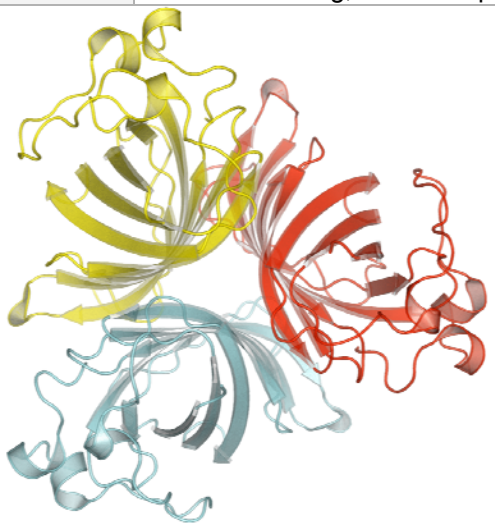
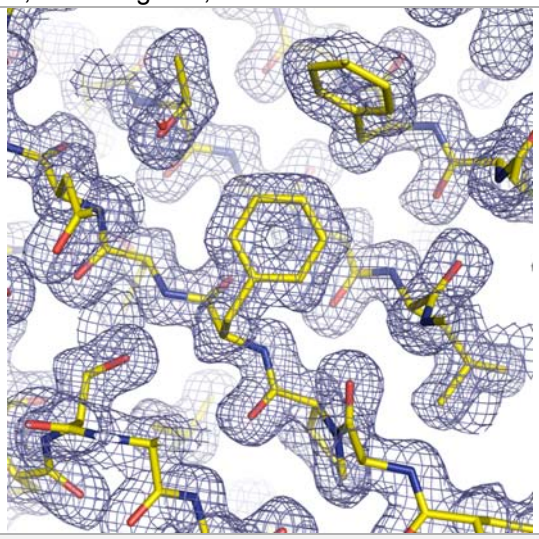
Center for Eukaryotic Structural Genomics

Protein Structure Initiative

Target ID	GO.15839	
Source Organism	*Arabidopsis thaliana*	
Target Name	At3g25770.1	
PDB Entry	1Z8K	Deposition: 30-Mar-2005
Function	allene oxide cyclase (FF/Refine: 2Q4I)	
Produced From	*E. coli* B834 p(RARE2) pVP-16	
Structure by X-ray	Resolution: 1.71Å	R-value (R-free): 15.0% (18.0%)
	No. of Residues/ASU: 522	Monomers/ASU: 3
Data Collected At	Advanced Photon Source 22-ID 12-Mar-2005	
Authors	G.E. Wesenberg, G.N. Phillips, Jr., E. Bitto, C.A. Bingman, S.T.M. Allard	





Structural Features

Arabidopsis thaliana gene At3g25770.1 encodes an isoform of allene oxide cyclase (AOC2), a key enzyme involved in biosynthesis of jasmonates. Jasmonates are plant hormones with growth-inhibiting and senescence-promoting activities. They also act as signaling molecules in plant defense by inducing the expression of protease inhibitors and antimicrobial agents. The biosynthesis of jasmonates starts with linolenic acid. Allene oxide cyclase catalyzes the cyclization of an unstable epoxide precursor of jasmonate, generating the first biologically active compound of the pathway, 12-oxo-phytodienoic acid (OPDA). The crystal structure of AOC2 reveals an eight-stranded antiparallel beta-barrel with a C-terminal helical extension. The hydrophobic center of the barrel forms a binding site of a substrate. AOC2 is trimeric both in crystals and in solution. The closest structural homologues of AOC are the proteins of the lipocalin family involved in transport of various small molecules. Recently solved crystal structure of AOC2 with competitive inhibitor vernolic acid provided insight into a catalytic mechanism of this enzyme. The hydrophobic part of the inhibitor is buried inside the central barrel while the charged carboxylic headgroup is located on the protein surface. The substrate specificity and stereoselectivity of the reaction is dictated by the shape of the central cavity. The initial opening of the epoxide ring is promoted by a conserved glutamate. The transition state is stabilized by a tightly bound water molecule and favorable interactions with aromatic residues in the cavity. All the residues involved in catalysis are strictly conserved

References: (1) Hofmann, E., Zerbe, P., Schaller, F. (2006) The crystal structure of *Arabidopsis thaliana* allene oxide cyclase: insights into the oxylipin cyclization reaction. *Plant Cell* 18:3201-3217.

Percent Identity with Nearest PDB Structure at Time Solved	93% (1ZVC)
Pfam Cluster	Allene_oxide_cyclase
Sequence Cluster Size	36

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