How To MorphOT MAP594

Arthur Ecoffet

August 2020

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`

- 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

  See the user manual for more existing parameters and how they affect computation