



wwPDB EM Validation Summary Report ⓘ

Feb 24, 2024 – 06:27 PM EST

PDB ID : 7LT3
EMDB ID : EMD-23510
Title : NHEJ Long-range synaptic complex
Authors : He, Y.; Chen, S.
Deposited on : 2021-02-18
Resolution : 4.60 Å (reported)
Based on initial models : 2R9A, 1JEY, 6ZHA, 5Y3R, 3II6, 5LUQ, 6ERH

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.dev70
Mogul : 1.8.5 (274361), 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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

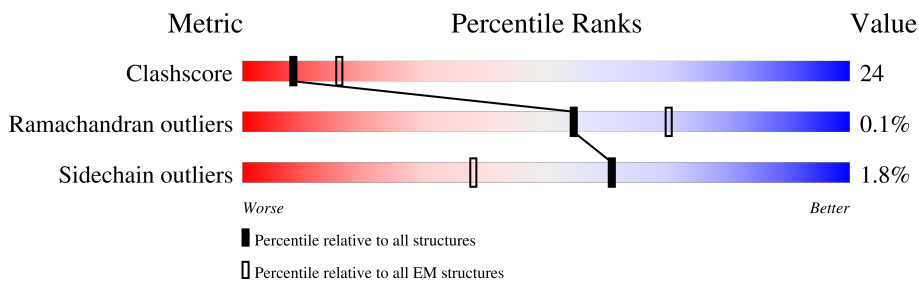
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	609	
1	J	609	
2	B	732	
2	K	732	
3	C	4128	
3	L	4128	
4	Q	20	
4	R	20	

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Mol	Chain	Length	Quality of chain
5	D	31	52% 45%
5	M	31	48% 48%
6	E	30	50% 47%
6	N	30	53% 43%
7	F	336	42% 48% 12% 37%
7	G	336	34% 42% 14% 42%
7	O	336	38% 42% 14% 42%
7	P	336	38% 51% 11% 37%
8	H	299	70% 61% 10% 25%
8	I	299	62% 60% 10% 27%
9	X	911	14% 19% 8% 72%
9	Y	911	16% 20% 8% 72%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 93244 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	497	Total	C	N	O	S	0	0
			4021	2577	680	746	18		
1	J	497	Total	C	N	O	S	0	0
			4021	2577	680	746	18		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	531	Total	C	N	O	S	0	0
			4259	2723	711	801	24		
2	K	531	Total	C	N	O	S	0	0
			4259	2723	711	801	24		

- Molecule 3 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	3720	Total	C	N	O	S	0	0
			29811	19106	5059	5451	195		
3	L	3720	Total	C	N	O	S	0	0
			29811	19106	5059	5451	195		

- Molecule 4 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	Q	20	Total	C	N	O	0	0
			101	60	20	21		
4	R	20	Total	C	N	O	0	0
			101	60	20	21		

- Molecule 5 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	31	Total	C	N	O	P	0	0
			634	304	113	186	31		
5	M	31	Total	C	N	O	P	0	0
			634	304	113	186	31		

- Molecule 6 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	30	Total	C	N	O	P	0	0
			616	295	110	181	30		
6	N	30	Total	C	N	O	P	0	0
			616	295	110	181	30		

- Molecule 7 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	213	Total	C	N	O	S	0	0
			1736	1093	308	327	8		
7	G	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		
7	O	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		
7	P	213	Total	C	N	O	S	0	0
			1736	1093	308	327	8		

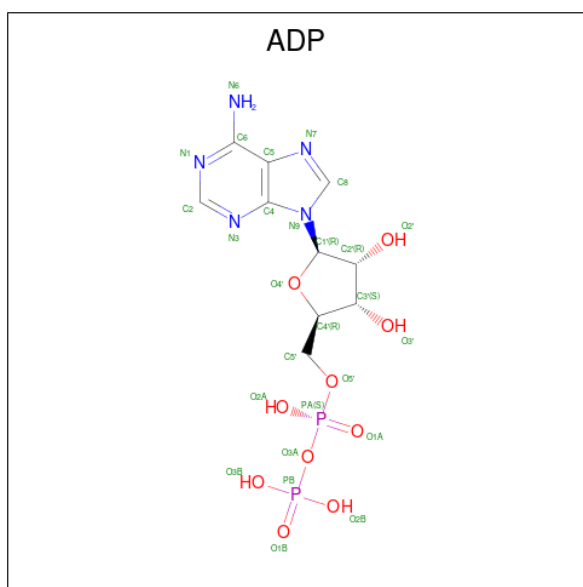
- Molecule 8 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	223	Total	C	N	O	S	0	0
			1779	1140	298	326	15		
8	I	218	Total	C	N	O	S	0	0
			1737	1111	290	321	15		

- Molecule 9 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	254	Total	C	N	O	S	0	0
			2064	1314	348	389	13		
9	Y	254	Total	C	N	O	S	0	0
			2064	1314	348	389	13		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

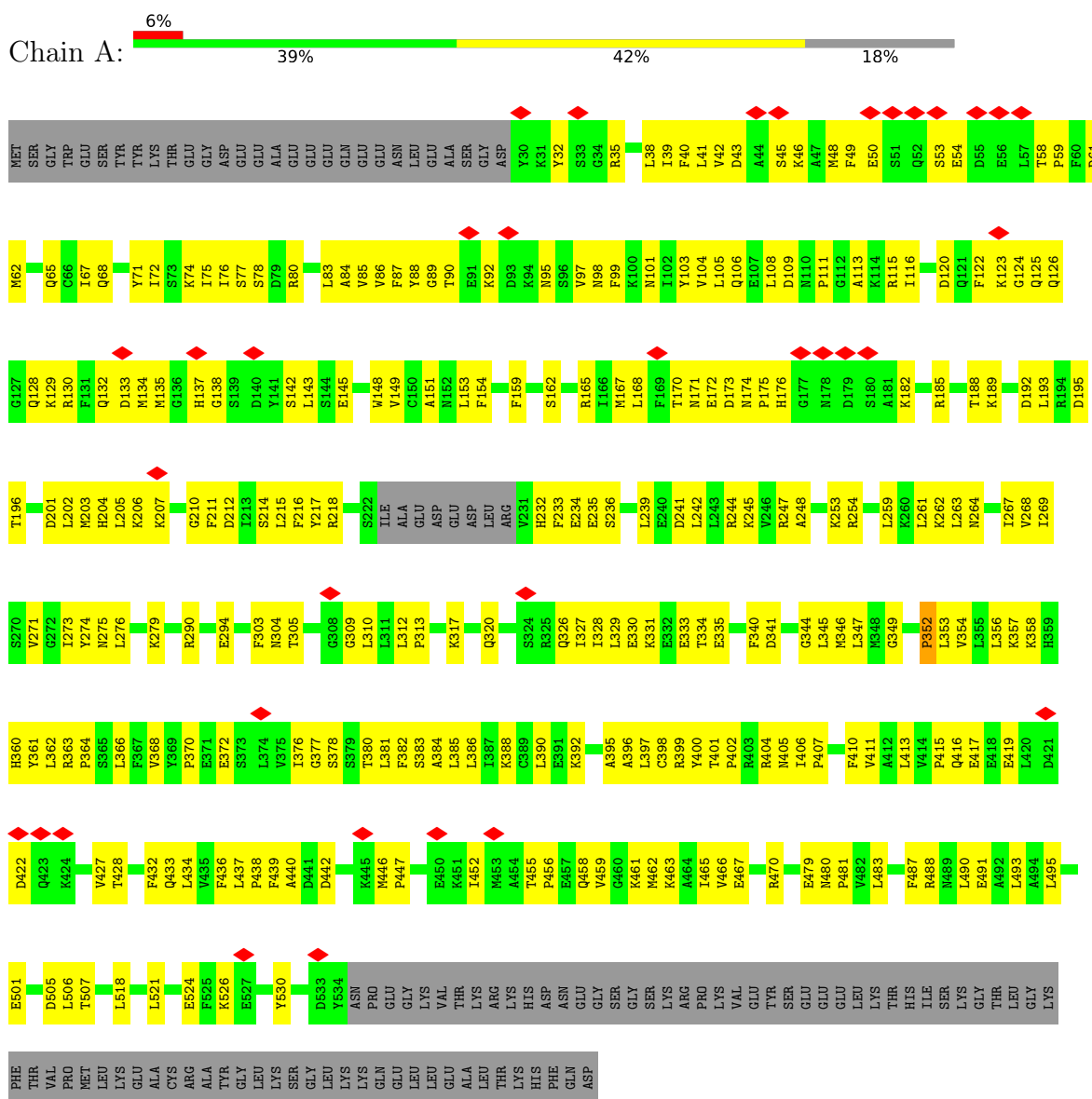


Mol	Chain	Residues	Atoms				AltConf	
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

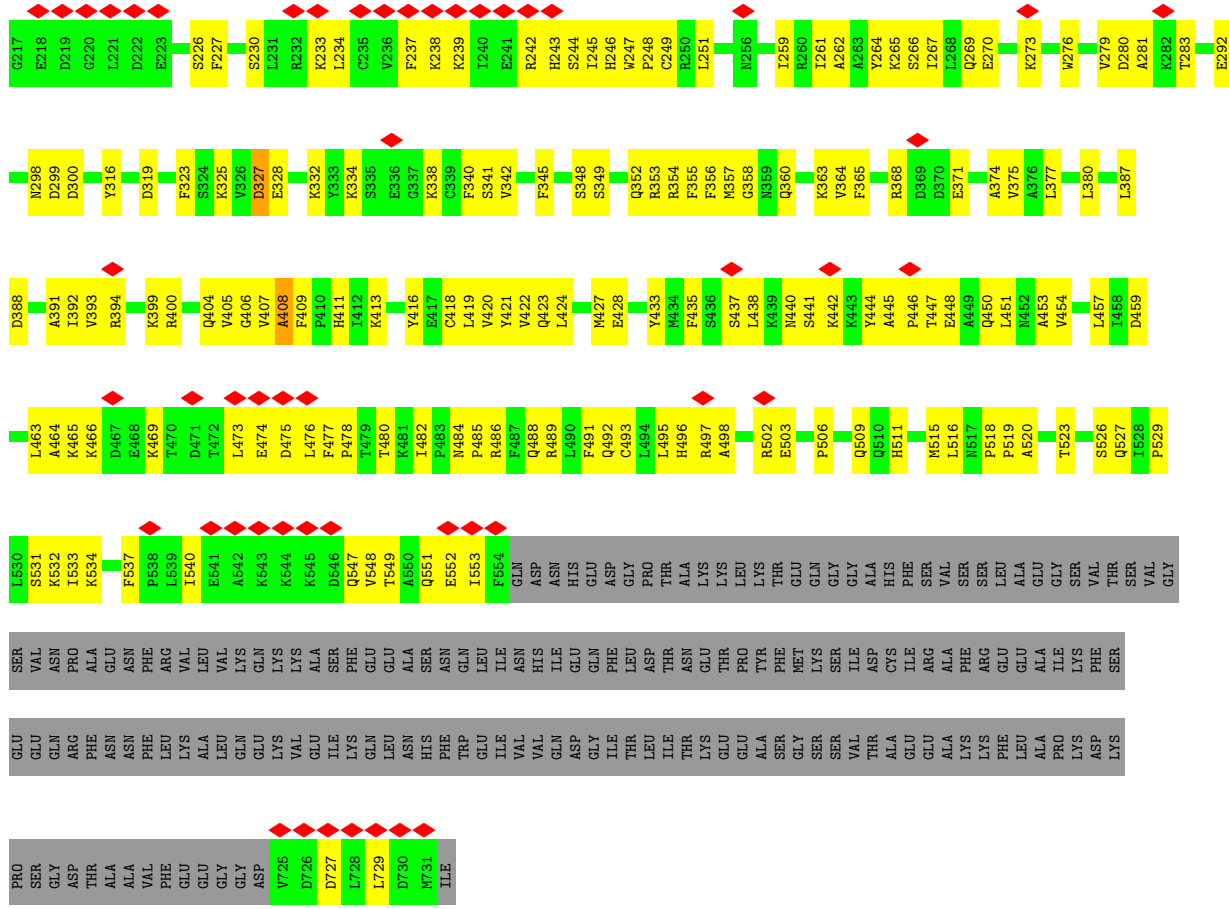
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

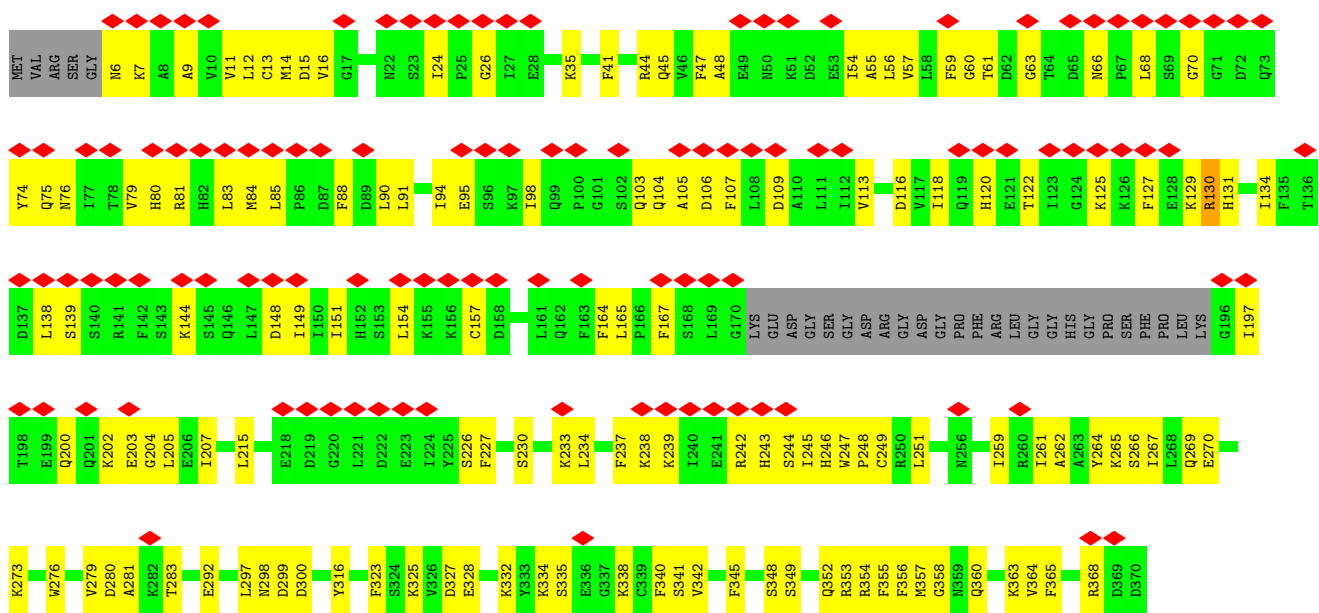
- Molecule 1: X-ray repair cross-complementing protein 6

