

Supplementary figure legends

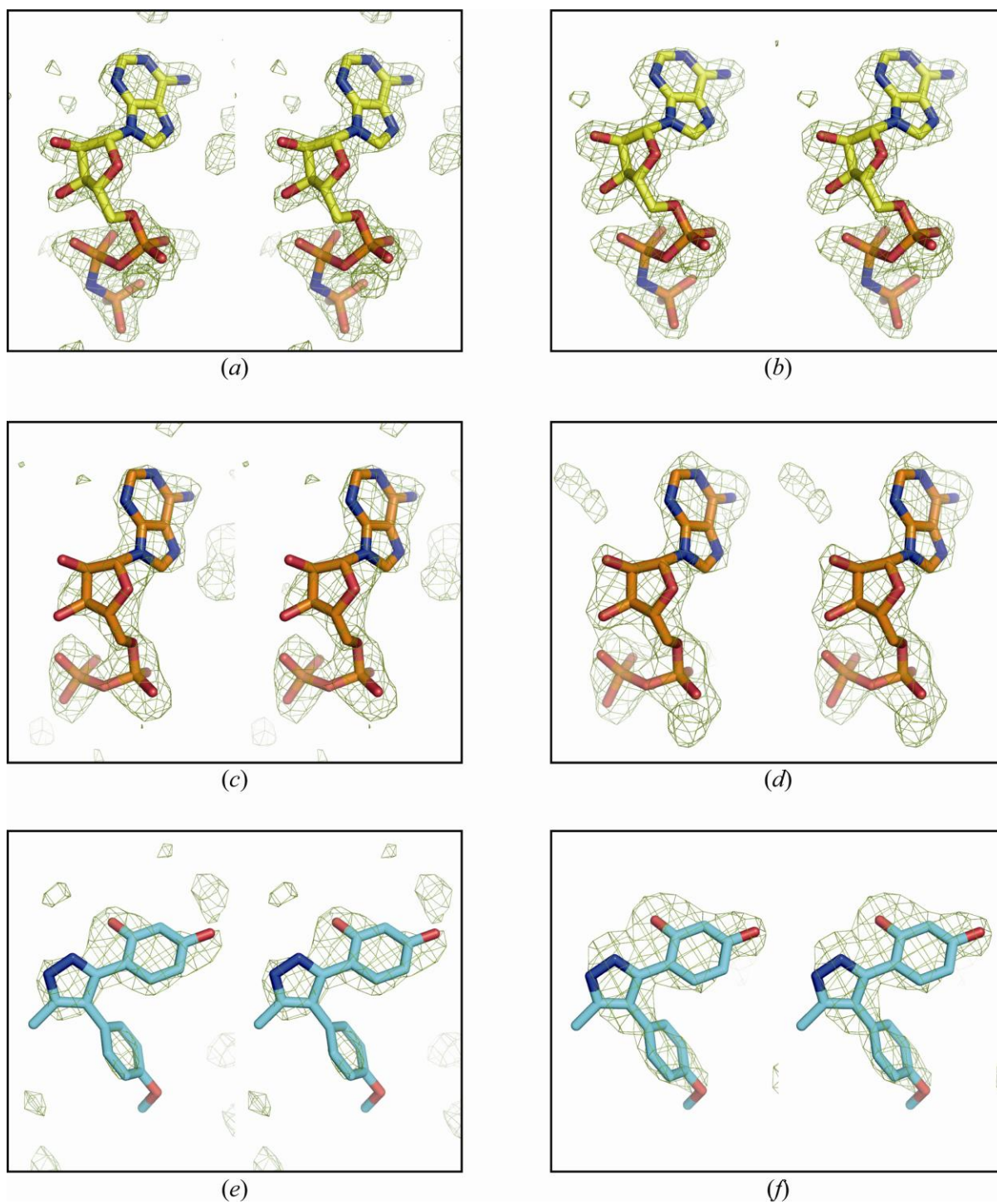


Figure S1 Fo-Fc omit maps for the bound inhibitors. Stereo views of the maps for (a) (b) AMPPNP, (c) (d) ADP, and (e) (f) M77976 calculated before (a, c, e) and after (b, d, f) refinement. The final models for the bound inhibitors are shown as sticks.

