

Supporting Figures

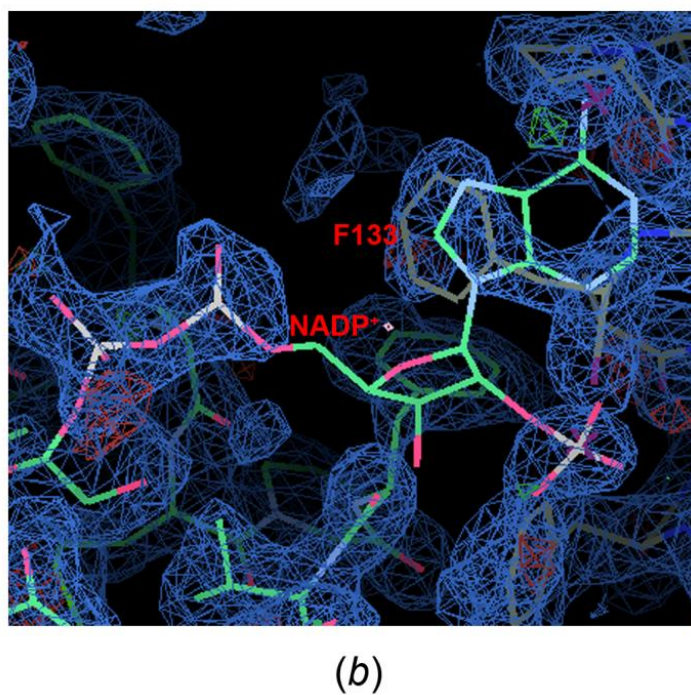
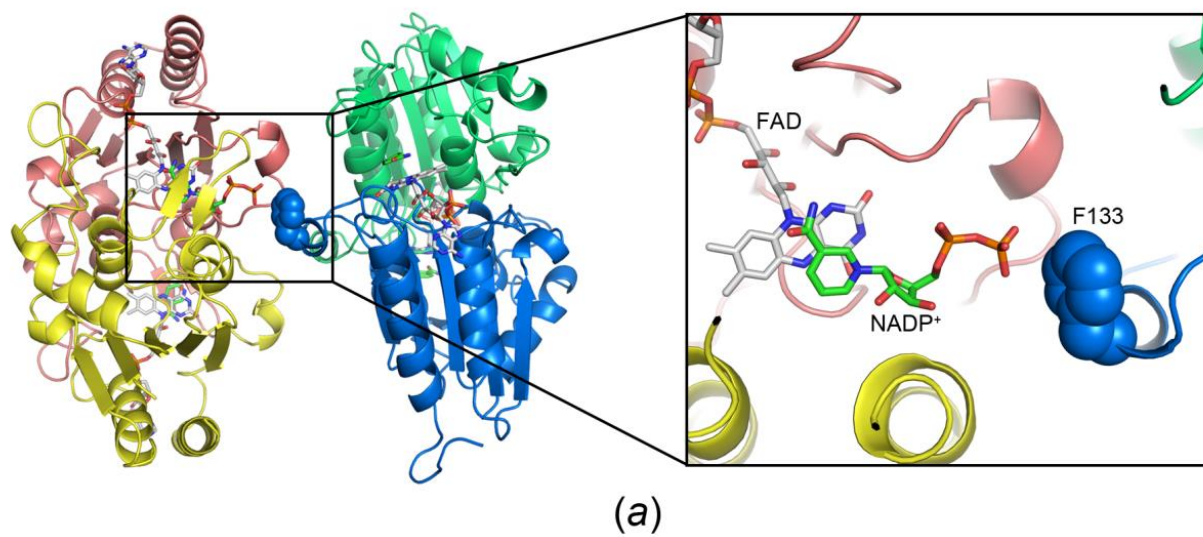


Figure S1. The environment of NADP⁺ binding pocket. **(a)** A phenylalanine residue from a neighboring molecule protrudes above the NADP⁺ binding pocket. **(b)** Fully-built NADP⁺ molecule has a steric clash with a phenylalanine residue from the adjacent protein chain.

