

New and Updated Phenix features

Billy Poon¹, Paul Adams², Pavel Afonine³, Dorothee Liebschner⁴, Nigel Moriarty⁵, Oleg Sobolev⁶,
Christopher Schlicksup⁷

¹*Lawrence Berkeley National Lab* ²*Lawrence Berkeley National Lab*, ³*N/A*, ⁴*Lawrence Berkeley National Lab*, ⁵*Lawrence Berkeley National Lab*, ⁶*Lawrence Berkeley National Lab*, ⁷*Lawrence Berkeley National Lab*

bkpoon@lbl.gov

Phenix is a comprehensive software package for macromolecular structure determination that handles data from diffraction experiments and electron cryo-microscopy. Tasks performed with Phenix include data-quality assessment, map improvement, model building, the validation/rebuilding/refinement cycle and deposition. Each tool caters to the type of experimental data. The design of Phenix emphasizes the automation of procedures, where possible, to minimize repetitive and time-consuming manual tasks, while default parameters are chosen to encourage best practice. A graphical user interface provides access to many command-line features of Phenix and streamlines the transition between programs, project tracking and re-running of previous tasks. Some of the new features in Phenix, like utilizing predicted models from AlphaFold and a viewer for reciprocal space data, are highlighted in this poster.