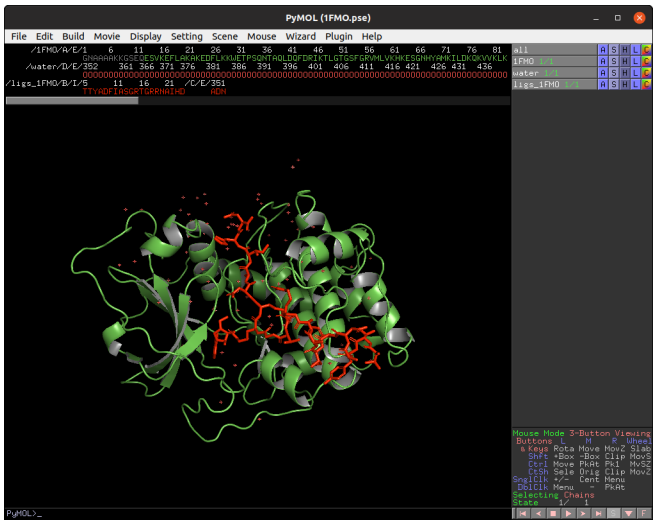
Tutorial

On this tutorial, we are going to demonstrate some features of the parKVFinder, including the graphical user interface (*parKVFinder PyMOL Tools*) and the command-line interface.

All files used on this tutorial can be found under **input** directory, on the **parKVFinder** directory.

parKVFinder PyMOL Tools

First, load **input/1FMO.pse** into PyMOL, which loads two objects in your scene. The **1FMO** is a subunit of a protein kinase A and the **ligs_1FMO** is an adenosine (ADN) and a peptide kinase inhibitor (PKI).

