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Supporting information for article:

Crystal structure and kinetic analysis of *N*-acetylmannosamine-6-phosphate 2-epimerase from *Fusobacterium nucleatum* and *Vibrio cholerae*

Lavanyaa Manjunath, Sai Rohit Guntupalli, Michael J. Currie, Rachel A. North, Renwick C. J. Dobson, Vinod Nayak and Ramaswamy Subramanian

Supplementary information

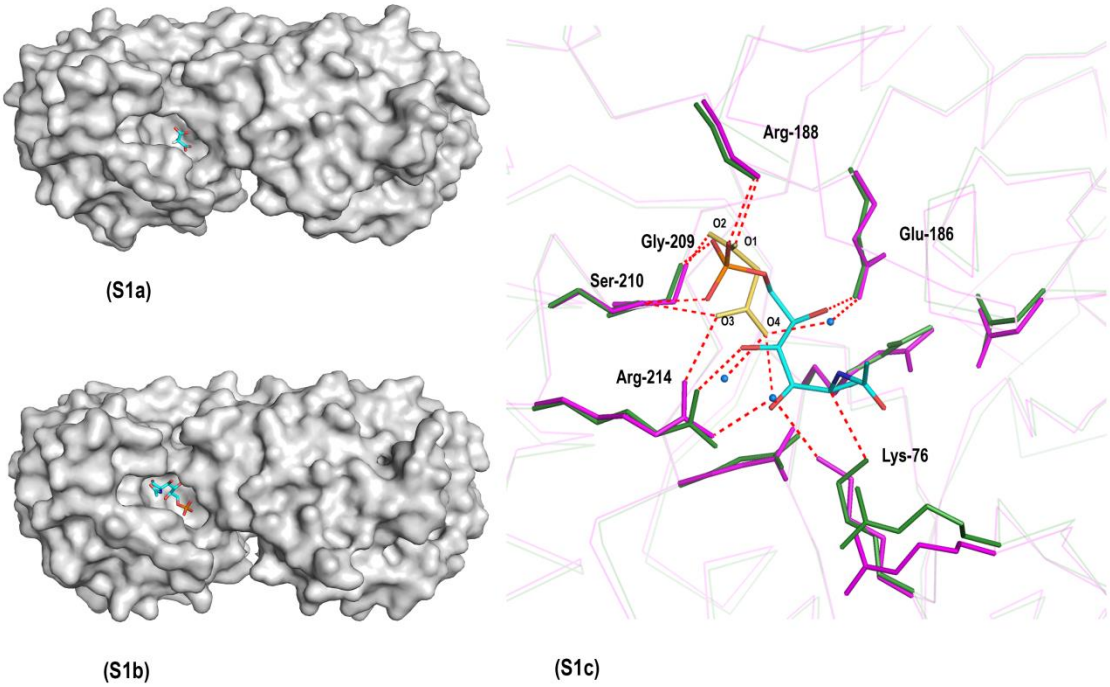

Figure S1 (S1a) Malonate (a component of the crystallization buffer condition) in the binding pocket of VcNanE **(S1b)** ManNAc-6-P in the binding site of VcNanE **(S1c)** Comparison of active site interactions with malonate and ManNAc-6-P. The O1 and O2 of malonate hydrogen bond with amide backbones of R188 and G209, O3 can hydrogen bond with guanidinium group of R214. The O4 can hydrogen bond with ε-amine K76 via a water molecule (depicted as a blue spheres) and can also hydrogen bond with carboxyl group of E186 via a water molecule. Amino acids of apo- VcNanE and VcNanE/ManNAc-6-P are depicted in green and magenta respectively. Hydrogen bonds are represented as dashed red lines. Figures were made using Pymol.

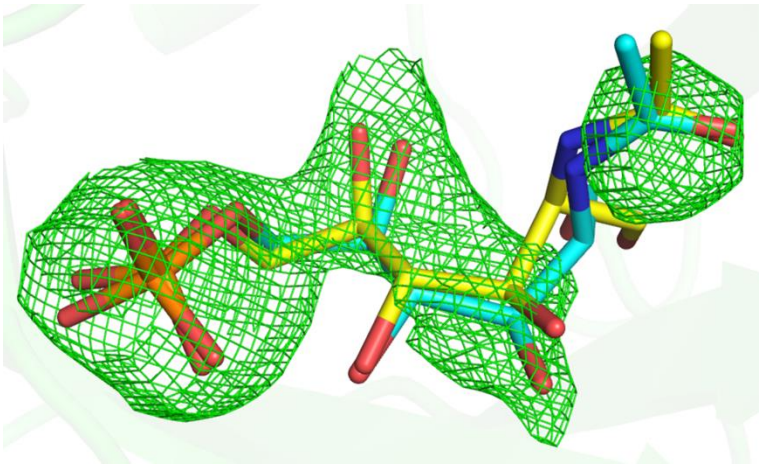

Figure S2 Electron density for open chain sugar phosphate in VcNanE co crystallized with GlcNAc-6-P. The Fo-Fc electron density modeled with both ManNAc-6-P and GlcNAc-6-P (depicted in cyan and yellow respectively). The density is contoured at 2σ. Figure was made using Pymol.

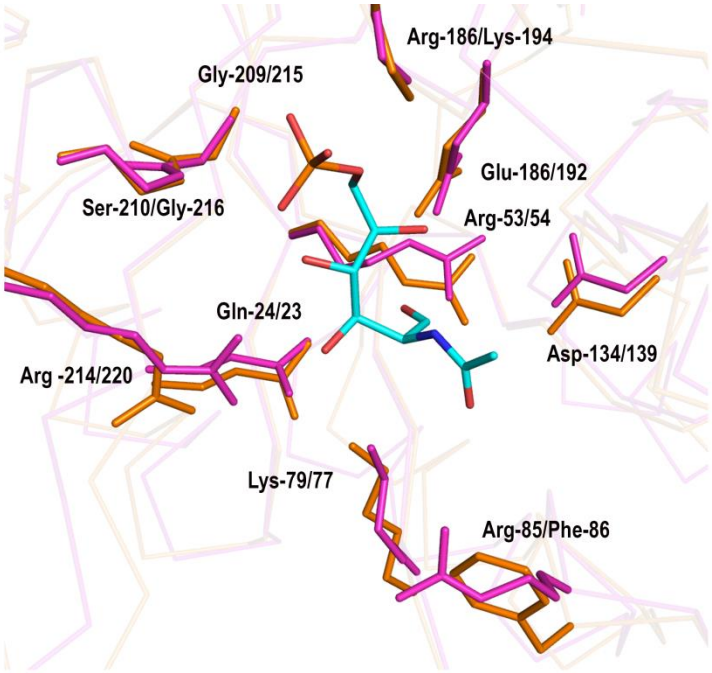

Figure S3 Active site is rigid. Superposition of apo SpNanE (1YXY) with VcNanE-ManNAc-6-P shows the spatial orientations of the active site amino acids. Arg-220 of SpNanE has moved away from the ligand binding site as there is no ligand for it to anchor. Amino acids of VcNanE-ManNAc-6-P and SpNanE are represented in magenta and orange respectively. ManNAc-6-P is depicted in cyan. Figures were made using Pymol.