



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 02:11 AM UTC

PDB ID : 7LT3 / pdb_00007lt3
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 : 6ERH, 6ZHA, 1JEY, 5LUQ, 5Y3R, 2R9A, 3II6

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

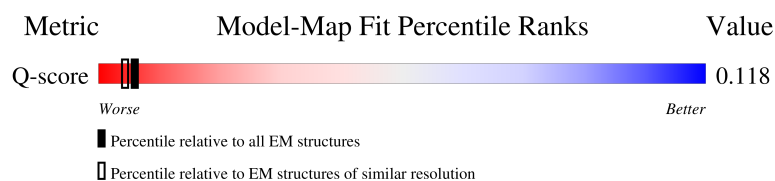
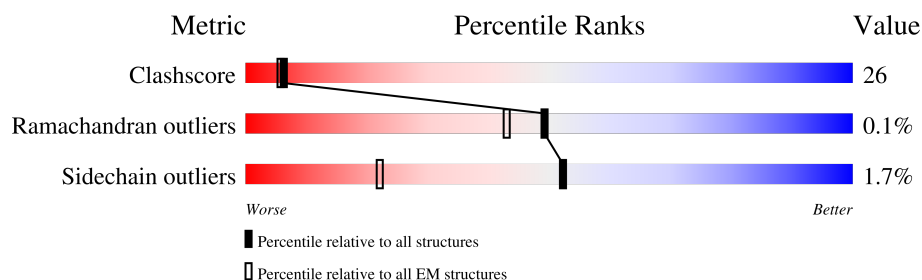
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	

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Mol	Chain	Length	Quality of chain
3	C	4128	
3	L	4128	
4	Q	20	
4	R	20	
5	D	31	
5	M	31	
6	E	30	
6	N	30	
7	F	336	
7	G	336	
7	O	336	
7	P	336	
8	H	299	
8	I	299	
9	X	911	
9	Y	911	

2 Entry composition

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
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
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
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
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		

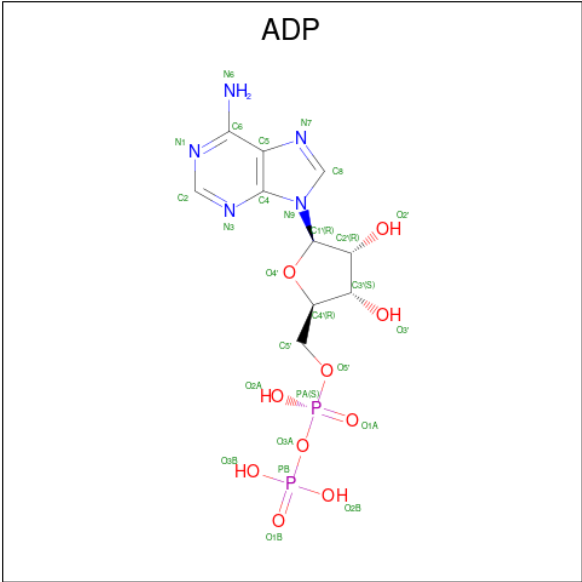
- Molecule 8 is a protein called Non-homologous end-joining factor 1.

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.

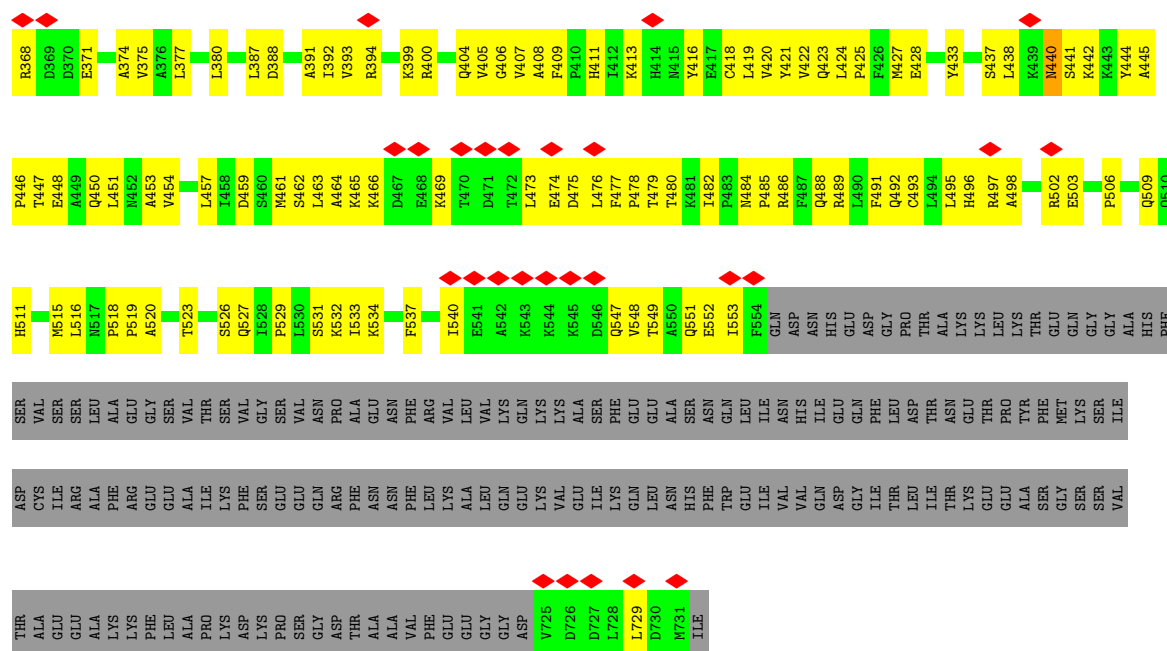
Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	254	Total	C	N	O	S	0	0
			2064	1314	348	389	13		
9	Y	254	Total	C	N	O	S	0	0
			2064	1314	348	389	13		

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

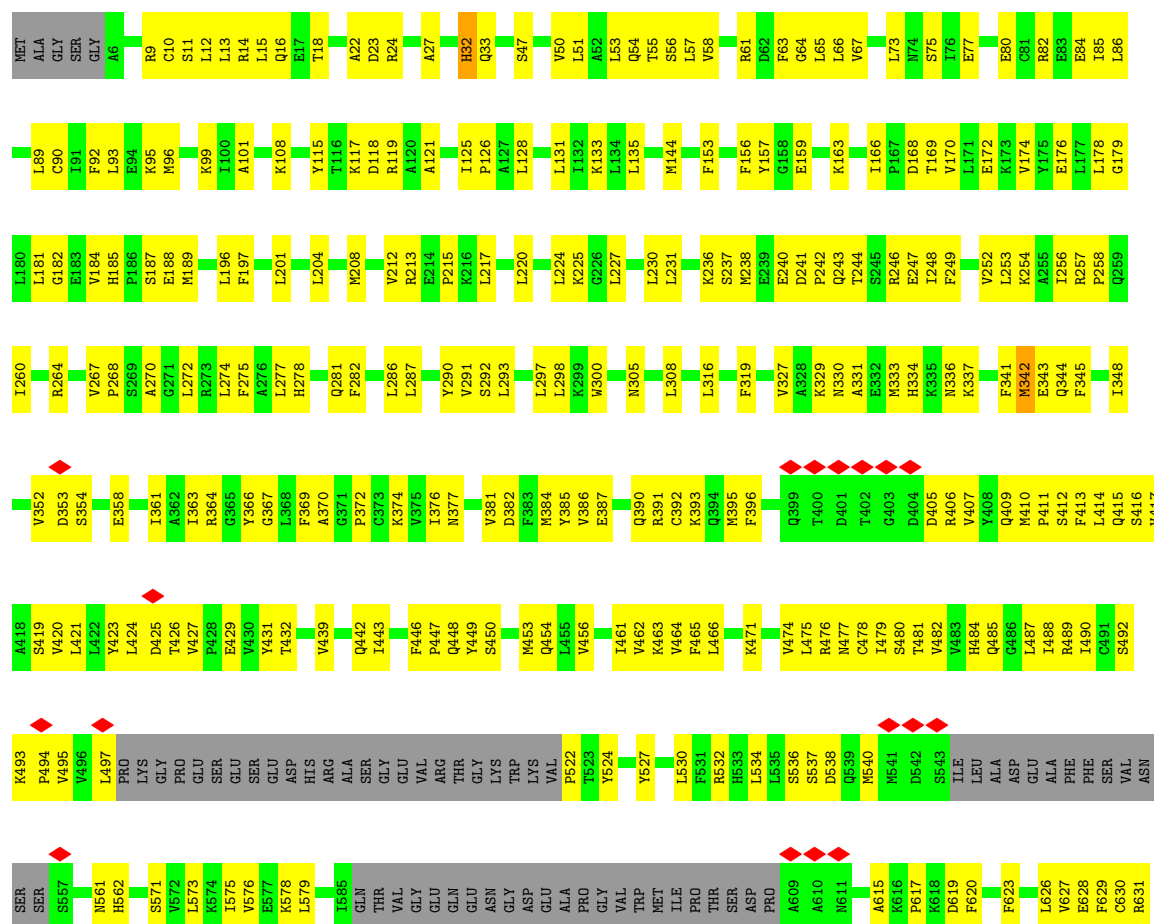


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	





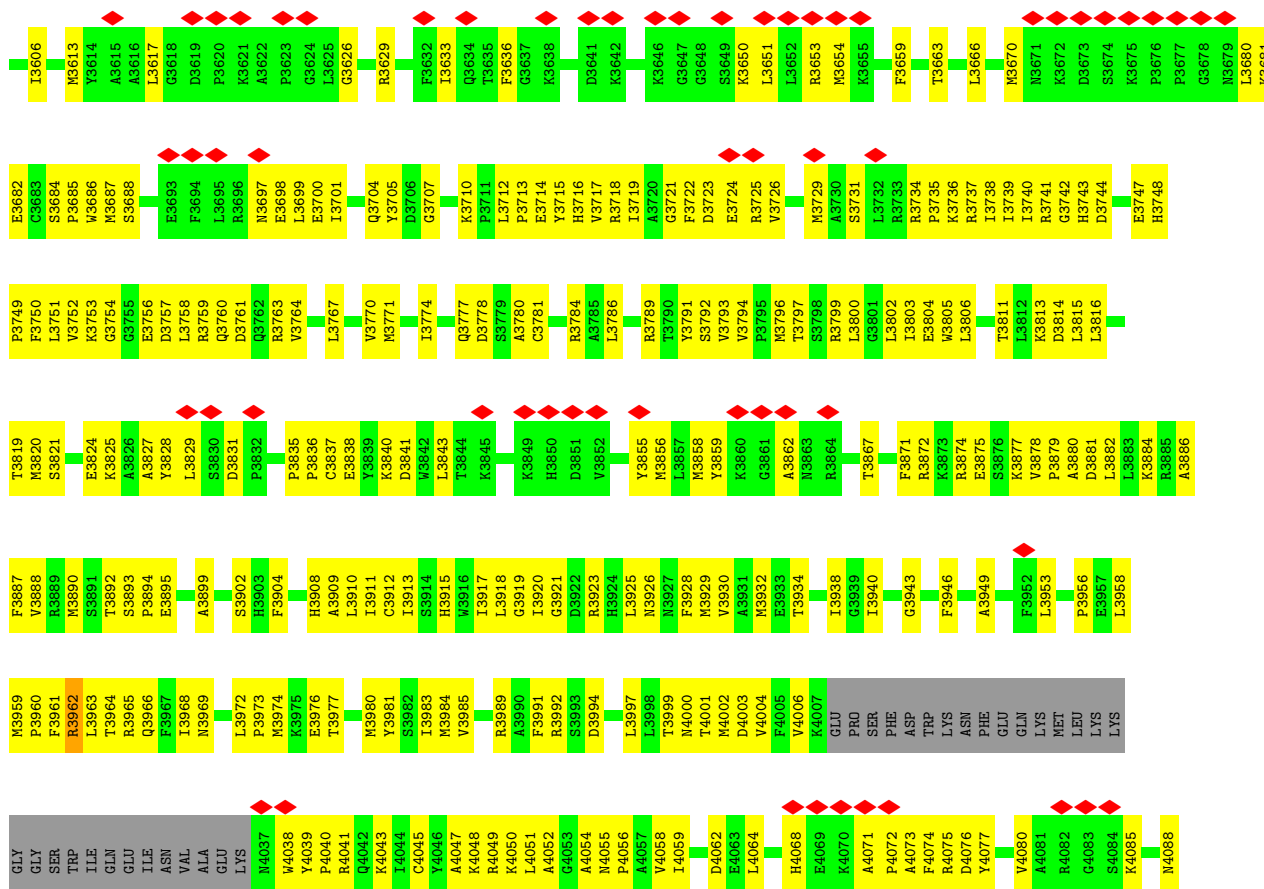
• Molecule 3: DNA-dependent protein kinase catalytic subunit



