# *Readme for installing "3D-printer" or "Build struts" PyMOL plugin and a tutorial on how to use it*

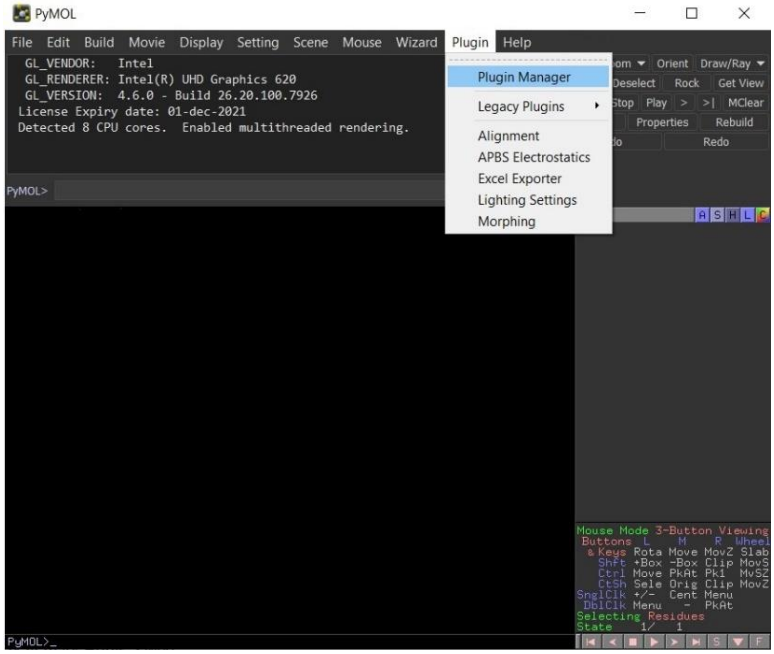
## Steps to install the plugin:

The following steps are applicable to both windows and macOS systems

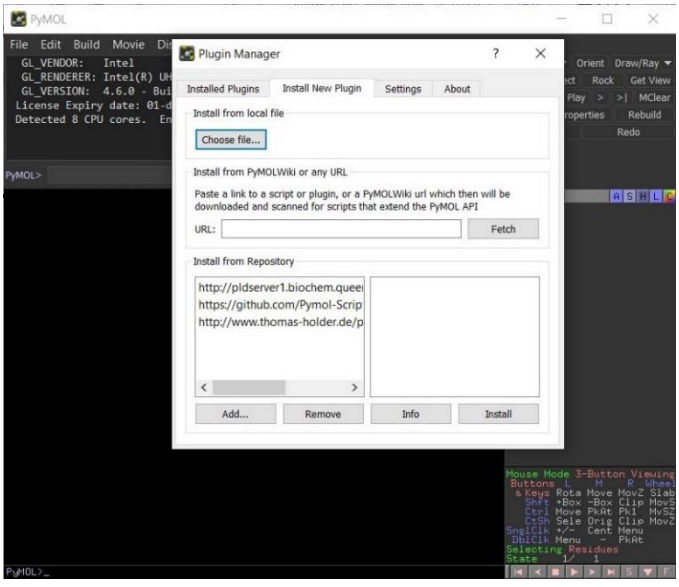
I. Download the '.zip' file and save it in your home directory. Once you unzip the file, you should see a directory named '3D_strut_plugin' containing three files:

   i) __init__.py  ii) struts.py  iii) build_struts.py

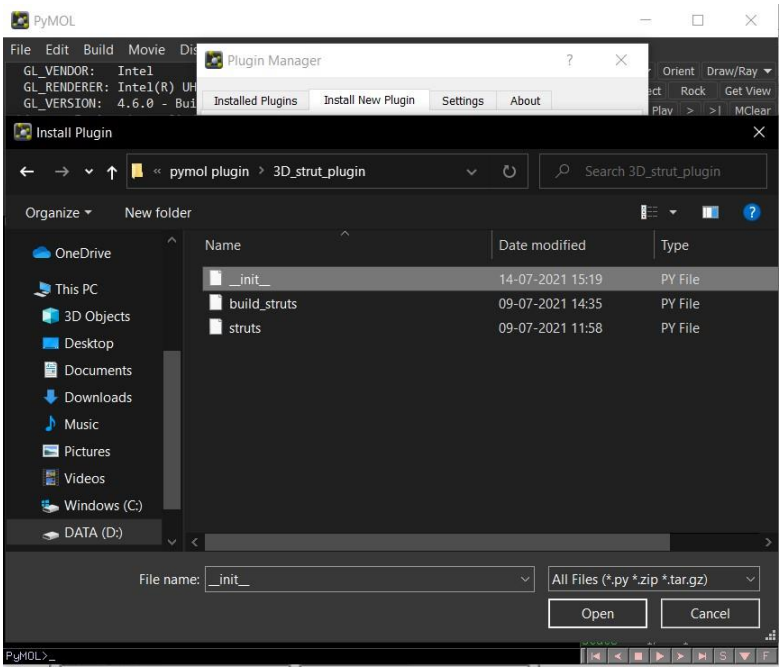
II. Open PyMOL and go to Plugin → Plugin manager.



