



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 29, 2020 – 10:10 PM EST

PDB ID : 7K17
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.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

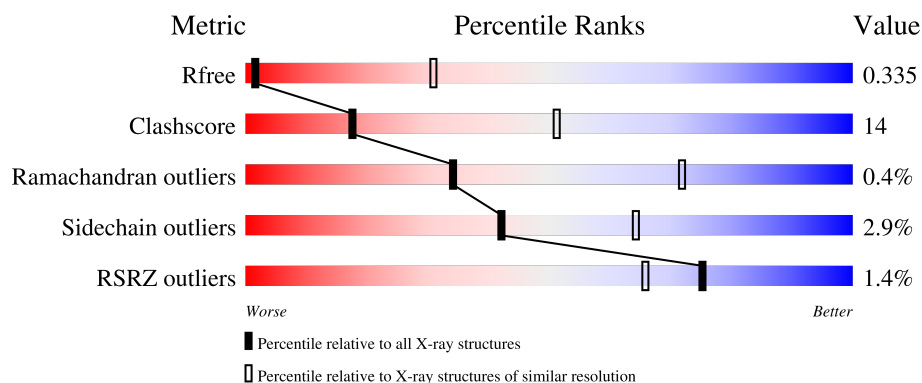
1 Overall quality at a glance

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}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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	
1	B	3986	
2	C	192	
2	D	192	

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			

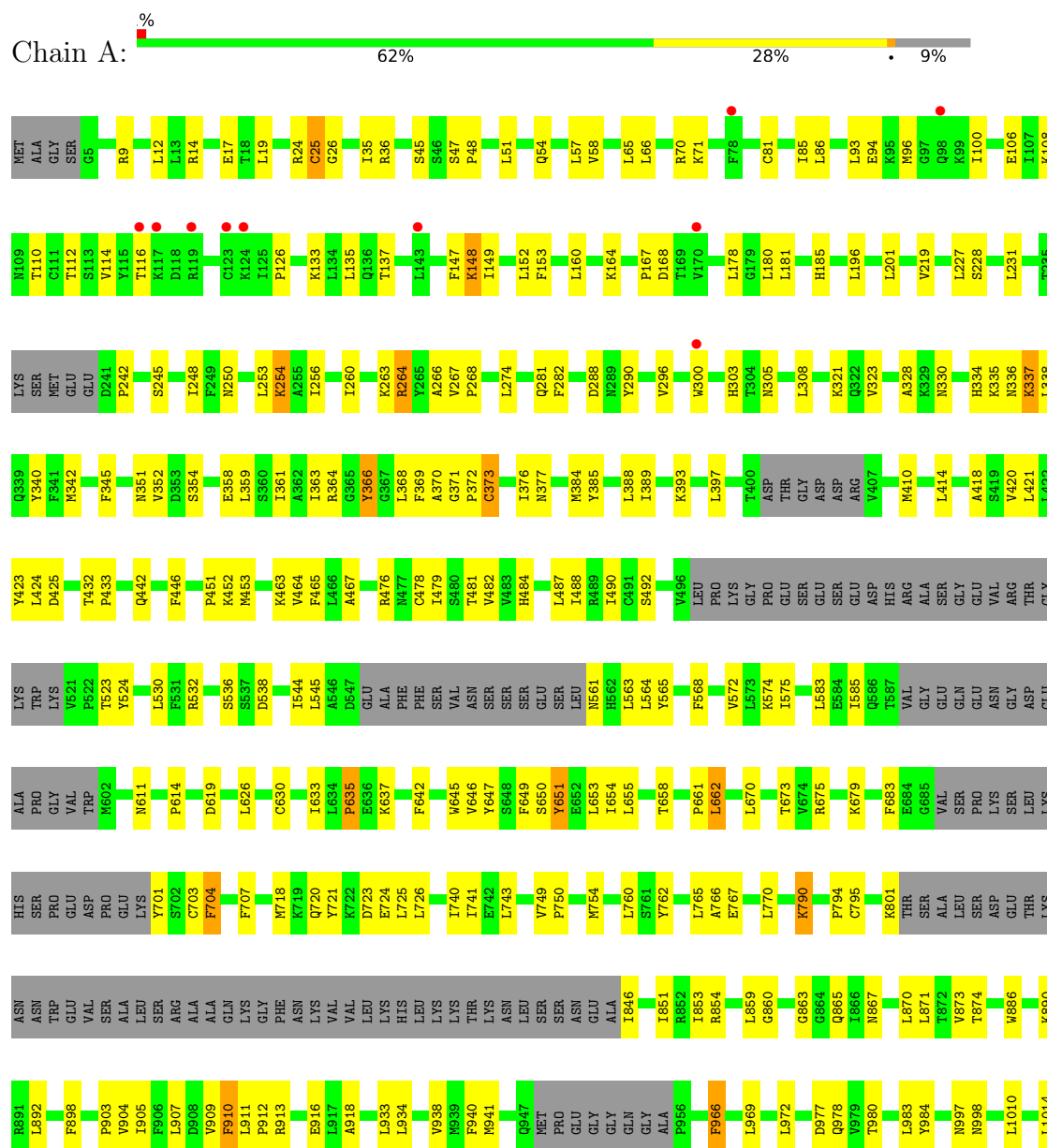
- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

