



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:01 AM GMT

PDB ID : 3KGV
Title : Crystal Structure of Human DNA-dependent Protein Kinase Catalytic Subunit (DNA-PKcs)
Authors : Sibanda, B.L.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2009-10-29
Resolution : 6.60 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
<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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

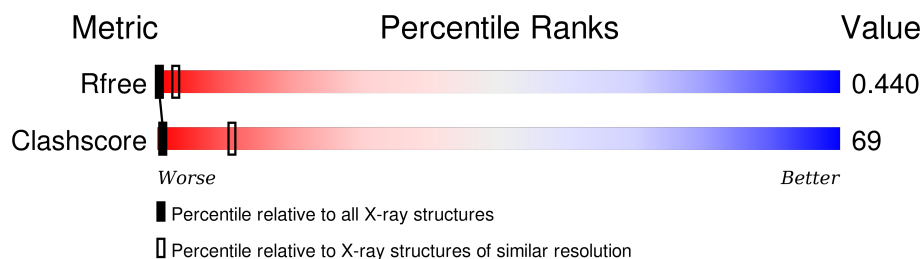
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION










The reported resolution of this entry is 6.60 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	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 91%
1	B	4128	 93%
1	C	4128	 90%
1	D	4128	 96%
1	E	4128	 98%
1	F	4128	 87%
1	O	4128	 91%
1	P	4128	 93%
1	Q	4128	 90%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	R	4128	 96%
1	S	4128	 98%
1	T	4128	 87%
1	X	4128	 95%
1	Y	4128	 95%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20320 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.

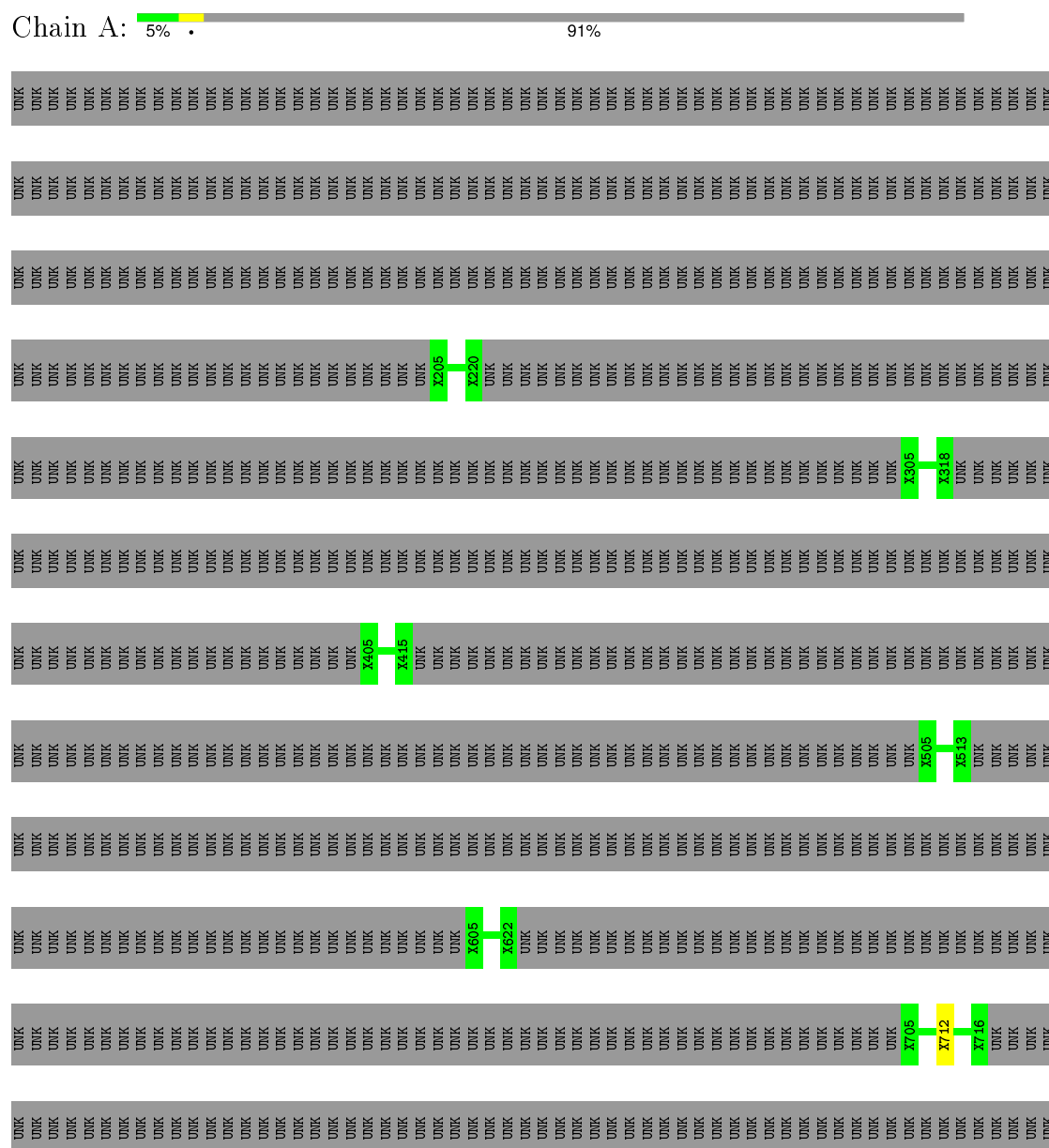
- Molecule 1 is a protein called DNA-dependent Protein Kinase Catalytic Subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	0	0	0
			1770	1062	354	354			
1	B	283	Total	C	N	O	0	0	0
			1415	849	283	283			
1	C	406	Total	C	N	O	0	0	0
			2030	1218	406	406			
1	D	182	Total	C	N	O	0	0	0
			910	546	182	182			
1	E	65	Total	C	N	O	0	0	0
			325	195	65	65			
1	F	531	Total	C	N	O	0	0	0
			2655	1593	531	531			
1	X	211	Total	C	N	O	0	0	0
			1055	633	211	211			
1	O	354	Total	C	N	O	0	0	0
			1770	1062	354	354			
1	P	283	Total	C	N	O	0	0	0
			1415	849	283	283			
1	Q	406	Total	C	N	O	0	0	0
			2030	1218	406	406			
1	R	182	Total	C	N	O	0	0	0
			910	546	182	182			
1	S	65	Total	C	N	O	0	0	0
			325	195	65	65			
1	T	531	Total	C	N	O	0	0	0
			2655	1593	531	531			
1	Y	211	Total	C	N	O	0	0	0
			1055	633	211	211			

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 ($RSRZ > 2$). 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.

