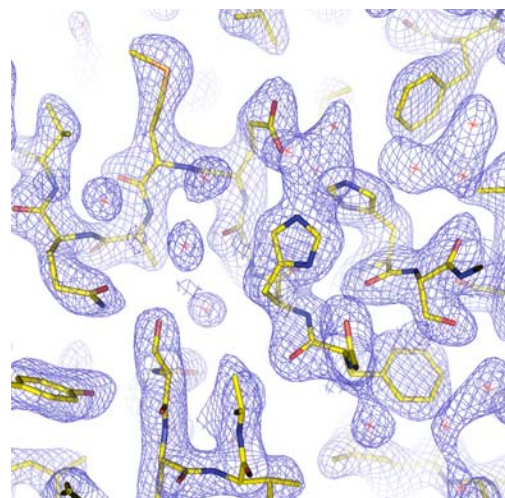


# Center for Eukaryotic Structural Genomics

## Protein Structure Data Summary

<b>Target ID</b>	GO.13167	
<b>Source Organism</b>	<i>Arabidopsis thaliana</i>	
<b>Target Name</b>	At3g21360.1	
<b>PDB Entry</b>	1Y0Z	Deposition: 16-Nov-2004
<b>Function</b>	non-heme iron $\alpha$ -ketoglutarate-dependent dioxygenase (FF/Refine: 2Q4A)	
<b>Produced From</b>	<i>E. coli</i> B834(DE3) p(LacI+RARE)	
<b>Structure by X-ray</b>	Resolution: 2.4Å	R-value (R-free): 26.5% (33.7%)
	No. of Residues: 330 (74,000)	Subunits/Molecule: 2
<b>Data Collected At</b>	Advanced Photon Source Bio-CARS 14-ID-B Oct-2004	
<b>Authors</b>	E. Bitto, G.N. Phillips, Jr., S.T.M. Allard, D.W. Smith, G.E. Wesenberg, C.A. Bingman	



### Structural Features

Based on profile-profile sequence analysis, At3g21360.1 is a member of the non-heme Fe(II)  $\alpha$ -ketoglutarate-dependent dioxygenase superfamily. These enzymes catalyze energetically demanding biosynthetic and degradative reactions (desaturation of unactivated aliphatic bonds, oxidative ring closures and hydroxylation). At3g21360.1 maps to an almost exclusively eukaryotic cluster in Protonet. Pfam-B\_9752 spans AA 54-105, Pfam-B\_6756 spans residues 106-325. A remarkable structural feature of this superfamily is the presence of Fe(II) coordinated by two conserved histidine and glu/asp residues. The catalytic site is unambiguously identified, and the Fe(II) shows strong anomalous signal. Two monomers are found in the asymmetric unit, and show significant differences near the active site that probably show order-disorder transitions related to substrate binding.

*References:* (1) Müller, I., Kahnert, A., Pape, T., Sheldrick, G.M., Meyer-Klaucke, W., Dierks, T., Kertesz, M., Usón, I. (2004) Crystal structure of the alkylsulfatase AtsK: insights into the catalytic mechanism of the Fe(II)  $\alpha$ -ketoglutarate-dependent dioxygenase superfamily. *Biochemistry* 43(11):3075-88; (2) Zhang, Z., Ren, J., Stammers, D.K., Baldwin, J.E., Harlos, K., Schofield, C.J. (2000) Structural origins of the selectivity of the trifunctional oxygenase clavaminic acid synthase. *Nature Struct Biol* 7(2):127-33. (3) Bitto, E., Bingman, C.A., Allard, S.T., Wesenberg, G.E., Aceti, D.J., Wrobel, R.L., Frederick, R.O., Sreenath, H., Vojtik, F.C., Jeon, W.B., Newman, C.S., Primm, J., Sussman, M.R., Fox, B.G., Markley, J.L., Phillips, G.N., Jr. (2005) The structure at 2.4 Å resolution of the protein from gene locus At3g21360, a putative Fe(II)/2-oxoglutarate-dependent enzyme from *Arabidopsis thaliana*. *Acta Crystallogr Sect F Struct Biol Cryst Commun* 61(Pt 5):469-72

<b>Percent Identity with Nearest PDB Structure at Time Solved</b>	22.8% over 214aa (1JQ0)
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<b>Pfam Cluster</b>	Pfam-B_9752,6756
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<b>Protonet Cluster Size : Structures in PDB</b>	19 : 1
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Center for Eukaryotic Structural Genomics (CESG), University of Wisconsin-Madison Biochemistry Department, 433 Babcock Drive, Madison, WI 53706-1549; phone: 608.263.2183; fax: 608.890.1942; email: [cesginfo@biochem.wisc.edu](mailto:cesginfo@biochem.wisc.edu); website: <http://www.uwstructuralgenomics.org>. This research funded by NIH / NIGMS Protein Structure Initiative grants U54 GM074901 and P50 GM064598.