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Supplemental Data

Structural Basis of Transcription:

Mismatch-Specific Fidelity Mechanisms

and Paused RNA Polymerase II with Frayed RNA

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Table S1. Amino acid residues contacting the frayed nucleotides in fraying site I (EC III) and fraying site II (EC IV) and their conserved counterparts in human Pol II and bacterial RNA polymerase

Fraying site I				
Pol II atom	RNA atom	Distance (Å)	<i>H. sapiens</i>	<i>T. thermophilus</i>
RPB2 R766 NH1	Frayed U C4	3.0	R721	R557
RPB1 D483 OD2	Frayed U O4'	2.4	D497	D741
RPB2 R1020 CZ	Frayed U C4	3.8	R975	R879
RPB1 D483 CG	Frayed U C1'	3.5	D497	D741
RPB2 K987 CE	Frayed U C2'	3.5	K942	K846
RPB2 K987 CD	Frayed U C2'	3.8	K942	K846
RPB1 D483 CG	Frayed U C4'	3.7	D497	D741
RPB1 D481 CG	Frayed U C5'	3.8	D495	D743
Fraying site II				
Pol II atom	RNA atom	Distance (Å)	<i>H. sapiens</i>	<i>T. thermophilus</i>
RPB1 R446 NH2	Frayed G O1P	3.2	R460	R704
RPB2 E529 OE1	Frayed G N1	2.8	E516	E445
Penultimate RNA base U C5'	Frayed G C2'	3.8	-	-
Penultimate RNA base U C5'	Frayed G C3'	3.1	-	-
RPB2 K987 CE	Frayed G C1'	3.4	K942	K846
RPB2 K987 CE	Frayed G C2'	3.4	K942	K846
RPB2 Y769 CZ	Frayed G C6	3.8	Y724	M560
RPB2 Y769 CZ	Frayed G C5	3.8	Y724	M560
RPB2 Y769 CE2	Frayed G C6	3.2	Y724	M560
RPB2 Y769 CE2	Frayed G C5	3.7	Y724	M560
RPB2 Y769 CD2	Frayed G C6	3.4	Y724	M560
RPB2 Y769 CD2	Frayed G C2	3.5	Y724	M560
RPB2 Y769 CG	Frayed G C2	3.4	Y724	M560
RPB2 Y769 CB	Frayed G C2	3.6	Y724	M560
RPB2 Y769 CA	Frayed G C2	3.8	Y724	M560
RPB2 E529 CB	Frayed G C6	3.9	E516	E445
RPB1 D483 CG	Frayed G C4'	3.7	D497	D741

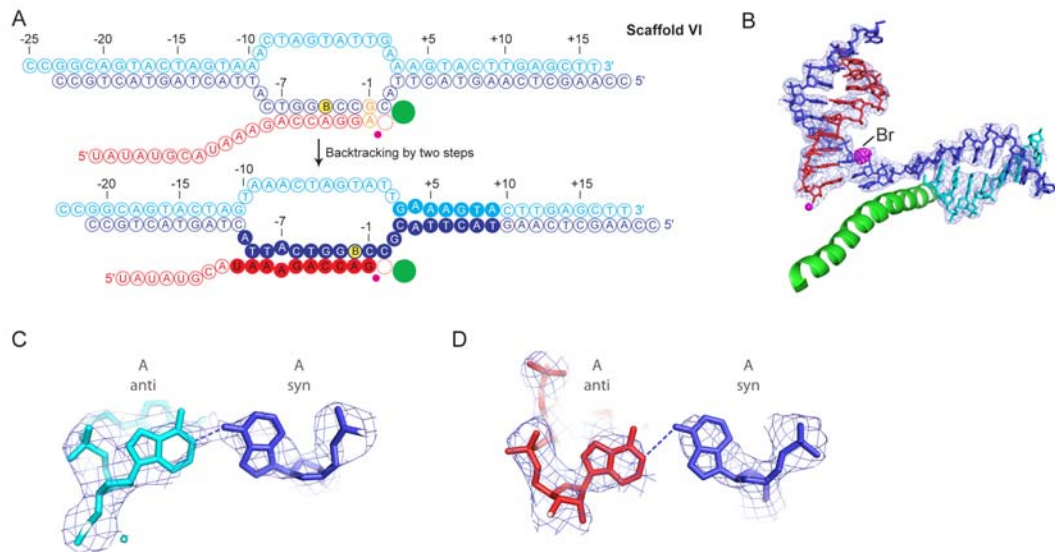


Figure S1. Structure of EC VI at 3.4 Å resolution

(A) Scaffold VI containing a G•A mismatch at the designed position -1 (top) and as observed in the crystal after backtracking by two steps (bottom).

(B) Structure of nucleic acids. The final 2F_o-F_c electron density map is shown as a blue mesh, contoured at 1.0σ. A peak in the anomalous difference Fourier map (magenta, contoured at 4.4σ) reveals the location of the bromine atom at position -2 of the template strand, indicating that Pol II had backtracked by two steps.

(C) Detailed view of the 2F_o-F_c map in (A) around the A•A *anti-syn* bps at position +4 in the downstream DNA duplex. A putative hydrogen bond is indicated by a dashed line.

(D) Detailed view of the 2F_o-F_c map in (A) contoured at 1.2 σ around the A•A *anti-syn* bp at position -7 in the RNA-DNA hybrid. A putative hydrogen bond is indicated by a dashed line.