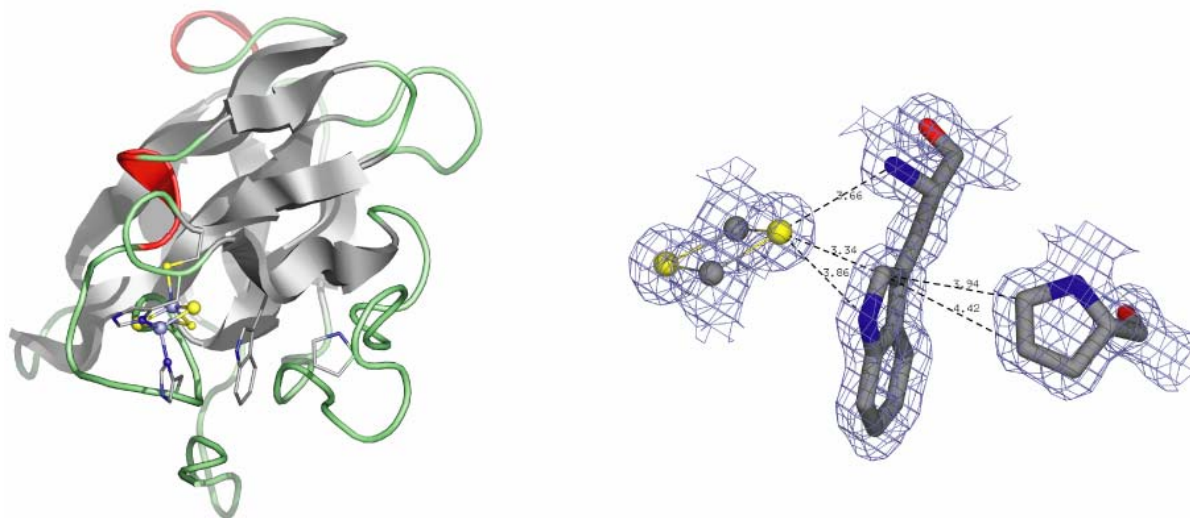


Center for Eukaryotic Structural Genomics

Protein Structure Data Summary

Target ID	GO.34660	
Source Organism	<i>Pseudomonas mendocina</i> KR1	
Target Name	GI: 1174721	
PDB Entry	1VM9	Deposition: 13-Sep-2004
Function	electron transfer component of toluene 4-monooxygenase complex (FF/Refine: 2Q3W)	
Produced From	<i>Escherichia coli</i> BL21 (DE3)	
Structure by X-ray	Resolution: 1.48 Å, Fe-SAD	R-value (R-free): 15.6% (17.6%)
	No. of Residues: 112 12,262	Subunits/Molecule: 1
Data Collected At	UW-Madison and Advanced Photon Source, COM-CAT 32-ID	
Authors	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 CESP. T4moC is the Rieske ferredoxin component of the toluene 4-monooxygenase complex, which catalyzes the NADH- and O_2 -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.

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

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