We are pleased to announce the release of PyRx 0.9. The following are new features and bug fixes implemented for 0.9 release:

Vina Wizard is now using the number of CPUs (--cpu option). Please use Edit > Preferences and enter Available CPUs to specify this number. By default, PyRx sets it to the number of available CPUs minus one, or just one if there is only one CPU available.

Implemented hydrogen bond visualization. Users can now click on icon on the toolbar or right-click on a molecule and select Display > Hydrogen Bonds. The former displays only intramolecular hydrogen bonding, while the latter shows intermolecular hydrogen bonding between all molecules in PyRx (unless there is only one molecule in 3D Scene, in which case we show intramolecular hydrogen bonding for that molecule).

You can now explicitly set search box dimensions. This was previously read-only and users could change it only by using handles of BoxWidget.
Implemented a new GUI for non-standard residues (HETATM) when making macromolecule pdbqt, available through Make Macromolecule menu. If input macromolecule contains non-standard residues, such as in the case of 1hsg, users can now select what to do with non-standard residues as shown in the GUI below:

Added cleanup='nphs_lps_waters' to AD4ReceptorPreparation to handle DNA's which otherwise was failing because the default was cleanup='nphs_lps_waters_nonstdres'.

Removed unbound ligand mode from AutoDock 4.2 parameters list. See Bug: Unbound ligand mode not respected.

Fixed Import > Workspace Tarball - Local File.

Users can now open multiple molecules at once. We copy input pdbqt files to ~/.mgltools/PyRx/Ligands by default. If there are more than 100 input files to open, we don't add pdbqt inputs to 3D Scene. This is done to allow "Add Ligand" to handle large number of input pdbqt files.

Updated atom color scheme to include new atom types.

Added an option to render secondary structures as ribbons thanks to ePMV. To use this, right-click (Control-click on Mac) on the molecule and select Display > Ribbons. To use this:

Fixed PyRx -> Help -> Check for Updates... for Windows.

Fixed alternate conformations selection when making pdbqt for macromolecules.

Fixed the histogram icon in the Tables toolbar.

See also: List of Changes in PyRx Version 0.8.