

Getting Started

These instructions will get a copy of the project working on your local machine.

Prerequisites

Software

To install this software you will need:

- keras
- tensorflow
- matplotlib
- scikit-learn
- Pillow
- numpy
- scipy
- mrcfile
- logging
- argparse

These should all be installed (or already were installed) when the environment is setup (see [here](#)). However, sometimes there are issues when installing and using tensorflow and keras. CHECK WHICH VERSIONS.

python3 must also be set up on your machine in order to work.

Data

For this program to work, the map files need to be stored in one directory. This layout is automatically created by the Topaz program designed to prepare the map files for eclips.

If using RunTrain or EP_success, there must also be a directory with a sub-directory for each of the protein names. Each of these sub directories must have a log file (each one with the same name). These log files (default is simple_xia2_to_shelxcde.log) need to contain the characters: "Best space group: " followed by a space group. In the same sub-directory there must also be a directory named this space group. In there there must be a .lst file with the same name as the protein (with _i if inverse). This file must contain the characters "with CC " followed by a percentage, between the last 1000 and last 700 characters. Alternatively, it can contain the words "CC is less than zero - giving up", or "Pseudo-free CC = ". This is to that EP_success can assign scores to the proteins for training.

A diagram of this:

```

MapDirectory
- ProteinName1.map
- ProteinName1_i.map
- ProteinName2.map
.
.
.

EP_phasing
- ProteinName1
  - SpaceGroup
    - ProteinName.lst
    - 'simple_xia2_to_shelxcde.log'
- ProteinName2
.
.
.
```

The SQLite database must have a table called "**Phasing**", with column names:

- pdb_id_id
- ep_success_o
- ep_percent_o
- ep_score_o
- ep_score_rawo
- ep_confidence_o
- ep_confidence_rawo

- ep_success_i
- ep_success_rawi
- ep_confidence_i
- ep_confidence_rawi
- ep_img_o
- ep_raw_o
- ep_img_i
- ep_raw_i

Installing

To get a development environment running, first download the package. The code can be found on the github repository [here](#). Then go to the directory containing setup.py and type the following into the command line:

```
python3 setup.py develop --user  
export PATH=$PATH:~/.local/bin
```

The functions should then be available to use in command line.