



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 01:11 PM EDT

PDB ID : 5LUQ
Title : Crystal Structure of Human DNA-dependent Protein Kinase Catalytic Subunit (DNA-PKcs)
Authors : Sibanda, B.L.; Chirgadze, D.Y.; Ascher, D.B.; Blundell, T.L.
Deposited on : 2016-09-09
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 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

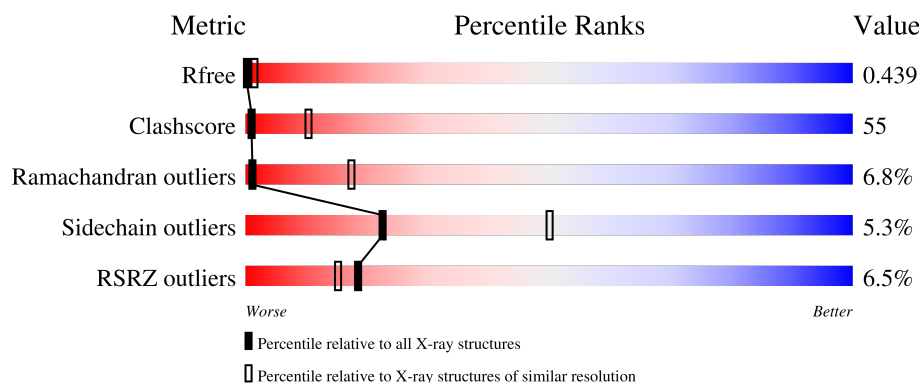
1 Overall quality at a glance

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	4128	<div> <div>5%</div> <div>29%</div> <div>53%</div> <div>8%</div> <div>10%</div> </div>
1	B	4128	<div> <div>6%</div> <div>28%</div> <div>53%</div> <div>8%</div> <div>10%</div> </div>
2	K	194	<div> <div>23%</div> <div>5%</div> <div>72%</div> </div>
2	S	194	<div> <div>23%</div> <div>5%</div> <div>72%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59694 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,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	3725	Total	C	N	O	S	Se	0	0	0
			29574	18907	5016	5460	81	110			
1	B	3725	Total	C	N	O	S	Se	0	0	0
			29574	18907	5016	5460	81	110			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP P78527
A	4128	MSE	-	expression tag	UNP P78527
B	1	MSE	-	expression tag	UNP P78527
B	4128	MSE	-	expression tag	UNP P78527

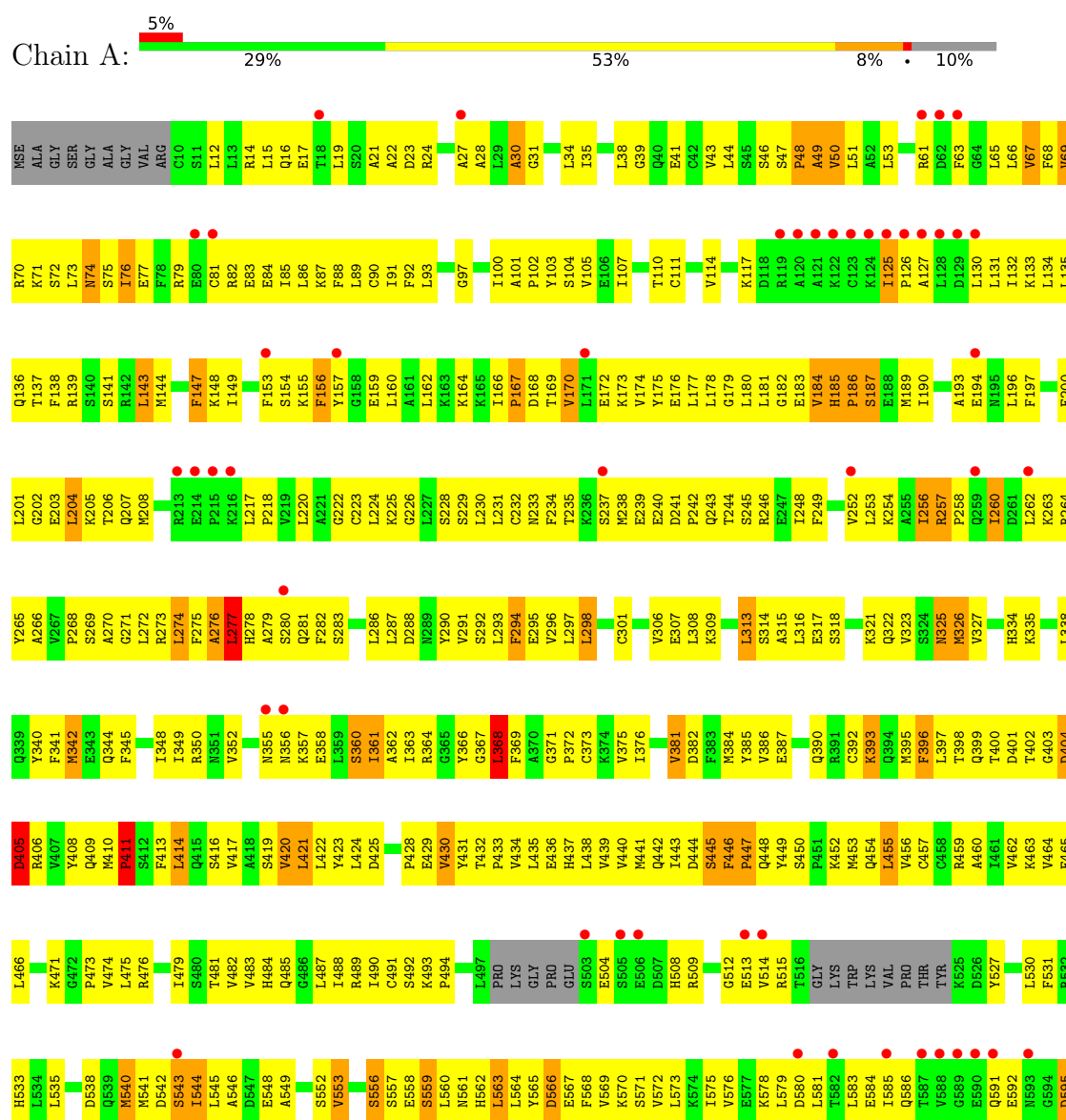
- Molecule 2 is a protein called C-terminal fragment of KU80 (KU80ct194).

