Supplementary Fig.4 A structural illustration for K403, K171, and K386 within the G6PD protein

Cartoon representation of dimeric G6PD structure (PDB ID: 2BH9 and 2BHL) (Kotaka et al, 2005) made by using Pymol [www.pymol.org]. (A) An overview of K171, K386, or K403 position within the G6PD protein structure. Upper left, electrostatic (G6PD) and stick (G6P) representation of the crystal structure of G6P bound to G6PD; Lower left, K386 lies to the interface of G6PD dimer; Right panel, shown is a ribbon (G6PD) and stick (structural and catalytic NADP⁺) representation of G6PD bound to NADP⁺. The protein and NADP⁺ are colored in green and yellow, respectively. Red dotted circle indicates the 3D location of K171, K386, and K403.

(B-C) K171 interacts with both G6P and catalytic NADP⁺. The protein is colored in green, and G6P (B) and NADP⁺ (C) are marked in yellow, with the interacting residues in G6PD being highlighted in magenta.