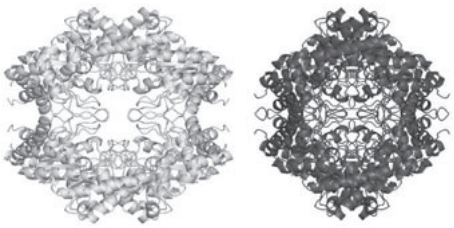
After the transition, the crystal totally recovers its crystalline state and diffraction power. The symmetry is reduced from space-group $I222$ to its subgroup $P2_12_12$ but the effects of this symmetry breaking on the structure are subtle.
The decrease of the unit-cell volume by more that 15 percents produces more intense and interesting structural rearrangements in the crystal (see figure).



Keywords: phase transitions, enzyme structure, polymorphism

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A comparison of hydrated protein models obtained by crystallography, SAXS and other techniques

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Crystallographic or NMR techniques provide information on the precise 3D structure of proteins and reveal the position of some water molecules preferentially bound to certain amino acids. Knowledge of the hydration sites is required for understanding behavior and interactions of hydrated proteins in context with flexibility, dynamics and functionality. A critical comparison of anhydrous and hydrated protein models obtained by crystallography with models from quite different experimental techniques and calculation approaches allows comparing the quality of the models under analysis. Both models and molecular parameters were analyzed: (i) Conventional and ab initio modeling approaches signify satisfactory agreement between crystal- and SAXS-based protein models, provided hydration contributions are taken into account. (ii) Recourse to crystallographic data also allows hydrodynamic modeling; in the case of multibead assemblages efficient bead reductions have to be adopted. (iii) The creation of hydrated models from cryo-electron microscopy data necessitates qualified assumptions regarding hydration. (iv) Combining surface calculation programs and our recent hydration algorithms allows the prediction of individual water molecules; a critical comparison of the water sites on the surface or buried in crevices and channels proves far-reaching identity of crystallographic data and predictions. The good agreement of the results found for hydrated models offers the possibility to complement different techniques and to predict details such as the localization of potential water sites (even in those cases where no crystallographic waters have been identified). Examples presented include proteins ranging from simple proteins to complex, multisubunit, liganded proteins.

Keywords: protein water analysis, small-angle X-ray scattering, modelling

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Flagellar and SOS structural genomics of *Xanthomonas campestris*

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Structural genomics is crucial for understanding the intricate interactions among proteins in a whole organism. We have studied the structural genomics of Xanthomonas campestris (Xcc), a gram-negative bacterium that is phytopathogenic to cruciferous plants and causes worldwide agricultural loss. Currently we are working on its flagellar and SOS structural genomics. In the flagellar system, we have solved the first crystal structure of a hook-capping protein FlgD. The core structure reveals a novel hybrid comprising a tudor-like domain interdigitated with a fibronectin type III domain. In the crystal, the monomers form an annular pentamer of dimers of pseudo five-fold symmetry. The resulting asymmetrical star-like decamer complex has a outer dimensions of approximately 110 Å × 90 Å × 65 Å, and a shortest diameter of approximately 20 Å in the center. The outer dimensions of the atomic Xcc hook-capping FlgD complex turn out to be very similar to those of the Salmonella filament cap complex observed by electron microscopy. SOS has been the most intensively studied system induced under DNA damage, and is characterized by the induction of more than 20 genes, which are under the control of LexA. In response to DNA damage, RecA is activated to induce the auto-cleavage of LexA, resulting in de-repression of genes in the SOS regulon. The recX gene is co-transcribed with recA and its product is suggested to regulate RecA function by directly interacting with RecA protein. We have solved the first RecX structure to a resolution of 1.6 Å. It comprise three tandem repeats R1, R2 and R3 of three-helix bundles. Model studies indicate RecX can fit into the helical groove of the RecA filament very well, similar to that reported for the cryoEM image of the RecA/RecX/ATP/ssDNA complex.

Keywords: RecA, RecX, three-helix bundle

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The structural basis of calcium transport by the calcium pump

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The sarcoplasmic reticulum Ca^{2+}-ATPase 1a (SERCA) actively pumps calcium across the SR membrane through formation and break-down of a phosphoenzyme intermediate. The pumping of Ca^{2+} from the muscle cell cytoplasm induces muscle relaxation and the SERCA pump consumes about 25% of the ATP hydrolyzed during muscle activity. The protein has 10 membrane spanning helices, with a cytoplasmic head consisting of three domains (A-actuator, P-phosphorylation and N-nucleotide binding). The vectorial translocation of two Ca^{2+} ions is secured by stringent movements of the cytoplasmic domains coupled to movements of