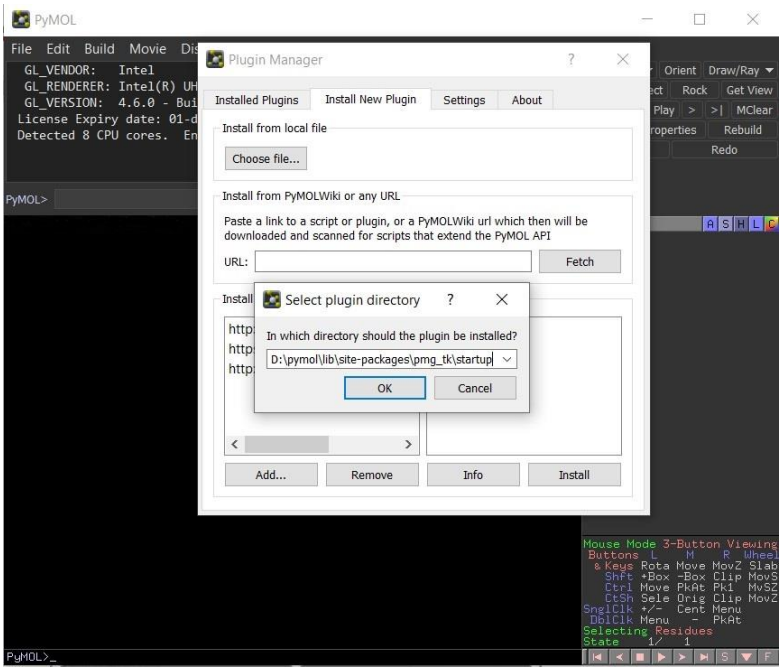

III. Select the 'Install new Plugin' tab and click on the choose button, a window will popup.



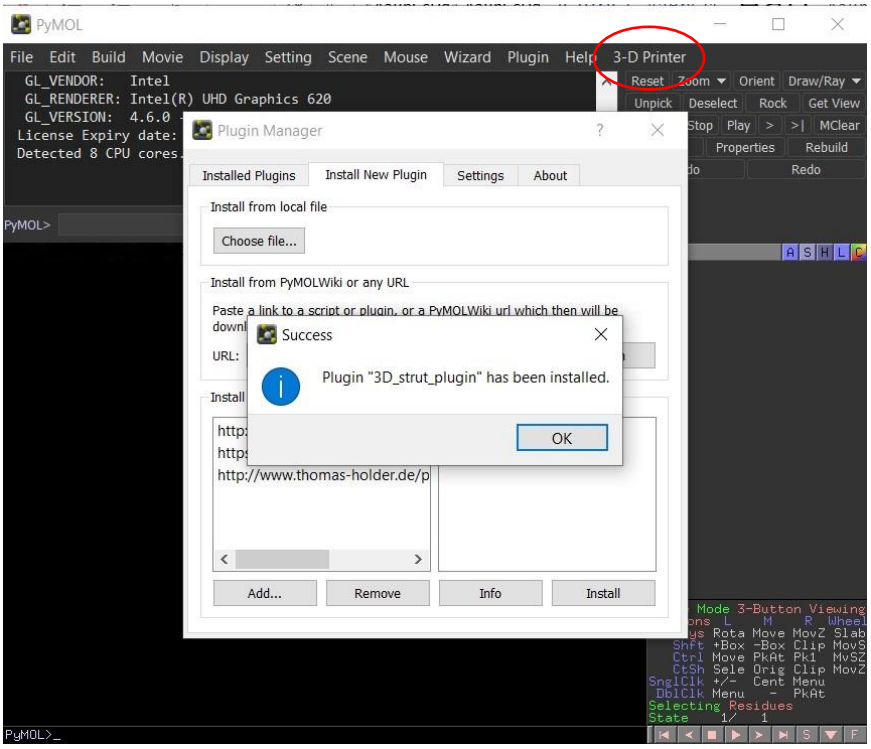
IV. Navigate to where you extracted the '.zip' file and select the '__init__.py' file. Click open.

