



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:35 PM UTC

PDB ID : 7K17 / pdb_00007k17
Title : Re-refined crystal structure of DNA-dependent protein kinase catalytic subunit complexed with Ku80 C-terminal helix
Authors : Chen, X.; Gellert, M.; Yang, W.
Deposited on : 2020-09-07
Resolution : 4.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

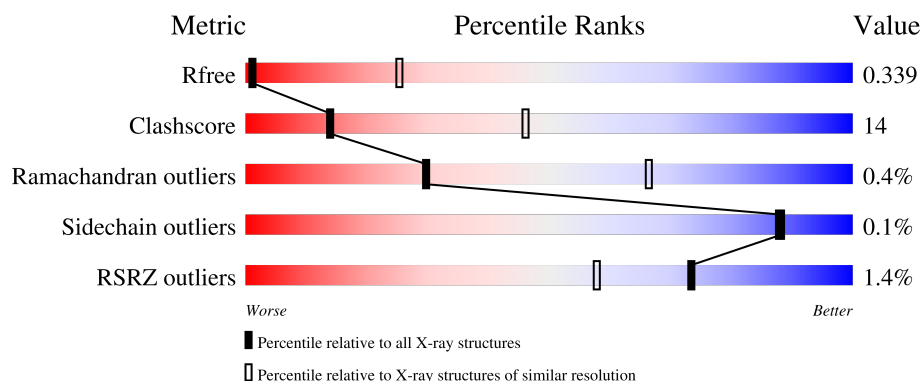
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3986	62% 29% 9%
1	B	3986	63% 28% 9%
2	C	192	95%
2	D	192	95%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 56895 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	3629	Total	C	N	O	S	0	0	0
			28238	18117	4751	5184	186			
1	B	3645	Total	C	N	O	S	0	0	0
			28521	18300	4815	5221	185			

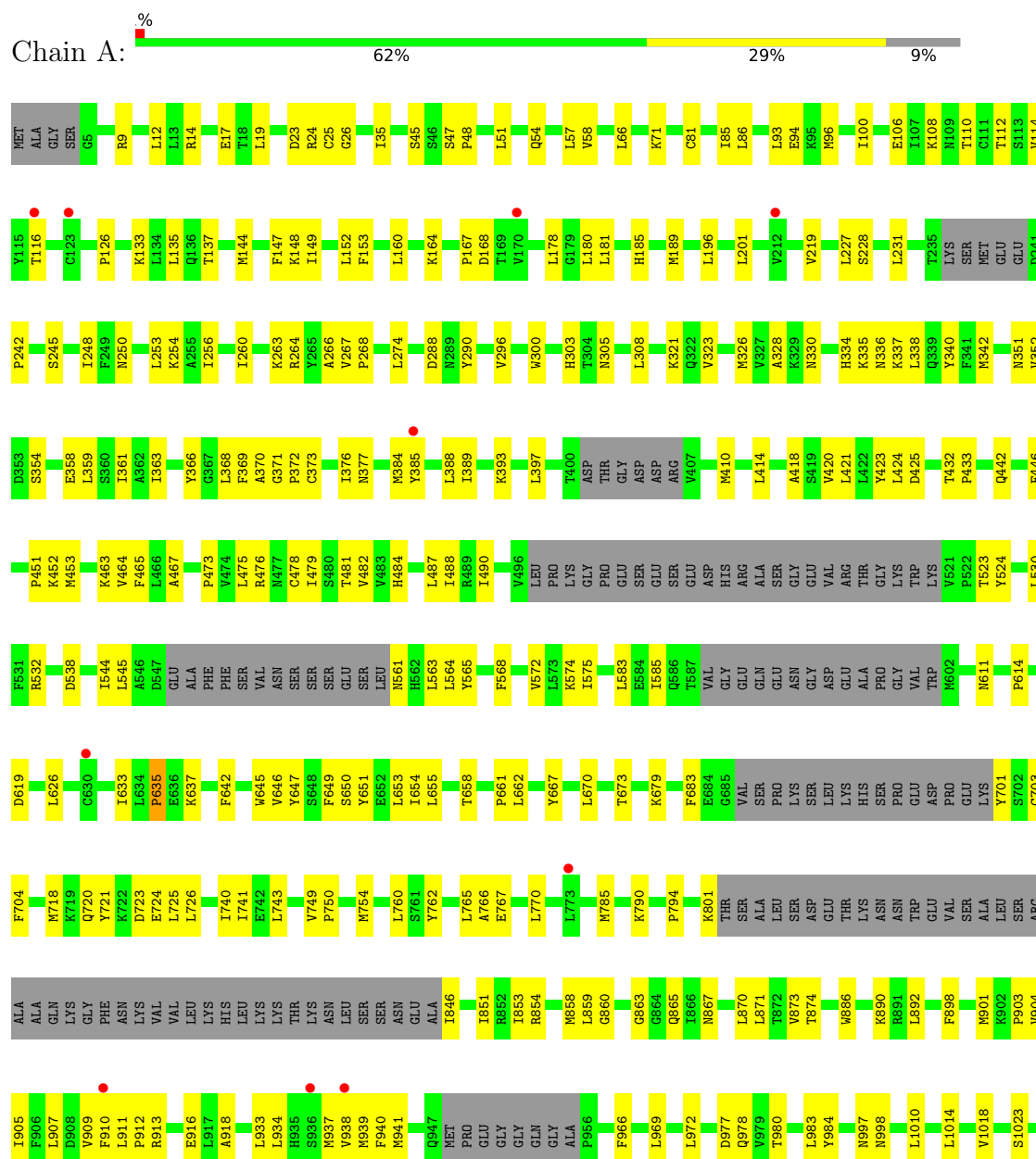
- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	S	0	0	0
			68	43	9	15	1			
2	C	9	Total	C	N	O	S	0	0	0
			68	43	9	15	1			