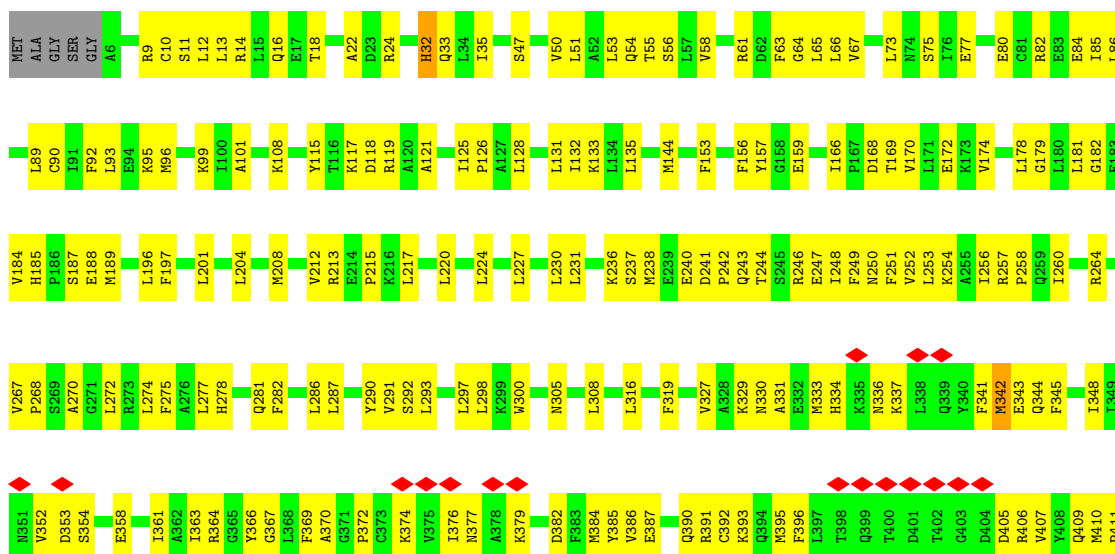


K2360	L2274	T2201	E2135	PRO	ALA	V1889	L1952	V1889	L1827	L1758	L1688	R1608
Q2353	Q2275	P2202	T2136	THR	ALA	H1890	I1952	H1890	L1828	L1759	L1689	A1609
M2356	L2276	G2204	I2137	VAL	ASN	A1891	V1955	A1891	V1693	E1760	V1693	M1610
E2357	L2277	T2203	V2138	HIS	GLY	K1892	F1956	K1892	H1829	T1763	V1693	Q1611
D2358	G2278	G2204	P2139	ASP	ASP	E1893	N1957	E1893	H1830	E1764	L1695	L2450
K2359	L2140	V2205	L2140	ASP	SER	E1893	N1957	E1893	H1830	V1765	L1696	K2452
F2360	N2141	P2206	N2141	GLY	GLY	K1895	E1958	K1895	S1832	L1766	P1697	E2463
L2454	T2142	K2207	T2142	PRO	PRO	L1959	L1959	L1959	S1832	C1767	F1698	L2464
	R2143	D2208	R2143	SER	SER	K1960	K1960	I1896	L1833	F1698	F1699	
		E2209		TYR	TYR	F1961	F1961	I1896	D1834	R1768	F1699	A1619
	L2146			GLU	GLU	Y1962	Y1962	N1897	D1834	E1769	T1700	
	A2147	N2210		GLU	GLU	Y1962	Y1962	Q1898	A1835	Q1770	S1701	I1622
	K2148	L2285		GLU	MET	Y1962	Y1962	V1899	L1836	Q1771	L1702	K1628
	L2149	P2286		GLU	SER	Q1963	Q1963	F1899	L1836	H1772	T1703	C1629
	V2150	P2287		GLU	SER	G1964	G1964	F1900	E1838	H1772	T1703	
	I2151	D2214		GLU	LEU	F1965	F1965	F1900	E1838	V1773	G1704	
	N2152	N2215		GLU	SER	F1967	F1967	G1902	F1840	M1774	G1705	
	T2153	N2217		GLU	TYR	F1967	F1967	S1903	F1840			
	E2154	F2218		GLU	ALA	S1968	S1968	C1904	S1841	F1778	S1706	
	E2155	L2288		GLU	ALA	S1968	S1968	I1905	T1842		S1707	
	V2156	P2286		GLU	ASP	E1969	E1969	I1905	V1844		E1708	
	F2157	P2287		GLU	SER	E1969	E1969	I1905	V1844		E1708	
	P2159	N2221		GLU	THR	P1970	P1970	T1906	I1848		E1709	
	Y2160	K2227		GLU	THR	P1971	P1971	E1907	D1849		L1710	
	A2161	R2228		GLU	LEU	E1972	E1972	E1907	R1783		L1710	
	K2162	N2234		GLU	SER	K1973	K1973	G1908	R1784		R1711	
	H2163			GLU	MET	N1974	N1974	N1909	I1785		H1713	
	L2165			GLU	MET	L1975	L1975	E1910	A1786		Q1716	
	S2166			GLU	SER	L1976	L1976	E1910	R1787		L1717	
	T2167			GLU	GLN	F1977	F1977	E1910	R1788		I1718	
	L2168			GLU	ASP	E1979	E1979	K1913	G1789		F1722	
	L2169			GLU	PHE	N1980	N1980	L1915	S1789		P1723	
				GLU	SER	L1981	L1981	L1916	S1790		M1724	
				GLU	THR	L1982	L1982	R1917	C1791			
				GLU	GLY	D1983	D1983	L1918	Q1794		Q1725	
				GLU	VAL	L1984	L1984	C1919	V1795		S1726	
				GLU	GLN	K1985	K1985	C1919	G1796		R1727	
				GLU	SER	L1986	L1986	Y1920	L1797		E1728	
				GLU	TYR	R1987	R1987	D1921	L1798		F1729	
				GLU	SER			A1922	E1799		V1659	
				GLU	TYR			F1923	S1800		P1730	
				GLU	SER				Y1801		P1731	
				GLU	SER				E1802		S1660	
				GLU	GLN				E1803		F1661	
				GLU	ASP				M1804		N1662	
				GLU	PRO				F1805		T1663	
				GLU	ARG				K1870		F1736	
				GLU	PRO				E1930		N1737	
				GLU	VAL				M1871			
				GLU	VAL				G1872			
				GLU	VAL				Y1873		D1741	
				GLU	ALA				D1809			
				GLU	THR				P1809			
				GLU	THR				D1809			
				GLU	THR				P1810			
				GLU	THR				R1811			
				GLU	THR				L1812			
				GLU	THR				S1813			
				GLU	THR				F1814			
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				GLU	THR				A1749			
				GLU	THR				L1750			
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V3530	A3461	S3386	Q3296	Q3074	W2994	ARG	ASN	L2519
Y3531	F3532	V3389	V3297	R3075	W2994	VAL	LYS	L2520
F3532	L3462	V3390	V3300	A3076	L2803	PHE	VAL	L2521
L3463	F3533	Q3390	V3300	I3077	L2804	ASP	LYS	
L3464	K3464	A3391	L3301	E3078	L2808	TRP	GLY	
F3465	F3465	A3392	K3302	E3079	L2809	LEU	ALA	
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S3537	L3467	ALA	V3304	Y3089	S2811	GLY	ALA	
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S3541	Q3470	PRO	D3325	L3091	S2813	GLY	ALA	
F3542	L3471	PRO	M3326	Y3102	S2814	THR	ALA	
L3472	L3472	PRO	K3327	Y3107	S2815	THR	ALA	
F3543	E3477	PRO	N3328	M3111	S2816	THR	ALA	
D3544	E3478	PRO	L3329	Y3114	S2817	THR	ALA	
T3545	E3478	PRO	L3330	S3115	S2818	THR	ALA	
S3546	E3478	PRO	L3330	S3116	S2819	THR	ALA	
K3550	L3482	PRO	T3333	Y3117	S2820	THR	ALA	
N3551	M3483	PRO	Y3334	L3178	S2821	THR	ALA	
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V3555	E3486	PRO	A3338	D3180	S2823	THR	ALA	
A3556	S3487	PRO	L3339	L3183	S2824	THR	ALA	
R3557	S3488	PRO	A3340	T3184	S2825	THR	ALA	
L3558	S3489	PRO	L3341	N3185	S2826	THR	ALA	
K3559	V3490	PRO	S3342	R3186	S2827	THR	ALA	
S3560	A3412	PRO	S3343	F3189	S2828	THR	ALA	
K3561	Y3413	PRO	E3344	L3190	S2829	THR	ALA	
L3562	F3492	PRO	F3345	T3193	S2830	THR	ALA	
D3563	Q3494	PRO	A3346	H3122	S2831	THR	ALA	
Q3564	F3495	PRO	C3347	Q3123	S2832	THR	ALA	
L3568	L3496	PRO	L3348	L3126	S2833	THR	ALA	
I3572	S3497	PRO	L3348	T3127	S2834	THR	ALA	
N3573	W3498	PRO	T3351	K3128	S2835	THR	ALA	
A3574	L3499	PRO	E3352	L3129	S2836	THR	ALA	
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L3578	M3502	PRO	R3357	Y3132	S2839	THR	ALA	
S3579	A3504	PRO	R3358	Q3133	S2840	THR	ALA	
N3580	L3505	PRO	L3359	A3134	S2841	THR	ALA	
F3581	L3506	PRO	L3360	L3135	S2842	THR	ALA	
L3583	D3507	PRO	S3363	VAL	S2843	THR	ALA	
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F3585	D3509	PRO	S3365	ASP	S2845	THR	ALA	
W3588	Q3510	PRO	S3366	GLN	S2846	THR	ALA	
R3593	V3511	PRO	E3371	ASP	S2847	THR	ALA	
L3596	V3512	PRO	L3374	GLY	S2848	THR	ALA	
A3597	V3513	PRO	A3375	ASP	S2849	THR	ALA	
K3598	V3514	PRO	L3378	ASP	S2850	THR	ALA	
T3599	V3447	PRO	Y3379	ASP	S2851	THR	ALA	
S3600	E3448	PRO	Q3291	ASP	S2852	THR	ALA	
V3601	K3449	PRO	C3292	ASP	S2853	THR	ALA	
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	V3601	PRO	Q3383	ASP	S2856	THR	ALA	
		PRO	H3384	ASP	S2857	THR	ALA	
		PRO	L3385	ASP	S2858	THR	ALA	



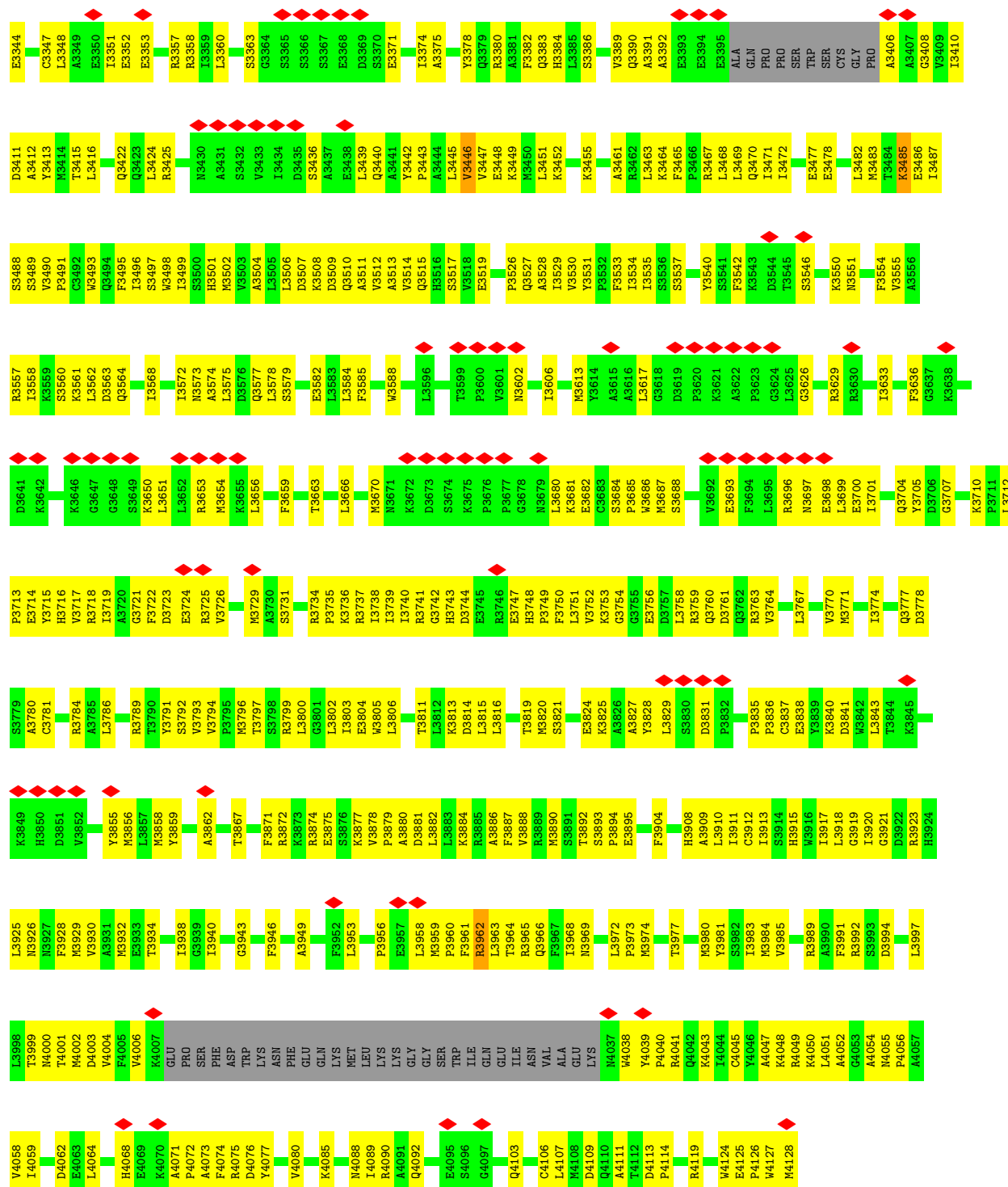
• Molecule 3: DNA-dependent protein kinase catalytic subunit



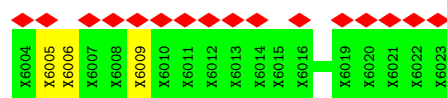
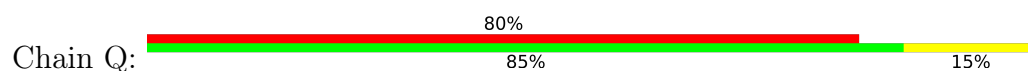
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A1309	L1241	G1163	L1014	E844	A766	E699	E628	ASN	S492	V417
E1310	L1242	Q1098	D1015	A845	E767	E699	F629	SER	K493	A418
K1311	Y1243	L1165	G1016	I846	V768	C703	C630	SER	P494	S419
CYS	LEU	L1166	I1017	S847	G769	L706	R631	ASP	V495	V420
PHE	ARG	F1101	V1018	L848	L770	F707	E632	GLU	V496	L421
GLY	ARG	E1102	D1022	1851	A771	V708	I633	PRO	L497	L422
THR	PHE	A1103	L1025	1853	A772	K709	E640	LYS	L497	Y423
ALA	GLY	I1106	F1028	1855	E774	F710	F642	GLY	PRO	L424
ALA	GLY	M1108	C1029	1856	E775	G711	F643	PRO	GLY	D425
GLY	ALA	E1109	C1032	1858	I778	K712	P644	SER	GLU	T426
ASN	ALA	S1110	C1033	1859	I779	E713	Y647	SER	GLU	V427
ARG	ALA	L1111	I1033	1861	R782	V716	S648	GLU	SER	P428
THR	ALA	A1112	R1034	1862	Y788	K717	F649	GLU	ASP	Y430
S1323	W1256	L1113	E1035	1863	Y789	M718	S650	GLU	ASP	Y431
E1326	L1259	A1114	F1036	1865	K790	Y721	Y651	GLU	ASP	T432
N1331	L1260	L1117	L1037	1866	D791	K722	E652	GLU	ASP	Y439
Y1332	L1261	P1178	L1038	1867	I792	K722	L653	GLU	ASP	Q442
S1333	A1263	P1179	W1039	1868	I793	D723	I654	GLU	ASP	I443
K1334	L1264	Q1180	I1040	1869	L794	E724	L655	GLU	ASP	Y446
C1335	E1265	L1121	I1041	1870	C795	L725	L655	GLU	ASP	F447
T1336	C1266	L1122	P1046	1871	L796	L726	L655	GLU	ASP	Q448
V1337	Y1267	I1123	Q1047	1872	D797	C729	L655	GLU	ASP	Y449
N1338	N1268	G1124	Q1048	1873	G798	Y732	L655	GLU	ASP	S450
V1339	T1269	Q1125	Q1049	1874	Y799	F732	L655	GLU	ASP	M453
R1340	F1270	C1127	Q1050	1875	Y799	F732	L655	GLU	ASP	Q454
I1341	V1194	D1129	E1050	1876	Y799	F732	L655	GLU	ASP	L455
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E1343	L1196	D1132	K1051	1878	Y799	F732	L655	GLU	ASP	I461
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G1355	P1199	D1132	F1060	1887	Y799	F732	L655	GLU	ASP	R476
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N1365	P1199	D1132	F1060	1893	Y799	F732	L655	GLU	ASP	V483
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A1405	H1465	M1598	V1671	N1737	K1807	Y1873	R1937	LYS	LYS	L2122	V2186
L1406	M1466	G1599	Y1675	D1741	D1808	Y1874	R1938	GLU	GLU	P2123	V2187
K1407	I1467	M1600	I1676	K1744	D1809	I1875	R1939	ILE	ILE	S2124	E2188
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K1412	S1472	V1537	D1681	D1748	F1814	M1880	E1944	LYS	LYS	L2129	G2197
D1413	T1473	L1538	T1682	K1750	R1816	Y1881	A1945	GLU	GLU	H2130	G2198
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G1438	L1500	L1572	E1709	R1782	K1852	F1910	I1977	SER	SER	N2160	N2234
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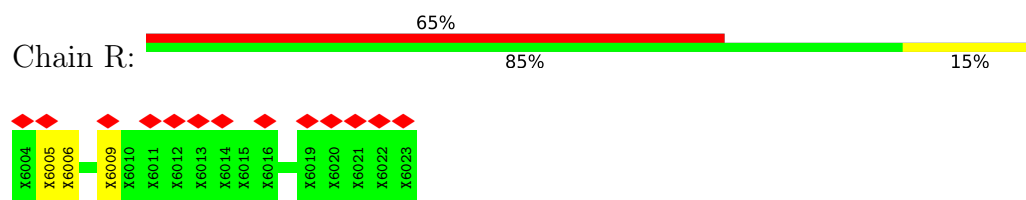
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GLU	ASP	ASN	SER	MET	ASN	VAL	ASP	GLN	ASP	GLY	ASP	SER	ASP	PRO	SER	ASP	MET	GLU	VAL	GLN	GLU	GLU	GLU	GLU	ASP	I3227	S3228	S3229	L3320	I3321	T3322	D3323	S3234	S3245	A3246	R3247	K3248	Q3249	N3250	N3251	F3252	A3255	M3256	K3257	L3258	L3259	L3262	H3263	K3264	E3265
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VAL	ALA	GLY	GLN	ILE	ARG	ALA	THR	GLN	GLN	HIS	ASP	PHE	THR	LEU	THR	GLN	THR	ALA	ASP	ARG	SER	SER	PHE	ASP	THR	TRP	LEU	GLY	LEU	VAL	THR	GLN	HIS	ASP	THR	GLN	THR	LEU	PHE	ALA	HIS	ARG	SER	GLU	ARG	GLN	ARG			
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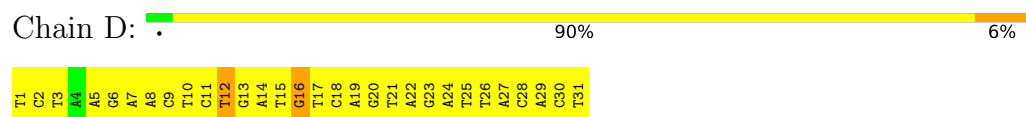
• Molecule 4: Unknown peptide



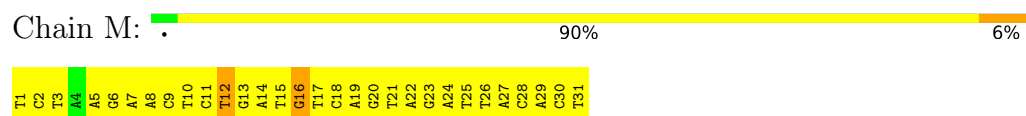
- Molecule 4: Unknown peptide



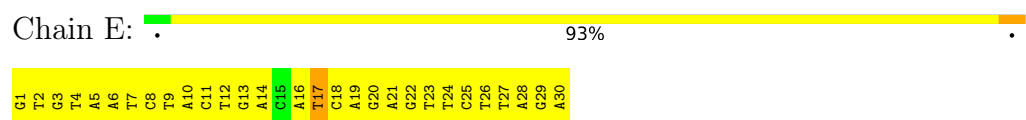
- Molecule 5: DNA (31-MER)



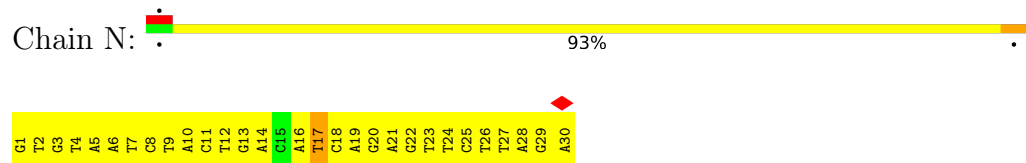
- Molecule 5: DNA (31-MER)



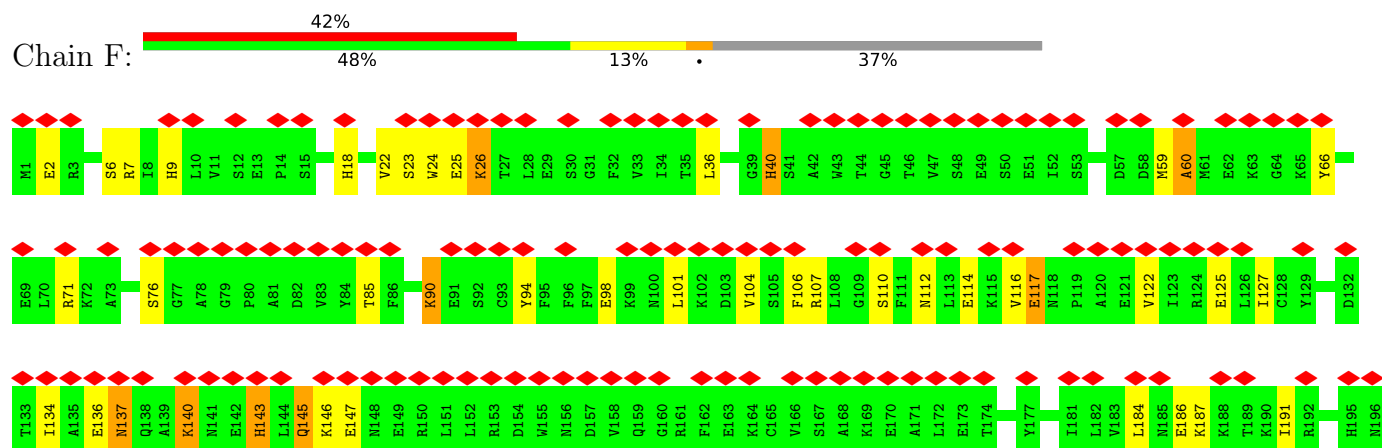
- Molecule 6: DNA (30-MER)

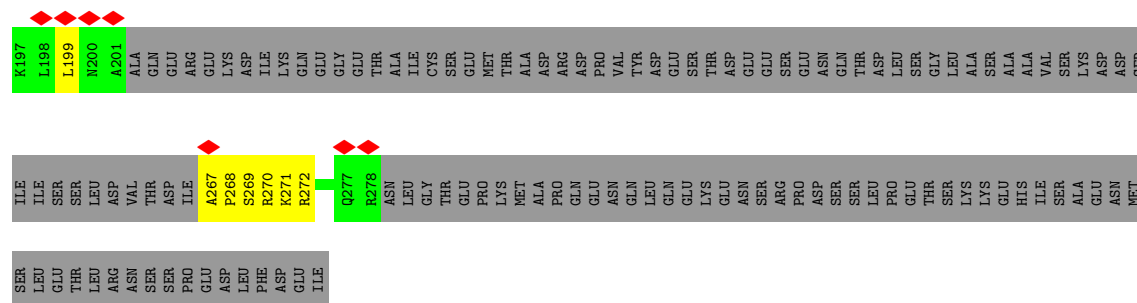


- Molecule 6: DNA (30-MER)

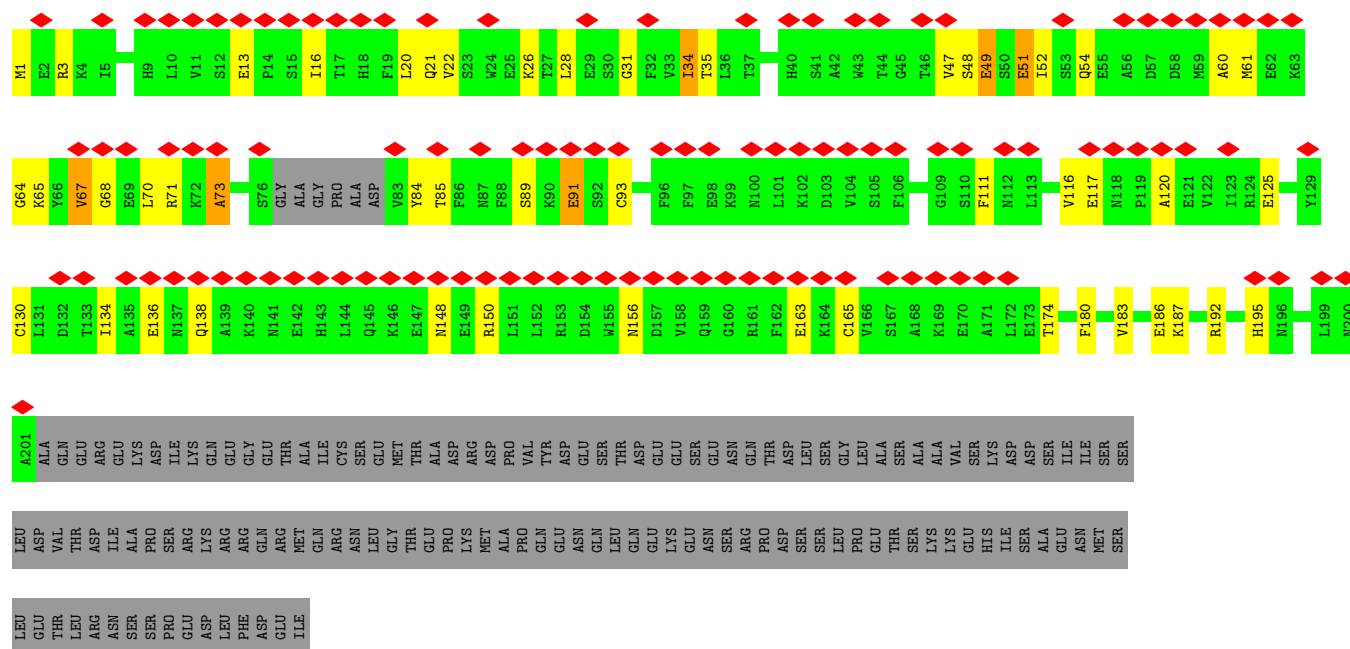


- Molecule 7: DNA repair protein XRCC4

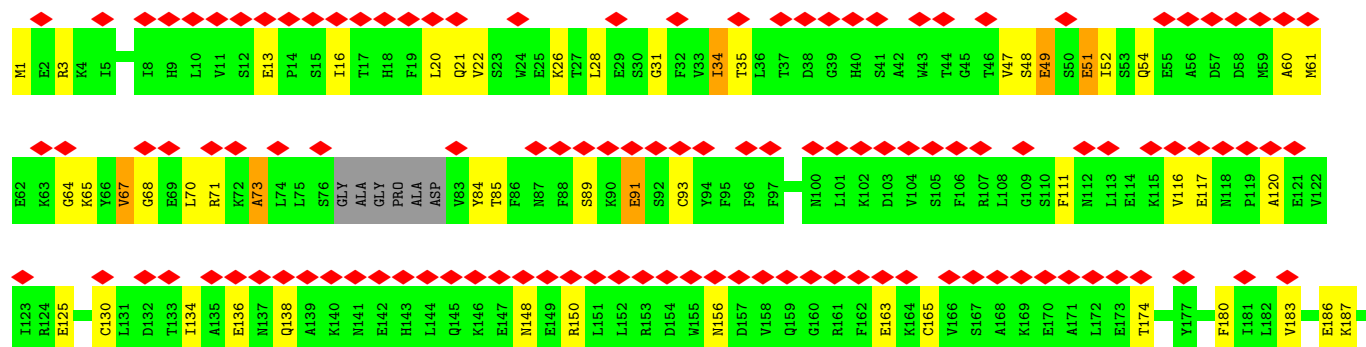
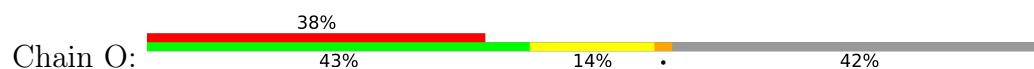




