



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:22 AM UTC

PDB ID : 5LUQ / pdb_00005luq
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

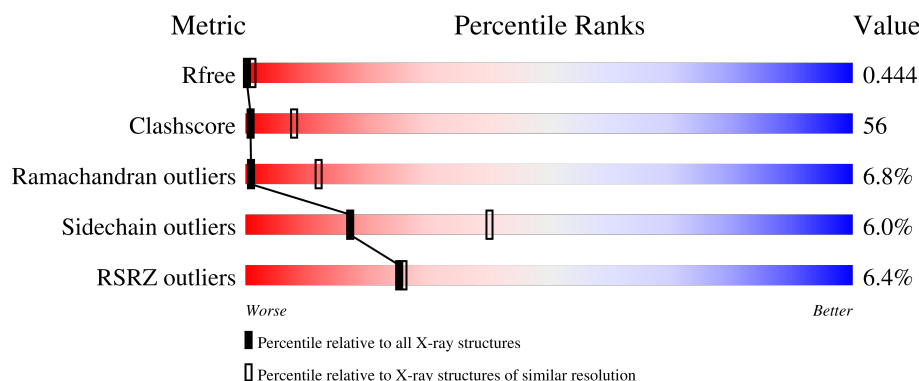
1 Overall quality at a glance

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	4128	5% 28% 54% 8% 10%
1	B	4128	6% 28% 54% 8% 10%
2	K	194	23% 5% 72%
2	S	194	23% 5% 72%

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

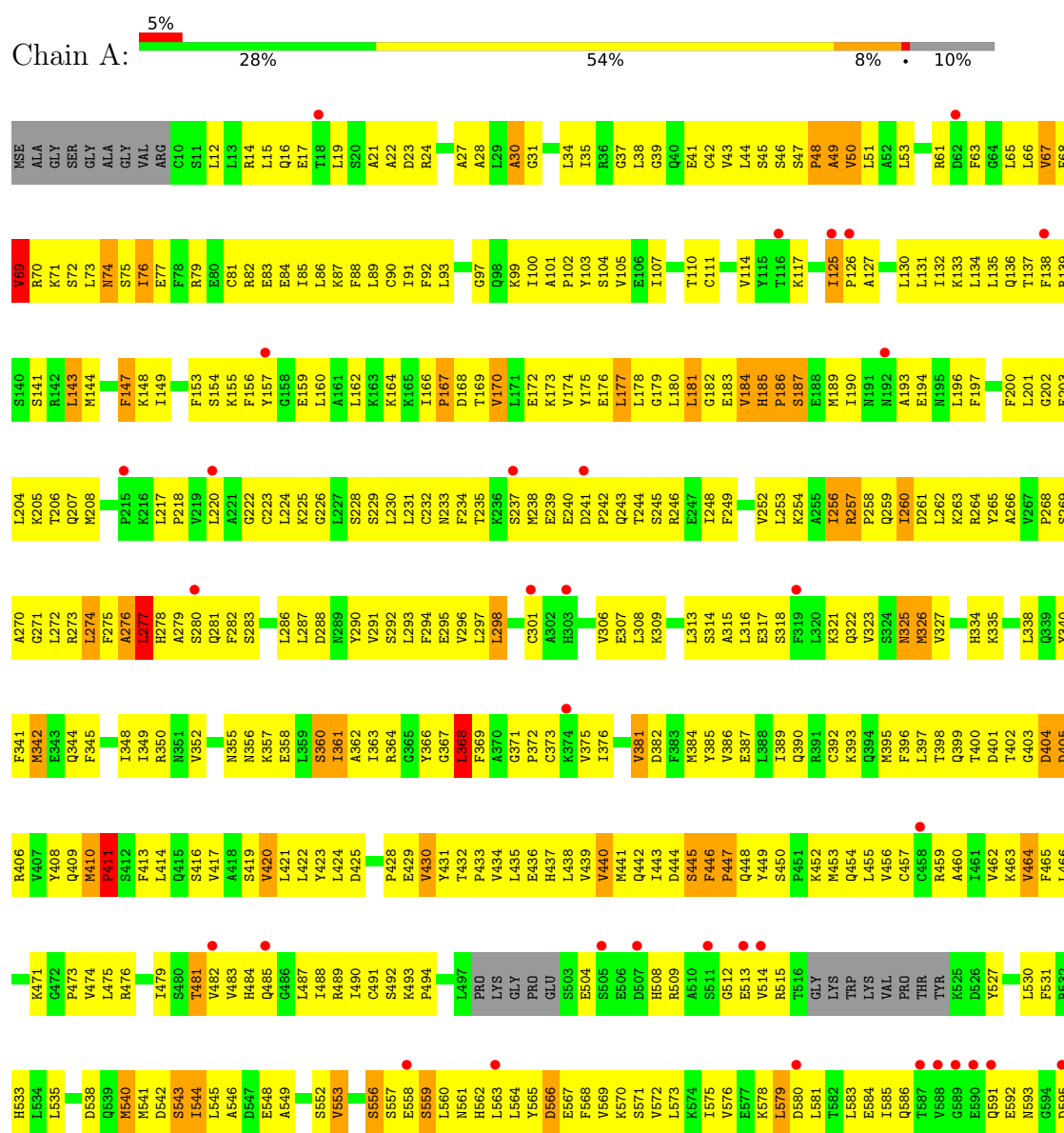
- Molecule 2 is a protein called C-terminal fragment of KU80 (KU80ct194).

