wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 06:38 am BST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

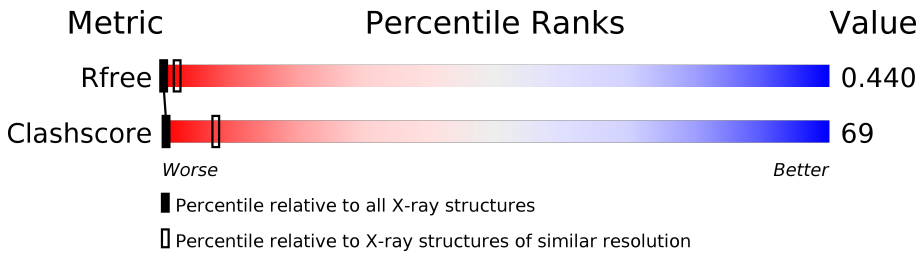
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)

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 on 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 <=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% • 91%
1	B	4128	• • 93%
1	C	4128	5% 5% 90%
1	D	4128	• • 96%
1	E	4128	•• 98%
1	F	4128	7% 6% 87%
1	O	4128	5% • 91%
1	P	4128	• • 93%
1	Q	4128	5% 5% 90%

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Mol	Chain	Length	Quality of chain
1	R	4128	96%
1	S	4128	98%
1	T	4128	7% 6% 87%
1	X	4128	95%
1	Y	4128	95%

2 Entry composition (i)

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.

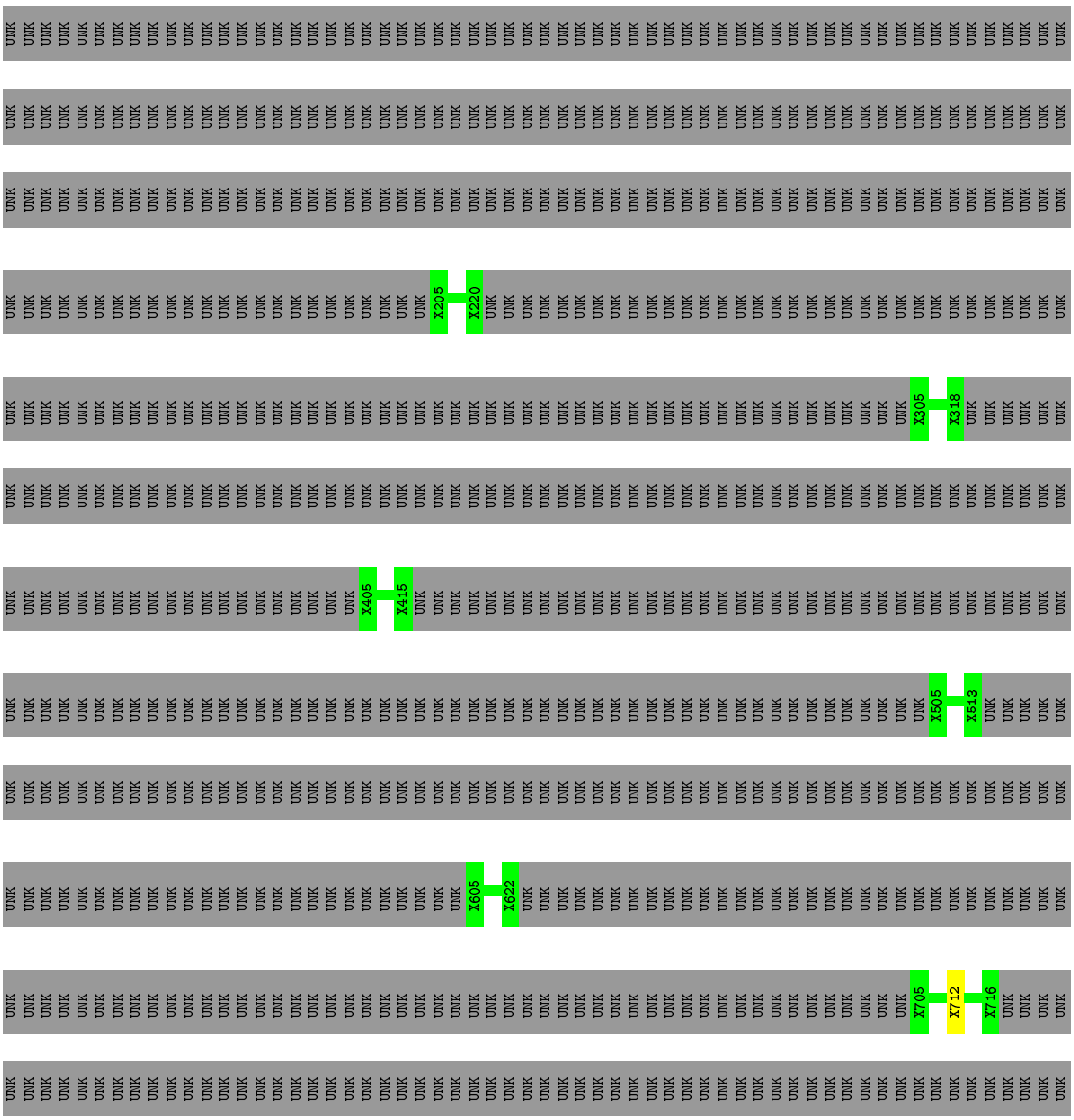
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	354	1770	1062	354	354	0	0	0
1	B	283	1415	849	283	283	0	0	0
1	C	406	2030	1218	406	406	0	0	0
1	D	182	910	546	182	182	0	0	0
1	E	65	325	195	65	65	0	0	0
1	F	531	2655	1593	531	531	0	0	0
1	X	211	1055	633	211	211	0	0	0
1	O	354	1770	1062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

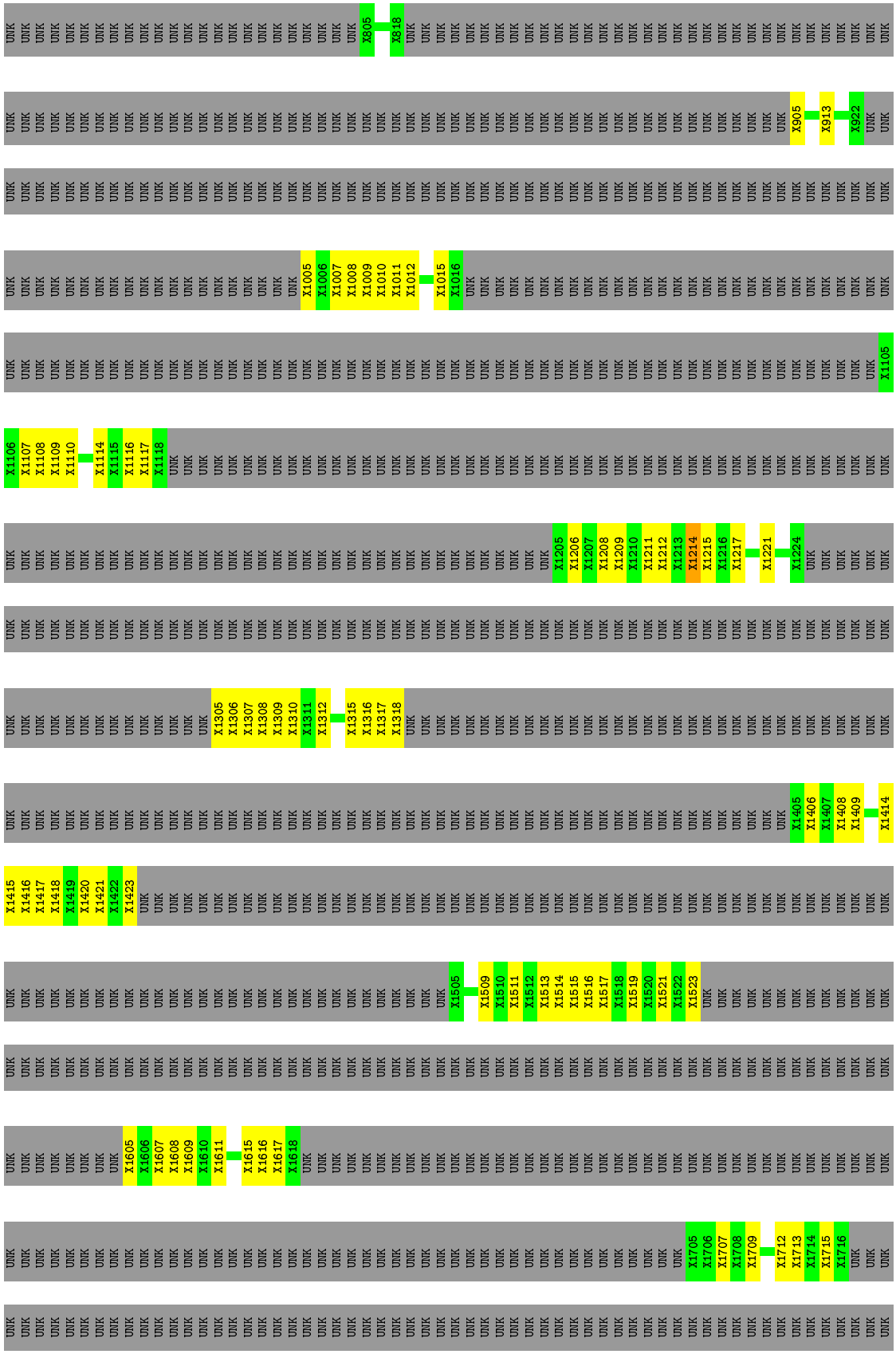
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

Chain A: 5% • 91%

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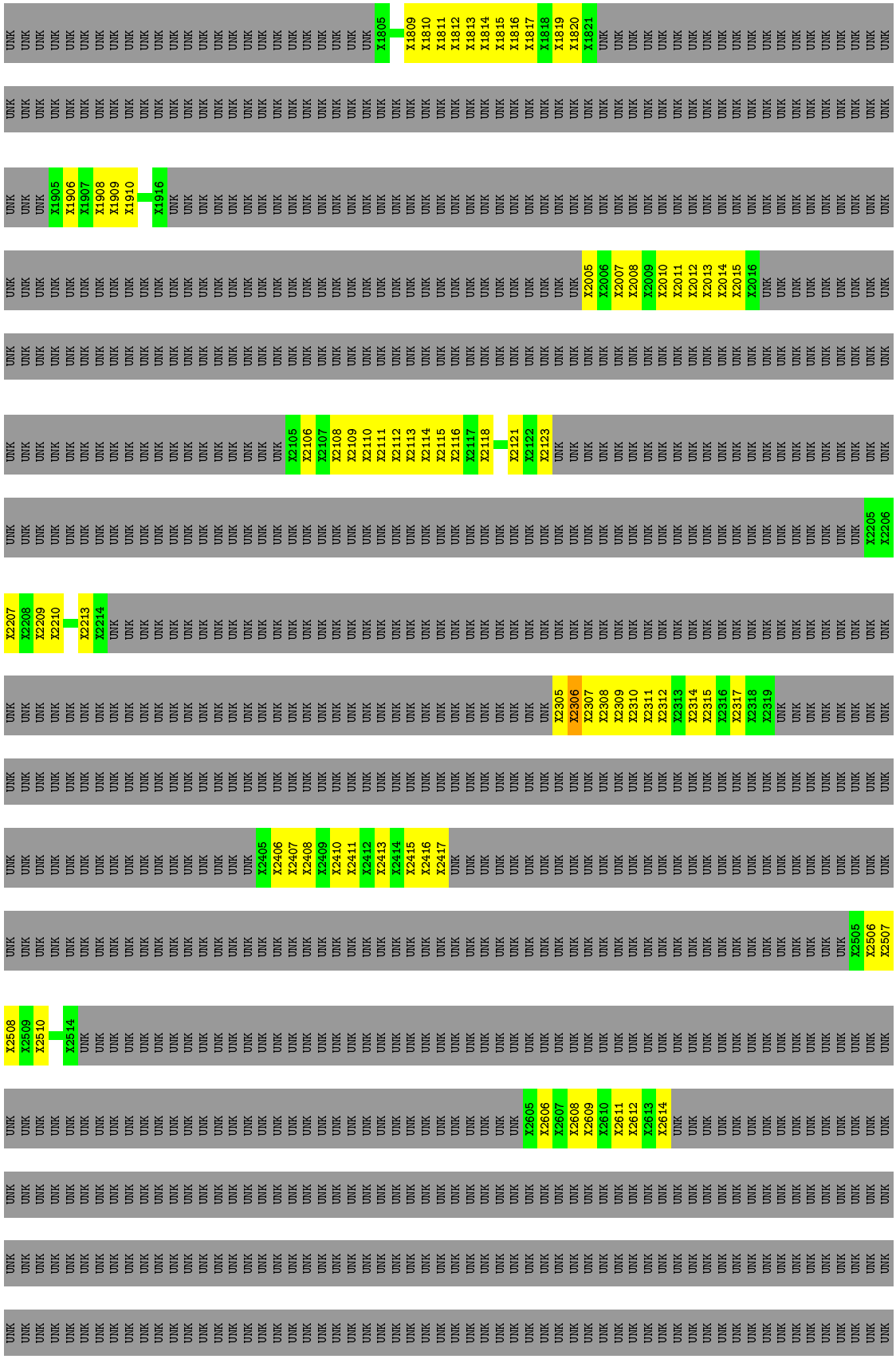
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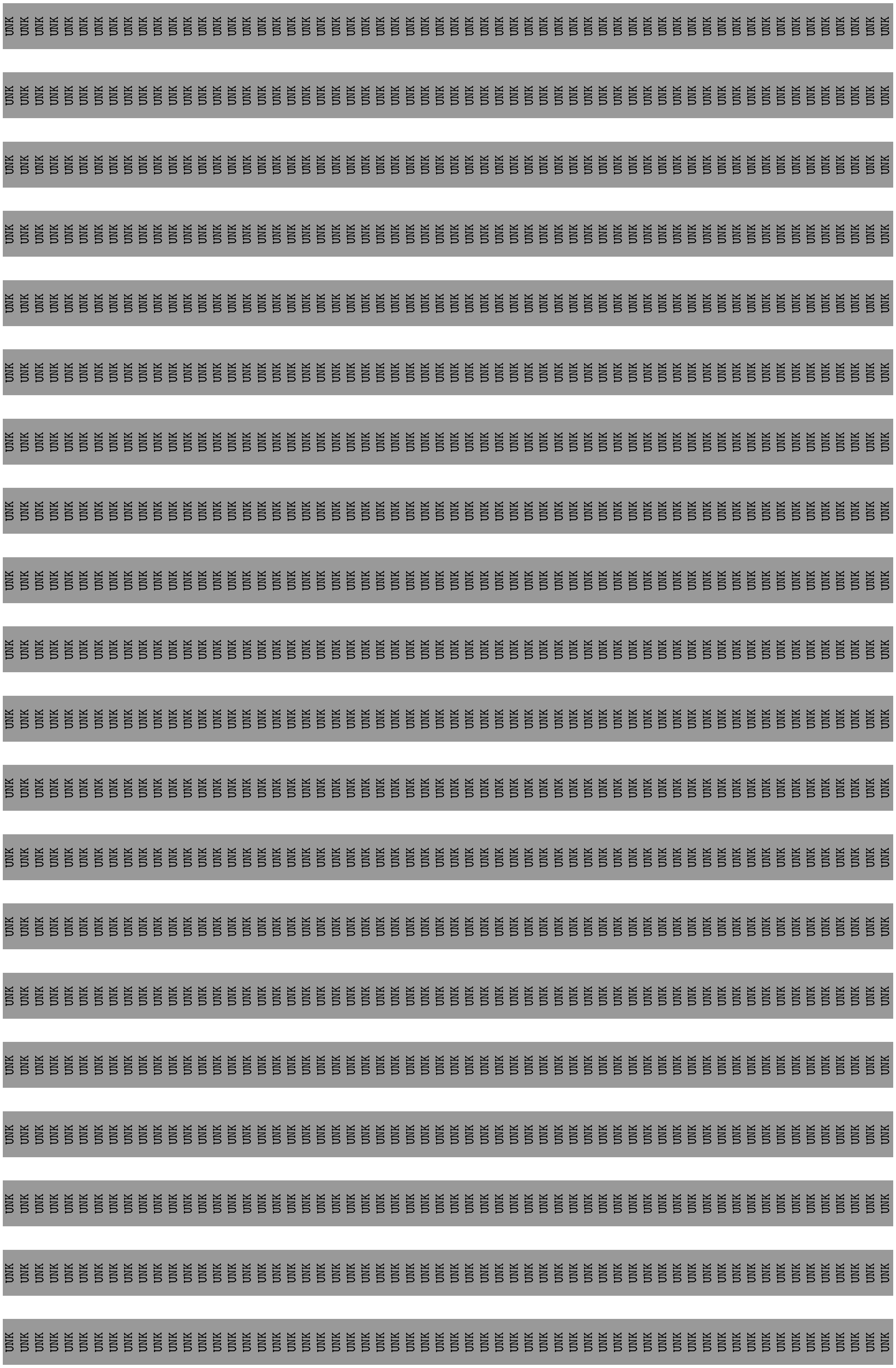
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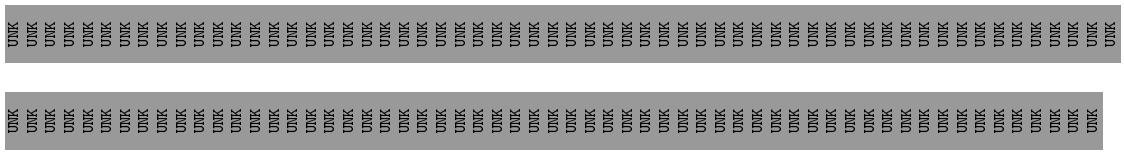
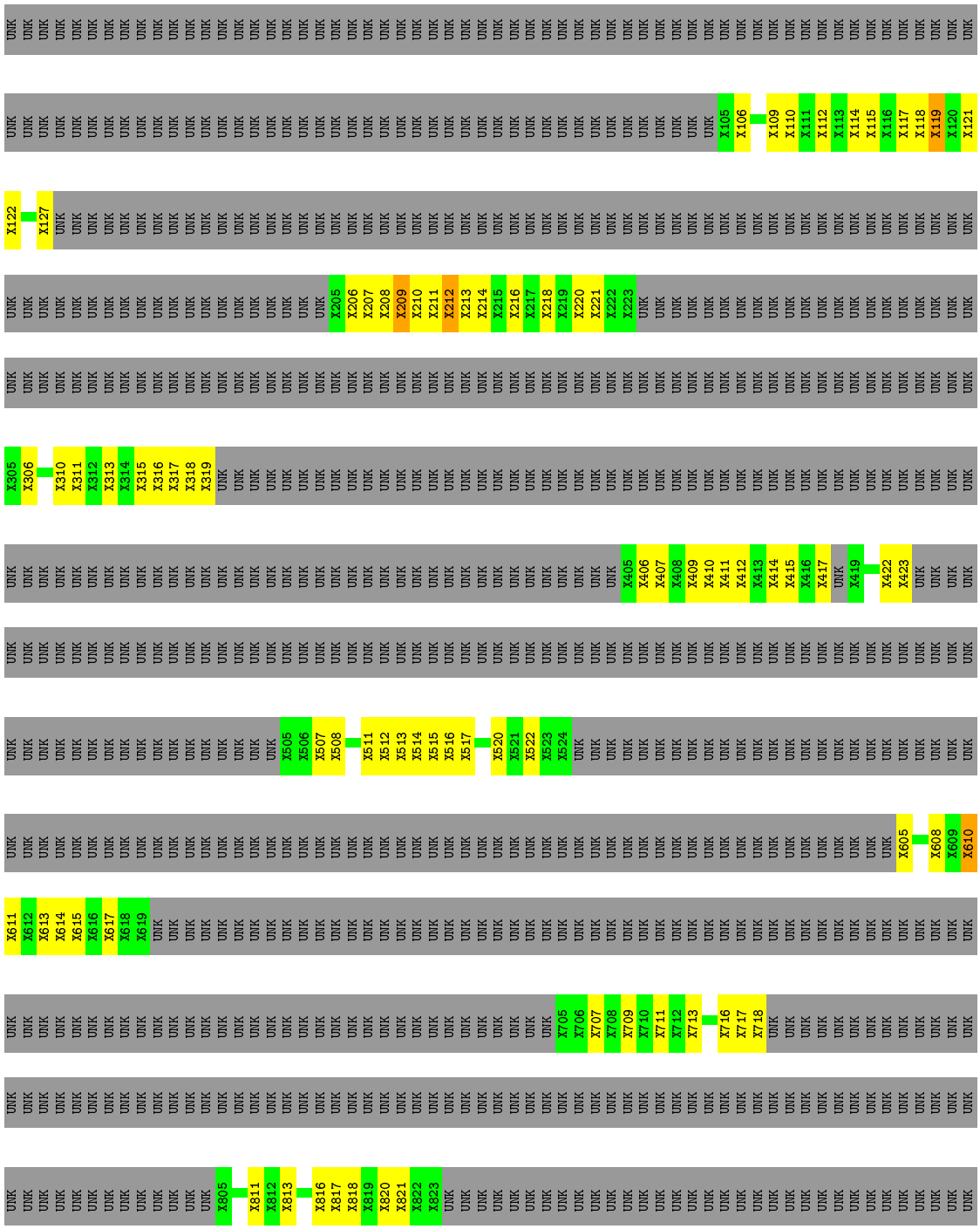
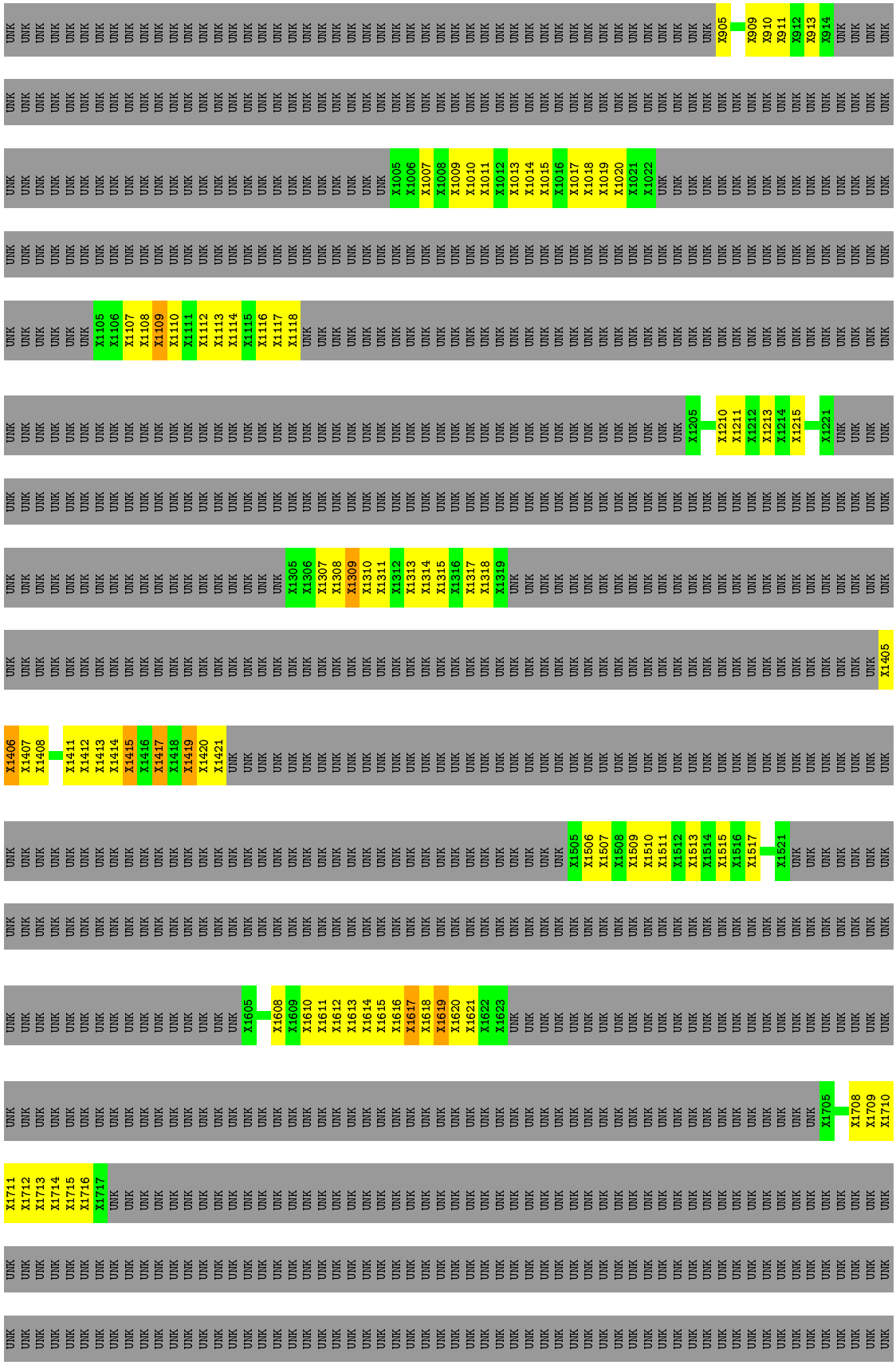


• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain B: 93%

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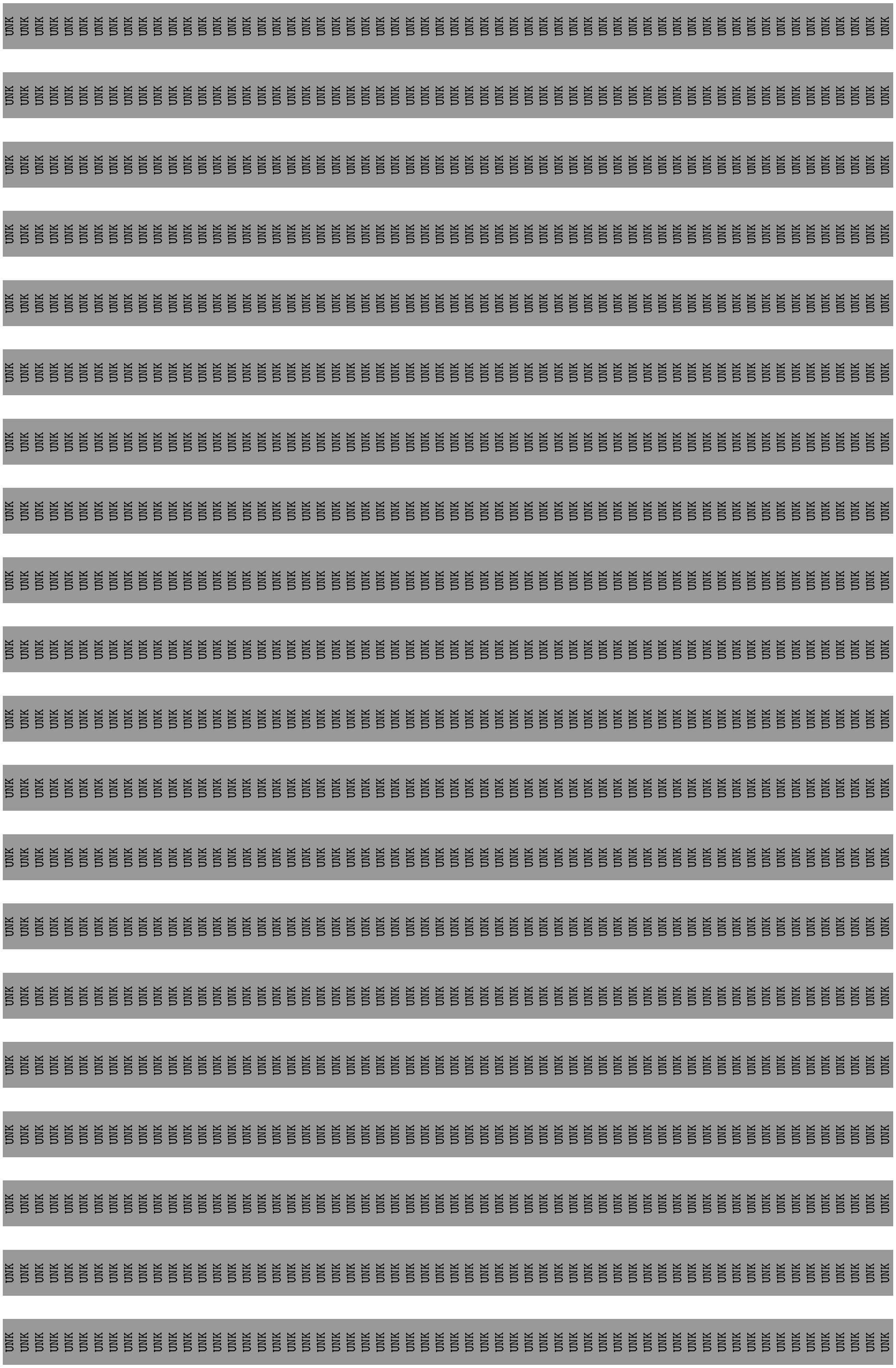
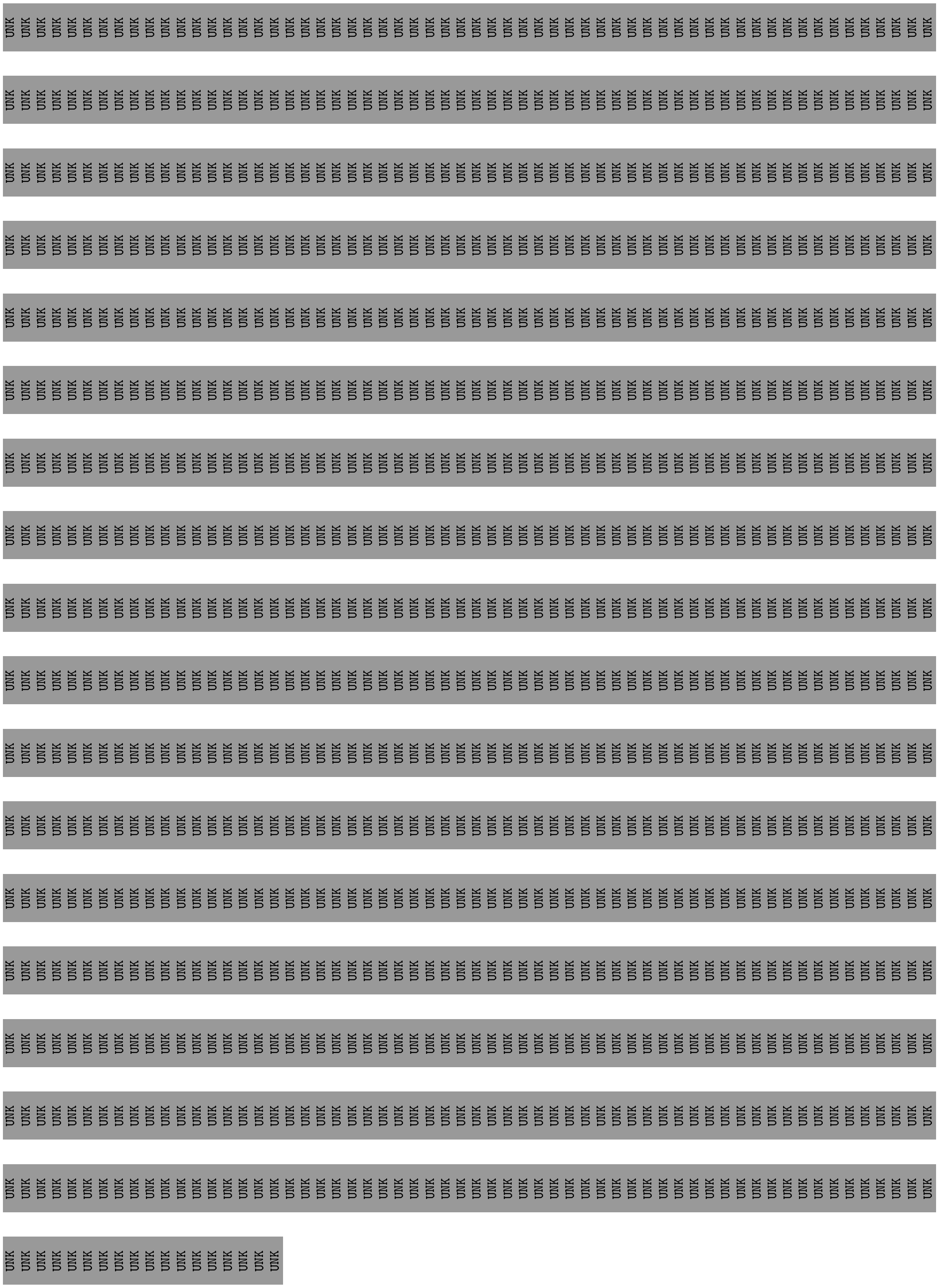
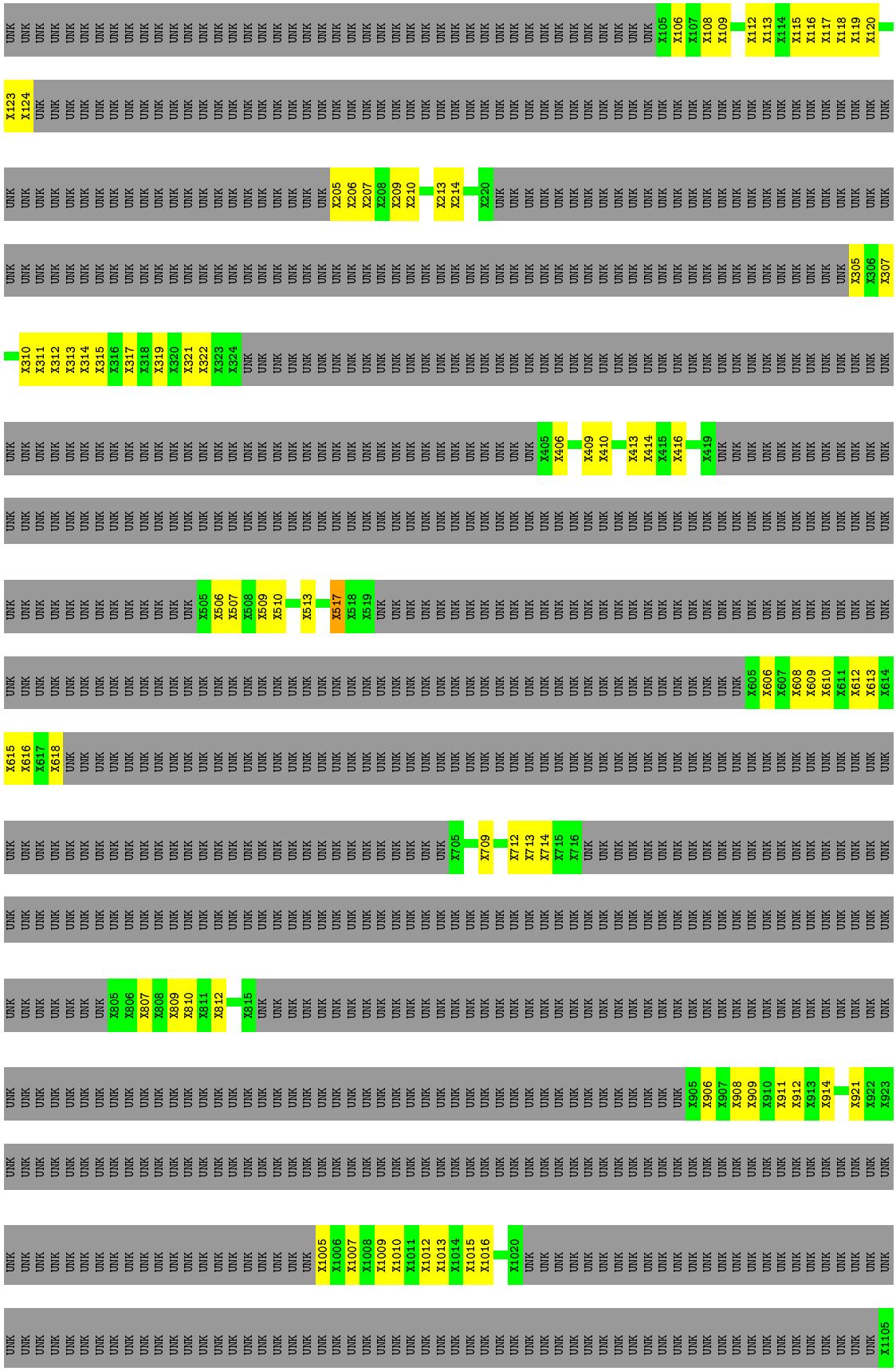




• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain C: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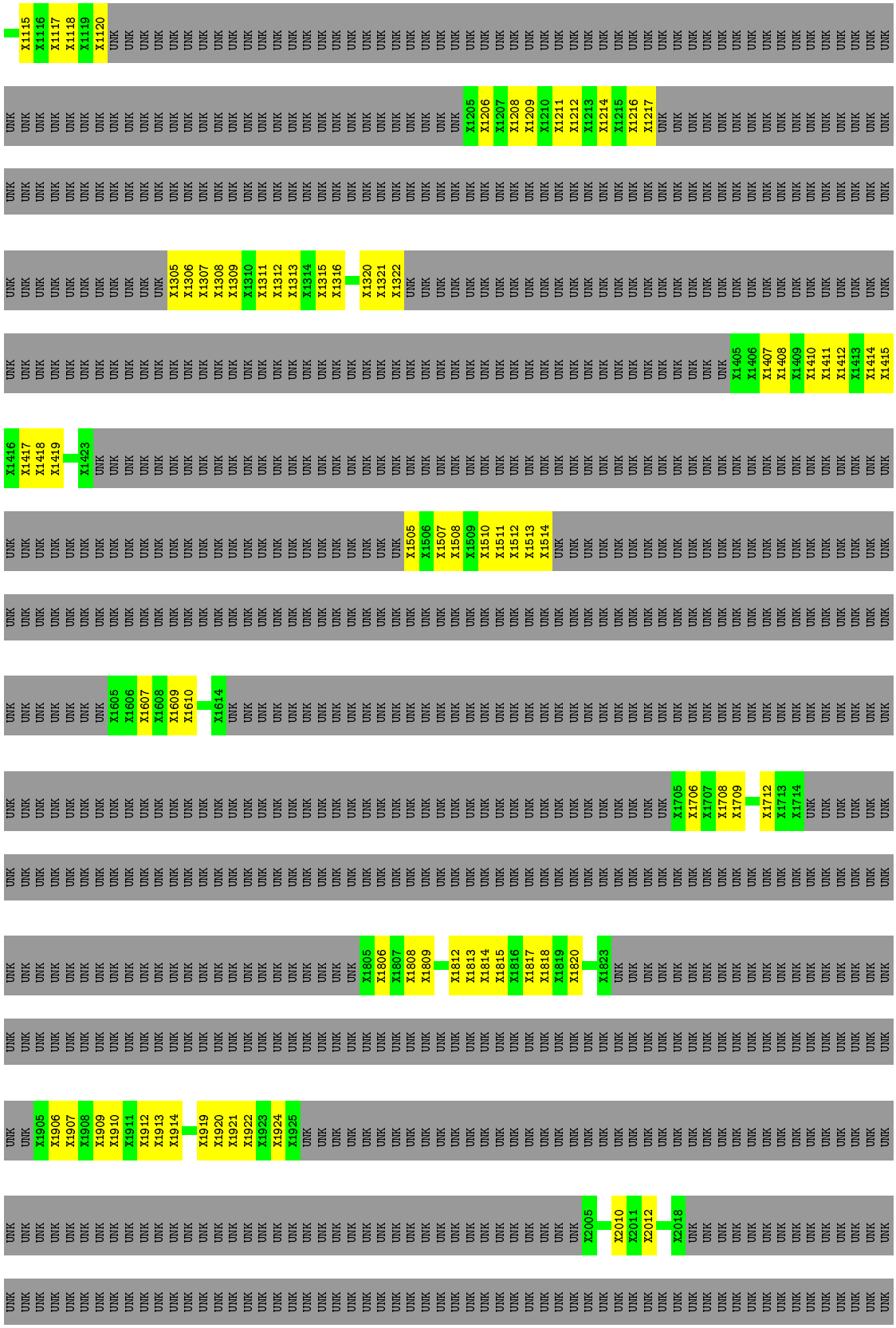
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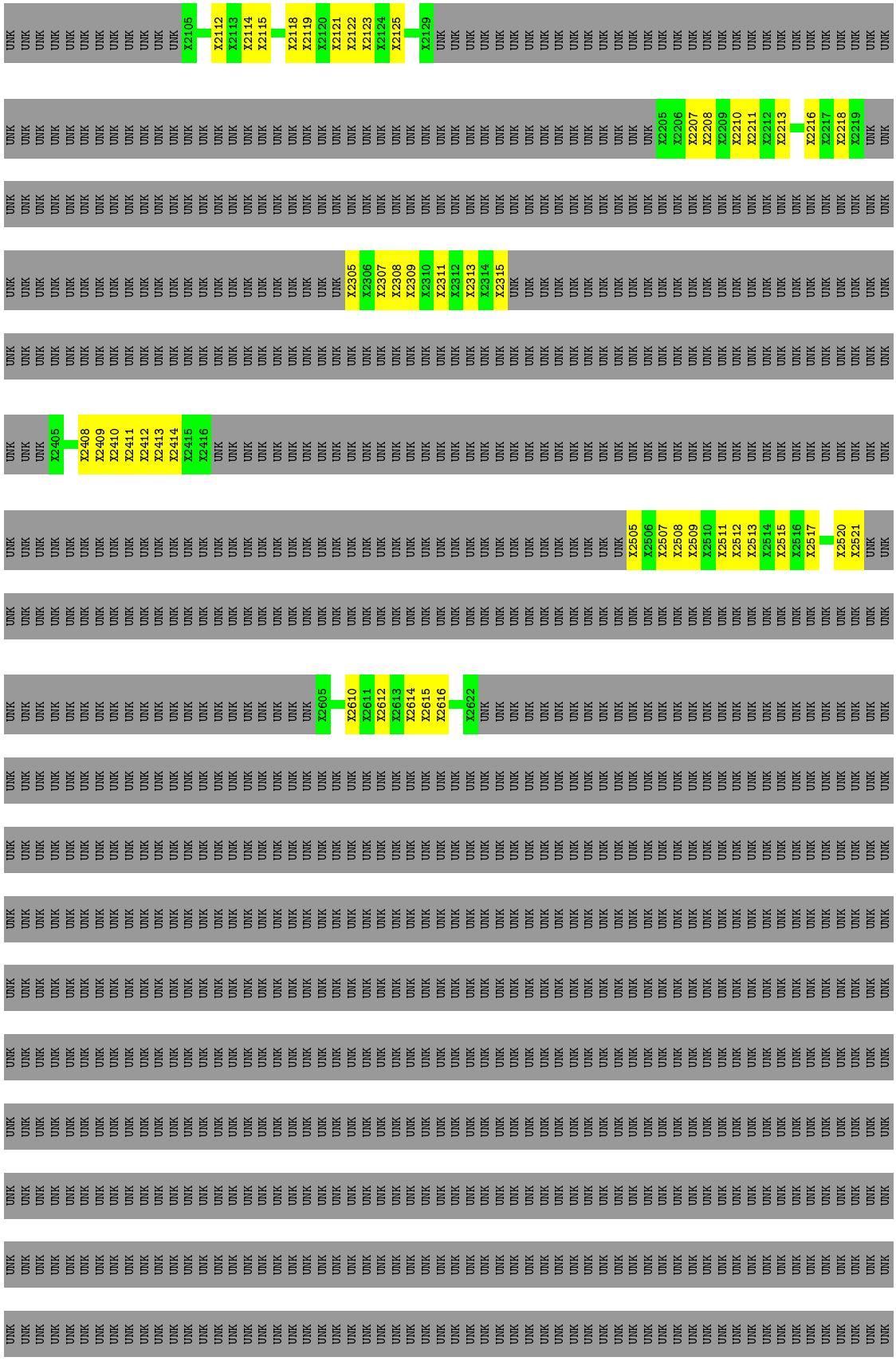
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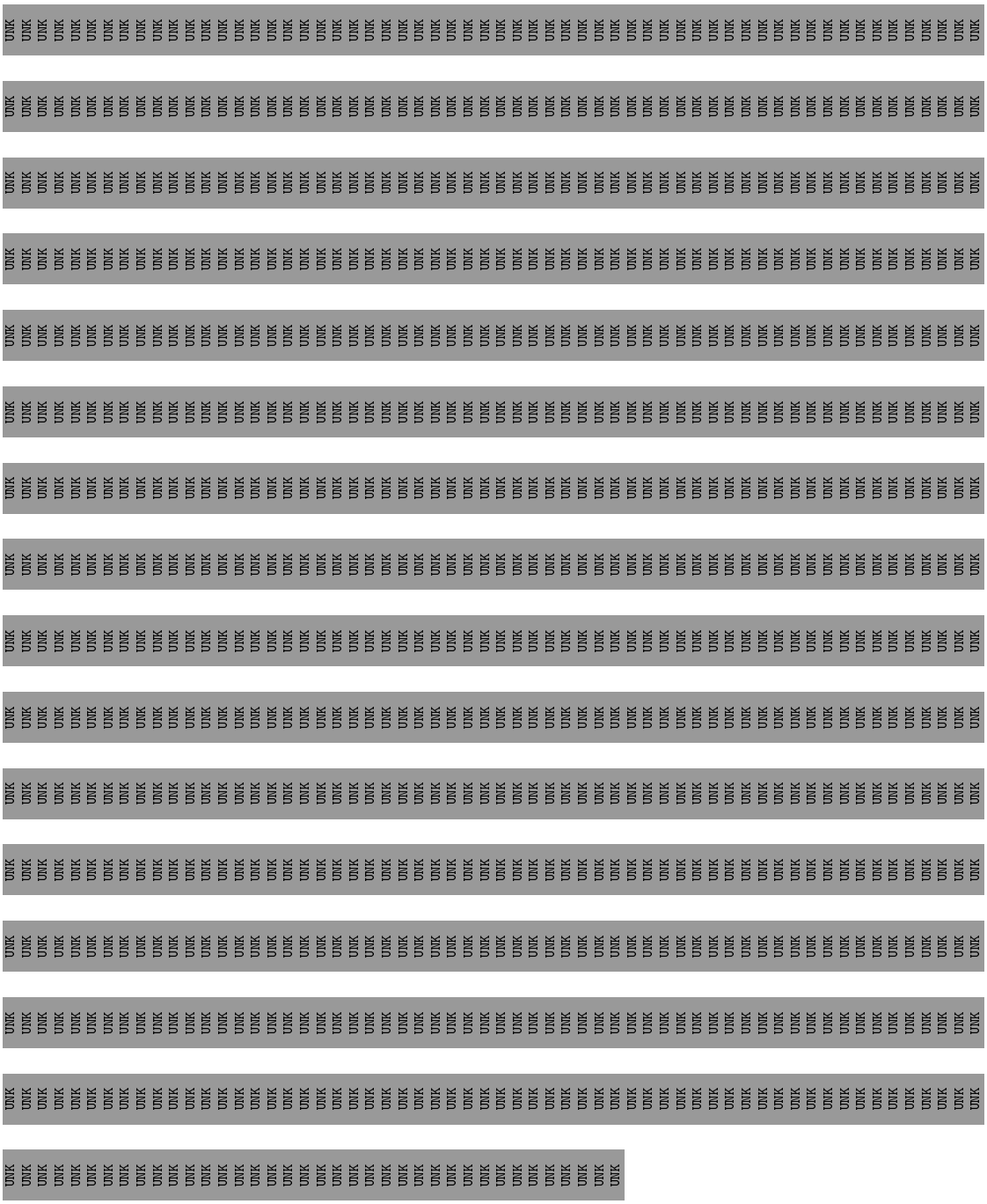
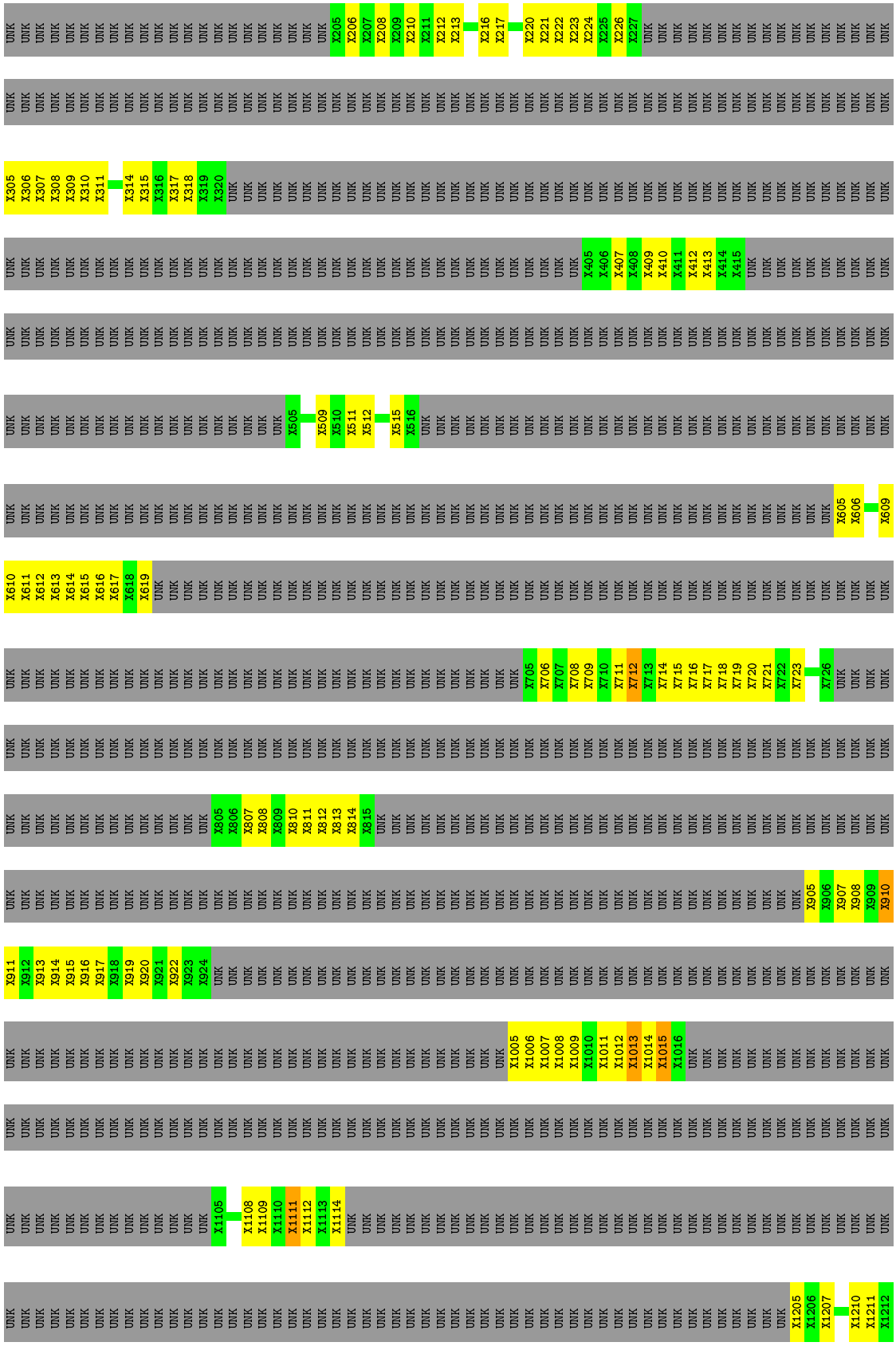


- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain D: 96%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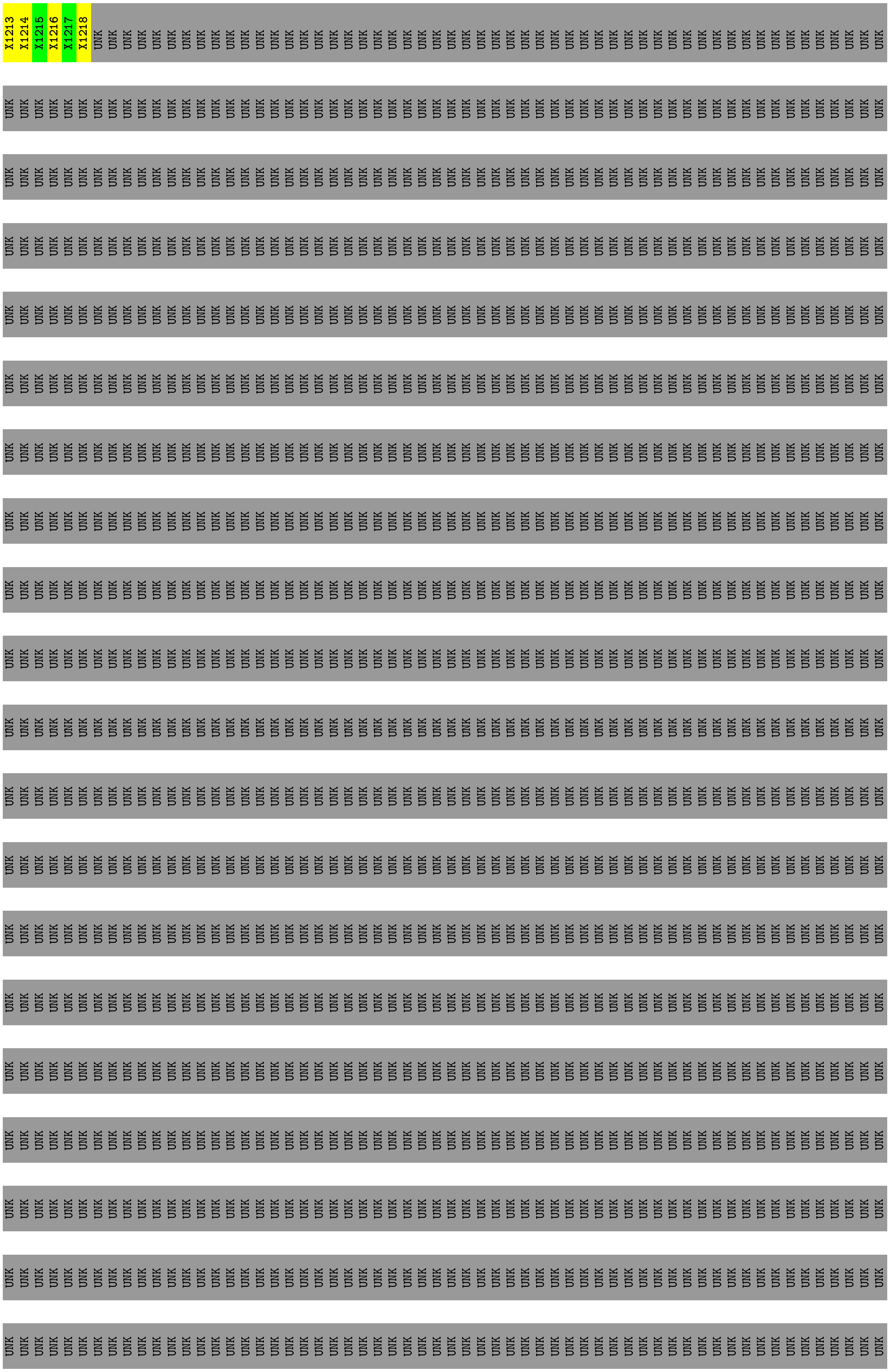
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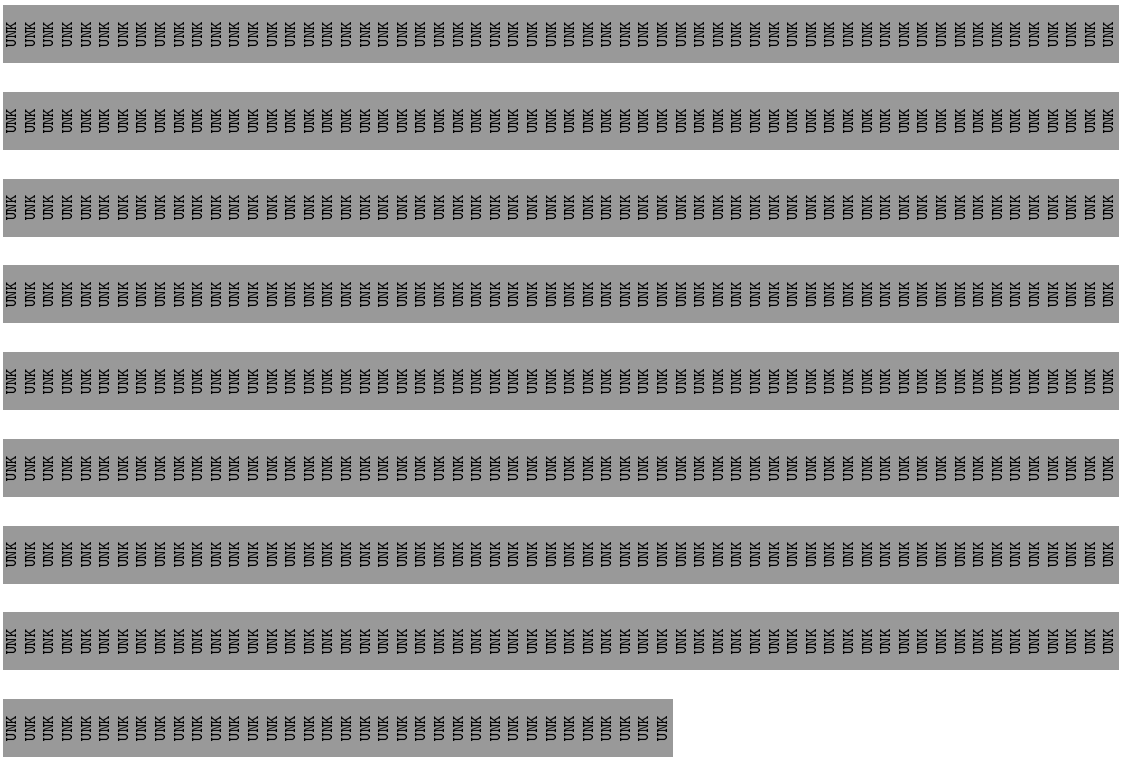
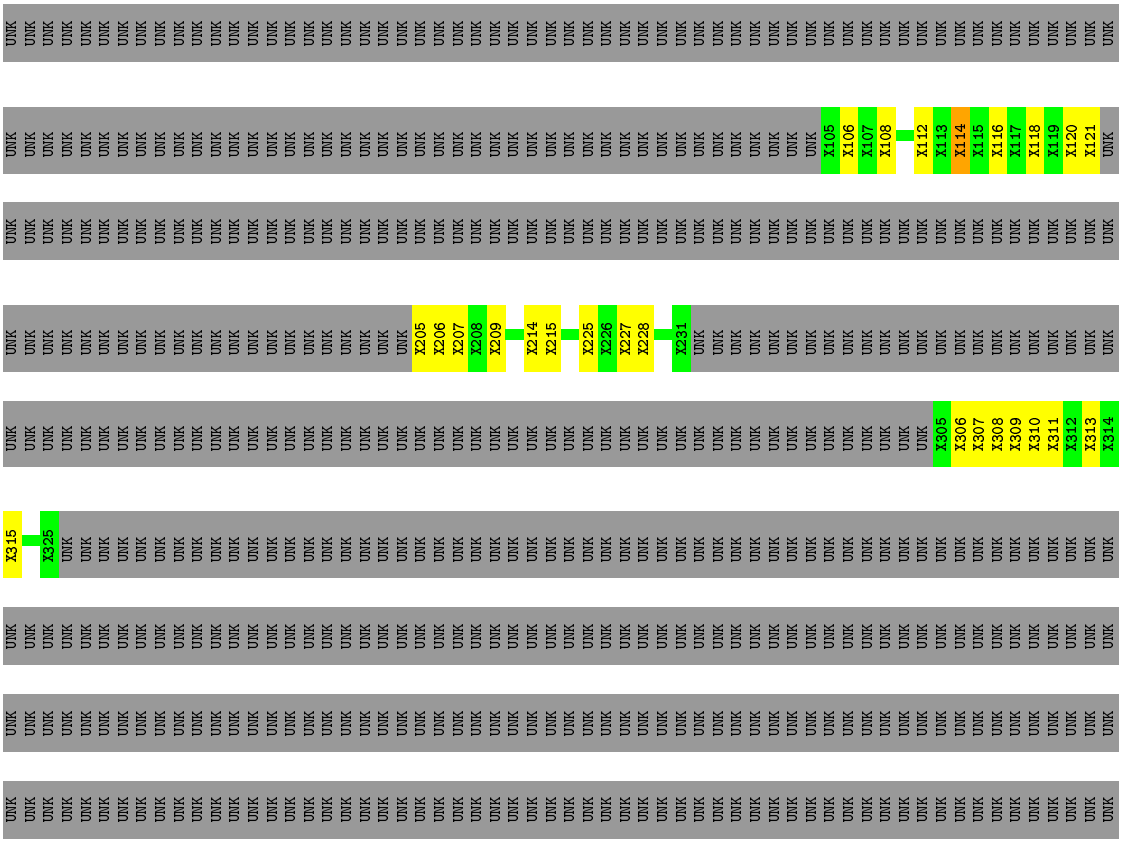
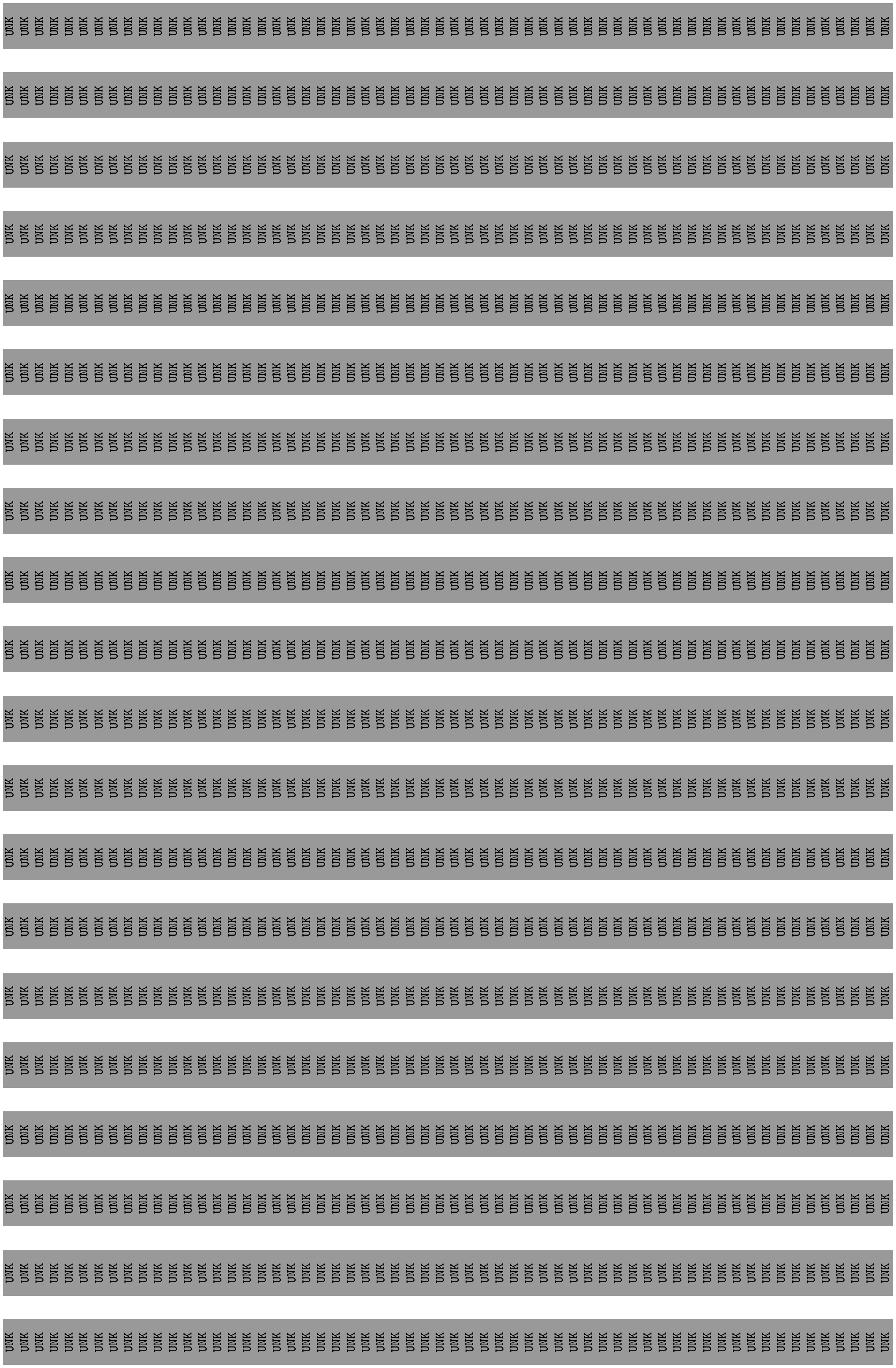
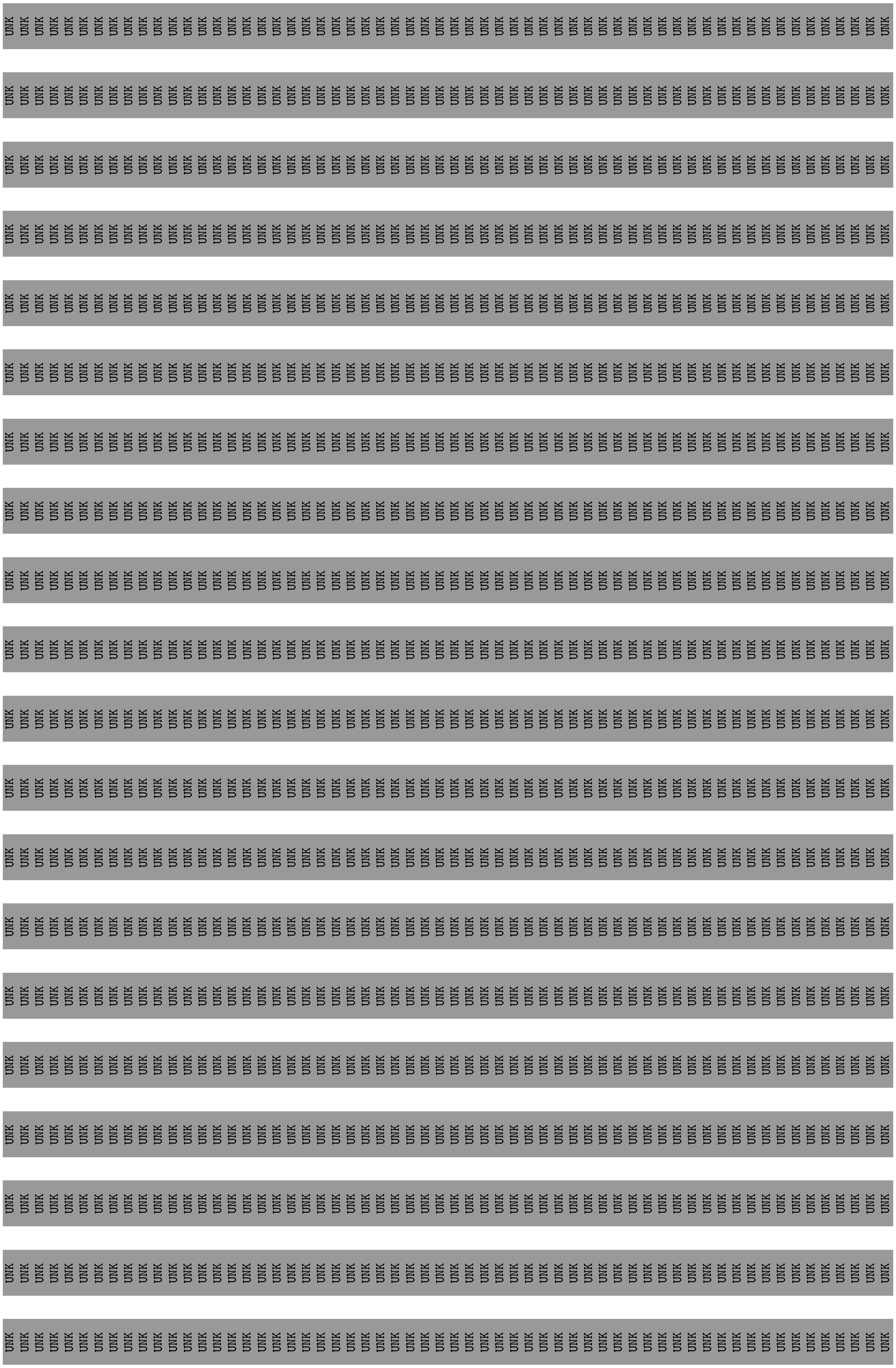


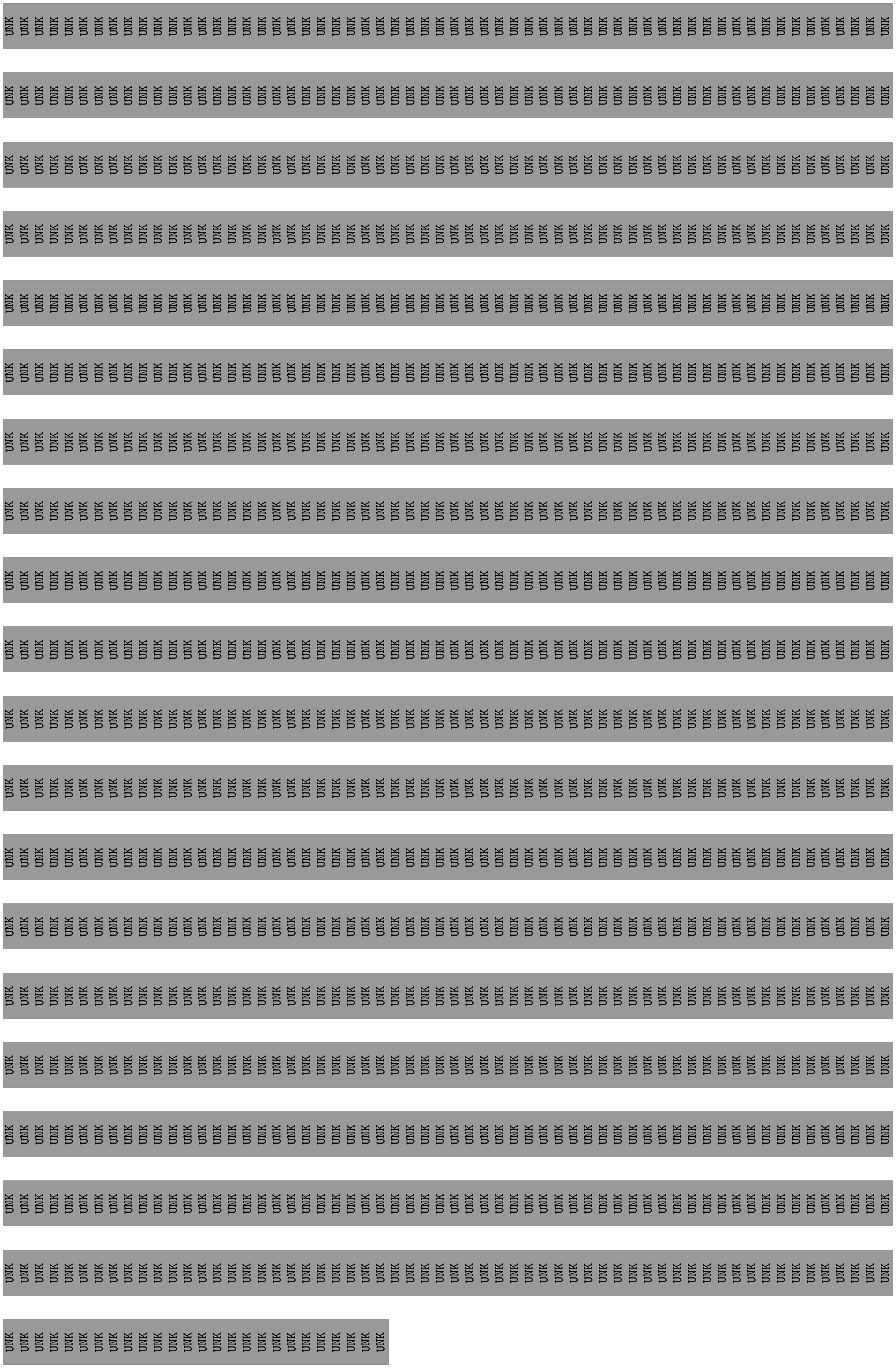
- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain E: 98%



