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Self -assembly of the S-layer protein SbsC. Tea Pavkov-Keller[a], Janet Vonck[b], Eva M. Egelseer[c], Uwe B. Sleytr[c], Werner Kühlbrandt[b], Walter Keller[a], [a]*Institute of Molecular Biosciences, Karl-Franzens University, Graz, Austria.* [b]*Structural Biology, Max-Planck Institute of Biophysics, Frankfurt, Germany.* [c]*Department of Nanobiotechnology, University of Natural Resources and Applied Life Sciences, Vienna, Austria.*
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Crystalline bacterial cell surface layer (S-layer) proteins are one of the most abundant cellular proteins with the ability to form crystalline arrays on prokaryotic cells. Different biological functions and promising nanobiotechnological applications have been demonstrated. However, detailed structural information on S-layer proteins is very scarce. For determining the structure-function relationship of SbsC, the S-layer protein from *Geobacillus stearothermophilus* ATCC 12980, deletion mutants were produced. It was shown that the N-terminal part is responsible for binding to a secondary cell wall polymer (SCWP) and that the C-terminal part is essential for self-assembly.
Combining X-ray crystallography and electron microscopy we could, for the first time, describe how the S-layer self-assembles. We present three X-ray structures of the different truncated forms of the S-layer protein SbsC. The protein consists of 9 domains: one coiled-coil domain and 8 Ig-like domains. The domains are connected via short linkers forming an elongated molecule with a great flexibility. These high resolution structures could be fit in an electron density map obtained by 3D-reconstruction of negatively stained 2D-crystals of a full length SbsC, showing which domains are involved in the self-assembly process.

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SAXS Modeling of Structural Changes of DNA-Gadolinium Complexes. Vladimir Volkov[a], Eleonora Shtykova[a], Yuri Yevdokimov[b]. [a]*Institute of Crystallography, Russian Academy of Sciences, Moscow, Russia.* [b]*Institute of Molecular Biology, Russian Academy of Sciences, Moscow, Russia.*
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Structure of cholesteric liquid-crystalline dispersions (CLCDs) formed by double-stranded DNA molecules and treated with gadolinium salts (i), and those with embedded gold nanoparticles (ii) were studied by small-angle X-ray scattering (SAXS). The obtained SAXS data were used for step by step structural modeling of the spatial organization of DNA complexes to give the comprehensive consideration of structural changes caused by the DNA modifications. This modeling provided a reasonable explanation for the increasing of the abnormal negative band in the CD spectra, accompanied by the disappearance of the diffraction peak in the experimental small-angle X-ray scattering curves, which was observed at the treatment of the CLCD by gadolinium salts. Computer simulations also allowed us to obtain structural characteristics of incorporated gold nanoparticles, such as their average size, size distributions and localization in DNA CLCDs. The novel SAXS data analysis methods in combination with early developed complementary modeling approaches were used [1 - 2]. The low resolution three-dimensional structural models of the DNA CLCD particles on the different stages of their modifications were obtained. This work was supported, in part, by the Federal Scientific Program No. 02.740.11.0218.

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