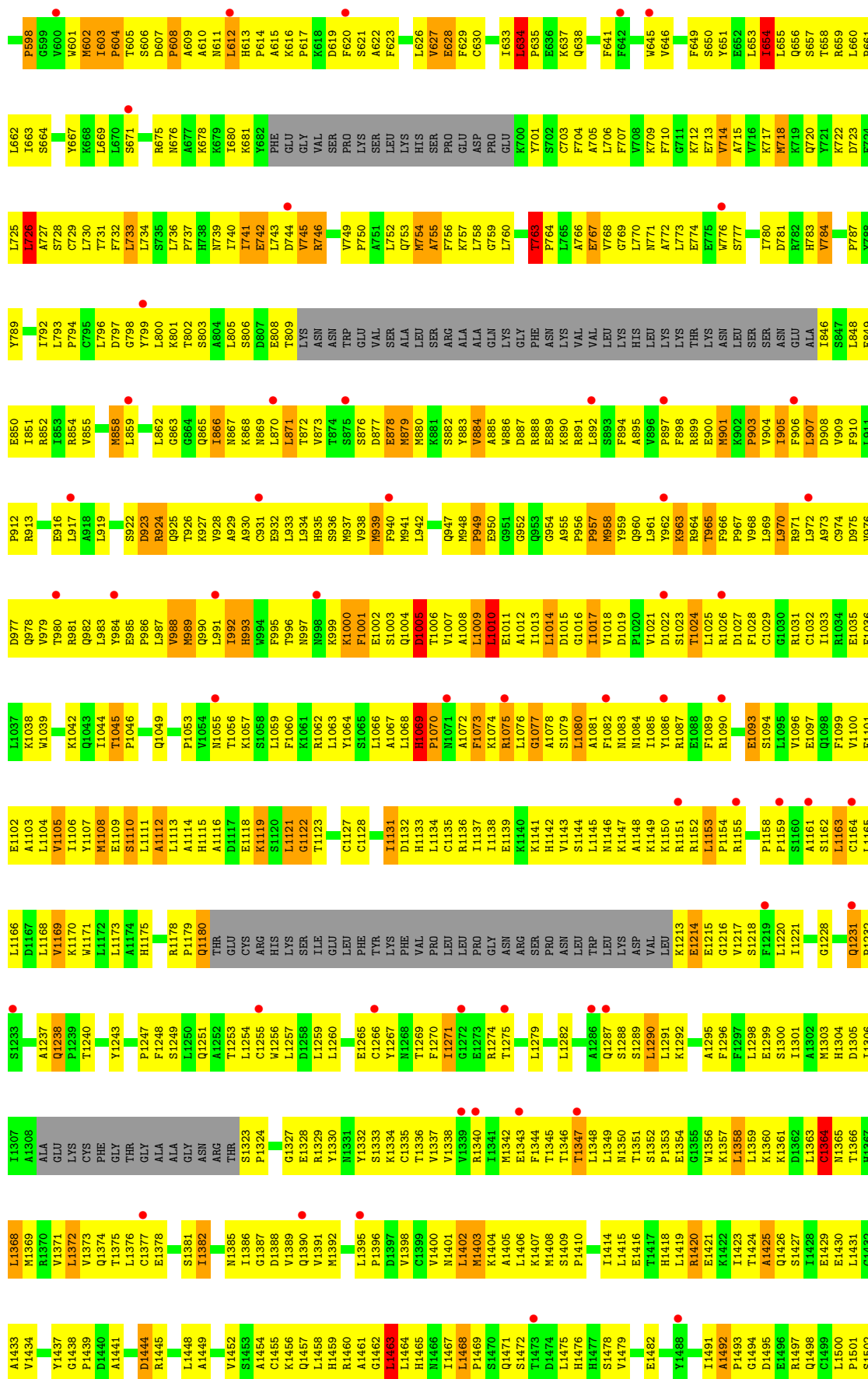
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			
2	S	54	Total	C	N	O	Se	0	0	0
			273	164	54	54	1			

