1 – Linux Terminal, PHENIX, and Coot

(handout created by Susanna Huang on August 14th, 2024, for STARS collegiate branch located at the Georgia Tech campus)

INTRODUCTION

As you may know, there are four stages of crystallography:

1. **Protein expression and purification**
    a. Where the desired protein manufacturing instructions (or essentially the DNA coding the desired protein) is given to bacterial strains in the form of plasmids for the bacteria to mass produce the proteins, so that the high quantities of proteins can be obtained for crystallography experiments
    b. (but if you are working with just crystallizing nucleic acids, one advantage is that you can simply purchase the nucleic acid sequences and not have to worry about the expression and purification part)

Figure 1. Left flask: an example of bacteria, which are manufacturing the desired protein, growing well in broth. Right flask: an example of bacteria that has just started to grow or is growing poorly in the broth. Source for photos and further reading: https://bitesizebio.com/28882/optimize-bacterial-protein-expression-by-considering-these-4-variables/

2. **Crystallization and crystal-growth optimization**
    a. Where the protein and/or DNA samples are used for crystallization into beautiful crystals and where their crystal-growing conditions (experimental conditions) need to be optimized for best crystal quality growth (this is what we had worked on during the spring 2024 semester)

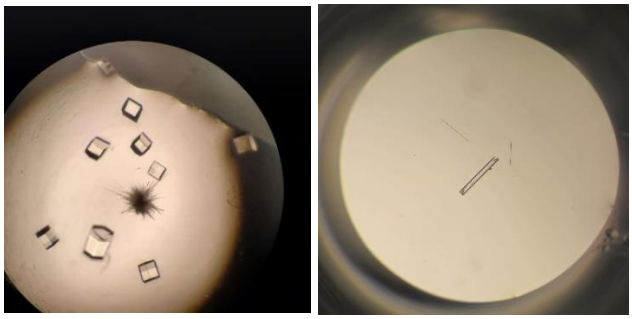


Figure 2. Left photo: lysozyme crystals grown for a STARS experiment (week 7, set up on March 14, 2024 by Susanna). Right photo: DNA crystals (CGCGCG) grown for an outside project (set up on 7/5/2024 and checked on 8/5/2024 by Susanna).

3. Crystal harvesting and diffraction of crystals

a. Where the good crystals are harvested, cryo-protected, and shipped off to a synchrotron facility and where the crystals are then diffracted at the beamline for X-ray diffraction data collection on the crystals' structures

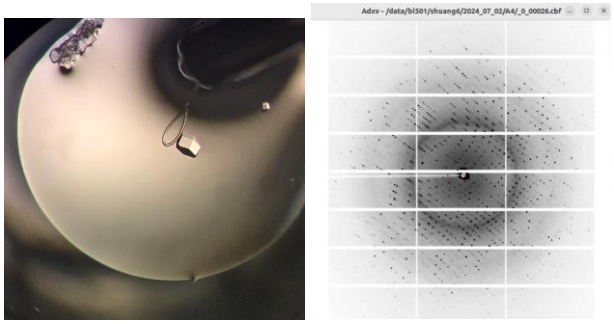


Figure 3. Left photo: a lysozyme crystal being harvested onto a loop. Right photo: An example of good lysozyme diffraction data (one snap) from a different lysozyme crystal. (photo credit: Susanna Huang with the support of LBNL)

4. Diffraction data solving, model building, and model refinement

a. Where the diffraction data is scaled and integrated into electron density maps, and where these electron density maps are used in conjunction with model sequences to build the protein and/or DNA models and refine these models

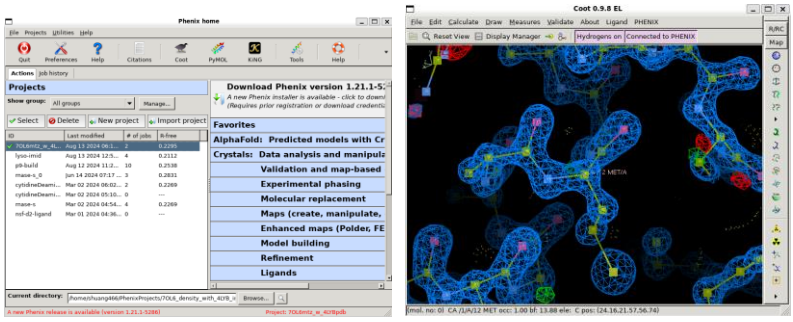


Figure 4. Left photo: Example of PHENIX GUI interface. Right photo: Example of Coot GUI interface, specifically for a 12-position methionine residue on lysozyme. (Susanna Huang)

AIMS FOR THIS HANDOUT

This handout aims to:

- Contextualize PHENIX and Coot with respect to the other three steps of crystallography (INTRODUCTION)
- Provide a general introduction of model building and refinement in the crystallography process and its significance
- Guide students through the download, installation, and set-up process for a Linux subsystem
- Provide students with the basic understanding on how to navigate through a Linux subsystem, such as basic commands and typing into the Linux terminal
- Guide students through the download, installation, and set-up process for PHENIX, Coot, Python3, and Rosetta

This handout can be used for initial instruction to students and can be used for students' self-guided download of these important programs.

MODEL BUILDING AND REFINEMENT and THEIR SIGNFICANCE

You have your beautiful crystal, which is a co-crystal of HDAC6, a cancer target protein, and a small molecule inhibitor of HDAC6. You wanted to see how the small molecule inhibitor was interacting with HDAC6, in terms of its mechanism (or essentially, what is occurring at the atomic level). You had decided to go with crystallography because the other two prominent methods for structure determination: (1) Solution NMR and (2) cryoEM just did not quite seem suitable for this specific system. Solution NMR is only really good for high atomic resolution for smaller systems that are around less than 100 kDa in mass (but HDAC6 on its own is already 130-150 kDa, so Solution NMR would not be possible here). cryoEM is really good for obtaining the general structure of large macromolecular systems, requiring the studied system to be at least 50 kDa, which is good news, but only at relatively low resolution (only around 10 Å and maybe 3 Å resolution at best for most cases), which would not be useful for obtaining atomic resolution (1 Å) information of the molecular interactions occurring between the HDAC6 and the small molecule inhibitor. X-ray crystallography was the best bet here because it frequently provides atomic or near-atomic resolution and can work for small systems as well as larger macromolecular systems.

You have your beautiful crystal, and you harvested it, cryoprotected it, plunged it in liquid nitrogen, and shipped it off in a black puck (a hockey puck-sized puck, which has little holes for placing the crystal pins into), packed the pucks inside of a dewar (a shipping

container that is filled with a stack of pucks and lots of liquid nitrogen to keep it cold), and shipped it off to a synchrotron facility, such as the Advanced Light Source (ALS) at the Berkeley Lab.

Several months later, when the ALS notifies you about available beamtime that you can use, you hop onto your computer, open a remote connection, obtained access to one of their macromolecular crystallography beamlines (such as 5.0.1 or 5.0.3, further reading here: https://bcsb.als.lbl.gov/beamline-overview/), and shot your crystal with X-rays to get some pretty diffraction patterns.

ALS automatically helped you integrate and scale the diffraction patterns into an electron density map. You now have the **HDAC6 sequence information** in a **.fasta file format**, your crystal **electron density information** (with phasing information as well) in a **.mtz format**.

What do you do now?

Currently, the .fasta file is a string of alphabetical numbers that are each associated with an amino acid in HDAC6. This file needs to be converted into a **.dat file format** before it can be used in conjunction with the phase information (.mtz file) by PHENIX and Coot to create a **new HDAC6 protein model** based on your HDAC6 diffraction data.

Why do we need this specific model? Other HDAC6 models will not have your special inhibitor compound, so the HDAC6 protein model may not adopt a specific conformation that we are investigating into. This HDAC6 co-crystallized with small molecule model can provide great information and insight on how the small molecule inhibitor affects HDAC6's protein and residue conformation at the atomic level, providing insight on if the small molecule may be doing its job or if the small molecule can be improved to have better binding with HDAC6 for improved protein inhibition.

DOWNLOADING LINUX SUBSYSTEMS:

Before we can do PHENIX and Coot work, we need to prepare the system format that they are compatible with: Linux.

This will be a step-by-step guide on how to download and install everything for a Windows 11 system, but each of the steps are largely applicable to Mac systems and other Windows systems as well.

Here are the main instructions websites that will be referenced:

1. https://github.com/phenix-project/phenix_html/blob/master/wsl_instructions.md
2. https://phenix-online.org/
3. https://phenix-online.org/download
4. https://phenix-online.org/documentation/install-setup-run.html
5. https://phenix-online.org/documentation/reference/rosetta_install.html
6. https://rosettacommons.org/download/
7. https://downloads.rosettacommons.org/software/academic/

Most of these pages are linked pages to each other. I just put them here to delineate them clearly.

Other documentation:

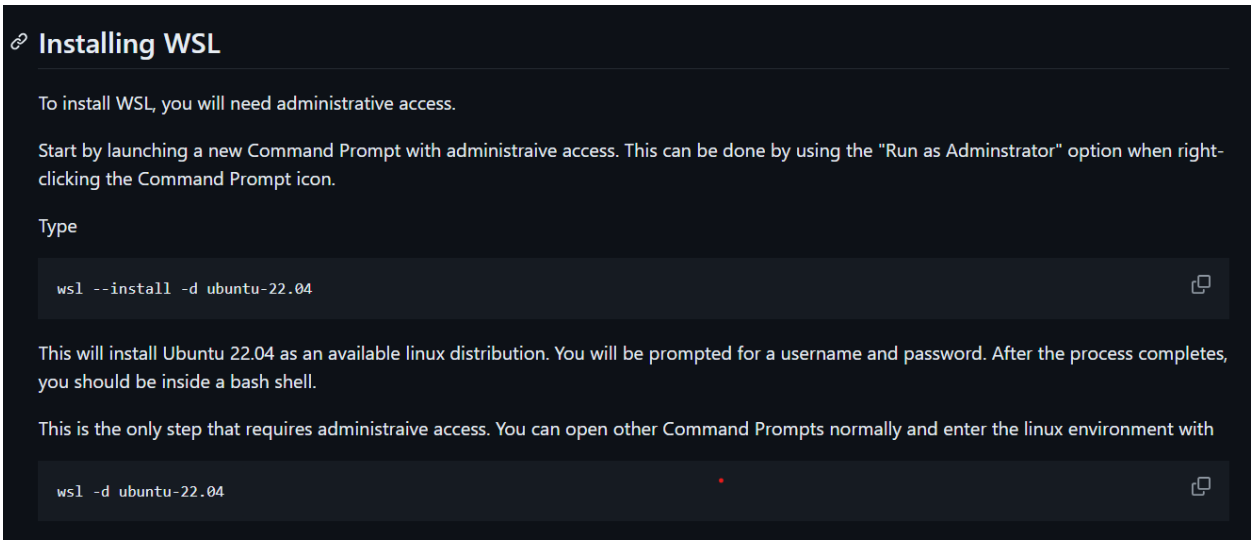
Phenix Documentation (phenix-online.org)

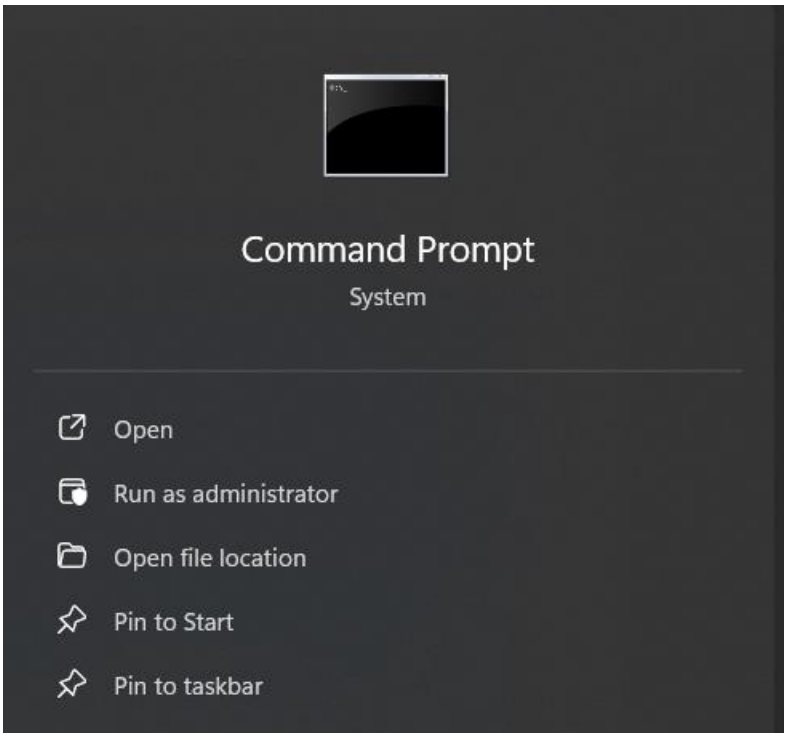
Main steps:

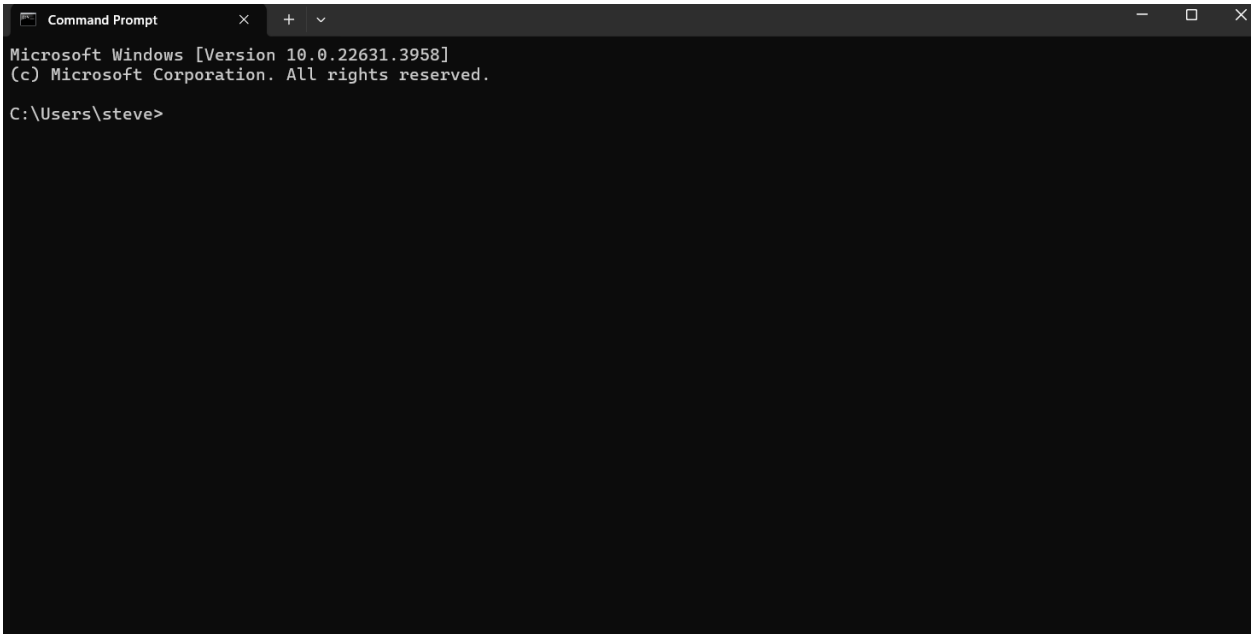
- How to download Linux
- How to use Linux subsystem
- How to download Phenix
- How to download Coot
- How to download Python3

To start, we first need WSL to run Linux on Windows:

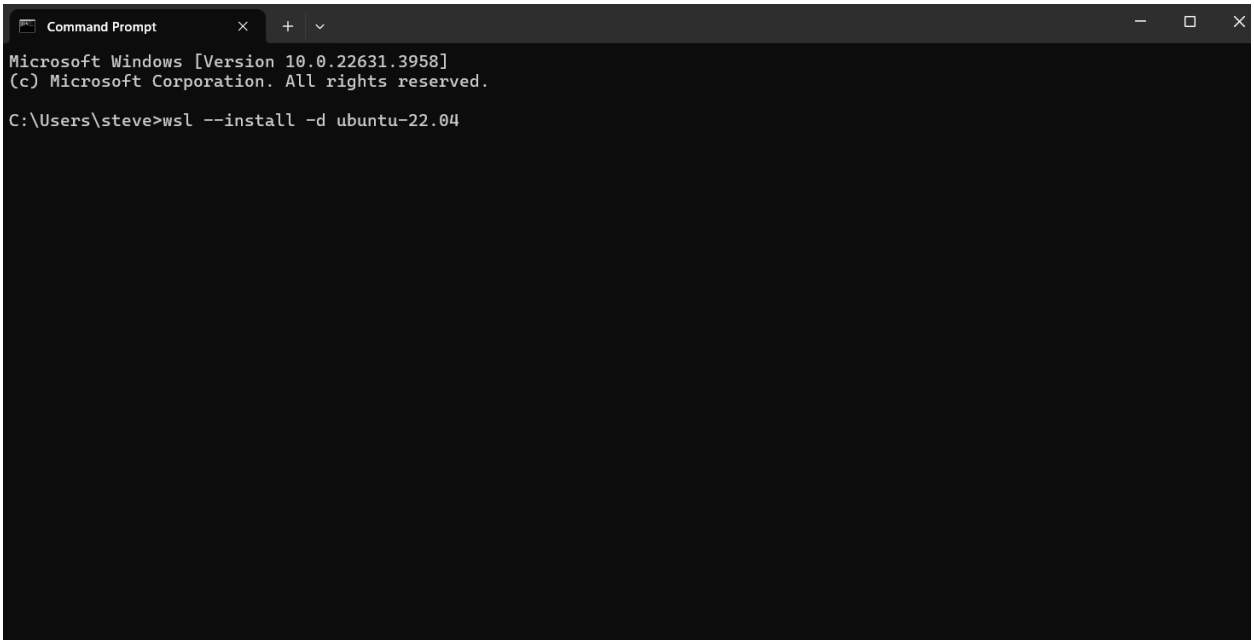
1. Reference website 1 (https://github.com/phenix-project/phenix_html/blob/master/wsl_instructions.md):



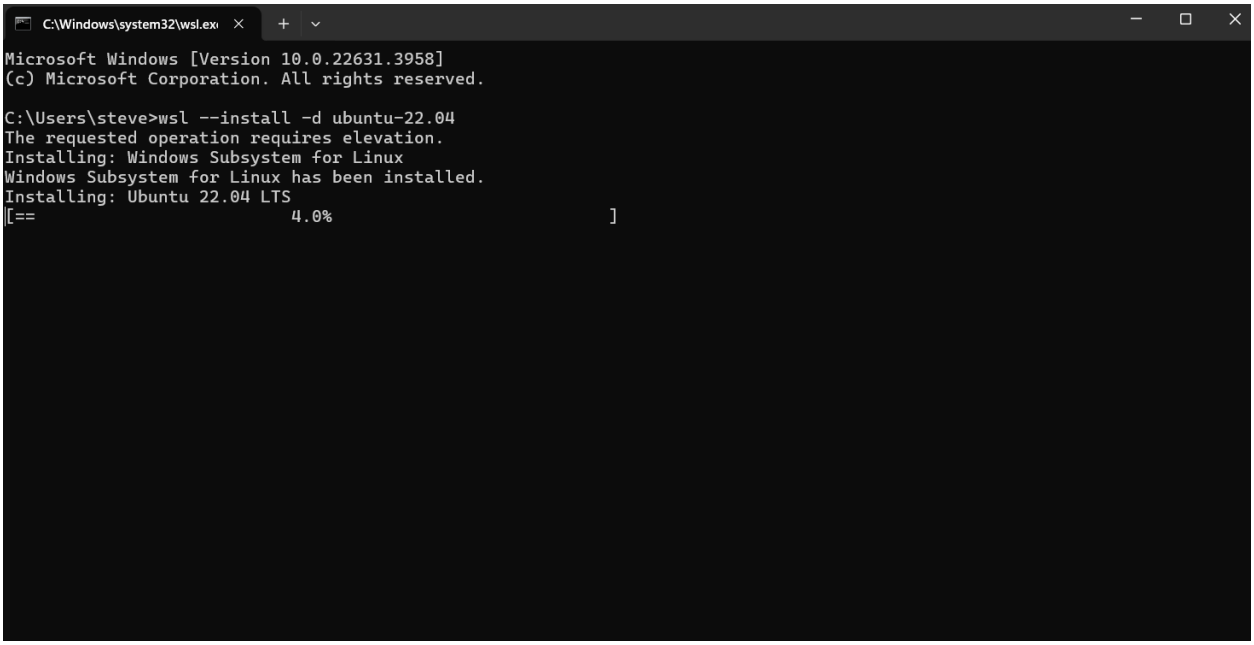


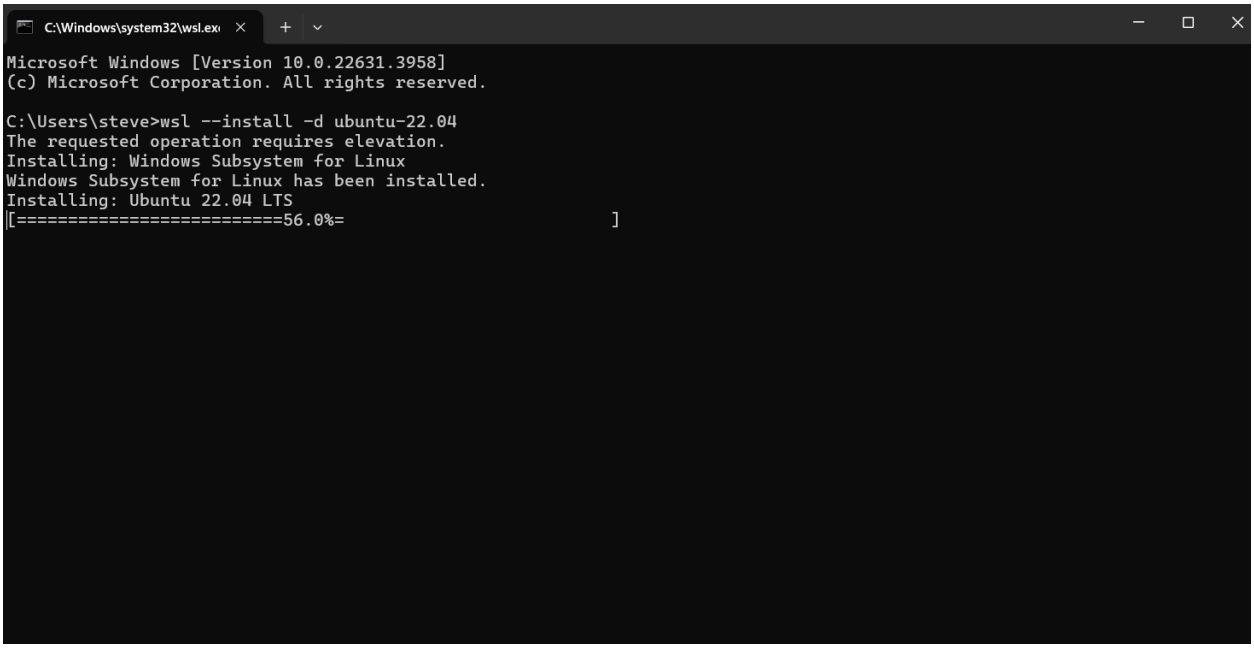


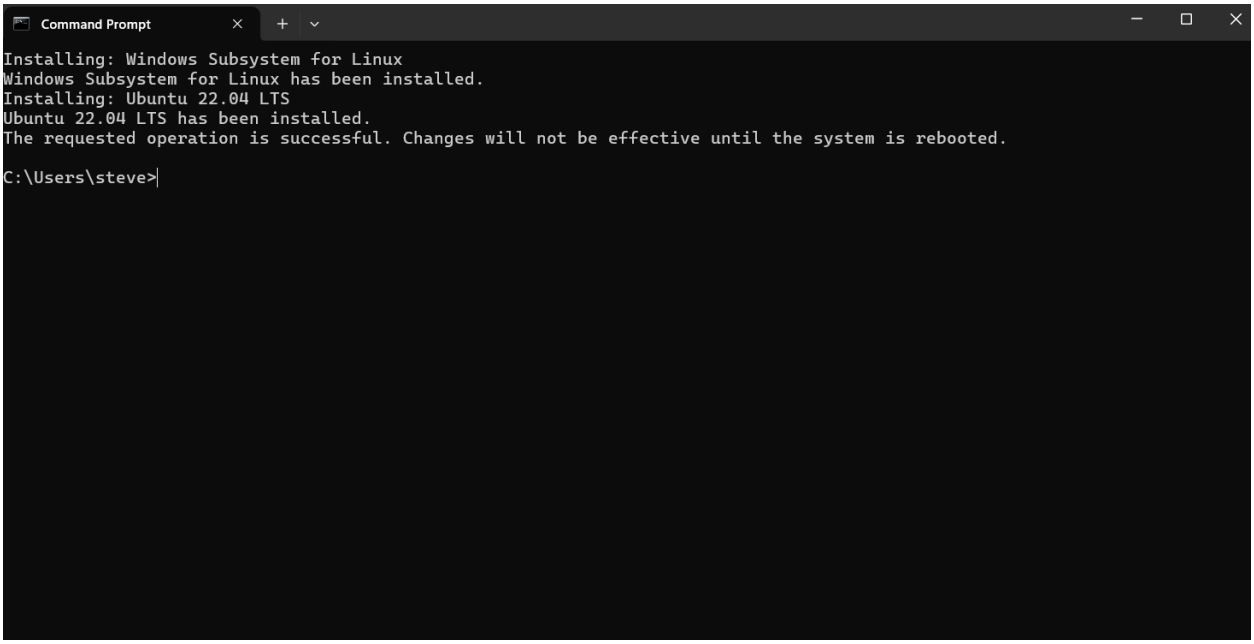
Open Command Prompt and type **wsl --install -d ubuntu-22.04**



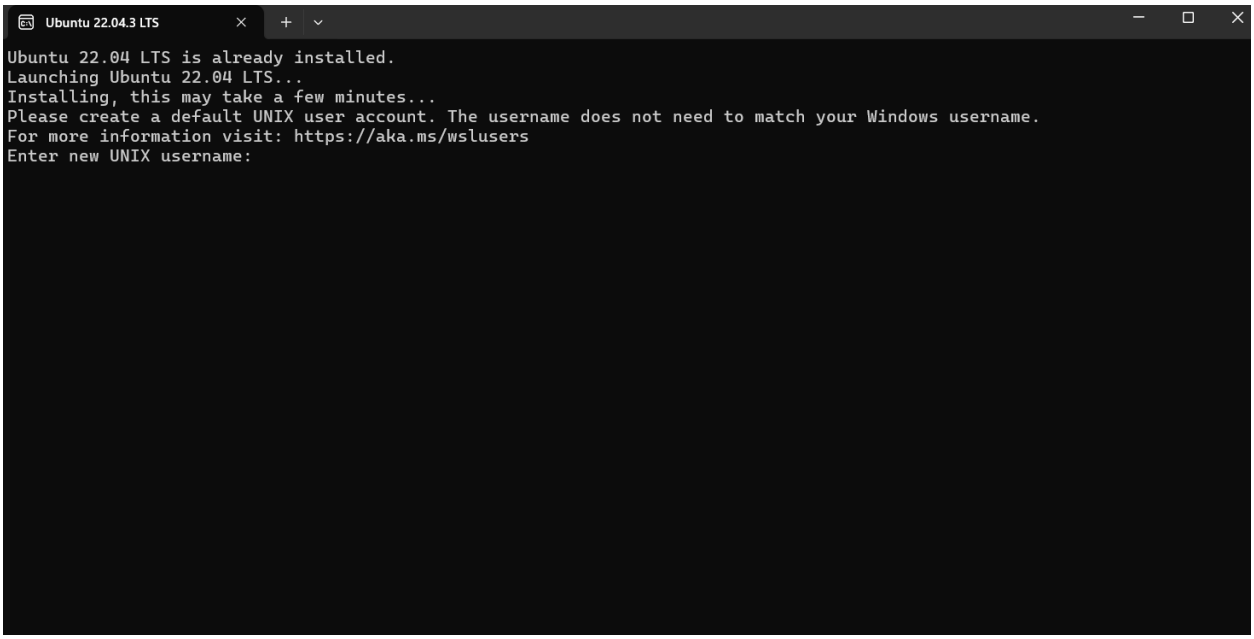
This will be Windows Subsystem for Linux, as the host process for Linux service on Windows.

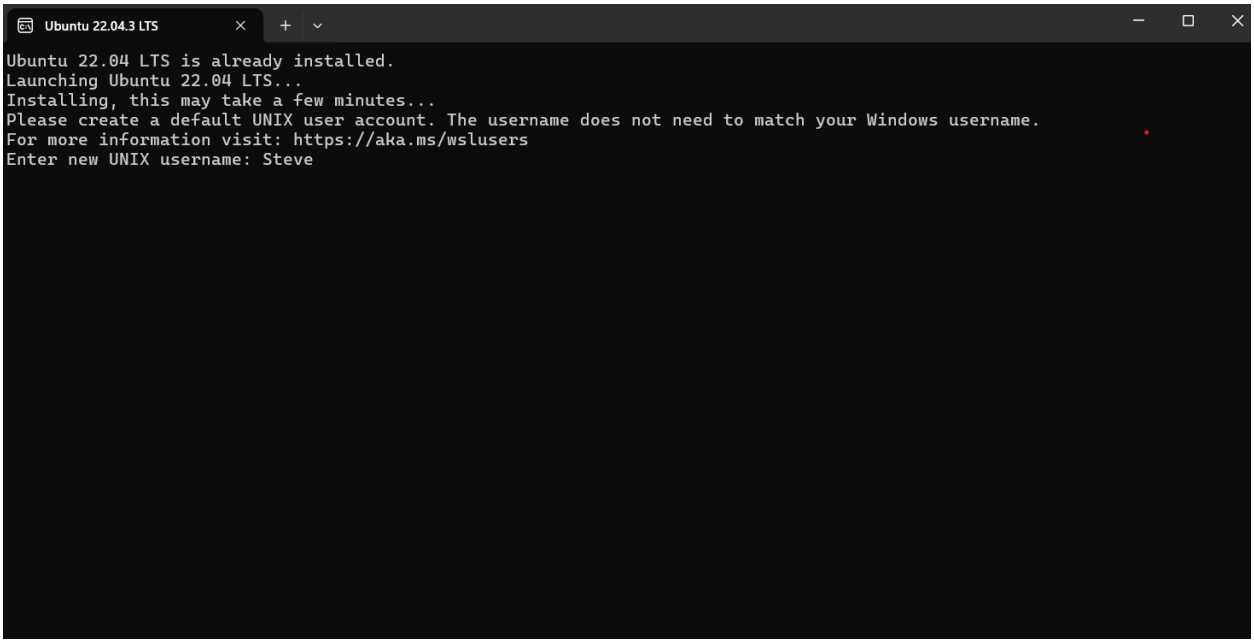

C:\Windows\system32\wsl.exe
Microsoft Windows [Version 10.0.22631.3958]
(c) Microsoft Corporation. All rights reserved.
C:\Users\steve>wsl --install -d ubuntu-22.04
The requested operation requires elevation.
Installing: Windows Subsystem for Linux
Windows Subsystem for Linux has been installed.
Installing: Ubuntu 22.04 LTS
[== 4.0%]


C:\Windows\system32\wsl.exe
Microsoft Windows [Version 10.0.22631.3958]
(c) Microsoft Corporation. All rights reserved.
C:\Users\steve>wsl --install -d ubuntu-22.04
The requested operation requires elevation.
Installing: Windows Subsystem for Linux
Windows Subsystem for Linux has been installed.
Installing: Ubuntu 22.04 LTS
[==========56.0%=]



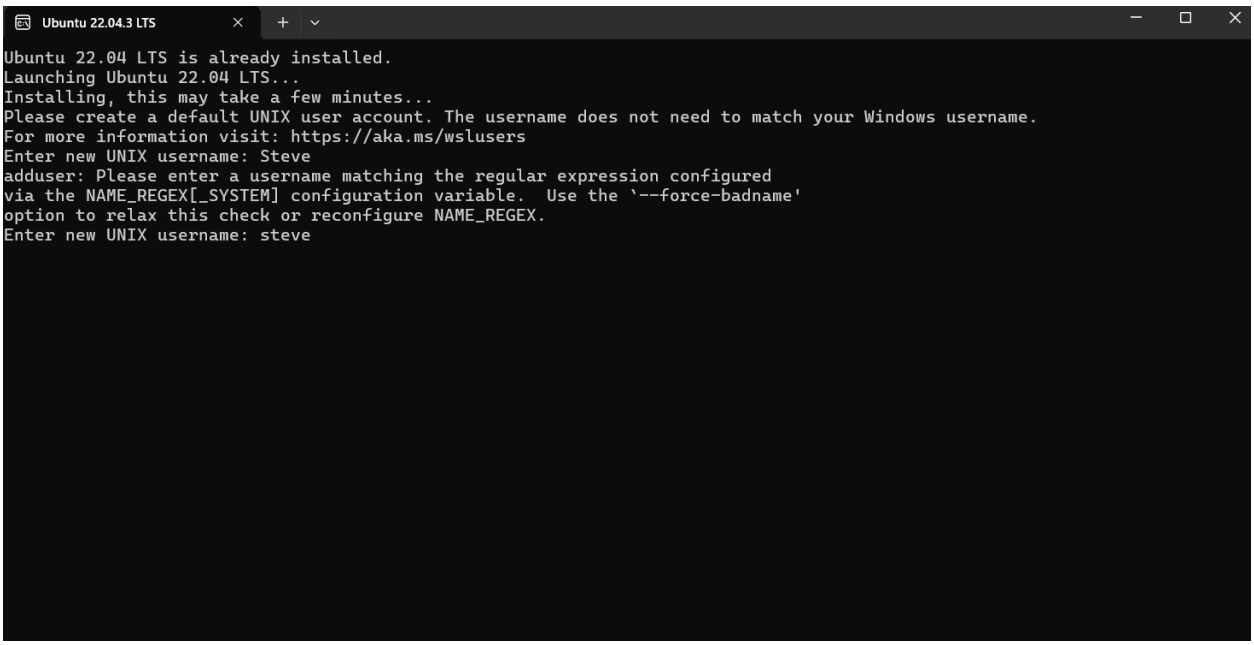
Now it will ask for the creation of your username and password. Beware, your password will not have anything show up when you are typing into it (but the computer is remembering what you are typing).



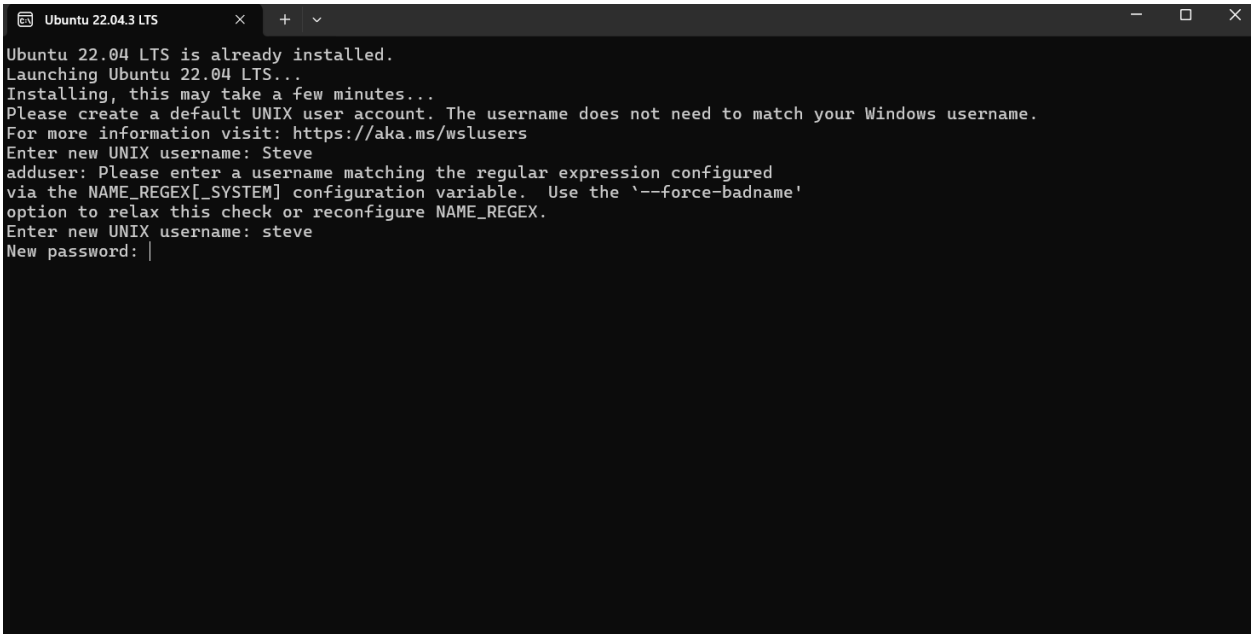


Click enter

Lower case letters only



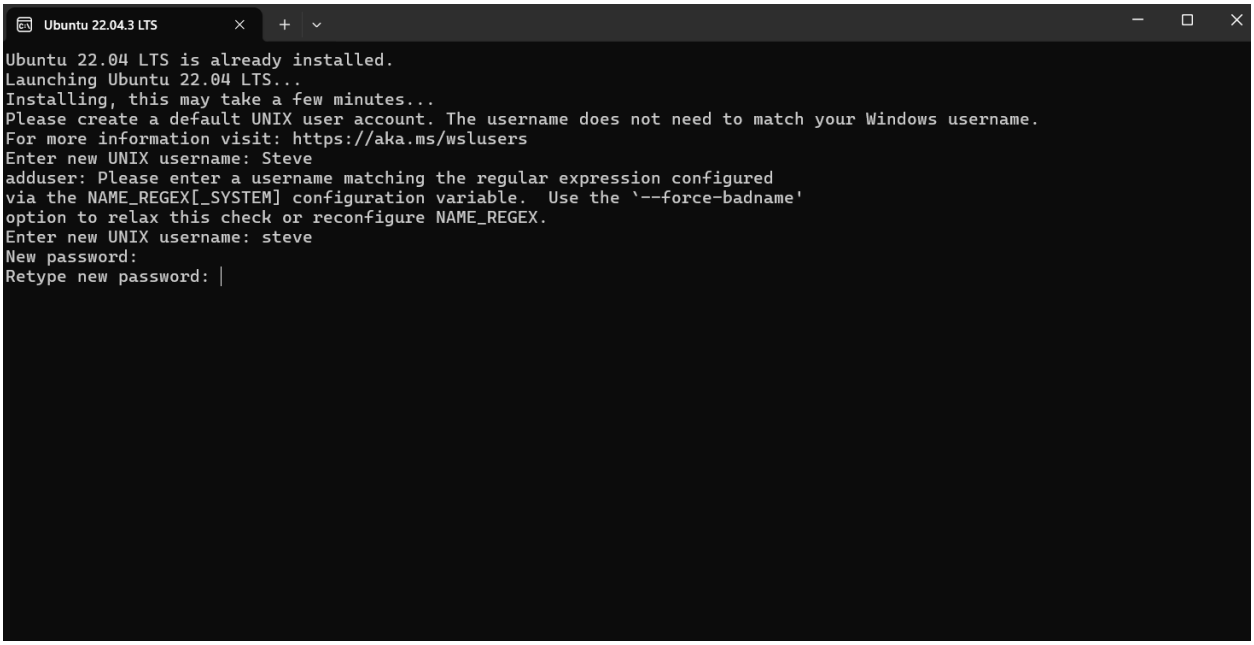
Click enter

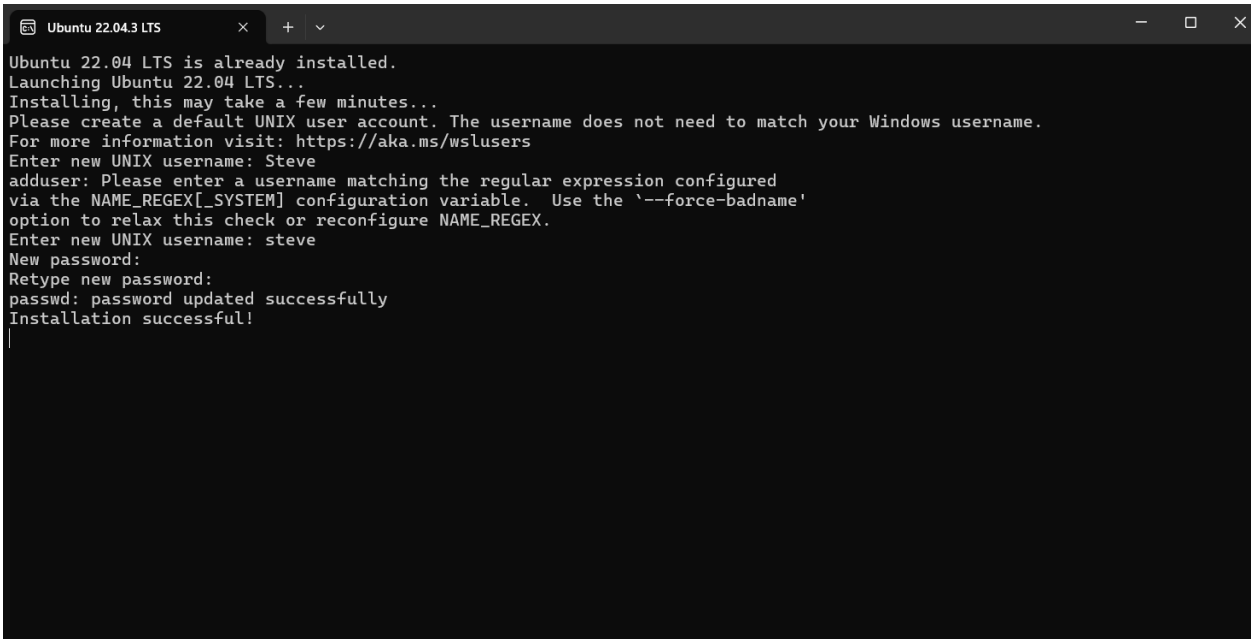


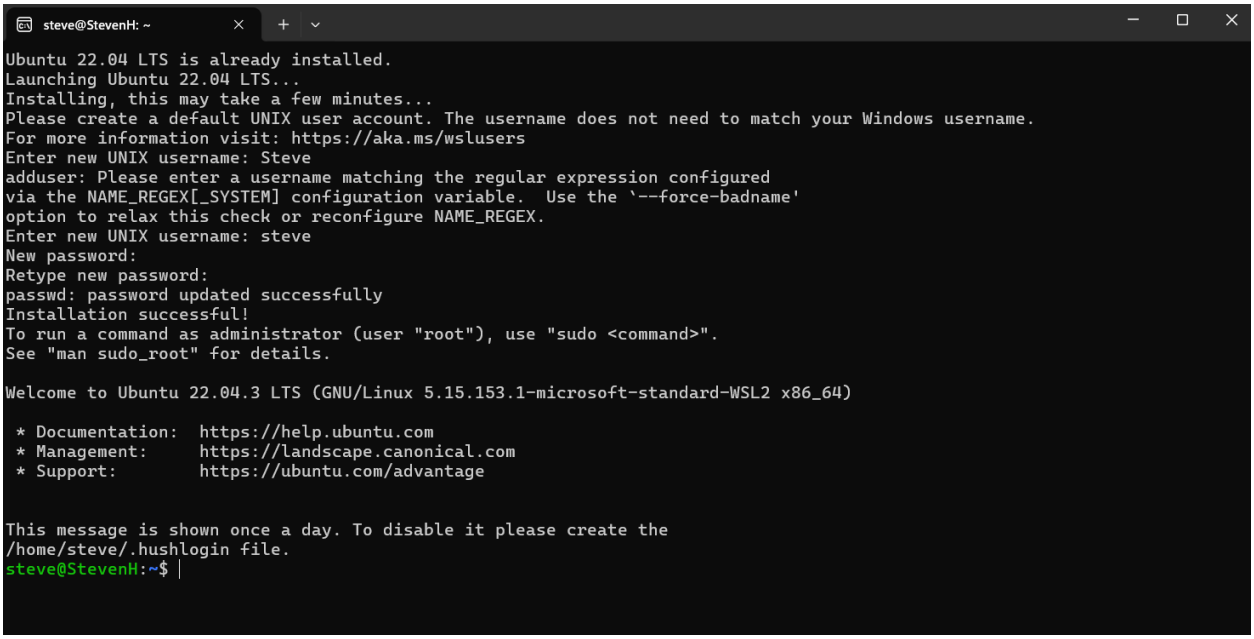
Now enter a new password

We know it looks very weird when the cursor stays in the same place, but trust it, it is recording your new password, press enter

