How To MorphOT MAP594

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1 Introduction

This document is a short supplementary material for my jury to test my USCF ChimeraX MorphOT bundle if they feel like it.

2 Step-by-step explanation

- Download UCSF ChimeraX on this page.
- Clone this github repository containing the bundle itself, a more thorough user manual and some input data
- Launch ChimeraX and install the plugin by typing in ChimeraX's command line :

```
devel build Path/To/GitHub/Repo/otmorph-bundle devel install Path/To/GitHub/Repo/otmorph-bundle
```

- Open the two files emd5140_preprocessed.mrc and emd5138_preprocessed_aligned.mrc
- In the Volume Viewer panel on the bottom right, set the level of each volume to approximately 0.15. You can do this either by typing it in the "Level" box, or by sliding the vertical bar on the histogram below.
- Type in one of the following commands in the command line :

```
MorphOT morphOT #1 #2
MorphOT semiMorphOT #1 #2 frames 100 otframes 10
MorphOT barycenterSave #1 #2 Path/to/save/folder
```

Note: the "numbers" correspond to volumes IDs you can see in the **Volume Viewer** panel. They are the only required parameters.

See the user manual for the different function parameters and how they affect computation.