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: DNA-dependent protein kinase catalytic subunit

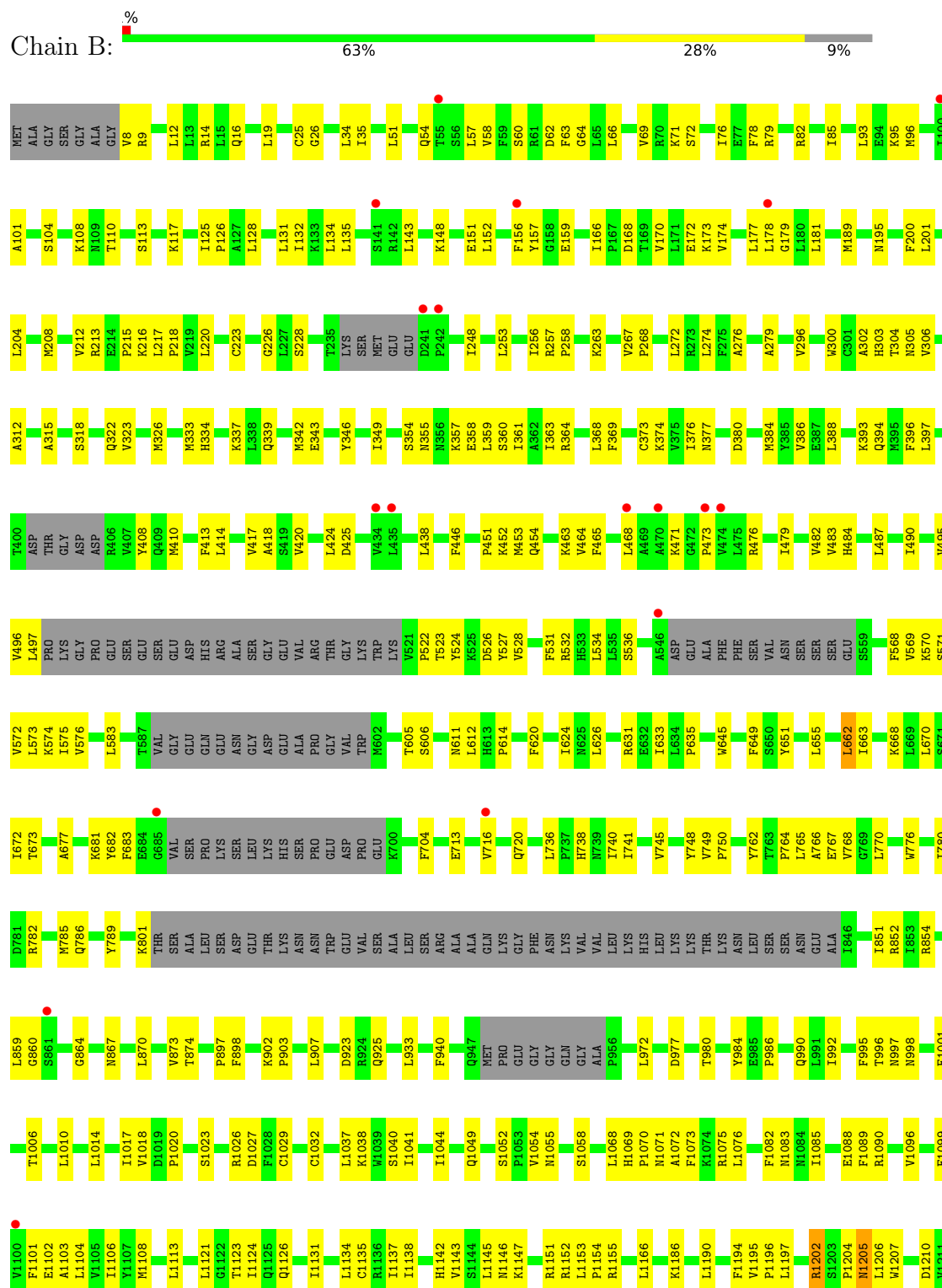


P2226	M2126	F1978	D1878	R1783	F1698	D1602	F1519	L1415	ALA	GLY	ILE	R1026
K2227	G2131	E1979	V1879	R1787	F1699	Q1603	A1520	E1416	GLY	ILE	LEU	C1029
V2230	N1880	N1980	M1880	R1788	S1701	S1604	A1520	R1420	ASN	ALA	ARG	C1032
N2234	N2135	D1983	L1884	G1789	T1703	K1612	L1528	E1421	THR	GLN	PRO	L1037
T2237	T2137	L1984	L1884	S1790	L1707	H1613	L1532	K1422	S1323	THR	THR	K1038
P2138	P2138	F1990	H1890	T1793	L1707	G1615	L1533	A1425	S1333	LEU	LEU	W1039
P2139	P2139	P1991	A1891	Q1794	R1712	L1616	M1534	E1426	K1334	LEU	LEU	K1039
L2140	L2140	P1992	K1892	Q1794	R1712	K1617	P1535	E1427	C1335	TYR	TYR	S1040
R2143	R2143	E1993	K1895	L1797	W1713	L1618	A1536	I1428	S1336	LEU	LEU	I1041
L2144	L2144	E1995	I1896	L1797	Q1716	T1621	LEU	E1429	V1337	ARG	ARG	K1042
K2148	K2148	V1996	V1899	V1801	L1717	H1625	SER	E1430	V1338	GLY	GLY	S1052
S2250	S2250	PRO	E1803	Y1802	I1718	H1625	THR	L1431	V1339	PRO	PRO	N1055
T2151	T2151	MET	T1906	M1804	H1721	W1633	THR	A1432	M1342	PHE	PHE	K1057
N2152	N2152	GLU	T1906	M1804	F1722	W1633	SER	A1433	E1343	SER	SER	T1056
V2156	V2156	ARG	M1909	V1820	M1723	E1640	GLY	L1436	F1344	LEU	LEU	K1057
R2254	R2254	LYS	E1910	D1821	M1724	T1641	SER	D1440	T1345	P1154	P1154	F1089
L2255	L2255	LYS	L1911	R1822	Q1725	K1642	SER	V1443	T1346	R1178	R1178	K1074
L2256	L2256	LYS	T1912	S1823	M1724	M1643	SER	V1443	T1347	P1179	P1179	R1075
F2257	F2257	TYR	K1913	L1824	P1730	M1643	GLN	L1448	L1348	Q1180	Q1180	L1076
L2163	L2163	ASP	T1914	L1825	T1733	L1646	SER	L1448	L1349	T1275	T1275	G1077
N2177	N2177	GLU	L1915	D1834	M1743	SER	G1556	L1448	S1352	L1279	L1279	A1078
G2178	G2178	ILE	I1916	W1829	F1734	L1653	ILE	H1459	P1353	L1279	L1279	N1071
Q2275	Q2275	ARG	R1917	H1830	R1735	Q1654	HIS	H1459	P1353	L1279	L1279	A1072
L2276	L2276	LYS	L1918	C1831	F1736	I1655	THR	L1463	G1354	L1282	L1282	F1073
G2180	G2180	GLU	C1919	S1832	M1739	D1656	SER	L1463	G1354	G1283	G1283	K1074
