Supporting Information

1. Simulation Condition Summary

Template	Experiments		Model T (original)		Model T (replicated)		Model B	
	T (ºC)	[NTP] (μM)	*T* (ºC)	[NTP] (μM)	*T* (ºC)	[NTP] (μM)	*T* (ºC)	[NTP] (μM)
10	37	ACGU: 40	37	ACGU: 40	37	ACGU: 40	25	ACGU: 40
11, 12, 13	37	ACGU: 30	37	ACGU: 30	37	ACGU: 30	25	ACGU: 30
D104, D111, D112, D123, D167, D387	30	ACGU: 10	37	ACGU: 10	37	ACGU: 10	25	ACGU: 10
pKA2	25	ACGU: 1000	NA	NA	25	ACGU: 1000	25	ACGU: 1000
pTS147	25	ACG: 1000 U: 200	NA	NA	25	ACG: 1000 U: 200	25	ACG: 1000 U: 200
λtR1	25	ACGU: 100	NA	NA	25	ACGU: 100	25	ACGU: 100
his, *ops*	25	ACU: 1000 G: 250	NA	NA	25	ACU: 1000 G: 250	25	ACU: 1000 G: 250
For transcription gel simulations (Figure 2 and Supplementary Materials)								
D104, D111, D112, D123, D167, D387	30	ACGU: 10	NA	NA	25	ACGU: 25	25	ACGU: 25

For sequence information, see Material and Methods under Supporting Information.

2. Comparison of Pause Location Predictions at Low [NTP]

The following tables show the measured (column 1) and predicted (column 2-4) pause locations on ten sequences used in Tadigotla et al. (2006). The pause locations were identified on these sequences at low [NTP] (also see Supplementary Materials under Simulation Condition Summary).Using the same treatment as in Tadigotla et al., all pauses within 3 bp are considered as a single pause cluster.

Column 2 shows predictions by the original Model T. Pause threshold $\xi = 0.015$.
Column 3 shows predictions by the replicated Model T. Pause threshold $\xi = 0.015$.
Column 4 shows predictions by Model B (2007). Pause threshold $\eta = 0.050$.
Column 5 shows predictions by Model B (2004). Pause threshold $\eta = 0.055$.

Seq. 10

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
27				
34	31-32	31-32, 37	31-32, 37	31-32, 37
	47	47		
56	57-58	57-58	56	56
			63	63
67	69-70	69-70		
			74	74
80	81-84	81-85	81-83	83
	93	93	92-93	
	97-100	97-102		

Seq. 11

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
25-27				
33-35	31-32	31-32	31-32	31-32
38	37	37		
	42	42	43	43
47,48	48	48	47	47
53	53	53	50-53	50-53
		62	58	58
			67	67
73	68-73	67-73		
	78-79	78-79	77-78	77-78
		83	83	83
	93-94	93-94	90	
100			102-103	102

Seq. 12

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
35		33	32	32
37,39	37	37		
			43	43
	53-55	53-56		53
61	57-58	57-58	63	63

Seq. 13

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
	33	33	32	33
39	37	37		
45			43	43
55	57-60	57-61	57	
63			66	
72	68-75	68-76	69, 75	69
			81	
89	85-89	85-89	85-88	85-88
			94-99	95-100

Seq. D112

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
32	31-32	31-32	31-32	31-32
37	38	37	37	37
	47-48	47-48	50	47-49
	58-61	58-61	58-59	58-59
76	71-76	71-78	69, 72-73	69, 73-74
	80-87	80-88	80	80, 83
95	93, 96-98	92-93, 96-98	92, 96	92, 96
			103, 106	102-106
111	113			
116	115	115		
120	117-120	117-120		

Seq. D104

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
32	31-32	31-32	31-32	31-32
37	38	37	37	37
	47-48	47-48	50	47-49
	58-61	58-61	58-59	58-59
75,77	71-76	71-76	69, 72-73	69, 73-74
78,80	78, 81-87	77-89	80	80
90,91,92				
94, 96	95-96	95-96	97	
104,107	103-108	103-109	103-104	103-104
115,118	116-117	116-117	113-116	113-116
128	125	125	125	125

