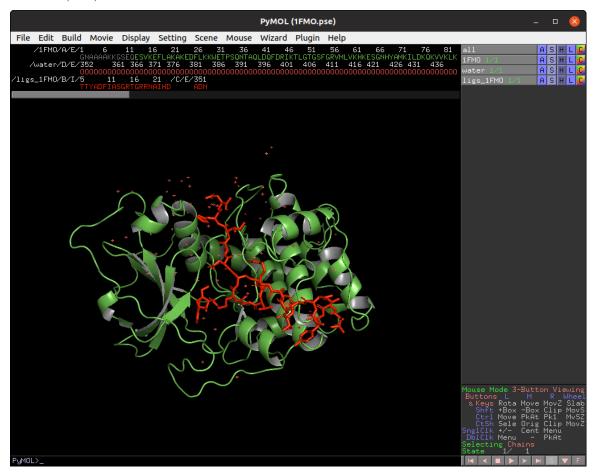
Tutorial

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

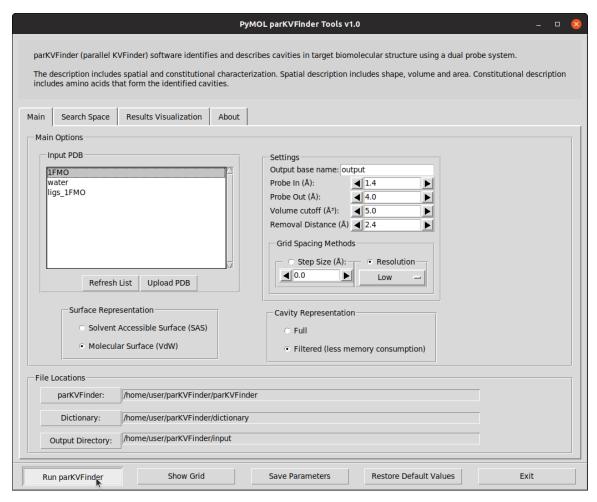
The default parameters are designed to make a simple and fast whole protein prospection.

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

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