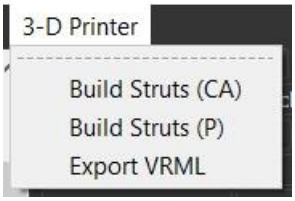



V. Make sure that the path in the 'Select Plugin directory' popup box is similar to the one in the figure below and then click ok.




VI. A new window will pop up with the message 'Plugin "3D_Strut_plugin" has been installed." and a new menu named "3-D printer" will be added to the menu bar. If you do not see the new menu immediately, close the plugin manager window quit and re-open PyMOL.



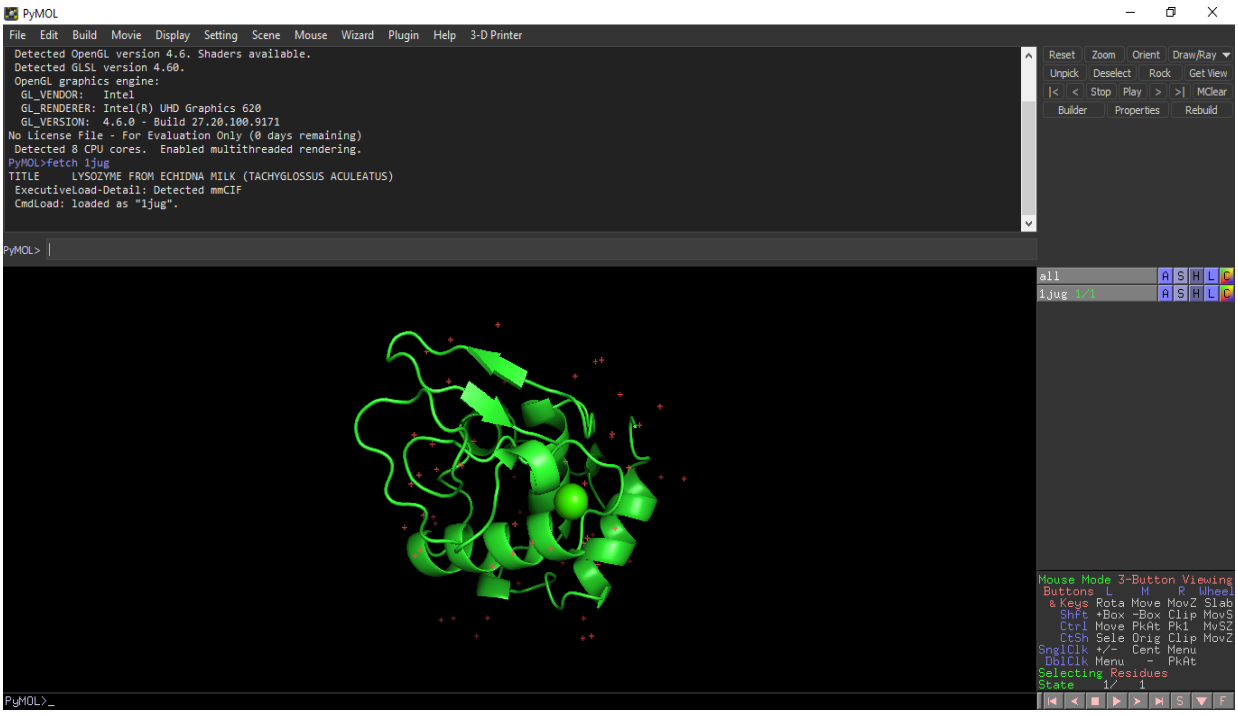




## Error after installation:

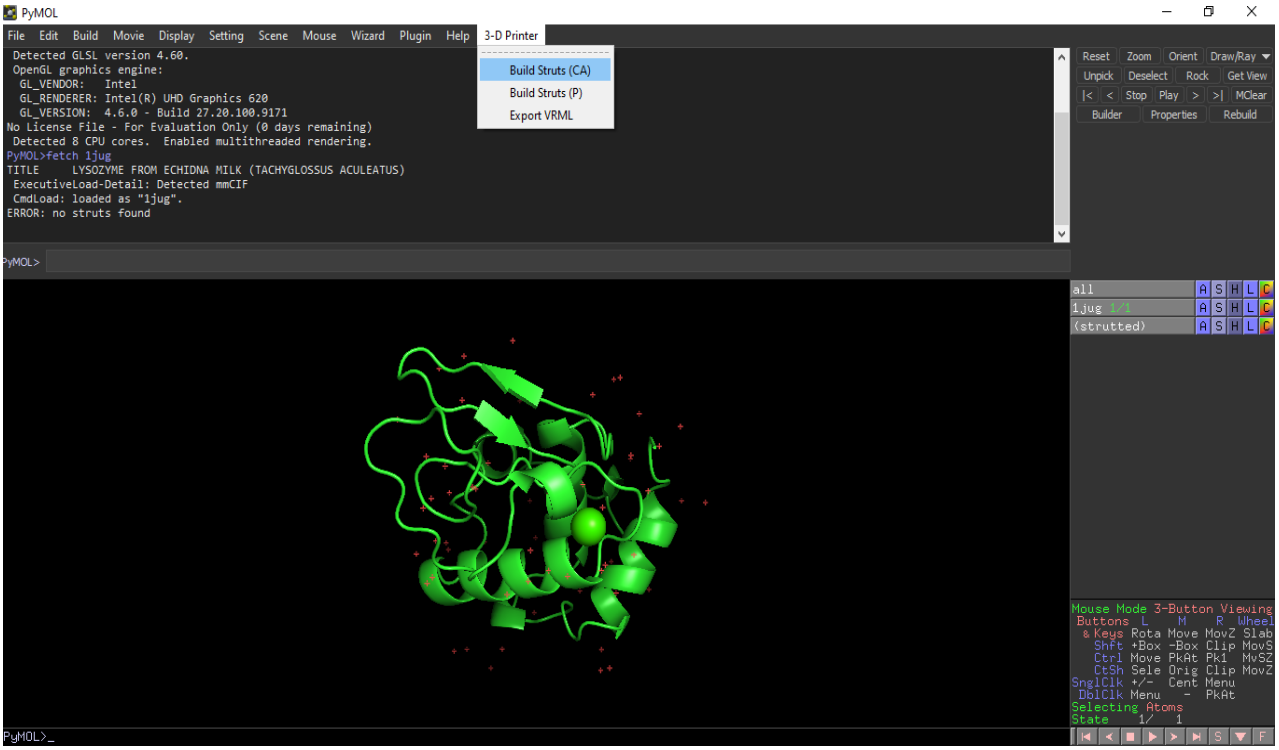
If you get ‘Plugin “3D_strut_plugin” has been installed but failed to initialise’ message after installing the plugin, check the command line in the main window of PyMOL and install any missing dependency files. Redo the installation steps.