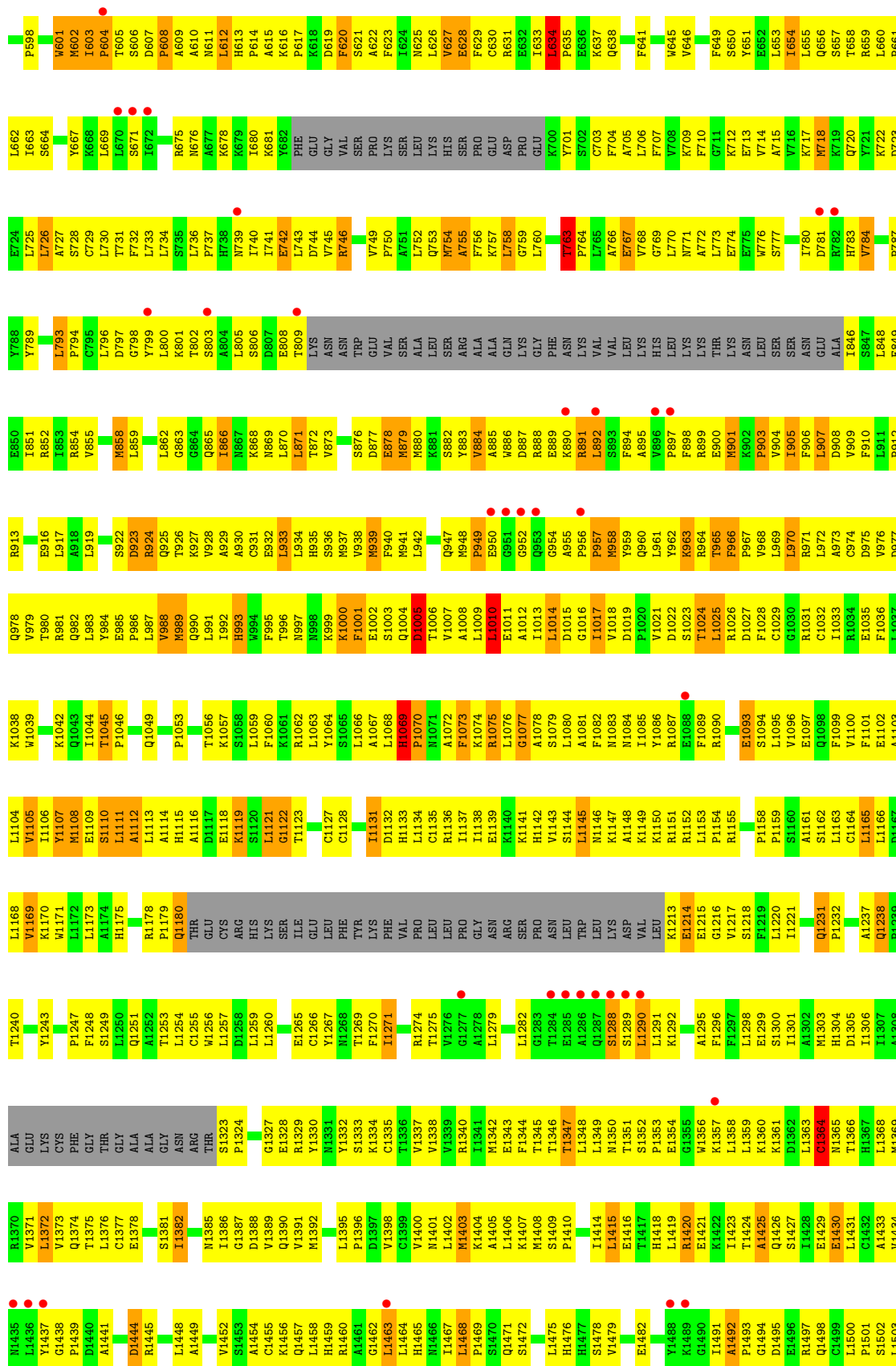
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			
2	S	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			

