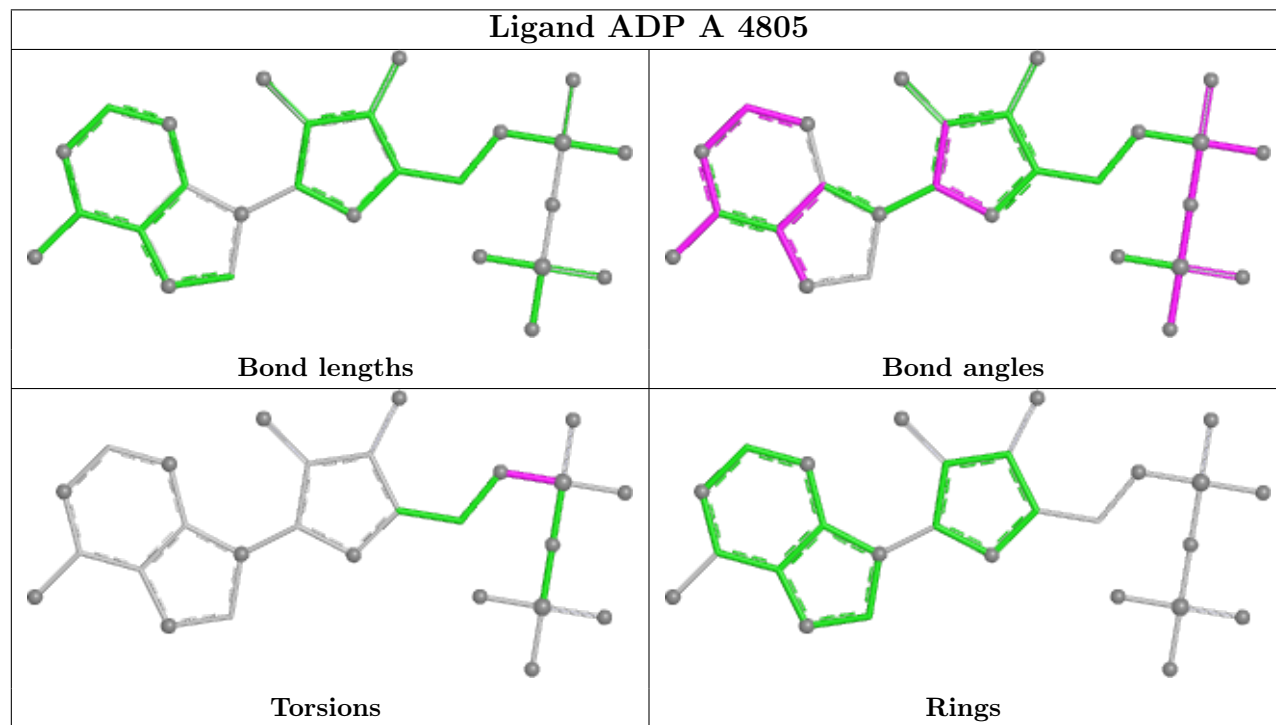
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4801	ADP	11	0
3	B	4802	ATP	4	0
3	A	4802	ATP	4	0

