

Gromacs 2023.3 installation tutorial ubuntu (Unix)

To download gromacs on your Unix machine (Ubuntu)

\$ wget <https://ftp.gromacs.org/gromacs/gromacs-2023.3.tar.gz>

1. \$ tar xzf gromacs-2023.3.tar.gz

2. \$ cd gromacs-2023.3/

3. gromacs-2023.3\$ mkdir build

4. gromacs-2023.3\$ cd build

5. gromacs-2023.3/build\$ cmake .. -DREGRESSIONTEST_DOWNLOAD=on -
DGMX_BUILD_OWN_FFTW=on

6. gromacs-2023.3/build\$ make -j 8

7. gromacs-2023.3/build\$ make check

8. gromacs-2023.3/build\$ sudo make install

9. source *usr/local/gromacs/bin/GMXRC*