merohedral (twin law matching a symmetry operation in the crystal system, but not crystal point group) and pseudo-merohedral (where the twin law belongs to a higher symmetry lattice than the structure obeys). The most common type of merohedral twinning is hemihedral involving two twin domains. We have also observed two cases with four twin domains (tetartohedral; PDBids 2PRX and 3NUZ). Improvements in software have simplified the detection and treatment of twinned data. When the project was started, twin refinement was limited to SHELXL and CNS or using detwinned data in cases of low twin fractions. The addition of twin refinement to phenix.refine and refmac has expanded the options for refining twinned data. A review of the twinning cases at the JCSG provides a guide for the characterization, solution and refinement of twinned structures.

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Keywords: twinning, structural genomics, macromolecular crystallography

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Advances in the CRANK software suite for automated crystal structure solution

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CRANK is a suite for automated macromolecular crystal structure solution that enables different crystallographic programs to seamlessly communicate. The current release can build structures automatically from single- and multiple-wavelength anomalous diffraction data and single isomorphous replacement with anomalous scattering data [1]. The latest release of CRANK includes several new algorithms which both increase robustness and speed up the automatic structure solution process.

Several improvements were made in substructure determination. While most programs use the absolute value of Bijvoet differences, $\Delta F=|F^{+}|-|F^{-}|$, as an estimate of $|F_A|$, a multivariate joint probability distribution, implemented in the AFRO program, is used in CRANK to obtain more accurate values for $|F_A|$. The substructure determination process was sped up substantially by allowing substructure detection to be terminated early without running all trials and by quickly evaluating whether a correct solution for the substructure was located.

In density modification it is often assumed that the initial and density-modified map are independent. We have developed a multivariate function for phase combination that rectifies this assumption by considering the observed Friedel pairs directly from a SAD experiment, accounting for the correlation between the initial and density-modified maps and refining the errors that can occur in a single-wavelength anomalous diffraction experiment. The maps produced by this multivariate phase combination program lead to many more structures being built automatically [2]. We also recently implemented a new cross-validated scheme for accurate error-parameter estimation in likelihood-based phase combination that results in improved phase probability and figure of merit estimates [3].

The use of experimental phase information in refinement is known to improve automated model building results. For SAD and SIRAS [4] experiments CRANK uses a multivariate likelihood function implemented in the program REFMAC [5], that takes as input the diffraction data, heavy atom coordinates and the calculated structure factors and accounts for the correlation between them. By using all experimental information directly, the multivariate functions overcome limitations of the function that uses Hendrickson–Lattman coefficients to incorporate experimen-tal phase information in refinement.

CRANK can be run either via a command line program GCX or through a *ccp4i* graphical user interface: both require only minimal input to run. Users however may also set-up a custom-made pipeline using any program at each step, customize variables for the individual steps and define the start and end step for a pipeline.

CRANK is licensed under GPL v2 and available from the CCP4 suite (www.ccp4.ac.uk) or www.bfsc.leidenuniv.nl/software/crank

[1] N.S. Pannu et al., *Acta Cryst.,* **2011**, *D67*, 331-337. [2] W.-J. Waterreus, P. Skubák et al., *Acta Cryst.,* **2010**, *D66*, 783-788. [3] P. Skubák, N.S. Pannu, *Acta Cryst.,* **2011**, *D67*, 345-354. [4] P. Skubák, G.N. Murshudov, N.S. Pannu, *Acta Cryst.,* **2009**, *D65*, 1051-1061. [5] Murshudov et al., *Acta Cryst.*, **2011**, *D67*, 355-367.

Keywords: automation, phasing, software

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Novel Approach to Automatic Scoring of Protein Drop Images Using UV Fluorescence

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Analyzing vast numbers of images is a time consuming bottleneck that affects most protein crystallization experiments. So far, software based image analysis tools for automatic scoring and ranking these images have generally failed because of various image artifacts caused by plates, lighting, and drop geometry. The recent commercial introduction of UV fluorescence imaging for protein crystallization has brought new opportunities for simpler and more reliable approaches to image analysis. Most existing analysis tools rank images using methods such as edge, shape, intensity, and frequency analysis.