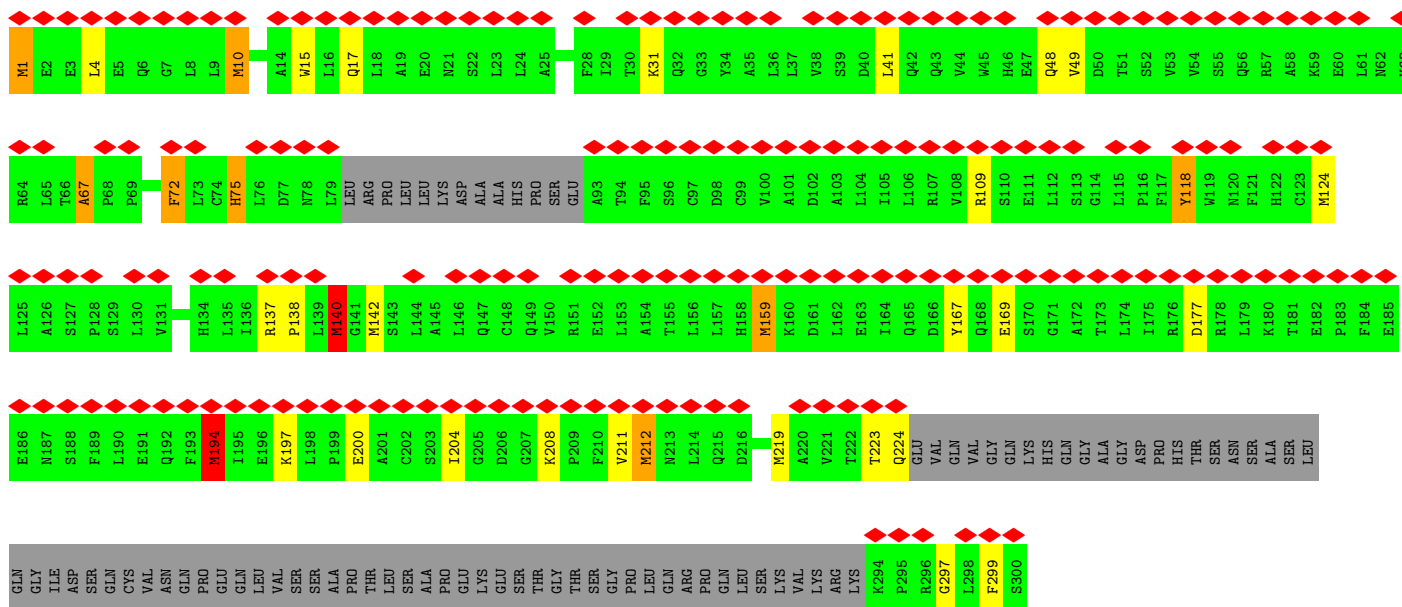
• Molecule 7: DNA repair protein XRCC4



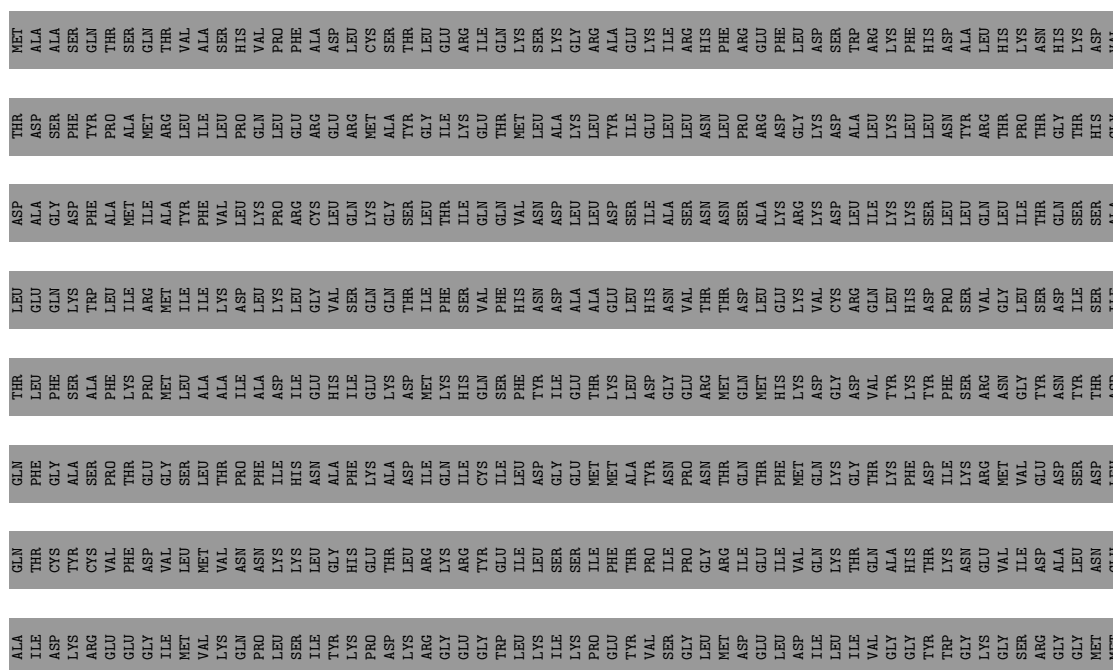
• Molecule 7: DNA repair protein XRCC4



Chain I: 62% 61% 8% 27%



Chain X: 14% 19% 8% 72%





GLY	THR	GLU	GLY	PRO	GLU	GLU	TYR	ILE	GLU	PRO	CYS	ASN	SER	ASN	VAL	ILE	VAL	GLN	ILE	LYS	ALA	GLU	GLU	VAL	PRO	SER	ASP	MET	TYR	LYS	THR	GLY	CYS	THR	LEU	ARG	PHE	PRO	ARG	ILE	ILE	GLU	GLY	LYS	LYS	LYS	ARG	ASP	LYS	THR	LEU	ASP	ASP	LEU	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
E663	F664	C665	S668	G669	T670	ASP	SER	Q673	P674	K675	P676	D677	L678	E679	N680	R681	I682	A683	E684	F685	G686	S687	Y688	I689	V690	N691	N692	P693	G694	P695	D696	T697	Y698	G703	S704	E705	N706	I707	R708	I713	H718	D719	V720	V721	K722	P723	A724	W725	L726	L727	E728	C729	F730	K731																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
V736	Q739	F740	R741	F742	T750	K751	E752	H753	F754	A755	R756	E757	Y758	D759	C760	Y761	D762	D763	S764	Y765	F766	I767	D768	T769	D770	L771	N772	Q773	L774	K775	E776	V777	F778	S779	G780	I781	K782	N783	S784	N785	E786	Q787	T788	F789	E790	E791	N792	A793	S794	L795	I796	A797	D798	L799	E800	Y801	R802																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
Y803	S804	W805	D806	C807	S808	P809	L810	S811	N812	F813	R814	R815	H816	T817	W818	Y819	L820	D821	S822	Y823	A824	W825	I826	N827	D828	L829	S830	T831	K832	N833	E834	G835	T836	R837	L838	A839	T840	K841	A842	L843	E844	L845	R846	F847	H848	G849	A850	K851	V852	W853	S854	C855	L856	A857	E858	G859	V860	S861	H862																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
V863	I864	I865	H869	S870	R871	W872	A873	D874	F875	K876	A877	F878	R879	R880	T881	F882	K883	R884	K885	F886	K887	I888	E891	V894	T895	D896	S897	I898	D899	K900	C901	E902	L903	Q904	E905	E906	N907	L910	I911																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							</

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 ($\text{\AA}$)	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 ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.59	0/4101	0.71	2/5523 (0.0%)
1	J	0.59	0/4101	0.71	2/5523 (0.0%)
2	B	0.44	0/4340	0.60	5/5853 (0.1%)
2	K	0.44	0/4340	0.61	5/5853 (0.1%)
3	C	0.62	2/30414 (0.0%)	0.74	22/41079 (0.1%)
3	L	0.62	2/30414 (0.0%)	0.74	22/41079 (0.1%)
5	D	0.95	0/710	0.79	1/1093 (0.1%)
5	M	0.95	0/710	0.79	1/1093 (0.1%)
6	E	0.98	0/690	0.73	0/1063
6	N	0.98	0/690	0.73	0/1063
7	F	0.77	0/1765	1.43	9/2367 (0.4%)
7	G	0.85	0/1622	1.55	15/2178 (0.7%)
7	O	0.84	0/1622	1.55	14/2178 (0.6%)
7	P	0.77	0/1765	1.42	9/2367 (0.4%)
8	H	0.94	17/1814 (0.9%)	1.39	10/2454 (0.4%)
8	I	0.95	16/1771 (0.9%)	1.33	2/2395 (0.1%)
9	X	0.75	1/2112 (0.0%)	1.27	14/2851 (0.5%)
9	Y	0.77	1/2112 (0.0%)	1.30	17/2851 (0.6%)
All	All	0.66	39/95093 (0.0%)	0.86	150/128863 (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

Continued on next page...

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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 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	342	MET	CA-C	-8.41	1.40	1.52
3	C	342	MET	CA-C	-8.34	1.40	1.52
8	H	1	MET	CG-SD	6.99	1.98	1.80
8	H	159	MET	SD-CE	6.63	1.96	1.79
8	I	140	MET	SD-CE	6.63	1.96	1.79

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	18	LEU	CD1-CG-CD2	9.94	132.66	110.80
1	A	352	PRO	CA-N-CD	-9.60	98.57	112.00
1	J	352	PRO	CA-N-CD	-9.59	98.57	112.00
7	F	143	HIS	CB-CG-CD2	-8.96	119.55	131.20
7	P	143	HIS	CB-CG-CD2	-8.68	119.92	131.20

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 ⓘ

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	291	0
1	J	4021	0	4100	289	0
2	B	4259	0	4301	269	0
2	K	4259	0	4301	265	0
3	C	29811	0	30286	1694	0
3	L	29811	0	30286	1674	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	65	0
6	E	616	0	339	63	0
6	N	616	0	339	60	0
7	F	1736	0	1739	45	0
7	G	1595	0	1592	40	0
7	O	1595	0	1592	38	0
7	P	1736	0	1739	34	0
8	H	1779	0	1797	34	0
8	I	1737	0	1744	16	0
9	X	2064	0	2012	42	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	4750	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 26.

The worst 5 of 4750 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%)	12	47
7	G	191/336 (57%)	176 (92%)	12 (6%)	3 (2%)	7	37
7	O	191/336 (57%)	176 (92%)	12 (6%)	3 (2%)	7	37
7	P	209/336 (62%)	203 (97%)	5 (2%)	1 (0%)	24	63
8	H	217/299 (73%)	201 (93%)	15 (7%)	1 (0%)	24	63
8	I	212/299 (71%)	200 (94%)	11 (5%)	1 (0%)	24	63
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%)	49	83

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 ⓘ

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%)	481 (100%)	0	100	100
2	K	481/649 (74%)	481 (100%)	0	100	100
3	C	3325/3671 (91%)	3325 (100%)	0	100	100
3	L	3325/3671 (91%)	3325 (100%)	0	100	100
7	F	191/303 (63%)	165 (86%)	26 (14%)	3	15
7	G	178/303 (59%)	155 (87%)	23 (13%)	4	17
7	O	178/303 (59%)	155 (87%)	23 (13%)	4	17
7	P	191/303 (63%)	165 (86%)	26 (14%)	3	15
8	H	198/262 (76%)	185 (93%)	13 (7%)	15	37
8	I	193/262 (74%)	178 (92%)	15 (8%)	11	32
9	X	230/808 (28%)	211 (92%)	19 (8%)	10	30
9	Y	230/808 (28%)	208 (90%)	22 (10%)	8	25
All	All	10105/13088 (77%)	9938 (98%)	167 (2%)	52	67

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	P	117	GLU
9	X	894	VAL
7	P	140	LYS
9	X	792	MET
9	Y	786	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
8	I	21	ASN

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Mol	Chain	Res	Type
7	P	159	GLN
3	L	339	GLN
7	P	145	GLN
3	L	3787	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	28,29,29	1.55	5 (17%)	43,45,45	1.96	8 (18%)
10	ADP	C	4201	-	28,29,29	1.54	5 (17%)	43,45,45	1.94	8 (18%)

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	-	-	2/16/32/32	0/3/3/3
10	ADP	C	4201	-	-	2/16/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	4201	ADP	C5-N7	-3.68	1.32	1.39
10	L	4201	ADP	C5-N7	-3.66	1.32	1.39
10	L	4201	ADP	C5-C4	3.38	1.45	1.39
10	C	4201	ADP	C5-C4	3.33	1.45	1.39
10	L	4201	ADP	C8-N9	-3.25	1.32	1.37

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	4201	ADP	C5-C4-N3	-6.13	118.27	126.72
10	C	4201	ADP	C5-C4-N3	-6.06	118.38	126.72
10	C	4201	ADP	N3-C4-N9	5.30	136.17	127.17
10	L	4201	ADP	N3-C4-N9	5.30	136.17	127.17
10	L	4201	ADP	C1'-N9-C8	-3.36	119.64	127.09

