Supplementary Material

Overview of Free Energy Surfaces and Transition State Geometries for the Hydrolysis of a Series of dGTP Analogues Modified at the β,γ-Bridging Position

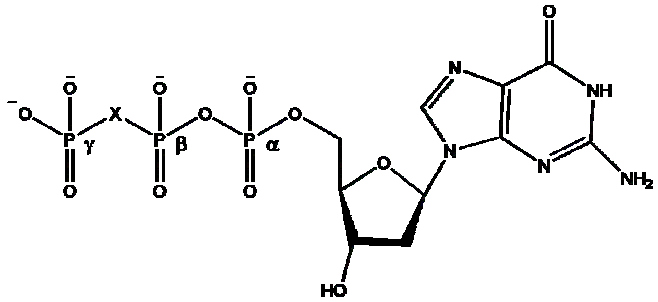

Figure S1: Structure of dGTP and β,γ-substituted analogues. X=CF_2, CFCl, CCl_2, O, CHF, CBr_2, CHCl, CHBr and CH_2[12,16].

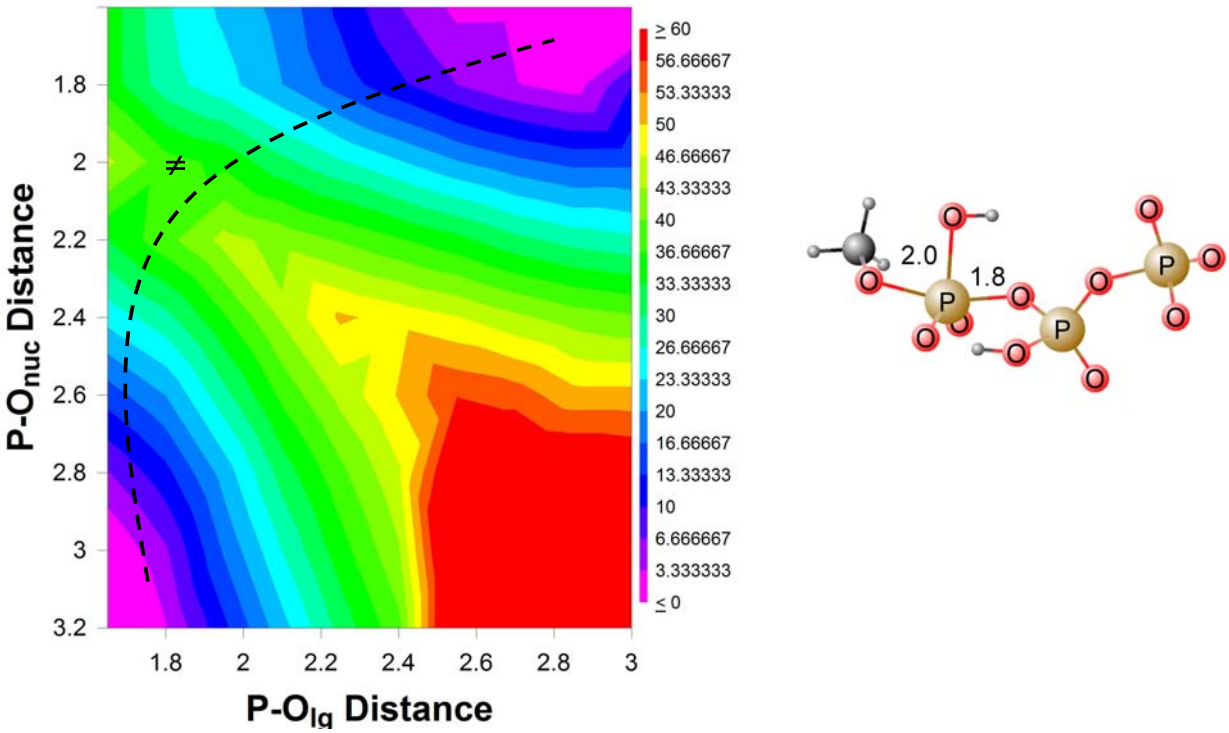

Figure S2: Free energy surface and transition state geometry for the dGTP analog where X=O. All distances are in Å, and ≠ denotes a transition state.