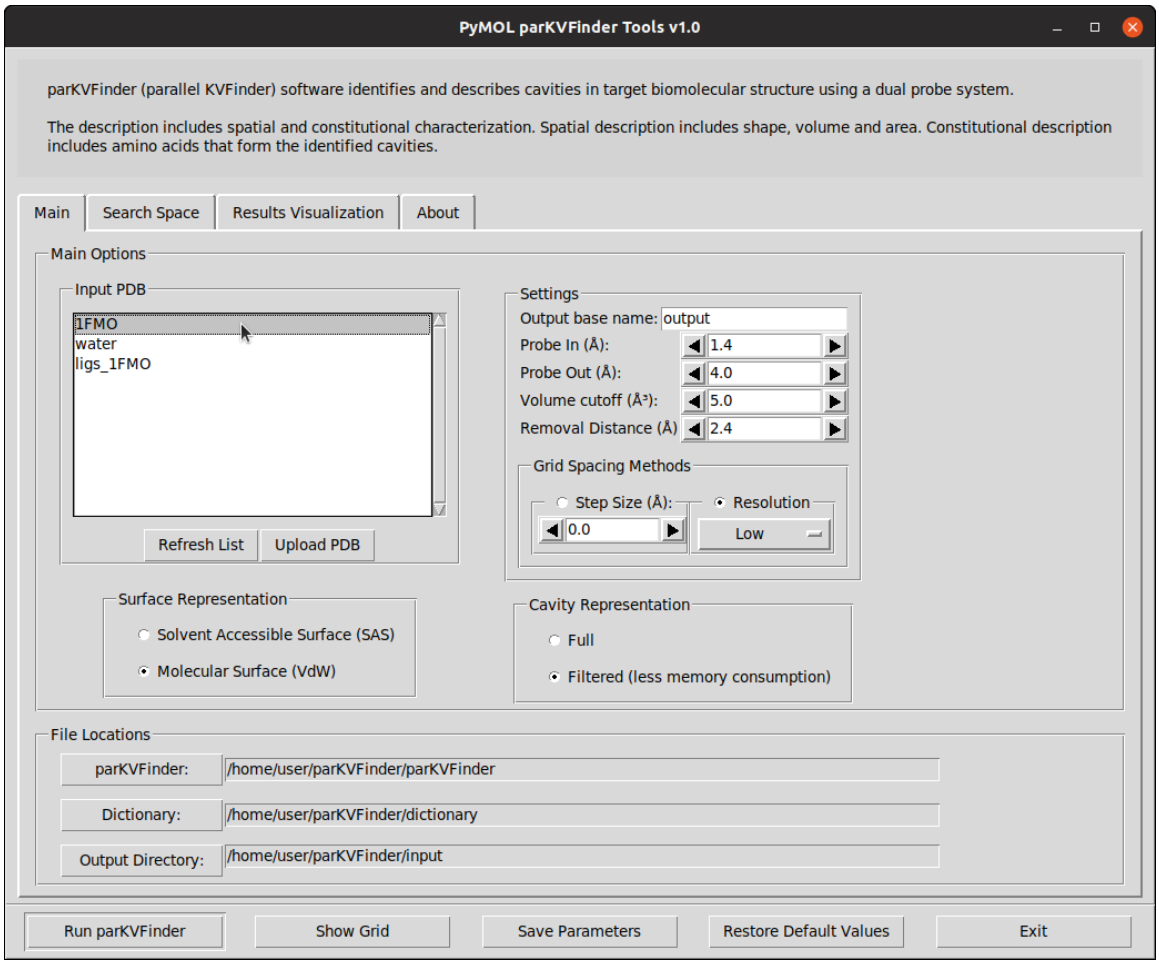


Default parameters

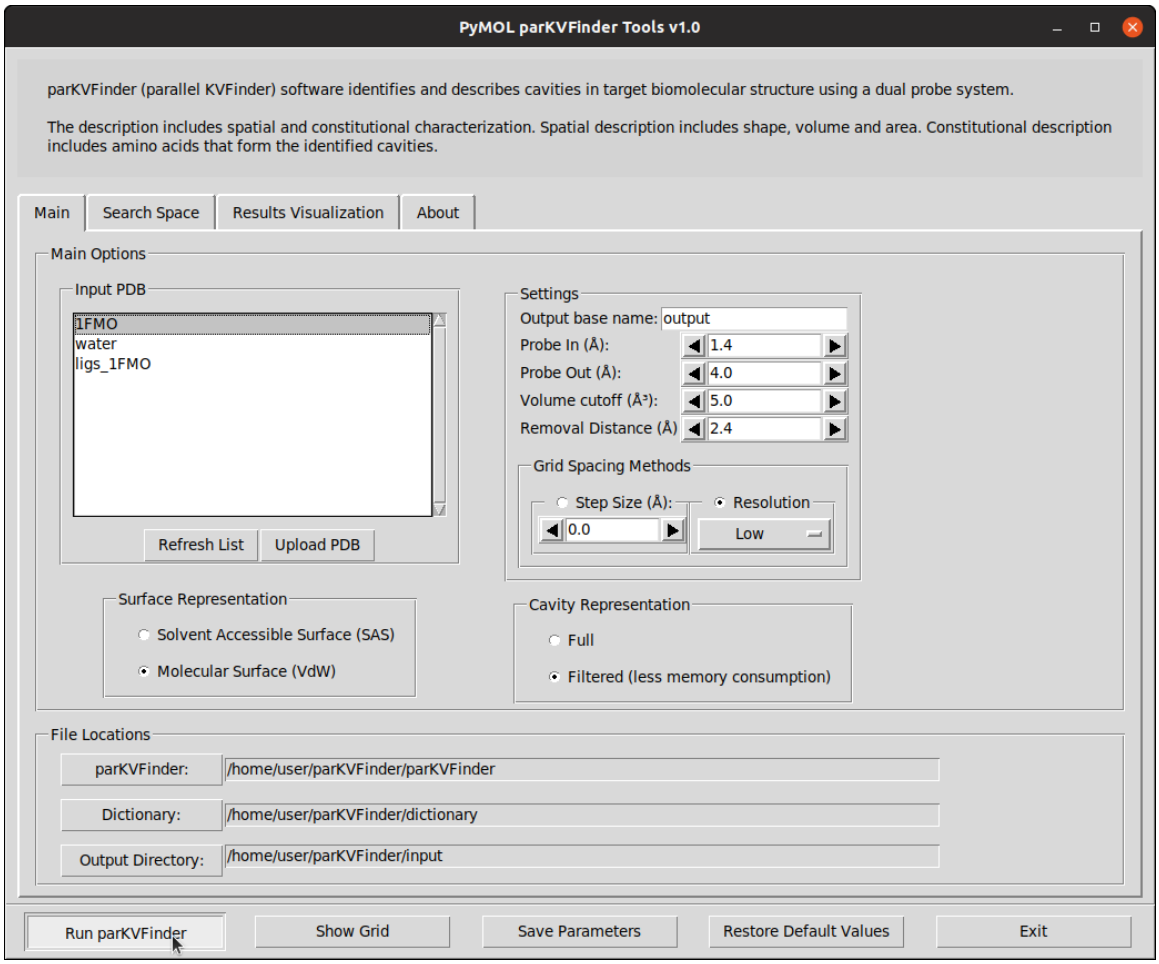
The default parameters are designed to make a simple and fast whole protein prospection.

On PyMOL, open **parKVFinder PyMOL Tools** under **Plugin** tab. The objects on the scene will be listed on the **Input PDB** listbox, on the **Main** tab. If not, press the **Refresh List**

The **Input PDB** selection sets which object will be analyzed by parKVFinder. Select **1FMO** on the listbox.



To run parKVFinder with the default parameters, just click **Run parKVFinder** button or press **Enter**.



After finish running, cavities PDB and results file are automatically loaded on **Results Visualization** tab.

Command line interface

parKVFinder has a command-line interface, which can be useful for molecular dynamics and high-throughput analysis. It also handles the same parameters available in parKVFinder PyMOL Tools, except for box rotations in box adjustment mode.
