Use of polysterism analysis to probe the conformational landscape and residue networks within an α-D-phosphohexomutase

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The transmission of information across a protein structure is of fundamental importance to biology. Here we use analyses of polysterism (pre-existing conformational diversity) to identify functionally important residue networks within a protein from the α-D-phosphohexomutase superfamily. These enzymes play key roles in carbohydrate biosynthesis in organisms from archaea to humans. In the present study, crystals of phosphoglucomutase from *Xanthomonas citrii* were employed due to their high-resolution diffraction, a pre-requisite for identification of minor conformers in electron density maps. Both cryogenic (1.5 Å or better resolution) and room temperature (2.1 Å or better resolution) data sets were obtained for a variety of enzyme states, including apo-enzyme, enzyme-ligand complexes, and the phospho- and dephospho-states of its catalytic serine. Computational analyses of low population side chain conformers in the electron density maps were used to identify networks of residues associated with different enzyme states. Relationships between these coupled networks and enzyme function will be discussed.