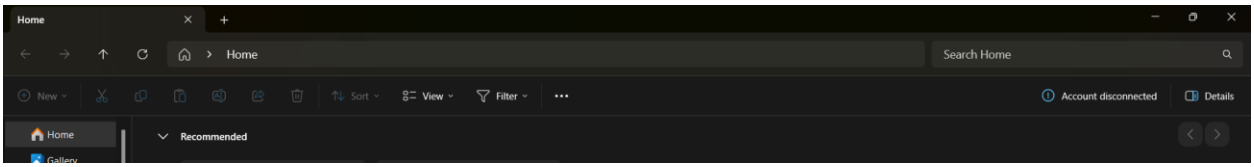
Now retype the password again, and press enter:

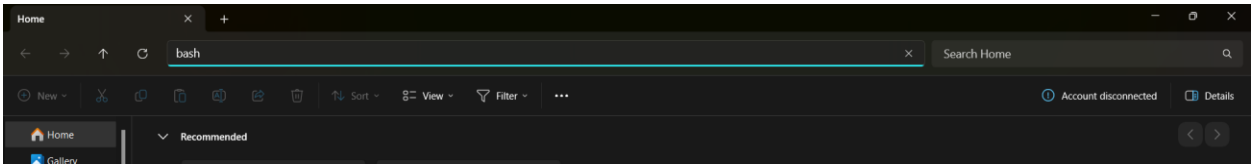


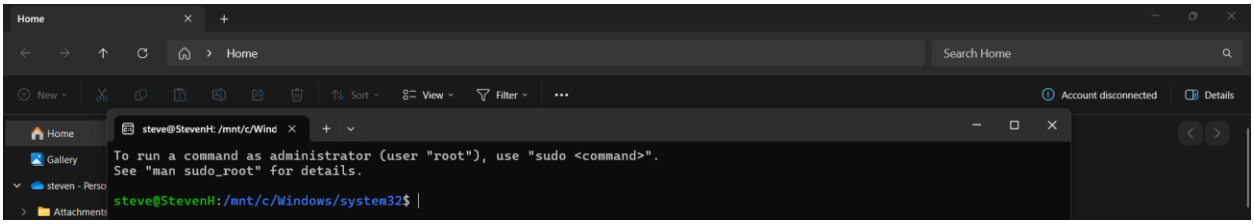




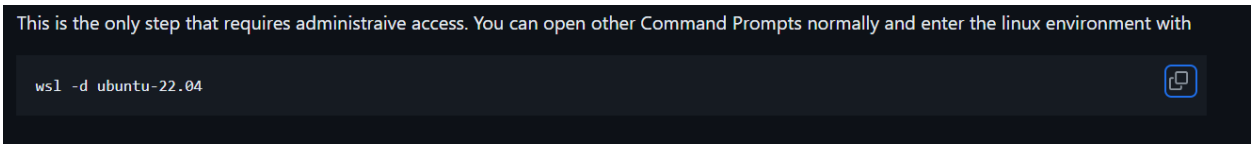
Now, do the second command on the website, you can enter into the Linux subsystem by typing bash into the top:



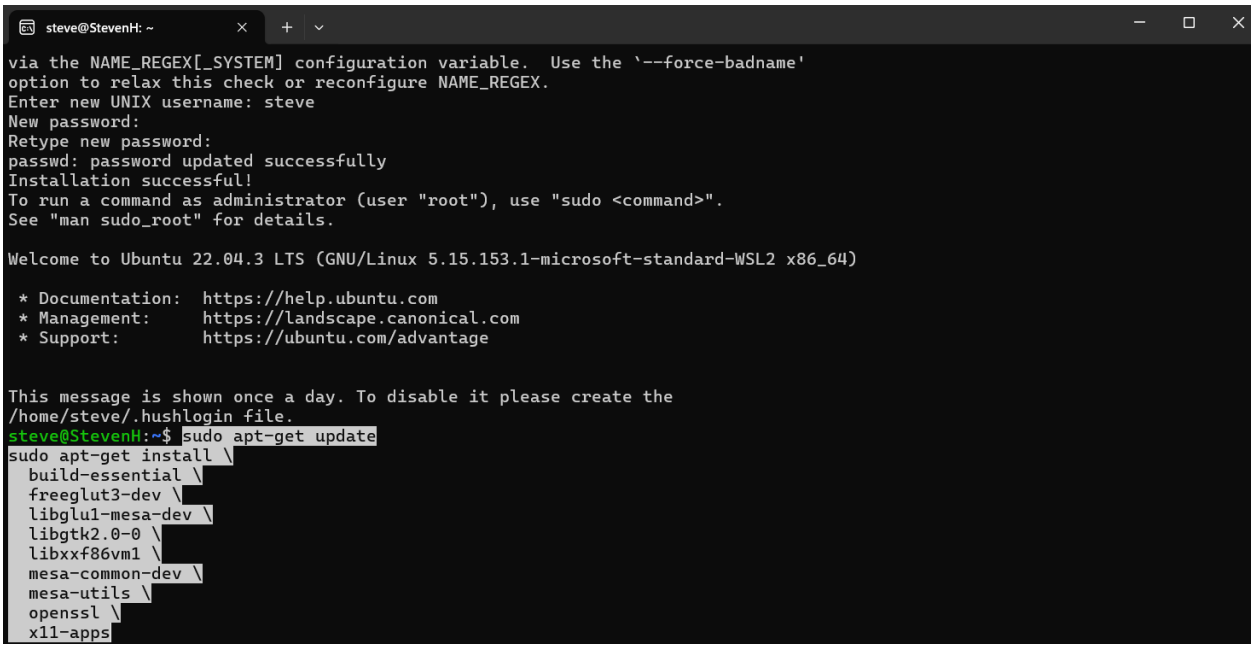


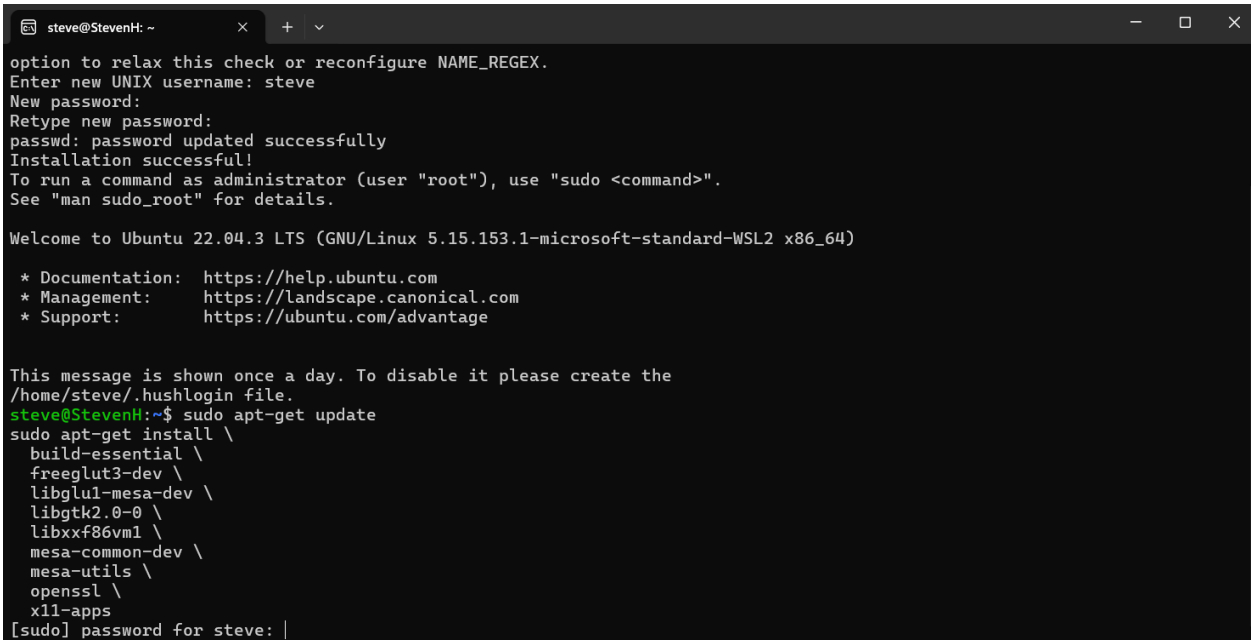


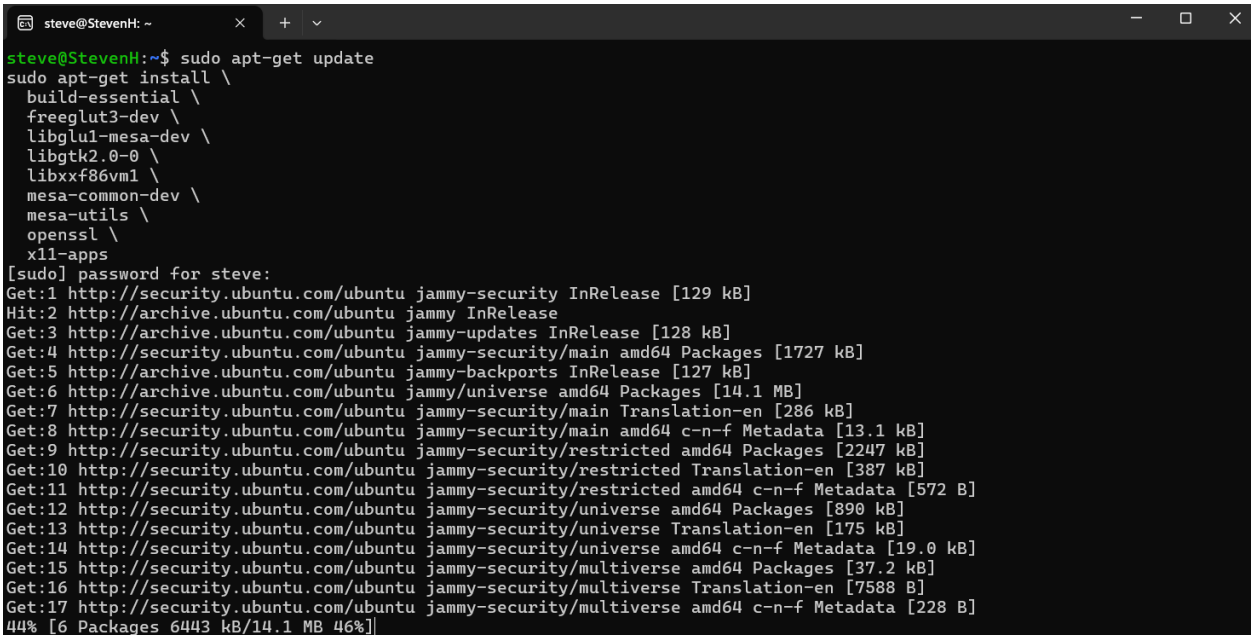
You can also enter by going into the command prompt this way:



Follow other steps on website:




steve@StevenH: ~
option to relax this check or reconfigure NAME_REGEX.
Enter new UNIX username: steve
New password:
Retype new password:
passwd: password updated successfully
Installation successful!
To run a command as administrator (user "root"), use "sudo <command>".
See "man sudo_root" for details.
Welcome to Ubuntu 22.04.3 LTS (GNU/Linux 5.15.153.1-microsoft-standard-WSL2 x86_64)
* Documentation: https://help.ubuntu.com
* Management: https://landscape.canonical.com
* Support: https://ubuntu.com/advantage
This message is shown once a day. To disable it please create the
/home/steve/.hushlogin file.
steve@StevenH:~$ sudo apt-get update
sudo apt-get install \
build-essential \
freeglut3-dev \
libglu1-mesa-dev \
libgtk2.0-0 \
libxxf86vm1 \
mesa-common-dev \
mesa-utils \
openssl \
x11-apps
[sudo] password for steve:


steve@StevenH: ~
steve@StevenH:~$ sudo apt-get update
sudo apt-get install \
build-essential \
freeglut3-dev \
libglu1-mesa-dev \
libgtk2.0-0 \
libxxf86vm1 \
mesa-common-dev \
mesa-utils \
openssl \
x11-apps
[sudo] password for steve:
Get:1 http://security.ubuntu.com/ubuntu jammy-security InRelease [129 kB]
Hit:2 http://archive.ubuntu.com/ubuntu jammy InRelease
Get:3 http://archive.ubuntu.com/ubuntu jammy-updates InRelease [128 kB]
Get:4 http://security.ubuntu.com/ubuntu jammy-security/main amd64 Packages [1727 kB]
Get:5 http://archive.ubuntu.com/ubuntu jammy-backports InRelease [127 kB]
Get:6 http://archive.ubuntu.com/ubuntu jammy/universe amd64 Packages [14.1 MB]
Get:7 http://security.ubuntu.com/ubuntu jammy-security/main Translation-en [286 kB]
Get:8 http://security.ubuntu.com/ubuntu jammy-security/main amd64 c-n-f Metadata [13.1 kB]
Get:9 http://security.ubuntu.com/ubuntu jammy-security/restricted amd64 Packages [2247 kB]
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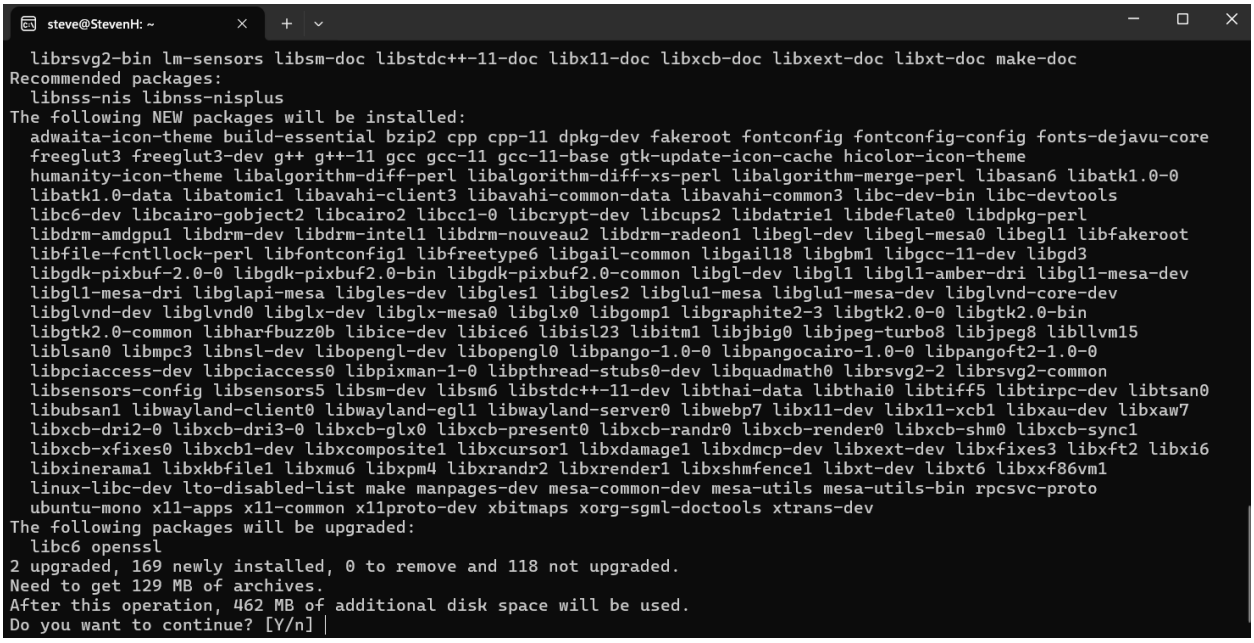
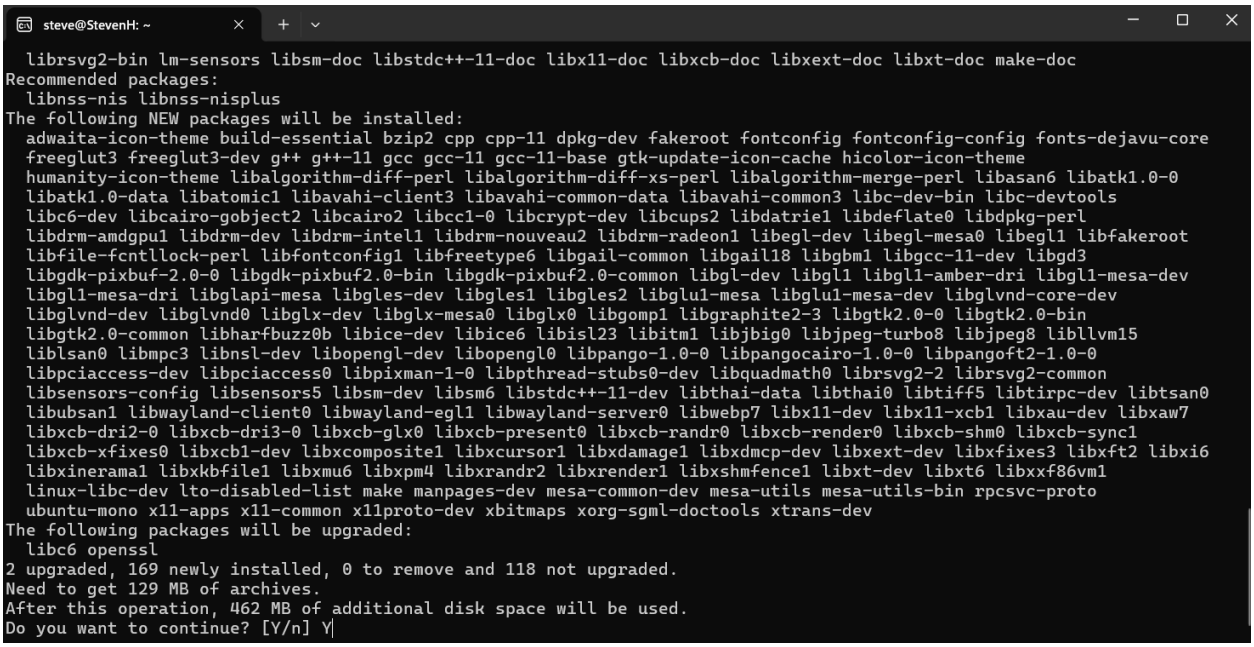
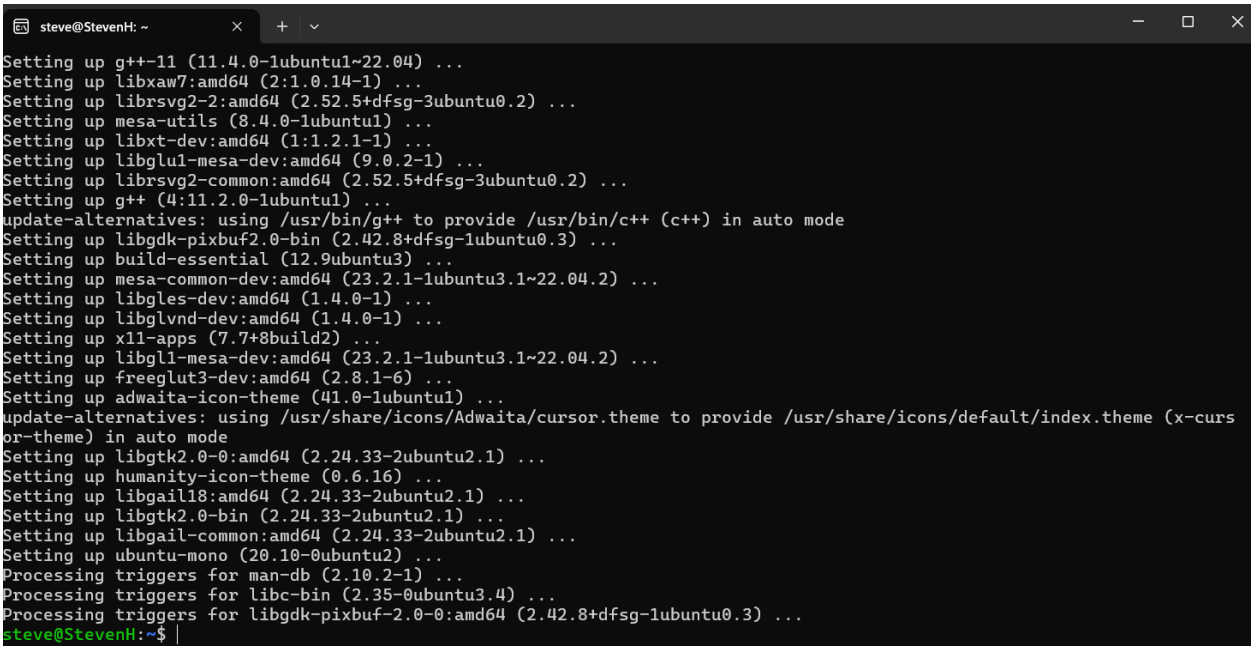
Get:11 http://security.ubuntu.com/ubuntu jammy-security/restricted amd64 c-n-f Metadata [572 B]
Get:12 http://security.ubuntu.com/ubuntu jammy-security/universe amd64 Packages [890 kB]
Get:13 http://security.ubuntu.com/ubuntu jammy-security/universe Translation-en [175 kB]
Get:14 http://security.ubuntu.com/ubuntu jammy-security/universe amd64 c-n-f Metadata [19.0 kB]
Get:15 http://security.ubuntu.com/ubuntu jammy-security/multiverse amd64 Packages [37.2 kB]
Get:16 http://security.ubuntu.com/ubuntu jammy-security/multiverse Translation-en [7588 B]
Get:17 http://security.ubuntu.com/ubuntu jammy-security/multiverse amd64 c-n-f Metadata [228 B]
44% [6 Packages 6443 kB/14.1 MB 46%]

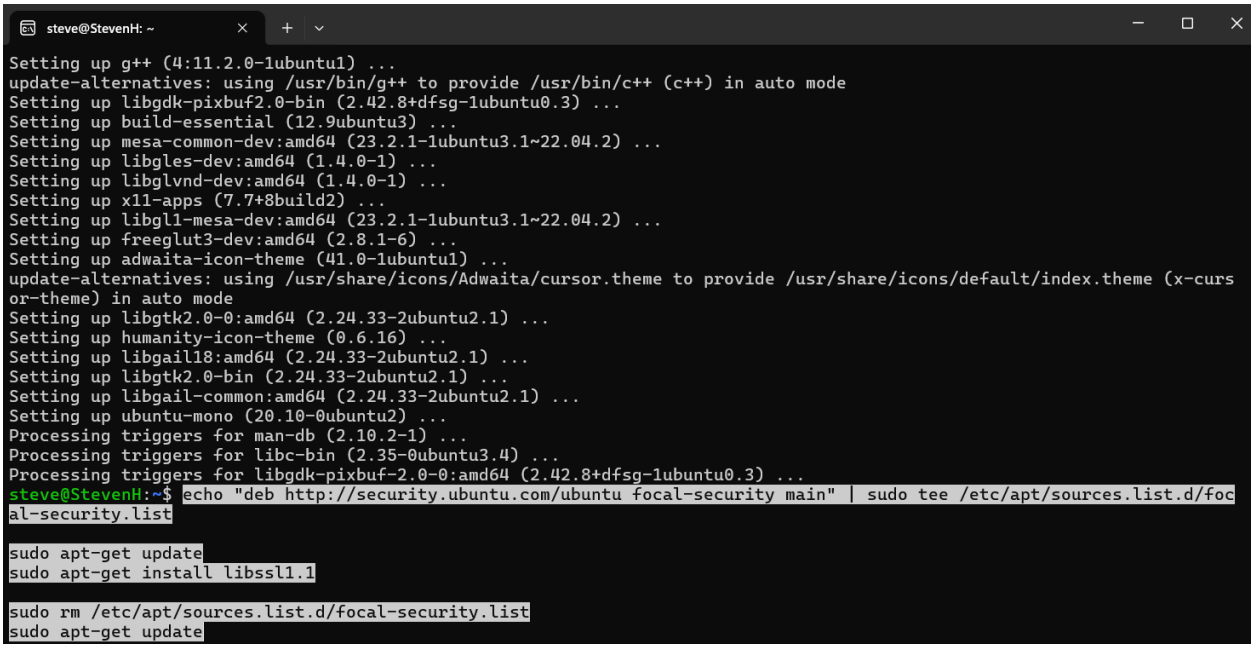


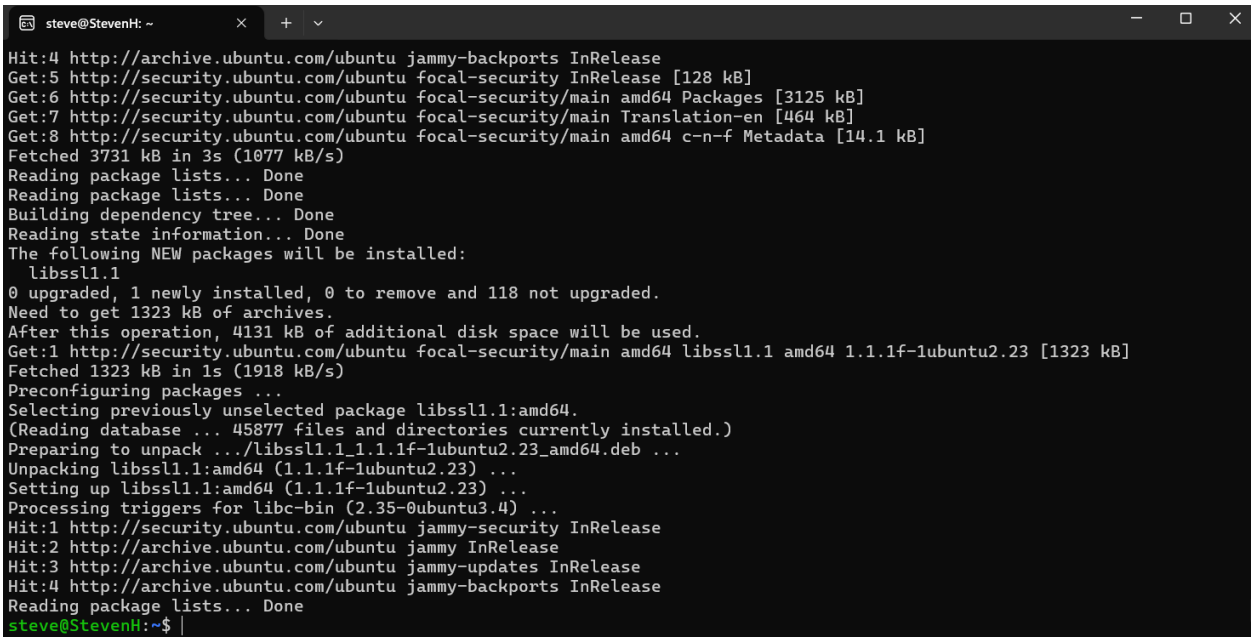
Y or n, so of course say Y, click enter

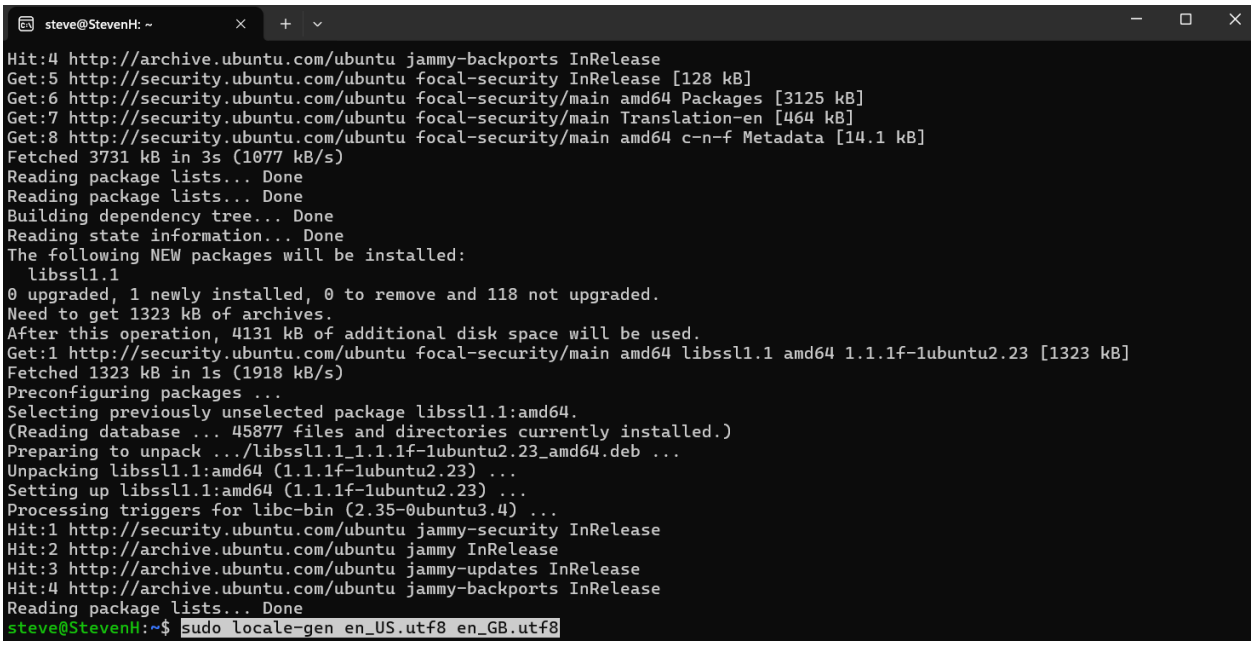


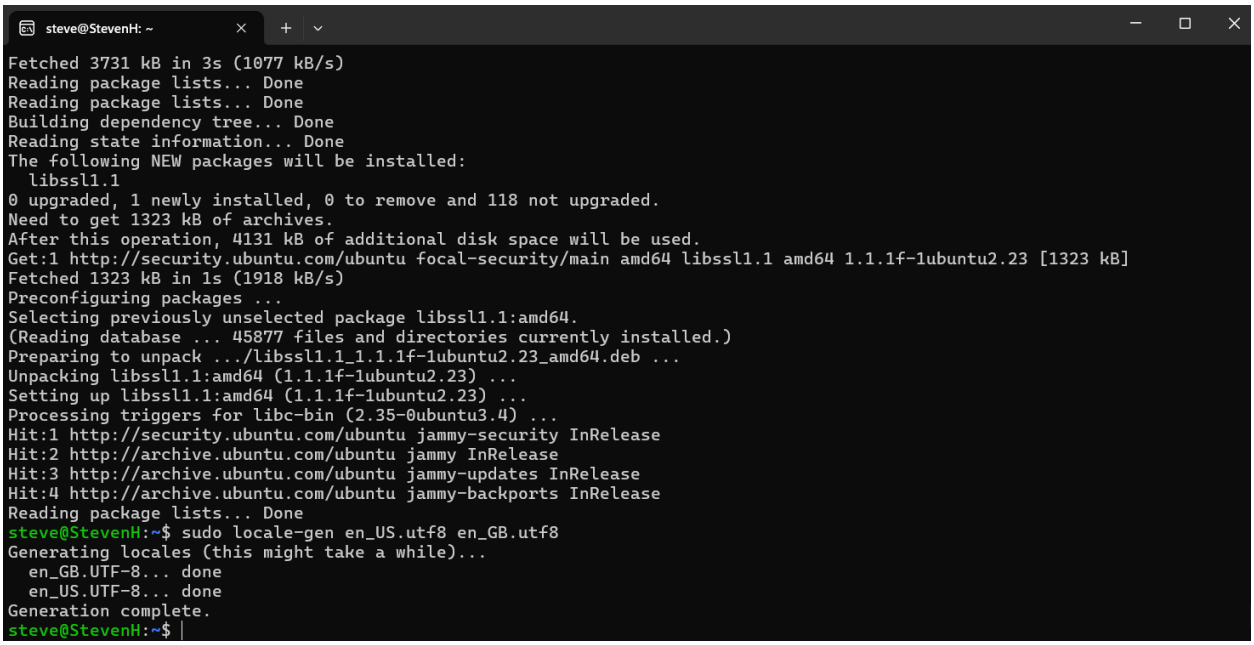
It is now done:


steve@StevenH: ~
Setting up g++-11 (11.4.0-1ubuntu1~22.04) ...
Setting up libxaw7:amd64 (2:1.0.14-1) ...
Setting up librsvg2-2:amd64 (2.52.5+dfsg-3ubuntu0.2) ...
Setting up mesa-utils (8.4.0-1ubuntu1) ...
Setting up libxt-dev:amd64 (1:1.2.1-1) ...
Setting up libglu1-mesa-dev:amd64 (9.0.2-1) ...
Setting up librsvg2-common:amd64 (2.52.5+dfsg-3ubuntu0.2) ...
Setting up g++ (4:11.2.0-1ubuntu1) ...
update-alternatives: using /usr/bin/g++ to provide /usr/bin/c++ (c++) in auto mode
Setting up libgdk-pixbuf2.0-bin (2.42.8+dfsg-1ubuntu0.3) ...
Setting up build-essential (12.9ubuntu3) ...
Setting up mesa-common-dev:amd64 (23.2.1-1ubuntu3.1~22.04.2) ...
Setting up libgles-dev:amd64 (1.4.0-1) ...
Setting up libglvnd-dev:amd64 (1.4.0-1) ...
Setting up x11-apps (7.7+8build2) ...
Setting up libgl1-mesa-dev:amd64 (23.2.1-1ubuntu3.1~22.04.2) ...
Setting up freeglut3-dev:amd64 (2.8.1-6) ...
Setting up adwaita-icon-theme (41.0-1ubuntu1) ...
update-alternatives: using /usr/share/icons/Adwaita/cursor.theme to provide /usr/share/icons/default/index.theme (x-cursor-theme) in auto mode
Setting up libgtk2.0-0:amd64 (2.24.33-2ubuntu2.1) ...
Setting up humanity-icon-theme (0.6.16) ...
Setting up libgail18:amd64 (2.24.33-2ubuntu2.1) ...
Setting up libgtk2.0-bin (2.24.33-2ubuntu2.1) ...
Setting up libgail-common:amd64 (2.24.33-2ubuntu2.1) ...
Setting up ubuntu-mono (20.10-0ubuntu2) ...
Processing triggers for man-db (2.10.2-1) ...
Processing triggers for libc-bin (2.35-0ubuntu3.4) ...
Processing triggers for libgdk-pixbuf-2.0-0:amd64 (2.42.8+dfsg-1ubuntu0.3) ...
steve@StevenH:~$

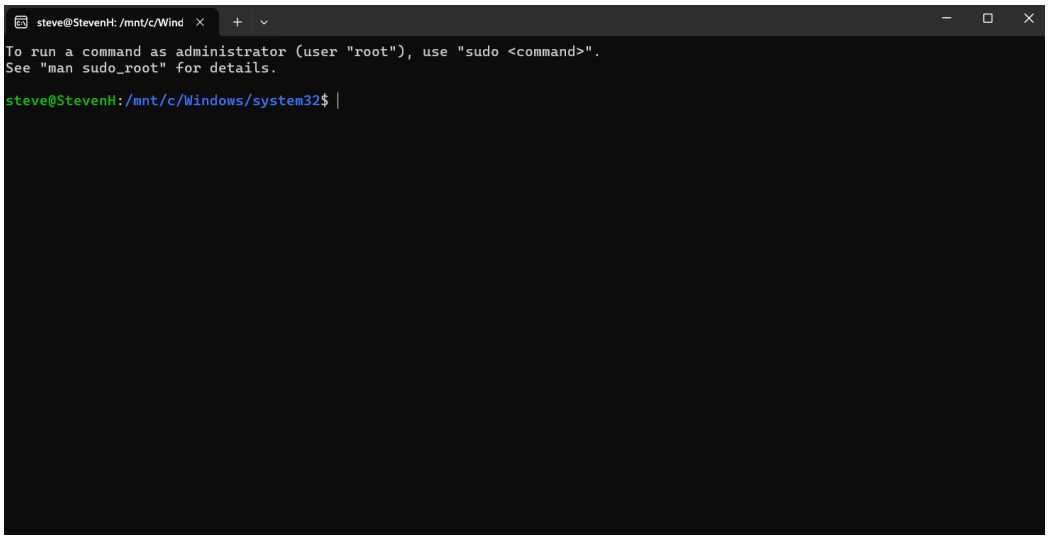

steve@StevenH: ~
Setting up g++ (4:11.2.0-1ubuntu1) ...
update-alternatives: using /usr/bin/g++ to provide /usr/bin/c++ (c++) in auto mode
Setting up libgdk-pixbuf2.0-bin (2.42.8+dfsg-1ubuntu0.3) ...
Setting up build-essential (12.9ubuntu3) ...
Setting up mesa-common-dev:amd64 (23.2.1-1ubuntu3.1~22.04.2) ...
Setting up libgles-dev:amd64 (1.4.0-1) ...
Setting up libglvnd-dev:amd64 (1.4.0-1) ...
Setting up x11-apps (7.7+8build2) ...
Setting up libgl1-mesa-dev:amd64 (23.2.1-1ubuntu3.1~22.04.2) ...
Setting up freeglut3-dev:amd64 (2.8.1-6) ...
Setting up adwaita-icon-theme (41.0-1ubuntu1) ...
update-alternatives: using /usr/share/icons/Adwaita/cursor.theme to provide /usr/share/icons/default/index.theme (x-cursor-theme) in auto mode
Setting up libgtk2.0-0:amd64 (2.24.33-2ubuntu2.1) ...
Setting up humanity-icon-theme (0.6.16) ...
Setting up libgail18:amd64 (2.24.33-2ubuntu2.1) ...
Setting up libgtk2.0-bin (2.24.33-2ubuntu2.1) ...
Setting up libgail-common:amd64 (2.24.33-2ubuntu2.1) ...
Setting up ubuntu-mono (20.10-0ubuntu2) ...
Processing triggers for man-db (2.10.2-1) ...
Processing triggers for libc-bin (2.35-0ubuntu3.4) ...
Processing triggers for libgdk-pixbuf-2.0-0:amd64 (2.42.8+dfsg-1ubuntu0.3) ...
steve@StevenH:~$ echo "deb http://security.ubuntu.com/ubuntu focal-security main" | sudo tee /etc/apt/sources.list.d/focal-security.list
sudo apt-get update
sudo apt-get install libssl1.1
sudo rm /etc/apt/sources.list.d/focal-security.list
sudo apt-get update

