

Figure S1: Potential energy of Productive and non productive confirmation of SmSirt2, -1.48293×10^{-6} KJ/mol and -1.2906×10^{-6} KJ/mol respectively.

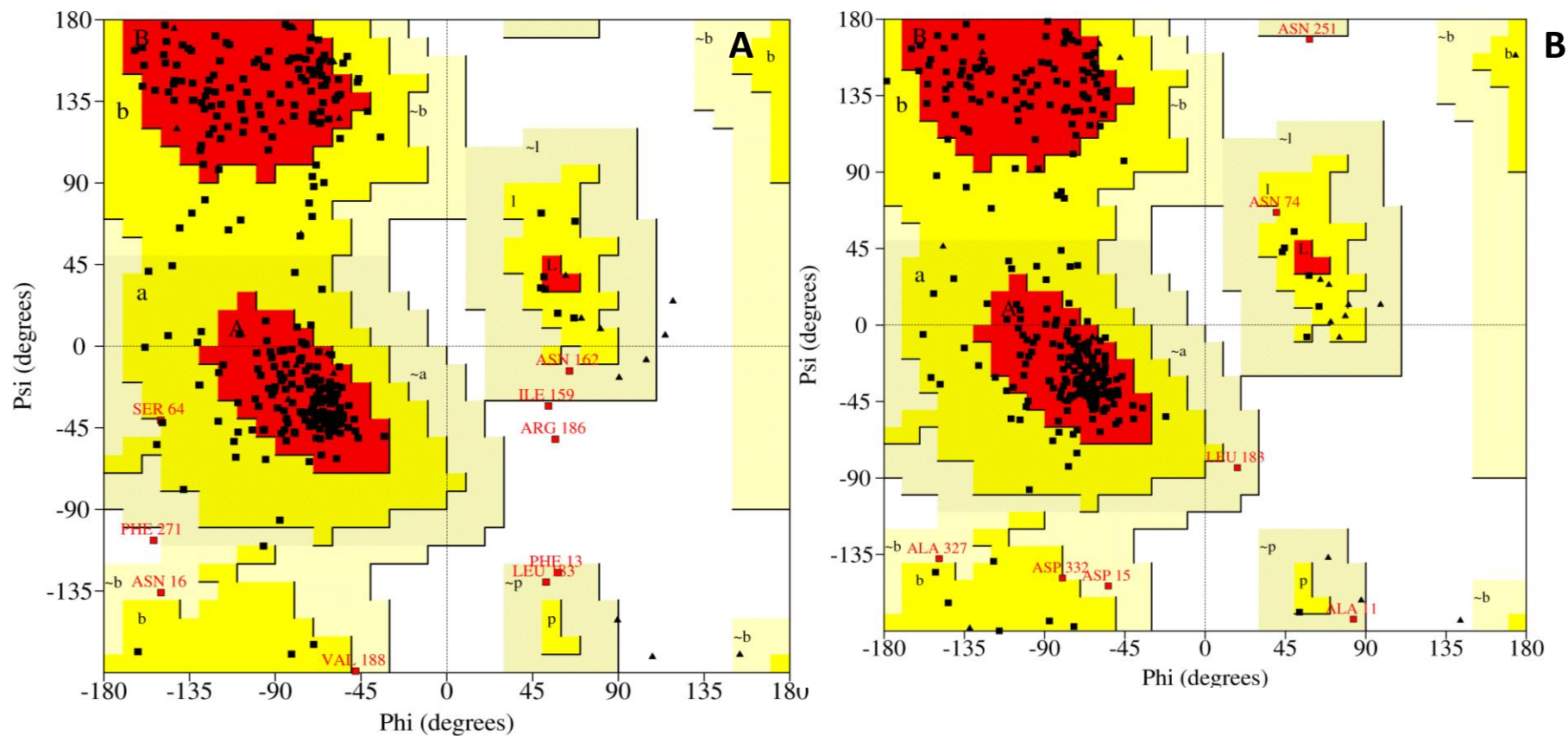


Figure S2: Quality assessment of the Ramachandran plot of productive conformation of SmSirt2 (A) and non-productive conformation of SmSirt2 (B).