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.

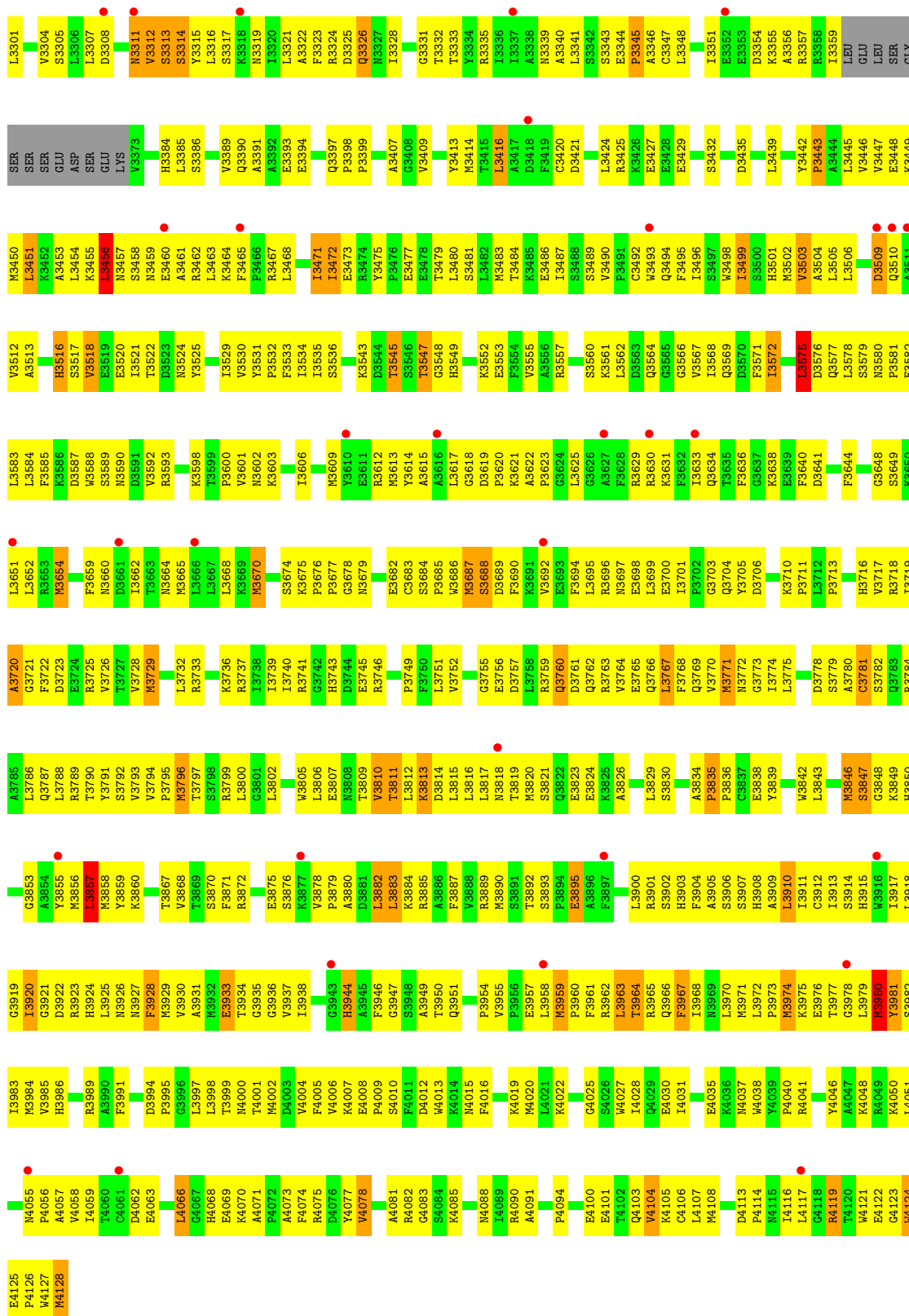
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit



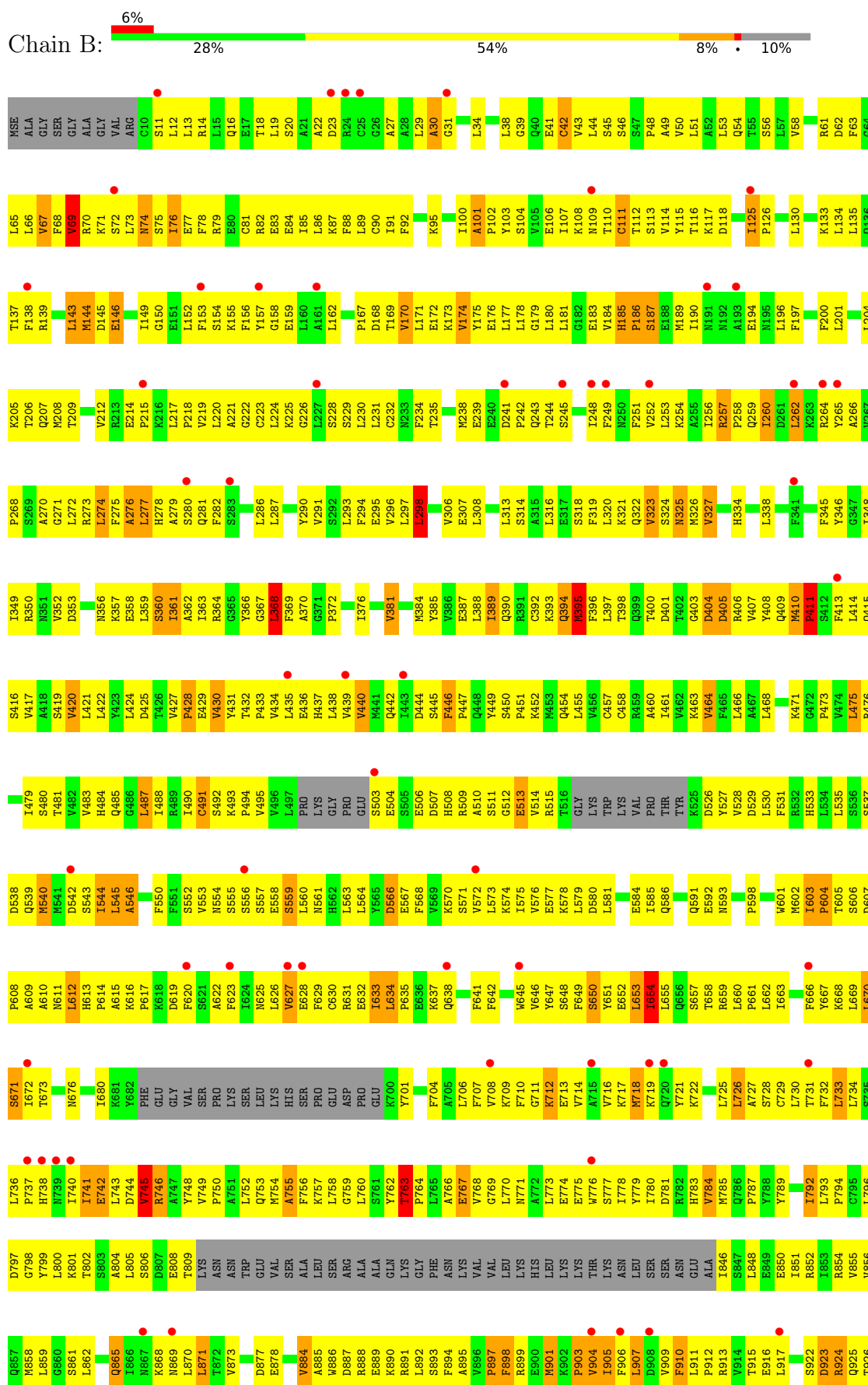








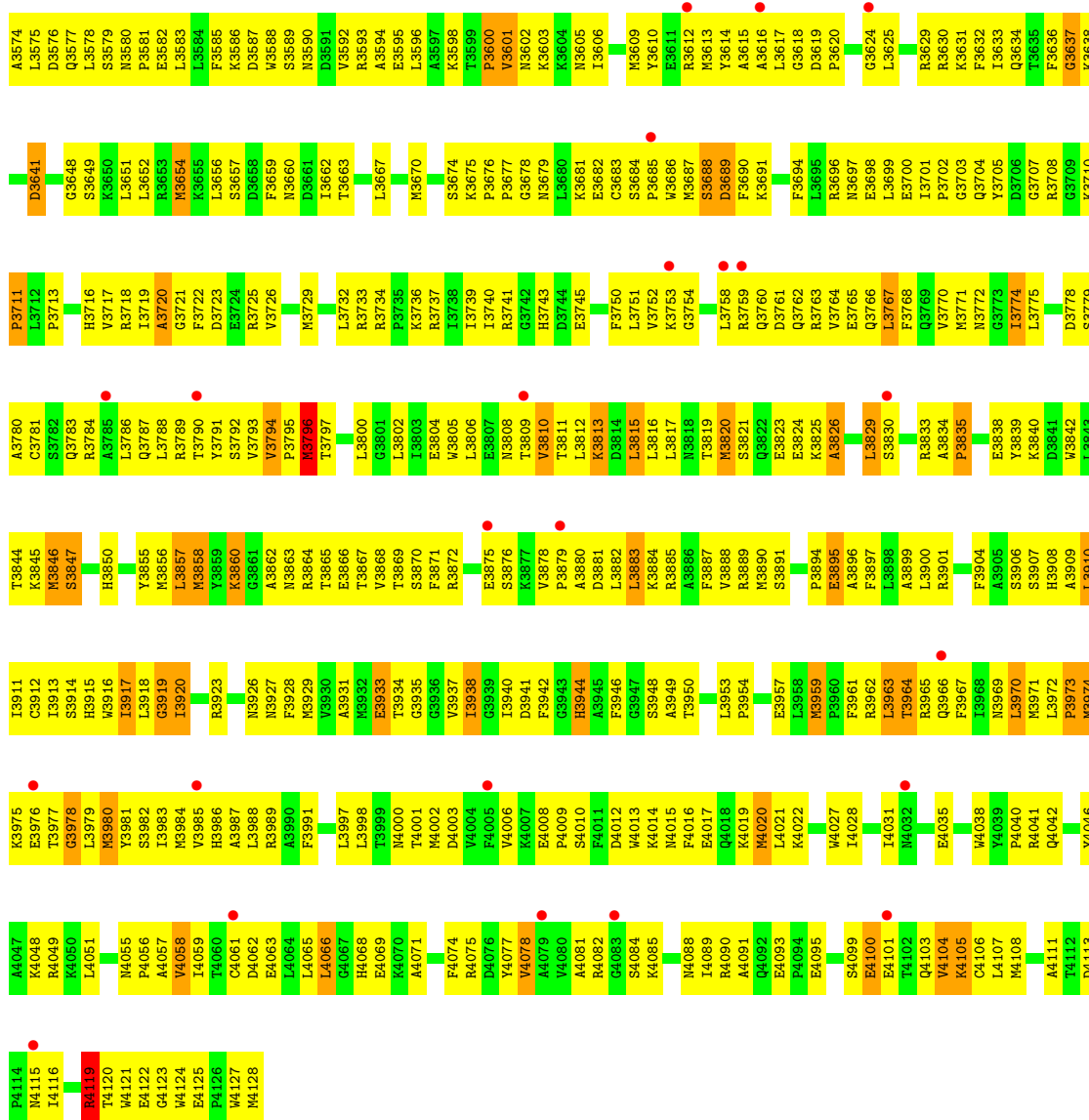
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit



L1696	P1697	F1698	F1699	T1700	S1701	L1702	G1705	S1706	L1707	E1708	E1709	L1710	R1711	R1712	L1713	L1714	E1715	L1716	L1717	L1718	F1722	P1723	H1724	Q1725	S1726	R1727	E1728	F1729	P1730	P1731	T1732	T1733	P1734	R1735	F1736	N1737	N1738	Y1739	D1740	D1741	C1742	M1743	K1744	K1745	F1746	L1747	L1750	E1751	L1752	L1753	Q1754	S1755	P1756	M1757	L1758	L1759			
W1632	L1633	A1634	K1635	L1636	S1637	P1638	L1639	E1640	M1643	A1644	V1645	L1646	A1647	L1648	L1649	A1650	K1651	L1652	L1653	Q1654	I1655	V1658	VAL	SER	PHE	ASN	THR	SER	HIS	GLY	SER	PHE	PRO	GLU	V1671	V1677	H1678	L1679	A1680	D1681	T1682	K1683	L1684	D1685	L1686	H1687	L1688	K1689	G1690	S1691	A1692	P1693	T1694	L1695					
L1572	K1573	N1574	L1575	D1576	L1577	A1578	V1579	L1580	E1581	L1582	M1583	L1584	S1585	S1586	V1587	D1588	M1589	T1590	K1591	M1592	V1593	S1594	A1595	V1596	L1597	N1598	S1599	M1600	L1601	D1602	G1603	S1604	F1605	R1606	E1607	R1608	A1609	ASN	GLN	L1610	H1611	L1612	L1613	F1614	L1615	L1616	L1617	L1618	L1619	L1620	D1630	S1631							
S1506	C1507	K1508	Q1509	L1510	G1513	A1514	L1515	A1516	A1517	A1520	L1521	C1522	ARG	LEU	VAL	SER	LEU	LEU	LEU	LEU	S1525	VAL	SER	GLY	SER	SER	GLN	G1548	S1549	V1550	H1551	H1552	F1553	S1554	H1555	G1556	E1557	Y1558	F1559	V1560	S1561	L1562	F1563	S1564	E1565	T1566	L1567	N1568	T1569	E1570	L1571								
A1441	Q1442	V1443	D1444	S1445	R1446	R1447	L1448	A1449	A1450	V1451	S1452	V1453	A1454	C1455	L1458	H1459	R1460	A1461	G1462	L1463	L1464	Q1465	H1466	T1467	D1474	L1475	H1476	V1479	L1483	L1484	S1485	L1486	V1487	K1488	G1489	G1490	I1491	A1492	P1493	G1494	D1495	E1496	R1497	L1500	P1501	S1502	L1503	P1439	L1505										
Q1374	T1375	L1376	C1377	E1378	P1379	L1382	N1385	L1386	G1387	D1388	V1389	Q1390	V1391	M1392	A1393	D1397	V1398	C1399	V1400	N1401	L1402	M1403	K1404	A1405	L1406	K1407	L1408	S1409	P1410	Y1411	K1412	D1413	L1414	L1415	T1417	H1418	L1419	R1420	E1421	K1422	T1423	T1424	A1425	Q1426	E1430	L1431	V1434	L1435	Y1437	G1438	P1439	D1440							
ALA	GLU	LYS	CYS	PHE	GLY	THR	GLY	ALA	ALA	GLY	ASN	ARG	THR	S1323	P1324	Y1330	S1333	K1334	C1335	T1336	V1337	V1338	V1339	R1340	T1341	M1342	E1343	F1344	T1345	T1346	T1347	L1348	N1350	T1351	S1352	P1353	E1354	G1355	V1356	K1357	L1358	K1360	K1361	D1362	C1364	M1365	T1366	H1367	L1368	M1369	R1370	V1371	L1372	V1373					