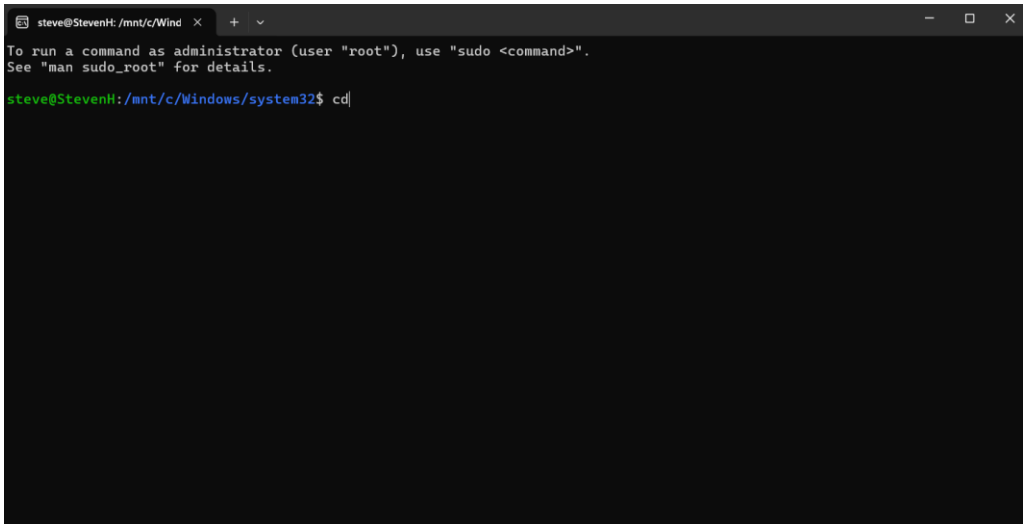

steve@StevenH: ~
Hit:4 http://archive.ubuntu.com/ubuntu jammy-backports InRelease
Get:5 http://security.ubuntu.com/ubuntu focal-security InRelease [128 kB]
Get:6 http://security.ubuntu.com/ubuntu focal-security/main amd64 Packages [3125 kB]
Get:7 http://security.ubuntu.com/ubuntu focal-security/main Translation-en [464 kB]
Get:8 http://security.ubuntu.com/ubuntu focal-security/main amd64 c-n-f Metadata [14.1 kB]
Fetched 3731 kB in 3s (1077 kB/s)
Reading package lists... Done
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
The following NEW packages will be installed:
libssl1.1
0 upgraded, 1 newly installed, 0 to remove and 118 not upgraded.
Need to get 1323 kB of archives.
After this operation, 4131 kB of additional disk space will be used.
Get:1 http://security.ubuntu.com/ubuntu focal-security/main amd64 libssl1.1 amd64 1.1.1f-1ubuntu2.23 [1323 kB]
Fetched 1323 kB in 1s (1918 kB/s)
Preconfiguring packages ...
Selecting previously unselected package libssl1.1:amd64.
(Reading database ... 45877 files and directories currently installed.)
Preparing to unpack .../libssl1.1_1.1.1f-1ubuntu2.23_amd64.deb ...
Unpacking libssl1.1:amd64 (1.1.1f-1ubuntu2.23) ...
Setting up libssl1.1:amd64 (1.1.1f-1ubuntu2.23) ...
Processing triggers for libc-bin (2.35-0ubuntu3.4) ...
Hit:1 http://security.ubuntu.com/ubuntu jammy-security InRelease
Hit:2 http://archive.ubuntu.com/ubuntu jammy InRelease
Hit:3 http://archive.ubuntu.com/ubuntu jammy-updates InRelease
Hit:4 http://archive.ubuntu.com/ubuntu jammy-backports InRelease
Reading package lists... Done
steve@StevenH:~$


steve@StevenH: ~
Hit:4 http://archive.ubuntu.com/ubuntu jammy-backports InRelease
Get:5 http://security.ubuntu.com/ubuntu focal-security InRelease [128 kB]
Get:6 http://security.ubuntu.com/ubuntu focal-security/main amd64 Packages [3125 kB]
Get:7 http://security.ubuntu.com/ubuntu focal-security/main Translation-en [464 kB]
Get:8 http://security.ubuntu.com/ubuntu focal-security/main amd64 c-n-f Metadata [14.1 kB]
Fetched 3731 kB in 3s (1077 kB/s)
Reading package lists... Done
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
The following NEW packages will be installed:
libssl1.1
0 upgraded, 1 newly installed, 0 to remove and 118 not upgraded.
Need to get 1323 kB of archives.
After this operation, 4131 kB of additional disk space will be used.
Get:1 http://security.ubuntu.com/ubuntu focal-security/main amd64 libssl1.1 amd64 1.1.1f-1ubuntu2.23 [1323 kB]
Fetched 1323 kB in 1s (1918 kB/s)
Preconfiguring packages ...
Selecting previously unselected package libssl1.1:amd64.
(Reading database ... 45877 files and directories currently installed.)
Preparing to unpack .../libssl1.1_1.1.1f-1ubuntu2.23_amd64.deb ...
Unpacking libssl1.1:amd64 (1.1.1f-1ubuntu2.23) ...
Setting up libssl1.1:amd64 (1.1.1f-1ubuntu2.23) ...
Processing triggers for libc-bin (2.35-0ubuntu3.4) ...
Hit:1 http://security.ubuntu.com/ubuntu jammy-security InRelease
Hit:2 http://archive.ubuntu.com/ubuntu jammy InRelease
Hit:3 http://archive.ubuntu.com/ubuntu jammy-updates InRelease
Hit:4 http://archive.ubuntu.com/ubuntu jammy-backports InRelease
Reading package lists... Done
steve@StevenH:~$ sudo locale-gen en_US.utf8 en_GB.utf8

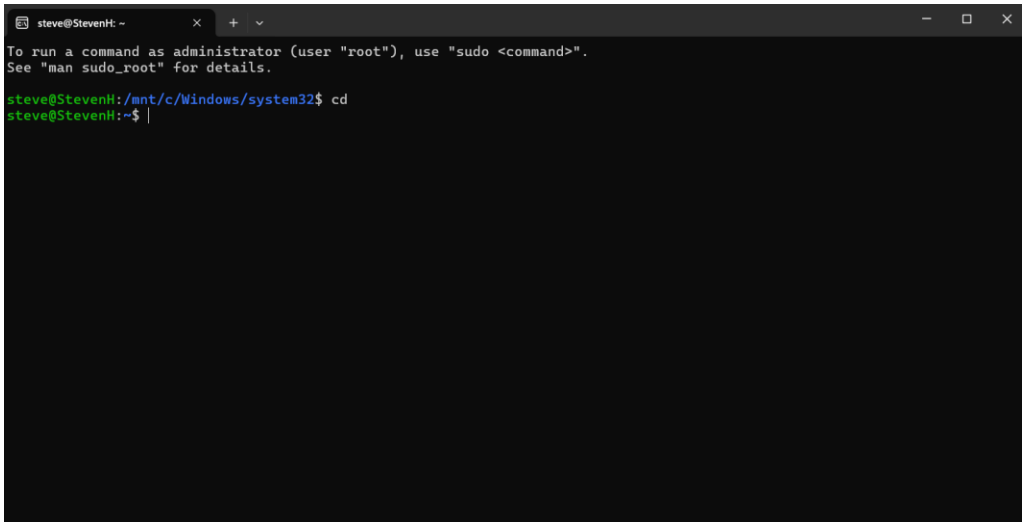


Time for some basics:

1. How to change directories (or go into different folders)
    a. To go to the root directory, you simply type “cd”:
        i. 

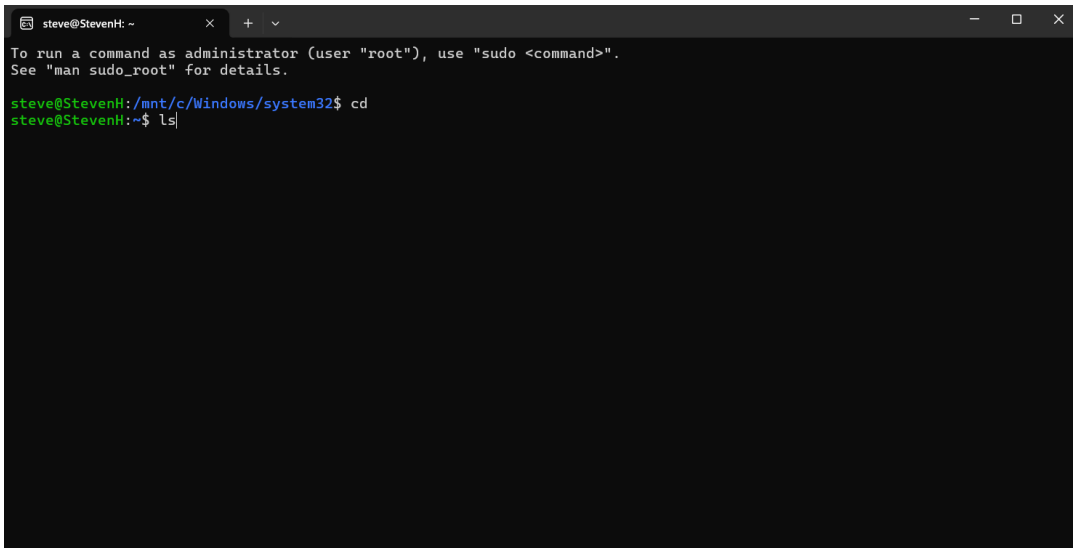
ii. 

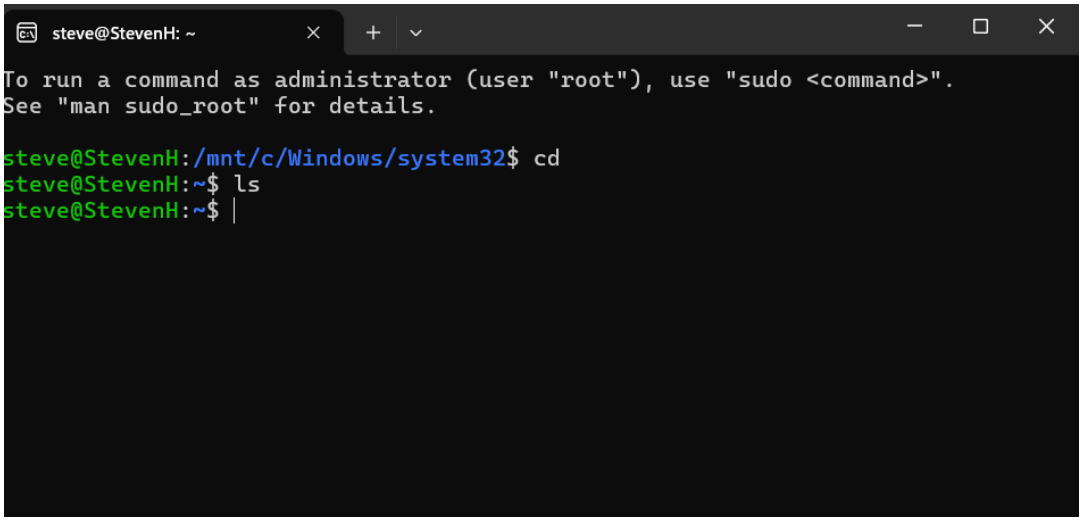
iii. "cd" means change directory, it will bring you to the root directory

iv. 

v.

2. How to list things out that are in a folder
    a. To see what is in the folder, simply type **ls** to list the items out:

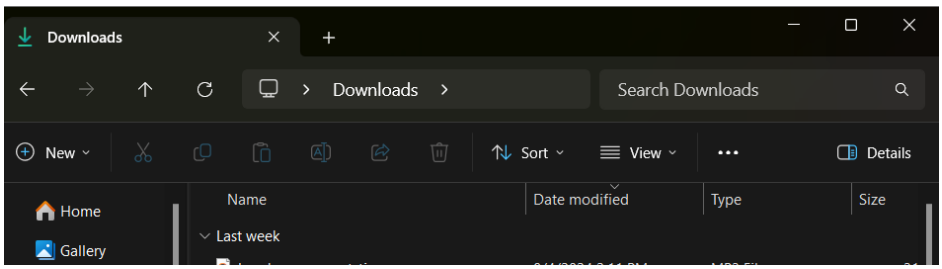
i. 

ii. 

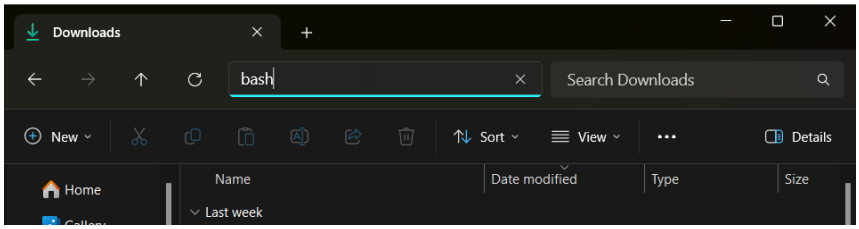
iii. There is nothing in the Linux subsystem folder just yet, which is why nothing is there.

iv. If you opened the downloads folder and wanted to go to the desktop folder, this is how you do it:

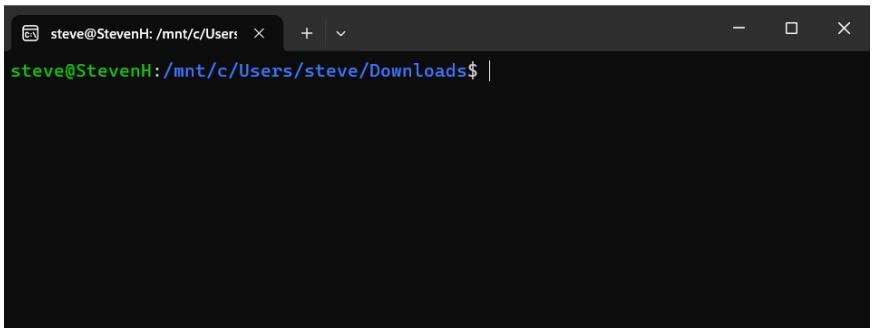
v. Open the downloads folder in Windows, type bash at the top, **cd ..** on folder below, like so:

vi. 

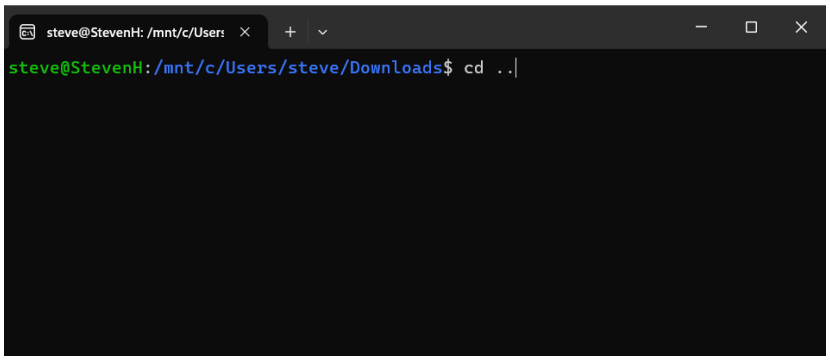
vii.



viii.

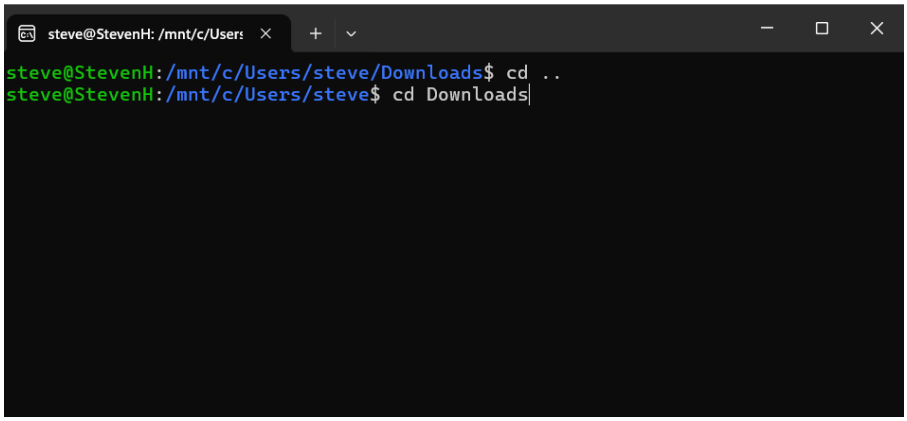


ix.

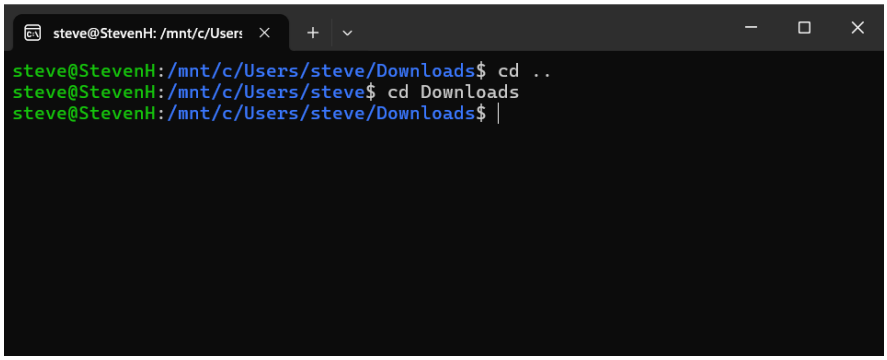


x.

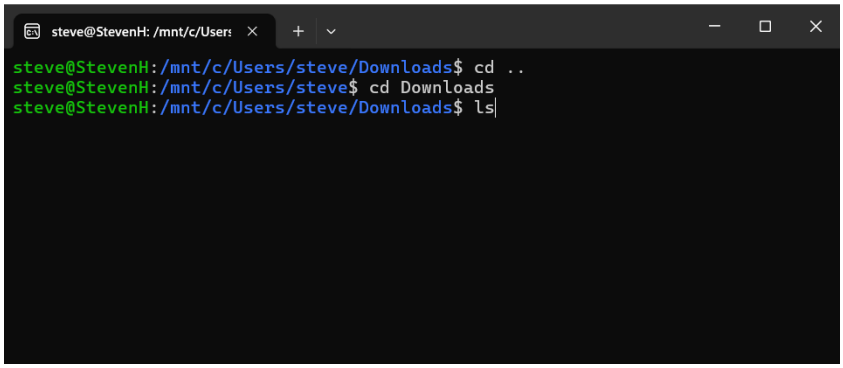
xi.



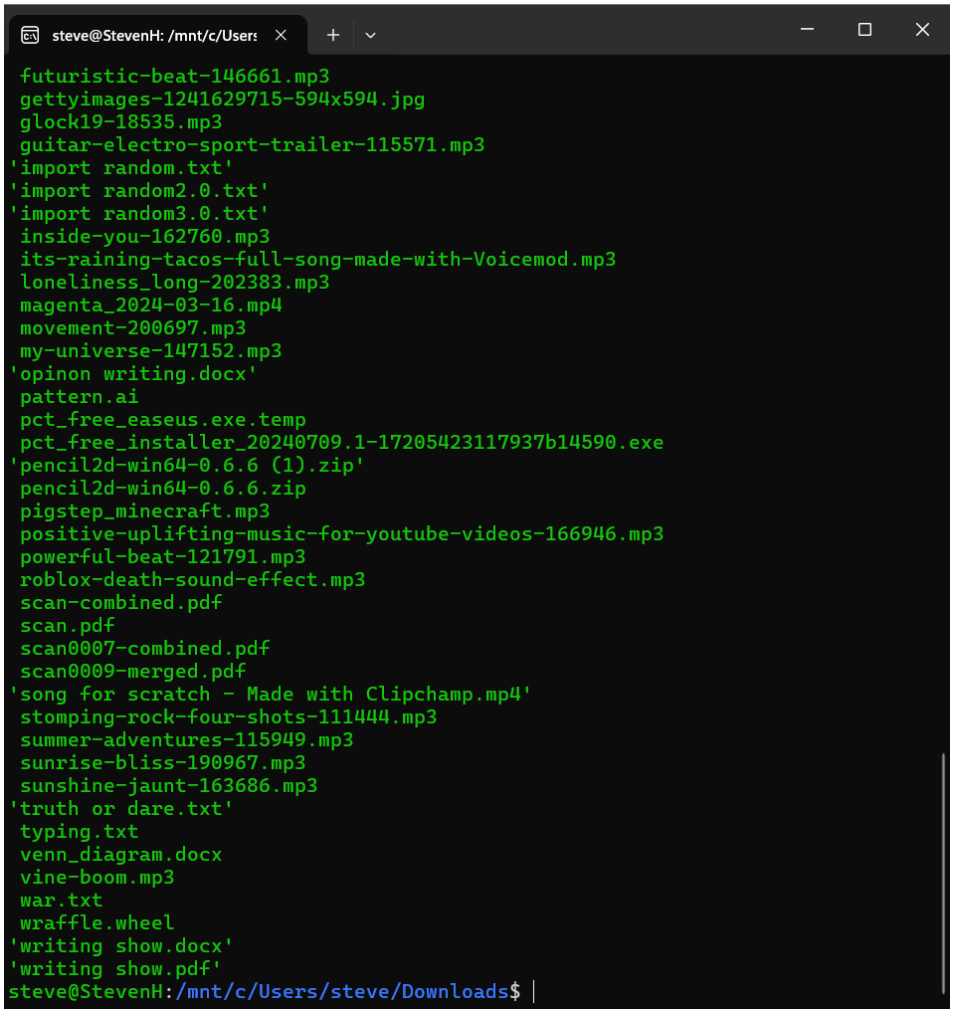
xii.


steve@StevenH: /mnt/c/Users
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd ..
steve@StevenH:/mnt/c/Users/steve$ cd Downloads
steve@StevenH:/mnt/c/Users/steve/Downloads$

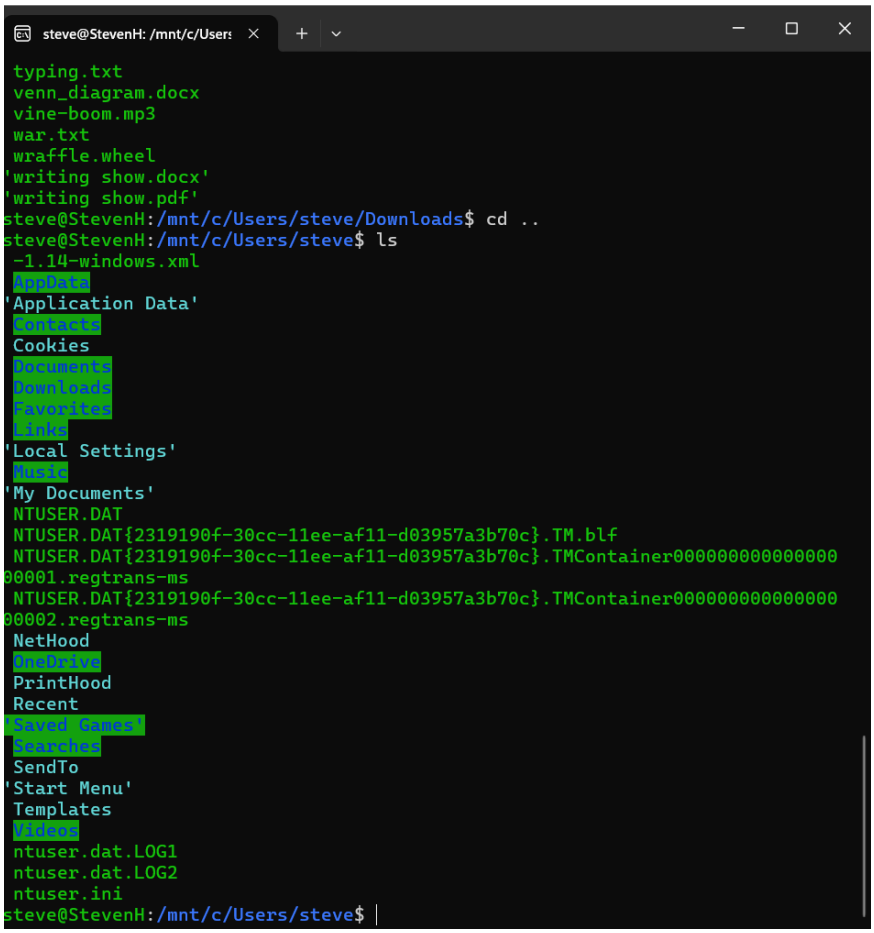
xiii.


steve@StevenH: /mnt/c/Users
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd ..
steve@StevenH:/mnt/c/Users/steve$ cd Downloads
steve@StevenH:/mnt/c/Users/steve/Downloads$ ls

xiv.

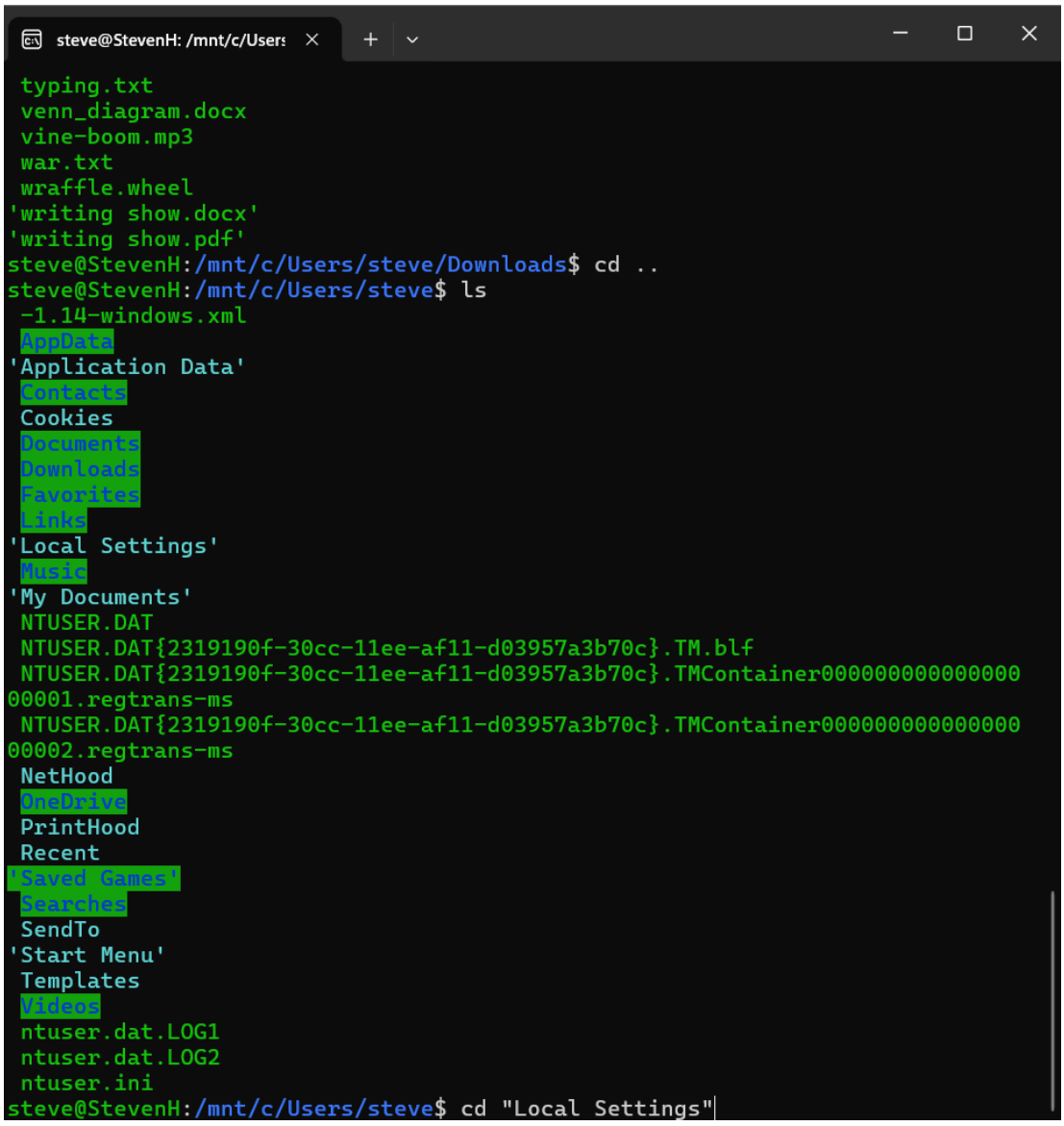

steve@StevenH: /mnt/c/Users
futuristic-beat-146661.mp3
gettyimages-1241629715-594x594.jpg
glock19-18535.mp3
guitar-electro-sport-trailer-115571.mp3
'import random.txt'
'import random2.0.txt'
'import random3.0.txt'
inside-you-162760.mp3
its-raining-tacos-full-song-made-with-Voicemod.mp3
loneliness_long-202383.mp3
magenta_2024-03-16.mp4
movement-200697.mp3
my-universe-147152.mp3
'opinon writing.docx'
pattern.ai
pct_free_easeus.exe.temp
pct_free_installer_20240709.1-17205423117937b14590.exe
'pencil2d-win64-0.6.6 (1).zip'
pencil2d-win64-0.6.6.zip
pigstep_minecraft.mp3
positive-uplifting-music-for-youtube-videos-166946.mp3
powerful-beat-121791.mp3
roblox-death-sound-effect.mp3
scan-combined.pdf
scan.pdf
scan0007-combined.pdf
scan0009-merged.pdf
'song for scratch - Made with Clipchamp.mp4'
stomping-rock-four-shots-111444.mp3
summer-adventures-115949.mp3
sunrise-bliss-190967.mp3
sunshine-jaunt-163686.mp3
'truth or dare.txt'
typing.txt
venn_diagram.docx
vine-boom.mp3
war.txt
wraffle.wheel
'writing show.docx'
'writing show.pdf'
steve@StevenH:/mnt/c/Users/steve/Downloads$

xv.

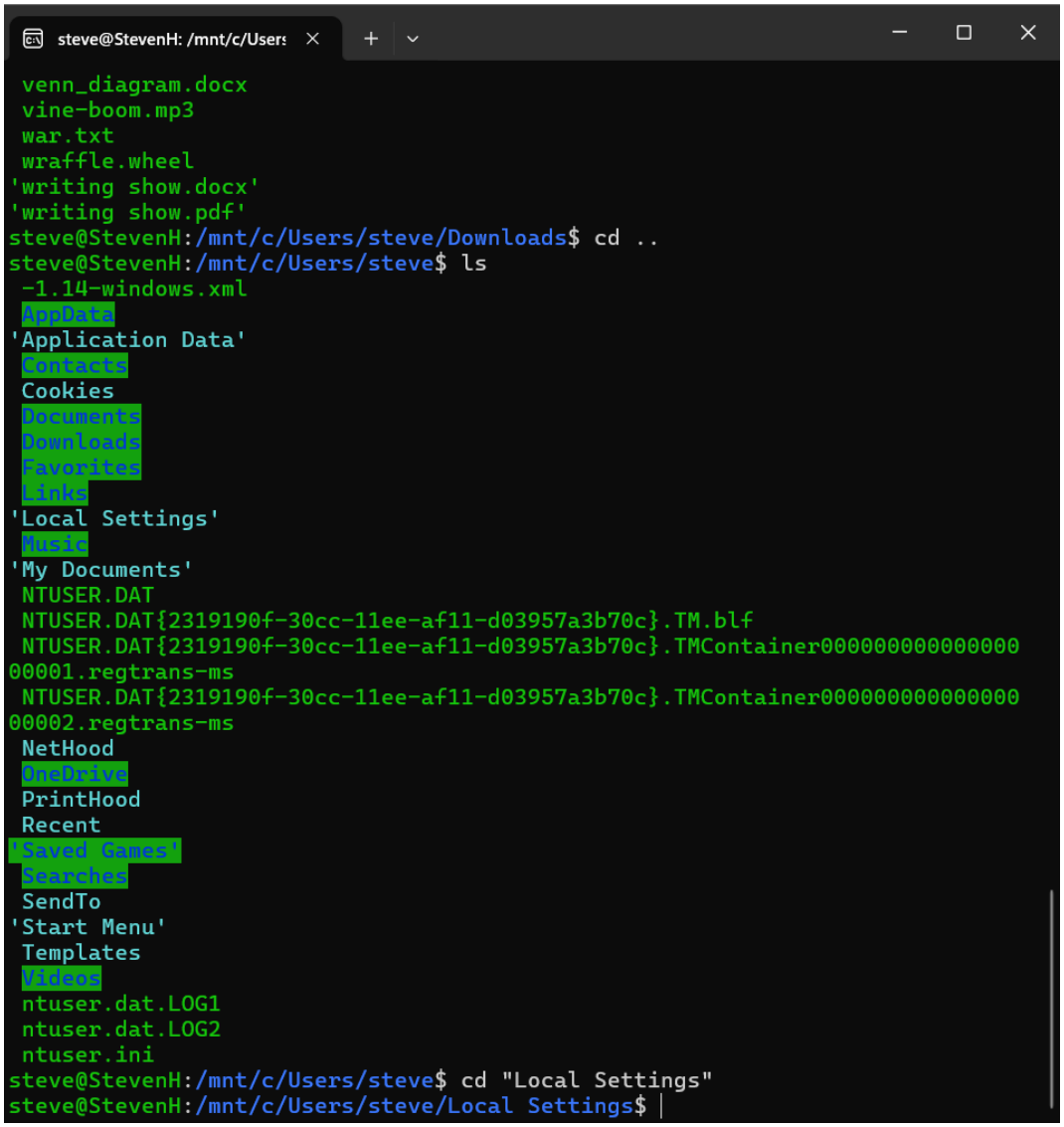


xvi. Notice that text with spaces have half quotations around them. If you wanted to cd into those folders, you would have to reference them with full quotation marks around the full term: ex: Local Settings is displaying as ‘Local Settings’ but if you wanted to cd into Local Settings, you would need to cd “Local Settings” with full quotation marks. Make sure to keep all the other capitalizations, punctuations exactly the same as listed.

xvii.


steve@StevenH: /mnt/c/Users
typing.txt
venn_diagram.docx
vine-boom.mp3
war.txt
wraffle.wheel
'writing show.docx'
'writing show.pdf'
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd ..
steve@StevenH:/mnt/c/Users/steve$ ls
-1.14-windows.xml
AppData
'Application Data'
Contacts
Cookies
Documents
Downloads
Favorites
Links
'Local Settings'
Music
'My Documents'
NTUSER.DAT
NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TM.blf
NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TMContainer00000000000000000001.regtrans-ms
NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TMContainer00000000000000000002.regtrans-ms
NetHood
OneDrive
PrintHood
Recent
'Saved Games'
Searches
SendTo
'Start Menu'
Templates
Videos
ntuser.dat.LOG1
ntuser.dat.LOG2
ntuser.ini
steve@StevenH:/mnt/c/Users/steve$ cd "Local Settings"

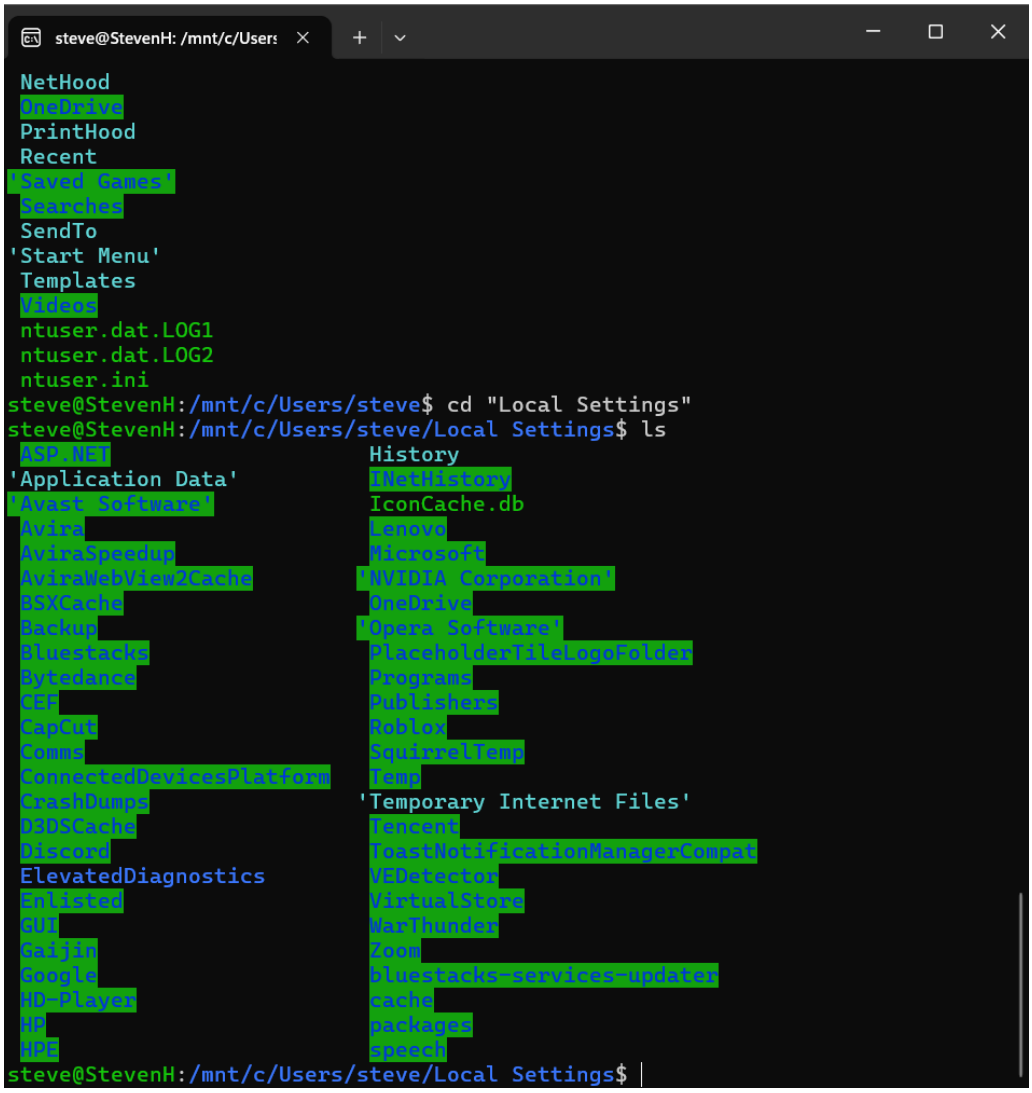
xviii.



xix. Now you are in your Local Settings folder

xx. You can ls in the local setting folder to see what is in it

xxi.



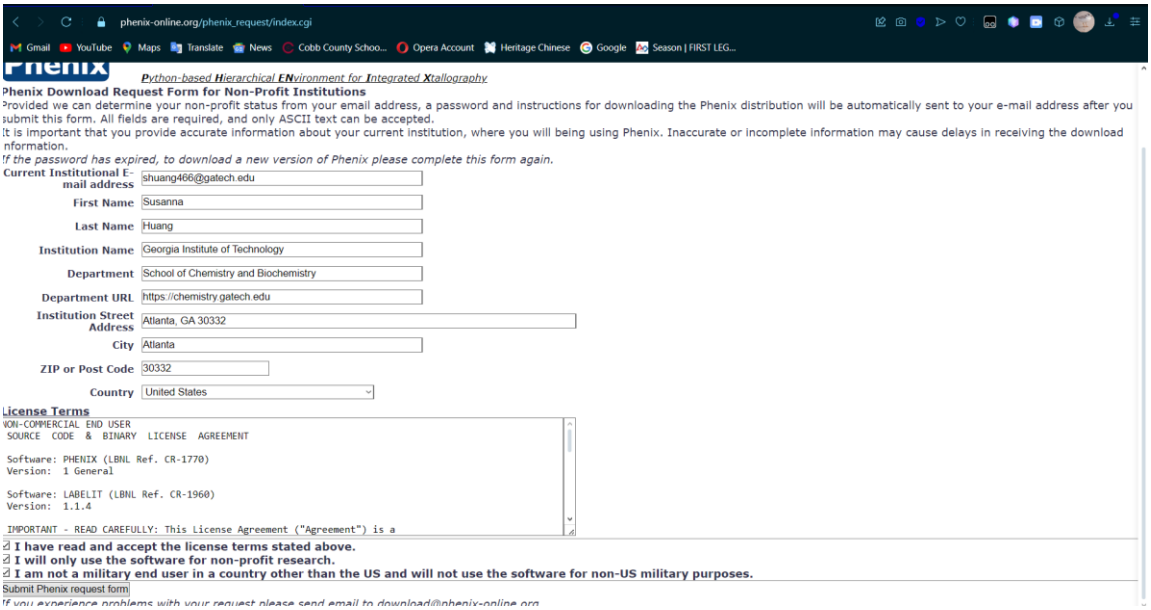
3. A list of key commands in your Linux Windows subsystem:

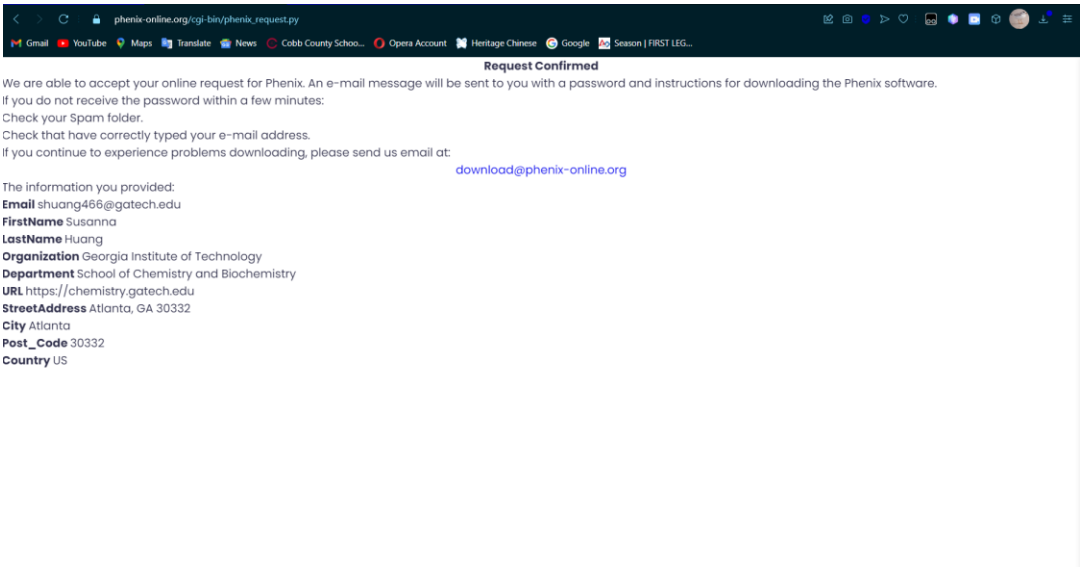
- **cd**
    - goes to the home directory
- **ls**
    - list out the items in the folder
- **cp**
    - the copy file or directory function
    - a file:
        - cd <file name> <copy-to-folder directory>
    - an entire directory
        - cd -r <file directory name> <copy-to-folder directory>
- **pwd**
    - print current directory name, useful for copying the directory name for cp'ing things

- **mkdr**
    - makes a new directory or folder
    - Ex: **mkdr PhenixProjects**
        - This makes a new directory, called PhenixProjects, in your current directory

Now you just need to download the PHENIX files:

Go to the third link.





