

How to run the script

Suppose you have on the Desktop:

- a python script, called **algo.py**;
- an example directory called **protein** which contains:
 - the **pdb** directory;
 - the **edges** directory.

Now let's create a new directory, called **new**, and insert in it **algo.py** and the directory **protein**.

In order to run the script is necessary:

1. Open Anaconda Prompt (on Windows) or Command Prompt (on Linux);
2. Set in the directory **new** with:

```
(base) C:\Users\name> cd Desktop/new
```

3. Run the script by writing on the command line:

```
(base) C:\Users\name\Desktop\new> python algo.py protein/pdb/snapshot_0.pdb protein/edges protein
```

Where:

- `./snapshot_0.pdb` is just an example name of the first pdb file to pass to the procedure to extract the residues list;
 - `protein` (the last argument to pass) indicates the folder where the output directory will be created.
4. After running the script it will automatically create an **output** folder containing all the files returned by the procedure.

It is necessary to remember that inside **protein there must not be other folders called **output**.**