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Supporting information for article:

***Bacillus licheniformis* trehalose-6-phosphate hydrolase
structures suggest keys to substrate specificity**

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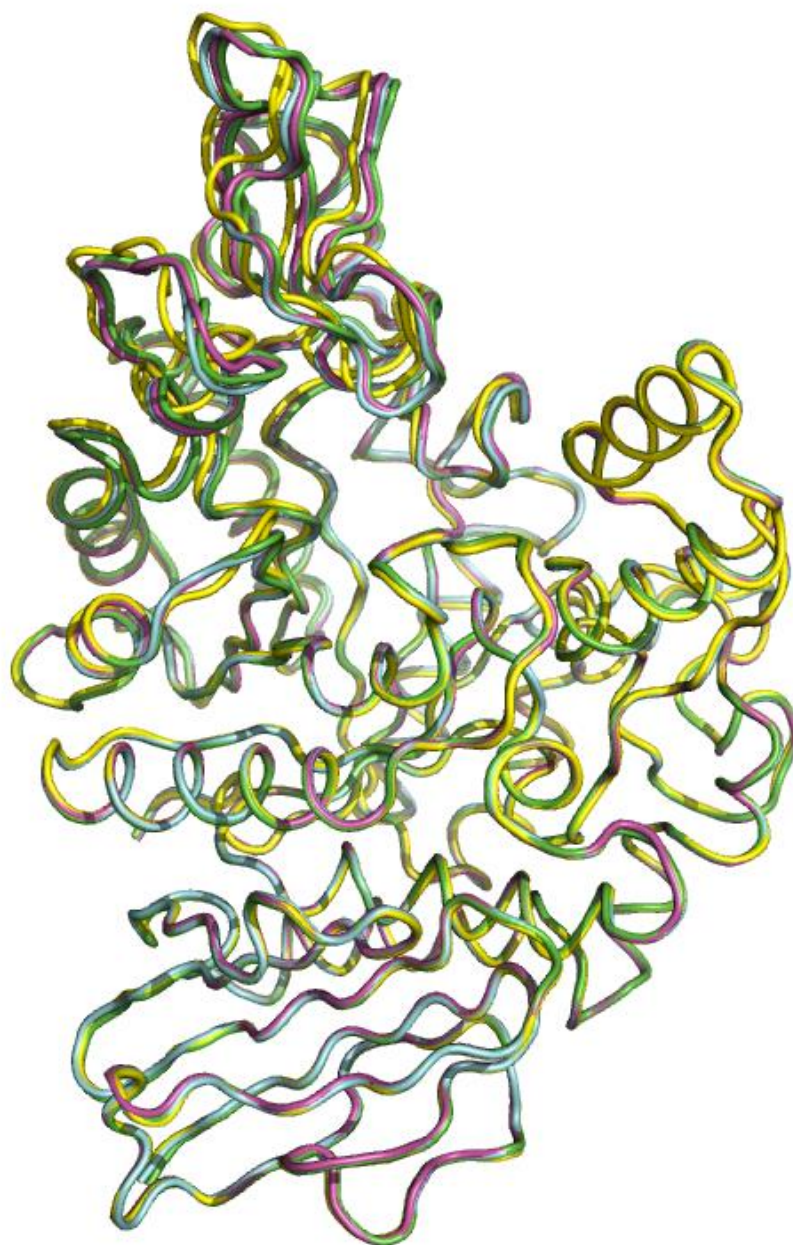


Figure S1 The alignment of four *B/TreAs* in the crystallographic asymmetric unit. Chains A, B, C, and D are colored in green, cyan, yellow, and magenta, respectively.

