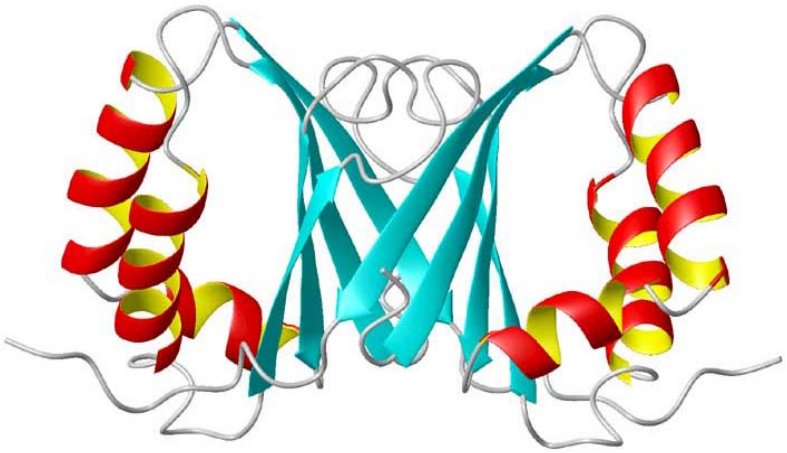
Center for Eukaryotic Structural Genomics

Protein Structure Initiative

Target ID	GO.22997	
Source Organism	*Arabidopsis thaliana*	
Target Name	At5g22580.1	
PDB Entry	1RJJ	Deposition: 19-Nov-2003
BMRB Entry	6011	Deposition: 19-Nov-2003
Function	monooxygenase	
Produced From	*E. coli* Rosetta(DE3)/pLysS	
Structure by NMR	Restraints/Residue: 21.5	Subunits/Molecule: 2
	No. of Residues: 222	Molecular Weight: 24.7 kDa
	Backbone RMSD(6–102): 0.61Å	All Heavy Atoms RMSD(6–102): 1.25 Å
Data Collected At	Nuclear Magnetic Resonance Facility at Madison (NMRFAM)	
Authors	G. Cornilescu, C.C. Cornilescu, Q. Zhao, R.O. Frederick, F.C. Peterson, S. Thao, J. L. Markley	



Structural Features

The structure of homodimeric (111 residues/monomer) At5g22580.1 was solved by starting with a monomeric structure obtained using CANDID/CYANA in the XPLOR simulated annealing protocol. A dimeric model with the correct relative orientation of its monomeric subunits was obtained using ambiguous inter-subunit NOE assignments, radius of gyration and RDC constraints. The dimeric NOE contacts were then refined by consideration of incompatibility of distances within the monomer. Each monomer adopts a *β-α-β-(3_{10})-β-α-α-β fold.* The most similar structure in the PDB shows 36% sequence identified over 88 aligned residues (1Q53 and 1Q4R). Additionally, the bacterial monooxygenase from *Streptomyces coelicolor* (1LQ9) and a protein of unknown function from *Thermus thermophilus* (1IUJ) show structural similarity. This target aligns to Pfam-B domain of Pfam-B_3438 over residues 7–98.

References: (1) Cornilescu, G., Cornilescu, C.C., Zhao, Q., Frederick, R.O., Peterson, F.C., Thao, S., Markley, J.L.(2004) Solution structure of a homodimeric hypothetical protein, At5g22580, a structural genomics target from *Arabidopsis thaliana*. *J Biomol NMR* (3):387-90.

Percent Identity with Nearest PDB Structure at Time Solved	36% over 88 aa (1Q53)
Pfam Cluster	B_3438
Protonet Cluster Size : Structures in PDB	582 : 2

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