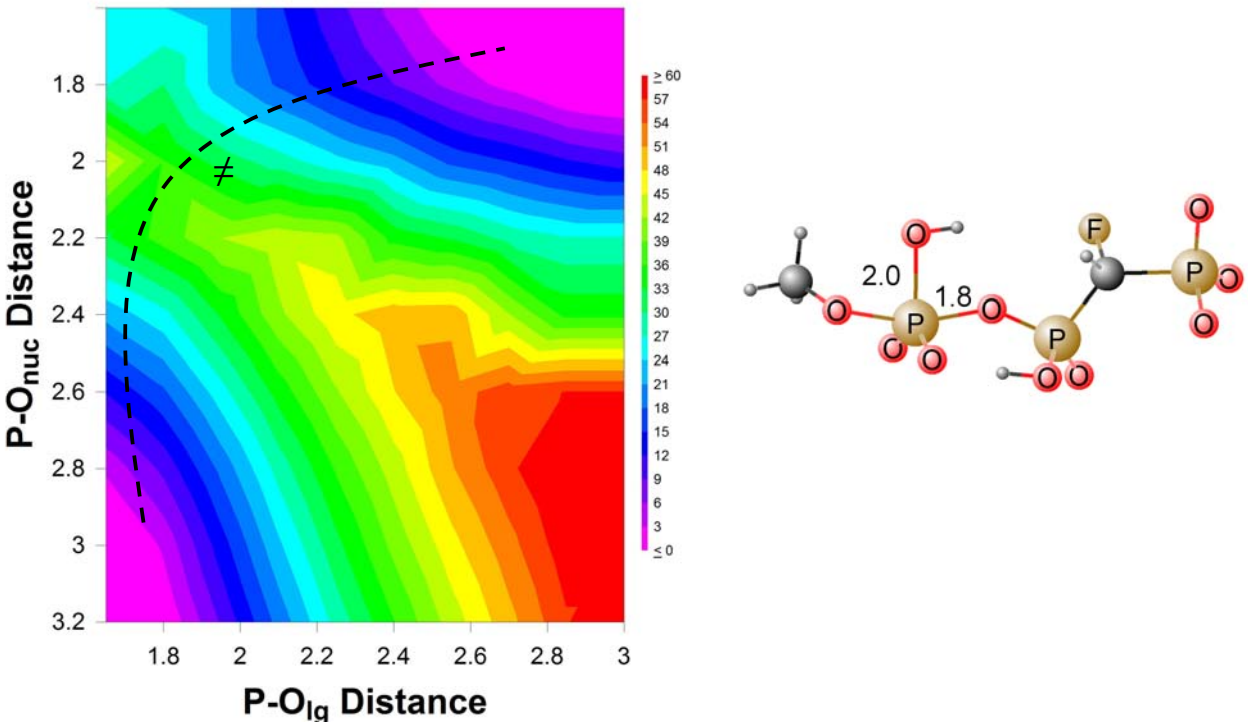

Figure S3: Free energy surface and transition state geometry for the dGTP analog where X=CHF. All distances are in Å, and ≠ denotes a transition state.