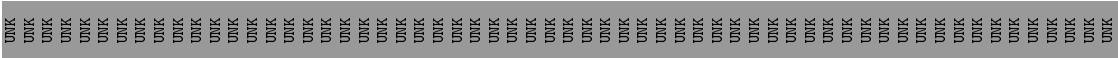
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit





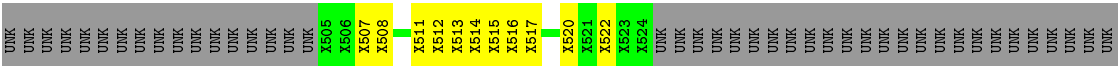
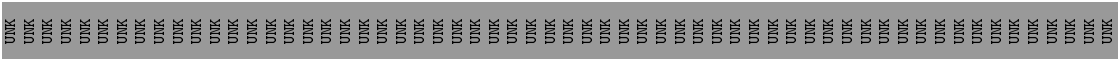
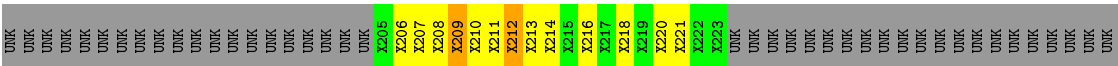






● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain B: . . 93%

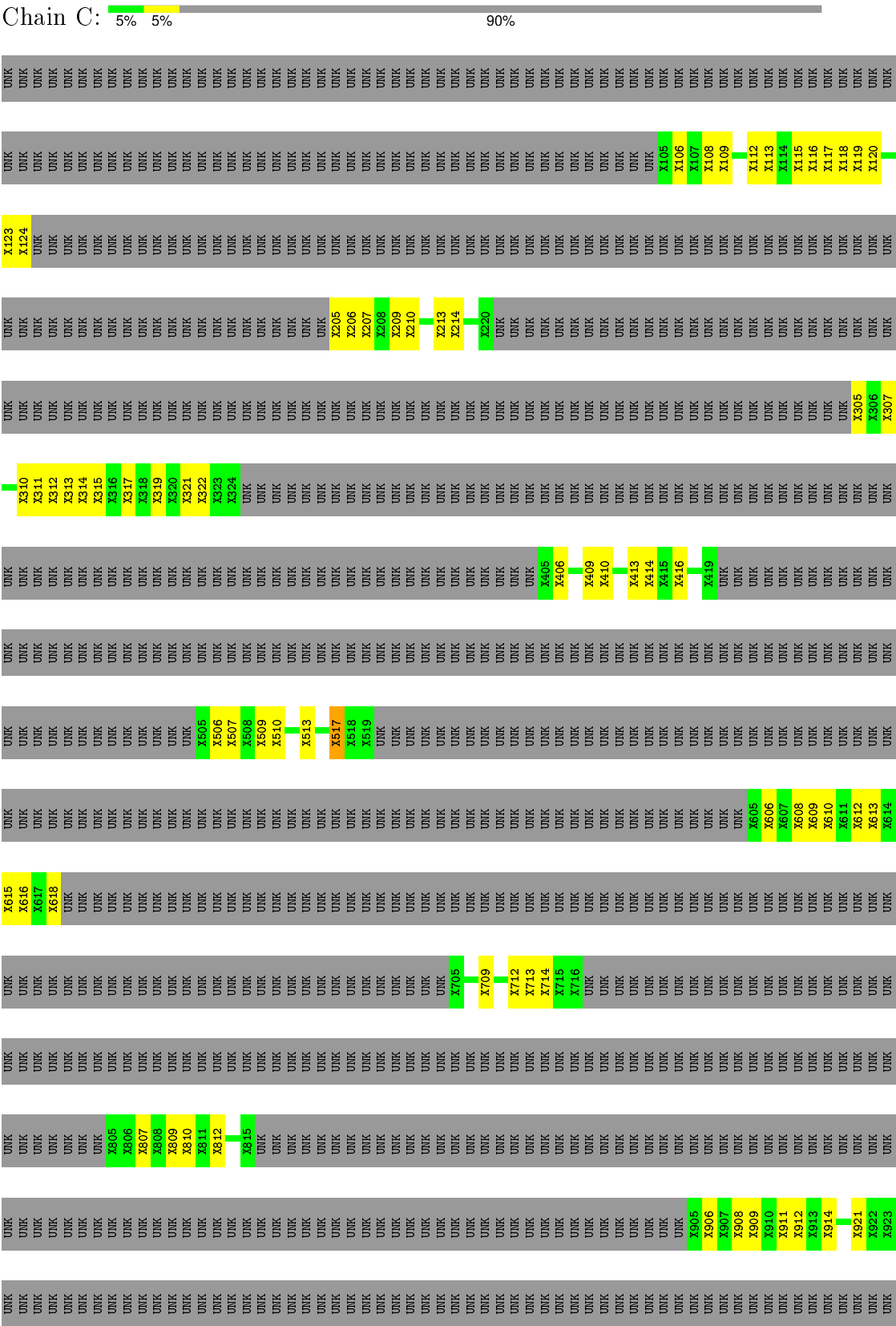






[illegible]

● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit





[illegible]

