

Online Supporting Information

Insights into Base Selectivity from the 1.8 Å Resolution Structure of an RB69 DNA Polymerase Ternary Complex

Mina Wang, Shuangluo, Xia, Gregor Blaha, Thomas A. Steitz, William H. Konigsberg, and Jimin Wang

Online Supplementary Figure Captions

Figure S1. Experimental Evidence for five buried water molecules mediating the polymerase-DNA duplex interactions. (A) Stereodiagram of final 2Fo-Fc maps contoured at 0.75 σ superimposed on the refined model showing five buried water molecules. (B) Stereodiagram of the 2Fo-Fc maps contoured 0.7 σ superimposed on the refined model (edited to remove non-solvent density for clarity). (C) Stereodiagram of the superposition of this complex (golden, red) onto the ϕ 29 pol ternary complex (cyan, and green, Berman *et al.*, 2007, EMBO J. 26, 3496-3505).

Figure S2. Solvation of the nascent base pair. (A-B) Two orthogonal views of the final 2Fo-Fc maps contoured at 1.2 σ superimposed on the refined RB69 pol (cyan) and the nascent base-pair (golden). (C) Stereodiagram of solvent structure around the edge of the nascent base pair.

Figure S3. Distribution of the geometry of ribonucleotide residues in the 50S ribosome structure (1VQ0, Schmeing *et al.*, 2005, Mol. Cell 20, 437-448). (A) Distribution of the O5'-C6 (U or C) or O5'-C8 (A or G) distances versus the projected angles between the glycosidic bond and the C5'-O5' bond. (B) Distribution of the O5'-C6 or O5'-C8 distances versus the unsigned pseudo dihedral torsion angles of from O5'-C5' to the glycosidic bond C1'-N1 (U or C) or to C1'-N9 (A or G) atoms. Source codes for this analysis are available upon request (to. J.W.).

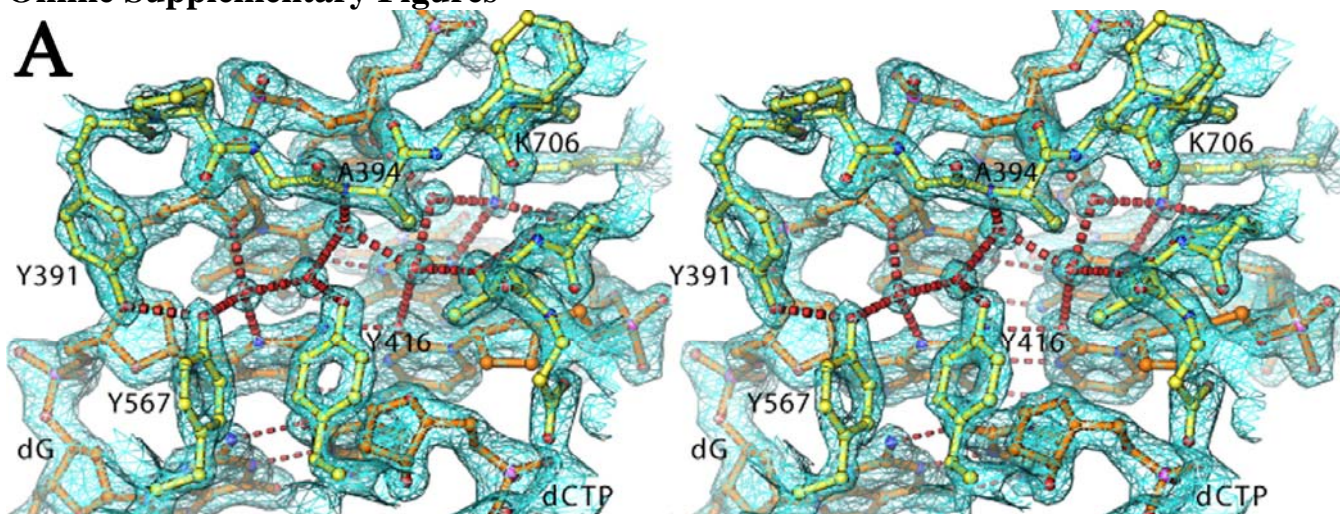
Figure S4. Rigidity of the templating nucleotide binding pocket. (A) Interactions of 5' and 3'-phosphodiester of the dG with RB69 pol. (B). Space-filling model of the binding pockets for 5' and 3'-phosphodiester of the dG.

