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Supporting information for article:

Structures of substrate- and nucleotide-bound propionate kinase from *Salmonella typhimurium*: substrate specificity and phosphate-transfer mechanism

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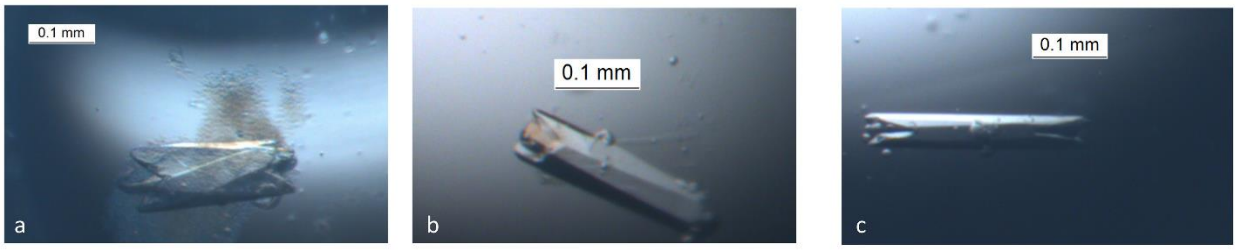

Figure S1 Crystal of *Salmonella typhimurium* (a) wild type StTdcD and mutants (b) A88G and (c) A88V in complex with AMPPNP and propionate.

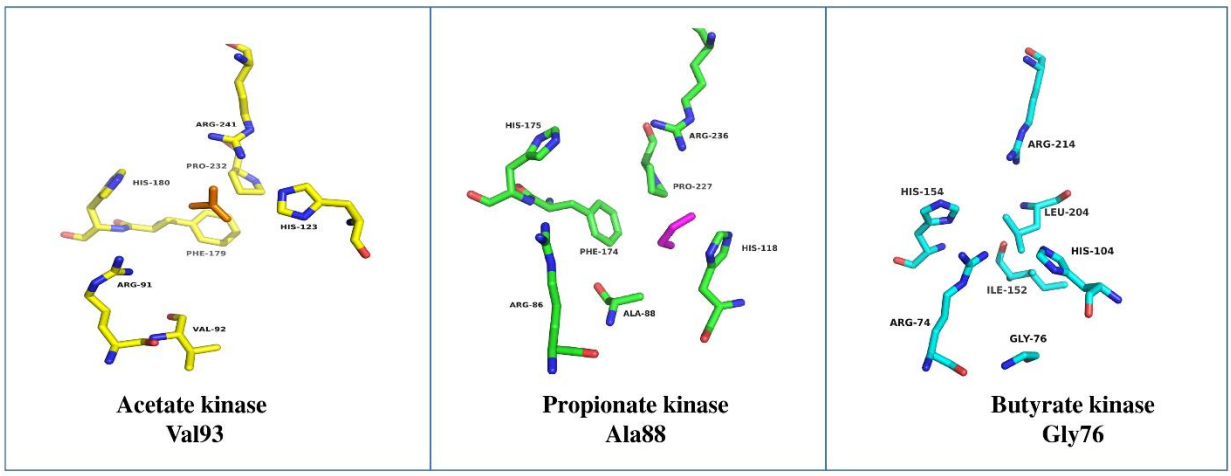

Figure S2 Representation of substrate binding pocket in acetate, propionate and butyrate kinases.(a) Acetate (orange) bound in *Methanosarcina thermophila* acetate kinase (MtAckA) (PDB code: 1TUY) (b) EDO (magenta) bound in the proposed site of propionate binding in *St*TdcD (PDB code:1X3N) (c) Proposed butyrate binding pocket from *Thermotoga maritima* butyrate kinase 2 (TmBuk2) (PDB code: 1SAZ)