G2181	G2181	ALA	Y1920	L1833	Y1739	S1657	HIS	M1466	P1356	L1291	L1291	R1075
T2182	T2182	ARG	F1923	D1834	M1743	SER	G1556	M1466	K1357	L1291	L1291	L1076
L2183	L2183	GLU	F1923	A1835	M1743	VAL	F1559	D1474	L1358	L1291	L1291	G1077
Y2184	Y2184	ALA	E1930	F1840	D1747	SER	Y1560	L1475	L1359	L1291	L1291	A1078
N2185	N2185	ASN	L1934	I1843	A1749	THR	S1564	H1476	K1360	L1291	L1291	F1082
V2186	V2186	GLY	L1934	V1844	L1750	SER	S1564	H1476	D1362	L1291	L1291	I1085
E2092	E2092	ASP	R1937	V1845	L1750	SER	S1564	H1476	C1363	L1291	L1291	F1089
C2093	C2093	SER	R1937	V1845	L1750	SER	S1564	H1476	C1364	L1291	L1291	R1090
L2100	L2100	ASP	R1937	V1845	L1750	SER	S1564	H1476	N1365	L1291	L1291	V1096
V2101	V2101	GLY	R1937	V1845	L1750	SER	S1564	H1476	T1366	L1291	L1291	V1096
H2105	H2105	PRO	M1946	T1848	Q1754	G1666	L1572	G1494	L1368	L1291	L1291	F1099
L2194	L2194	TYR	C1947	D1849	S1755	F1668	N1574	ASP	L1371	L1291	L1291	V1100
S2195	S2195	MET	M1757	L1851	P1756	P1669	L1575	GLU	L1372	L1291	L1291	F1101
W2196	W2196	SER	L1949	L1852	M1757	E1670	D1575	ARG	V1373	L1291	L1291	E1102
Q2293	Q2293	GLY	S1950	S1853	L1759	V1671	D1575	GLN	A1302	L1291	L1291	A1103
L2294	L2294	PRO	V1951	T1856	E1760	T1674	L1577	LEU	H1303	L1291	L1291	L1104
S2296	S2296	LEU	I1952	T1856	E1760	I1676	L1578	CYS	V1389	L1291	L1291	V1105
T2203	T2203	GLN	V1955	L1858	E1764	I1676	L1581	LEU	M1392	L1291	L1291	I1106
D2208	D2208	GLU	F1956	L1858	V1765	L1679	E1581	P1501	A1393	L1291	L1291	Y1107
L2216	L2216	ASP	N1957	S1861	L1766	A1680	M1583	S1502	H1394	L1291	L1291	A1114
L2219	L2219	VAL	Y1962	T1862	G1767	D1681	L1582	D1504	P1396	L1291	L1291	E1225
L2219	L2219	GLN	F1967	D1864	R1769	K1683	M1589	C1507	L1402	L1291	L1291	G1226
M2220	M2220	SER	T1865	T1865	E1772	L1686	M1592	M1509	L1402	L1291	L1291	G1227
V2223	V2223	TYR	K1870	K1870	M1774	L1686	V1593	D1509	L1402	L1291	L1291	E1118
F2224	F2224	TYR	Y1873	Y1873	M1774	L1686	V1593	D1509	L1402	L1291	L1291	G1229
H2225	H2225	SER	Y1873	Y1873	M1774	L1686	V1593	D1509	L1402	L1291	L1291	G1230
												L1121
												G1122
												T1123
												I1124

