



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2017 – 10:35 PM EST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

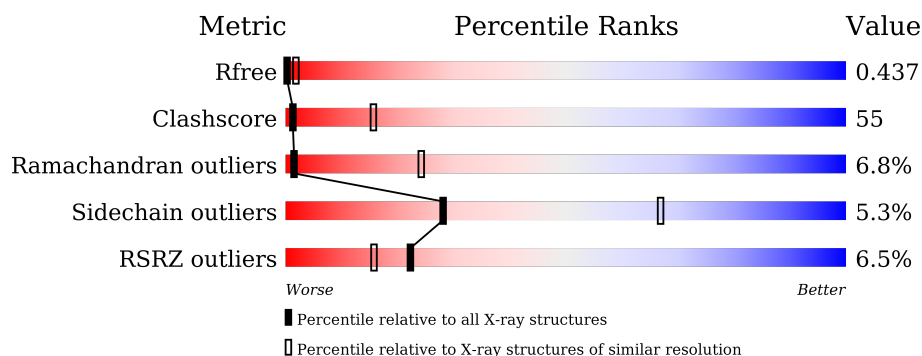
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	4128	
2	K	194	
2	S	194	

## 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

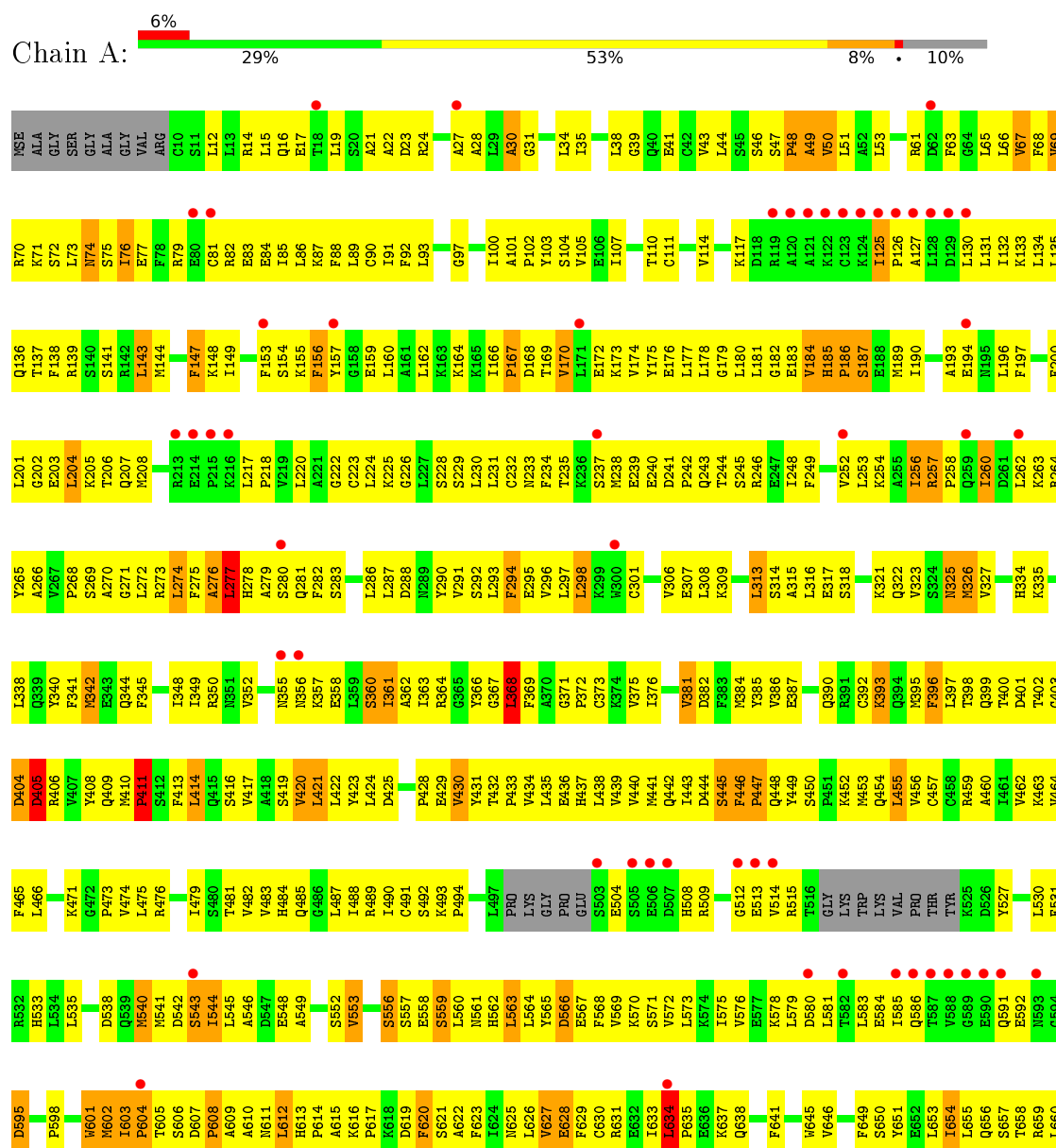
- Molecule 2 is a protein called C-terminal fragment of KU80 (KU80ct194).

