



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 02:21 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, 6ERH, 5Y3R, 1JEY, 3II6, 6ZHA, 5LUQ

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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

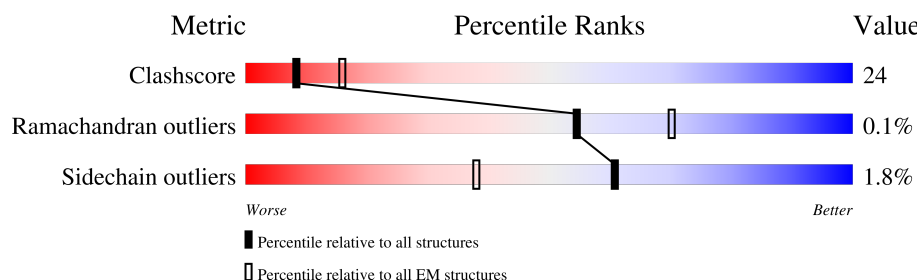
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.








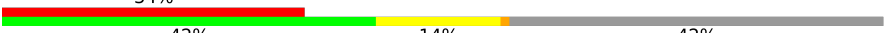
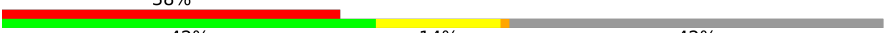





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

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		

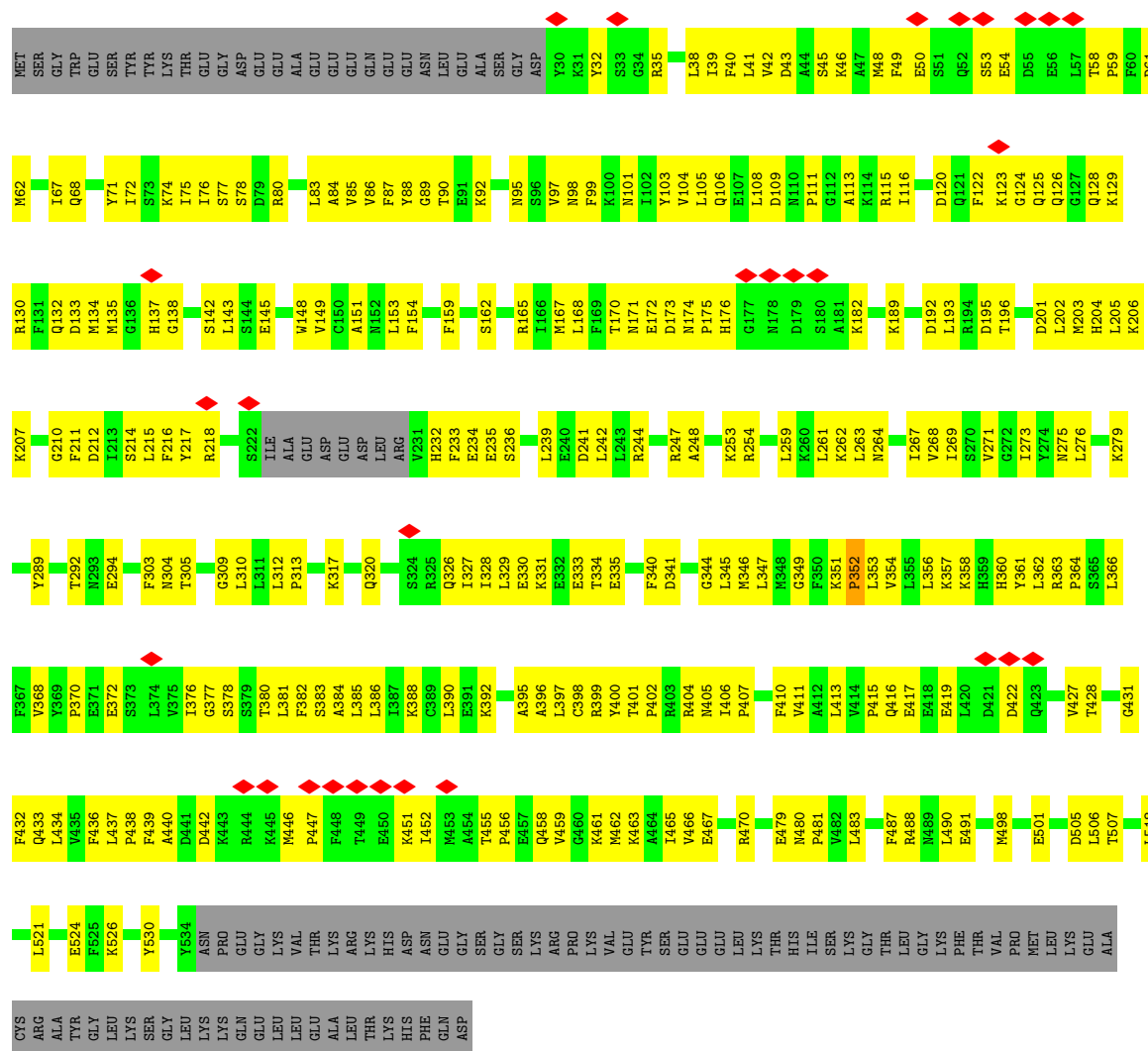
- Molecule 9 is a protein called DNA ligase 4.

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		

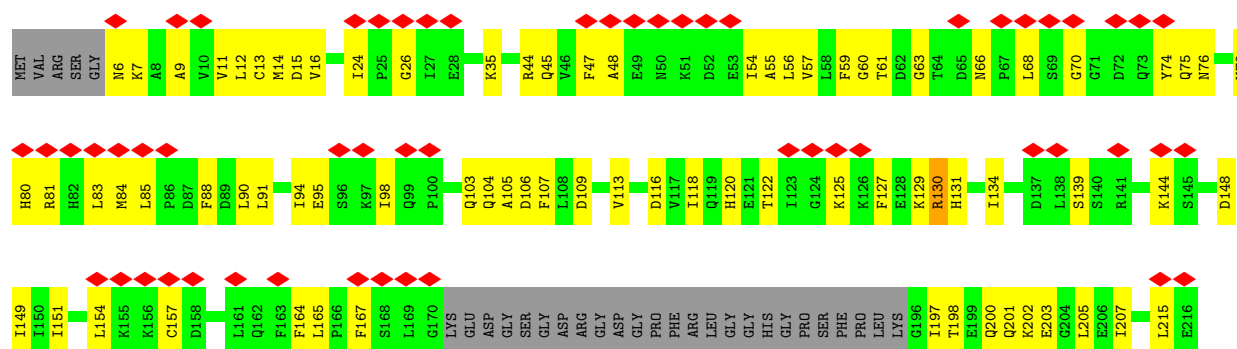
- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