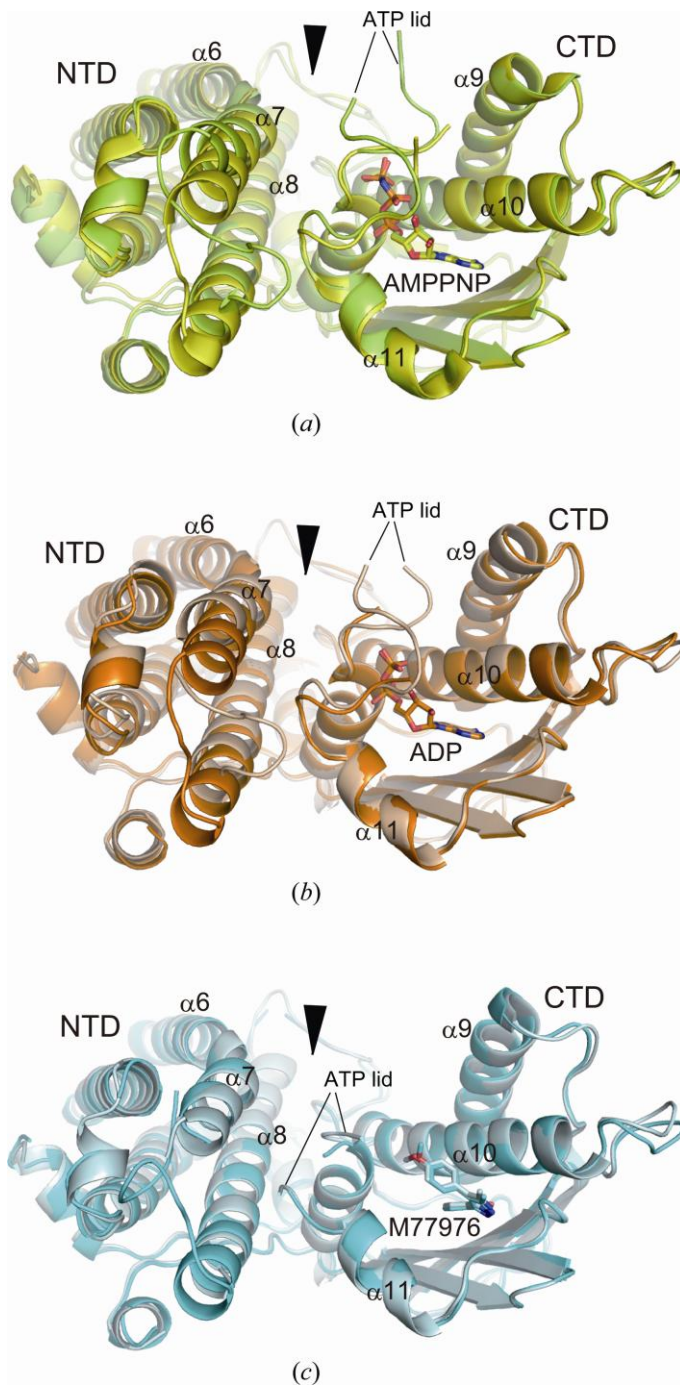


Figure S2 Superimposition of two subunits of (a) PDK4•AMPPNP, (b) PDK4•ADP, and (c) PDK4•M77976. PDK4•AMPPNP is colored lemon (subunit A) and yellow (subunit B), PDK4•ADP is wheat (subunit A) and orange (subunit B), and PDK4•M77976 is green-cyan (subunit A) and pale-cyan (subunit B), as in Figure 2. NTD and CTD denote the N-terminal and C-terminal domains, respectively. The arrowhead indicates the active-site cleft. Bound ligands are shown as stick models.

