anhydrous and hydrated models for the complex, the subunits, and the assembly from the constituents [4-8]. Moreover, the crystallographic availability of this MDa complex provides the opportunity to apply modern scattering and hydrodynamic modeling approaches to such huge entities, including assemblage of the complex from its constituents, and to check the extensive reduction steps to be adopted for modeling.
We tackled the following problems: (i) comparison of the SAXS- or EM-based conventional or *ab initio* models for the HBL complex with up-to-date crystallographic data, (ii) modelling the HBL complex from constituents, (iii) realistic assumptions or predictions regarding the contribution of hydration, (iv) search for any discrepancies between solution and crystal data. For modelling, primarily the programs DAMMIN, HYDRO, HYDCRYST and several modifications of the approaches were applied, in addition to usage of templates and superimpositions; results were checked by prediction of structural and hydrodynamic data. The most serious problems arose from amino acids missing in the crystallographic data base. We eventually managed to explain the observed discrepancies by the residues absent in the crystal structure of the linker chains; these residues are obviously located in the central core of the complex.

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Keywords: complex protein models, data reduction, hydration

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A Hybrid Pixel Detector in the Home Laboratory: Prospects for Better Data. Joseph D. Ferrara, Colin Acheson, Angela Criswell, Pierre Le Magueres, James W. Pflugrath, Katsunari Sasaki. *Rigaku Americas Corp., The Woodlands, TX, USA.*
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We have begun using a hybrid pixel detector (HPD), specifically the Dectris Pilatus 100K, in home lab single crystal X-ray diffraction experiments. In order to assess the utility of such a device for the home lab, we have studied the performance of this device for both small molecule and protein data collection experiments with copper radiation. We will present results comparing HPD data collection to conventional CCD data collection as well as results comparing conventional data collection to “shutterless” data collection in terms of data quality and increased throughput.

Keywords: area detector, hybrid pixel detector, data collection methods

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Bacterial conjugation in Gram-positive bacteria: Impact of Tra proteins from plasmid pIP501. N. Gössweiner-Mohr[a], E.-K. Çelik[a,b], M.Y. Abajy[a,b], K.Arends [b], E.Grohmann[b], W.Keller[a]. [a]*Institute for Molecular Biosciences, Karl-Franzens-University Graz, Humboldtstrasse 50/III, 8010 Graz, Austria.* [b]*Environmental Microbiology/Genetics, Technical University Berlin, Franklinstr. 29, 10587 Berlin, Germany.*
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Conjugative plasmid transfer is an important way for horizontal gene spread (e.g. antibiotic resistance genes) [1]. It can lead to the increase of bacteria with multiple antibiotic resistances. The plasmid conjugation process in Gram-negative bacteria has been studied in detail, whereas little information is available about the corresponding mechanisms in Gram-positive bacteria [2]. The transfer region of our Gram-positive multiple antibiotic resistance plasmid pIP501 is organized in an operon encoding fifteen putative transfer proteins. The transfer region of pIP501 encodes a putative simplified type IV secretion system (T4SS), as three pIP501-encoded Tra proteins show significant sequence similarity to the Agrobacterium tumefaciens T-DNA transfer system proteins. The homologues are an ATPase (ORF5 homologue of VirB4) [3], a coupling protein (ORF10 homologue of VirD4) and a lytic transglycosylase (ORF7 homologue of VirB1) [4].
One priority of the project is to determine the structure of ORF11 and ORF14, two members of the T4SS for whom neither homologues exist in the Agrobacterium tumefaciens T-DNA transfer system, nor detailed structure information is available. The focus on these exclusive members of the conjugation complex will further facilitate the understanding of the bacterial conjugation process in Gram-positive bacteria. 7xHis-fusion proteins of ORF11 and ORF14 have already been successfully expressed, purified and used in first crystallisation- and optimization screens. The purified proteins have also been examined for their secondary structure content, folding status and temperature stability by far UV circular dichroism.
As the aim of solving the structure of some individual key tra-region proteins gets closer, we will start to focus on the interaction of the core complex members and the detailed study of the complex structure as a whole.

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Keywords: crystallization, conjugation, pIP501