



Using PyMOL to create suitable model for print

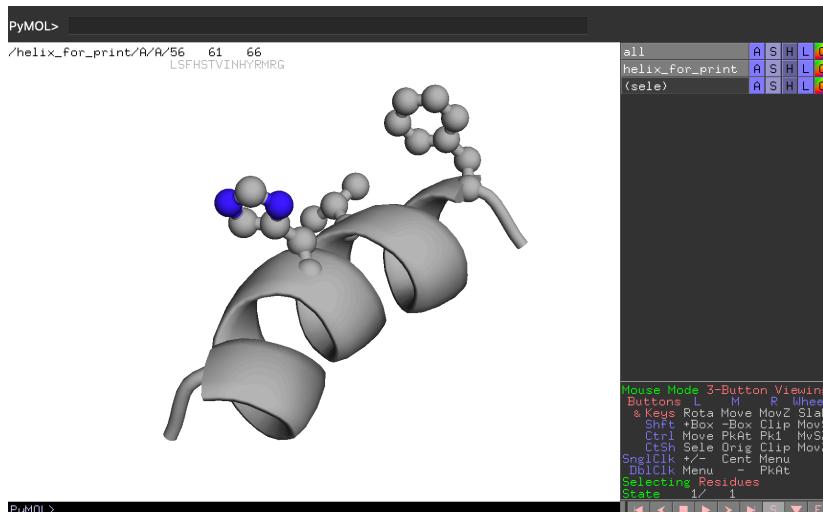
Lena Quambusch - Mar 13, 2023 at 7:12 PM GMT

1. PyMOL

Printing 3D structures of Proteins can be challenging. Most details are too delicate for the printer or might lack stability in the end. Protein surfaces might be a lot easier than secondary structures. Since we don't print with *soluble* support, but the structures depend on solid support during printing, it might be very tricky to get rid of the material inside those folded structures.

Therefore one needs to adjust the size and volume of the structure in PyMOL. Probably it will work in a 3D modeling software as well, but this might be more complicated.

The Helix pictured below has some altered setting compared to the default presentation. The width and length of the cartoon was increased as well as the stick and ball radius/size. (Not sure if those are optimal parameters. Try and error I guess...)



settings:

```
stick_radius, 0.28
sphere_scale, 0.38
cartoon_oval_width, 0.45
cartoon_oval_length, 1.6
cartoon_loop_radius, 0.3
```

(In case of side chains and sticks, turn off valences)

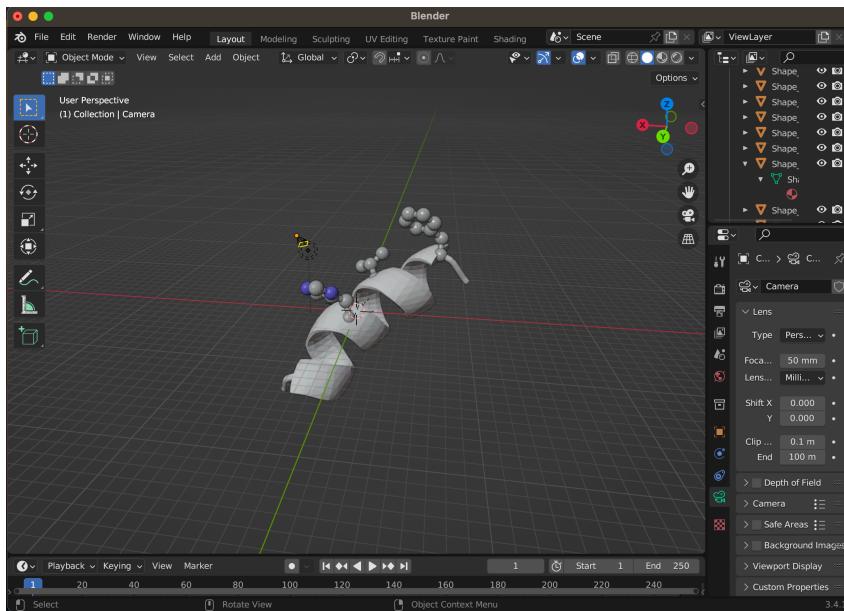
PyMol can export images as .stl directly under > file > export image as > STL...

Some versions don't support that command (like the Open-Source one). In that case one can export the image (so the visible molecule) as VRML 2 under the same directory. This file format is not compatible with every 3D modeling software, but with Blender for example (see next step).

