

resolution of 1.4 Å using a synchrotron radiation source. Crystals belong to the orthorhombic space group  $P2_12_12_1$ , with unit-cell parameters  $a = 25.76$ ,  $b = 45.38$  and  $c = 56.77$  Å. Initial phases were calculated by molecular replacement using an edited rhodniin molecule as the search model. Currently the structure is under the final stages of refinement with an  $R = 0.203$  and  $R_{\text{free}} = 0.214$ . We shall discuss the implications of this structure in the light of its biological inhibitory function against factor XIIa.

[1] Campos I.T.N., et al., *Insect Biochem. Mol. Biol.*, 2002, **32**, 991.

**Keywords:** infestin, *Triatoma infestans*, serine-protease inhibitor

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#### Structural Studies on 3-hydroxyanthranilate-3,4-dioxygenase

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3-Hydroxyanthranilate-3,4-dioxygenase (HAD) catalyzes the oxidative ring opening of 3-hydroxyanthranilate in the tryptophan-based quinolinate biosynthetic pathway. The enzyme requires  $\text{Fe}^{2+}$  as a cofactor and is inactivated by 4-chloro-3-hydroxyanthranilate (CIHAA). The structure of HAD from *Ralstonia metallidurans* was determined at 1.9 Å resolution. The structures of HAD complexed with the inhibitor CIHAA and either molecular oxygen or nitrous oxide were determined at 2.0 Å resolution, and the structure of HAD complexed with the substrate 3-hydroxyanthranilate was determined at 3.2 Å resolution. HAD is a homodimer with a subunit topology that is characteristic of the cupin barrel fold. Each monomer contains two iron binding sites. The catalytic iron is buried deep inside the cupin barrel. The other iron site forms an  $\text{FeS}_4$  center close to the solvent surface. The two iron sites are separated by about 24 Å. Based on the crystal structures of HAD, mutagenesis studies were carried out and a new mechanism for the enzyme inactivation by 4-chloro-3-hydroxyanthranilate is proposed.

**Keywords:** dioxygenase, cupin, enzyme mechanism

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#### Structure of *S. typhimurium* Formylglycinamide Ribonucleotide amidotransferase

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Formylglycinamide ribonucleotide amidotransferase (FGAR-AT) catalyzes the ATP-dependent conversion of formylglycinamide ribonucleotide, and glutamine to formylglycinamidine ribonucleotide (FGAM) and glutamate in the purine biosynthetic pathway. In eukaryotes and Gram negative bacteria, FGAR-AT is encoded by the *purL* gene as a multidomain protein. In Gram positive bacteria and archaeobacteria FGAR-AT is a complex of three proteins: PurS, PurL and PurQ. We have determined the structure of FGAR-AT from *Salmonella typhimurium* at 1.9 Å resolution. The structure reveals four domains: an N-terminal domain structurally homologous to a PurS dimer, a linker region, an FGAM synthetase domain homologous to an aminoimidazole ribonucleotide synthetase dimer, and a triad glutaminase domain. A structural ADP molecule was found bound. A glutamylthioester intermediate was found in the glutaminase domain at C1135. The N-terminal domain is hypothesized to form the channel through which ammonia passes from the glutaminase domain to the FGAM synthetase domain.

**Keywords:** formylglycinamide ribonucleotide amidotransferase, ATP-grasp motif, protein evolution

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#### Towards the Structure of the Bchl Hexameric Complex of Magnesium Chelatase

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The insertion of  $\text{Mg}^{2+}$  into protoporphyrin IX is catalyzed by the enzyme magnesium chelatase and represents the first committed step in the chlorophyll and bacteriochlorophyll biosynthetic pathways. Magnesium chelatase, in organisms that synthesize bacteriochlorophyll, consists of three subunits, known as Bchl, BchD and BchH. The structure of the monomeric Bchl has been determined by X-Ray crystallography and it belongs to the chaperone-like, ATPase associated with a variety of cellular activities, (AAA) family of ATPases. Examination by electron microscopy of Bchl solutions in the presence of ATP demonstrated that Bchl, like other AAA proteins, forms oligomeric ring structures, [1]. The ATP hydrolysis is proposed to trigger major conformational changes in the hexamer, as has been shown for other AAA modules, [2]. Thus, it is crucial to fixate the complex in one single conformational state using non-hydrolysable substrates to create a homogenous environment. Needle shaped protein crystals have been obtained in different conditions. Ongoing optimization of crystallization conditions will hopefully give single crystals suitable for X-ray diffraction.

[1] Fodje M. N., Hansson A., Hansson M., Olsen J. G., Gough S., Willows R. D., Al-Karadaghi S., *J. Mol. Biol.*, 2002, **311**, 111-122. [2] Rouiller I., DeLaBarre B., May A.P., Weis W.I., Brunger A.T., Milligan R.A., Wilson-Kubalek E.M., *Nat. Struct. Biol.*, 2002, **9**(12), 950-7.

**Keywords:** AAA-domain, ATPase, biosynthesis

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#### Crystal Structure of Glutaredoxin of CxxC1 Type from Poplar

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Glutaredoxins are small ubiquitous oxidoreductases of the thioredoxin family. The major function of glutaredoxin and thioredoxin is to selectively reduce disulfide bridges of target proteins. One of the major differences between glutaredoxin and thioredoxin is that the latter is reduced by various thioredoxin reductases whereas the former requires glutathione. The functions of plant glutaredoxins are not well understood compared to those of *E. coli* and animals. Nineteen poplar glutaredoxins have been annotated based on its genome information and they are classified into three classes [1]. We started crystal structure analysis of poplar glutaredoxin of CxxC1 type belonging to one of the three classes for deepening our understanding of plant glutaredoxins.

The glutaredoxin was overexpressed in *E. coli* cells and crystals were obtained by the hanging drop vapor diffusion method. X-ray diffraction data with three wavelengths were collected at 100K on beam line BL5A of the Photon factory, Tsukuba up to 2.3 Å resolution. The crystals belonged to space group P6<sub>1</sub> with unit cell dimensions  $a=b=97.5$  Å and  $c=91.7$  Å. The structure has been determined by the multiple-wavelength anomalous dispersion method. The polypeptide chain was traced in the electron density map and is now being refined. The molecule has a structure typical of the glutaredoxin fold but contains several new features.

[1] Rouhier N., Gelhaye E., Jacquot J.P., *Cell Mol Life Sci*, 2004, **61**, 1.

**Keywords:** redox enzyme, protein structure determination, MAD

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#### The Structure of *Yersinia pestis* Dehydroquinase

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