# Tutorial:

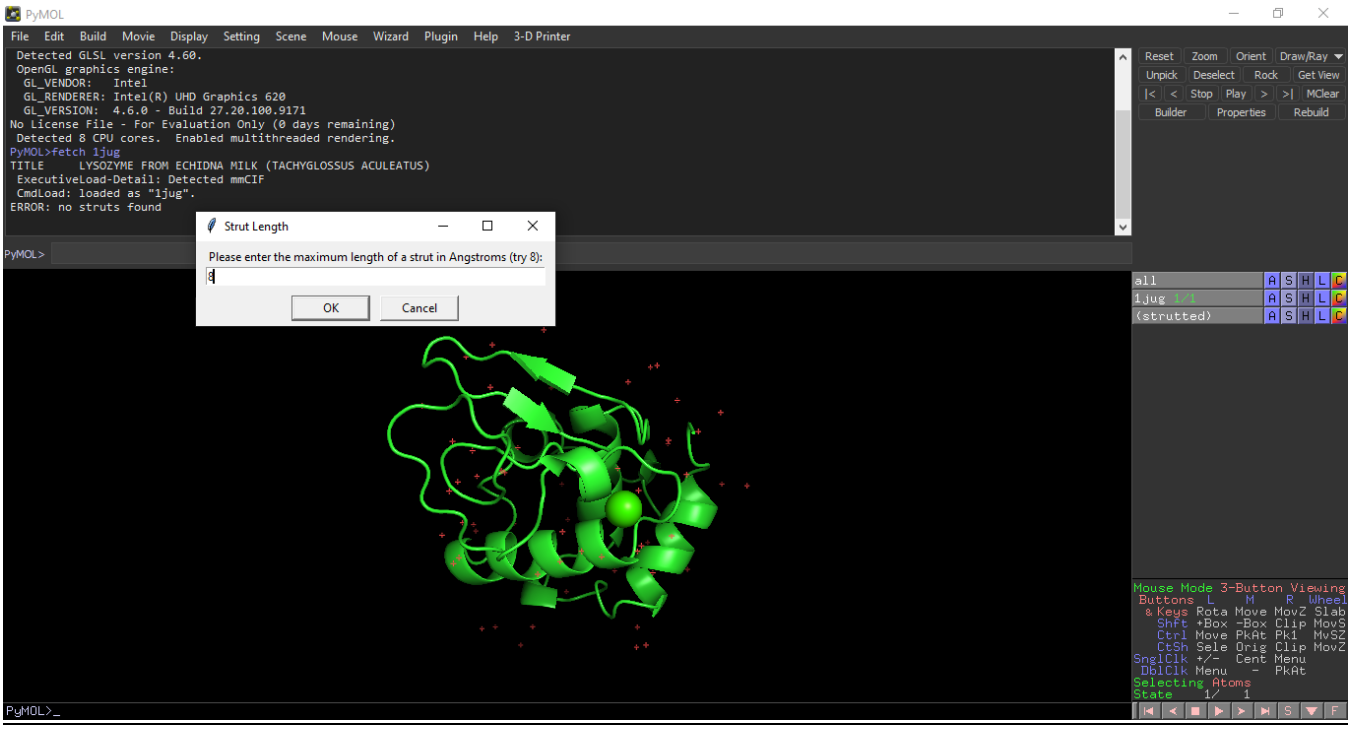
Open a pdb file of your choice



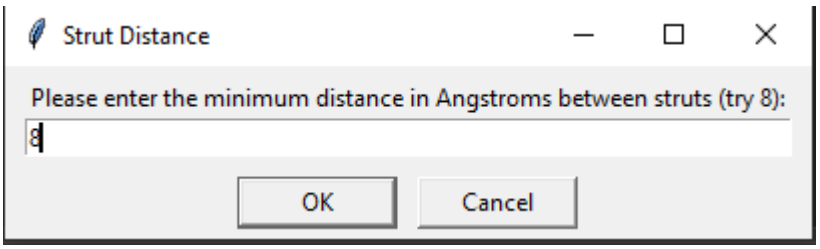

3D Printer -> Build Struts (CA)



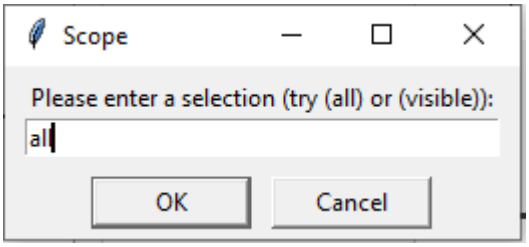
A popup will ask you to enter a value for the maximum length a strut can be. Try 8. Click OK to proceed to next step/popup.