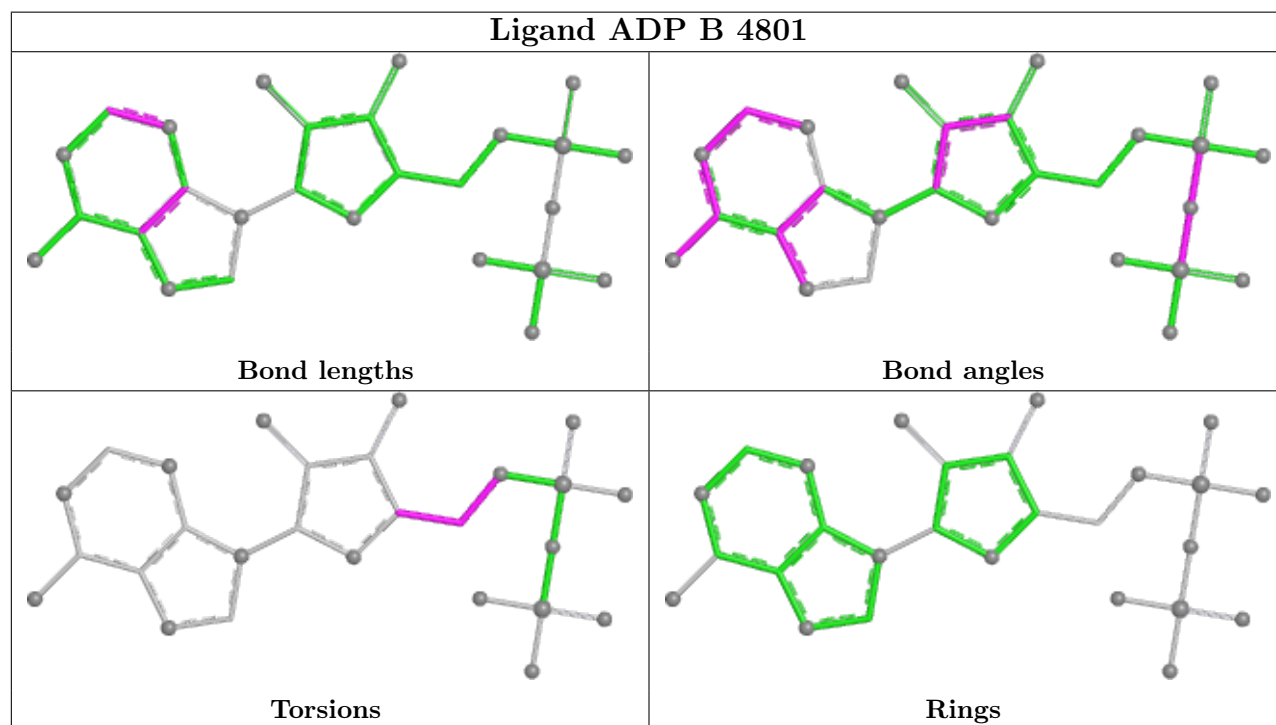
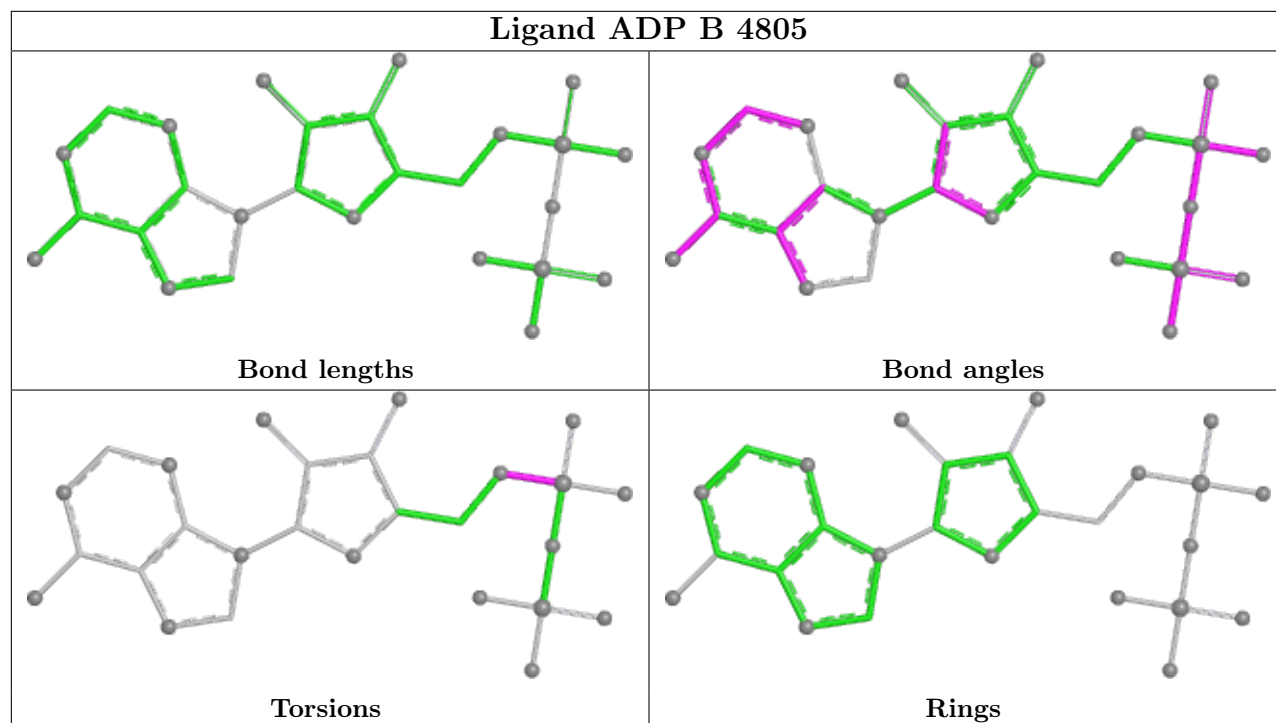
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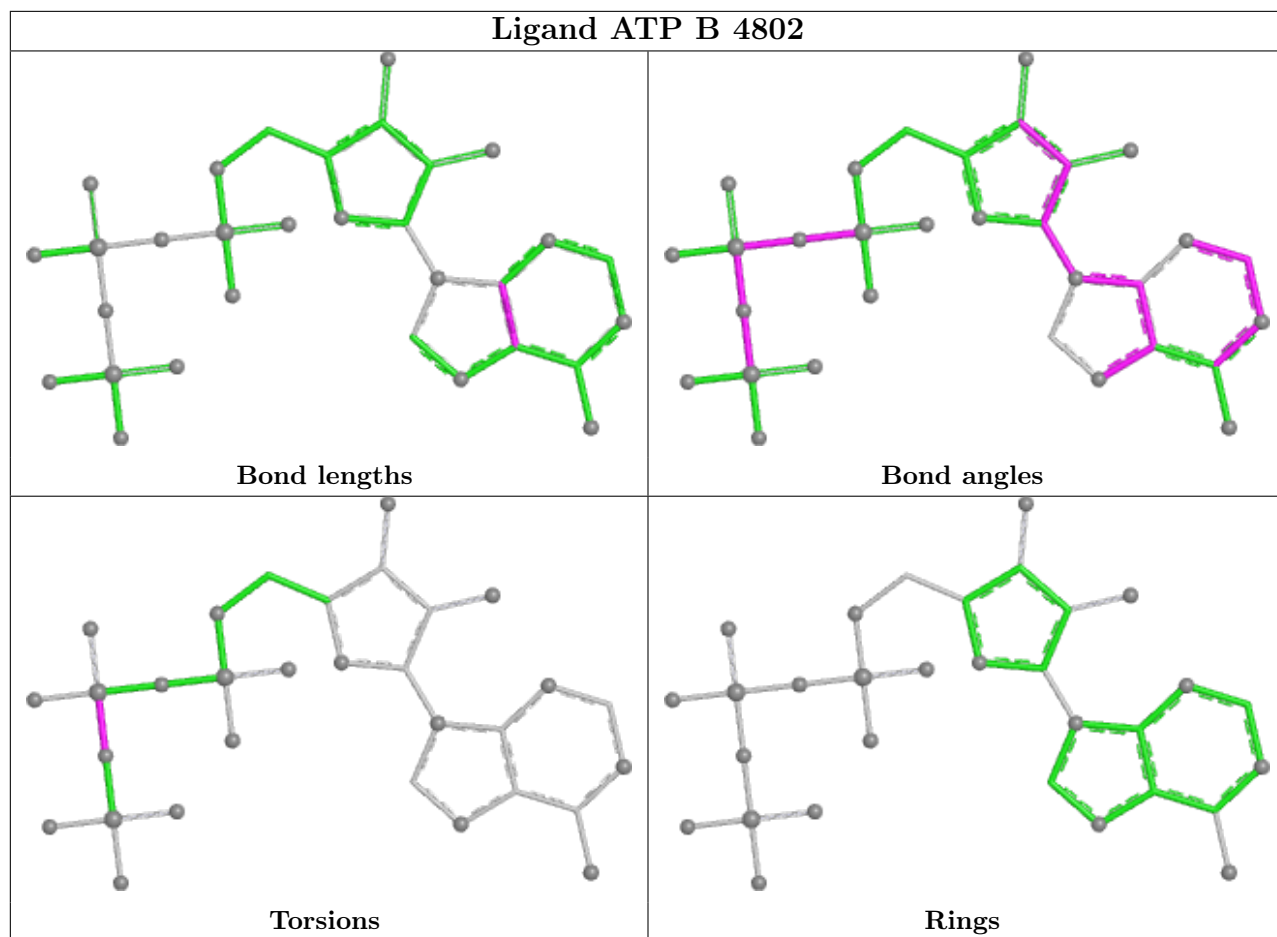