Email that is received:

To download the Phenix distribution with a web browser go to:

https://phenix-online.org/download

When prompted for a user name and password enter:

User Name: download

Password: 3c55hyu

The password is changed on the 1st of each month at 00:05 PST/PDT.

If the password is expired, simply request a new one at: https://phenix-online.org/

This is an automatically generated message. Please do not reply to this email. If you experience problems please contact:

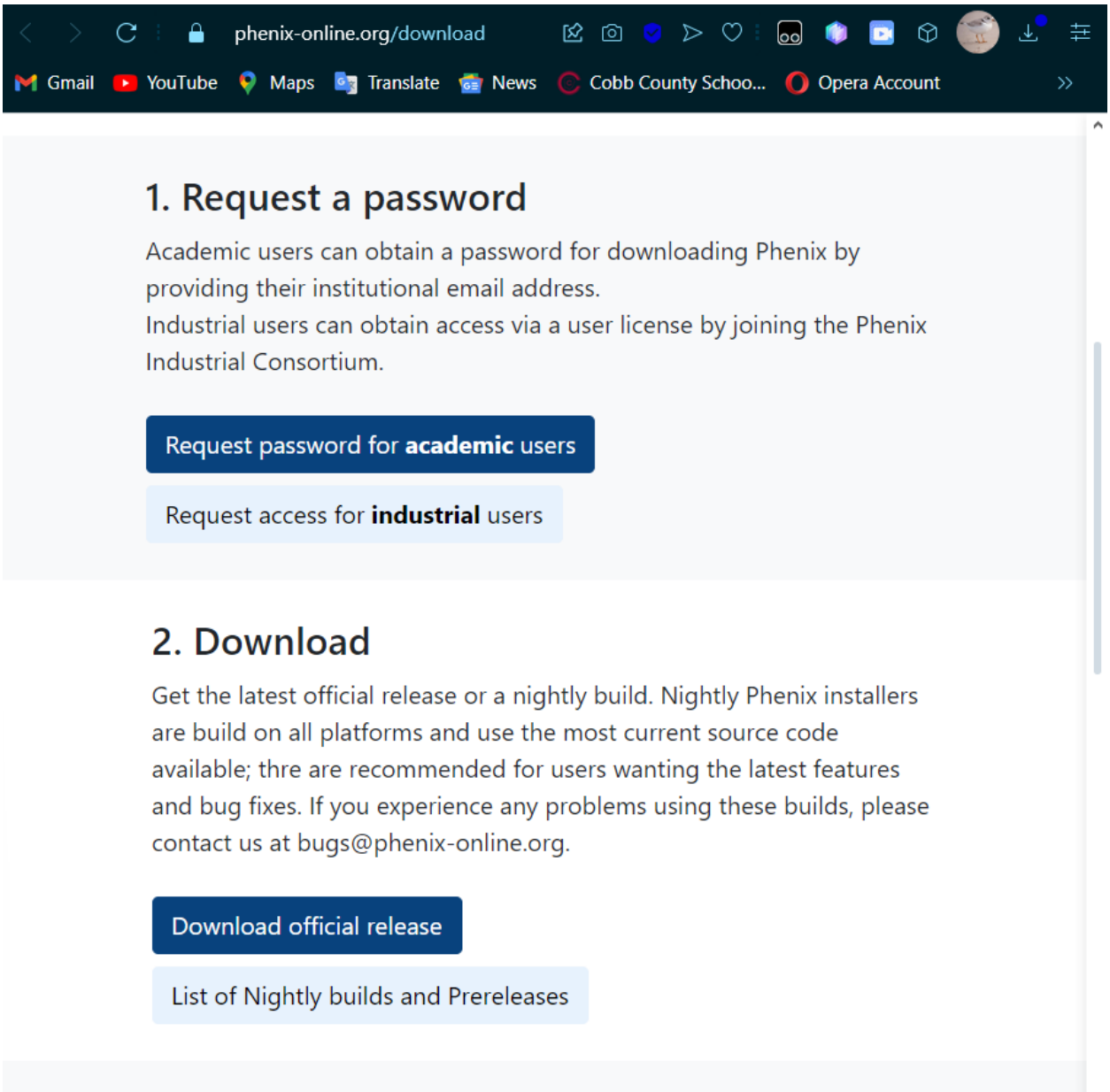
download@phenix-online.org

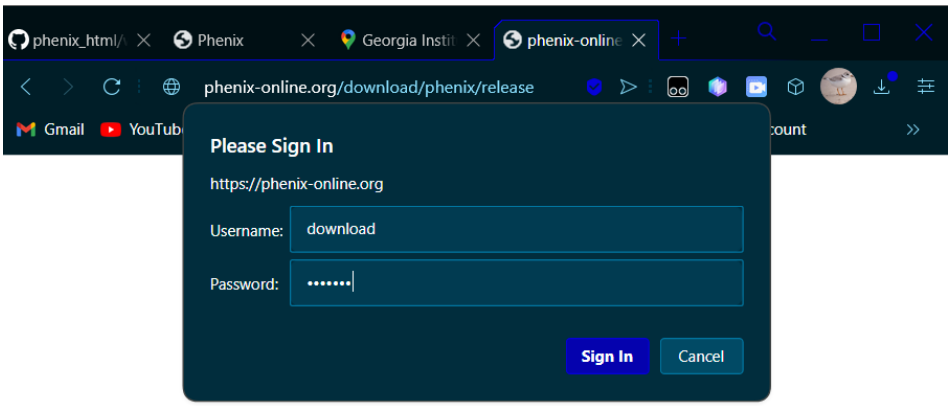
Citing Phenix:
Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. Liebschner D., Afonine P.V., Baker M.L., Bunkoczi G., Chen V.B., Croll T.I., Hintze B., Hung L.W., Jain S., McCoy A.J., Moriarty N.W., Oeffner R.D., Poon B.K., Prisant M.G., Read R.J., Richardson J.S., Richardson D.C., Sammito M.D., Sobolev O.V., Stockwell D.H., Terwilliger T.C., Urzhumtsev A.G., Videau L.L., Williams C.J., and Adams P.D. Acta Cryst. D75, 861-877 (2019).

This software is controlled by the U.S. Government and authorized for export only to the country of ultimate destination for use by the ultimate consignee or end-user(s) herein identified. Software may not be resold, transferred, or otherwise disposed of, to any other country or to any person other than the

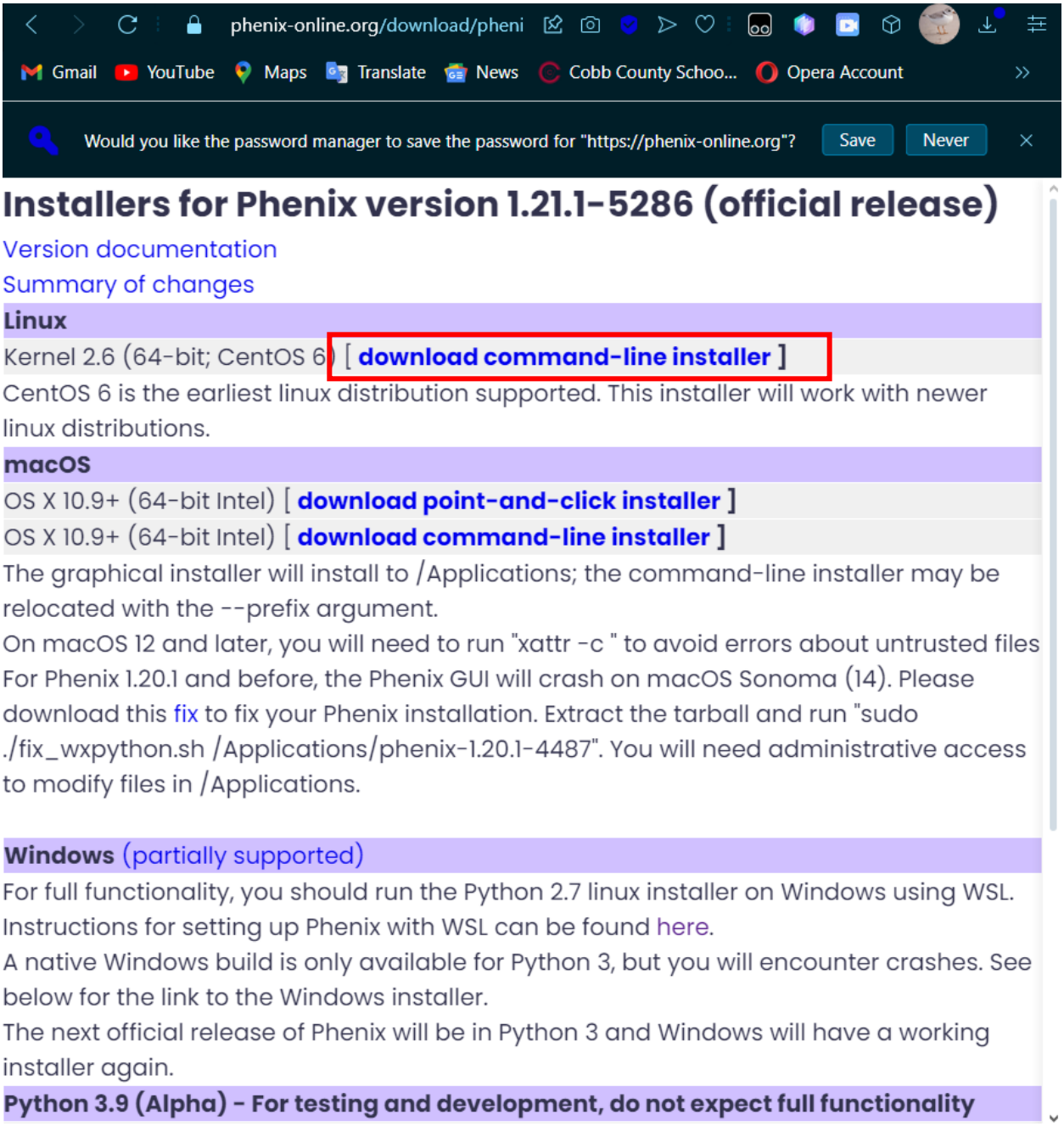
authorized ultimate consignee or end-user(s), either in their original form or after being incorporated into other items, without first obtaining approval from the U.S. government or as otherwise authorized by U.S. law and regulations.

With the temporary username and password, you can now go back to website 3 and click “Download official release” and paste the login information inside

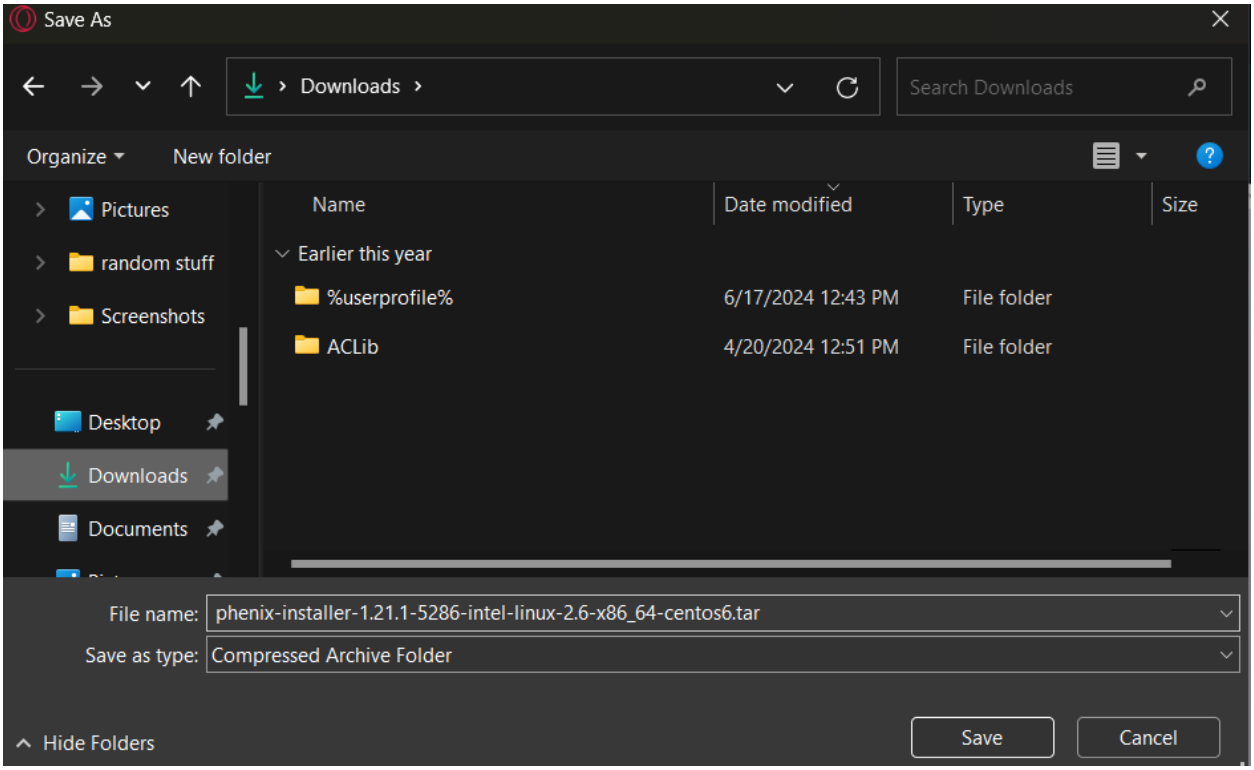


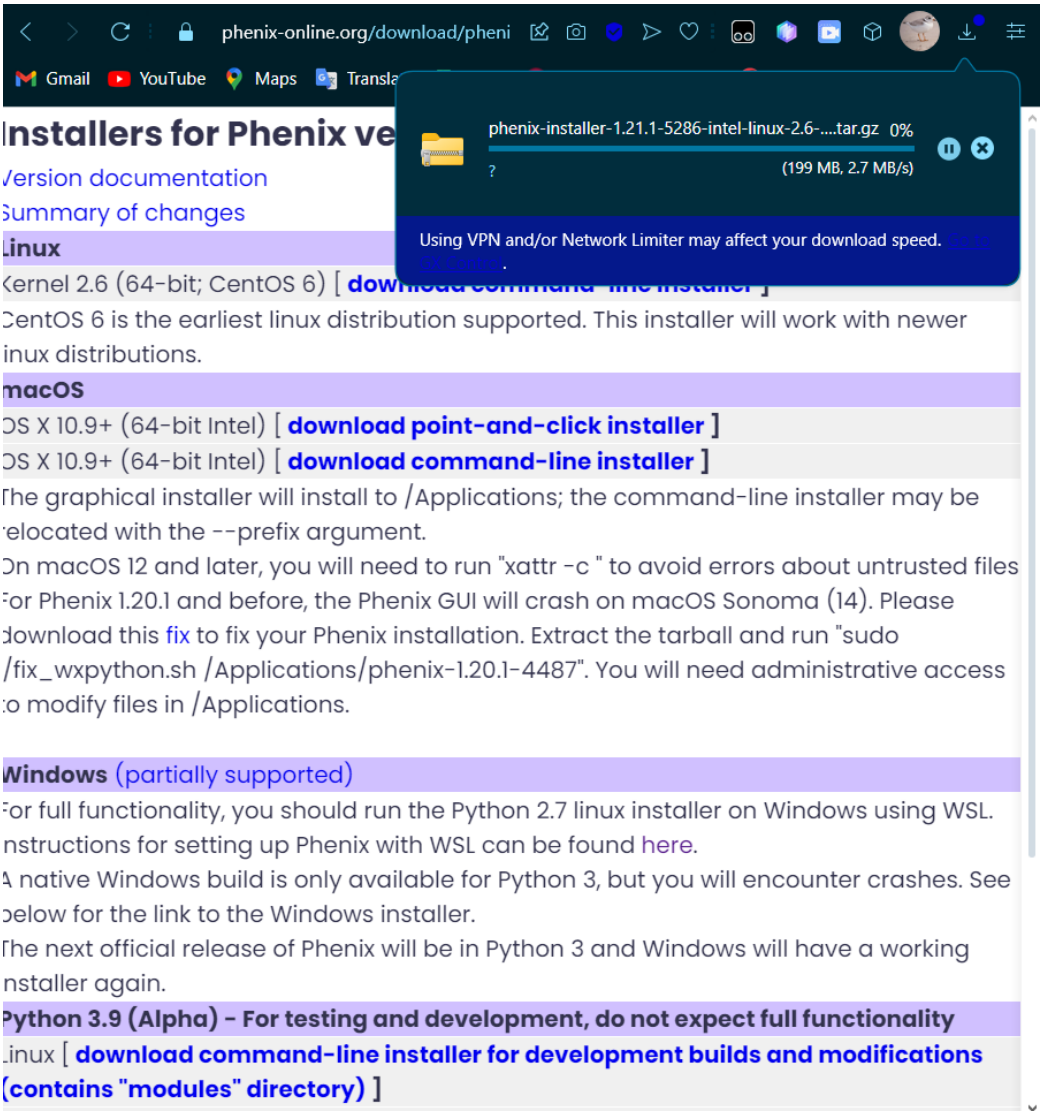


It will bring you to the below page. Click on the Linux download command-line installer at the top of the page.



Save the downloaded tar.gz file into the downloads folder:


Save As
Downloads
Search Downloads
Organize
New folder
Pictures
random stuff
Screenshots
Desktop
Downloads
Documents
Name
Date modified
Type
Size
Earlier this year
%userprofile%
6/17/2024 12:43 PM
File folder
ACLib
4/20/2024 12:51 PM
File folder
File name:
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar
Save as type:
Compressed Archive Folder
Hide Folders
Save
Cancel

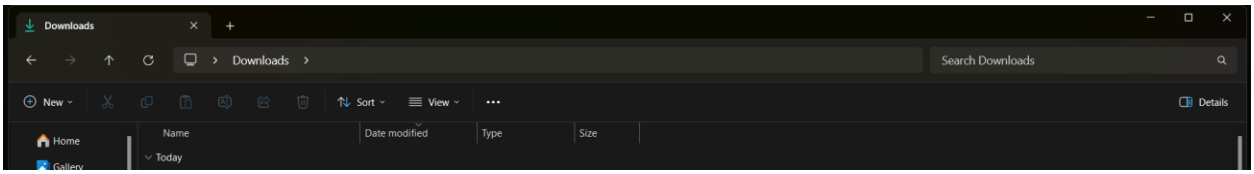


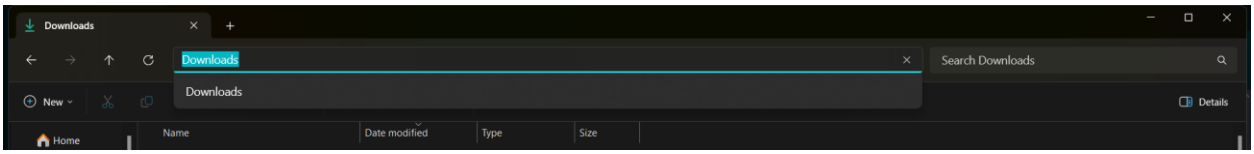
Meanwhile, while we get the phenix thing working, we can go ahead and download Coot:

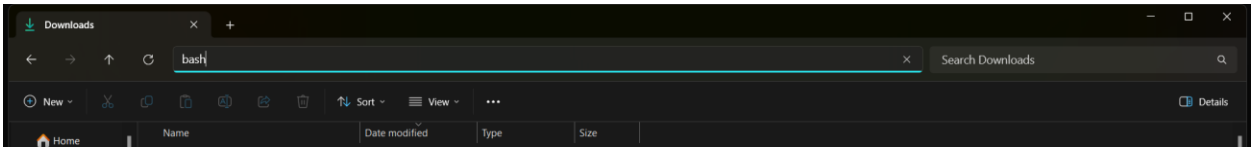
https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/binaries/release/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz and save it into the downloads folder. This link will directly download the Coot directory

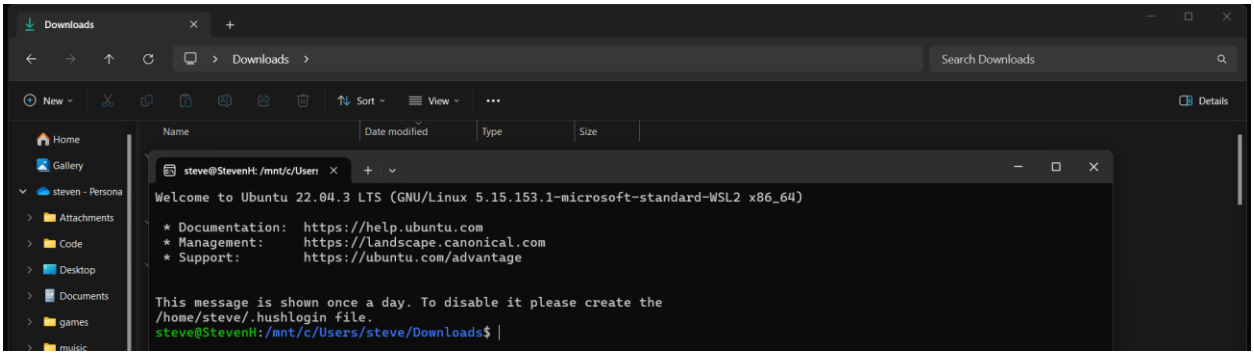
While that is installing

go to the downloads folder



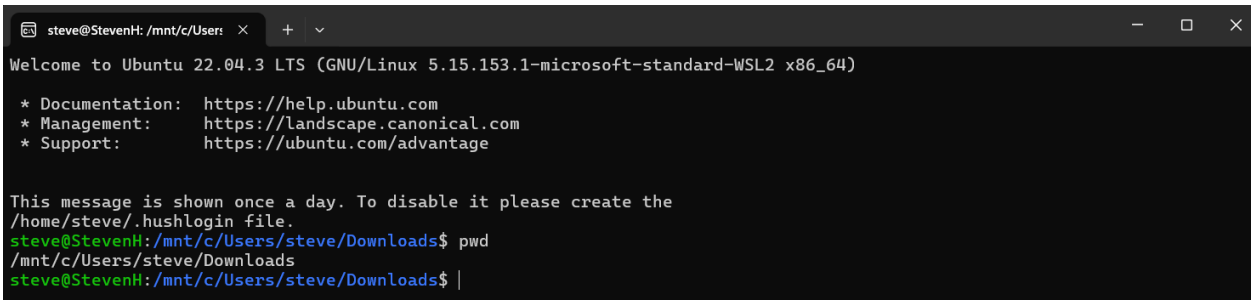






Now, type **pwd** into the terminal to print the working directory (essentially the directory that you are currently in)

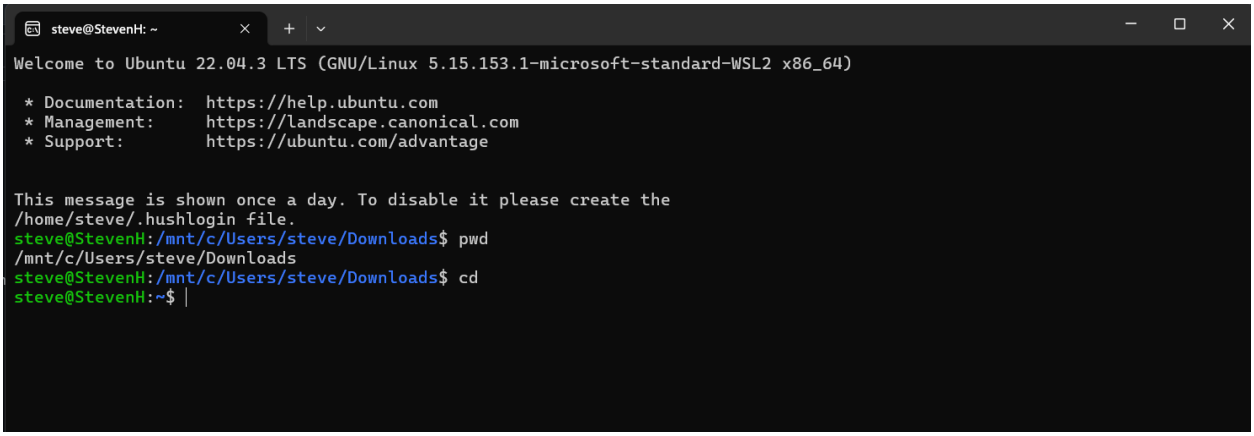
We need this working directory so that when we go to the root directory, we can extract the tar ball file (which is currently in the downloads directory) into the root directory, where the PHENIX program can reside in the Linux subsystem and operate correctly.



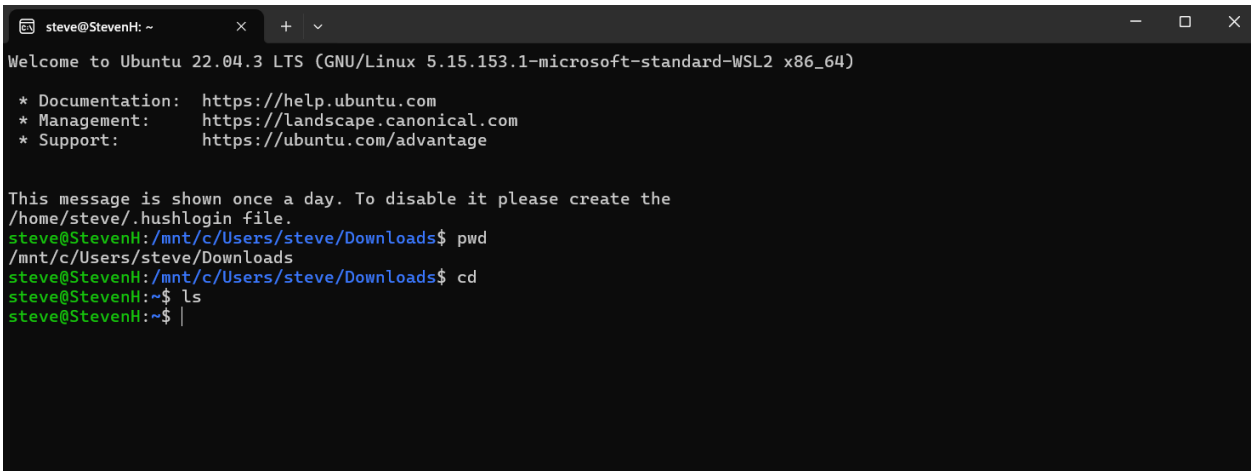
In this case, the operating directory is /mnt/c/Users/steve/Downloads

This will be used in the next step:

Go to the root directory, this is where you will extract your PHENIX file into.



There most likely is nothing in it right now:



While you are in this root directory, extract the Linux installer:

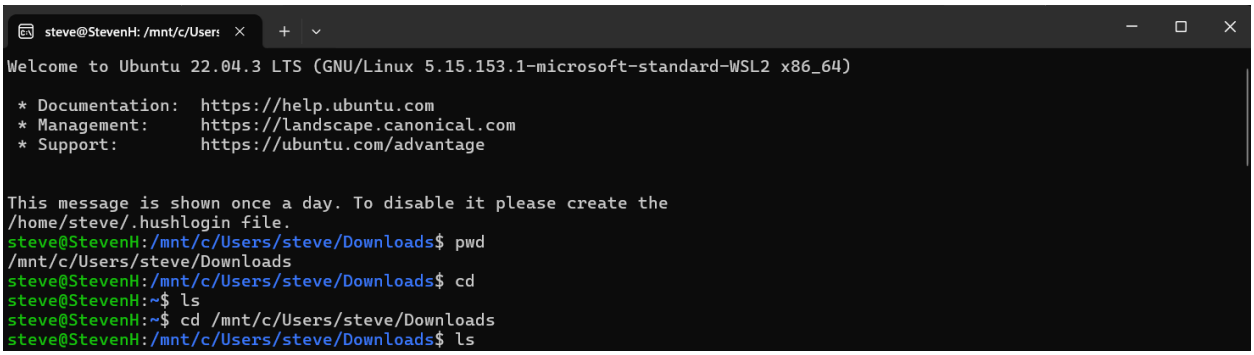
tar -xf /mnt/c/Users/<Windows username>/Downloads/<Phenix installer file>

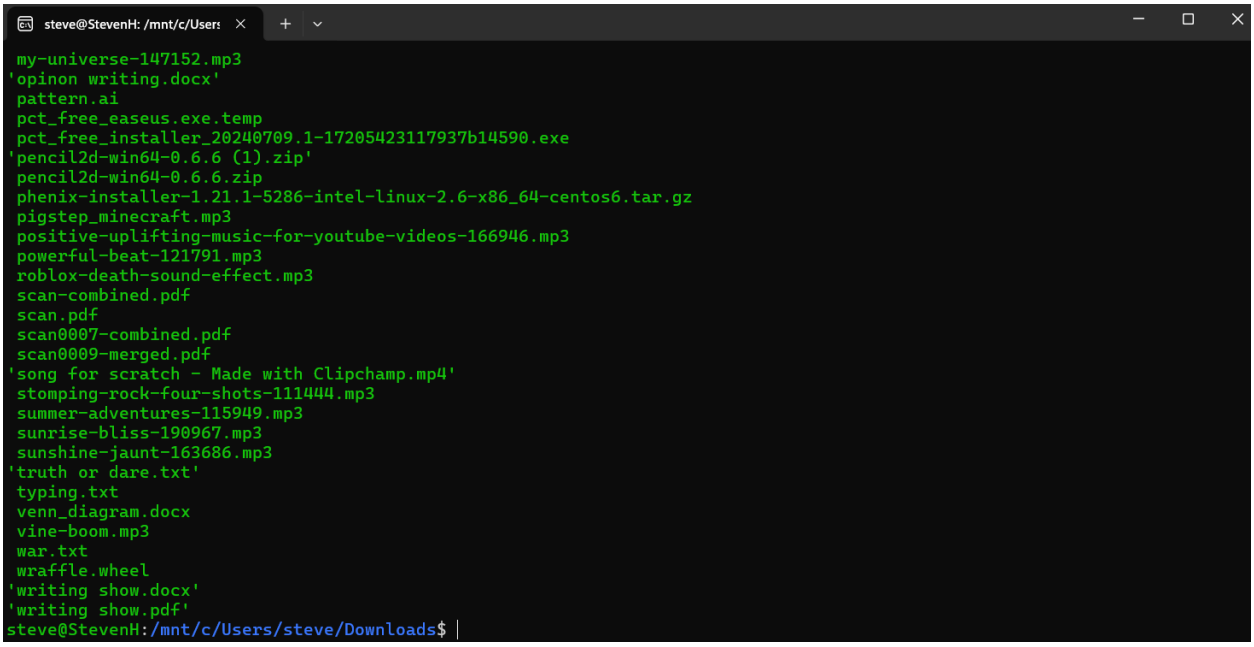
where <Windows username> would be “steve” in this case.

Where <Phenix installer file> is … well we don’t know

How do we find the file name?

Go to the downloads folder and type “ls”:





In this case, it was listed as “phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz”

Copy the name of this directory (which in this case is /mnt/c/Users/steve/Downloads), the name of the file (which in this case is phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz)

Next, navigate back to the root directory and type in this into the terminal:

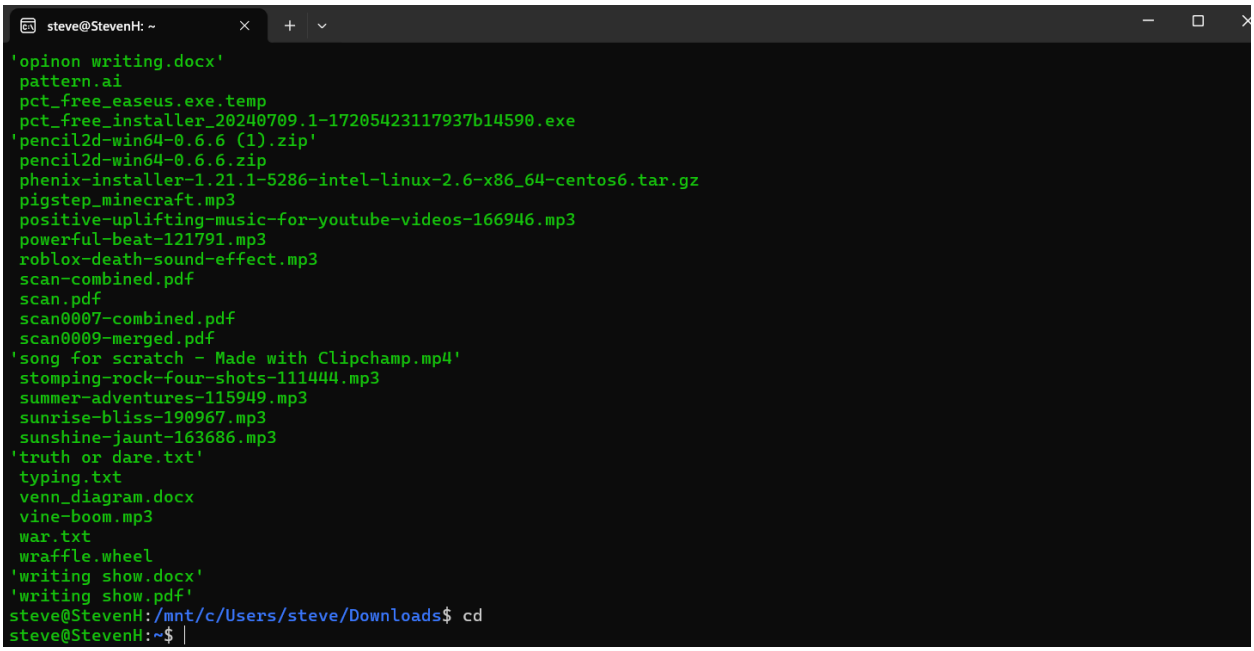
cd

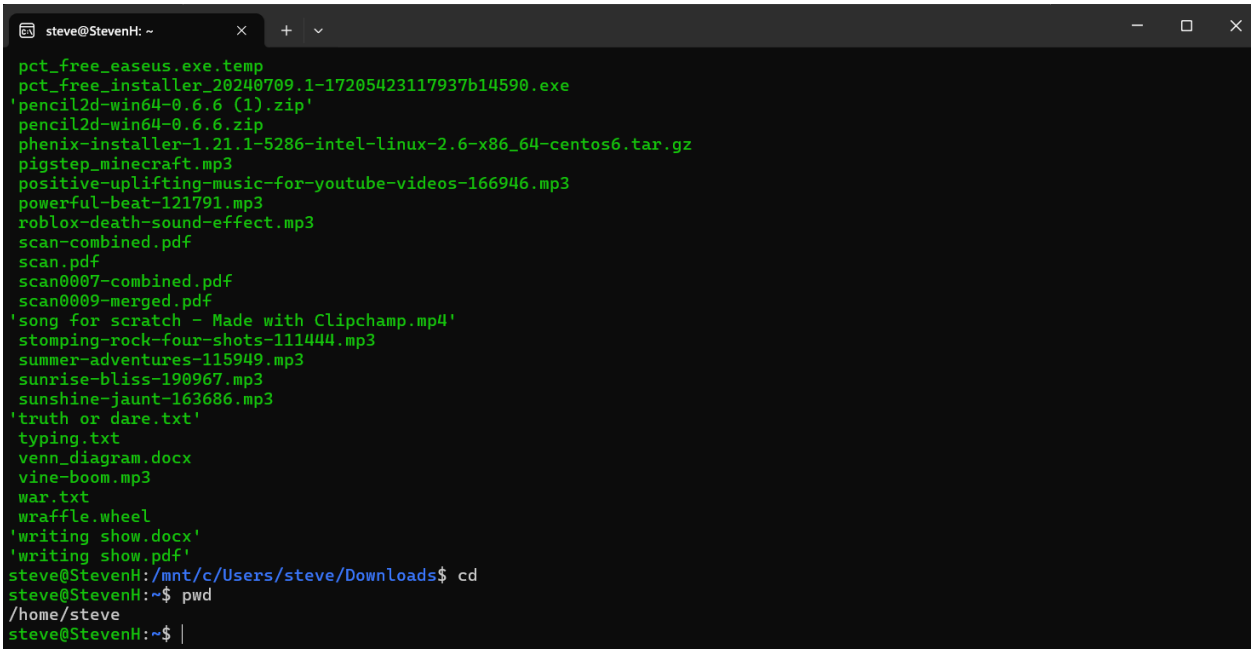
tar -xf /mnt/c/Users/<Windows username>/Downloads/<Phenix installer file>

or in this specific case:

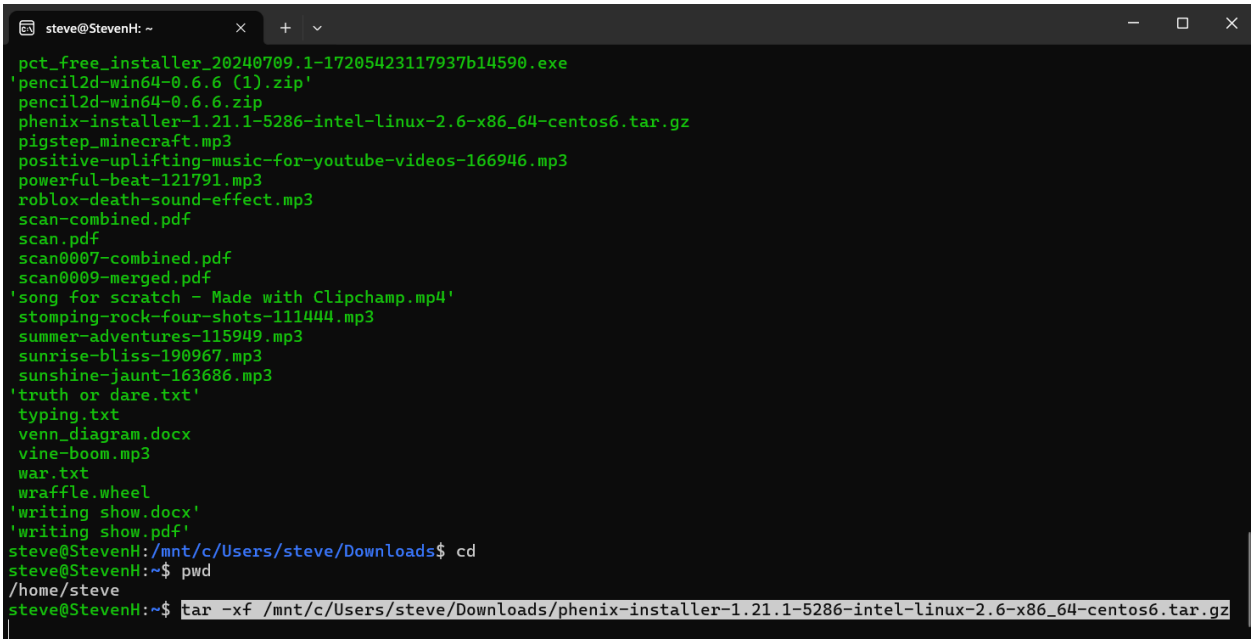
cd

tar -xf /mnt/c/Users/steve/Downloads/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz



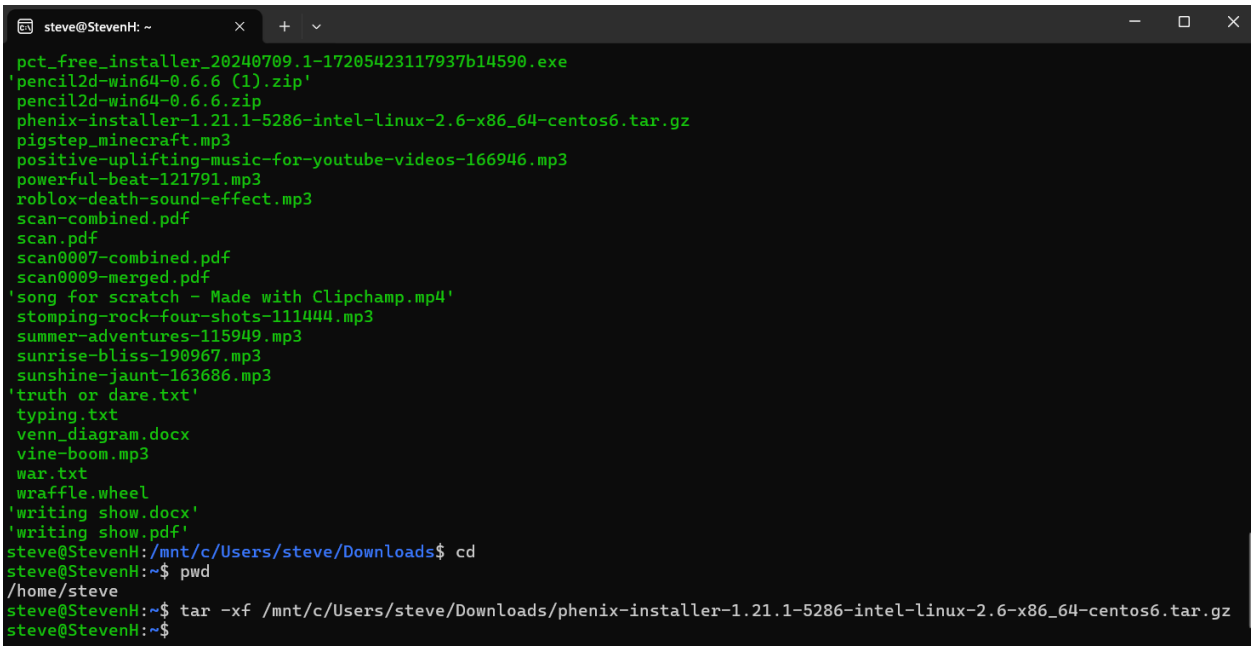


Now type in your command

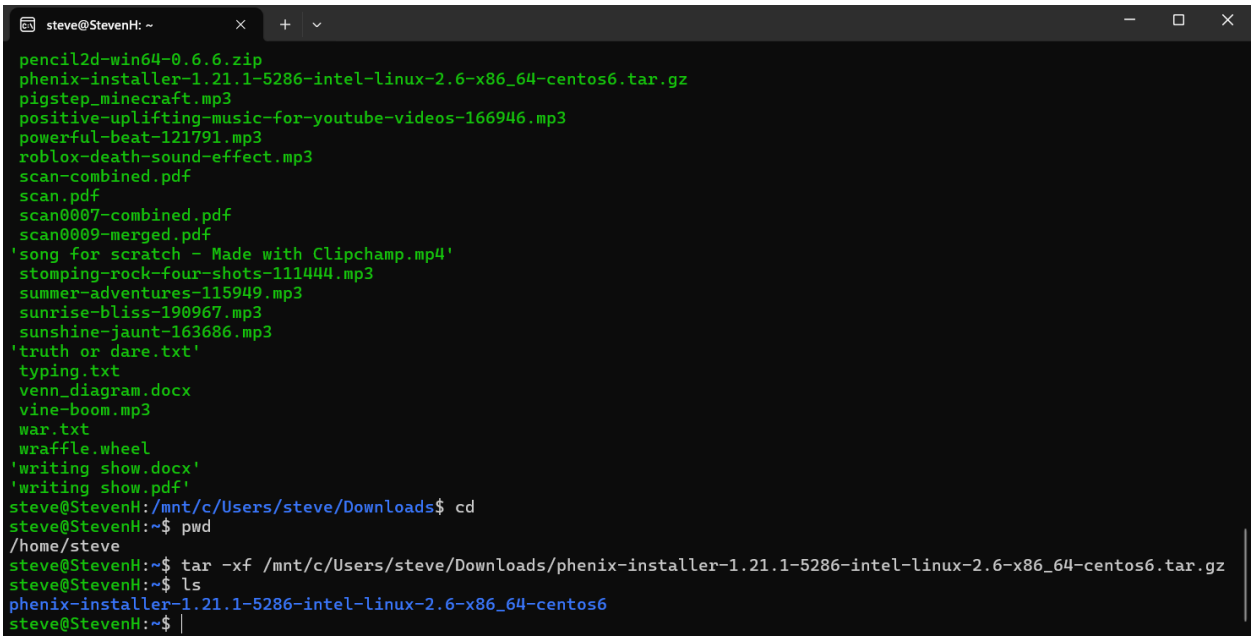


This might take a quick second or a bit of a while. It is just extracting the zip file (or in the case of Linux, the tar file) into the root directory. This process may be fast or slow depending on your computer (this example computer had Windows 11, 6 cores, 8 processors, 8 GB of memory, 4 GB of dedicated GPU and it only took a couple of minutes)

You will know when it is done when the “$” comes back again:



Now you can check to see if it successfully copied over by typing ls



If it copied over successfully, now you can run the installation process:

cd phenix-installer-<version>-<platform>

./install --prefix ${HOME}

You need to cd into this folder. You can do so by typing “cd phenix” and then click tab to autofill the rest. If you don’t want to autofill, you can simply type the full folder name.

```
positive-uplifting-music-for-youtube-videos-166946.mp3
 powerful-beat-121791.mp3
 roblox-death-sound-effect.mp3
 scan-combined.pdf
 scan.pdf
 scan0007-combined.pdf
 scan0009-merged.pdf
'song for scratch - Made with Clipchamp.mp4'
 stomping-rock-four-shots-111444.mp3
 summer-adventures-115949.mp3
 sunrise-bliss-190967.mp3
 sunshine-jaunt-163686.mp3
'truth or dare.txt'
 typing.txt
 venn_diagram.docx
 vine-boom.mp3
 war.txt
 wraffle.wheel
'writing show.docx'
'writing show.pdf'
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd
steve@StevenH:~$ pwd
/home/steve
steve@StevenH:~$ tar -xf /mnt/c/Users/steve/Downloads/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz
steve@StevenH:~$ ls
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd
steve@StevenH:~$ ^C
steve@StevenH:~$ cd
steve@StevenH:~$ cd phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6/
```

```
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd
steve@StevenH:~$ pwd
/home/steve
steve@StevenH:~$ tar -xf /mnt/c/Users/steve/Downloads/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz
steve@StevenH:~$ ls
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd
steve@StevenH:~$ ^C
steve@StevenH:~$ cd
steve@StevenH:~$ cd phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6/
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
```

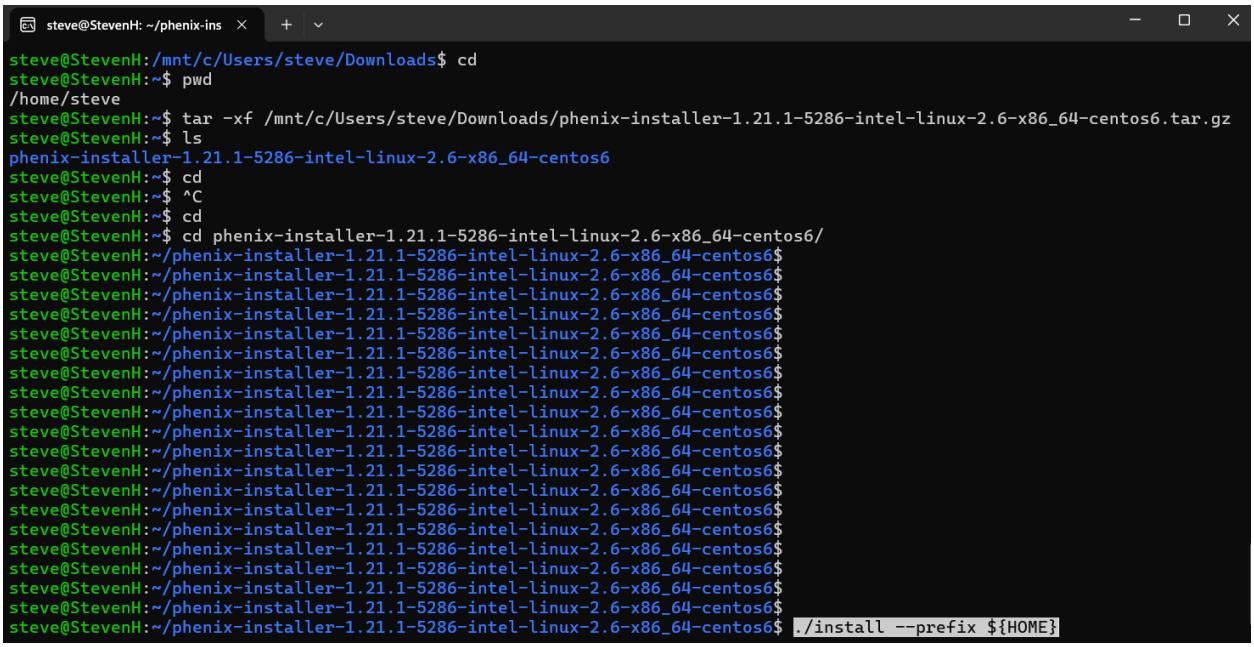
If you hold it down, this accidently happens:

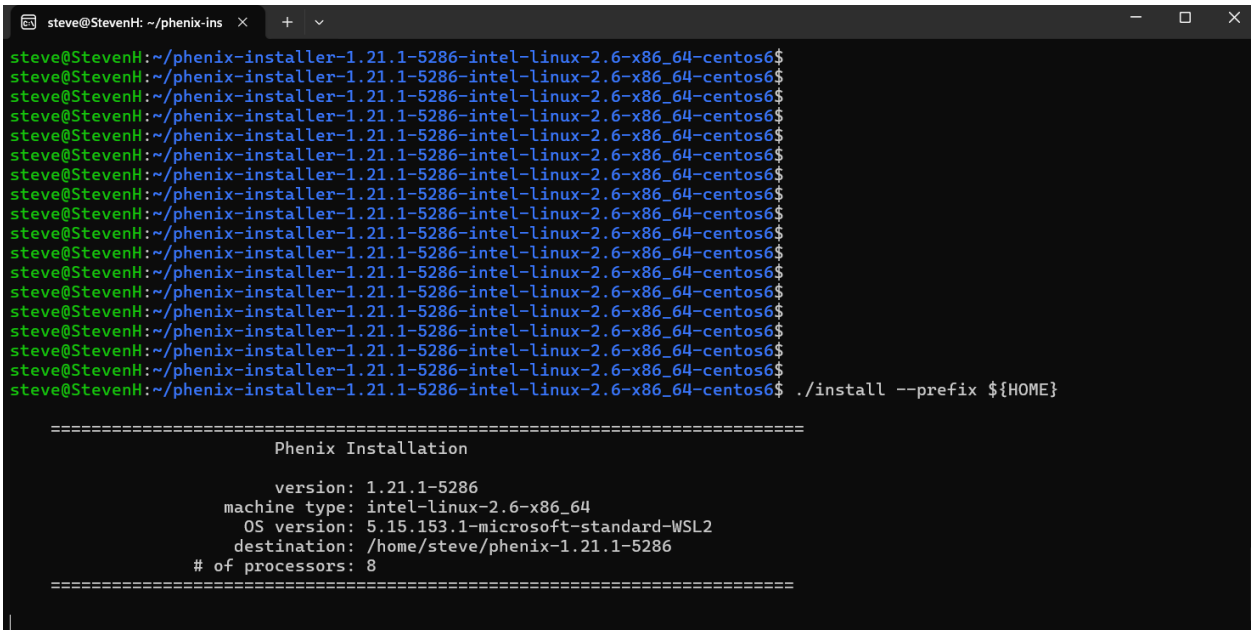
```
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd
steve@StevenH:~$ pwd
/home/steve
steve@StevenH:~$ tar -xf /mnt/c/Users/steve/Downloads/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz
steve@StevenH:~$ ls
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd
steve@StevenH:~$ ^C
steve@StevenH:~$ cd
steve@StevenH:~$ cd phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6/
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$
```

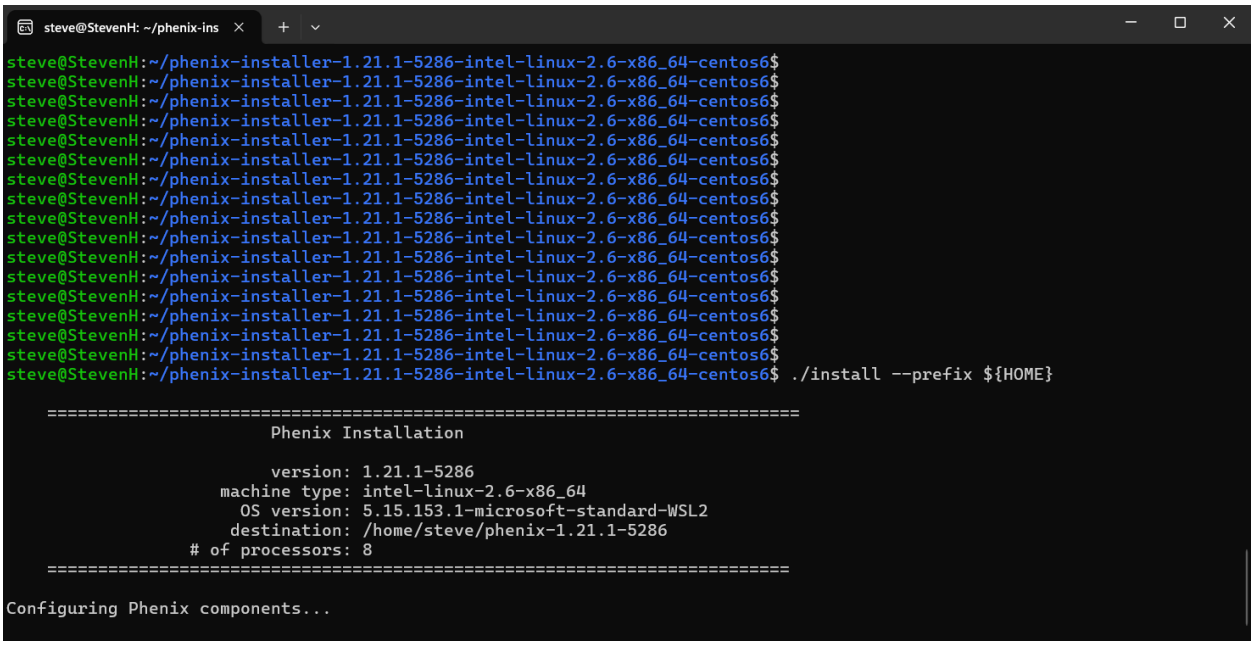
But don’t worry if that happens, there is nothing wrong with it.

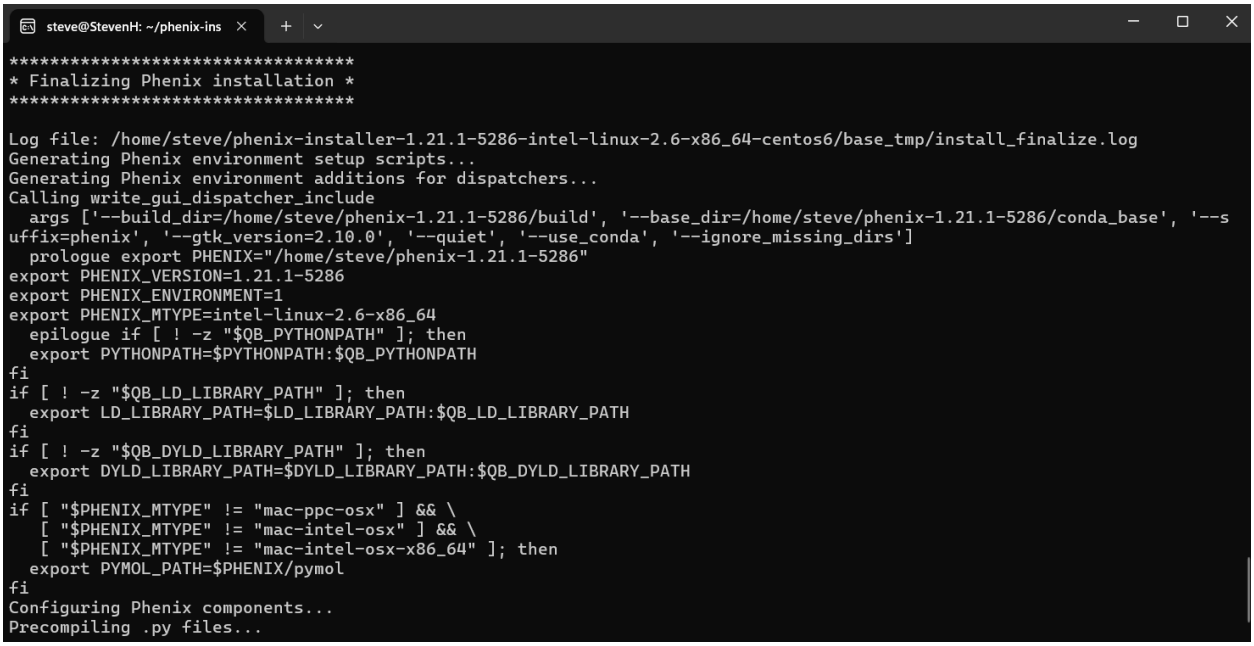
Now that you are in the correct folder, start the installation process by typing:

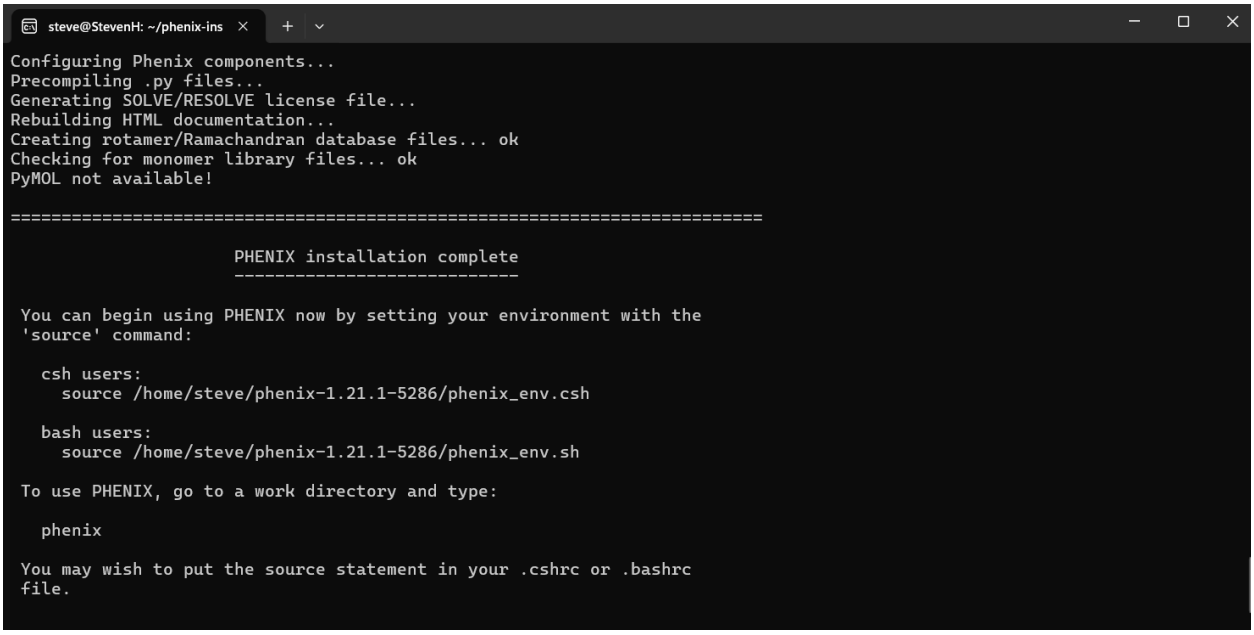
./install --prefix ${HOME}

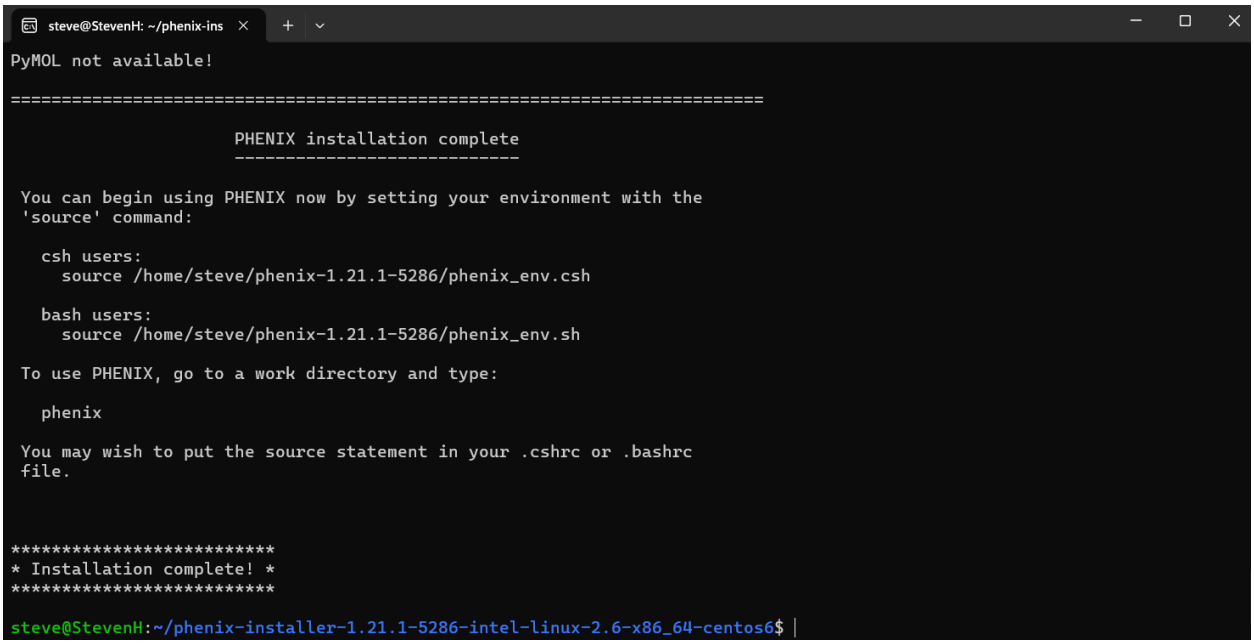





steve@StevenH: ~/phenix-ins
steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$ ./install --prefix ${HOME}
Phenix Installation
version: 1.21.1-5286
machine type: intel-linux-2.6-x86_64
OS version: 5.15.153.1-microsoft-standard-WSL2
destination: /home/steve/phenix-1.21.1-5286
# of processors: 8
Configuring Phenix components...


steve@StevenH: ~/phenix-ins
* Finalizing Phenix installation *
Log file: /home/steve/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6/base_tmp/install_finalize.log
Generating Phenix environment setup scripts...
Generating Phenix environment additions for dispatchers...
Calling write_gui_dispatcher_include
export PHENIX_VERSION=1.21.1-5286
export PHENIX_ENVIRONMENT=1
export PHENIX_MTYPE=intel-linux-2.6-x86_64
export PYMOL_PATH=$PHENIX/pymol
Configuring Phenix components...
Precompiling .py files...

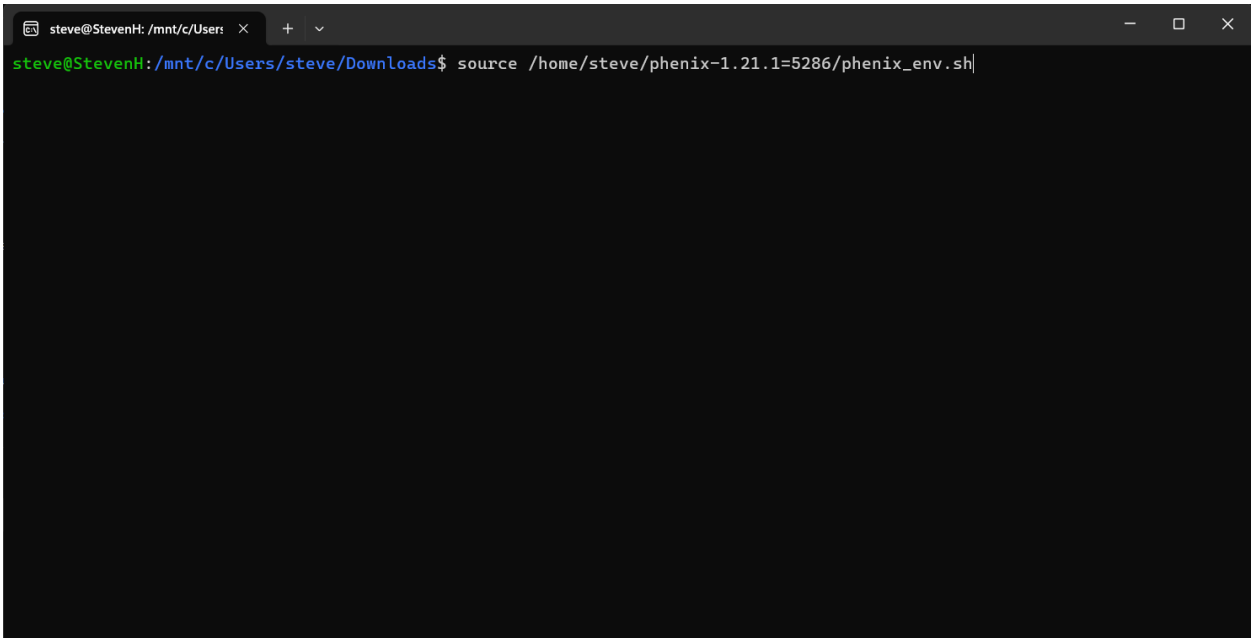


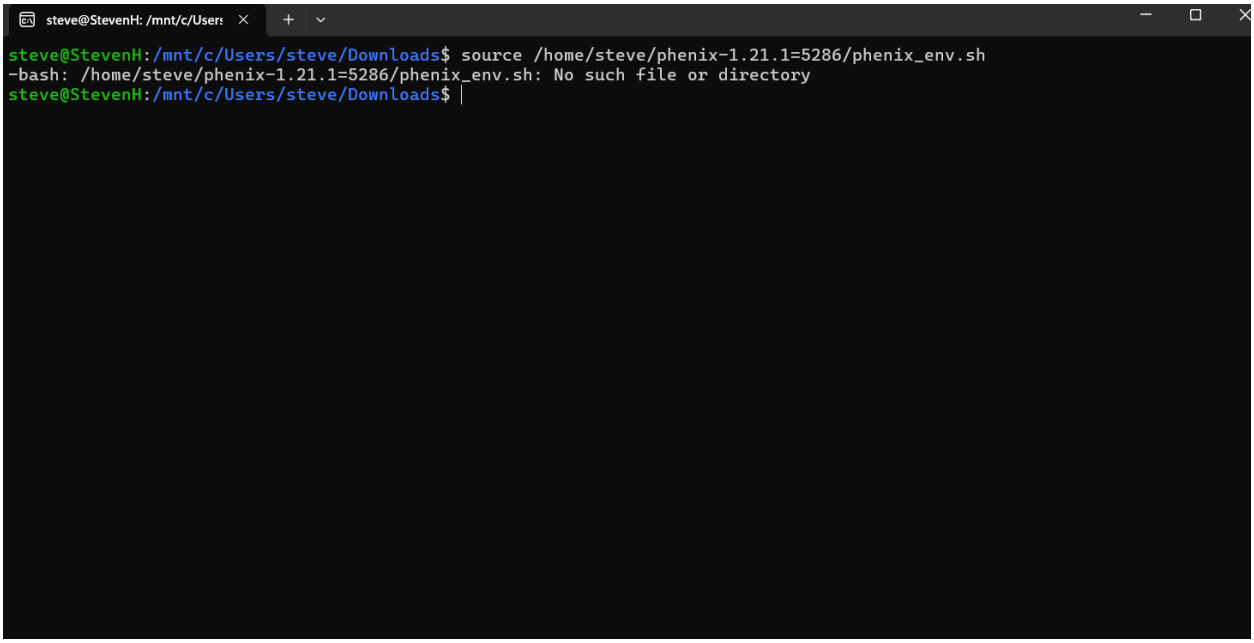


So, now if you want to open PHENIX, you just bash into any folder, for this example, type:

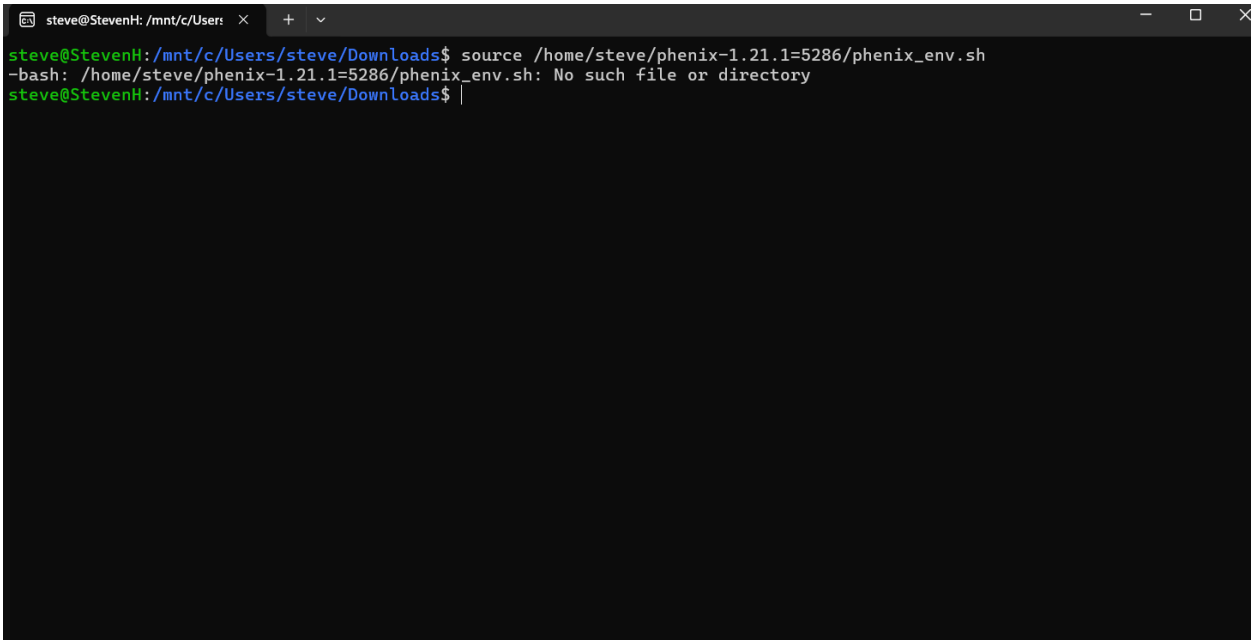
source /home/steve/phenix-1.21.1=5286/phenix_env.sh

Then type **phenix**

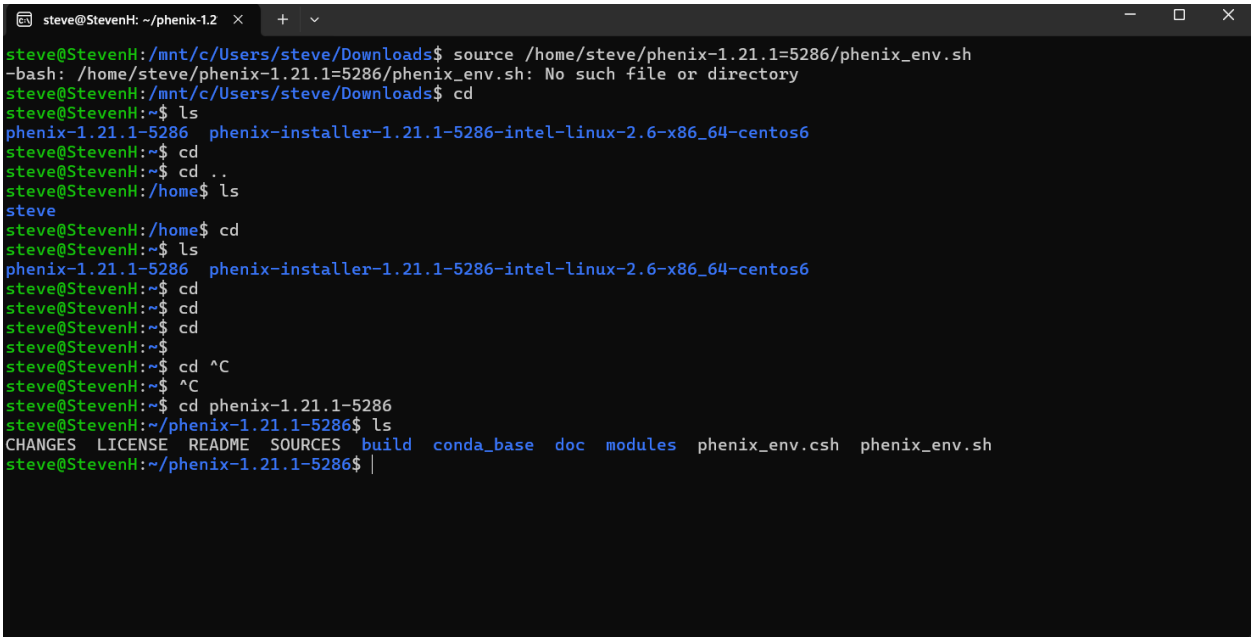




If it doesn't work, **cd** to the root directory, go into the phenix folder and find out the list of items in the directory.



It seems that it is here:

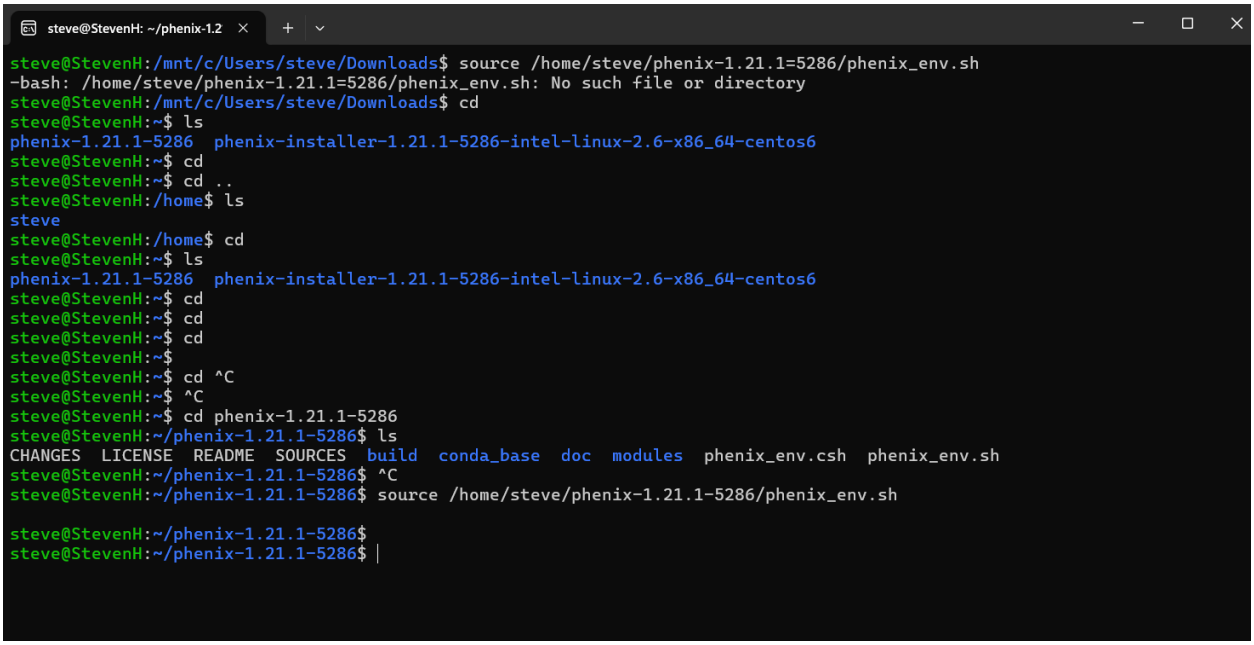


You just need to make sure that the directory is correct, in the first command, an equals sign was used when a dash was supposed to be used. When you fix this error, it can be fixed:

Get the new one: **source /home/steve/phenix-1.21.1-5286/phenix_env.sh**

And then type **phenix**

This time it worked because there was no error:



Now type **phenix**

The Phenix GUI shows up, but not the full screen. This may be because it is missing code or may be because of limited memory space.

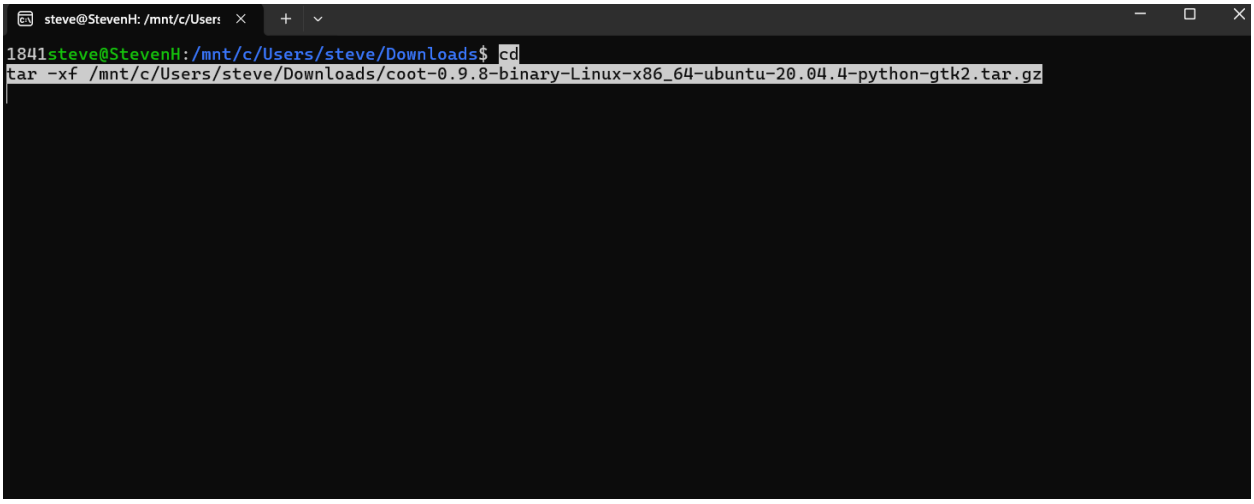
We are just going to go ahead and install coot:

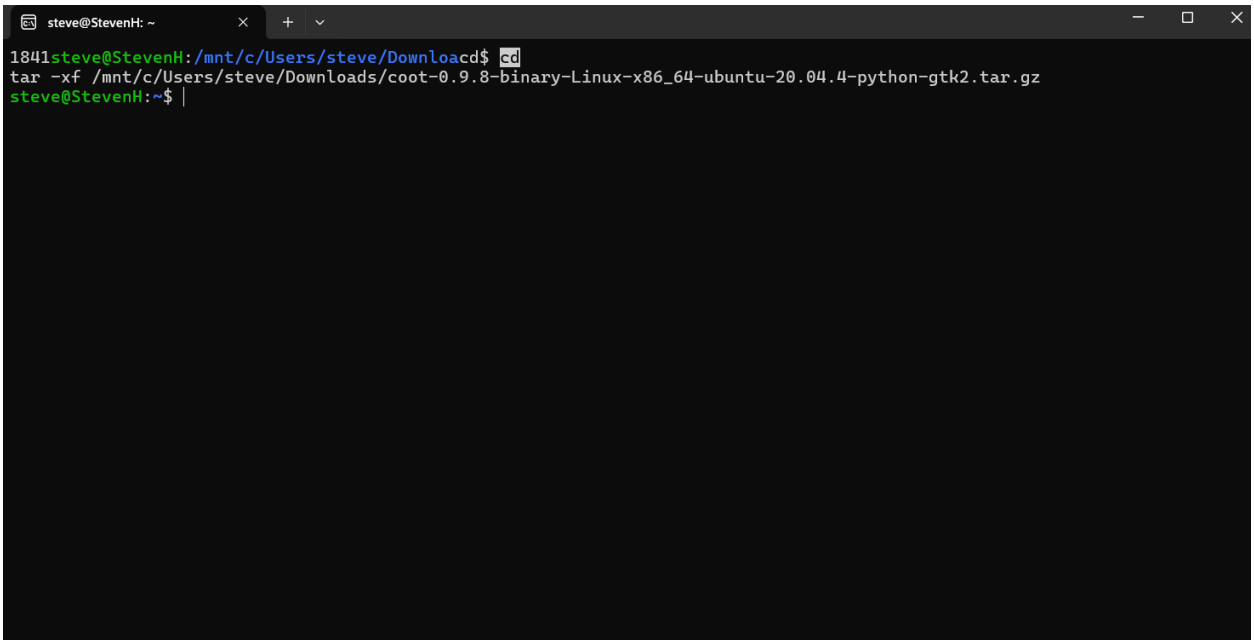
cd

tar -xf /mnt/c/Users/<Windows username>/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz

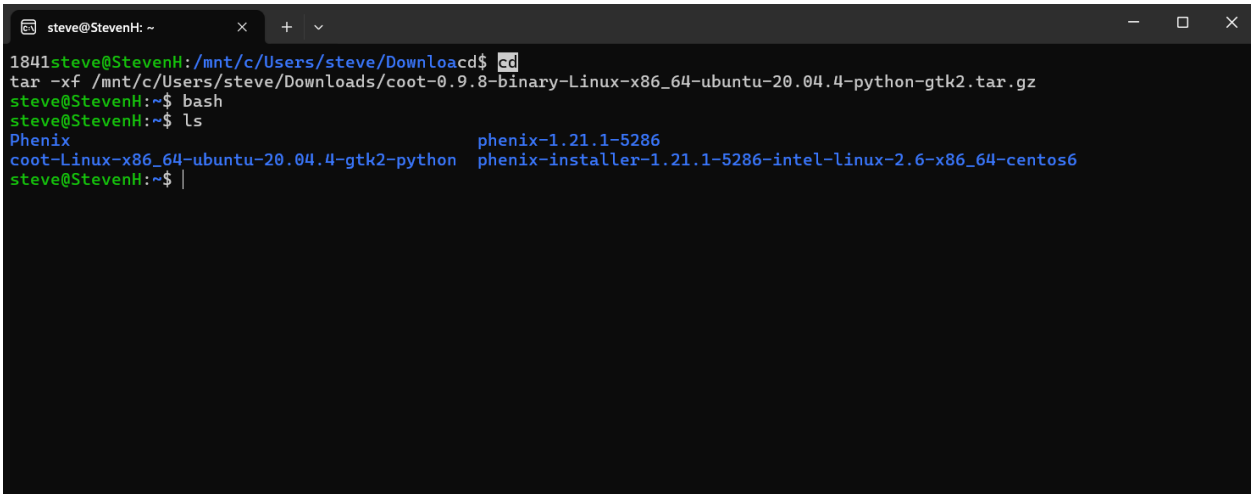
cd

tar -xf /mnt/c/Users/steve/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz

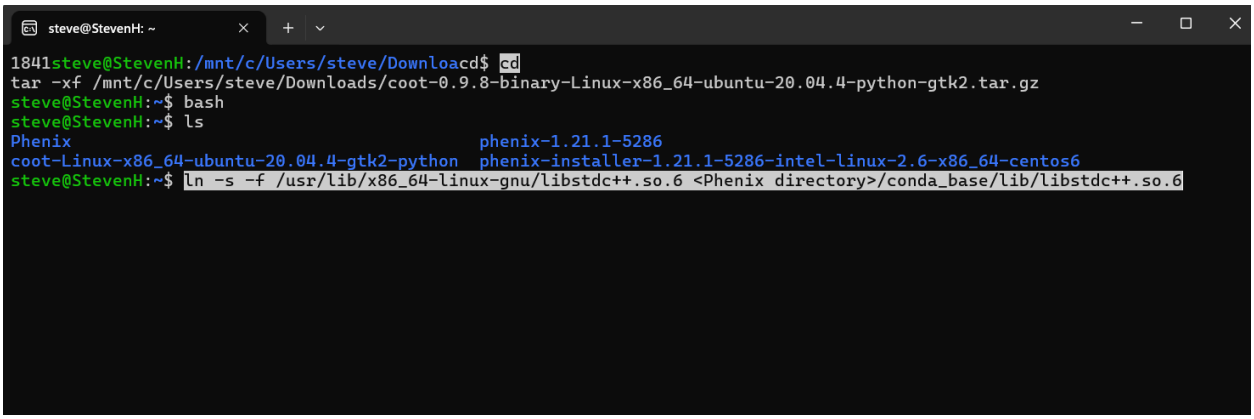


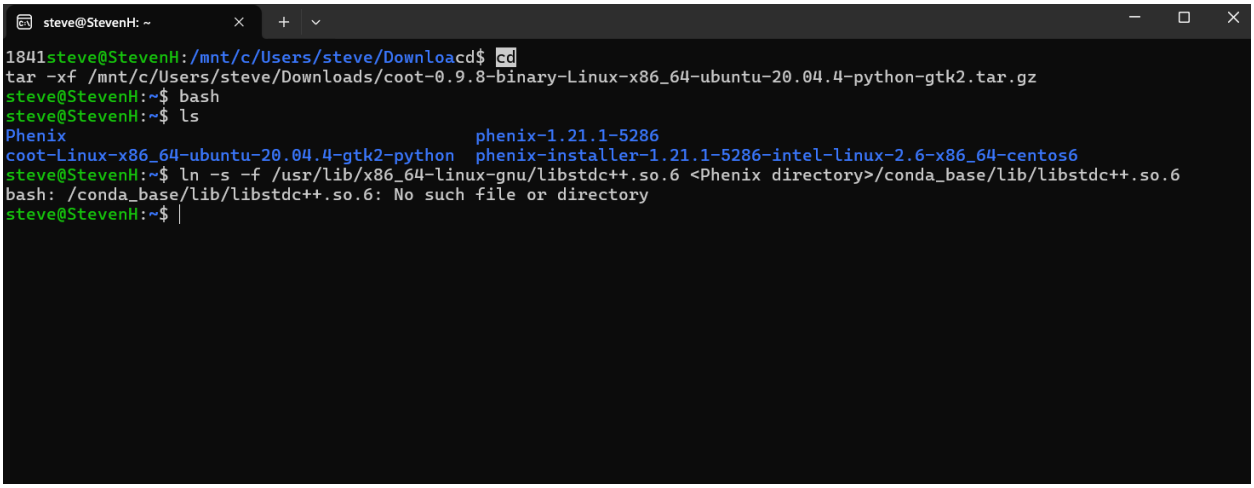


It has extracted the files successfully into the root directory you can check:



Coot is extracted now.

