SUPPLEMENTAL MATERIAL

FIG. S1. UV-visible absorption spectra of purified wild-type CYP105P1. Spectra were measured in 50 mM sodium phosphate buffer (pH 7.5) containing 10% (v/v) glycerol, 0.05 mM dithiothreitol, and 0.05 mM EDTA at room temperature. The concentration of CYP105P1 protein was 10.2 μM. Resting (———), dithionite-reduced (- - -), and dithionite-reduced plus CO (– – –). *Inset*, (dithionite-reduced plus CO) minus (dithionite-reduced). The resting state exhibits a typical low spin state spectrum with the Soret peak maximum at 420 nm, and β and α peaks at 540 and 571 nm, respectively. The dithionite-reduced state shows Soret peak maximum at 418 nm with decreased intensity, and its CO-ligated state yielded a spectral species with peaks at 447 and 548 nm. The feature of UV-visible absorption spectra of purified H72A mutant was almost identical with that of wild-type CYP105P1 (data not shown).

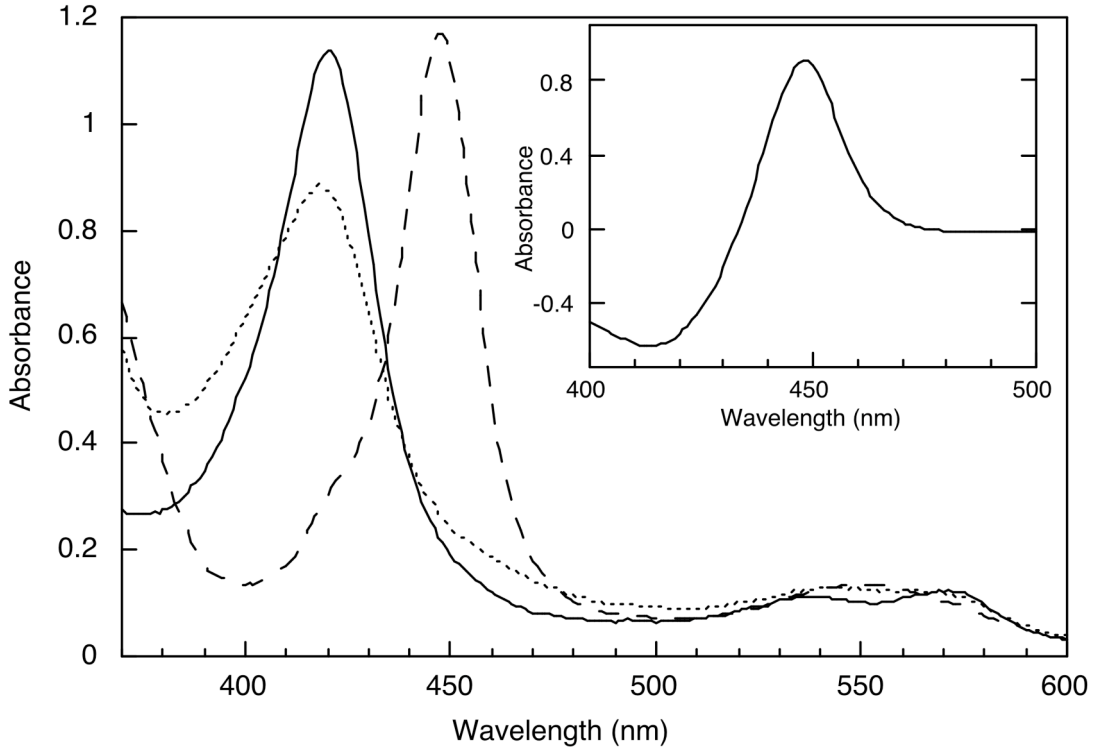
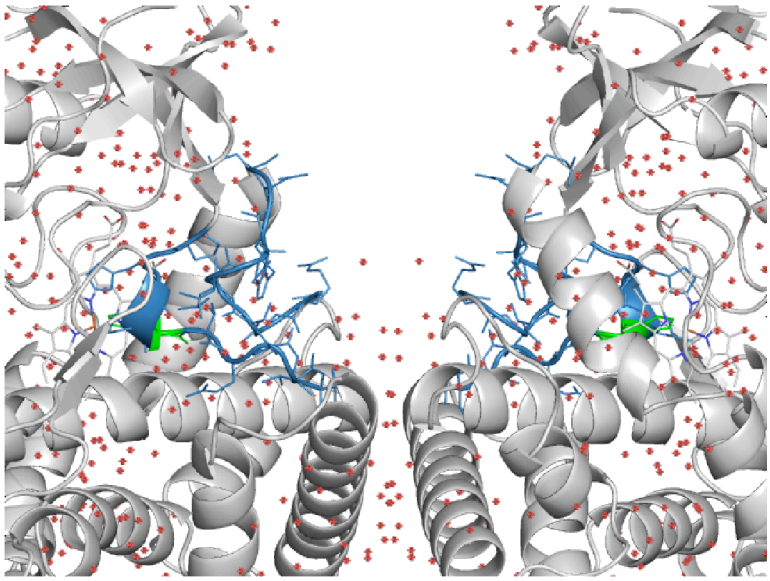


FIG. S2. Crystal packing interactions of the symmetry-related molecules in the crystals of WT-free (*A*) and H72A-free (*B*) forms. The BC loop regions (blue) and His72 or Ala72 residue (green) are differently colored. Water molecules are shown as red asterisks.

A



B