Figure S5. Hydration structure of DNA duplex within the ternary complex. (A). Superposition of the observed DNA duplex (primer stand in yellow and template strand in gold) on an idealized B form (cyan and green). (B). Same as (A) but observed DNA is superimposed on an idealized A form (cyan

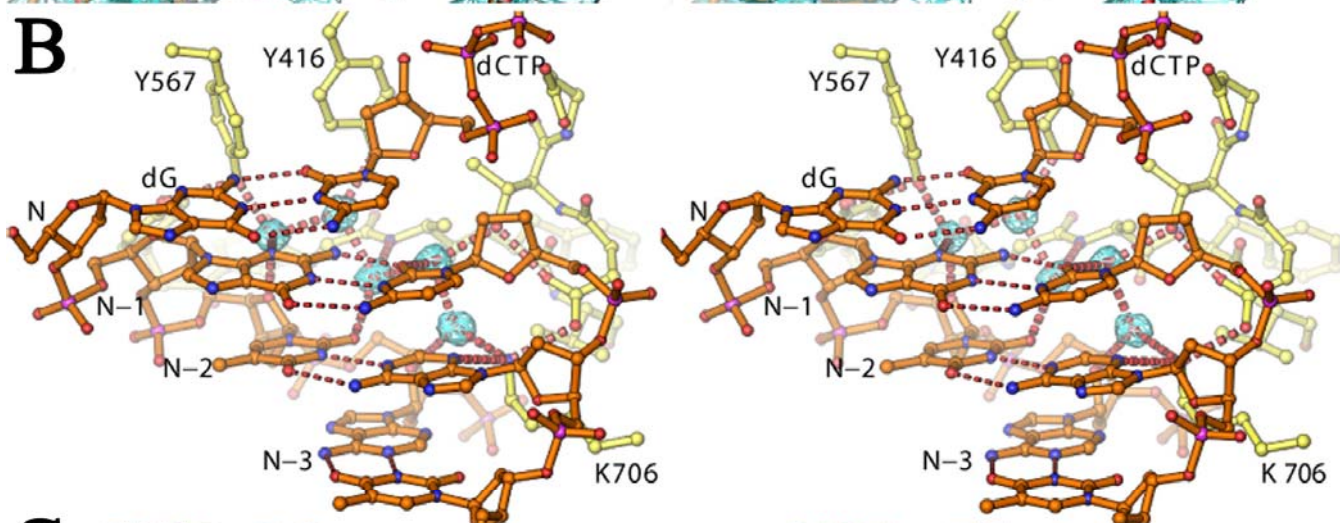
and green). (C). A stereodiagram of superposition of the final 2Fo-Fc maps for hydration shells (cyan, the first shell, magenta, the second shell, and blue, the third shell) onto the DNA duplex. Two spines of hydration are in circle. (D). A rear-view of (C) with five buried water molecules encircled.