١٨٨٨	١٨٨٩	١٨٩٠	١٨٩١	١٨٩٢	١٨٩٣	١٨٩٤	١٨٩٥	١٨٩٦	١٨٩٧	١٨٩٨	١٨٩٩	١٩٠٠	١٩٠١	١٩٠٢	١٩٠٣	١٩٠٤	١٩٠٥	١٩٠٦	١٩٠٧	١٩٠٨	١٩٠٩	١٩١٠	١٩١١	١٩١٢	١٩١٣	١٩١٤	١٩١٥	١٩١٦	١٩١٧	١٩١٨	١٩١٩	١٩٢٠	١٩٢١	١٩٢٢	١٩٢٣	١٩٢٤	١٩٢٥	١٩٢٦	١٩٢٧	١٩٢٨	١٩٢٩	١٩٣٠	١٩٣١	١٩٣٢	١٩٣٣	١٩٣٤	١٩٣٥	١٩٣٦	١٩٣٧	١٩٣٨	١٩٣٩	١٩٤٠	١٩٤١	١٩٤٢	١٩٤٣	١٩٤٤	١٩٤٥	١٩٤٦	١٩٤٧	١٩٤٨	١٩٤٩	١٩٥٠	١٩٥١	١٩٥٢	١٩٥٣	١٩٥٤	١٩٥٥	١٩٥٦	١٩٥٧	١٩٥٨	١٩٥٩	١٩٦٠	١٩٦١	١٩٦٢	١٩٦٣	١٩٦٤	١٩٦٥	١٩٦٦	١٩٦٧	١٩٦٨	١٩٦٩	١٩٧٠	١٩٧١	١٩٧٢	١٩٧٣	١٩٧٤	١٩٧٥	١٩٧٦	١٩٧٧	١٩٧٨	١٩٧٩	١٩٨٠	١٩٨١	١٩٨٢	١٩٨٣	١٩٨٤	١٩٨٥	١٩٨٦	١٩٨٧	١٩٨٨	١٩٨٩	١٩٩٠	١٩٩١	١٩٩٢	١٩٩٣	١٩٩٤	١٩٩٥	١٩٩٦	١٩٩٧	١٩٩٨	١٩٩٩	٢٠٠٠	٢٠٠١	٢٠٠٢	٢٠٠٣	٢٠٠٤	٢٠٠٥	٢٠٠٦	٢٠٠٧	٢٠٠٨	٢٠٠٩	٢٠١٠	٢٠١١	٢٠١٢	٢٠١٣	٢٠١٤	٢٠١٥	٢٠١٦	٢٠١٧	٢٠١٨	٢٠١٩	٢٠٢٠	٢٠٢١	٢٠٢٢	٢٠٢٣	٢٠٢٤	٢٠٢٥	٢٠٢٦	٢٠٢٧	٢٠٢٨	٢٠٢٩	٢٠٣٠	٢٠٣١	٢٠٣٢	٢٠٣٣	٢٠٣٤	٢٠٣٥	٢٠٣٦	٢٠٣٧	٢٠٣٨	٢٠٣٩	٢٠٤٠	٢٠٤١	٢٠٤٢	٢٠٤٣	٢٠٤٤	٢٠٤٥	٢٠٤٦	٢٠٤٧	٢٠٤٨	٢٠٤٩	٢٠٥٠	٢٠٥١	٢٠٥٢	٢٠٥٣	٢٠٥٤	٢٠٥٥	٢٠٥٦	٢٠٥٧	٢٠٥٨	٢٠٥٩	٢٠٦٠	٢٠٦١	٢٠٦٢	٢٠٦٣	٢٠٦٤	٢٠٦٥	٢٠٦٦	٢٠٦٧	٢٠٦٨	٢٠٦٩	٢٠٧٠	٢٠٧١	٢٠٧٢	٢٠٧٣	٢٠٧٤	٢٠٧٥	٢٠٧٦	٢٠٧٧	٢٠٧٨	٢٠٧٩	٢٠٨٠	٢٠٨١	٢٠٨٢	٢٠٨٣	٢٠٨٤	٢٠٨٥	٢٠٨٦	٢٠٨٧	٢٠٨٨	٢٠٨٩	٢٠٩٠	٢٠٩١	٢٠٩٢	٢٠٩٣	٢٠٩٤	٢٠٩٥	٢٠٩٦	٢٠٩٧	٢٠٩٨	٢٠٩٩	٢١٠٠	٢١٠١	٢١٠٢	٢١٠٣	٢١٠٤	٢١٠٥	٢١٠٦	٢١٠٧	٢١٠٨	٢١٠٩	٢١١٠	٢١١١	٢١١٢	٢١١٣	٢١١٤	٢١١٥	٢١١٦	٢١١٧	٢١١٨	٢١١٩	٢١٢٠	٢١٢١	٢١٢٢	٢١٢٣	٢١٢٤	٢١٢٥	٢١٢٦	٢١٢٧	٢١٢٨	٢١٢٩	٢١٣٠	٢١٣١	٢١٣٢	٢١٣٣	٢١٣٤	٢١٣٥	٢١٣٦	٢١٣٧	٢١٣٨	٢١٣٩	٢١٤٠	٢١٤١	٢١٤٢	٢١٤٣	٢١٤٤	٢١٤٥	٢١٤٦	٢١٤٧	٢١٤٨	٢١٤٩	٢١٥٠	٢١٥١	٢١٥٢	٢١٥٣	٢١٥٤	٢١٥٥	٢١٥٦	٢١٥٧	٢١٥٨	٢١٥٩	٢١٦٠	٢١٦١	٢١٦٢	٢١٦٣	٢١٦٤	٢١٦٥	٢١٦٦	٢١٦٧	٢١٦٨	٢١٦٩	٢١٧٠	٢١٧١	٢١٧٢	٢١٧٣	٢١٧٤	٢١٧٥	٢١٧٦	٢١٧٧	٢١٧٨	٢١٧٩	٢١٨٠	٢١٨١	٢١٨٢	٢١٨٣	٢١٨٤	٢١٨٥	٢١٨٦	٢١٨٧	٢١٨٨	٢١٨٩	٢١٩٠	٢١٩١	٢١٩٢	٢١٩٣	٢١٩٤	٢١٩٥	٢١٩٦	٢١٩٧	٢١٩٨	٢١٩٩	٢٢٠٠	٢٢٠١	٢٢٠٢	٢٢٠٣	٢٢٠٤	٢٢٠٥	٢٢٠٦	٢٢٠٧	٢٢٠٨	٢٢٠٩	٢٢١٠	٢٢١١	٢٢١٢	٢٢١٣	٢٢١٤	٢٢١٥	٢٢١٦	٢٢١٧	٢٢١٨	٢٢١٩	٢٢٢٠	٢٢٢١	٢٢٢٢	٢٢٢٣	٢٢٢٤	٢٢٢٥	٢٢٢٦	٢٢٢٧	٢٢٢٨	٢٢٢٩	٢٢٣٠	٢٢٣١	٢٢٣٢	٢٢٣٣	٢٢٣٤	٢٢٣٥	٢٢٣٦	٢٢٣٧	٢٢٣٨	٢٢٣٩	٢٢٤٠	٢٢٤١	٢٢٤٢	٢٢٤٣	٢٢٤٤	٢٢٤٥	٢٢٤٦	٢٢٤٧	٢٢٤٨	٢٢٤٩	٢٢٥٠	٢٢٥١	٢٢٥٢	٢٢٥٣	٢٢٥٤	٢٢٥٥	٢٢٥٦	٢٢٥٧	٢٢٥٨	٢٢٥٩	٢٢٦٠	٢٢٦١	٢٢٦٢	٢٢٦٣	٢٢٦٤	٢٢٦٥	٢٢٦٦	٢٢٦٧	٢٢٦٨	٢٢٦٩	٢٢٧٠	٢٢٧١	٢٢٧٢	٢٢٧٣	٢٢٧٤	٢٢٧٥	٢٢٧٦	٢٢٧٧	٢٢٧٨	٢٢٧٩	٢٢٨٠	٢٢٨١	٢٢٨٢	٢٢٨٣	٢٢٨٤	٢٢٨٥	٢٢٨٦	٢٢٨٧	٢٢٨٨	٢٢٨٩	٢٢٩٠	٢٢٩١	٢٢٩٢	٢٢٩٣	٢٢٩٤	٢٢٩٥	٢٢٩٦	٢٢٩٧	٢٢٩٨	٢٢٩٩	٢٣٠٠	٢٣٠١	٢٣٠٢	٢٣٠٣	٢٣٠٤	٢٣٠٥	٢٣٠٦	٢٣٠٧	٢٣٠٨	٢٣٠٩	٢٣١٠	٢٣١١	٢٣١٢	٢٣١٣	٢٣١٤	٢٣١٥	٢٣١٦	٢٣١٧	٢٣١٨	٢٣١٩	٢٣٢٠	٢٣٢١	٢٣٢٢	٢٣٢٣	٢٣٢٤	٢٣٢٥	٢٣٢٦	٢٣٢٧	٢٣٢٨	٢٣٢٩	٢٣٣٠	٢٣٣١	٢٣٣٢	٢٣٣٣	٢٣٣٤	٢٣٣٥	٢٣٣٦	٢٣٣٧	٢٣٣٨	٢٣٣٩	٢٣٤٠	٢٣٤١	٢٣٤٢	٢٣٤٣	٢٣٤٤	٢٣٤٥	٢٣٤٦	٢٣٤٧	٢٣٤٨	٢٣٤٩	٢٣٥٠	٢٣٥١	٢٣٥٢	٢٣٥٣	٢٣٥٤	٢٣٥٥	٢٣٥٦	٢٣٥٧	٢٣٥٨	٢٣٥٩	٢٣٦٠	٢٣٦١	٢٣٦٢	٢٣٦٣	٢٣٦٤	٢٣٦٥	٢٣٦٦	٢٣٦٧	٢٣٦٨	٢٣٦٩	