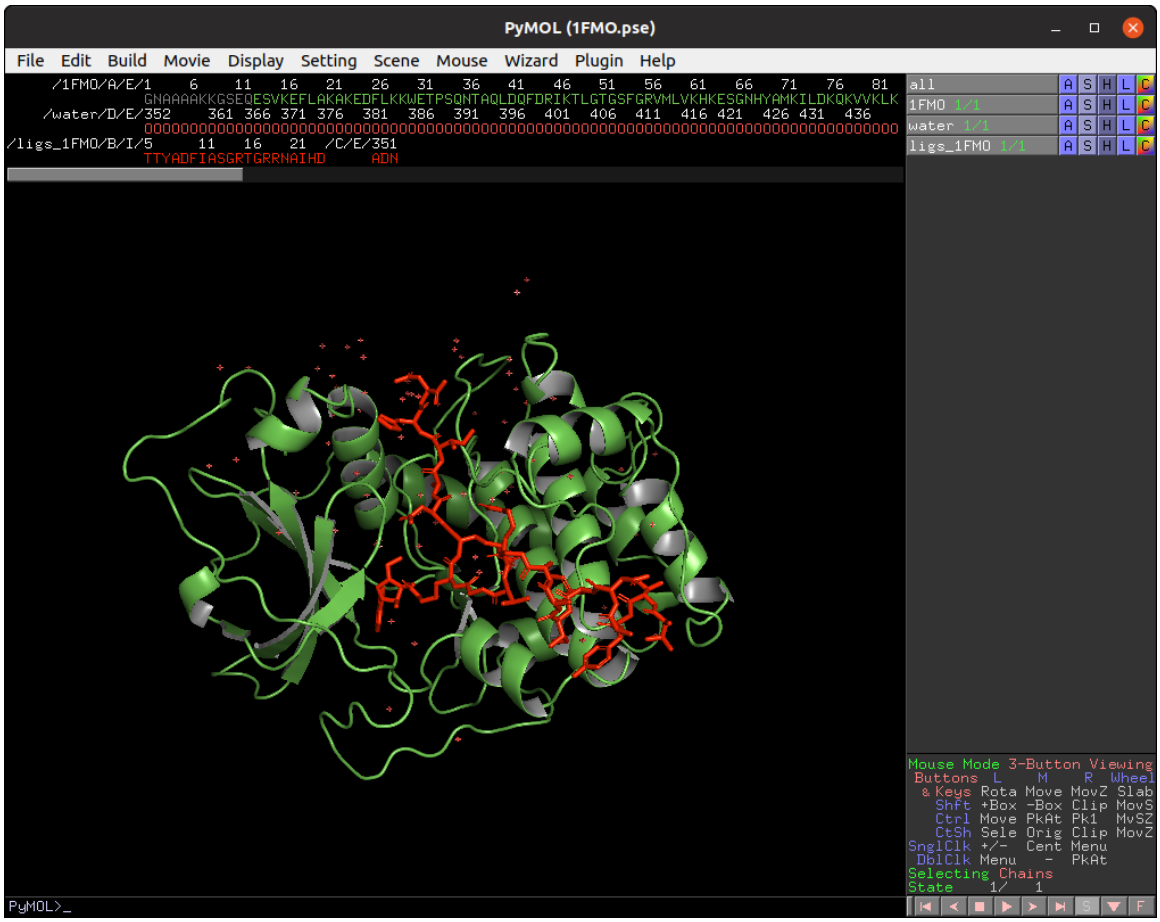
Tutorial

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 viewer, 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).