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.

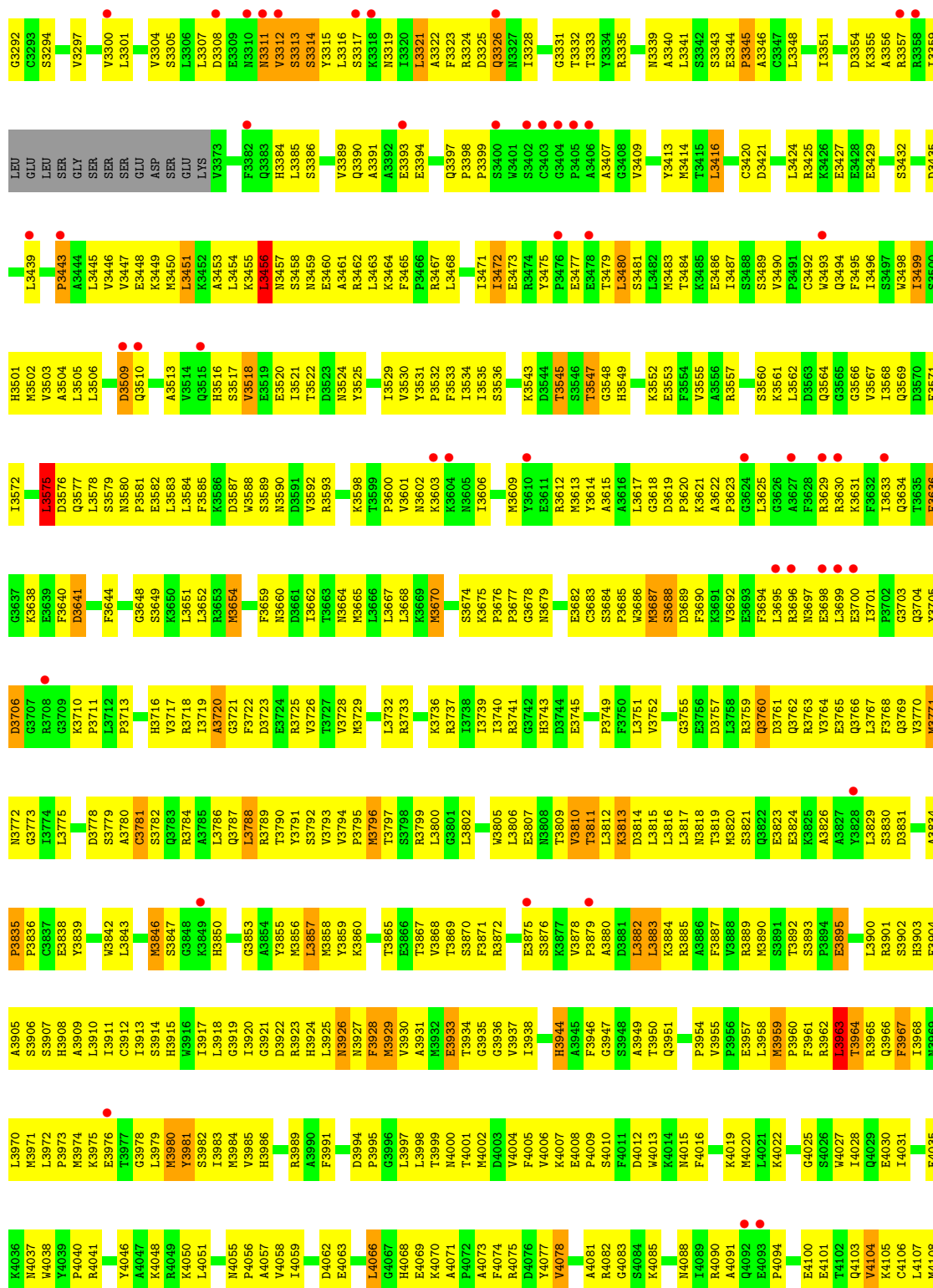
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit