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

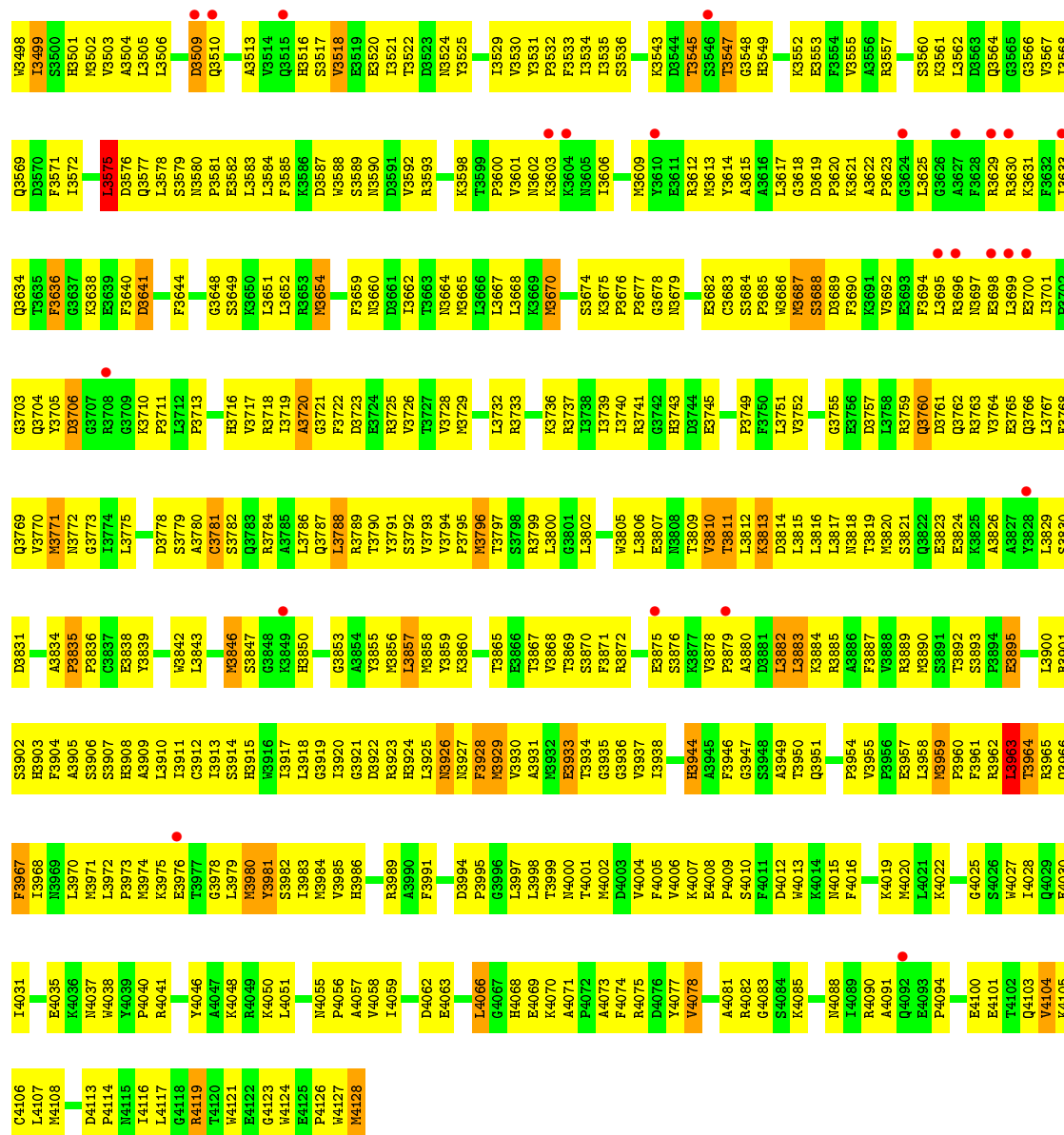
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit



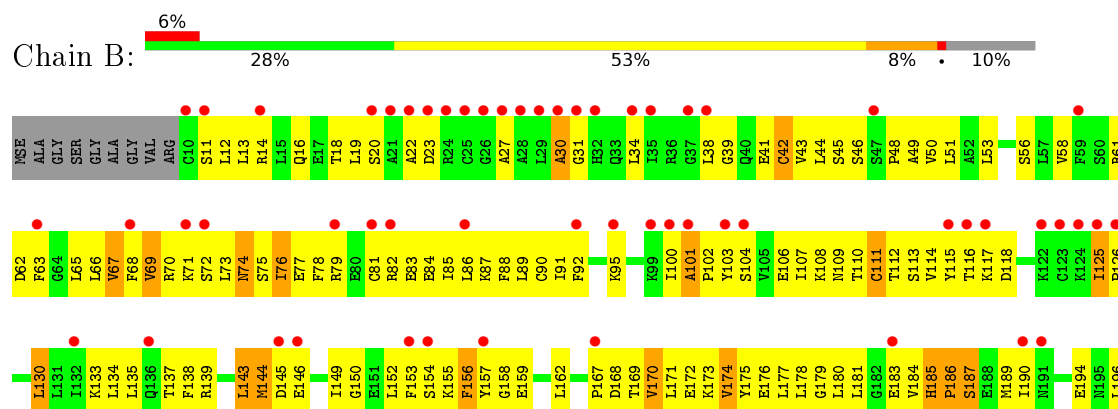
E1565	L1503	V1434	M1369	A1308	P1289	D1467	A1103	L1037	D977	P912	E849	P787	D723	P661
T1566	D1504	M1435	R1370	ALA	T1240	L1168	L1104	K1038	Q978	R913	E850	L788	E724	L662
L1567	L1505	L1436	V1371	GLU	Y1243	V1169	V1105	W1039	V979	R851	R852	Y789	L725	S664
M1568	S1506	Y1437	L1372	LVS	Y1243	L1170	LVS	LVS	T980	E916	R853	L793	L726	Y667
L1569	C1507	G1438	V1373	CYS	P1247	M1171	M1108	K1042	R981	Q917	I854	R794	S728	K668
E1570	K1508	P1439	V1374	PHE	F1248	L1172	E1109	Q1043	Q982	Q918	R854	C795	C729	L689
L1571	Q1509	D1440	T1375	GLY	S1249	L1173	E1109	L1044	L983	L919	L796	L796	L730	K668
L1572	L1510	A1441	L1376	THR	A1174	A1174	S1110	T1045	L984	S922	M858	D797	L731	L671
L1573	L1511	A1442	L1377	GLY	L1250	A1175	L1111	P1046	P986	L859	L859	L799	F732	L672
M1574	S1512	D1444	E1378	ALA	Q1251	R1178	A1112	Q1049	L987	L862	L862	L733	F733	L672
D1576	G1513	L1445	E1378	GLY	T1253	A1252	L1113	P1053	L988	L862	L862	L734	L734	R675
L1577	G1513	L1448	E1378	ASN	L1254	Q1180	H1115	P1053	Q989	G863	G863	L736	L736	M676
A1578	L1517	A1449	I1382	ARG	C1255	THR	A1116	P1053	Q990	Q864	Q864	P737	P737	A677
L1582	A1518	V1452	M1385	THR	W1256	GLU	D1117	T1056	L991	R928	Q865	L800	L736	R675
M1583	F1519	I1386	I1386	CYS	L1257	CYS	E1118	T1056	L992	R928	Q866	K801	L736	M676
L1584	A1520	G1387	D1387	P1324	D1258	ARG	L1119	S1058	R993	R929	I866	L804	L736	A677
C1585	A1454	D1388	D1388	P1324	D1258	ARG	L1119	S1058	R993	R929	I866	L804	L736	A677
S1585	V1389	V1389	V1389	HIS	L1259	HIS	S1120	S1058	R993	R929	I866	L804	L736	A677
S1586	Q1390	Q1390	Q1390	LVS	L1260	LVS	L1121	F1060	R995	R929	I866	L804	L736	A677
S1587	R1391	R1391	R1391	ILE	L1260	LVS	G1122	K1061	R996	R929	I866	L804	L736	A677
D1588	L1458	L1458	L1458	GLU	E1285	ILE	T1123	K1061	R997	R929	I866	L804	L736	A677
M1589	H1459	H1459	H1459	GLU	Y1287	GLU	C1127	L1063	R998	R929	I866	L804	L736	A677
T1590	ARG	R1460	L1395	PHE	N1288	THR	C1128	S1065	K1000	R929	I866	L804	L736	A677
L1591	LEU	A1461	P1396	THR	T1269	LVS	I1131	L1066	K1001	R929	I866	L804	L736	A677
M1592	VAL	G1462	D1397	LVS	F1270	LVS	I1131	A1067	E1002	R929	I866	L804	L736	A677
S1593	SER	L1463	C1398	PHE	I1271	PHE	D1132	L1068	Q1003	R929	I866	L804	L736	A677
S1594	LEU	L1464	C1398	VAL	I1271	VAL	H1133	H1069	Q1004	R929	I866	L804	L736	A677
L1597	LEU	H1465	V1400	PRO	T1274	PRO	L1134	P1070	D1005	R929	I866	L804	L736	A677
M1598	LEU	H1466	N1401	LEU	T1275	LEU	C1135	N1071	T1006	R929	I866	L804	L736	A677