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

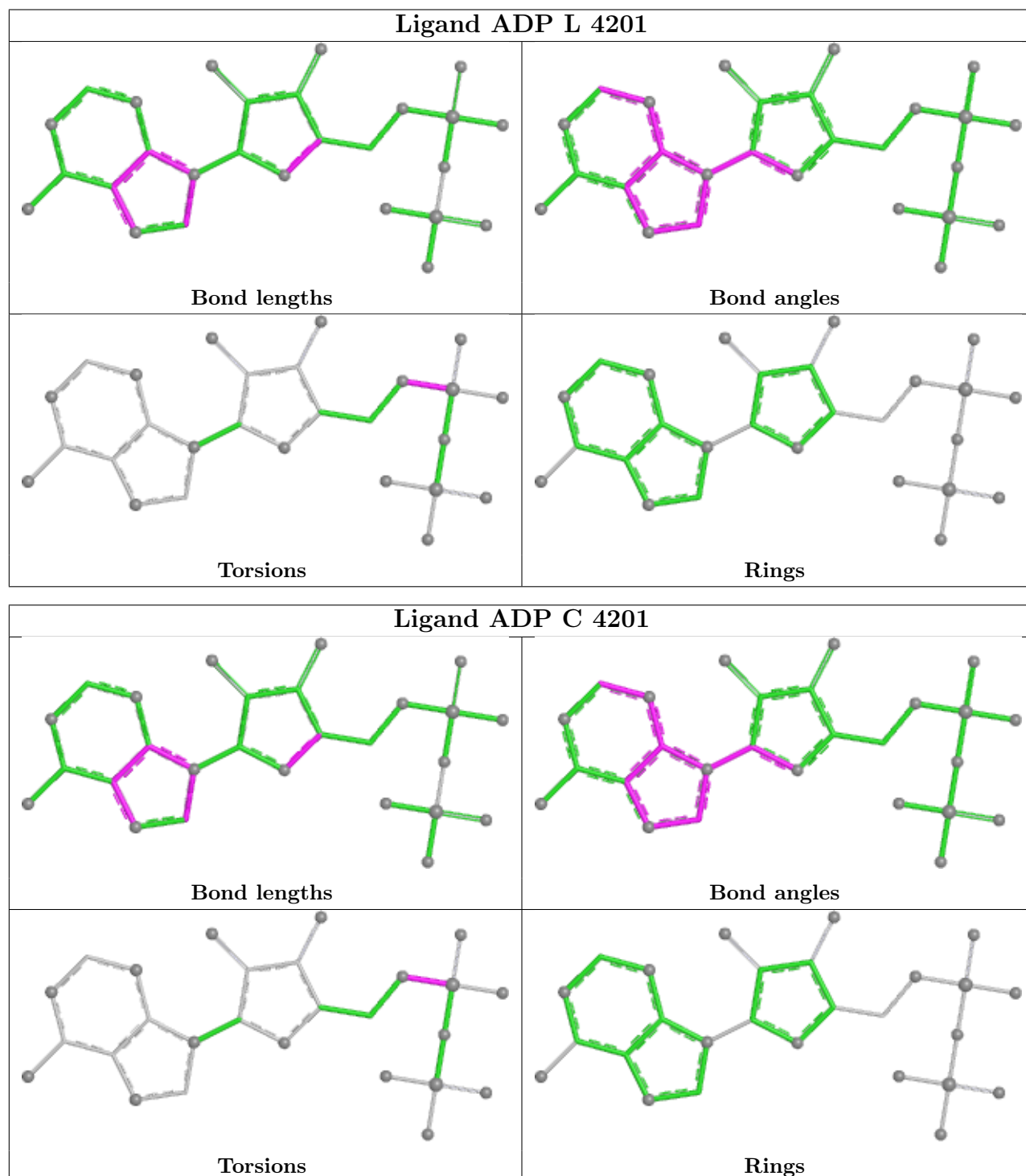
There are no ring outliers.

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.

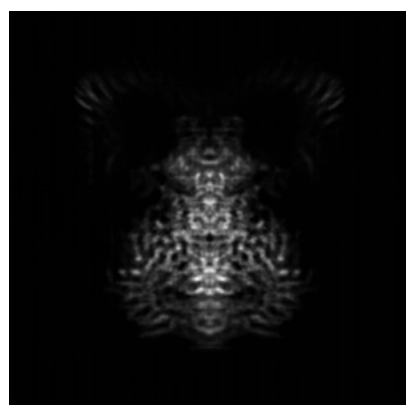
6 Map visualisation [i](#)

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.

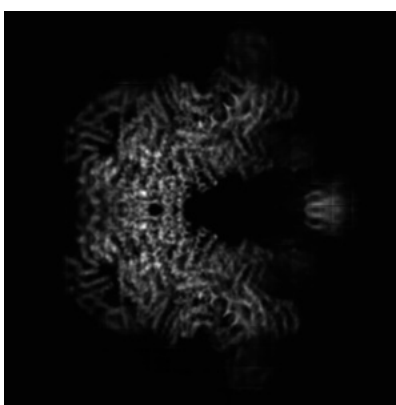
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

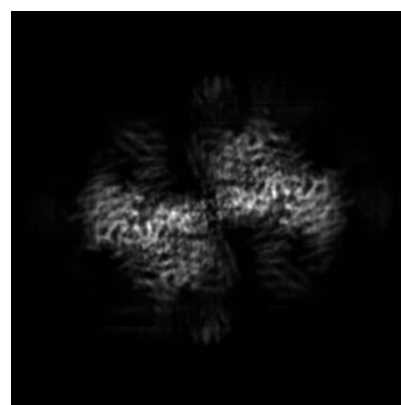
6.1.1 Primary map



X



Y

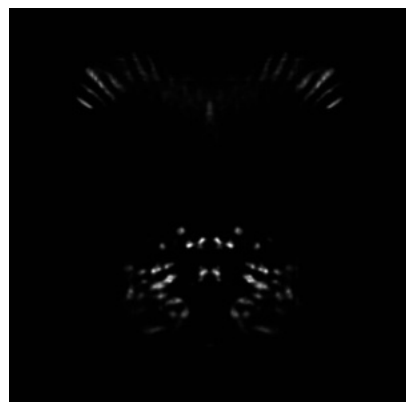


Z

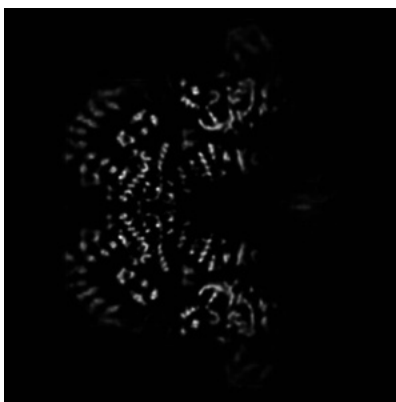
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

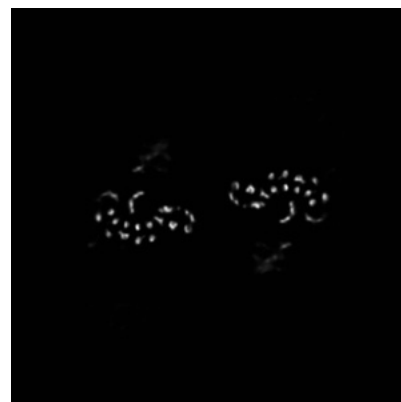
6.2.1 Primary map



X Index: 145



Y Index: 145



Z Index: 145

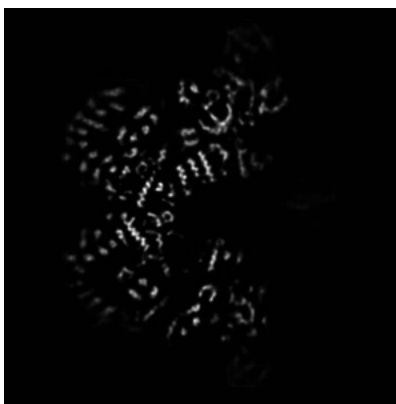
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

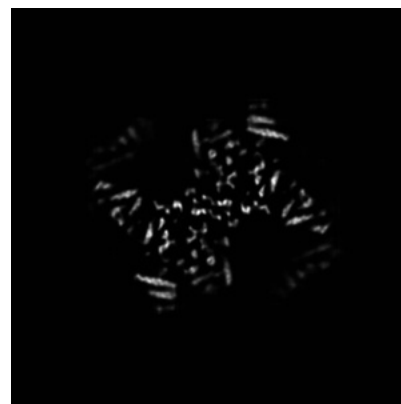
6.3.1 Primary map



X Index: 185



Y Index: 147

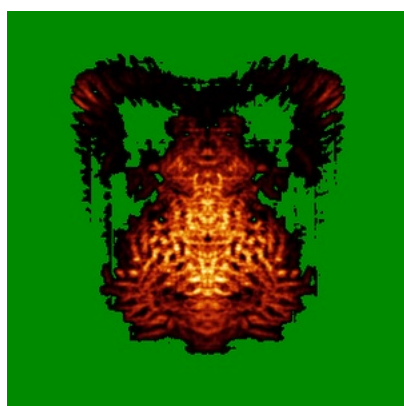


Z Index: 100

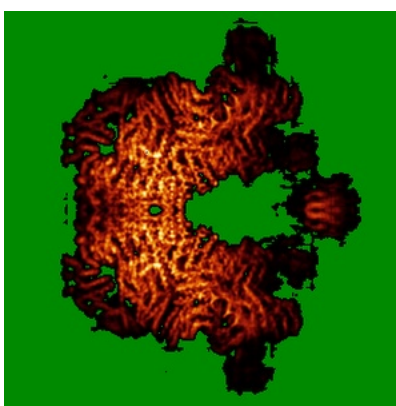
The images above show the largest variance slices of the map in three orthogonal directions.

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

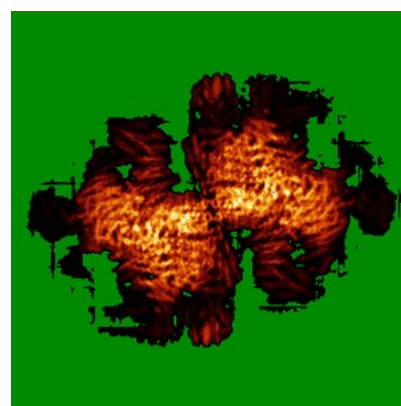
6.4.1 Primary map



X



Y

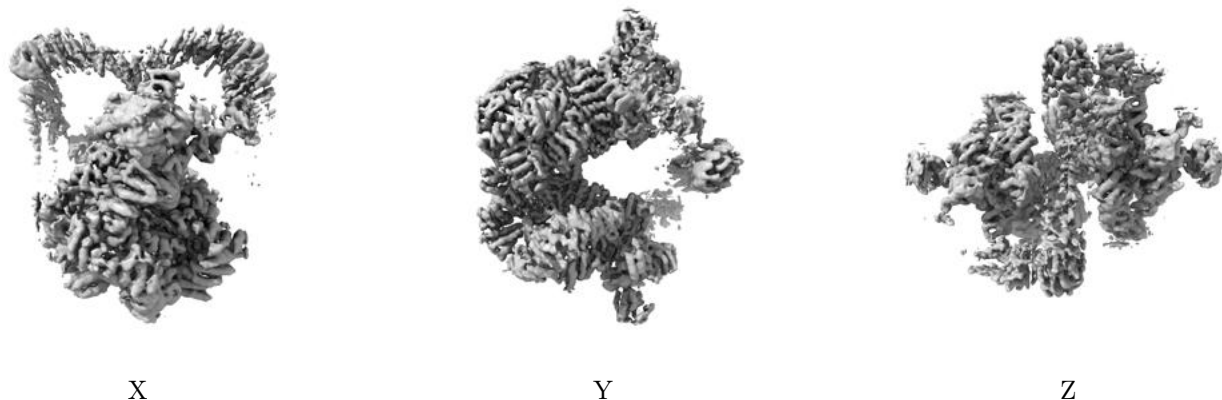


Z

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.

