Crystal Structures of DAH7PS Synthase from *Pyrococcus Furiosus*

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The enzyme 3 deoxy-D-arabino-heptulosate 7-phosphate synthase (DAH7PS) catalyses the condensation reaction between phosphoenol pyruvate (PEP) and the 4 carbon saccharide D-erythrose-4-phosphate (E4P). This reaction is the first step in the shikimate pathway used in plants and microorganisms to synthesize aromatic amino acids and many secondary aromatic metabolites.

DAH7PS from *P furiosus* requires a metal ion for activity and, unlike DAH7PS from other species, is not subject to regulation by aromatic amino acids, It is also able to utilize both 4-carbon and 5-carbon phosphorylated monosaccharides with similar K_{cat} but increased K_m values. This broad substrate specificity and lack of regulation indicates it may be the closest protein to the ancestral enzyme of the type 1 DAH7PS enzymes.

Two crystal structures will be presented. The first – the apo form of the molecule, crystallizes in space group I222 with *a*=87.23Å, *b*=110.02Å, *c*=144.35Å. There are two molecules in the asymmetric unit (the biological unit) which associate with a 2-fold related pair to form distinct tetramers. The structure was solved by molecular replacement using a hybrid model formed from elements of two related structures with low sequence identity (26% and 30%). Maps show the presence of PEP at low occupancy.

The second form, the Cd loaded derivative crystallizes in space group $P2_1$, *a*=48.94Å, *b*=84.33Å, *c*=139.16Å, β=92.60° with two intact tetramers in the unit cell. Current maps show a greatly expanded metal binding site, the presence of PEP at low occupancy, and the presence of some ribose 5-phosphate.

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