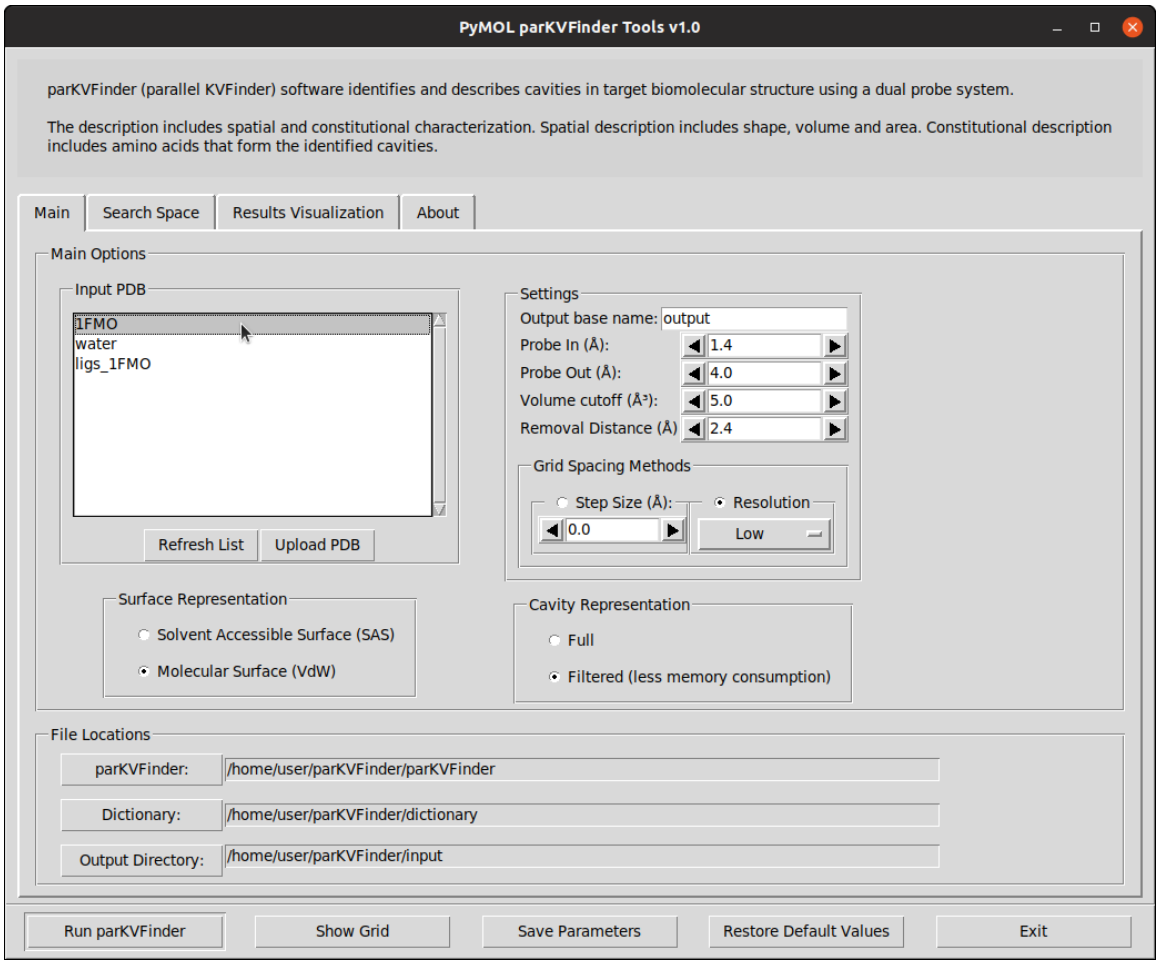


Default parameters

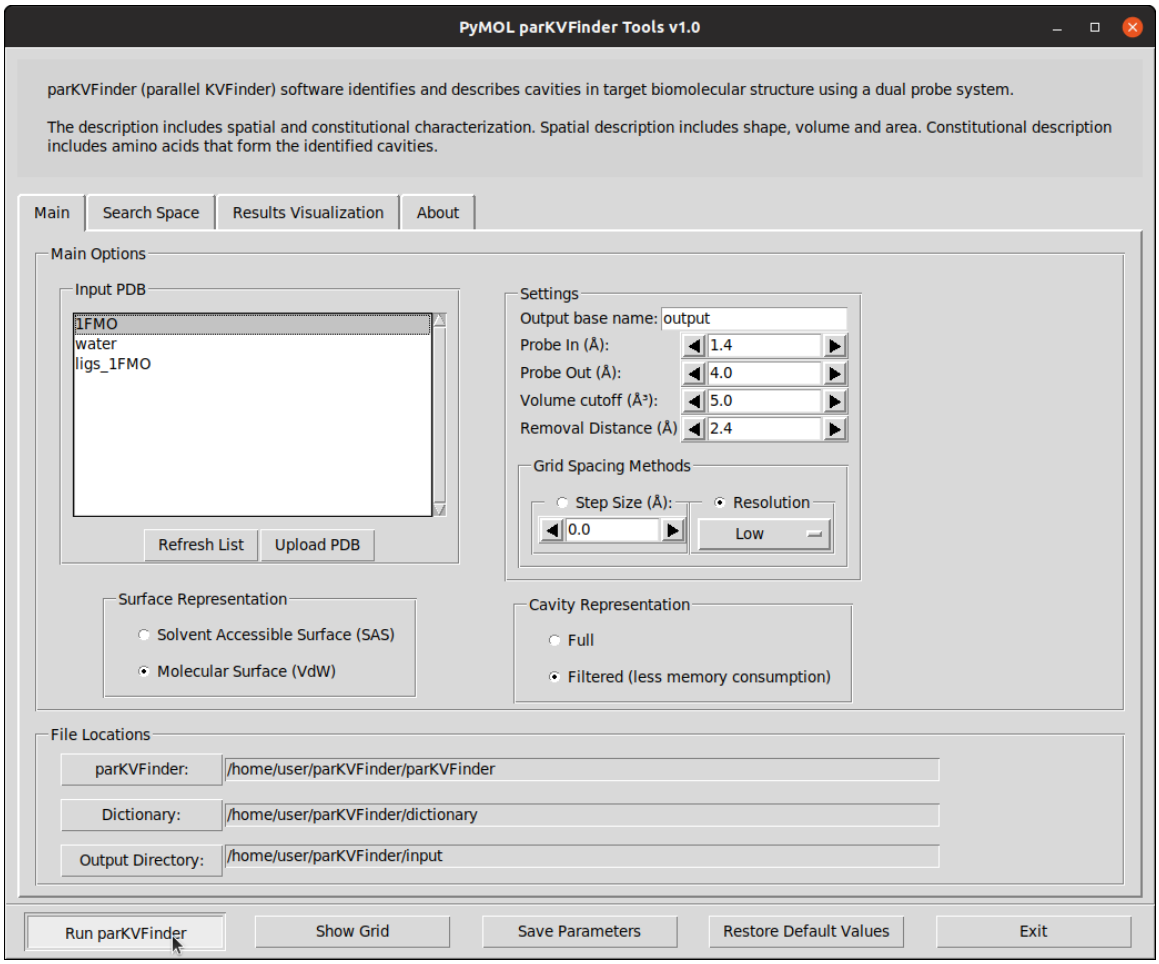
The default parameters are designed to make a simple and fast whole protein prospection.