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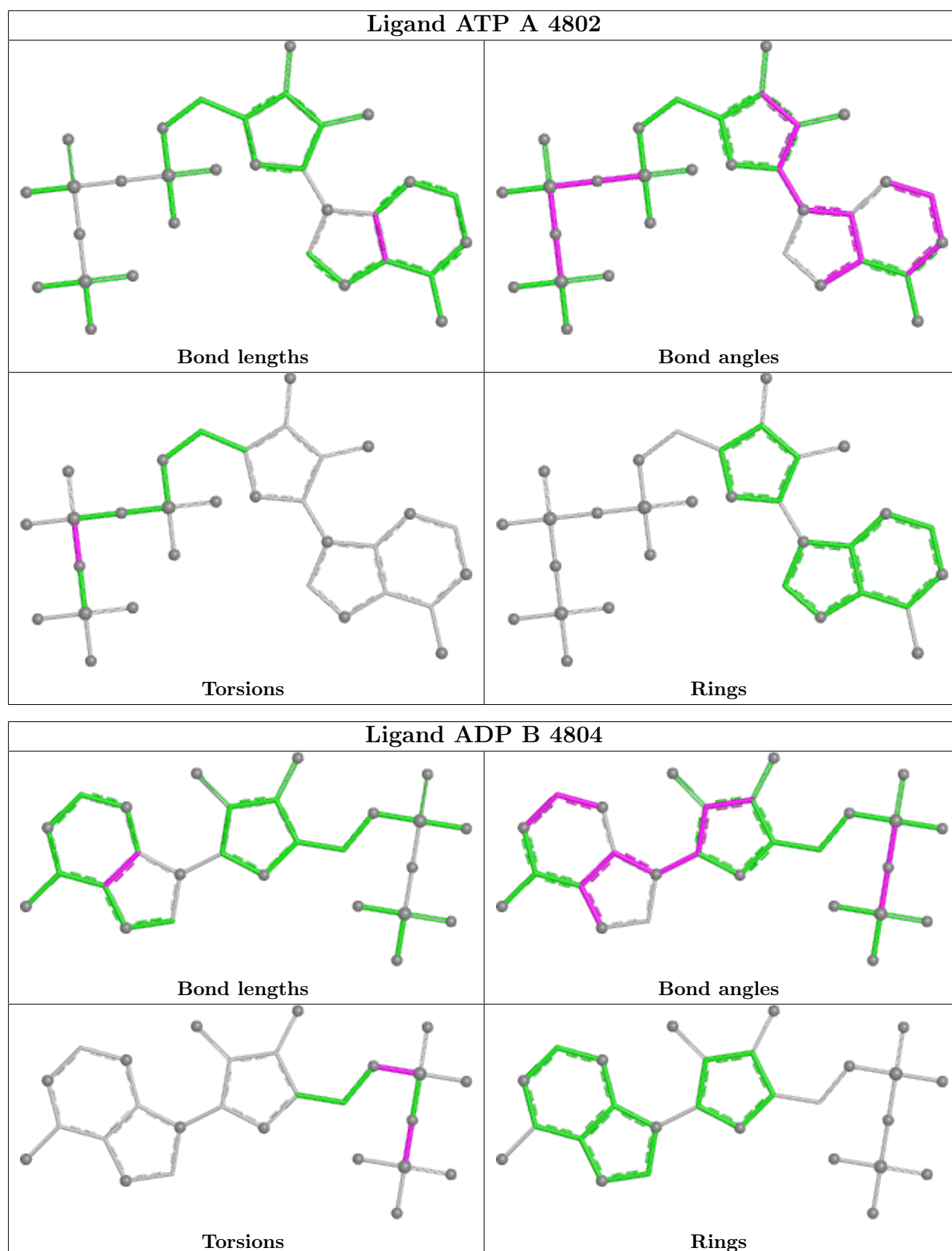
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4804	ADP	2	0
2	A	4801	ADP	11	0
2	A	4804	ADP	2	0

