3DP-Jmol
an automatic tool for generating 3D printable molecular models from structural data

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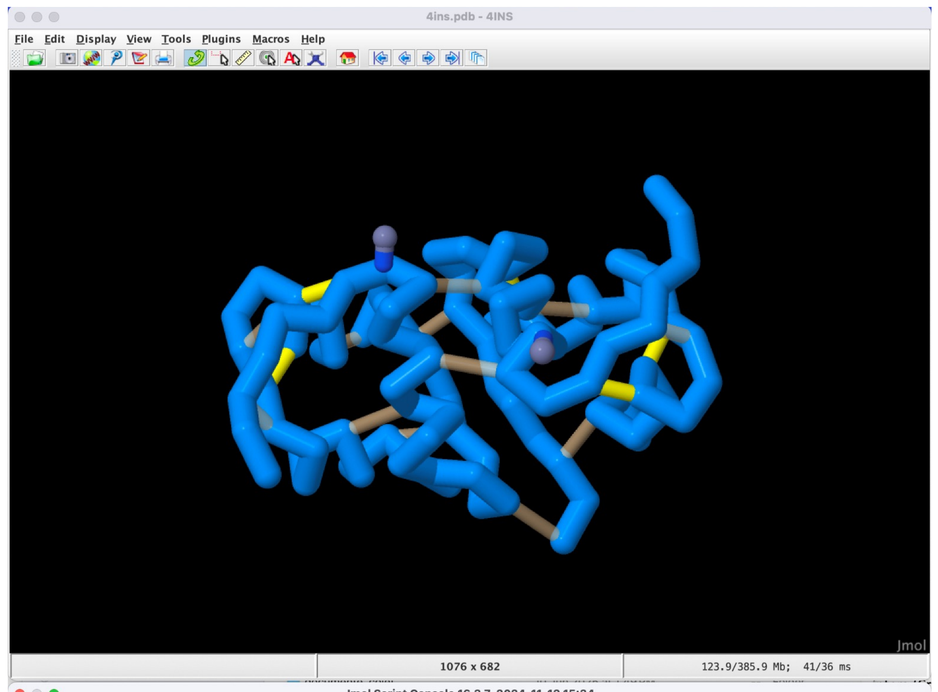
Introduction

Physical models of macromolecules have been shown to improve learning gains under various settings and to be well received by students and educators alike. Various systems to produce physical models are available, but coupling the available structural databases with 3D printing is by far the most flexible. Hypothetically, any life-science educator would be able to select any PDB entry, generate a custom physical model adapted to his teaching goals and fabricate it using consumer-grade 3D printers. The major bottleneck in this approach is the conversion of the structural data into reliable printable files. This step requires knowledge in structural biology and 3D printing technology and is key not only for the printability, but also for the model's success as an educational or demonstration material. To automate the process, **3DP-Jmol** was created.

How it works

3DP-Jmol is a script that can be run in the Jmol console and can:

- automatically **loads structural data** from known databases (RCSB PDB, PubChem)
- **evaluates the size of the model**, atom types and bond lengths
- **calculates** maximum and minimum **printable size** of the final physical model
- **indicates** suitable **rendering styles** depending on the user selected model size
- automatically **generates struts** for improved printability, including for ligands
- **generates** printable **.stl** (monochrome) or **.obj** (multi-colour) **files**.

