

LABELIT is a set of programs to assist with automated data processing. An autoindexing program is available which corrects three commonly experienced problems: getting the wrong beam center, finding a unit cell that is too large, and improperly identifying the allowed Bravais symmetry. This requires minimal user input, typically just 2 diffraction images, results are returned within 30-60 seconds. We are currently developing tools for automated determination of space group symmetry once some frames of data have been collected.

Any user can use the LABELIT autoindexing software using a web server, which can be found at:

<http://cci.lbl.gov/labelit>

The LABELIT software is available for download by academic groups at:

<http://cci.lbl.gov/labelit/download.cgi>

To assess the quality of each crystal, two diffraction images are collected. These images are then analyzed (summarized in Figure 1) using the LABELIT software developed by Component VI of the BSGC. Briefly, this consists of locating spots on each image using the DISTL software developed by the Joint Center for Structural Genomics, autoindexing of each image, determining the Bravais lattice, and finally integrating the images automatically with the program MOSFLM (Leslie, 2001) to produce an accurate estimate of the diffraction limit. The foremost consideration in LABELIT's development was the necessity in an automated system to index a diffraction pattern without the usual requirement for a graphical user interface. It was determined that new methods were required to correct failures commonly experienced during indexing, and increase the overall success rate of the process. Novel procedures include a more robust way to verify the position of the incident X-ray beam on the detector, an algorithm to verify that the deduced lattice basis is consistent with the observations, and an alternative approach to identify the metric symmetry of the lattice

The development of the automated crystal screening system, in combination with robotic hardware (Snell et al., 2004), has made it possible to automatically screen up to 112 crystals at the sector 5.0 beamlines at the ALS without the need to enter the experimental hutch. For each crystal, the mounting of the cryo-pin, loop centering, and collection of two images takes approximately 1 minute. The automated diffraction analysis with LABELIT takes approximately 45 seconds. The collection of images and diffraction analysis can be performed concurrently, with analysis of the first crystal being completed while data are being collected from the second crystal. Therefore the screening of a 100 crystals takes approximately 100 minutes, representing less than 1/12 of a standard ALS 24 hour shift. All results of crystal screening are saved in a MySQL relational database.

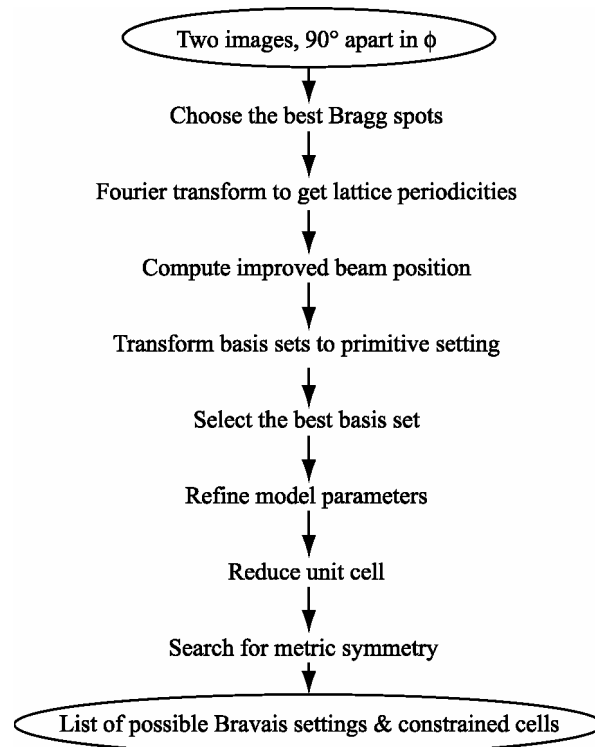


Figure 1: Overview of the LABELIT autoindexing procedure.

LABELIT makes use of the following packages:

- The DISTL package for identifying Bragg spots, developed by A. Deacon, Z. Zhang and H. van den Bedem at Stanford Synchrotron Radiation Laboratory.
- The cmtz library and MOSFLM, components of the CCP4 package.
- The CBF library for reading diffraction images.

References

- Leslie, A.G.W. (2001). In *International Tables for Crystallography: Volume F, Crystallography of Biological Macromolecules*, Rossmann, M.G. & Arnold, E., eds. Dordrecht: Kluwer Academic Publishers, pp. 212-217.
- Snell, G., Cork, C., Nordmeyer, R., Cornell, E., Meigs, G., Yegian, D., Jaklevic, J., Jin, J., & Earnest, T. (2004). Automated sample mounting and alignment system for biological crystallography at a synchrotron source. *Structure*, 12: 537-545.