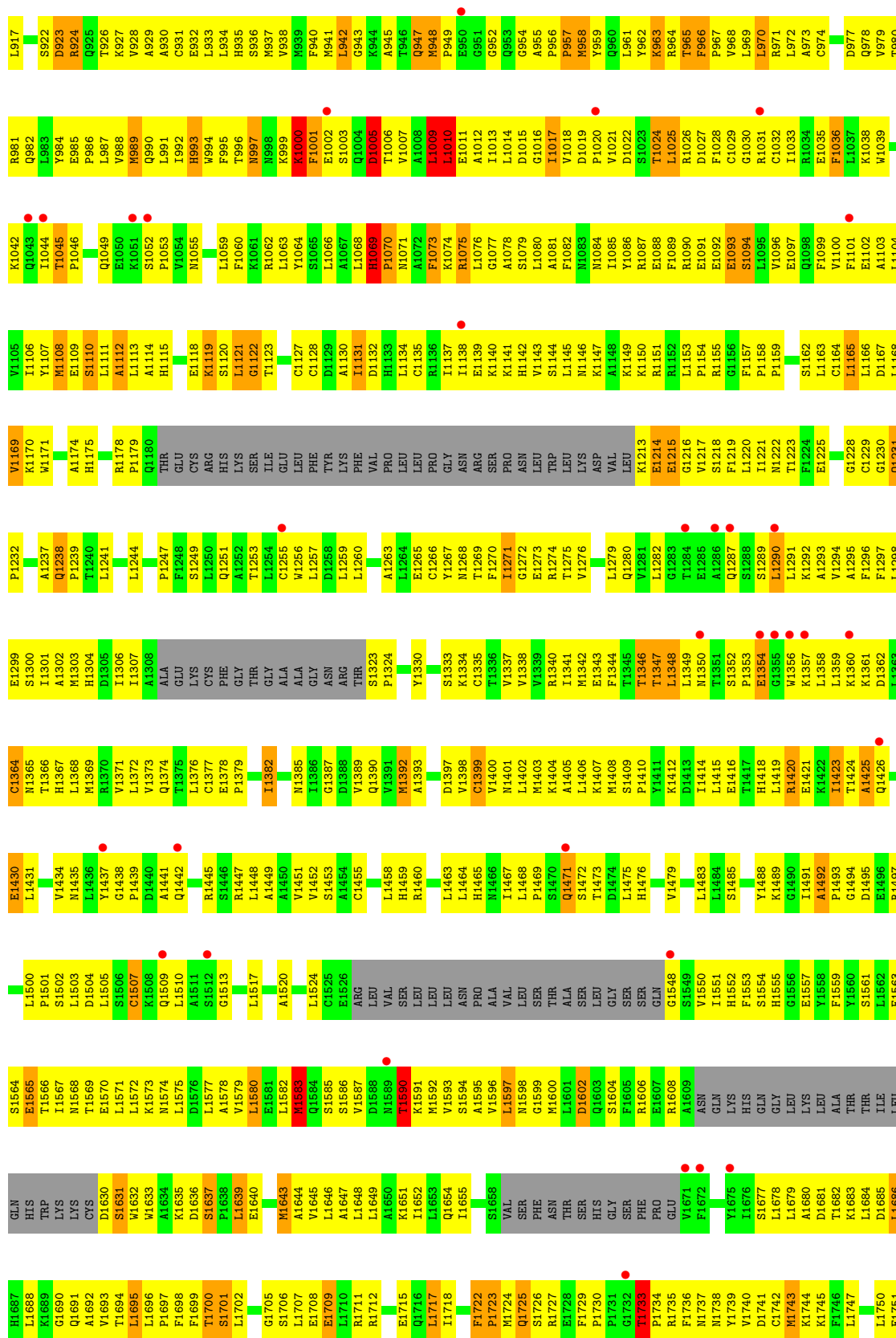


MSE	S3152	A3076	L3011	C2941	V2876	F2813	UNK	UNK	UNK	L2551	P2457	E2332
GLU	S3153	I3077	L3011	T2942	S2877	S2814	UNK	UNK	UNK	P2532	V2458	R2333
VAL	Q3154	L3078	T2943	T2943	A2878	Q2815	UNK	UNK	UNK	P2532	E2459	R2333
GLN	Q3155	E3079	T2944	T2944	A2879	L2816	UNK	UNK	UNK	P2533	E2460	N2335
GLU	P3156	L3080	S2945	S2945	C2880	L2817	UNK	UNK	UNK	N2534	F2461	L2336
GLU	R3159	H3081	S3015	S2949	L2881	L2818	UNK	UNK	UNK	T2535	V2462	L2337
GLU	L3160	Q3084	I3019	T2949	A2882	E2819	UNK	UNK	UNK	L2536	S2463	E2338
ASP	R3167	L3089	D3020	K2950	S2883	E2820	UNK	UNK	UNK	D2537	P2465	E2339
ASP	R3167	L3090	Q2951	T2952	L2884	F2822	UNK	UNK	UNK	L2540	S2466	S2340
ASP	R3170	L3091	L2952	S2955	Q2885	L2823	MSE	UNK	UNK	L2541	T2467	L2341
ASP	R3171	L3092	L2952	S2956	Q2886	F2823	UNK	UNK	UNK	L2542	T2468	C2342
ASP	R3172	L3092	L2952	S2957	P2887	K2824	UNK	UNK	UNK	L2543	R2470	E2343
ASP	R3173	L3092	L2952	S2958	V2888	T2825	UNK	UNK	UNK	L2544	C2469	L2344
ASP	R3174	L3092	L2952	S2959	Q2889	L2826	UNK	UNK	UNK	L2545	R2471	V2345
ASP	R3175	L3092	L2952	S2960	L2890	E2827	UNK	UNK	UNK	L2546	E2472	A2346
ASP	R3176	L3092	L2952	S2961	R2891	L2828	UNK	UNK	UNK	L2547	M2473	Q2348
ASP	R3177	L3092	L2952	S2962	L2892	K2830	UNK	UNK	UNK	L2548	Y2474	L2349
ASP	R3178	L3092	L2952	S2963	L2893	E2831	UNK	UNK	UNK	L2549	N2475	Q2350
ASP	R3179	L3092	L2952	S2964	L2894	L2832	UNK	UNK	UNK	L2550	L2476	Q2351
ASP	R3180	L3092	L2952	S2965	L2895	T2833	UNK	UNK	UNK	L2551	L2477	H2352
ASP	R3181	L3092	L2952	S2966	L2896	Q2834	UNK	UNK	UNK	L2552	M2478	Q2353
ASP	R3182	L3092	L2952	S2967	L2897	L2837	UNK	UNK	UNK	L2553	Y2479	N2354
ASP	R3183	L3092	L2952	S2968	L2898	L2838	UNK	UNK	UNK	L2554	L2480	T2355
ASP	R3184	L3092	L2952	S2969	L2899	E2840	UNK	UNK	UNK	L2555	H2481	M2356
ASP	R3185	L3092	L2952	S2970	L2900	R2841	UNK	UNK	UNK	L2556	F2482	E2357
ASP	R3186	L3092	L2952	S2971	L2901	N2842	UNK	UNK	UNK	L2557	R2485	D2358
ASP	R3187	L3092	L2952	S2972	L2902	L2843	UNK	UNK	UNK	L2558	Q2422	K2359
