Supporting material:

Sampoli et al.
How DNA polymerase X preferentially accommodates incoming dATP opposite 8-oxoguanine on the template

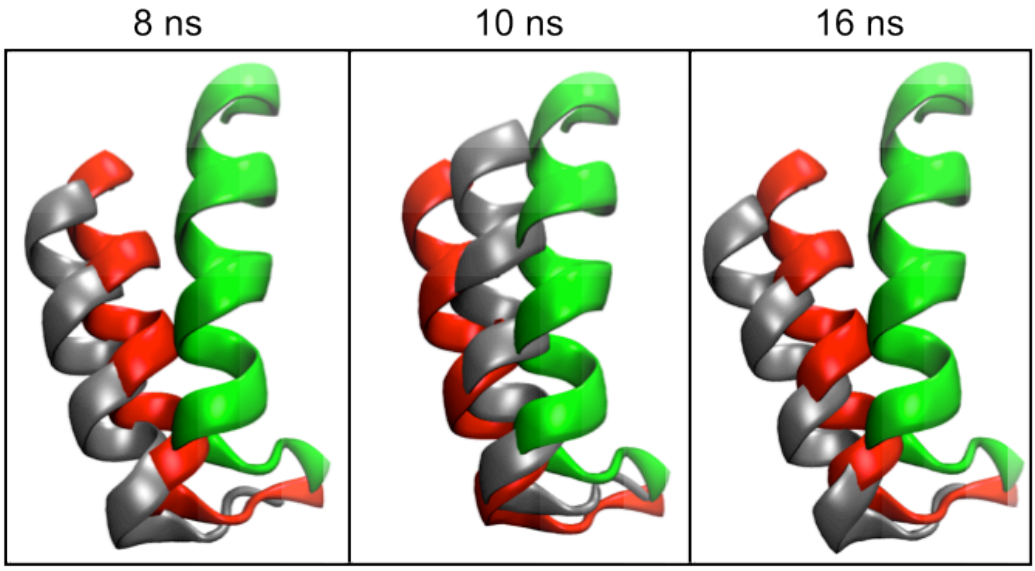

Figure S1. *VMD snapshots of the oxoG$_{syn}$:A system*. Movement of αE in the oxoG$_{syn}$:A system (grey) with respect to the open (green) and closed (red) structures. The panels above show three snapshots taken at different points during the dynamics trajectory While the simulated grey structure oscillates around the closed (red) structure, it appears to deviate significantly from the open (green) structure, giving rise to high RMSD values (See **Figure 3**).

