obtained by irradiating the crystals for 10 min. with a blue laser (508 nm). Diffraction data were collected at the PXII beamline of the Swiss Light Source at 100K using a MarResearch CCDC detector.

The structures were solved in space group $P2_12_12_1$ by molecular replacement using the monomer of Dronpa (pdb code 2z1o) as search model. The asymmetric unit contains 12 monomers, associated in three tetramers. The structures were refined at an effective resolution of 3.0 Å for the *on*-state and 3.15 Å for the *off*-state. R/R_{free} values converged at 21.1/25.7% for the *on*-state and 21.3/25.0% for the *off*-state.

PDM1-4 exhibits a β-barrel structure typical for GFP-like proteins. Furthermore, a light-driven *cis-trans* isomerization of the chromophore is observed. From the structures of the *on*- and *off*-states we elucidate that the presence of nickel ions, interacting with His 194 and His 212, decreases the flexibility of the β-strands, resulting in the slower switching kinetics of PDM1-4. The photoswitching mechanism of reversible photoswitchable fluorescent proteins not only arises from the flexibility of the chromophore accompanied by a rearrangement of the proximate residues, but is also influenced by the flexibility of the β-strands.

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Keywords: fluorescence, nickel, protein

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Crystal Structures of Bacterial Peptidoglycan Amidase AmpD and an Unprecedented Activation Mechanism

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AmpD is a cytoplasmic peptidoglycan (PG) amidase involved in bacterial cell-wall recycling and in induction of *β*-lactamase, a key enzyme of *β*-lactam antibiotic resistance [1], [2]. AmpD belongs to the amidase_2 family that includes zinc-dependent amidases and the peptidoglycan-recognition proteins (PGRPs), highly conserved pattern-recognition molecules of the immune system [3], [4]. Crystal structures of *Citrobacter freundii* AmpD were solved for the apoenzyme, for the holoenzyme at two different pH values, and for the complex with the reaction products, providing insights into the PG recognition and the catalytic process. These structures are significantly different compared to the previously reported NMR structure for the same protein [5]. The NMR structure does not possess an accessible active site and shows the protein in what is proposed herein as an inactive "closed" conformation. The transition of the protein from this inactive conformation to the active "open" conformation, as seen in the X-ray structures, was studied by targeted molecular dynamics simulations, which revealed large conformational rearrangements (as much as 17 Å) in four specific regions representing one third of the entire protein. It is proposed that the large conformational change that would take the inactive NMR structure to the active X-ray structure represents an unprecedented mechanism for activation of AmpD. Analysis is presented to argue that this activation mechanism might be representative of a regulatory process for other intracellular members of the bacterial amidase_2 family of enzymes.

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Structure of a novel bacterial small molecule sensor domain with two ligands

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Chemoreceptors play important roles in the adaptation of bacteria to changing environmental conditions. For most chemoreceptors the cognate signal molecules are unknown. Receptors can be classified according to the size of their ligand-binding domain (LBD) into cluster I and cluster II. Several structures of cluster I domains are available, but structural information on the larger cluster II domains is lacking. Here we report the structure of *P. Putida* McpS-LBD in complex with two strong chemoattractants, succinate and malate. Crystals were initially grown using the counter-diffusion method to be further improved by the vapor diffusion technique. Malate crystals diffracted up to 1.8 Å and the structure was solved by wavelength Anomalous Scattering (SAS) using Se-methionine derivatized protein. The McpS-LBD structure together with succinate was solved at 1.9 Å resolution by Molecular Replacement (MR). In the solved structures McpS-LBD is a dimer in which each monomer folds as 6 α-helices (2 long and 4 short) organized in two four-helix bundles located at opposite sites or their long bundle axis.These structures are the first examples of cluster II domains and identifies McpS-LBD as a novel small molecule binding domain. Moreover, despite low sequence similarity, both bundles share high structural similarities with *E. Coli* Tar-LBD. In McpS-LBD, as in the case of Tar, the binding of ligand molecules is accomplished by amino acids from both monomers. Site-directed mutagenesis of amino acids involved in ligand binding causes loss of binding activity. It is proposed that Tar-LBD and McpS-LBD are the result of convergent evolution.

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Non-catalytic glycogen-binding site and its functional role in glycogen synthase

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Glycogen is a polymer of α-1,4- and α-1,6-linked glucose residues