Commands for Gromacs build

The following commands in the terminal, to download, check build instructions, build the software, test installation path, source the path and test the installation of Gromacs. After each command press the **Enter** key to execute the command.

1. **sudo apt-get update** .

2. Enter the **sudo password**.

3. If desired press **Ctrl+L** to clear the screen after the process is complete.

4. **sudo apt-get upgrade** .

5. If desired press **Ctrl+L** to clear the screen after the process is complete.

6. **sudo apt-get upgrade** .

7. **sudo apt-get install -y build-essential make cmake gcc** .

8. **mkdir gromacs** .

9. **cd gromacs** .

10. **wget https://ftp.gromacs.org/gromacs/gromacs-2021.2.tar.gz** .

11. **tar -xvf gromacs-2021.2.tar.gz** .

12. **cd gromacs-2021.2** .

13. **vim INSTALL** .

14. Read the installation instructions.

15. **:q!** to quit vim text editor.

16. **mkdir build** .

17. **cd build** .

18. **sudo cmake .. -DGMX_BUILD_OWN_FFTW=ON** .

19. **sudo make** and press the **Enter**.

20. **sudo make install** and press the **Enter**.

21. **ls** and press **Enter**.

22. See the files in the **build** directory.

23. **cd bin** .

24. **ls** and press **Enter**.

25. **cd** and press **Enter**.

26. **whereis gromacs** .

27. Notice the path as **/usr/local/gromacs/** . If different, note down the path.

28. Check if **gmx** file path is in **/usr/local/gromcs/** directory, **ls /usr/local/gromcs/bin/** will have the **gmx** file.

29. **vim .bashrc** and press the **Enter**.

30. Scroll to the bottom of the file using down arrow key or page down key.

31. Press the **Insert** key.

32. Use the arrow key to start a new line.

33. **alias gmx='/usr/local/gromacs/bin/gmx'**

34. Press the **Esc** key.

35. **:wq** .

36. **source .bashrc** .

37. **gmx help grompp** .