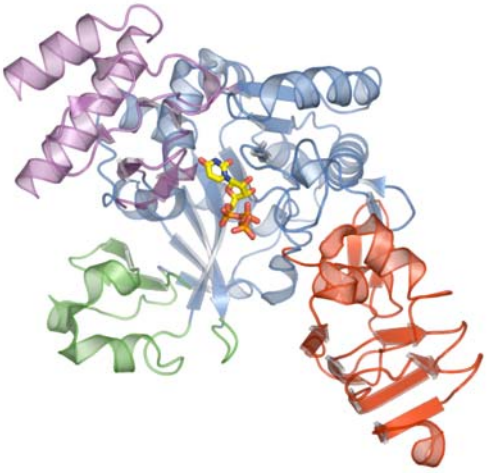
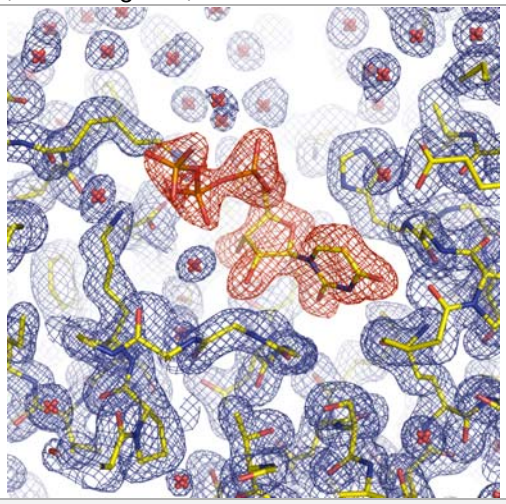
Center for Eukaryotic Structural Genomics

Protein Structure Initiative

Target ID	GO.14914	
Source Organism	*Arabidopsis thaliana*	
Target Name	At3g03250.1	
PDB Entry	1Z90	Deposition: 31-Mar-2005
Function	UDP-glucose pyrophosphorylase-like protein (FF/Refine: 2ICX, 2ICY, 2Q4J)	
Produced From	*E. coli* B834 p(RARE2) pVP-16	
Structure by X-ray	Resolution: 1.86 Å	R-value (R-free): 20.3% (24.9%)
	No. of Residues/ASU: 915	Monomers/ASU: 2
Data Collected At	Advanced Photon Source 22-BM 13-Mar-2005, 22-ID 13-Mar-2005	
Authors	G.E. Wesenberg, G.N. Phillips, Jr ., E. Bitto, C.A. Bingman, S.T.M. Allard	





Structural Features

The structure of the UDP–glucose pyrophosphorylase encoded by *Arabidopsis thaliana* gene At3g03250.1 has been solved to a nominal resolution of 1.86 Å. In addition, the structure has been solved in the presence of the substrates/products UTP and UDP–glucose to nominal resolutions of 1.64 Å and 1.85 Å (1). The three structures revealed a catalytic domain similar to that of other nucleotidyl-glucose pyrophosphorylases with a carboxy-terminal β-helix domain in a unique orientation. Conformational changes are observed between the native and substrate-bound complexes. The nucleotide-binding loop and the carboxy-terminal domain, including the suspected catalytically important Lys360, move in and out of the active site in a concerted fashion. TLS refinement was employed initially to model conformational heterogeneity in the UDP–glucose complex followed by the use of multiconformer refinement for the entire molecule. Normal mode analysis generated atomic displacement predictions in good agreement in magnitude and direction with the observed conformational changes and anisotropic displacement parameters generated by TLS refinement. The structures and the observed dynamic changes provide insight into the ordered mechanism of this enzyme and previously described oligomerization effects on catalytic activity.

References: (1) McCoy, J.G., Bitto, E., Bingman, C.A., Wesenberg, G.E., Bannen, R.M., Kondrashov, D.A., Phillips, G.N., Jr. (2007) Structure and dynamics of UDP-glucose pyrophosphorylase from *Arabidopsis thaliana* with bound UDP-glucose and UTP. *J Mol Biol* 366(3):830-41.

Percent Identity with Nearest PDB Structure at Time Solved	38% (1EEP)
Pfam Cluster	UDPGP
Sequence Cluster Size	250

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