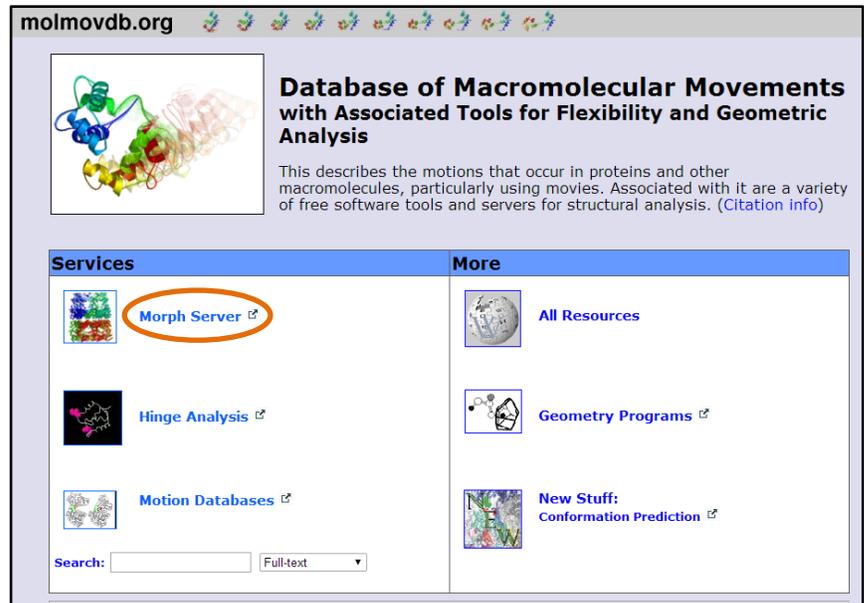


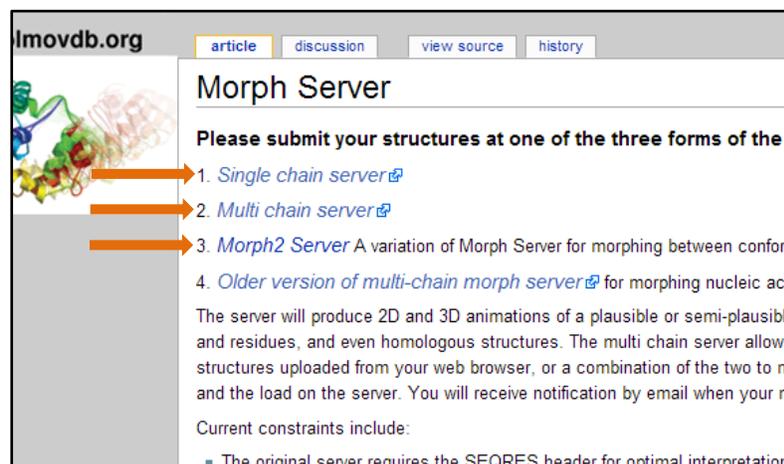
How to Morph a Protein

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.)

The image shows a web form for protein morphing on molmovdb.org. Several callout boxes with orange arrows point to specific fields:

- Protein Name – see their description for what this should include**: Points to the "Protein Name (*)" text input field.
- Type in the 2 PDB files of what you want to morph between**: Points to the "PDB ID1" and "PDB ID2" input fields.
- Select which chain you want to show for each PDB file**: Points to the "Chain:" dropdown menus for each PDB file.
- A description of your morph is optional**: Points to the "Description:" text area.
- Enter your name**: Points to the "Your name (*)" text input field.
- Enter your email address**: Points to the "Your e-mail address (*)" text input field.

The form includes the following fields and options:

- Protein Name (*)**: Text input field.
- Number of frames between solved structures (default:8 max:30)**: Text input field with value 8.
- Morph Type**: Dropdown menu set to "Yale (modified XPLOR)".
- Include heteroatoms? (DISABLED)**: Disabled checkbox.
- Private ? (Strongly discouraged)**: Disabled checkbox.
- Number of conformations to morph (minimum 2, max 10): (*)**: Text input field.
- PDB identifiers or PDB files for upload: (*)**: Two sets of "PDB ID#" or "PDB File #:" with "Choose File" buttons.
- Description:**: Text area for a paragraph-length description.
- Your name (*)**: Text input field.
- Your e-mail address (*)**: Text input field.

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!

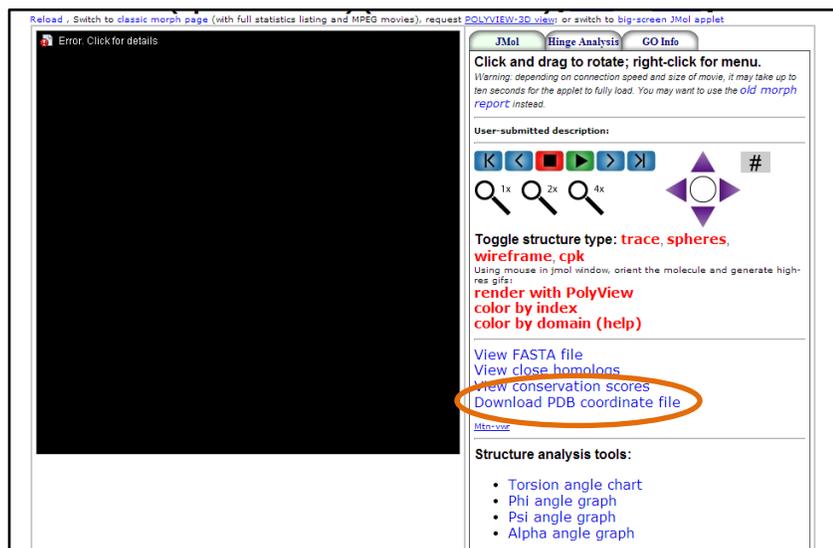
The screenshot shows a "Server message:" page from molmovdb.org. The message content is as follows:

```

Server message:
The submission is being processed. Your confirmation ID is:
870418-11230
Computation time varies from a few minutes to a day or so. Please wait a bit and then go to this URL to view your results or check on your job:
http://molmovdb.org/cgi-bin/morph.cgi?ID=870418-11230
Note that we are not providing confirmation emails at the moment, with apologies for any inconvenience.

protein_name : Hexokinase (open to closed)
nframes : 8
MOVIE TYPE : Yale
ncoeffs : 2
pdbID1 : 3o80
input_file1 :
chain1 : A
pdbID2 : 3o8m
input_file2 :
chain2 :
description :
user_name :
email :
submit : Submit
    
```

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.msoc.edu/crest/crestJmolResources.php> and view the Interactive Jmol Training materials on various topics.*