protein crystallized in space group P2₁, with unit-cell parameter a = 34.538, b = 56.772, c = 71.710 Å. The overall structure contains three alpha-helix and four beta-strands. In refined model, we can suggest that the very electrostatically positive surface of SMRD is a possible site of interaction between SMRD and DNA substrate. To define the mechanism of DNA recombination and repair, this structural insight will have to be complemented by new cell-based and complexed approaches.

Keywords: SMRD, B3BP, nicking endonuclease

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Crystal structure of the Fab fragment of antibody against p-bromophenylalanine

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 mass spectrum of Fab fragment of antibody is also used to perform the specific monitoring and analytical immunoassay system of BPA including determination of BPA concentration. We have started an analysis for the crystal structure of anti-BPA to clarify the structural features participating in antigen recognition of anti-BPA. Fab fragment of anti-BPA was prepared by papain digestion. Fab was purified by MonoQ column. The solution of Fab was concentrated to 8 mg/ml in 20 mM Tris-HCl (pH 7.5) prior to crystallization. Fab was crystallized by sitting drop vapor diffusion method at 293 K using PEG4000 as a precipitant. A crystal structure of oxidized C-cyt c₅ was obtained by the Fe-SAD method and refined to 1.3 Å resolution. The N-terminal 20 residues of C-cyt c₅ are disordered and additional 8 residues form a loop structure. This feature may explain the flexibility between the transmembrane and the periplasmic domains of cytochrome c₅, which makes it possible to mediate the direct electron transfer between cytochrome c₅ and RC. C-cyt c₅ shows structural similarities with cytochrome c₅₅ from Pseudomonas aeruginosa and cytochrome c₅ from Monoraphidium braunii. Despite of the overall structural similarities with the class I cytochrome proteins, the coordination pattern of the heme iron is different between C-cyt c₅ and other members in this class. On the other hand, unusual paramagnetic NMR shifts were observed for the oxidized form of C-cyt c₅. This may be attributed to the unique coordination environment of the heme c as revealed from the crystal structure.

Keywords: cytochromes, photosynthesis-related proteins, paramagnetic NMR

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Isopeptide bonds stabilize Gram-positive bacterial pilus structure and assembly

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Bacterial pili are long, slender appendages that mediate adhesion to host cells, and thus promote colonisation and infection. Gram positive organisms such as Streptococcus pyogenes have extremely thin (~30 Å) pili, formed by covalently-linked pilin subunits. We have determined the crystal structure of the major S. pyogenes pilin protein, and have derived an atomic model for pilus assembly which explains the extraordinary strength and stability of this structure. The 2.2 Å crystal structure reveals an extended structure comprising two all-beta domains. The molecules associate in columns through the pilus, providing a model for pilus structure and assembly. The 2.2 Å crystal structure reveals an extended structure comprising two all-beta domains. The molecules associate in columns through the pilus, providing a model for pilus structure and assembly.

Keywords: antibody, boron compound, crystal structure

P04.25.467

Structural studies of the cytochrome c₅ from the green photosynthetic bacterium Chlorobium tepidum

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Green sulfur photosynthetic bacteria have a reaction center (RC) with a Fe-S cluster as the terminal electron acceptor. The RC consists of five subunits: PscA containing a special pair (P840), PscB containing Fe-S clusters A and B (F₆/F₆), PscC containing a heme c (cytochrome c₅), PscD binding to the FMO, and the BChl-a protein FMO. Two molecules of cytochrome c₅ bind to the RC and each of them has been reported to directly transport an electron from cytochrome b₅₅ to the P840. Cytochrome c₅ is supposed to consist of an N-terminal transmembrane domain and a C-terminal periplasmic domain which contains one heme c. In order to determine the crystal structure of the functional domain, we constructed a soluble variant of cytochrome c₅ from the green sulfur photosynthetic bacterium Chlorobium tepidum (residues 111-206; C-cyt c₅). We determined the crystal structure of oxidized C-cyt c₅ by the Fe-SAD method and refined to 1.3 Å resolution. The N-terminal 20 residues of C-cyt c₅ are disordered and additional 8 residues form a loop structure. This feature may explain the flexibility between the transmembrane and the periplasmic domains of cytochrome c₅, which makes it possible to mediate the direct electron transfer between cytochrome b₅₅ and RC. C-cyt c₅ shows structural similarities with cytochrome c₅₅ from Pseudomonas aeruginosa and cytochrome c₅ from Monoraphidium braunii. Despite of the overall structural similarities with the class I cytochrome proteins, the coordination pattern of the heme iron is different between C-cyt c₅ and other members in this class. On the other hand, unusual paramagnetic NMR shifts were observed for the oxidized form of C-cyt c₅. This may be attributed to the unique coordination environment of the heme c as revealed from the crystal structure.