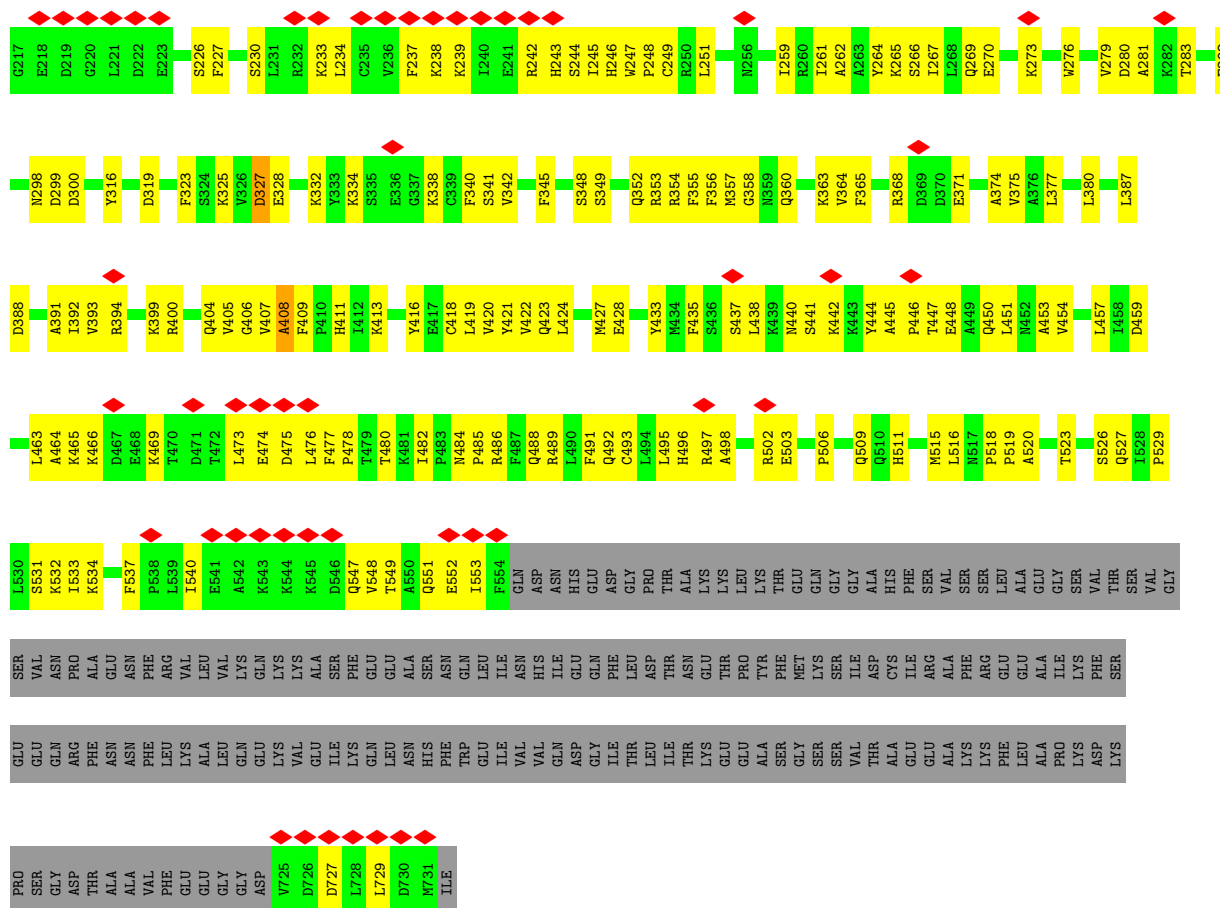


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

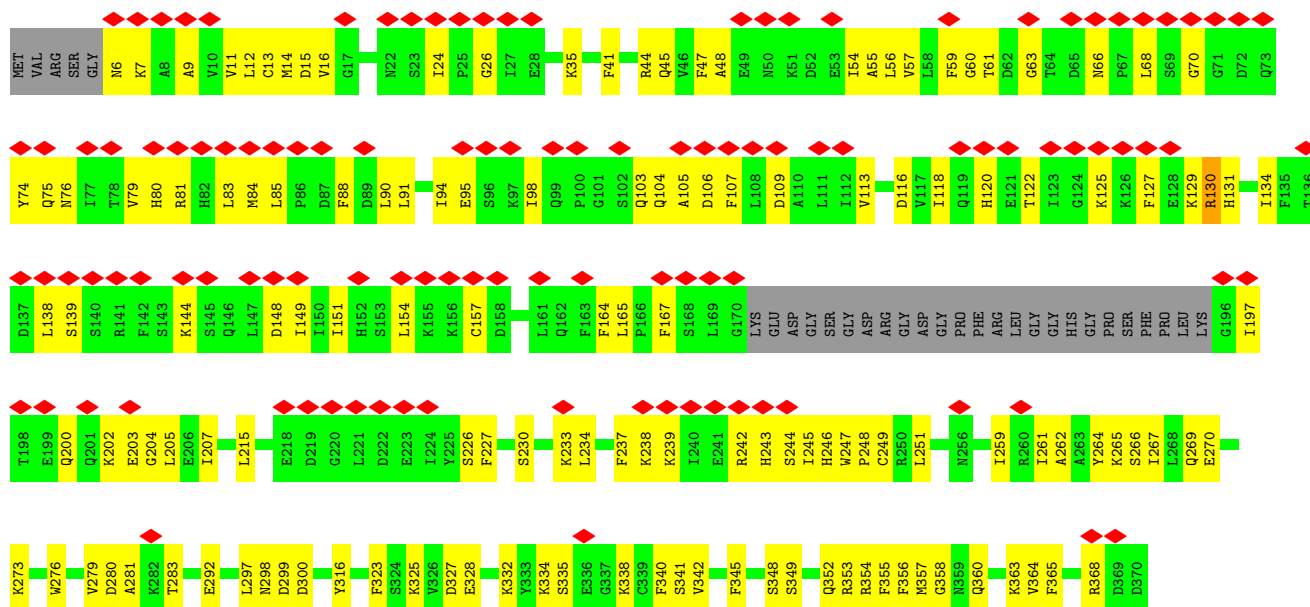


• Molecule 2: X-ray repair cross-complementing protein 5





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





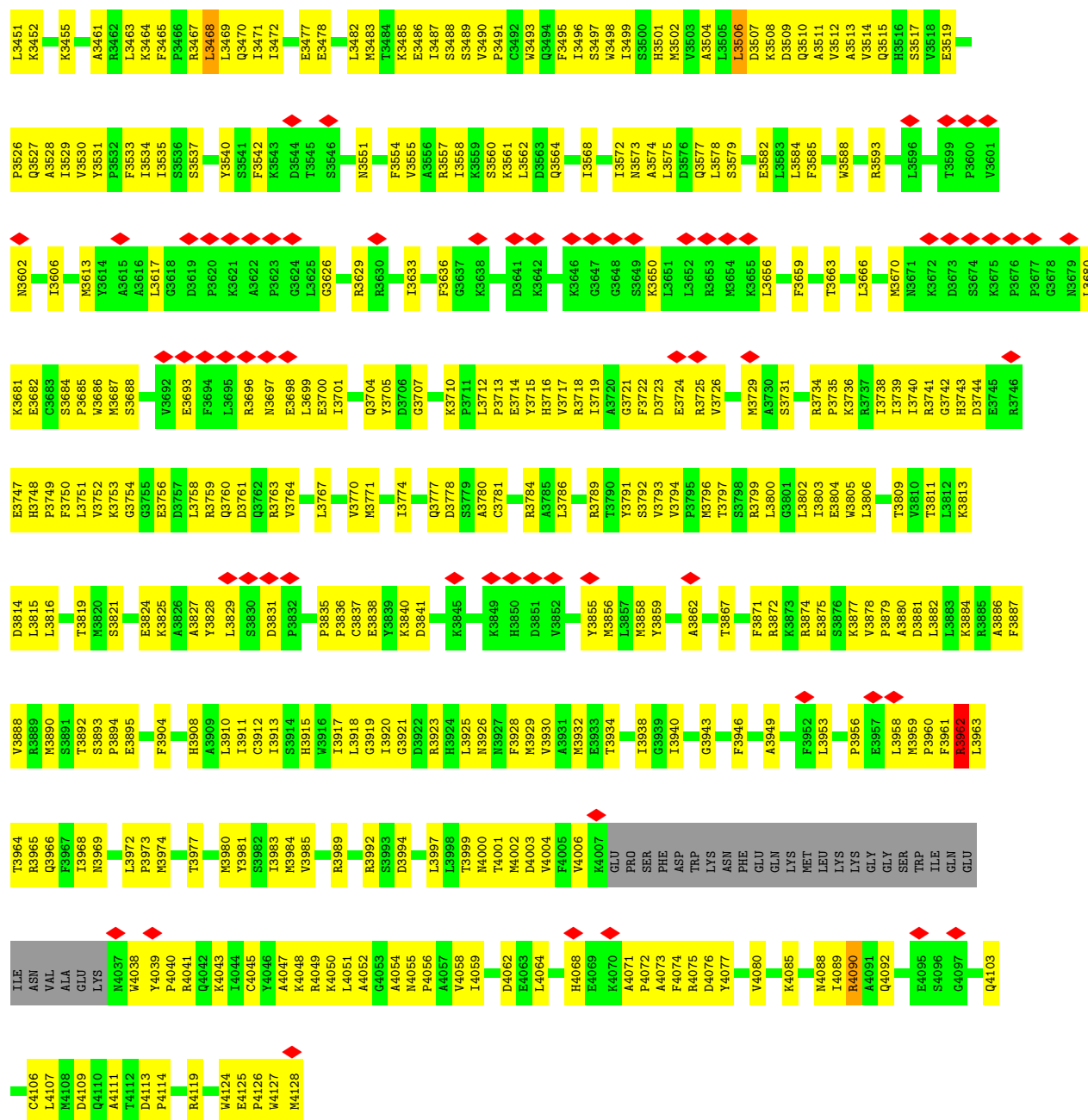
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S2489		L2303	K2162	A2161	A2099	F1977	T1912		I1785	L1710	L1639
E2490	L2402	N2305	I2237	K2163	L2100	E1979	K1913	K1852	I1786	R1711	E1640
T2491	C2403	N2306	I2238	W2164	M2104	N1980	T1914	S1853	R1787	V1713	T1641
T2492	R2404	N2307	K2239	L2165	L2105	L1981	L1915	R1854	R1788		K1642
N2493	E2405	S2308	T2240	S2166	R2106	D1982	L1916	F1855	G1789	Q1716	L1649
D2494	L2241	M2309	V2242	P2167	S2107	D1983	L1918	T1856	G1790	L1718	A1650
Q2495	G2407	R2311	L2168	L2169	S2107	L1984	C1919	K1857	S1790	I1718	K1651
Q2496	M2408	L2108	THR	THR	THR	K1985	Y1920	L1858	C1791	F1722	I1652
K2500	L2411	GLY	GLY	GLY	GLY	R1986	D1921	D1921	Q1794	P1723	L1653
K2503	Q2414	PRO	VAL	VAL	VAL	R1987	A1922	E1860	V1795	M1724	Q1654
K2506	L2415	GLN	GLN	GLN	GLN	F1990	F1923	S1861	G1796	Q1725	I1655
L2506	S2416	GLY	TYR	TYR	TYR	P1991	M1927	F1863	L1797	R1727	D1656
L2507	K2417	GLY	TYR	TYR	TYR	V1992	A1928	D1864	L1798	R1727	S1657
L2508	T2418	GLY	TYR	TYR	TYR	GLU	G1929	T1865	L1799	E1728	S1658
Q2509	D2419	ASP	SER	SER	SER	VAL	E1930	Q1866	V1801	F1729	V1659
L2510	F2420	SER	SER	SER	SER	GLU	I1867	Q1867	I1867	P1730	S1660
L2511	Q2421	VAL	GLN	GLN	GLN	VAL	N1931	T1868	M1803	P1731	F1661
D2512	Q2422	PRO	ASP	ASP	ASP	PRO	Q1932	K1869	F1805	G1732	N1662
N2514	H2426	PRO	ARG	ARG	ARG	MET	L1933	K1870	R1806		T1663
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G2516	M2443	LYS	ARG	ARG	ARG	ARG	E1935	G1872	D1808	N1737	H1665
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Q2518		LYS	GLY	GLY	GLY	LYS	R1937	Y1874	P1810		S1667
L2519	L2446	THR	THR	THR	THR	THR	R1938	I1875	R1811	K1744	F1668
L2520		ARG	ARG	ARG	ARG	THR	R1939	I1876	K1745	K1746	P1669
L2521		PHE	PHE	PHE	PHE	ILE	Y1940	I1877	L1812	L1747	E1670
F2524	E2450	ARG	ARG	ARG	ARG	GLU	H1941	D1878	F1814	D1748	V1671
W2525	L2451	ARG	GLU	GLU	GLU	ILE	C1942	V1879	T1815	A1749	Y1675
T2529	R2452	GLN	GLN	GLN	GLN	LYS	A1943	I1880	R1816	L1750	I1676
L2531	L2454	ASP	ASP	ASP	ASP	ALA	A1944	L1883	F1819	E1751	S1677
	P2457	PRO	PRO	PRO	PRO	ARG	N1945	L1884	V1820	L1678	L1678
	V2458	THR	THR	THR	THR	ALA	C1947	L1885	D1821		D1681
	V2459	VAL	VAL	VAL	VAL	ASN	V1951	K1886	R1822	S1785	T1682
	H2464	HTS	HTS	HTS	HTS	ASP	I1952	D1887	S1823		K1683
	P2465	ASP	ASP	ASP	ASP	GLY	V1955	V1888	L1824	L1768	L1684
	S2466	VAL	VAL	VAL	VAL	ASP	F1956	H1899	L1827	L1759	
		LEU	LEU	LEU	LEU	SER	N1957	H1890	L1828	E1760	
		GLU	GLU	GLU	GLU	GLY	E1958	A1891	W1829	T1763	
		LEU	LEU	LEU	LEU	PRO	L1959	K1892	H1830	E1764	
		GLU	GLU	GLU	GLU	SER	K1960	E1893	C1831	V1765	
		GLU	GLU	GLU	GLU	TYR	F1961	S1894	H1831	L1766	V1693
		M2085	M2085	M2085	M2085	MET	Y1962	K1895	C1832	C1767	T1694
		D2086	D2086	D2086	D2086	SER	Q1963	I1896	S1832	R1768	L1695
		E2087	E2087	E2087	E2087	SER	G1964	N1897	L1833	E1769	L1696
		R2090	R2090	R2090	R2090	LEU	F1965	Q1898	D1834	Q1770	P1697
		H2091	H2091	H2091	H2091	SER	V1899	A1835	F1699		F1699
		E2092	E2092	E2092	E2092	TYR	L1966	L1836	T1700		S1700
		C2093	C2093	C2093	C2093	LEU	F1967	L1837	S1701		S1701
		M2094	M2094	M2094	M2094	ALA	S1968	E1838	H1772		L1702
		A2095	A2095	A2095	A2095	ASP	G1902	F1839	V1773		T1703
		P2096	P2096	P2096	P2096	SER	E1969	F1840	M1774		
		R2157	R2157	R2157	R2157	THR	K1970	S1903	F1778		G1704
		R2158	R2158	R2158	R2158		P1971	C1904	T1842		S1705
							E1972	I1905	S1706		L1707
							K1973	E1907	V1844		
							N1974	G1908			
								N1909			



