

Supplementary Information

Structural basis for the bypass of the major oxaliplatin-DNA adducts by human DNA polymerase η

Hala Ouzon-Shubeita, Meghan Baker, Myong-Chul Koag and Seongmin Lee*

Division of Chemical Biology and Medicinal Chemistry, College of Pharmacy,

The University of Texas at Austin, Austin, TX 78750, USA

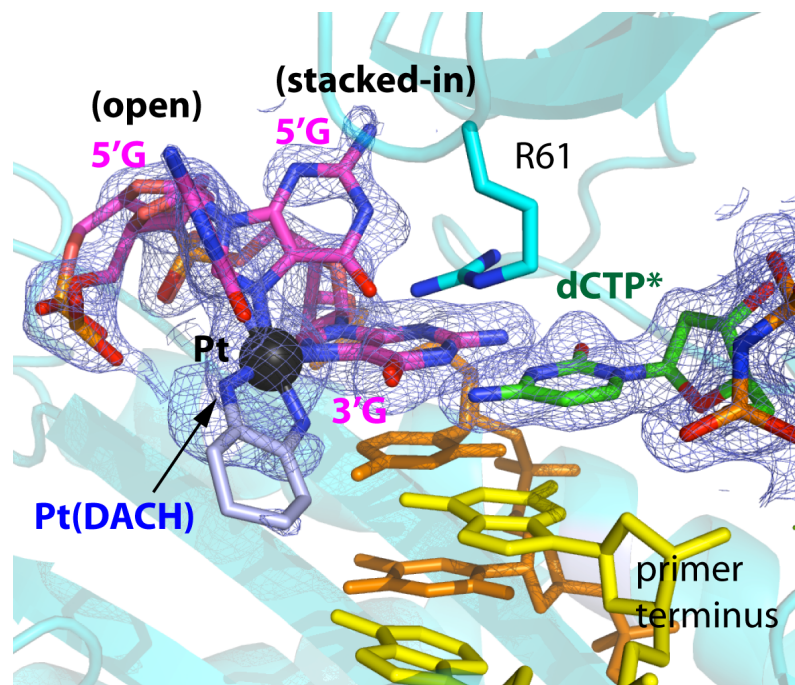


Figure S1. Structure of Polη incorporating dCTP opposite the 3'G of the Pt(DACH)GpG adducts. A $2F_o - F_c$ electron density map contoured at 1σ around the Pt(DACH):dCTP* base pair. Pt is shown in black sphere. The 5'G of the Pt(DACH)GpG exists as a mixture of an “open” and “stacked-in” conformations.

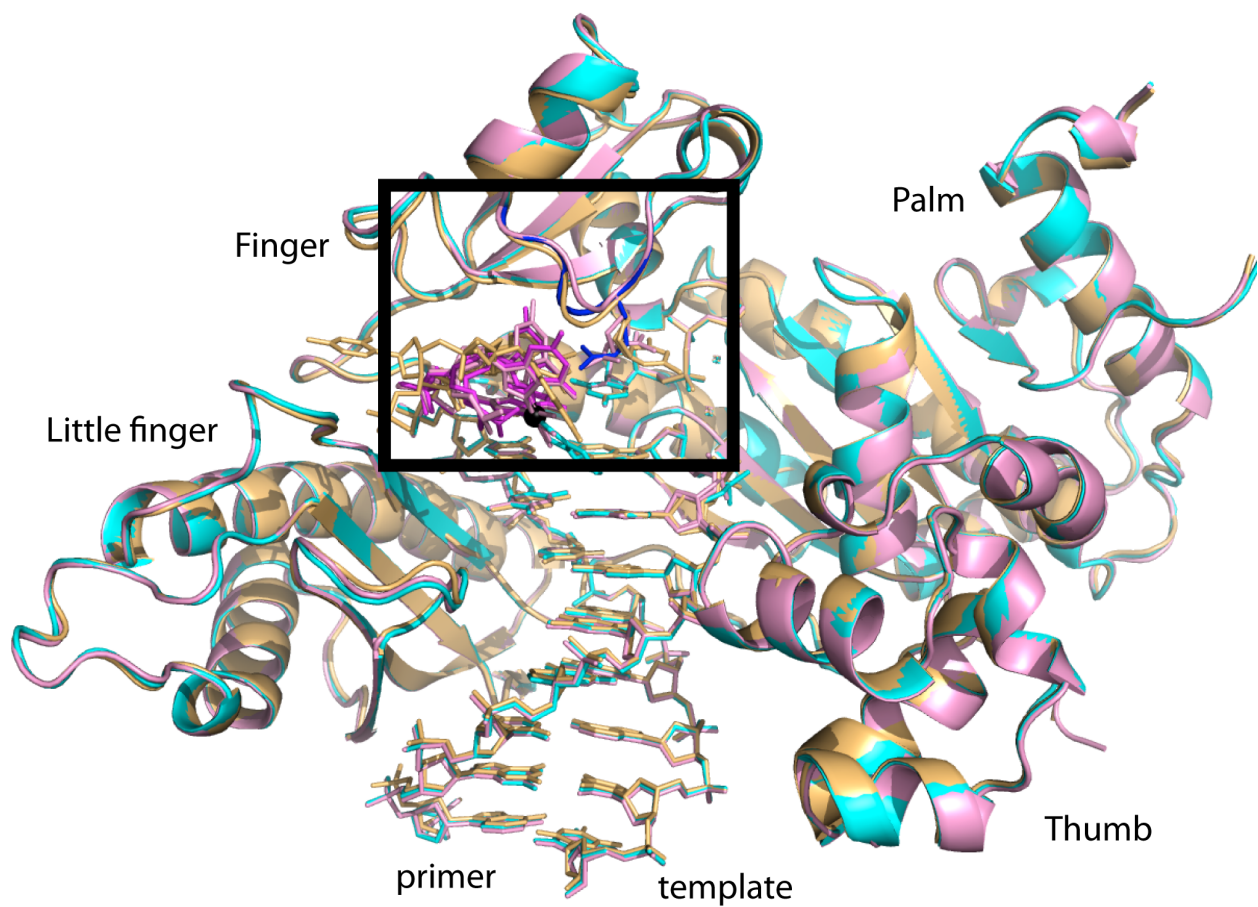


Figure S2. Superposition of structures of Polη incorporating dCTP opposite the 3'G, Pt(NH₃)₂-3'G, and Pt(DACH)-3'G. Pt(DACH)-3'G·dCTP* (cyan), Pt(NH₃)₂-3'G·dCTP* (pink, PDB ID: 4DL4 [39]), and normal-3'G·dCTP* (green, PDB ID: 4DL2 [39]) are colored in cyan, pink, and gold, respectively. Pt(DACH)GpG is shown in magenta. The region containing the Val59-Trp64 loop of the finger domain, platinumated GpG, and incoming dCTP is shown in a box.