Keywords: cytochromes, photosynthesis-related proteins, paramagnetic NMR
Poster Sessions

Keywords: bacterial pili, isopeptide bonds, oligomer assembly

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Recognition of an unusual peroxisomal targeting signal 1 by the import receptor Pex5p
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The structure of the peroxisomal receptor Pex5p in the presence of a small model cargo revealed a large conformational change of the receptor upon cargo binding (Stanley et al., 2006). It, however, remained unknown whether the binding was cargo-specific and only indirect methods were applicable to test cargo activity during the translocation process. In order to investigate whether the previously observed type of cargo binding is generally applicable, we have determined the structure of Pex5p in complex with alanine-glyoxylate aminotransferase (AGT). The complex reveals how the unusual C-terminal KKL receptor recognition motif can be accommodated within the previously characterized central binding cavity. The present structure, similarly to the Pex5p-mSC2 complex, reveals a secondary interaction site. From the receptor side the motif that participates in the interaction is the very same than the one in the Pex5p-mSCP2 structure. A common feature of all the available Pex5p crystal structures is that of one the seven TPR repeats of the receptor (TPR4) is not visible and thus can be considered as a highly flexible part of the molecule. Since most TPR proteins participate in various interactions it would not be surprising if the TPR4 segment was serving as an interaction site and stabilized by a binding partner in a later step of peroxisomal translocation. Important to note that TPR4 and the secondary binding motif are located on the opposite sides of the receptor. It is intriguing to hypothesize that secondary interactions are playing a role in the correct orientation of the cargo to ensure the accessibility of the TPR4 region during translocation process. Our structural and biochemical data also consistently show that AGT remains fully active when bound to the receptor.

Keywords: peroxisome, transport, Pex5p

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Crystal structure of L-CKS from *Haemophilus influenzae* in complex with KDO
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The enzyme 3-deoxy-manno-octulosonate cytidylyltransferase (CMP-KDO synthetase; CKS) catalyzes the activation of 3-deoxy-D-manno-octulosonate (or 2-keto-3-deoxy-manno-octonic acid, KDO) by forming L-CKS. In order to determine the structure of L-CKS from *H. influenzae*, we have crystallized it by hanging drop vapour-diffusion method at 296 K. The crystal of L-CKS is orthorhombic, belonging to the space group *P2_12_2_1* with unit cell parameters of *a* = 48.42, *b* = 82.61, *c* = 115.71 Å. The presence of two monomers in the asymmetric unit gives a reasonable *V_m* of 2.05 Å³ Da⁻¹, with a solvent content of 40.0%. We determined the crystal structure of L-CKS from *H. influenzae* in complex with KDO at 2.30 Å resolution by the multiwavelength anomalous diffraction method. The overall protein structure is similar to that of K-CKS from *E. coli*. The C-terminal alpha-helix (Ala230-Asn254) of monomer A has a unique conformation. The structure of L-CKS from *H. influenzae* in complex with KDO will be useful in structure-based inhibitor design.

Keywords: antibacterial target, CKS, KDO

**P04.26.472**

Structure and function of the human histone chaperone CIA complexed with the bromodomain from TFIID
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Histone modifications frequently function as a mark to induce nucleosome structure changes in a site-specific manner. Although many domains that specifically recognize histone modification have been identified, the molecular mechanism of the change in the nucleosome structure induced by histone modification remains elusive. We have therefore studied the functional interaction between the histone chaperone CIA, which has histone-(H3-H4)₄-tetramer disrupting activity, and an acetylated histone-recognizing...