

Supplementary information

Replication through an Abasic DNA Lesion: Structural Basis for Adenine

Selectivity

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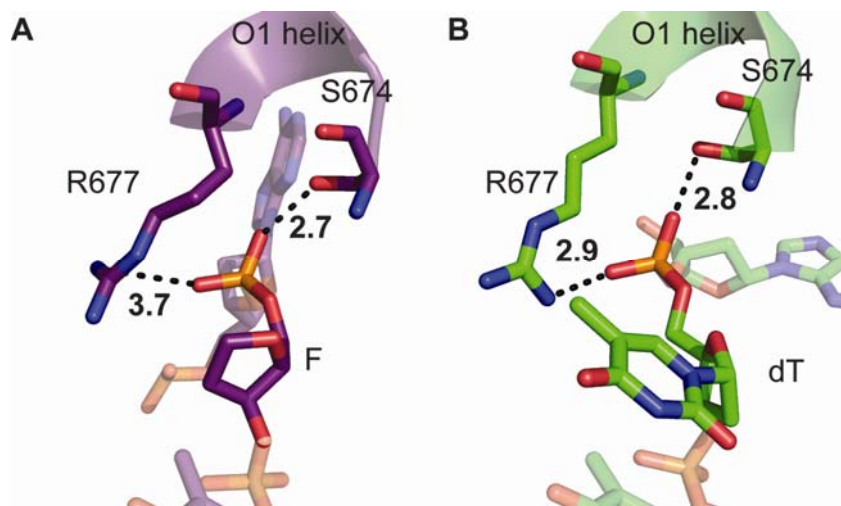


Figure S1 Close-up view of the positioning of the abasic site F in *KlenTaq_{AP}*. (A) Orientation of F in *KlenTaq_{AP}*. (B) Orientation of template dT in *KlenTaq* (PDB 1QSY). All distances are in Å.

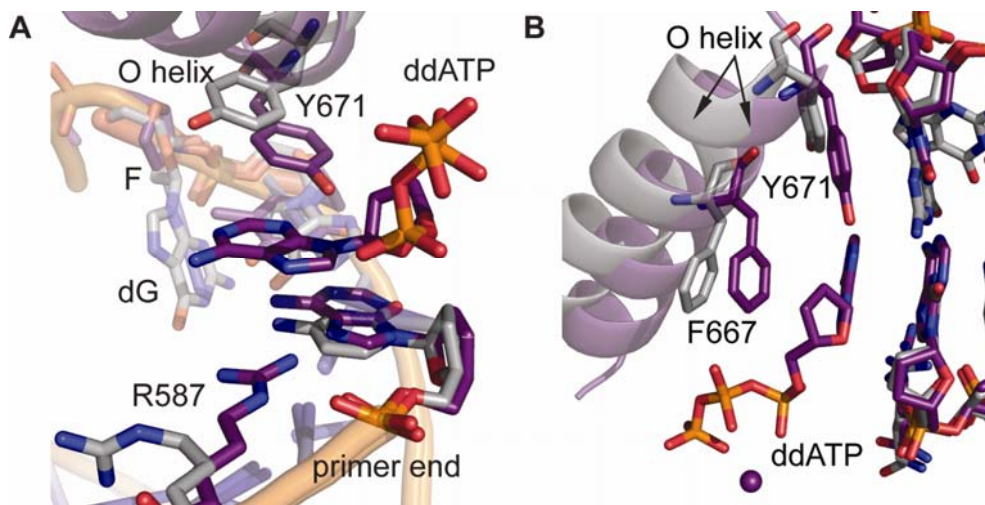


Figure S2 Comparison of *KlenTaq_{AP}* with *KlenTaq* in binary complex with primer / template without incoming dNTP (PDB 4KTQ). (A) Superimposed structures of *KlenTaq_{AP}* (purple) and *KlenTaq* in binary complex (grey) show the difference in orientation of residues R587 and Y671. (B) Superimposed structures of *KlenTaq_{AP}* (purple) and *KlenTaq* in binary complex (grey) show the difference in orientation of the O helix, residues Y671 and F667.

