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Title

LABELIT: Robust Indexing for Automatic Data Collection

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LABELIT: Robust Indexing for Automatic Data Collection. Nicholas K. Sauter, Ralf W. Grosse-Kunstleve & Paul D. Adams, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 USA.

A new program, LABELIT (*Lawrence Berkeley Lab Indexing Toolbox*), implements new methods for indexing diffraction patterns from macromolecular crystals. The program represents an improvement over existing programs 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 that can better accommodate experimental errors. These methods help to correct failures commonly experienced during indexing, and increase the overall success rate of the process. Rapid indexing, without the need for visual inspection, will play an important role as beamlines at synchrotron sources prepare for high-throughput automation.

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