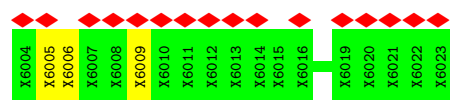
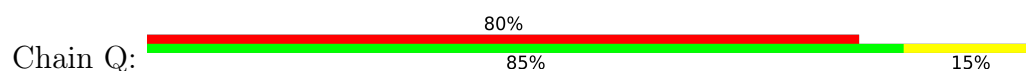




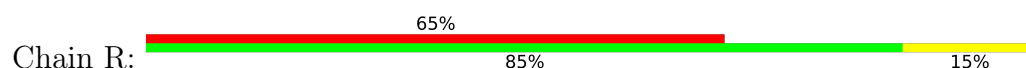
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L2446	E2450	L2451	L2454	P2457	V2458	V2459	H2464	P2465	S2466	R2470	E2471	Q2472	M2473	N2474	L2475	L2476	E2477	M2478	V2479	I2480	R2485	D2486	P2487	E2488	S2489	E2490	L2402	T2491	D2492	N2493	D2494	Q2407	S2495	Q2408	L2411	K2500	L2501	Q2414	L2415	K2503	L2506	I2507	Q2508	G2509	L2510	I2511	D2512	E2513	N2514	P2515	L2517	Q2518				
F2597	R2598	S2599	V2600	L2601	L2602	T2603	P2604	M2605	PHE	VAL	GLU	THR	GLN	ALA	GLN	GLY	THR	THR	LEU	GLN	THR	THR	ALA	ARG	TRP	ARG	VAL	PRO	ALA	GLY	GLN	ILE	ARG	ALA	THR	GLN	PHE	GLN	GLN	HIS	LYS	ASP	PHE	THR	LEU	THR	PRO	GLY	ASP	GLU	VAL	ASP	ASN	LYS	SER	VAL
L2521	F2524	W2525	T2529	R2530	L2531	T2535	L2536	D2537	R2538	L2539	L2542	N2543	S2544	L2545	P2548	K2549	L2550	E2551	H2552	H2553	F2554	L2555	S2556	L2562	L2563	E2564	M2565	S2566	S2567	N2568	S2569	F2570	T2571	Y2572	M2576	F2577	E2578	H2579	P2580	L2581	S2582	F2583	C2584	E2585	F2586	Q2587	E2588	Y2589	D2594	W2595	R2596					
L2804	L2808	F2809	S2810	S2811	L2812	L2817	M2820	T2825	L2826	F2840	N2841	R2842	F2843	F2848	F2851	P2852	P2853	F2854	V2855	S2856	Q2859	D2860	L2861	D2872	S2877	S2883	L2884	Q2885	Q2886	P2887	L2898	L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	W2994														
ARG	GLY	LYS	ALA	R2915	S2916	P2917	P2918	V2924	K2928	L2929	T2930	R2931	S2932	L2933	Y2936	R2940	G2941	I2942	F2943	T2944	S2945	E2946	I2947	K2950	Q2954	A2955	A2956	L2957	L2958	A2959	E2960	A2961	R2962	Y2965	Q2971	Y2972	D2973	E2974	A2975	L2976	N2977	W2981	G2984	E2985	P2986	L2989	Q3071	Q3074	R3075	A3076	L3077					
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Y3168	P3169	K3172	P3175	I3178	W3179	D3180	I3183	T3184	N3185	R3186	F3189	S3190	L3193	K3196	L3197	T3198	P3199	LEU	PRO	GLU	ASP	ASN	GLN	ASP	GLY	ASP	ASP	PRO	SER	ASP	ARG	MET	GLU	VAL	GLN	GLU	GLN	GLU	GLU	ASP	L3227	S3228	S3229	L3230	T3231	R3232	S3233									
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N3311	V3312	L3316	S3317	K3318	N3319	L3320	R3324	D3325	N3326	N3327	L3328	L3329	L3330	T3333	Y3334	R3335	A3338	N3339	A3340	L3341	S3342	K3343	E3344	C3347	L3348	A3349	E3350	L3351	E3352	E3353	R3357	R3358	L3359	S3363	G3364	S3365	S3366	S3367	E3368	D3369	S3370	E3371	I3374	A3375	Y3378	Q3379	R3380	A3381	F3382							
Q3383	H3384	L3385	S3386	V3389	Q3390	A3391	A3392	E3393	E3394	E3395	ALA	GLN	PRD	PRD	TRP	SER	CYS	GLY	PRD	A3406	A3407	G3408	V3409	T3410	D3411	Y3412	Y3413	N3414	T3415	L3416	Q3422	Q3423	L3424	R3425	N3430	A3431	S3432	V3433	L3434	L3435	S3436	S3437	E3438	Q3440	A3441	Y3442	P3443	A3444	V3446	V3447	E3448	K3449	N3450			

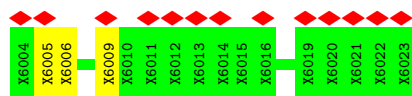


• Molecule 4: Unknown peptide



• Molecule 4: Unknown peptide





• Molecule 5: DNA (31-MER)

Chain D: . 52% 45%



• Molecule 5: DNA (31-MER)

Chain M: . 48% 48%



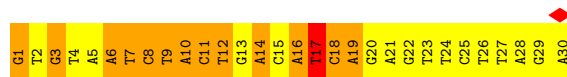
• Molecule 6: DNA (30-MER)

Chain E: 50% 47% .



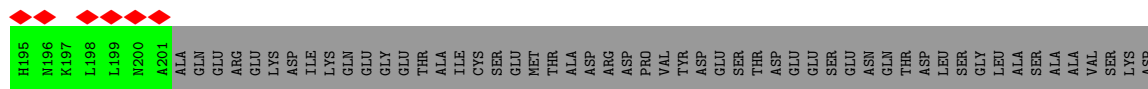
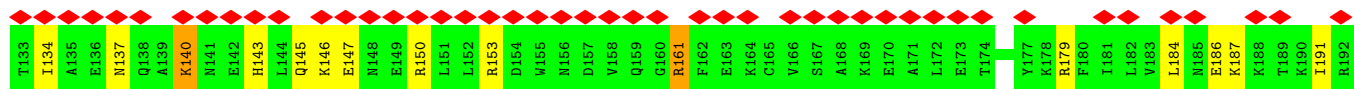
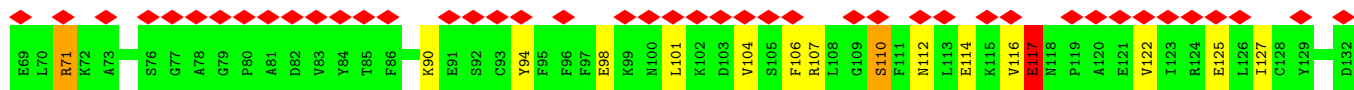
• Molecule 6: DNA (30-MER)

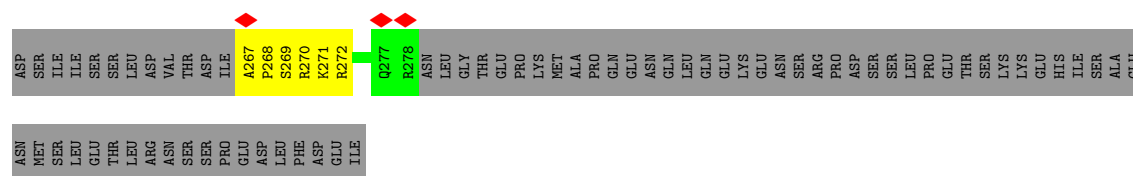
Chain N: . 53% 43% .



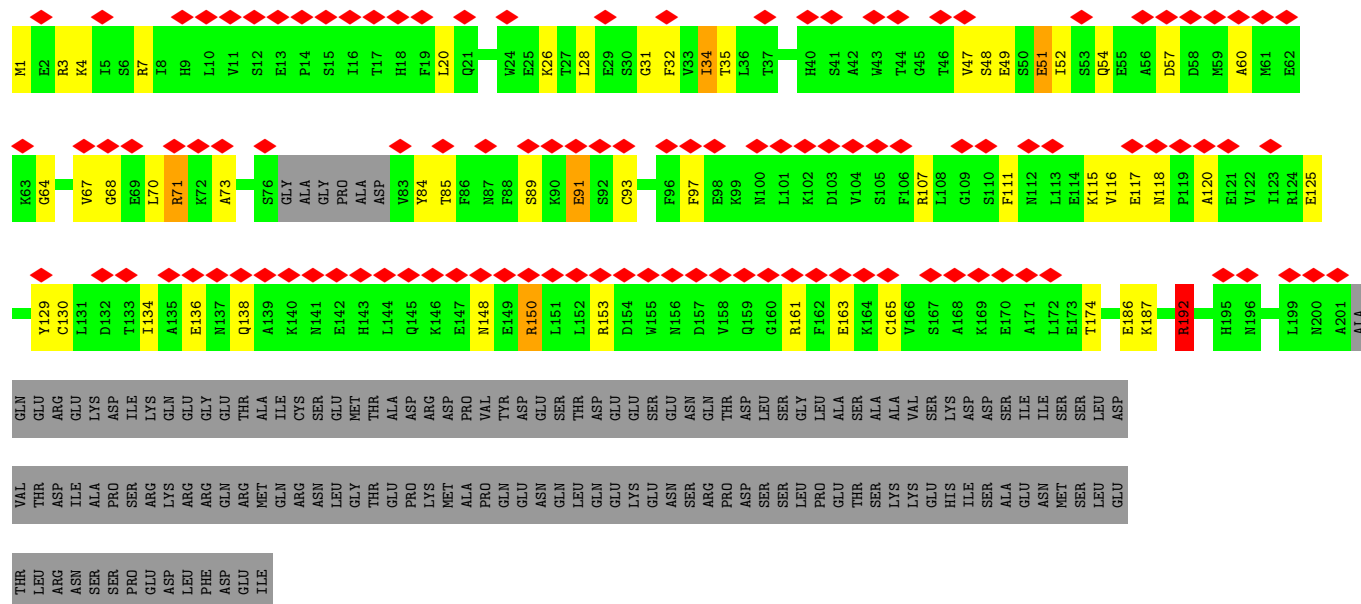
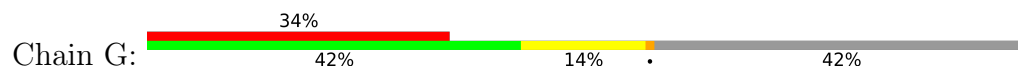
• Molecule 7: DNA repair protein XRCC4

