wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2026 – 04:46 AM UTC

PDB ID	:	3KGV / pdb_00003kgv
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

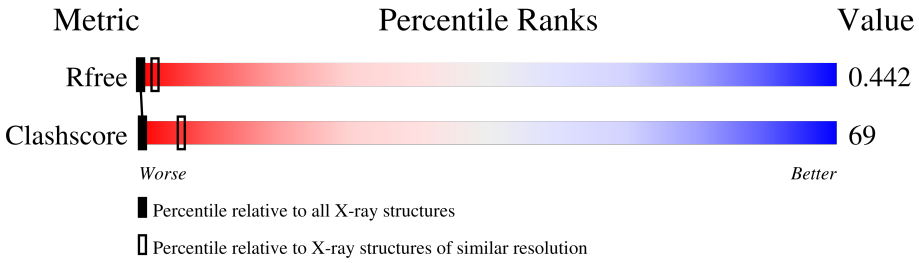
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (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}	180053	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

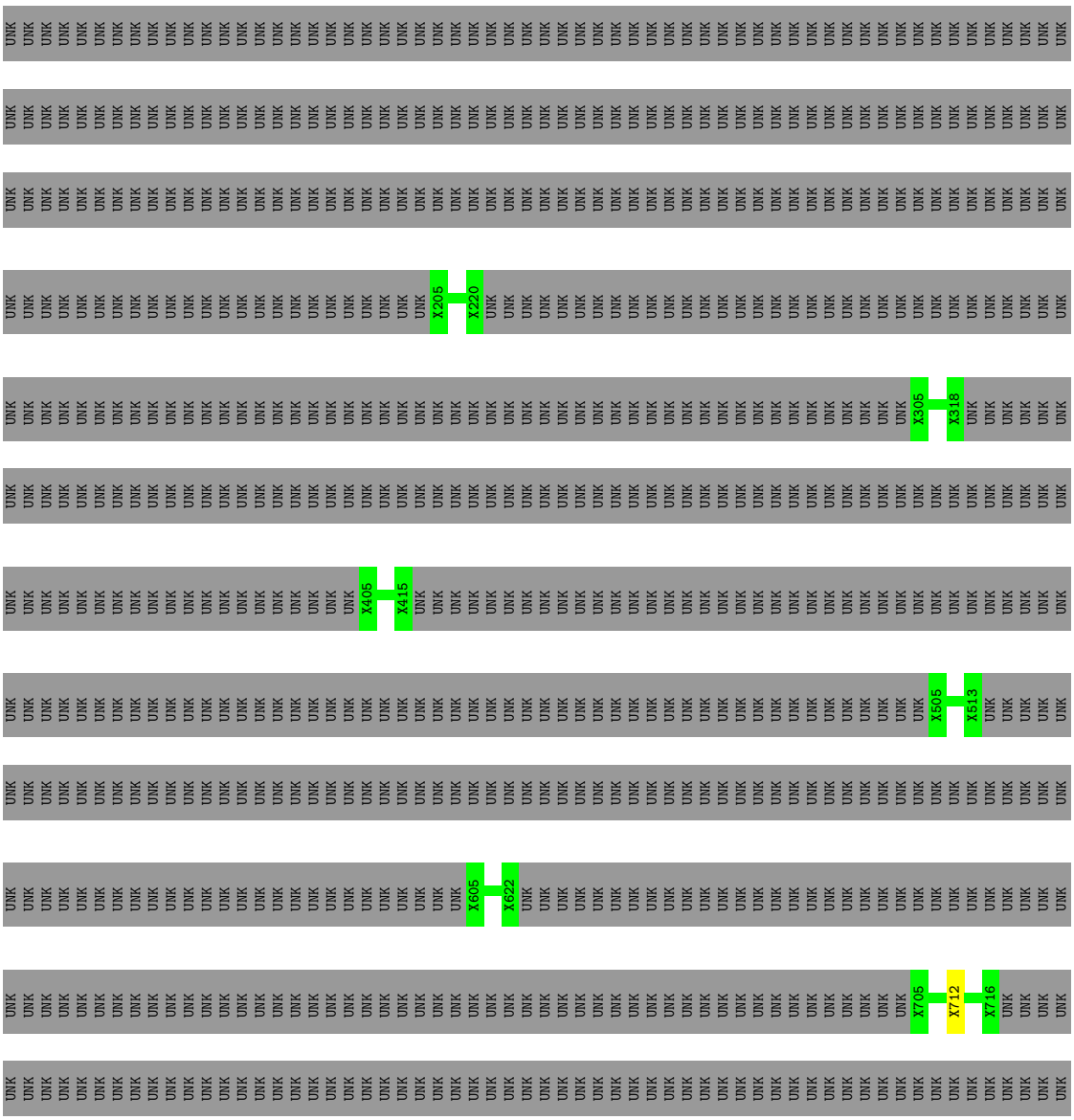
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	0	0	0
			1770	1062	354	354			
1	B	283	Total	C	N	O	0	0	0
			1415	849	283	283			
1	C	406	Total	C	N	O	0	0	0
			2030	1218	406	406			
1	D	182	Total	C	N	O	0	0	0
			910	546	182	182			
1	E	65	Total	C	N	O	0	0	0
			325	195	65	65			
1	F	531	Total	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			

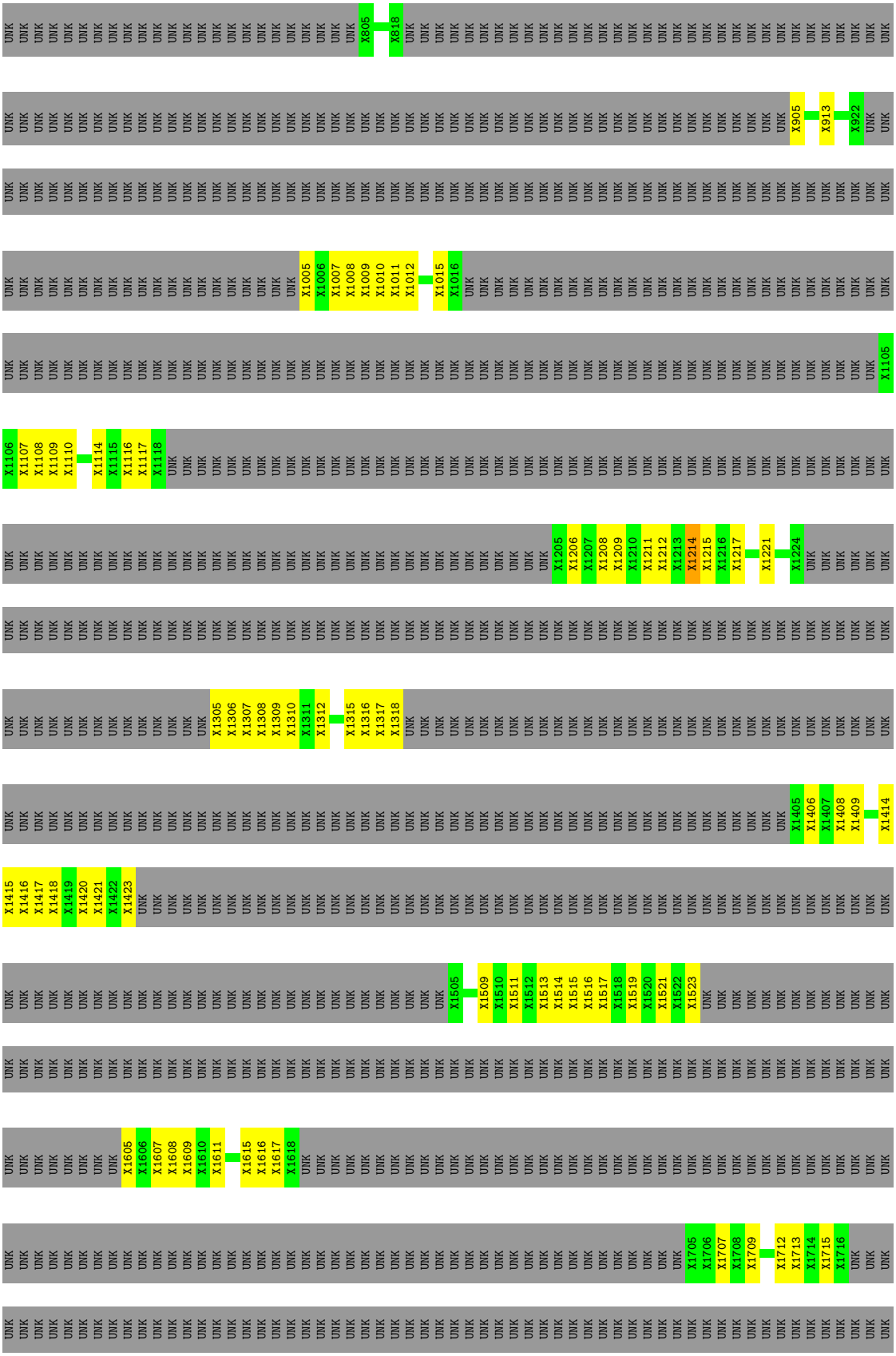
3 Residue-property plots (i)

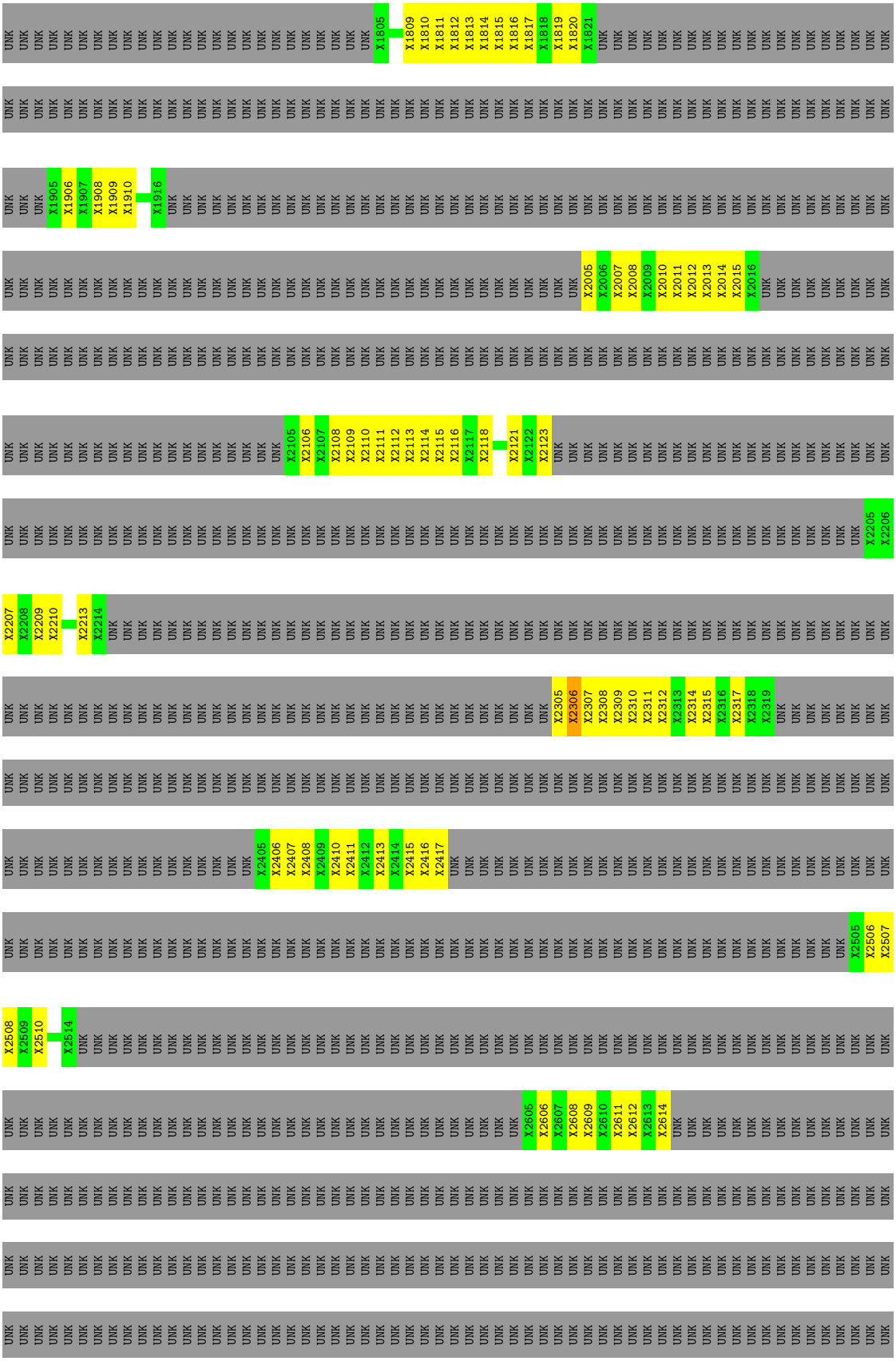
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

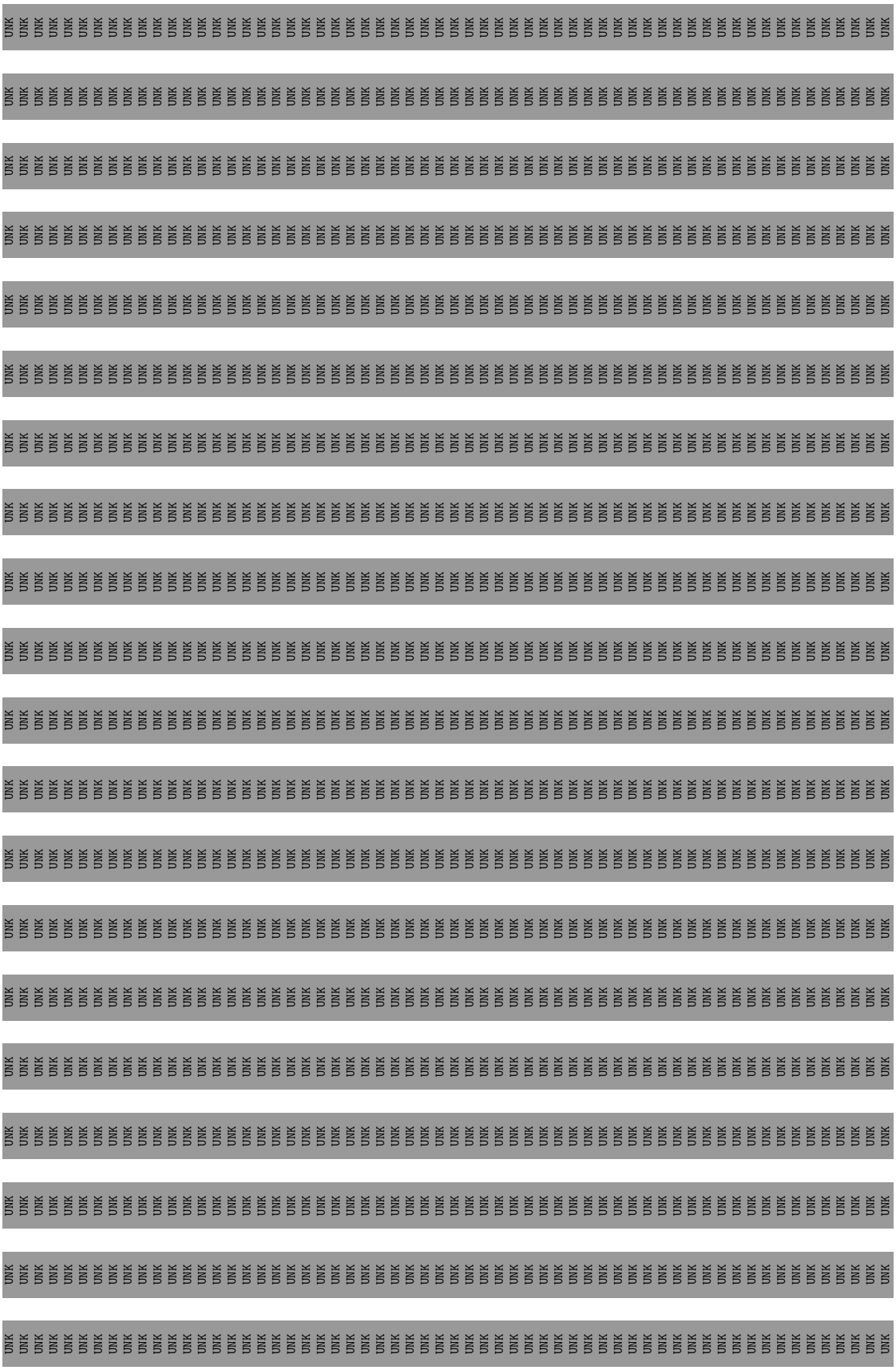
- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

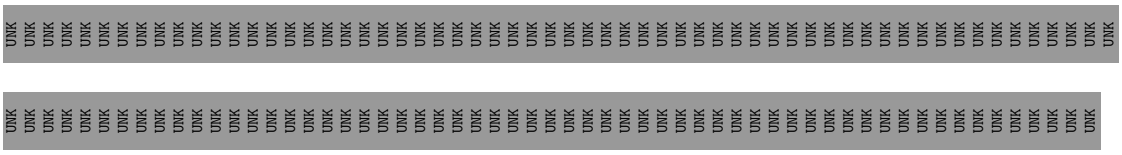
Chain A: 5% · 91%




UNK X805 X818 UNK
UNK X905 X913 X922 UNK
UNK X1005 X1006 X1007 X1008 X1009 X1010 X1011 X1012 X1015 X1016 UNK
UNK X1105
X1106 X1107 X1108 X1109 X1110 X1114 X1115 X1116 X1117 X1118 UNK
UNK X1205 X1206 X1207 X1208 X1209 X1210 X1211 X1212 X1213 X1214 X1215 X1216 X1217 X1221 X1224 UNK
UNK X1305 X1306 X1307 X1308 X1309 X1310 X1311 X1312 X1315 X1316 X1317 X1318 UNK
UNK X1405 X1406 X1407 X1408 X1409 X1414
X1415 X1416 X1417 X1418 X1419 X1420 X1421 X1422 X1423 UNK
UNK X1505 X1509 X1510 X1511 X1512 X1513 X1514 X1515 X1516 X1517 X1518 X1519 X1520 X1521 X1522 X1523 UNK
UNK X1605 X1606 X1607 X1608 X1609 X1610 X1611 X1615 X1616 X1617 X1618 UNK
UNK X1705 X1706 X1707 X1708 X1709 X1712 X1713 X1714 X1715 X1716 UNK

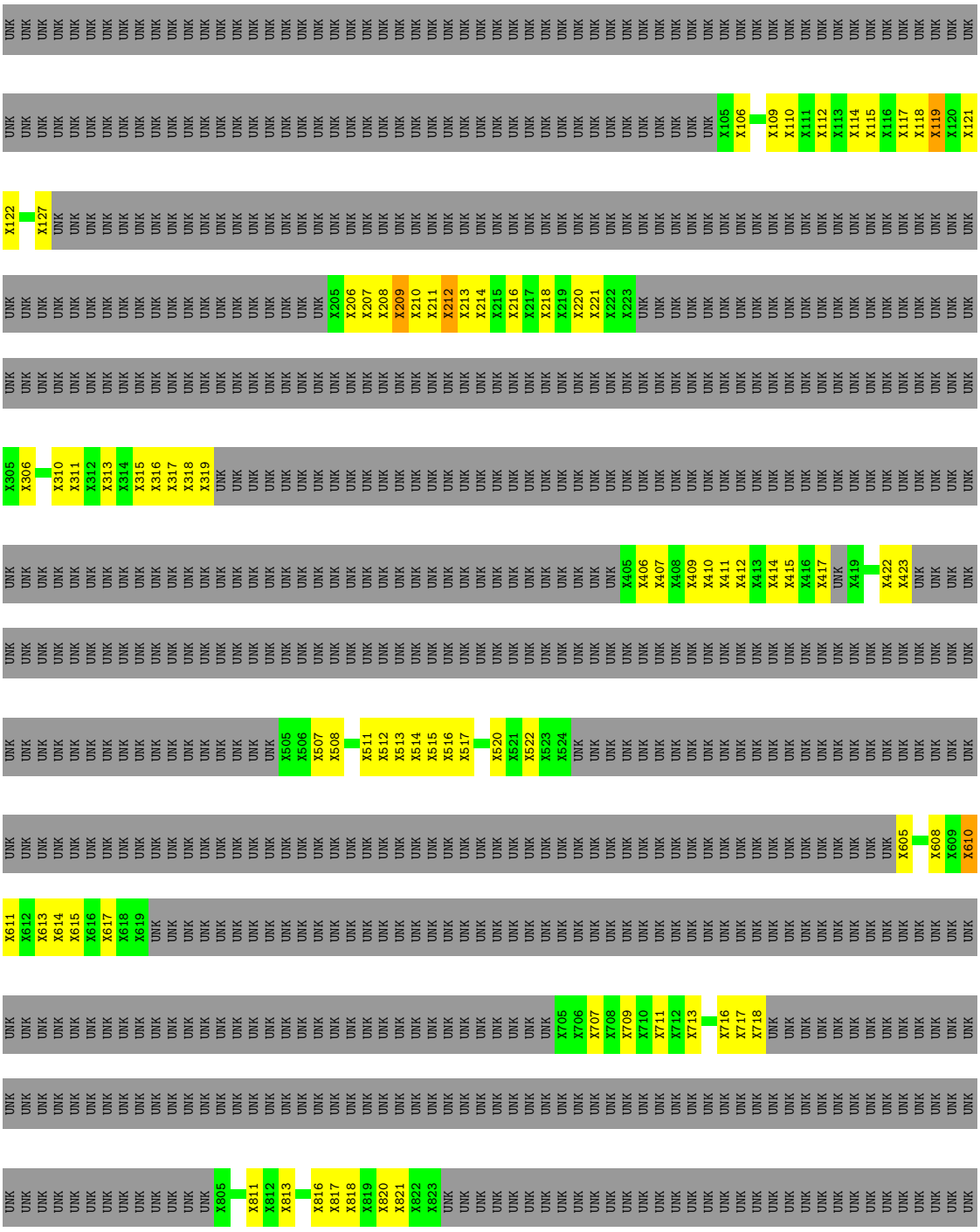


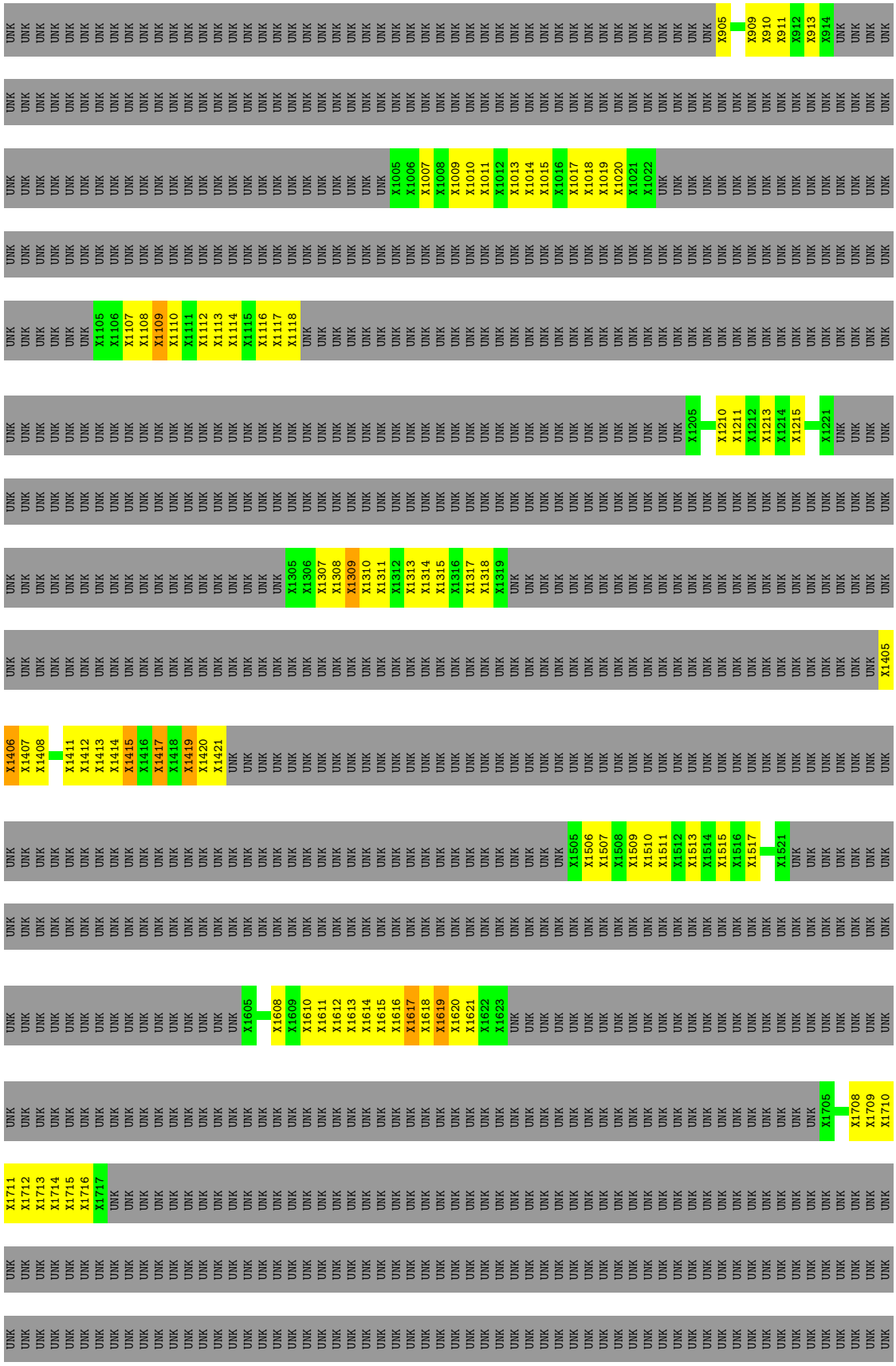

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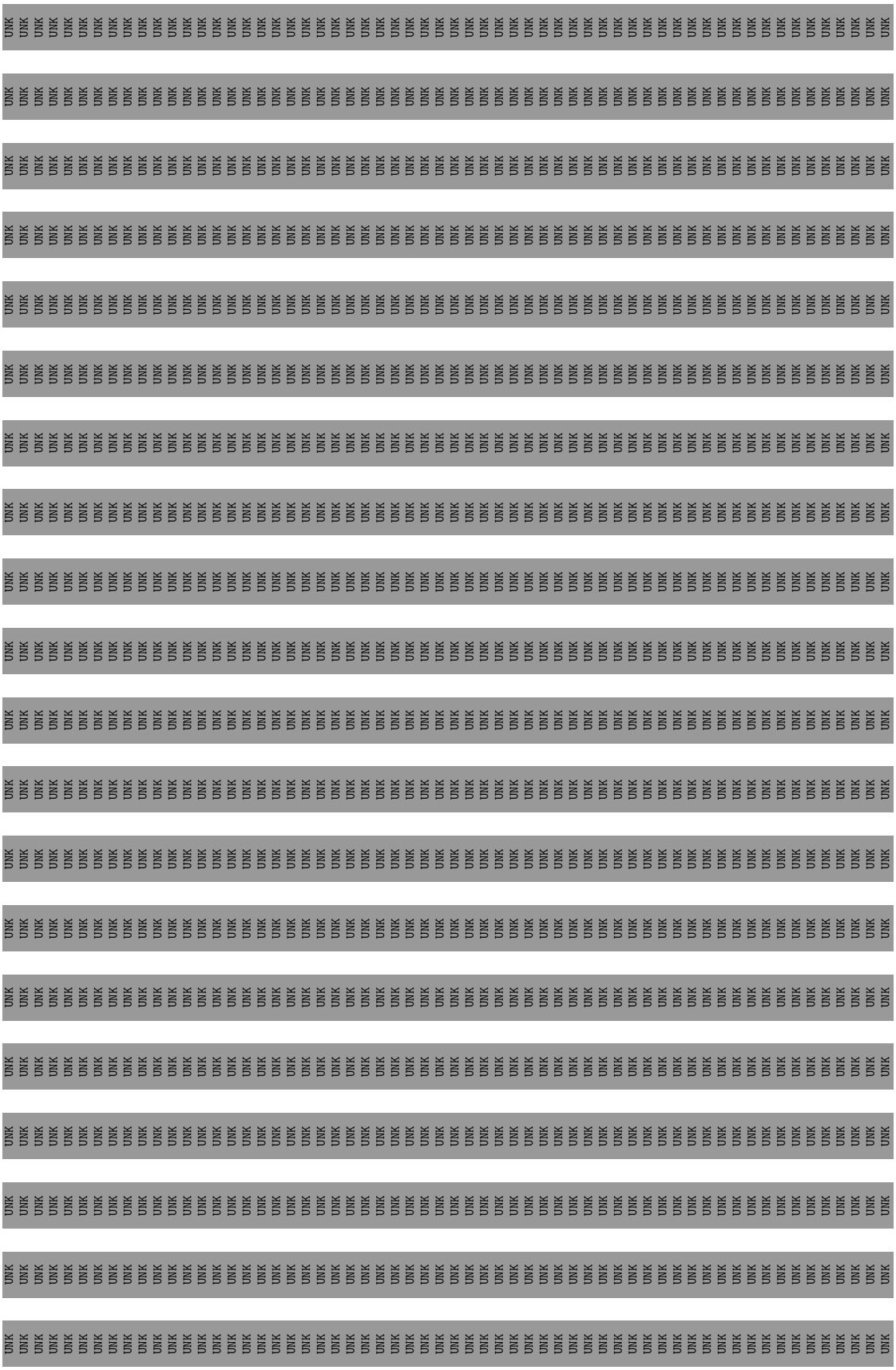