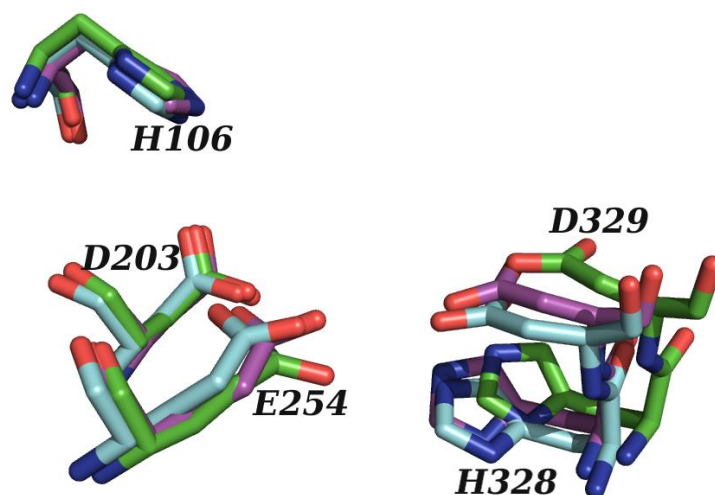


Figure S2 Structural comparison between *B/TreA* and its neighbor. Magnified view of the highly conserved catalytic residues in the active pocket of *B/TreA* (green), *BcOgl* (magenta) and NX-5 (cyan), Residues from *B/TreA* are labeled.

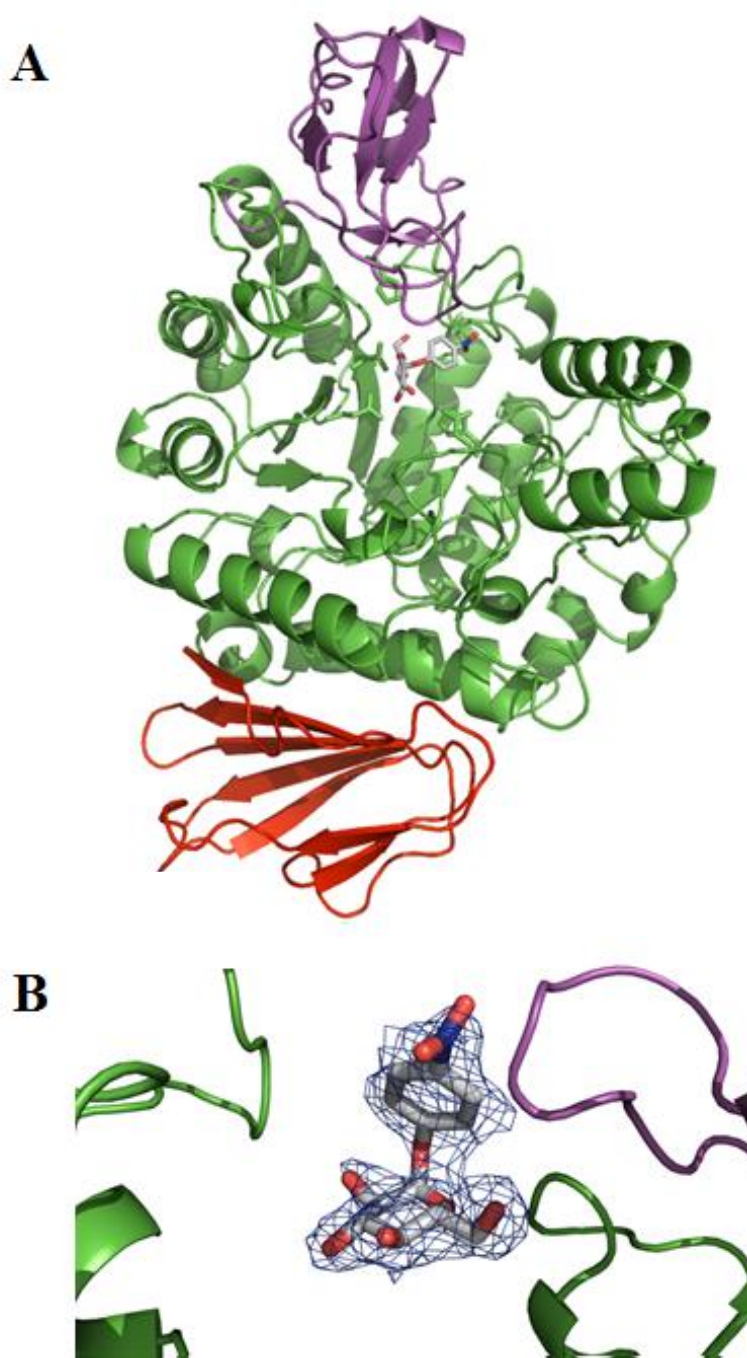


Figure S3 The overall structure of *B/TreA* in complex with *pPNG*. *A*, Schematic representation of the overall structure of *B/TreA*. The *B/TreA* subdomain is indicated in magenta, N-domain in green, and C-domain in red. *pPNG* (white) and the five conserved residues are shown as a stick model. *B*, The *pPNG* molecule in the active site. The $2F_o - F_c$ omit electron density maps are contoured at 1σ level and are shown in blue.