Chain F: 42% 48% 12% 37%

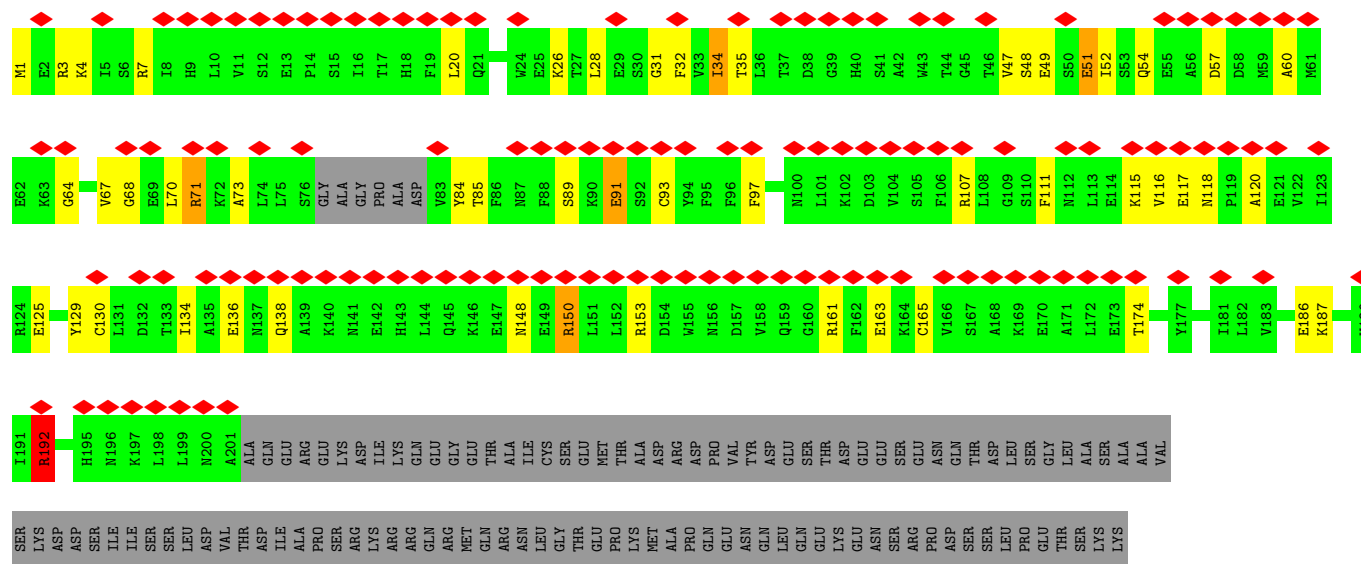
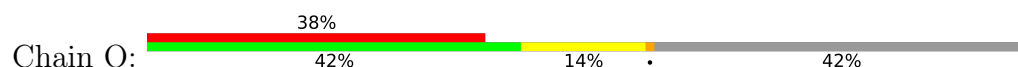




● Molecule 7: DNA repair protein XRCC4



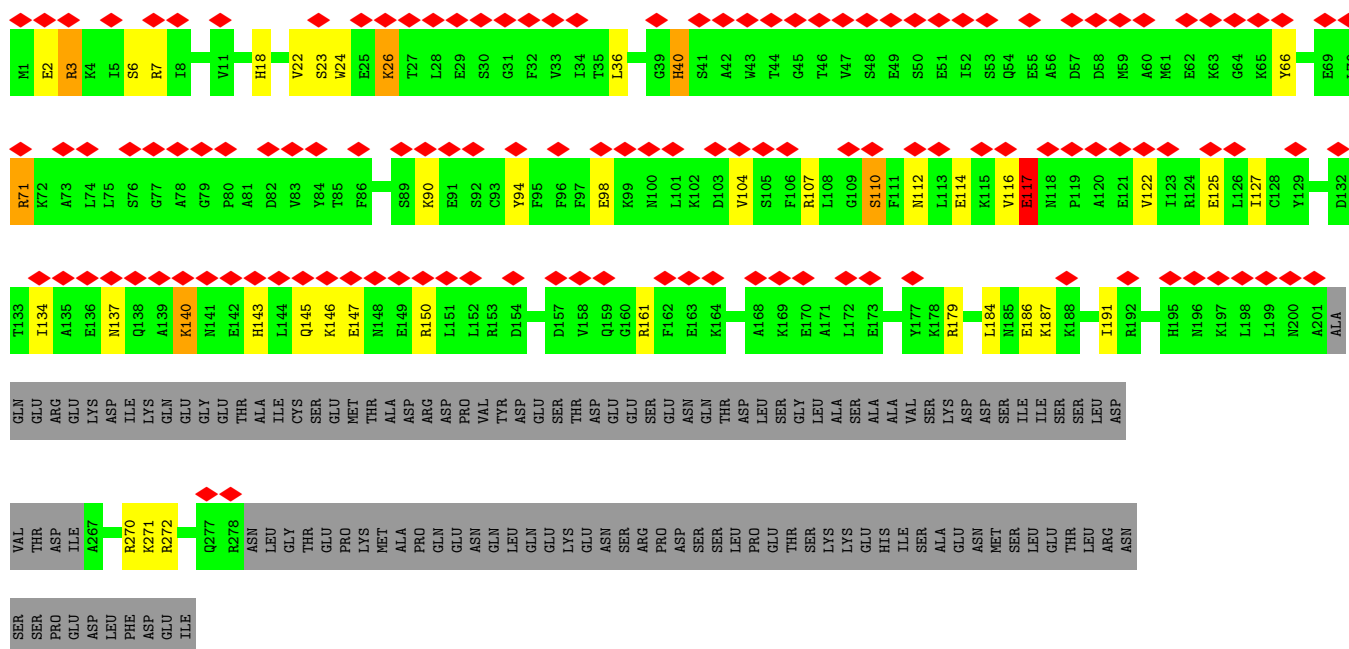
● Molecule 7: DNA repair protein XRCC4



GLU
HIS
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GLU
ASN
MET
SER
LEU
GLU
THR
LEU
ARG
ASN
SER
SER
PRO
GLU
ASP
LEU
PHE
ASP
GLU
ILE

