

GROMACS installation guide

1) Downloading GROMACS

To check the latest version, visit:

<https://manual.gromacs.org/current/download.html>

Steps:

wget <https://ftp.gromacs.org/gromacs/gromacs-2024.3.tar.gz>

```
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS$ wget https://ftp.gromacs.org/gromacs/gromacs-2024.3.tar.gz
--2024-09-22 22:56:06-- https://ftp.gromacs.org/gromacs/gromacs-2024.3.tar.gz
Resolving ftp.gromacs.org (ftp.gromacs.org)... 2001:6b0:1:1191:216:3eff:fec7:6e30, 130.237.11.165
Connecting to ftp.gromacs.org (ftp.gromacs.org)|2001:6b0:1:1191:216:3eff:fec7:6e30|:443... failed: Connection timed out.
Connecting to ftp.gromacs.org (ftp.gromacs.org)|130.237.11.165|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 42373103 (40M) [application/x-gzip]
Saving to: 'gromacs-2024.3.tar.gz'

gromacs-2024.3.tar.gz      100%[=====>] 40.41M  1.31MB/s   in 31s

2024-09-22 22:58:54 (1.32 MB/s) - 'gromacs-2024.3.tar.gz' saved [42373103/42373103]
```

Check the downloaded file:

ls -lrth

```
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS$ ls -lrth
total 41M
-rw-rw-r-- 1 rejwana rejwana 41M Aug 29 17:49 gromacs-2024.3.tar.gz
```

Unzip tar file:

tar -zxvf gromacs-2024.3.tar.gz

```
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS$ ls -lrth
total 41M
-rw-rw-r-- 1 rejwana rejwana 41M Aug 29 17:49 gromacs-2024.3.tar.gz
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS$ tar -zxvf gromacs-2024.3.tar.gz
gromacs-2024.3/
gromacs-2024.3/scripts/
gromacs-2024.3/scripts/GMXRC.bash.cmakein
gromacs-2024.3/scripts/grompplog2top
gromacs-2024.3/scripts/GMXRC.zsh.cmakein
gromacs-2024.3/scripts/xplor2gmx.pl
```

ls

```
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS$ ls
gromacs-2024.3  gromacs-2024.3.tar.gz
```

2) Installing GROMACS

<https://manual.gromacs.org/documentation/current/install-guide/index.html>

```
cd gromacs-2024.3/
```

```
ls -lrth
```

```
mkdir build
```

```
cd build
```

```
cmake .. -DGMX_BUILD_OWN_FFTW=ON -
DREGRESSIONTEST_DOWNLOAD=ON
```

```
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS$ ls
gromacs-2024.3  gromacs-2024.3.tar.gz
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS$ cd gromacs-2024.3/
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS/gromacs-2024.3$ ls -lrth
total 204K
-rw-rw-r-- 1 rejwana rejwana 4.7K Aug 29 17:47 README
-rw-rw-r-- 1 rejwana rejwana 2.0K Aug 29 17:47 CTestConfig.cmake
-rw-rw-r-- 1 rejwana rejwana 3.7K Aug 29 17:47 CPackInit.cmake
-rw-rw-r-- 1 rejwana rejwana 26K Aug 29 17:47 COPYING
-rw-rw-r-- 1 rejwana rejwana 43K Aug 29 17:47 CMakeLists.txt
-rw-rw-r-- 1 rejwana rejwana 2.8K Aug 29 17:47 CITATION.cff
-rw-rw-r-- 1 rejwana rejwana 1.8K Aug 29 17:47 AUTHORS
-rw-rw-r-- 1 rejwana rejwana 71K Aug 29 17:48 INSTALL
drwxrwxr-x 3 rejwana rejwana 4.0K Aug 29 17:48 tests
drwxrwxr-x 4 rejwana rejwana 4.0K Aug 29 17:48 share
drwxrwxr-x 2 rejwana rejwana 4.0K Aug 29 17:48 scripts
drwxrwxr-x 6 rejwana rejwana 4.0K Aug 29 17:48 python_packaging
drwxrwxr-x 4 rejwana rejwana 4.0K Aug 29 17:48 cmake
drwxrwxr-x 7 rejwana rejwana 4.0K Aug 29 17:48 src
drwxrwxr-x 6 rejwana rejwana 4.0K Aug 29 17:48 api
drwxrwxr-x 15 rejwana rejwana 4.0K Aug 29 17:49 docs
drwxrwxr-x 5 rejwana rejwana 4.0K Aug 29 17:49 admin
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS/gromacs-2024.3$ mkdir build
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS/gromacs-2024.3$ cd build/
(base) rejwana@bioinfo:~/Documents/REJWANA/GROMACS/gromacs-2024.3/build$ cmake .. -DGMX_BUILD_OWN_FFTW=ON -DREGRESSIONTEST_DOWNLOAD=ON
-- The C compiler identification is GNU 11.4.0
-- The CXX compiler identification is GNU 11.4.0
-- Detecting C compiler ABI info
-- Detecting C compiler ABI info - done
-- Check for working C compiler: /usr/bin/cc - skipped
-- Detecting C compile features
```

```
make
```

```
make check
```

```
sudo make install
```

```
source /usr/local/gromacs/bin/GMXRC
```

3. Cheing the installation of GROMACS

```
gmx
```

```

(base) rejwana@bioinfo:~$ gmx
:~) GROMACS - gmx, 2024.3 (-:

Executable:  /usr/local/gromacs/bin/gmx
Data prefix: /usr/local/gromacs
Working dir: /home/rejwana
Command line:
    gmx

SYNOPSIS

gmx [-[no]h] [-[no]quiet] [-[no]version] [-[no]copyright] [-nice <int>]
    [-[no]backup]

OPTIONS

Other options:

-[no]h          (no)
                Print help and quit
-[no]quiet      (no)
                Do not print common startup info or quotes
-[no]version    (no)
                Print extended version information and quit
-[no]copyright  (no)
                Print copyright information on startup
-nice <int>    (19)
                Set the nicelevel (default depends on command)
-[no]backup     (yes)
                Write backups if output files exist

Additional help is available on the following topics:
    commands    List of available commands
    selections   Selection syntax and usage
To access the help, use 'gmx help <topic>'.
For help on a command, use 'gmx help <command>'.

GROMACS reminds you: "Science is a wonderful thing if one does not have to earn one's living at it." (Albert E

```

Note: Make sure to use the path always>

source /usr/local/gromacs/bin/GMXRC