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**A POSSIBLE MODEL FOR FILAMENT EXTENSION OF THE *E. COLI* RECA PROTEIN IN HOMOLOGOUS RECOMBINATION**

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The RecA proteins of *E. coli* form a filamentous complex around a single-stranded (ss) DNA prior to homology search in homologous recombination. The filament pitches are 95 Å and 65 Å in the presence of ATP and ADP, respectively. NMR studies revealed recently a novel RecA/Rad51-induced extended ssDNA structure including deoxyribose-base stacking (PNAS, 95 (1997), 6623) and the authors propose two models of deoxyribose for the ATP (C3' endo) and ADP (C2' endo) forms with alternative puckers. X-ray crystal analysis of RecA protein shows a filament of 83 Å pitch with a 61 screw symmetry (Nature, 355 (1992), 318). We succeeded in the present study to crystallize the RecA protein in a different pitch of 72 Å and analyzed at 2.8 Å resolution using BL44B2 of SPring-8. Its crystal parameters were very similar to those previously reported except the c-axis. The overall monomer structures also resemble each other except two DNA-binding loops highly ordered in the current crystals. The loops protruded from monomers toward the filament axis and constructed two continuous side-walls of a spiral gutter. The gutter was expected as the ssDNA-binding site. Comparing the filament structures in crystals, we found a small rotation of monomer around a hinge point near the N-terminal helix. Since the differences on monomer structures were small, we rotated the monomer further so as to realize a putative filament structure of 95 Å pitch for the ATP form. The DNA-binding loops thus rearranged seem to fit very well with the ssDNA proposed from the NMR studies.

**Keywords: RECA FILAMENT CRYSTAL STRUCTURE**

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**PHOTOACTIVATION PROCESS OBSERVED AROUND THE REACTION CENTER OF PHOTOREACTIVE NITRILE HYDRATASE**

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Nitrile hydratase (NHase) from Rhodococcus sp. N-771 consists of α- and β-subunits and contains a mononuclear non-heme iron as the reaction center. The center is photo-reactive, inactivated by nitrosylation and activated by photo-driven NO release. Mass spectrometry and crystal structure determination of the nitrosylated NHase revealed that two ligand residues of the iron, αCys112 and αCys114, are post-translationally modified to Cys-$SO_2$H and Cys-SOH, respectively [Nat. Struct. Biol. 5 (1998), 347]. To study the function of the post-translational modifications in the photo-activation, we determined four structures on different states of photoactivation using BL44B2 at SPring-8. Three of them were obtained from one single nitrosylated NHase crystal with cumulative exposure to a Xe lamp of 150W at 100K for 0min(A), 75min(B) and 195min(C). Remaining state D was analyzed using another crystal exposed to a fluorescent lamp at 25°C for 8h with subsequent storage in liquid nitrogen without light for one day before the X-ray diffraction data collection. After rigorous structure refinements, the NO molecule was found replaced by a solvent ligand in each state, except for state A. Electron densities for two oxygens of αCys112-$SO_2$H remained firmly in all states. However, the density for Oδ of αCys114-SOH gradually disappeared along with the light irradiation (A to C), while the density remained in the state D. The light irradiation process of NHase might include not only the replacement from NO to a solvent ligand on the iron center but also the rearrangement of Oδ at αCys114-SOH.

**Keywords**: **NITRILE HYDRATASE, PHOTO-REACTIVE, CYSTEINE SULFENIC ACID (CYS-SOH)**

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**CRYSTAL STRUCTURE OF RAT BILIVERDIN-IX A REDUCTASE**

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In mammals, heme is degraded to biliverdin-IXα and subsequently, it is reduced to bilirubin-IXα by biliverdin-IXα reductase (BVR). The bilirubin play a key role in oxidative stress defense in vivo, but it is also neurotoxic. We have determined the crystal structure of rat BVR at 1.4 Å resolution.

**Keywords: HEME DEGRADATION, BILIVERDIN, REDUCTASE**

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**BACTERIOFERRITIN FROM *DESULFOVIBRIO DESULFURICANS:* THE IDENTIFICATION OF THE FERROXIDASE CENTRE**

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Essential for the growth and development of most organisms, iron is also potentially toxic and, due to its high insolubility under physiological conditions, in short supply in biological systems (1). Ferritins fulfill the need of iron storage in a biologically accessible and harmless form in organisms as diverse as bacteria, fungi, plants and vertebrates. The oxidized and reduced structures of a new type of bacterioferritin, isolated from *D. desulfuricans* ATCC 27774 (2), were determined at 1.95Å and 2.05Å resolution respectively. Crystals were reduced by soak with sodium dithionite prior to cryo-cooling. Data for MAD phasing were collected at three different wavelengths at the ESRF beamline BM 14 (Grenoble, France) from a single crystal frozen at 100 K (3). This bacterioferritin has the typical ferritin molecular architecture in the form of a roughly spherical hollow shell made up from 24 interlocking subunit monomers. Each subunit contains the diiron site inserted in a four-helix bundle and 12 Fe-coproporphyrin III groups are embedded at the interfaces between pairs of subunits. This is the first case of such a prosthetic group in a biological system (4). It is also the first example of a bacterioferritin from an anaerobe and the first time that the iron atoms from the diiron site were located on a ferritin native protein.

**Keywords: IRON STORAGE, DIIRON CENTRE, DESULFOVIBRIO**