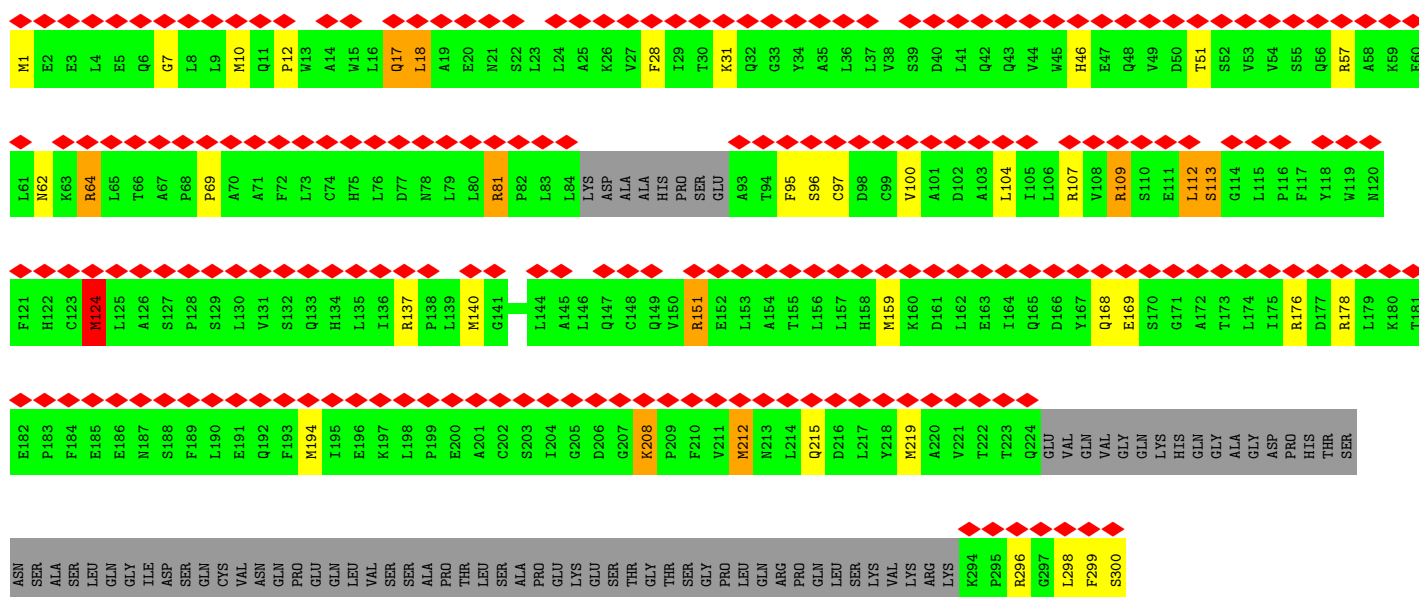
• Molecule 7: DNA repair protein XRCC4

Chain P: 38% 51% 11% 37%



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

Chain H: 70% 61% 10% 25%

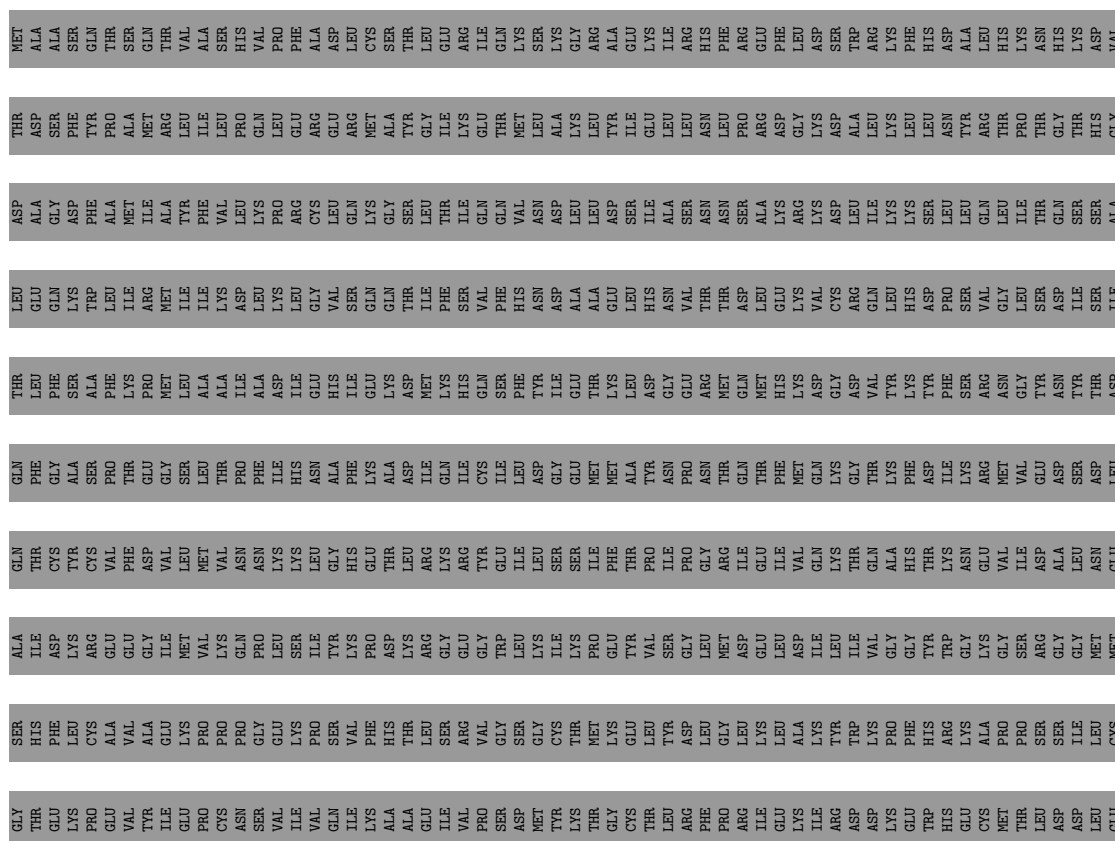


• Molecule 8: Non-homologous end-joining factor 1

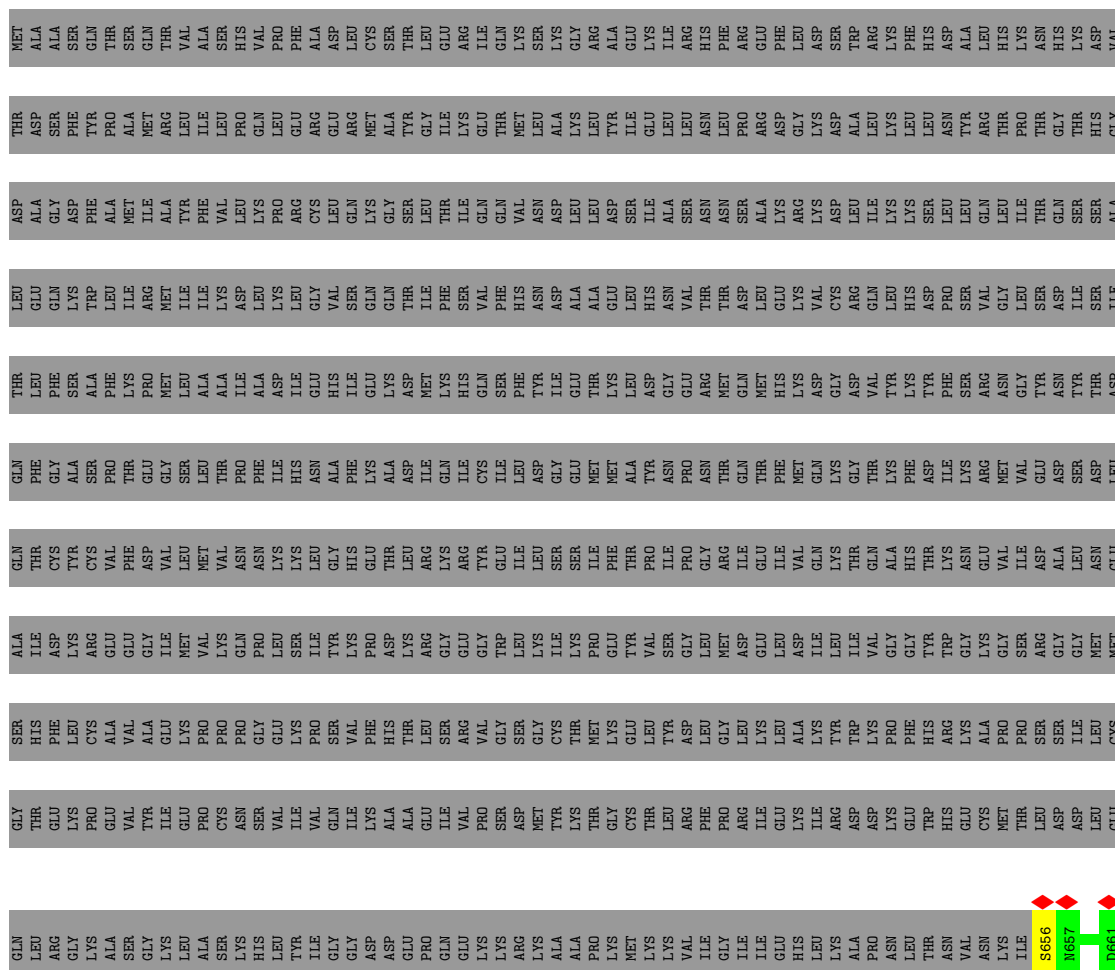
Chain I:

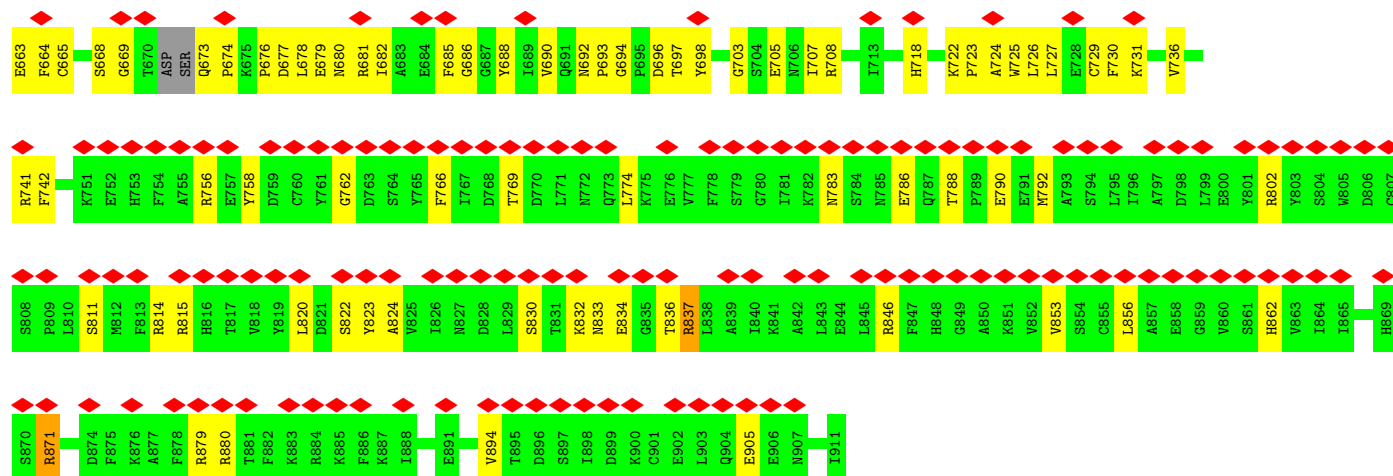
- Molecule 9: DNA ligase 4

Chain X:



- 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 ⓘ

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	0.58	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 ⓘ

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 ⓘ

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

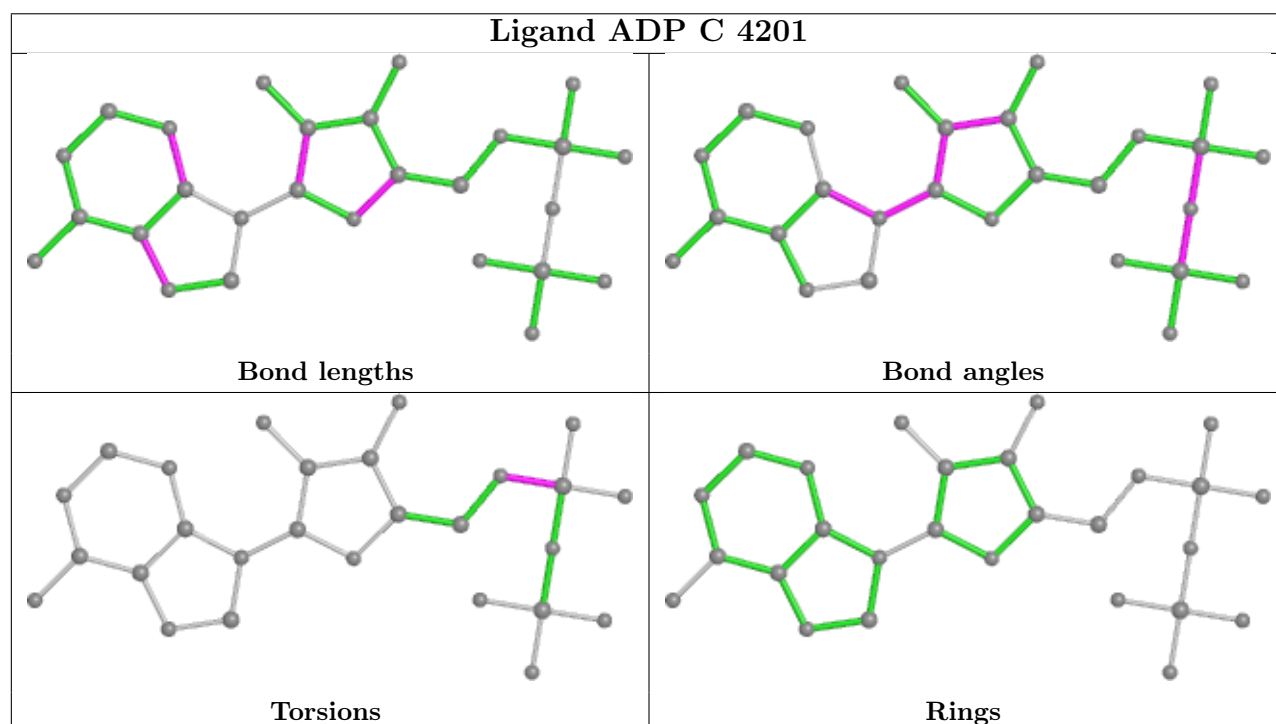
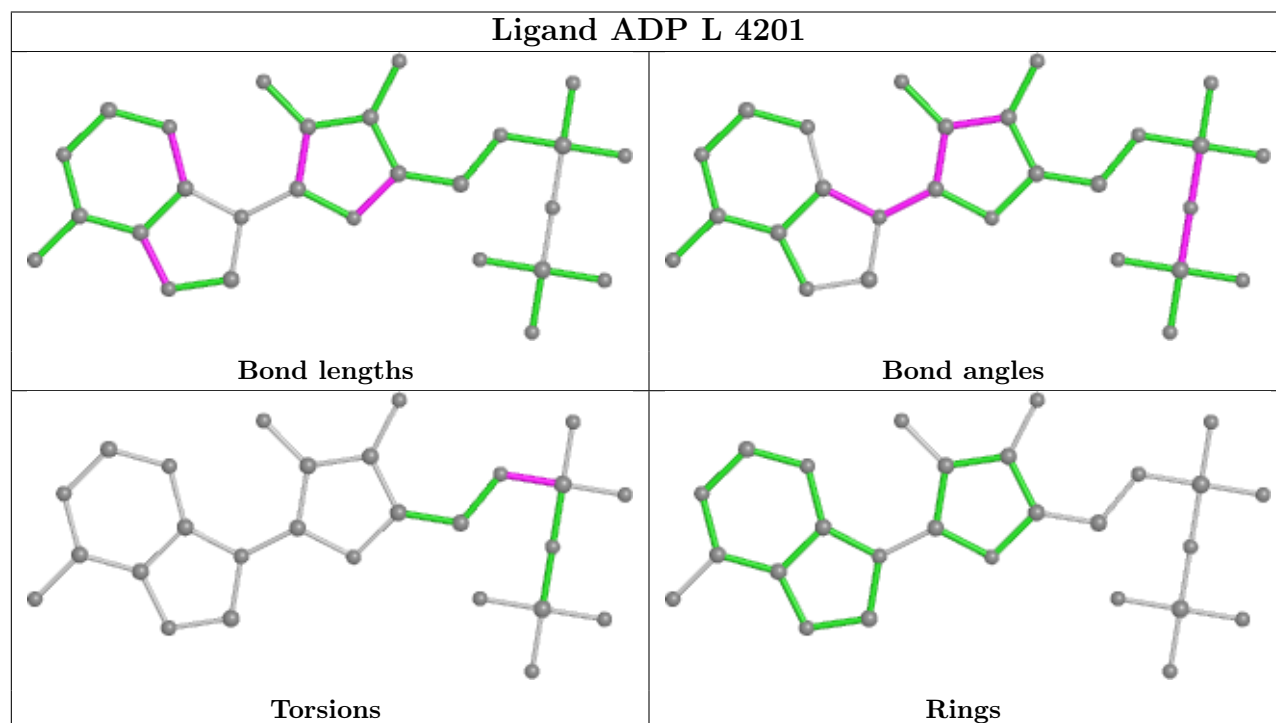
There are no ring outliers.