٢٣٧٠	٢٣٧١	٢٣٧٢	٢٣٧٣	٢٣٧٤	٢٣٧٥	٢٣٧٦	٢٣٧٧	٢٣٧٨	٢٣٧٩	٢٣٨٠	٢٣٨١	٢٣٨٢	٢٣٨٣	٢٣٨٤	٢٣٨٥	٢٣٨٦	٢٣٨٧	٢٣٨٨	٢٣٨٩	٢٣٩٠	٢٣٩١	٢٣٩٢	٢٣٩٣	٢٣٩٤	٢٣٩٥	٢٣٩٦	٢٣٩٧	٢٣٩٨	٢٣٩٩	٢٤٠٠	٢٤٠١	٢٤٠٢	٢٤٠٣	٢٤٠٤	٢٤٠٥	٢٤٠٦	٢٤٠٧	٢٤٠٨	٢٤٠٩	٢٤١٠	٢٤١١	٢٤١٢	٢٤١٣	٢٤١٤	٢٤١٥	٢٤١٦	٢٤١٧	٢٤١٨	٢٤١٩	٢٤٢٠	٢٤٢١	٢٤٢٢	٢٤٢٣	٢٤٢٤	٢٤٢٥	٢٤٢٦	٢٤٢٧	٢٤٢٨	٢٤٢٩	٢٤٣٠	٢٤٣١	٢٤٣٢	٢٤٣٣	٢٤٣٤	٢٤٣٥	٢٤٣٦	٢٤٣٧	٢٤٣٨	٢٤٣٩	٢٤٤٠	٢٤٤١	٢٤٤٢	٢٤٤٣	٢٤٤٤	٢٤٤٥	٢٤٤٦	٢٤٤٧	٢٤٤٨	٢٤٤٩	٢٤٥٠	٢٤٥١	٢٤٥٢	٢٤٥٣	٢٤٥٤	٢٤٥٥	٢٤٥٦	٢٤٥٧	٢٤٥٨	٢٤٥٩	٢٤٦٠	٢٤٦١	٢٤٦٢	٢٤٦٣	٢٤٦٤	٢٤٦٥	٢٤٦٦	٢٤٦٧	٢٤٦٨	٢٤٦٩	٢٤٧٠	٢٤٧١	٢٤٧٢	٢٤٧٣	٢٤٧٤	٢٤٧٥	٢٤٧٦	٢٤٧٧	٢٤٧٨	٢٤٧٩	٢٤٨٠	٢٤٨١	٢٤٨٢	٢٤٨٣	٢٤٨٤	٢٤٨٥	٢٤٨٦	٢٤٨٧	٢٤٨٨	٢٤٨٩	٢٤٩٠	٢٤٩١	٢٤٩٢	٢٤٩٣	٢٤٩٤	٢٤٩٥	٢٤٩٦	٢٤٩٧	٢٤٩٨	٢٤٩٩	٢٥٠٠	٢٥٠١	٢٥٠٢	٢٥٠٣	٢٥٠٤	٢٥٠٥	٢٥٠٦	٢٥٠٧	٢٥٠٨	٢٥٠٩	٢٥١٠	٢٥١١	٢٥١٢	٢٥١٣	٢٥١٤	٢٥١٥	٢٥١٦	٢٥١٧	٢٥١٨	٢٥١٩	٢٥٢٠	٢٥٢١	٢٥٢٢	٢٥٢٣	٢٥٢٤	٢٥٢٥	٢٥٢٦	٢٥٢٧	٢٥٢٨	٢٥٢٩	٢٥٣٠	٢٥٣١	٢٥٣٢	٢٥٣٣	٢٥٣٤	٢٥٣٥	٢٥٣٦	٢٥٣٧	٢٥٣٨	٢٥٣٩	٢٥٤٠	٢٥٤١	٢٥٤٢	٢٥٤٣	٢٥٤٤	٢٥٤٥	٢٥٤٦	٢٥٤٧	٢٥٤٨	٢٥٤٩	٢٥٥٠	٢٥٥١	٢٥٥٢	٢٥٥٣	٢٥٥٤	٢٥٥٥	٢٥٥٦	٢٥٥٧	٢٥٥٨	٢٥٥٩	٢٥٦٠	٢٥٦١	٢٥٦٢	٢٥٦٣	٢٥٦٤	٢٥٦٥	٢٥٦٦	٢٥٦٧	٢٥٦٨	٢٥٦٩	٢٥٧٠	٢٥٧١	٢٥٧٢	٢٥٧٣	٢٥٧٤	٢٥٧٥	٢٥٧٦	٢٥٧٧	٢٥٧٨	٢٥٧٩	٢٥٨٠	٢٥٨١	٢٥٨٢	٢٥٨٣	٢٥٨٤	٢٥٨٥	٢٥٨٦	٢٥٨٧	٢٥٨٨	٢٥٨٩	٢٥٩٠	٢٥٩١	٢٥٩٢	٢٥٩٣	٢٥٩٤	٢٥٩٥	٢٥٩٦	٢٥٩٧	٢٥٩٨	٢٥٩٩	٢٦٠٠	٢٦٠١	٢٦٠٢	٢٦٠٣	٢٦٠٤	٢٦٠٥	٢٦٠٦	٢٦٠٧	٢٦٠٨	٢٦٠٩	٢٦١٠	٢٦١١	٢٦١٢	٢٦١٣	٢٦١٤	٢٦١٥	٢٦١٦	٢٦١٧	٢٦١٨	٢٦١٩	٢٦٢٠	٢٦٢١	٢٦٢٢	٢٦٢٣	٢٦٢٤	٢٦٢٥	٢٦٢٦	٢٦٢٧	٢٦٢٨	٢٦٢٩	٢٦٣٠	٢٦٣١	٢٦٣٢	٢٦٣٣	٢٦٣٤	٢٦٣٥	٢٦٣٦	٢٦٣٧	٢٦٣٨	٢٦٣٩	٢٦٤٠	٢٦٤١	٢٦٤٢	٢٦٤٣	٢٦٤٤	٢٦٤٥	٢٦٤٦	٢٦٤٧	٢٦٤٨	٢٦٤٩	٢٦٥٠	٢٦٥١	٢٦٥٢	٢٦٥٣	٢٦٥٤	٢٦٥٥	٢٦٥٦	٢٦٥٧	٢٦٥٨	٢٦٥٩	٢٦٦٠	٢٦٦١	٢٦٦٢	٢٦٦٣	٢٦٦٤	٢٦٦٥	٢٦٦٦	٢٦٦٧	٢٦٦٨	٢٦٦٩	٢٦٧٠	٢٦٧١	٢٦٧٢	٢٦٧٣	٢٦٧٤	٢٦٧٥	٢٦٧٦	٢٦٧٧	٢٦٧٨	٢٦٧٩	٢٦٨٠	٢٦٨١	٢٦٨٢	٢٦٨٣	٢٦٨٤	٢٦٨٥	٢٦٨٦	٢٦٨٧	٢٦٨٨	٢٦٨٩	٢٦٩٠	٢٦٩١	٢٦٩٢	٢٦٩٣	٢٦٩٤	٢٦٩٥	٢٦٩٦	٢٦٩٧	٢٦٩٨	٢٦٩٩	٢٧٠٠	٢٧٠١	٢٧٠٢	٢٧٠٣	٢٧٠٤	٢٧٠٥	٢٧٠٦	٢٧٠٧	٢٧٠٨	٢٧٠٩	٢٧١٠	٢٧١١	٢٧١٢	٢٧١٣	٢٧١٤	٢٧١٥	٢٧١٦	٢٧١٧	٢٧١٨	٢٧١٩	٢٧٢٠	٢٧٢١	٢٧٢٢	٢٧٢٣	٢٧٢٤	٢٧٢٥	٢٧٢٦	٢٧٢٧	٢٧٢٨	٢٧٢٩	٢٧٣٠	٢٧٣١	٢٧٣٢	٢٧٣٣	٢٧٣٤	٢٧٣٥	٢٧٣٦	٢٧٣٧	٢٧٣٨	٢٧٣٩	٢٧٤٠	٢٧٤١	٢٧٤٢	٢٧٤٣	٢٧٤٤	٢٧٤٥	٢٧٤٦	٢٧٤٧	٢٧٤٨	٢٧٤٩	٢٧٥٠	٢٧٥١	٢٧٥٢	٢٧٥٣	٢٧٥٤	٢٧٥٥	٢٧٥٦	٢٧٥٧	٢٧٥٨	٢٧٥٩	٢٧٦٠	٢٧٦١	٢٧٦٢	٢٧٦٣	٢٧٦٤	٢٧٦٥	٢٧٦٦	٢٧٦٧	٢٧٦٨	٢٧٦٩	٢٧٧٠	٢٧٧١	٢٧٧٢	٢٧٧٣	٢٧٧٤	٢٧٧٥	٢٧٧٦	٢٧٧٧	٢٧٧٨	٢٧٧٩	٢٧٨٠	٢٧٨١	٢٧٨٢	٢٧٨٣	٢٧٨٤	٢٧٨٥	٢٧٨٦	٢٧٨٧	٢٧٨٨	٢٧٨٩	٢٧٩٠	٢٧٩١	٢٧٩٢	٢٧٩٣	٢٧٩٤	٢٧٩٥	٢٧٩٦	٢٧٩٧	٢٧٩٨	٢٧٩٩	٢٨٠٠	٢٨٠١	٢٨٠٢	٢٨٠٣	٢٨٠٤	٢٨٠٥	٢٨٠٦	٢٨٠٧	٢٨٠٨	٢٨٠٩	٢٨١٠	٢٨١١	٢٨١٢	٢٨١٣	٢٨١٤	٢٨١٥	٢٨١٦	٢٨١٧	٢٨١٨	٢٨١٩	٢٨٢٠	٢٨٢١	٢٨٢٢	٢٨٢٣	٢٨٢٤	٢٨٢٥	٢٨٢٦	٢٨٢٧	٢٨٢٨	٢٨٢٩	٢٨٣٠	٢٨٣١	٢٨٣٢	٢٨٣٣	٢٨٣٤	٢٨٣٥	٢٨٣٦	٢٨٣٧	٢٨٣٨	٢٨٣٩	٢
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	---



