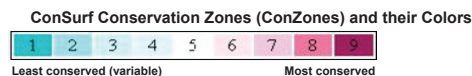


ConSurf Phylogenetic Models on “Scaffold” PDB-Sequences of Three Enzymes: Phosphoglucose Isomerase (PGI), Triose Isomerase (TPI) and Glyceraldehyde-3-phosphate Dehydrogenase (GAPDH)



*RAA = “recovered amino acid(s)” represent data “points” with four-components: 1) an amino acid ID of an MSA modal-consensus site using a taxonomically varied homologous enzymatic unique protein sequence set (Edgar, 2004), 2) the amino acid's chain position (MSA site number), 3) the MSA site's conservation value (determined by ConSurf analyses using the MSA and a PDB-structural model (“Scaffold”) sequence included in the MSA as the programmatically required query) and 4) the Euclidean distance from each of the MSA chain's amino acids Cαs to our choice of a PDB identified atom (“anchor-atom” = AA) found in an amino acid of the chain and reported as a catalytic residue (see, Methods). The three enzyme sets each of four figures show the respective RAAs superimposed on a protein structure (“Scaffold”) at their corresponding chain sites colored according to their conservation zone (ConZone) by the ConSurf program (Landau et al., 2005; Ashkenazy et al., 2010). The average distances of the RAAs to their respective C/CAC were calculated by the Yasara program (Krieger et al., 2002). (see, original article for further details)

**The PDB sequences and their localized anchor-amino acids (AAA) and their specific anchor-atom's (AA) are: (PDB-) 1b0z-R202NH1, 1btm-G172N, 1gd1-H176ND1. The three conservation models in this figure are each built upon the single designated PDB structure (“PDB-scaffold”), according to the ConSurf program. Their site-associated CZ1 and CZ9 RAA distance measures are averages of data calculated in separate analyses using RAAs and different homologous enzyme Scaffolds for each enzyme. The distances for the PDB PGI-1b0z set, for example, are the average of six distance analyses with six different PGI Scaffold sequences, 1b0z, 1z3g, 2q8n, 2wu8, 2f1 and 3hjb. For the PDB TPI-1btm set, the average was of four analyses using as Scaffolds: 1btm, 1aw1, 1lmh and 1yya, and for the PDB GAPDH-1gd1 figures, the average was of seven analyses using as Scaffolds: 1gd1, 1cer, 1dc3, 1obf, 2ep7, 3hja and 3l0d (see, Methods and references in original article).