Online Supplementary Figures

A



B



C

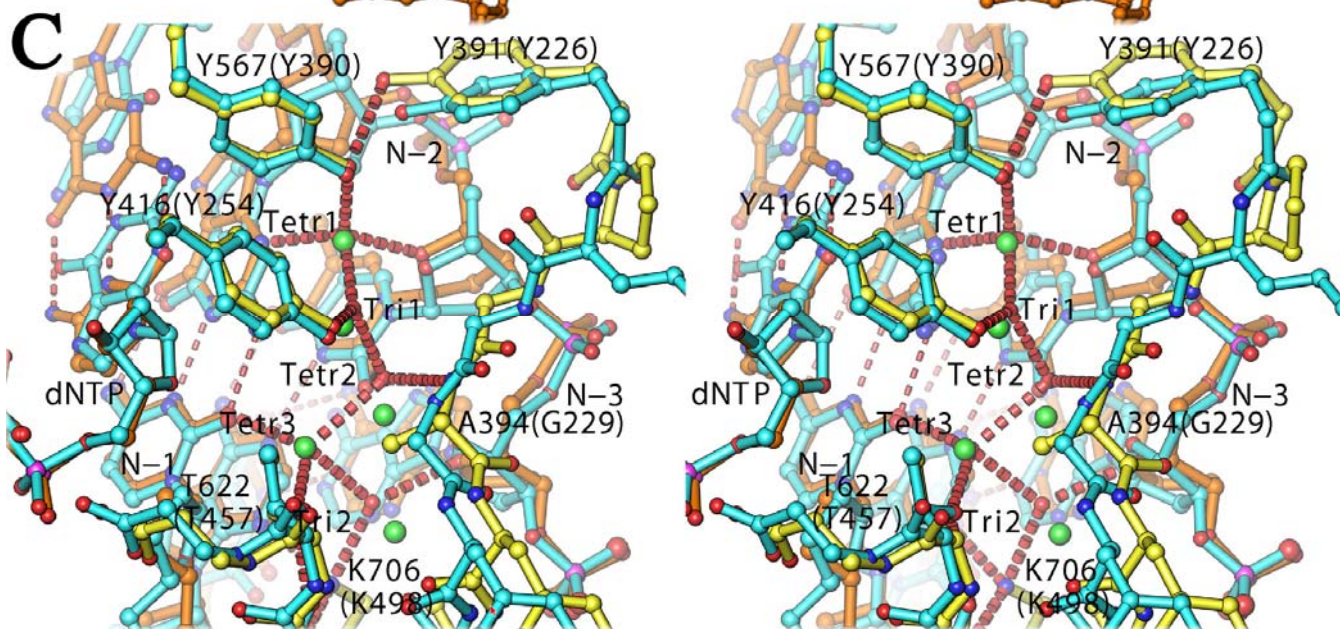


Figure S1.

