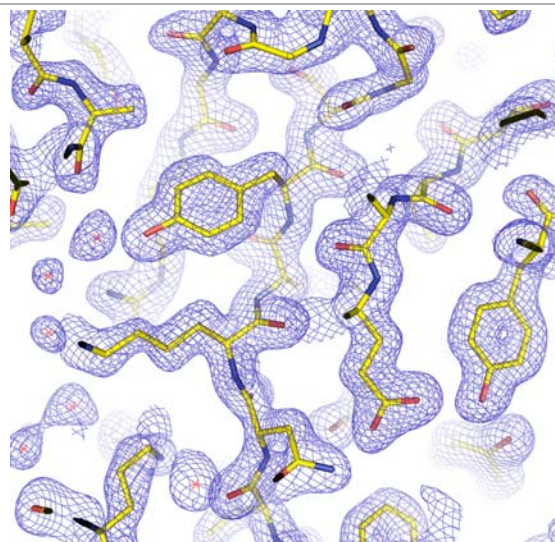
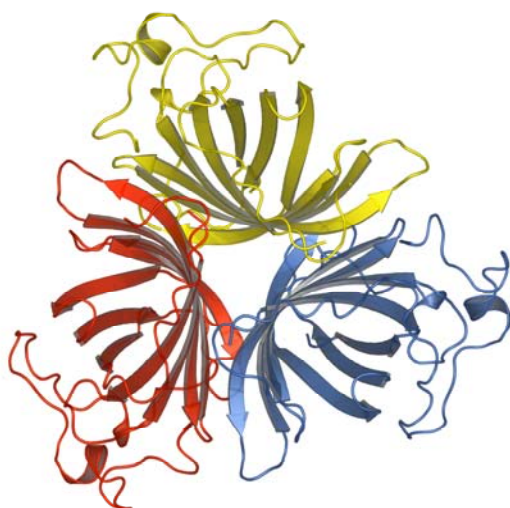




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|---------------------------|---|---------------------------------|
| Target ID | GO.15838 | |
| Source Organism | <i>Arabidopsis thaliana</i> | |
| Target Name | At3g25760.1 | |
| PDB Entry | 1ZVC | Deposition: 01-Jun-2005 |
| Function | Allene oxide cyclase | |
| Produced From | <i>E. coli</i> B834 p(RARE2) pVP-16 | |
| Structure by X-ray | Resolution: 1.79 Å | R-value (R-free): 23.9% (28.3%) |
| | No. of Residues/ASU: 171 | Monomers/ASU: 1 |
| Data Collected At | Advanced Photon Source 22-BM 12-Mar-2005 | |
| Authors | G.E. Wesenberg, G.N. Phillips, Jr., B.W. Han, E. Bitto, C.A. Bingman, S.T.M. Allard | |



Structural Features

Arabidopsis thaliana gene At3g25770.1 encodes an isoform of allene oxide cyclase (AOC1), 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 AOC1 reveals the same fold as AOC2, another AOC isoform solved by CESG (PDB ID 1Z8K). The two isoforms superimpose very well with RMSD of 0.30 Å for 162 atoms. Sequence comparison of AOC1 and AOC2 shows total of ten mutations. Most of them are conservative changes on the protein surface with no differences in ligand binding site. This is in agreement with the results of an *in vitro* assay that showed similar activity and substrate specificity for all four AOC isoforms found in *A. thaliana* (1). However, differences in expression pattern point toward a specific function of each AOC isoform. AOC2 is upregulated upon wounding whereas AOC1 is strongly expressed during senescence. Small structural differences between AOC1 and AOC2 might facilitate the interaction with different regulatory proteins resulting in functional specificity of those two proteins.

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.

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|---|----------------------|
| Percent Identity with Nearest PDB Structure at Time Solved | 93% (1Z8K) |
| Pfam Cluster | Allene_oxide_cyclase |
| Sequence Cluster Size | 36 |

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