G1599	ASN	L1467	L1402	V1338	V1276	PRO	R1136	A1072	V1007	R929	I866	L804	L736	A677
M1600	PRO	L1468	M1403	V1340	G1277	PRO	L1137	F1073	A1008	R929	I866	L804	L736	A677
L1601	ALA	P1469	K1404	I1341	A1278	GLY	L1138	K1074	L1009	R929	I866	L804	L736	A677
D1602	VAL	S1470	A1405	M1342	L1279	ASN	K1139	R1075	E950	R929	I866	L804	L736	A677
Q1603	LEU	Q1471	L1406	E1343	L1279	ARG	K1140	L1076	E951	R929	I866	L804	L736	A677
S1604	SER	S1472	K1407	F1344	L1279	ASN	K1141	G1077	E951	R929	I866	L804	L736	A677
F1605	ALA	L1475	M1408	T1345	L1282	PRO	H1142	A1078	I1013	R929	I866	L804	L736	A677
L1606	SER	H1476	S1409	T1346	L1283	ASN	V1143	S1079	L1014	R929	I866	L804	L736	A677
E1607	LEU	H1477	P1410	T1347	L1284	LEU	L1144	L1080	D1015	R929	I866	L804	L736	A677
A1608	GLY	S1478	L1414	L1348	E1285	THR	L1145	A1081	G1016	R929	I866	L804	L736	A677
A1609	SER	V1479	L1415	N1349	Q1287	LEU	M1146	F1082	T1017	R929	I866	L804	L736	A677
ASN	SER	E1482	E1416	T1351	S1289	ASP	A1148	N1084	D1019	R929	I866	L804	L736	A677
GLN	GLN	E1482	T1447	S1352	L1290	VAL	K1149	I1085	P1020	R929	I866	L804	L736	A677
LVS	LVS	E1482	H1418	P1353	L1291	LEU	K1150	Y1086	V1021	R929	I866	L804	L736	A677
HIS	G1548	Y1488	L1419	E1354	K1292	K1213	R1151	R1087	D1022	R929	I866	L804	L736	A677
GLN	S1549	K1489	R1420	G1355	L1292	E1214	L1152	E1088	S1023	R929	I866	L804	L736	A677
HIS	V1550	G1490	E1421	K1357	L1296	E1215	L1153	F1089	T1024	R929	I866	L804	L736	A677
GLY	L1551	I1491	K1422	K1357	F1296	G1216	P1154	R1090	L1025	R929	I866	L804	L736	A677
LEU	H1552	A1492	K1423	L1358	F1297	V1217	R1155	R1090	R1026	R929	I866	L804	L736	A677
LVS	S1554	P1493	T1424	L1359	L1298	S1218	P1158	E1093	D1027	R929	I866	L804	L736	A677
LEU	L1555	G1494	A1426	K1360	E1299	F1220	P1159	S1094	D1028	R929	I866	L804	L736	A677
ALA	G1556	D1495	Q1426	K1361	S1300	L1220	P1160	L1095	C1029	R929	I866	L804	L736	A677
THR	E1557	E1496	S1427	D1362	I1301	I1221	S1160	V1096	G1030	R929	I866	L804	L736	A677
THR	E1557	E1496	S1427	D1362	I1301	I1221	S1160	V1096	G1030	R929	I866	L804	L736	A677
ILE	F1558	Q1497	E1428	C1364	M1303	Q1231	A1161	Q1097	R1031	R929	I866	L804	L736	A677
LEU	F1559	Q1498	E1430	C1364	M1303	Q1231	A1161	Q1097	R1031	R929	I866	L804	L736	A677
GLN	Y1560	C1499	E1430	M1365	H1304	P1232	S1162	Q1098	C1032	R929	I866	L804	L736	A677
HIS	L1500	H1501	L1431	T1366	D1305	P1232	L1163	F1099	I1033	R929	I866	L804	L736	A677
TRP	F1563	C1432	C1432	H1367	I1306	A1237	L1165	V1100	R1034	R929	I866	L804	L736	A677
LVS	S1564	S1502	A1433	L1368	I1307	Q1238	L1166	E1102	F1036	R929	I866	L804	L736	A677







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



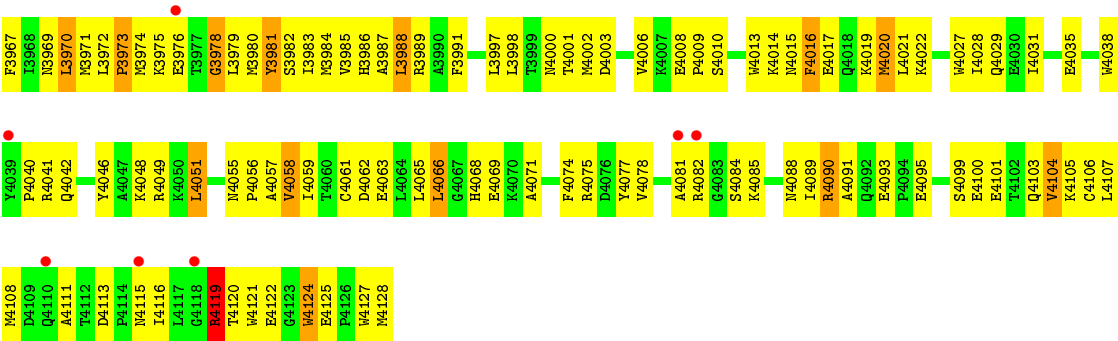


Y1107	M1108	E1109	S1110	L1111	A1112	L1113	A1114	H1115	E1118	K1119	S1120	L1121	T1122	C1127	D1128	D1129	A1130	I1131	D1132	H1133	L1134	C1135	I1136	L1137	I1138	E1139	K1140	K1141	L1142	V1143	S1144	L1145	N1146	K1147	A1148	K1149	K1150	R1151	L1152	L1153	P1154	R1155	G1156	F1157	P1158	P1159	S1162	L1163	C1164	L1165	L1166	D1167	V1168	K1170												
I1044	Y984	E985	P986	L987	V988	M989	Q990	L991	Y992	H993	Y994	F995	T996	N997	R998	K999	L1000	F1001	E1002	S1003	Q1004	D1005	T1006	V1007	A1008	L1009	L1010	I1011	A1012	R1013	L1014	D1015	G1016	I1017	P1018	F1082	H1083	D1019	N988	L1019	P1020	V1021	D1022	T1023	L1024	L1025	R1026	L1027	F1028	C1029	G1030	L1031	C1032	I1033	H1034	E1035	F1036	L1037	F1101	L1102	W1039	K1042	Q1043			
S922	R852	L853	R854	R855	V856	Q857	L858	G859	S860	L861	E862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917
Y792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L475	R476	L479	S480	T481	Y482	H483	R484	Q485	G486	L424	Y425	L426	P428	E429	V430	Y431	T432	P433	V434	L435	E436	H437	G371	P372	I376	V381	M384	Y385	V386	E387	L388	I389	Q390	S391	C392	K393	Q394	R395	F396	T397	T398	Q399	T400	D401	S402	G403	D404	D405	R406	V407	Y408	Q409	M410	P411					
L792	T731	F666	I603	L534	P473	V474	L																																																											

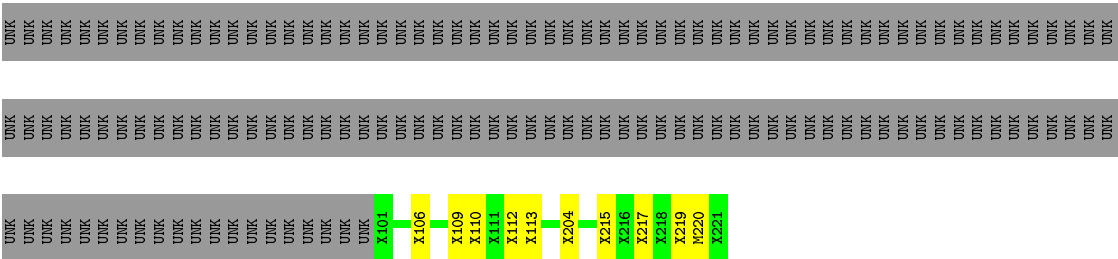
E2012	V1951	K1886	THR	Q1891	TRP	T1566	P1501	V1434	T1366	I1301	A1237	W1171
E2013	I1952	D1887	LEU	A1692	LYS	I1567	S1502	V1435	H1367	A1302	Q1238	
A2014	C1953	D1888	LEU	V1693	LYS	T1568	D1503	L1436	L1368	M1303	P1239	A1174
A2015	V1889	L1758	TRP	V1694	CYS	M1569	D1504	L1437	M1369	H1304	T1240	H1175
N2016	V1955	E1760	HIS	L1695	D1630	E1570	L1506	G1438	A1370	D1305	L1241	
G2017	F1956	L1761	CYS	L1696	S1631	L1571	S1507	G1439	V1371	I1306	L1244	R1178
D2018	M1957	M1762	SER	F1697	V1632	K1572	K1508	P1439	L1372	P1179		
S2019	E1958	T1763	LEU	F1698	V1633	K1573	C1507	D1440	V1373	A1908		
	K1895	GLU	ASP	F1699	A1634	M1574	Q1509	Q1441	Q1374	ALA	P1247	Q1180
P2022	K1960	VAL	ALA	T1700	D1636	L1575	A1511	Q1442	L1376	GLY	F1248	GLU
S2023	F1961	LEU	LEU	S1701	K1636	D1576	G1512	Q1443	L1377	LYS	S1249	CYS
	Y1962	ARG	ARG	L1702	S1637	L1577	G1513	R1445	C1377	CYS	L1250	ARG
S2026	Q1963	GLU	GLU	G1705	L1639	A1578		R1446	E1378	PHE	Q1251	HIS
S2027	G1964	ARG	ARG	S1706	L1640	V1579	L1517	R1447	P1379	GLY	A1252	LYS
L2028	F1965	GLN	PHE	L1707	E1640			A1449		THR	T1253	SER
S2029	L1966	GLN	SER	E1581	E1581			L1448		GLY	L1254	ILE
Y2030	F1967	HIS	THR	M1582	M1582			A1450		ALA	L1255	GLU
L2031	C1968	ILE	ILE	M1583	M1583			V1451		ALA	W1256	LEU
A2032	T1906	VAL	VAL	Q1584	Q1584			V1452		GLY	L1257	PHE
E1907	E1907	VAL	VAL	S1585	S1585			S1453		ASN	D1258	THR
G1908	G1908	ASP	ASP	S1586	S1586			A1454		ARG	L1259	LYS
M1909	M1909	ILE	ILE	L1648	L1648			C1455		THR	L1260	PHE
E1972	E1972	ALA	ALA	L1649	L1649					VAL	S1323	VAL
K1973	K1973	ASP	ASP	E1715	E1715			L1458		PRO	A1263	PRO
N1974	N1974	GLN	GLN	Q1716	Q1716			H1459		LEU	L1264	LEU
L1911	L1911	SER	SER	L1717	L1717			M1392		LEU	E1265	LEU
T1912	T1912	SER	SER	I1718	I1718			A1393		PRO	C1266	PRO
K1913	K1913	PHE	PHE	F1722	F1722			D1397		GLY	Y1267	GLY
T1914	T1914	PHE	PHE	P1723	P1723			V1398		ASN	N1268	ASN
L1915	L1915	ARG	ARG	M1724	M1724			C1399		ARG	T1269	ARG
I1916	I1916	ILE	ILE	T1725	T1725			V1400		SER	F1270	SER
K1917	K1917	ALA	ALA	S1726	S1726			L1401		PRO	I1271	PRO
L1918	L1918	ALA	ALA	L1857	L1857			L1402		ASN	G1272	ASN
C1919	C1919	THR	THR	L1797	L1797			M1403		LEU	E1273	LEU
Y1920	Y1920	THR	THR	L1798	L1798			K1404		TRP	R1274	TRP
				E1860	E1860			A1405		LEU	T1275	LEU
F1923	F1923	S1861	S1861	E1799	E1799			M1342		LYS	V1276	ASP
T1924	T1924	T1862	T1862	S1800	S1800			E1343		VAL	L1279	VAL
E1925	E1925	F1863	F1863	V1801	V1801			F1344		LEU	Q1280	LEU
M1926	M1926	Y1802	Y1802	Y1802	Y1802			T1345		K1213	V1281	K1213
M1927	M1927	F1805	F1805	F1734	F1734			T1346		E1214	L1282	E1214
A1928	A1928	R1735	R1735	R1735	R1735			L1347		O1215	G1283	O1215
G1929	G1929	PHE	PHE	F1736	F1736			L1348		G1216	T1284	G1216
N1930	N1930	PRO	PRO	M1737	M1737			M1350		V1217	E1285	V1217
E1931	E1931	GLU	GLU	K1807	K1807			T1351		F1218	Q1287	F1218
K1869	K1869	V1671	V1671	D1808	D1808			L1412		L1220	S1288	L1220
Q1932	Q1932	F1672	F1672	D1809	D1809			L1413		N1221	S1289	N1221
L1933	L1933	S1677	S1677	P1810	P1810			L1414		T1222	L1290	T1222
M1871	M1871	L1678	L1678	R1811	R1811			L1415		T1223	L1291	T1223
G1872	G1872	K1812	K1812	C1742	C1742			L1416		F1224	K1292	F1224
Y1873	Y1873	S1813	S1813	M1743	M1743			L1417		E1225	L1292	E1225
L1874	L1874	F1814	F1814	K1744	K1744			L1418		G1228	L1293	G1228
K1875	K1875	T1815	T1815	K1745	K1745			L1419		C1229	V1294	C1229
L1876	L1876	L1816	L1816	F1746	F1746			L1420		G1230	A1295	G1230
L1877	L1877	Q1817	Q1817	L1747	L1747			L1421		Q1231	F1297	Q1231
D1878	D1878	S1818	S1818	L1748	L1748			L1422		P1232	L1298	P1232
M1880	M1880	F1819	F1819	L1750	L1750			L1423		E1232	E1299	E1232
Y1881	Y1881	K1822	K1822	L1751	L1751			L1424		G1233	L1299	G1233
S1882	S1882	SER	SER	L1752	L1752			L1425				
K2009	K2009	LEU	LEU	S1753	S1753			L1426				
E2010	E2010	LEU	LEU	Q1754	Q1754			L1427				
A2011	A2011	LEU	LEU	S1755	S1755			L1428				
								L1429				
								L1430				
								L1431				
								L1432				
								L1433				
								L1434				
								L1435				
								L1436				
								L1437				
								L1438				
								L1439				
								L1440				
								L1441				
								L1442				
								L1443				
								L1444				
								L1445				
								L1446				
								L1447				
								L1448				
								L1449				
								L1450				
								L1451				
								L1452				
								L1453				
								L1454				
								L1455				
								L1456				
								L1457				
								L1458				
								L1459				
								L1460				
								L1461				
								L1462				
								L1463				
								L1464				
								L1465				
								L1466				
								L1467				
								L1468				
								L1469				
								L1470				
								L1471				
								L1472				
								L1473				
								L1474				
								L1475				
								L1476				
								L1477				
								L1478				
								L1479				
								L1480				
								L1481				
								L1482				
								L1483				
								L1484				
								L1485				
								L1486				
								L1487				
								L1488				
								L1489				
								L1490				
								L1491				
								L1492				
								L1493				
								L1494				
								L1495				
								L1496				
								L1497				
								L1498				
								L1499				
								L1500				