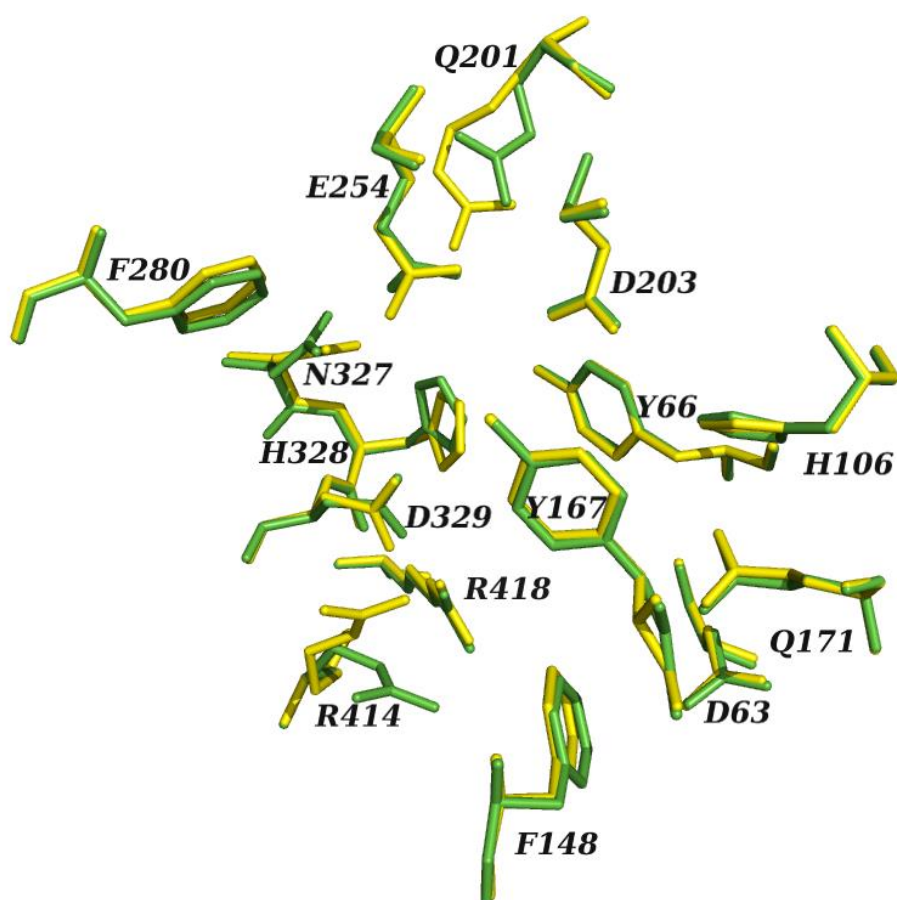


Figure S4 Structural comparison of the interacting residues between native *B/TreA* and R201Q/*pPNG*. The native *B/TreA* and R201Q/*pPNG* are colored in green and yellow, respectively. Residues from R201Q are labeled.

