of biological molecules whose structures may be determined from x-ray diffraction data.

Here, we describe a novel approach for the structure analysis of 2D IMP crystals using x-ray powder diffraction data [3]. We apply our method to the recovery of the structure of the bacteriorhodopsin molecule to a resolution of 7Å.

We use a priori information about unit cell lattice parameters, space group transformations and chemical composition in a bootstrap process that resolves the ambiguities associated with overlapping reflections. The measured ratios of reflections that can be resolved experimentally are used to refine the position, shape and orientation of low-resolution molecular structures within the unit cell, leading to the resolution of the remaining overlapping reflections. The molecular model is then made progressively more sophisticated as additional diffraction information is included in the analysis. Our approach can be used to provide reliable low-resolution phase information that can be further refined by the conventional methods of protein crystallography.

Keywords: integral membrane proteins, 2D crystals, powder diffraction

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Towards more complete models in macromolecular crystal structure determination

Tim Wiegels,[a] Marco Biasini,[b] Victor Lamzin,[a] [a]*European Molecular Biology Laboratory (EMBL) - Hamburg Unit, Hamburg (Germany).* [b]*Swiss Institute of Bioinformatics, Biozentrum, University of Basel, Basel (Switzerland).* E-mail: wiegels@embl-hamburg.de

Macromolecular machines play central roles in life processes and present important targets in biomedical and pharmaceutical research. However, determining the three-dimensional structures of large molecular assemblies is a challenging task in macromolecular crystallography (MX). Crystals of such structures rarely diffract to high resolution and often only noisy and inaccurate electron density maps are obtained. Computational approaches for model building in MX have historically been focused on high-resolution data, thus their application at lower than 3.0 Å resolution data is limited and typically results in incomplete and highly fragmented models. Hence, robust methods that would improve the completeness and the accuracy of models are urgently needed for the automated determination of low-resolution MX structures.

To address this aim within the ARP/wARP software project [1], we exploit the fact that 50% of all crystal structures deposited in the PDB [2] contain multiple copies of subunits or their assemblies in the asymmetric unit "non-crystallographic symmetry or NCS". We noticed that during automated model building with ARP/wARP, particularly in its initial steps, NCS-related parts of the structure are rarely built in exactly the same way. The reasons for that are manifold - including limited resolution of the data and poor initial phases. However, a beneficial side effect of differently built NCS-related copies is that each provides information that is not present in another copy; combining this (which we call *intrinsic*) information improves the model building process and increases the overall completeness of built structures at low resolution. The use of NCS during model building with ARP/wARP provides a significant improvement in many cases, and often requires less model-building cycles. In the best case, at 3.2 Å resolution, the model completeness improves from 55% to 73%, more side chains can be docked in sequence, and the length of the built fragments increases.

Density that cannot be easily interpreted as part of a protein chain can be regarded as a poorly defined connection between two built chain fragments. Such connection generally contains not only loops but also helices or strands. In an approach using *complementary* information, we use structural fragments from the PDB for the interpretation of such density. Tests are currently underway, with very promising preliminary results. Rebuilding of 10-residue long gaps in high-resolution structures can already be achieved with an r.m.s.d. of under 0.5 Å. Further results and application to model building will be presented at the conference.

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ShelXle – A Qt GUI for SHELXL

Christian B. Huebschle,[a] George M. Sheldrick,[b] Birger Dittrich,[a] [a]*Institute of Inorganic Chemistry, Georg-August-Unviversity of Goettingen (Germany).* [b]*Department of Structural Chemistry, Georg-August-Unversity of Goettingen (Grermany).* E-mail: chuebsch@moliso.de

ShelXle is a graphical user interface (GUI) for small-molecule least-squares refinements of single-crystal diffraction data with SHELXL[1]. It is designed like a integrated development environment and combines an editor with syntax highlighting and auto completer with a graphical representation of the three dimensional structure. ShelXle is a tool for expert users of SHELXL giving full control over the *.res/*.ins input file. Non expert users can rapidly learn how to appreciate the full capability of SHELXL by exploring the functionality of ShelXle. The electron density and difference electron density maps (F_o and F_o-F_c) can be visualized as wire framed isosurfaces. A 'rename mode' provides the ability to re label atoms including residues and/or parts and assigning free variables for occupation constraints. Molecules can be moved so that their centers of gravity lie inside the unit cell by just one click. If there is more than one chemical identical molecule present in the asymmetric unit then one can inherit labels semi-automatically from a previously labeled molecule. The 'auto HFIX' function uses electron density (F_o-F_c) for the placement of Hydrogen atoms with suitable constraints/restraints. For convenience functions to update the number of atoms in the cell (UNIT) and the weighting scheme (WGHT) are build in. A refinement history and a save history allow to go back to previous file versions.

The three dimensional representation of the molecule is drawn using OpenGL. Several stereoscopic projection modes are available including one for Zalman Monitors. The GUI is written entirely in C++ using Qt. Some tools are written in Fortran using Intel's MKL library. The program has been thoroughly tested prior to this launch. ShelXle is available for Windows (XP/Vista/7),

MacOS X (10.5/10.6), Linux (SuSE [11.1-11.4] / Debian) and as source. On all systems it is easy to install. ShelXle is licensed under LGPL(2.1) and can be downloaded free of charge at http://ewald.ac.chemie.uni-goettingen.de/shelx/ .

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