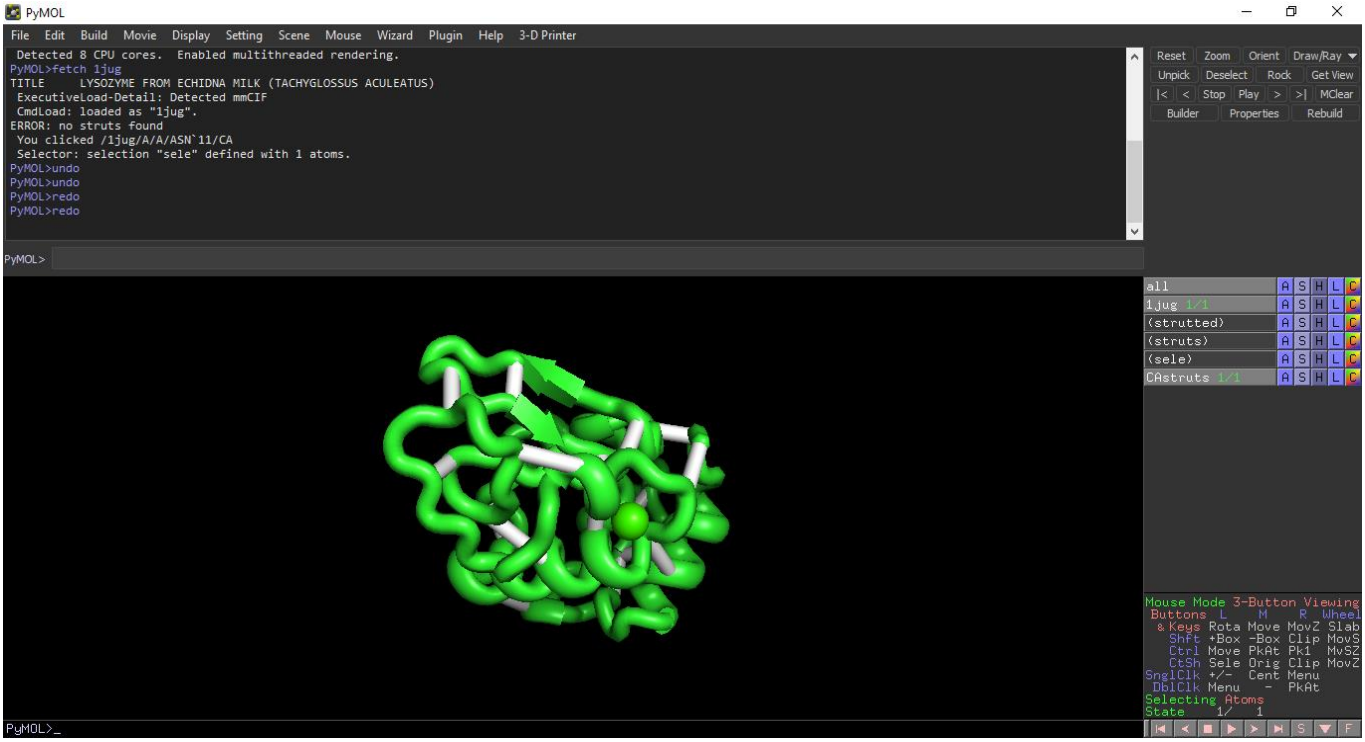

Then, enter the value for the minimum distance between struts. Try 8.