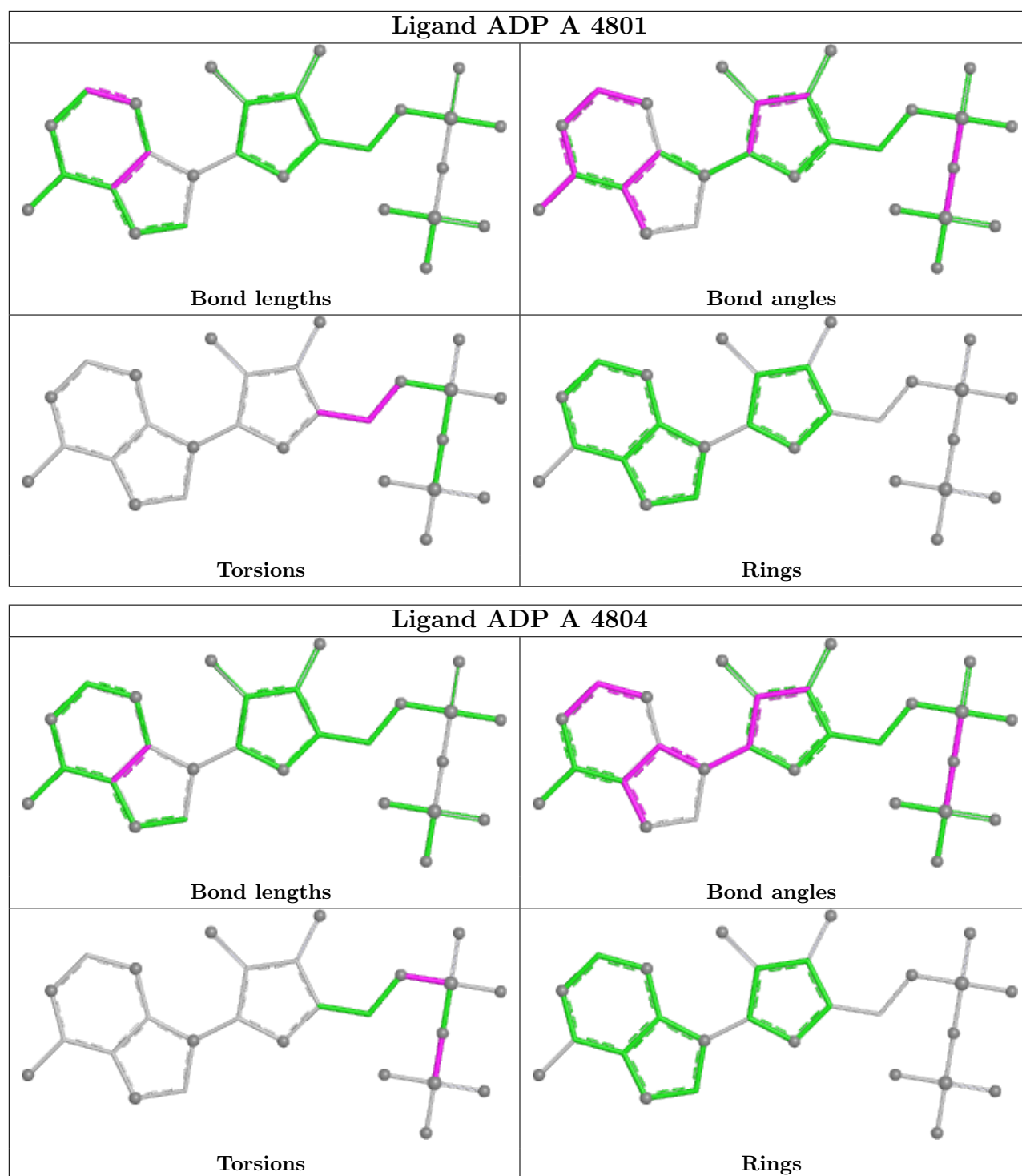
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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

