



Fig. S2: Molecular surface representation with emphasis on the deep cleft within the catalytic domain. The substrate binding pocket is designed to perfectly position APS and PP_i in adequate proximity. The calculation of the electrostatic potential of the surface using the program APBS (Baker, N. A., Sept. D. et al. (2001). "Electrostatics of nanosystems: application to microtubules and the ribosome." Proc Natl Acad Sci USA 98: 10037-41.) revealed an overall negative potential on the surface (red) and around the substrate binding pocket a positive charge (blue).