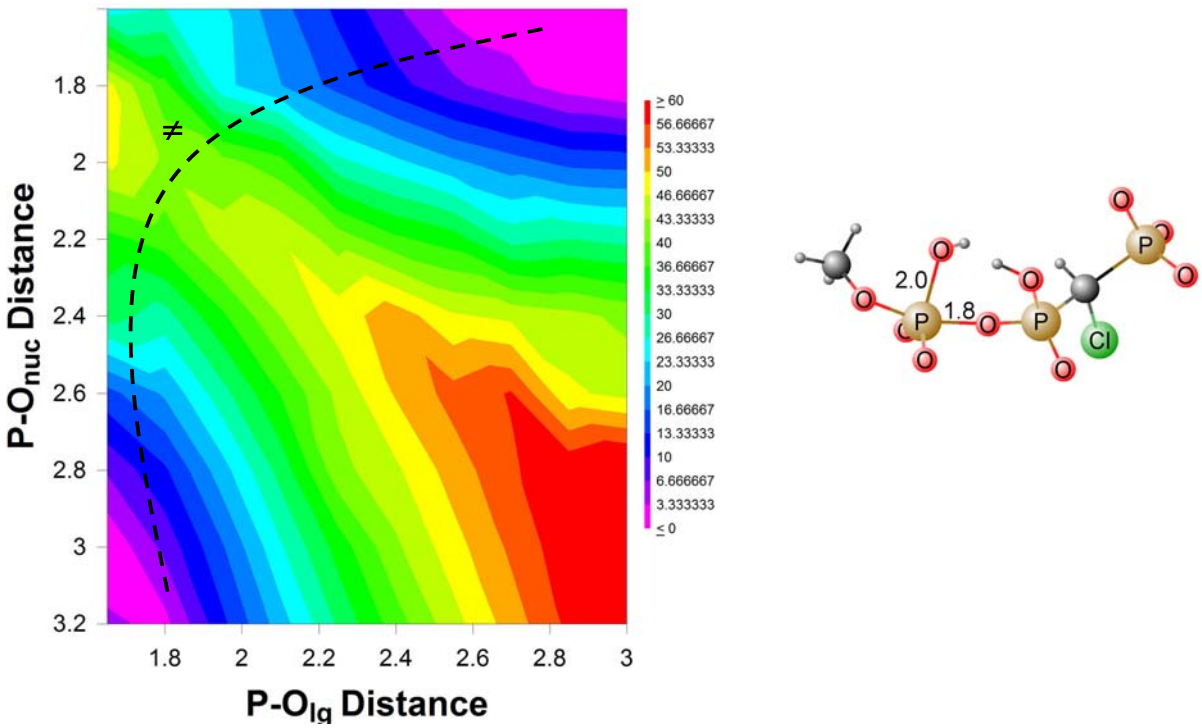

Figure S4: Free energy surface and transition state geometry for the dGTP analog where X=CHCl. All distances are in Å, and ≠ denotes a transition state.