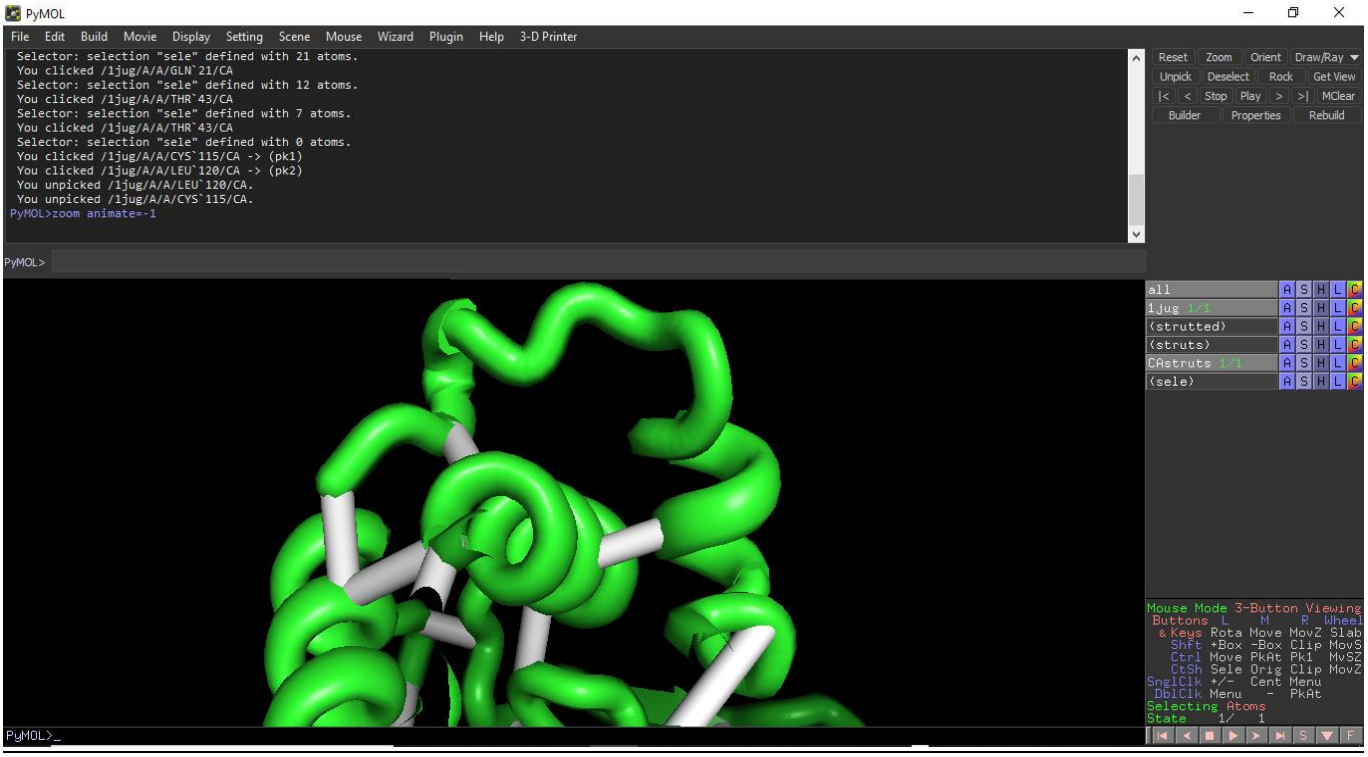

If you want to build struts for everything opened in pymol, type “all”. Otherwise, if you want only one chain to be built, select that particular chain, make a new object, and hide the rest of the protein. In this case, you will type “visible”