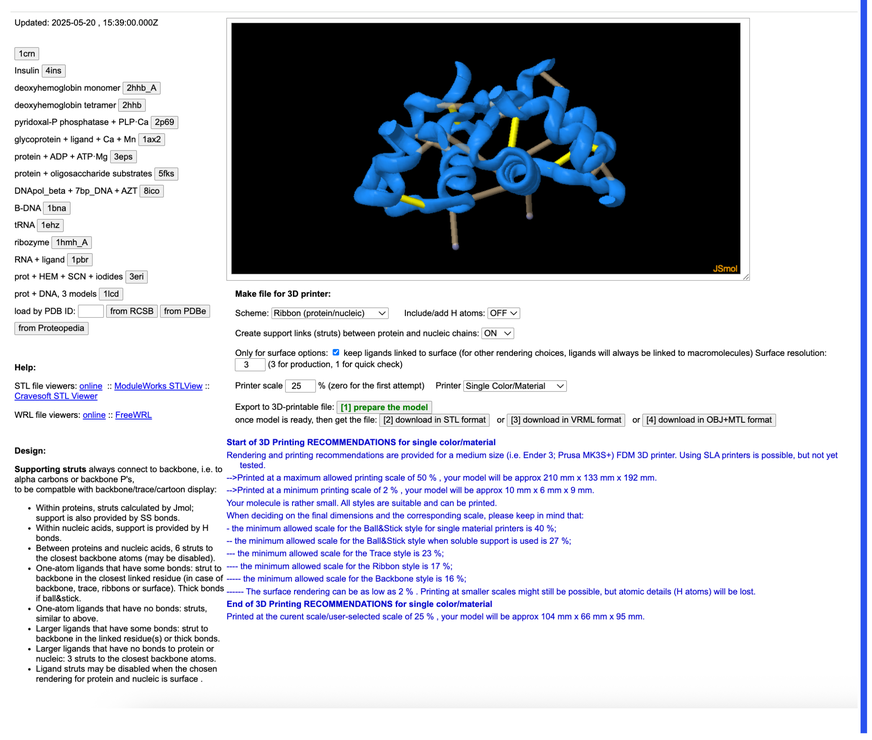


Easy to integrate into web-pages

3DP-Jmol can be run with JSmol too and can be easily integrated into web-pages.