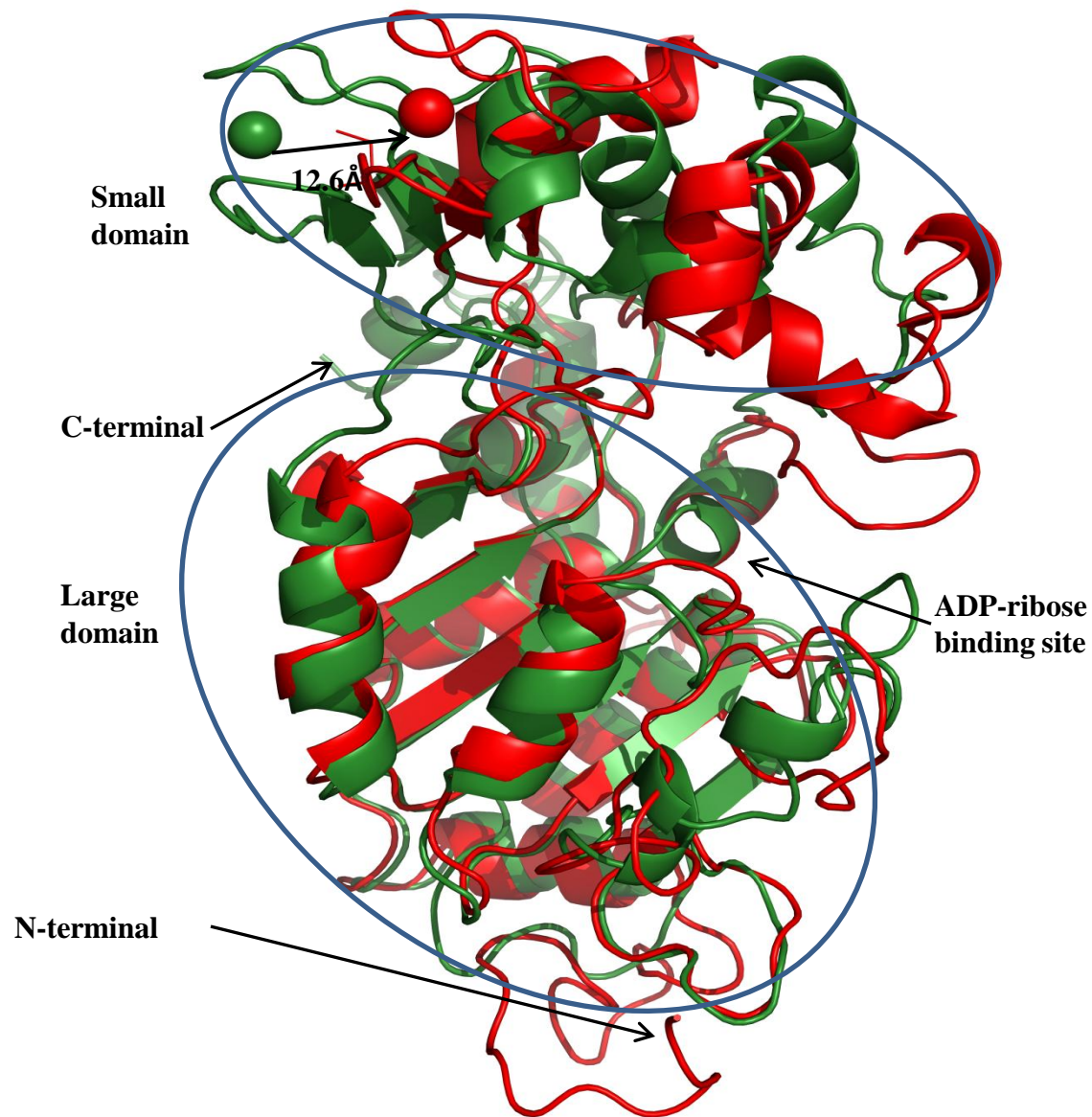


Figure S3:3D structure of SmSirt2 Non-productive (green) and a productive (red) conformation is superimposed. Lower large circle represents a large domain contain Rossmann fold of SmSirt2 proteins and the upper small circle represents small domain which is consist of the Zn ion binding site.