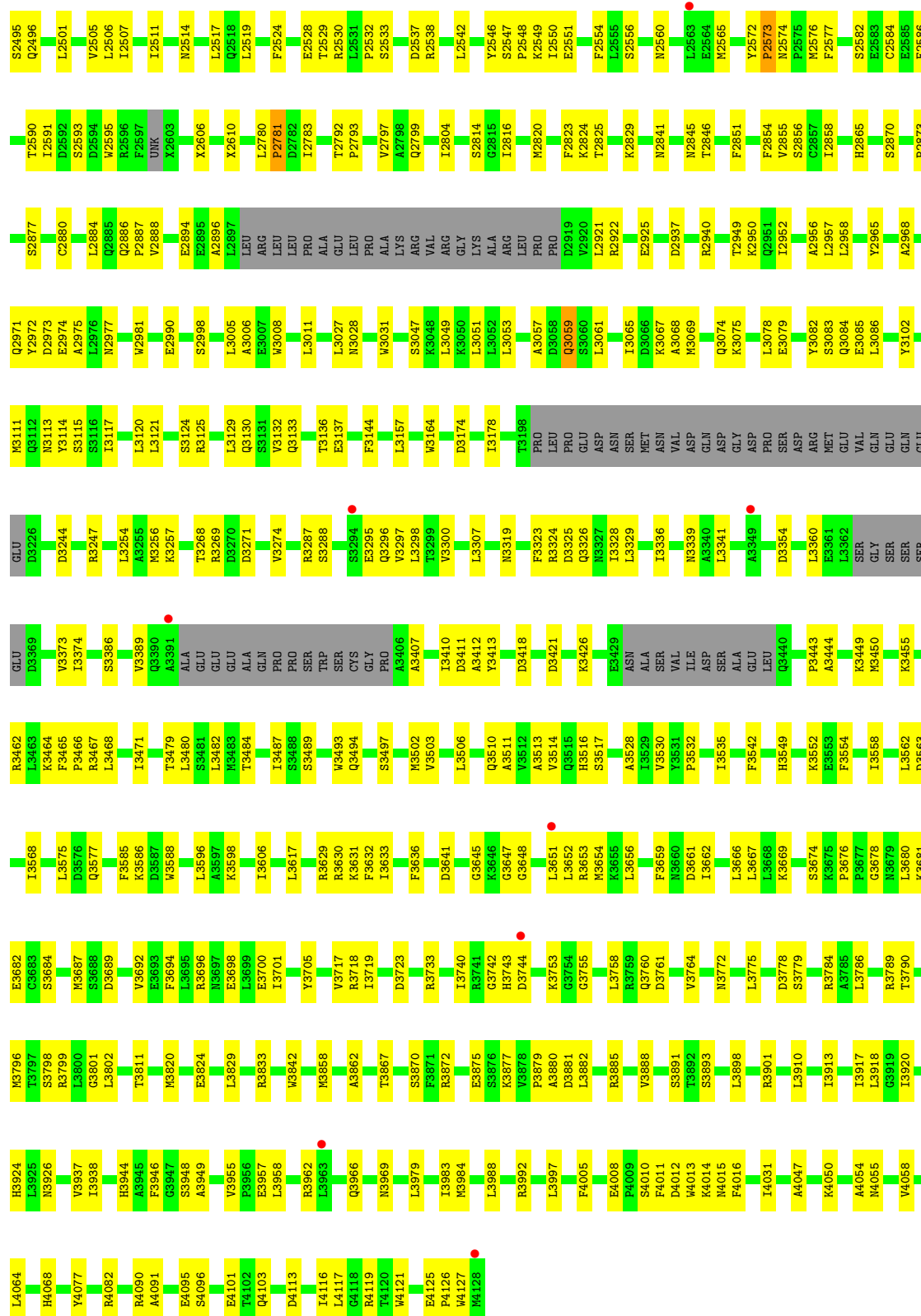
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H3924	T3797	F3554	L3451	GLY	Q3137	K3029	LYS	F2813	F2554	D2437	I2326
I3925	S3798	V3555	R3462	SER	I3138	I3030	ARG	L2555	L2556	I2439	L2327
M3929	L3800	I3558	K3463	GLU	F3144	W3031	ARG	I2816	S2556	M2443	R2328
V3930	L3802	K3559	K3464	GLU	N3150	T3039	LYS	E2819	F2561	L2446	Y2329
V3937	L3665	L3562	R3467	H3384	N3156	Y3043	ALA	F2823	L2562	L2446	E2338
I3938	L3666	V3567	L3468	L3385	L3157	K3248	ARG	K2824	L2563	K2447	L2341
G3939	L3667	I3471	S3386	L3258	L3157	L3049	LEU	T2825	Y2572	P2448	P2449
I3940	L3668	P3476	D3369	L3259	W3164	K3050	PRO	L2826	W2574	E2450	L2344
F3946	L3669	L3480	Q3390	E3261	R3167	L3053	D2919	L2829	P2575	L2451	K2350
G3947	L3670	S3481	A3391	T3268	R3167	A3057	V2920	Q2351	M2576	Q2351	Q2351
A3949	L3671	L3482	GLU	R3269	D3170	Q3058	R2922	L2837	F2577	V2459	T2355
V3955	L3672	K3483	GLU	V3274	A3171	Q3059	W2923	N2841	E2588	H2464	M2356
F3956	L3673	L3484	GLU	S3275	D3174	S3060	E2925	Y2589	Y2589	P2465	K2359
E3957	L3674	L3485	ALA	W3276	D3181	L3061	L2926	W2845	T2590	C2469	K2366
R3962	L3675	S3488	GLN	Q3278	D3186	L3062	R2931	S2849	I2591	Q2472	T2368
K3975	L3676	P3494	PRO	Q3278	R3186	F3063	R2931	S2852	D2594	M2473	F2371
E3976	L3677	Q3494	SER	H3285	F3189	I3065	G2934	P2853	TRP	L2476	P2372
T3977	L3678	S3497	CYS	C3286	K3192	L3077	E2935	S2856	ARG	L2477	P2373
I3983	L3679	W3498	GLY	E3295	K3196	L3078	R2940	I2861	PHE	W2479	L2374
K3989	L3680	M3502	PRO	L3298	K3197	H3081	I2942	S2862	X2603	D2492	A2375