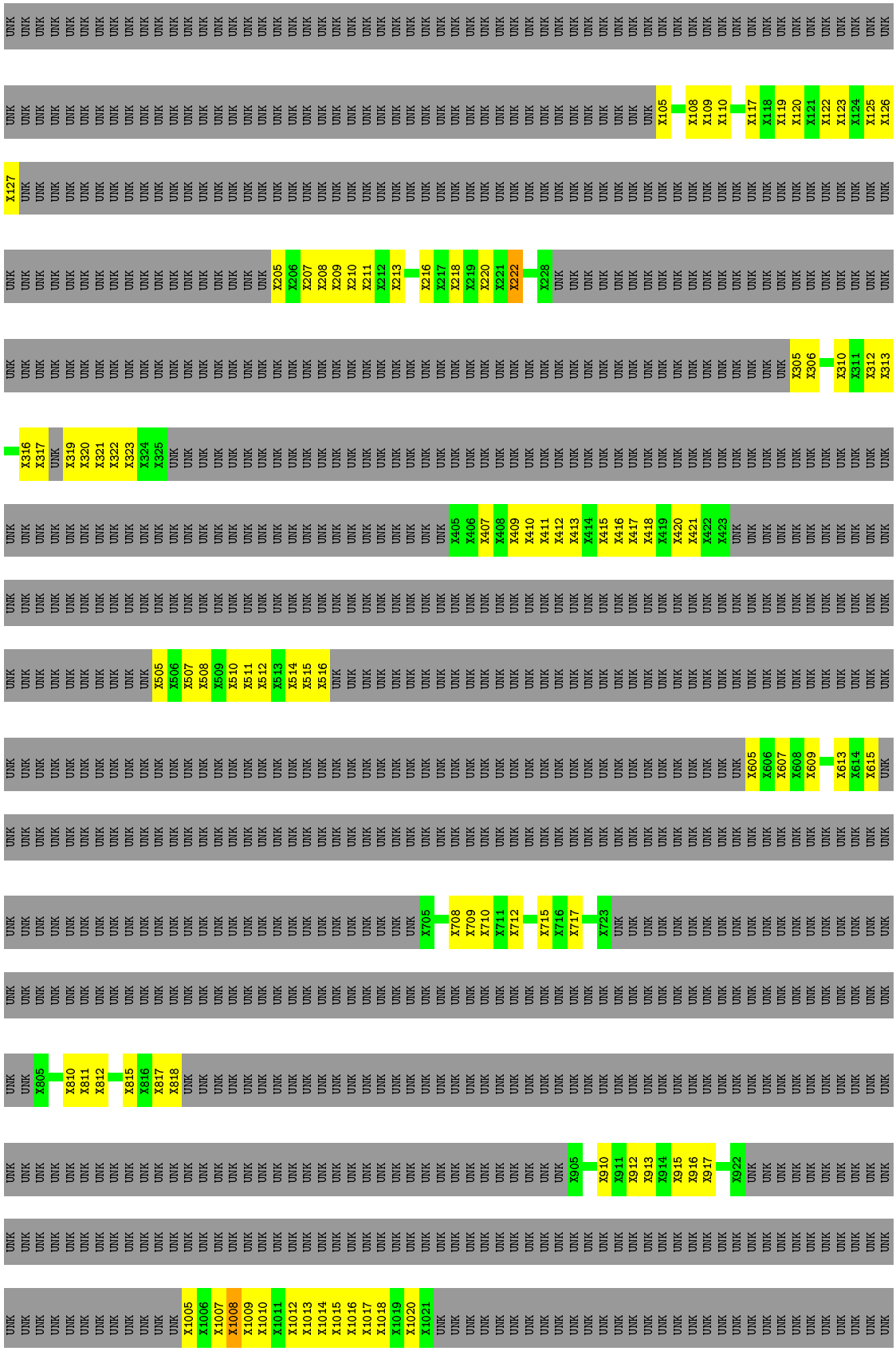






- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain F: 7% 6% 87%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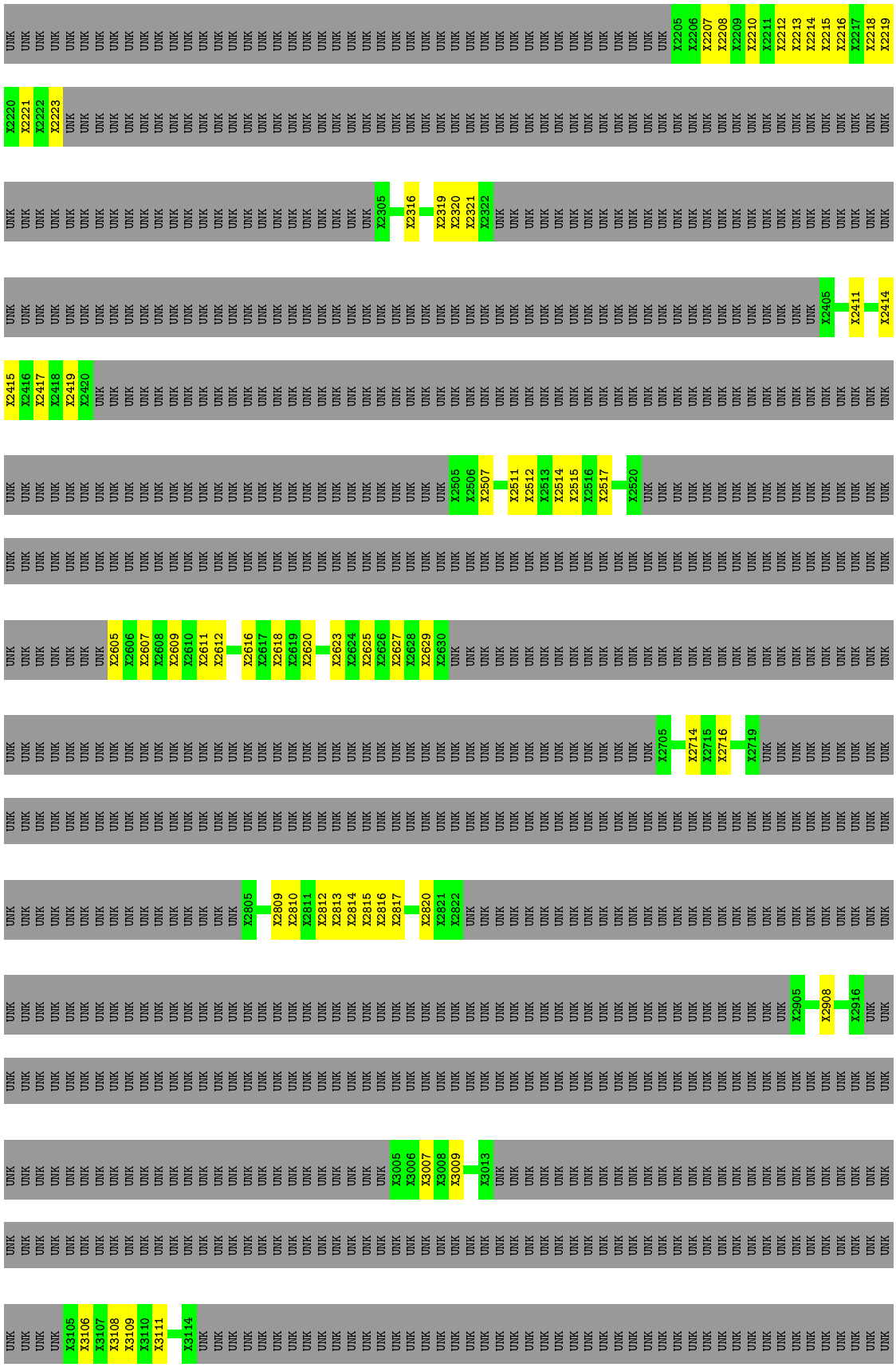
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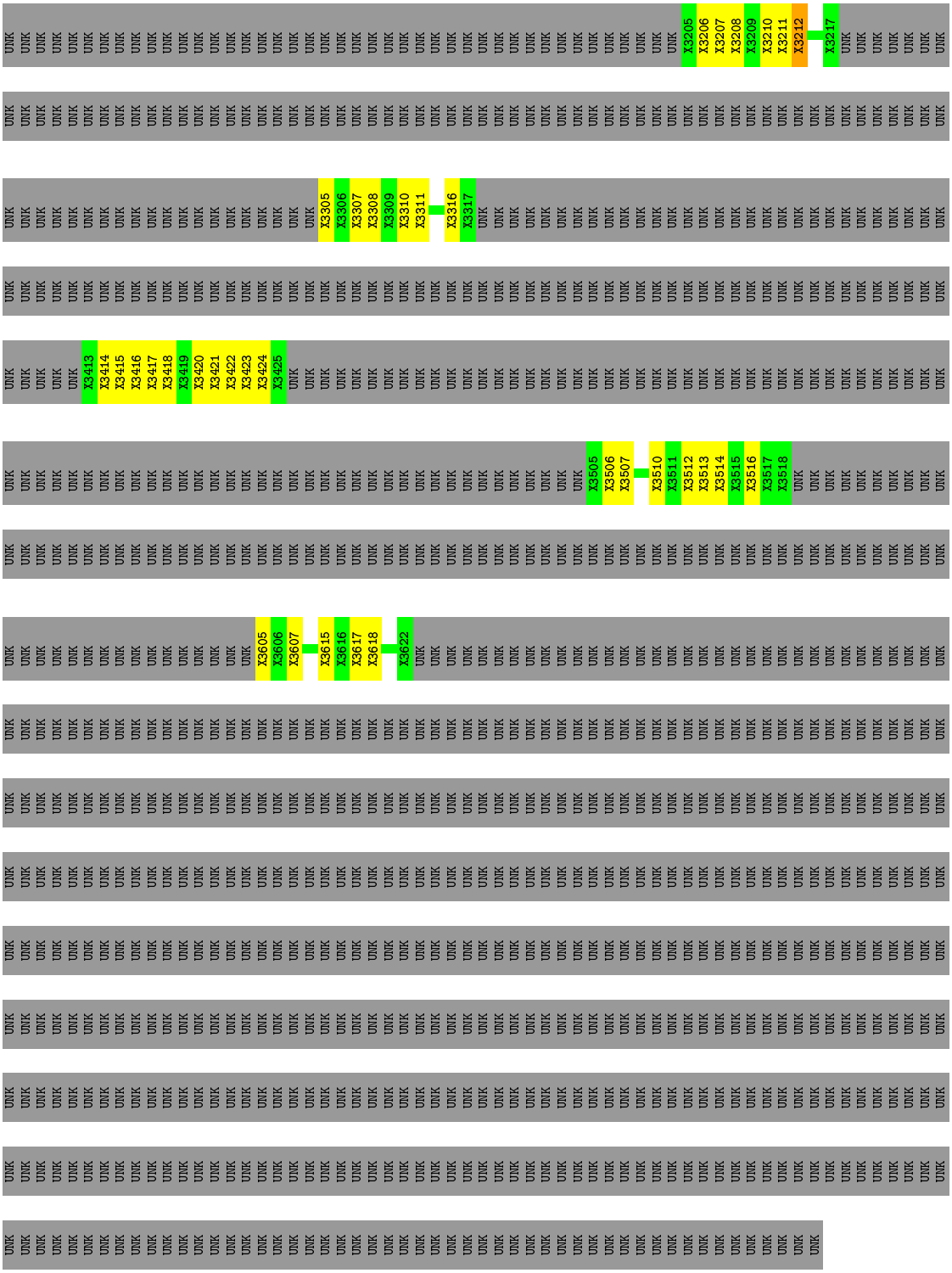
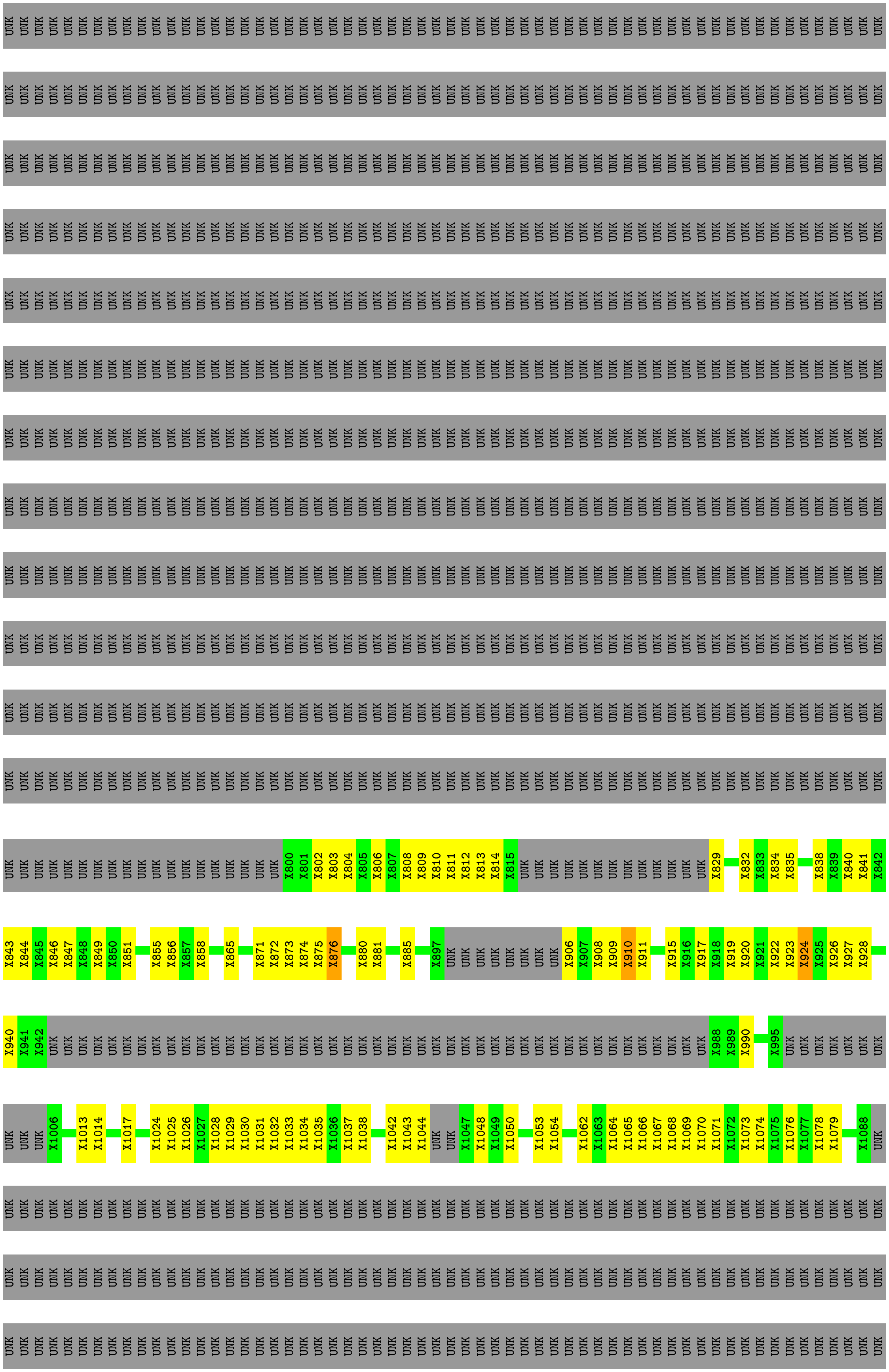


- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain X: 95%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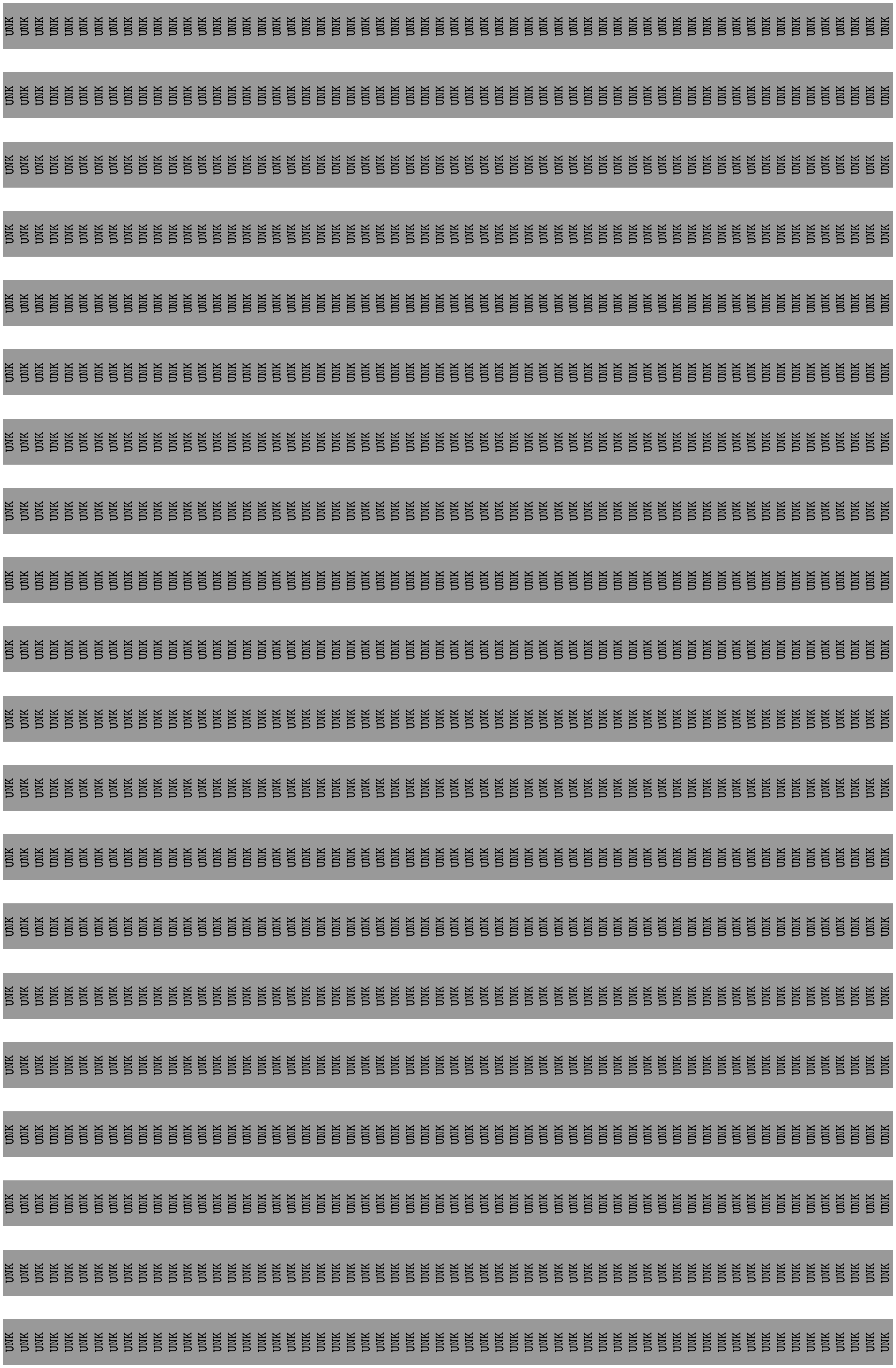