ASP	R3188	L3092	L2952	S2973	L2903	F2843	UNK	UNK	UNK	L2559	N2423	F2360
ASP	R3189	L3092	L2952	S2974	L2904	L2844	UNK	UNK	UNK	L2560	M2424	L2361
ASP	R3190	L3092	L2952	S2975	L2905	E2845	UNK	UNK	UNK	L2561	R2425	V2362
ASP	R3191	L3092	L2952	S2976	L2906	T2846	UNK	UNK	UNK	L2562	H2426	C2363
ASP	R3192	L3092	L2952	S2977	L2907	L2847	UNK	UNK	UNK	L2563	L2427	L2364
ASP	R3193	L3092	L2952	S2978	L2908	T2848	UNK	UNK	UNK	L2564	R2428	N2365
ASP	R3194	L3092	L2952	S2979	L2909	F2850	UNK	UNK	UNK	L2565	E2430	K2366
ASP	R3195	L3092	L2952	S2980	L2910	R2851	UNK	UNK	UNK	L2566	V2367	V2367
ASP	R3196	L3092	L2952	S2981	L2911	P2852	UNK	UNK	UNK	L2567	T2368	T2368
ASP	R3197	L3092	L2952	S2982	L2912	L2853	UNK	UNK	UNK	L2568	K2369	K2369
ASP	R3198	L3092	L2952	S2983	L2913	F2854	UNK	UNK	UNK	L2569	S2370	S2370
ASP	R3199	L3092	L2952	S2984	L2914	P2855	UNK	UNK	UNK	L2570	P2371	P2371
ASP	R3200	L3092	L2952	S2985	L2915	L2856	UNK	UNK	UNK	L2571	D2372	D2372
ASP	R3201	L3092	L2952	S2986	L2916	C2857	UNK	UNK	UNK	L2572	L2373	L2373
ASP	R3202	L3092	L2952	S2987	L2917	L2858	UNK	UNK	UNK	L2573	L2374	L2374
ASP	R3203	L3092	L2952	S2988	L2918	Q2859	UNK	UNK	UNK	L2574	A2375	A2375
ASP	R3204	L3092	L2952	S2989	L2919	L2860	UNK	UNK	UNK	L2575	F2378	F2378
ASP	R3205	L3092	L2952	S2990	L2920	L2861	UNK	UNK	UNK	L2576	M2379	M2379
ASP	R3206	L3092	L2952	S2991	L2921	S2862	UNK	UNK	UNK	L2577	V2382	V2382
ASP	R3207	L3092	L2952	S2992	L2922	C2863	UNK	UNK	UNK	L2578	F2383	F2383
ASP	R3208	L3092	L2952	S2993	L2923	L2864	UNK	UNK	UNK	L2579	L2384	L2384
ASP	R3209	L3092	L2952	S2994	L2924	H2865	UNK	UNK	UNK	L2580	L2385	L2385
ASP	R3210	L3092	L2952	S2995	L2925	A2866	UNK	UNK	UNK	L2581	L2386	L2386
ASP	R3211	L3092	L2952	S2996	L2926	L2867	UNK	UNK	UNK	L2582	P2387	P2387
ASP	R3212	L3092	L2952	S2997	L2927	L2868	UNK	UNK	UNK	L2583	L2451	L2451
ASP	R3213	L3092	L2952	S2998	L2928	L2869	UNK	UNK	UNK	L2584	F2388	F2388
ASP	R3214	L3092	L2952	S2999	L2929	S2870	UNK	UNK	UNK	L2585	H2390	H2390
ASP	R3215	L3092	L2952	S3000	L2930	L2871	UNK	UNK	UNK	L2586	G2391	G2391