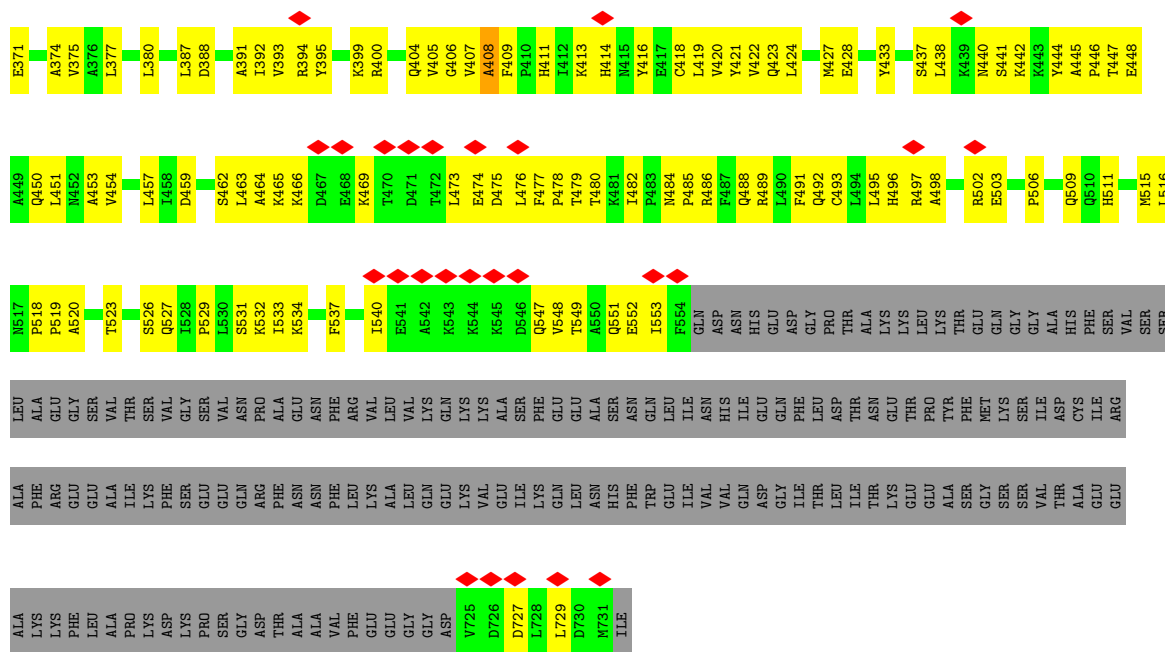


- Molecule 1: X-ray repair cross-complementing protein 6

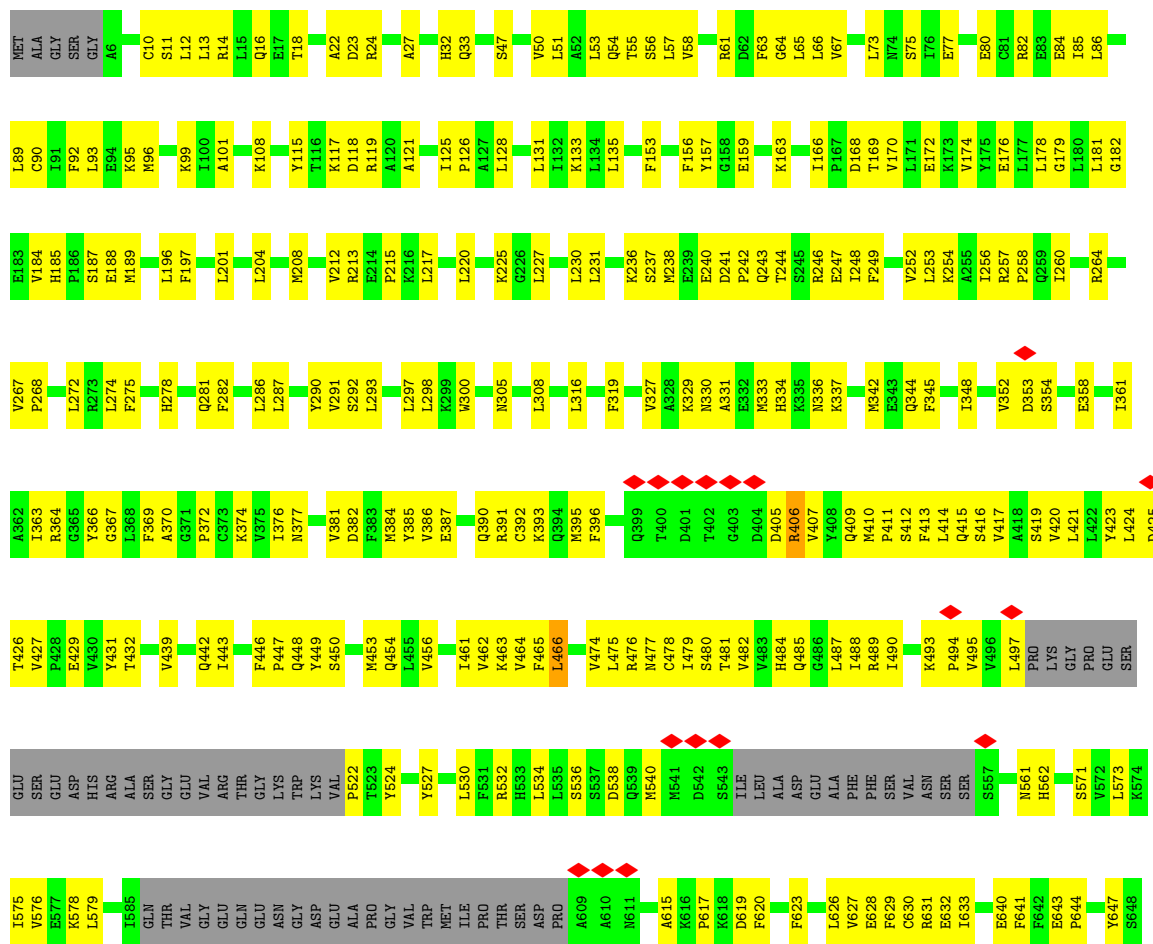


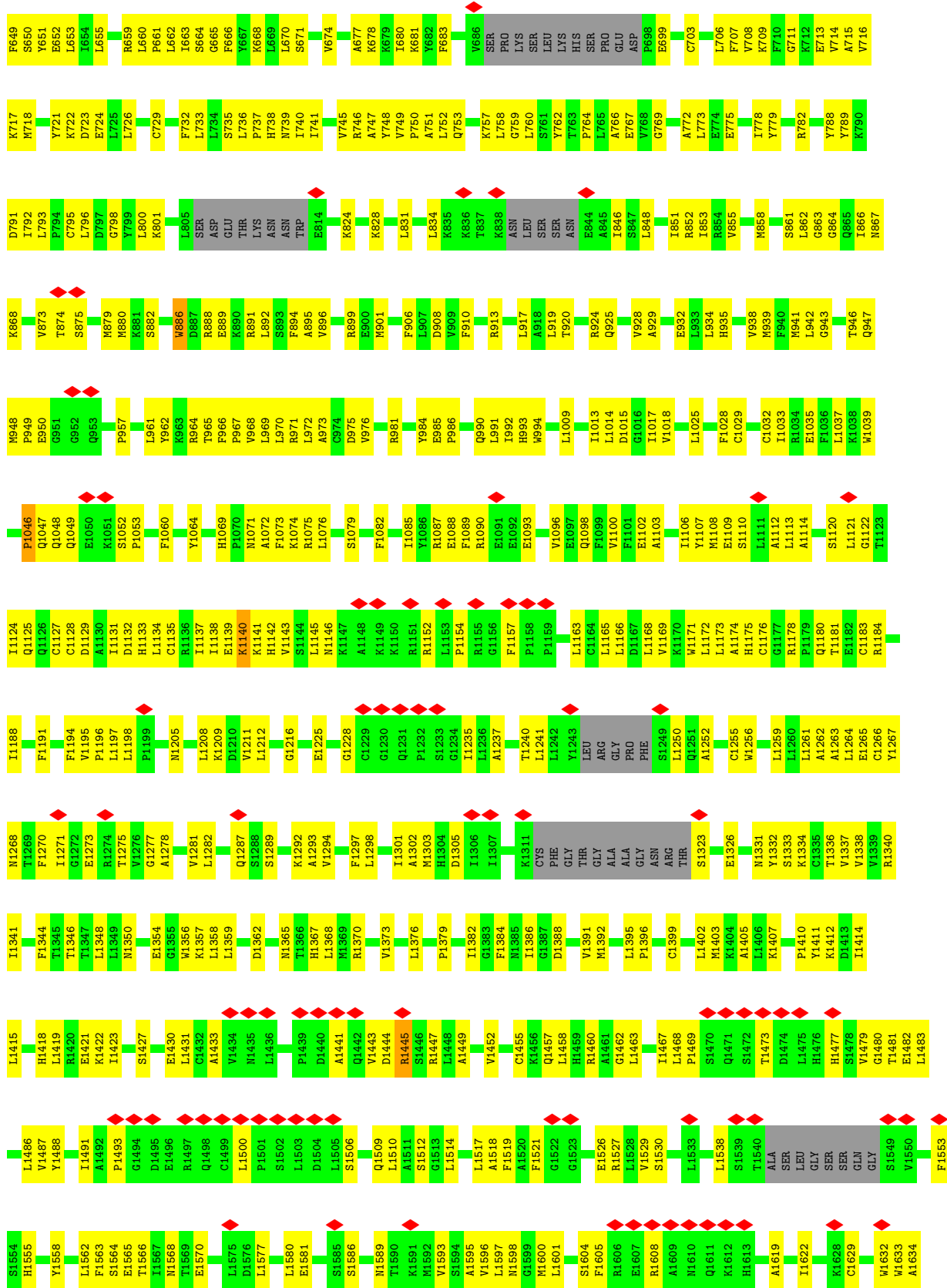
• Molecule 2: X-ray repair cross-complementing protein 5