L1244	P1247	F1248	S1249	L1250	Q1251	A1252	T1253	L1254	C1255	W1256	L1257	D1258	L1259	L1260	L1261	A1262	A1263	L1264	C1265	Y1267	N1268	T1269	F1270	I1271	L1272	L1273	R1274	T1275	V1276	L1279	Q1280	V1281	L1282	Q1287	S1288	S1289	L1290	L1291	K1292	A1293	V1294	A1295	F1296	F1297	L1298	E1299	S1300	I1301	A1302	H1303	M1304	D1305	I1306	I1307	A1308				
P1179	Q1180	THR	GLU	CYS	ARG	HIS	LYS	SER	ILE	GLU	LEU	PHE	TTR	S1323	LYS	PHE	VAL	PRO	LEU	LEU	PRO	ASN	GLY	ASN	ARG	SER	PRO	LEU	VAL	K1213	E1214	E1215	G1216	V1217	S1218	F1219	L1220	I1221	N1222	T1223	F1224	E1225	G1228	C1229	Q1231	P1232	Q1233	C1234	A1237	Q1238	P1239	T1241	L1241						
L1113	A1114	H1115	E1118	K1119	S1120	L1121	G1122	T1123	C1127	K1128	D1129	A1130	T1131	L1132	H1133	L1134	C1135	R1136	T1137	I1138	E1139	K1140	K1141	H1142	V1143	TRP	L1144	L1145	N1146	K1147	A1148	K1149	K1150	R1151	L1152	L1153	P1154	L1155	G1156	F1157	P1158	P1159	S1162	L1163	C1164	L1165	L1166	D1167	L1168	V1169	K1170	W1171	A1174	H1175	R1178				
S1052	V1053	Y1054	N1055	L1059	F1060	K1061	L1062	L1063	S1064	L1065	L1066	A1067	L1068	H1069	P1070	N1071	A1072	K1073	L1074	R1075	L1076	G1077	A1078	S1079	L1080	A1081	F1082	N1083	N1084	I1085	Y1086	R1087	E1088	E1089	R1090	E1091	E1092	E1093	S1094	L1095	V1096	E1097	Q1098	F1099	V1100	F1101	E1102	A1103	L1104	V1105	T1106	Y1107	M1108	E1109	S1110	L1111	A1112		
V988	M989	Q990	L991	I992	H993	W994	F995	T996	N997	N998	N999	K1000	F1001	E1002	S1003	L1004	D1005	T1006	A1007	L1008	L1009	L1010	E1011	A1012	L1013	L1014	L1015	P956	P957	L1016	V1017	L1018	D1019	P1020	V1021	D1022	S1023	T1024	L1025	D1027	F1028	C1029	G1030	R1031	C1032	I1033	R1034	E1035	F1036	L1037	D1038	W1039	K1042	Q1043	L1044	T1045	P1046	Q1049	
K927	V928	A929	A930	C931	E932	L933	L934	H935	S936	N937	V938	M939	F940	M941	L942	G943	K944	A945	T946	Q947	M948	P949	G952	Q953	G954	A955	P956	P957	L958	M959	Y960	Q961	L961	Y962	K963	R964	T965	F966	P967	V968	L969	L970	R971	L972	A973	C974	D975	V976	D977	Q978	V979	T980	R981	Q982	L983	Y984	E985	P986	L987