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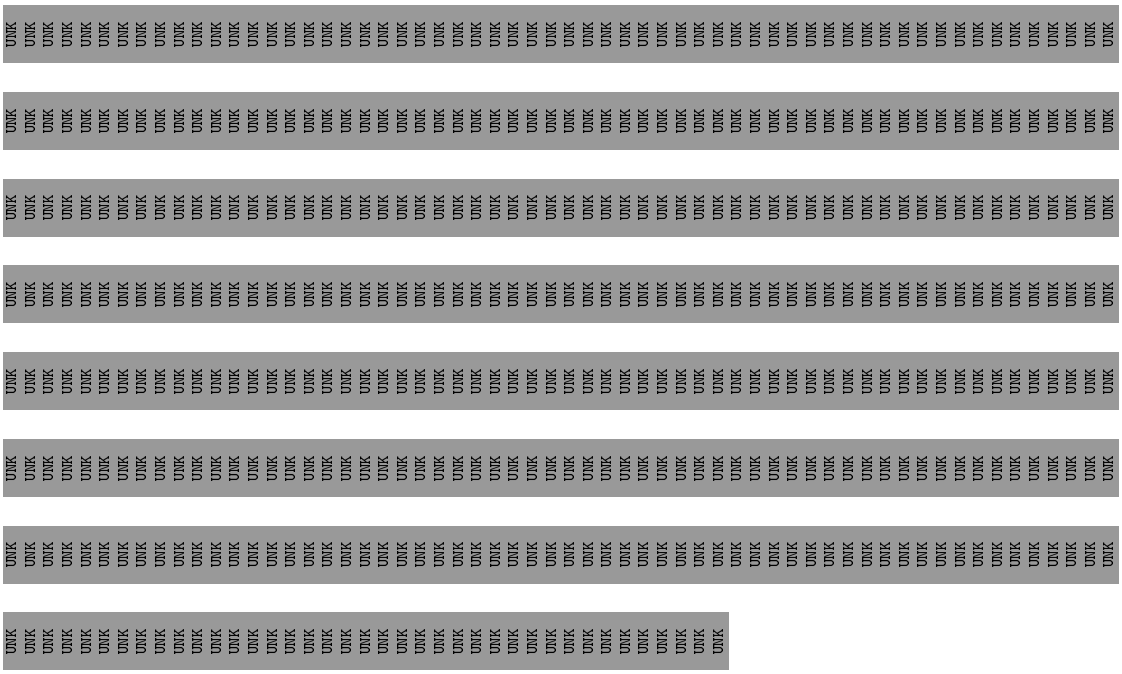
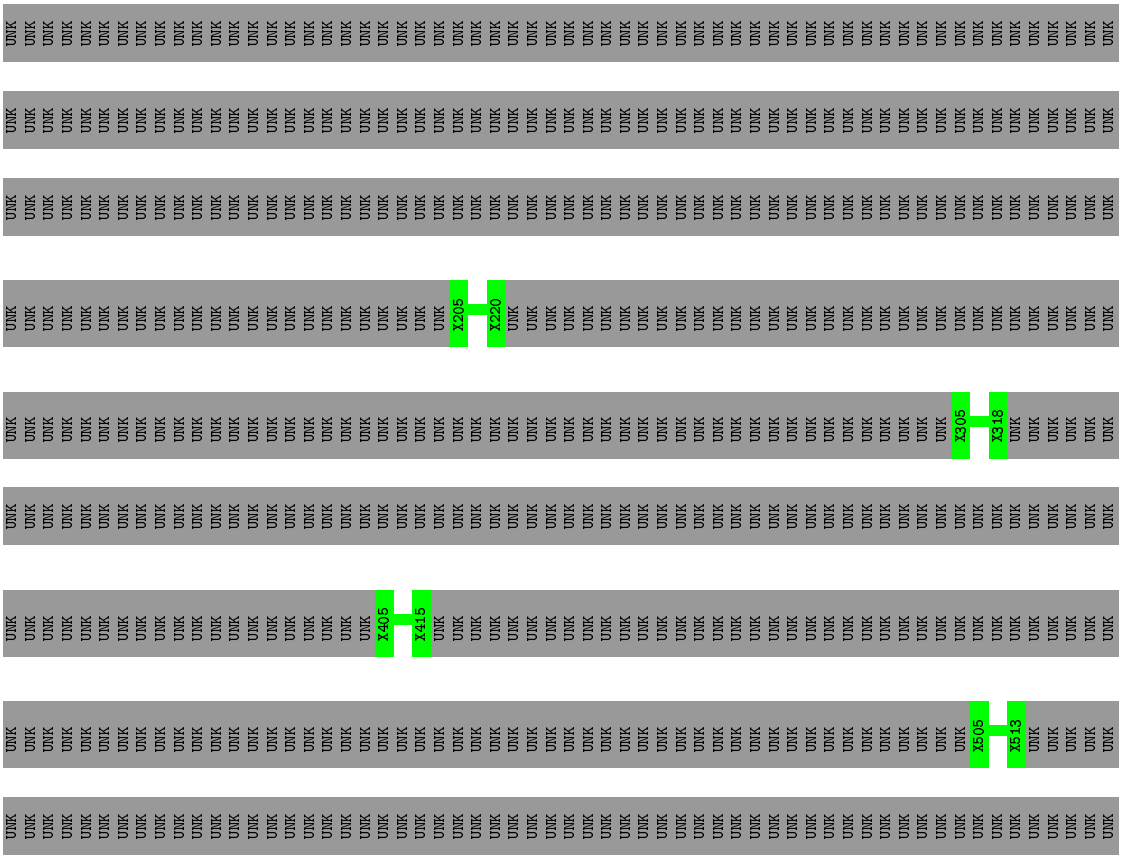
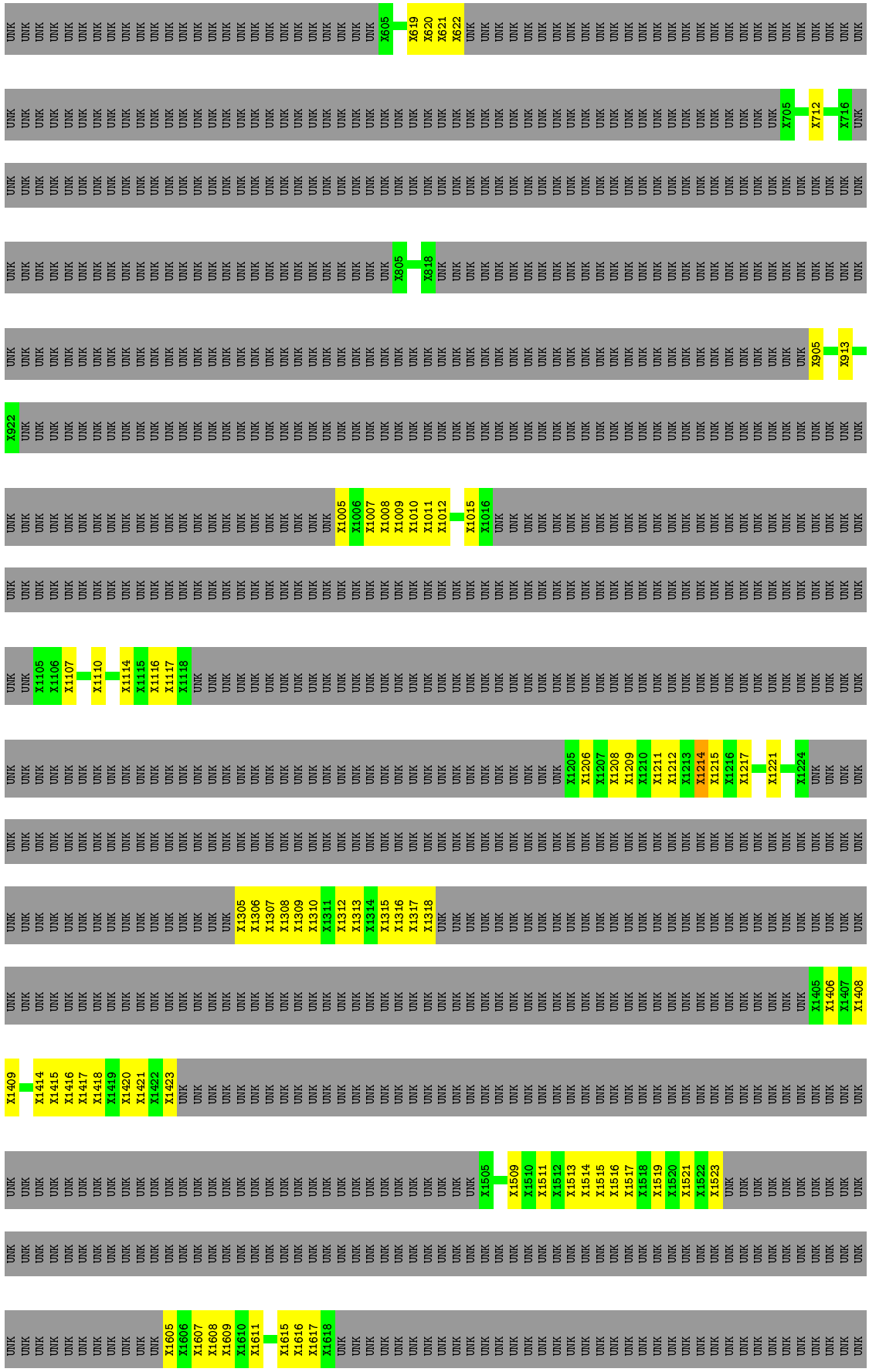


- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain O: 5% • 91%

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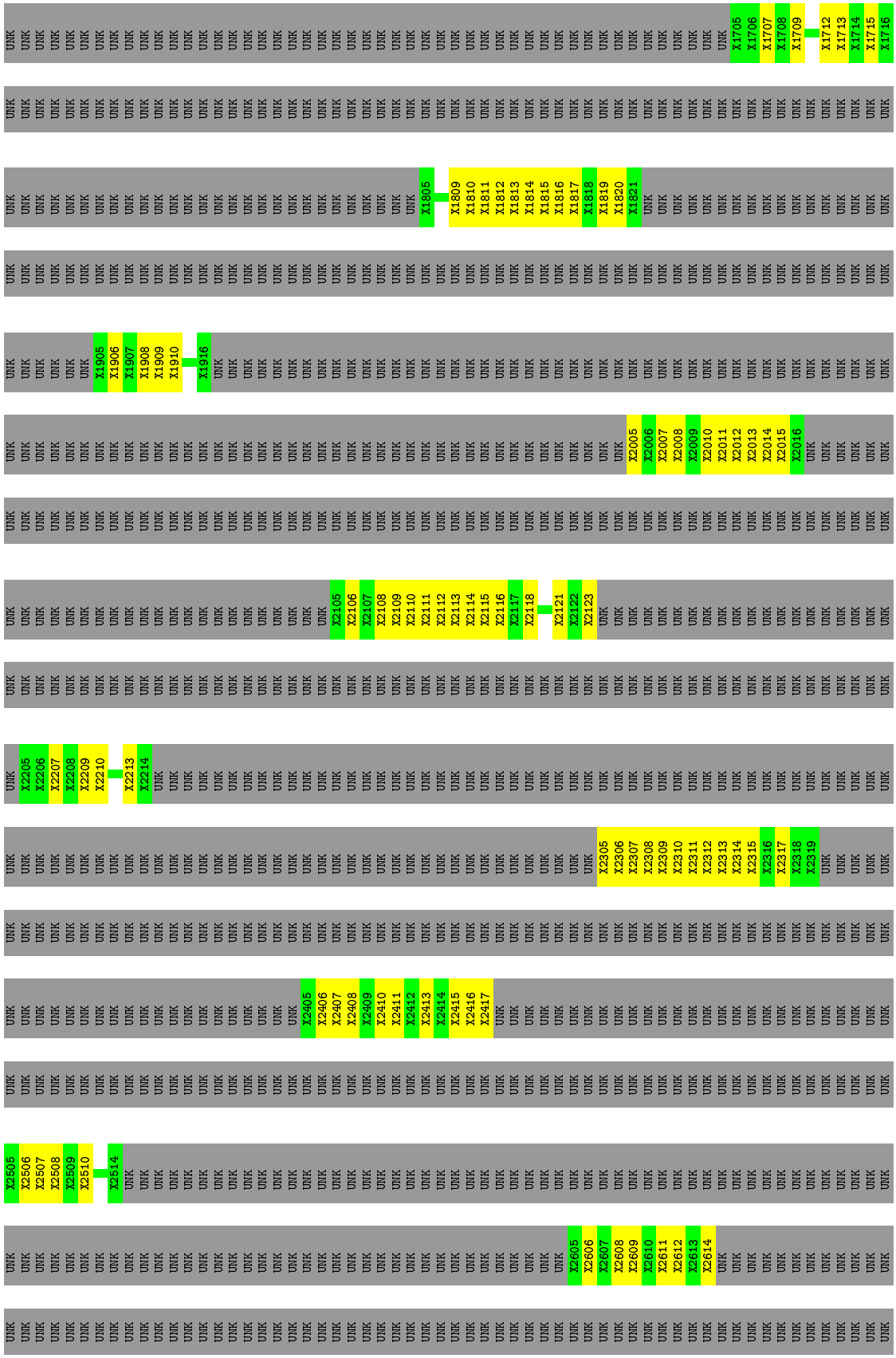
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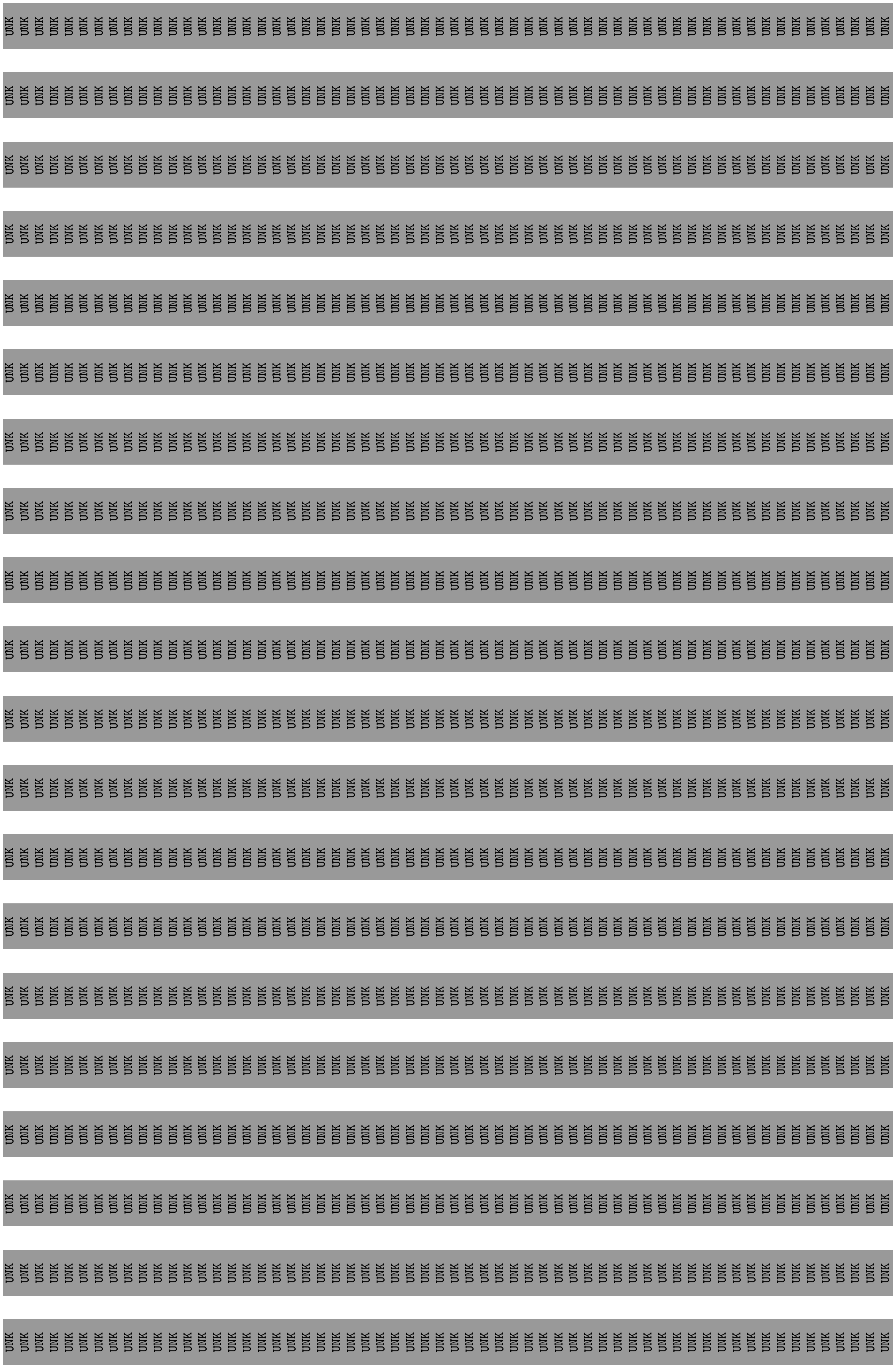
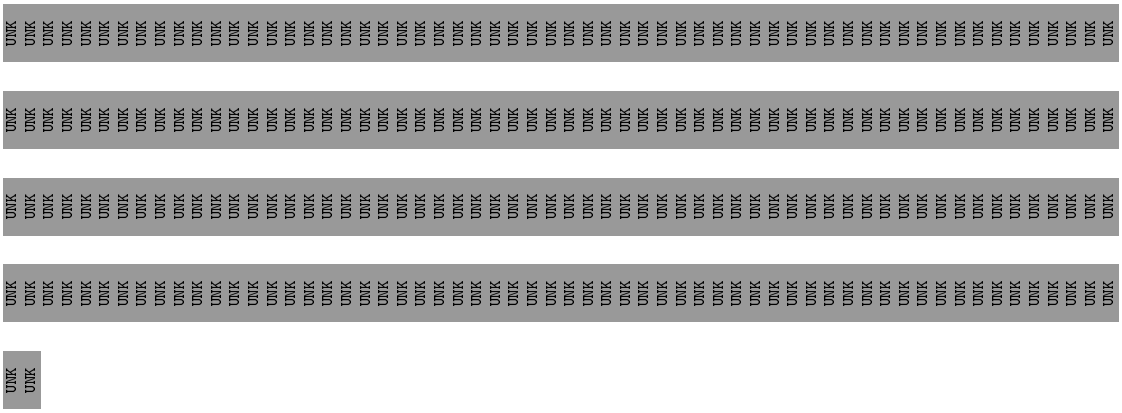
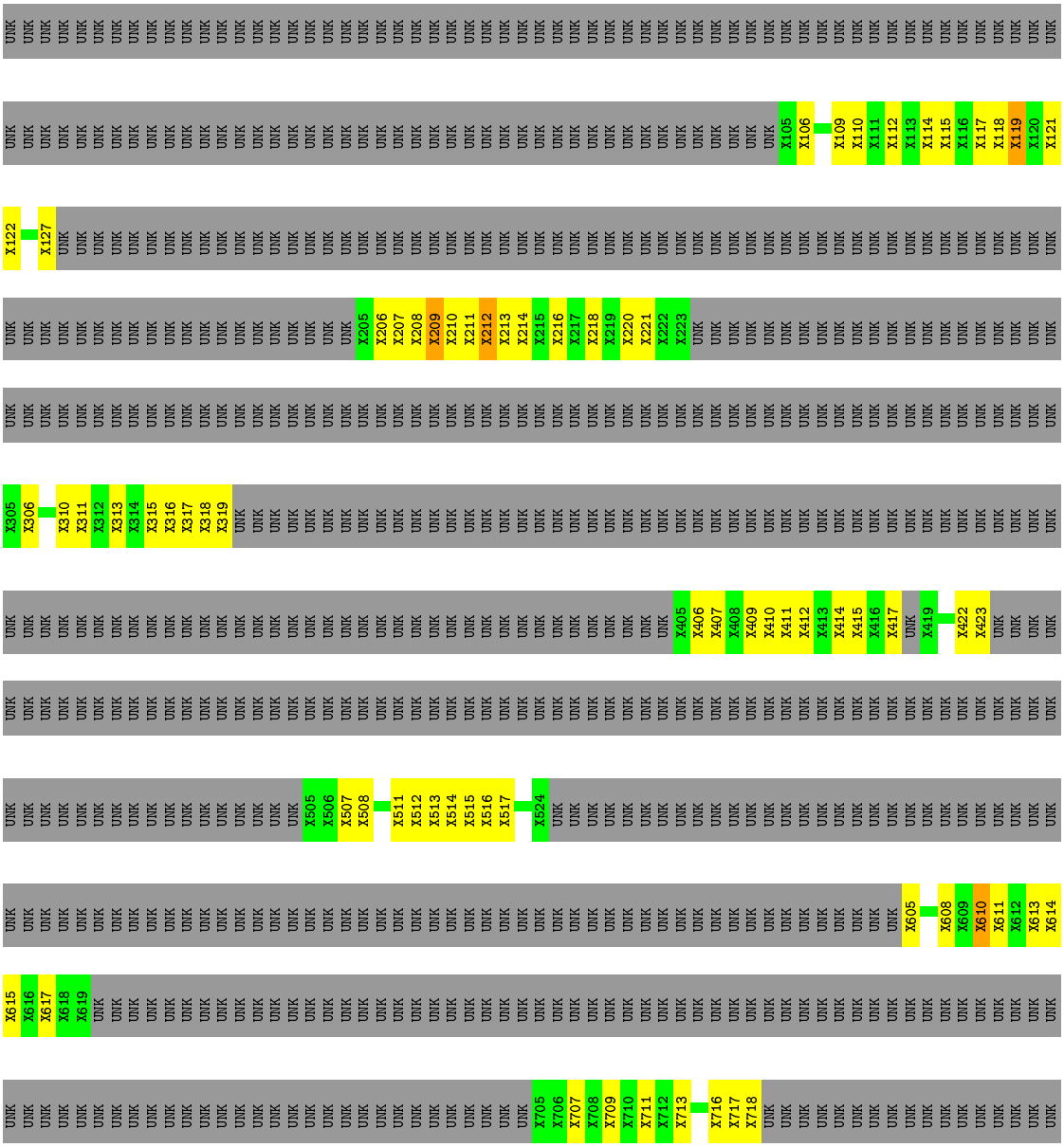
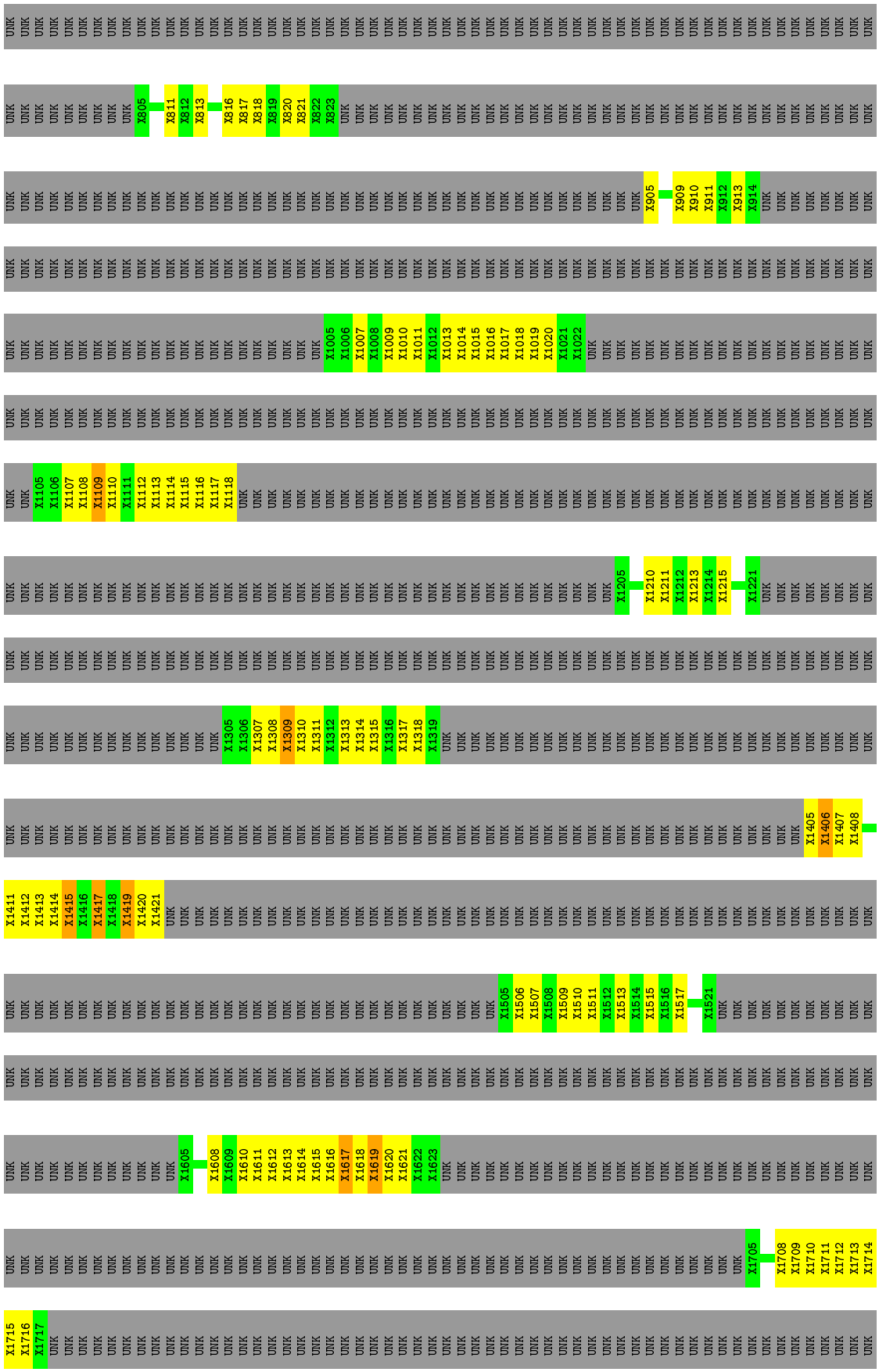




- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain P: 93%




X1715 X1716 X1717
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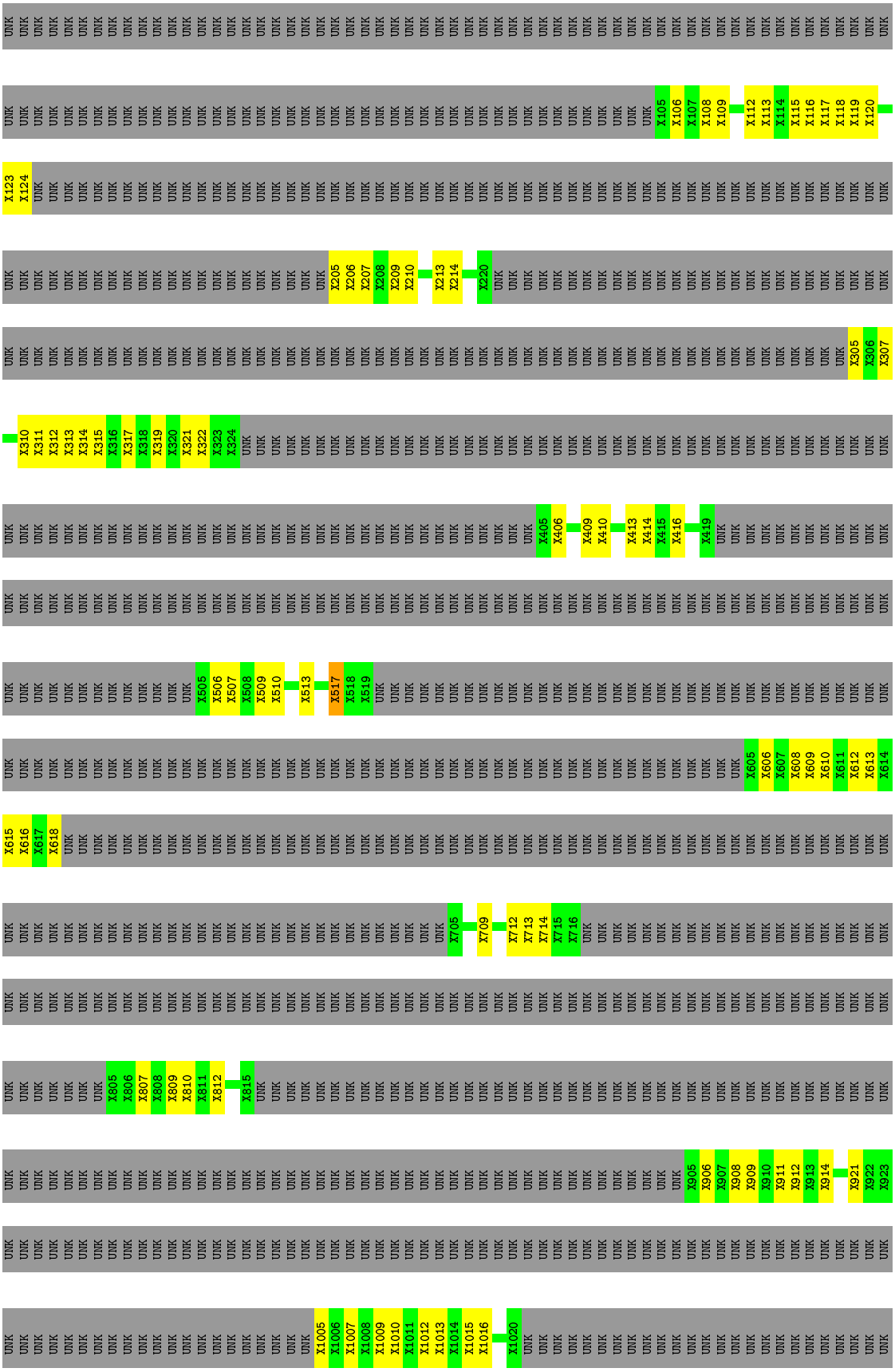
X1005 X1006 X1007 X1008 X1009 X1010 X1011 X1012 X1013 X1014 X1015 X1016 X1017 X1018 X1019 X1020 X1021 X1022
X905 X909 X910 X911 X912 X913 X914
X805 X811 X812 X813 X816 X817 X818 X819 X820 X821 X822 X823

UNK UNK UNK

UNK UNK UNK

Chain Q: 5% 5% 90%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X310 X311 X312 X313 X314 X315 X316 X317 X318 X319 X320 X321 X322 X323 X324
X405 X406 X409 X410 X413 X414 X415 X416 X419
X505 X506 X507 X508 X509 X510 X513 X517 X518 X519
X605 X606 X607 X608 X609 X610 X611 X612 X613 X614
X615 X616 X617 X618
X705 X709 X712 X713 X714 X715 X716
X805 X806 X807 X808 X809 X810 X811 X812 X815
X905 X906 X907 X908 X909 X910 X911 X912 X913 X914 X921 X922 X923
X1005 X1006 X1007 X1008 X1009 X1010 X1011 X1012 X1013 X1014 X1015 X1016 X1020

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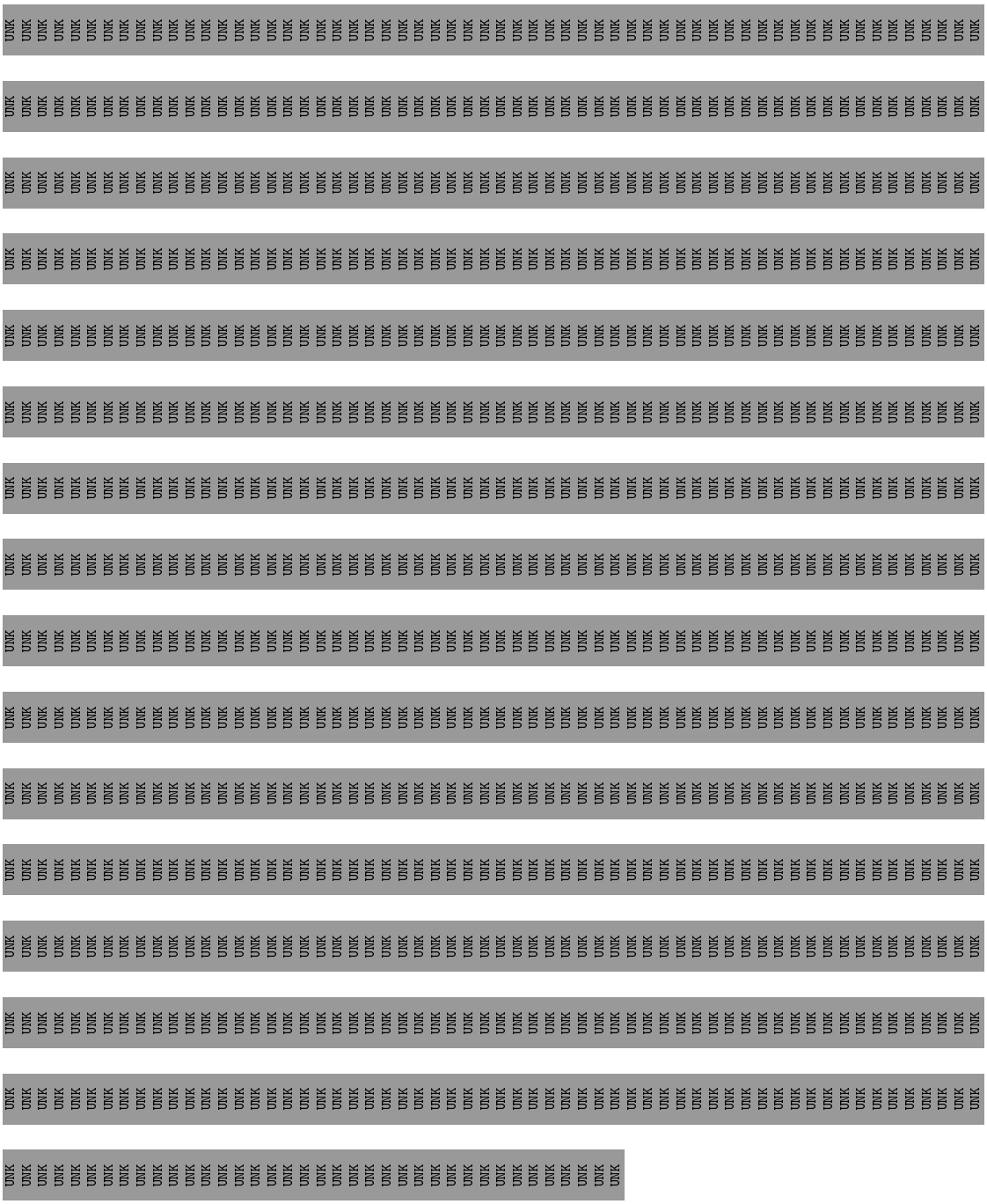
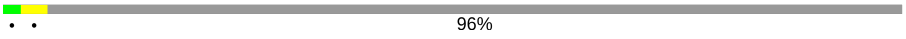
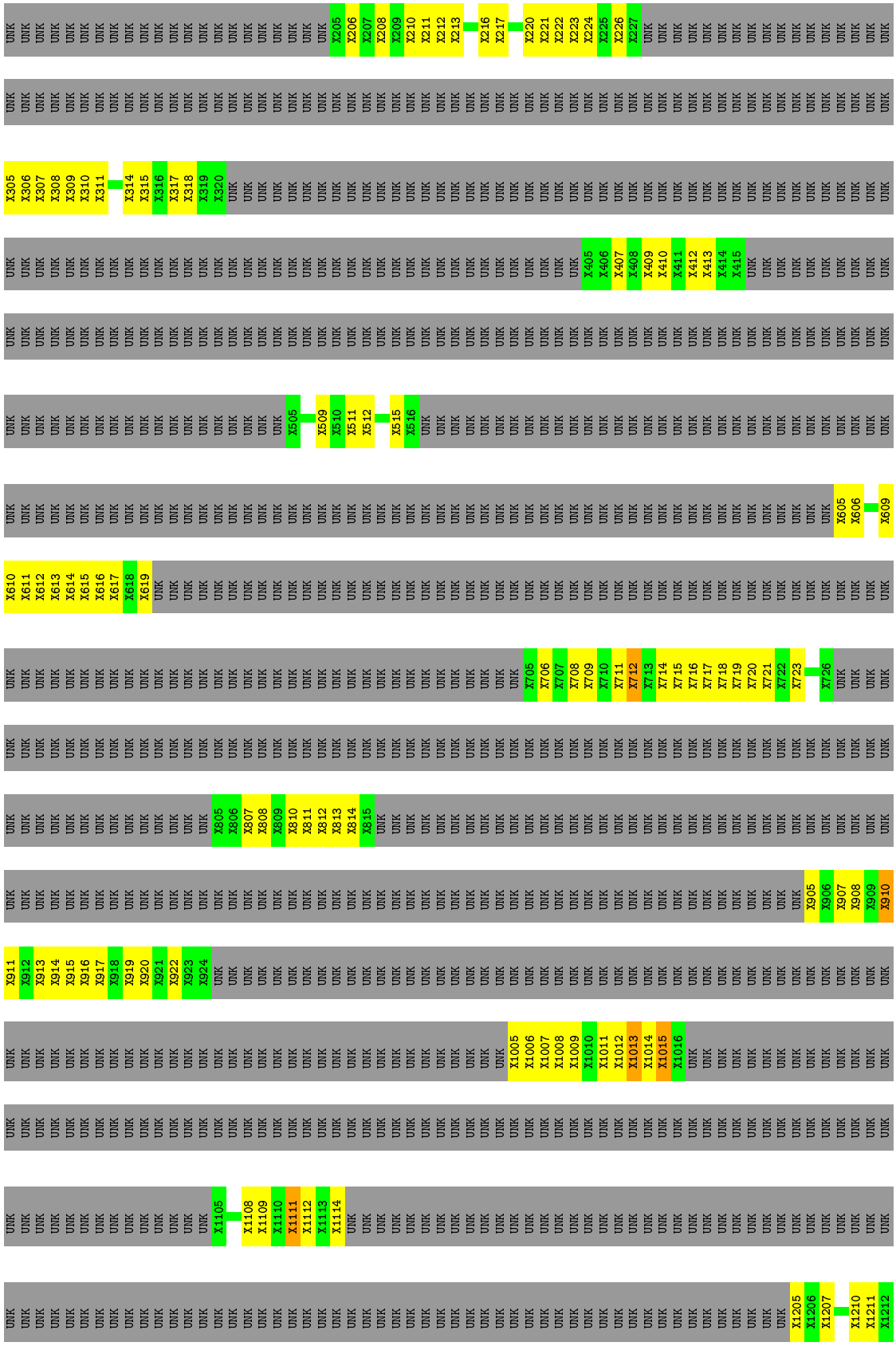


- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain R:

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X505 X509 X510 X511 X512 X515 X516
X605 X606 X609
X610 X611 X612 X613 X614 X615 X616 X617 X618 X619
X705 X706 X707 X708 X709 X710 X711 X712 X713 X714 X715 X716 X717 X718 X719 X720 X721 X722 X723 X726
X805 X806 X807 X808 X809 X810 X811 X812 X813 X814 X815
X905 X906 X907 X908 X909 X910
X911 X912 X913 X914 X915 X916 X917 X918 X919 X920 X921 X922 X923 X924
X1005 X1006 X1007 X1008 X1009 X1010 X1011 X1012 X1013 X1014 X1015 X1016
X1105 X1108 X1109 X1110 X1111 X1112 X1113 X1114
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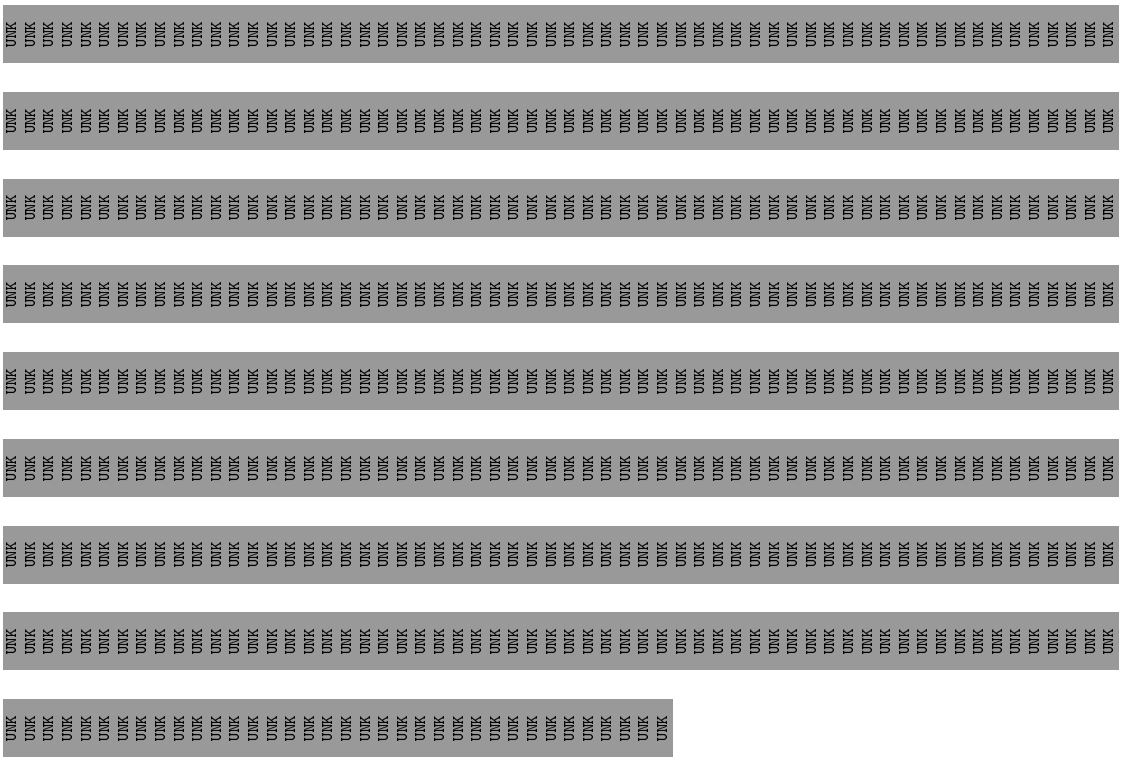
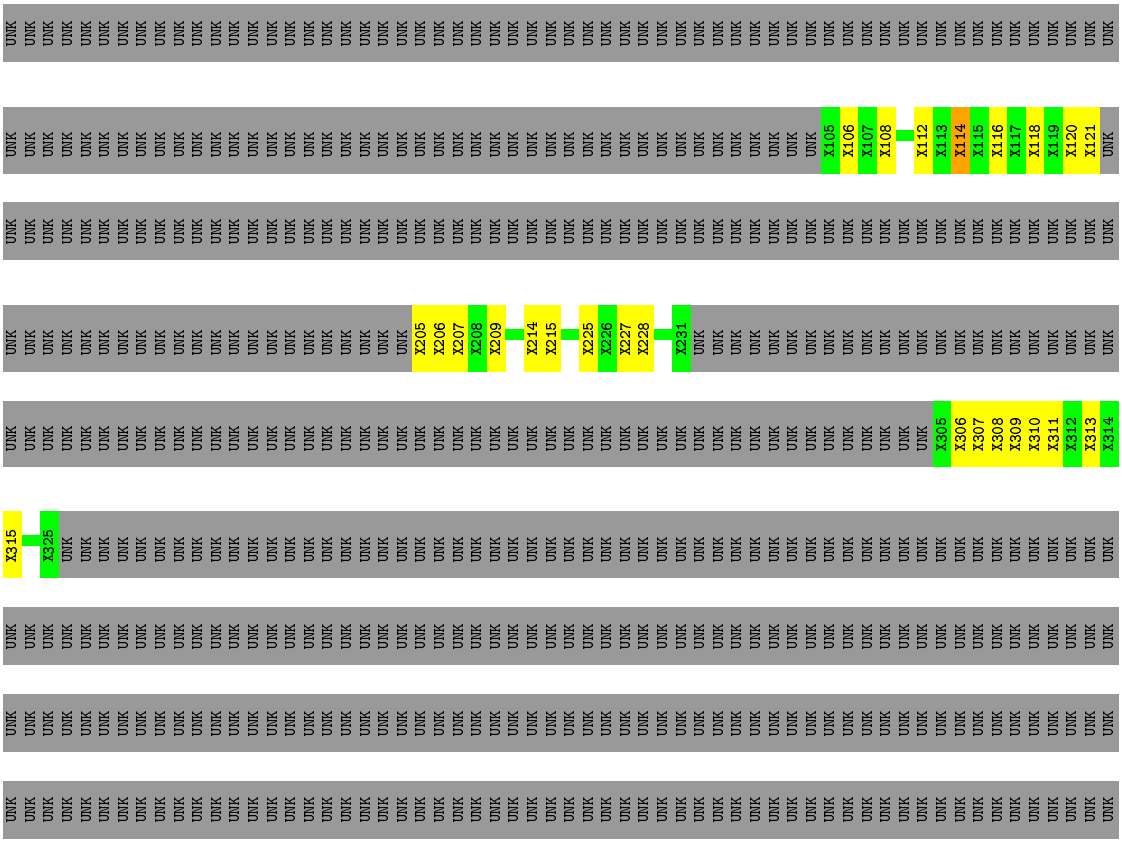
X1213 X1214 X1215 X1216 X1217 X1218 UNK UNK UNK

UNK UNK UNK



- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain S: 98%

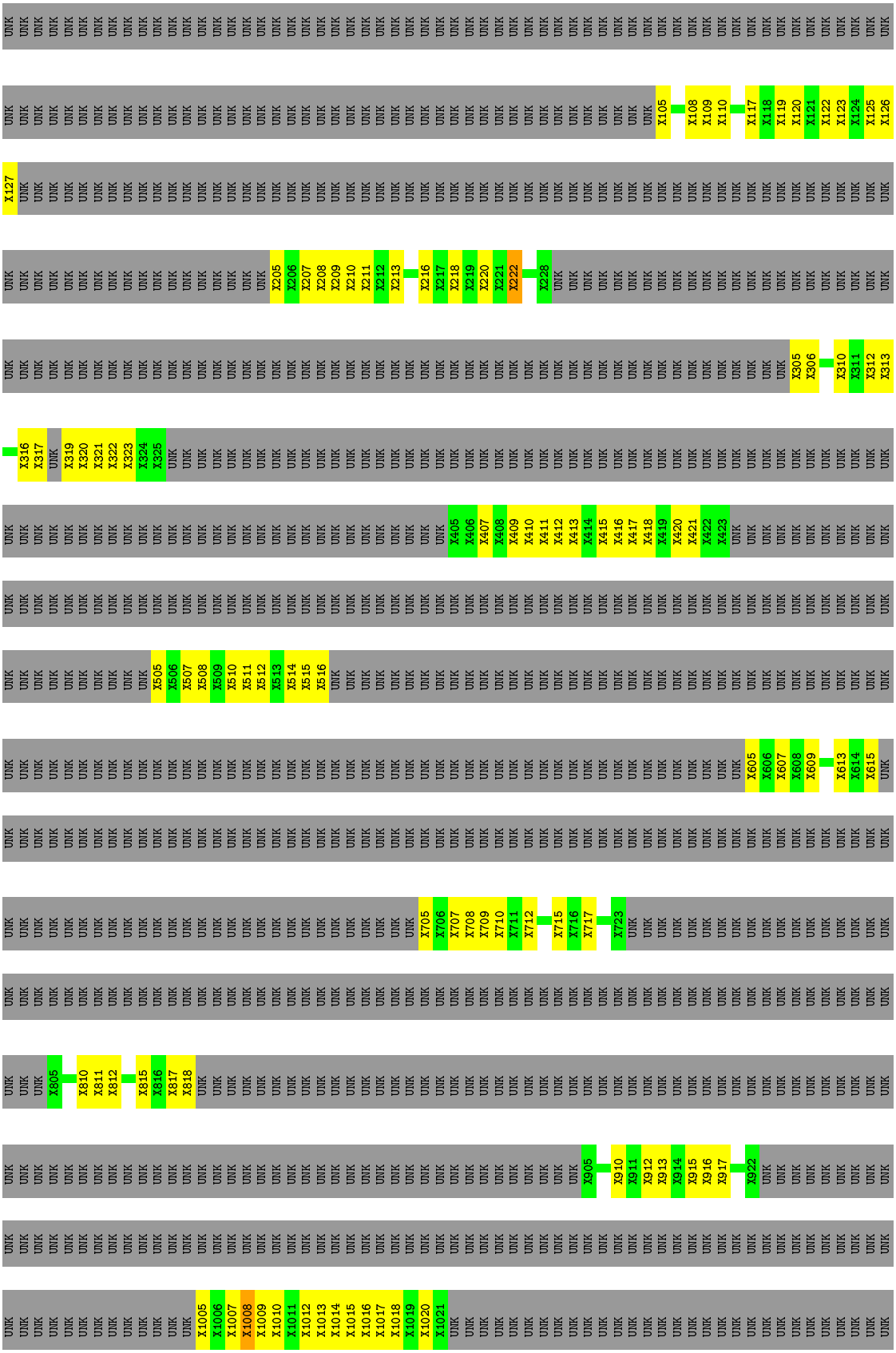


UNK UNK UNK

UNK UNK UNK

UNK UNK UNK

Chain T: 7% 6% 87%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X1005 X1006 X1007 X1008 X1009 X1010 X1011 X1012 X1013 X1014 X1015 X1016 X1017 X1018 X1019 X1020 X1021
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X805 X810 X811 X812 X815 X816 X817 X818
X705 X706 X707 X708 X709 X710 X711 X712 X715 X716 X717 X723
X605 X606 X607 X608 X609 X613 X614 X615
X505 X506 X507 X508 X509 X510 X511 X512 X513 X514 X515 X516
X405 X406 X407 X408 X409 X410 X411 X412 X413 X414 X415 X416 X417 X418 X419 X420 X421 X422 X423
X316 X317 X319 X320 X321 X322 X323 X324 X325
X305 X306 X310 X311 X312 X313
X127 X205 X206 X207 X208 X209 X210 X211 X212 X213 X216 X217 X218 X219 X220 X221 X222 X228
X105 X108 X109 X110 X117 X118 X119 X120 X121 X122 X123 X124 X125 X126

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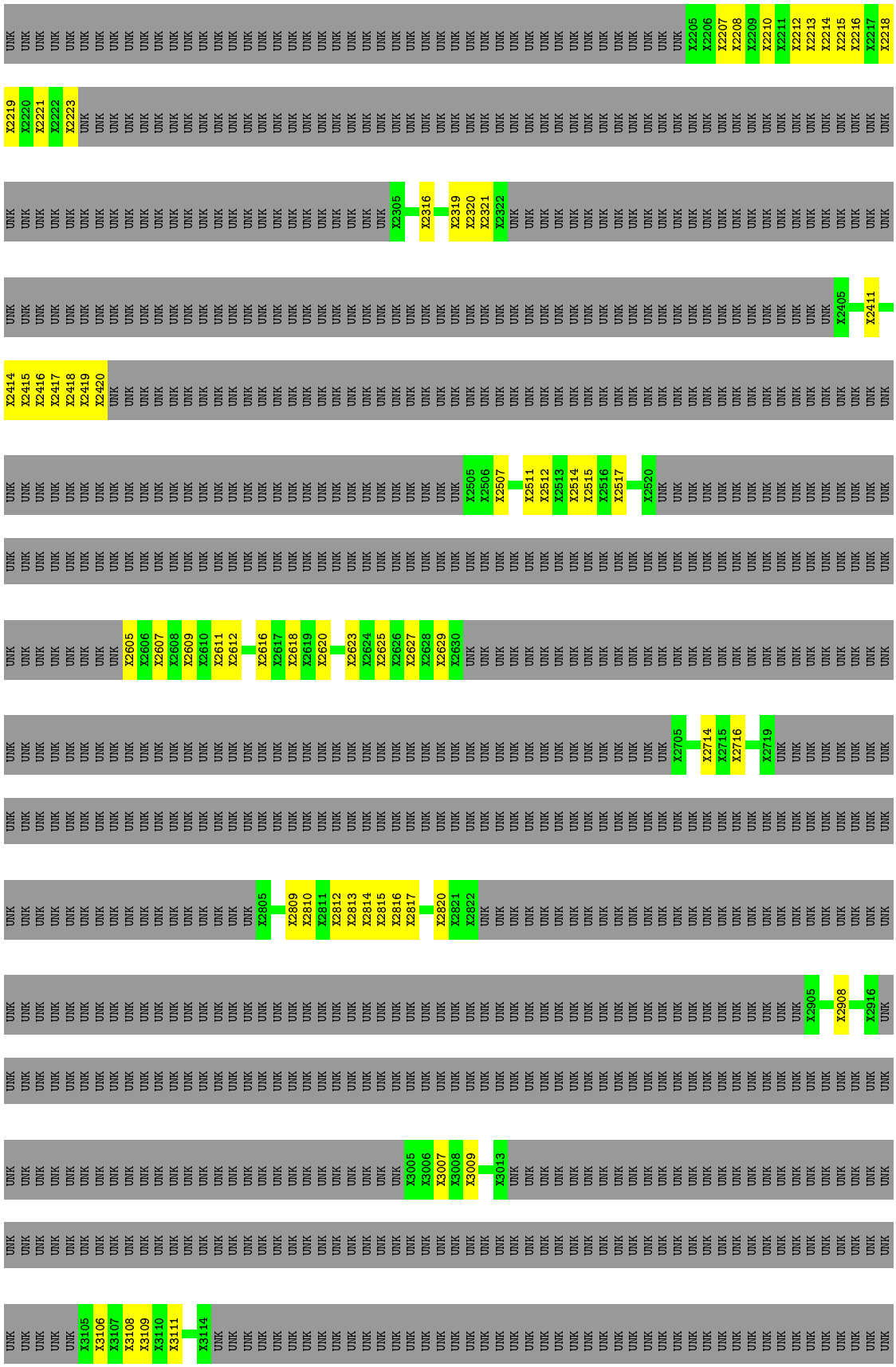
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X3005 X3006 X3007 X3008 X3009 X3013
X2905 X2908 X2916
X2805 X2809 X2810 X2811 X2812 X2813 X2814 X2815 X2816 X2817 X2820 X2821 X2822
X2705 X2714 X2715 X2716 X2719
X2605 X2606 X2607 X2608 X2609 X2610 X2611 X2612 X2616 X2617 X2618 X2619 X2620 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2630
X2505 X2506 X2507 X2511 X2512 X2513 X2514 X2515 X2516 X2517 X2520
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X2405 X2411
X2305 X2316 X2319 X2320 X2321 X2322
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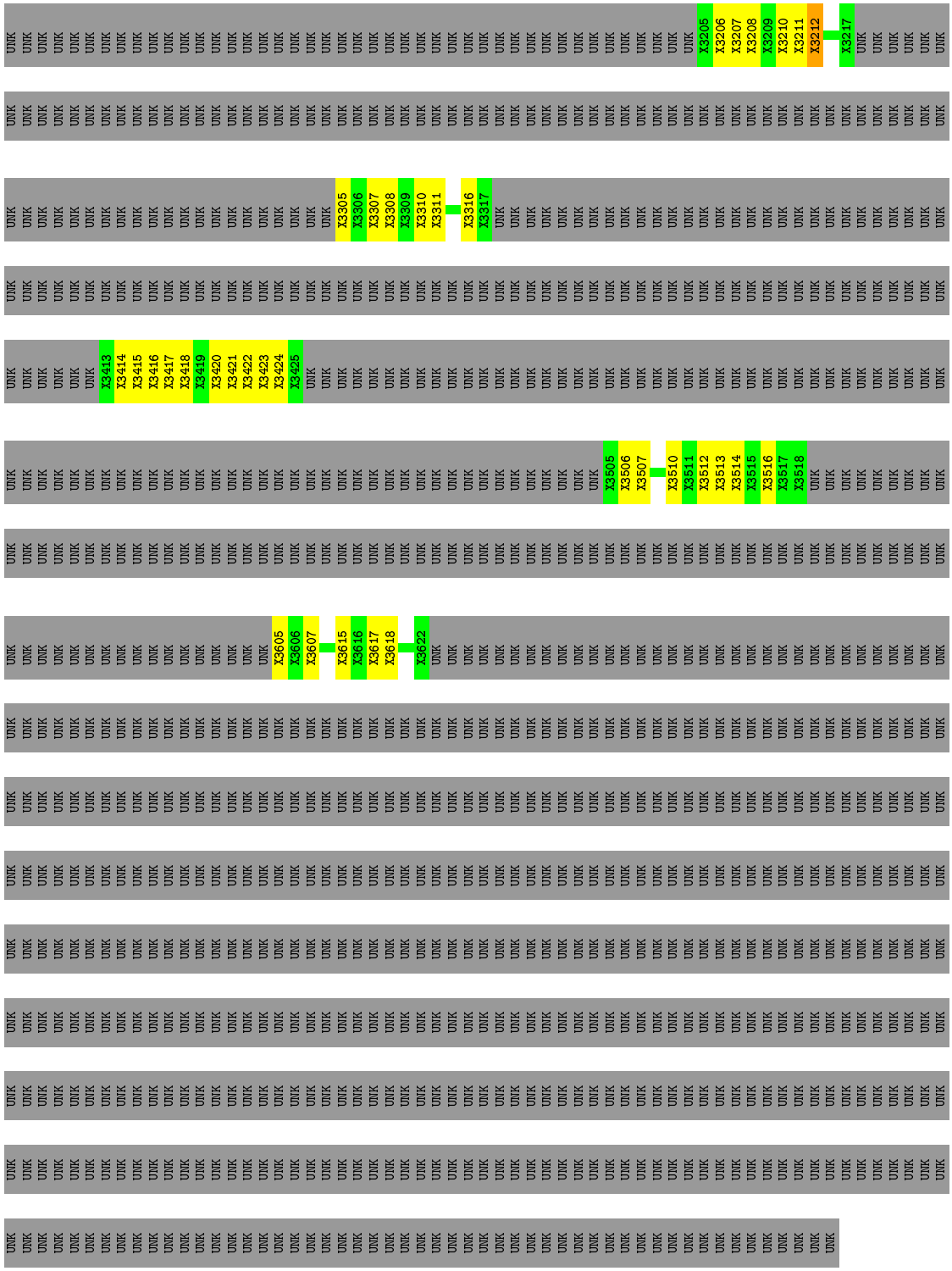

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain Y: 95%

UNK
X940 X941 X942
X843 X844 X845 X846 X847 X848 X849 X850 X851 X855 X856 X857 X858 X865 X871 X872 X873 X874 X875 X876 X880 X881 X885 X897 X906 X907 X908 X909 X910 X911 X915 X916 X917 X918 X919 X920 X921 X922 X923 X924 X925 X926 X927 X928
X800 X801 X802 X803 X804 X805 X806 X807 X808 X809 X810 X811 X812 X813 X814 X815 X829 X832 X833 X834 X835 X838 X839 X840 X841 X842
X988 X989 X990 X995
X1006 X1013 X1014 X1017 X1024 X1025 X1026 X1027 X1028 X1029 X1030 X1031 X1032 X1033 X1034 X1035 X1036 X1037 X1038 X1042 X1043 X1044 X1047 X1048 X1049 X1050 X1053 X1054 X1062 X1063 X1064 X1065 X1066 X1067 X1068 X1069 X1070 X1071 X1072 X1073 X1074 X1075 X1076 X1077 X1078 X1079 X1088

UNK UNK UNK

UNK UNK UNK

UNK UNK UNK

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	1223 reflections (5.12%)	wwPDB-VP
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 , 606.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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).

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...

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Mol	Chain	Res	Type	Group
1	B	209	UNK	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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 (i)

There are no chain breaks in this entry.

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	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 (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.