

Supplementary Information for Structural Insights into Phosphorylation-Mediated Activity Loss in DNA Polymerase β Binding to Gapped DNA

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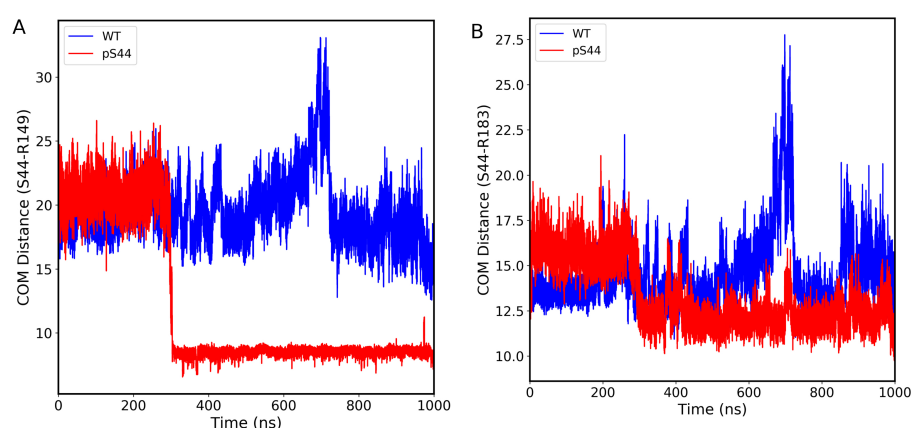


Figure S1. Distance *vs* simulation time (A) Center of mass distance between S44-R149. (B) Center of mass distance between S44-R183.

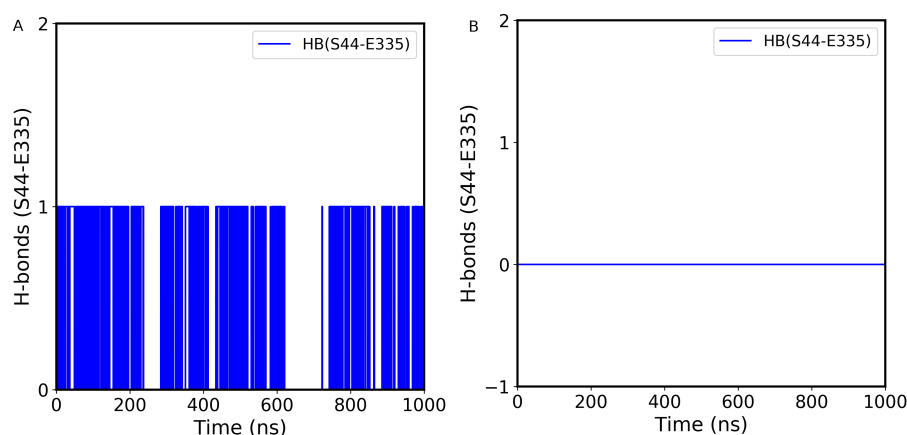


Figure S2. Time evolution of hydrogen bond between S44-E335 (A) WT, (B) pS44

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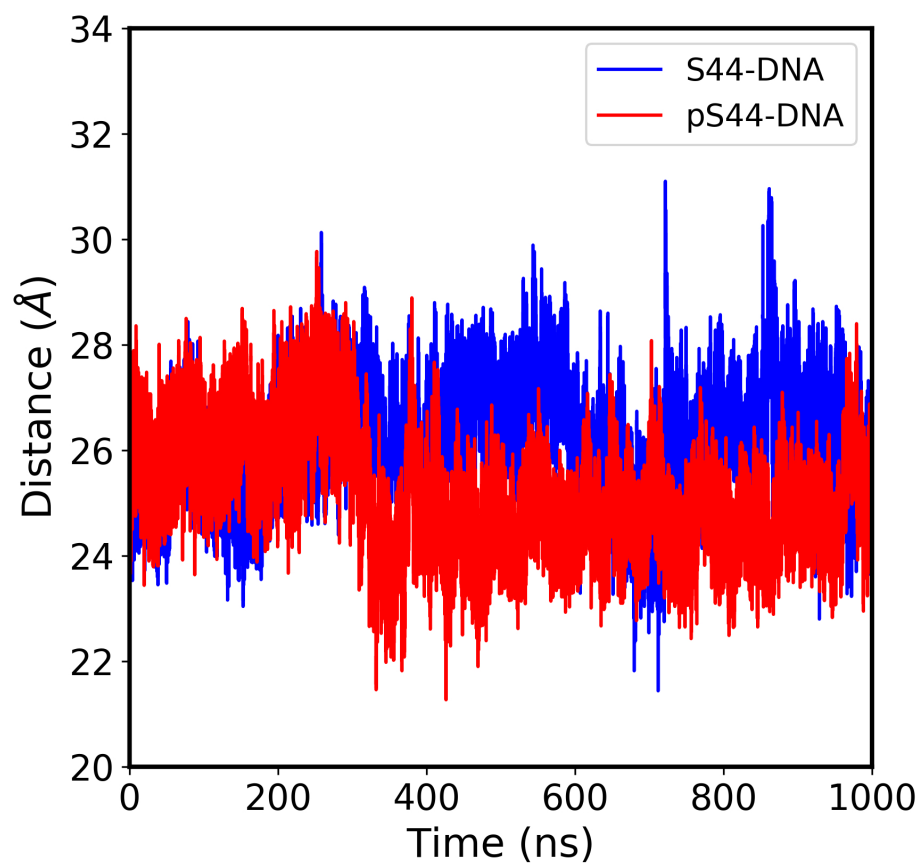