L3988	L3681	V3503	A3406	L3301	T3198	Q3083	L2946	C2863	X2614	S2495	F2378
R3989	L3682	L3506	D3411	L3307	PRO	Q3084	E2946	L2868	X2743	L2506	K2379
R3992	L3683	A3511	A3412	D3308	LEU	Q3085	I2952	L2869	X2753	N2514	L2396
L3998	L3684	A3511	F3419	N3310	GLU	L3088	L2957	S2870	X2757	L2517	L2397
T3999	L3685	V3514	L3416	N3311	ASP	L3091	L2967	S2877	X2781	L2402	C2403
F4005	L3686	Q3515	D3417	L3316	ASN	D3094	E2967	L2881	D2782	R2404	R2404
V4006	L3687	H3516	D3418	R3324	SER	D3095	Q2971	A2882	I2783	T2528	T2409
K4007	L3688	S3517	F3419	D3325	MET	R3098	Y2972	Q2885	I2785	T2529	E2410
E4008	L3689	T3522	Q3422	Q3326	ASN	Q3108	D2973	Q2886	I2786	L2531	L2411
P4009	L3690	Q3527	Q3423	N3327	VAL	S3109	E2974	P2887	K2786	R2538	L2415
S4010	L3691	P3532	E3429	I3328	GLN	F3110	A2975	V2888	H2787	E2528	D2419
F4011	L3692	F3533	ASN	L3329	ASP	S3115	N2977	L2892	L2790	T2529	F2420
V3888	L3693	I3534	SER	L3330	GLY	D3118	K2978	L2893	I2791	R2530	V2421
T3892	L3694	L3535	VAL	L3333	PRO	V3119	W2981	E2894	P2793	L2531	Q2422
S3891	L3695	F3542	TLE	Y3334	ASP	L3120	T2987	E2895	L2794	R2538	Y2546
S3893	L3696	R3543	ASP	R3335	ARG	L3121	E2988	A2896	Q2795	A2541	S2547
P3894	L3697	D3544	ALA	N3339	MET	S3124	A2989	R2899	A2796	L2542	P2548
E3895	L3698	T3545	GLU	D3354	VAL	K3128	L2996	LEU	V2797	L2542	K2549
L4015	L3699	S3546	LEU	R3358	GLN	L3129	I3019	PRO	A2798	Y2546	Q2422
F4016	L3700	H3549	Q3440	I3359	GLU	L3129	D3020	ALA	R2800	Y2546	Q2422
E4017	L3701	K3550	V3447	L3362	GLU	V3132	P3024	LEU	D2801	P2548	V2434
Q4018	L3702	K3552	K3449	L3362	D3226			PRO	I2804	I2550	C2435