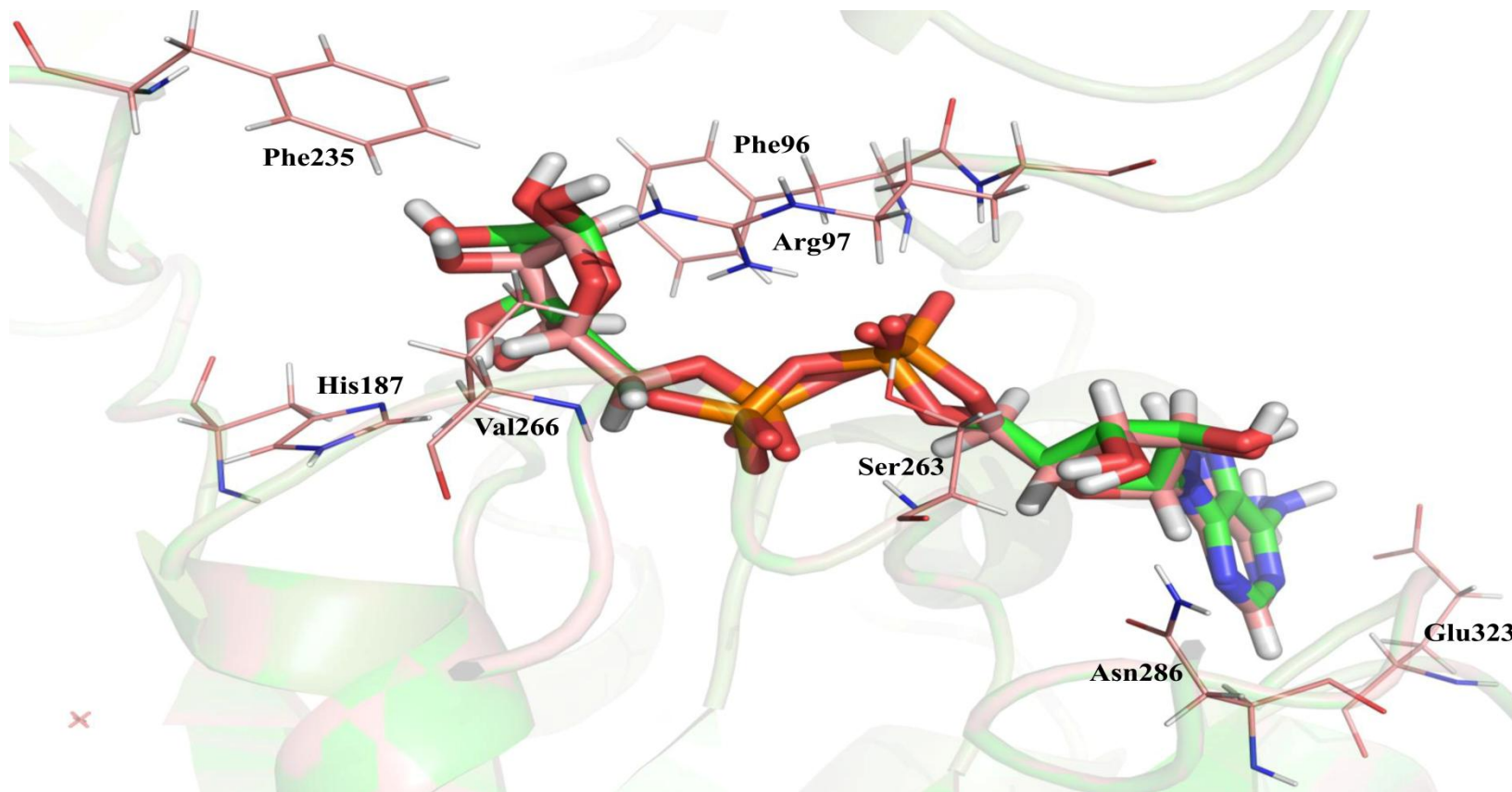


Figure S4: Crystallographic pose of ADP-ribose (in C=brown, N=blue and O=red with stick representation) and re-docked ADP-ribose (C=green, N=blue and O=red stick representation) with hSirt2 (PDB id: 3ZGV).