With the new UV technologies it is now possible to rank based on protein fluorescence which also has the advantage of differentiating protein versus salt. We have developed a new analysis tool that when integrated with the CrystalTrak software provides the user with a fluorescence score which can be used to filter images from the image viewer those images with little to no fluorescence. This greatly reduces the number of images needing review. Due to the fact that the UV fluorescence images are free of many of the artifacts found in visible images the algorithm has been shown to be very reliable at eliminating clear drops with no false negatives. The methods used produce a score that is fundamentally a ratio of fluorescence signal versus background noise. The user then has the ability to set their own threshold based on this score determining how sensitive they want the algorithm to be and filter as many images as desired. Due to the fact that the Rigaku Minstrel HT UV uses the same optics for the visible and UV images the analysis tool also provides the ability to overlay the detected fluorescence signal over top of the visible images to highlight the items of interest in the visible image.

Keywords: biomacromolecule, crystallization, microscopy

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Fully Automated Cryogenic Crystal Screening System

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The handling of cryo-cooled protein crystals has been automated by robotics systems, where samples are kept in liquid-nitrogen storage, to be loaded on the goniometer for the experiment and retrieved afterwards. Crystals are automatically centered in the X-ray beam by means of an automated goniometer head and software that applies algorithms that determine the crystal position in three-dimensional space from images taken with high resolution digital microscopes. For the steps that follow, we report on the development of XPRESSO, a new crystal screening and data collection system for macromolecular samples.

The screening process starts out by taking short series of X-ray diffraction images from which the general quality of the crystal is judged by the resolution limit, the mosaicity, the ability to find the unit cell, and the presence of ice rings. User input limits for the unit cell help distinguish between the actual sample and unwanted crystals, such as from buffers or salts co-crystallized with a protein.

For the data collection a strategy is determined based on the screening results. It takes into account the exposure time, sample to detector distance, scan width, and resolution limit, among others. The data is integrated in parallel to the data acquisition, followed by data scaling. Space group determination is the final step. Results are provided as HTML reports, including Matthews coefficient probabilities.

Keywords: automation, protein, software

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New Tools for Biological Crystallography in the Home Lab.

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Advances in crystallographic hardware and software have enabled structural biologists to investigate more challenging projects. Recent developments have greatly increased the capabilities of in-house diffraction systems providing increased productivity for synchrotron trips and home-lab studies.

We have made recent improvements in source and detector technology which have significantly improved the capability of home-lab systems for both screening and data collection. Developments include next generation microfocus sources which exhibit significantly higher intensity as well as enhanced beam stability. Combined with a new sensor-based active pixel detector, these systems provide a significant improvement in overall performance while offering extremely low maintenance and cost of ownership. A new feature in our PROTEUM software, XPRESSO, offers a completely automated data acquisition and analysis pipeline for macromolecular crystallography. New developments in hardware and software will be discussed.

Keywords: microfocus source, detector, automated data acquisition

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Graphical user interface for automated crystallography data reduction.

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With the advances in throughput at synchrotron facility sites capable of yielding up to 15 data sets an hour the automatic reduction of single crystal diffraction data is becoming a routine component on synchrotron beamlines. For the past three years at Diamond Light Source, packages such as fast_dp (in house development) and xia2[1] have been employed to carry out data reduction immediately after data collection and are automatically triggered without user interaction. Here we describe how our first implementation which was geared towards processing single sweeps of data with no user interaction has been integrated with a graphical user interface that provides finer control to these programs and the ability to process multiple or partial sweeps of data.

[1] G. Winter, *J. Appl. Cryst.* **2010**, *43*, 186-190.

Keywords: data processing, automation, GUI

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Readiness evaluation method for X-ray difraction data collection systems

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High quality diffraction data is critical for structure determinations. For macromolecular crystallography, there are many factors that may compromise the final data quality. In addition to crystal quality and data collection strategy, the instrumentation factors, such as x-ray beam quality, goniometry and the quality of detectors, are important for data quality too. Since the data collection systems are composed of many electronic and mechanical units and they have to work synegically at their at least normal performance. But this may not always be true.

In order to develop a quick and simple method to access the overall performance of the X-ray data collection system, we proposed a protocol to test X-ray diffraction facilities' readiness. In this protocol, cubic insulin crystals are used to quickly collect anomalous data at long wavelength such 1.54Å. The weak anomalous signals from the 3 disulfide bonds are used to indicat the acuracy of the whole data collection system. This method has been tested at different data collection systems including both rotating anode based home labs and synchrotron beam lines. The detailed results and analysis will be presented.

Keywords: data collection, readiness

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New version of CrysAlisPro optimized for automatic macromolecular data collection and processing

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While the majority of macromolecular X-ray data are currently collected using highly-efficient beam lines on an ever increasing number of synchrotrons, there is still a need for low-maintenance, reliable systems for in-house experiments. In addition to crystal screening and optimization of x-ray experiments before a successful synchrotron trip,