S2966	R2989	L2826	UNK	L2542	Q2472	G2407	L2341	G2378	L2216	L2149	E2077
E2967	L2900	•	UNK	N2543	M2473	M2408	L2344	I2279	L2219	V2150	•
A2968	•	T2833	UNK	S2544	T2409	T2409	L2345	V2280	I2151	I2151	D2078
A2969	E2904	•	UNK	N2545	M2475	E2410	•	N2280	N2152	N2152	D2079
Q2970	L2905	•	UNK	S2546	L2476	L2411	•	N2281	N2153	N2153	•
Q2971	L2906	•	UNK	S2547	L2477	Y2412	•	N2282	N2154	N2154	E2082
Q2972	A2907	•	UNK	S2548	M2478	F2413	•	N2283	N2155	N2155	L2083
D2973	R2908	•	UNK	K2549	•	K2416	•	N2284	N2156	N2156	•
E2974	•	UNK	UNK	K2550	•	•	•	L2285	F2157	F2157	E2084
A2975	S2774	•	UNK	E2551	H2481	•	•	L2286	R2158	R2158	E2085
L2976	R2775	•	UNK	E2552	H2482	•	•	F2287	R2159	R2159	D2086
N2977	R2776	•	UNK	H2553	•	D2419	•	R2158	R2159	R2159	D2087
N2978	R2777	•	UNK	H2554	•	F2420	•	R2159	R2159	R2159	L2088
Q2979	G2778	•	UNK	L2555	•	V2421	•	R2159	R2159	R2159	L2089
•	•	•	UNK	S2556	•	Q2422	•	R2159	R2159	R2159	•
E2980	P2781	•	UNK	S2557	•	V2423	•	R2159	R2159	R2159	E2091
E2981	D2782	•	UNK	L2557	•	M2424	•	R2159	R2159	R2159	E2092
D2982	L2783	•	UNK	A2558	•	R2425	•	R2159	R2159	R2159	Q2093
Q2983	L2783	•	UNK	T2559	•	H2426	•	R2159	R2159	R2159	M2094
Q2984	Q2784	•	UNK	N2560	•	R2427	•	R2159	R2159	R2159	A2095
E2985	I2785	•	UNK	F2561	•	E2430	•	R2159	R2159	R2159	F2096
F2986	I2786	•	UNK	L2562	•	•	•	R2159	R2159	R2159	L2097
T2987	H2787	•	UNK	L2563	•	K2433	•	R2159	R2159	R2159	L2098
E2988	S2788	•	UNK	E2564	•	V2434	•	R2159	R2159	R2159	A2099
A2989	S2789	•	UNK	M2565	•	L2435	•	R2159	R2159	R2159	L2100
E2990	L2790	•	UNK	T2567	•	L2436	•	R2159	R2159	R2159	•
•	•	•	UNK	•	•	D2437	•	R2159	R2159	R2159	E2101
E2991	I2791	•	UNK	M2568	•	•	•	R2159	R2159	R2159	K2102
•	•	•	UNK	•	•	•	•	R2159	R2159	R2159	E2103
E2992	T2792	•	UNK	S2569	•	I2438	•	R2159	R2159	R2159	•
F2993	P2793	•	UNK	P2570	•	I2439	•	R2159	R2159	R2159	E2104
E2994	L2794	•	UNK	N2571	•	Y2440	•	R2159	R2159	R2159	P2110
E2995	Q2795	•	UNK	Q2509	•	K2441	•	R2159	R2159	R2159	P2111
•	•	•	UNK	•	•	•	•	R2159	R2159	R2159	Q2112
S2998	S2982	•	UNK	P2573	•	M2442	•	R2159	R2159	R2159	•
L2999	A2798	•	UNK	•	•	M2443	•	R2159	R2159	R2159	P2119
D3000	Q2799	•	UNK	P2575	•	K2444	•	R2159	R2159	R2159	R2120
C3001	R2800	•	UNK	N2576	•	K2445	•	R2159	R2159	R2159	R2121
Y3002	D2801	•	UNK	UNK	•	L2446	•	R2159	R2159	R2159	L2122
N3003	P2802	•	UNK	UNK	•	K2447	•	R2159	R2159	R2159	•
H3004	L2803	•	UNK	UNK	•	•	•	R2159	R2159	R2159	P2125
L3005	I2804	•	UNK	UNK	•	•	•	R2159	R2159	R2159	M2126
A3006	S2877	•	UNK	UNK	•	•	•	R2159	R2159	R2159	•
E3007	A2878	•	UNK	UNK	•	•	•	R2159	R2159	R2159	W2125
•	Q2941	•	UNK	UNK	•	•	•	R2159	R2159	R2159	W2126
N3008	Q2880	•	UNK	UNK	•	•	•	R2159	R2159	R2159	•
•	L2942	•	UNK	UNK	•	•	•	R2159	R2159	R2159	W2127
S3010	F2943	•	UNK	UNK	•	•	•	R2159	R2159	R2159	•
E3011	A2882	•	UNK	UNK	•	•	•	R2159	R2159	R2159	L2128
•	S2945	•	UNK	UNK	•	•	•	R2159	R2159	R2159	L2129
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	•
Y3013	T2949	•	UNK	UNK	•	•	•	R2159	R2159	R2159	N2135
C3014	K2950	•	UNK	UNK	•	•	•	R2159	R2159	R2159	P2136
S3015	Q2951	•	UNK	UNK	•	•	•	R2159	R2159	R2159	T2137
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	Q2204
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	V2138
I3019	Q2954	•	UNK	UNK	•	•	•	R2159	R2159	R2159	F2139
D3020	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	L2140
S3021	L2957	•	UNK	UNK	•	•	•	R2159	R2159	R2159	R2207
E3022	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	D2208
N3023	L2891	•	UNK	UNK	•	•	•	R2159	R2159	R2159	N2141
•	L2892	•	UNK	UNK	•	•	•	R2159	R2159	R2159	T2270
P3024	L2893	•	UNK	UNK	•	•	•	R2159	R2159	R2159	S2271
•	L2894	•	UNK	UNK	•	•	•	R2159	R2159	R2159	V2210
F3025	L2895	•	UNK	UNK	•	•	•	R2159	R2159	R2159	G2272
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	L2211
D3026	L2896	•	UNK	UNK	•	•	•	R2159	R2159	R2159	G2273
•	L2897	•	UNK	UNK	•	•	•	R2159	R2159	R2159	L2212
L3028	L2898	•	UNK	UNK	•	•	•	R2159	R2159	R2159	A2212
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	F2145
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	L2146
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	L2147
•	•	•	UNK	UNK	•	•	•	R2159	R2159	R2159	K2148

