

CMPyMOL User Guide ¹

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¹<https://goo.gl/VyMXPd>

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About the companion website

The website¹ contains the source code and brief instructions for running CMPyMOL:

- This software is provided under The MIT License (MIT).

Acknowledgements

- A special word of thanks goes to Professor Markus Deserno² for his useful and insightful discussions about this software in particular and science in general.

¹<https://goo.gl/VyMXPd>

²<https://www.cmu.edu/physics/people/faculty/deserno.html>

1

Installation Instructions

“Only Mac OS X and Linux operating systems are fully supported at this time.”

—

1.1 Mac OS X

1.1.1 Prerequisites and Initial Setup

PyMOL

PyMOL binaries can be installed using HomeBrew by following the below instructions.

```
# Open Terminal.app and enter the following commands

# Installing HomeBrew
ruby -e "$(curl -fsSL
  https://raw.githubusercontent.com/Homebrew/install/master/install)"

# Installing PyMOL
brew tap homebrew/science
brew install python --with-brewed-tk --enable-threads --with-x11
brew install pymol
brew link pymol

# While installing PyMOL you might have to enter your superuser
  password to complete installation successfully.
```

Python Dependencies

Installing python dependencies wxpython, matplotlib, python imaging library and numpy.

```
# Open Terminal.app and enter the following commands
brew install wxmac
brew install wxpython
pip install matplotlib
pip install pillow
pip install numpy
```

Installing Stride (*optional*)

Skipping this step will automatically disable certain features in CMPyMOL.

```
# Download Stride
wget http://webclu.bio.wzw.tum.de/stride/stride.tar.gz

# Unzip the downloaded file
tar xvfz stride.tar.gz

# Compile Stride
cd stride
make

# Open the .profile file from your ‘home’ directory with your
  favorite text editor
# Add the following line at the end of the .profile file by
  appropriately replacing the <directory stride> to the
  downloaded stride package path.
export PATH=$PATH:<directory stride>

# source the .profile file changes
source ~/.profile
```

1.1.2 Running CMPyMOL

Download git package from the CMPyMOL repository and run it.

```
# Download the git repository
git clone https://github.com/emptyewer/CMPyMOL
cd CMPyMOL

# Executing the below command will automatically launch PyMOL. Then
  follow on screen instructions.
python CMPyMOL1.5.py
```

1.2 Linux

1.2.1 Prerequisites and Initial Setup

PyMOL binaries can be installed using `aptitude` that is provided by default in Ubuntu by following the below instructions.

```
# Installing PyMOL
```

```
sudo apt-get install pymol
```

```
# While installing PyMOL you might have to enter your superuser  
password to complete installation sucessfully.
```

Python Dependencies

Installing python dependencies wxpython, matplotlib, python imaging library and numpy.

```
sudo apt-get install python-wxgtk2.8
```

```
sudo pip install matplotlib
```

```
sudo pip install pillow
```

```
sudo pip install numpy
```

Installing Stride (*optional*)

Skipping this step will automatically disable certain features in CMPyMOL.

```
# Download Stride
```

```
wget http://webclu.bio.wzw.tum.de/stride/stride.tar.gz
```

```
# Unzip the downloaded file
```

```
tar xvfz stride.tar.gz
```

```
# Compile Stride
```

```
cd stride
```

```
make
```

```
# Open the .bashrc file from your ‘home’ directory with your  
favorite text editor
```

```
# Add the following line at the end of the .bashrc file by  
appropriately replacing the <directory stride> to the  
downloaded stride package path.
```

```
export PATH=$PATH:<directory stride>
```

```
# source the .bashrc file changes
```

```
source ~/.bashrc
```

1.2.2 Running CMPyMOL

Download git package from the CMPyMOL repository and run it.

```
# Download the git repository
git clone https://github.com/emptyewer/CMPyMOL
cd CMPyMOL

# Executing the below command will automatically launch PyMOL. Then
  follow on screen instructions.
python CMPyMOL1.5.py
```

1.3 Windows

Currently not supported.

2

Load PDB and Contact Map

*“Single frame and multi-frame PDB files are currently supported
by CMPyMOL”*

2.1 Loading a Single-frame or Multi-frame PDB file/trajectory