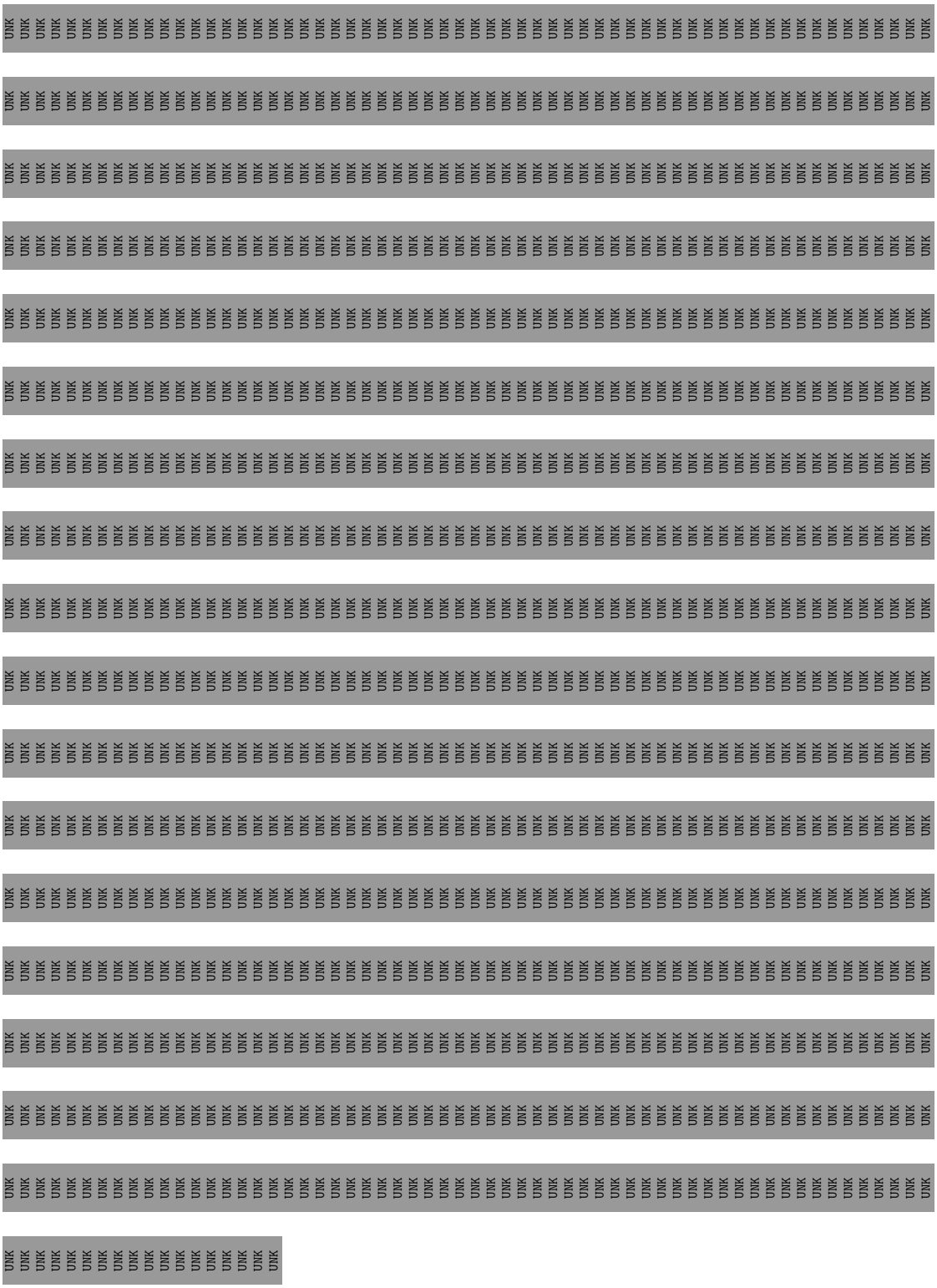
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain B: 93%




UNK
X905
X909
X910
X911
X912
X913
X914
X1005
X1006
X1007
X1008
X1009
X1010
X1011
X1012
X1013
X1014
X1015
X1016
X1017
X1018
X1019
X1020
X1021
X1022
X1105
X1106
X1107
X1108
X1109
X1110
X1111
X1112
X1113
X1114
X1115
X1116
X1117
X1118
X1205
X1210
X1211
X1212
X1213
X1214
X1215
X1221
X1305
X1306
X1307
X1308
X1309
X1310
X1311
X1312
X1313
X1314
X1315
X1316
X1317
X1318
X1319
X1405
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X1418
X1419
X1420
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X1509
X1510
X1511
X1512
X1513
X1514
X1515
X1516
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X1521
X1605
X1608
X1609
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X1614
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X1617
X1618
X1619
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X1622
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X1715
X1716
X1717

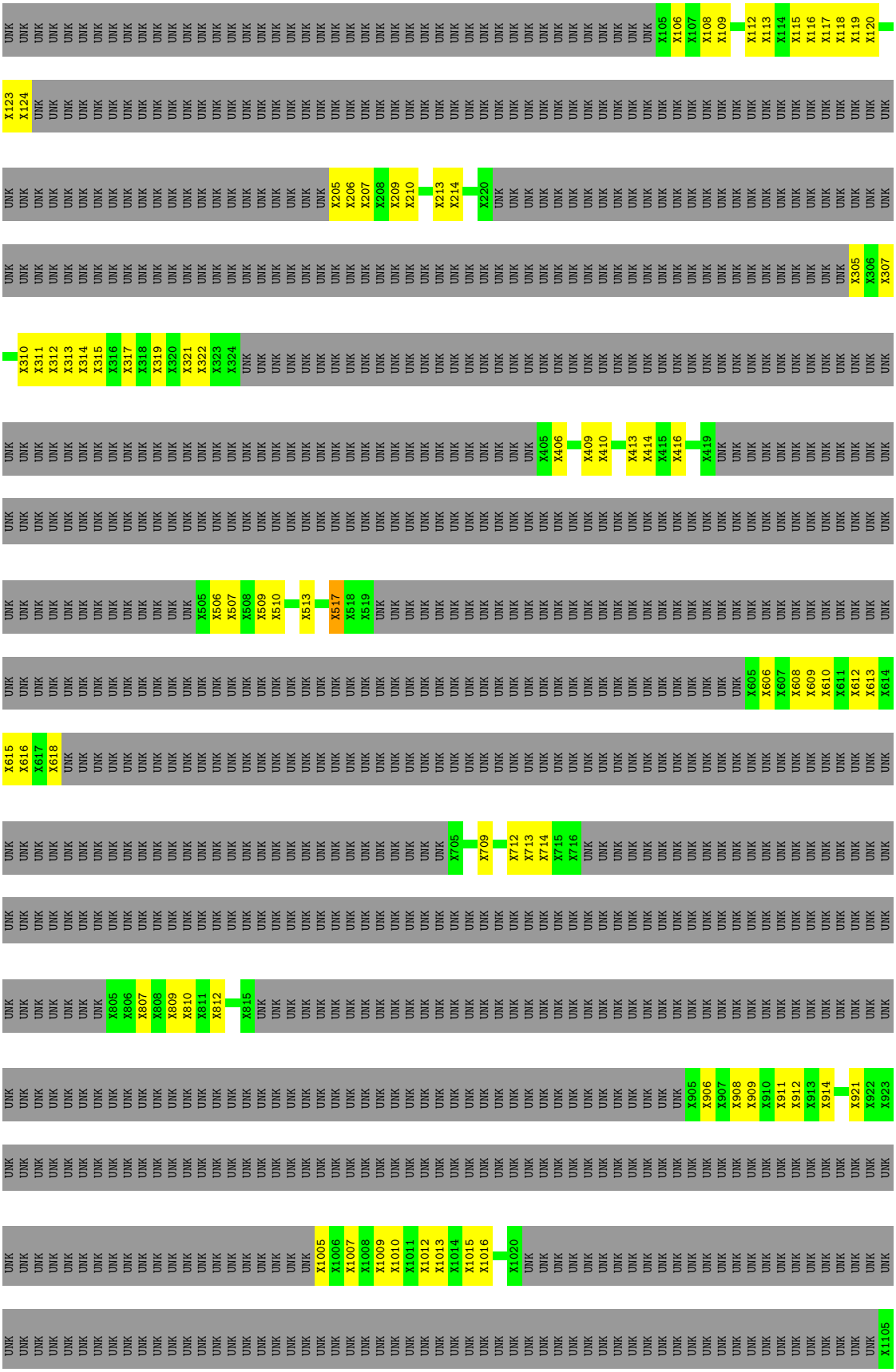

UNK

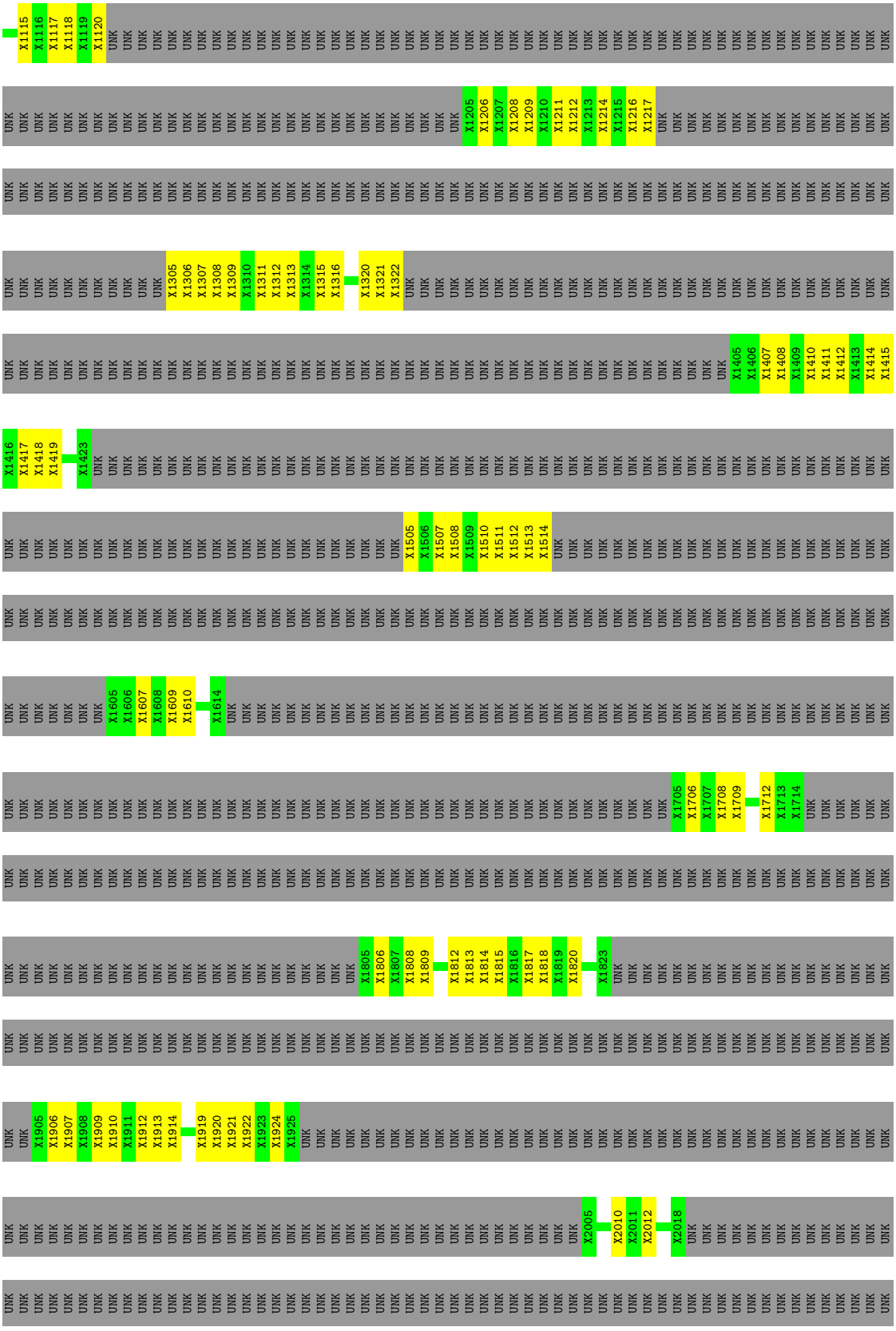


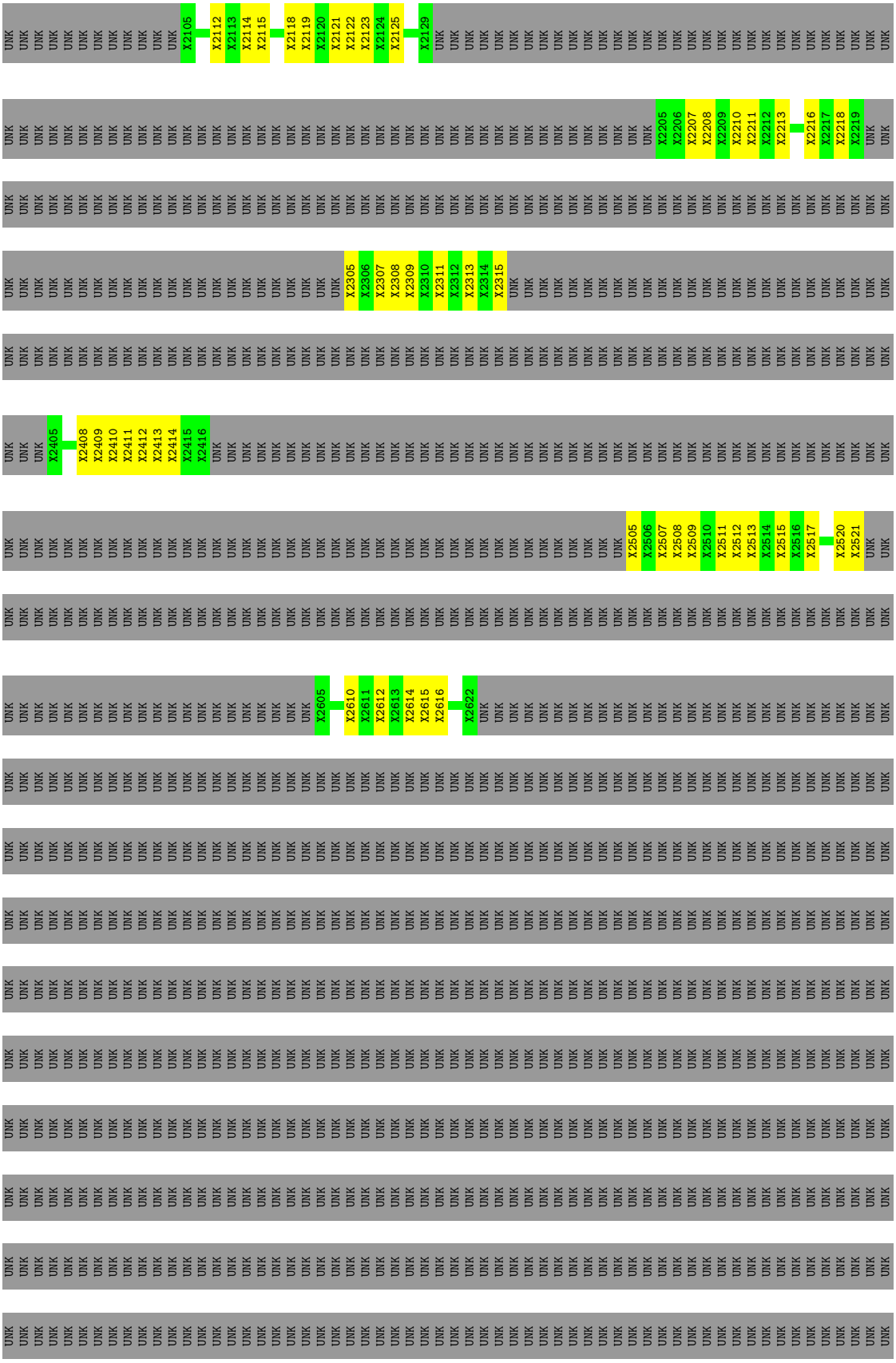
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

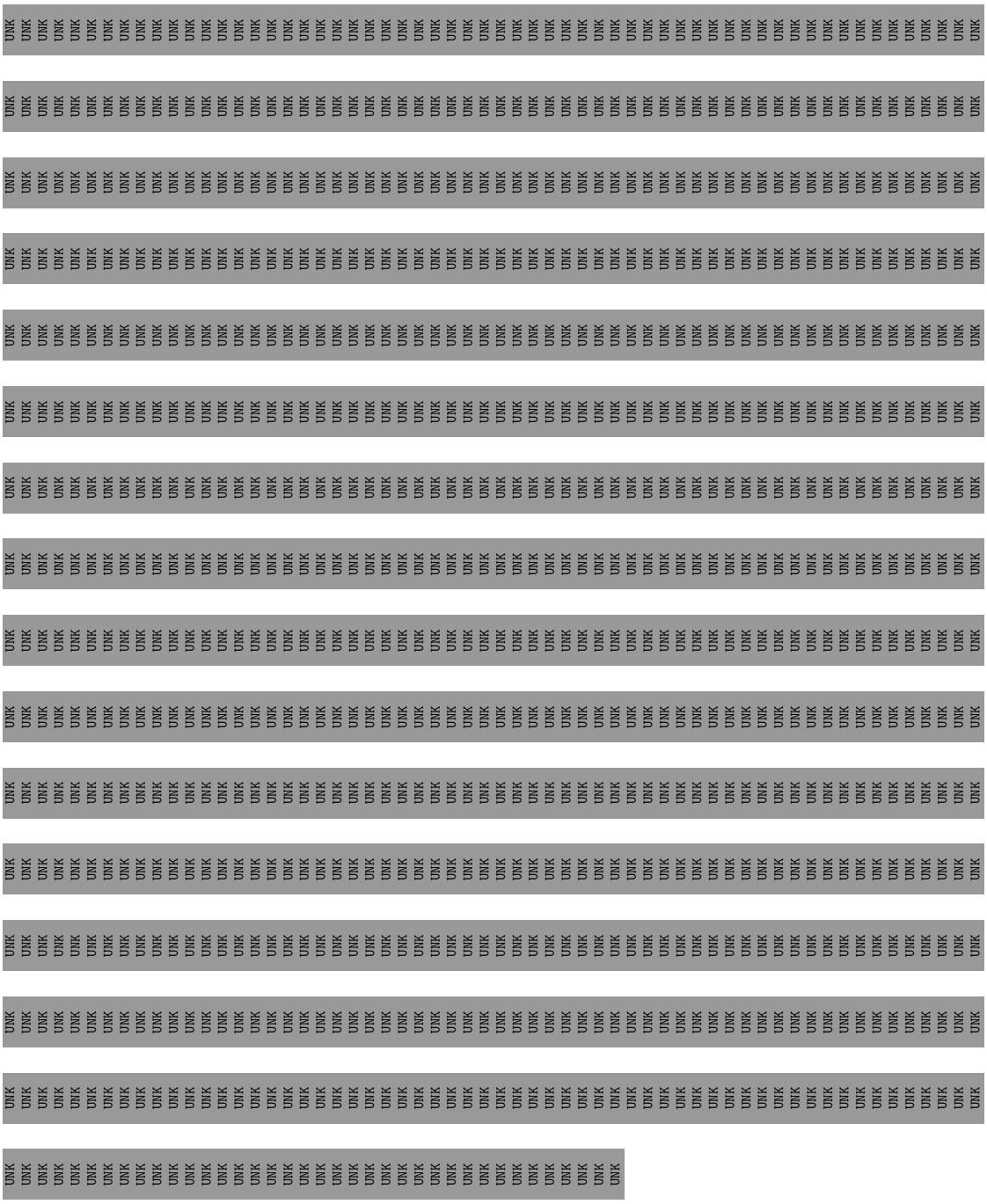
Chain C: 5% 5% 90%





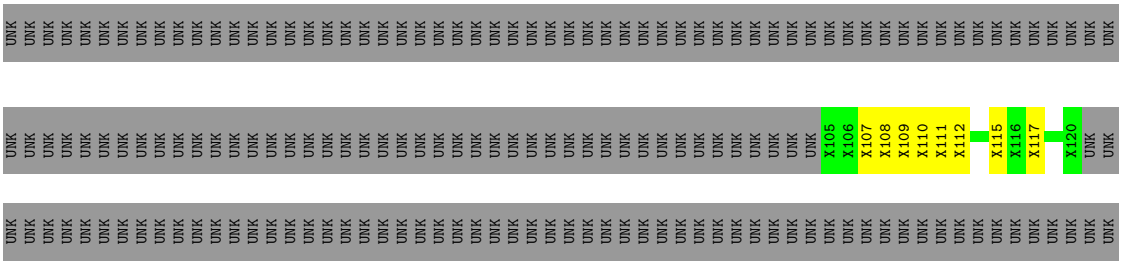

X1115 X1116 X1117 X1118 X1119 X1120
X1205 X1206 X1207 X1208 X1209 X1210 X1211 X1212 X1213 X1214 X1215 X1216 X1217
X1305 X1306 X1307 X1308 X1309 X1310 X1311 X1312 X1313 X1314 X1315 X1316 X1320 X1321 X1322
X1405 X1406 X1407 X1408 X1409 X1410 X1411 X1412 X1413 X1414 X1415
X1416 X1417 X1418 X1419 X1423
X1505 X1506 X1507 X1508 X1509 X1510 X1511 X1512 X1513 X1514
X1605 X1606 X1607 X1608 X1609 X1610 X1614
X1705 X1706 X1707 X1708 X1709 X1712 X1713 X1714
X1805 X1806 X1807 X1808 X1809 X1812 X1813 X1814 X1815 X1816 X1817 X1818 X1819 X1820 X1823
X1905 X1906 X1907 X1908 X1909 X1910 X1911 X1912 X1913 X1914 X1919 X1920 X1921 X1922 X1923 X1924 X1925
X2005 X2010 X2011 X2012 X2018