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.

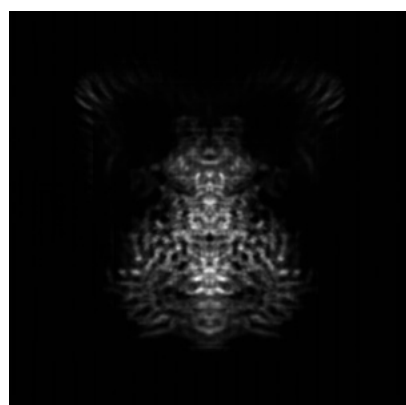
6 Map visualisation [i](#)

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.

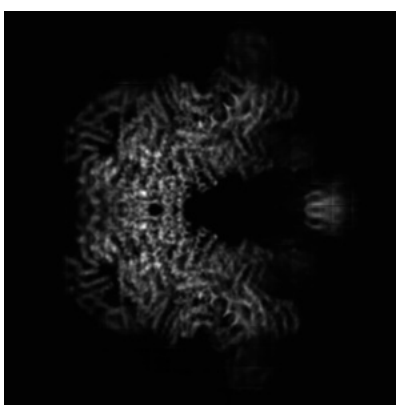
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

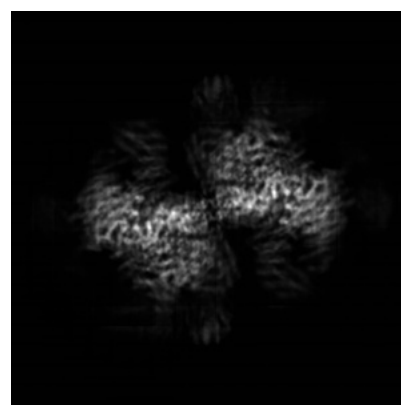
6.1.1 Primary map



X



Y

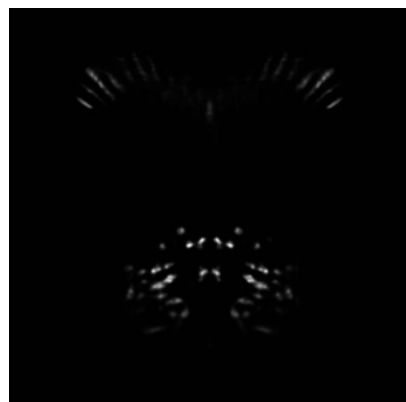


Z

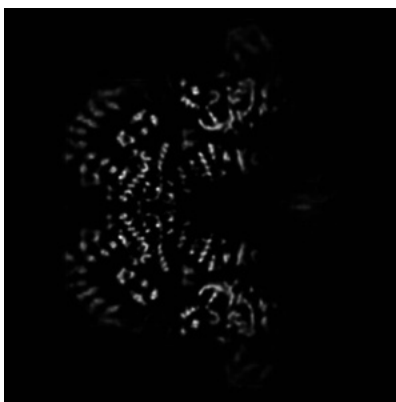
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

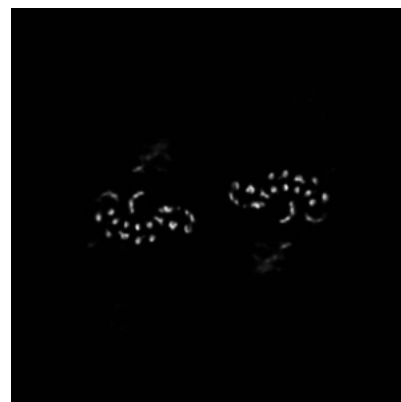
6.2.1 Primary map



X Index: 145



Y Index: 145



Z Index: 145

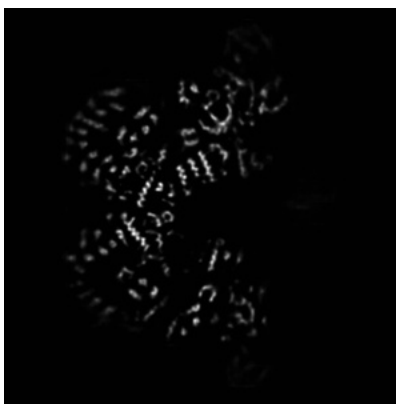
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

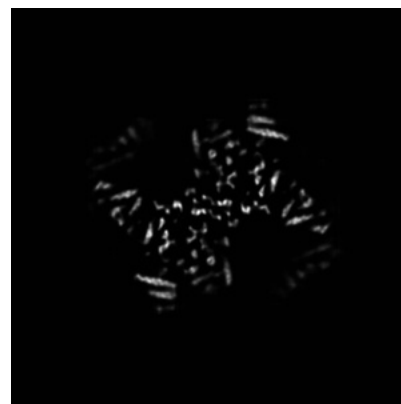
6.3.1 Primary map



X Index: 185



Y Index: 147



Z Index: 100

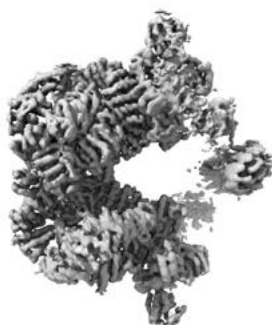
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

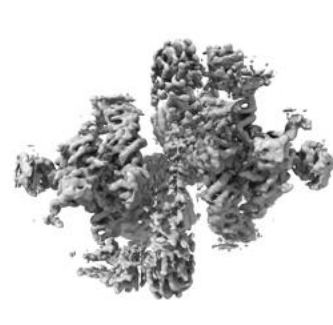
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