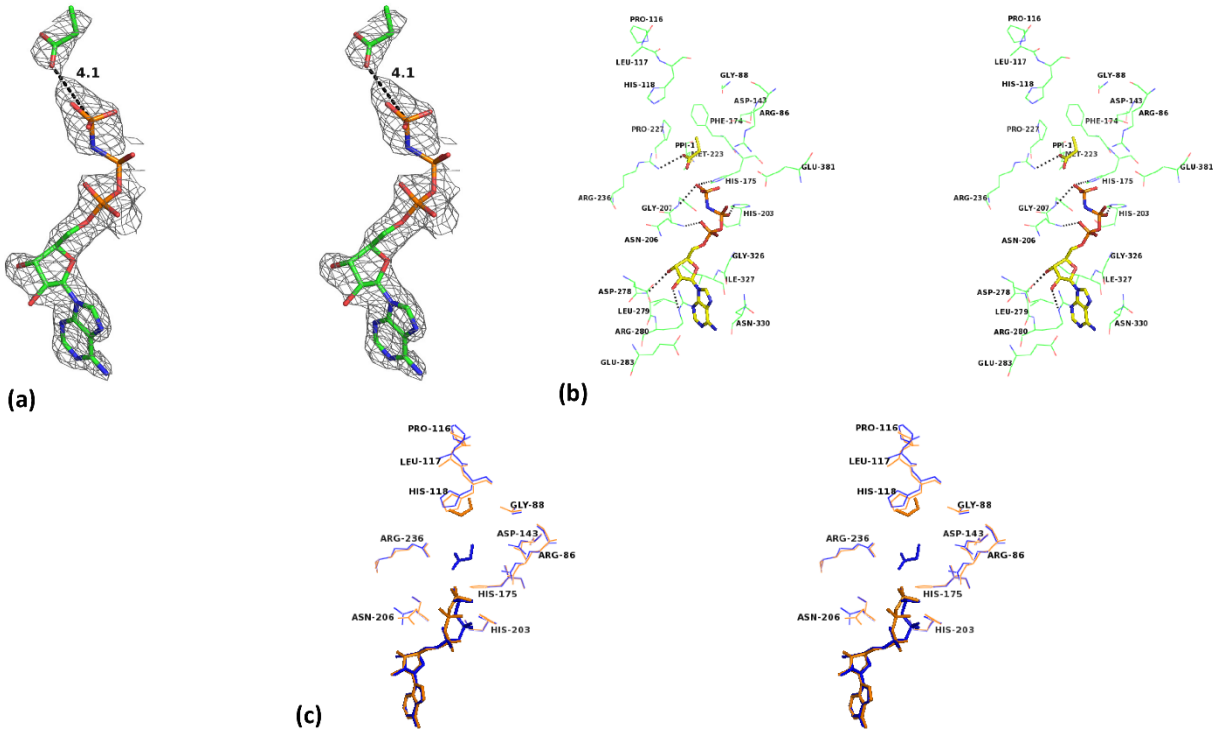

Figure S3 Ligand binding in A88G TdcD in complex with AMPPNP. (a) Stereo view of electron density corresponding to AMPPNP and propionate from a $2F_o$-F_c map countered at 1.0 σ. (b) Stereo representation of the A88G TdcD active site cavity highlighting interactions with bound SCFA and nucleotide. Grey broken lines indicate hydrogen bonds. Ligands are represented in ball and stick. (c) Stereo image of structural superposition of active site pocket and the surrounding interacting residues of propionate bound A88G-AMPPNP complex (blue) upon *St*TdcD-AMPPNP (orange).

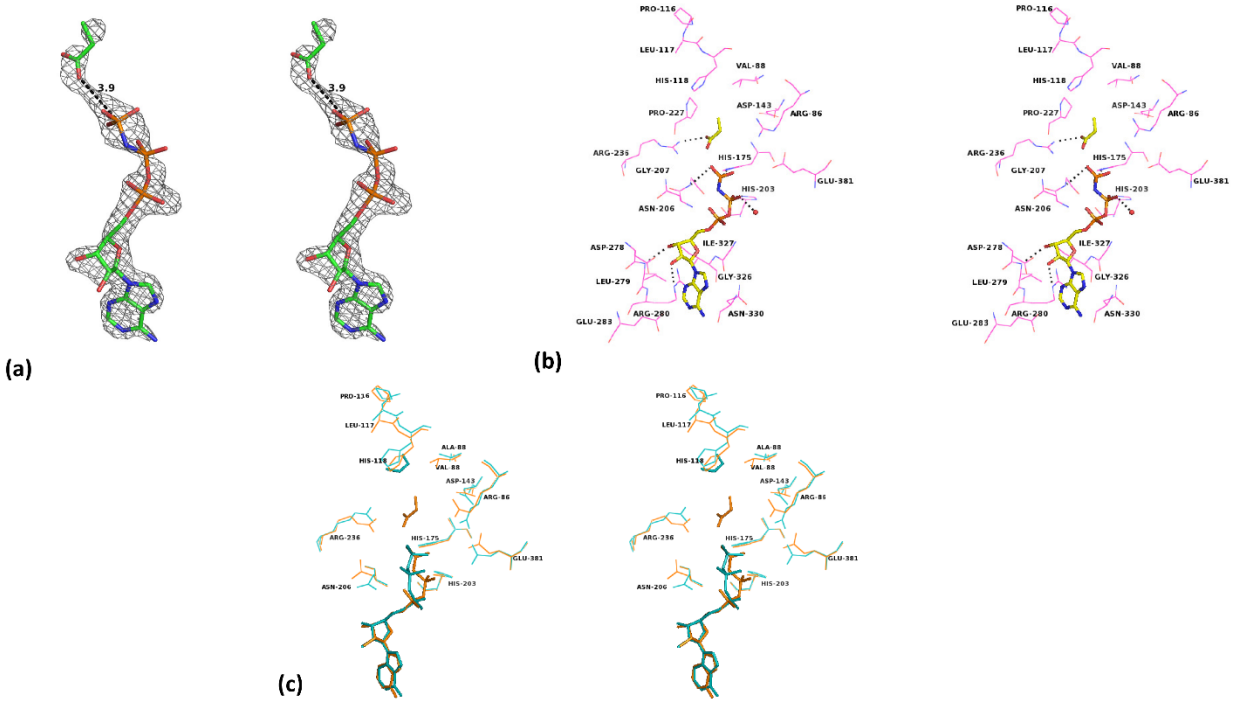

Figure S4 Propionate binding in A88V-AMPPNP complex. (a) Stereo diagram of electron density corresponding to AMPPNP and propionate from a $2F_o$-F_c map countered at 1.0 σ. (b) Stereo diagram of ligand bound A88V-TdcD-AMPPNP complex active site featuring interactions with propionate and nucleotide. AMPPNP and propionate are represented in ball and stick whereas hydrogen bonds are represented by broken grey lines. (c) Stereo view of structural superposition of active site pocket of ligand bound A88V propionate AMPPNP (cyan) complex upon *St*TdcD-AMPPNP (orange). Propionate is depicted in cyan and EDO in orange.