Figure S3. Distance between S44 and DNA fragment *vs* simulation time. The blue solid line shows the distance between S44 and DNA, whereas, the red line shows the distance between phosphorylated S44 residue and DNA.

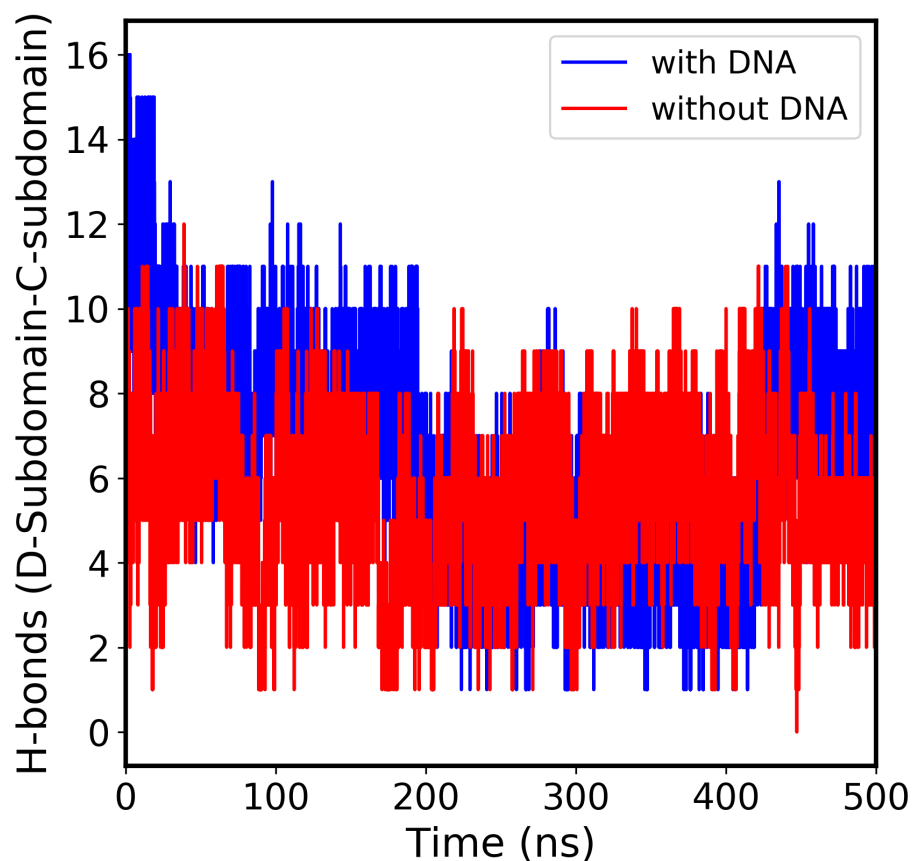


Figure S4. Time evolution of hydrogen bond between DNA binding -Catalytic subdomains in presence and absence of DNA.