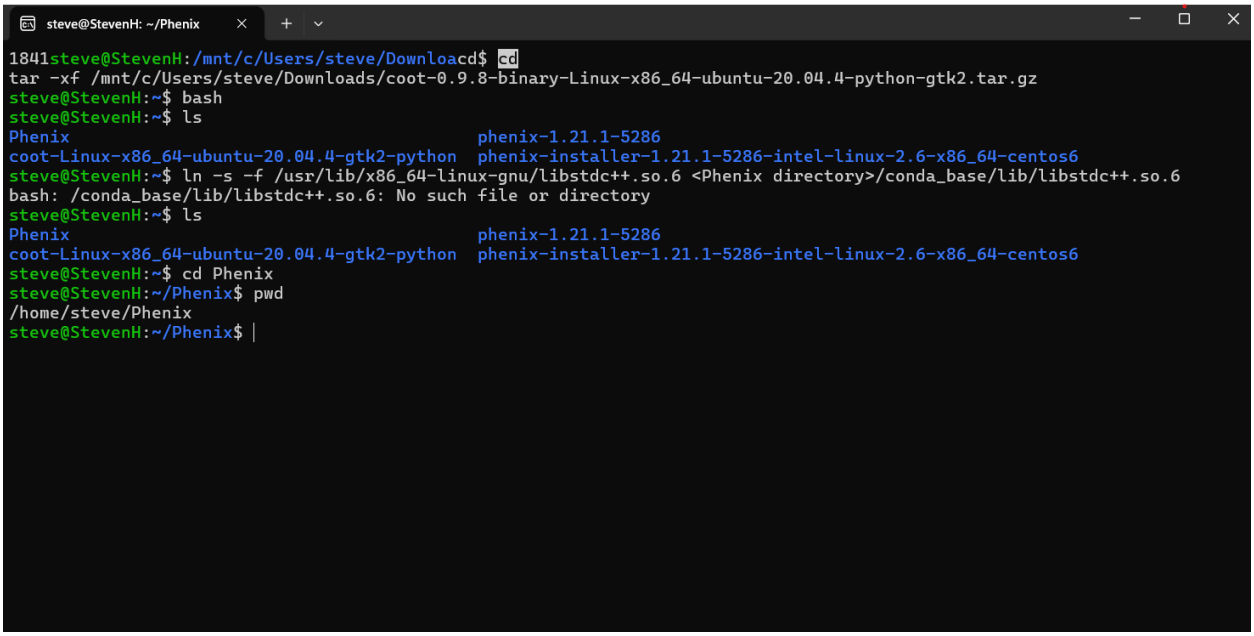




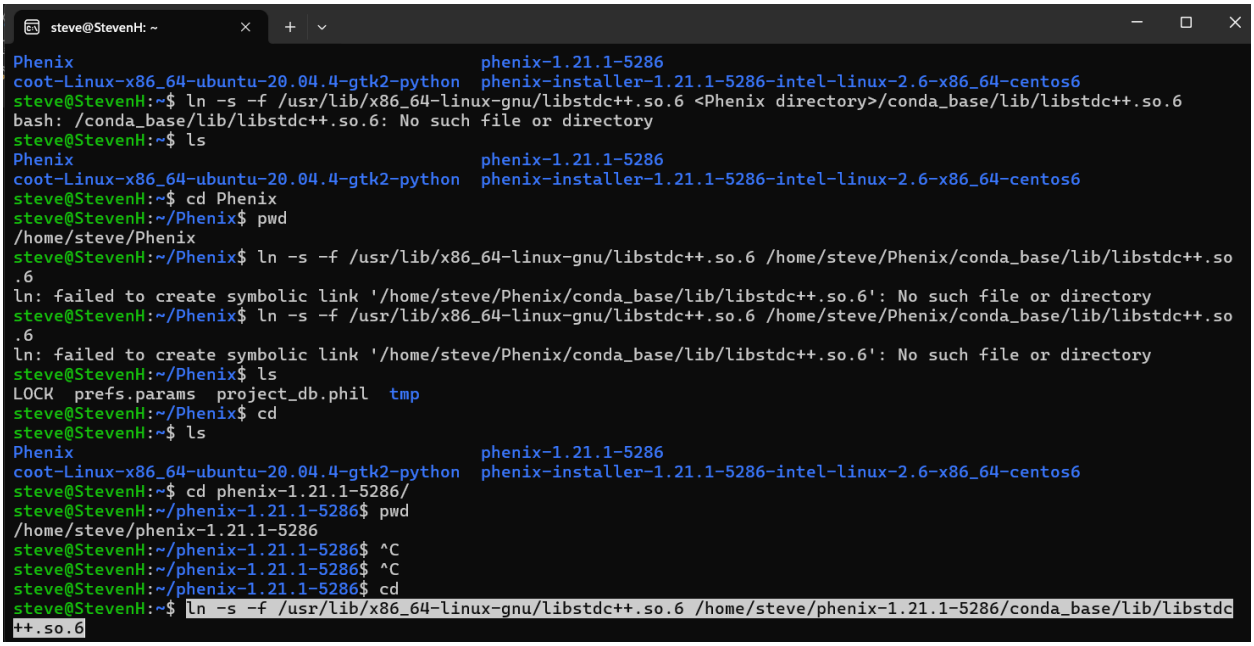
As you can see, it says no lib libstdc++ available, so we are going to download this library.

Actually no it is because the <*phenix directory*> was not replaced.

ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 <User>/conda_base/lib/libstdc++.so.6



ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 /home/steve/phenix-1.21.1-5286/conda_base/lib/libstdc++.so.6



It has to be the full phenix folder

So that is done.

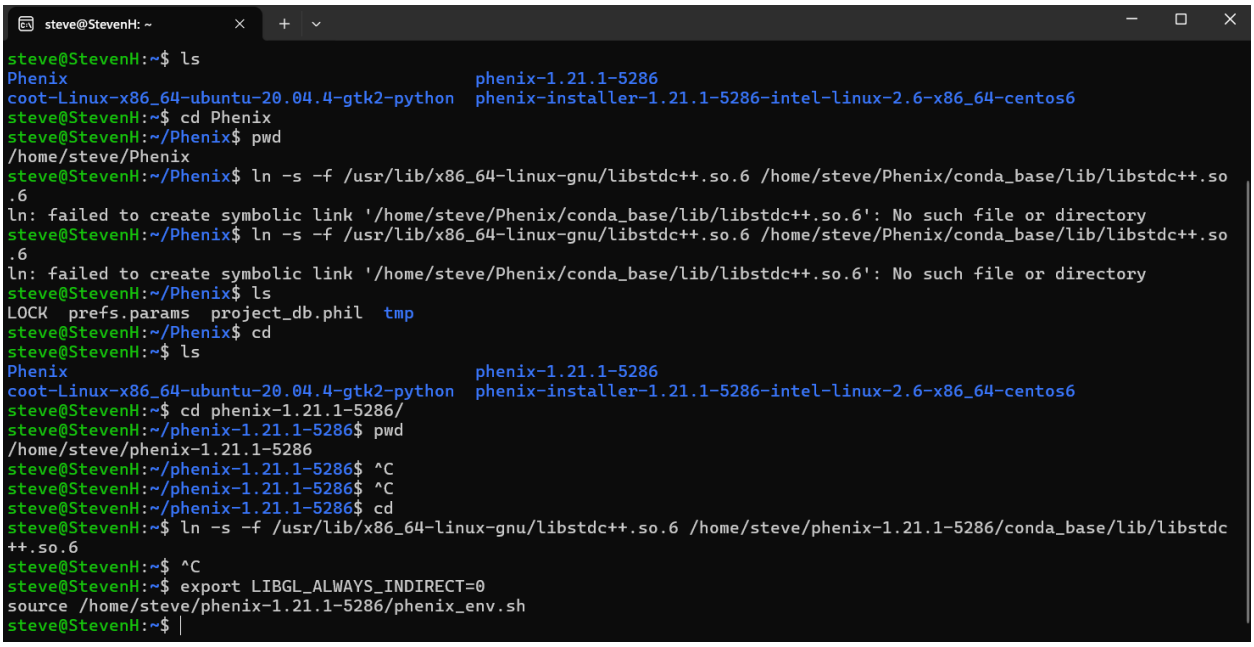
Then this part:

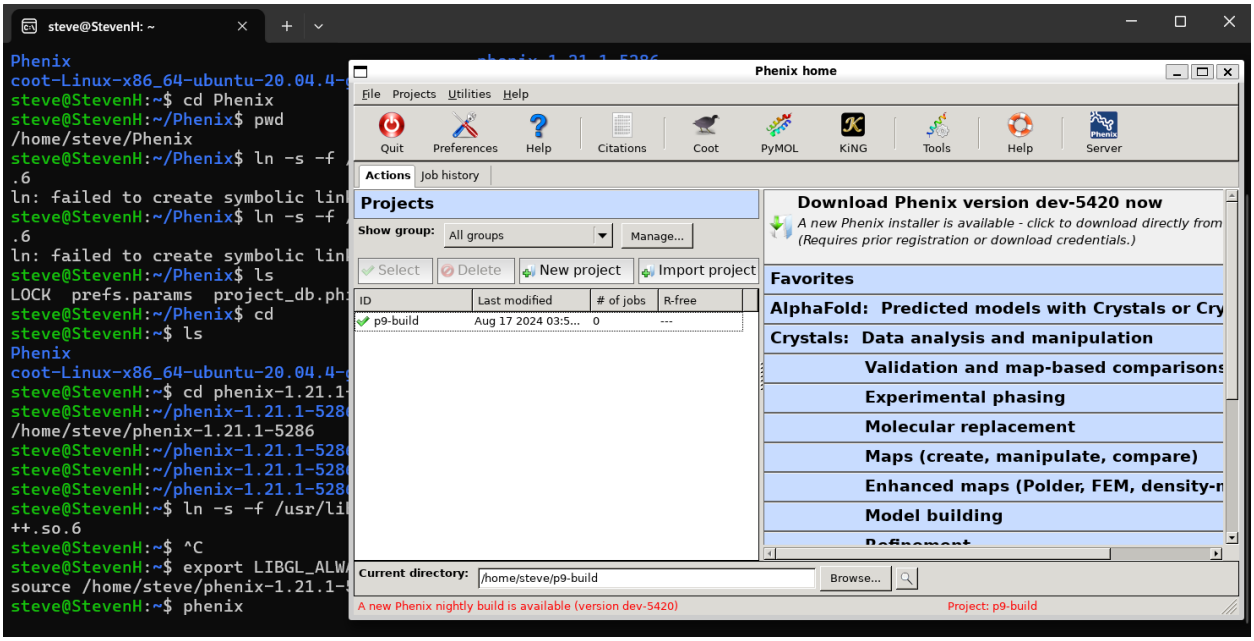
export LIBGL_ALWAYS_INDIRECT=0

source <Phenix directory>/phenix_env.sh

export LIBGL_ALWAYS_INDIRECT=0

source /home/steve/phenix-1.21.1-5286/phenix_env.sh



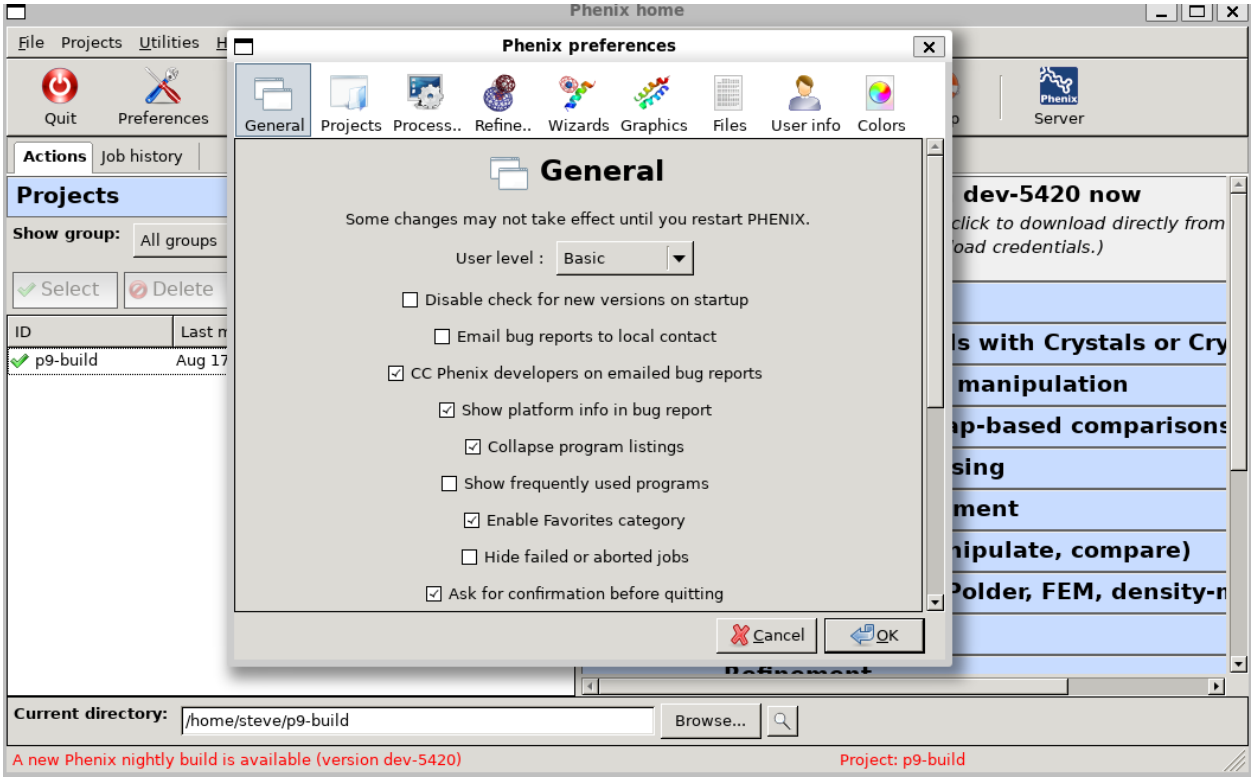


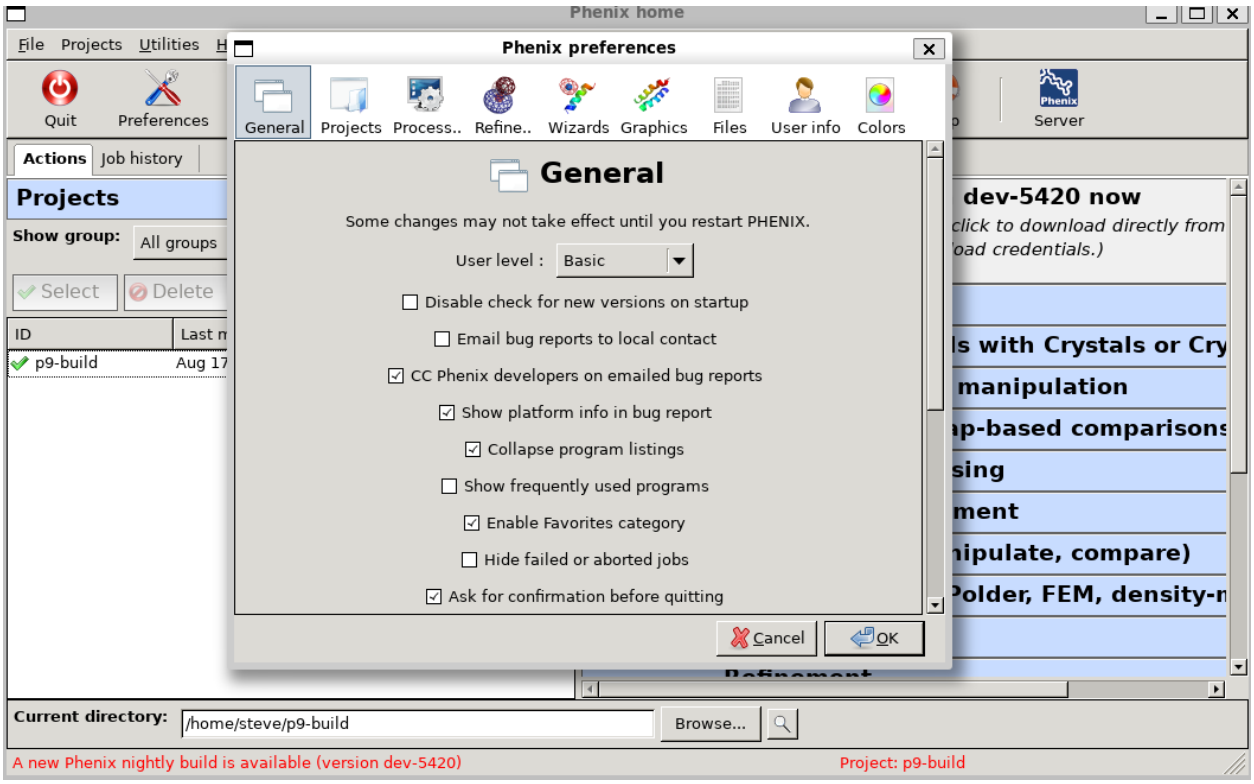
And you may have to set up tutorial data first before you can open the phenix window, but now the phenix window is working perfectly fine.

And now you just need to link Coot to Phenix:

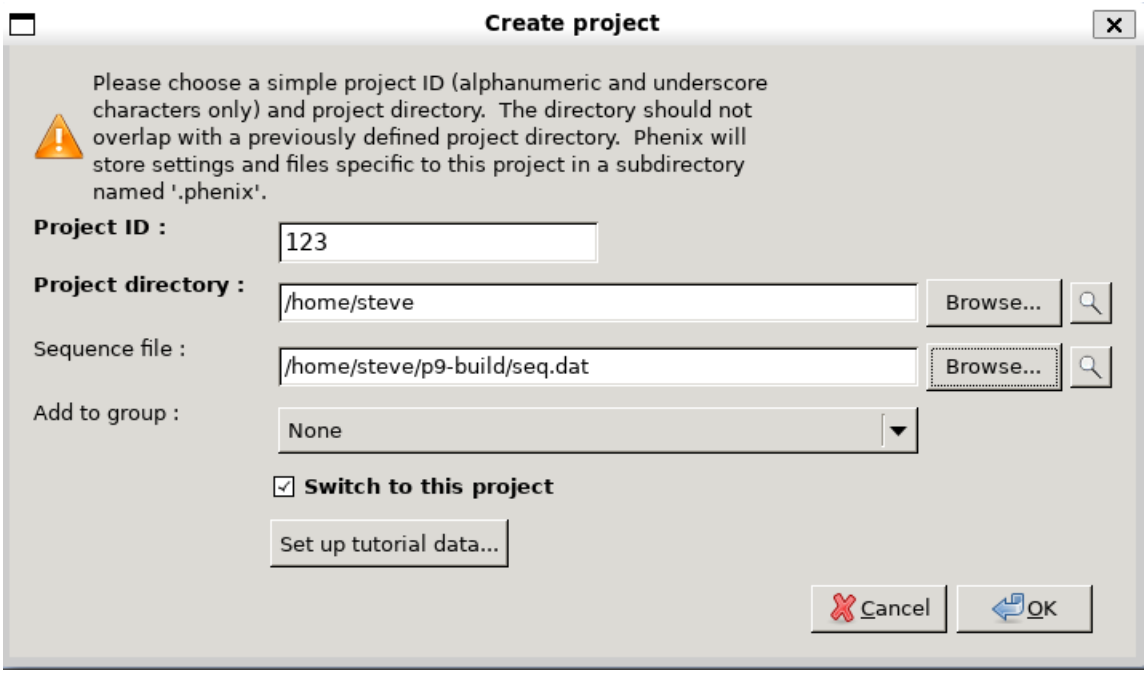
/home/<linux username>/coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python/bin/coot

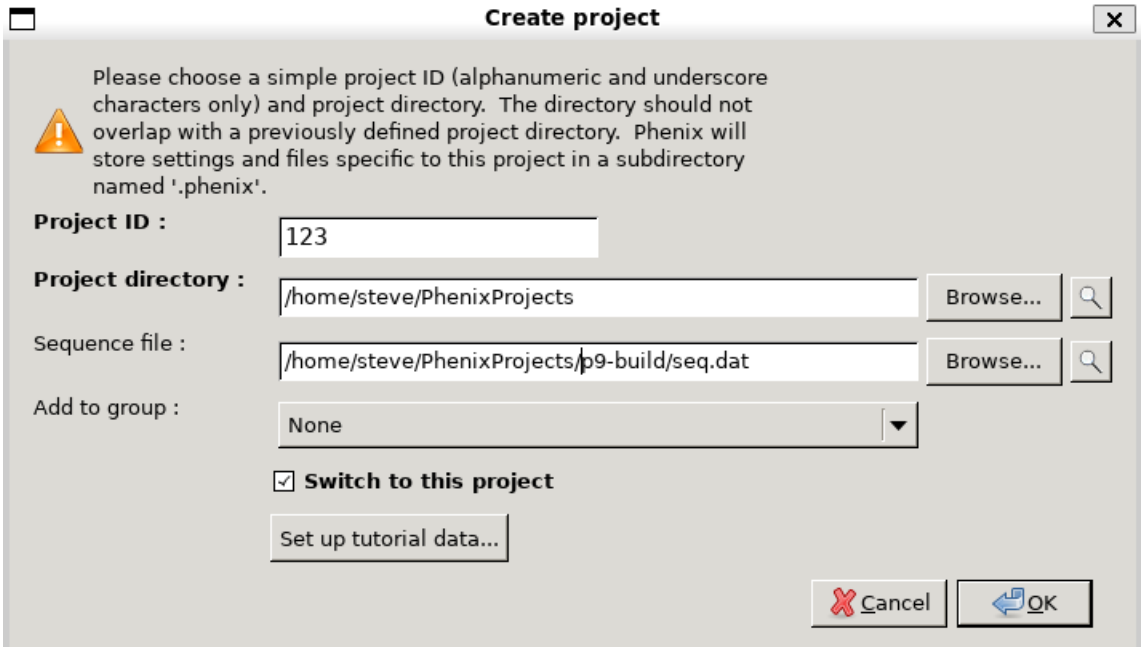
/home/steve/coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python/bin/coot

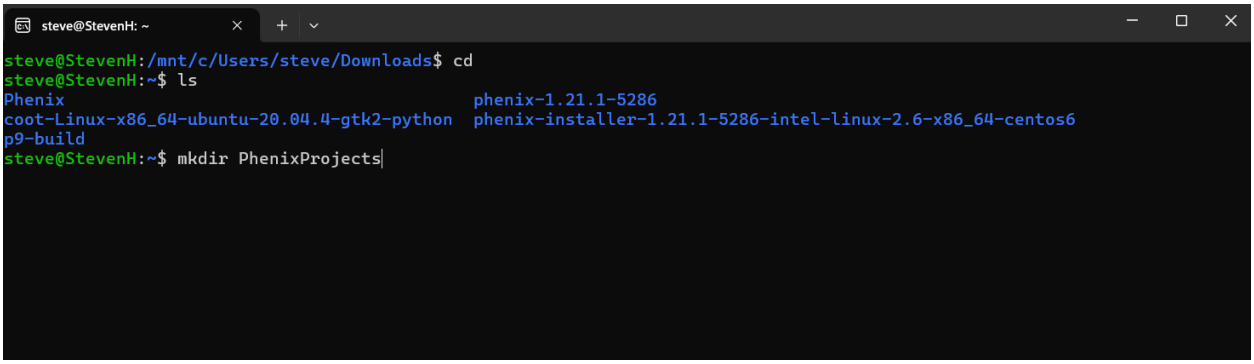




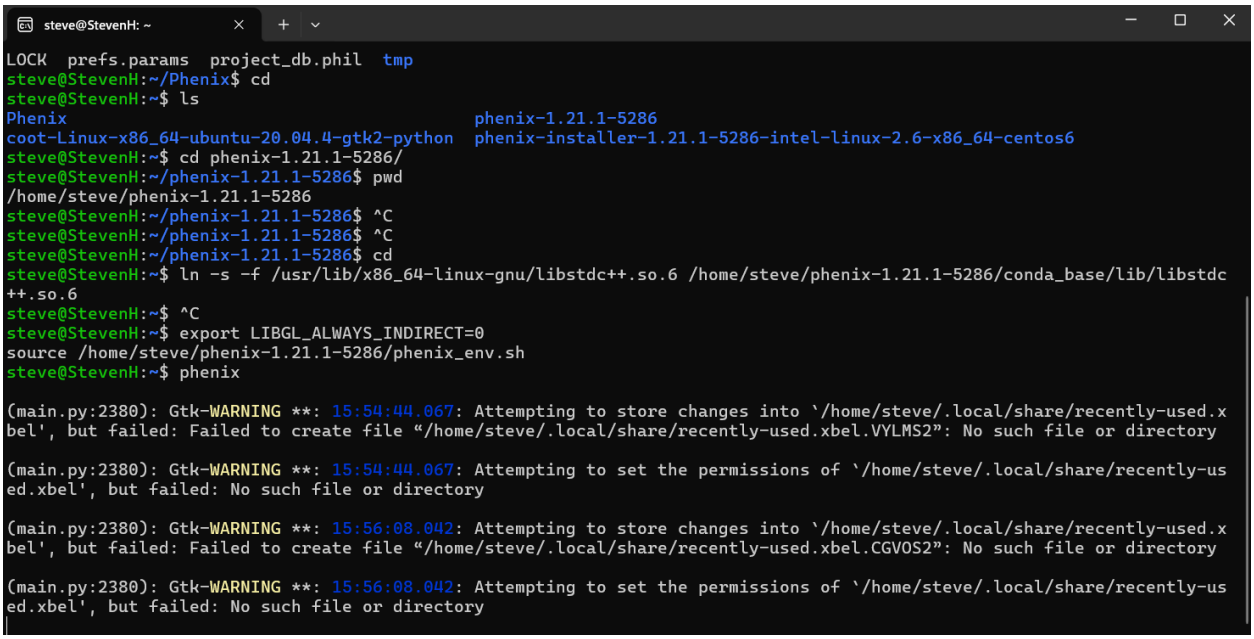
To check to see if Phenix is running properly, you can run the p9 build tutorial data model building project.

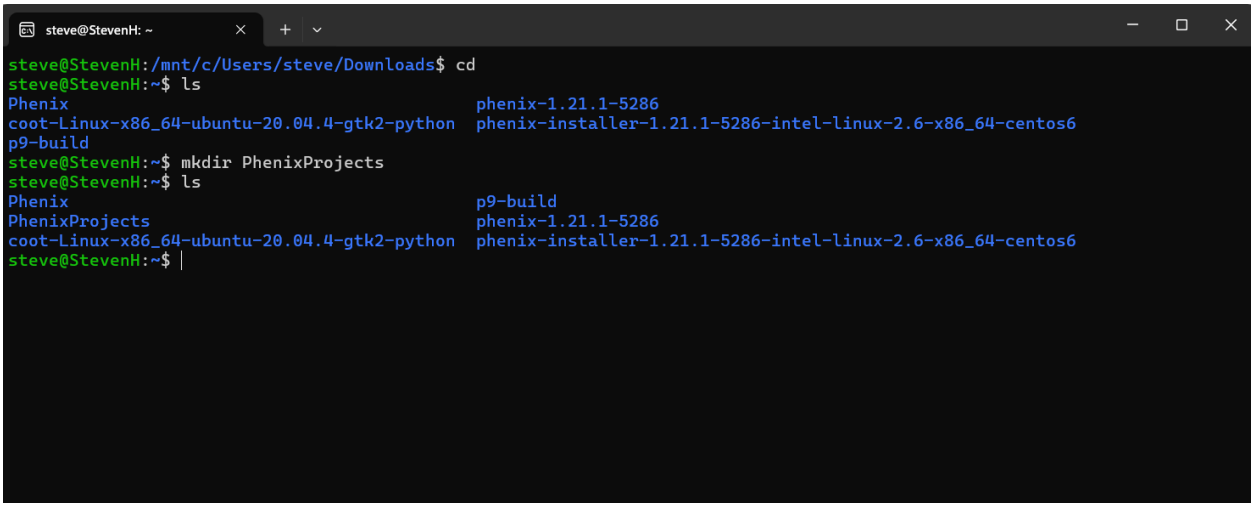






And you can see that while you were doing the Phenix stuff, there were errors that occurred:

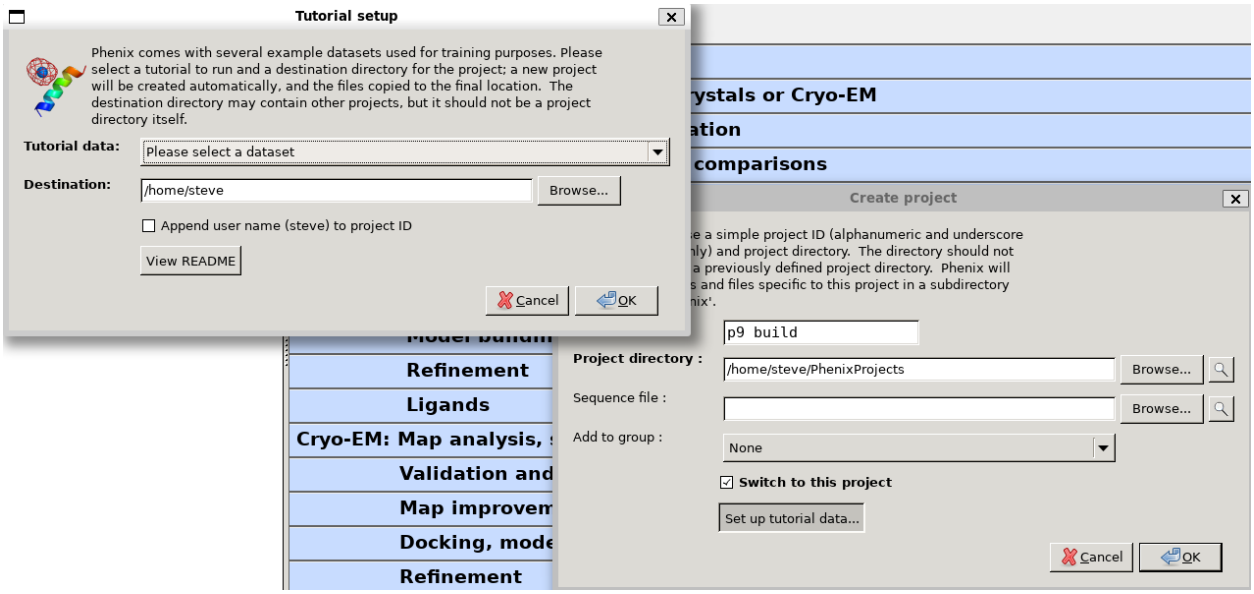




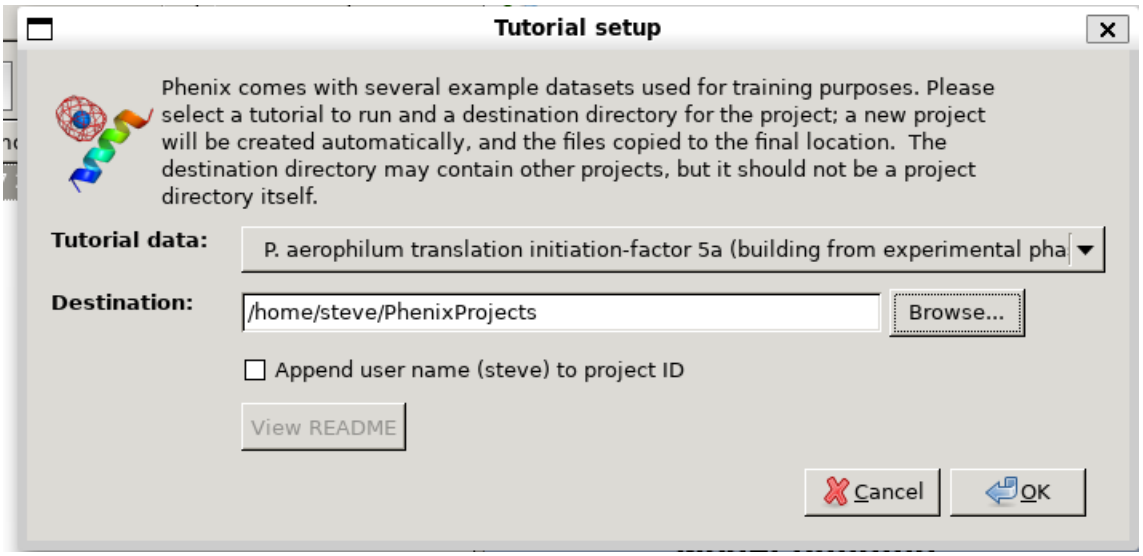
This PhenixProjects folder is where you will put your PHENIX projects into (because they cannot be out in the open in your root directory)

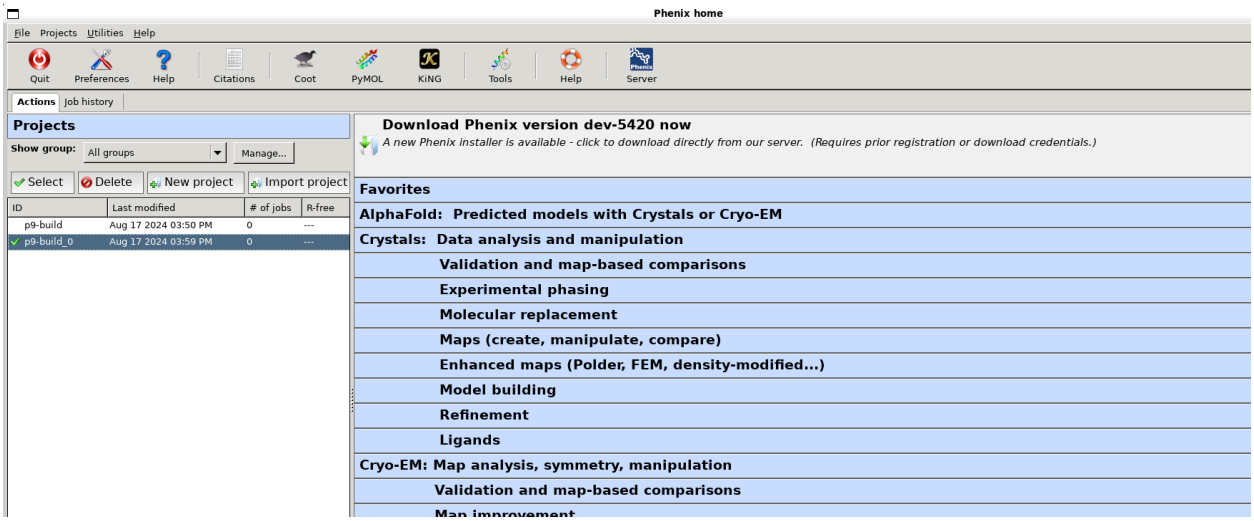
You cane make a new directory in your root directory by typing: **mkdir PhenixProjects**

Now your new directory is called PhenixProjects. You can save your Phenix Project folders in here.



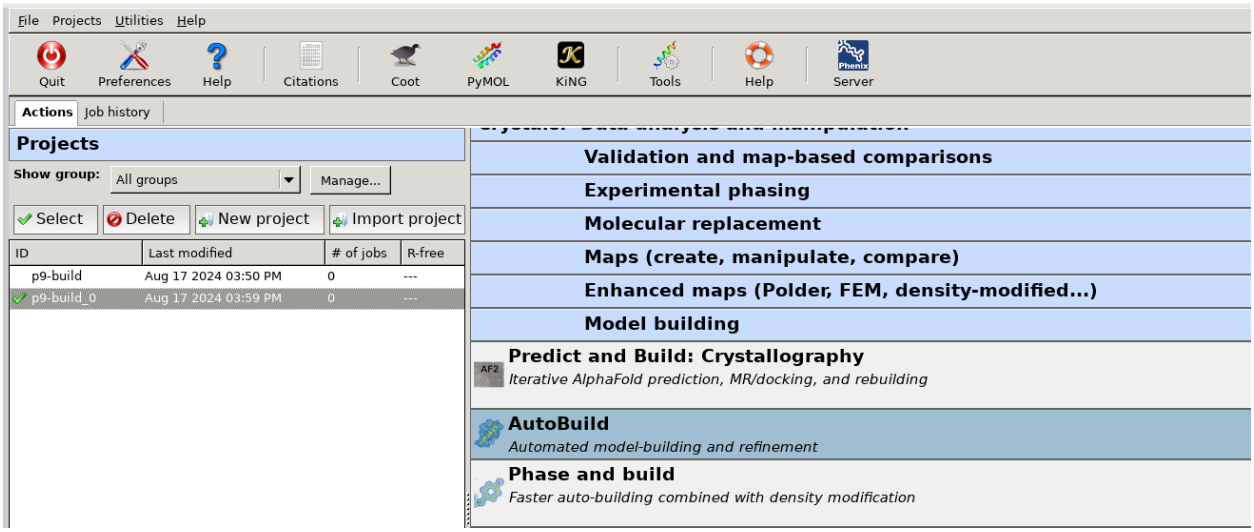
The only tutorial data under BUILDING:



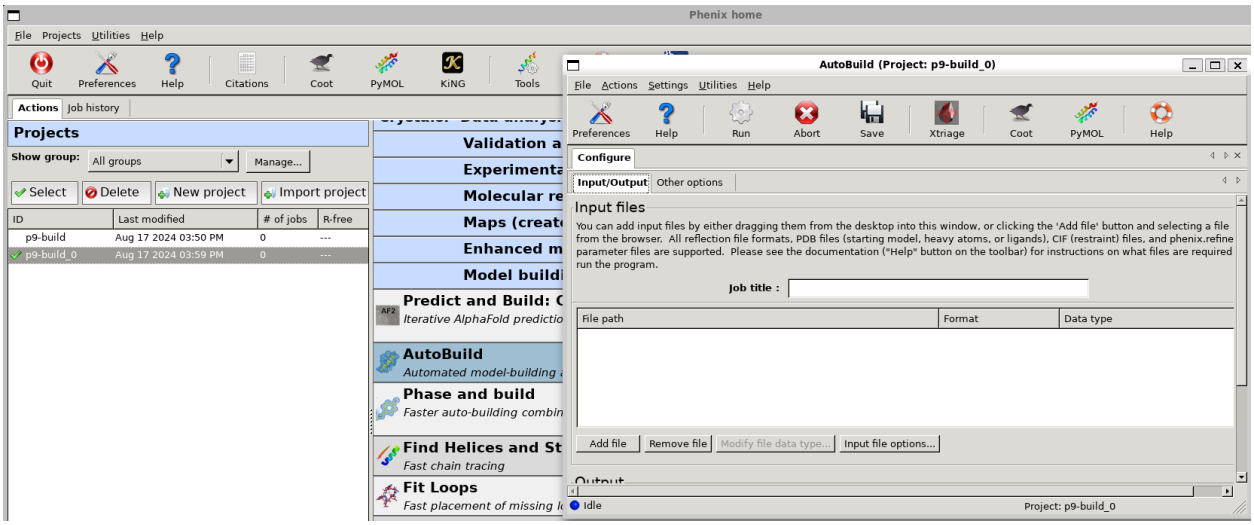


Now click ok and go to this one, double click.