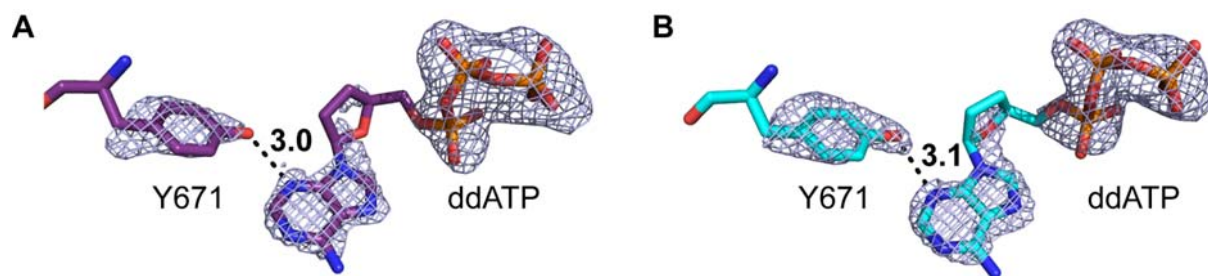


Figure S3 The F_o-F_c simulated annealing electron density omit map (after omitting ddATP and Y671) contoured at 3.5σ for the ddATP and residue Y671 is shown in grey. (A) *KlenTaq_{AP}*. (B) *KlenTaq_{BE}*. All distances are in Å.

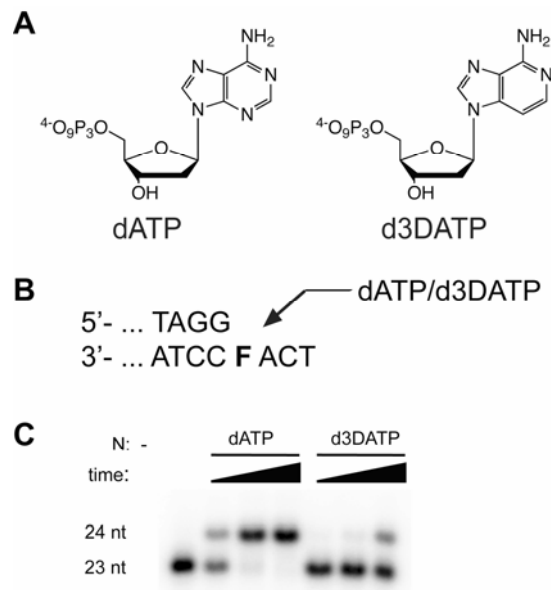


Figure S4 Incorporation of dATP and 3-deaza-2'-deoxyadenosine-5'-triphosphate opposite an abasic site. (A) Structures of dATP and 3-deaza-2'-deoxyadenosine-5'-triphosphate (d3DATP). (B) Partial primer template sequence used in primer extension experiments. (C) Single nucleotide incorporation of *KlenTaq* opposite **F** for 2, 10, or 60 min, respectively. The respective dNTP is indicated. The dATP analogue d3DATP was prepared as described from commercially available d3DA. The reactions are conducted as described in “Materials and methods”.

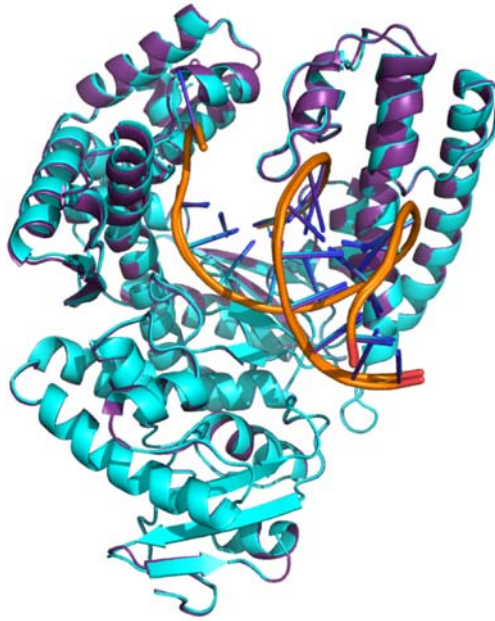


Figure S5 Structures of *KlenTaq* in complex with substrates. Structure of *KlenTaq*_{AP} (purple) superimposed with *KlenTaq*_{BE} (cyan).