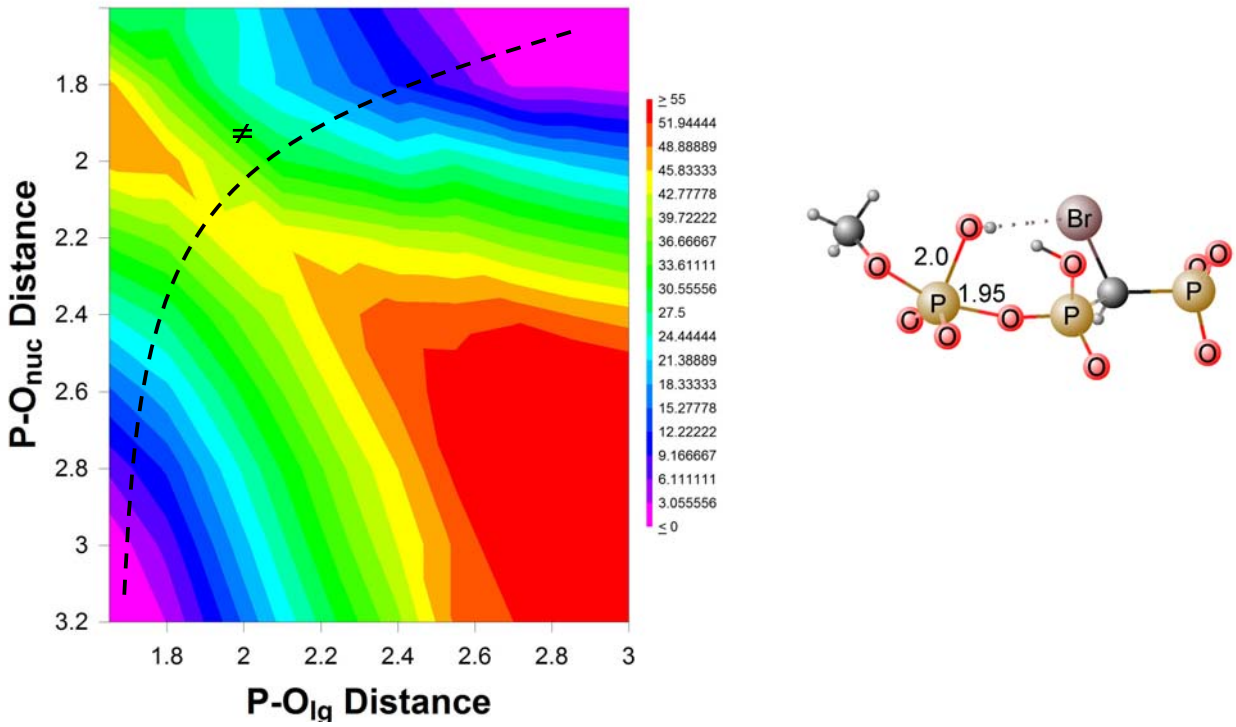

Figure S5: Free energy surface and transition state geometry for the dGTP analog where X=CHBr. All distances are in Å, and ≠ denotes a transition state.

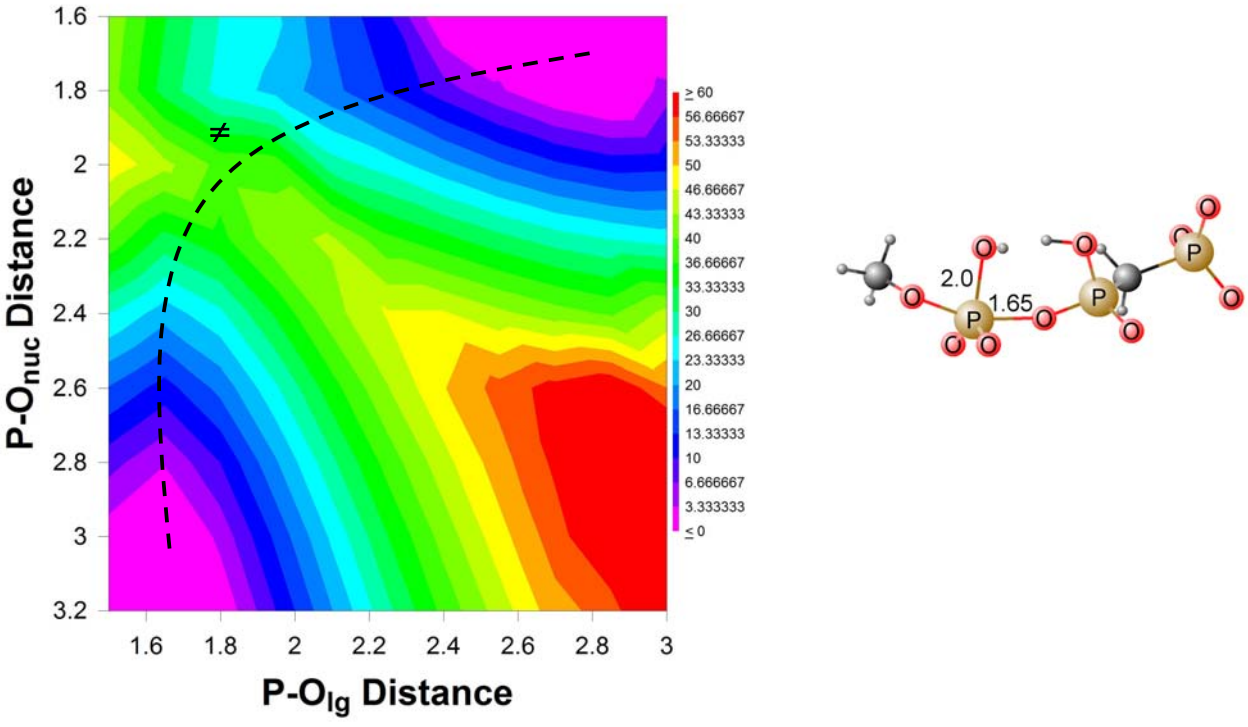

Figure S6: Free energy surface and transition state geometry for the dGTP analog where X=CH_2. All distances are in Å, and ≠ denotes a transition state.