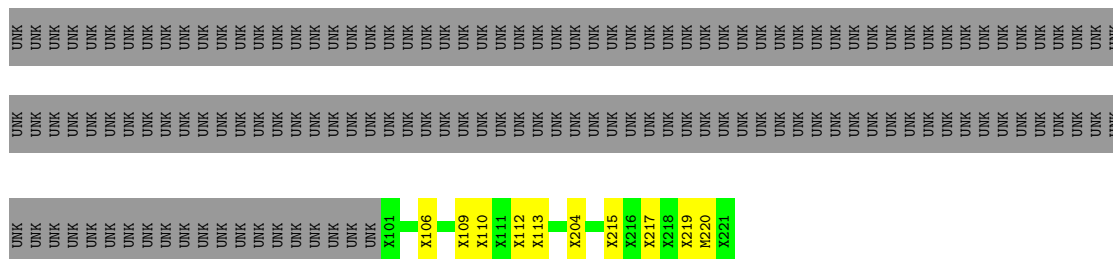






- Molecule 2: C-terminal fragment of KU80 (KU80ct194)

Chain K: 23% 5% 72%



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

Chain S: 23% 5% 72%

[illegible]

UNK

[illegible]

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 , 0.444	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)	0.31 , 290.8	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	0.44	3/29743 (0.0%)	0.85	24/40014 (0.1%)
1	B	0.44	4/29743 (0.0%)	0.84	25/40014 (0.1%)
2	K	0.22	0/7	0.43	0/7
2	S	0.44	0/7	0.39	0/7
All	All	0.44	7/59500 (0.0%)	0.84	49/80042 (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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3847	SER	CA-C	-12.16	1.46	1.52
1	A	1069	HIS	C-N	-7.66	1.16	1.33
1	B	146	GLU	CA-C	-6.88	1.49	1.52
1	B	3794	VAL	C-N	-6.53	1.18	1.33
1	B	1069	HIS	C-N	6.43	1.48	1.33

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1998	MSE	N-CA-C	-9.53	99.77	111.40
1	B	1880	MSE	N-CA-C	-7.59	103.01	111.28
1	B	2371	PHE	CA-C-N	-7.41	112.74	120.38
1	B	2371	PHE	C-N-CA	-7.41	112.74	120.38
1	A	3980	MSE	N-CA-C	-7.35	103.57	112.54

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	3318	0
1	B	29574	0	29642	3380	0
2	K	273	0	70	9	0
2	S	273	0	73	9	0
All	All	59694	0	59427	6706	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 56.

The worst 5 of 6706 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	12
1	B	3631/4128 (88%)	2657 (73%)	723 (20%)	251 (7%)	1	11
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	12

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%)	3064 (94%)	195 (6%)	17	40
1	B	3259/3384 (96%)	3062 (94%)	197 (6%)	17	40
2	K	-	1 (100%)	0	100	100
2	S	-	1 (100%)	0	100	100
All	All	6520/6768 (96%)	6128 (94%)	392 (6%)	17	40

5 of 392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	898	PHE
1	B	1950	SER
1	B	970	LEU
1	B	1347	THR
1	B	2137	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	GLN
1	B	1238	GLN
1	B	3154	GLN
1	B	351	ASN
1	B	508	HIS

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

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%)	0.64	210 (5%) 28 28	83, 248, 332, 443	0
1	B	3551/4128 (86%)	0.72	246 (6%) 23 24	117, 251, 358, 507	0
2	K	0/194	-	-	-	-
2	S	0/194	-	-	-	-
All	All	7102/8644 (82%)	0.68	456 (6%) 25 26	83, 249, 343, 507	0

The worst 5 of 456 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3976	GLU	8.1
1	A	591	GLN	8.0
1	A	1586	SER	7.3
1	B	157	TYR	7.3
1	B	1874	TYR	7.2

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.