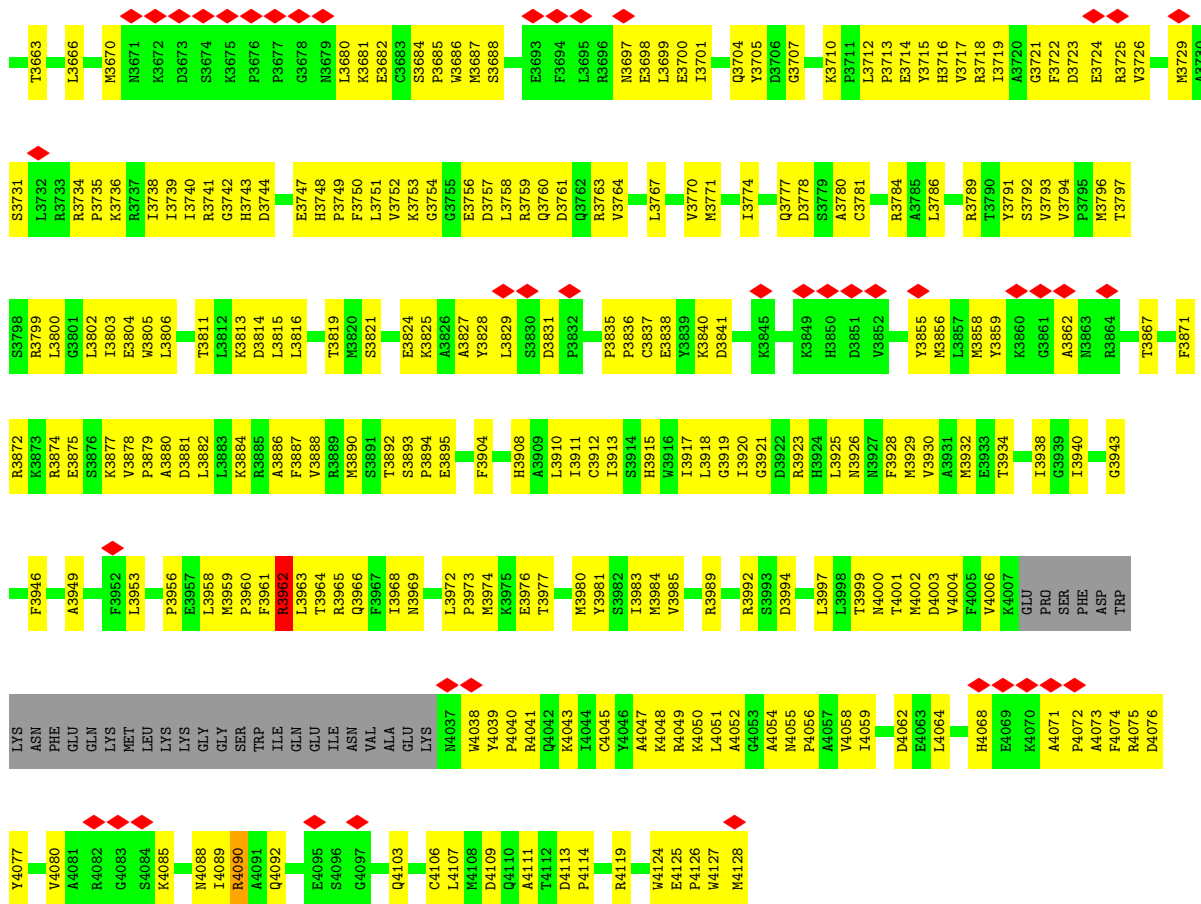


• Molecule 3: DNA-dependent protein kinase catalytic subunit

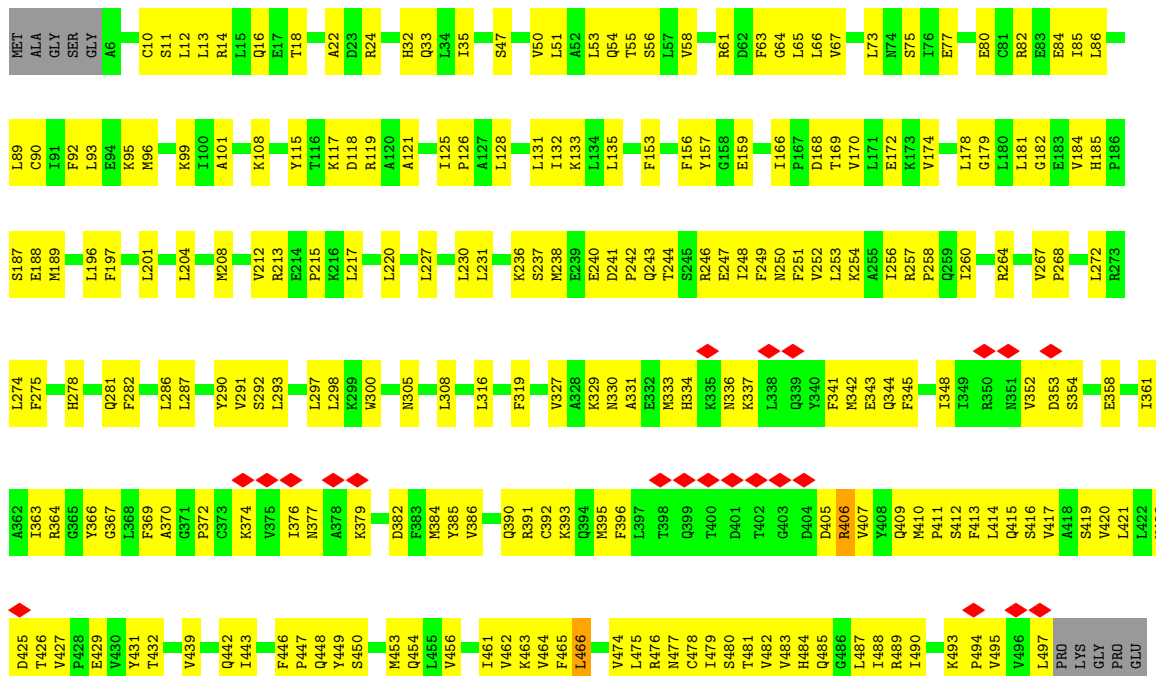




F2487	T3395	Y2289	R2228	P2159	L2097	E1910	I1848	R1783	E1708	S1637
E2488	L2398	A2302	M2234	Y2160	T2098	L1911	D1849	R1784	E1709	P1638
S2489	L2399	L2303	N2234	A2161	A2099	L1912	K1852	R1785	L1710	L1639
E2490	L2402	N2304	I2237	K2162	F1977	K1913	S1853	I1785	R1711	E1640
T2491	L2403	N2305	L2238	H2163	E1979	L1914	R1854	A1786	R1712	T1641
N2493	R2404	N2306	K2239	M2164	M1960	L1915	F1855	R1787	V1713	K1642
D2494	E2405	M2307	T2240	L2165	L1981	L1916	T1856	R1788	Q1716	L1649
S2495	E2406	S2308	L2241	S2166	D1982	K1917	T1857	G1789	L1717	A1650
Q2496	M2408	E2243	V2242	L2168	L1984	C1919	K1857	C1791	I1718	K1651
L2411	L2411	R2311	G2244	L2108	K1985	Y1920	M1859	Q1794	F1722	I1652
Q2414	Q2414	E2175	G2245	PRO	R1987	D1921	E1860	V1795	M1724	L1653
L2415	D2247	N2176	K2246	PRO	F1990	A1922	S1861	G1796	P1725	Q1654
K2416	C2248	N2177	L2249	GLN	F1991	F1923	T1862	L1797	Q1726	I1655
S2417	L2249	G2178	GLY	GLY	V1992	M1927	D1863	L1798	Q1727	D1656
K2418	L2250	G2179	GLY	VAL	GLU	A1928	F1864	L1799	R1727	S1657
D2419	L2251	E2180	GLU	VAL	VAL	G1929	T1865	S1800	E1728	S1658
F2420	P2252	G2181	ASP	GLU	GLU	E1930	Q1866	V1801	F1729	V1659
L2421	Y2253	I2182	SER	GLU	GLU	M1931	I1867	I1802	P1730	S1660
L2422	I2256	I2183	VAL	GLN	VAL	Q1932	K1869	E1803	P1731	F1661
H2426	F2257	Y2184	PRO	PRO	PRO	L1933	K1870	M1804	G1732	N1662
D2437	E2258	Y2186	ARG	MET	MET	L1934	M1871	R1806	F1736	N1663
M2443	K2259	E2188	PRO	GLU	GLU	E1935	G1872	K1807	N1737	S1664
L2446	F2260	G2262	ALA	LYS	ARG	R1936	Y1873	D1808	F1736	H1665
L2454	S2261	G2263	THR	LYS	LYS	R1937	K1875	D1809	K1744	G1666
E2457	K2263	D2264	GLY	LYS	THR	R1938	I1876	P1810	F1746	S1677
R2458	D2265	T2192	PHE	ILE	ILE	Y1940	L1877	R1811	D1748	F1668
V2459	L2193	L2129	ARG	GLU	GLU	H1941	D1878	L1812	K1744	F1669
H2464	K2268	L2133	ARG	GLU	ALA	C1942	I1879	F1814	A1749	E1670
P2465	D2269	G2134	THR	ASP	ARG	A1944	V1879	F1815	L1750	L1676
S2466	S2271	G2135	VAL	GLN	ALA	Y1945	M1880	R1816	L1752	L1678
R2470	T2274	N2136	HIS	ARG	ALA	V1951	R1883	R1822	S1785	D1681
E2471	Q2275	R2137	ASP	ASP	ASN	I1952	L1884	R1823	L1766	T1682
Q2472	L2276	V2138	ASP	ASP	GLY	V1955	F1885	L1824	L1759	K1683
M2473	L2277	V2139	VAL	VAL	ASP	F1956	K1886	S1825	E1760	L1684
Y2474	G2278	L2140	HIS	HIS	GLY	N1957	D1887	R1827	L1688	K1689
N2475	V2280	M2141	ASP	ASP	ASP	F1962	V1889	L1828	V1693	T1694
L2476	A2282	M2142	LEU	LEU	ASP	Y1963	D1892	H1830	L1695	L1696
L2477	M2283	L2143	LEU	LEU	PRO	G1964	K1892	L1833	P1697	P1697
M2478	D2284	A2146	THR	THR	SER	F1965	M1892	D1834	F1698	F1699
W2479	L2285	K2148	H2091	H2091	TYR	L1966	V1899	A1835	Q1770	F1699
F2378	P2286	L2210	E2092	E2092	TYR	F1967	L1836	L1836	Q1771	T1700
L2480	P2287	L2211	M2094	M2094	LEU	S1968	H1901	L1837	V1773	S1701
R2485	Q2292	R2214	A2095	A2095	LEU	E1969	G1902	F1839	M1774	L1702
D2486	Q2295	E2154	P2096	P2096	ASP	K1970	S1903	F1840	F1778	T1703
L2557	E2298	E2155	R2157	R2157	THR	P1971	C1904	T1842	G1705	G1705
						K1974	T1906	S1844	F1782	L1707



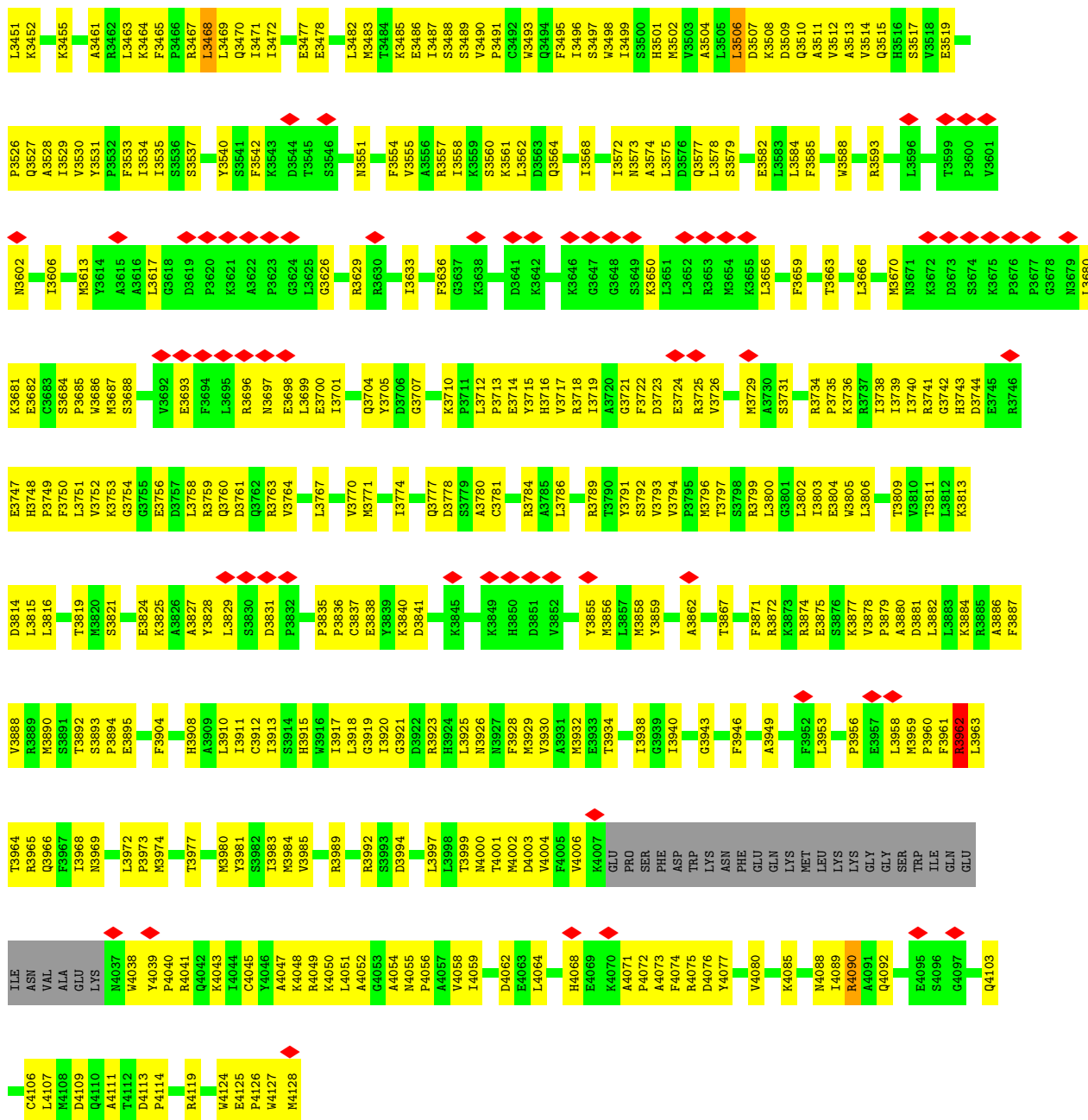
● Molecule 3: DNA-dependent protein kinase catalytic subunit



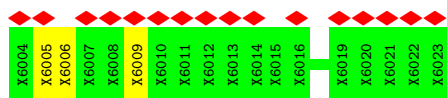
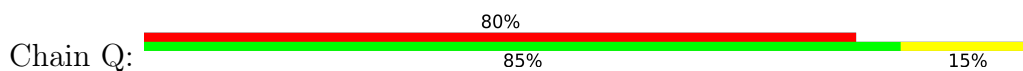
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W1256	G1177	R1178	Q1179	Q1180	T1181	E1182	C1183	R1184	I1188	F1191	F1194	V1195	P1196	L1197	L1198	F1199	G1200	M1201	M1205	L1208	K1209	D1210	V1211	S1212	G1216	E1225	G1228	C1229	G1230	Q1231	P1232	S1233	G1234	I1235	L1236	A1237	T1240	L1241	L1242	Y1243	LEU	PHE	ARG	GLY	PRO	PHE	S1249	L1250	Q1251	A1252	C1255	W1256				
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L1942	G943	T946	Q947	M948	P949	E950	G951	R952	Q953	P957	L961	Y962	R963	R964	T965	F966	P967	V968	L969	R971	L972	A973	G974	D975	V976	R981	Y884	E985	Q990	L991	I992	H993	W994	L1009	L1010	I1013	L1014	D1015	G1016	I1017	V1018	L1025	F1028	C1029	C1032	I1033										
M658	S861	G862	G863	G864	Q865	R866	R867	K868	V873	T874	S875	M879	M880	W886	D887	R888	E889	K890	R891	L892	S893	F894	A895	V896	R899	E900	M901	F906	L907	D908	V909	F910	R913	L919	T920	R824	Q925	V928	A929	E932	H935	V938	M939	F940	M941											
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V714	A715	K717	M718	Y721	D722	E724	L725	L726	C729	F732	L733	G734	S735	L736	P737	H738	N739	I740	I741	E742	L743	D744	R745	R746	A747	Y748	V749	P750	L752	Q753	K757	G759	L760	S761	T762	P764	L765	A766	E767	V768	G769	A772	L773	E774	E775	I778	Y779	I780								
V672	L573	K574	I575	S576	V577	K578	L579	I585	THR	VAL	ARG	THR	GLY	GLU	GLN	GLU	TRP	LYS	VAL	P522	T523	Y524	Y527	L530	F531	R532	H533	L534	L535	S536	S537	D538	Q539	M540	H541	D542	S543	ILE	LEU	ALA	ASP	GLU	ALA	PHE	PHE	SER	VAL	ASN	SER	S557	H561	H562	E567	E643	P644	

Table with 12 columns of residue identifiers (e.g., G2262, V2190, L1463, S1590, M1598, Y1675, D1741, K1807, Y1873, L1938, LYS, THR, W2125, V2190, G2262, R2288, D2284, L2285, P2286, L2210, L2211, R2214, L2215, L2216, R2217, L2218, L2219, M2220, K2221, H2222, R2228, M2234, I2237, L2238, K2239, L2240, V2242, E2243, C2244, W2245, K2246, D2247, L2249, S2250, I2251, P2252, Y2253, I2256, F2257, E2258, K2259, L2260, S2261, R2333, Y2312, K2313, E2314, V2315, K2316, A2317, A2318, A2319, L2323, L2325, L2326, Y2329, R2333).