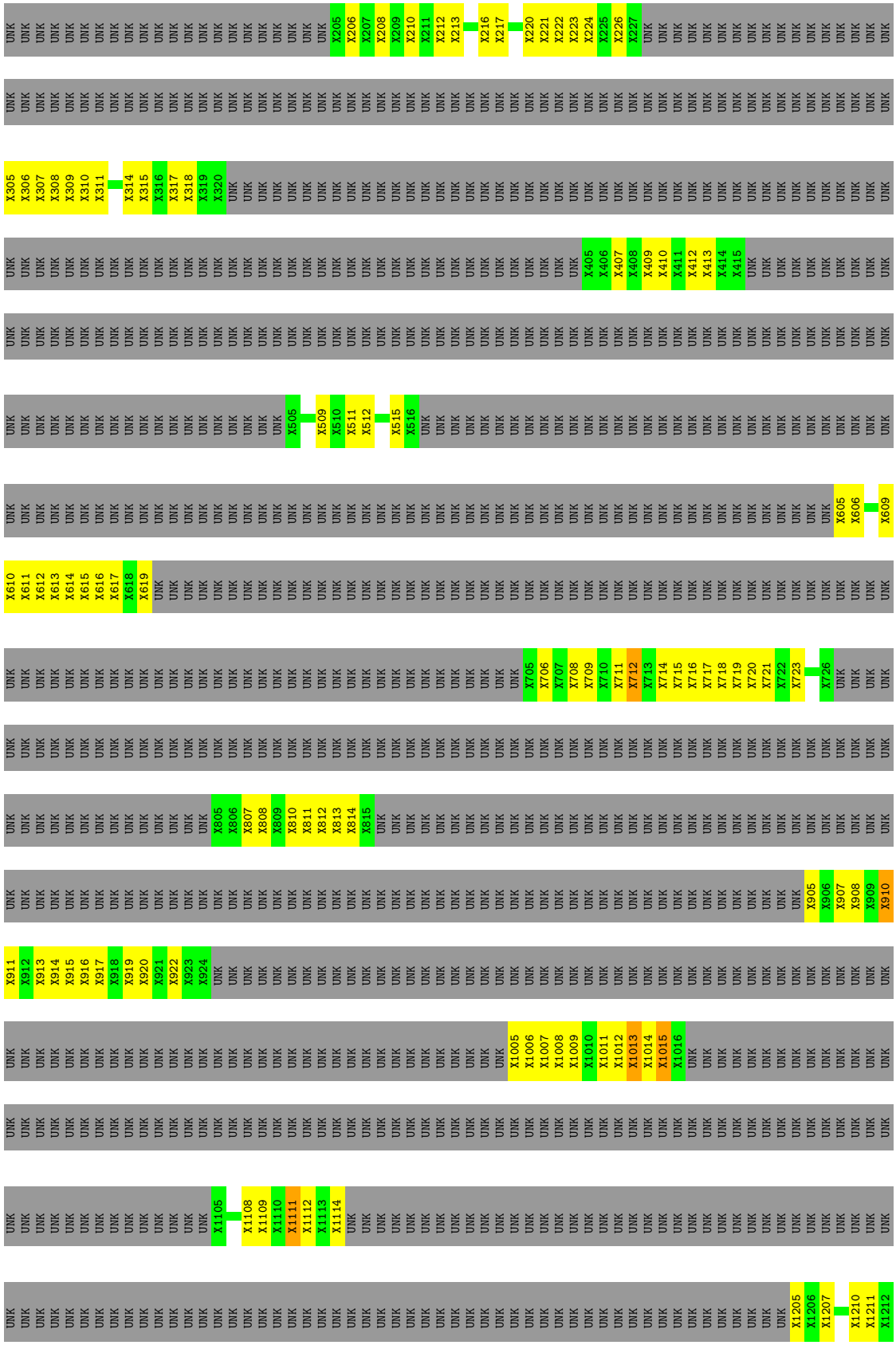

UNK X2105 X2112 X2113 X2114 X2115 X2118 X2119 X2120 X2121 X2122 X2123 X2124 X2125 X2129 UNK
UNK X2205 X2206 X2207 X2208 X2209 X2210 X2211 X2212 X2213 X2216 X2217 X2218 X2219 UNK UNK
UNK X2305 X2306 X2307 X2308 X2309 X2310 X2311 X2312 X2313 X2314 X2315 UNK
UNK X2405 X2408 X2409 X2410 X2411 X2412 X2413 X2414 X2415 X2416 UNK
UNK X2505 X2506 X2507 X2508 X2509 X2510 X2511 X2512 X2513 X2514 X2515 X2516 X2517 X2520 X2521 UNK UNK
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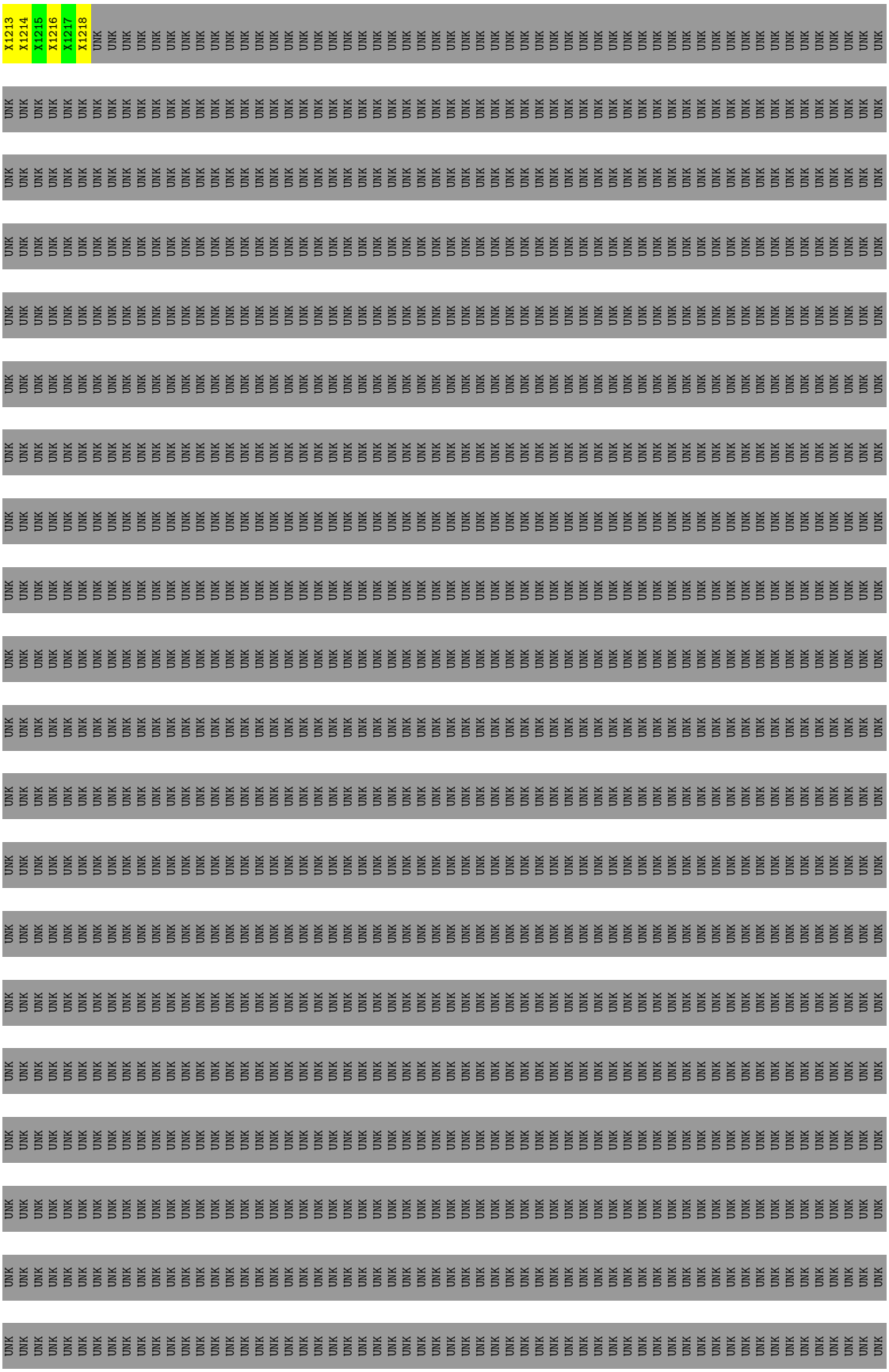


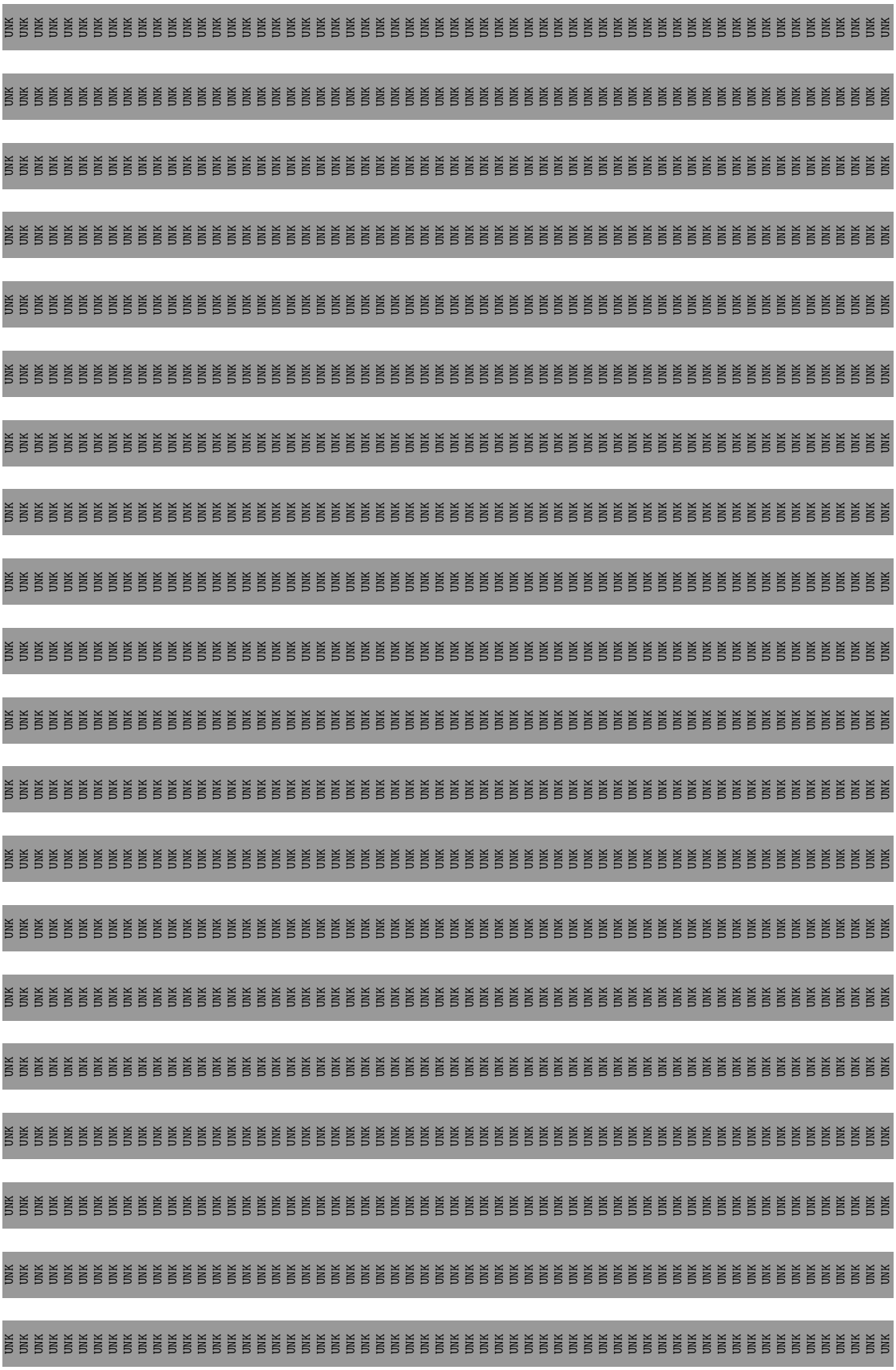
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

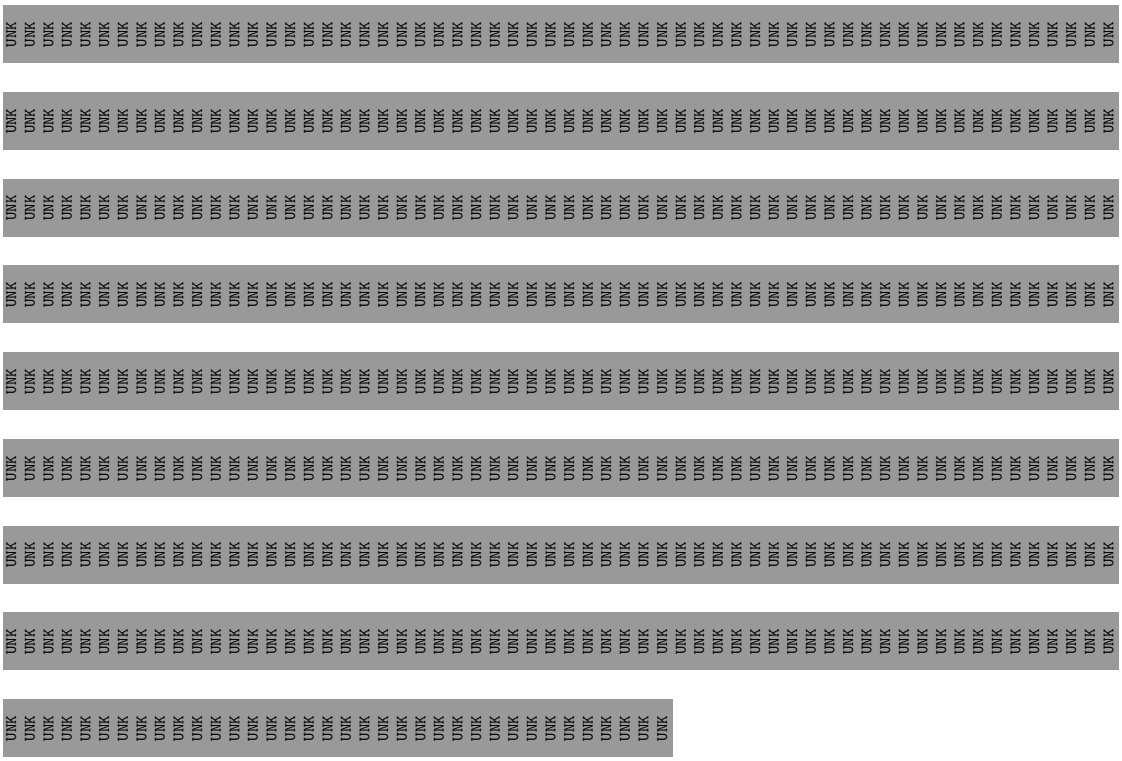
Chain D: 96%





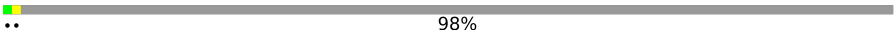

X1213
X1214
X1215
X1216
X1217
X1218
UNK

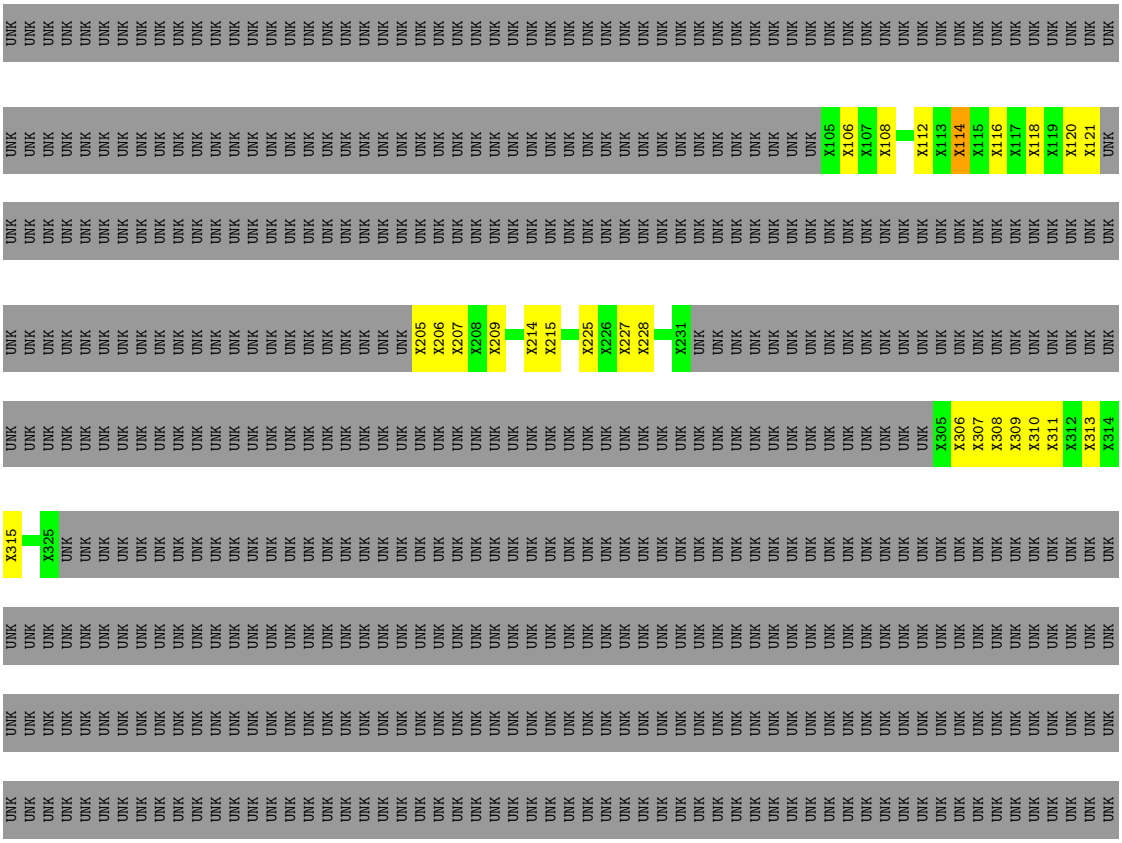

UNK

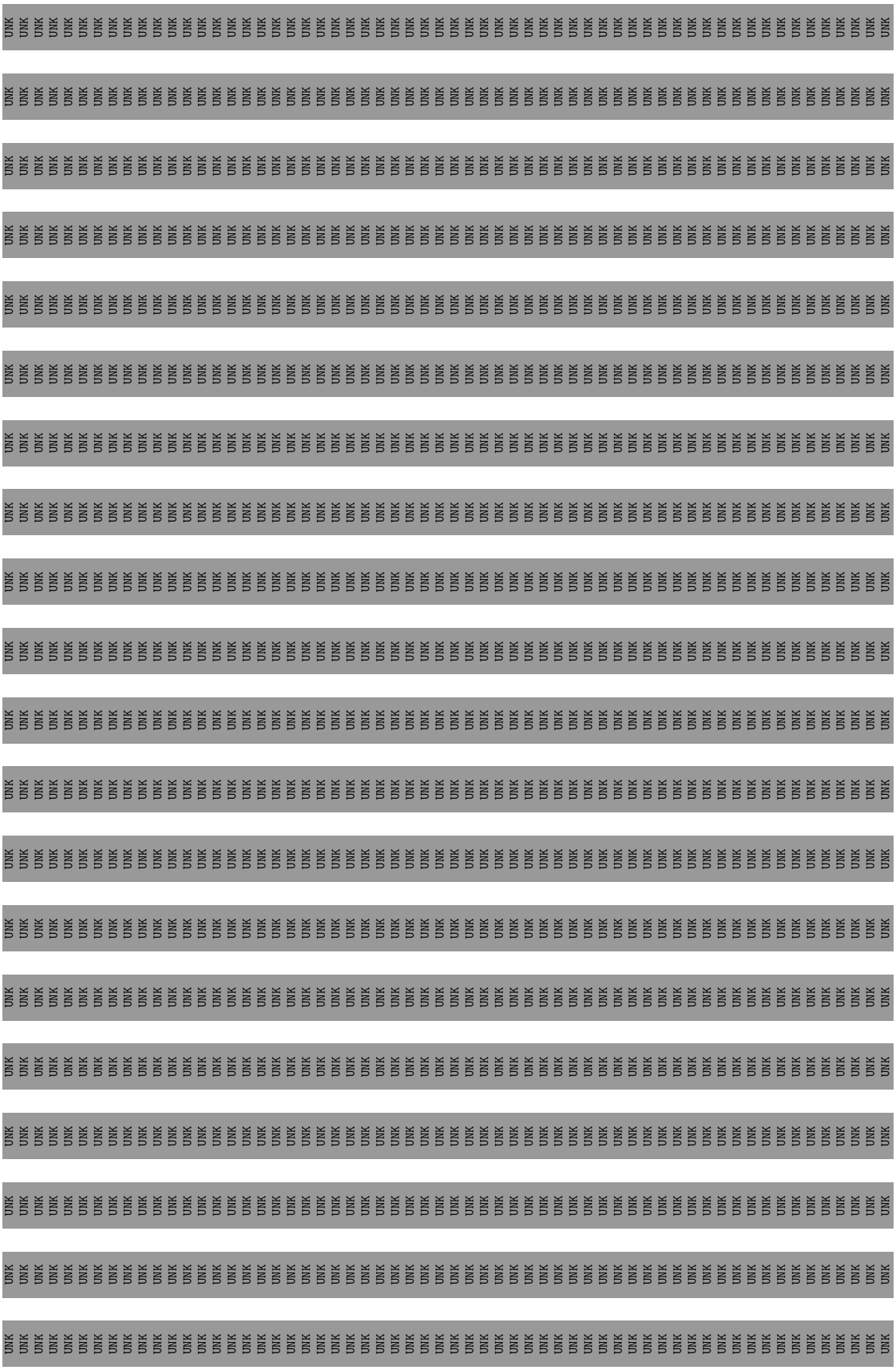


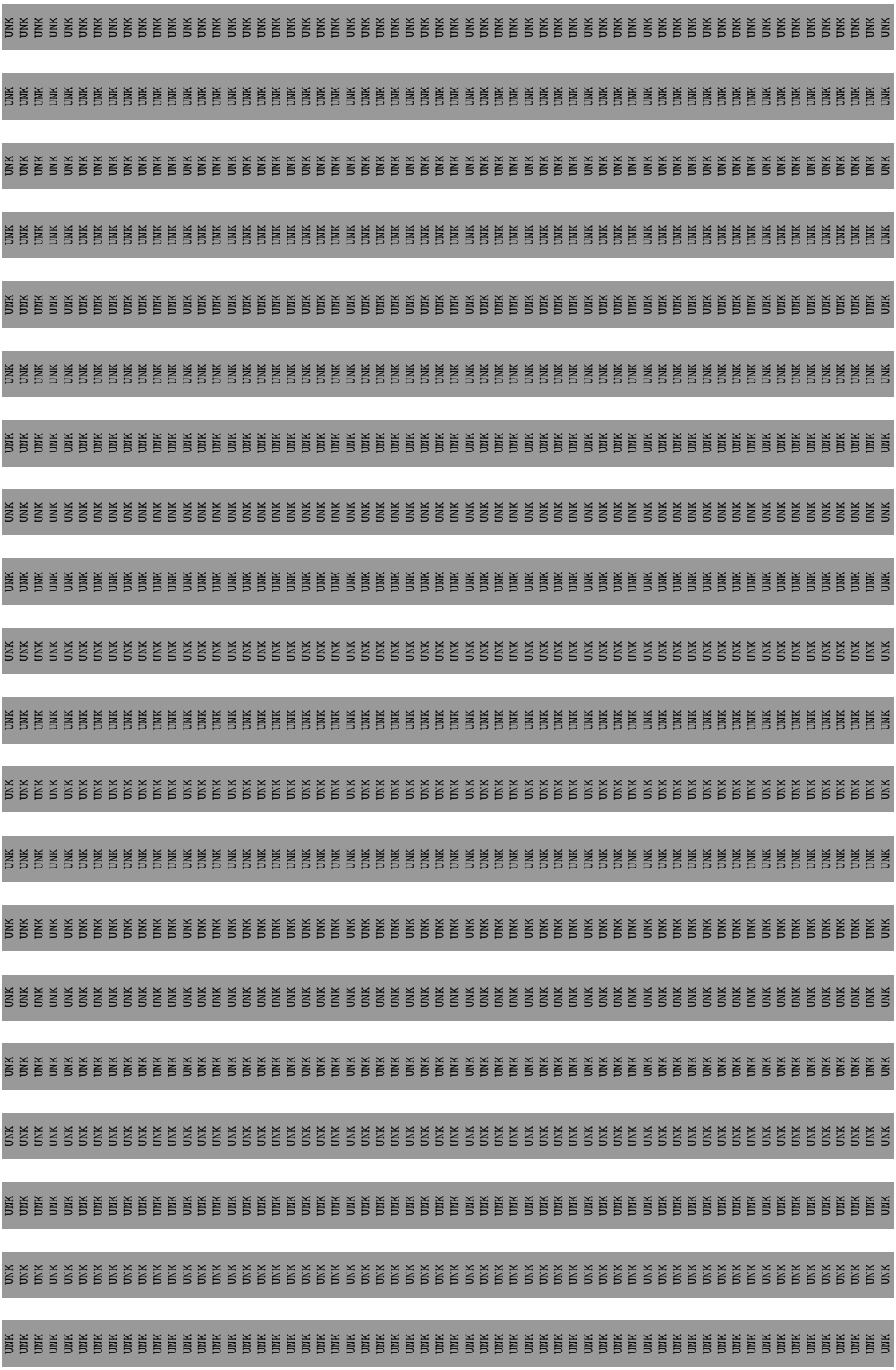
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

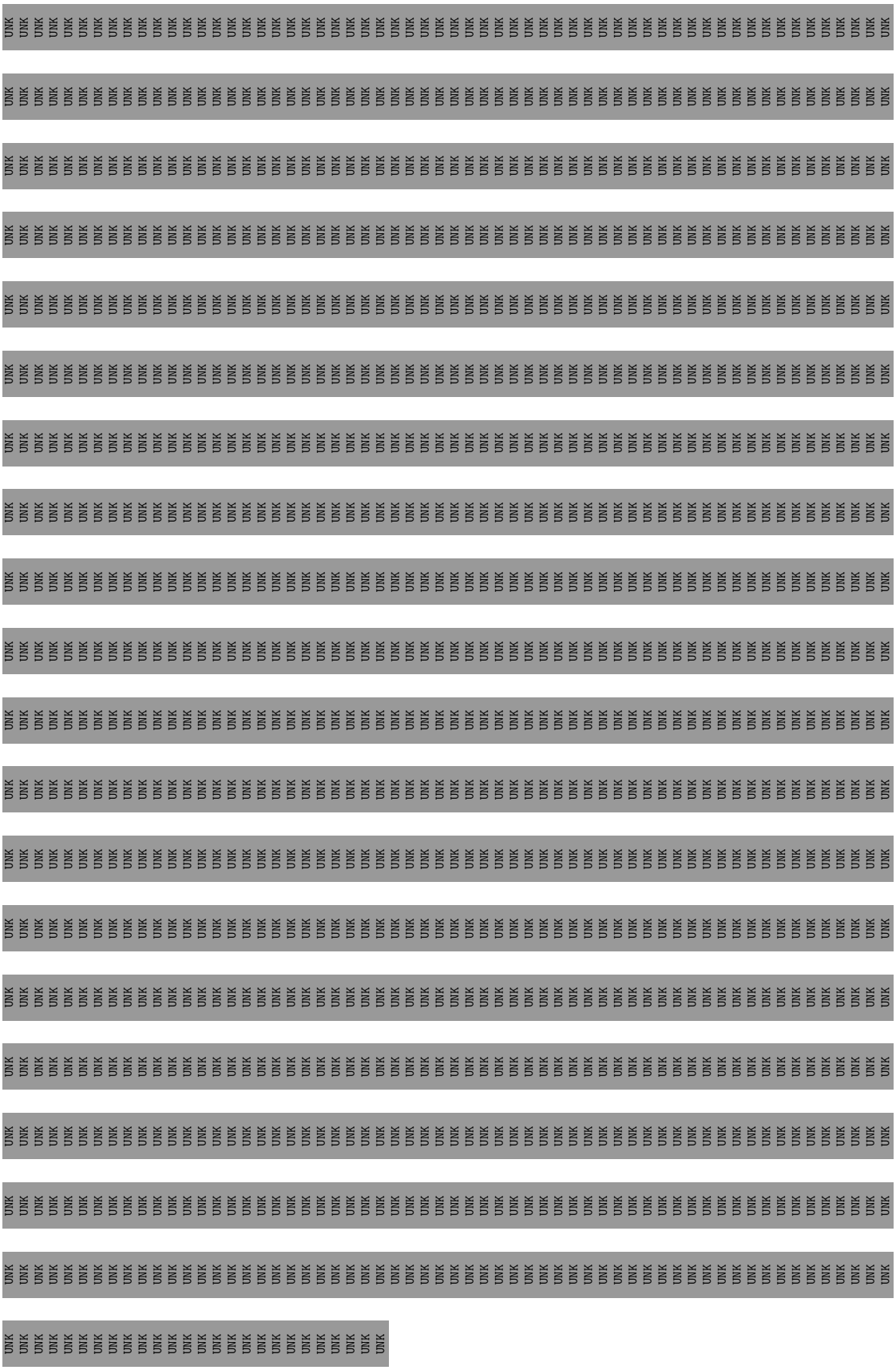
Chain E:





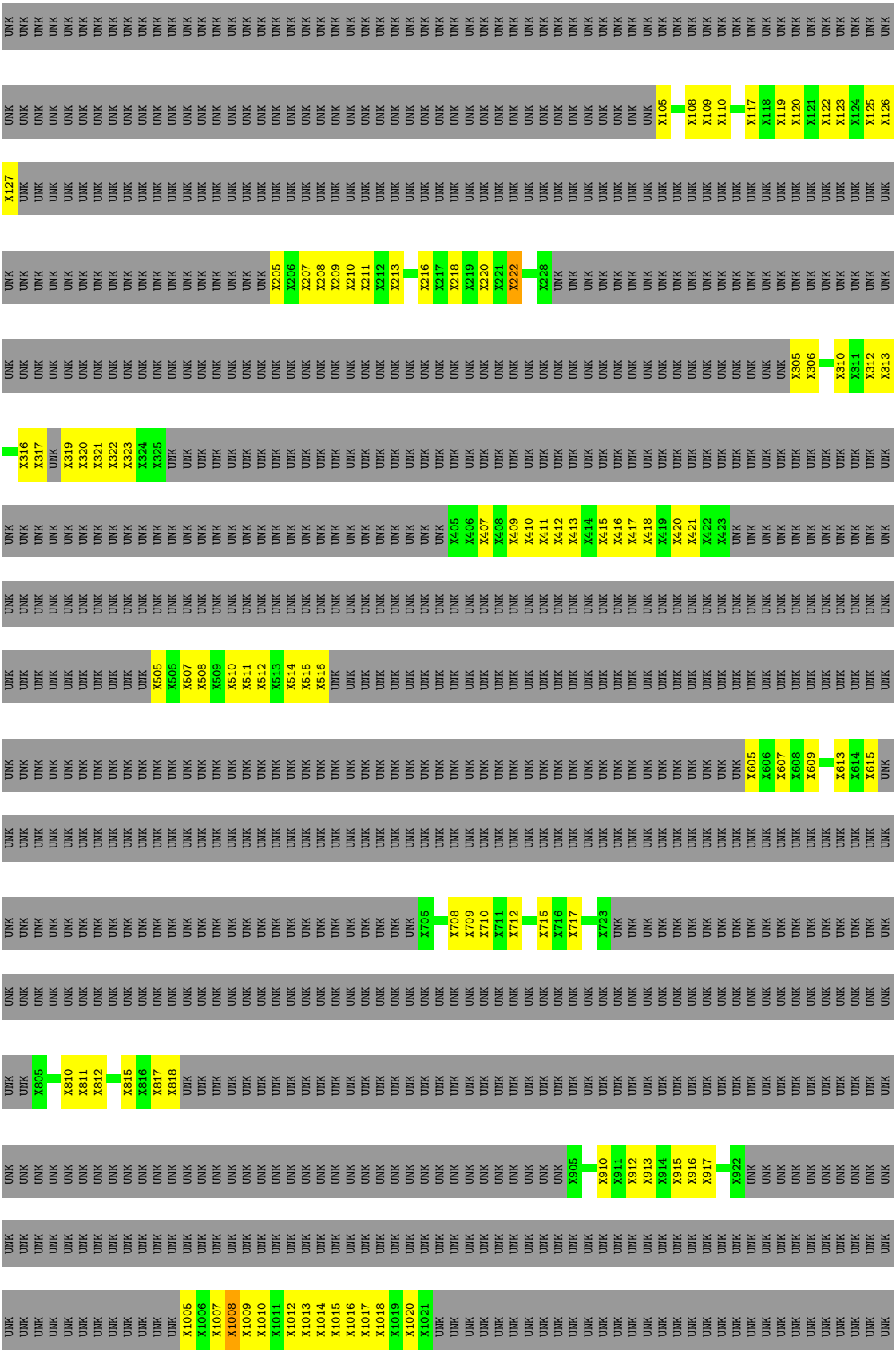

UNK

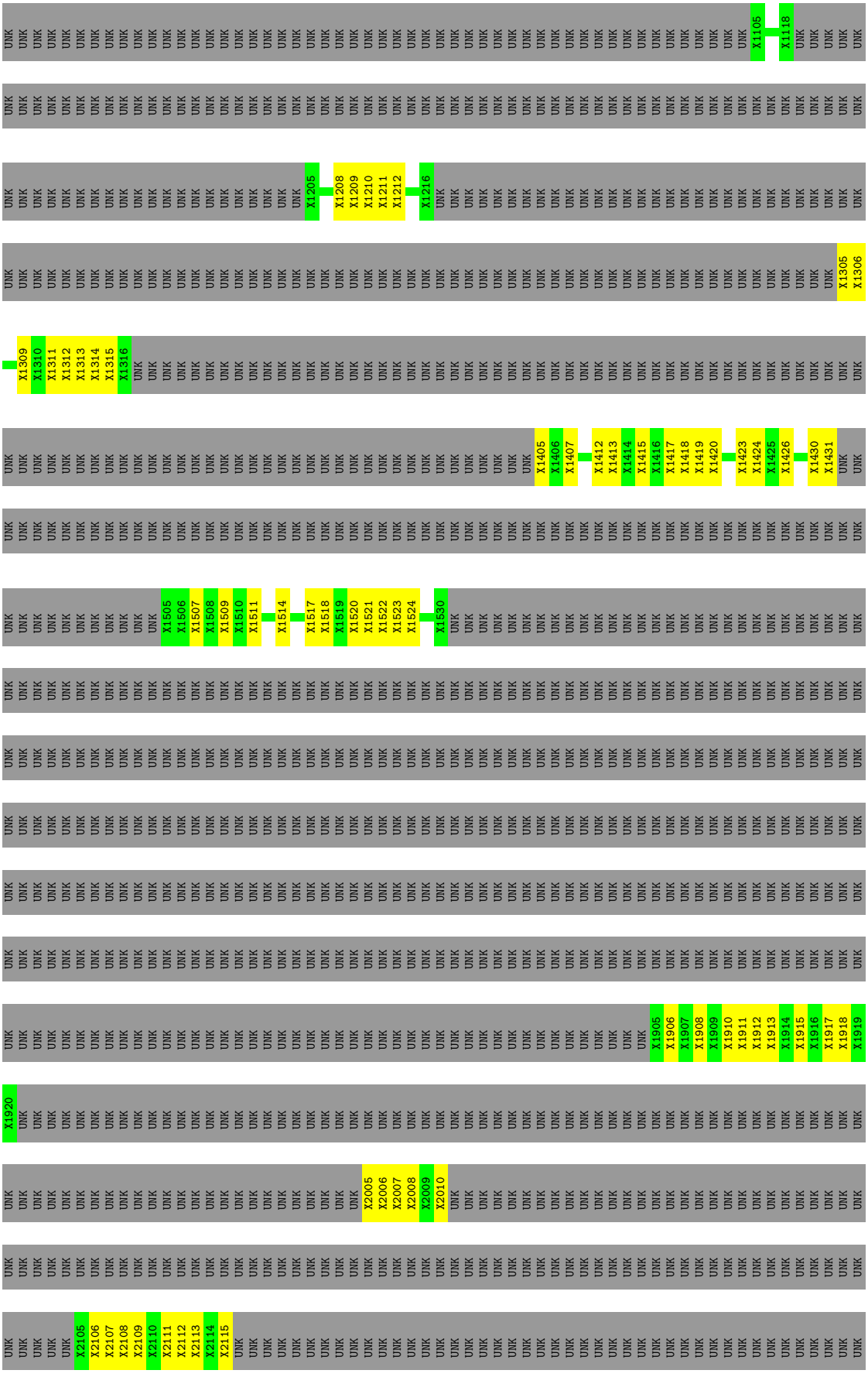

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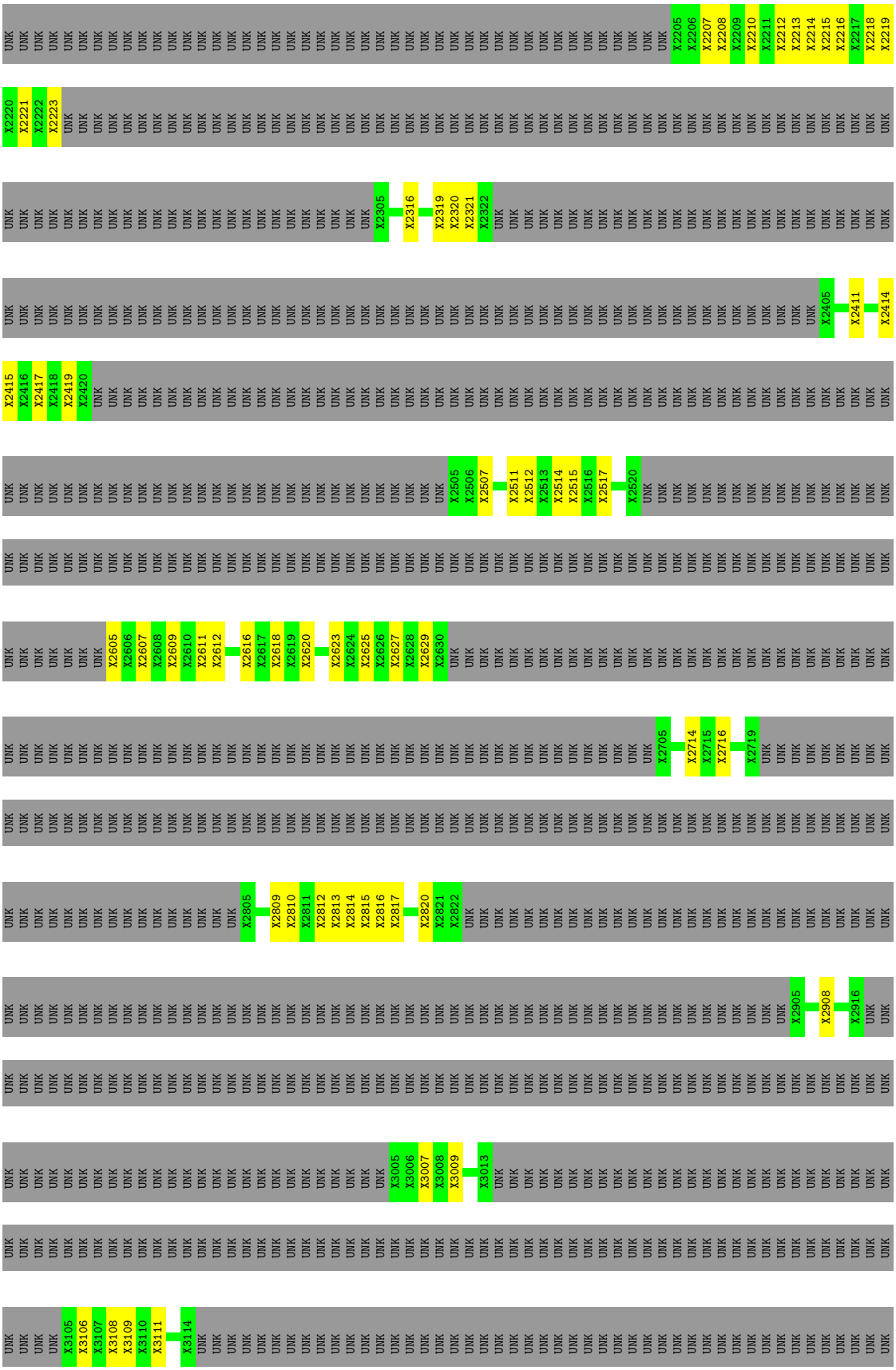


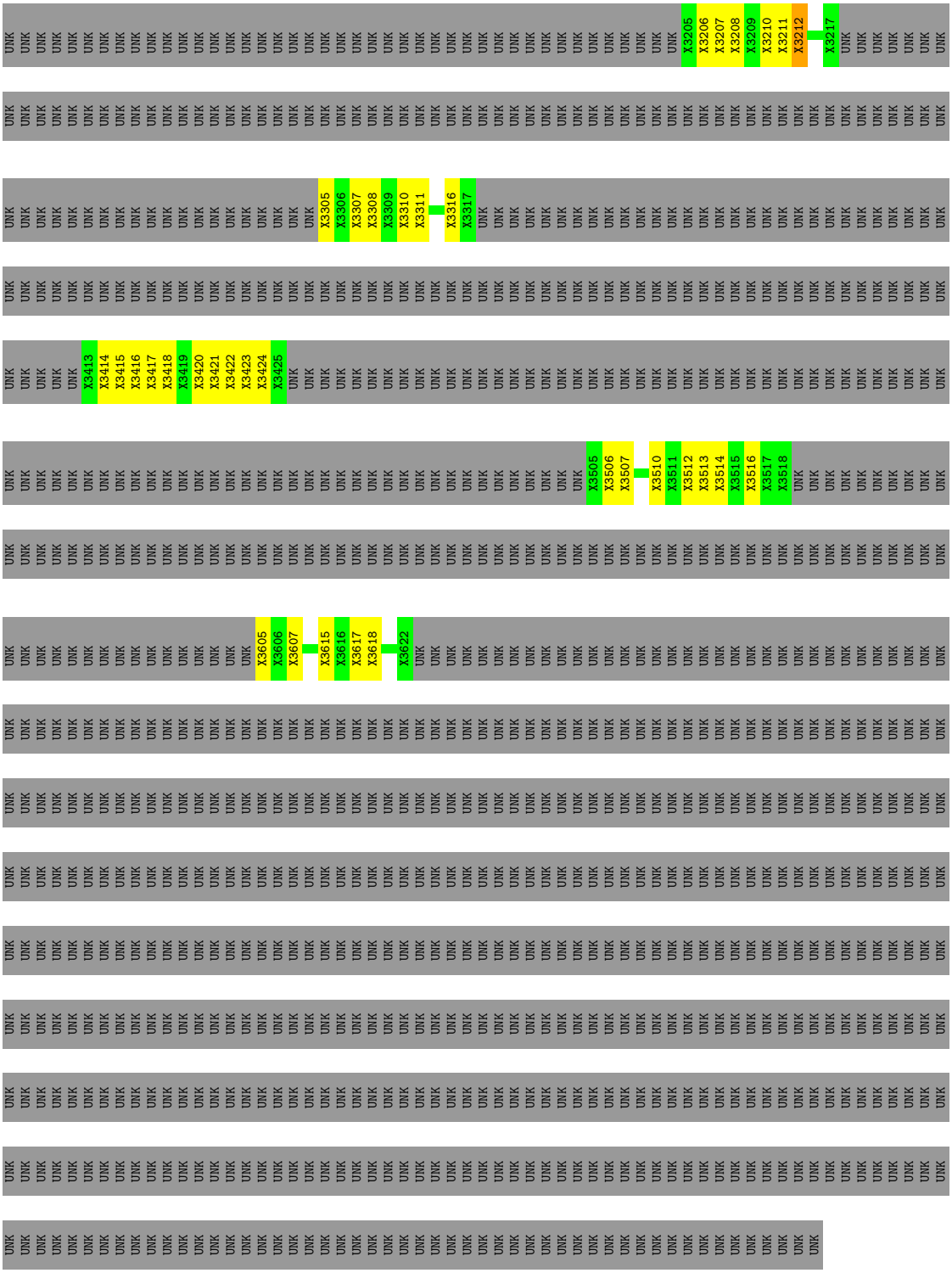
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain F: 7% 6% 87%




X1105
X1118
X1205
X1208
X1209
X1210
X1211
X1212
X1216
X1305
X1306
X1309
X1310
X1311
X1312
X1313
X1314
X1315
X1316
X1405
X1406
X1407
X1412
X1413
X1414
X1415
X1416
X1417
X1418
X1419
X1420
X1423
X1424
X1425
X1426
X1430
X1431
X1505
X1506
X1507
X1508
X1509
X1510
X1511
X1514
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X1518
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X1910
X1911
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X2113
X2114
X2115

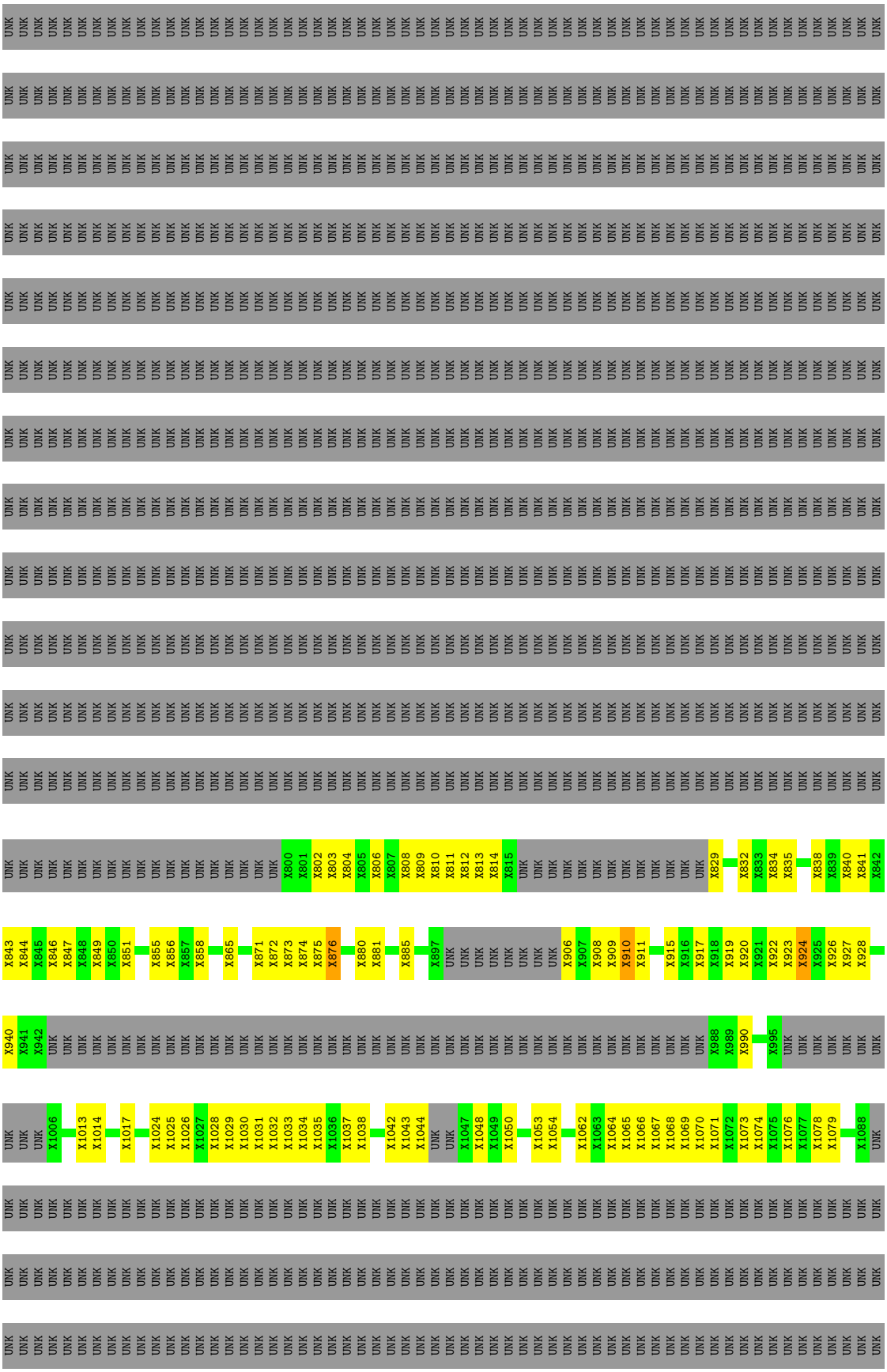

UNK
X2205
X2206
X2207
X2208
X2209
X2210
X2211
X2212
X2213
X2214
X2215
X2216
X2217
X2218
X2219
X2220
X2221
X2222
X2223
X2305
X2316
X2319
X2320
X2321
X2322
X2405
X2411
X2414
X2415
X2416
X2417
X2418
X2419
X2420
X2505
X2506
X2507
X2511
X2512
X2513
X2514
X2515
X2516
X2517
X2520
X2605
X2606
X2607
X2608
X2609
X2610
X2611
X2612
X2616
X2617
X2618
X2619
X2620
X2623
X2624
X2625
X2626
X2627
X2628
X2629
X2630
X2705
X2714
X2715
X2716
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X2812
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X2815
X2816
X2817
X2820
X2821
X2822
X2905
X2908
X2916
X3005
X3006
X3007
X3008
X3009
X3013
X3105
X3106
X3107
X3108
X3109
X3110
X3111
X3114

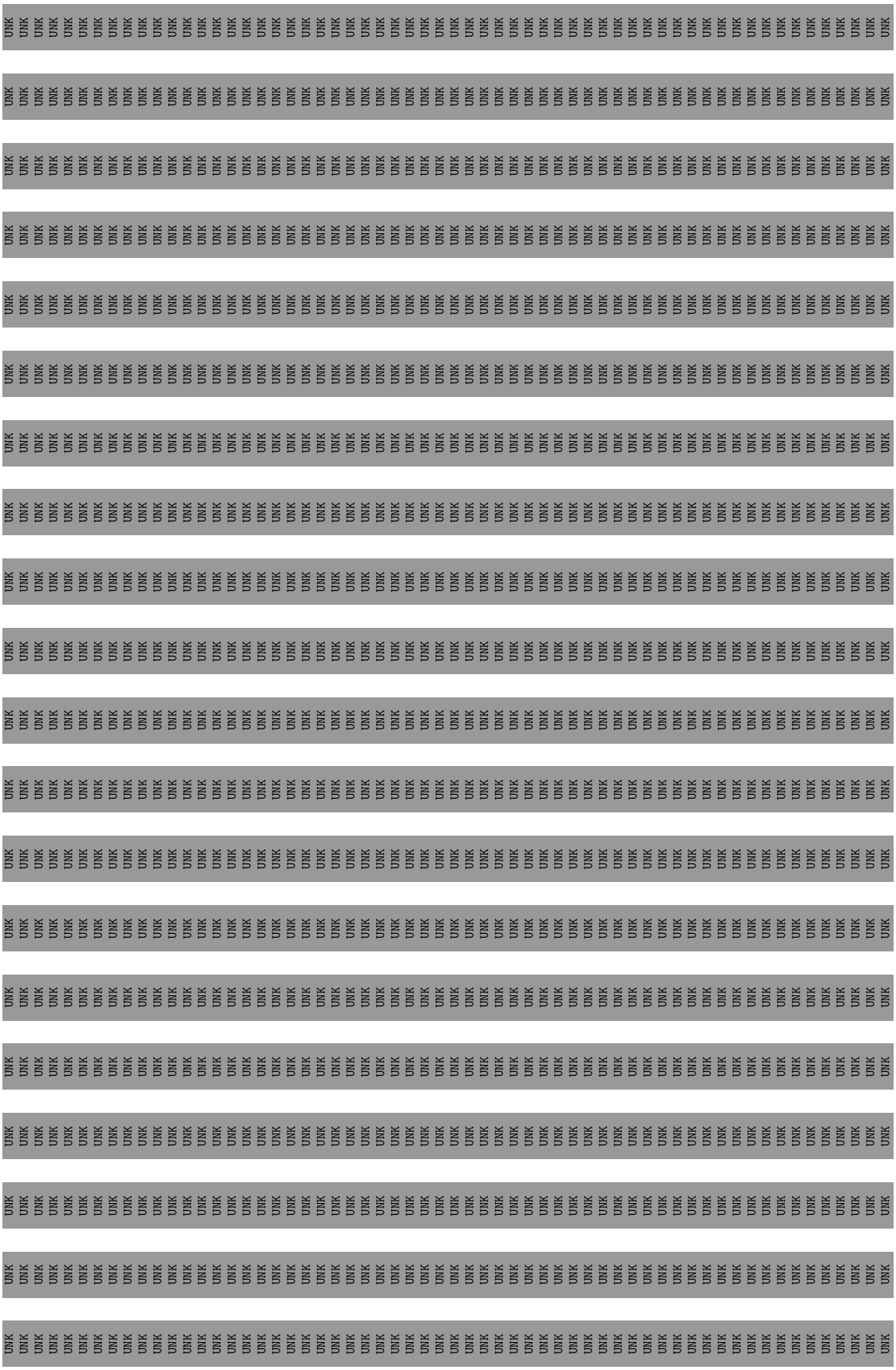


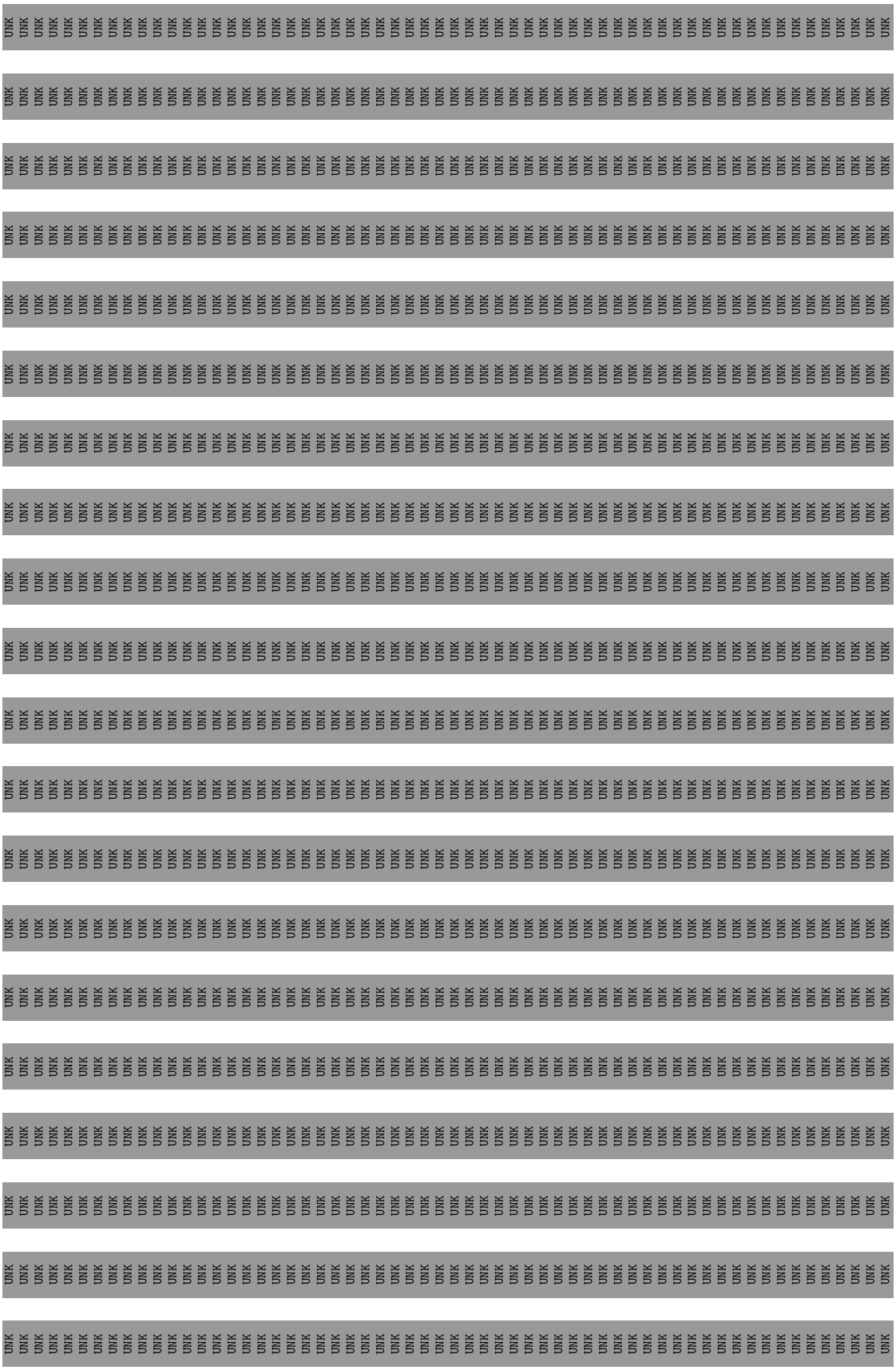
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

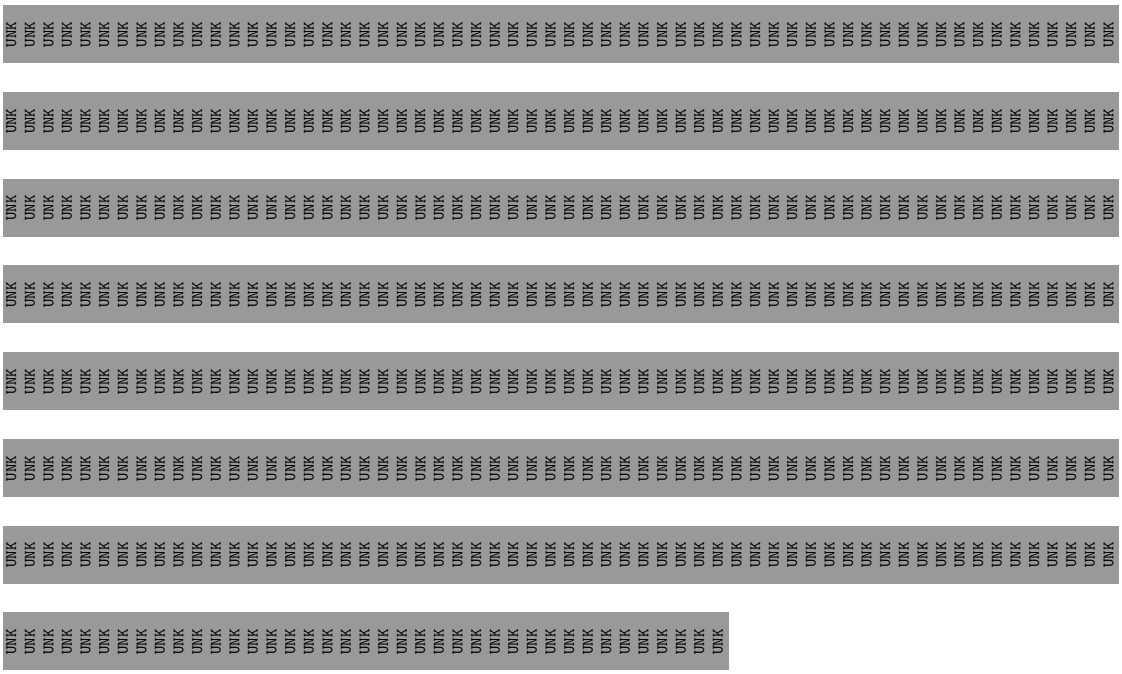
Chain X: 95%




UNK
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
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
X940 X941 X942 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