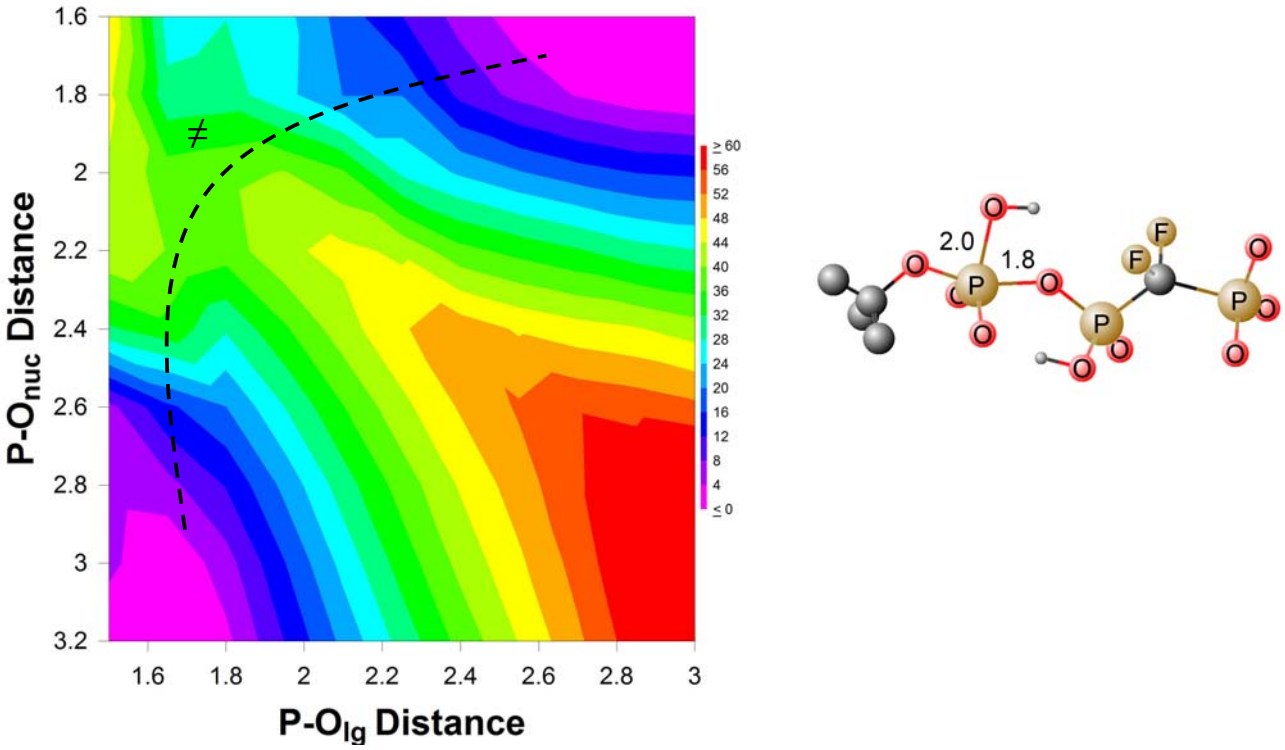

Figure S7: Free energy surface and transition state geometry for the dGTP analog where X=CF_2. All distances are in Å, and ≠ denotes a transition state.

