

W0424

Diffraction Image Ranking and Data Collection Strategy. J.W. Pflugrath, T.J. Niemeyer, Angela R. Criswell, Robert Bolotovskiy, Rigaku Americas, Corp., 9009 New Trails Drive, The Woodlands, TX 77381 USA.

While the minimum requirements for a diffraction data set are completeness in the unique Miller indexes to a given resolution, many other factors play a role in achieving good statistics and good redundancy required for optimal phasing and crystal structure refinement. Two synergistic programs, dtranker and dtmultistrategy have been developed which fulfill the role of an experienced crystallographer in evaluating diffraction images and determining the best data collection strategy. These programs allow for screening and automated diffraction data collection from crystalline samples in both manual and robotic experimental setups. Many aspects of optimizing the diffraction data collection experiment with 2D detectors are dealt with, including choice of crystal, exposure time, rotation width per image, axes to scan, scan setting angles, multiple scans, rotation ranges, potential collisions, multiple detector positions, spot overlap, and tolerance for completeness. These new programs are now available in the d*TREK suite. d*TREK is flexible, customizable, device-independent software and toolkit which collects and processes single crystal X-ray diffraction images from two-dimensional position sensitive detectors such as IP and CCD detectors.