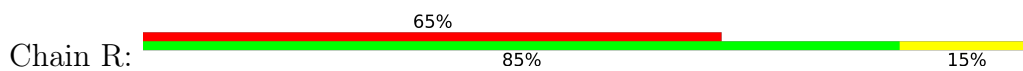
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F3236	S3237	M3238	K3239	M3242	L3243	D3244	R3247	K3248	Q3249	N3250	M3251	F3252	A3255	M3256	K3257	L3258	L3259	L3262	H3263	K3264	E3265	S3266	K3267	T3268	R3269	W3272	L3273	V3274	V3277	C3281	H3285	C3286	R3287	S3290	Q3291	G3292	C3293	S3294	E3295	Q3296	V3297	L3298	T3299	V3300	L3301	K3302	L3303	T3303	V3304	M3310				
N3311	V3312	L3316	S3317	K3318	M3319	L3320	R3324	K3324	Q3325	N3325	Q3326	N3327	L3328	L3329	L3330	T3333	Y3334	R3335	A3338	M3339	A3340	L3341	S3342	K3343	E3344	C3347	L3348	A3349	E3350	L3351	E3352	E3353	R3357	R3358	L3360	S3363	G3364	S3365	S3366	S3367	E3368	D3369	S3370	E3371	I3374	A3375	Y3378	Q3379	R3380	A3381	F3382			
L2446	E2450	L2451	L2454	P2457	V2458	V2459	H2464	P2465	S2466	R2470	Q2472	M2473	Y2474	L2475	L2476	L2477	M2478	V2479	I2480	R2485	D2486	P2487	E2488	S2489	E2490	L2491	D2492	N2493	D2494	G2497	S2495	Q2496	K2500	L2501	A2502	K2503	L2506	I2507	Q2508	G2509	L2510	I2511	D2512	E2513	N2514	P2515	G2516	L2517	Q2518					
L2521	F2524	W2525	L2526	T2529	R2530	L2531	T2535	V2536	D2537	R2538	L2539	L2542	W2543	S2544	L2545	P2548	K2549	L2550	E2551	W2552	H2553	F2554	L2555	S2556	L2562	L2563	E2564	M2565	T2566	S2567	W2568	S2569	F2570	D2571	Y2572	M2576	F2577	E2578	H2579	P2580	L2581	P2582	E2583	C2584	E2585	L2586	Q2587	Y2588	Y2589	D2594	W2595	R2596		
F2597	R2598	S2599	T2600	L2601	L2602	R2603	P2604	M2605	PHE	VAL	GLU	THR	THR	GLN	ALA	SER	GLN	GLY	THR	THR	LEU	GLN	GLN	ALA	ARG	TRP	VAL	VAL	ALA	GLY	GLY	GLN	GLN	GLN	GLN	HIS	ASP	PHE	THR	LEU	THR	PRO	GLY	ASP	GLU	VAL	ASP	ASN	SER	LYS	VAL			
ASP	TRP	LEU	THR	GLY	SER	SER	THR	ASP	PRO	VAL	VAL	THR	HIS	THR	ALA	SER	PRO	SER	SER	LEU	SER	LEU	LEU	ALA	ARG	GLN	ARG	ALA	VAL	PRO	ALA	GLY	GLN	LYS	SER	GLY	ASP	PHE	GLY	LYS	LYS	ARG	LEU	VAL	ASP	ASN	LYS	VAL						
L2804	L2808	F2809	S2810	S2811	L2812	L2817	M2820	T2825	L2826	F2840	M2841	R2842	F2843	F2848	F2851	F2852	F2853	F2854	E2855	S2856	Q2859	D2860	L2861	D2872	S2877	S2883	L2884	Q2885	Q2886	P2887	L2890	R2891	E2894	L2898	L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL										
ARG	GLY	LYS	ALA	R2915	L2916	P2917	P2918	V2924	K2928	L2929	T2930	R2931	S2932	L2933	Y2936	R2940	G2941	I2942	F2943	T2944	S2945	E2946	I2947	K2950	Q2954	S2955	A2956	L2957	L2958	A2959	E2960	A2961	R2962	Y2965	Q2971	Y2972	D2973	E2974	A2975	L2976	M2977	W2981	G2984	E2985	P2986	Q3074	R3075	A3076	L3077	W3094				
E2995	L2996	A2997	L2999	L3005	A3006	W3008	E3012	Y3013	T3016	L3019	S3115	S3116	L3121	H3122	Q3123	L3126	T3127	K3128	L3129	Q3130	S3131	Q3037	L3041	F3042	Y3043	M3044	L3045	R3046	S3047	K3048	L3049	K3050	L3053	D3058	Q3059	S3060	L3061	L3062	T3063	F3064	L3065	H3070	G3071	Q3074	R3075	A3076	L3077							
L3078	E3079	Y3082	L3089	Y3090	D3097	R3098	Y3101	T3107	Y3114	S3115	S3116	L3121	H3122	Q3123	L3126	T3127	K3128	L3129	Q3130	S3131	Q3037	L3041	F3042	Y3043	M3044	L3045	R3046	S3047	K3048	L3049	K3050	L3053	D3058	Q3059	S3060	L3061	L3062	T3063	F3064	L3065	H3070	G3071	Q3074	R3075	A3076	L3077								
Y3168	P3169	K3172	P3175	L3178	W3179	D3180	L3183	T3184	N3185	R3186	F3189	L3190	L3193	K3196	L3197	T3198	P3199	LEU	PRO	GLU	ASP	ASN	SER	MET	ASN	VAL	ASP	GLN	ASP	GLY	ASP	PRO	SER	ARG	MET	GLU	VAL	GLN	GLU	GLN	GLN	GLU	GLU	GLU	ASP	L3227	S3228	S3229	L3230	W3164	T3165	N3166	S3233	
F3236	S3237	M3238	K3239	M3242	L3243	D3244	R3247	K3248	Q3249	N3250	M3251	F3252	A3255	M3256	K3257	L3258	L3259	L3262	H3263	K3264	E3265	S3266	K3267	T3268	R3269	W3272	L3273	V3274	V3277	C3281	H3285	C3286	R3287	S3290	Q3291	G3292	C3293	S3294	E3295	Q3296	V3297	L3298	T3299	V3300	L3301	K3302	L3303	T3303	V3304	M3310				
N3311	V3312	L3316	S3317	K3318	M3319	L3320	R3324	K3324	Q3325	N3325	Q3326	N3327	L3328	L3329	L3330	T3333	Y3334	R3335	A3338	M3339	A3340	L3341	S3342	K3343	E3344	C3347	L3348	A3349	E3350	L3351	E3352	E3353	R3357	R3358	L3360	S3363	G3364	S3365	S3366	S3367	E3368	D3369	S3370	E3371	I3374	A3375	Y3378	Q3379	R3380	A3381	F3382			

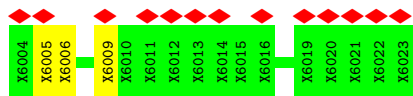


● Molecule 4: Unknown peptide

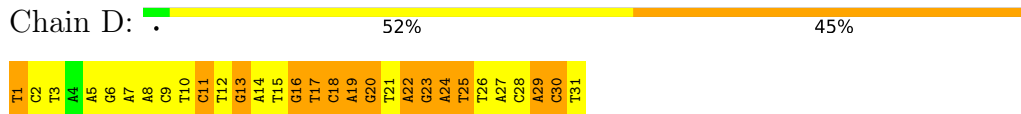


● Molecule 4: Unknown peptide

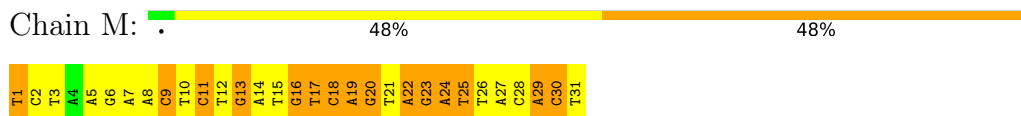




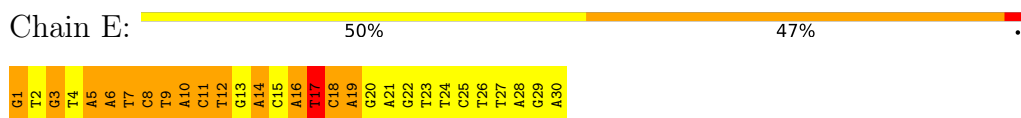
• Molecule 5: DNA (31-MER)



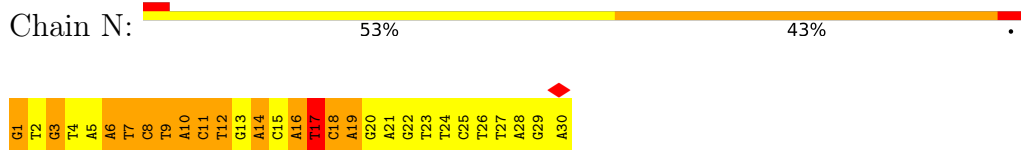
• Molecule 5: DNA (31-MER)



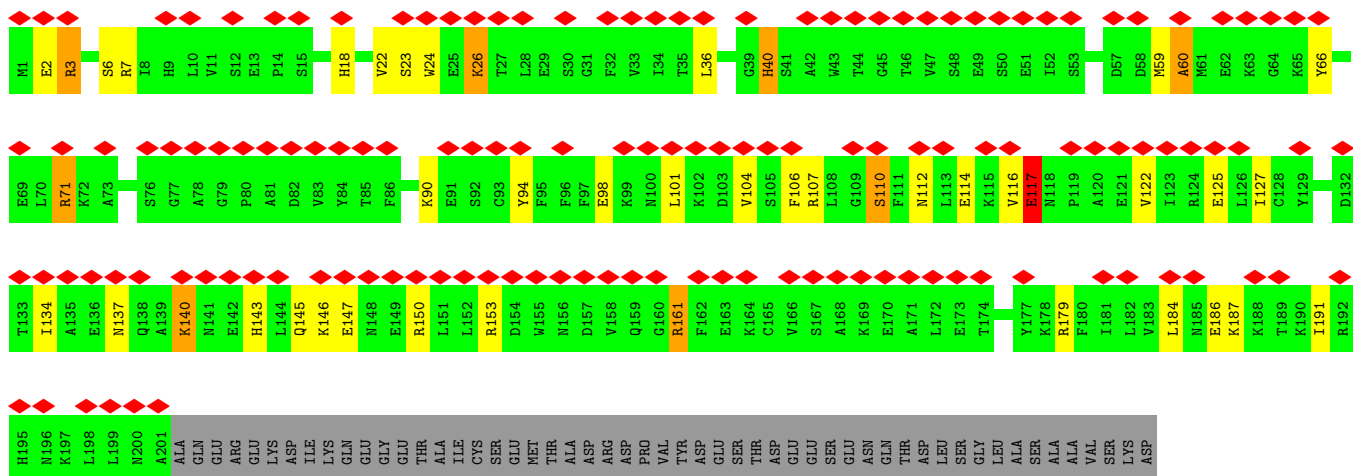
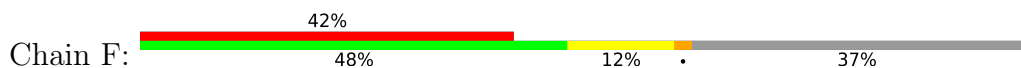
• Molecule 6: DNA (30-MER)

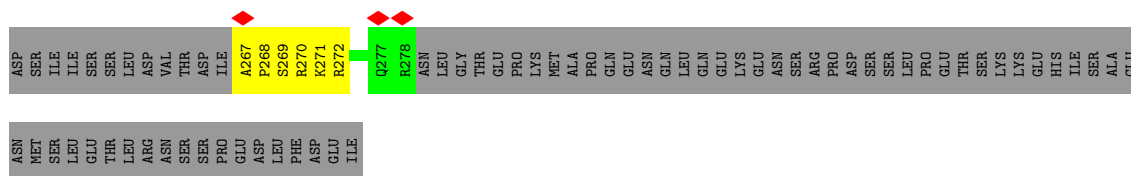


• Molecule 6: DNA (30-MER)

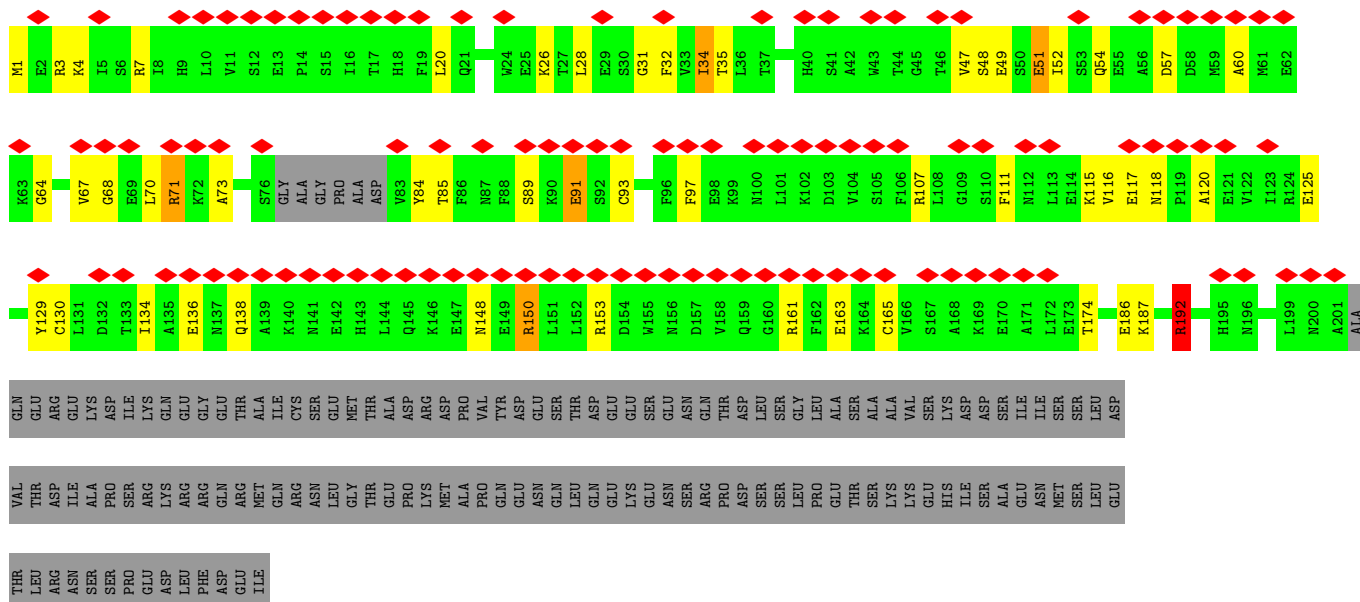
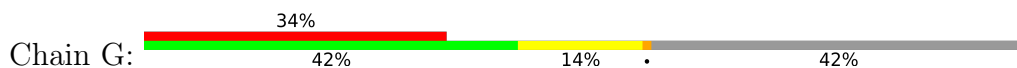