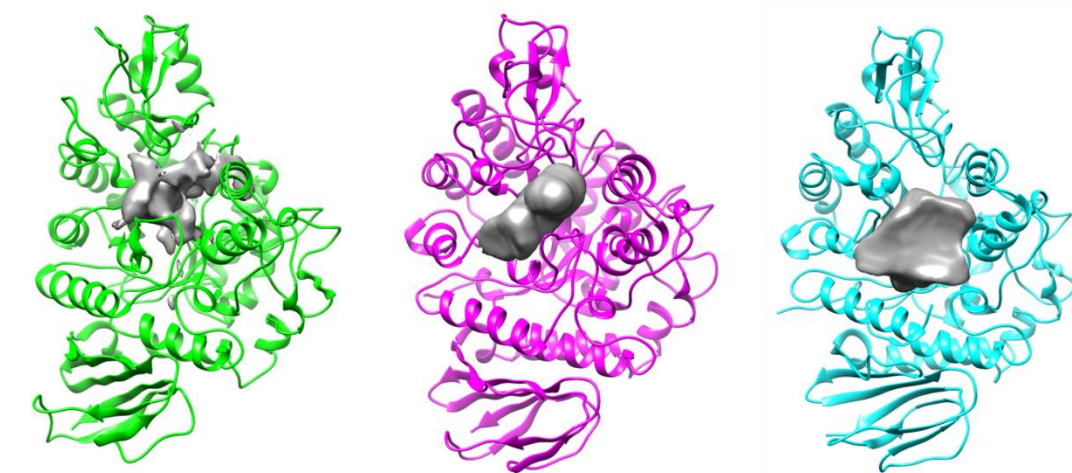


Figure S5 The models highlighting the binding cavity for *B/TreA*, *BcOgl* and *NX-5*. The enzymes are color coded with *B/TreA* in green, *BcOgl* in magenta, and *NX-5* in cyan. The visualization of active site pockets are colored in gray.

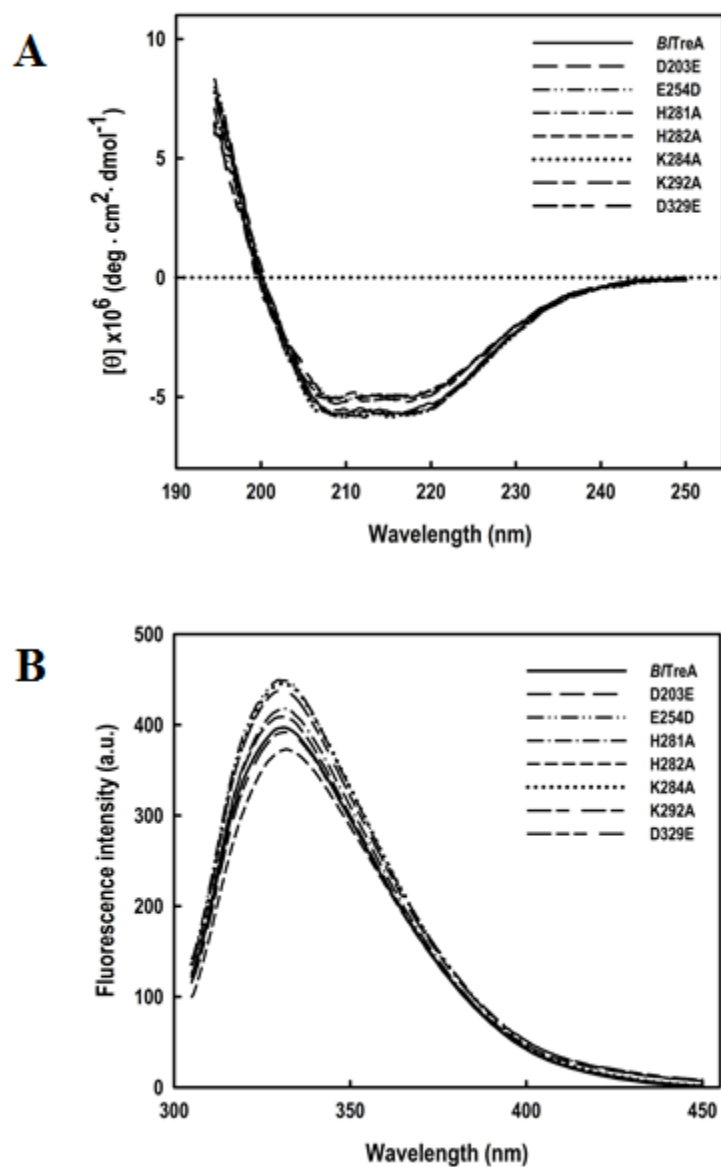


Figure S6 The far-UV CD and fluorescence spectra of *B/TreA* and several mutants. Far-UV CD (A) and fluorescence (B) spectra were obtained with a protein concentration of approximately 0.2 mg/ml at 25°C.