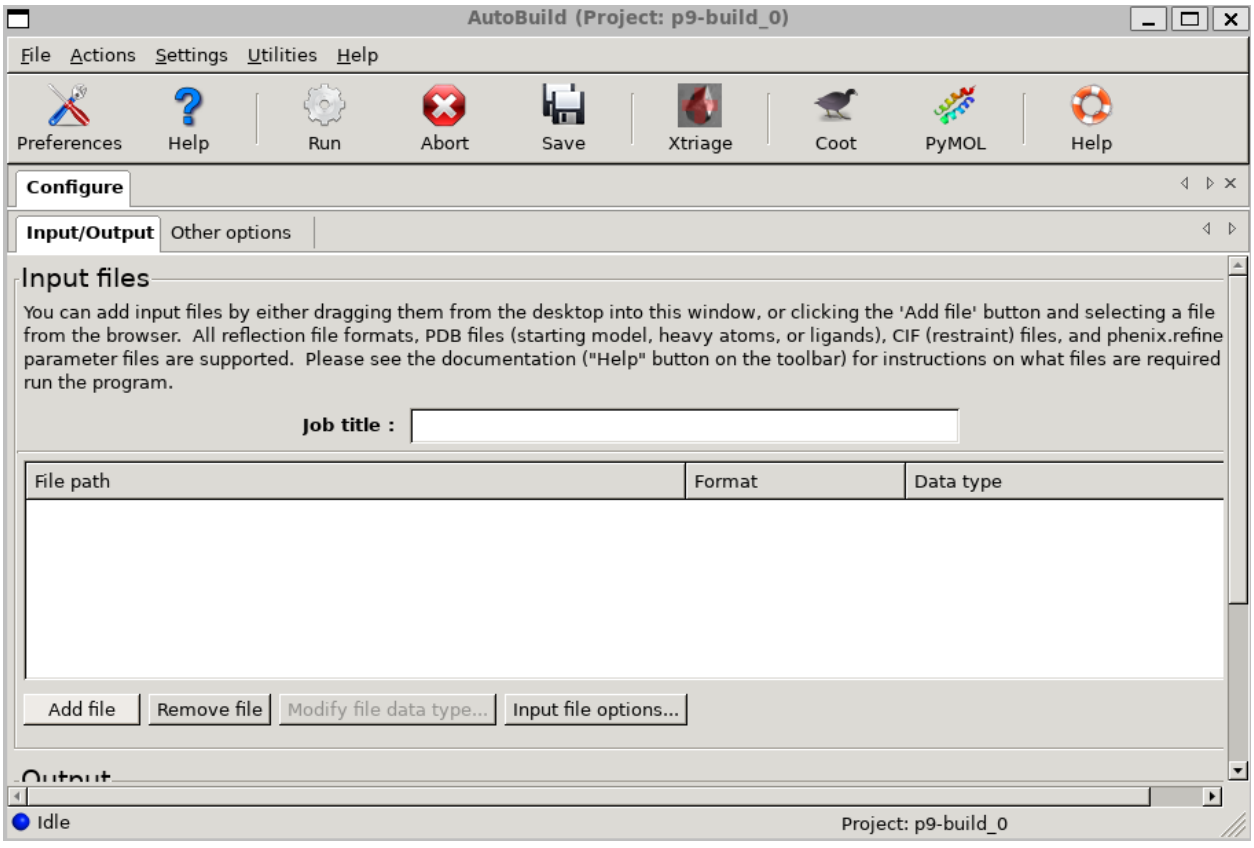
Then click Model Building and go to AutoBuild:

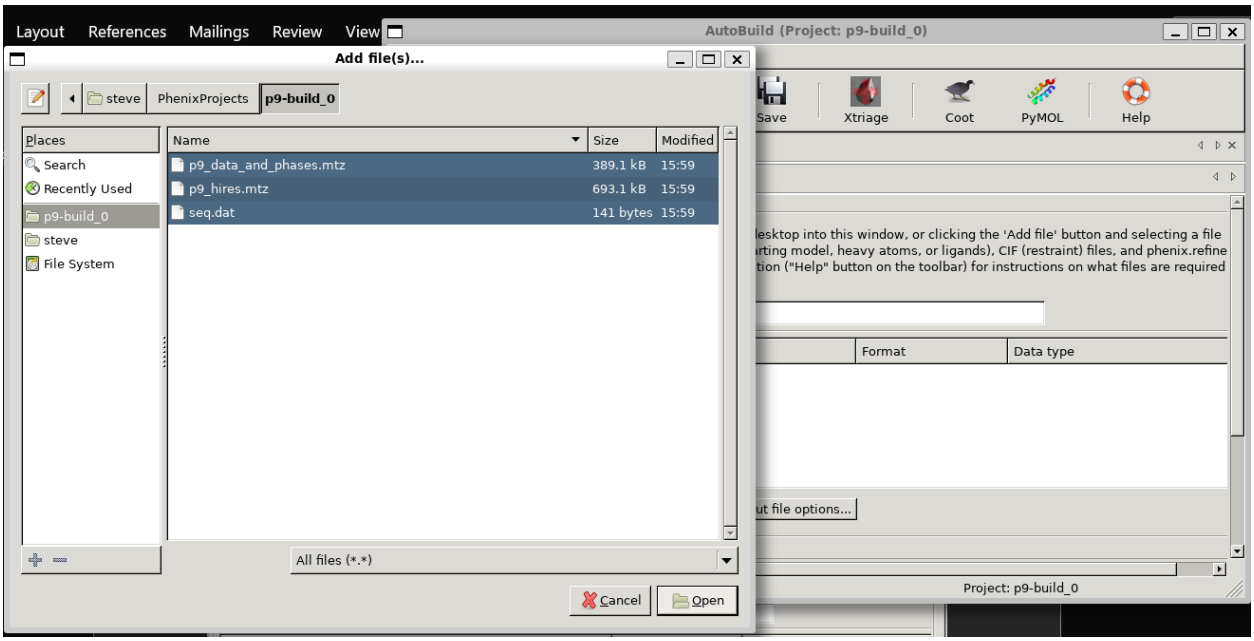


and click on it

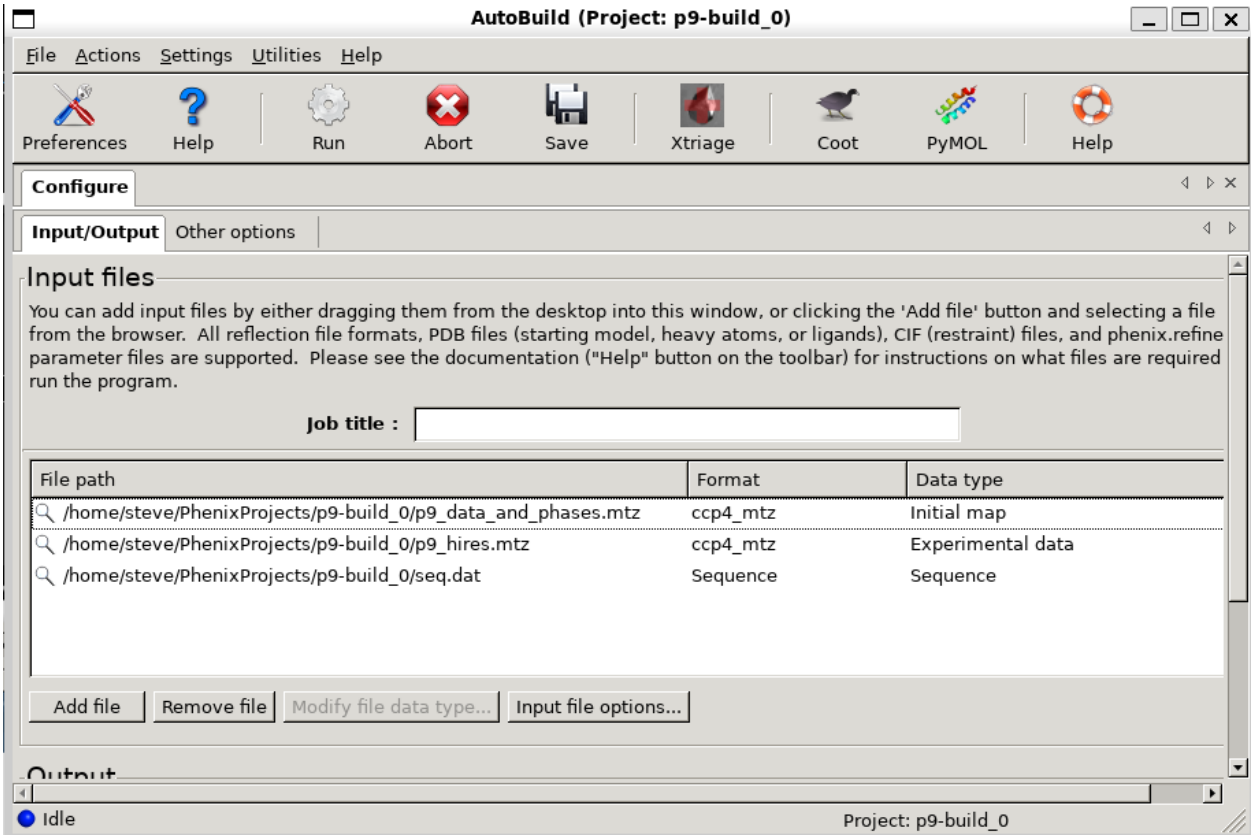


Follow the tutorial here: https://youtu.be/og3TM9Cwve0?si=iqtepsk4G8bu0VZ1 or follow along on this document as well:



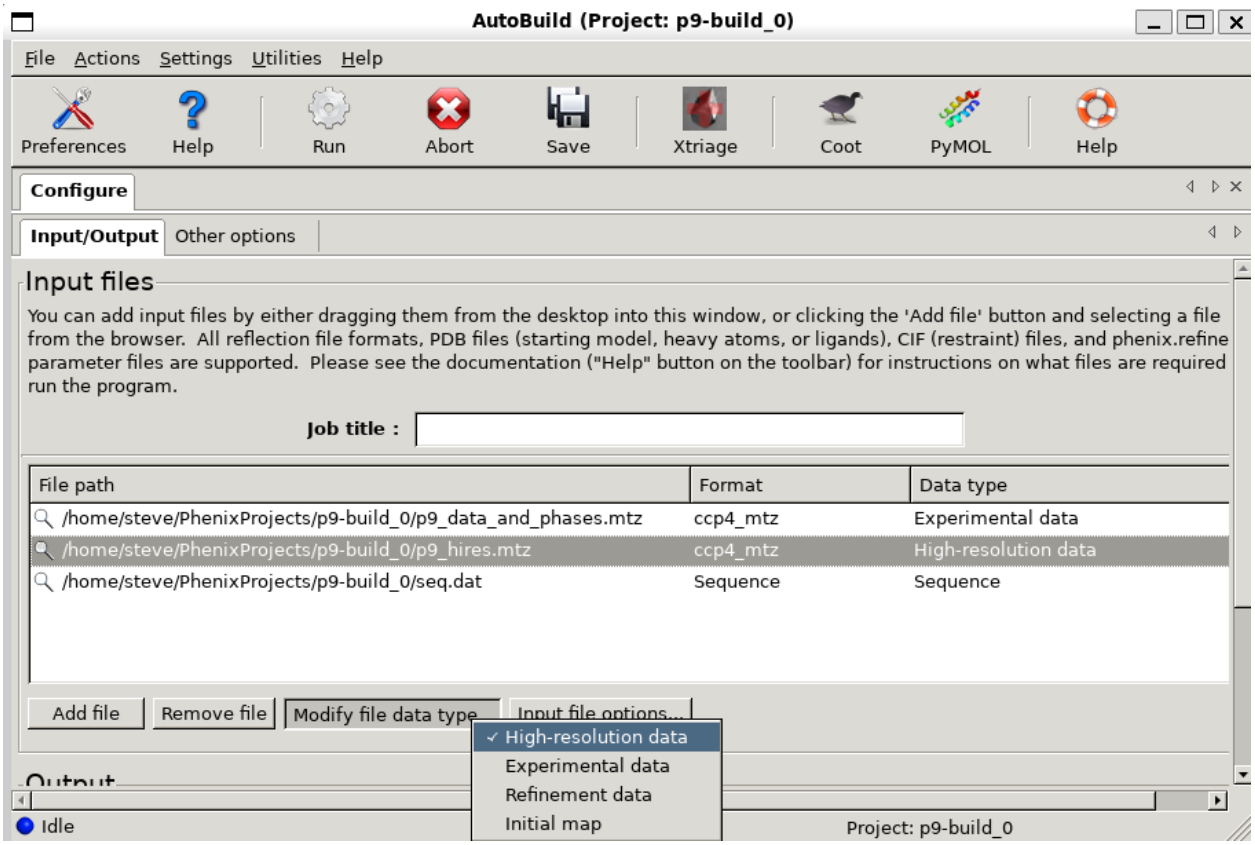


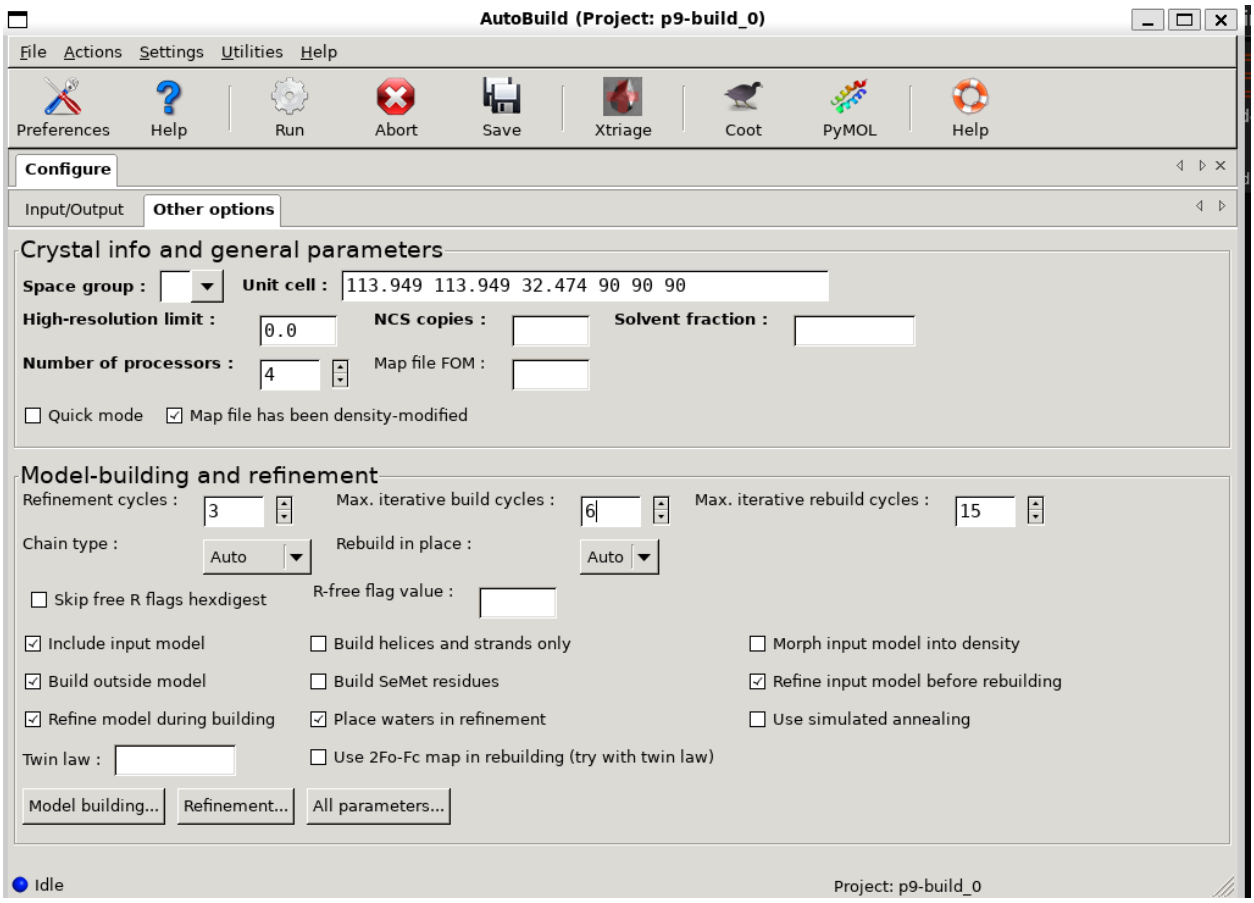
And click open



Now you will modify the file data type so that the pd_data_and_phases.mtz will be the experimental data (where the phases are)

And change the setting so that the p9_hires.mtz will be the high resolution map data type:





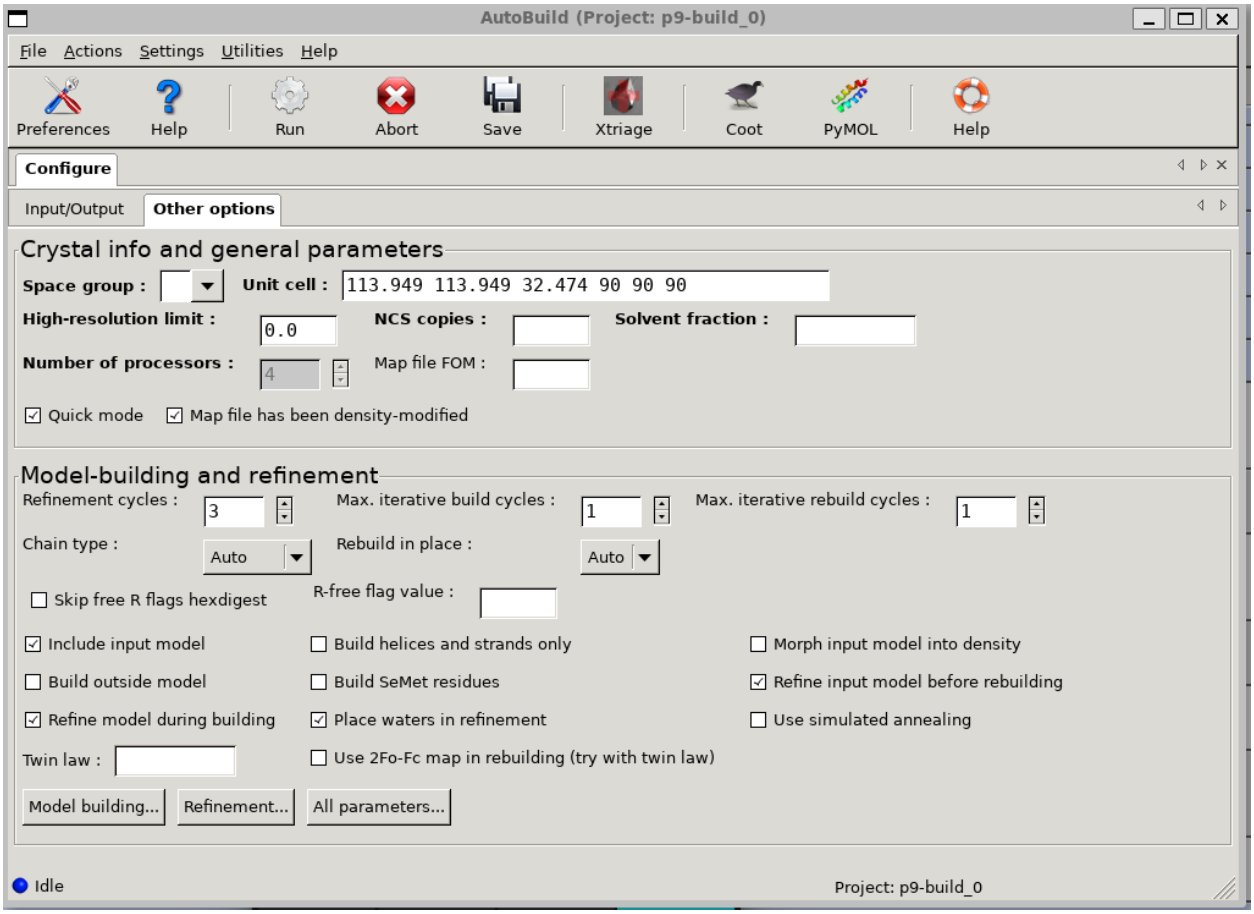
This is the original

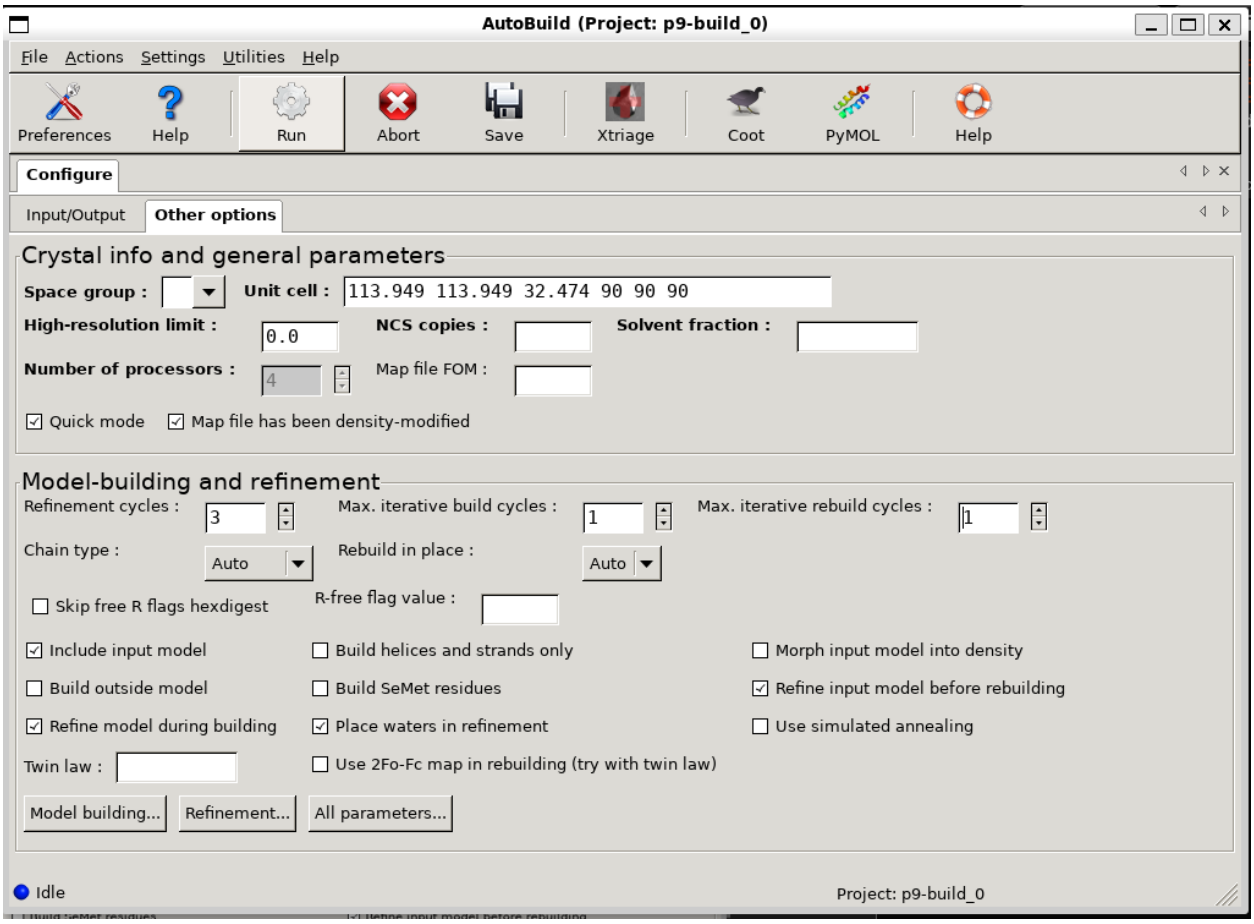
Just check “quick mode”

Change the “max iterative build cycles” to 1 from 6

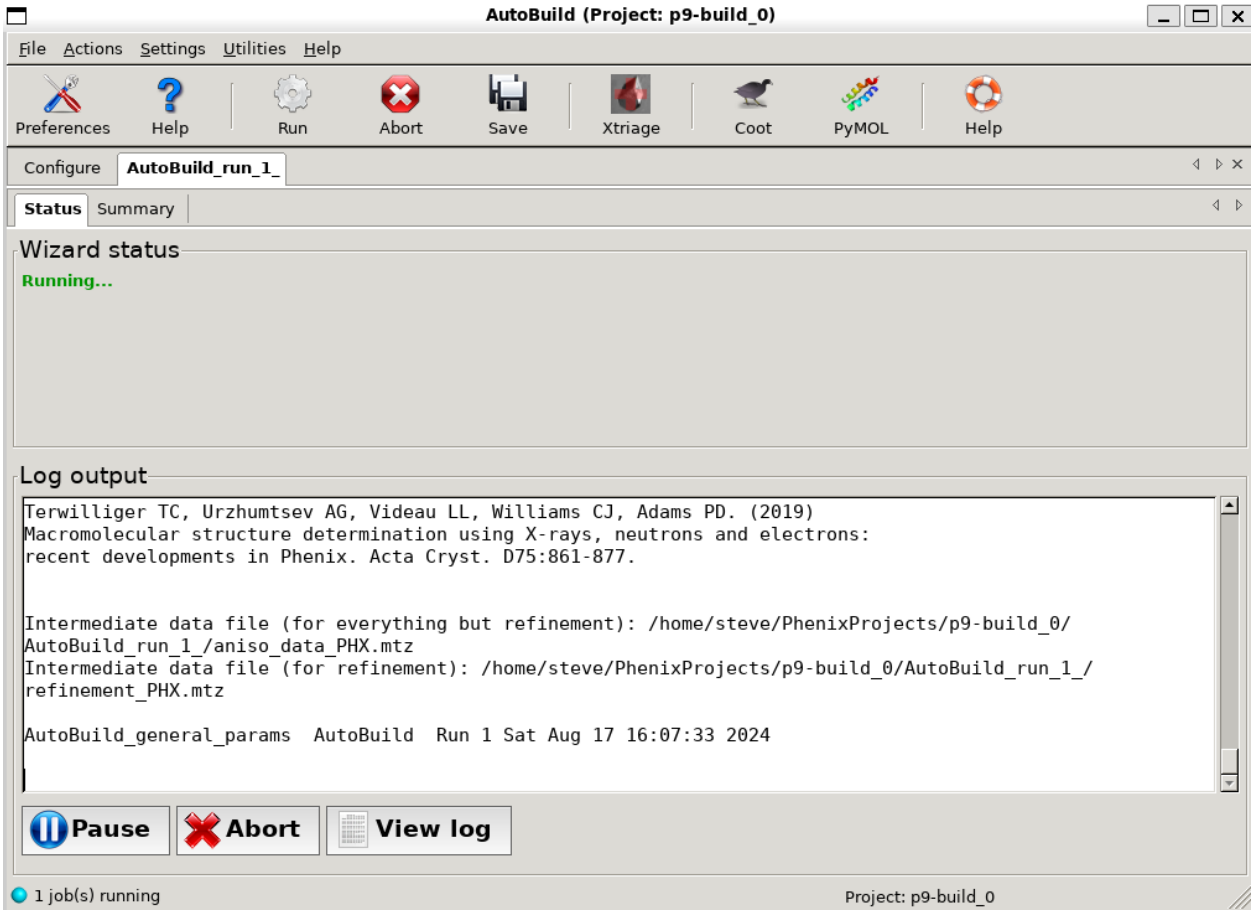
Change the “max iterative rebuild cycles” to 1 from 15

Un-check “build outside model”

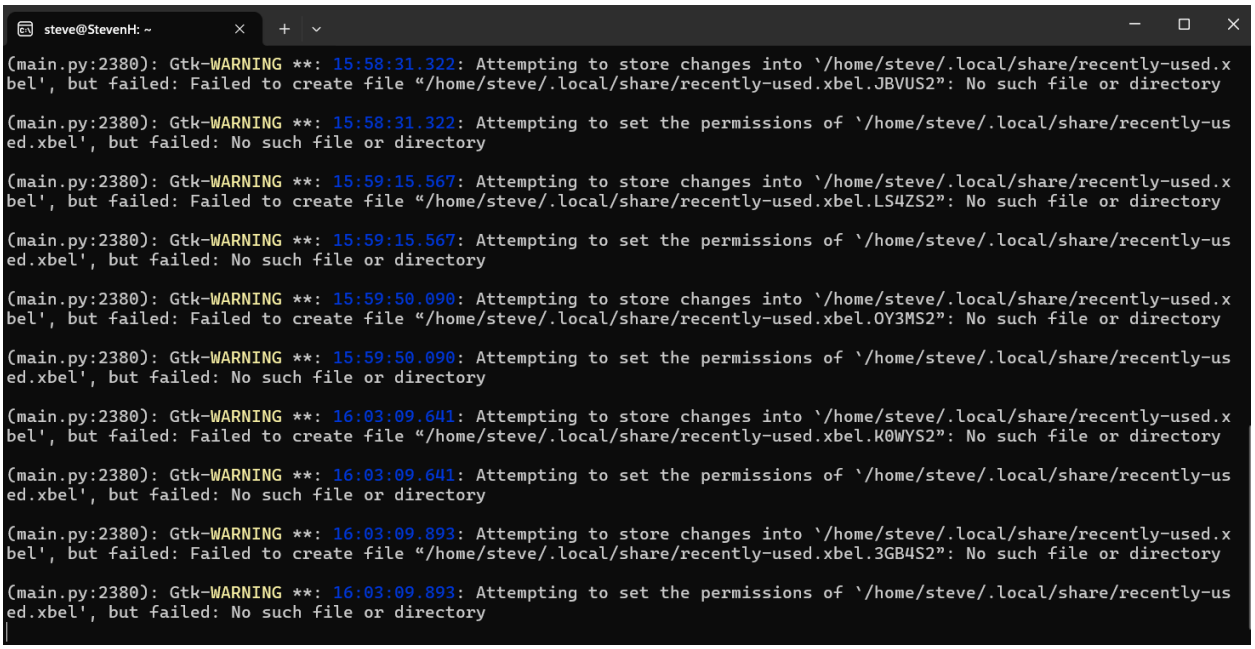

AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure
Input/Output Other options
Crystal info and general parameters
Space group :
Unit cell : 113.949 113.949 32.474 90 90 90
High-resolution limit : 0.0
NCS copies :
Solvent fraction :
Number of processors : 4
Map file FOM :
Quick mode
Map file has been density-modified
Model-building and refinement
Refinement cycles : 3
Max. iterative build cycles : 1
Max. iterative rebuild cycles : 1
Chain type : Auto
Rebuild in place : Auto
Skip free R flags hexdigest
R-free flag value :
Include input model
Build helices and strands only
Morph input model into density
Build outside model
Build SeMet residues
Refine input model before rebuilding
Refine model during building
Place waters in refinement
Use simulated annealing
Twin law :
Use 2Fo-Fc map in rebuilding (try with twin law)
Model building...
Refinement...
All parameters...
Idle
Project: p9-build_0

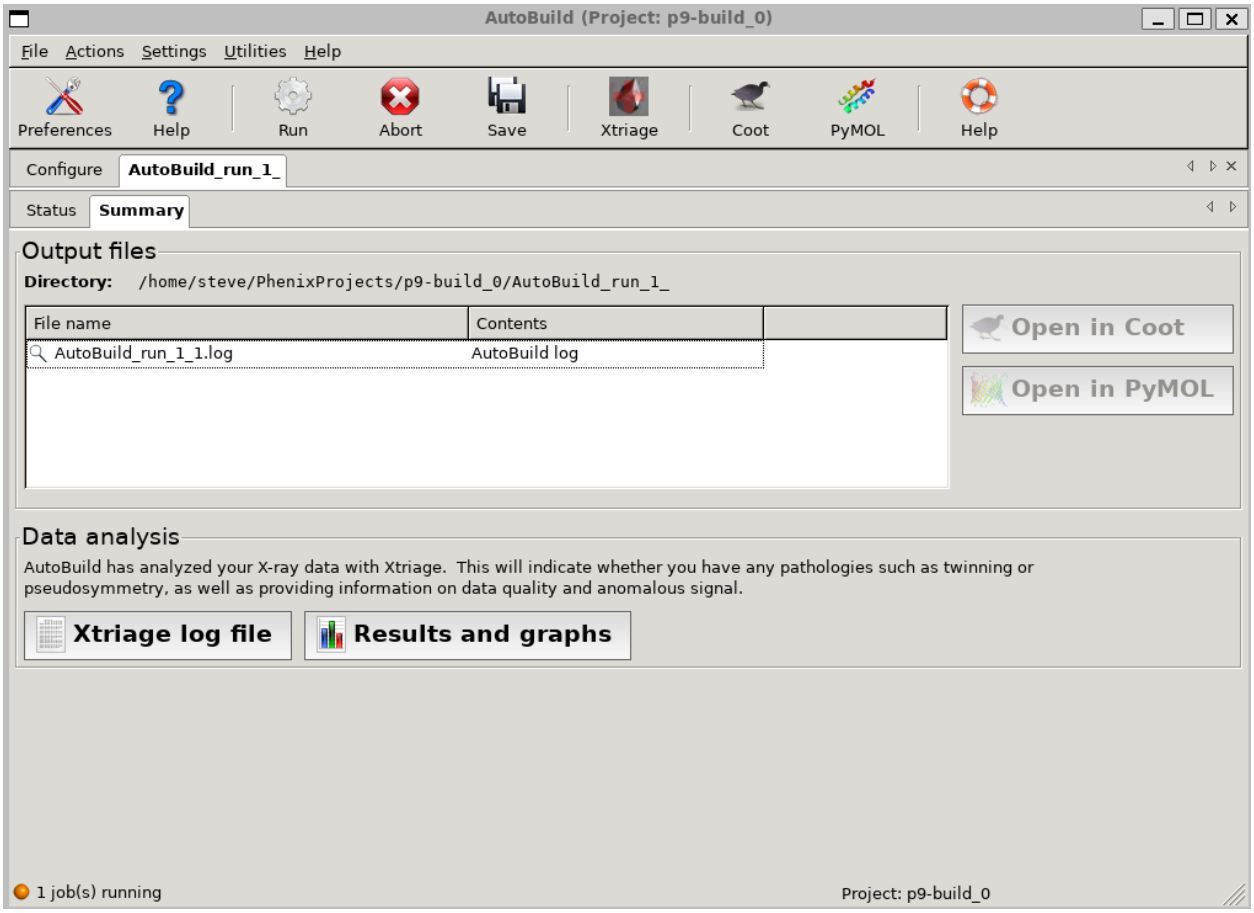


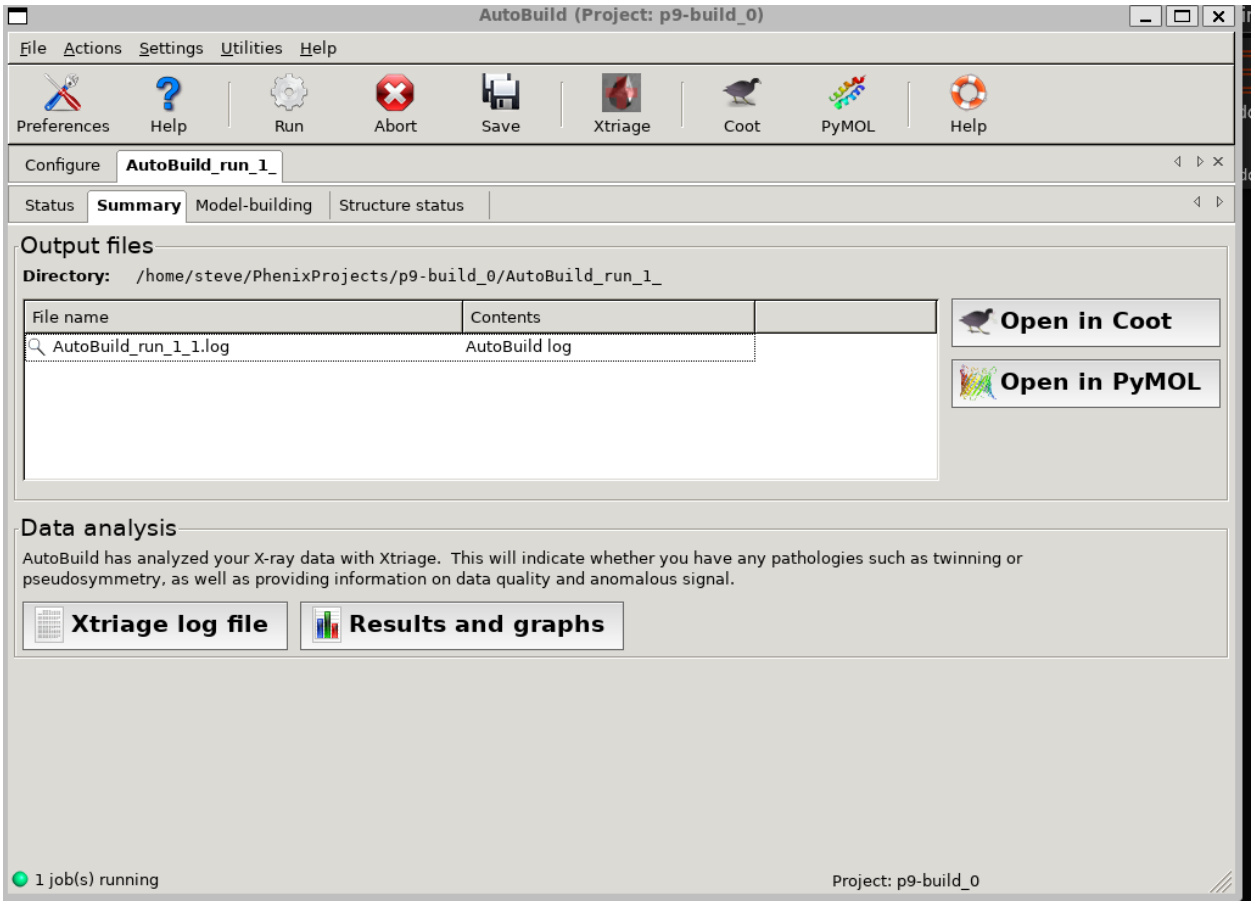
Now click run

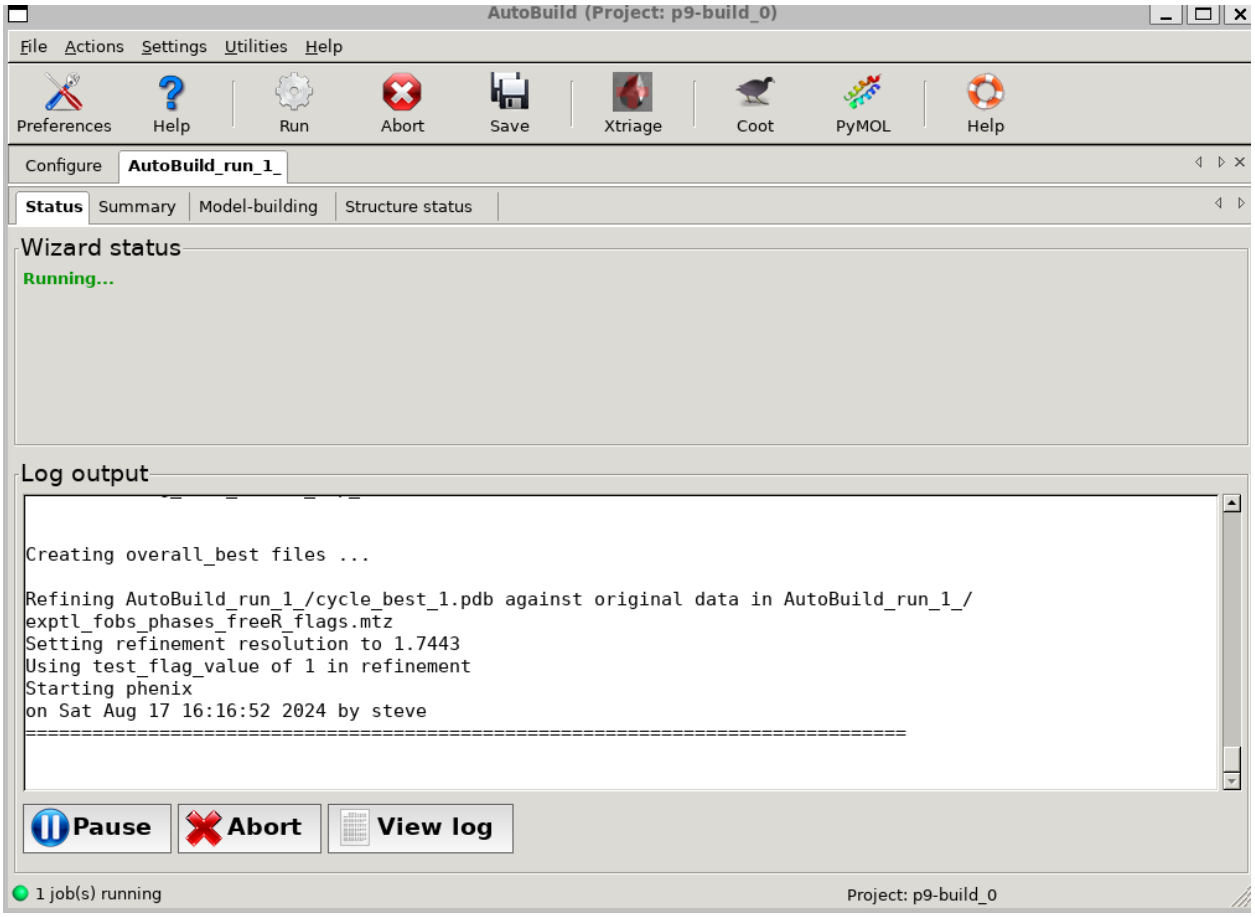


While this is loading, you can check the terminal, and there might be a lot of errors:

