April 2014

How to Morph a Protein

Using the Yale Morph Server tool, you can morph between two PDB files of the same or similar proteins to see conformational changes, flexible regions, etc.

1. To morph between two PDB files, go to http://molmovdb.org/

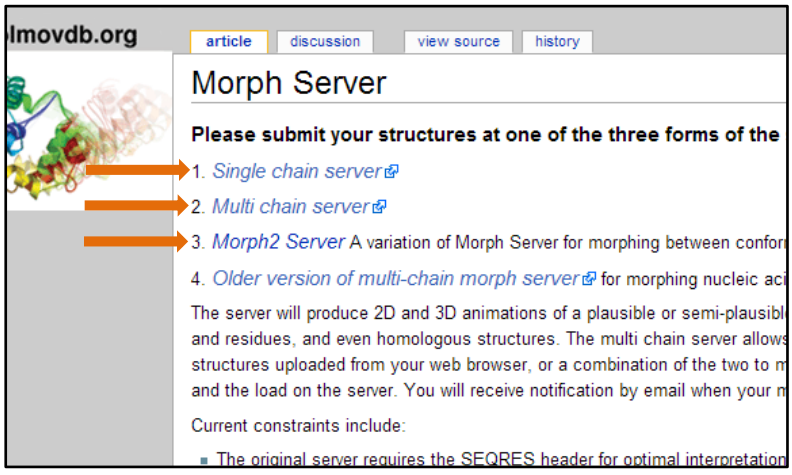
2. Click on "Morph Server".

3. Select the type of morph you want to do:

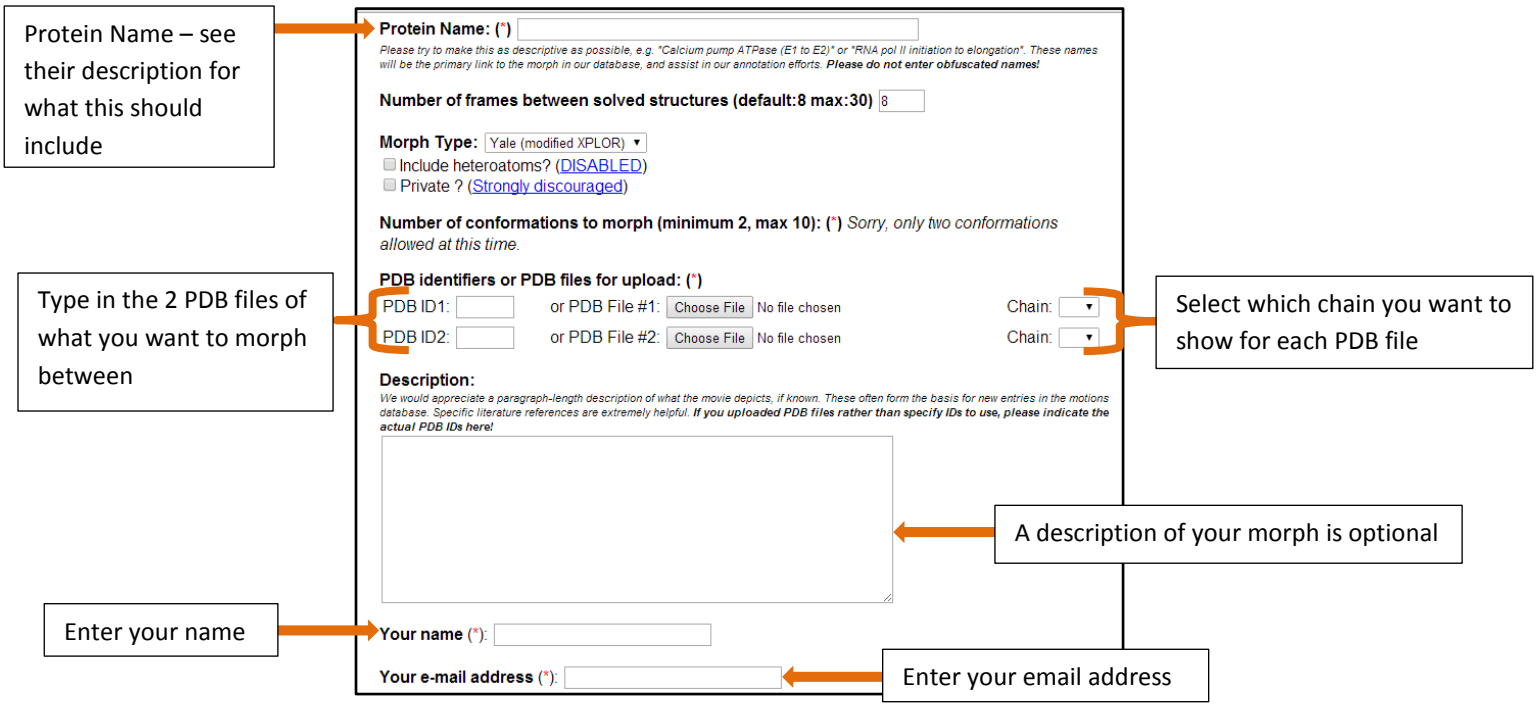
   a. **Single chain server** – use if you want to morph a single chain of a protein (or if a protein only has one chain)

   b. **Multi chain server** – for morphing multiple chains of a protein

   c. **Morph2 Server** – to morph between conformations of different but related proteins