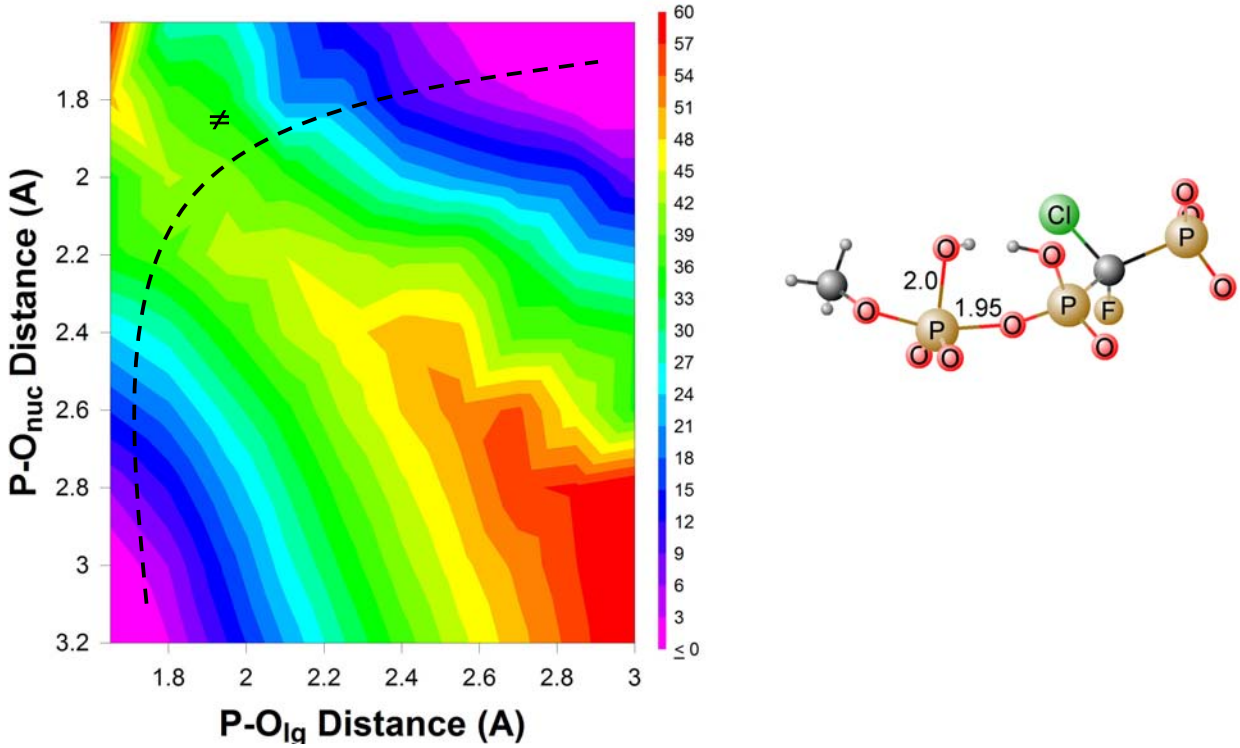

Figure S8: Free energy surface and transition state geometry for the dGTP analog where X=CFCl. All distances are in Å, and ≠ denotes a transition state.