• Molecule 7: DNA repair protein XRCC4

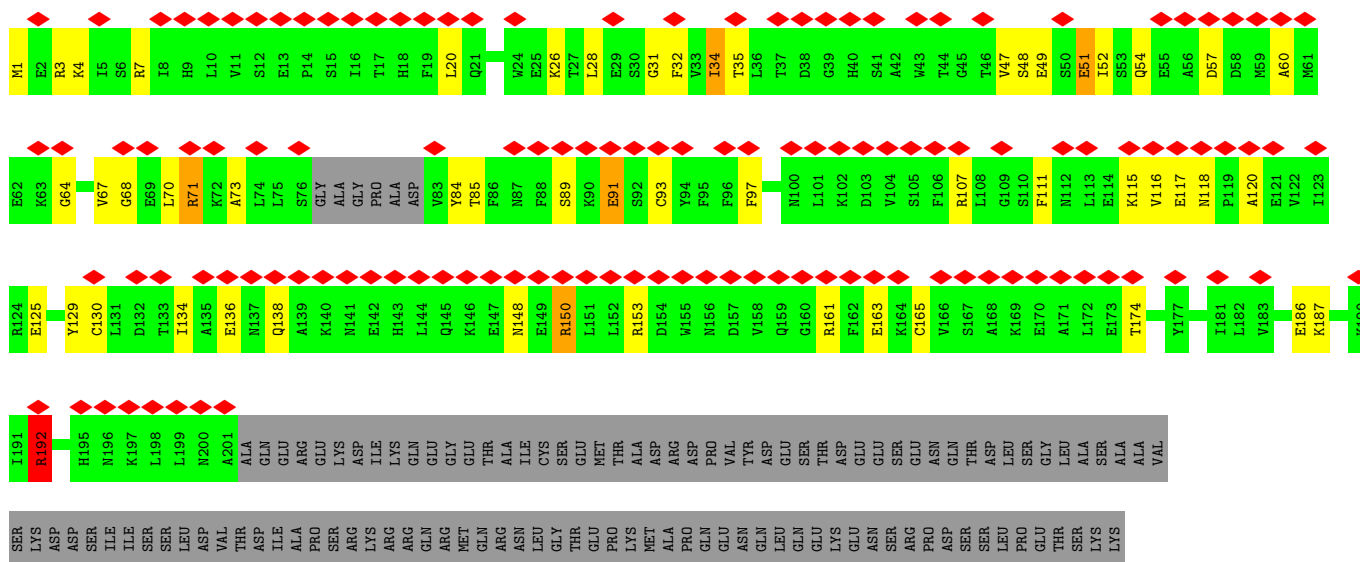




• Molecule 7: DNA repair protein XRCC4

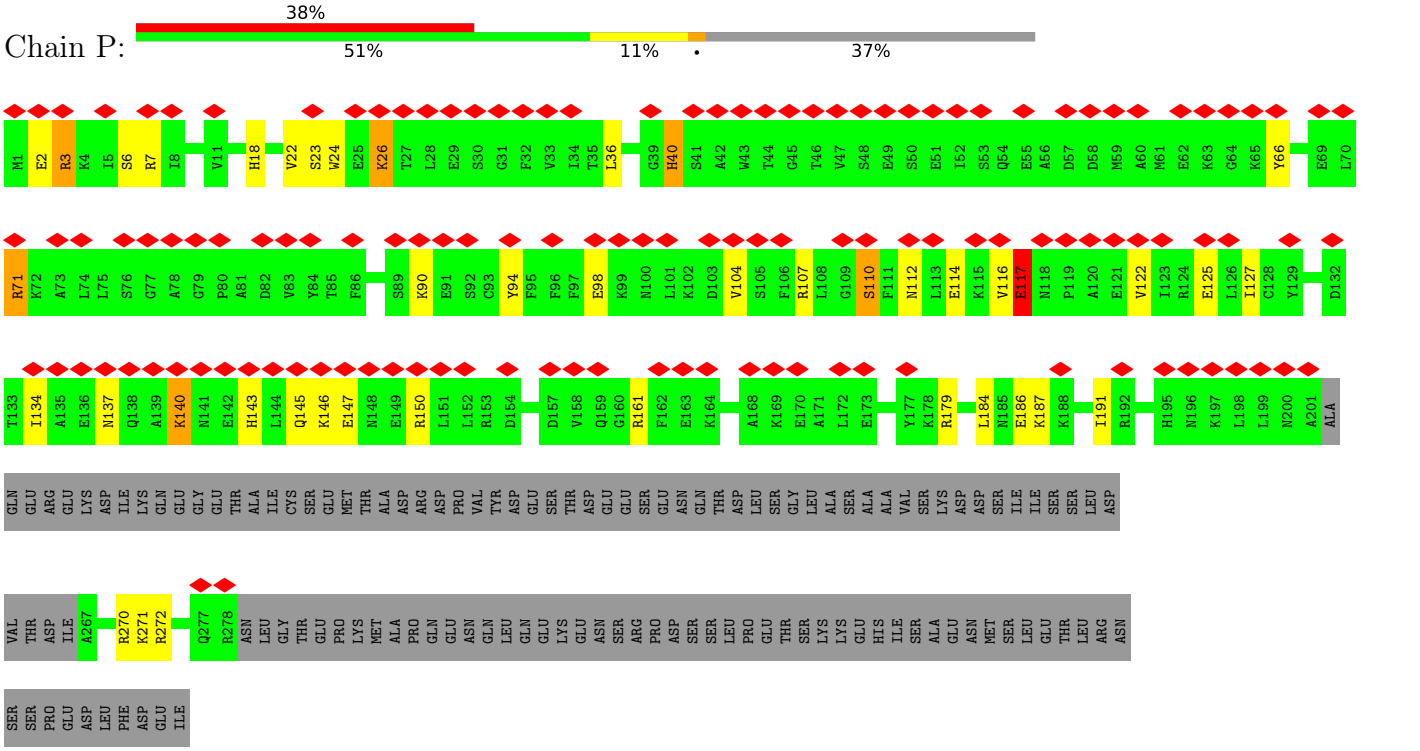


• Molecule 7: DNA repair protein XRCC4

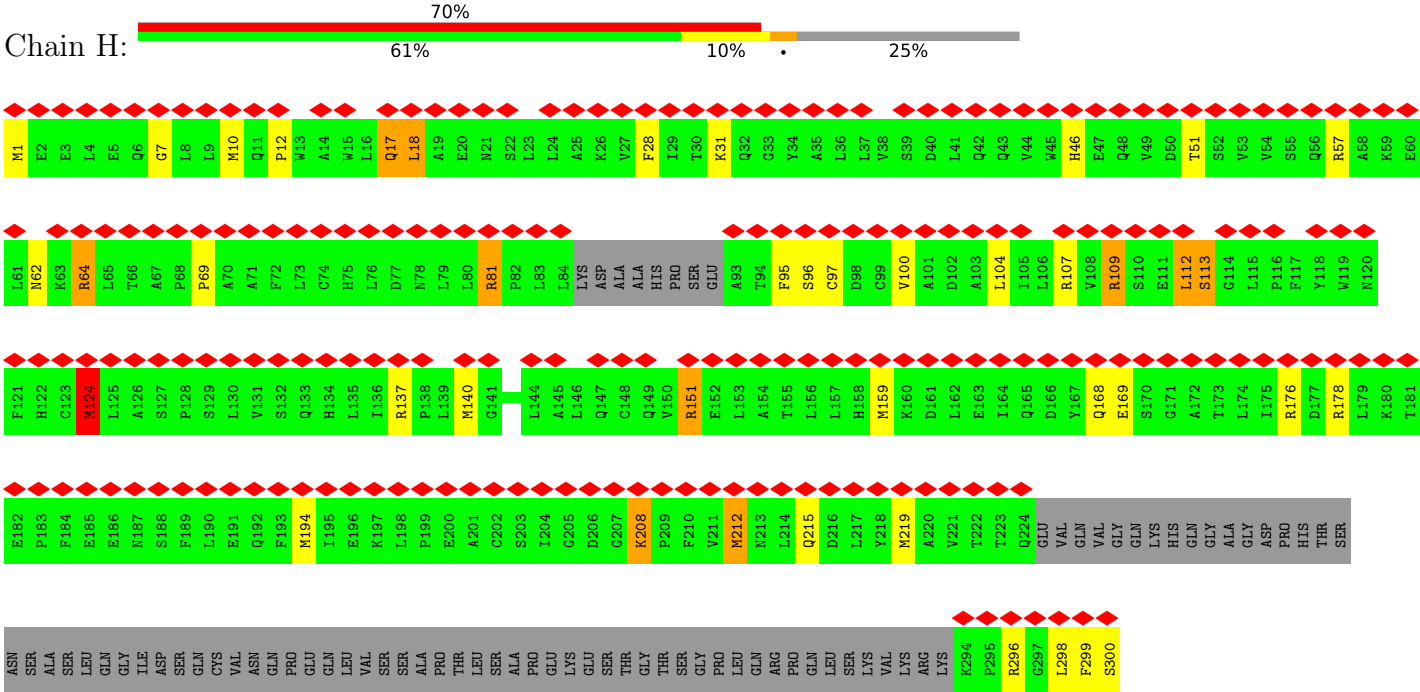


GLU	HIS	LEU	THR	LEU	ARG	ASN	SER	PRO	GLY	ILE
HIS	ILE	ALA	GLU	ASN	MET	LEU	GLU	THR	LEU	ARG
SER	SER	ALA	GLU	ASN	MET	LEU	GLU	THR	LEU	ARG
LEU	THR	LEU	ARG	ASN	SER	PRO	GLY	ILE		
ILE										

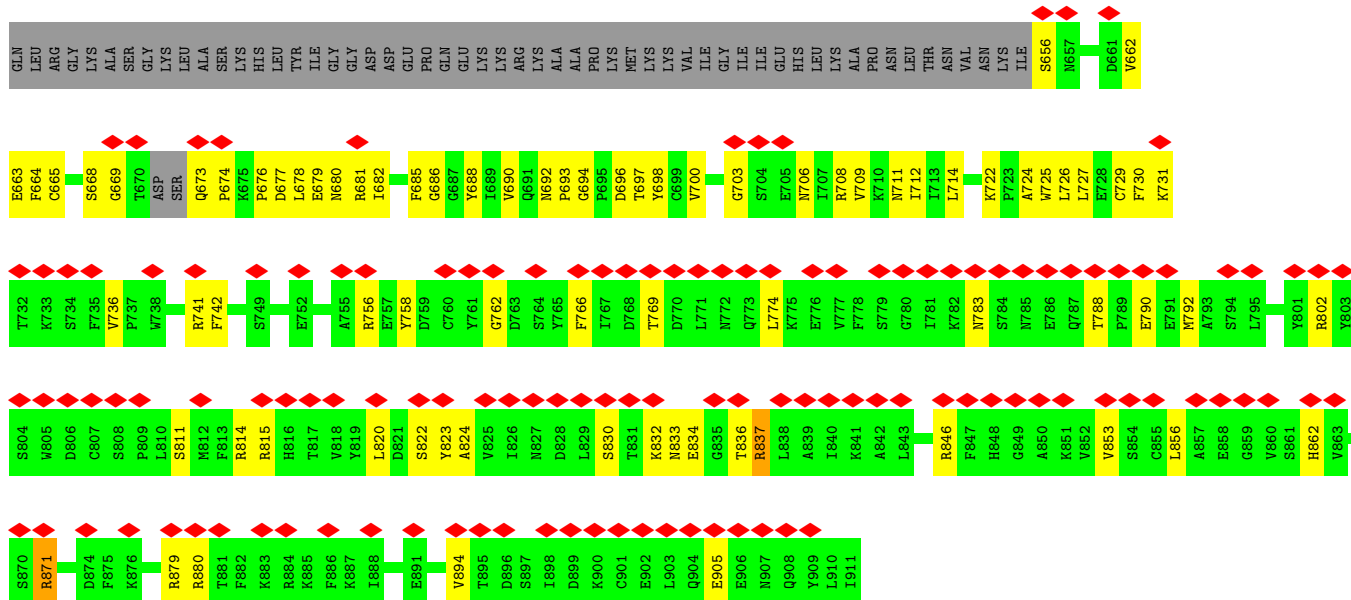
● Molecule 7: DNA repair protein XRCC4



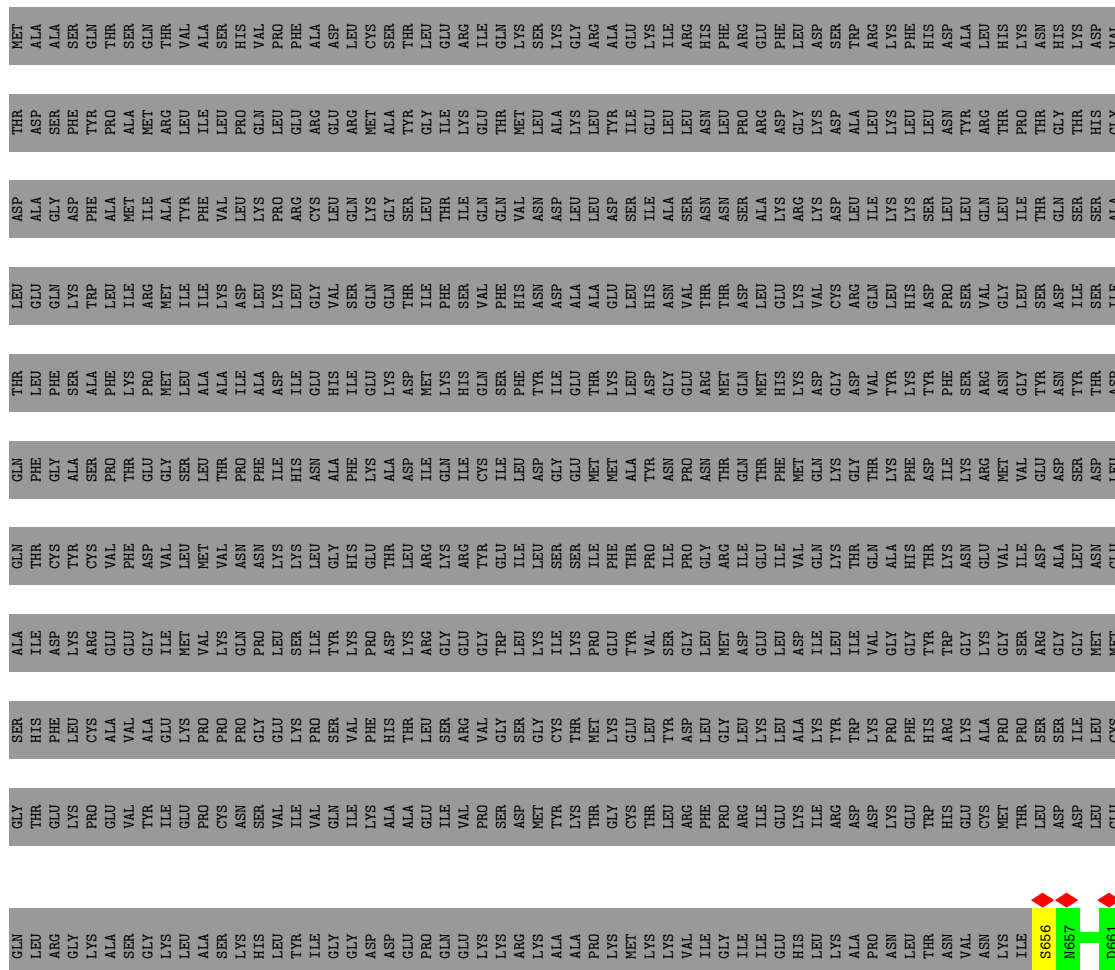
● Molecule 8: Non-homologous end-joining factor 1

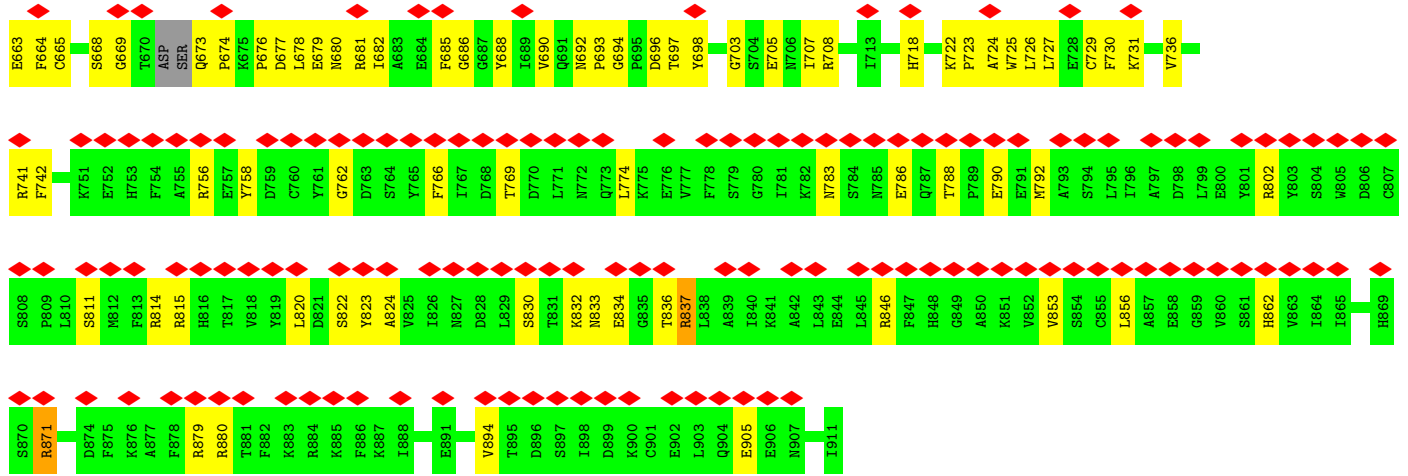


● Molecule 8: Non-homologous end-joining factor 1



• Molecule 9: DNA ligase 4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	329784	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76.5	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	30000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.874	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	319.0, 319.0, 319.0	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.58	0/4101	0.68	1/5523 (0.0%)
1	J	0.58	0/4101	0.68	1/5523 (0.0%)
2	B	0.46	0/4340	0.56	1/5853 (0.0%)
2	K	0.46	0/4340	0.56	1/5853 (0.0%)
3	C	0.57	2/30414 (0.0%)	0.63	8/41079 (0.0%)
3	L	0.57	2/30414 (0.0%)	0.64	8/41079 (0.0%)
5	D	2.09	13/710 (1.8%)	1.37	7/1093 (0.6%)
5	M	2.10	14/710 (2.0%)	1.37	6/1093 (0.5%)
6	E	2.15	19/690 (2.8%)	1.32	5/1063 (0.5%)
6	N	2.15	18/690 (2.6%)	1.32	5/1063 (0.5%)
7	F	0.71	2/1765 (0.1%)	1.13	7/2367 (0.3%)
7	G	0.74	0/1622	1.22	11/2178 (0.5%)
7	O	0.74	0/1622	1.22	11/2178 (0.5%)
7	P	0.71	2/1765 (0.1%)	1.12	7/2367 (0.3%)
8	H	0.77	7/1814 (0.4%)	1.17	14/2454 (0.6%)
8	I	0.78	6/1771 (0.3%)	1.11	6/2395 (0.3%)
9	X	0.69	2/2112 (0.1%)	1.06	14/2851 (0.5%)
9	Y	0.70	2/2112 (0.1%)	1.08	16/2851 (0.6%)
All	All	0.69	89/95093 (0.1%)	0.76	129/128863 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
3	L	0	2
5	D	0	4
5	M	0	4
6	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	N	0	1
7	F	0	4
7	G	0	3
7	O	0	3
7	P	0	4
8	H	0	2
8	I	0	4
9	X	0	1
9	Y	0	1
All	All	0	36

