



**Fig. S7. Topology diagram of SaM1PDH, its structural comparison with *Shigella flexneri* (SfM1PDH); and multiple sequence alignment of SaM1PDH with its homologs in other bacterial species.** (A) Topology diagram showing the overall fold of SaM1PDH wherein cylinders (blue) and arrows (gray) represent  $\alpha$ -helices and  $\beta$ -strands, respectively; whereas solid lines (black) represents loops and turns. Figure was adapted from that generated by PDBsum (<http://www.ebi.ac.uk/pdbsum>). The  $\alpha$ -helices and  $\beta$ -strands are numbered in accordance with their orders found in SaM1PDH crystal structure. The N- and C-termini of SaM1PDH are annotated by N and C, respectively. (B) Structural superimposition of SaM1PDH (blue) and SfM1PDH (orange; PDB: 3H2Z) in (left) front view and (right) side view. Protein structures are displayed as ribbon diagrams. The N- and C-terminal domains are indicated. (C) Structural superimposition of the active sites of SaM1PDH (blue) and SfM1PDH (orange). (D) Electrostatic potential surfaces (contouring level of  $\pm 8 \text{ kTe}^{-1}$ ) of substrate-binding sites of (left) SaM1PDH and (right) SfM1PDH. Structures of SaM1PDH and SfM2DH are superimposed as shown in (B). Electrostatic properties (positive charge, blue; neutral, white; negative, red) were calculated using APBS and PDB2PQR Server ([http://nbc-222.ucsd.edu/pdb2pqr\\_2.0.0/](http://nbc-222.ucsd.edu/pdb2pqr_2.0.0/)). In (C) and (D), sulfate, phosphate, and key residues in substrate-binding sites are drawn in ball-and-stick models. Dashed lines represent bonds between interacting atoms. Figures were prepared using PyMOL (<http://www.pymol.org>). (E) Multiple sequence alignment of SaM1PDH with its homologs in other bacterial species showing amino acid sequences of M1PDHs collected from four Gram-positive bacteria (*S. aureus*, GenBank: ABD20823.1; *Bacillus subtilis*, GenBank: AQR80339.1; *Clostridium acetobutylicum*, GenBank: AAC12851.1; *Streptococcus pneumoniae*, GenBank: AAK99163.1) and four Gram-negative bacteria (*Vibrio cholerae*, GenBank: AAF96940.1; *Escherichia coli*, GenBank: AAG58744.1; *Klebsiella pneumoniae*, GenBank: AIE00851.1; *Shigella flexneri*, GenBank: AAP19108.1). Strictly conserved residues are colored yellow and boxed in black, whereas highly similar residues are colored white and boxed in blue. Secondary structures of *S. aureus* M1PDH (blue; PDB: 5JNM) and *S. flexneri* M1PDH (black; PDB: 3H2Z) are shown above and below the alignment, respectively. Residues involved in binding to cofactors (NAD<sup>+</sup>/NADH), substrate (mannitol), and phosphate moieties of substrates are denoted by black, blue, and orange arrows, respectively. Amino acid sequences of M1PDHs were aligned using T-Coffee Multiple Sequence Alignment Server (<http://tcoffee.org.cat>). Alignment figure was adapted from that generated by ESPript 3 (<http://esprpt.ibcp.fr>).