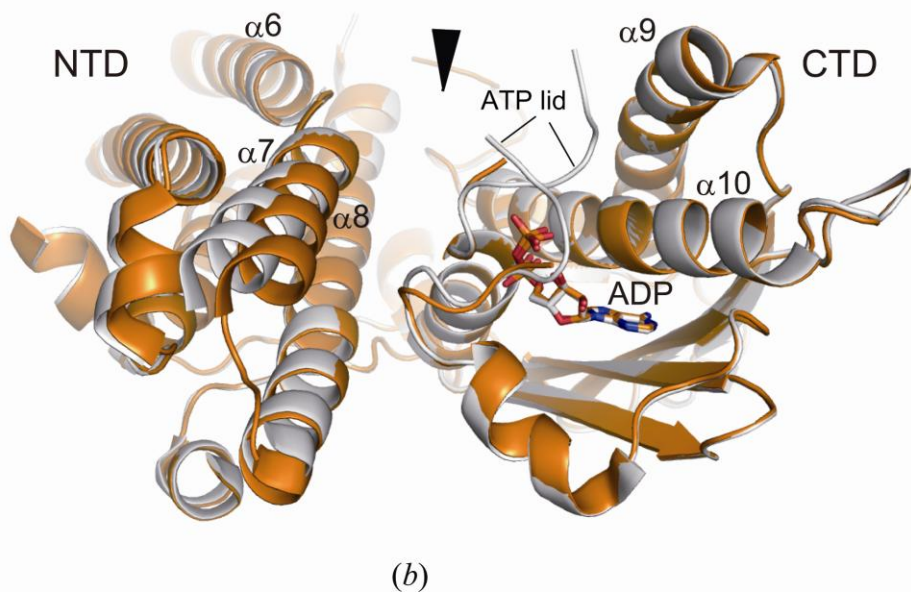
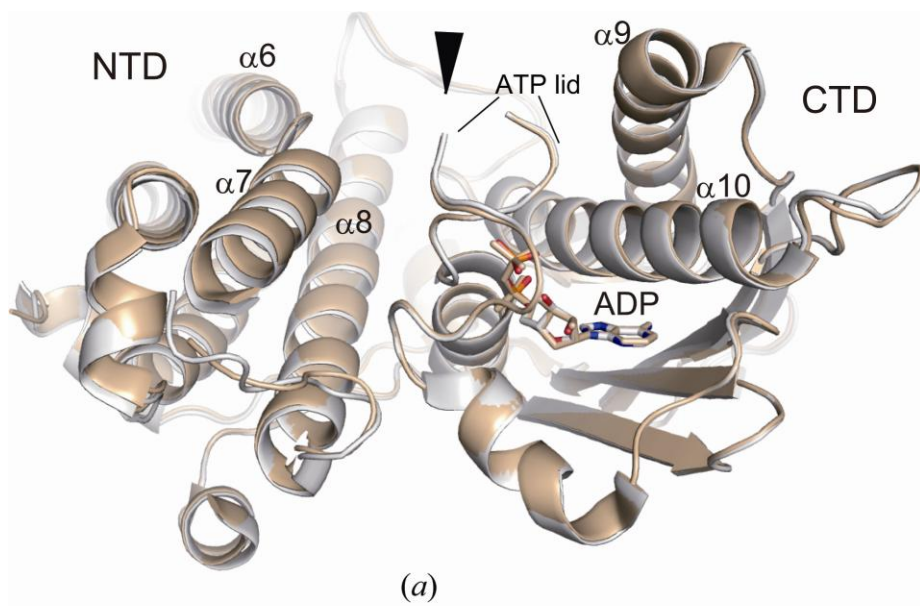


Figure S3 Superposition of the reported PDK4•ADP structure (white) (PDB ID: 3D2R) on our PDK4•ADP structure, in which (a) subunit A is colored wheat and (b) subunit B is colored orange.