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	29	DA	C3'-O3'	-7.31	1.34	1.44
5	M	24	DA	C3'-O3'	-7.30	1.34	1.44
5	D	24	DA	C3'-O3'	-7.20	1.34	1.44
5	D	29	DA	C3'-O3'	-7.19	1.34	1.44
6	E	10	DA	C3'-O3'	-7.09	1.34	1.44

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	150	ARG	NE-CZ-NH1	9.79	125.19	120.30
7	F	150	ARG	NE-CZ-NH1	9.76	125.18	120.30
8	H	109	ARG	NE-CZ-NH1	9.58	125.09	120.30
8	I	176	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	352	PRO	CA-N-CD	-9.24	98.57	111.50

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	3962	ARG	Sidechain
3	C	4090	ARG	Sidechain
5	D	13	DG	Sidechain
5	D	16	DG	Sidechain
5	D	17	DT	Sidechain

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	4021	0	4100	278	0
1	J	4021	0	4100	278	0
2	B	4259	0	4301	254	0
2	K	4259	0	4301	259	0
3	C	29811	0	30286	1585	0
3	L	29811	0	30286	1583	0
4	Q	101	0	23	2	0
4	R	101	0	23	2	0
5	D	634	0	352	65	0
5	M	634	0	352	66	0
6	E	616	0	339	64	0
6	N	616	0	339	60	0
7	F	1736	0	1739	44	0
7	G	1595	0	1592	38	0
7	O	1595	0	1592	37	0
7	P	1736	0	1739	33	0
8	H	1779	0	1797	30	0
8	I	1737	0	1744	16	0
9	X	2064	0	2012	41	0
9	Y	2064	0	2012	41	0
10	C	27	0	12	5	0
10	L	27	0	12	5	0
All	All	93244	0	93053	4499	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 24.

The worst 5 of 4499 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)
7:O:130:CYS:CA	7:P:134:ILE:HD11	1.44	1.46
7:F:134:ILE:HD11	7:G:130:CYS:CA	1.44	1.45
7:F:134:ILE:CD1	7:G:130:CYS:HA	1.60	1.31
7:O:130:CYS:HA	7:P:134:ILE:CD1	1.60	1.31
7:F:134:ILE:HG12	7:G:134:ILE:HG13	1.22	1.16

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	493/609 (81%)	424 (86%)	69 (14%)	0	100	100
1	J	493/609 (81%)	424 (86%)	69 (14%)	0	100	100
2	B	525/732 (72%)	465 (89%)	60 (11%)	0	100	100
2	K	525/732 (72%)	466 (89%)	59 (11%)	0	100	100
3	C	3686/4128 (89%)	3269 (89%)	416 (11%)	1 (0%)	100	100
3	L	3686/4128 (89%)	3269 (89%)	416 (11%)	1 (0%)	100	100
7	F	209/336 (62%)	202 (97%)	5 (2%)	2 (1%)	15	54
7	G	191/336 (57%)	176 (92%)	12 (6%)	3 (2%)	9	45
7	O	191/336 (57%)	176 (92%)	12 (6%)	3 (2%)	9	45
7	P	209/336 (62%)	203 (97%)	5 (2%)	1 (0%)	29	68
8	H	217/299 (73%)	201 (93%)	15 (7%)	1 (0%)	29	68
8	I	212/299 (71%)	200 (94%)	11 (5%)	1 (0%)	29	68
9	X	250/911 (27%)	230 (92%)	20 (8%)	0	100	100
9	Y	250/911 (27%)	231 (92%)	19 (8%)	0	100	100
All	All	11137/14702 (76%)	9936 (89%)	1188 (11%)	13 (0%)	54	85

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	F	26	LYS
7	P	26	LYS
7	G	26	LYS
7	G	64	GLY
8	H	208	LYS

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	452/548 (82%)	452 (100%)	0	100	100
1	J	452/548 (82%)	452 (100%)	0	100	100
2	B	481/649 (74%)	478 (99%)	3 (1%)	86	92
2	K	481/649 (74%)	478 (99%)	3 (1%)	86	92
3	C	3325/3671 (91%)	3316 (100%)	9 (0%)	92	95
3	L	3325/3671 (91%)	3316 (100%)	9 (0%)	92	95
7	F	191/303 (63%)	166 (87%)	25 (13%)	4	20
7	G	178/303 (59%)	153 (86%)	25 (14%)	3	19
7	O	178/303 (59%)	153 (86%)	25 (14%)	3	19
7	P	191/303 (63%)	167 (87%)	24 (13%)	4	21
8	H	198/262 (76%)	188 (95%)	10 (5%)	24	50
8	I	193/262 (74%)	177 (92%)	16 (8%)	11	36
9	X	230/808 (28%)	212 (92%)	18 (8%)	12	38
9	Y	230/808 (28%)	211 (92%)	19 (8%)	11	36
All	All	10105/13088 (77%)	9919 (98%)	186 (2%)	61	77

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	O	115	LYS
7	P	140	LYS
7	O	150	ARG
7	P	40	HIS
9	X	774	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
8	I	56	GLN

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Mol	Chain	Res	Type
3	L	1909	ASN
7	P	40	HIS
1	J	204	HIS
3	L	16	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	ADP	L	4201	-	24,29,29	1.20	4 (16%)	29,45,45	1.59	3 (10%)
10	ADP	C	4201	-	24,29,29	1.20	4 (16%)	29,45,45	1.58	3 (10%)

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
10	ADP	L	4201	-	-	2/12/32/32	0/3/3/3
10	ADP	C	4201	-	-	2/12/32/32	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)
10	L	4201	ADP	C2'-C1'	-2.88	1.49	1.53
10	C	4201	ADP	C2'-C1'	-2.83	1.49	1.53
10	C	4201	ADP	C4-N3	-2.18	1.32	1.35
10	C	4201	ADP	O4'-C4'	-2.13	1.40	1.45
10	L	4201	ADP	C4-N3	-2.12	1.32	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	4201	ADP	PA-O3A-PB	-4.85	116.19	132.83
10	C	4201	ADP	PA-O3A-PB	-4.84	116.22	132.83
10	C	4201	ADP	C3'-C2'-C1'	2.65	104.97	100.98
10	L	4201	ADP	C1'-N9-C4	2.62	131.25	126.64
10	L	4201	ADP	C3'-C2'-C1'	2.61	104.90	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	4201	ADP	C5'-O5'-PA-O3A
10	L	4201	ADP	C5'-O5'-PA-O3A
10	C	4201	ADP	C5'-O5'-PA-O1A
10	L	4201	ADP	C5'-O5'-PA-O1A

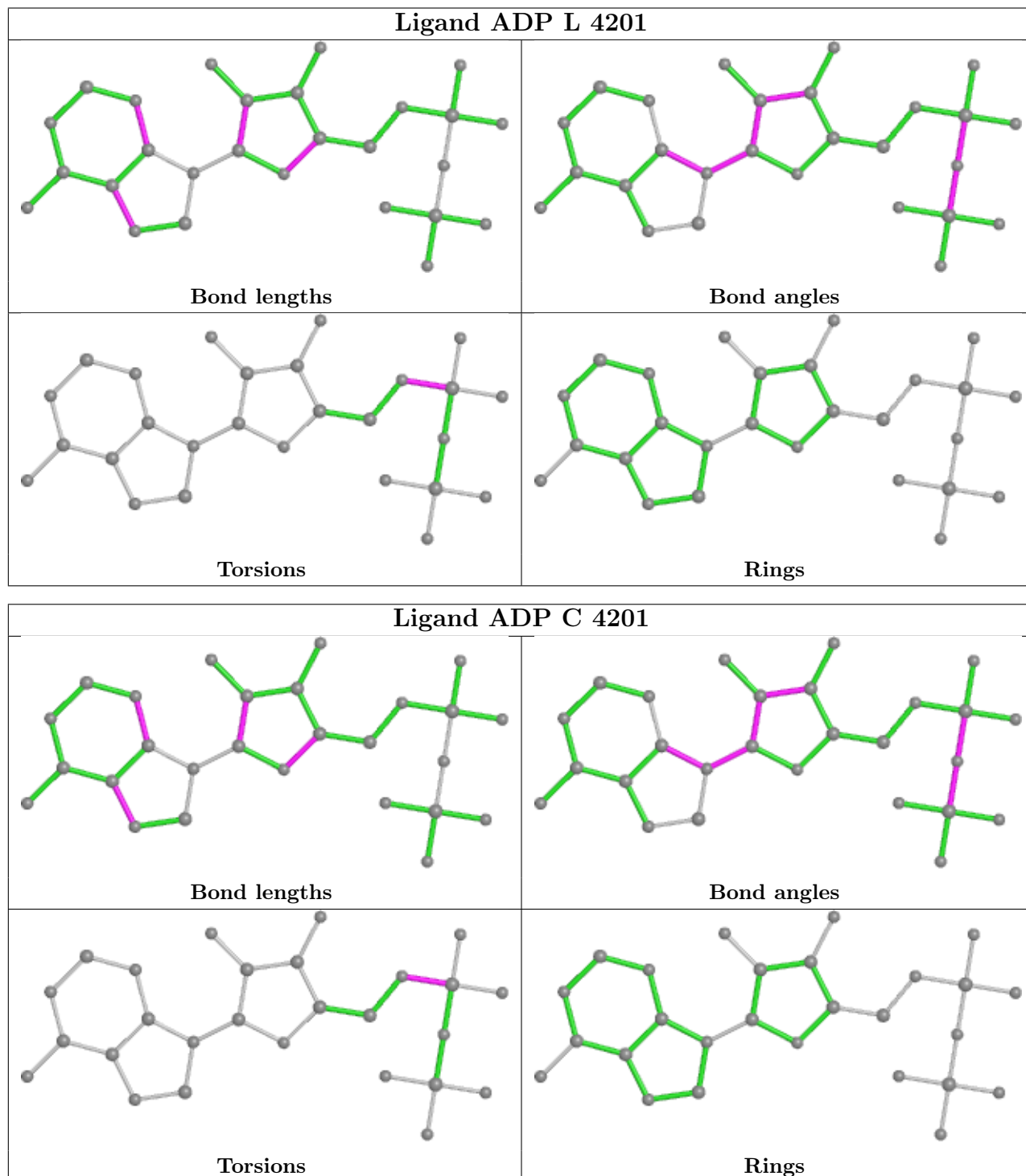
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	4201	ADP	5	0
10	C	4201	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

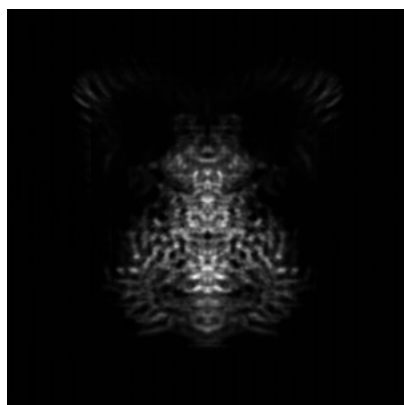
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23510. These allow visual inspection of the internal detail of the map and identification of artifacts.

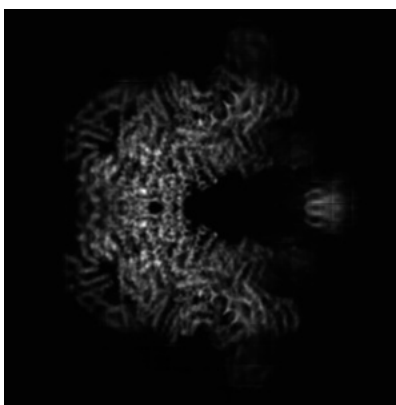
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

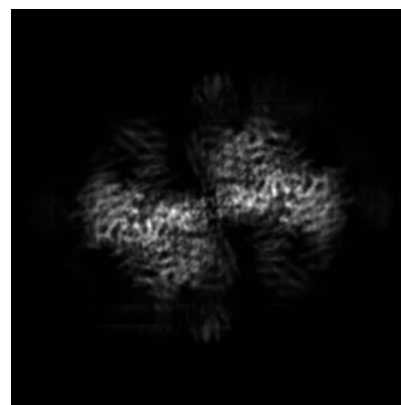
6.1.1 Primary map



X



Y

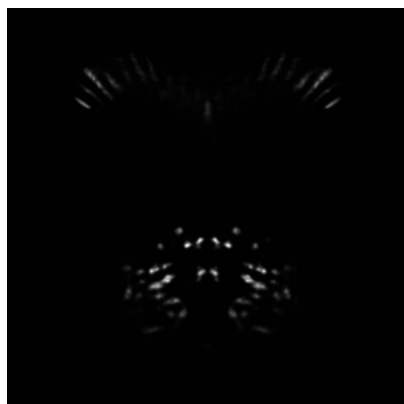


Z

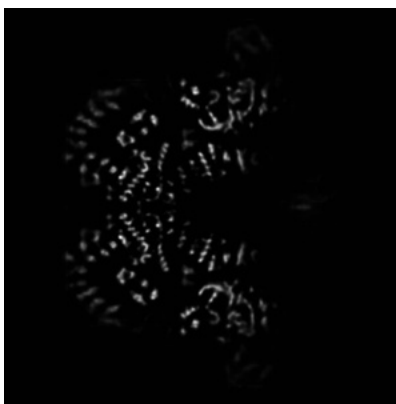
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