ASP	R3216	L3092	L2952	S3001	L2931	D2872	UNK	UNK	UNK	L2587	V2392	V2392
ASP	R3217	L3092	L2952	S3002	L2932	P2873	UNK	UNK	UNK	L2588	L2456	L2456
ASP	R3218	L3092	L2952	S3003	L2933	L2874	UNK	UNK	UNK	L2589	N2456	N2456
ASP	R3219	L3092	L2952	S3004	L2934	A2875	UNK	UNK	UNK	L2590		
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ASP	R3221	L3092	L2952	S3006	L2936		UNK	UNK	UNK	L2592		
ASP	R3222	L3092	L2952	S3007	L2937		UNK	UNK	UNK	L2593		
ASP	R3223	L3092	L2952	S3008	L2938		UNK	UNK	UNK	L2594		
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ASP	R3227	L3092	L2952	S3012	L2942		UNK	UNK	UNK	L2598		
ASP	R3228	L3092	L2952	S3013	L2943		UNK	UNK	UNK	L2599		
ASP	R3229	L3092	L2952	S3014	L2944		UNK	UNK	UNK	L2600		
ASP	R3230	L3092	L2952	S3015	L2945		UNK	UNK	UNK	L2601		
ASP	R3231	L3092	L2952	S3016	L2946		UNK	UNK	UNK	L2602		
ASP	R3232	L3092	L2952	S3017	L2947		UNK	UNK	UNK	L2603		
ASP	R3233	L3092	L2952	S3018	L2948		UNK	UNK	UNK	L2604		
ASP	R3234	L3092	L2952	S3019	L2949		UNK	UNK	UNK	L2605		
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ASP	R3236	L3092	L2952	S3021	L2951		UNK	UNK	UNK	L2607		
ASP	R3237	L3092	L2952	S3022	L2952		UNK	UNK	UNK	L2608		
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ASP	R3244	L3092	L2952	S3029	L2959		UNK	UNK	UNK	L2615		
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ASP	R3252	L3092	L2952	S3037	L2967		UNK	UNK	UNK	L2623		
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ASP	R3258	L3092	L2952	S3043	L2973		UNK	UNK	UNK	L2629		
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ASP	R3271	L3092	L2952	S3056	L2986		UNK	UNK	UNK	L2642		
ASP	R3272	L3092	L2952	S3057	L2987		UNK	UNK	UNK	L2643		
ASP	R3273	L3092	L2952	S3058	L2988		UNK	UNK	UNK	L2644		
ASP	R3274	L3092	L2952	S3059	L2989		UNK	UNK	UNK	L2645		
ASP	R3275	L3092	L2952	S3060	L2990		UNK	UNK	UNK	L2646		
ASP	R3276	L3092	L2952	S3061	L2991		UNK	UNK	UNK	L2647		
ASP	R3277	L3092	L2952	S3062	L2992		UNK	UNK	UNK	L2648		
ASP	R3278	L3092	L2952	S3063	L2993		UNK	UNK	UNK	L2649		
ASP	R3279	L3092										