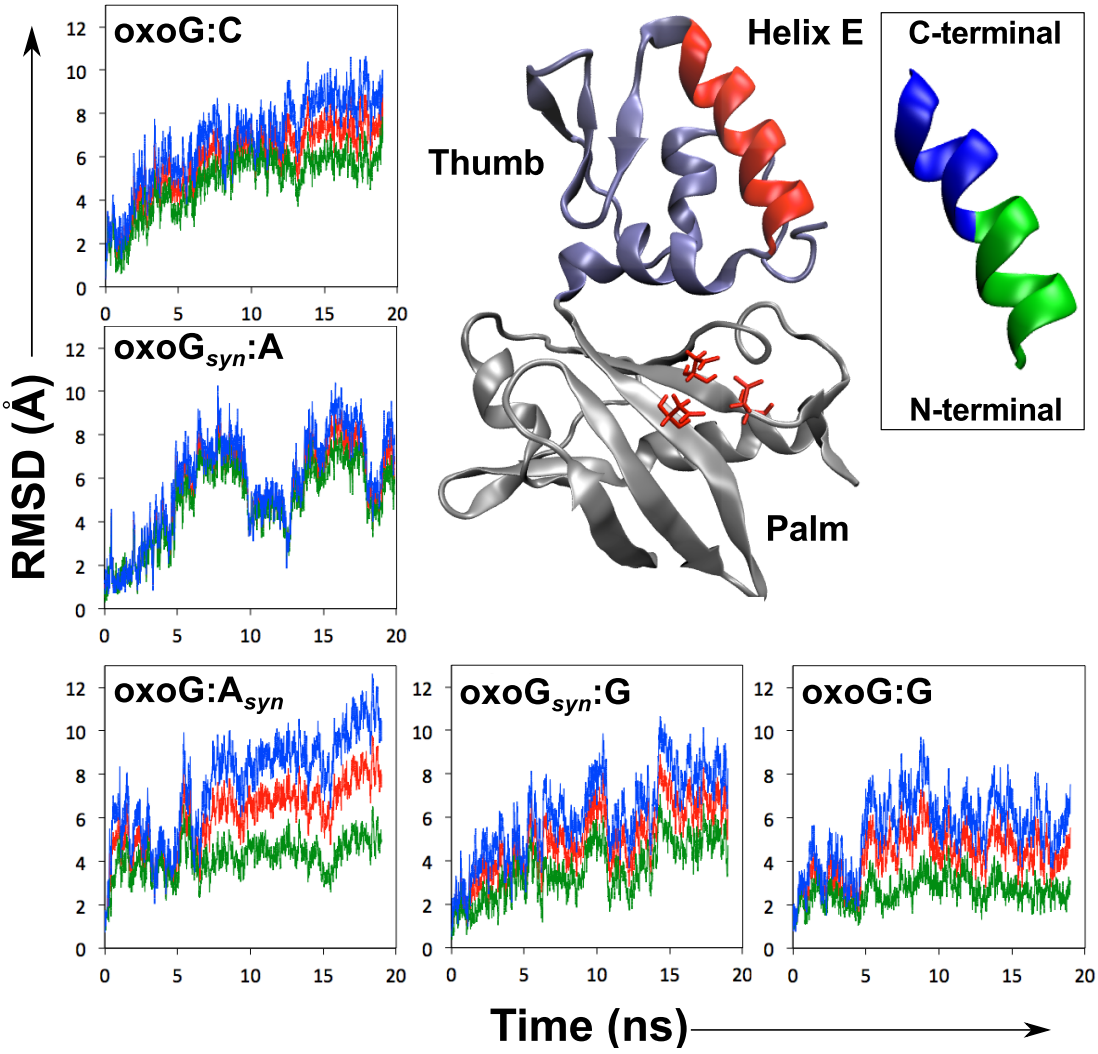

Figure S2. *Segmentation of αE motion in the simulated trajectories.* Time evolution of the root-mean square deviations (RMSD) for αE (red), N-terminal αE segment (120-126) (green) and C-terminal αE segment (127-132) (blue) are shown for all five oxoG systems. These data were generated using VMD RMSD trajectory tool aligning the thumb (107-174) and αE (120-132) to the palm subdomain (1-105) of their initial structures. The y-axis represents RMSD in Å and the x-axis is time (ns). In the top right panel, Pol X is represented as a cartoon model with the palm subdomain (grey), thumb subdomain (purple), and αE (red). The catalytic triad is also displayed as stick-lines in red. The division of αE is magnified, where the N-terminal segment of αE (120-126) is shown in green and the C-terminal segment is in blue.

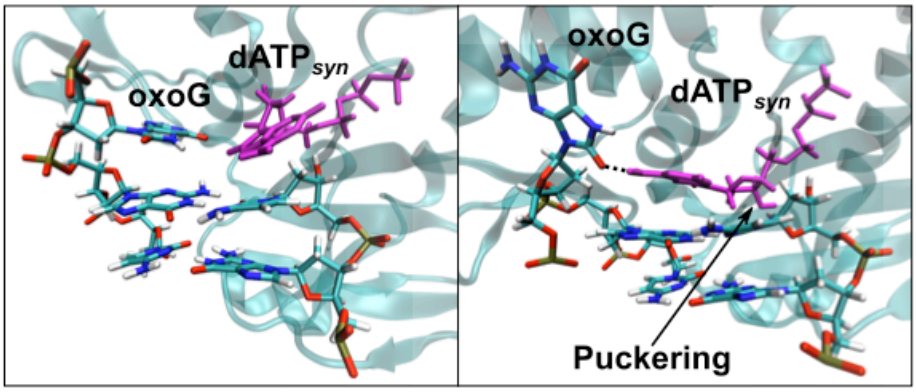

Figure S3: *VMD snapshots of the oxoG:A_{syn} system*. (A) At the beginning of the simulation and (B) after 9 ns, when the incoming dATP (magenta) rotates over its glycosidic dihedral angle. The oxoG on the template strand (gray) also flips towards a *syn* conformation.