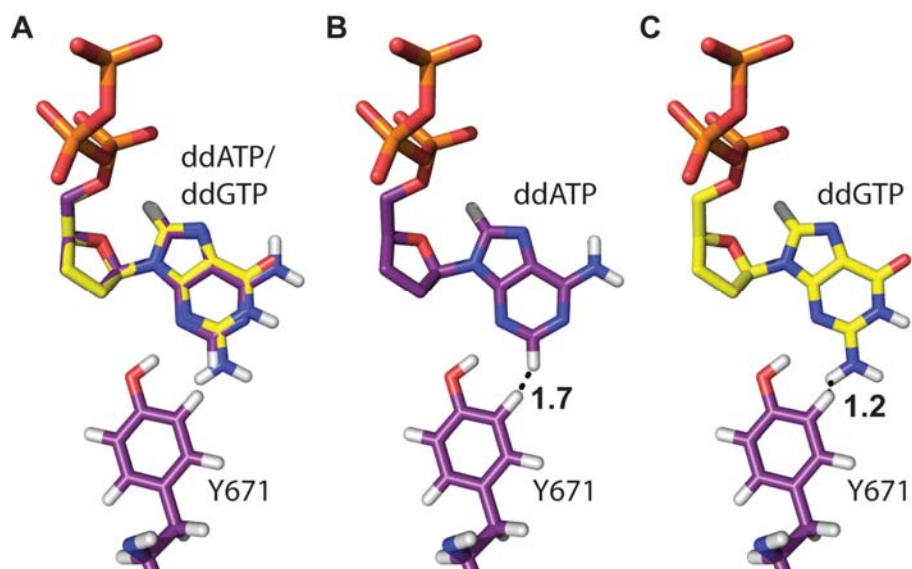


Figure S6 Modeling of ddGTP at position of ddATP in *KlenTaq_{AP}*. (A) Overlay of the modeled ddGTP (yellow) with ddATP opposite to Y671. (B) Shown is distance between C2-H of ddATP and C-H *ortho* to the OH-group of Y671. (C) Shown is theoretical distance between C2-NH-H of the modeled ddGTP (yellow) and C-H *ortho* to the OH-group of Y671. All distances are in Å.

Table SI Data collections and refinement statistics for *KlenTaq* DNA polymerases

Crystal	<i>KlenTaq</i>_{AP}	<i>KlenTaq</i>_{BE}
Data Collection		
Wavelength (Å)	1.000	1.000
Resolution (Å)	50.0-2.25 (2.38-2.25)	50.0-2.20 (2.33-2.2)
Total reflections	331791	341959
Unique reflections	30775	32238
Completeness (%) ^a	99.7 (98.5)	98.9 (93.4)
Mean I/σ ^a	16.1 (2.5)	19.0 (2.5)
R _{meas} (%) ^a	12.4 (97.1)	10.5 (86.4)
Refinement		
Resolution range (Å)	47.8-2.25 (2.32-2.25)	47.5-2.19 (2.25-2.19)
R _{cryst} (%) ^a	18.8 (25.0)	18.3 (26.1)
R _{free} (%) ^a	23.4 (28.3)	22.8 (30.8)
<i>Composition of the model</i>		
Protein residues	534	538
DNA nucleotides (primer/template)	12/14	12/12
ddNTP	ddATP	ddATP
Water molecules	162	154
Mg ²⁺ ions	1	1
Na ⁺ ions	4	4
<i>Average B factors (Å²)</i>		
protein	45.4	45.3
DNA	34.1	35.2
dNTP	81.7	51.3
Mg ²⁺ ion	68.4	56.1
<i>Rms. deviations</i>		
Bond length (Å)	0.016	0.006
Bond angle (°)	0.929	0.851
Max. likelihood estimate for coord. error (Å)	0.28	0.29
Ramachandran outliers	1	1

^aValues in parentheses correspond to those in the outer resolution shell.