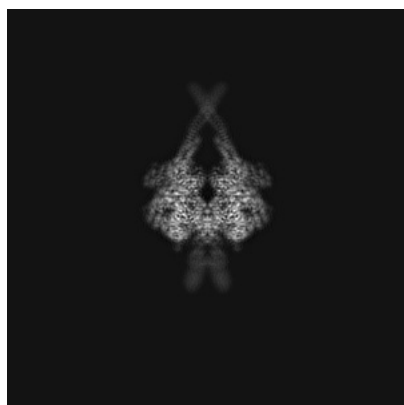
6 Map visualisation [i](#)

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.

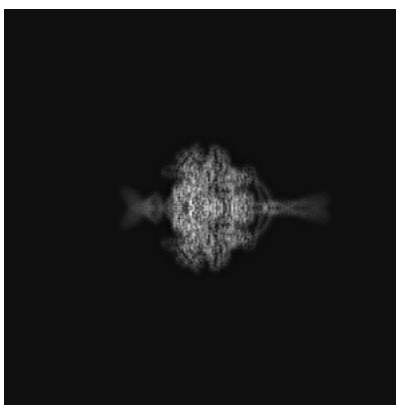
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

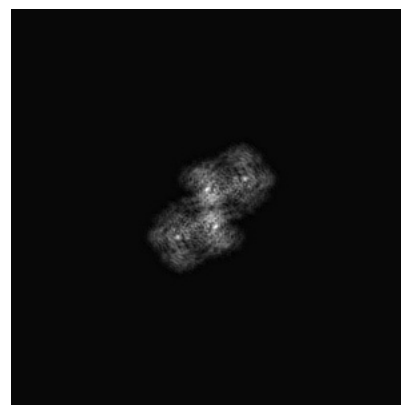
6.1.1 Primary map



X



Y

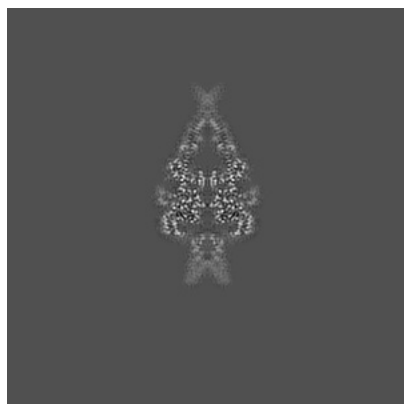


Z

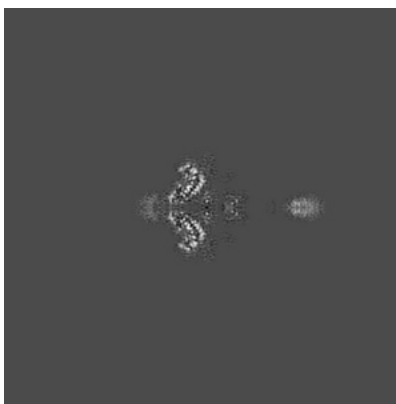
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

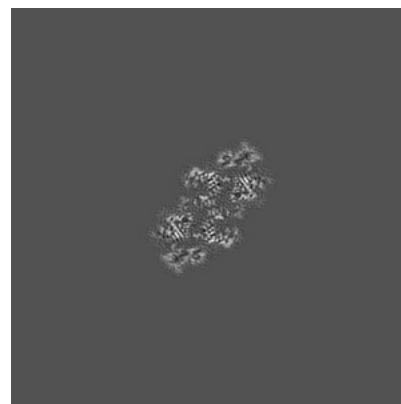
6.2.1 Primary map



X Index: 200



Y Index: 200

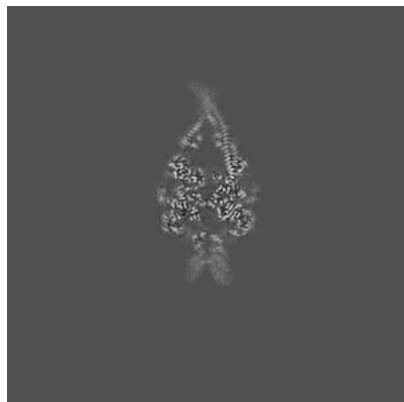


Z Index: 200

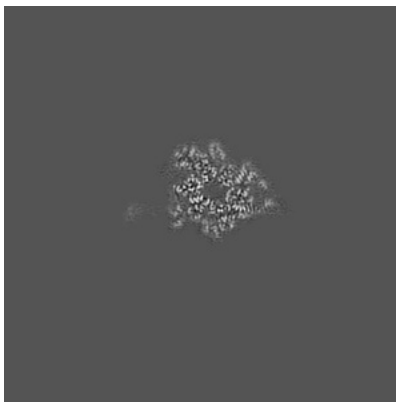
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