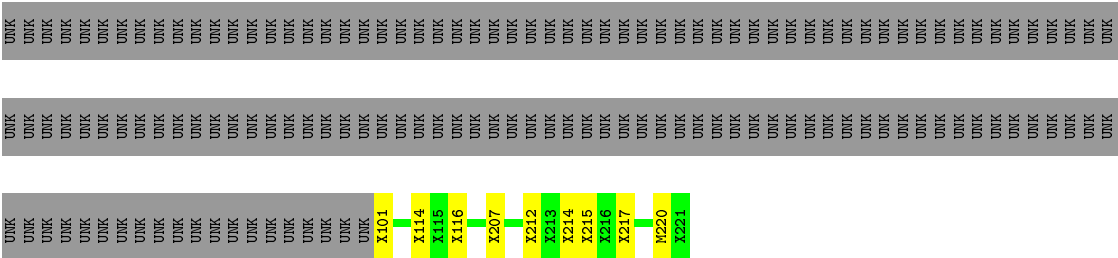




● Molecule 2: C-terminal fragment of KU80 (KU80ct194)



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.386 , 0.437 0.384 , 0.437	Depositor DCC
$R_{free}$ test set	1973 reflections (2.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	184.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 187.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	3631/4128 (88%)	2664 (73%)	724 (20%)	243 (7%)	1	25
1	B	3631/4128 (88%)	2657 (73%)	723 (20%)	251 (7%)	1	24
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	24

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 [i](#)

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%)	29	67
1	B	3259/3384 (96%)	3084 (95%)	175 (5%)	27	66
2	K	-	1 (100%)	0	100	100
2	S	-	1 (100%)	0	100	100
All	All	6520/6768 (96%)	6175 (95%)	345 (5%)	28	67

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

Mol	Chain	Res	Type
1	A	3893	SER
1	B	559	SER
1	B	3636	PHE
1	A	3929	MSE
1	B	274	LEU

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

Mol	Chain	Res	Type
1	A	3524	ASN
1	B	442	GLN
1	B	3524	ASN
1	A	3762	GLN
1	A	4068	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 carbohydrates 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
1	B	1
1	A	1
2	K	1
2	S	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	3551/4128 (86%)	0.24	229 (6%) 23 16	83, 248, 332, 443	0
1	B	3551/4128 (86%)	0.30	236 (6%) 22 15	117, 251, 358, 507	0
2	K	0/194	-	-	-	-
2	S	0/194	-	-	-	-
All	All	7102/8644 (82%)	0.27	465 (6%) 22 16	83, 249, 343, 507	0

The worst 5 of 465 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	LYS	12.9
1	B	31	GLY	9.7
1	B	1355	GLY	9.6
1	A	126	PRO	9.1
1	A	123	CYS	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 carbohydrates 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.