Seq. D111

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
31	31-32	31-32	31-32	31-32
37	37	37	37	37
39,40			43-44	44
48	47	47	46	46
56,57,59	53-59	53-61	55-58	57-58
63			63	63
69	70-71	70-71	70	
	74			
	80-81	79-84	79-80	79-80, 85
	93	93		
	96-99	96-99	96, 98	96-98
	103-104	103-104	102, 105	
109	108	107-108	107-108	107-108
	114-117	114-117	113-116	113-116
121			124	123-124
128	125		125	125

Seq. D123

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
	31-32	31-32	31-32	31-32
37				
43,44	41-45	41-47	41	41
49			47	47
53	53-56	53-56	53	54
	60-61	60-62		
71			69-70	70
78	80-82	80-82	75, 79-81	80
85	85	85-86	84	84
	97-99	97-99	96	96
103	102-104	102-104	102	102
				108
	114-116	114-116	116	114-117
127	128	128-130	126-129	127-132

Seq. D167

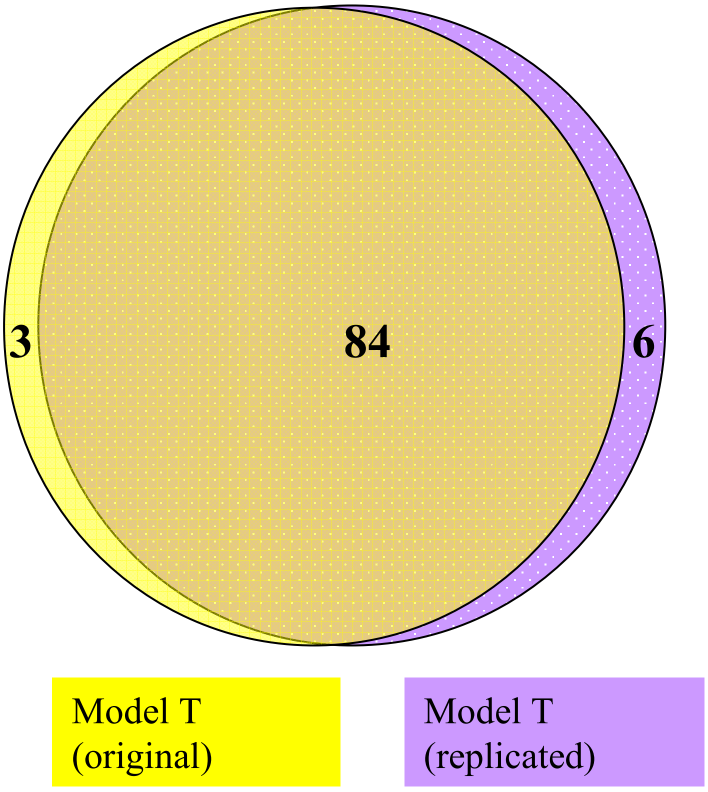
Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
31-33	31-32	31-32	31-32	31-32
37		37	37	37
41		42	42	42
	48	47-48	47-48	47-49
56	54-57	54-57	57	54, 57
	67-69	67-70	67, 71	67, 71
81	77-82	76-82	77-78, 81	77-78, 81
	89-91	89-91	89	89
100	99-100	98-101	98-99	98-99
	104-107	104-107	104, 106	104-110
114	115-116	115-116	114	

Seq. D387

Experiment	Model T (original)	Model T (replicated)	Model B (2007)	Model B (2004)
32	31-32	31-32	31-32	31-32
37	38	37	37	37
	47-48	47-48	50	47-49
	58-61	58-61	58-59	58-59
72,74,76	71-78	71-79	69, 72-73	69, 73-74
	82-85	80-86	83-84	83-84
90,91	87	87-88, 93	93	
100	96-99	96-99	96, 101	96, 101
107,108	108-110	108-110	108-109	108-109
116	114-116	114-116	114-115	114, 119

Summary of Comparison of Pause Location Predictions at Low [NTP]

Predictions of pause locations by the replicated Model T agree well with those by the original Model T of Tadigotla et al. (2006). On the ten DNA templates examined, the original Model T predicted a total of 87 pause clusters and the replicated Model T predicted 90 pause clusters. The predictions have 84 clusters in common. Therefore, the replicated Model T reproduced ~ 97 % of the pauses predicted by the original Model T.



