Title
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Robust Indexing & Automatic Data Collection at the Advanced Light Source.
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With structural genomics programs and drug discovery efforts producing large
numbers of macromolecular crystals, increasing demands are being placed on
synchrotron beamlines. To facilitate high-throughput crystallography, we are
developing new methods for achieving automation. One such development is LABELIT
(the Lawrence Berkeley Lab Indexing Toolbox), a program with new procedures for
autoindexing diffraction patterns. Specifically, the program represents an improvement
in three areas: 1) LABELIT can tolerate inaccuracies in the given position of the incident
beam of up to several millimeters; 2) A check is made to confirm that the deduced unit
cell is not an integer multiple of the true unit cell; and 3) A different approach is used to
identify the Bravais symmetry to better accommodate experimental uncertainty. These
methods help to correct failures commonly experienced during indexing, and increase
the overall success rate of the process. Moreover, LABELIT produces its results without
any requirement for computer graphics intervention. It is presently running as a
background process at beamlines 5.0.1, 5.0.2, and 5.0.3 of the Advanced Light Source,
and will soon be available at beamlines 8.2.1 and 8.2.2. Beamline users can see the
results through a simple web interface. General users can upload data and experiment

Rapid indexing without the need for visual inspection is just one important
ingredient for overall automation. Beamlines 5.0.1, 5.0.2, and 5.0.3 have been equipped
with robotic mounters to transfer cryocooled samples to the goniometer. Software tools
to complement the robot are in place at the beamline, and are also still evolving. These
include high-level graphical controls to rapidly screen 96 samples, rank them by
diffraction quality, and proceed with the collection of full data sets. It is intended that
minimal input will be required for this type of operation, as diffraction experiments can
be automatically orchestrated by underlying software modules. Unattended, the
AutoScreen module will center each crystal in the X-ray beam by analyzing
videomicrographs, acquire two diffraction snapshots, index the lattice with LABELIT,
and compute the Bravais symmetry. An AutoCollect module is under development to
automatically deduce and set the optimal data collection parameters, while an
AutoProcess module will evaluate the diffraction in real time to confirm the Laue
symmetry and monitor radiation damage. We anticipate that these tools will increase
experimental efficiency for both individual users and large-scale efforts alike.

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