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**

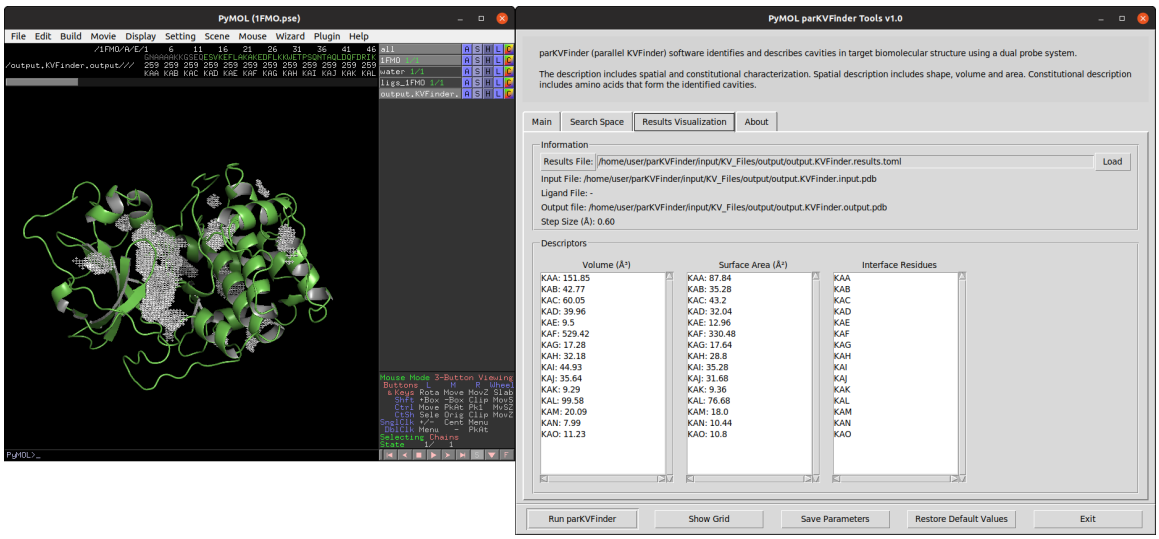
The **Input PDB** selection sets which object will be analyzed by parKVFinder. Select **1FMO** on the listbox.



