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## Recent Work

### Title

Protein crystallography automation software at the Advanced Light Source

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## Protein Crystallography Automation Software at the Advanced Light Source

**Conference Topic:** Future challenges in synchrotron radiation instrumentation

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### ABSTRACT

The use of synchrotron X-ray diffraction to determine the atomic structures of protein crystals is well established. However, new demands are being placed on synchrotron facilities by Structural Genomics programs and drug discovery efforts which propose to investigate hundreds of protein structures in a high-throughput fashion. We have implemented a data collection environment at the Advanced Light Source to allow the beamline user to collect and process data automatically from dozens of crystals. Components include a robotic mounter to repeatedly transfer cryocooled samples to the goniometer, a database to remotely track high volumes of information, a facility to autocenter the crystal loop in the beam, and a graphical user interface to orchestrate the entire process. Minimal input is required, as data collection and reduction are automatically handled using scripted tools. Unattended, the system can screen up to 112 crystals. Diffraction snapshots are acquired to rank the crystals by quality, and crystal symmetry and optimal collection strategy are then determined. The user can then collect full datasets on the best crystals from the initial screen. This system is installed on branchlines 5.0.1, 5.0.2, and 5.0.3 of the ALS, and is suitable for either individual users or large-scale projects.

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