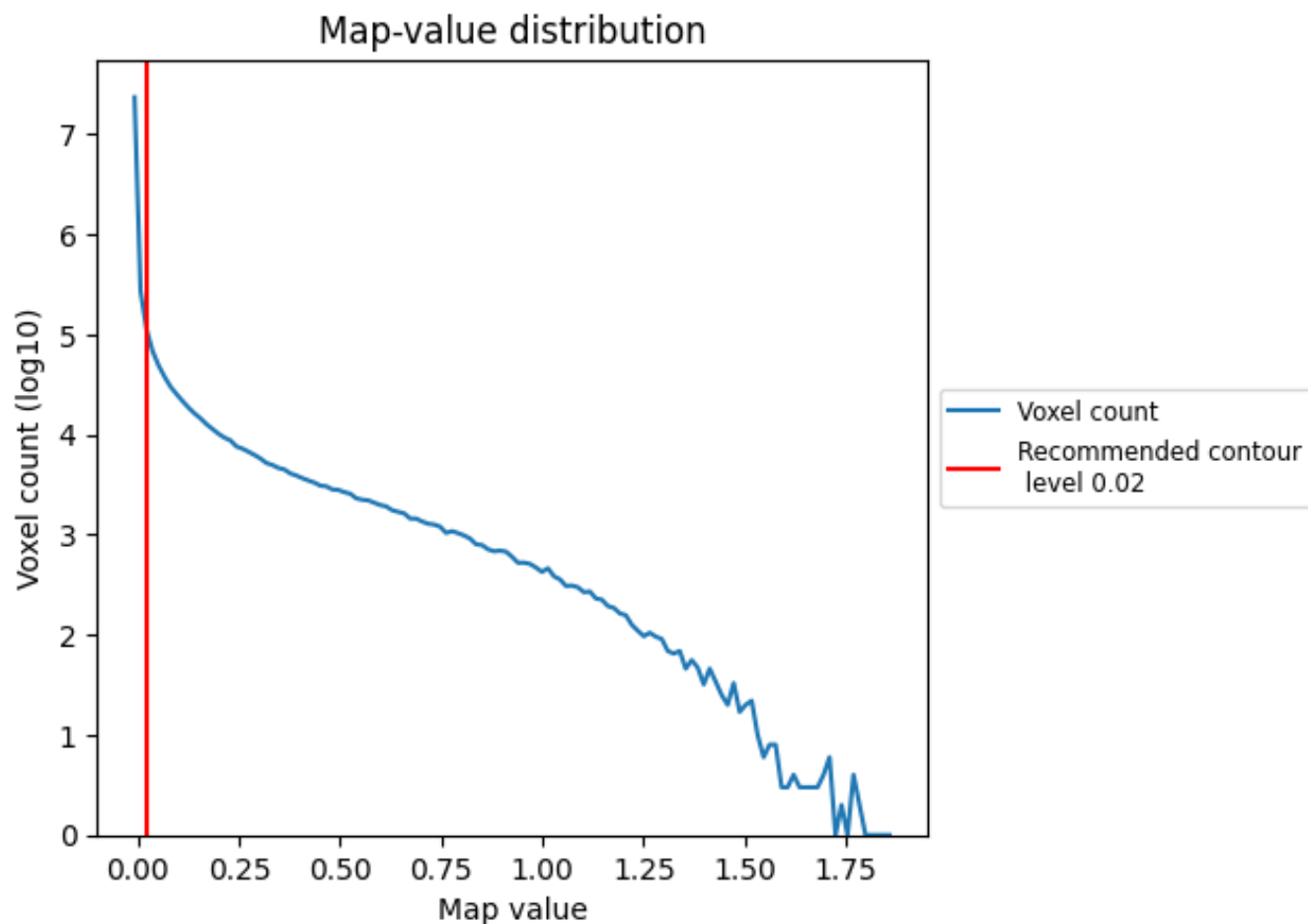
6.5 Mask visualisation

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

7 Map analysis [i](#)

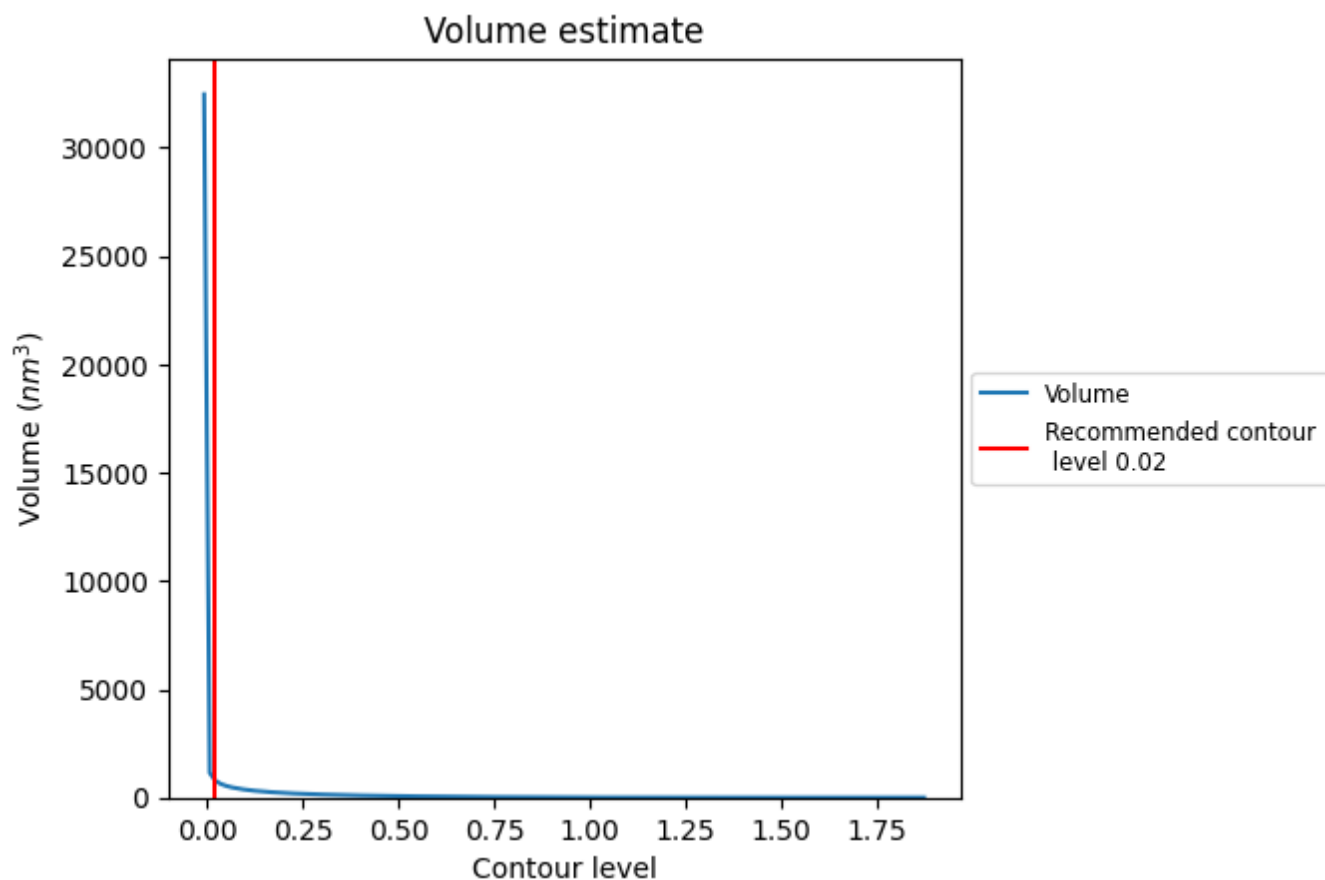
This section contains the results of statistical analysis of the map.

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.

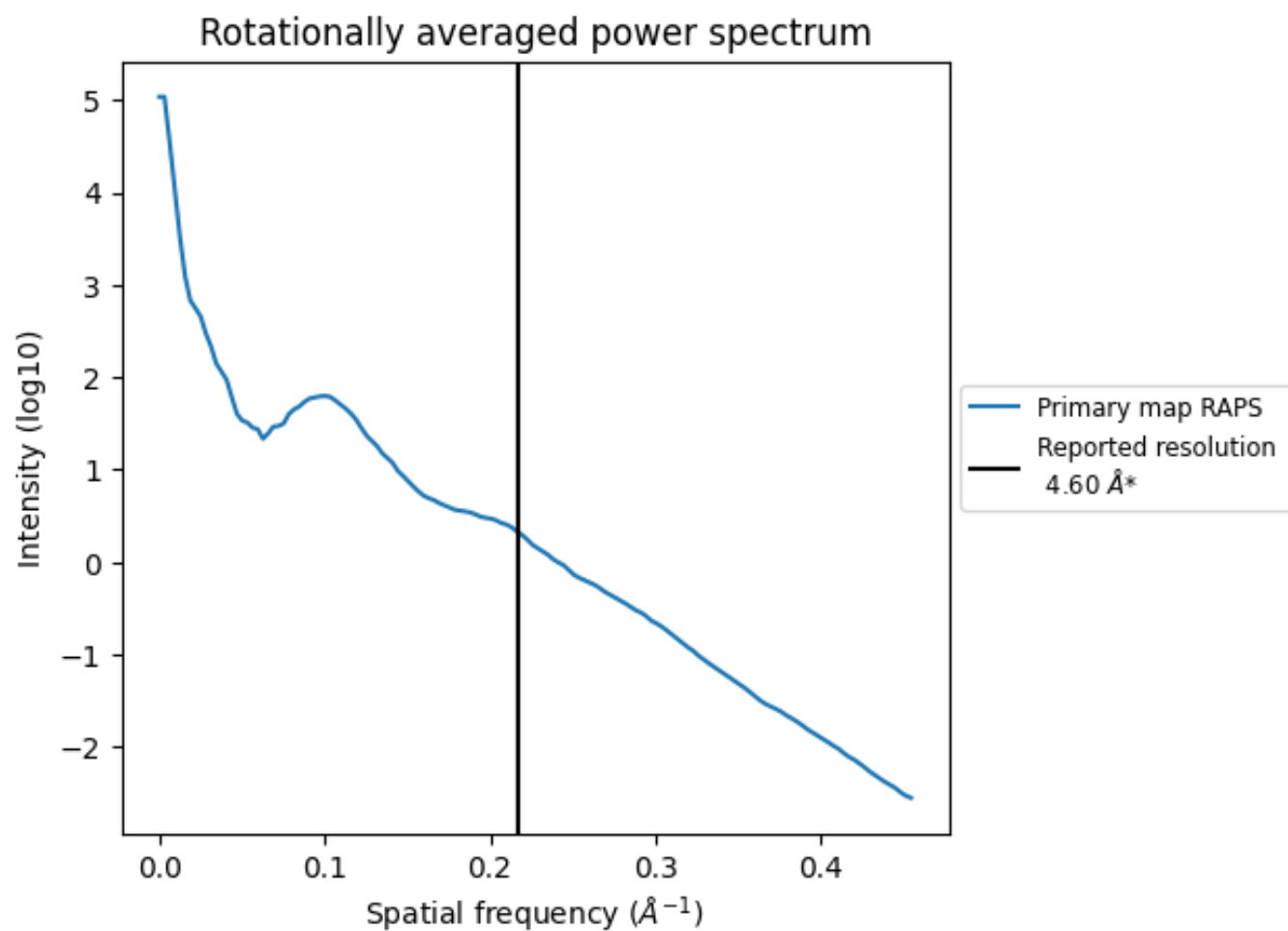
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

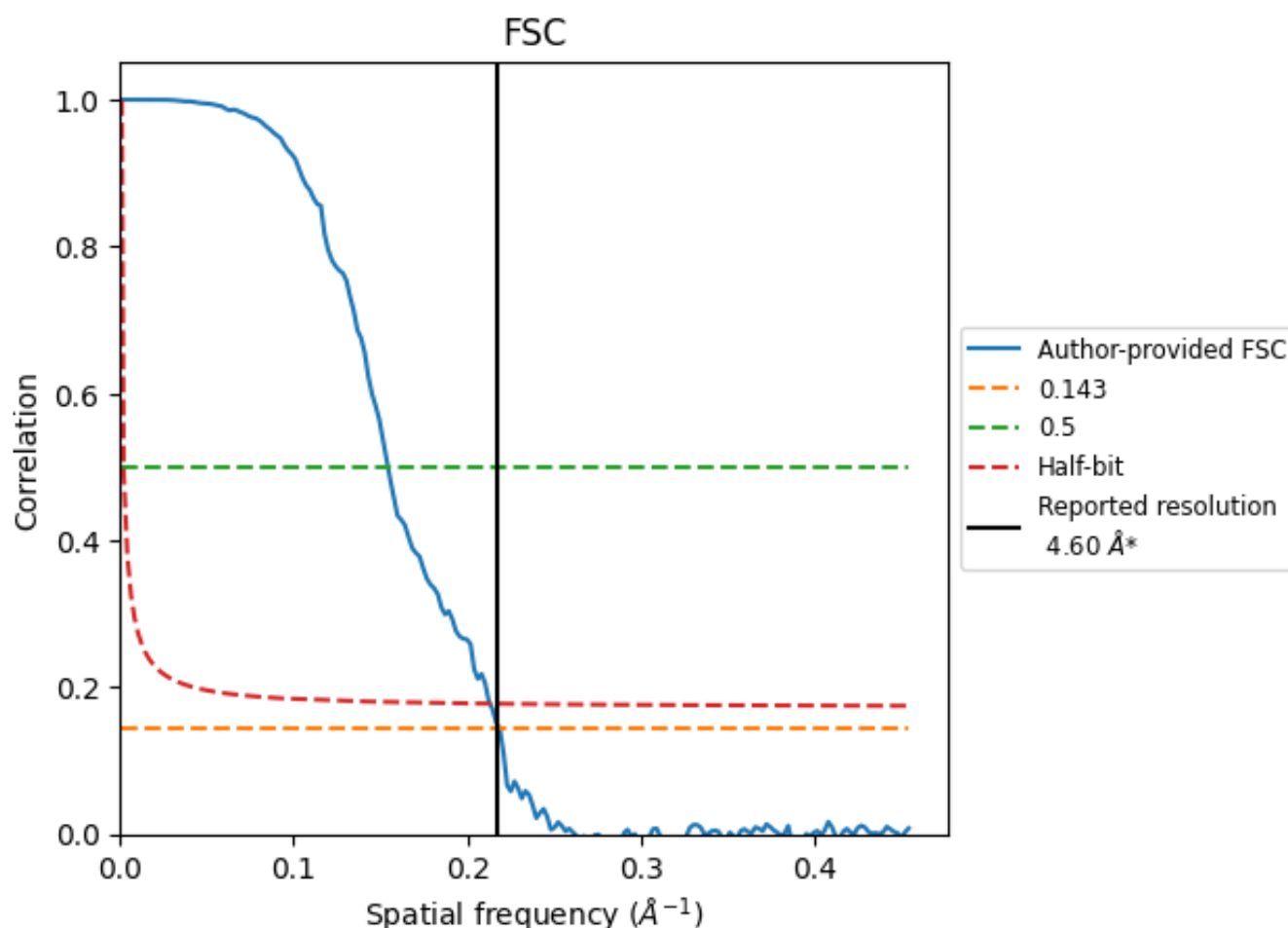


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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](#)

