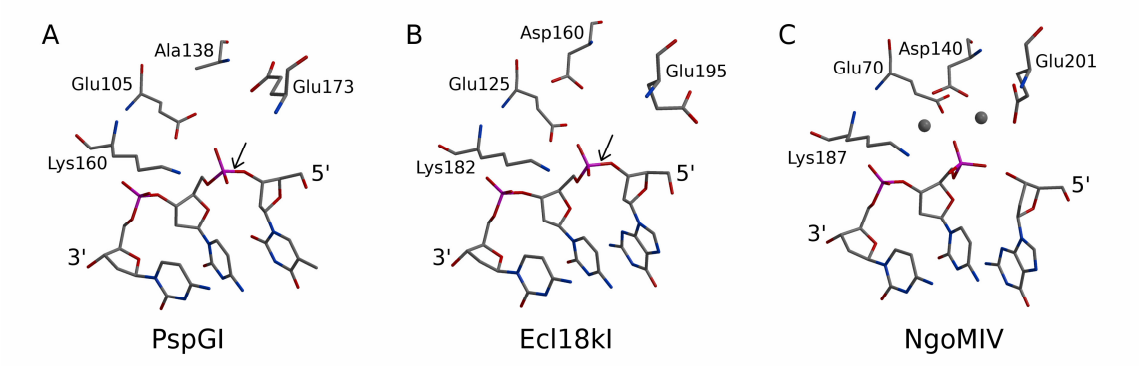
Supplementary Figure 1: Comparison of the active site regions of PspGI (A), Ecl18kI (B) and NgoMIV (C). In wild-type PspGI, Asp138 is expected to chelate two metal ions in the active site. In the crystal structure, this residue is mutated to alanine to prevent DNA cleavage during the process of crystallization. No metal ions are observed and the active site is slightly distorted. Ecl18kI was crystallized in the absence of metals (Bochtler et al, 2006). In the NgoMIV structure the metal ions are present (marked by gray balls in the figure), but product DNA was used for crystallization (Deibert et al, 2000).



Supplementary Figure 2: The superposition of guanine base on top of the flipped adenine in the pockets of (A) PspGI and (B) Ecl18kI. The contacts of the 2-amino group with the protein that are shorter than 3.5 Å are shown as the potential steric clashes. In each panel the structure on the right is ~90° horizontally rotated relatively to the one on the left.