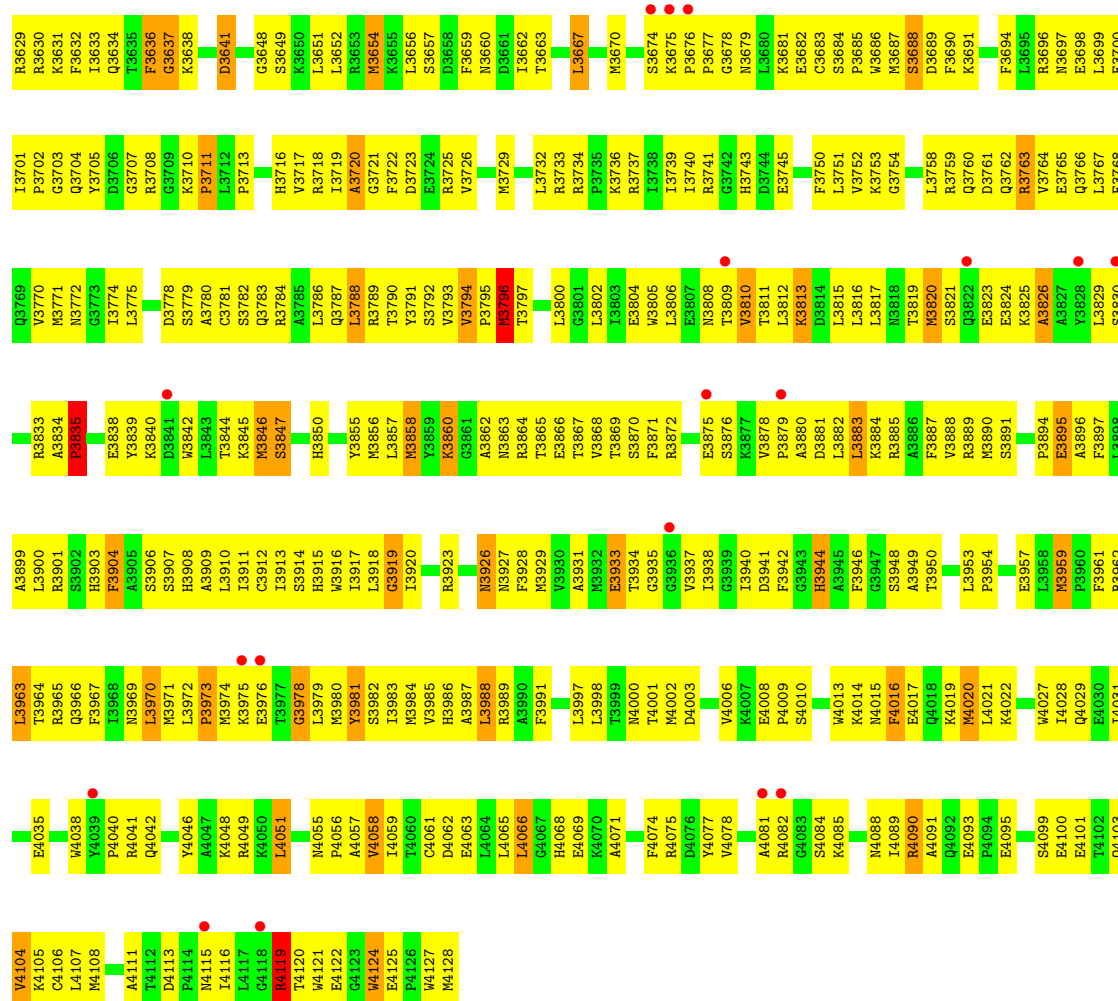
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit