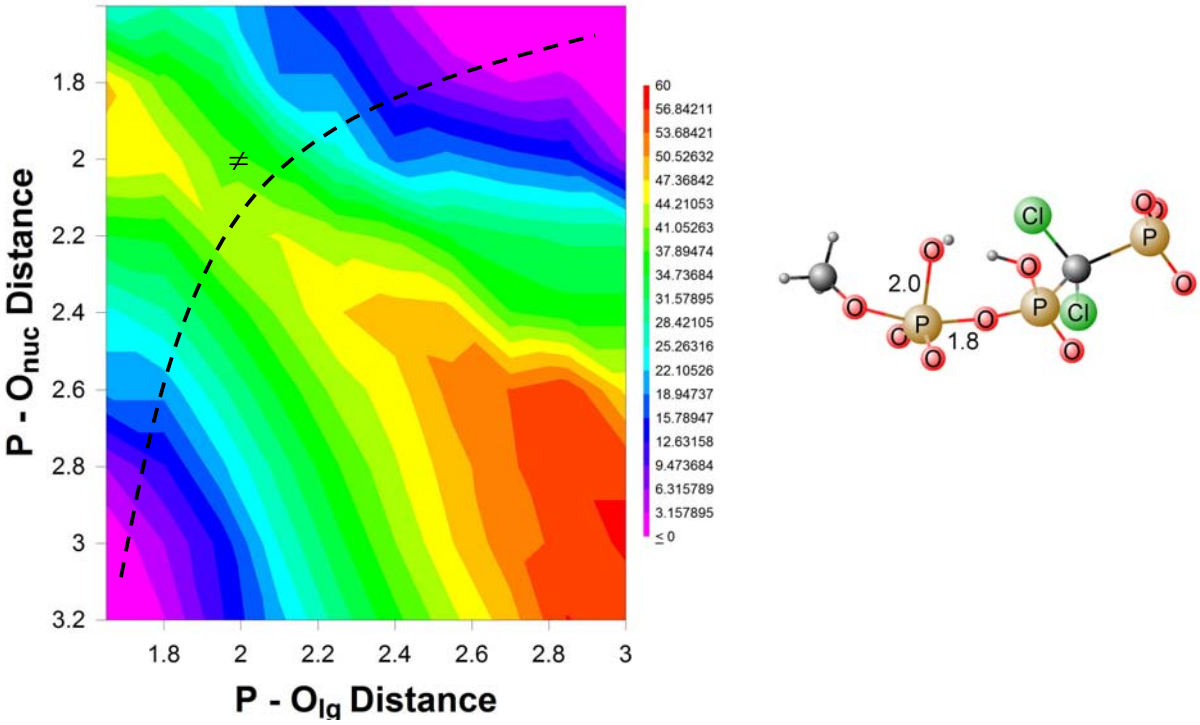

Figure S9: Free energy surface and transition state geometry for the dGTP analog where X=CCl_2. All distances are in Å, and ≠ denotes a transition state.

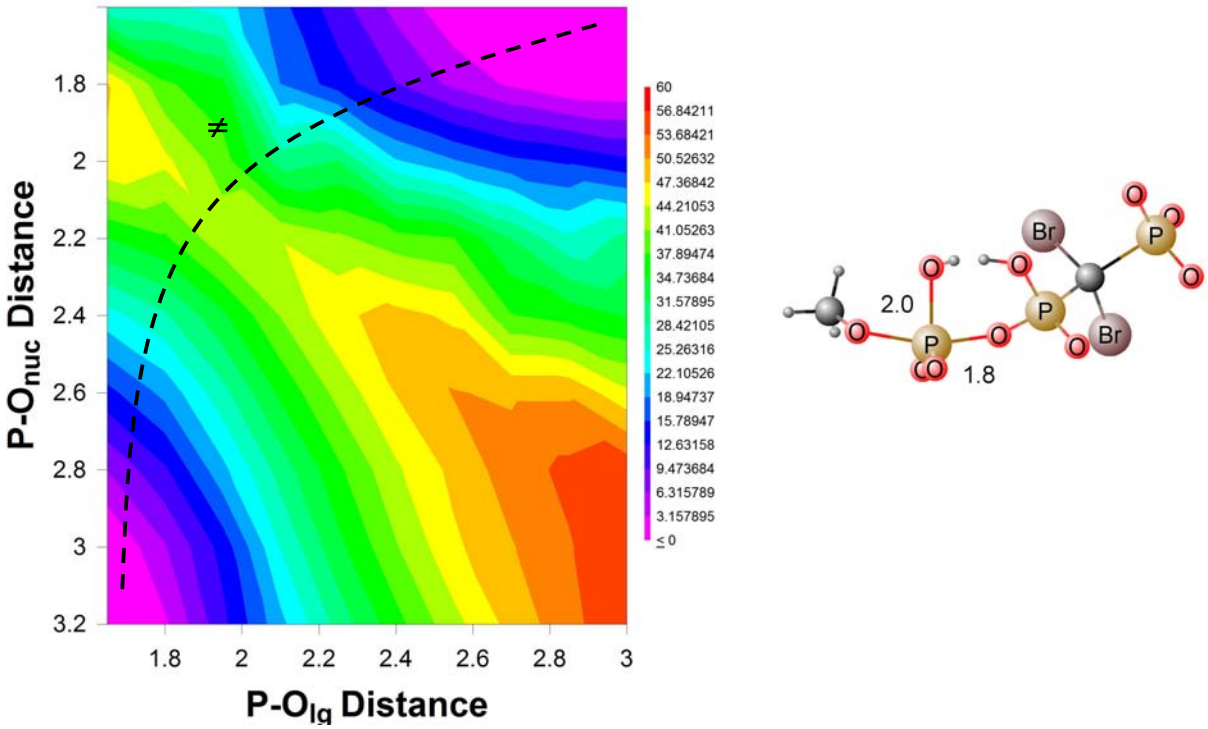

Figure S10: Free energy surface and transition state geometry for the dGTP analog where X=CBr_2. All distances are in Å, and ≠ denotes a transition state.