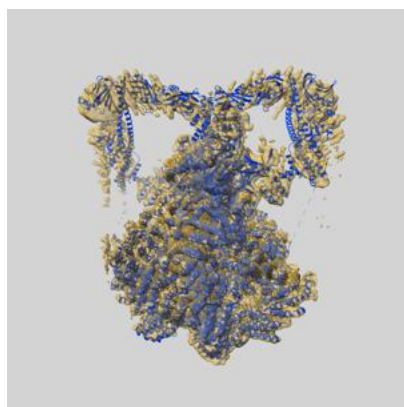
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.57	6.48	4.69
Unmasked-calculated*	-	-	-

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

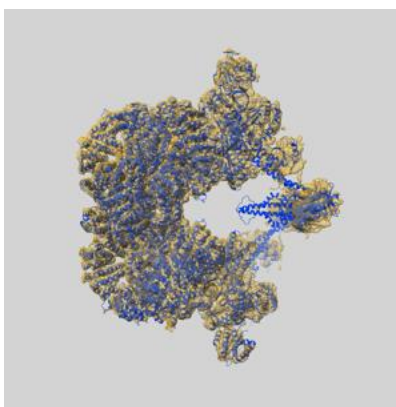
9 Map-model fit [i](#)

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](#).

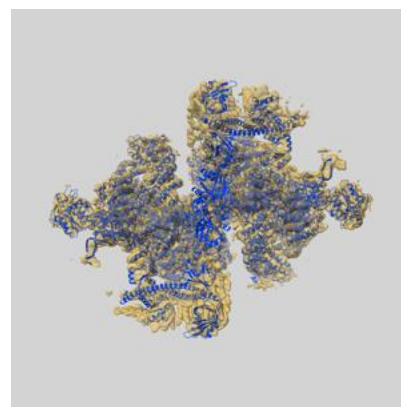
9.1 Map-model overlay [i](#)



X



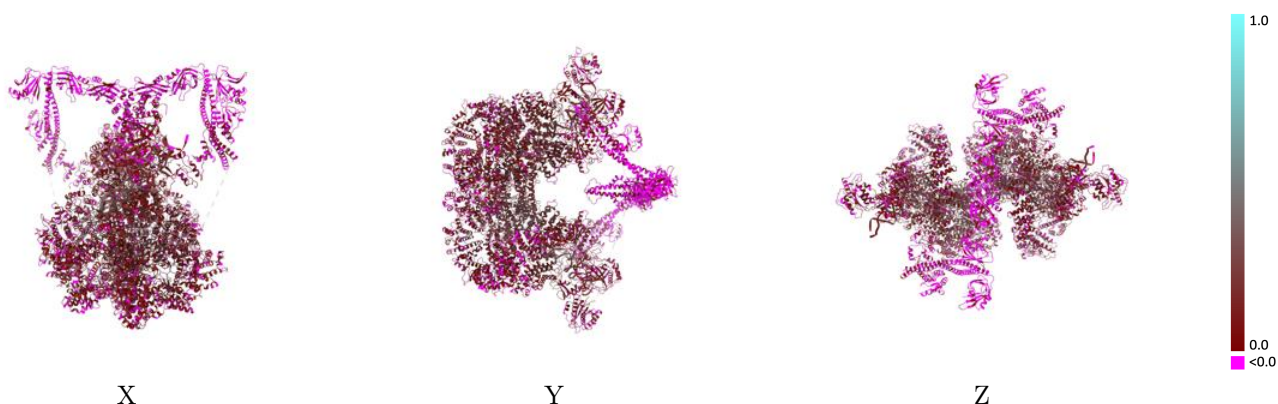
Y



Z

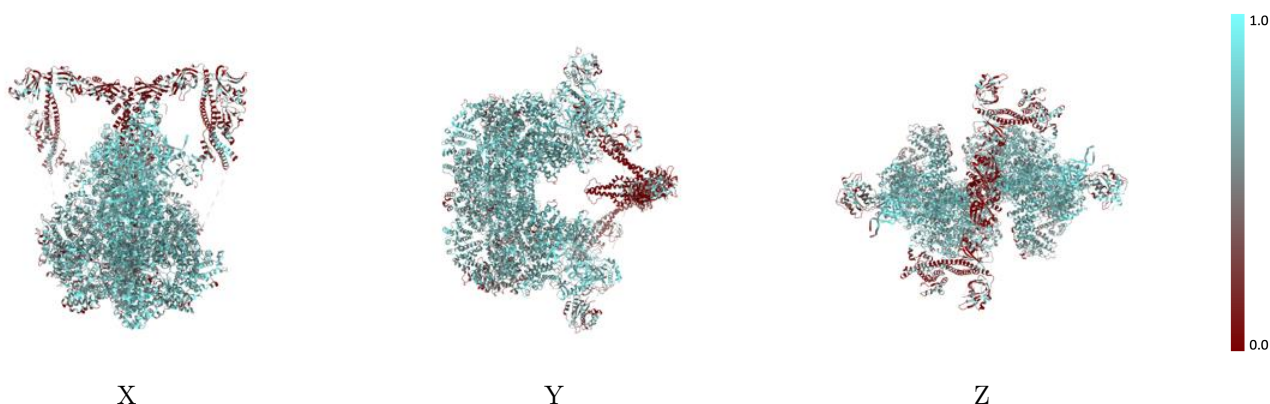
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



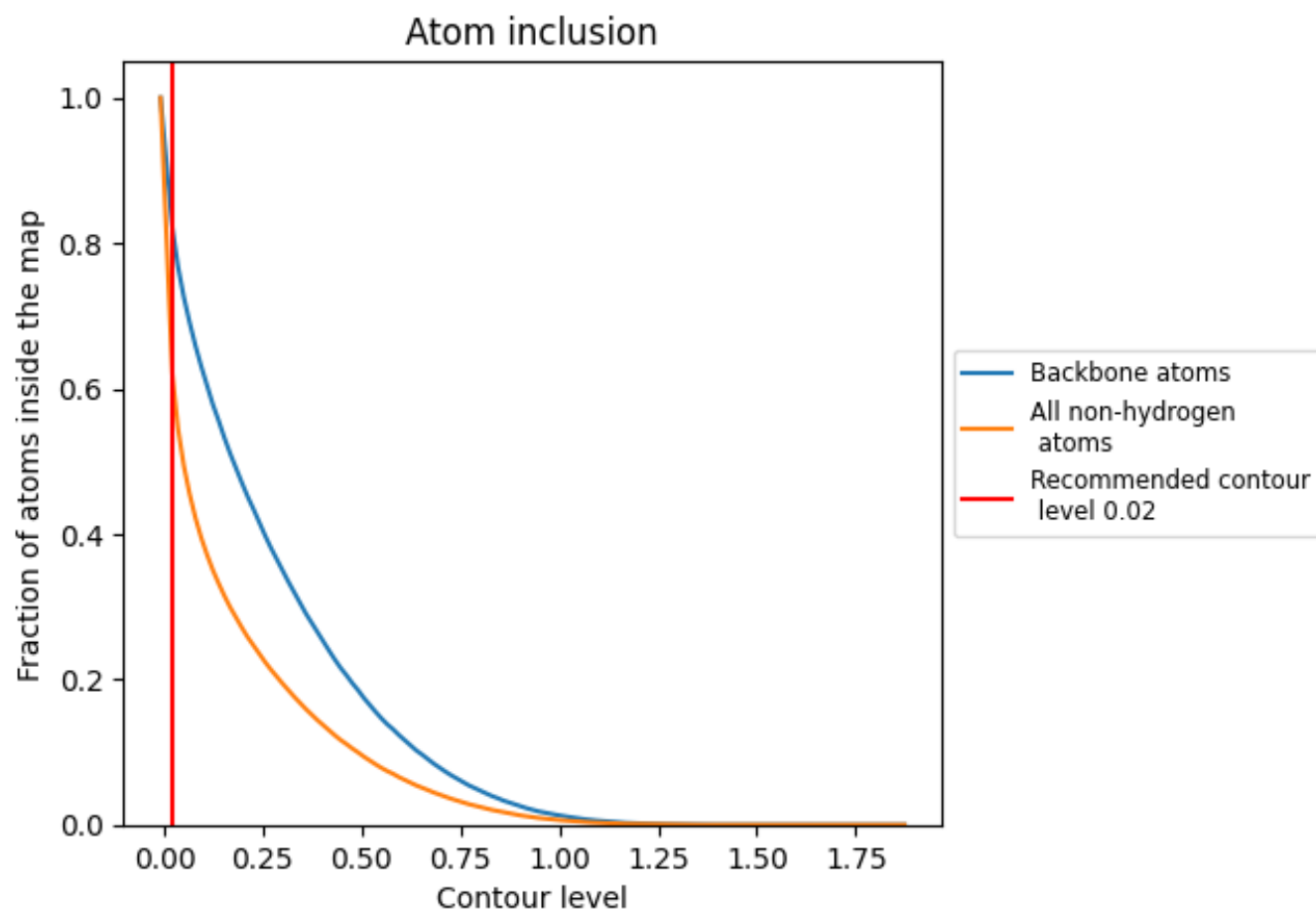
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6249	 0.1180
A	 0.6924	 0.1410
B	 0.6194	 0.1190
C	 0.6939	 0.1450
D	 0.9338	 0.2740
E	 0.9367	 0.2930
F	 0.3068	 -0.0340
G	 0.3669	 -0.0580
H	 0.0794	 -0.0220
I	 0.1362	 -0.0420
J	 0.7071	 0.1420
K	 0.5616	 0.1120
L	 0.6813	 0.1410
M	 0.9038	 0.2740
N	 0.9042	 0.2910
O	 0.3133	 -0.0650
P	 0.3469	 -0.0230
Q	 0.2475	 0.1700
R	 0.3663	 0.1090
X	 0.4101	 0.0050
Y	 0.3701	 -0.0030

