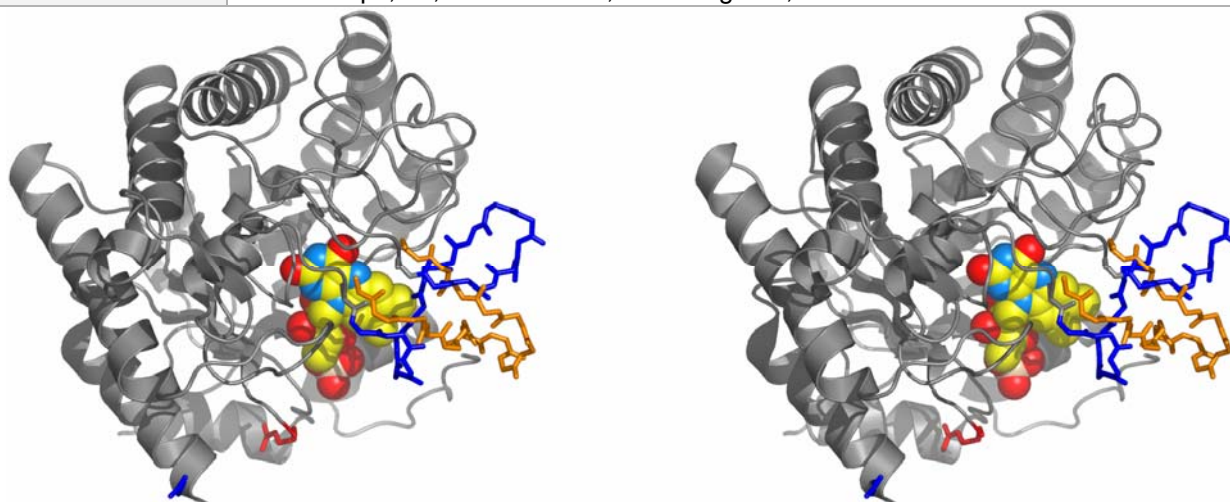


Center for Eukaryotic Structural Genomics

Protein Structure Data Summary

Target ID	GO.8210	
Source Organism	<i>Arabidopsis thaliana</i>	
Target Name	At2g06050.1	
PDB Entry	1Q45	Deposition: 1-Aug-2003
Function	12-oxophytodienoate reductase isoform 3 (FF/Refine: 2G5W, 2Q3O)	
Produced From	<i>Escherichia coli</i> Rosetta pLacI RARE	
Structure by X-ray	Resolution: 2.0 Å, Mol rep	R-value (R-free): 18.6% (23.6%)
	No. of Residues: 391 (42,691)	Subunits/Molecule: 1
Data Collected At	Advanced Photon Source, BioCARS 14-ID-B	
Authors	G.N. Phillips, Jr., K.A. Johnson, C.A. Bingman, D.W. Smith	



Structural Features

In *Arabidopsis*, 12-oxophytodienoate reductase isoform 3 (At2g06050.1, OPR3) catalyzes the NADPH-dependent reduction of 9S, 13S-12-oxo-10,15(*Z*)-phytydienoic acid in an essential, stereospecific reaction of the jasmonic acid biosynthetic pathway. The central role of 9S, 13S-OPDA, which has structural similarity to mammalian prostaglandins, lends significance to characterization of the enzyme(s) responsible for its biosynthesis. In *Arabidopsis*, five OPR isoforms have been identified by genome analysis. OPR1 and OPR2 preferentially react with NADPH to give reduction of the non-physiological 9*R*, 13*R*- stereoisomer of OPDA, while OPR3 alone preferentially reduces the physiologically relevant 9*S*, 13*S*-OPDA but can also reduce the 9*R*, 13*R*- diastereomer. The biological functions of the alternative diastereomers of OPDA are presently not known. Furthermore, the functions of both OPR4 and OPR5 are not known. CESG solved the 2.0 Å X-ray structure of *Arabidopsis* OPR3 (PDB accession number 1Q45) by molecular replacement with tomato OPR1 (PDB 1ICQ). Comparison of the two structures revealed a different backbone conformation at the putative substrate-binding loop (OPR1, *orange*; OPR3, *blue*), suggesting structural contributions leading to the observed stereoselectivity of a required reaction in plant secondary messenger signaling.

References: (1) Malone, T.E., Madson, S.E., Wrobel, R.L., Jeon, W.B., Rosenberg, N.S., Johnson, K.A., Bingman, C.A., Smith, D.W., Phillips, G.N. Jr, Markley, J.L., Fox, B.G. (2005). X-ray structure of *Arabidopsis* At2g06050, 12-oxophytodienoate reductase isoform 3. *Proteins* 58(1):243-5.

Percent Identity with Nearest PDB Structure at Time Solved	49% over 385 aa (1VJI)
Pfam Cluster	Oxidored_FMN, B_5997
Protonet Cluster Size : Structures in PDB	290 : 5

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