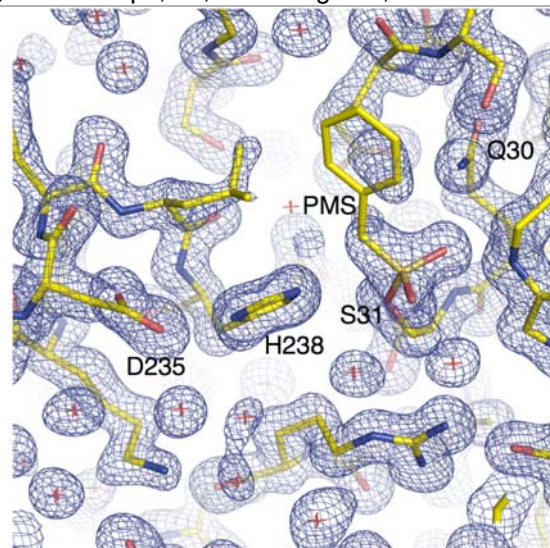
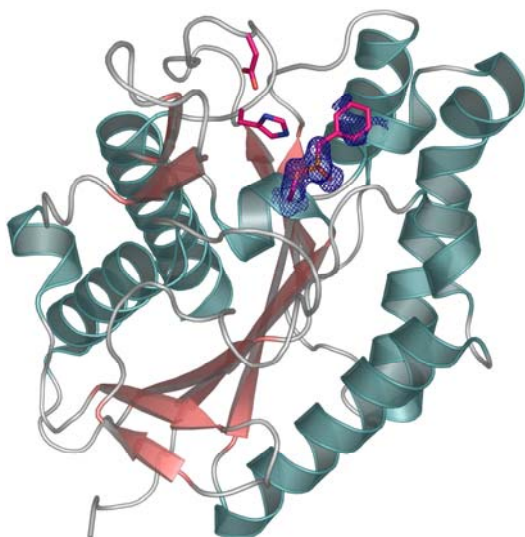


Center for Eukaryotic Structural Genomics

Protein Structure Initiative



Target ID	GO.22797	
Source Organism	<i>Arabidopsis thaliana</i>	
Target Name	At4g34215.1	
PDB Entry	2APJ (replaced 1AEA)	Deposition: 16-Aug-2005
Function	Putative esterase	
Produced From	<i>E. coli</i> B834 p(RARE2) pVP-16	
Structure by X-ray	Resolution: 1.60 Å	R-value (R-free): 14.7% (18.3%)
	No. of Residues/ASU: 966	Monomers/ASU: 4
Data Collected At	Advanced Photon Source 22-ID 10-Aug-2005, 10-Jul-2005	
Authors	E. Bitto, G.E. Wesenberg, J.G. McCoy, G.N. Phillips, Jr., C.A. Bingman, S.T.M. Allard	



Structural Features

The crystal structure of the At4g34215.1 protein of *Arabidopsis thaliana* was determined by molecular replacement and refined to 1.6Å resolution (1). The crystal structure confirms that At4g34215.1 belongs to the SGNH-hydrolase superfamily of enzymes with three-layer $\alpha\beta\alpha$ -sandwich architecture and Rossmann fold topology. The catalytic triad of the enzyme comprises residues Ser31, His238, and Asp235. The crystal structure revealed that the catalytic serine residue was covalently modified by phenylmethyl-sulfonyl fluoride. The structure also reveals a previously undescribed variation within the active site. A conserved asparagine, found in block III of conserved residues in the SGNH-hydrolase superfamily enzymes, which provides a hydrogen bond for an oxyanion hole, is missing in At4g34215.1 and is functionally replaced by Gln30 in block I. This residue is positioned in a catalytically competent conformation by nearby residues, including Gln159, Gly160, and Glu161, which are fully conserved in the carbohydrate esterase family 6 enzymes.

References: (1) Bitto, E., Bingman, C.A., McCoy, J.G., Allard, S.T.M., Wesenberg, G.E., Phillips, G.N., Jr. (2005) The structure at 1.6 Angstroms resolution of the protein product of the At4g34215 gene from *Arabidopsis thaliana*. *Acta Crystallogr D Biol Crystallogr* 61(Pt 12):1655-61.

Percent Identity with Nearest PDB Structure at Time Solved	27% (1ZMB)
Pfam Cluster	DUF303
Sequence Cluster Size	77

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