Center for Eukaryotic Structural Genomics

Protein Structure Initiative

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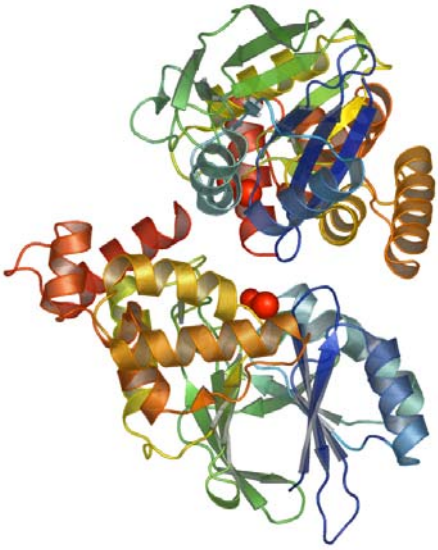
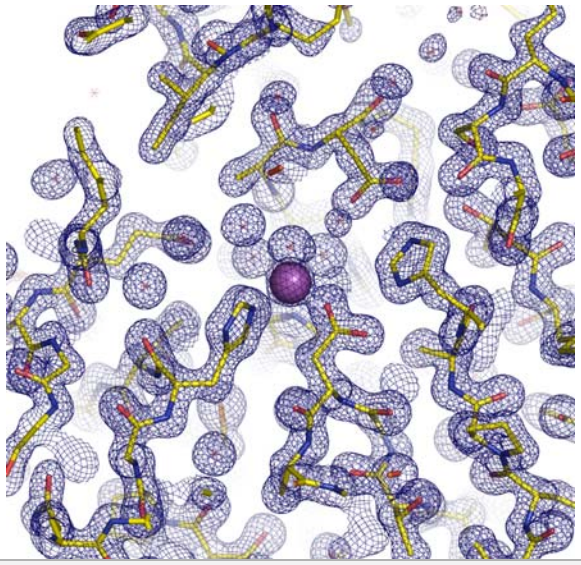
| **Target ID** | GO.4020 | |
| **Source Organism** | *Arabidopsis thaliana* | |
| **Target Name** | At1g53580.1 | |
| **PDB Entry** | 2GCU | Deposition: 14-Mar-2006 |
| **Function** | putative hydroxyacylglutathione hydrolase 3 (FF/Refine: 2Q4C) | |
| **Produced From** | *E. coli* BL21 | |
| **Structure by X-ray** | Resolution: 1.48Å | R-value (R-free): 17.6% (20.4%) |
| | No. of Residues/ASU: 982 (976) | Monomers/ASU: 4 |
| **Data Collected At** | Advanced Photon Source 22-ID 05-May-2005, 23-ID-D 11-Aug-2005 | |
| **Authors** | J.G. McCoy, G.E. Wesenberg, G.N. Phillips, Jr., E. Bitto, C.A. Bingman | |





## Structural Features

The protein product of At1g53580.1 from *Arabidopsis* belongs to the metallo-β-lactamase superfamily. It is closely related to the glyoxalase II enzymes, however, the enzyme does not possess glyoxalase II activity (hydrolysis of glutathione-based thioesters). The enzyme has been shown to bind two equivalents of iron. ICP analysis indicated that the iron/protein ration of our sample was roughly 0.5. This was confirmed in the crystal structure as well, although all of the residues necessary for binding a second metal atom were there. The enzyme possesses 54% identity to a human protein which has been implicated in the rare disorder ethylmalonic encephalopathy. The At1g53580.1 enzyme is currently the most closely related homolog to this enzyme that has been structurally characterized. The structure reveals a small dimeric interface, which is accessible due to a missing two-helix bundle found in glyoxalase II enzymes, as well as a C-terminal fold change which occludes the opening of the active site. The function of this enzyme is currently unknown.

*References:* (1) McCoy, J.G., Bingman, C.A., Bitto, E., Holdorf, M.M., Makaroff, C.A., Phillips, G.N., Jr. (2006) Structure of an ETHE1-like protein from *Arabidopsis thaliana*. *Acta Crystallogr D Biol Crystallogr* 62(Pt 9):964-70.

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| **Percent Identity with Nearest PDB Structure at Time Solved** | 30% (1QH3) |
| **Pfam Cluster** | Lactamase_B |
| **Sequence Cluster Size** | 1331 |

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