And Eureka!

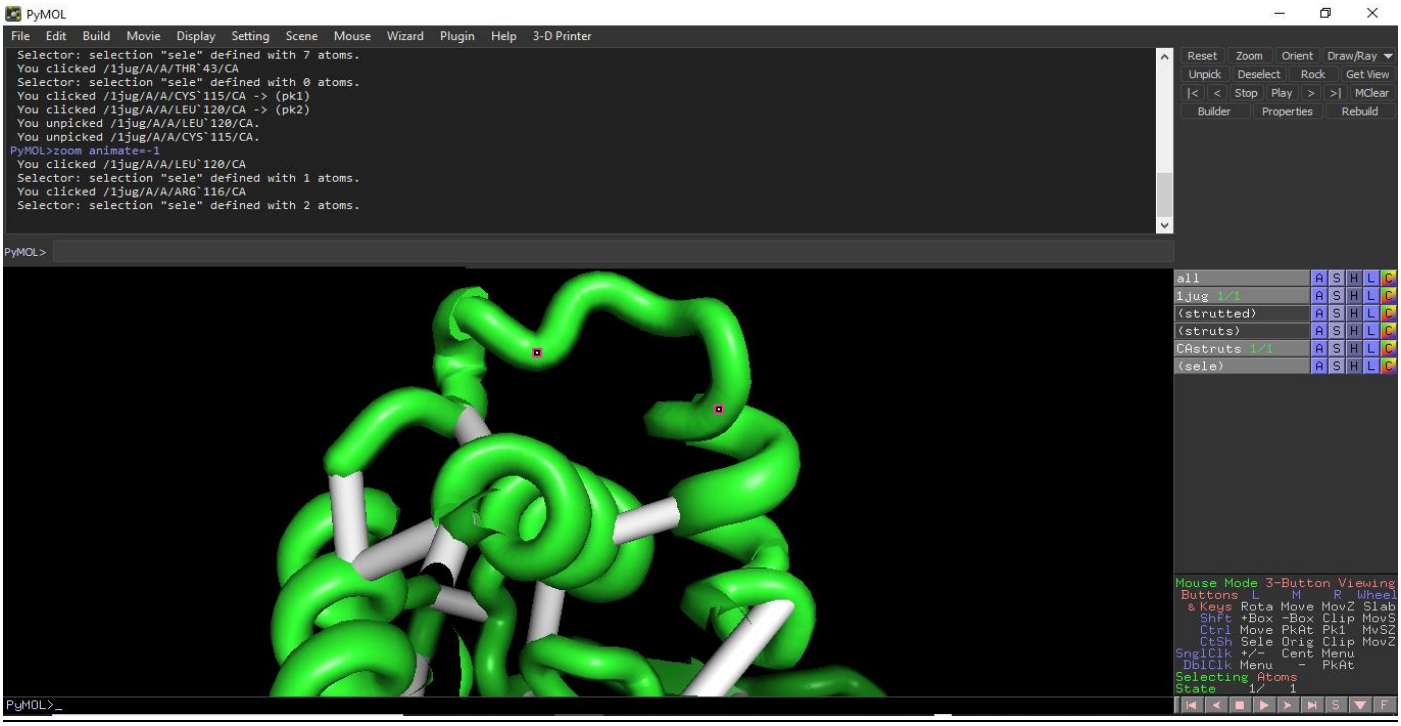



You should look for spots where building one more strut would make the printed model structurally stable. For example, in this case this loop will be unstable after printing and will crumble during processing of the model.