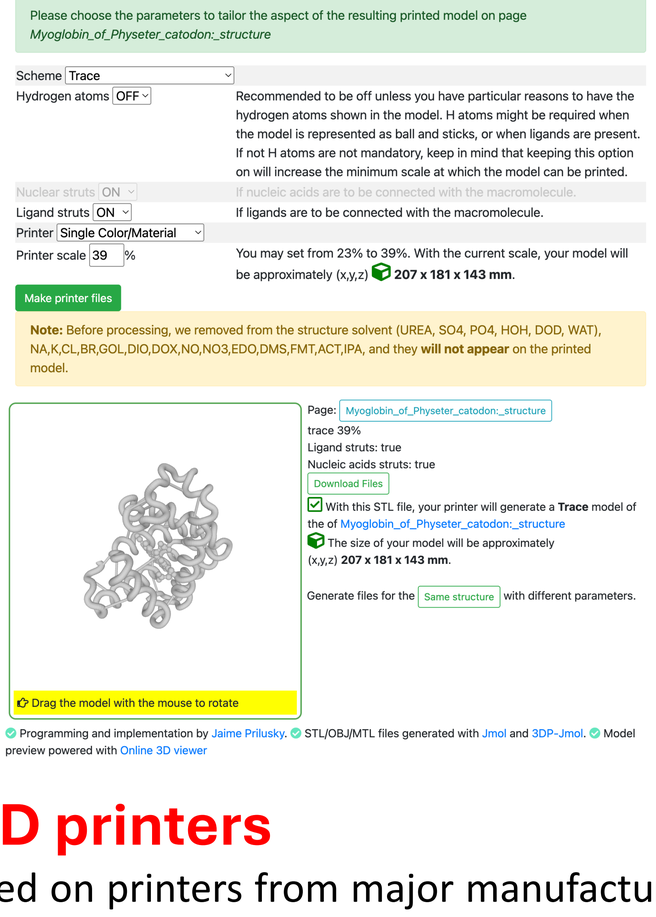
On biomodel.uah.es

https://biomodel.uah.es/JSmol16/3Dprint/3Dprint_2.htm



On Proteopedia

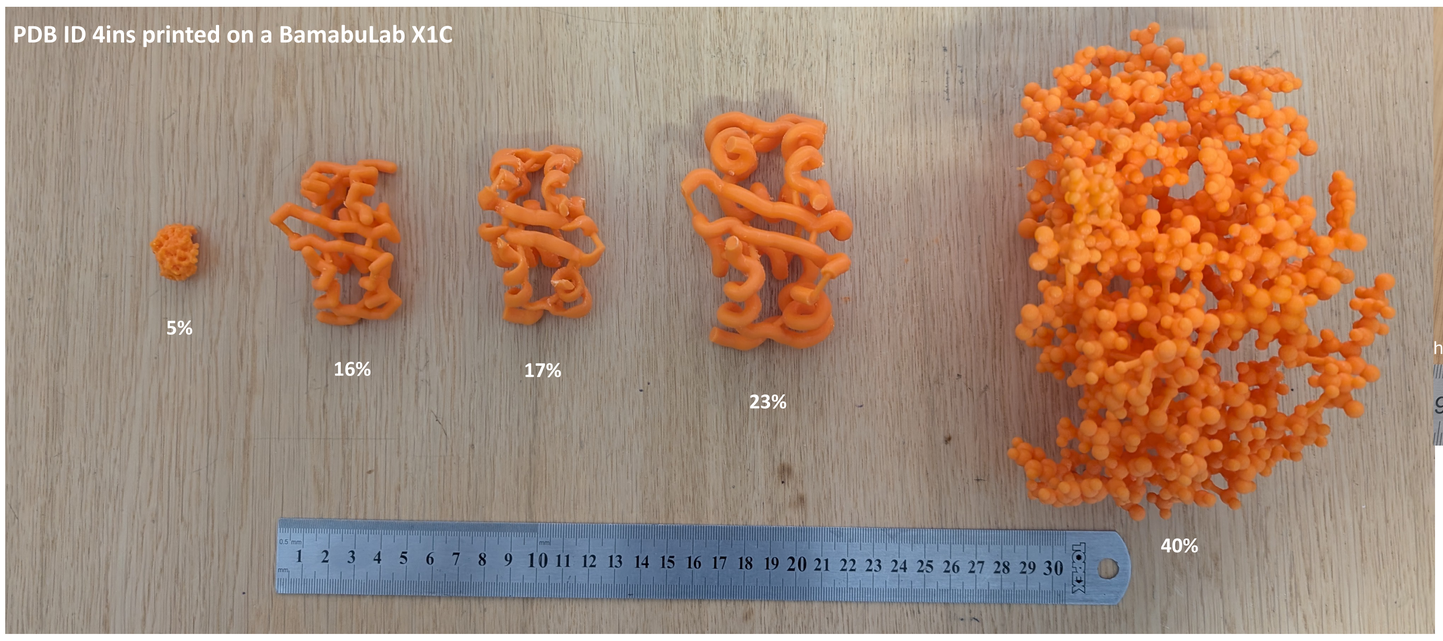
(experimental, not yet publicly available)

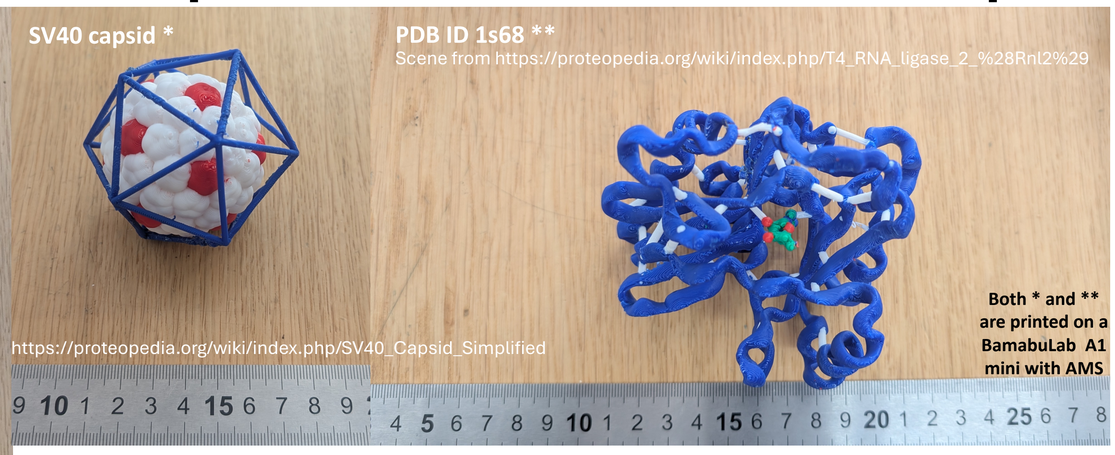


Output files tested on various 3D printers

The printability of 3DP-Jmol output files was tested on printers from major manufactures, including Prusa Research (MK3S+ and Core One), BambuLab (A1 mini and X1C), Creality (Ender 5 and Ender 3)

Experimental feature: color output





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3DP-Jmol: https://github.com/mariusmihasan/3DP-Jmol

3D printing profiles: https://github.com/mariusmihasan/molecularmodels-3d-printing-profiles

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