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.