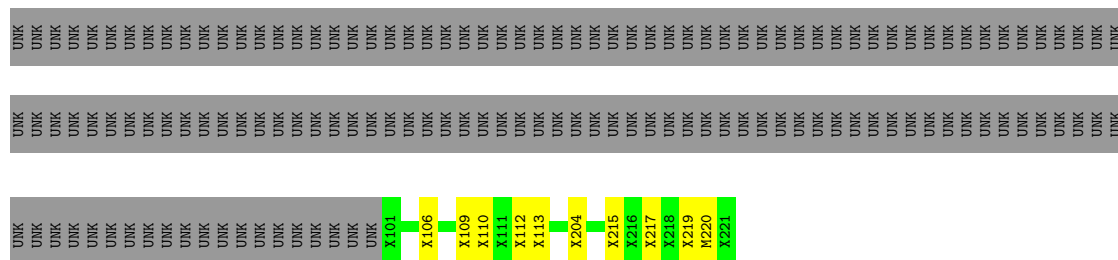






• Molecule 2: C-terminal fragment of KU80 (KU80ct194)

Chain K: 23% 5% 72%



• Molecule 2: C-terminal fragment of KU80 (KU80ct194)

Chain S: 23% 5% 72%





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 (1.10_2155: ???)	Depositor
R, R_{free}	0.386 , 0.437 0.388 , 0.439	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 , 188.9	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	0.83	EDS
Total number of atoms	59694	wwPDB-VP
Average B, all atoms (Å ²)	253.0	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	0.45	3/29743 (0.0%)	0.77	47/40014 (0.1%)
1	B	0.46	6/29743 (0.0%)	0.77	49/40014 (0.1%)
2	K	0.22	0/7	0.50	0/7
2	S	0.45	0/7	0.34	0/7
All	All	0.46	9/59500 (0.0%)	0.77	96/80042 (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
1	A	0	8
1	B	0	6
All	All	0	14

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1069	HIS	C-N	-9.65	1.16	1.34
1	B	3794	VAL	C-N	-8.26	1.18	1.34
1	B	1069	HIS	C-N	7.70	1.48	1.34
1	B	4124	TRP	CB-CG	-6.16	1.39	1.50
1	A	601	TRP	CB-CG	-5.75	1.40	1.50

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	LEU	CA-CB-CG	-10.22	91.80	115.30
1	B	3456	LEU	CA-CB-CG	9.67	137.54	115.30
1	B	1009	LEU	CB-CG-CD1	-9.35	95.11	111.00
1	A	3456	LEU	CA-CB-CG	9.33	136.75	115.30
1	B	726	LEU	CA-CB-CG	-9.12	94.32	115.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1323	SER	Peptide
1	A	2283	ASN	Peptide
1	A	2372	PRO	Peptide
1	A	411	PRO	Peptide
1	A	634	LEU	Peptide

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	29574	0	29642	3223	0
1	B	29574	0	29642	3283	0
2	K	273	0	70	9	0
2	S	273	0	73	8	0
All	All	59694	0	59427	6514	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 55.

The worst 5 of 6514 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:B:2183:HIS:O	1:B:2187:VAL:HB	1.30	1.31
1:B:662:LEU:O	1:B:666:PHE:HB2	1.28	1.30
1:A:3521:ILE:O	1:A:3525:TYR:HB2	1.32	1.28
1:B:3683:CYS:SG	1:B:3736:LYS:NZ	2.12	1.23
1:B:2167:PRO:O	1:B:2171:LEU:HB2	1.39	1.18

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	3631/4128 (88%)	2664 (73%)	724 (20%)	243 (7%)	1	18
1	B	3631/4128 (88%)	2657 (73%)	723 (20%)	251 (7%)	1	17
2	K	1/194 (0%)	1 (100%)	0	0	100	100
2	S	1/194 (0%)	1 (100%)	0	0	100	100
All	All	7264/8644 (84%)	5323 (73%)	1447 (20%)	494 (7%)	1	17

5 of 494 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ALA
1	A	76	ILE
1	A	147	PHE
1	A	167	PRO
1	A	184	VAL

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	3259/3384 (96%)	3089 (95%)	170 (5%)	23	50
1	B	3259/3384 (96%)	3084 (95%)	175 (5%)	22	50
2	K	-	1 (100%)	0	100	100
2	S	-	1 (100%)	0	100	100
All	All	6520/6768 (96%)	6175 (95%)	345 (5%)	22	50

5 of 345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1399	CYS
1	B	2788	SER
1	B	1602	ASP
1	B	1993	GLU
1	B	3120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2481	HIS
1	B	3251	ASN
1	B	3926	ASN
1	A	3081	HIS
1	A	3003	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 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	K	1
2	S	1
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	133:UNK	C	201:UNK	N	46.74
1	S	133:UNK	C	201:UNK	N	41.40
1	B	3794:VAL	C	3795:PRO	N	1.18
1	A	1069:HIS	C	1070:PRO	N	1.15

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	3551/4128 (86%)	0.25	220 (6%) 20 17	83, 248, 332, 443	0
1	B	3551/4128 (86%)	0.30	240 (6%) 17 14	117, 251, 358, 507	0
2	K	0/194	-	-	-	-
2	S	0/194	-	-	-	-
All	All	7102/8644 (82%)	0.28	460 (6%) 18 15	83, 249, 343, 507	0

The worst 5 of 460 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	LYS	12.8
1	B	31	GLY	9.6
1	B	1355	GLY	9.6
1	B	145	ASP	9.1
1	A	126	PRO	8.7

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 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.