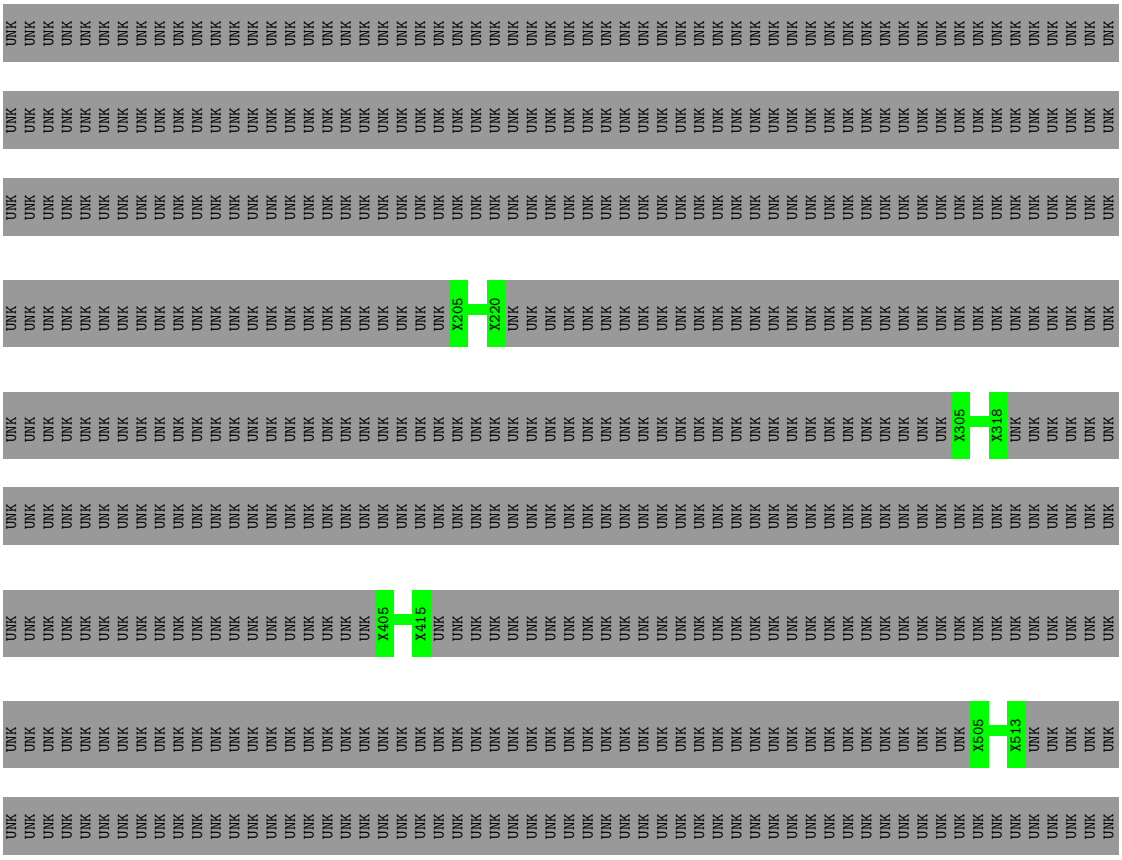

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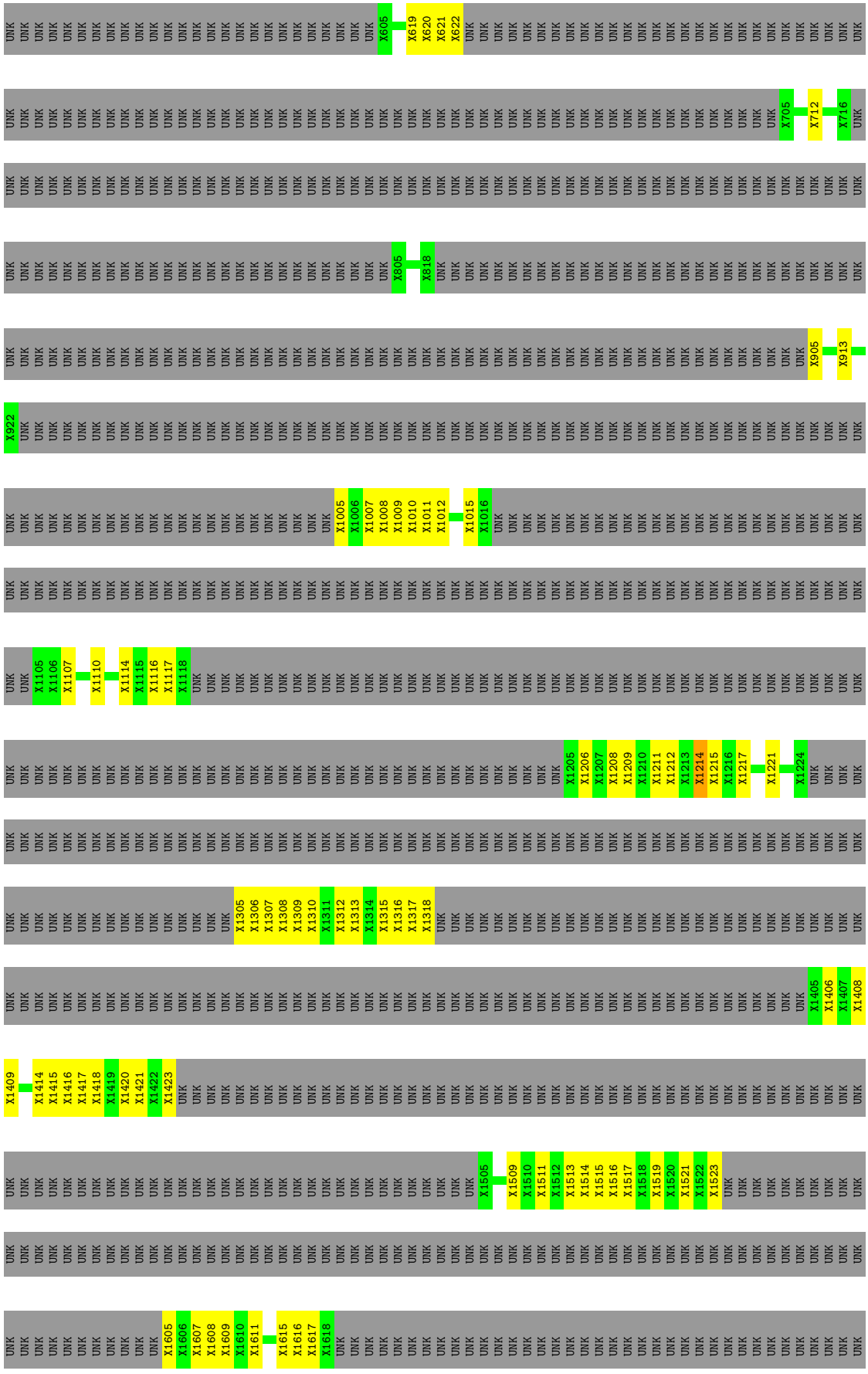

UNK

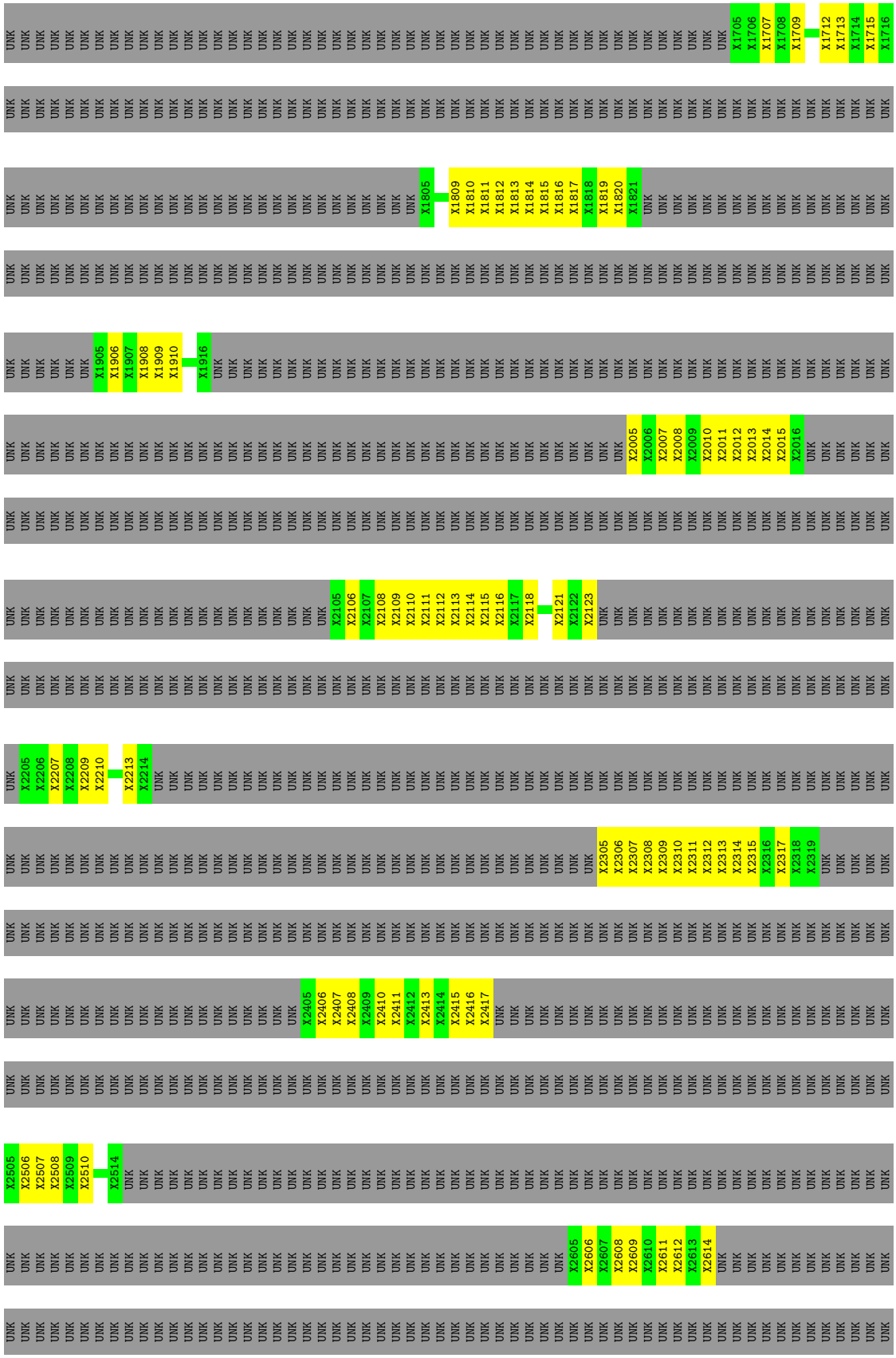


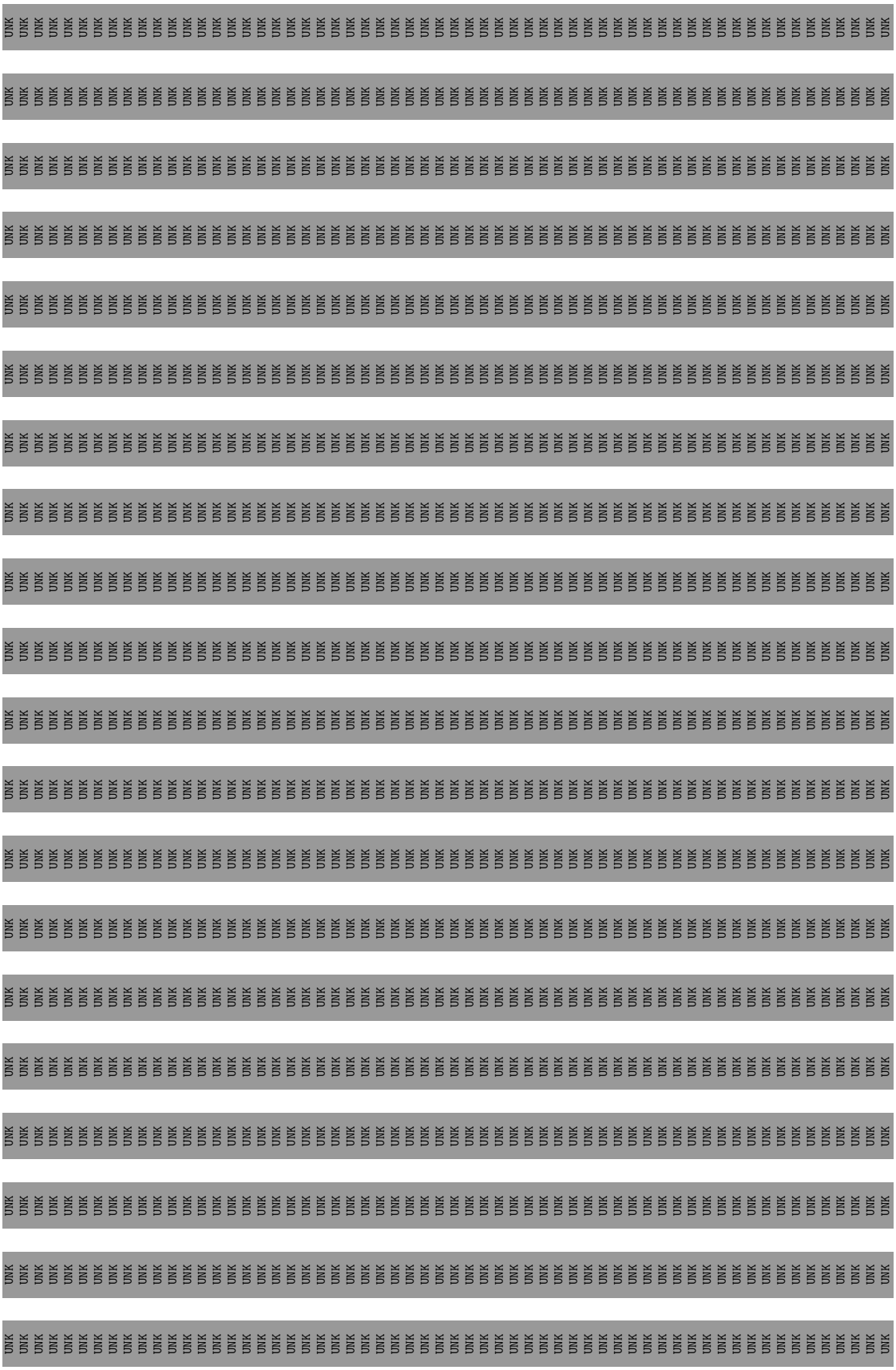
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

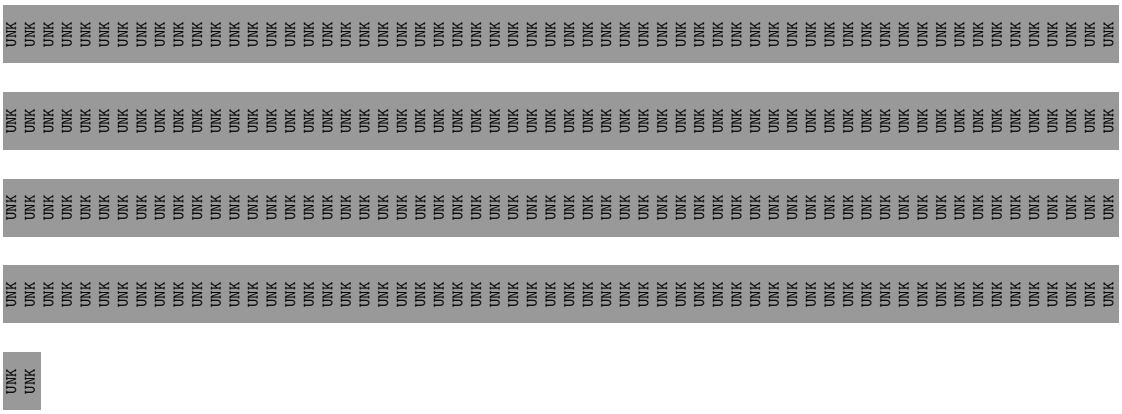
Chain O: 5% 91%




UNK
X605
X619
X620
X621
X622
X705
X712
X716
X805
X818
X905
X913
X922
X1005
X1006
X1007
X1008
X1009
X1010
X1011
X1012
X1015
X1016
X1105
X1106
X1107
X1110
X1114
X1115
X1116
X1117
X1118
X1205
X1206
X1207
X1208
X1209
X1210
X1211
X1212
X1213
X1214
X1215
X1216
X1217
X1221
X1224
X1305
X1306
X1307
X1308
X1309
X1310
X1311
X1312
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X1314
X1315
X1316
X1317
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X1510
X1511
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X1515
X1516
X1517
X1518
X1519
X1520
X1521
X1522
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X1616
X1617
X1618

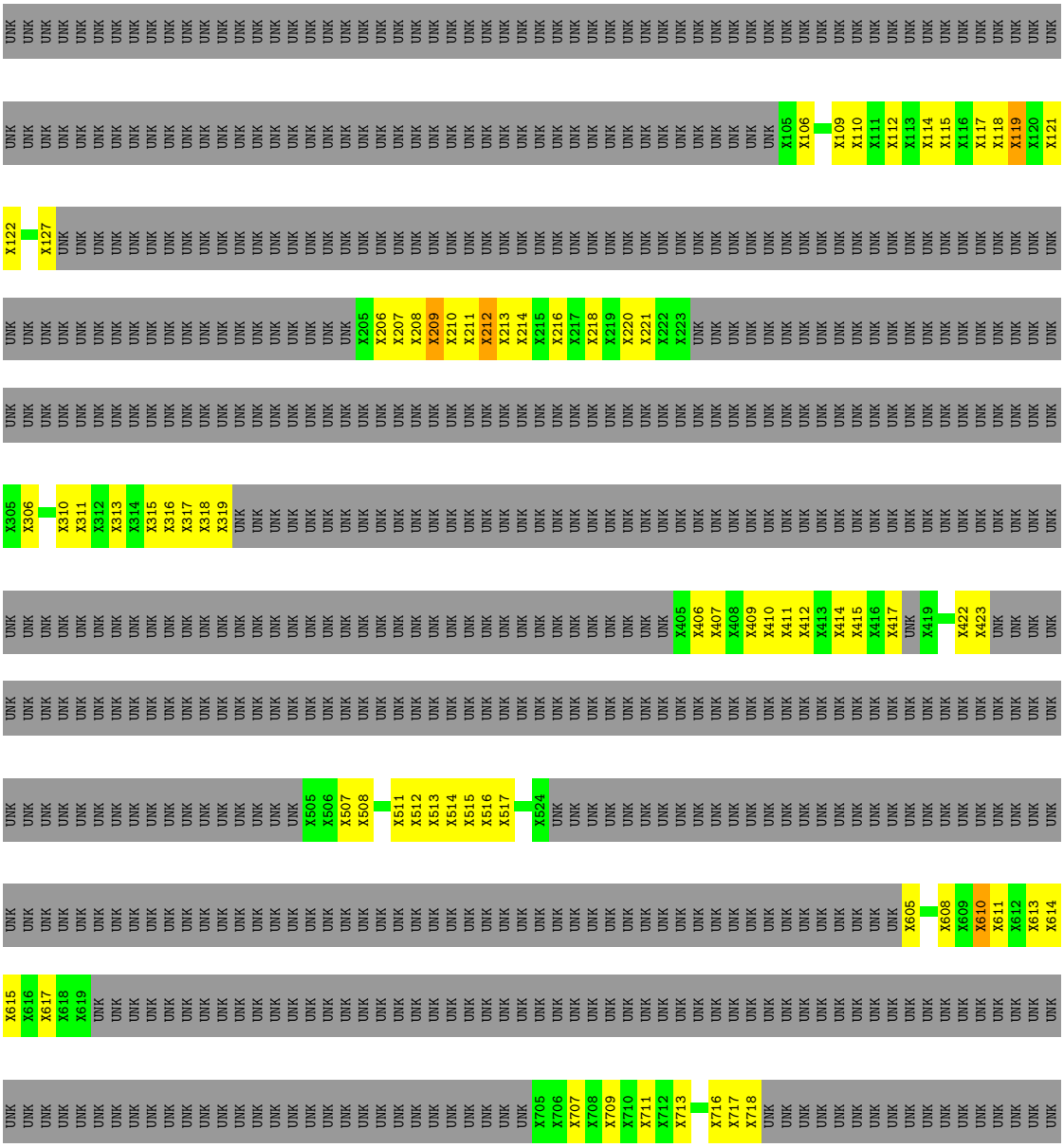

UNK X1705 X1706 X1707 X1708 X1709 X1712 X1713 X1714 X1715 X1716
UNK X1805 X1809 X1810 X1811 X1812 X1813 X1814 X1815 X1816 X1817 X1818 X1819 X1820 X1821
UNK X1905 X1906 X1907 X1908 X1909 X1910 X1916
UNK X2005 X2006 X2007 X2008 X2009 X2010 X2011 X2012 X2013 X2014 X2015 X2016
UNK X2105 X2106 X2107 X2108 X2109 X2110 X2111 X2112 X2113 X2114 X2115 X2116 X2117 X2118 X2121 X2122 X2123
UNK X2205 X2206 X2207 X2208 X2209 X2210 X2213 X2214
UNK X2305 X2306 X2307 X2308 X2309 X2310 X2311 X2312 X2313 X2314 X2315 X2316 X2317 X2318 X2319
UNK X2405 X2406 X2407 X2408 X2409 X2410 X2411 X2412 X2413 X2414 X2415 X2416 X2417
UNK X2505 X2506 X2507 X2508 X2509 X2510 X2514
UNK X2605 X2606 X2607 X2608 X2609 X2610 X2611 X2612 X2613 X2614