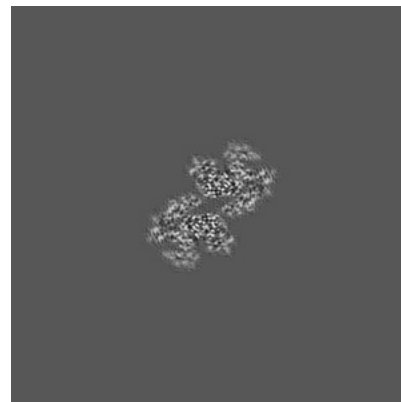
6.3.1 Primary map



X Index: 198



Y Index: 223



Z Index: 189

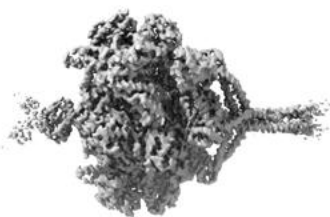
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

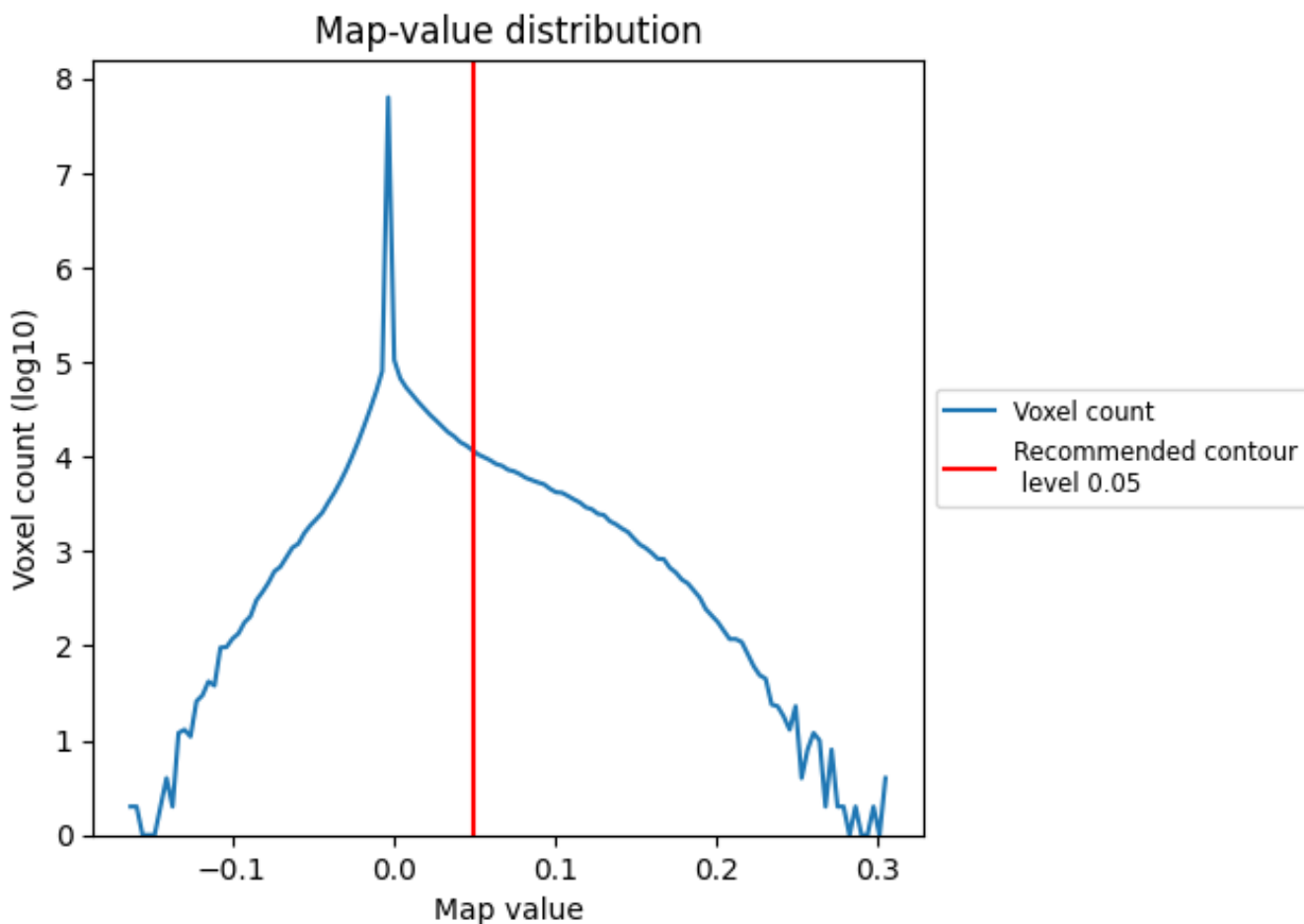
6.5 Mask visualisation

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

7 Map analysis [i](#)

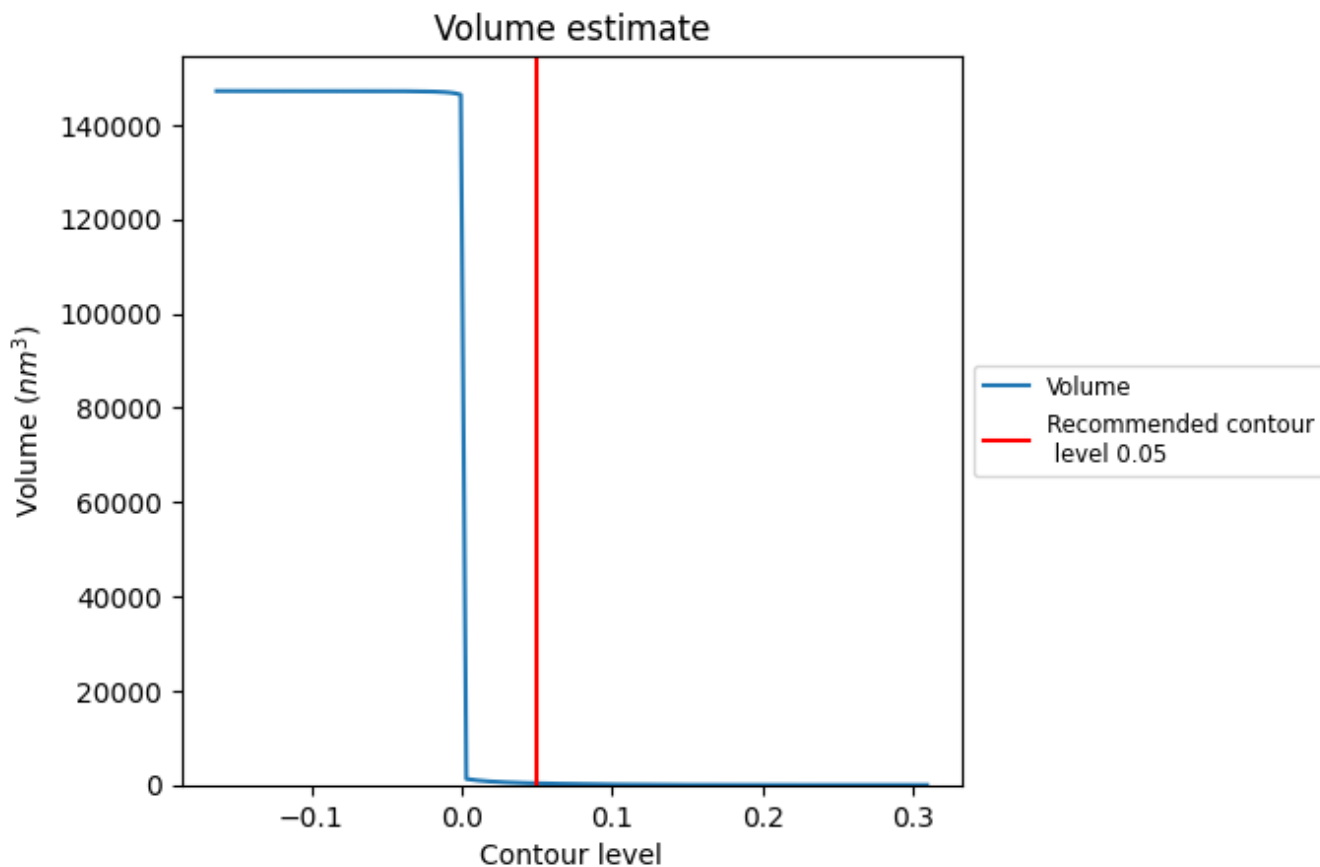
This section contains the results of statistical analysis of the map.

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.

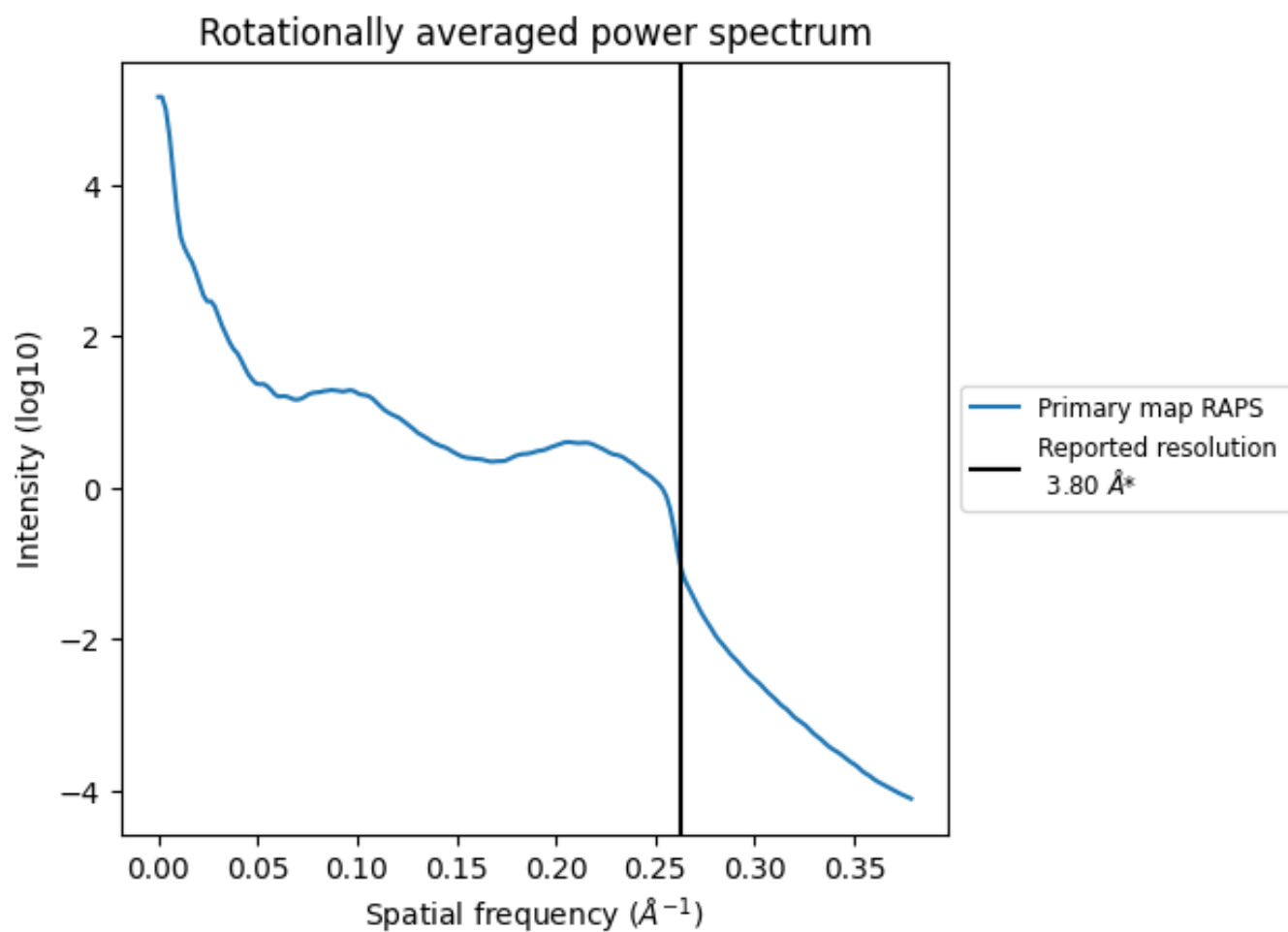
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm^3 ; 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 [i](#)