[illegible]



[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

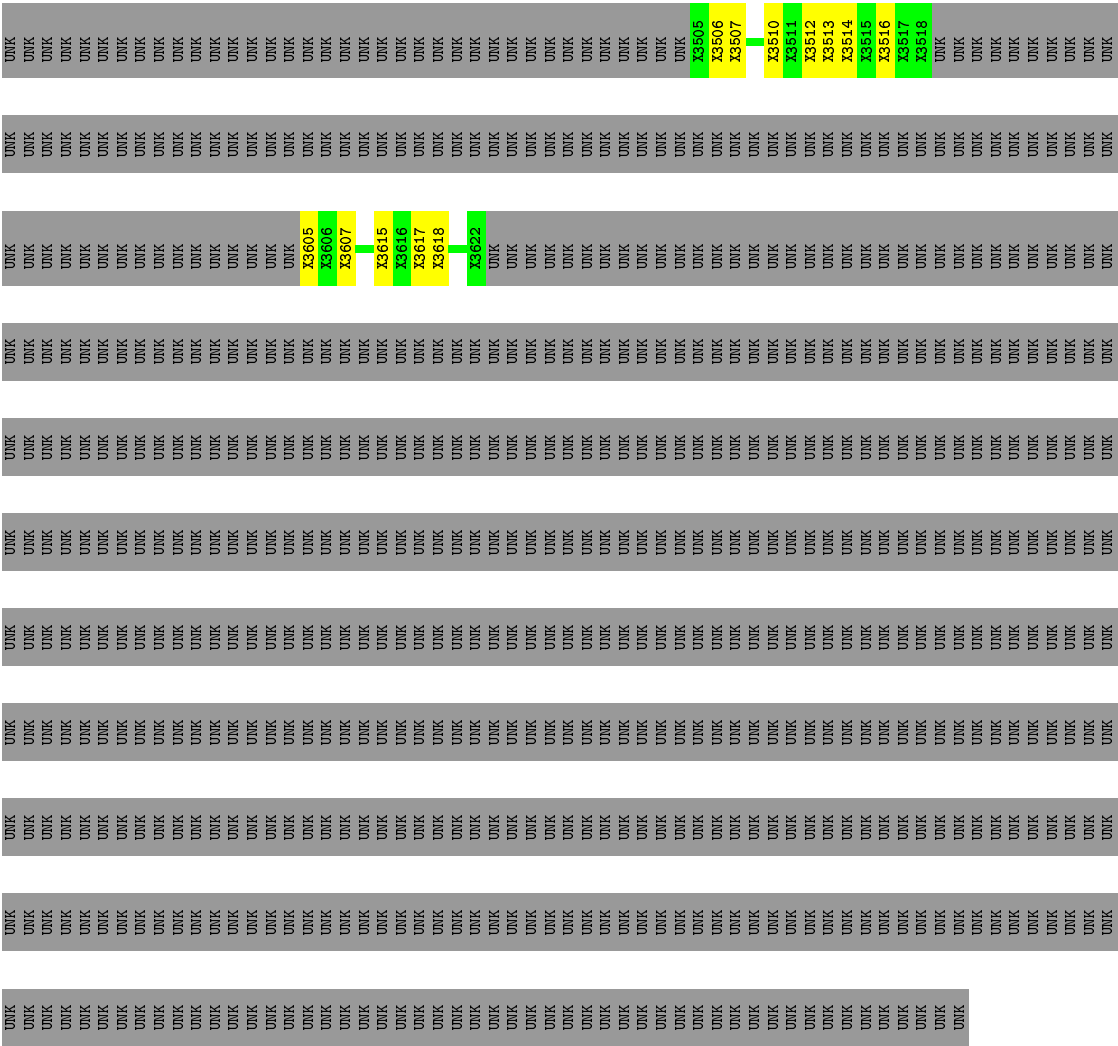
Chain F:  7% 6% 87%

[illegible]



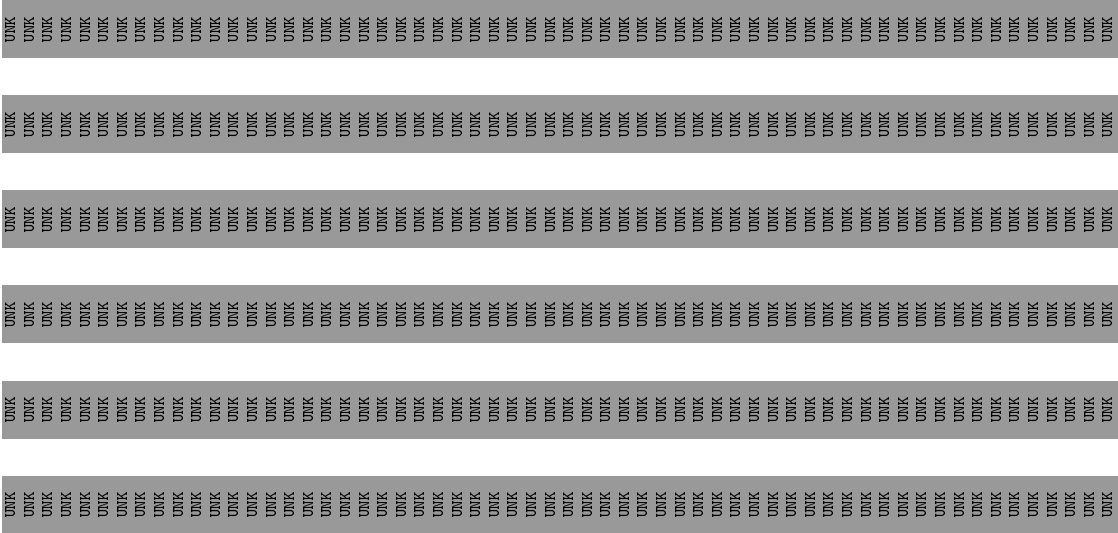
[illegible]





● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

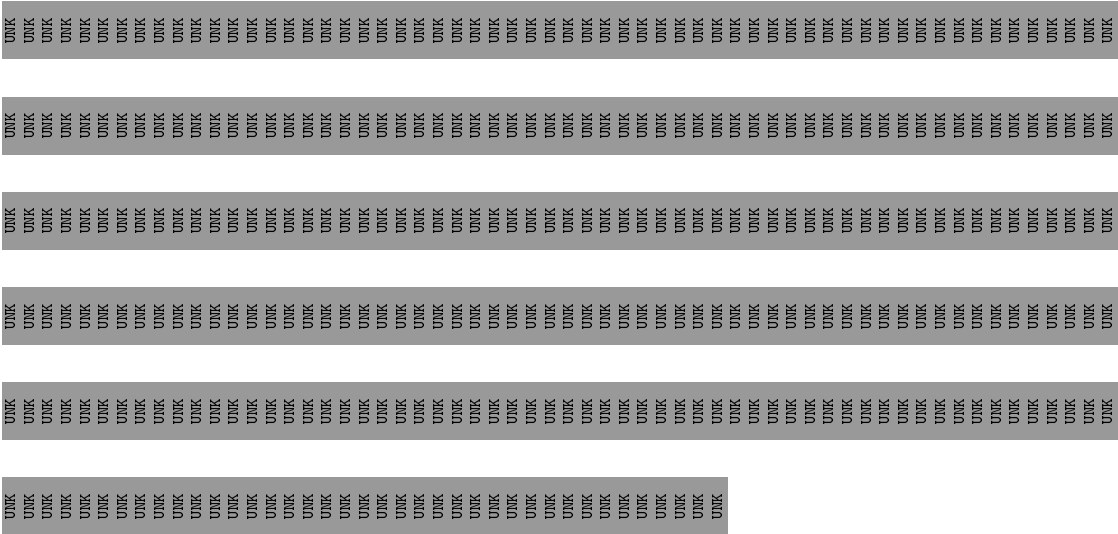
Chain X:  95%



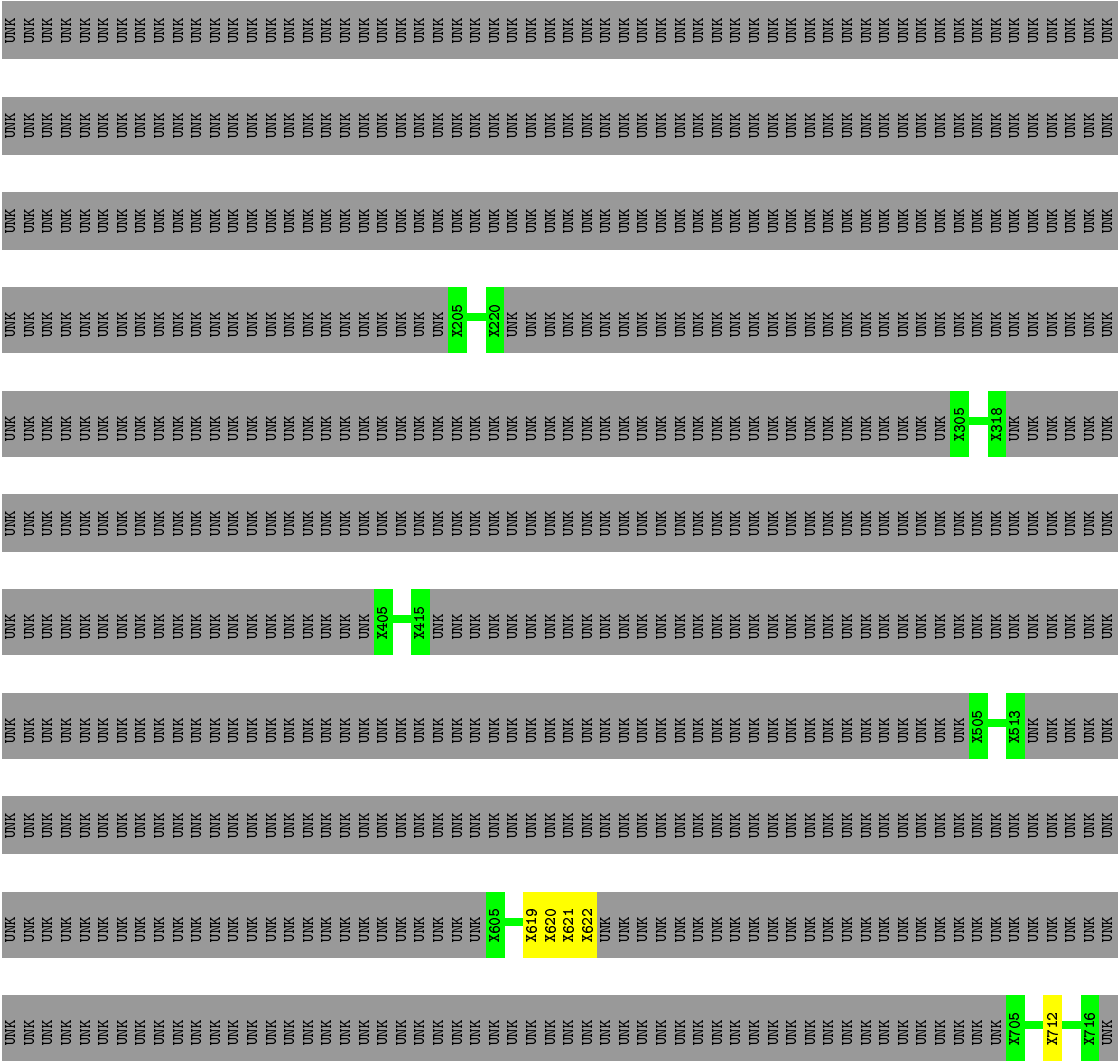


[illegible]





● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit





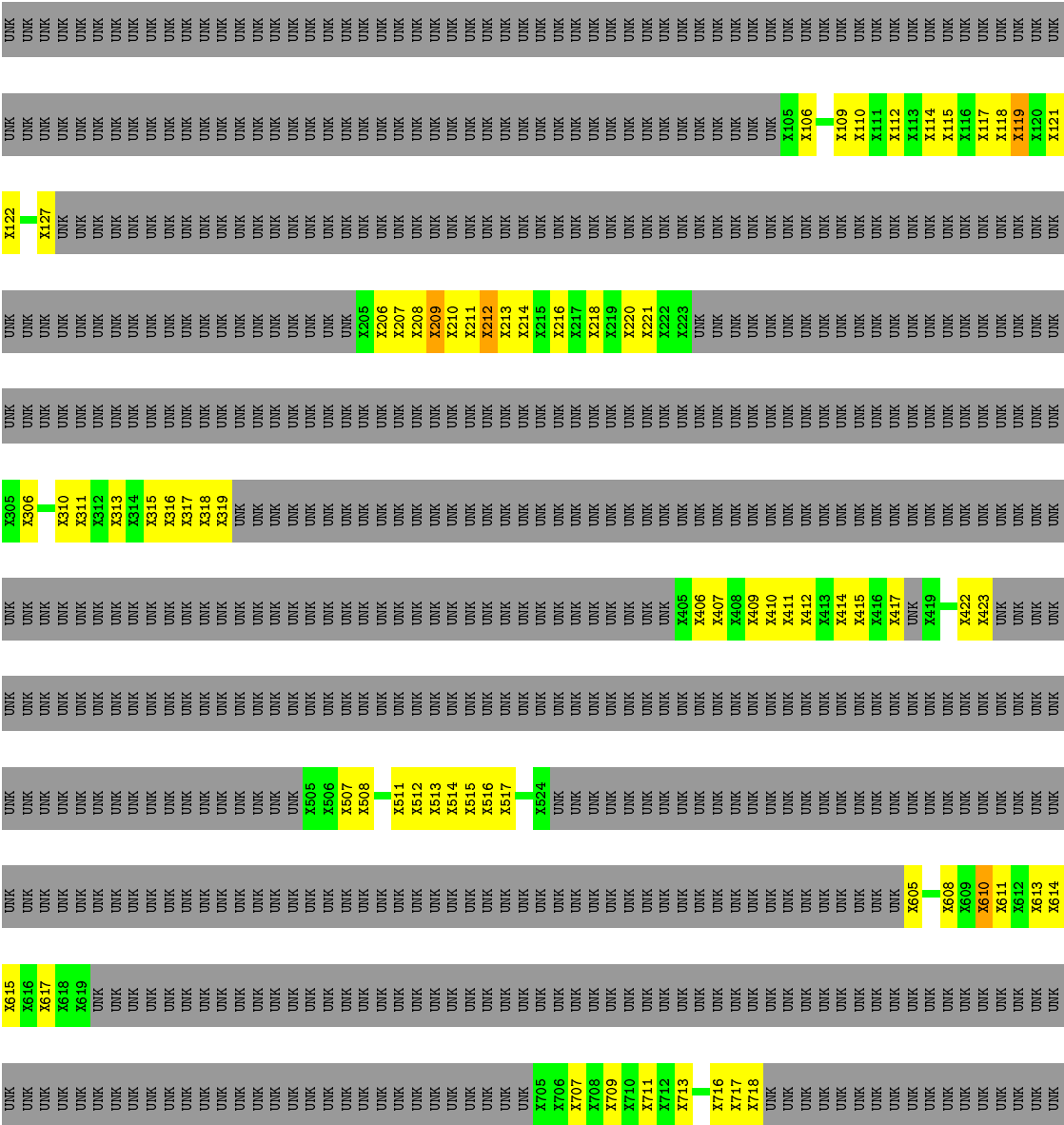


[illegible]



● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain P:  93%





[illegible]

[illegible]





[illegible]



[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain S:

98%





[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

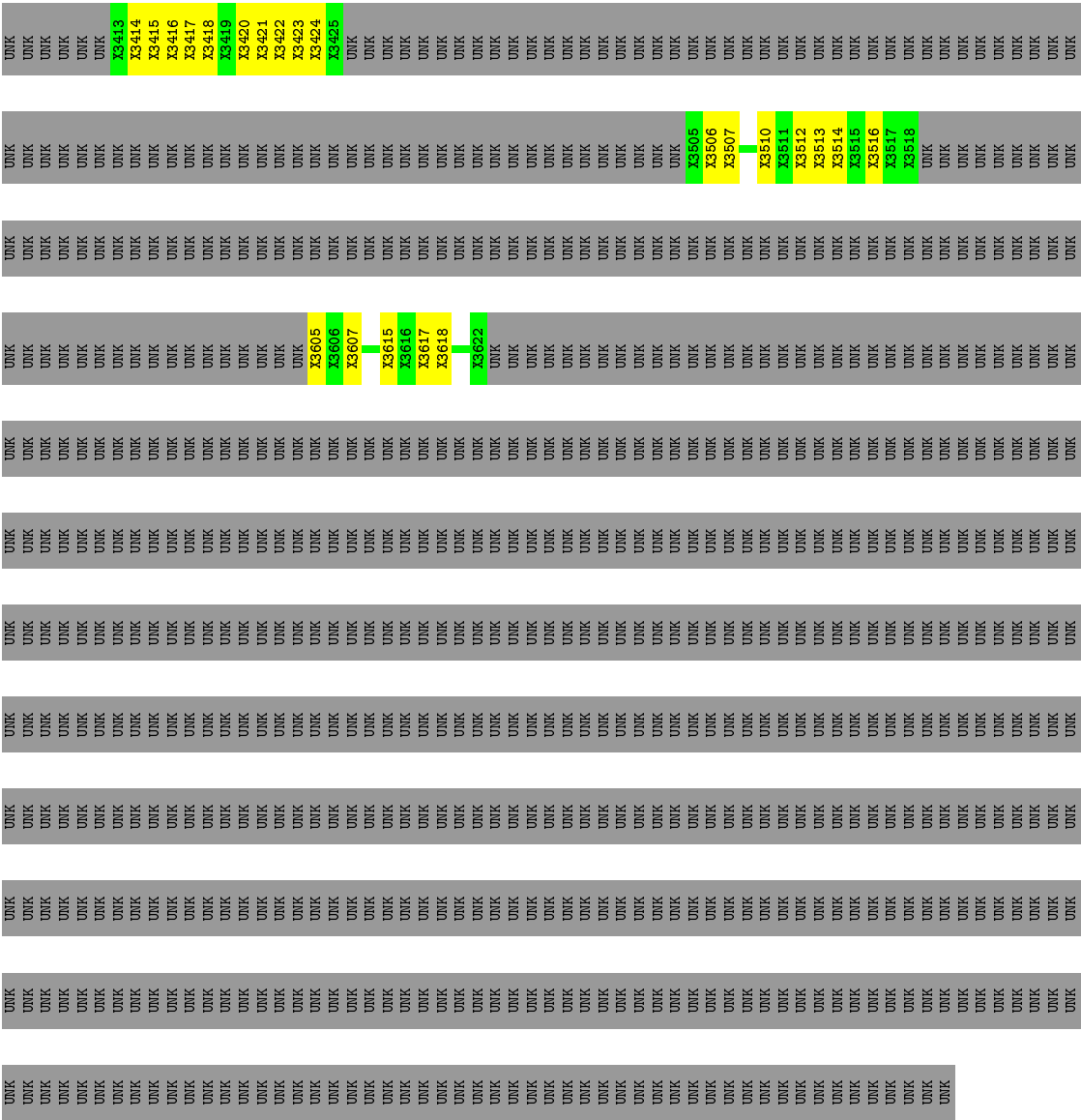
Chain T: 7% 6% 87%

X106	X107	X108	X109	X110	X111	X112	X113	X114	X115	X116	X117	X118	X119	X120	X121	X122	X123	X124	X125
X126	X127	X128	X129	X130	X131	X132	X133	X134	X135	X136	X137	X138	X139	X140	X141	X142	X143	X144	X145
X146	X147	X148	X149	X150	X151	X152	X153	X154	X155	X156	X157	X158	X159	X160	X161	X162	X163	X164	X165
X166	X167	X168	X169	X170	X171	X172	X173	X174	X175	X176	X177	X178	X179	X180	X181	X182	X183	X184	X185
X186	X187	X188	X189	X190	X191	X192	X193	X194	X195	X196	X197	X198	X199	X200	X201	X202	X203	X204	X205
X206	X207	X208	X209	X210	X211	X212	X213	X214	X215	X216	X217	X218	X219	X220	X221	X222	X223	X224	X225
X226	X227	X228	X229	X230	X231	X232	X233	X234	X235	X236	X237	X238	X239	X240	X241	X242	X243	X244	X245
X246	X247	X248	X249	X250	X251	X252	X253	X254	X255	X256	X257	X258	X259	X260	X261	X262	X263	X264	X265
X266	X267	X268	X269	X270	X271	X272	X273	X274	X275	X276	X277	X278	X279	X280	X281	X282	X283	X284	X285
X286	X287	X288	X289	X290	X291	X292	X293	X294	X295	X296	X297	X298	X299	X300	X301	X302	X303	X304	X305
X306	X307	X308	X309	X310	X311	X312	X313	X314	X315	X316	X317	X318	X319	X320	X321	X322	X323	X324	X325
X326	X327	X328	X329	X330	X331	X332	X333	X334	X335	X336	X337	X338	X339	X340	X341	X342	X343	X344	X345
X346	X347	X348	X349	X350	X351	X352	X353	X354	X355	X356	X357	X358	X359	X360	X361	X362	X363	X364	X365
X366	X367	X368	X369	X370	X371	X372	X373	X374	X375	X376	X377	X378	X379	X380	X381	X382	X383	X384	X385
X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X397	X398	X399	X400	X401	X402	X403	X404	X405
X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425
X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445
X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465
X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485
X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	X501	X502	X503	X504	X505
X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525
X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X540	X541	X542	X543	X544	X545
X546	X547	X548	X549	X550	X551	X552	X553	X554	X555	X556	X557	X558	X559	X560	X561	X562	X563	X564	X565
X566	X567	X568	X569	X570	X571	X572	X573	X574	X575	X576	X577	X578	X579	X580	X581	X582	X583	X584	X585
X586	X587	X588	X589	X590	X591	X592	X593	X594	X595	X596	X597	X598	X599	X600	X601	X602	X603	X604	X60

[illegible]

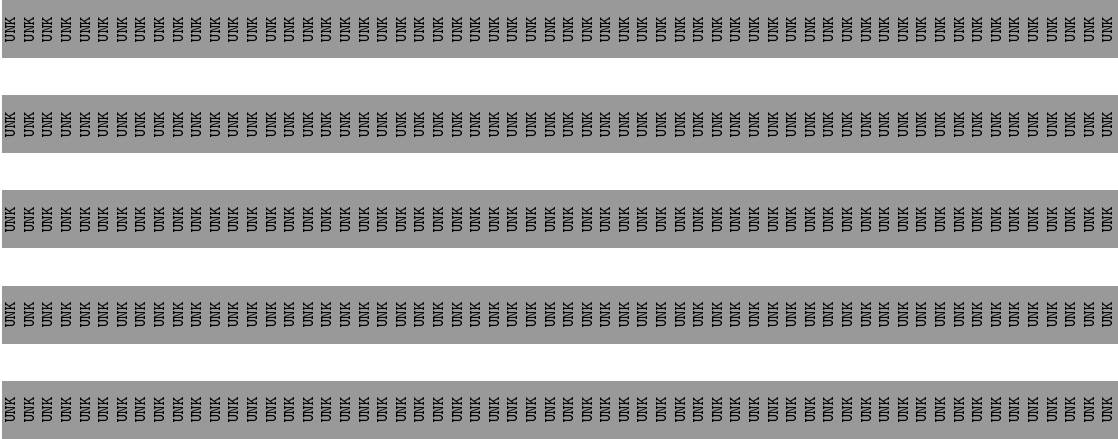






● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain Y:  95%





[illegible]

[illegible]

UNITED STATES DISTRICT COURT

UNIK

[illegible][illegible][illegible][illegible][illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.60Å 132.99Å 297.00Å 90.00° 105.58° 90.00°	Depositor
Resolution (Å)	100.00 – 6.60 91.97 – 6.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (100.00-6.60) 97.6 (91.97-6.58)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.86 (at 6.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.442 , 0.441 0.441 , 0.440	Depositor DCC
R_{free} test set	1214 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	269.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 633.9	EDS
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 23876 reflections	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	20320	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	18
1	C	0	8
1	D	0	8
1	E	0	3
1	F	0	6
1	O	0	2
1	P	0	18
1	Q	0	8
1	R	0	8
1	S	0	3
1	T	0	6
1	X	0	7
1	Y	0	7
All	All	0	104

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1214	UNK	Peptide
1	A	2306	UNK	Peptide
1	B	119	UNK	Peptide
1	B	122	UNK	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	209	UNK	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	1770	0	429	123	0
1	B	1415	0	356	149	0
1	C	2030	0	489	178	0
1	D	910	0	239	117	0
1	E	325	0	78	20	0
1	F	2655	0	648	203	0
1	O	1770	0	429	123	48
1	P	1415	0	358	153	0
1	Q	2030	0	489	180	0
1	R	910	0	239	119	0
1	S	325	0	78	19	0
1	T	2655	0	648	208	48
1	X	1055	0	263	74	0
1	Y	1055	0	264	75	0
All	All	20320	0	5007	1740	48

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 69.

The worst 5 of 1740 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:1412:UNK:CA	1:B:1412:UNK:C	1.75	1.64
1:P:1412:UNK:C	1:P:1412:UNK:CA	1.74	1.58
1:P:1412:UNK:HA	1:P:1415:UNK:CB	1.69	1.22
1:B:1412:UNK:HA	1:B:1415:UNK:CB	1.69	1.20
1:E:116:UNK:O	1:E:118:UNK:N	1.76	1.17

The worst 5 of 48 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:619:UNK:C	1:T:2418:UNK:O[1_545]	0.56	1.64
1:O:620:UNK:C	1:T:2419:UNK:CA[1_545]	0.57	1.63
1:O:622:UNK:N	1:T:2418:UNK:N[1_545]	0.67	1.53
1:O:622:UNK:C	1:T:2417:UNK:O[1_545]	0.68	1.52
1:O:621:UNK:O	1:T:2417:UNK:CA[1_545]	0.91	1.29

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	0/4128	-	-	-	-
1	B	0/4128	-	-	-	-
1	C	0/4128	-	-	-	-
1	D	0/4128	-	-	-	-
1	E	0/4128	-	-	-	-
1	F	0/4128	-	-	-	-
1	O	0/4128	-	-	-	-
1	P	0/4128	-	-	-	-
1	Q	0/4128	-	-	-	-
1	R	0/4128	-	-	-	-
1	S	0/4128	-	-	-	-
1	T	0/4128	-	-	-	-
1	X	0/4128	-	-	-	-
1	Y	0/4128	-	-	-	-
All	All	0/57792	-	-	-	-

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.