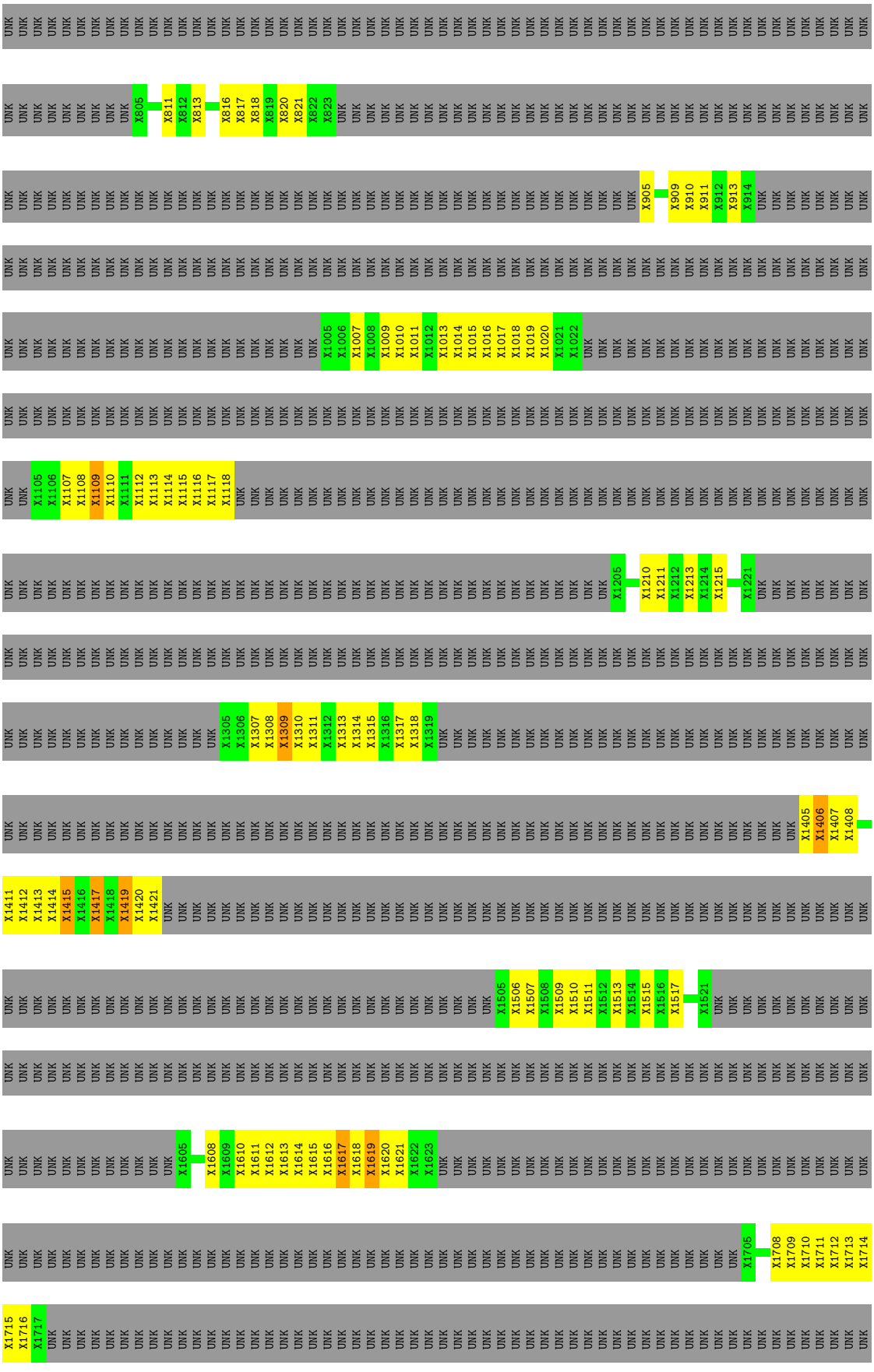

UNK

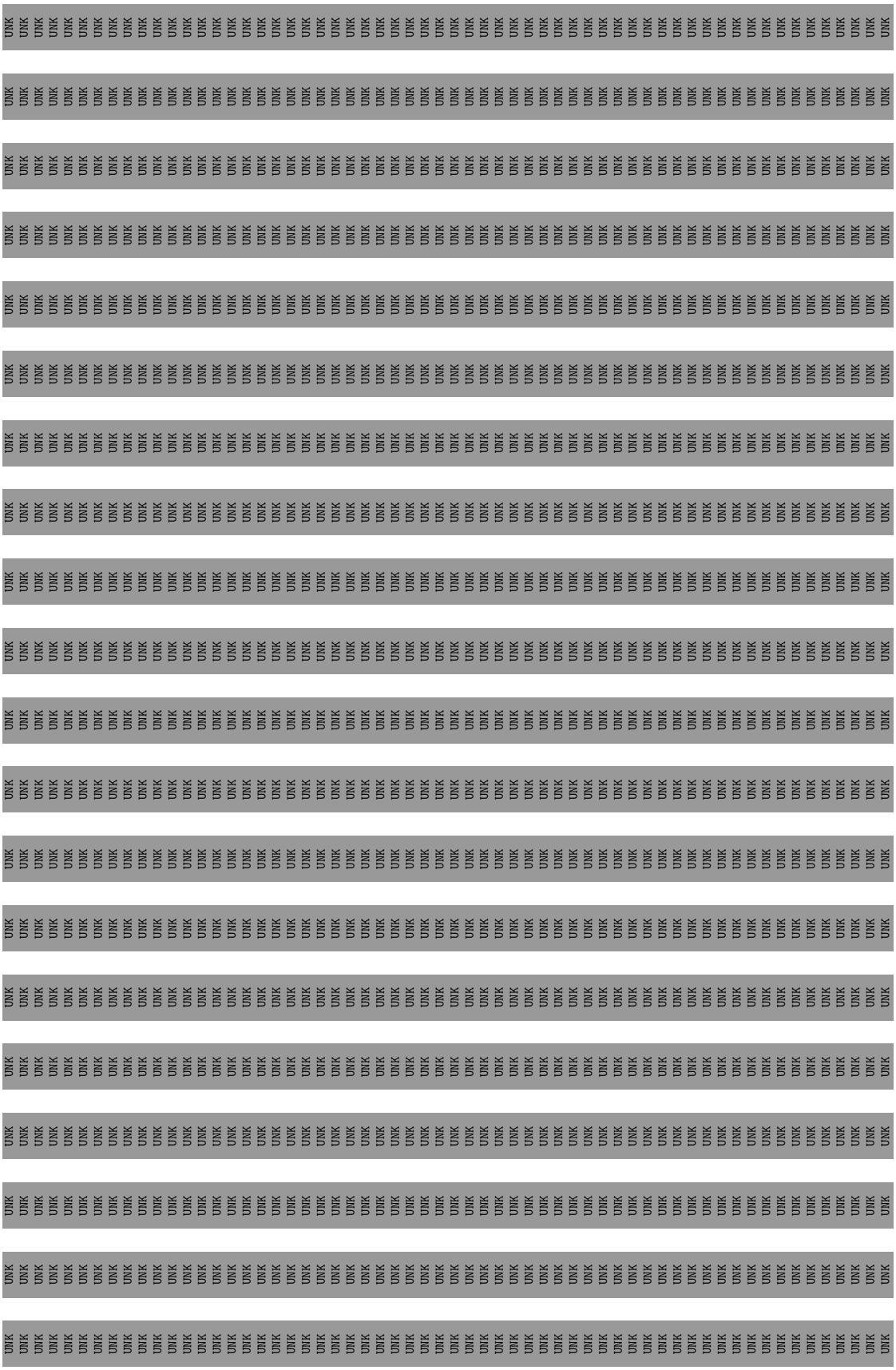


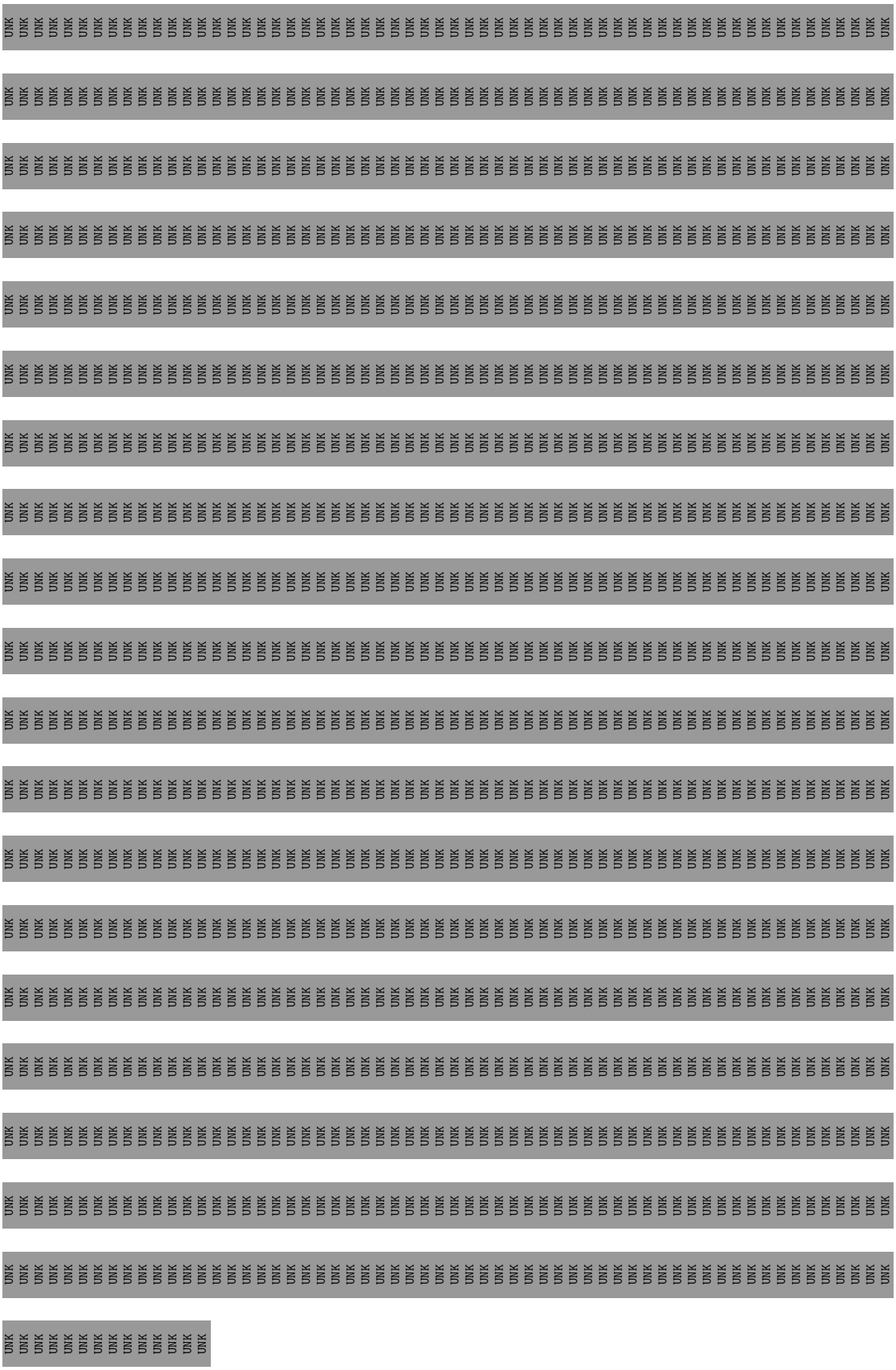
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain P: 93%



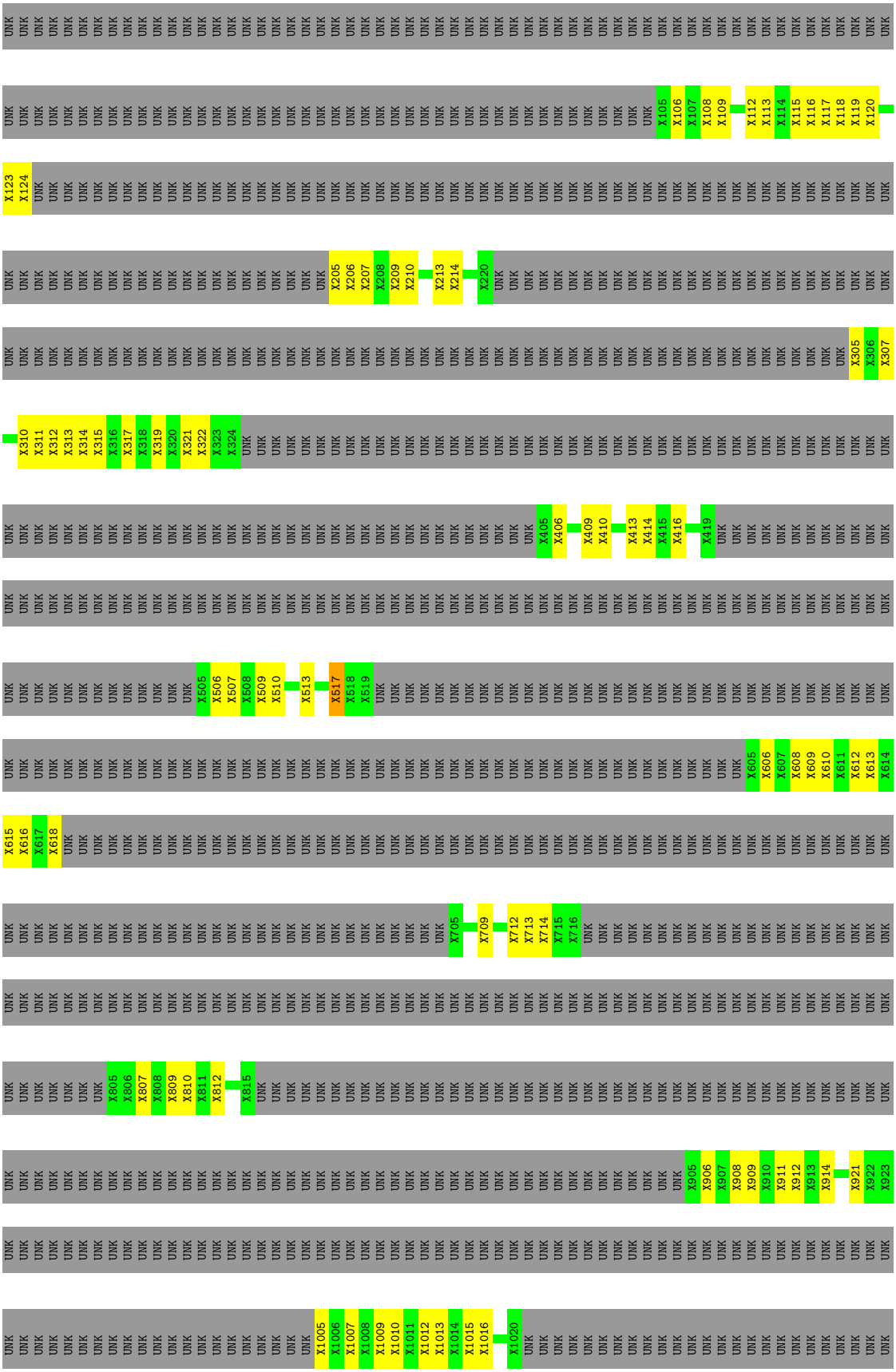


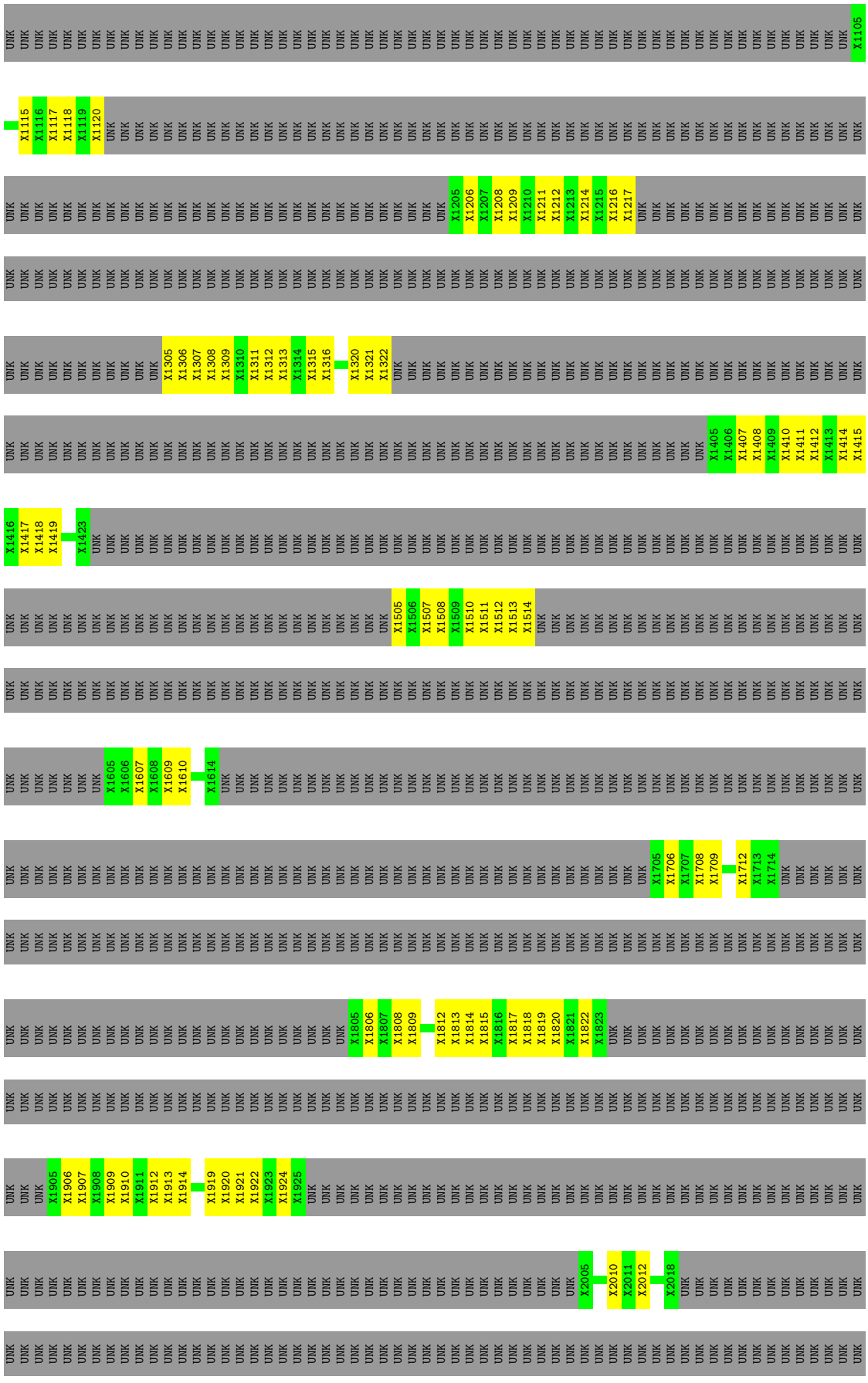

UNK

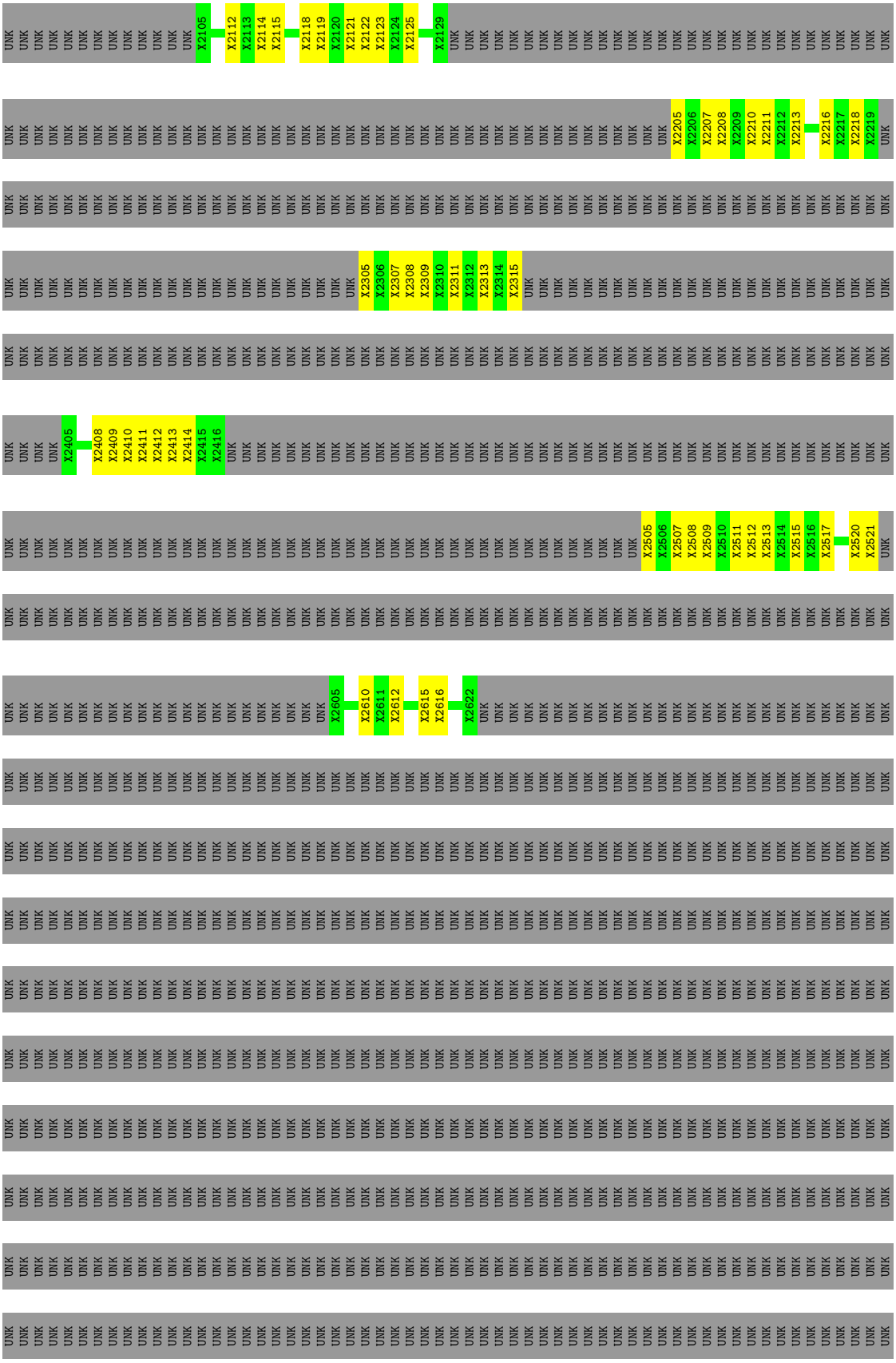


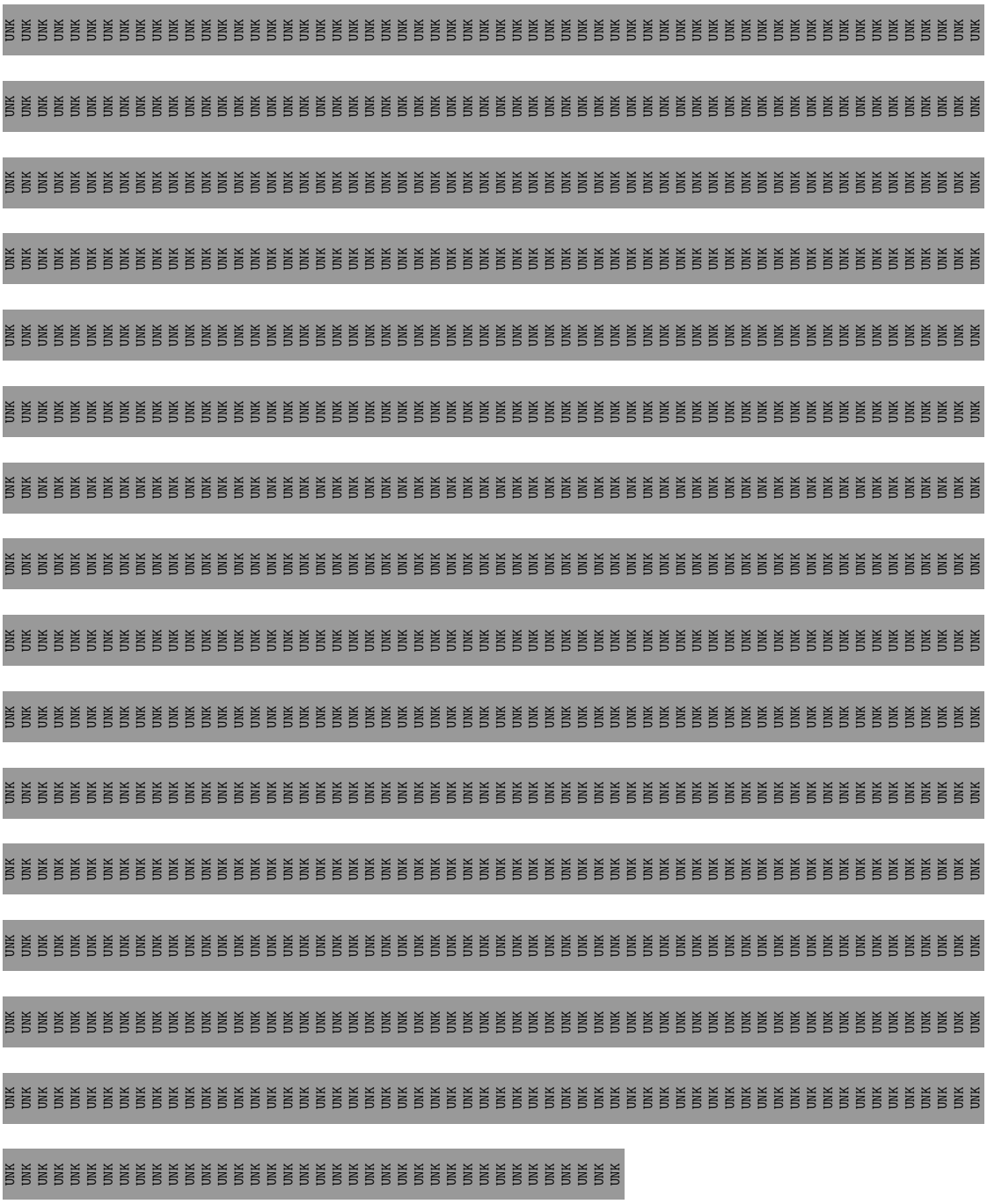
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain Q: 5% 5% 90%



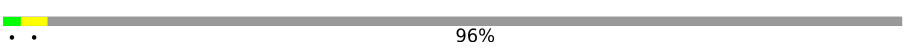


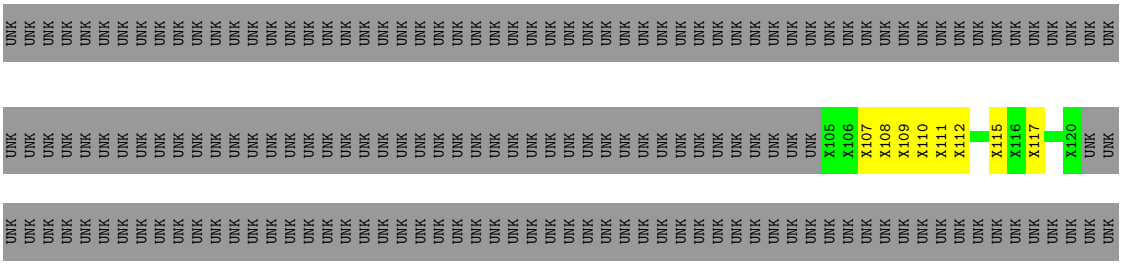

X2105
X2112
X2113
X2114
X2115
X2118
X2119
X2120
X2121
X2122
X2123
X2124
X2125
X2129
X2205
X2206
X2207
X2208
X2209
X2210
X2211
X2212
X2213
X2216
X2217
X2218
X2219
X2305
X2306
X2307
X2308
X2309
X2310
X2311
X2312
X2313
X2314
X2315
X2405
X2408
X2409
X2410
X2411
X2412
X2413
X2414
X2415
X2416
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X2615
X2616
X2622

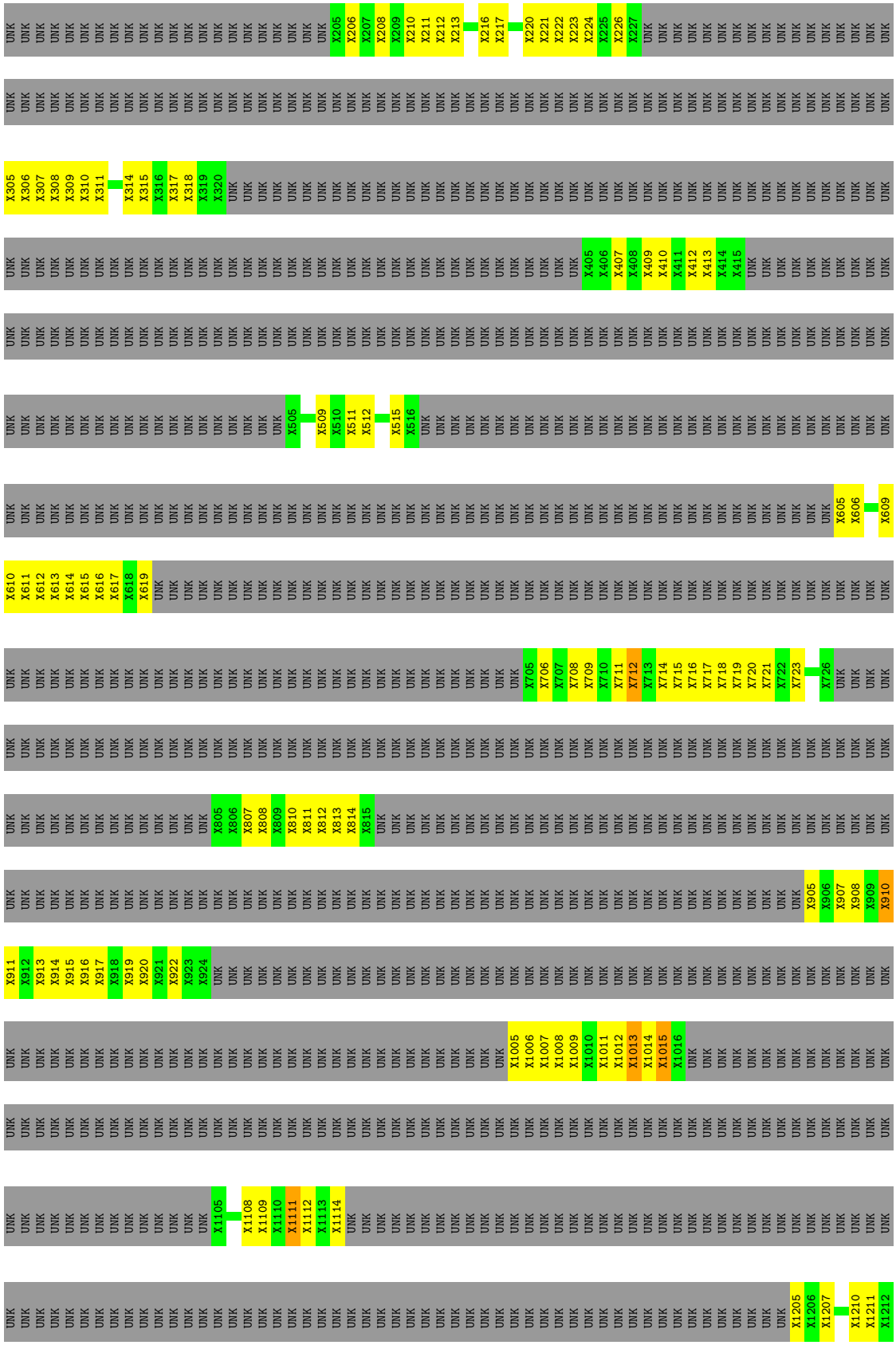


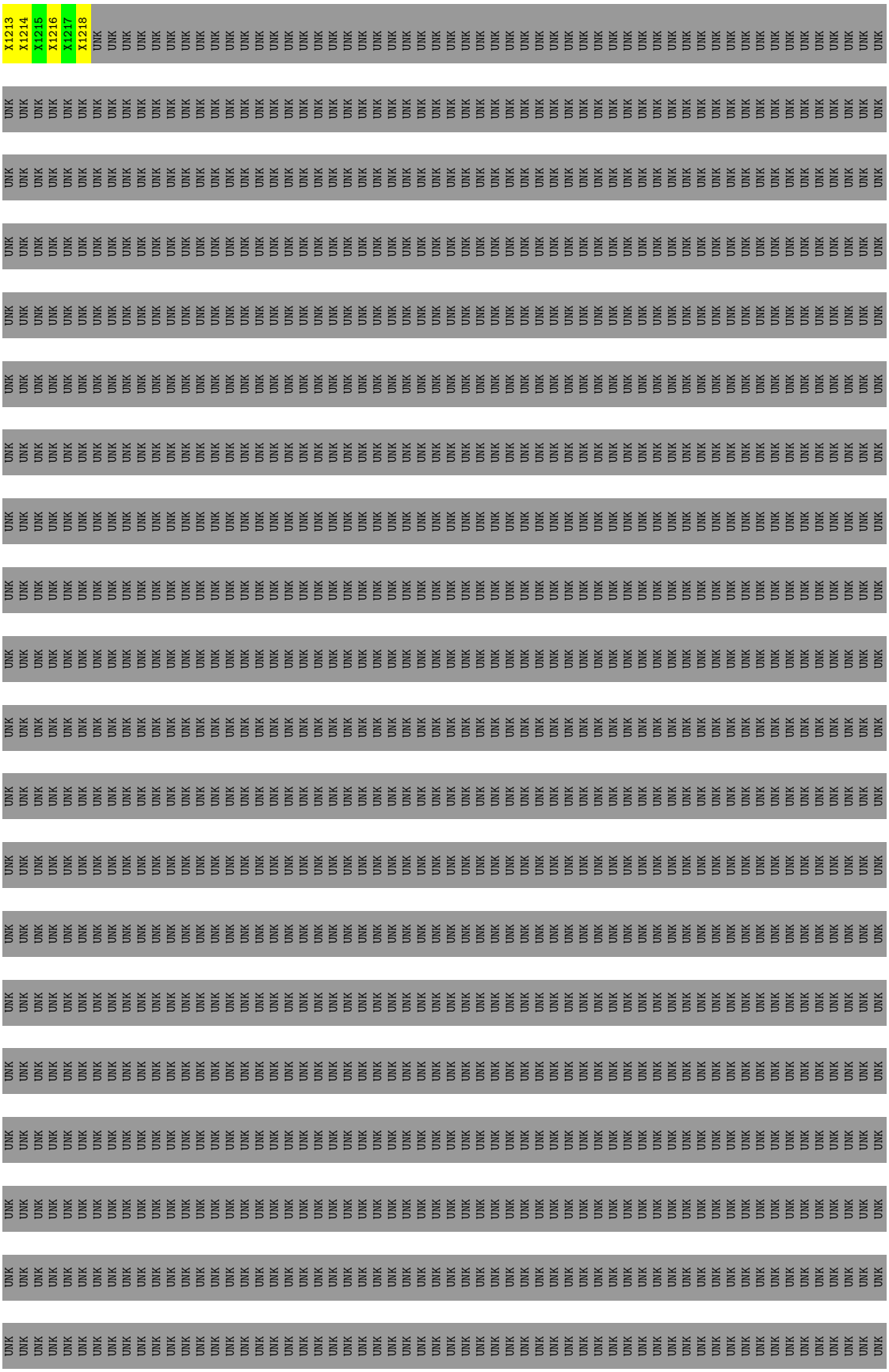
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