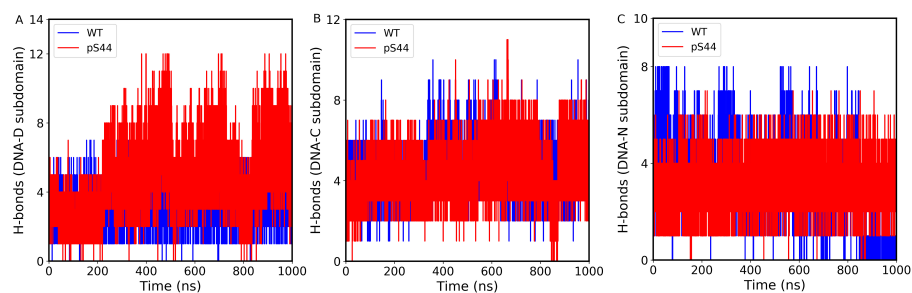


Figure S5. Time evolution of Hydrogen bonds (A) DNA and DNA binding subdomain, (B) DNA and Catalytic subdomain, and (C) DNA and N-base pairing subdomain. The blue solid line shows the hydrogen bond for WT, whereas, the red line shows the hydrogen bond for pS44.

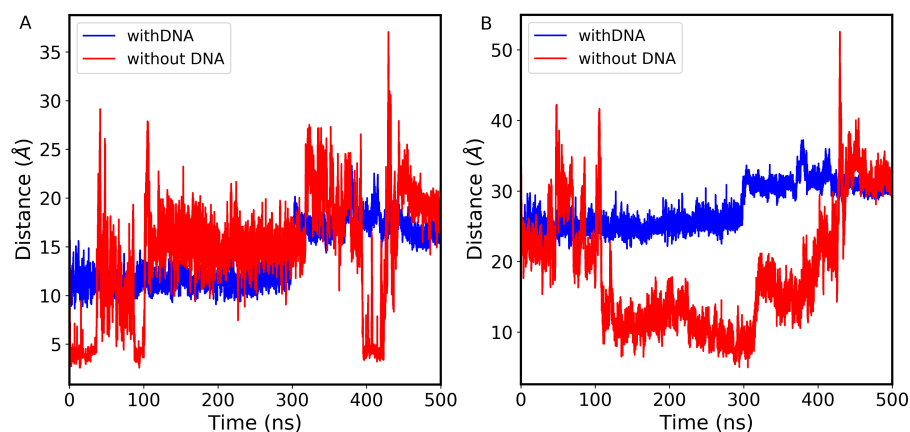


Figure S6. Distance *vs* time (A) pS44-K280; with and without DNA fragment, (B) pS44-R299; with and without DNA fragment.

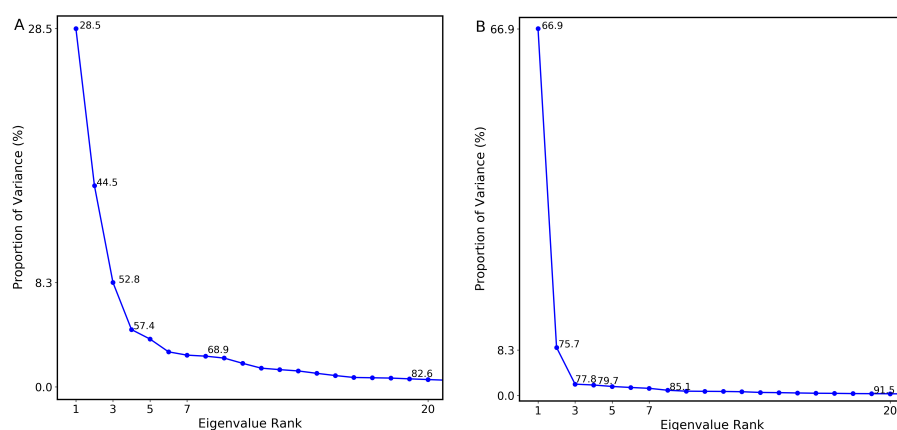


Figure S7. Scree plot for principal component analysis on the MD data of DNA pol β complex (A) WT, and (B) pS44.

