

ModelAngelo is an automatic atomic model building program for cryo-EM maps.

## Setup

```
ssh jmwadmin@pollux  
  
bash  
  
conda activate model_angelo
```

## Building a map with FASTA sequence

This is the recommended use case, when you have access to a medium-high resolution cryo-EM map (resolutions exceeding 4 Å) as well as a FASTA file with all of your protein sequences.

Let's say the map's name is *map.mrc* and the sequence file is *sequence.fasta*. To build your model in a directory named *output*, you run:

```
model_angelo build -v map.mrc -f sequence.fasta -o output
```

If the output of the program halts before the completion of *GNN model refinement, round 3 / 3*, there was a bug that you can see in *output/model\_angelo.log*. Otherwise, you can find your model in *output/output.cif*. The name of the mmCIF file is based on the output folder name, so if you specify, for example, *-o testing/test/model\_building*, the model will be in *testing/test/model\_building/model\_building.cif*.

## Building a map with no FASTA sequence

If you have a sample where you do not know all of the protein sequences that occur in the map, you can run *model\_angelo build\_no\_seq* instead. This version of the program uses a network that was not trained with input sequences, nor does it do post-processing on the built map.

Instead, in addition to a built model, it provides you with HMM profile files that you can use to search a database such as UniRef with HHblits.

You run this command:

```
model_angelo build_no_seq -v map.mrc -o output
```

The model will be in *output/output.cif* as before. Now there are also HMM profiles for each chain in HHsearch's format here: *output/hmm\_profiles*. To do a sequence search for chain A (for example), you should first install HHblits and download one of the databases. Then, you can run

```
hhblits -i output/hmm_profiles/A.hmm -d PATH_TO_DB -o A.hhr -oa3m A.a3m -M first
```

You will have your result as a multiple sequence alignment here: *A.a3m*.

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