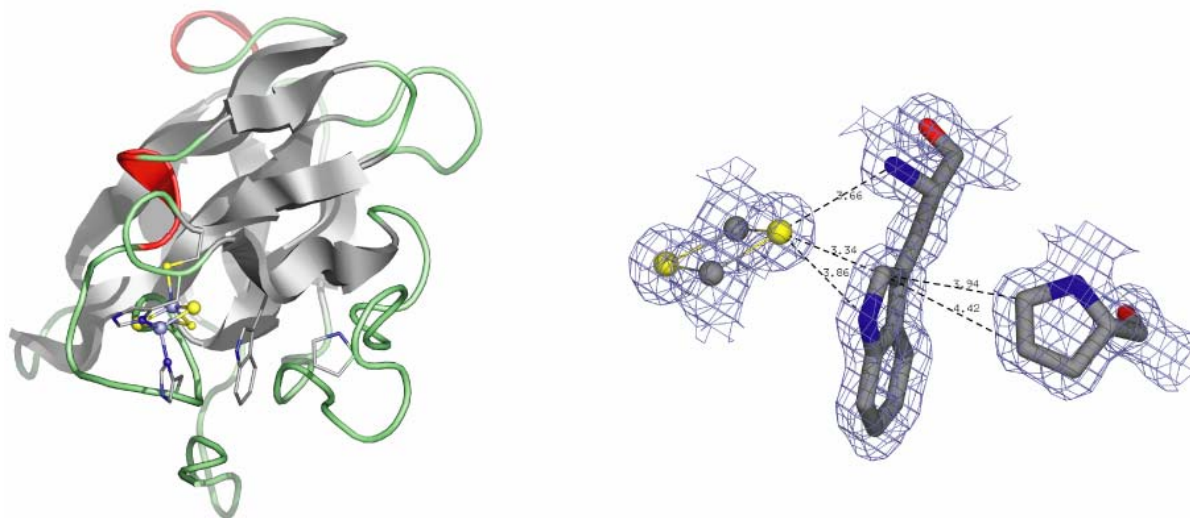


# Center for Eukaryotic Structural Genomics

## Protein Structure Data Summary

<b>Target ID</b>	GO.34660	
<b>Source Organism</b>	<i>Pseudomonas mendocina</i> KR1	
<b>Target Name</b>	Fe-Doxin	
<b>PDB Entry</b>	1VM9	Deposition: 13-Sep-2004
<b>Function</b>	electron transfer component of toluene 4-monooxygenase complex (FF/Refine: 2Q3W)	
<b>Produced From</b>	<i>Escherichia coli</i> BL21 (DE3)	
<b>Structure by X-ray</b>	Resolution: 1.48 Å, Fe-SAD	R-value (R-free): 15.6% (17.6%)
	No. of Residues: 112 12,262	Subunits/Molecule: 1
<b>Data Collected At</b>	UW-Madison and Advanced Photon Source, COM-CAT 32-ID	
<b>Authors</b>	C.A. Bingman, L.A. Moe, D. Smith, G.N. Phillips, Jr., B.G. Fox	



### Structural Features

The structure of T4moC in the  $[2\text{Fe-2S}]^{2+}$  (oxidized) state was determined by X-ray crystallography at a resolution of 1.48 Å with MAD phasing at Fe. This represents the first successful application of Fe phasing at CEGS. T4moC is the Rieske ferredoxin component of the toluene 4-monooxygenase complex, which catalyzes the NADH- and O<sub>2</sub>-dependent hydroxylation of toluene to form *p*-cresol. Phylogenetic analysis shows that T4moC is part of a clade of Rieske proteins specialized for reaction with diiron hydroxylases. The T4moC structure consists of ten β-strands arranged into the three anti-parallel β sheet topology observed in all Rieske  $[2\text{Fe-2S}]$  domain proteins. However, the well-defined region near to the  $[2\text{Fe-2S}]$  center revealed a unique positioning of Trp69 adjacent to the  $[2\text{Fe-2S}]$  center and an alternative configuration of the loop containing the conserved Pro residue. As *in vitro* complementation studies with Rieske ferredoxins from other phylogenetic clades lacking this Trp residue (1FQT, 1NYK) do not restore catalytic activity, this structural variation is implicated in an evolutionary specialization of the Rieske proteins for with different protein electron acceptors.

*References:* (1) Moe, L.A., Bingman, C.A., Wesenberg, G.E., Phillips, G.N., Jr., Fox, B.G. (2006) Structure of T4moC, the Rieske-type ferredoxin component of toluene 4-monooxygenase. *Acta Crystallogr D Biol Crystallogr* 62(Pt 5):476-82.

<b>Percent Identity with Nearest PDB Structure at Time Solved</b>	32.1% over 112 aa, (1FQT)
<b>Pfam Cluster</b>	PF00355
<b>Protonet Cluster Size : Structures in PDB</b>	22 : 0

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