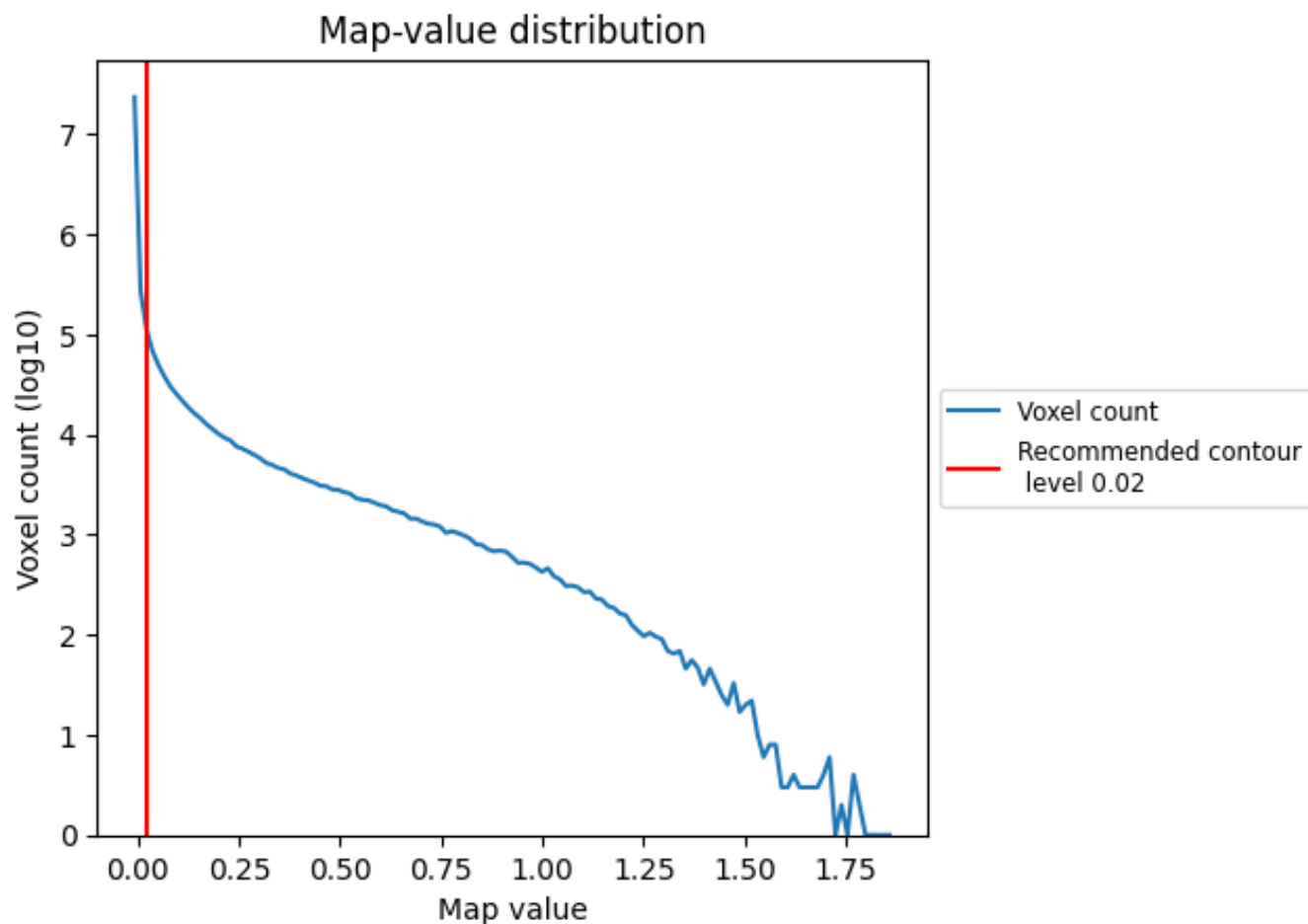
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

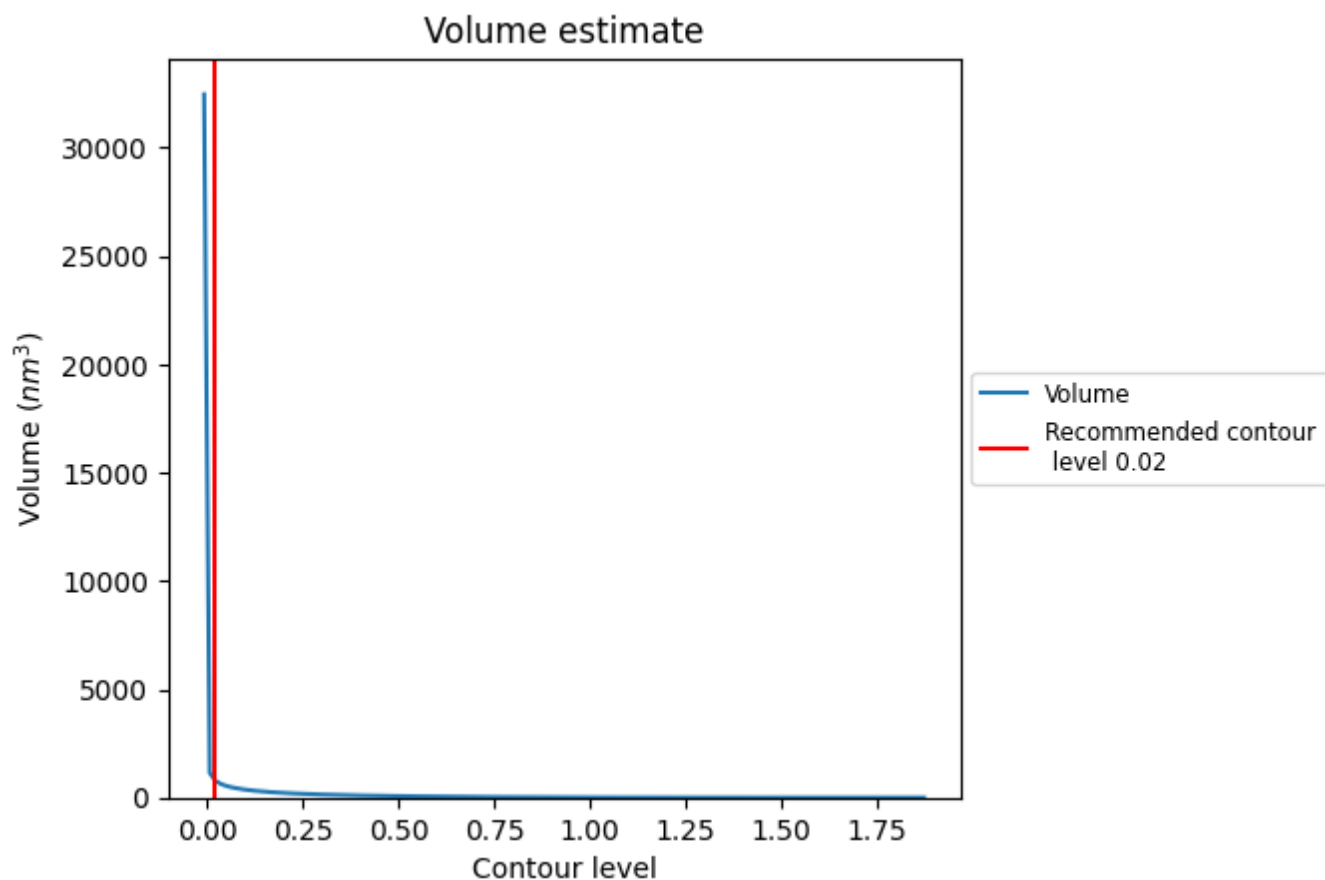
This section contains the results of statistical analysis of the map.

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.

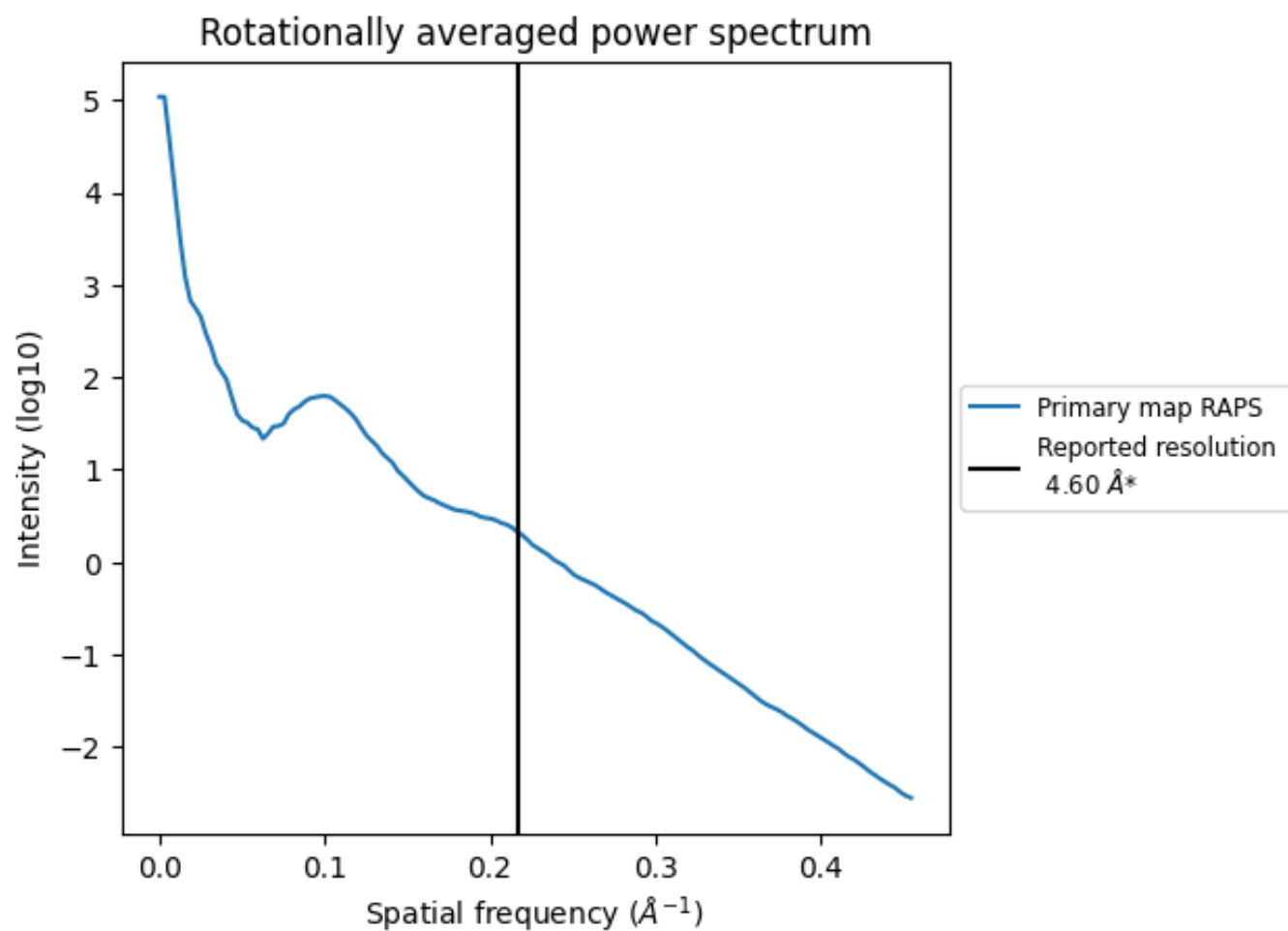
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 789 nm^3 ; 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 ⓘ