● Molecule 1: DNA-dependent protein kinase catalytic subunit



V2405	L2285	I2193	T2193	I1982	T1865	S1781	V1671	N1574	E1482	T1375	M1303	L1212
E2406	P2286	L2194	LEU	V1955	Q1866	F1782	F1672	L1575	L1483	T1375	HIS	L1220
M2407	P2287	S2195	ALA	F1956	R1783	R1784	T1673	D1576	G1494	I1382	ASP	F1224
M2408	P2288	N1957	ASP	N1958	R1785	A1786	T1674	V1579	ASP	F1384	ILE	E1225
T2409	D2289	E1958	S2034	K1870	I1785	D1684	L1684	F1581	GLU	G1387	ALA	G1226
E2410	P2290	N1958	GLN	M1871	A1786	D1685	D1685	F1581	ARG	G1387	ALA	G1227
L2411	Q2291	E1958	GLY	G1872	R1787	R1787	L1686	F1581	GLN	G1387	GLU	
Y2412	Q2291	E1958	GLY	G1872	R1787	R1787	L1686	F1581	GLN	G1387	GLU	
K2418	T2294	F1961	GLU	K1875	I1876	S1790	L1686	F1581	GLN	G1387	GLU	
D2419	P2295	Y1962	GLU	I1876	I1876	S1790	L1686	F1581	GLN	G1387	GLU	
F2420	S2296	F1967	ASP	L1877	L1877	S1790	L1686	F1581	GLN	G1387	GLU	
V2421	Q2301	S1968	VAL	D1878	D1878	S1790	L1686	F1581	GLN	G1387	GLU	
Q2422	Q2301	E1969	VAL	L1879	L1879	S1790	L1686	F1581	GLN	G1387	GLU	
V2423	V2304	N1974	GLN	M1880	M1880	S1790	L1686	F1581	GLN	G1387	GLU	
M2424	V2304	L1975	TYR	Y1881	Y1881	S1790	L1686	F1581	GLN	G1387	GLU	
F2309	F2309	S1882	TYR	Y1881	Y1881	S1790	L1686	F1581	GLN	G1387	GLU	
V2310	V2310	R1883	TYR	Y1881	Y1881	S1790	L1686	F1581	GLN	G1387	GLU	
Q2435	Q2311	I1976	TYR	Y1881	Y1881	S1790	L1686	F1581	GLN	G1387	GLU	
Q2435	Q2311	I1976	TYR	Y1881	Y1881	S1790	L1686	F1581	GLN	G1387	GLU	
L2436	V2312	F1978	SER	M1884	M1884	S1790	L1686	F1581	GLN	G1387	GLU	
K2313	K2313	F1978	SER	M1884	M1884	S1790	L1686	F1581	GLN	G1387	GLU	
E2314	E2314	F1978	SER	M1884	M1884	S1790	L1686	F1581	GLN	G1387	GLU	
Y2315	Y2315	F1978	SER	M1884	M1884	S1790	L1686	F1581	GLN	G1387	GLU	
V2316	V2316	F1978	SER	M1884	M1884	S1790	L1686	F1581	GLN	G1387	GLU	
K2320	K2320	F1978	SER	M1884	M1884	S1790	L1686	F1581	GLN	G1387	GLU	
L2446	L2325	P1991	THR	S1893	S1893	S1813	T1700	F1605	L1514	L1415	THR	