4. Fill out the form. Only enter the information explained here below. You don't need to enter/click on anything else. (NOTE: this example page is taken from the Single chain server.)

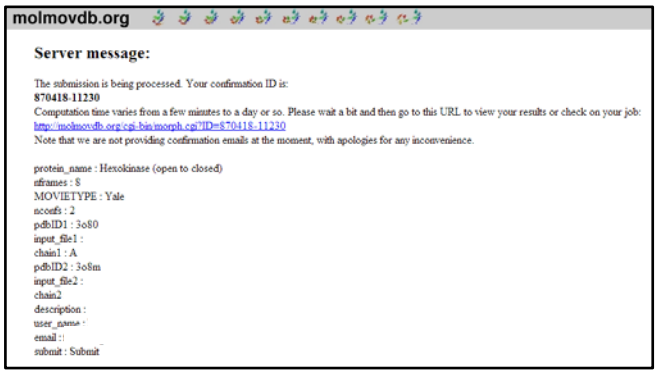


Then click "Submit" at the bottom of the page.

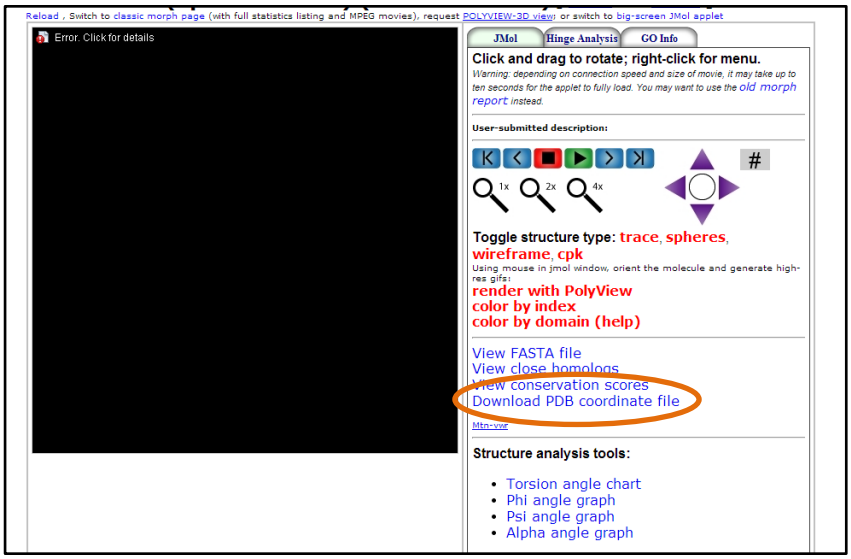
5. This will bring you to a new page with a link. This is the link to your morphing "job". It could take a couple minutes to a full day for your protein morph to be completed. **Wait a few minutes before you click on your link.**

-If the job is not done yet, the page will tell you so. Click on the "Back" button on your browser if this is the case. Wait a few more minutes before trying the link again.

-If the job is done, a Jmol viewer window will load. Be patient, this could take a few minutes!



5. Once the Jmol viewer window appears, click on “Download PDB coordinate file”.



6. Save this *.pdb.gz file onto your computer. You can now click and drag this file into the Jmol program on your desktop to view it (just like a regular PDB file).

7. In the script window of Jmol, first paste in your model design script. Then, include the following command at the *end* of your model design script to make your protein morph between the two models:

```
for (var i=0; i<15;i++){model next; delay 0.1;}
```

This command will only make your protein morph from the first PDB file to the second PDB file.

8. To morph from the first PDB file to the second PDB file, and then back again to the first PDB file, include the following script:

```
for (var i=0; i<15;i++){model next; delay 0.1;}; for (var i=0; i<15;i++){model -1; delay 0.1;}
```

9. Repeat the script in step #8 at the end of your model design as many times as you want to morph between the two PDB files.

**NOTE: Steps 6-9 assume you have knowledge of saving/opening PDB files, designing a model in Jmol, and creating a script. If you need to learn about these steps (or need a refresher course!), please visit http://cbm.msoe.edu/crest/crestJmolResources.php and view the Interactive Jmol Training materials on various topics.*