Ferredoxin-NADP+ reductase (FNR) catalyzes the redox reaction between NAD(P) and NAD(P)H with the electron carrier protein, Ferredoxin (Fd). Recently, new FNR subfamily that shares a structural homology to NADPH-dependent thioredoxin reductase (TrxR) was identified. We have solved the first crystal structure of the TrxR-like FNR from the green sulfur bacterium *Chlorobaculum tedium* and reported the several unique structural features of TrxR-like FNR [1]. The additional C-terminal sub-domain, that covers the re-face of the isoalloxazine ring of FAD, was newly found in *C. tedium* FNR. The unique asymmetric domain arrangement suggests the bending motion of the hinge region between the FAD and NADPH binding domains. Then, the crystal structure of *Bacillus subtilis* FNR, classified into TrxR-like FNR, was reported as with NADP+ [2]. On the basis of amino acid sequence analysis, it has been recently reported that photosynthetic purple bacterium *Rhodopseudomonas palustris* also has a TrxR-like FNR. In this study, we have examined the crystal structure of Rps. palustris FNR by X-ray crystallography in order to confirm the reported structural features of TrxR-like FNR.

The crystal structure of Rps. palustris FNR was determined by the molecular replacement method at 2.4 Å resolution. The C-terminal sub-domain containing the FAD stacking Tyr residue was confirmed in the Rps. palustris FNR structure. Rps. palustris FNR exists as a homodimer in the crystallographic asymmetric unit. When the FAD domain of one protomer is superimposed on that of the other, one NAD(P)H domain is rotated by 16.5° with respect to the other. The domain arrangements of Rps. palustris FNR is more open, when compared to those of *C. tepidum* FNR and *B. subtilis* FNR, Sequential comparison of the all NADPH domains of TrxR-like FNRs and TrxRs proposes the unique trajectory of the domain, which might be closely related to the replacement of the structurally conserved C-terminal sub-domain during the catalytic cycle.

References:


Keywords: flavoprotein, photosynthesis, reductase

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**Hydrolysis of the thioester intermediate in UDP-glucose dehydrogenases**


Keywords: dehydrogenase, exopolysaccharide, fibrosis

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**MS93.P21**


**Coenzyme binding in a highly specific isocitrate dehydrogenase**

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Isocitrate dehydrogenase catalyzes the first oxidative and dehydroxylation reactions in the citric acid cycle. It also lies at a branch point with the glyoxylate bypass, which makes it possible for some organisms to grow on acetate as the sole carbon source. The monomeric enzyme from *Corynebacterium glutamicum* is highly specific for its substrate isocitrate and coenzyme nicotinamide adenine dinucleotide phosphate (NADP), which it prefers to nicotinamide adenine dinucleotide by a factor of 50,000 [1]. Here, we present the 1.9 Å resolution crystal structure of the enzyme in complex with its coenzyme and the magnesium ion cofactor (Protein Data Bank accession code 3mbc). The overall structure is similar to the previously described structure of the monomeric enzyme from *Azotobacter vinelandii* in complex with isocitrate [2] and NADP [3], and that from *C. glutamicum* in the apo form [4]. In combination with the latter, we find that coenzyme binding in the holoenzyme may be approximately described by the lock-and-key mode even though a second molecule in the asymmetric unit in this family of sugar-nucleotide modifying enzymes. However, the catalytic residues responsible for last mechanistic step, the hydrolysis of a covalently bonded thioester intermediate, which is simultaneously the rate determining and the only irreversible step in the mechanism, have remained elusive.

References: