

"Automated structure determination with PHENIX"

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The advent of several large-scale pilot structural genomics projects leads to many new challenges in the field of macromolecular structure determination. Therefore, a novel software package called PHENIX (Python-based Hierarchical Environment for Integrated Xtallography) is being developed. This new software provides tools to go from reduced intensity data to a refined molecular model, and facilitate structure solution for both the novice and expert crystallographer. This software is being developed as part of an international collaboration between the groups of Paul Adams (Lawrence Berkeley Laboratory), Tom Terwilliger (Los Alamos National Laboratory), Randy Read (University of Cambridge, U.K.), and Tom Ioerger and Jim Sacchettini (Texas A&M University). The current features in PHENIX for automated and difficult structure solution will be presented.