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

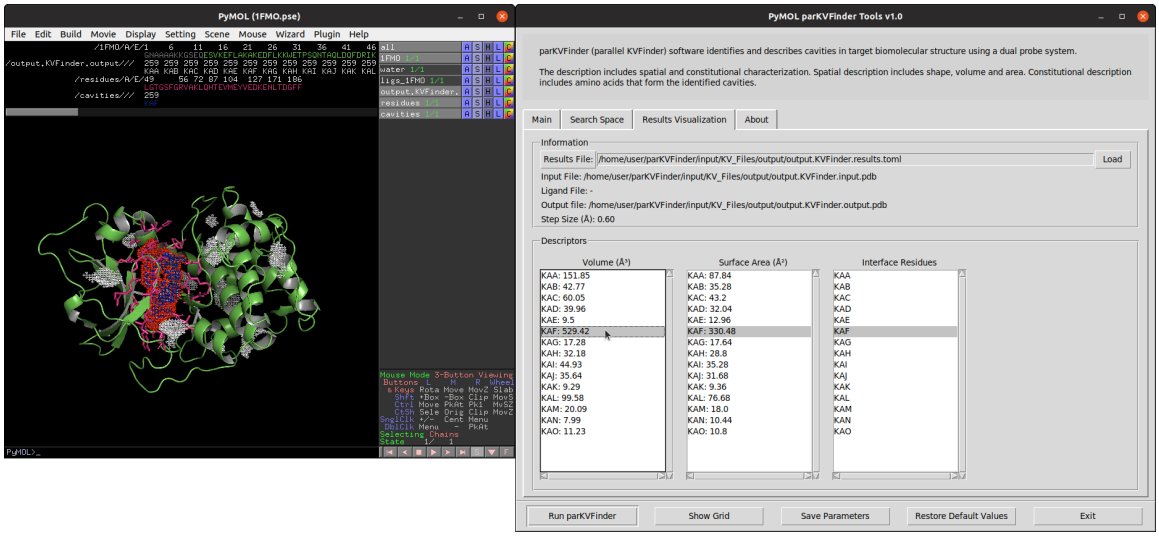


After execution is complete, cavities PDB is loaded into PyMOL viewer as <Output Base Name>.KVFinder.output object and the results file is loaded on the **Results Visualization** tab. In addition, the focus automatically shifts to **Results Visualization** tab.



You can select cavities in the **Volume** or **Surface Area** lists to highlight them on a new object called **cavities**, helping to identify each cavity. Also, you can select cavities in the **Interface Residues**

list to highlight the residues around the cavities on a new object named **residues**.



Changing cavity ceiling

parKVFinder is all about parameter customization. One of parKVFinder's most powerful assets is the ability to manually set the cavity ceiling. parKVFinder works with a double probe system. A smaller probe, called Probe In, and a bigger one, called Probe Out, that defines two molecular surfaces with different molecular accessibility. The space left between these surfaces is considered cavities.

Let's show the effect of varying **Probe Out** and **Removal Distance** on the cavity ceiling.

First, we should copy the adenosine to a new object using the following PyMOL commands:

```
# Copy adenosine
select resn ADN
create adenosine, sele
delete sele
```

Also, copy the adenosine cavity (KAF) to a new object to be able to compare cavity ceiling and prepare a new scene.

```
# Copy adenosine cavity
select resn KAF
create adnsite, sele
delete sele
# Prepare scene
color red, adnsite
disable
enable (adnsite, adenosine)
orient adnsite
```

Adjusting Probe Out

Adjusting Removal Distance

Exploring enclosed regions with box adjustment mode

Ligand adjustment mode

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.