L2446	L2325	P1991	THR	S1893	S1893	S1813	T1700	F1605	L1514	L1415	THR	
L2451	L2326	E1992	ARG	I1896	I1896	Q1817	L1702	R1606	F1519	L1419	THR	
R2452	L2326	E1992	ARG	I1896	I1896	Q1817	L1702	R1606	F1519	L1419	THR	
E2453	Y2329	V1994	ARG	F1900	F1900	V1820	H1721	L1524	L1524	L1423	THR	
K2334	K2334	V1994	ARG	F1900	F1900	V1820	H1721	L1524	L1524	L1423	THR	
V2458	L2344	GLU	GLU	C1904	C1904	L1828	M1737	L1617	L1532	E1429	THR	
E2460	L2344	GLU	GLU	C1904	C1904	L1828	M1737	L1617	L1532	E1429	THR	
F2461	K2359	GLU	GLU	C1904	C1904	L1828	M1737	L1617	L1532	E1429	THR	
G2469	K2366	THR	THR	L1915	L1915	D1834	M1743	L1623	L1541	A1434	THR	
Q2472	V2367	VAL	VAL	L1918	L1918	A1835	L1747	L1623	L1541	A1434	THR	
M2473	P2372	ASP	ASP	C1919	C1919	L1836	L1750	K1627	SER	D1440	THR	
L2476	P2373	ASP	ASP	C1919	C1919	L1836	L1750	K1627	SER	D1440	THR	
L2477	L2374	LEU	LEU	F1923	F1923	E1838	L1752	C1629	GLN	V1443	THR	
I2480	M2379	E2082	E2082	F1925	F1925	S1841	Q1754	S1631	VAL	L1448	THR	
H2481	F2383	L2083	L2083	N1926	N1926	T1842	L1758	W1632	ILE	L1448	THR	
D2482	F2383	E2084	E2084	E1930	E1930	I1843	L1758	W1632	ILE	L1448	THR	
N2483	P2387	M2085	M2085	E1930	E1930	I1843	L1758	W1632	ILE	L1448	THR	
H2485	P2387	N2089	N2089	L1934	L1934	D1846	M1762	L1648	S1554	L1458	THR	
D2486	L2393	H2091	H2091	F1935	F1935	A1847	L1765	T1652	E1557	L1458	THR	
P2487	L2393	E2092	E2092	R1936	R1936	I1848	L1766	L1653	L1562	G1462	THR	
E2488	L2398	C2093	C2093	A1937	A1937	L1851	R1768	I1655	F1563	L1463	THR	
S2489	V2401	L2097	L2097	H1941	H1941	R1854	M1773	S1658	T1565	N1466	THR	
E2490	L2402	E2188	E2188	C1947	C1947	R1854	M1773	S1658	T1565	N1466	THR	
D2491	C2403	I2189	I2189	A1948	A1948	E1860	M1774	F1661	I1567	L1467	THR	
L2492	L2492	V2190	V2190	I1949	I1949	E1860	M1774	F1661	I1567	L1467	THR	
		E2191	E2191	S1950	S1950	Q1779	Q1779	F1668	E1570	G1480	THR	
		R2106	R2106	SER	SER	T1862	S1780			T1481	THR	