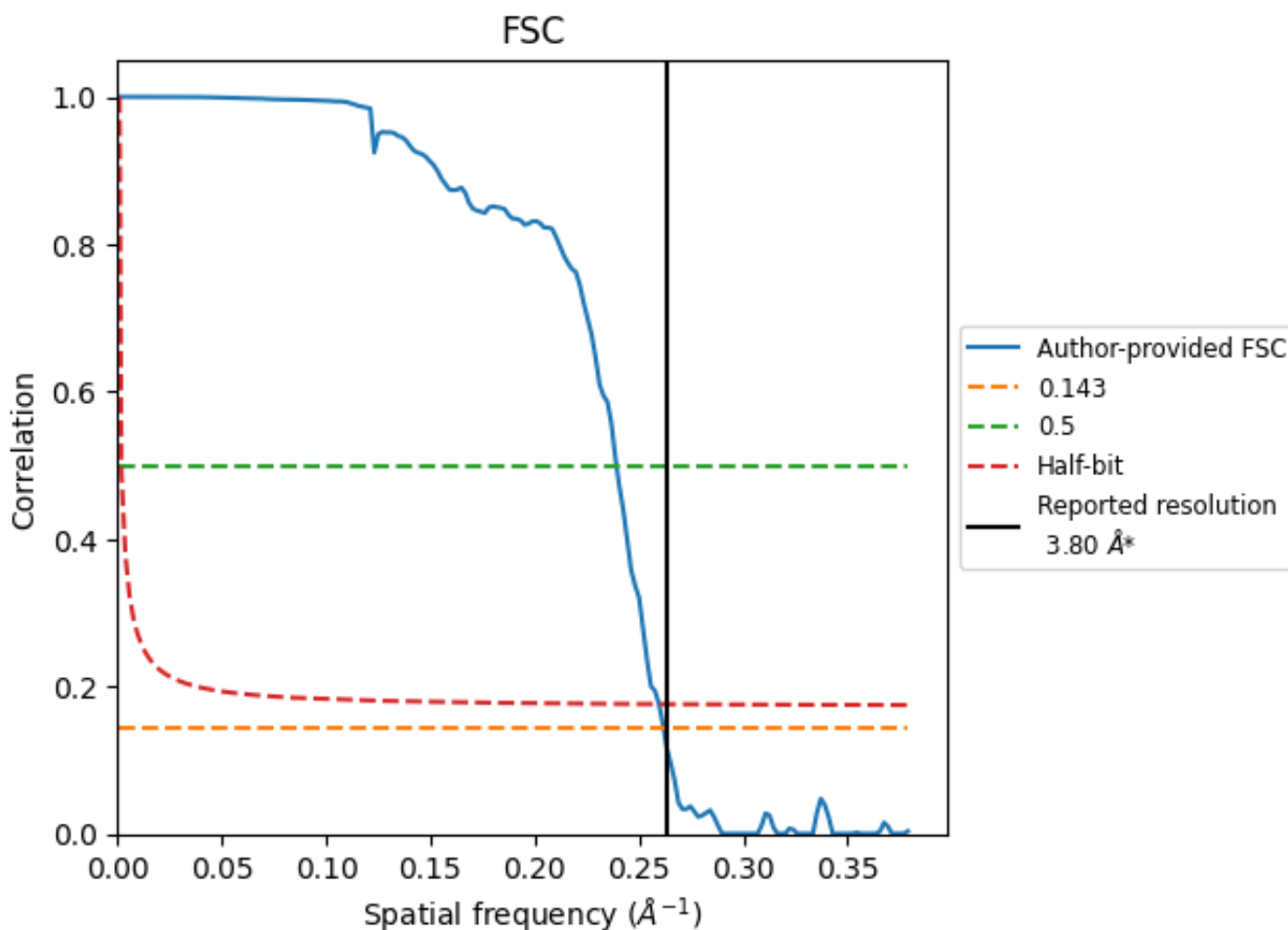


*Reported resolution corresponds to spatial frequency of 0.263\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

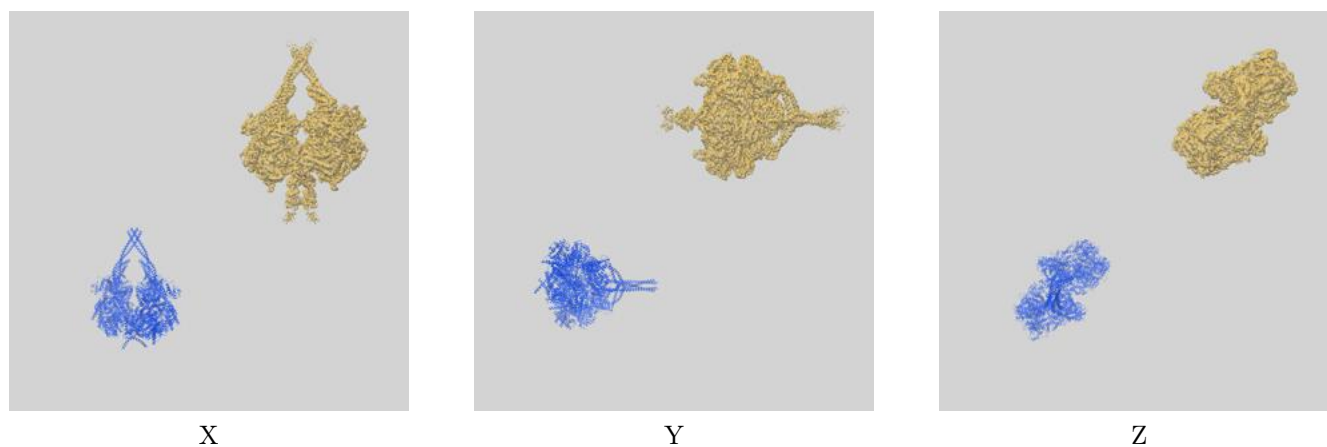
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.18	3.85
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

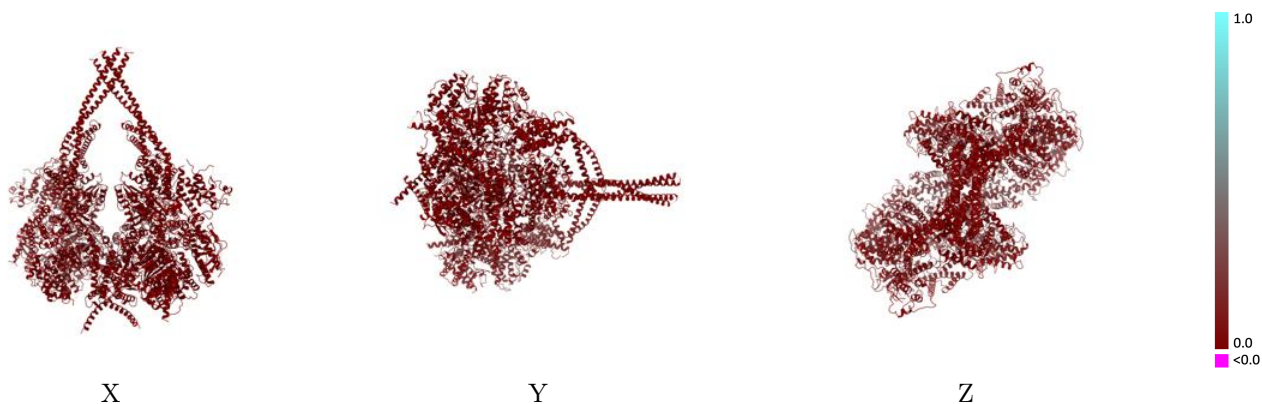
This section contains information regarding the fit between EMDB map EMD-3698 and PDB model 5NUG. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