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

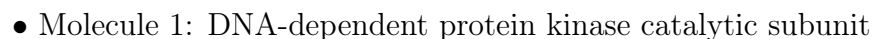
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



L2237	R2143	THR	G1789	L1702	H1800	Q1509	L1406	CYS	PRO	G1122	V1018
L2241	L2144	GLY	S1790	T1703	L1601	L1510	L1406	PHE	SER	T1123	V1018
K2246	K2148	ARG	T1793	L1707	D1602	L1514	Y1411	THR	GLY	I1124	S1023
C2248	E1993	ARG	Q1794	L1707	S1604	L1515	L1415	GLY	ALA	Q1125	R1026
L2249	V1994	ARG	L1797	R1712	K1612	F1519	E1416	ALA	ALA	L1134	C1029
S2250	E1995	PRO	V1801	V1713	H1613	A1520	R1420	GLY	PRO	I1137	C1029
L2251	E2155	GLU	Y1802	Q1716	K1617	L1528	R1420	ASN	THR	I1138	C1032
P2252	E2155	ASP	Y1802	L1717	L1618	L1528	K1422	ARG	LEU	E1139	C1032
R2254	V2156	PRO	V1820	I1718	T1621	L1533	A1425	LEU	LEU	K1140	L1037
L2255	L2165	THR	A1822	H1721	T1625	L1534	A1425	ARG	TYR	K1141	L1037
L2256	L2168	HIS	S1823	P1722	H1625	P1535	Q1426	ARG	LEU	H1142	K1038
F2257	L2168	ASP	S1823	P1722	T1641	A1536	S1427	GLY	ARG	V1143	V1039
F2260	N2177	ASP	L1825	M1724	W1633	V1537	E1429	PRO	PRO	N1146	I1041
D2269	C2178	VAL	L1825	Q1725	W1633	LEU	E1430	SER	PHE	K1147	K1042
D2269	C2178	LEU	W1829	P1730	D1636	THR	L1431	LEU	SER	R1151	S1052
I2274	E2180	ARG	H1830	P1730	E1640	ALA	A1432	M1342	LEU	Q1251	S1052
Q2275	G2181	LYS	E1831	T1733	E1640	SER	A1433	E1343	P1154	P1154	N1055
L2276	L2182	GLU	S1832	P1733	T1641	LEU	V1434	F1344	R1155	R1155	T1056
L2277	H2183	ALA	L1833	P1733	K1642	GLY	N1435	T1345	G1156	G1156	K1057
V2280	Y2184	ARG	D1834	R1735	L1646	SER	L1436	T1346	F1157	F1157	A1067
M2281	W2185	GLU	L1836	F1736	L1646	SER	F1439	T1347	C1164	C1164	A1067
D2284	V2186	ALA	R1837	Y1739	L1653	GLN	D1440	L1348	L1165	L1165	N1071
L2285	E2188	ALA	F1840	M1743	S1657	SER	V1443	L1349	L1166	L1166	A1072
P2286	A2191	ASP	F1840	L1747	S1657	ILE	V1443	S1352	C1255	C1255	F1073
F2287	T2192	ASP	V1843	L1747	VAL	ILE	V1443	S1352	A1263	A1263	R1074
D2288	L2193	GLY	V1845	L1750	VAL	PHE	L1448	E1354	R1178	R1178	R1075
P2290	S2195	PRO	V1849	L1750	SER	PHE	H1459	G1355	P1179	P1179	L1076
Q2291	W2196	SER	I1848	S1753	THR	HIS	H1459	W1356	Q1180	Q1180	G1077
C2292	T2197	TYR	D1849	Q1754	THR	G1556	L1463	L1357	T1181	T1181	G1077
G2293	G2198	MET	V1850	S1755	SER	GLN	N1466	L1358	E1182	E1182	A1078
L2294	L2199	SER	L1851	S1755	G1566	GLN	N1466	L1359	C1183	C1183	F1082
Q2295	A2200	LEU	K1852	L1758	S1667	Y1560	D1474	K1361	L1282	L1282	I1085
S2296	T2203	GLY	S1853	L1758	S1667	S1564	D1474	D1362	G1283	G1283	I1085
V2304	D2208	GLU	T1856	E1764	T1674	K1573	V1479	C1364	F1194	F1194	F1089
N2305	N2305	ASP	K1857	V1765	Y1675	L1574	V1487	N1365	V1195	V1195	R1090
N2306	N2306	SER	L1858	L1766	I1676	L1575	V1487	H1367	P1196	P1196	V1096
F2309	L2219	VAL	S1861	C1767	I1676	L1576	GLU	L1368	L1197	L1197	V1096
F2309	M2220	GLN	T1865	E1769	L1679	D1576	ASP	V1371	S1203	S1203	F1099
Y2312	V2223	SER	T1865	E1769	D1681	A1578	ASP	L1372	P1204	P1204	V1100
V2315	H2225	TYR	K1870	H1772	T1682	V1579	ARG	V1373	L1208	L1208	F1101
A2318	P2226	SER	Y1873	M1774	K1683	L1580	GLN	T1382	L1212	L1212	A1103
A2318	K2227	SER	D1878	F1778	L1686	E1581	CYS	H1382	K1213	K1213	L1104
E2321	V2230	GLN	Y1881	Q1779	A1692	M1583	LEU	V1389	L1220	L1220	V1105
V2322	F2231	ASP	L1981	Q1779	A1692	M1583	P1501	ASP	F1224	F1224	Y1107
V2138	V2138	PRO	I1982	R1783	L1695	L1503	L1503	ILE	A1114	A1114	A1114
P2139	P2139	ARG	D1983	R1783	L1695	L1503	D1504	ALA	G1228	G1228	D1117
L2326	L2326	PRO	H1890	R1787	L1695	V1593	D1504	ALA	E1118	E1118	E1118
L2327	L2327	ALA	A1891	R1787	L1695	V1593	C1507	GLU	G1230	G1230	G1230
			K1892	R1788	F1698	G1599	K1508	L1402	LYS	GLN	L1121

