



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

Updated: 2025-05-20, 15:59:00.000Z

10m

Insulin [4ns]

deoxyhemoglobin monomer [2hhb_A]

deoxyhemoglobin tetramer [2hhb]

pyridoxal-P phosphatase + PLP-Ca [2y69]

glycoprotein + ligand + Ca + Mn [1s62]

protein + ADP + ATP-Mg [3ap1]

protein + oligosaccharide substrates [5fks]

DNApol_beta + Topo_DNA + AZT [8co]

B-DNA [1bna]

IRNA [1ahz]

ribosome [1trh_A]

RNA + ligand [1tbr]

protein + DNA + 3 models [1icd]

used by PDB ID: [] from RCSB [] from PDBe [] from Proteopedia []

Help:

STL file viewers: [online](#) - [Module/Works STLView](#) - [Craveasoft STLViewer](#)

VRML file viewers: [online](#) - [ErosVRML](#)

Design:

Supporting struts always connect to backbone, i.e. to alpha carbons or backbone P_α, to be compatible with backbones/cartoon display:

- Within proteins, struts calculated by Jmol; support is also provided by SS bonds.
- Within nucleic acids, support is provided by H bonds.
- Between proteins and nucleic acids, 6 struts to the closest backbone atoms (may be disabled).
- One atom ligands that have some bonds: attach to backbone in the closest linked residue (in case of backbone, trace, ribbons or surface). Thick bonds if Ball&Stick.
- One atom ligands that have no bonds: struts similar to above.
- Larger ligands that have some bonds: struts to backbone in the linked residue(s) or thick bonds.
- Larger ligands that have no bonds: no protein or nucleic struts to the closest backbone atoms.
- Ligand struts may be disabled when the chosen rendering for protein and nucleic is surface.

Make file for 3D printer:

Scheme: [Ribbon (protein/nucleic)] Include/Hide H atoms: [OFF] [v]

Create support links (struts) between protein and nucleic chains: [ON] [v]

Only for surface options: [] keep ligands linked to surface (for other rendering choices, ligands will always be linked to macromolecules) Surface resolution: [3] [v] (3 for production, 1 for quick check)

Printer scale: [25] [%] (zero for the first attempt) Printer: [Single Color/Material] [v]

Export to 3D printable file: [1] [prepare the model](#) once model is ready, then get the file: [2] [download in STL format](#) or [3] [download in VRML format](#) or [4] [download in OBJ+MTL format](#)

Start of 3D Printing RECOMMENDATIONS for single color/material

Rendering and printing recommendations are provided for a medium size (i.e. Ender 3; Prusa MK3S+) FDM 3D printer. Using SLA printers is possible, but not yet tested.

-->Printed at a maximum allowed printing scale of 50 % , your model will be approx 210 mm x 133 mm x 192 mm.

-->Printed at a minimum printing scale of 2 % , your model will be approx 10 mm x 6 mm x 9 mm.

Your molecule is rather small. All styles are suitable and can be printed.

When deciding on the final dimensions and the corresponding scale, please keep in mind that:

- the minimum allowed scale for the Ball&Stick style for single material printers is 40 %;
- the minimum allowed scale for the Ball&Stick style when soluble support is used is 27 %;
- the minimum allowed scale for the Trace style is 23 %;
- the minimum allowed scale for the Ribbon style is 17 %;
- the minimum allowed scale for the Backbone style is 16 %;
- The surface rendering can be as low as 2 % . Printing at smaller scales might still be possible, but atomic details (H atoms) will be lost.

End of 3D Printing RECOMMENDATIONS for single color/material

Printed at the current scale/user-selected scale of 25 % , your model will be approx 104 mm x 66 mm x 95 mm.

On Proteopedia

(experimental, not yet publicly available)

Please choose the parameters to tailor the aspect of the resulting printed model on page

Myoglobin_of_Physeter_catodon_structure

Scheme: [Trace] [v]

Hydrogen atoms: [OFF] [v]

Recommended to be off unless you have particular reasons to have the hydrogen atoms shown in the model. H atoms might be required when the model is represented as ball and sticks, or when ligands are present. If not H atoms are not mandatory, keep in mind that keeping this option on will increase the minimum scale at which the model can be printed.

Nuclear struts: [ON] [v]

Ligand struts: [ON] [v]

Printer: [Single Color/Material] [v]

Printer scale: [39] [%]

You may set from 23% to 39%. With the current scale, your model will be approximately (x,y,z) **207 x 181 x 143 mm**.

Make printer files

Note: Before processing, we removed from the structure solvent (UREA, SO₄, PO₄, HOH, DOD, WAT), NA, K, CL, BR, GOL, DIQ, DOX, NO, NO₃, EDO, DMS, FMT, ACT, IPA, and they will **not appear** on the printed model.

Page: *Myoglobin_of_Physeter_catodon_structure*

trace 39%

Ligand struts: true

Nucleic acids struts: true

[Download Files](#)

☒ With this STL file, your printer will generate a Trace model of the of *Myoglobin_of_Physeter_catodon_structure*

☒ The size of your model will be approximately (x,y,z) **207 x 181 x 143 mm**.

Generate files for the [Same structure](#) with different parameters.

[Drag the model with the mouse to rotate](#)

Programming and implementation by [Jaime Prilusky](#). © STL/OBJ/MTL files generated with [Jmol](#) and [3DP-Jmol](#). Model preview powered with [Online 3D viewer](#)

4ins.pdb - 4INS

File Edit Display View Tools Plugins Macros Help

1076 x 682

123.9/385.9 Mb; 41/36 ms

Jmol Script Console 16.3.7 2024-11-12 15:34

1582 atoms selected
14 struts added
1584 atoms selected

--> Bond for one-atom linked ligand #1, ZN
--> Bond for one-atom linked ligand #2, ZN
--> Type 'checkStruts' to verify struts added for ligand support.
1584 atoms selected

--- Start of 3D Printing RECOMMENDATIONS for single color/material ---

Rendering and printing recommendations are provided for a medium size (ie. Ender 3; Prusa MK3S+) FDM 3D printer. Using SLA printers is possible, but not yet tested.

-->Printed at a maximum allowed printing scale of 48 % , your model will be approx 210 mm x 134 mm x 192 mm.

-->Printed at a minimum printing scale of 2 % , your model will be approx 10 mm x 6 mm x 9 mm.

Your molecule is rather small. All styles are suitable and can be printed.

When deciding on the final dimensions and the corresponding scale, please keep in mind that:

- the minimum allowed scale for the Ball and stick style for single material printers is 40 %;
- the minimum allowed scale for the Ball and stick style when soluble support is used is 28 %;
- the minimum allowed scale for the Trace style is 23 %;
- the minimum allowed scale for the Ribbon style is 17 %;
- the minimum allowed scale for the Cartoon style is 15 %;
- the minimum allowed scale for the Backbone style is 16 %;
- The surface rendering can be as low as 2 % . Printing at smaller scales might still be possible.

--- End of 3D Printing RECOMMENDATIONS for single color/material ---

Printed at the current scale/user selected scale of 20 % , your model will be approx 85 mm x 54 mm x 95 mm

OK 3200084 Stl /Users/mariusmihasan/test.stl

Time for running the script version alfa1.public: 1005ms

Editor Font Clear History State Undo Redo Close Variables Help

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



Released under MIT License

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

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

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