

How to perform protein model prediction with AlphaFold and visualize them

Workflow by Leander Rohr; last updated 03.11.2022 – 3.26 pm.

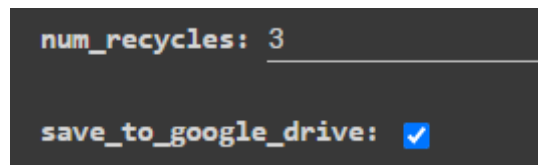
1. Prepare your amino acid sequence based on the one letter code in an extra text file (Word, Editor, ...)
2. For the prediction use the following link:
<https://colab.research.google.com/github/sokrypton/ColabFold/blob/main/AlphaFold2.ipynb>

Here you find a 'google colab' which is an executable notebook that includes the python-code to run the needed scripts. This 'colab' provides a modified version of AlphaFold that among other things fasten the prediction time. For more information see:

<https://www.nature.com/articles/s41592-022-01488-1>

The script itself is self-explanatory. The best option is to use the script during being logged in to your personal google account.

By checking this box in the advanced settings, you save the results directly to your Google Drive.



Run the script by following the instructions, starting with pasting your sequence (see point 1).

3. Finally, you receive a ZIP-File that contain all needed data to continue.
4. Models are ranked by the prediction probability. Use the model named with 'rank 1' for further processing.
5. Open the PDB-File with PyMOL.
PyMOL is a very overloaded software with many options.
A nice visualization is explained here:

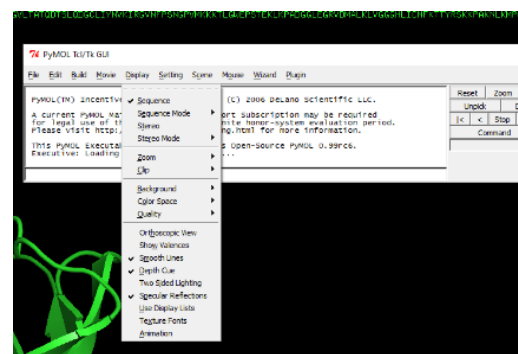
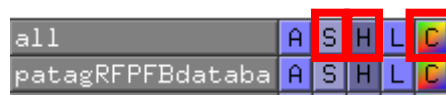
Click on 'S' and then on 'cartoon'.

Afterwards hide the lines by clicking 'H' and 'lines'.

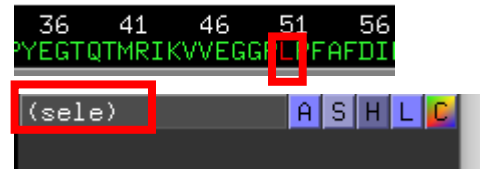
Colours can be changed by clicking on 'C'.

With 'Display' and 'Sequence' you can show the sequence within the viewer.

With this you can give certain amino acids a specific colour.



For this mark the amino acid in the sequence.
On the right '(sele)' appears for the selection.



With 'L' you can label the selection (e.g. with the name of the residue).
With 'C' you can change the colour.

6. In the viewer you can change the angle of view all the time.

All saving options are available *via* 'File' → [...]

It is recommended to save the session, molecule and images (image means the current view at the viewer).

7. Movies:

For many purposes its nice to have movies / animations.

By default this is quite complicated in PyMOL. However, there is a PlugIn that makes it easy to produce nice movies.