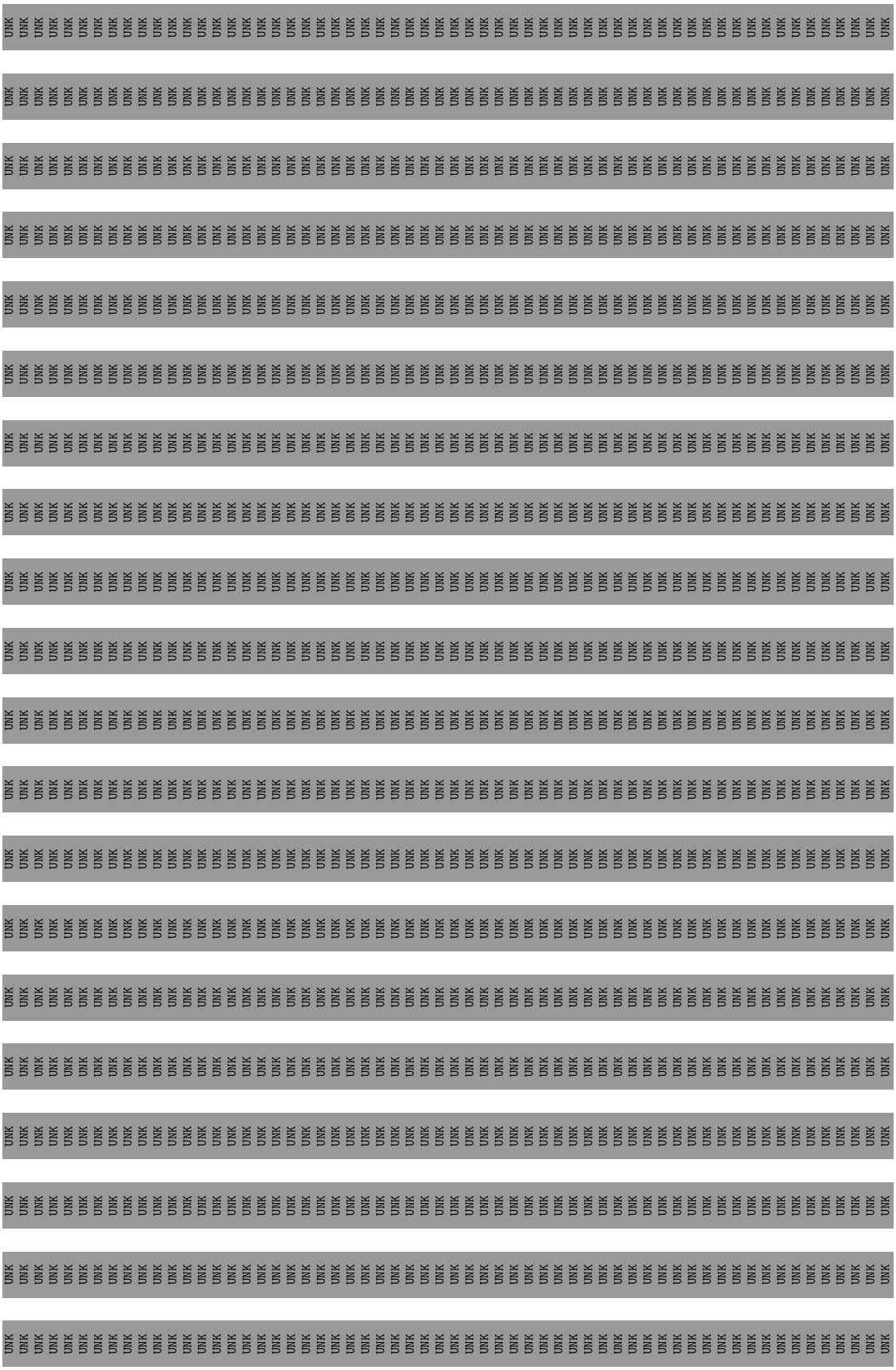
Chain R:

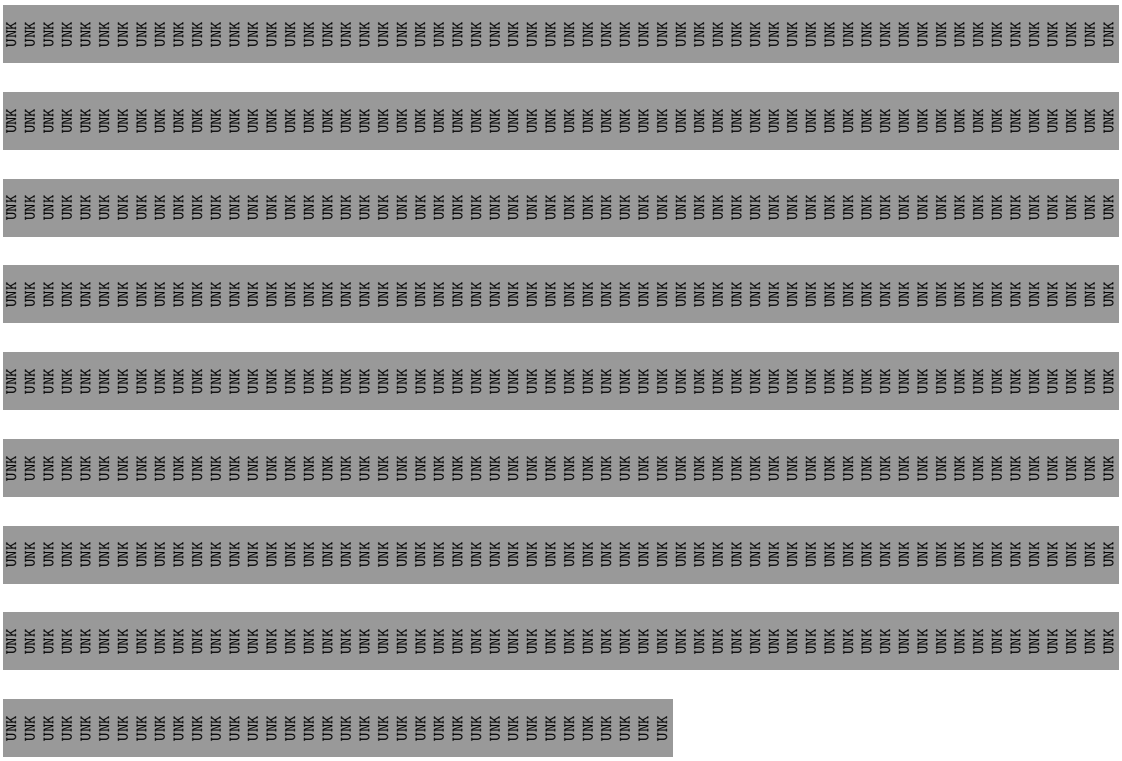






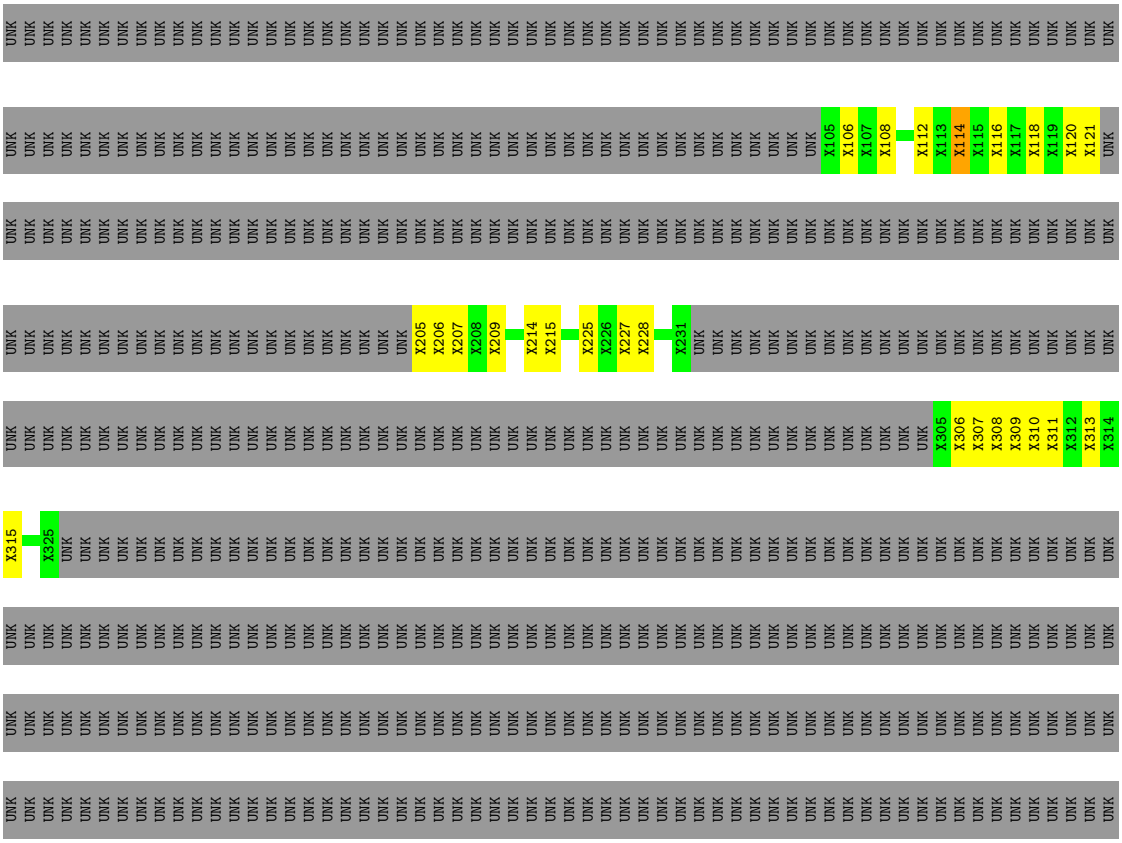

X1213
X1214
X1215
X1216
X1217
X1218
UNK

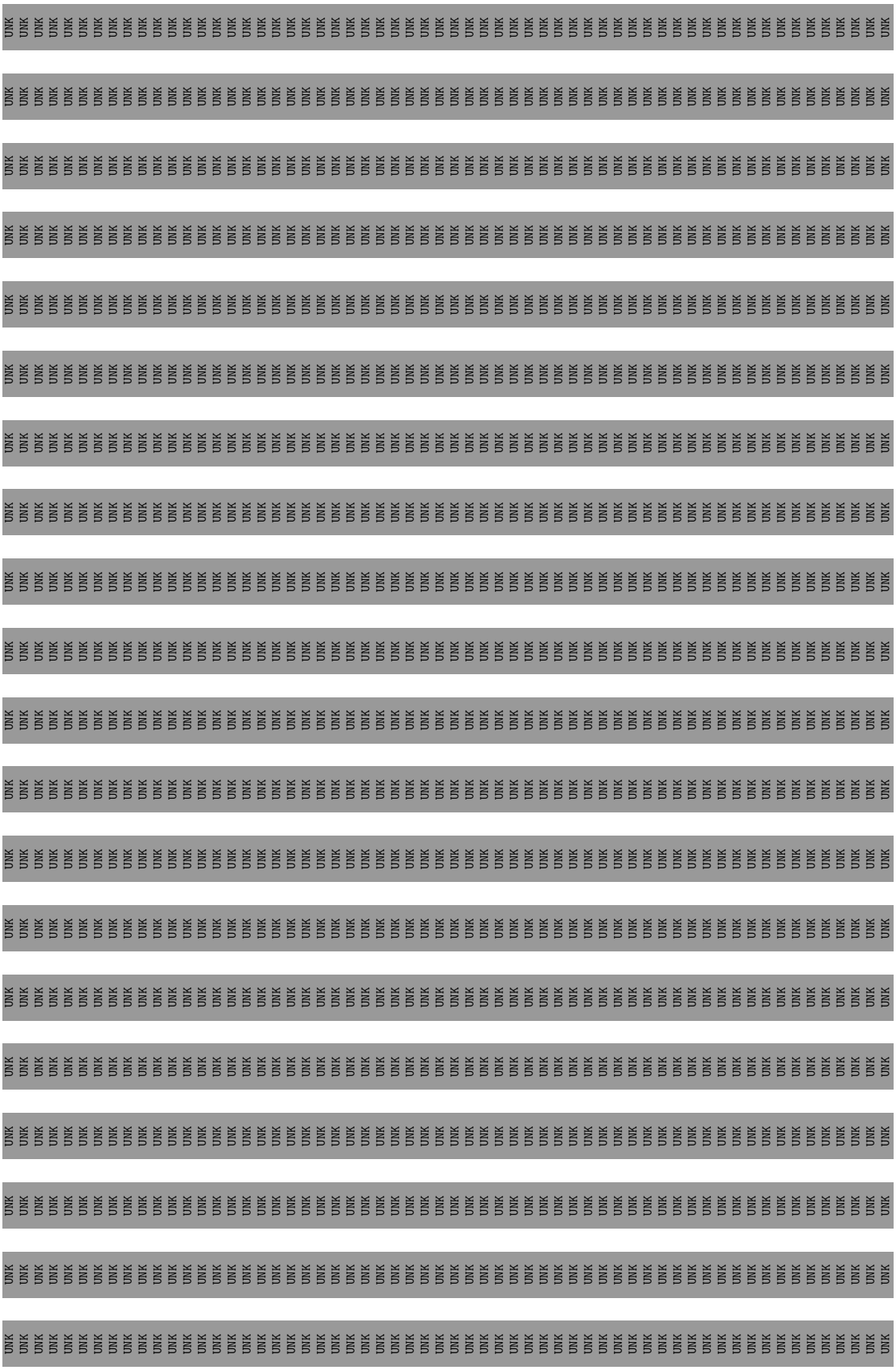

UNK

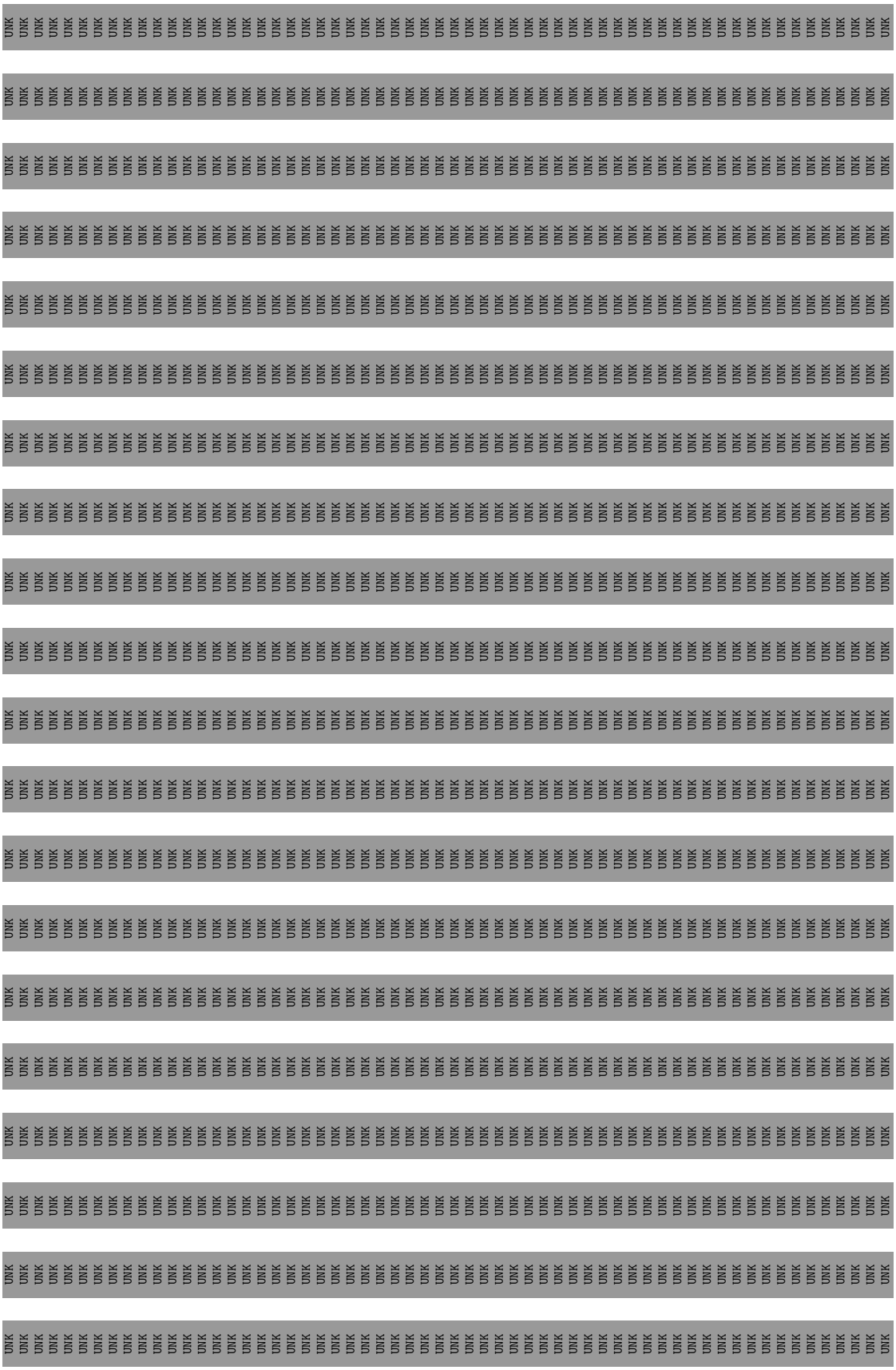


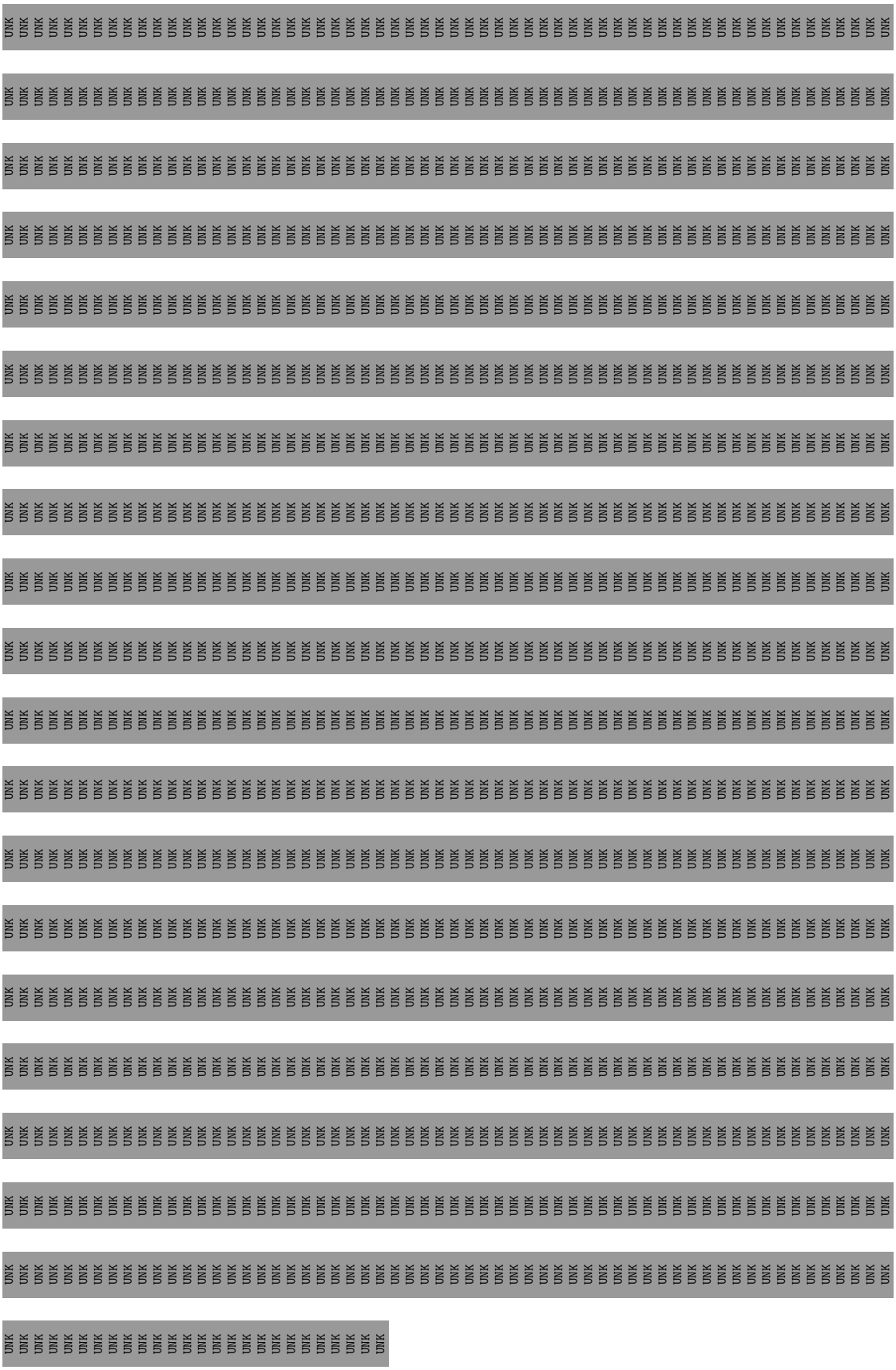
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain S: 98%