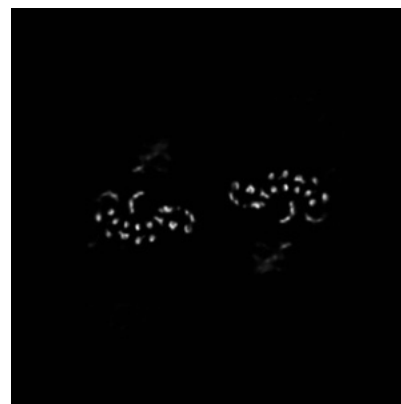
6.2.1 Primary map



X Index: 145



Y Index: 145



Z Index: 145

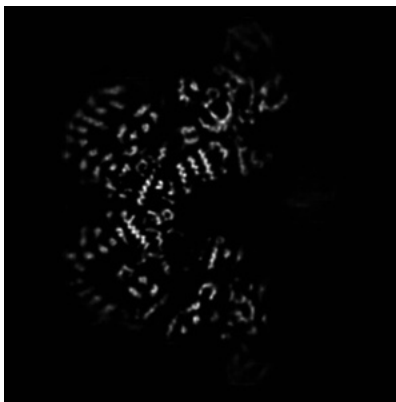
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

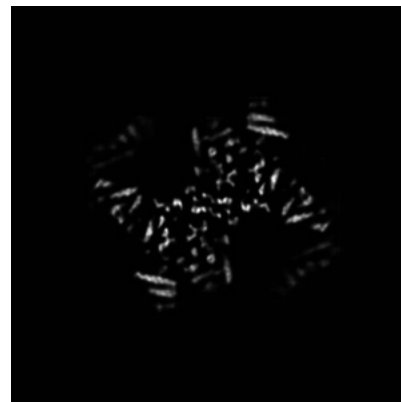
6.3.1 Primary map



X Index: 185



Y Index: 147

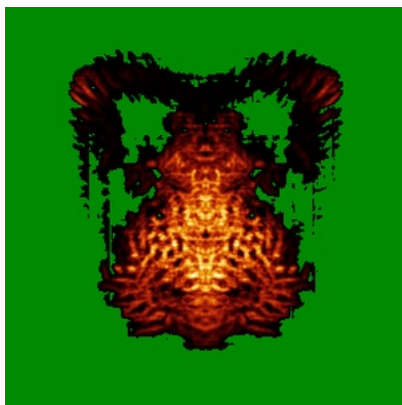


Z Index: 100

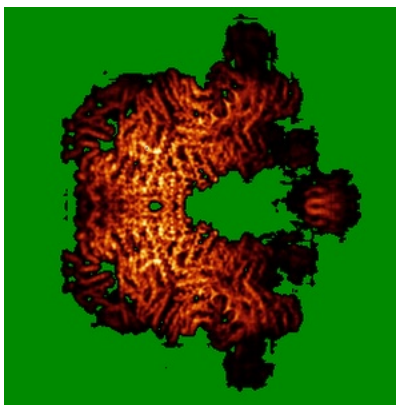
The images above show the largest variance slices of the map in three orthogonal directions.

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

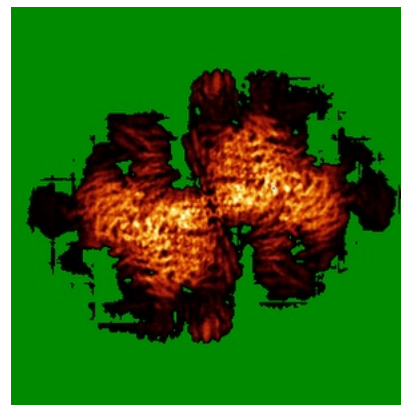
6.4.1 Primary map



X



Y

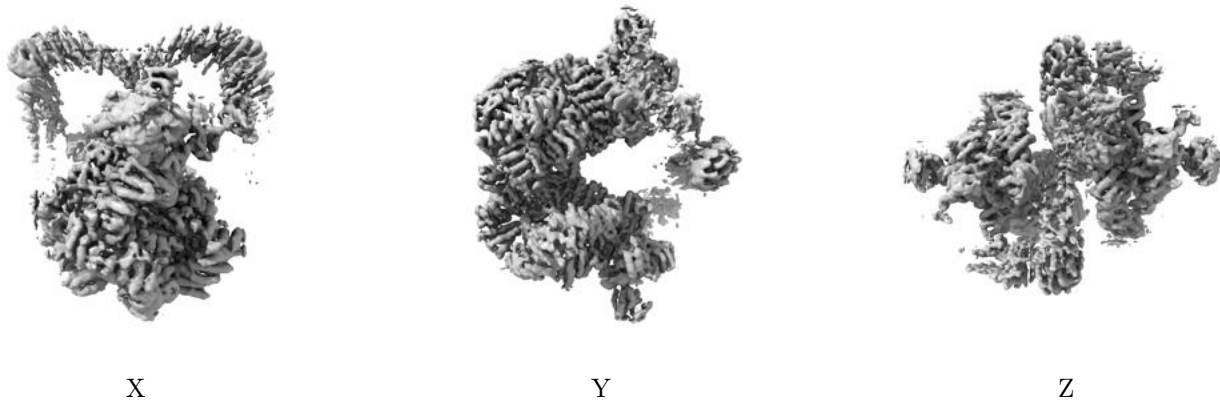


Z

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

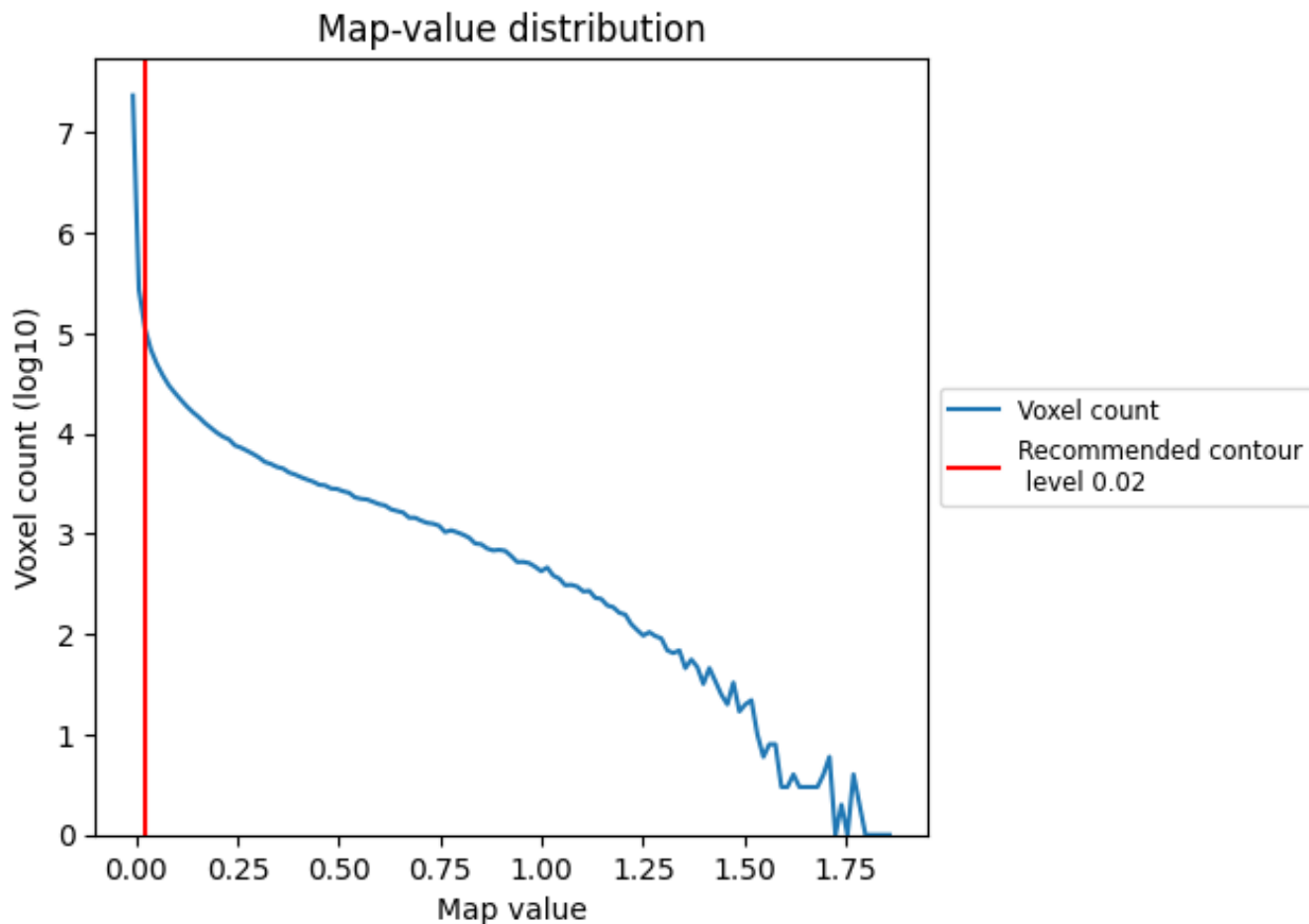
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

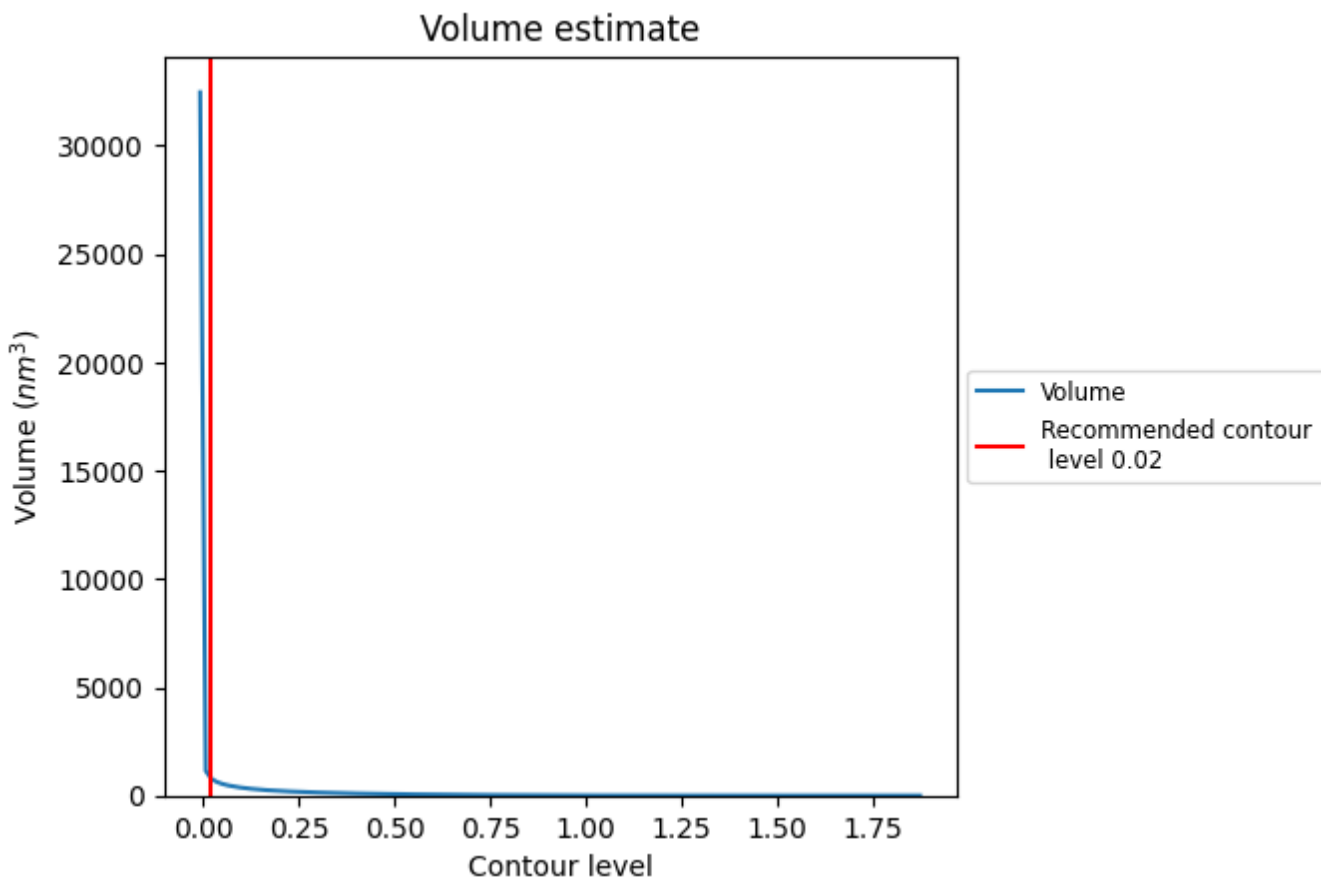
This section contains the results of statistical analysis of the map.

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.

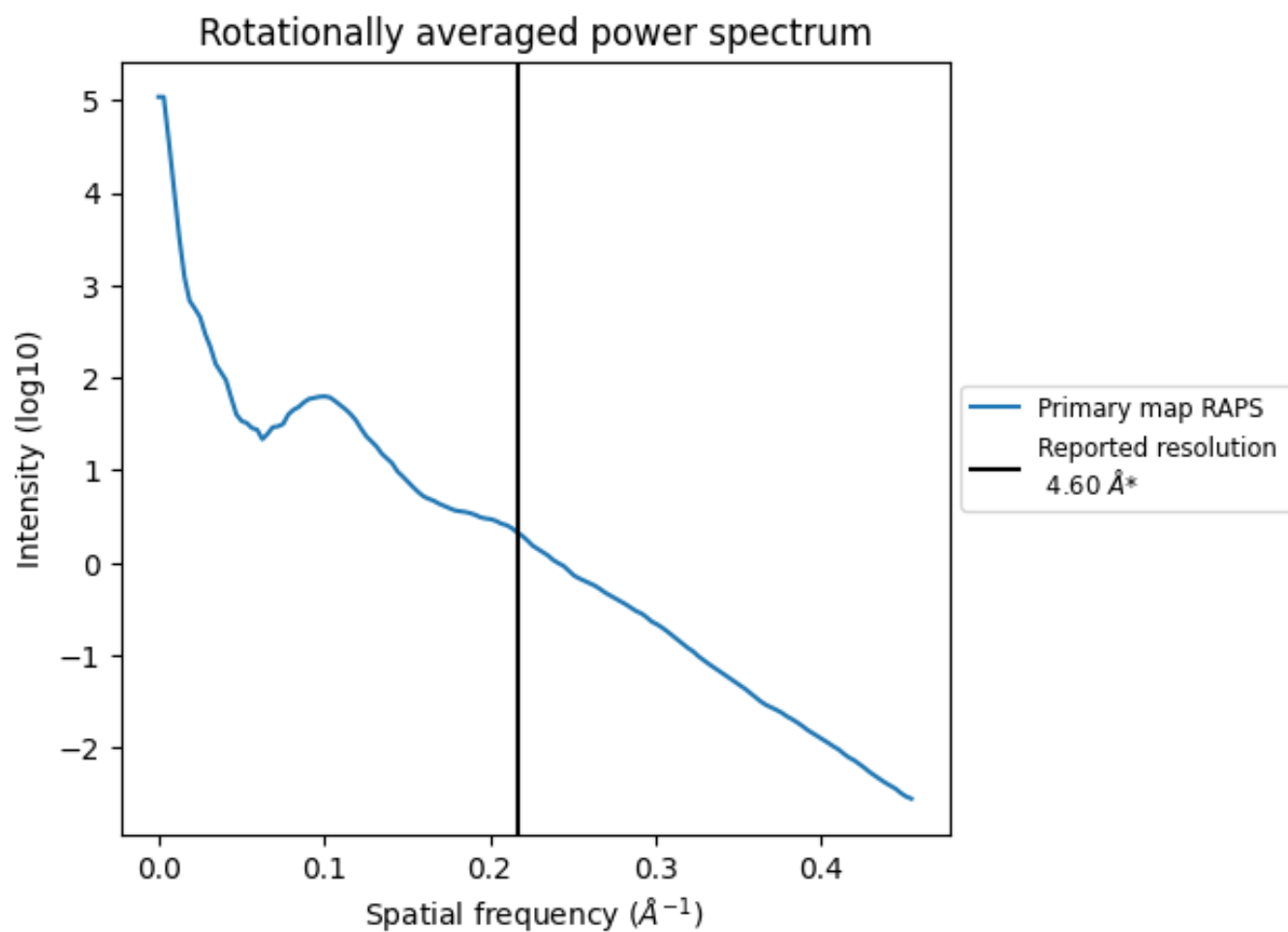
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 789 nm³; this corresponds to an approximate mass of 713 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](#)

