Updated Validation and Deposition Tools in the Phenix GUI

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The Phenix (**P**ython-based **H**ierarchical **En**vironment for **I**ntegrated **X**tallography) software package is a comprehensive collection of tools for determining macromolecular structures. Traditionally, the software used reciprocal-space data (e.g. X-ray/neutron crystallography) for structure determination, but with recent advances in cryo-electron microscopy (cryo-EM) providing higher resolution electron density maps, the software can be applied to real-space data as well. Previous updates to the graphical user interface for Phenix include functionality for validating cryo-EM maps and models, as well as a new unified interface for these validation tools.

With the most recent builds of Phenix, we applied this approach to the X-ray/neutron crystallography validation tools and added a new tool for preparing a model file in mmCIF format for deposition into the Protein Data Bank (PDB). The result is a consistent validation interface for both X-ray/neutron crystallography and cryo-EM structures that can export a table of statistics for publication (e.g. Table 1) and export an mmCIF model file suitable for deposition into the PDB.