Crystal Structure of Iron Superoxide Dismutase from Obligate Anaerobic Bacterium

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Superoxide dismutase scavenges the superoxide radical (O_2^-) to form molecular oxygen (O_2) and hydrogen peroxide (H_2O_2) and forms part of the defense mechanism of cells against free radical oxidative damages. We identified the iron superoxide dismutase from obligate anaerobic bacterium *Desulfovibrio vulgaris* Miyazaki F and constructed an expression system in *Escherichia coli* [1]. Crystallization was carried out using hanging drop vapor diffusion method with PEG6000 (space group $P2_1$; a=51.96 Å, b=83.07 Å, c=61.16 Å, â=114.5 ^{o}). The crystal structure has been determined by molecular replacement and refined to 1.0 Å resolution. The crystallographic R and free R are 17.9% and 19.2%, respectively. There are two identical monomers in the asymmetric unit. The monomer has a molecular weight of 22 kDa and consists of 205 amino acid residues of which 201 are visible in the electron density map. The overall fold of the monomer of *D. vulgaris* Fe-SOD is similar to that of other known Fe/Mn-SODs. The active site is composed of one iron, four metal ligand residues (His34, His84, Asp170 and His174) and one water molecule. The interaction of the dimer interface is also similar to that of other Fe/Mn-SODs. The structure differences compared with other Fe/Mn-SODs are at the loop regions on the surface of the molecule (Asp68-Ala72 and Gly143-Asp145).

[1] Nakanishi T., et. al., *J. Biochemistry*, 2003, **133**, 387-393.

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