M3846	G3707	I3606	L3416	Y3315	SER	L3121	A3006	GLU	K2549	C2435	R2398
M3858	R3708	E3607	A3417	L3316	ASP	H3122	E3007	LEU	I2590	L2436	Y2329
Y3859	I3719	E3618	D3418	N3319	ARG	H3123	I3019	ALA	E2551	D2437	E2338
K3860	G3727	G3618	G3420	R3324	GLU	S3124	D3020	LYS	S2556	I2439	L2341
A3862	T3727	D3619	D3421	D3325	VAL	K3128	P3024	ARG	F2561	L2446	C2342
T3867	R3733	A3622	Q3422	Q3326	GLN	L3129	N3028	VAL	I2562	K2447	E2343
Y3868	R3737	P3623	Q3423	I3327	GLN	V3132	I3030	ARG	L2563	P2448	L2344
R3872	T3740	P3623	R3425	I3328	GLU	Q3133	W3031	LYS	Y2572	P2449	K2350
K3877	I3740	R3629	E3428	L3330	D3226	E3137	Q3031	ALA	K2350	L2451	Q2351
D3881	R3759	K3630	ASN	T3333	I3243	I3138	T3039	ARG	P2573	Q2351	T2385
R3885	Q3760	K3631	ALA	R3334	D3244	F3144	Y3043	VAL	K2574	V2458	T2385
S3891	D3761	I3632	SER	R3335	R3247	F3144	Y3043	ARG	P2575	V2459	E2357
R3895	D3761	I3633	VAL	R3336	K3248	N3150	L3049	ARG	I2576	H2464	D2358
V3888	V3764	I3634	ILE	N3339	Q3249	P3156	K3050	ALA	E2578	P2465	K2359
V3888	V3764	I3635	ASP	D3354	Q3249	P3156	K3050	ALA	H2579	C2469	K2366
S3891	L3775	K3642	LEU	R3358	K3257	L3157	L3053	LEU	Y2589	Q2472	V2367
E3895	D3778	H3643	Q3440	I3359	L3258	K3158	A3057	PRO	I2590	M2473	T2368
A3896	S3779	H3643	A3441	D3362	L3259	R3159	D3058	PRO	I2591	Q2473	F2371
L3900	A3780	L3651	SER	SER	E3261	K3164	Q3059	PRO	D2594	I2476	P2372
R3901	C3781	L3652	GLY	GLY	T3268	R3167	S3060	ARG	TRP	L2477	P2373
L3910	R3784	M3654	SER	SER	R3269	R3167	L3061	ARG	PHE	Y2484	A2375
L3918	A3785	K3655	GLU	GLU	D3270	D3170	F3063	ARG	K2603	L2489	K2394
I3919	L3786	S3657	D3369	D3369	I3273	A3171	F3064	ARG	P2852	V2505	L2396
I3920	R3789	D3658	H3384	H3384	S3274	D3174	I3065	ARG	P2854	L2506	C2397
H3924	R3790	N3659	L3385	L3385	S3275	D3181	E3072	ARG	K2610	C2398	L2398
L3925	P3795	D3661	S3386	S3386	S3276	K3186	I3077	ARG	X2614	N2514	L2402
V3930	V3795	I3662	V3389	V3389	S3277	F3189	L3078	ARG	X2743	L2517	C2403
V3937	L3800	L3667	ALA	ALA	V3278	K3192	E3085	ARG	K2753	R2404	R2404
I3938	C3801	K3668	GLU	GLU	Q3291	K3196	L3088	ARG	X2757	M2408	T2409
F3946	D3814	M3670	GLU	GLU	G3292	L3197	L3091	ARG	H2787	H2527	T2410
G3947	T3811	S3674	ALA	ALA	E3295	T3198	D3094	ARG	V2888	E2528	E2410
S3948	L3812	K3675	GLN	GLN	L3298	PRD	D3095	ARG	L2790	T2529	L2411
A3949	D3814	P3676	PRO	PRO	L3301	LEU	R3098	ARG	L2791	P2530	L2415
V3955	D3814	F3690	SER	SER	L3301	ASP	Q3108	ARG	T2792	L2531	L2415
F3956	M3820	E3693	TRP	TRP	V3304	ASN	Q3109	ARG	L2793	R2538	D2419
E3957	E3824	F3694	SER	SER	L3307	SER	F3110	ARG	L2794	V2421	V2421
R3962	R3833	L3695	CYS	CYS	D3308	VAL	E2885	ARG	Q2795	A2541	Q2422
K3975	A3834	R3696	PRO	PRO	E3309	ASP	S3115	ARG	L2796	L2542	Q2422
E3976	P3835	E3698	A3406	A3406	N3310	GLN	D3118	LEU	V2797	Y2546	R2425
T3977	Y3839	L3699	D3411	D3411	H3311	ASP	V3119	PRO	A2798	S2547	V2434
I3983	V3842	I3701	A3412	A3412	V3312	GLY	L3120	ALA	Q2799	P2548	V2434
			Y3413	Y3413	S3313	ASP			D2800		
					S3314	PRO			D2801		



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K2246	H1613	Q1614	G1615	K1616	L1617	L1618	A1619	T1620	T1621	L1622	L1623	W1626	K1627	K1628	W1633	L1648	I1652	Q1653	I1655	S1658	F1661	S1667	F1668	V1671	F1672	T1673	T1674	L1684	D1685	H1686	H1687	L1688	K1689	G1690	V1693	T1694	L1695	L1696	P1697	F1698	L1702	H1721	R1727	P1730	L1828										
D2247	T1733	N1737	Y1739	M1743	L1747	L1750	E1751	L1752	S1753	Q1754	L1758	M1762	V1765	L1766	C1767	R1768	V1773	F1778	T1779	S1780	S1781	F1782	R1786	R1787	R1788	G1789	S1790	T1793	L1797	V1801	Y1802	L1803	L1804	P1805	V1809	K1892	E1893	S1894	K1895	I1896	M1897	F1900													
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L2249	VAL	PRO	GLU	MET	K2000	R2001	K2002	K2003	Y2004	T2007	E2010	A2011	A2014	ALA	ASN	GLY	ASP	SER	ASP	GLY	PRO	SER	TYR	MET	SER	LEU	LEU	ASP	ALA	ASP	S2034	Q2042	F2045	G2048	VAL	GLN	SER	TYR	SER	TYR	TYR	SER	SER	GLN	ASP	PRO	ARG	PRO	ALA	THR	GLY	ARG	PHE		
S2250	ARG	ARG	GLU	GLN	ARG	ASP	THR	THR	VAL	HIS	ASP	VAL	LEU	E2082	L2083	E2084	M2085	N2089	R2090	H2091	E2092	C2093	L2097	V2101	L2106	S2107	L2108	GLY	PRO	GLN	GLY	GLU	ASP	VAL	P2119	F2128	L2129	K2132	L2133	P2139	L2140	L2146	A2147	K2148	L2149	V2150	I2151								
P2251	W2152	T2153	E2154	E2155	V2156	F2157	H2163	W2164	L2168	L2169	A2172	G2178	G2179	T2182	T2183	T2184	W2185	V2186	V2187	E2188	T2189	V2190	A2191	T2192	L2193	L2194	S2195	W2196	T2201	V2205	P2206	K2207	D2208	A2212	L2219	V2223	F2224	H2225	P2226	K2227	V2230	F2231	H2232	W2233	W2234	T2237	I2238	K2239							
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I2256	E2154	E2155	V2156	F2157	H2163	W2164	L2168	L2169	A2172	G2178	G2179	T2182	T2183	T2184	W2185	V2186	V2187	E2188	T2189	V2190	A2191	T2192	L2193	L2194	S2195	W2196	T2201	V2205	P2206	K2207	D2208	A2212	L2219	V2223	F2224	H2225	P2226	K2227	V2230	F2231	H2232	W2233	W2234	T2237	I2238	K2239									
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F4005	D3881	G3742	F3632	S5437	V3300	W3164	L3049	K2823	E2550	V2460	E2334
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L3917	L3775	L3654	L3654	S3517	L3336	ASP	A3068	V2855	P2575	R2486	A2375
L3918	L3775	L3655	L3655	A3528	I3336	ASP	M3069	S2856	P2576	P2487	M2379
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L3920	L3775	L3657	L3657	V3530	L3336	ASP	Q3074	I2858	S2582	E2489	F2383
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L3928	L3775	L3665	L3665	F3554	L3361	ASP	E3085	P2873	T2590	L2501	L2398
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L3947	L3775	L3684	L3684	L3617	L3361	ASP	F3144	P2873	T2590	L2501	L2398
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L3966	L3775	L3703	L3703		L3361	ASP		P2873	T2590	L2501	L2398
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L3980	L3775	L3717	L3717		L3361	ASP		P2873	T2590	L2501	L2398
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L4010	L3775	L3747	L3747		L3361	ASP		P2873	T2590	L2501	L2398
L4011	L3775	L3748	L3748		L3361	ASP		P2873	T2590	L2501	L2398
L4012	L3775	L3749	L3749		L3361	ASP		P2873	T2590	L2501	L2398
L4013	L3775	L3750	L3750		L3361	ASP		P2873	T2590	L2501	L2398
L4014	L3775	L3751	L3751		L3361	ASP		P2873	T2590	L2501	L2398
L4015	L3775	L3752	L3752		L3361	ASP		P2873	T2590	L2501	L2398
L4016	L3775	L3753	L3753		L3361	ASP		P2873	T2590	L2501	L2398
L4017	L3775	L3754	L3754		L3361	ASP		P2873	T2590	L2501	L2398
L4018											