3. Comparison of Pause Location Predictions at High [NTP]

The following two tables show the measured (column 2) and predicted (column 3-5) pause locations on five sequences at high [NTP] (also see Supplementary Materials under Simulation Condition Summary).

Column 3 shows predictions by the replicated Model T. Pause threshold $\xi = 0.005$.
Column 4 shows predictions by Model B (2007). Pause threshold $\eta = 0.10$.
Column 5 shows predictions by Model B (2004). Pause threshold $\eta = 0.12$.

Template	Experiment	Model T (replicated)	Model B (2007)	Model B (2004)
pKA2	153		151-152	151-153
		178-181		
	235	235-236	233, 236	234
		261		261
ΔtR2	83, 84	83,84	83, 84	83, 84
		94-95		
λ sequence		91-94		
	96	97-104	97	97
		106-108	108, 109	108, 109
	115		118-119	118
		119-121		
	127	130-131	129	129
	135		136-137	136-137
	174	173-175	173	173
		179-181		
	185	184-186	183, 189	183, 189

Template	Experiment	Model T (replicated)	Model B (2007)	Model B (2004)
ops	5	5	5	5
			18	18
	30	27-28	28	28
			37	37
	63			
		83-86		
	90	87-88	88	88
			99, 101-102	99-102
	151, 153	147-152	150	
			162	162
his	5		5	5
			18	18
	30	27-28	28	28
			37	37
	63			
		83-86		
	90	87-88	88	88-89
			99, 101	100-102
			154	
	158			

4. Comparison of Pause Kinetics on Templates D167 and D387

Predicted Pause Durations by Model B (2007)

Note that the corresponding simulated transcription gels are shown in Figure 2.

Pause locations on D167	Duration (s)	Pause locations on D387	Duration (s)
31	8.4	31	5.3
32	11.1	32	21.7
37	5.1	37	4.7
42	4.8	50	1.8
47	2.6	59	3.3
48	4.5	69	2.4
57	5.1	72	1.5
67	3.1	73	4.3
71	4.7	84	1.9
77	3.6	96	1.5
78	36.4	101	2.1
89	1.6	109	2.2
98	2.7	114	3.9
99	58.5	115	1.5
104	15.9		
110	1.9		
114	1.5		

Predicted Pause Durations by Model T

Pause locations on D167	Duration (s)	Pause locations on D387	Duration (s)
31	4.3	31	1.8
32	120.5	32	26.2
37	0.6	37	1.8
42	2.1	47	0.3
47	0.3	58	0.6
48	0.8	59	36.2
54	3.2	60	6.4
55	0.3	61	0.5
67	1.0	71	1.9
68	10.0	72	26.7
69	2.0	73	186.5
76	0.3	74	1211.9
77	1.3	75	296.6
78	226.3	76	46.5
79	641.1	77	18.9
81	2.7	78	10.7
90	0.9	79	1.3
91	0.6	80	2.3

Predicted Pause Durations by Model T (continued)

Pause locations on D167	Duration (s)	Pause locations on D387	Duration (s)
98	0.4	81	5.0
99	147.8	82	3.6
100	98.3	84	1.7
101	5.8	85	0.9
104	5.7	86	0.4
105	49.9	87	0.6
115	0.8	96	0.4
116	1.0	97	2.7
		98	10.6
		99	1.3
		108	0.4
		109	9.5
		114	1.6
		115	24.5
		116	22.7

References

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