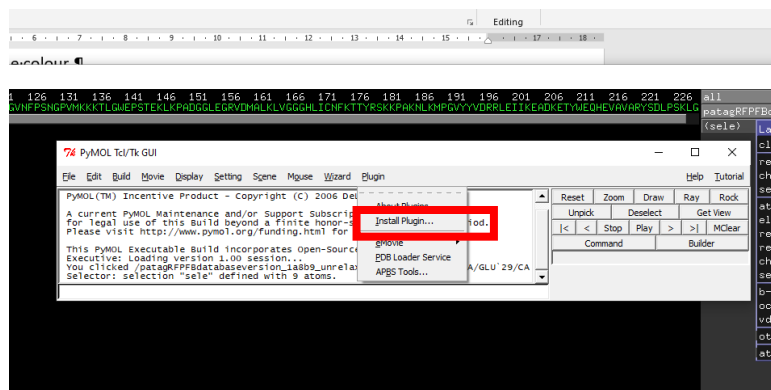
- 7.1. Download the eMovie PlugIn for PyMOL (recommended to use the 'package version'):

https://web.archive.org/web/20150923024429/http://www.weizmann.ac.il/ISPC/eMovie_download.html

For more information see:

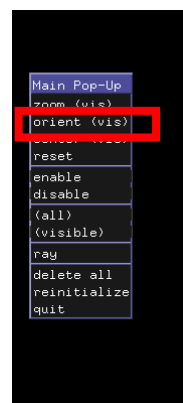
<https://web.archive.org/web/20150908061411/http://www.weizmann.ac.il/ISPC/eMovie.html>
(many examples, instructions, etc.)

- 7.2. Install the PlugIn in PyMOL (for this the content of the ZIP-folder has to be unpacked).



- 7.3. Follow the instructions and restart PyMOL by opening a PDB file you want to use for a video.

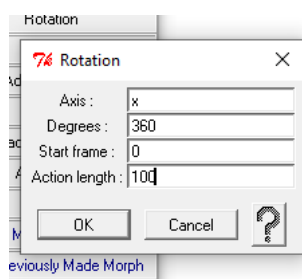
7.4. If you want to compare similar models later it is advisable to start at the same 'position'. For this right click in the viewer and chose 'orient (vis)' or any other suitable option.
(This option can be used for later movies again to have a better comparison).



7.5. With the Plugin installed the eMovie bar should appear.

This bar shows all important options.

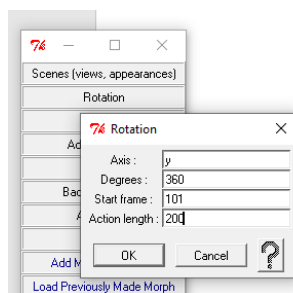
'Rotation' is a good option to make nice visualizations.



The here mentioned values will let the molecule rotate around its x-axis for 360° for 100 frames.



Press 'ok' and repeat this step by entering the following values to receive a y-axis rotation:

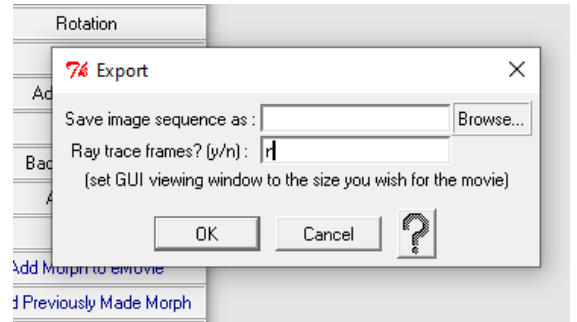


7.6. By 'View Storyboard' you can check if both commands were successfully added.

7.7. By clicking 'Save eMovie' you can save a file that can be edited later with PyMOL again.

7.8. By clicking 'Export eMovie' you can export your movie. Before exporting please check again if you are in the correct 'starting position', since this will be the start point of your movie (see point 7.4)

Chose a folder to save your image sequences.
Type in 'n' for 'ray trace frames'.



Note the images will be saved as single PNG files that need to be fused to a movie later. Due to this it is advisable to use an own folder for saving the images (e.g. here 300 images will be generated).

7.9. Fusing the single PNG files to an AVI movie

For this you can use FIJI (see <https://imagej.net/software/fiji/downloads>)

Click on File → Import → Image Sequence → Chose the Dir where your PNG's are saved and press 'ok'

Your Image Sequence will be imported.

Afterwards you can save this as AVI.

Click on File → Save as → AVI (30 fps are recommended)