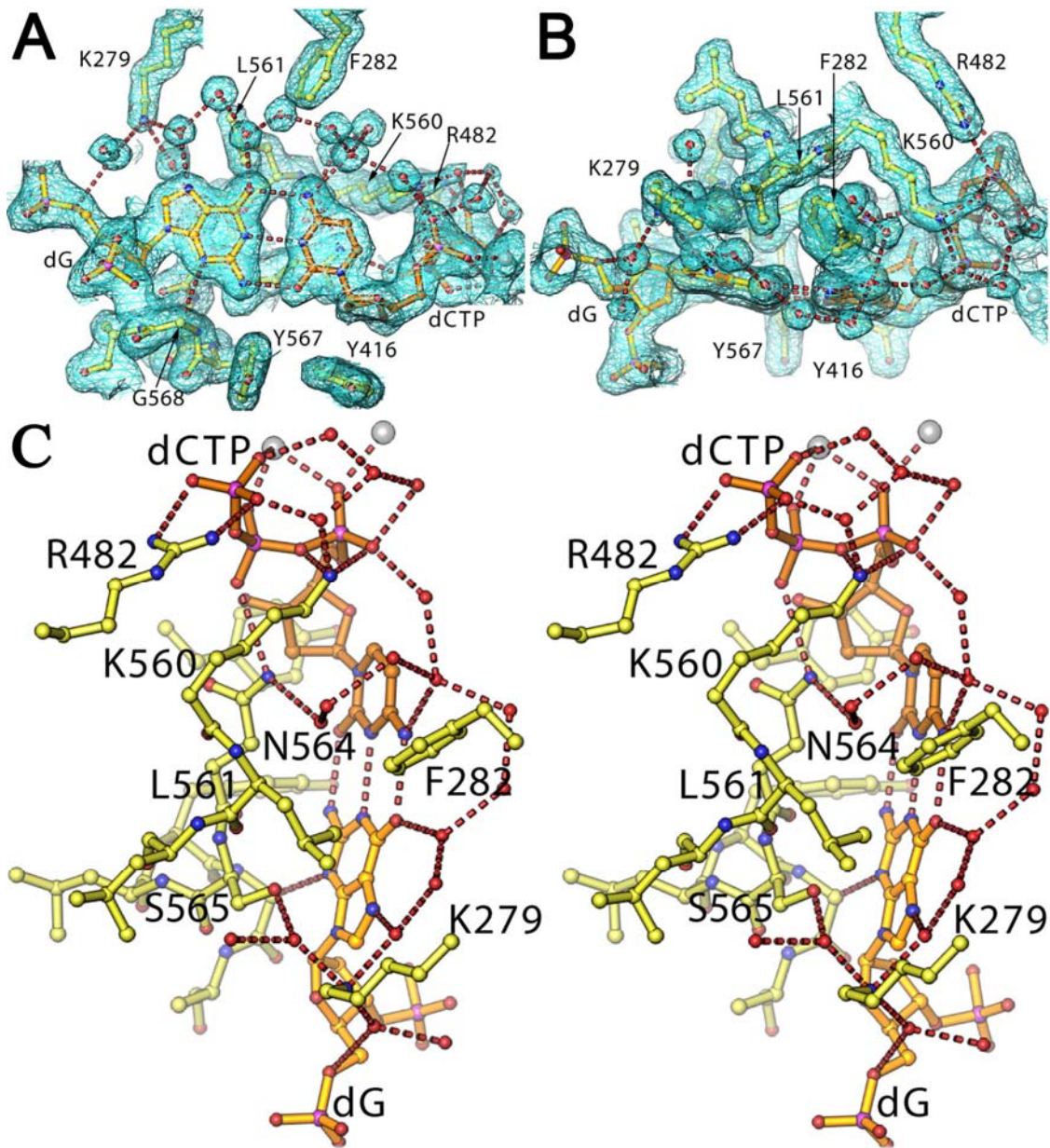


Figure S2.

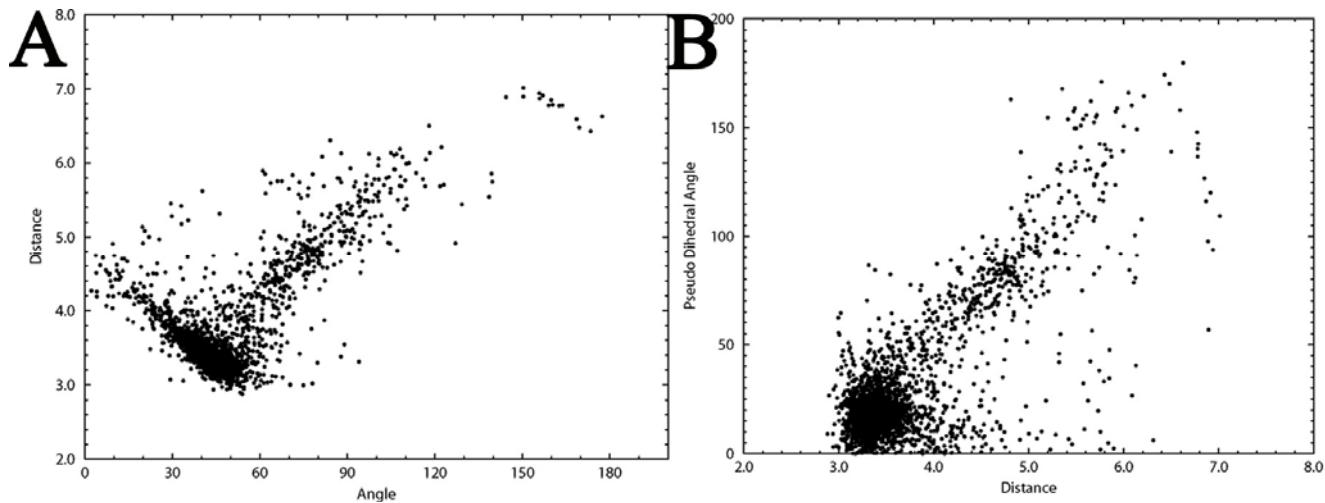


Figure S3.

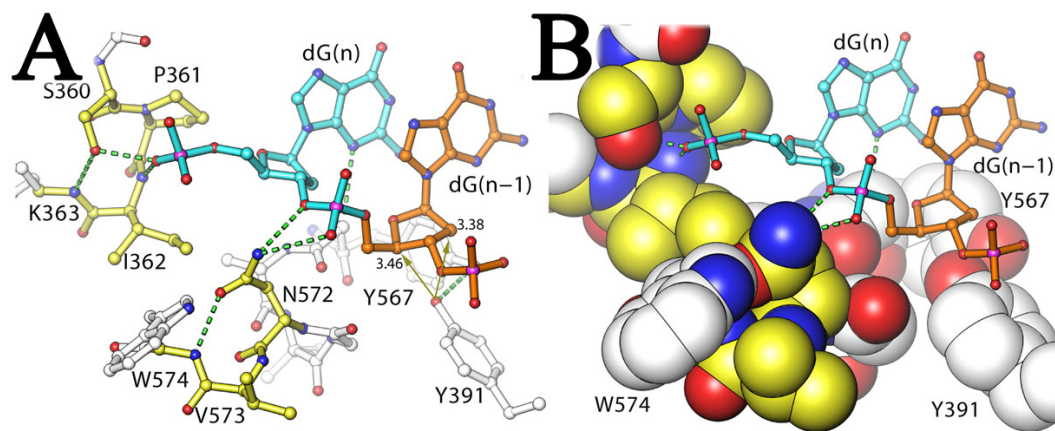


Figure S4.