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 0.286 , 0.335	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)	0.27 , 157.1	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

5.1 Standard geometry

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	0.29	0/28603	0.52	5/38757 (0.0%)
1	B	0.29	0/28898	0.51	8/39125 (0.0%)
2	C	0.25	0/67	0.43	0/90
2	D	0.28	0/67	0.50	0/90
All	All	0.29	0/57635	0.52	13/78062 (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.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3652	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	A	2781	PRO	N-CA-CB	6.49	111.08	103.30
1	B	1858	LEU	CB-CG-CD1	-6.17	100.51	111.00
1	B	1752	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	B	1752	LEU	CB-CG-CD2	5.72	120.72	111.00

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	774	0
1	B	28521	0	28367	774	0
2	C	68	0	64	1	0
2	D	68	0	64	1	0
All	All	56895	0	56458	1550	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 1550 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%)	34	72
1	B	3559/3986 (89%)	3069 (86%)	475 (13%)	15 (0%)	34	72
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%)	34	72

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%)	2953 (97%)	93 (3%)	40	63
1	B	3093/3515 (88%)	3005 (97%)	88 (3%)	43	65
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%)	5974 (97%)	181 (3%)	42	64

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3442	TYR
1	B	492	SER
1	B	3244	ASP
1	A	3632	PHE
1	A	3784	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4015	ASN
1	B	484	HIS
1	B	3278	GLN
1	A	3924	HIS
1	B	3130	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](#)

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%)	-0.14	46 (1%) 77 68	144, 217, 281, 339	0
1	B	3607/3986 (90%)	-0.11	55 (1%) 73 64	148, 210, 309, 413	0
2	C	9/192 (4%)	-0.39	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%)	-0.13	101 (1%) 75 66	144, 213, 288, 413	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	SER	5.7
1	B	46	SER	5.2
1	A	3310	ASN	5.0
1	B	55	THR	4.6
1	B	1994	VAL	4.3

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 monosaccharides 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.