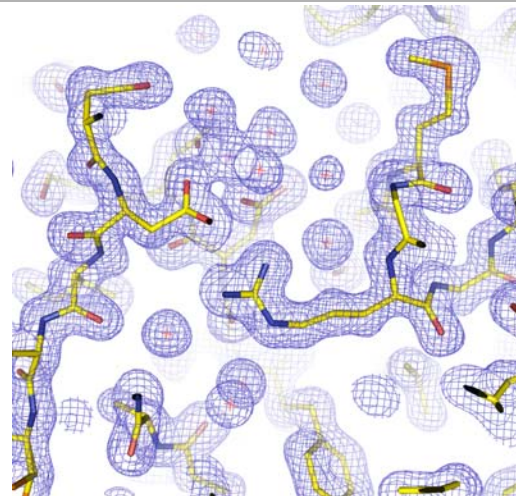
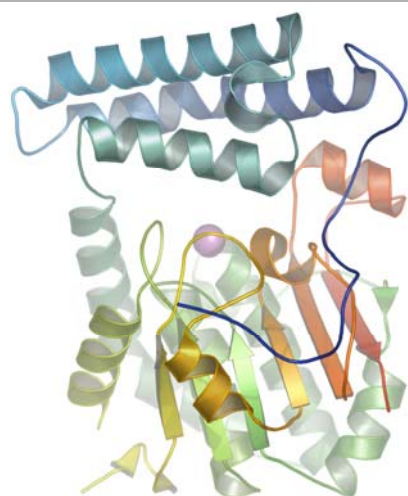


Center for Eukaryotic Structural Genomics

Protein Structure Data Summary

Target ID	GO.8195	
Source Organism	<i>Arabidopsis thaliana</i>	
Target Name	At2g17340.1	
PDB Entry	1XFI	Deposition: 14-Sep-2004
Function	pantothenate kinase-like (FF/Refine: 2Q40)	
Produced From	<i>E. coli</i> B834(DE3) p(LacI+RARE)	
Structure by X-ray	Resolution: 1.7 Å	R-value (R-free): 17.2% (22.1%)
	No. of Residues: 357 (40,813)	Subunits/Molecule: 1
Data Collected At	Advanced Photon Source SBC 19-BM, BioCARS 14-ID-B	
Authors	E. Bitto, C.A. Bingman, S.T.M. Allard, D.W. Smith, G.E. Wesenberg, G.N. Phillips, Jr.	



Structural Features

Sequence alignments strongly suggest that At2g17340.1 is the first structure of a pantothenate kinase (-like) protein (EC 2.7.1.33), with high identity (33-77%) to PK enzymes of eukaryotes including human, mouse, and rice. Pantothenate kinase is involved in coenzyme A biosynthesis, and defects are associated with a neurodegeneration syndrome (Hallervorden-Spatz syndrome). At2g17340.1 protein consists of two distinct domains. The larger C-terminal domain (green through red residues 113-343) shows 3-D similarity to a NADH+-dependent aldehyde dehydrogenase from *Vibrio Harveyi* (1EZO, RMSD 3.9). However, the aligned sequences for these regions show only 6 percent identity. The C-terminal domain shows further fold similarity over ~100 residues with several methyltransferase enzymes (1RJG, 1VID, 1P91, 1QYR). The magnesium site found within this domain is depicted in the electron density figure above, coordinating D220, N221, and D256. At2g17340.1 matches PFAM DUF89 ("unknown function" residues 47-362, COG1578), B_28918 (7-36) and B_81173 (243-266). DUF89 is represented all three kingdoms of life. The catalytic site of At2g17340.1 is likely to reside near the coordinated magnesium ion. The nicotinamide portion of NAD+ in 1EZO superposes to within a few angstroms of the magnesium binding site of At2g17340.1. The N-terminal domain is near the coordinated metal, and may act as a "lid" as it is connected by two short linker regions.

References: (1) Bitto, E., Bingman, C.A., Allard, S.T.M., Wesenberg, G.E., Phillips, G.N. Jr. (2005) The structure at 1.7 Å resolution of the protein product of the At2g17340 gene from *Arabidopsis thaliana*. *Acta Crystallogr Sect F Struct Biol Cryst Commun* 61(Pt 7):630-5.

Percent Identity with Nearest PDB Structure at Time Solved	22.7% over 225 aa (1QKK)
Pfam Cluster	DUF89, B_28918, B_81173
Protonet Cluster Size : Structures in PDB	58 : 0

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