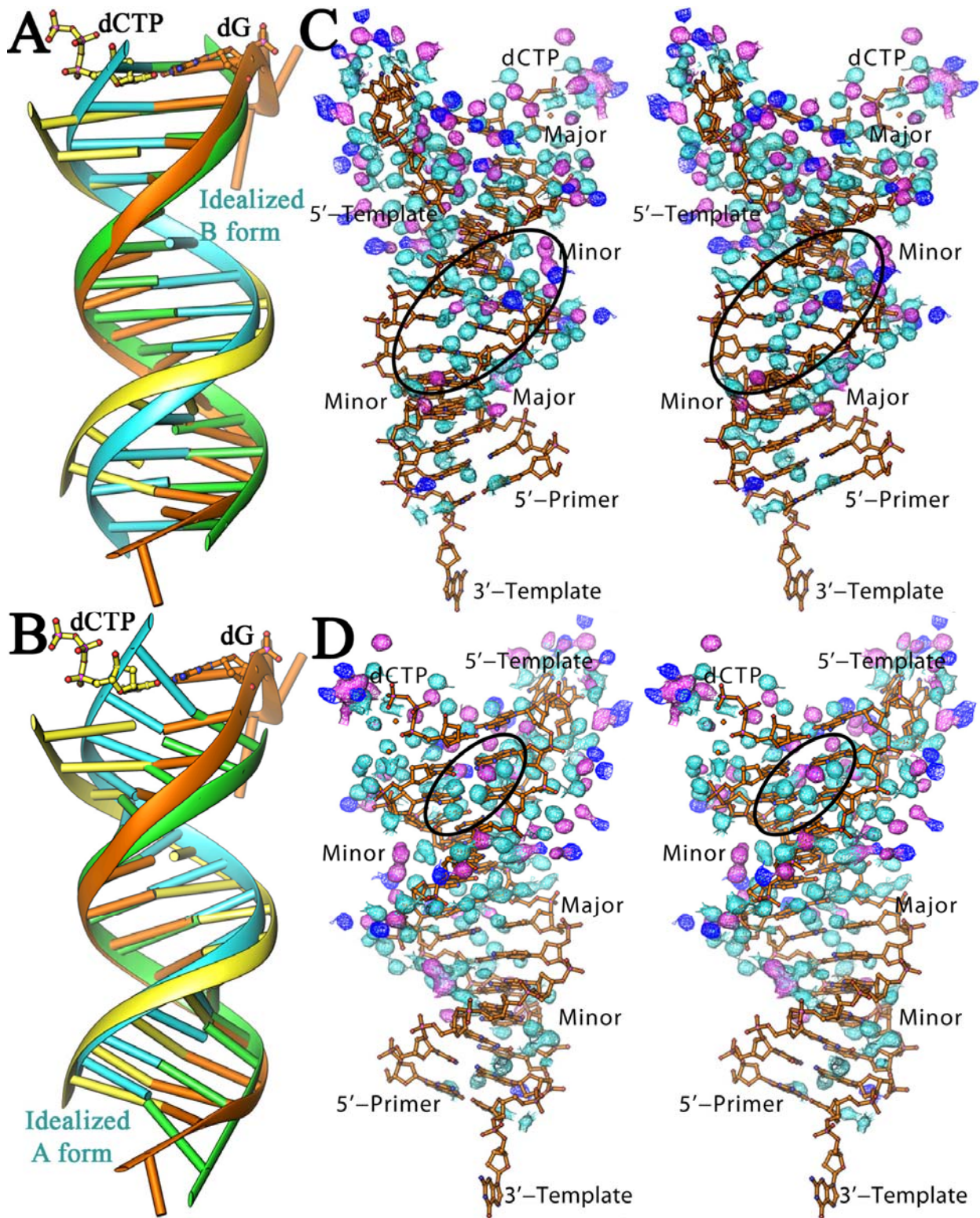


Figure S5.