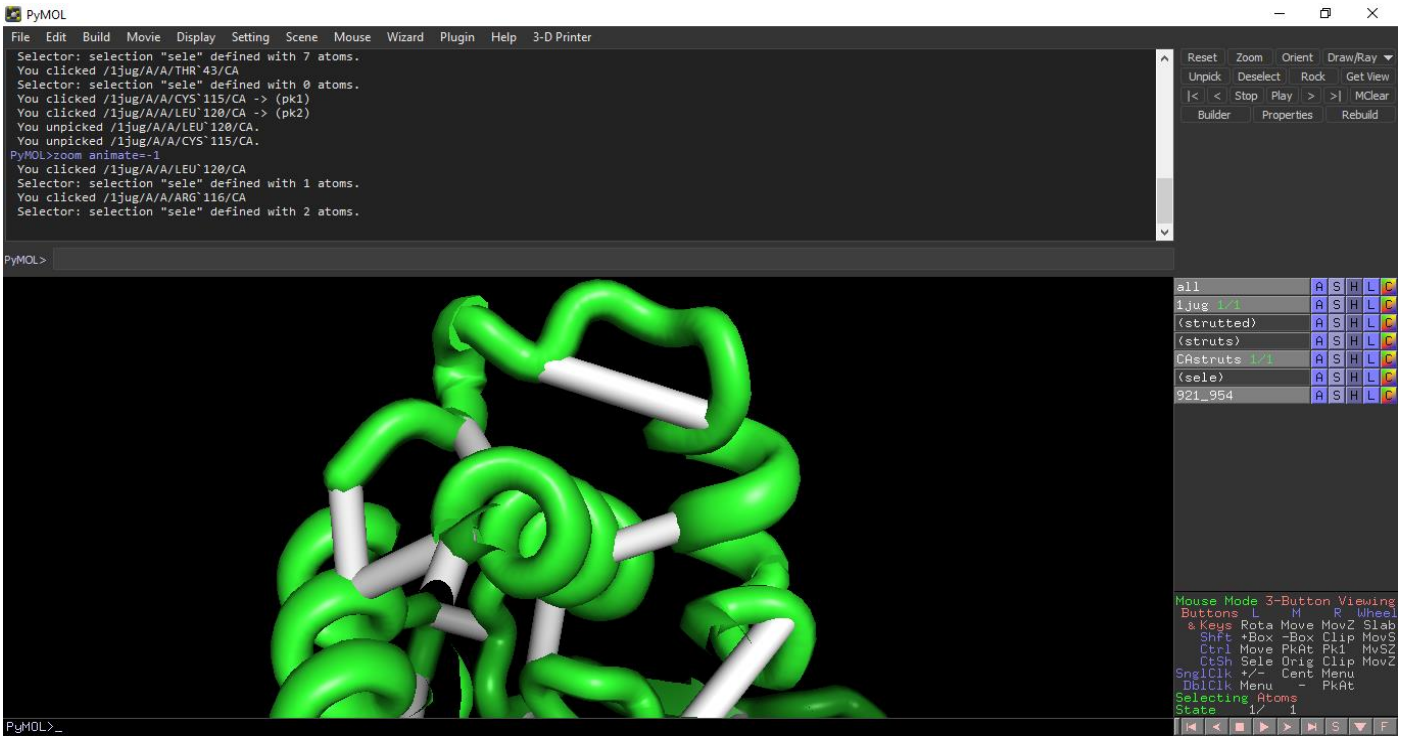



For the additional struts to be built, change the selection mode from “Residues” to “Atoms”.


_Pick the two atoms.




and press F1. (In some keyboards the “fn” button needs to be pressed while pressing F1).



Play around with parameters like “cartoon_rect_width”, “cartoon_rect_length”, “cartoon_oval_width”, “cartoon_oval_length”, and “cartoon_loop_radius”. Basically, the more fatter it looks on screen, the more stable it will be after printing. Once you are satisfied with the model save it as as pymol session file and as a .wrl file.

File-> Save Session As

File-> Save Image As-> VRML 2 (remember to save it with extension .wrl)

You are all set for printing.