GLU
GLY
GLY
D724
L728
M731
I732

Chain C: 95%

GLU
GLY
GLY
D724
L729
I732

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	169.12Å 132.64Å 296.59Å 90.00° 105.53° 90.00°	Depositor
Resolution (Å)	49.92 – 4.30 49.92 – 4.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.92-4.30) 97.6 (49.92-4.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.286 , 0.335 0.289 , 0.339	Depositor DCC
R_{free} test set	2009 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	184.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 196.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	56895	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.20	0/28603	0.49	2/38757 (0.0%)
1	B	0.20	0/28898	0.49	3/39125 (0.0%)
2	C	0.16	0/67	0.36	0/90
2	D	0.23	0/67	0.40	0/90
All	All	0.20	0/57635	0.49	5/78062 (0.0%)

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
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1846	ASP	N-CA-C	-7.62	103.05	113.18
1	A	2781	PRO	N-CA-CB	7.46	111.08	103.25
1	A	1995	GLU	N-CA-C	6.00	118.76	110.35
1	B	1611	GLN	CA-C-N	-5.27	111.47	121.54
1	B	1611	GLN	C-N-CA	-5.27	111.47	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1994	VAL	Peptide
1	A	2120	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	1202	ARG	Peptide

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	28238	0	27963	817	0
1	B	28521	0	28367	808	0
2	C	68	0	64	1	0
2	D	68	0	64	1	0
All	All	56895	0	56458	1627	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 14.

The worst 5 of 1627 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HG22	1:A:300:TRP:CZ2	1.96	1.00
1:B:3701:ILE:HD12	1:B:3740:ILE:HD11	1.50	0.94
1:A:645:TRP:O	1:A:649:PHE:HB2	1.71	0.91
1:A:1406:LEU:HB3	1:A:1415:LEU:HD11	1.51	0.89
1:B:2459:VAL:HB	1:B:2505:VAL:HG21	1.55	0.88

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 X-ray entries followed by that with respect to entries of similar resolution.

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	3544/3986 (89%)	3047 (86%)	482 (14%)	15 (0%)	30	66
1	B	3559/3986 (89%)	3069 (86%)	475 (13%)	15 (0%)	30	66
2	C	7/192 (4%)	7 (100%)	0	0	100	100
2	D	7/192 (4%)	7 (100%)	0	0	100	100
All	All	7117/8356 (85%)	6130 (86%)	957 (13%)	30 (0%)	30	66

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2182	ILE
1	A	2250	SER
1	A	2410	GLU
1	A	2781	PRO
1	B	1613	HIS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	3046/3515 (87%)	3046 (100%)	0	100	100
1	B	3093/3515 (88%)	3089 (100%)	4 (0%)	88	88
2	C	8/165 (5%)	8 (100%)	0	100	100
2	D	8/165 (5%)	8 (100%)	0	100	100
All	All	6155/7360 (84%)	6151 (100%)	4 (0%)	88	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	662	LEU
1	B	1205	ASN
1	B	1727	ARG
1	B	2489	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4015	ASN
1	B	3743	HIS
1	B	869	ASN
1	B	3664	ASN
1	B	4088	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2614:UNK	C	2740:UNK	N	43.02
1	A	2614:UNK	C	2739:UNK	N	37.67
1	B	2765:UNK	C	2779:ASP	N	14.02
1	A	2765:UNK	C	2779:ASP	N	13.16

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	3590/3986 (90%)	0.21	48 (1%) 75 59	144, 217, 281, 339	0
1	B	3607/3986 (90%)	0.23	52 (1%) 73 58	148, 210, 309, 413	0
2	C	9/192 (4%)	0.13	0 100 100	217, 221, 227, 228	0
2	D	9/192 (4%)	0.53	0 100 100	160, 169, 180, 182	0
All	All	7215/8356 (86%)	0.22	100 (1%) 73 58	144, 213, 288, 413	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1560	TYR	4.8
1	A	3301	LEU	4.3
1	A	1993	GLU	3.9
1	A	116	THR	3.8
1	B	1391	VAL	3.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.