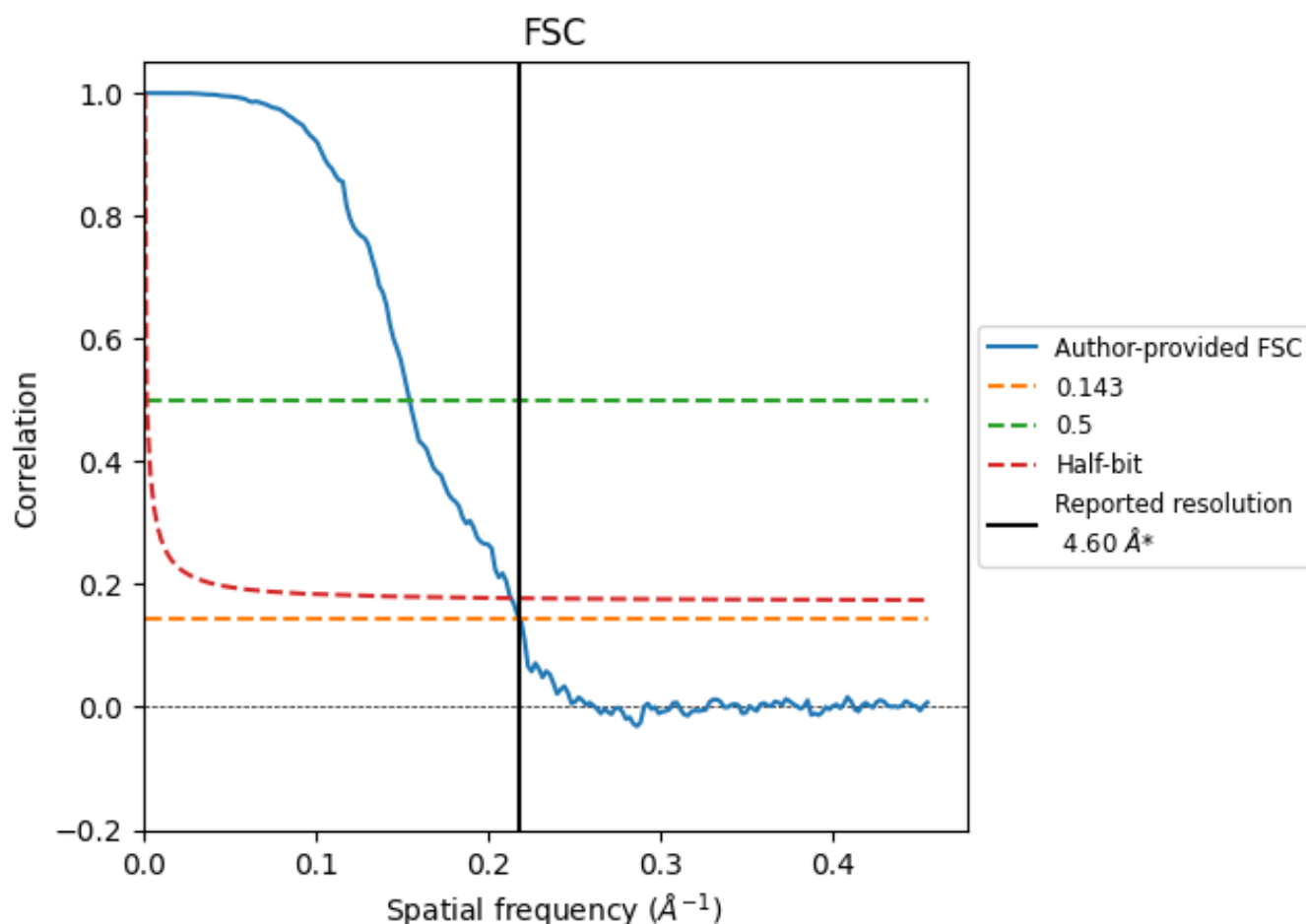


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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](#)

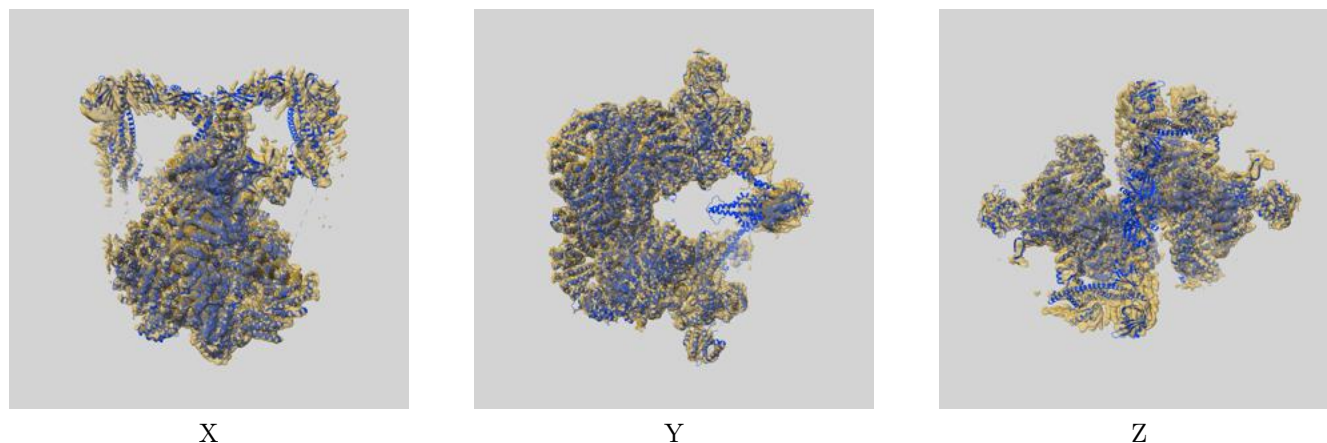
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.57	6.48	4.69
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

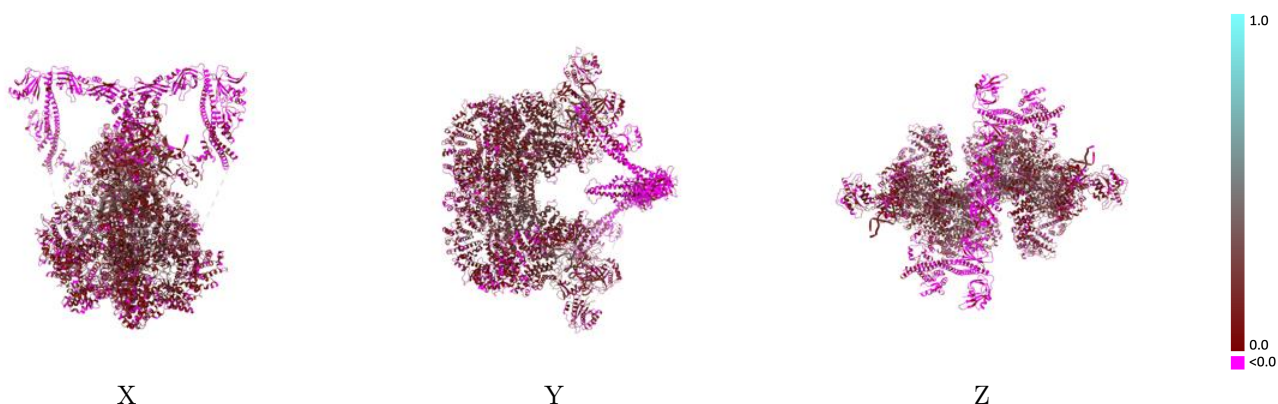
This section contains information regarding the fit between EMDB map EMD-23510 and PDB model 7LT3. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



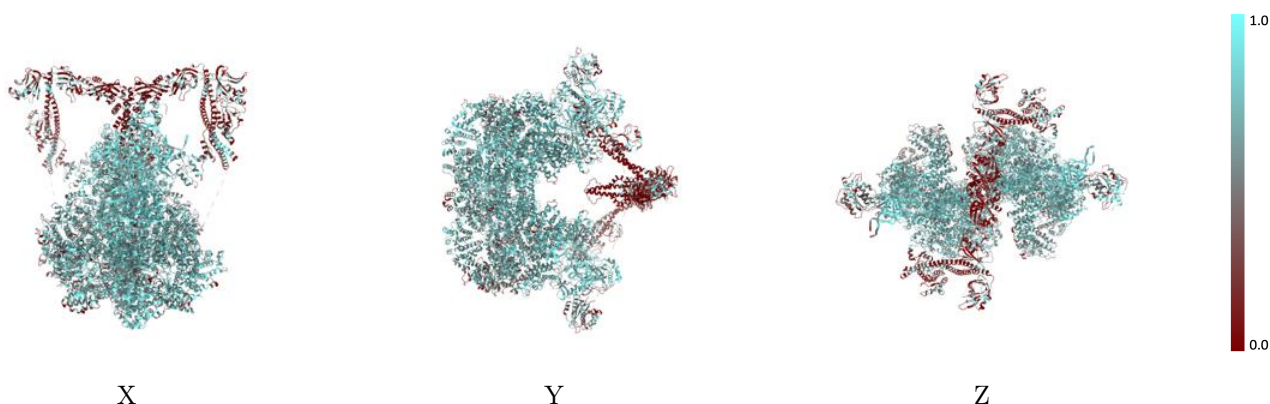
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



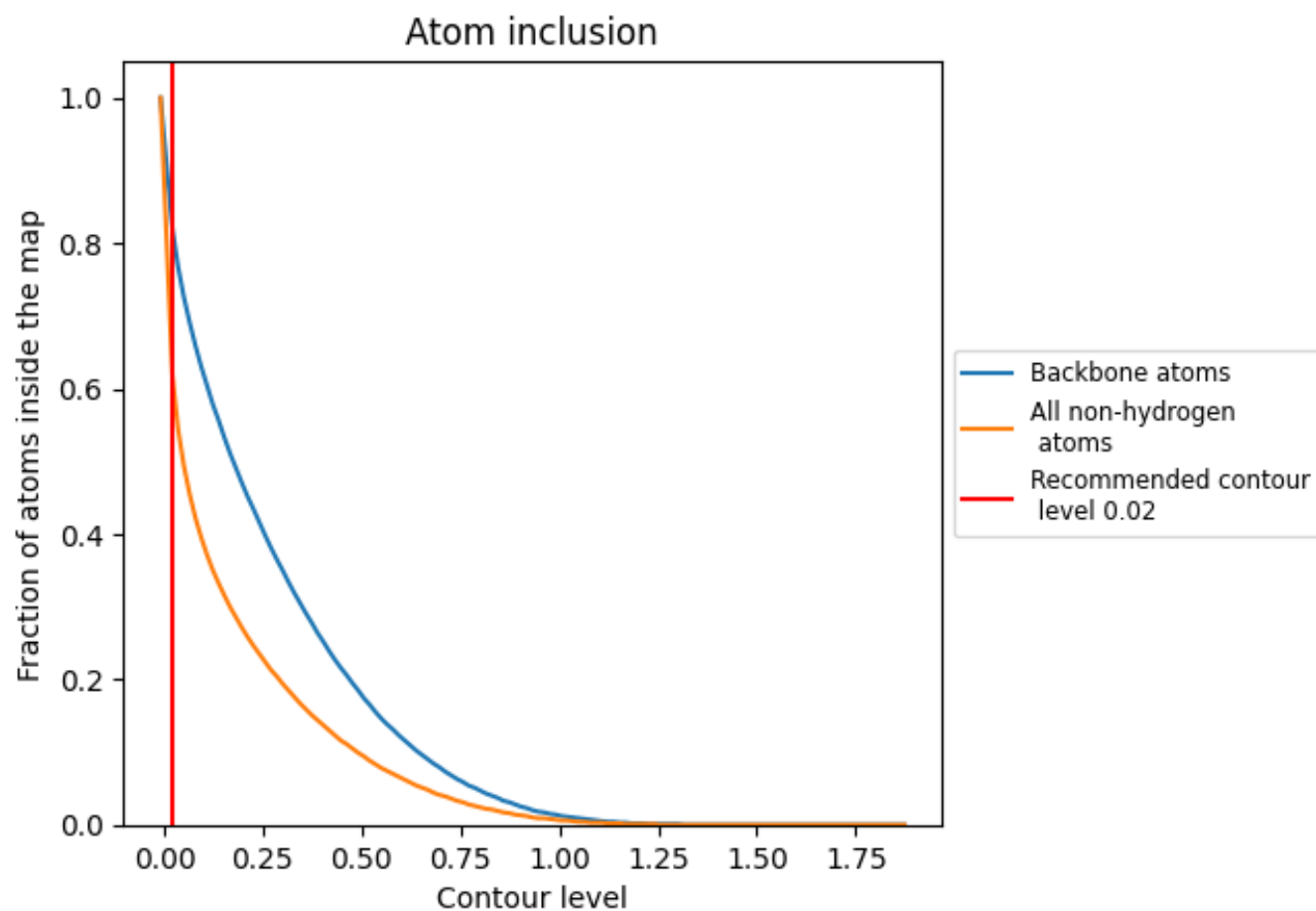
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