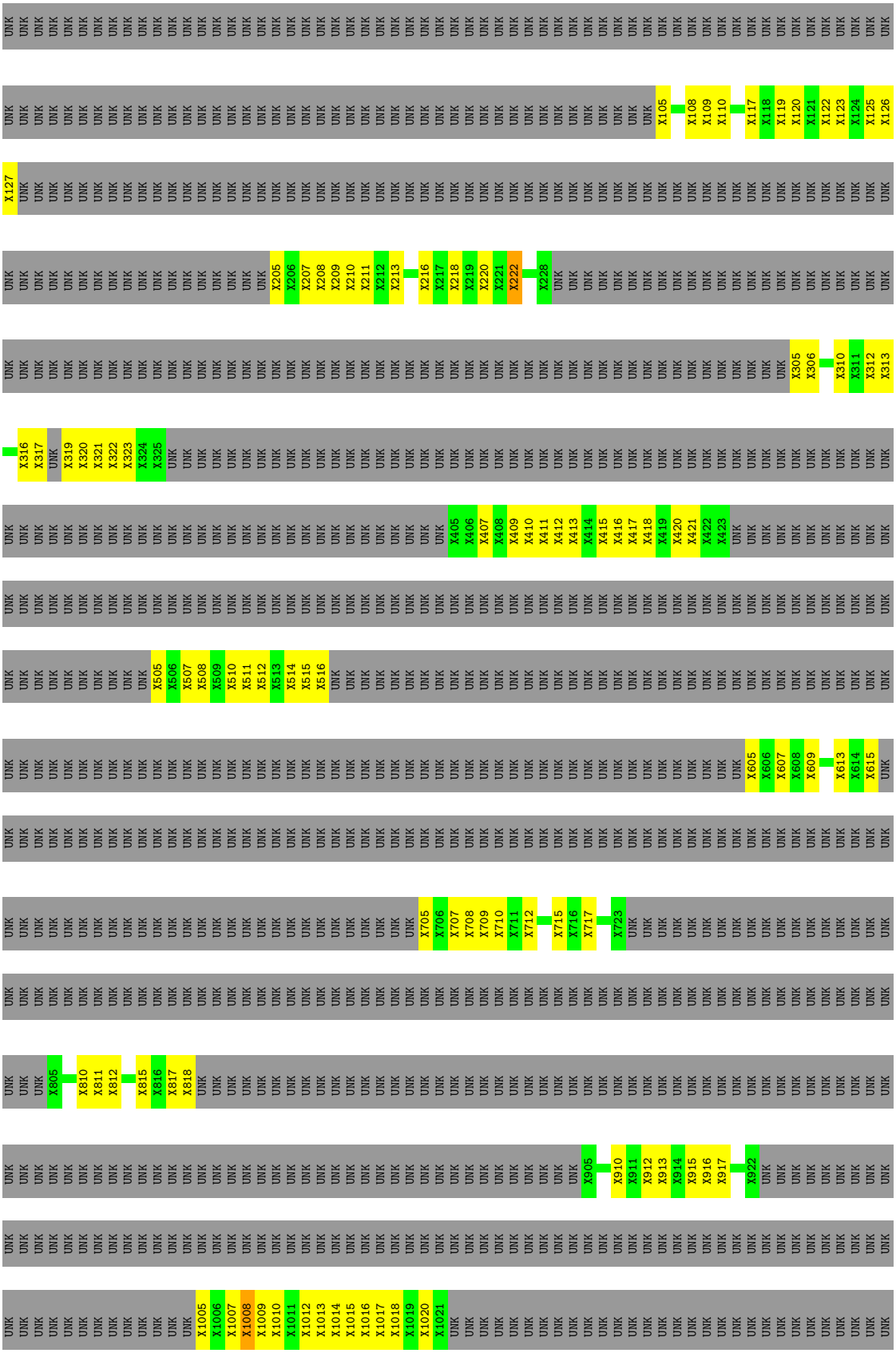

UNK

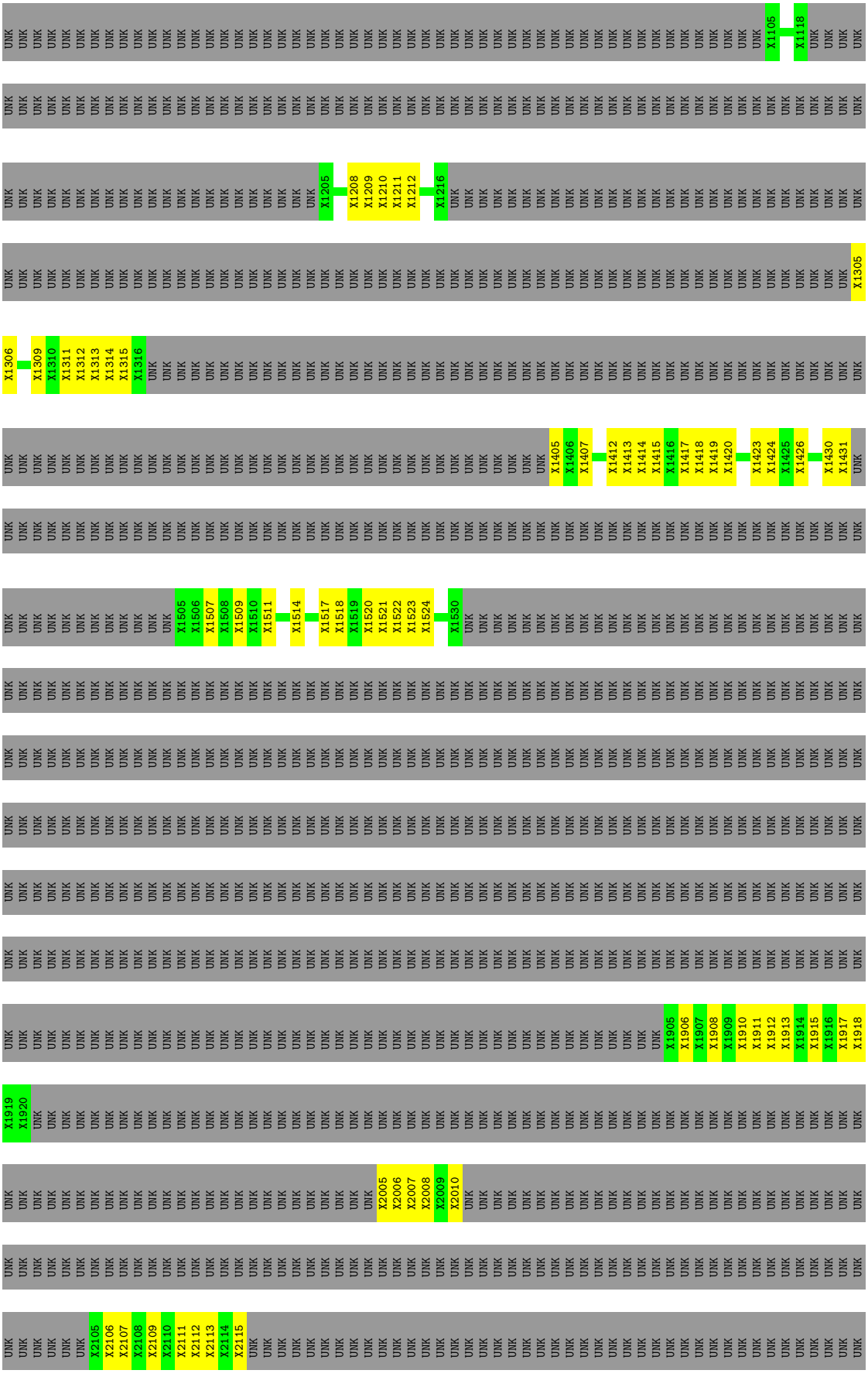

UNK

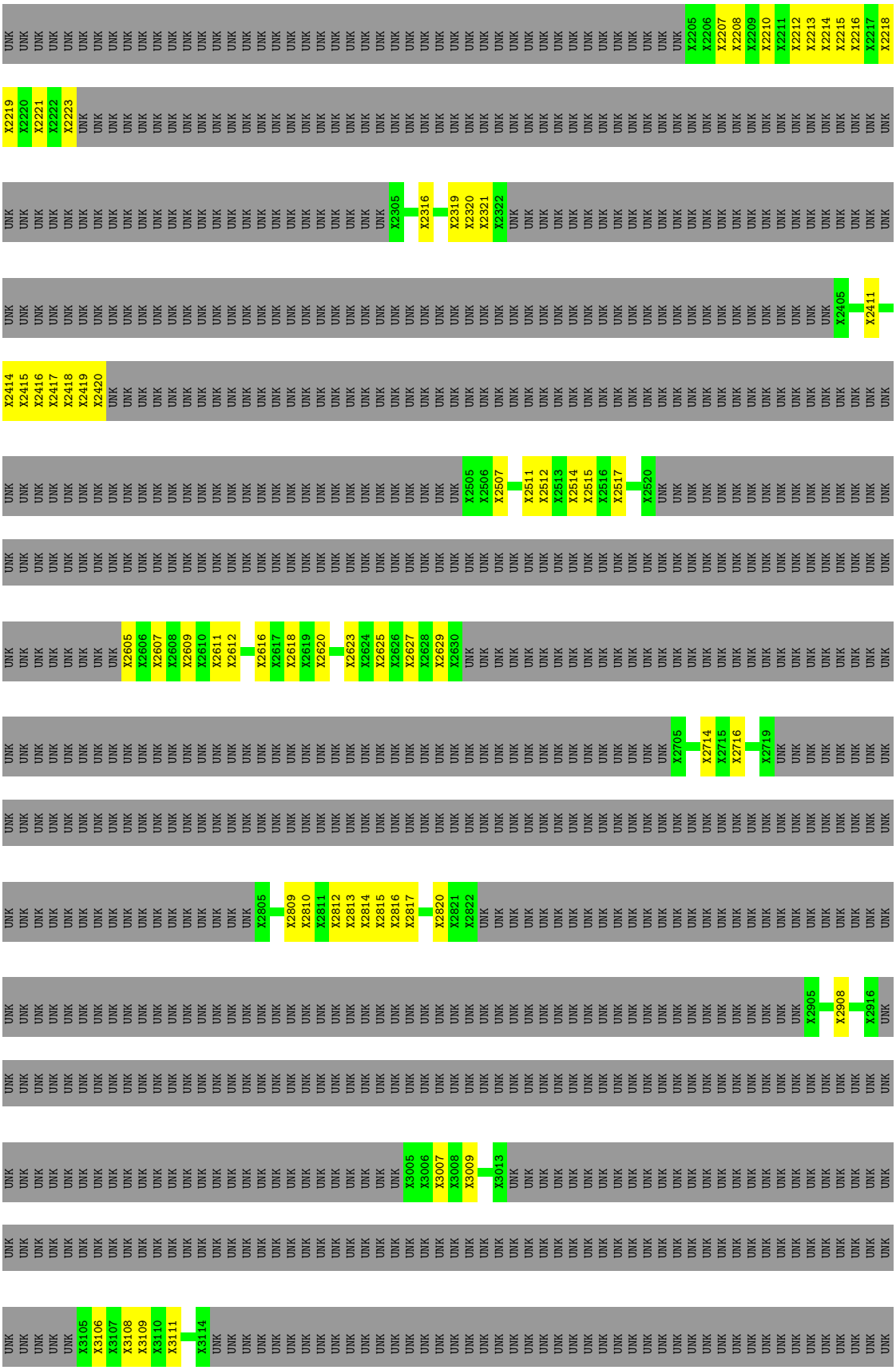


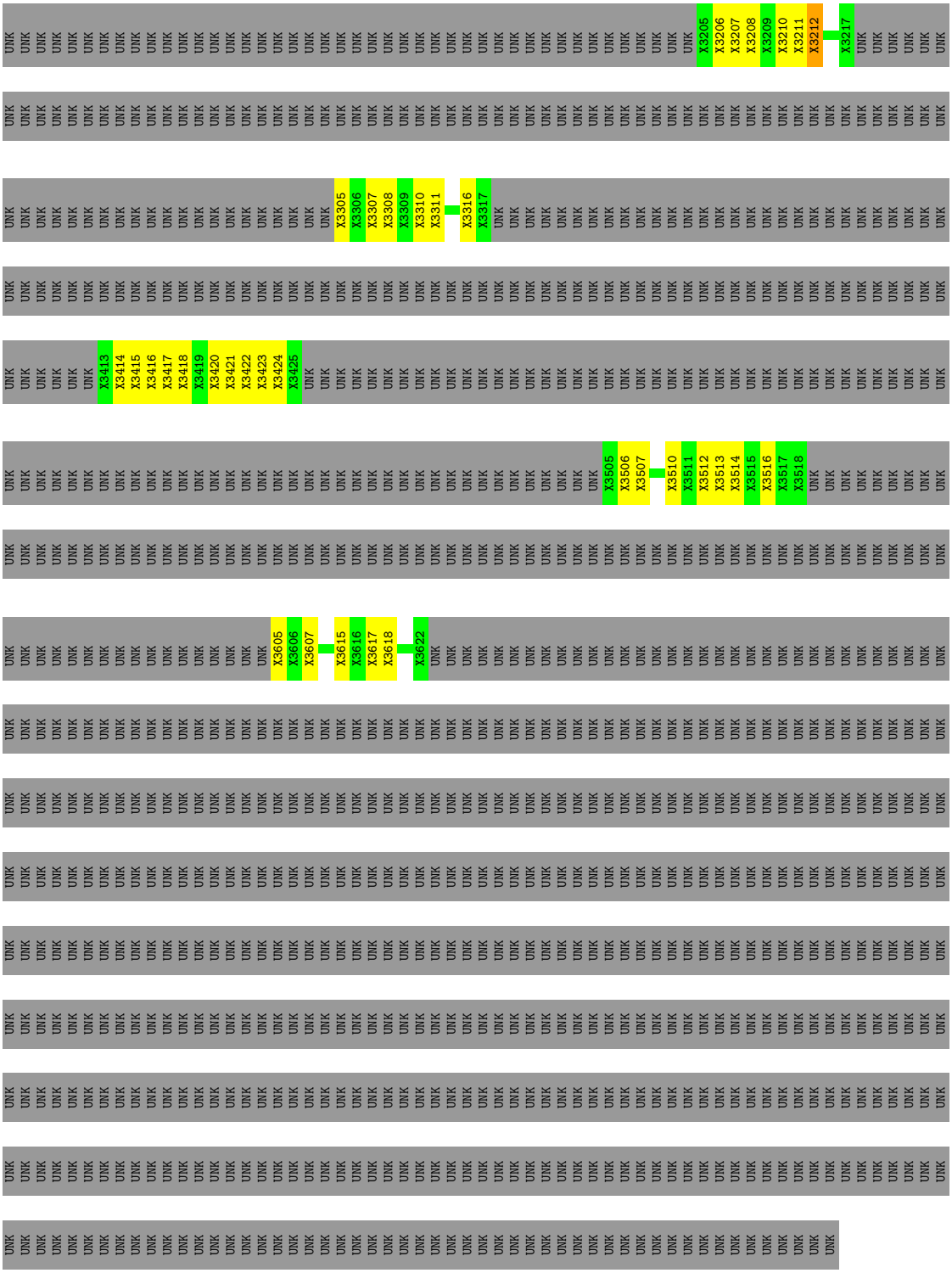
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain T: 7% 6% 87%




UNK
X1105
X1118
X1205
X1208
X1209
X1210
X1211
X1212
X1216
X1305
X1306
X1309
X1310
X1311
X1312
X1313
X1314
X1315
X1316
X1405
X1406
X1407
X1412
X1413
X1414
X1415
X1416
X1417
X1418
X1419
X1420
X1423
X1424
X1425
X1426
X1430
X1431
X1505
X1506
X1507
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X1509
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X1912
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X2006
X2007
X2008
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X2113
X2114
X2115

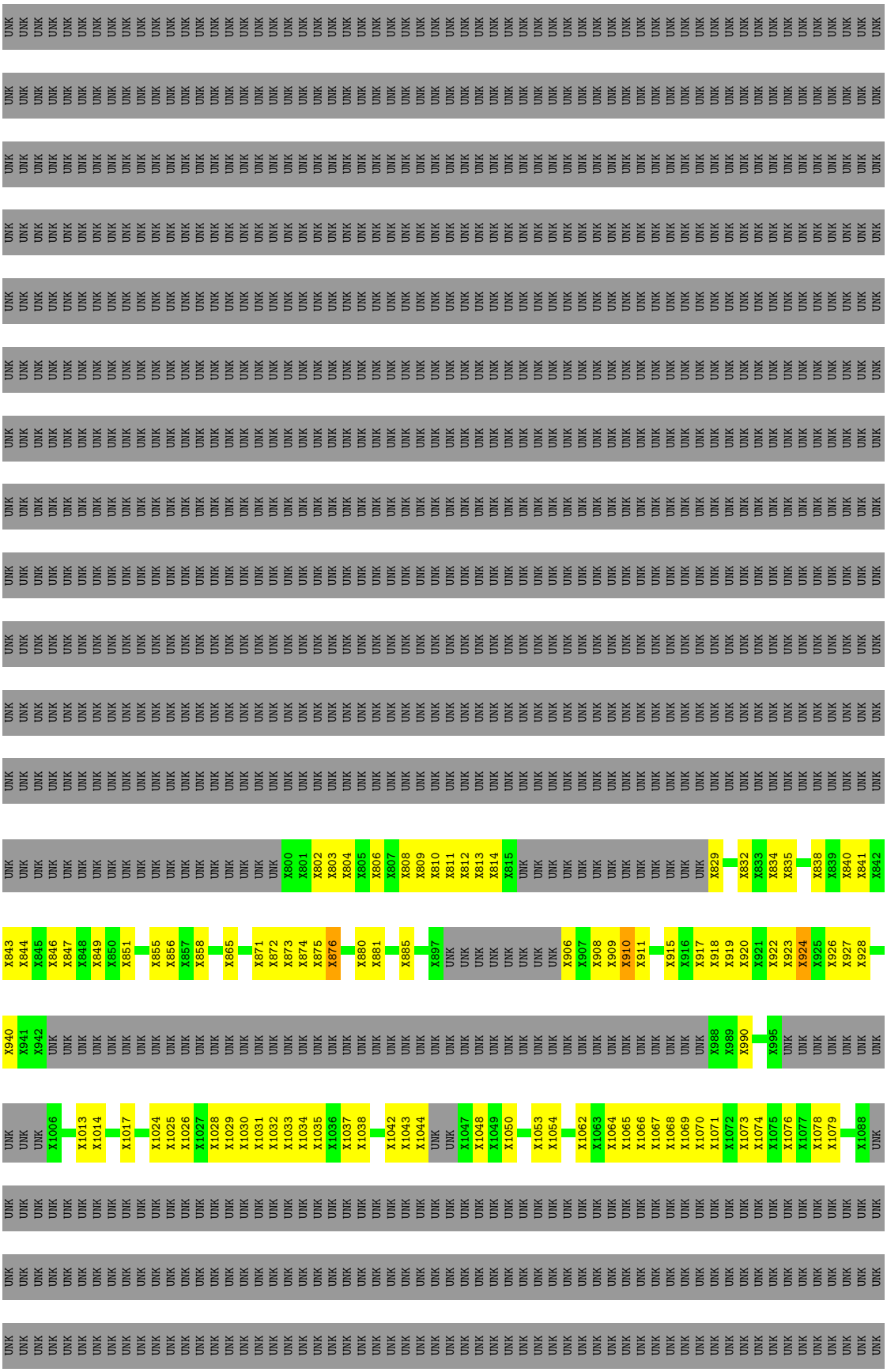

UNK X2205 X2206 X2207 X2208 X2209 X2210 X2211 X2212 X2213 X2214 X2215 X2216 X2217 X2218
X2219 X2220 X2221 X2222 X2223 UNK
UNK X2305 X2316 X2319 X2320 X2321 X2322
UNK X2405 X2411
X2414 X2415 X2416 X2417 X2418 X2419 X2420 UNK
UNK X2505 X2506 X2507 X2511 X2512 X2513 X2514 X2515 X2516 X2517 X2520
UNK X2605 X2606 X2607 X2608 X2609 X2610 X2611 X2612 X2616 X2617 X2618 X2619 X2620 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2630
UNK X2705 X2714 X2715 X2716 X2719
UNK X2805 X2809 X2810 X2811 X2812 X2813 X2814 X2815 X2816 X2817 X2820 X2821 X2822
UNK X2905 X2908 X2916
UNK X3005 X3006 X3007 X3008 X3009 X3013
UNK X3105 X3106 X3107 X3108 X3109 X3110 X3111 X3114

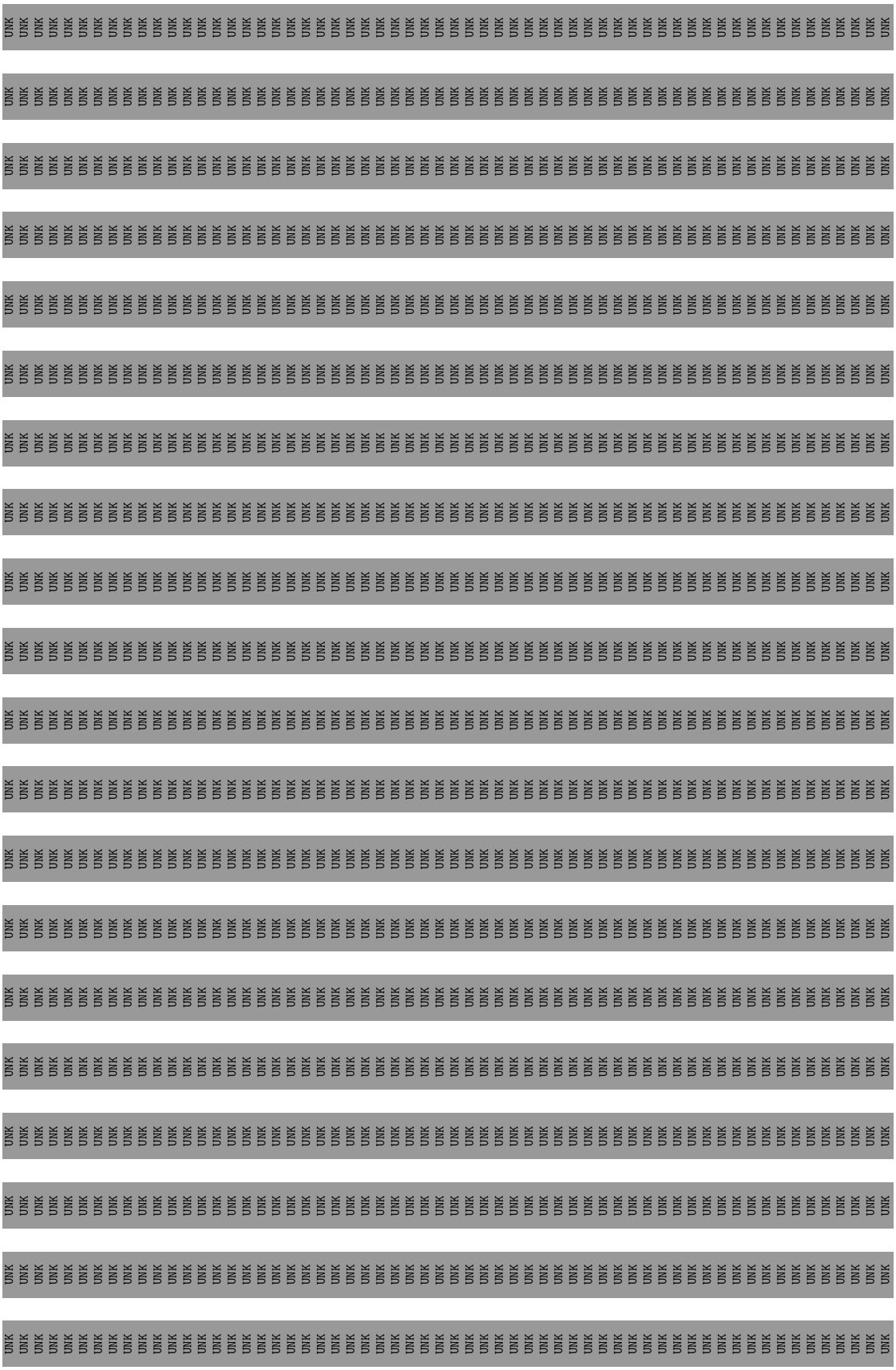


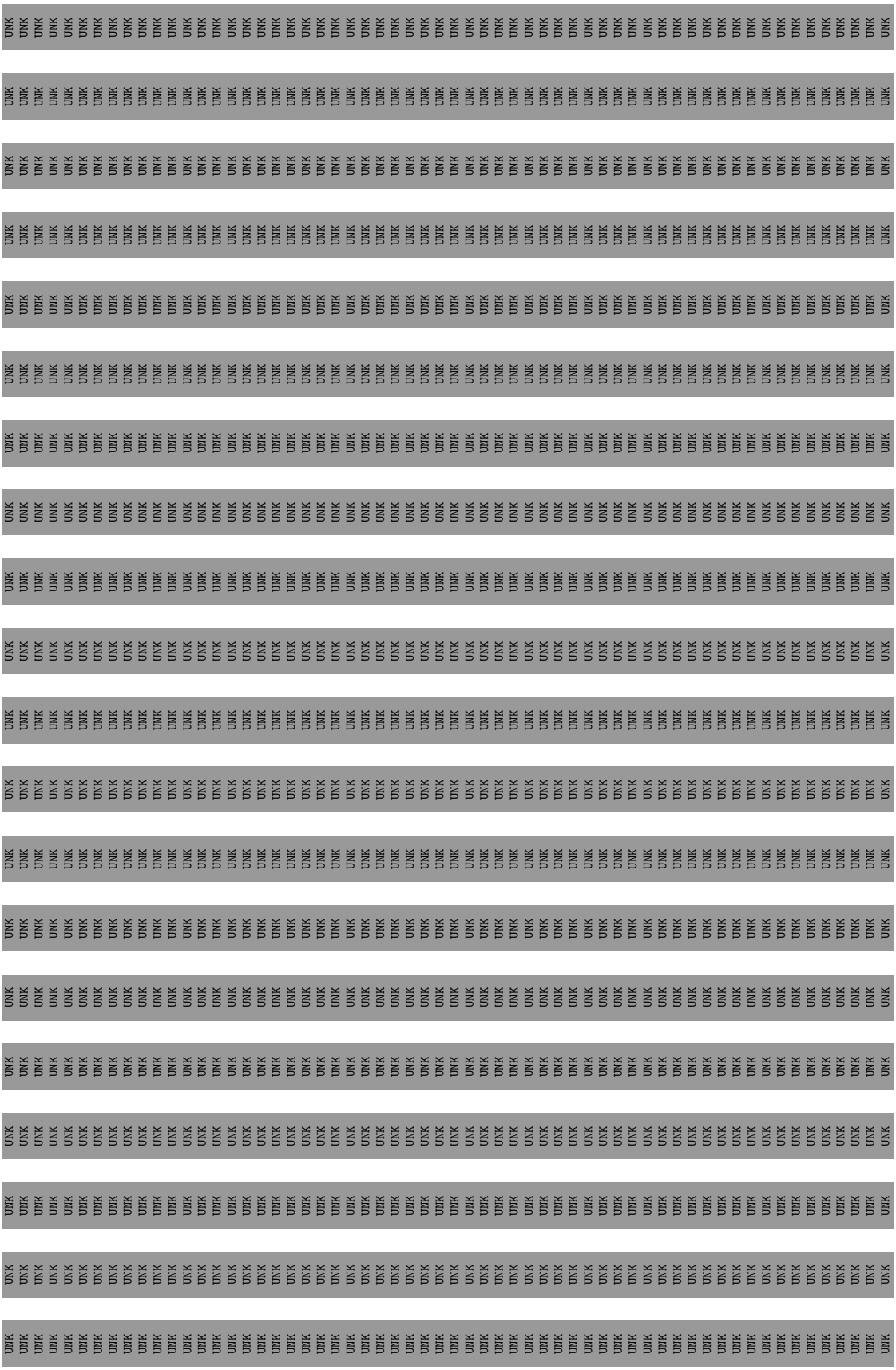
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

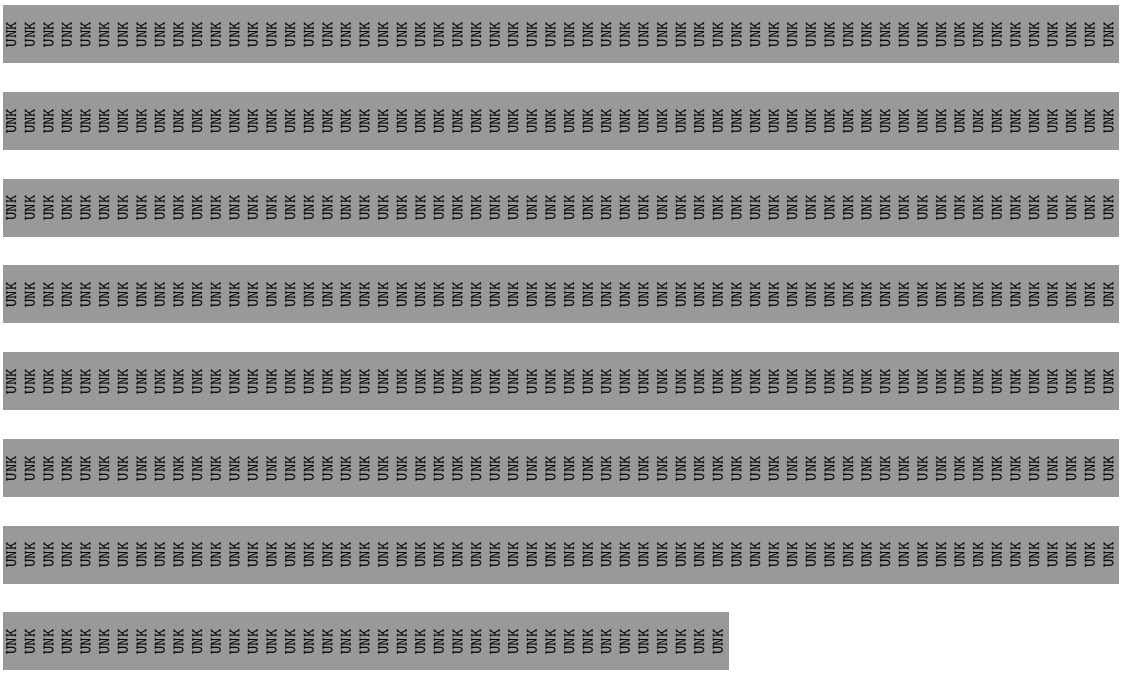
Chain Y: 95%




UNK
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
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
X940 X941 X942 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

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 – 6.60 100.00 – 6.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (100.00-6.60) 97.6 (100.00-6.60)	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 0.444 , 0.442	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 , 999.0	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	0.62	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

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

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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

5.3.1 Protein backbone

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

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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, 95^{th} 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 oligosaccharides 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.