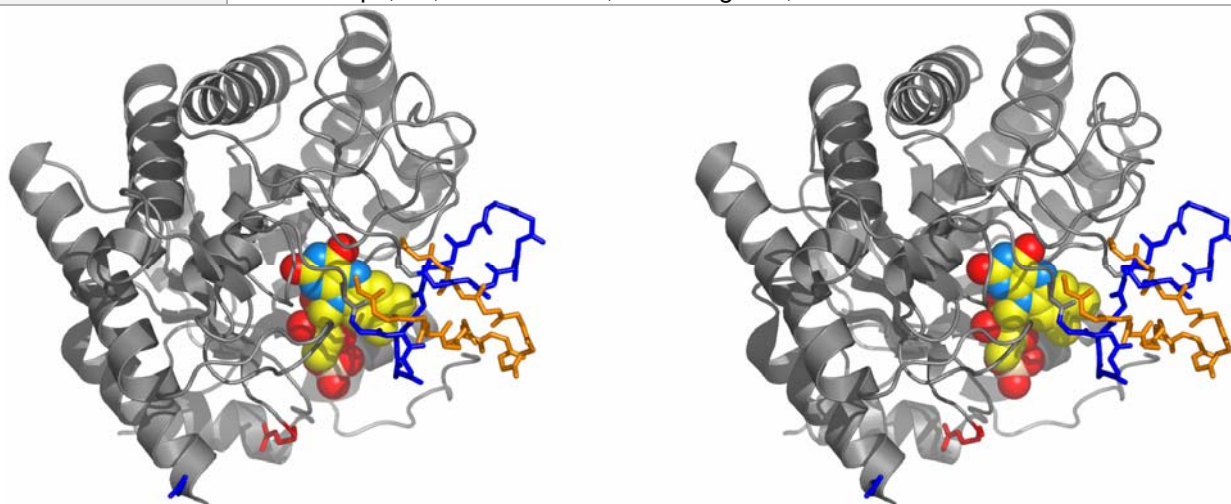


<b>Target ID</b>	GO.8210	
<b>Source Organism</b>	<i>Arabidopsis thaliana</i>	
<b>Target Name</b>	At2g06050.1	
<b>PDB Entry</b>	1Q45	Deposition: 1-Aug-2003
<b>Function</b>	12-oxophytodienoate reductase isoform 3 (FF/Refine: 2G5W, 2Q3O)	
<b>Produced From</b>	<i>Escherichia coli</i> Rosetta pLacI RARE	
<b>Structure by X-ray</b>	Resolution: 2.0 Å, Mol rep	R-value (R-free): 18.6% (23.6%)
	No. of Residues: 391 (42,691)	Subunits/Molecule: 1
<b>Data Collected At</b>	Advanced Photon Source, BioCARS 14-ID-B	
<b>Authors</b>	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)-phytyldienoic 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 9R, 13R- stereoisomer of OPDA, while OPR3 alone preferentially reduces the physiologically relevant 9S, 13S-OPDA but can also reduce the 9R, 13R- 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. CESH 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.

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

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