2. Blender

If PyMOL couldn't export the image as .stl file, the vrml2 (.wrl) file needs to be converted into the right format. Therefore open the file with Blender > file > import > X3D Extensible 3D (X3D/wrl).

There will be a little cube in the middle of the screen and loaded model, just right click on it to delete.

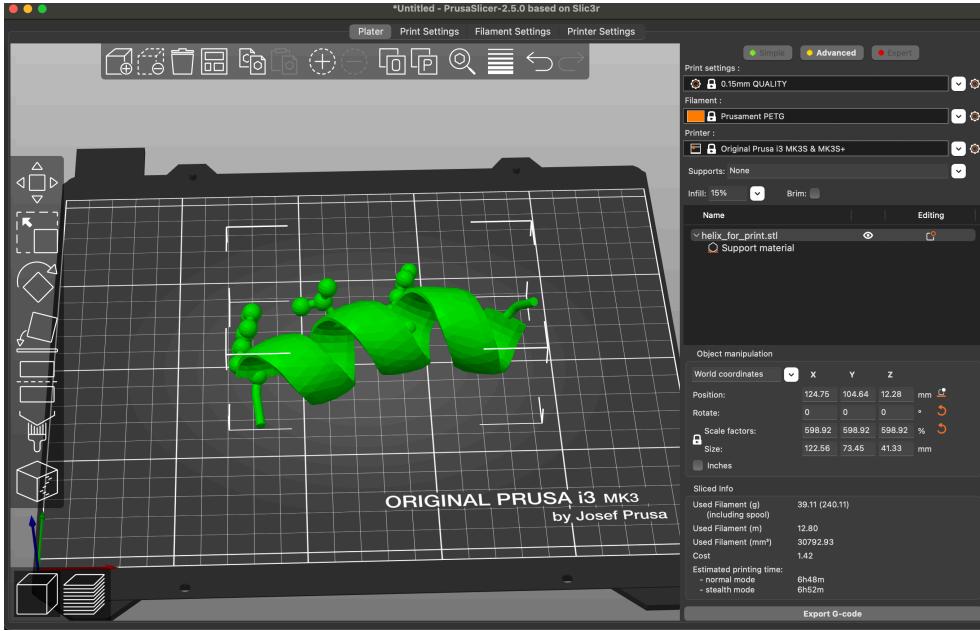


Already done for export > file > export > Stl (.stl).

3. PrusaSlicer

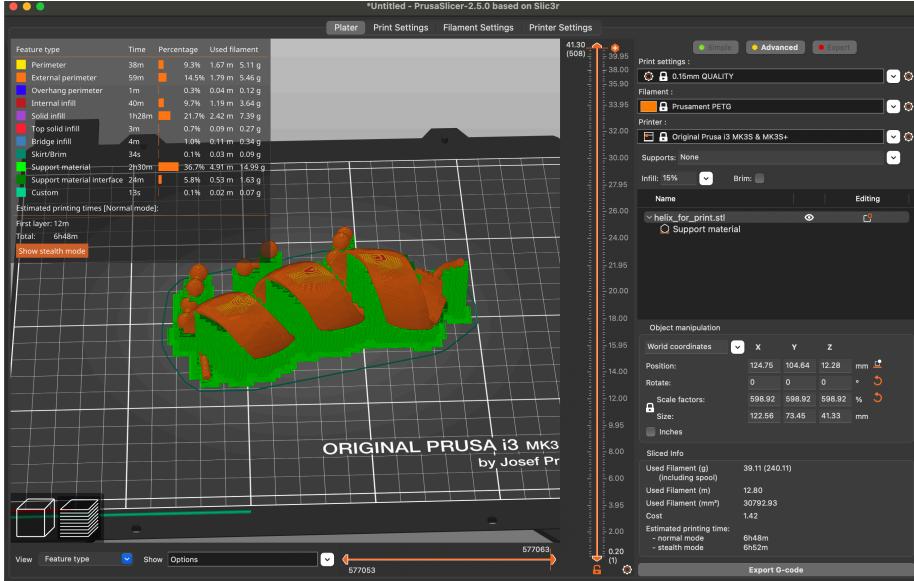
The .stl file is ready for printing now. Once loaded into PrusaSlicer the size needs to be adjusted. The model will be very small in size based on the original coordinates and scales.

1. Adjust size.
2. Select "Place on Face" to pick the orientation for the base of the model.



3. Adjust all the printing parameters and select Support material!

4. Generate G-Code of the model.



5. Once satisfied with all setting export the g-code.

Everything ready to print!