■ *E. coli* MdaB

■ SmMdaB

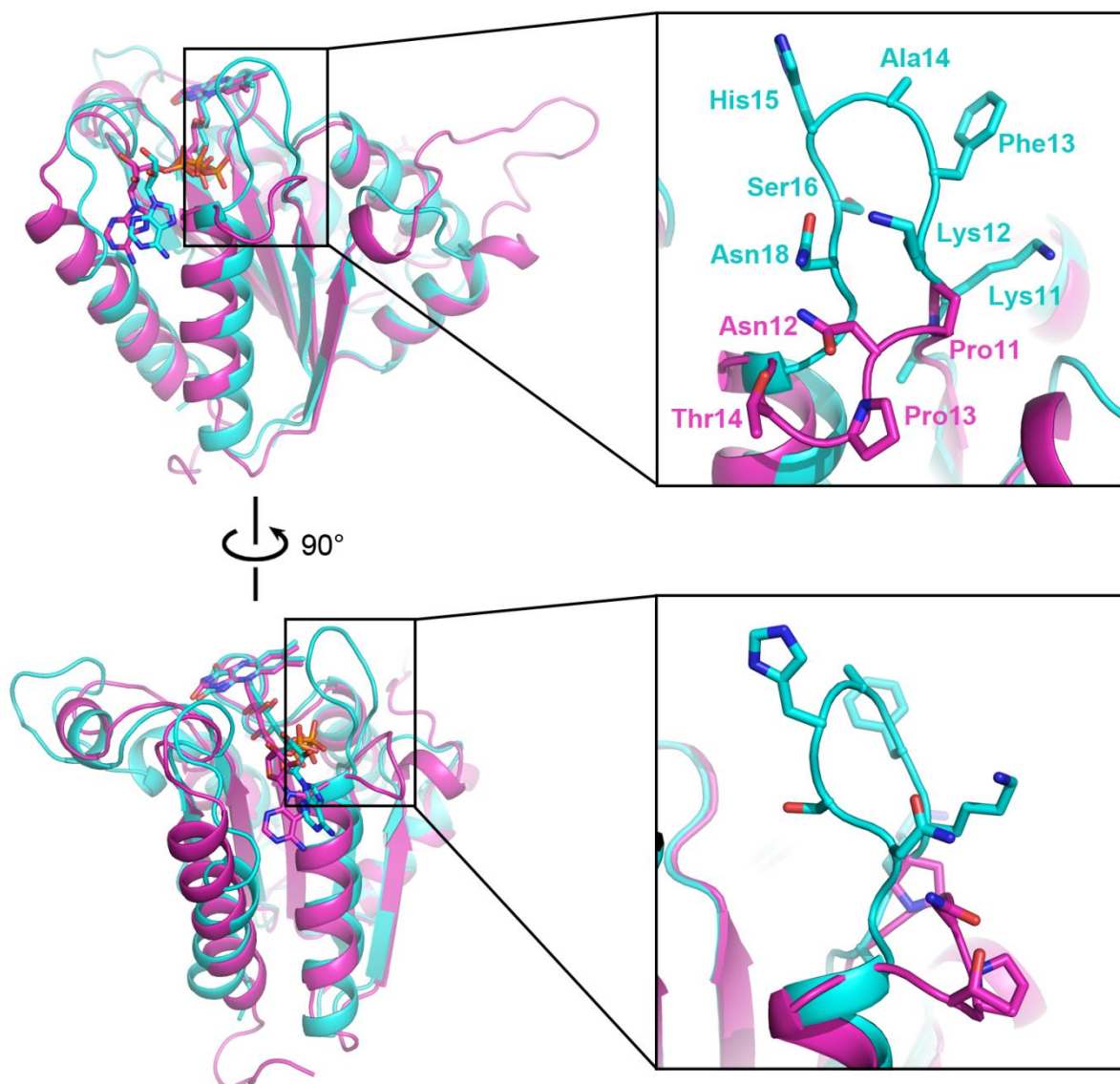


Figure S2. Structural comparison of the loop region connecting $\beta 1$ sheet and $\alpha 1$ helix. This loop in *E. coli* MdaB is relatively hydrophilic and probably covers the hydrophobic FAD binding site when FAD is absent, whereas that in SmMdaB is short and protrudes away from the FAD binding site, thus resulting in an exposure of a large hydrophobic area in the absence of FAD. *E. coli* MdaB (PDB: 2B3D) and SmMdaB (PDB: 3LCM) are colored cyan and magenta respectively.