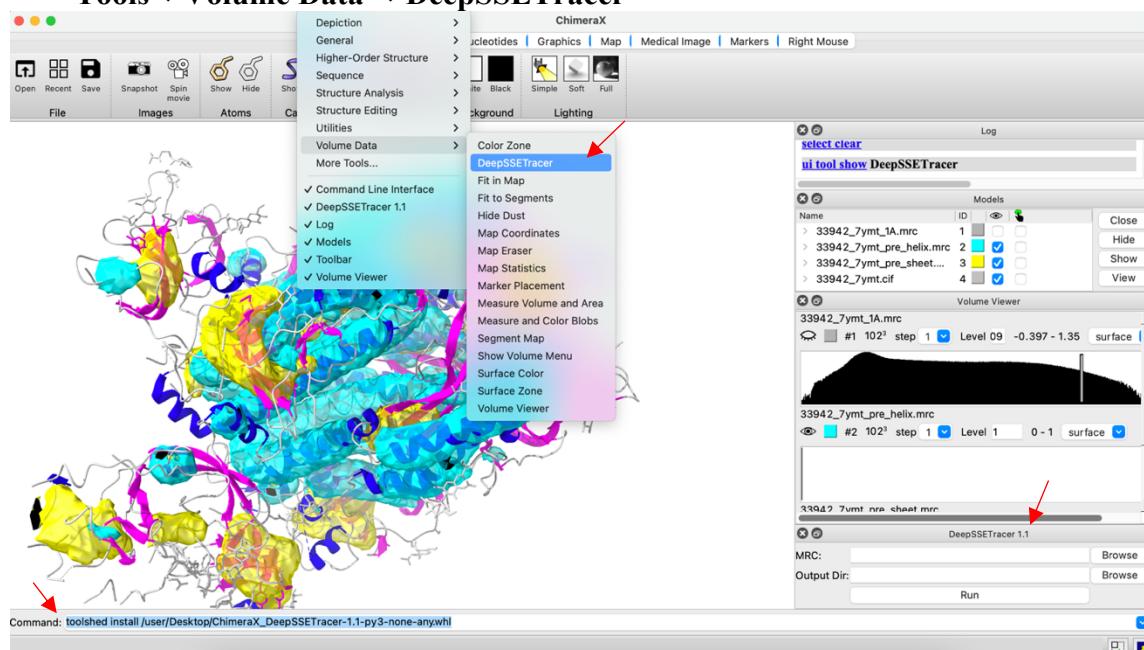


Manual for DeepSSETracer 1.1

Usage within UCSF ChimeraX

Download and Install:

1. Download and install UCSF [ChimeraX](#).
2. Download the zip file, the following files are provided:
|---DeepSSETracer
|---compiled_MacOS
|---compiled_Windows
|---DeepSSETracerBundle
|---sample_input_output
3. DeepSSETracer compiled files:
 - a. MacOS/Linux: ~/compiled_MacOS/ChimeraX_DeepSSETracer-1.1-py3-none-any.whl
 - b. Windows: ~/compiled_Windows/ChimeraX_DeepSSETracer-1.1-py3-none-any.whl
4. Uninstall the bundle using command line (Only if the bundle needs to be updated):
“toolshed uninstall DeepSSETracer”
5. Install the bundle using command line:
“toolshed install ~/path/to/compiled.whl”
6. DeepSSETracer will be available for using:
“Tools→ Volume Data → DeepSSETracer”



DeepSSETracer

DeepSSETracer is a tool for detecting secondary structures in medium-resolution cryo-EM density maps. The tool accepts any box-cropped cryo-EM maps; however, the map size may be limited depending on the device's resources. We are currently working on resolving the size limitation issue. The updated version will be able to accept maps of any size.

Required Input:

a. MRC/CCP4/MAP File:

The cryo-EM density map will be resampled automatically, click the browse button to select the file. (The density map can be cropped smaller using [Crop Volume Button](#), and [save the cropped density map](#) in ChimeraX)

b. Output Directory:

Click the browse button to select the Output folder path.

To Run:

After providing the necessary input, hit the “Run” button to start prediction. Once finished, the log information will be displayed.

Output:

1. “~/Output Directory/pre_helix.mrc”
2. “~/Output Directory /pre_sheet.mrc”
3. “~/Output Directory/pre_helix_cropped.mrc” (the 34 Å is cropped for each dimension)
4. “~/Output Directory /pre_sheet_cropped.mrc” (the 34 Å is cropped for each dimension)
5. “~/Output Directory/mrc_1A.mrc” (if the input density map is not resampled to 1Å)

Note:

The prediction may take several minutes or more without using a GPU; the time required depends on the size of the image.