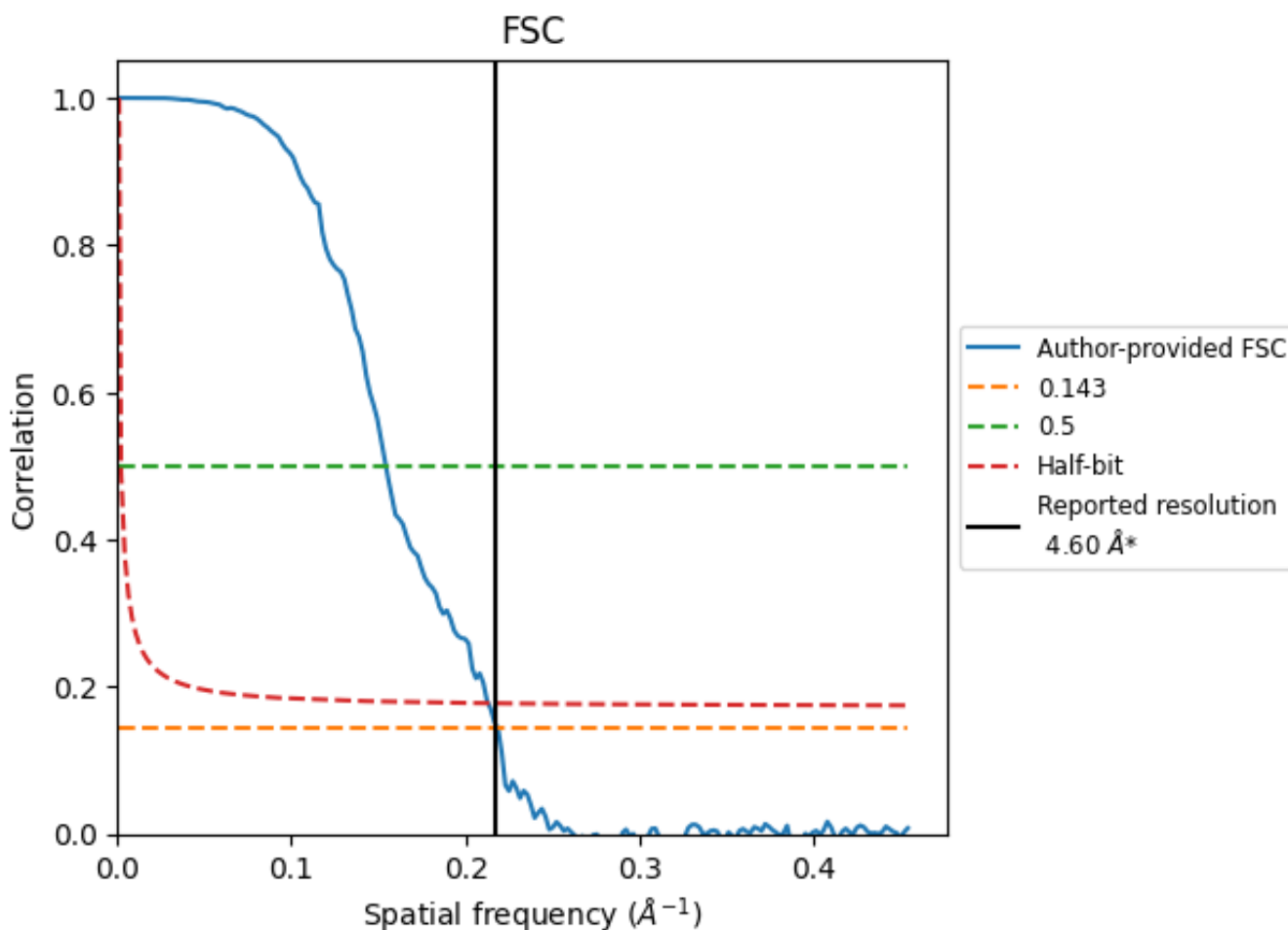


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

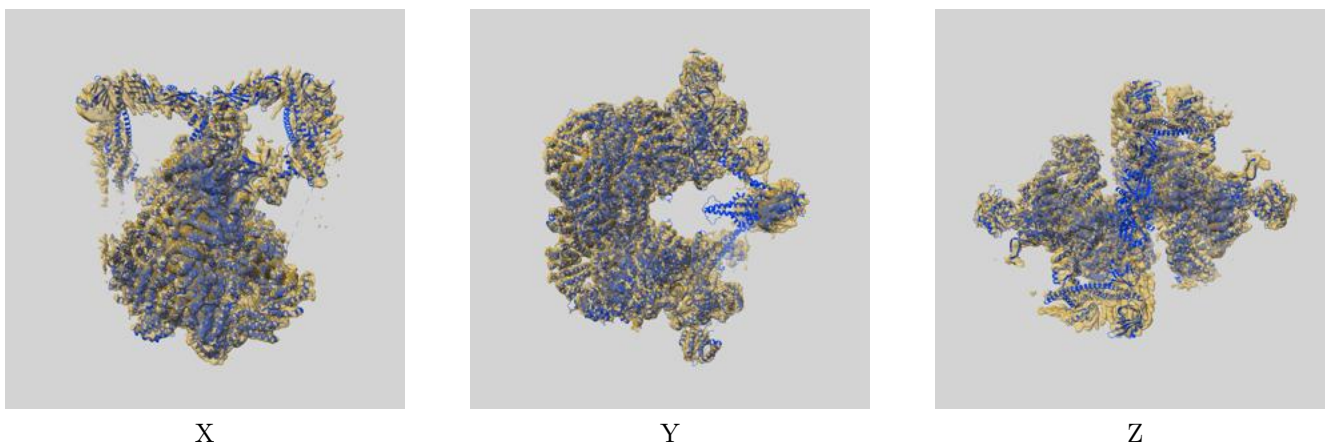
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.57	6.48	4.69
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

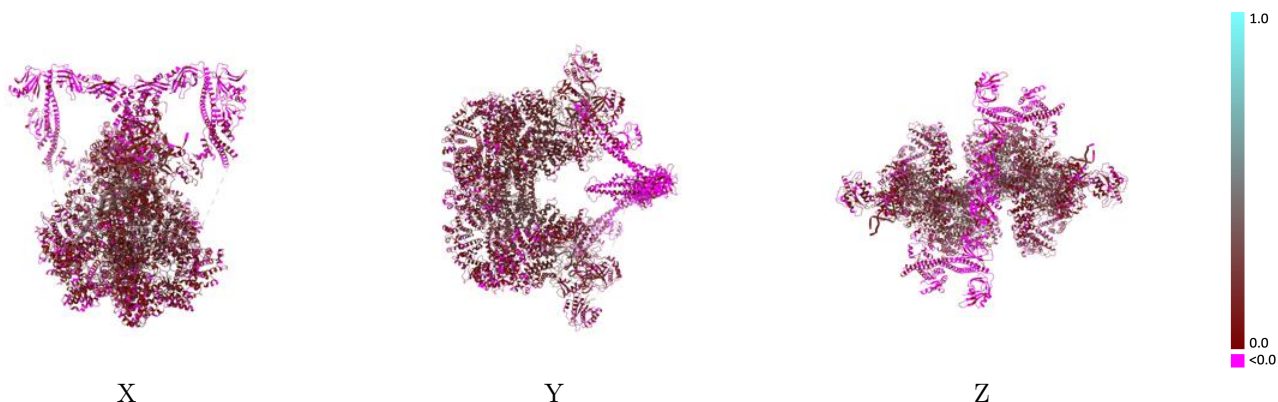
This section contains information regarding the fit between EMDB map EMD-23510 and PDB model 7LT3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



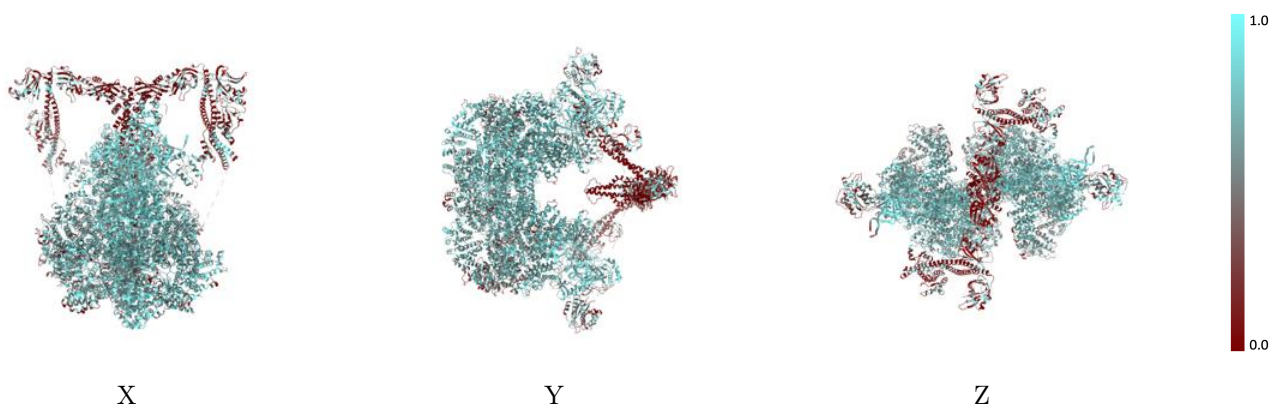
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



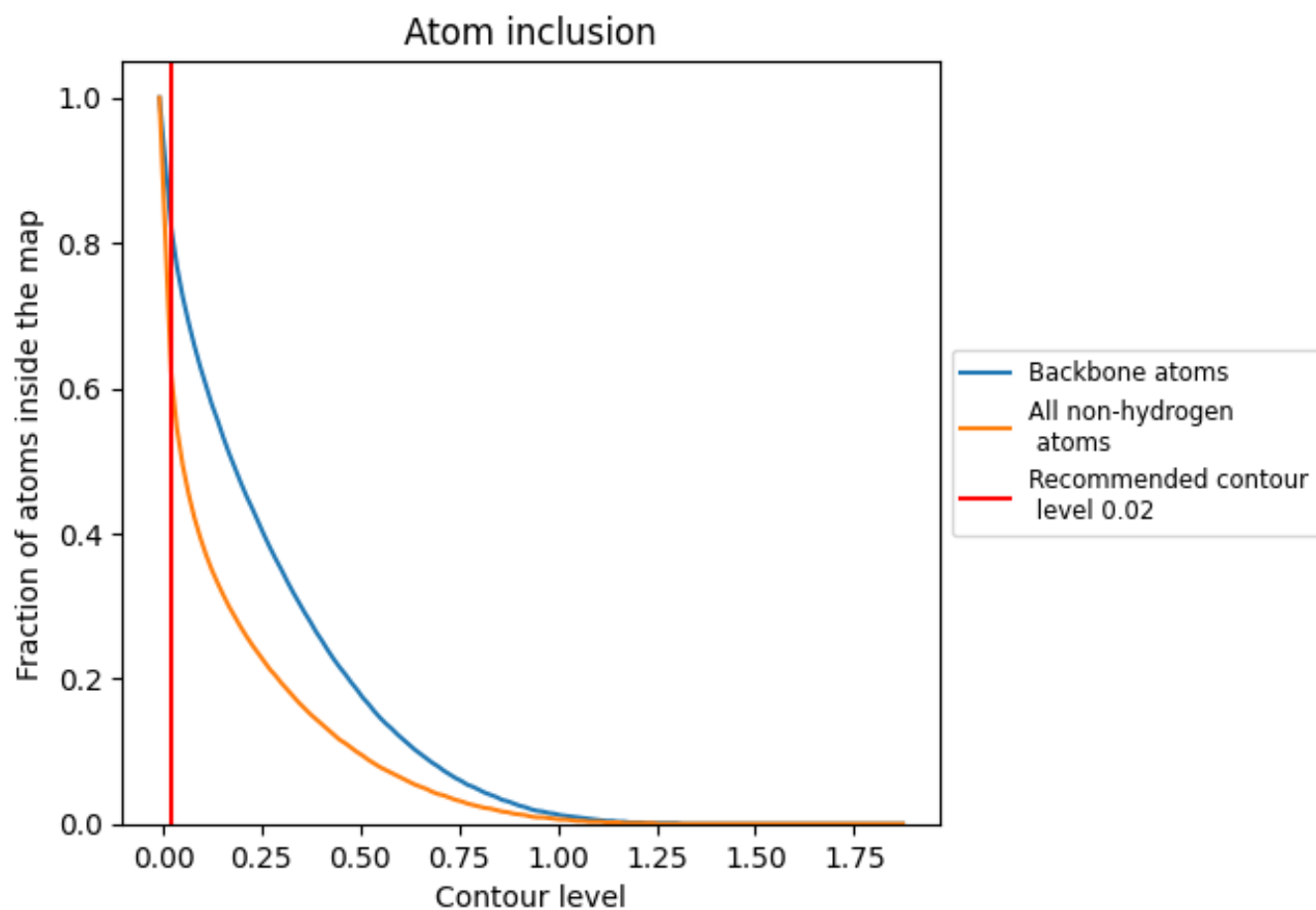
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 62% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.1180
A	 0.6920	 0.1410
B	 0.6190	 0.1190
C	 0.6940	 0.1450
D	 0.9340	 0.2740
E	 0.9370	 0.2930
F	 0.3070	 -0.0340
G	 0.3670	 -0.0580
H	 0.0790	 -0.0220
I	 0.1360	 -0.0420
J	 0.7070	 0.1420
K	 0.5620	 0.1120
L	 0.6810	 0.1410
M	 0.9040	 0.2740
N	 0.9040	 0.2910
O	 0.3130	 -0.0650
P	 0.3470	 -0.0230
Q	 0.2470	 0.1700
R	 0.3660	 0.1090
X	 0.4100	 0.0050
Y	 0.3700	 -0.0030

