

Volume 71 (2015)

Supporting information for article:

Ligand-bound structures of 3-deoxy-d-manno-octulosonate 8-phosphate phosphatase from *Moraxella catarrhalis* reveal a water channel connecting to the active site for the second step of catalysis

Sonali Dhindwal, Priyanka Priyadarshini, Dipak N. Patil, Satya Tapas, Pramod Kumar, Shailly Tomar and Pravindra Kumar

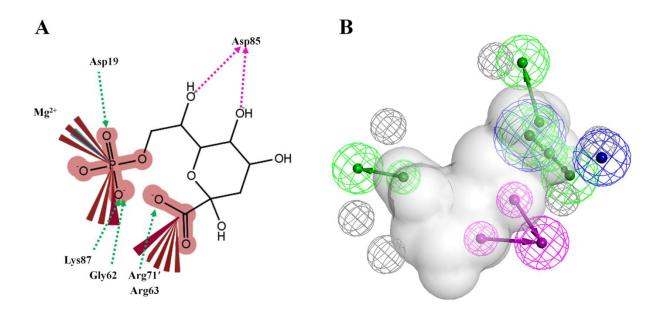


Figure S1 (A) The pharmacophore model generated by LigandScout. All the chemical features are shown along with the interacting residues. (B) The combined pharmacophore generated on the basis of chemical features and shape of the substrate, KDO8P. The hydrogen bond donors are indicated in magenta and hydrogen-bond acceptors are indicated in green dotted lines and spheres in (A) and (B), respectively. Negatively ionizable atoms are indicated by blue spheres and exclusion volumes are indicated as grey spheres in (B).