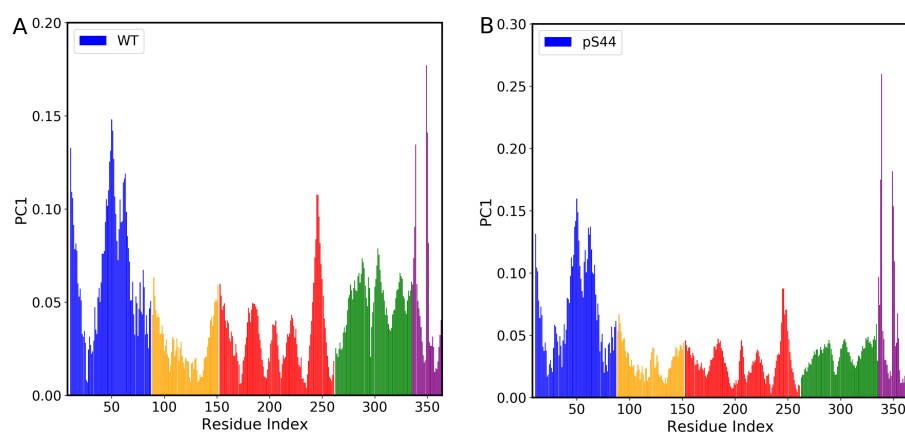


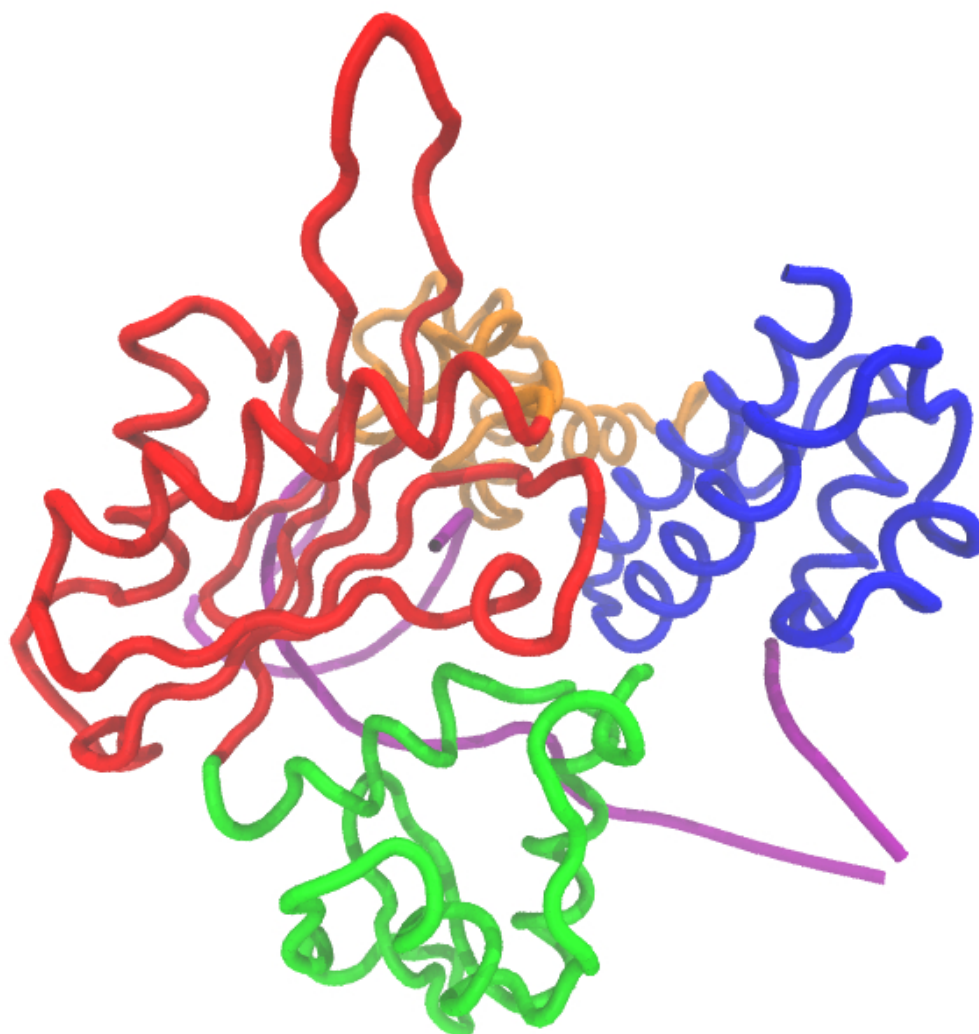
Figure S8. DNA polymerase β complex each residue and nucleotide contribution to principal component 1 (PC1) of (A) WT, and (B) pS44. Different colors in the figure represent the different domains and subdomains of DNA pol β complex as shown in figure 1 (in the main text).

Table S1. The donor-acceptor distance between S44 and E335 for three systems.

System	Average dist (Å)	St. Dev. (Å)
WT	6.18	2.10
phosphorylated S44	11.3	2.31
pS44	10.53	1.72

frame **Movie of Principal Component 1 for WT.**

1



frame Movie of Principal Component 1 for phosphorylated S44.