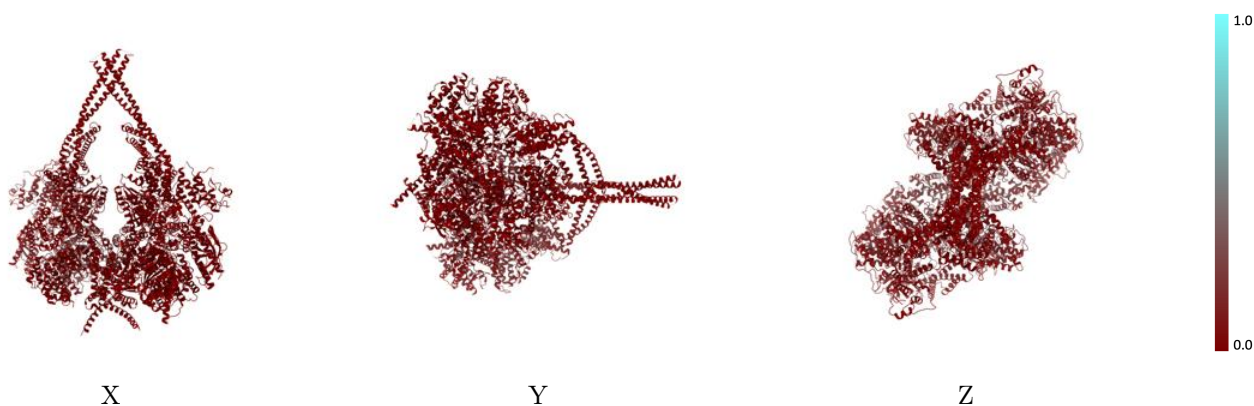
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



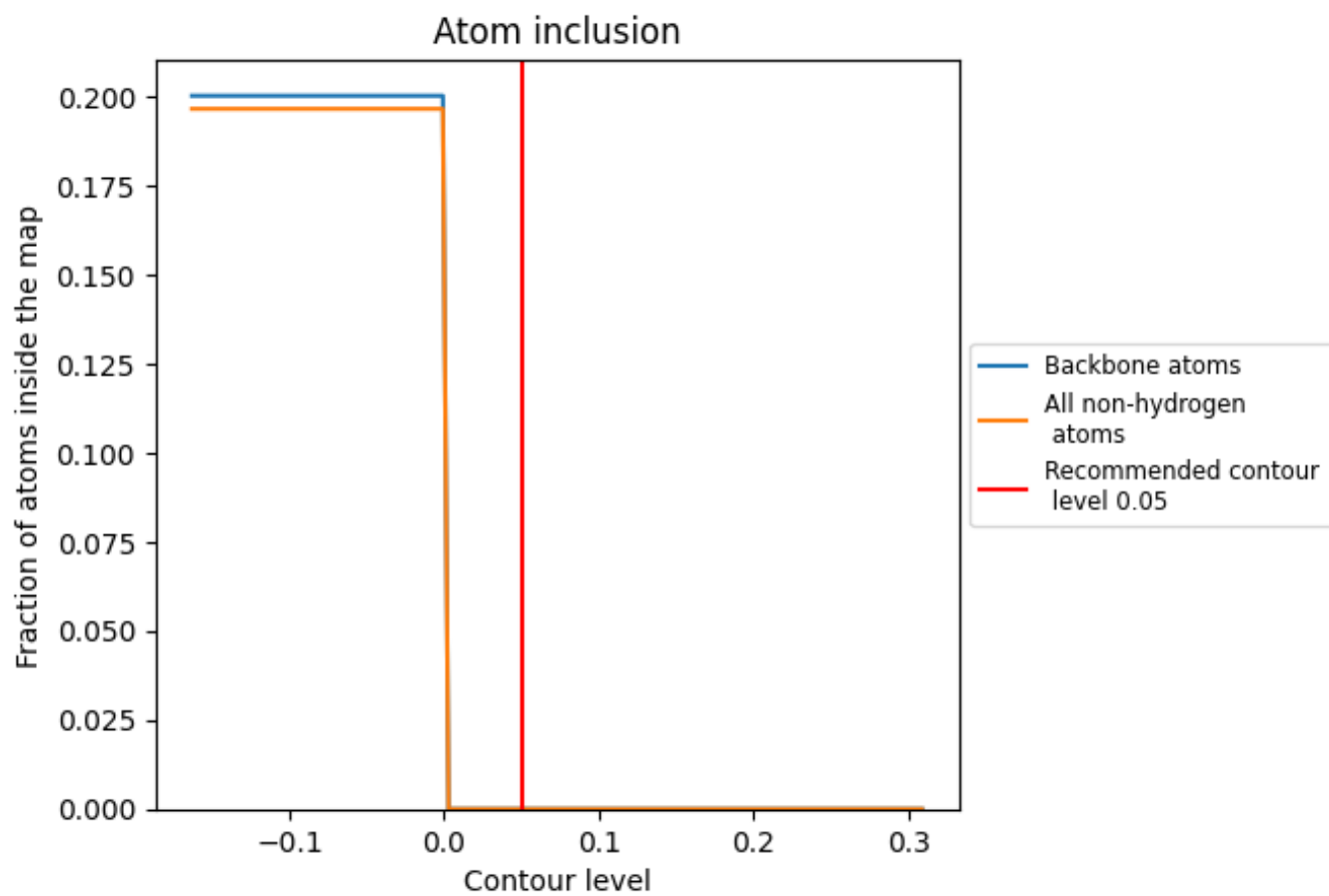
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.05).


9.4 Atom inclusion [i](#)



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 [i](#)

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