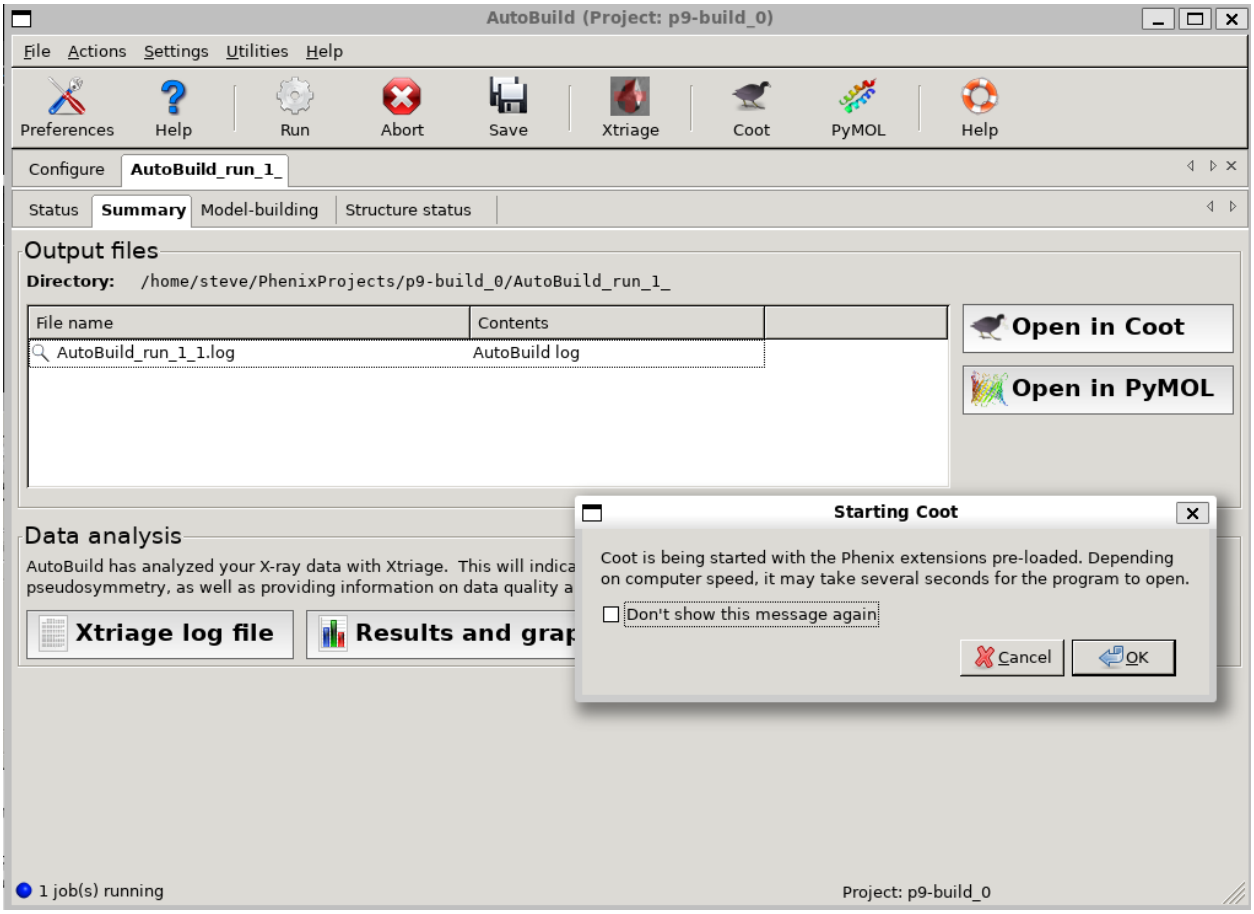


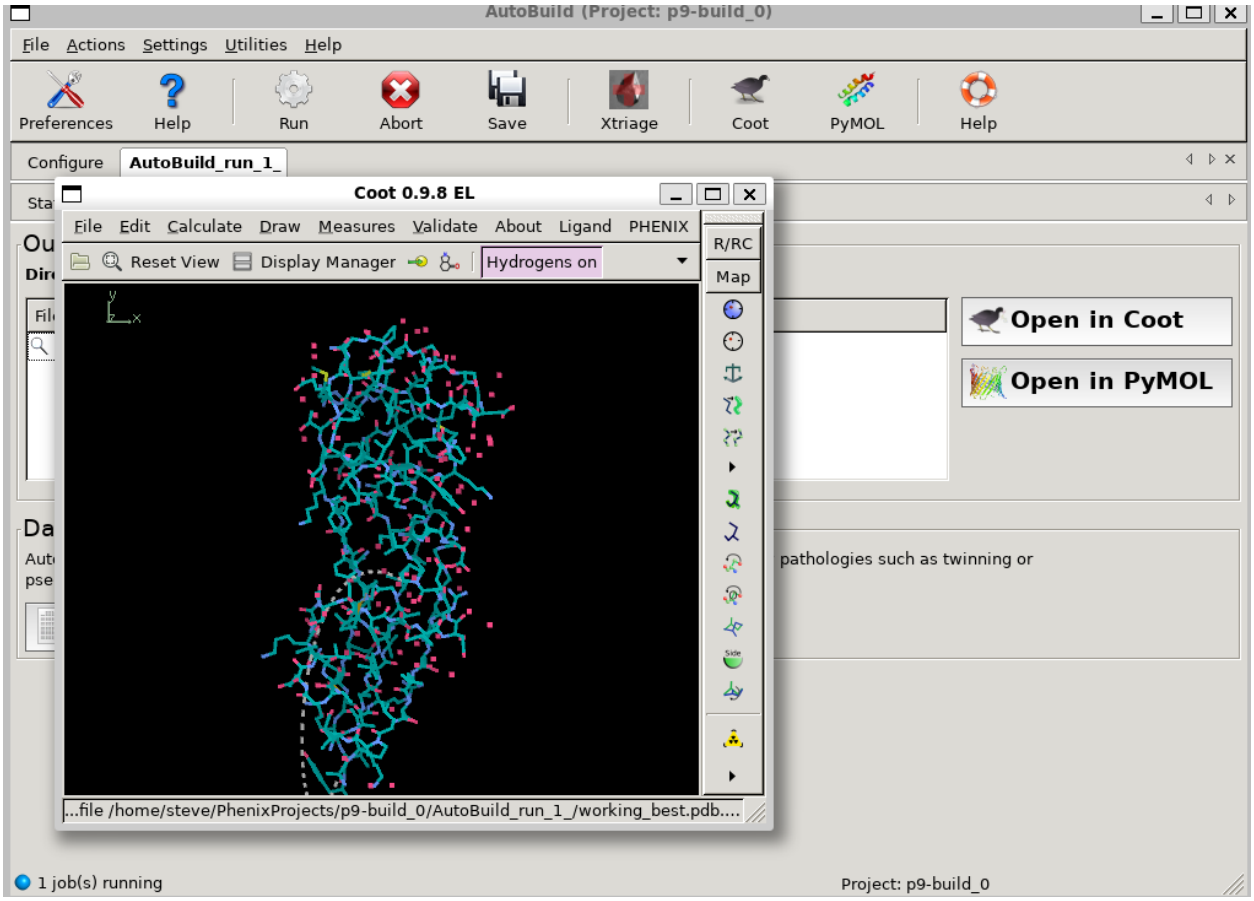

AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary
Output files
Directory: /home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1_
File name Contents
AutoBuild_run_1_1.log AutoBuild log
Open in Coot
Open in PyMOL
Data analysis
AutoBuild has analyzed your X-ray data with Xtriage. This will indicate whether you have any pathologies such as twinning or pseudosymmetry, as well as providing information on data quality and anomalous signal.
Xtriage log file
Results and graphs
1 job(s) running
Project: p9-build_0

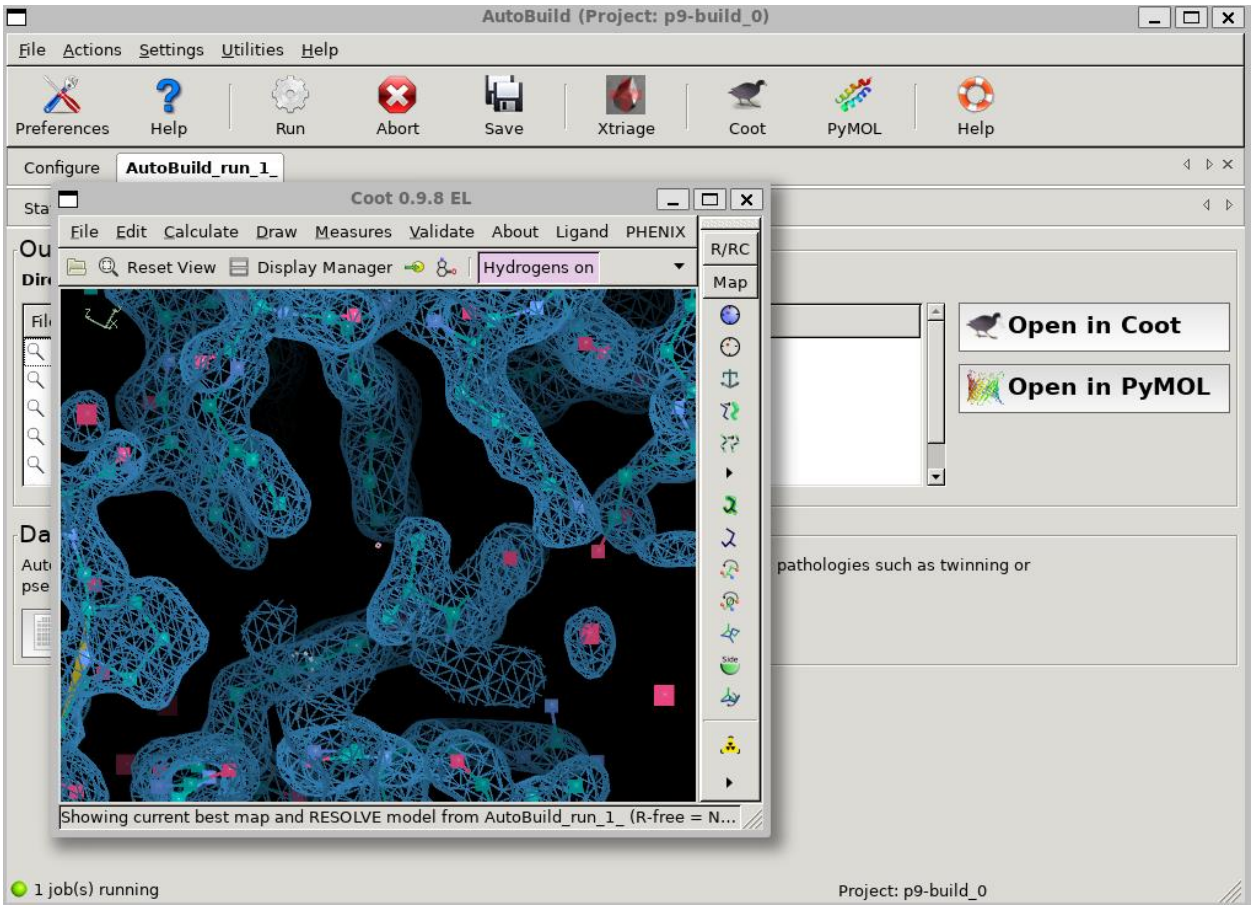

AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary Model-building Structure status
Output files
Directory: /home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1_
File name Contents
AutoBuild_run_1_1.log AutoBuild log
Open in Coot
Open in PyMOL
Data analysis
AutoBuild has analyzed your X-ray data with Xtriage. This will indicate whether you have any pathologies such as twinning or pseudosymmetry, as well as providing information on data quality and anomalous signal.
Xtriage log file
Results and graphs
1 job(s) running
Project: p9-build_0



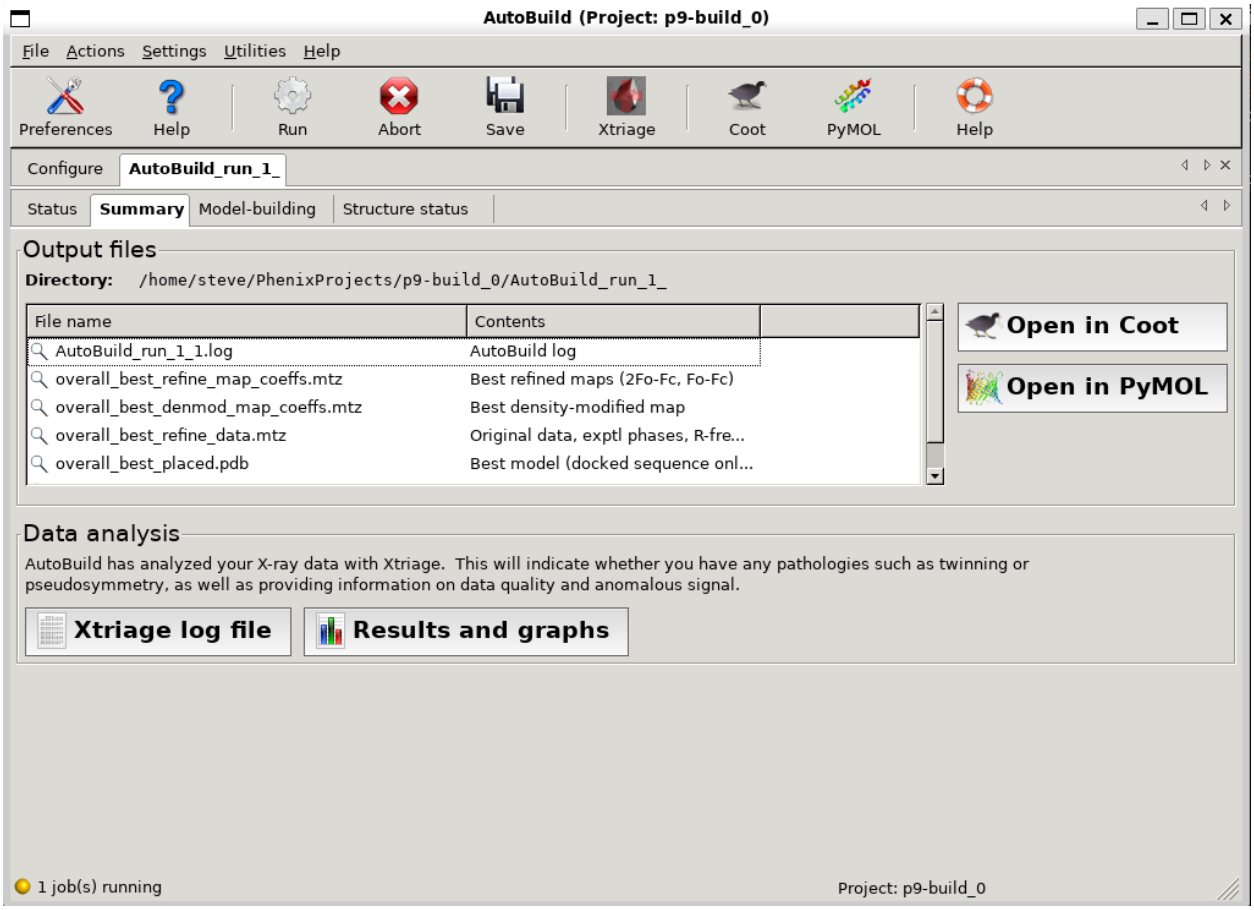
And now you can go to summary and open Coot to see what is going on to the model in Coot:

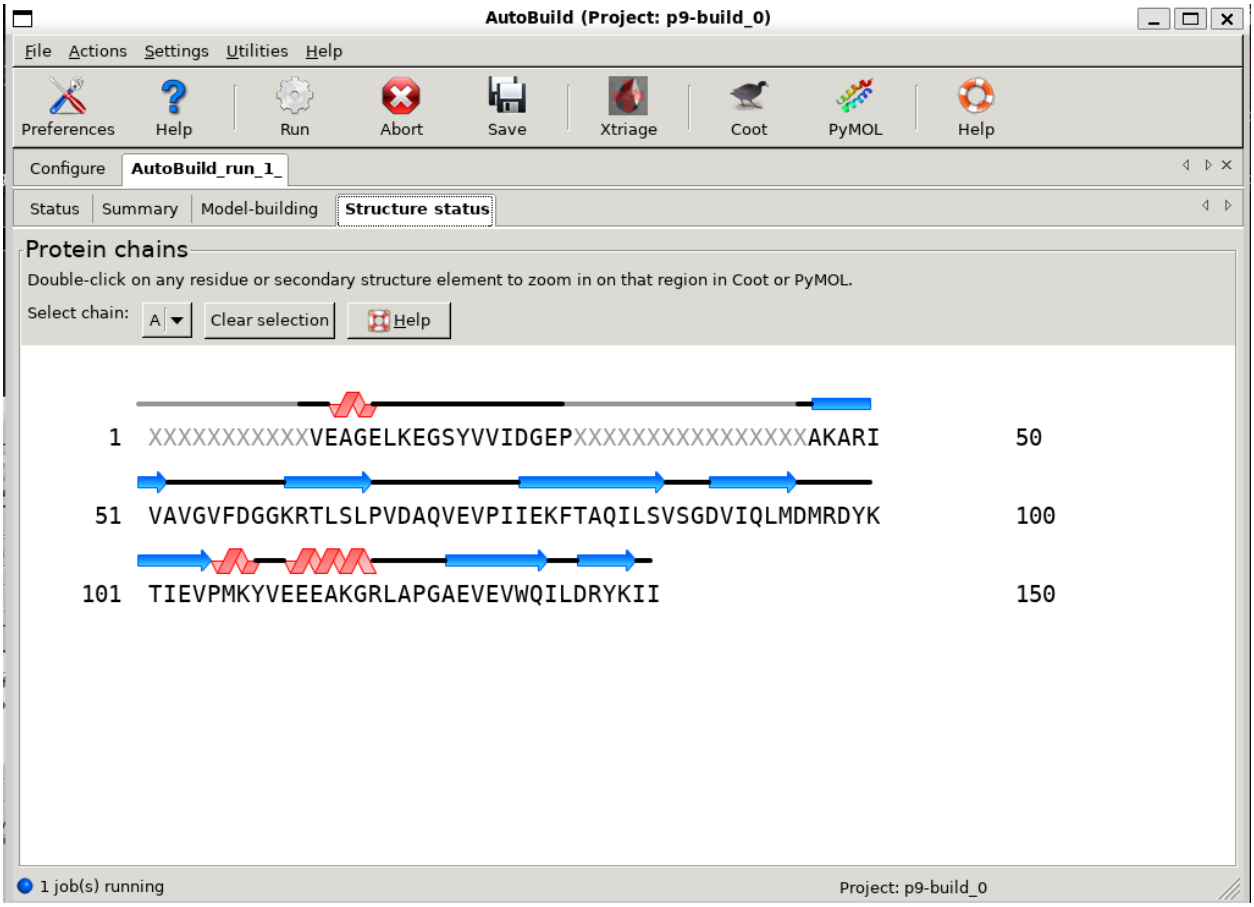

AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary Model-building Structure status
Output files
Directory: /home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1_
File name Contents
AutoBuild_run_1_1.log AutoBuild log
Open in Coot
Open in PyMOL
Data analysis
AutoBuild has analyzed your X-ray data with Xtriage. This will indica
pseudosymmetry, as well as providing information on data quality a
Xtriage log file
Results and grap
Starting Coot
Coot is being started with the Phenix extensions pre-loaded. Depending on computer speed, it may take several seconds for the program to open.
Don't show this message again
Cancel
OK
1 job(s) running
Project: p9-build_0

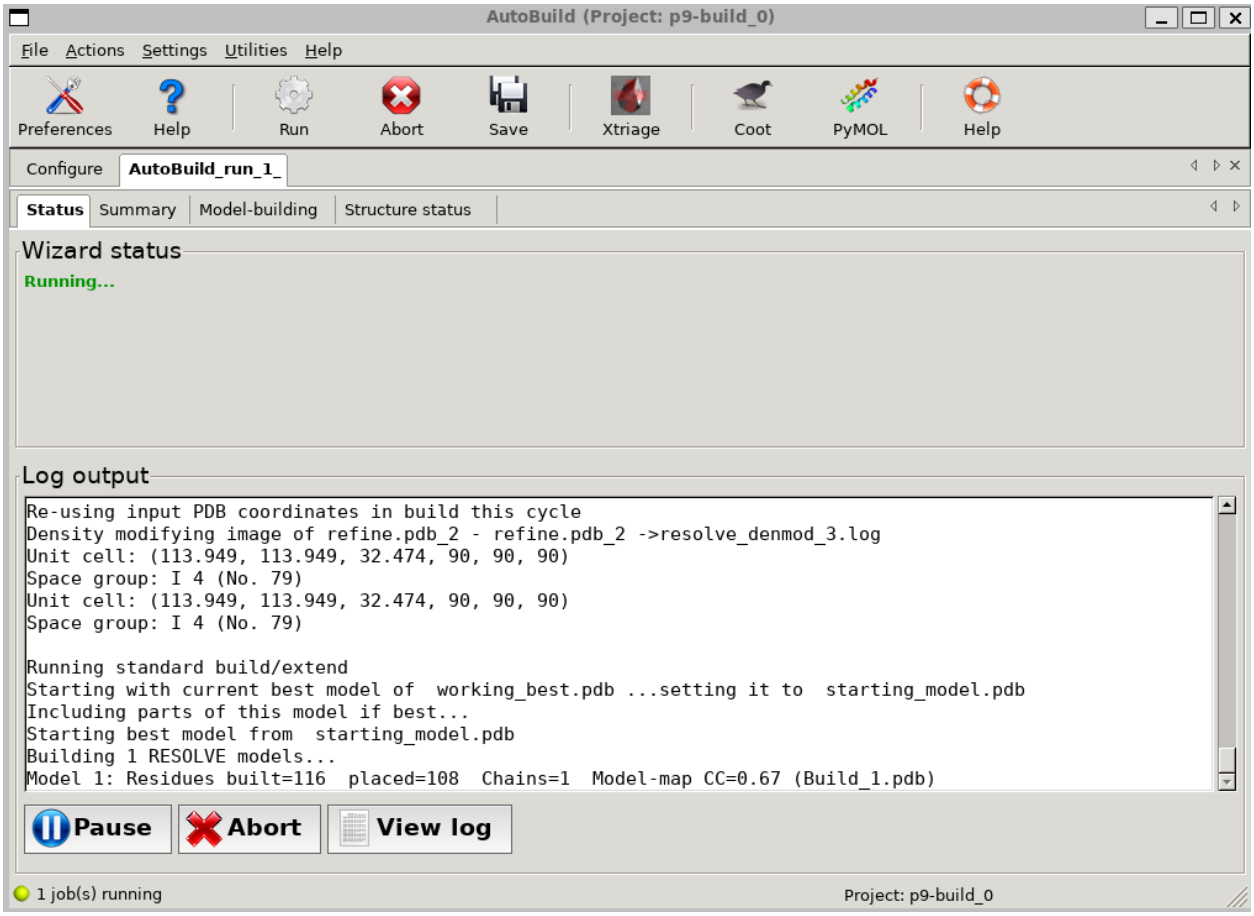

AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Coot 0.9.8 EL
File Edit Calculate Draw Measures Validate About Ligand PHENIX
Reset View Display Manager Hydrogens on
R/RC
Map
Open in Coot
Open in PyMOL
pathologies such as twinning or
...file /home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1_/working_best.pdb....
1 job(s) running
Project: p9-build_0

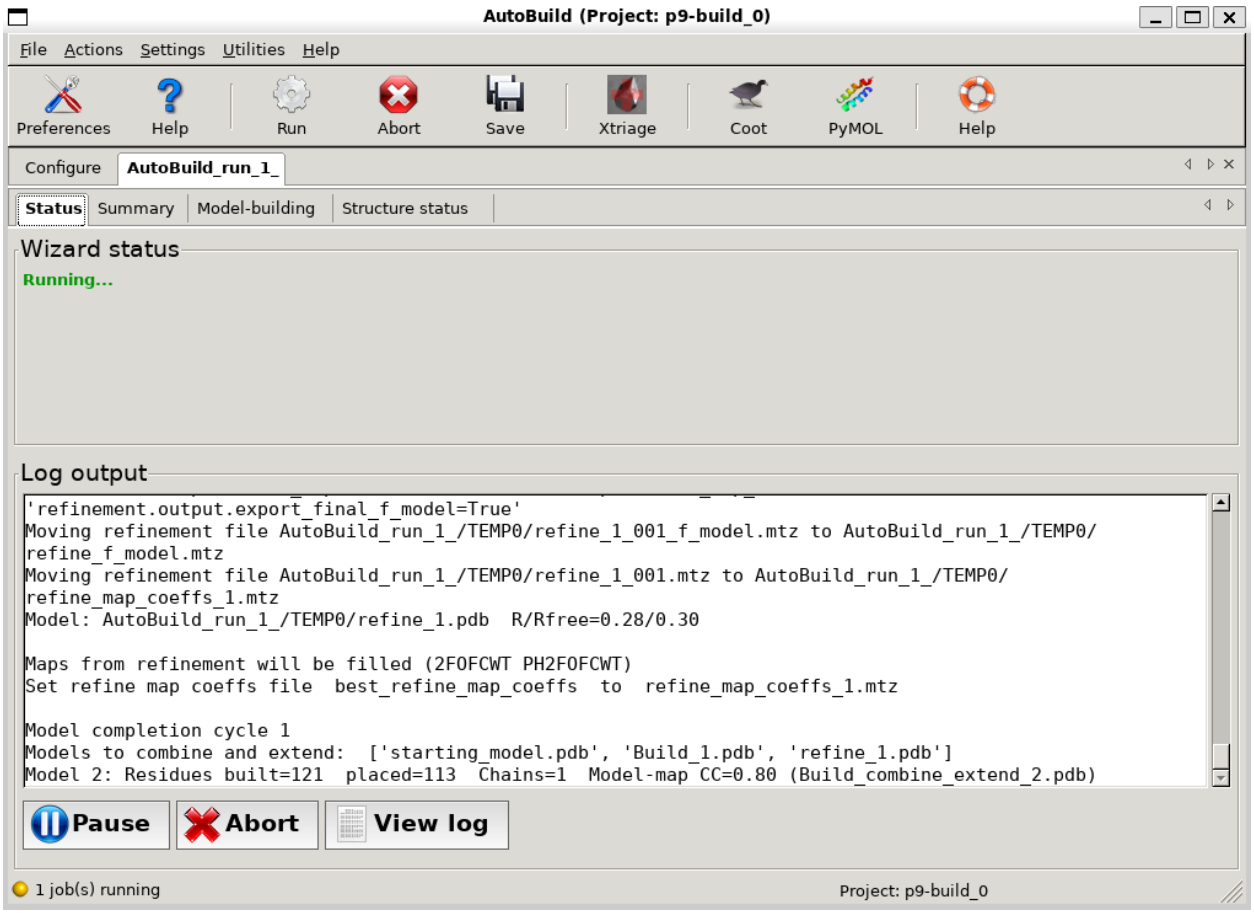


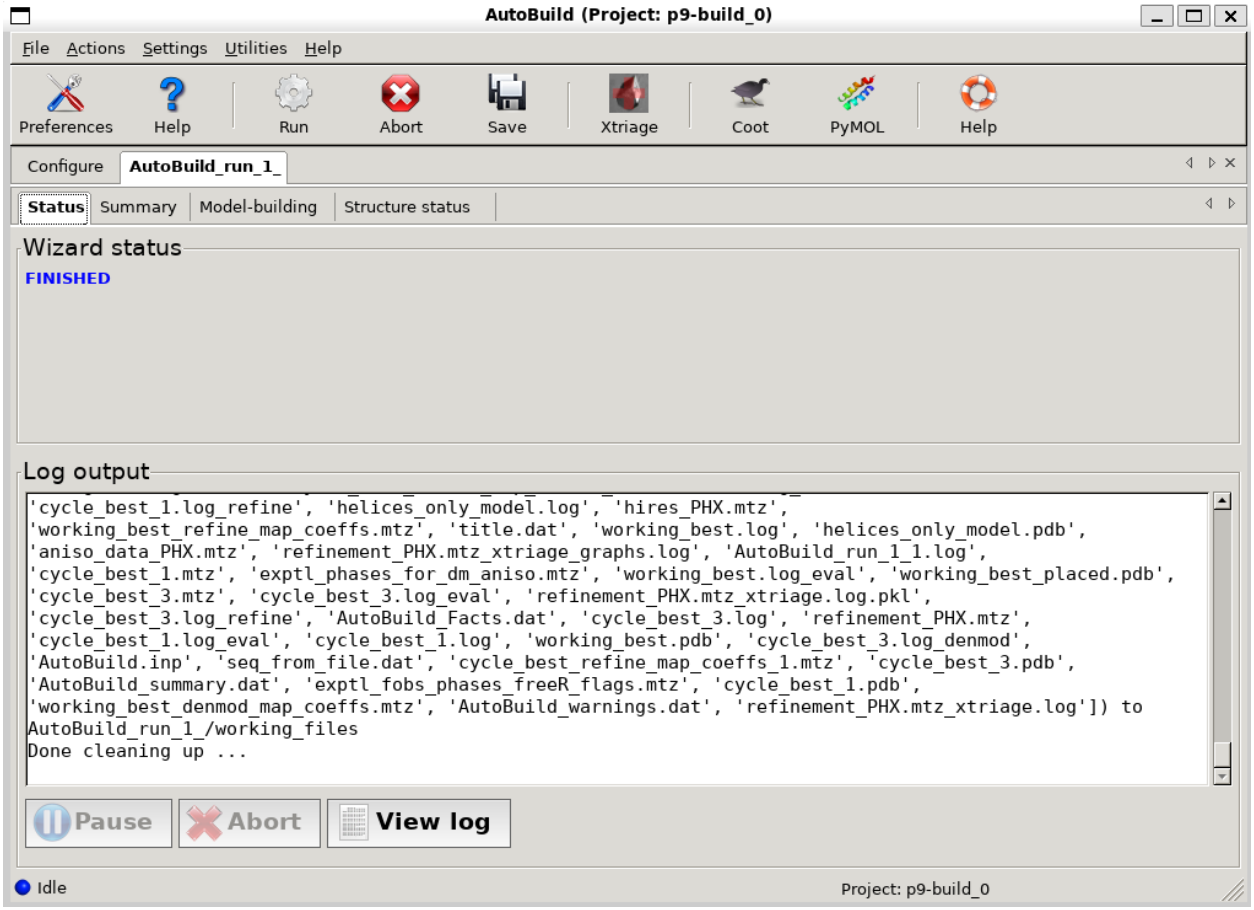
This run on average only takes around 20 to 30 minutes:

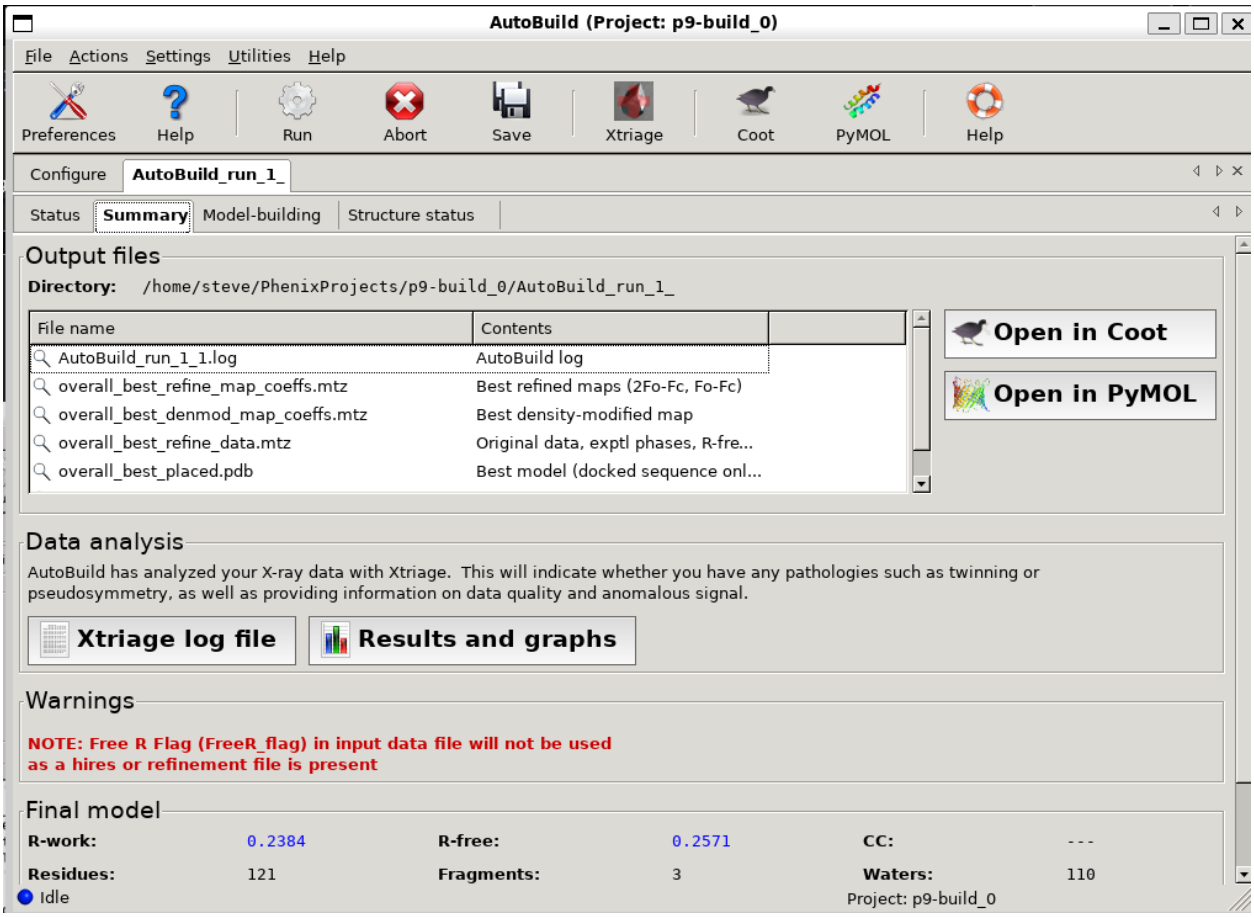

AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary Model-building Structure status
Output files
Directory: /home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1_
File name Contents
AutoBuild_run_1_1.log AutoBuild log
overall_best_refine_map_coeffs.mtz Best refined maps (2Fo-Fc, Fo-Fc)
overall_best_denmod_map_coeffs.mtz Best density-modified map
overall_best_refine_data.mtz Original data, exptl phases, R-fre...
overall_best_placed.pdb Best model (docked sequence onl...
Open in Coot
Open in PyMOL
Data analysis
AutoBuild has analyzed your X-ray data with Xtriage. This will indicate whether you have any pathologies such as twinning or pseudosymmetry, as well as providing information on data quality and anomalous signal.
Xtriage log file
Results and graphs
1 job(s) running
Project: p9-build_0


AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary Model-building Structure status
Protein chains
Double-click on any residue or secondary structure element to zoom in on that region in Coot or PyMOL.
Select chain: A Clear selection Help
1 XXXXXXXXXXXVEAGELKEGSYVVIDGEPXXXXXXXXXXXXXXXXXAKARI 50
51 VAVGVFDGGKRTLSLPVDAQVEVPIIEKFTAQILSVSGDVIQLMDMRDYK 100
101 TIEVPMKYVEEEAKGRLAPGAEVEVWQILDRYKII 150
1 job(s) running
Project: p9-build_0


AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary Model-building Structure status
Wizard status
Running...
Log output
Re-using input PDB coordinates in build this cycle
Density modifying image of refine.pdb_2 - refine.pdb_2 ->resolve_denmod_3.log
Unit cell: (113.949, 113.949, 32.474, 90, 90, 90)
Space group: I 4 (No. 79)
Unit cell: (113.949, 113.949, 32.474, 90, 90, 90)
Space group: I 4 (No. 79)
Running standard build/extend
Starting with current best model of working_best.pdb ...setting it to starting_model.pdb
Including parts of this model if best...
Starting best model from starting_model.pdb
Building 1 RESOLVE models...
Model 1: Residues built=116 placed=108 Chains=1 Model-map CC=0.67 (Build_1.pdb)
Pause
Abort
View log
1 job(s) running
Project: p9-build_0

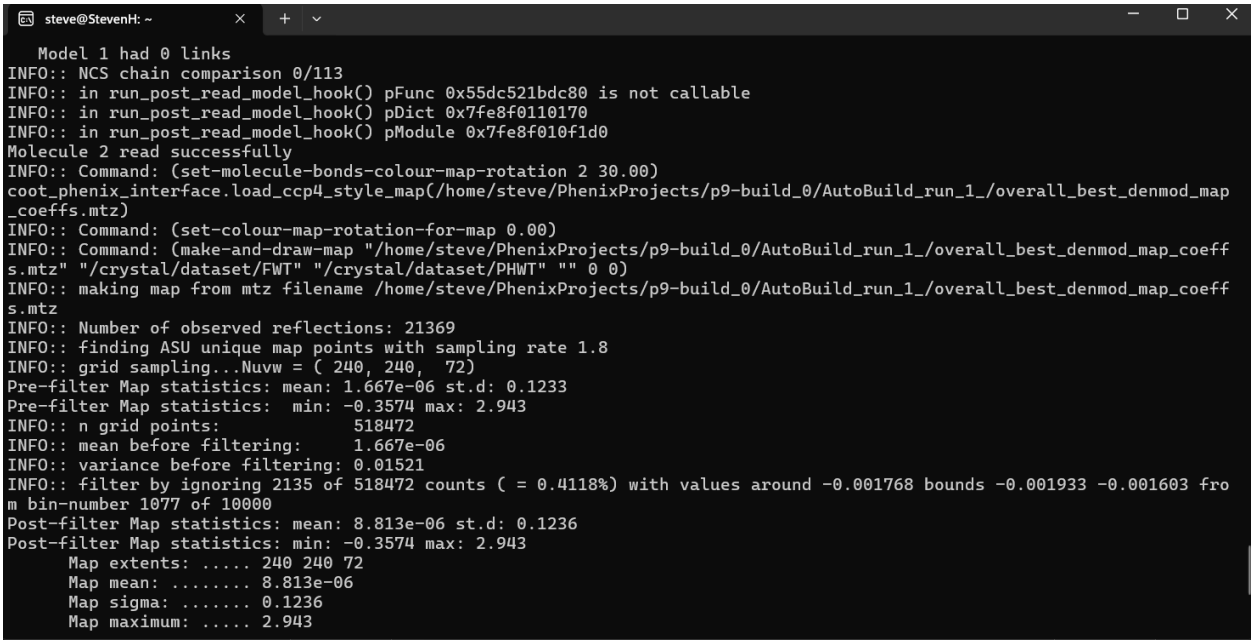

AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary Model-building Structure status
Wizard status
Running...
Log output
'refinement.output.export_final_f_model=True'
Moving refinement file AutoBuild_run_1_/TEMP0/refine_1_001_f_model.mtz to AutoBuild_run_1_/TEMP0/
refine_f_model.mtz
Moving refinement file AutoBuild_run_1_/TEMP0/refine_1_001.mtz to AutoBuild_run_1_/TEMP0/
refine_map_coeffs_1.mtz
Model: AutoBuild_run_1_/TEMP0/refine_1.pdb R/Rfree=0.28/0.30
Maps from refinement will be filled (2FOFCWT PH2FOFCWT)
Set refine map coeffs file best_refine_map_coeffs to refine_map_coeffs_1.mtz
Model completion cycle 1
Models to combine and extend: ['starting_model.pdb', 'Build_1.pdb', 'refine_1.pdb']
Model 2: Residues built=121 placed=113 Chains=1 Model-map CC=0.80 (Build_combine_extend_2.pdb)
Pause
Abort
View log
1 job(s) running
Project: p9-build_0


AutoBuild (Project: p9-build_0)
File Actions Settings Utilities Help
Preferences Help Run Abort Save Xtriage Coot PyMOL Help
Configure AutoBuild_run_1_
Status Summary Model-building Structure status
Wizard status
FINISHED
Log output
'cycle_best_1.log_refine', 'helices_only_model.log', 'hires_PHX.mtz',
'working_best_refine_map_coeffs.mtz', 'title.dat', 'working_best.log', 'helices_only_model.pdb',
'aniso_data_PHX.mtz', 'refinement_PHX.mtz_xtriage_graphs.log', 'AutoBuild_run_1_1.log',
'cycle_best_1.mtz', 'exptl_phases_for_dm_aniso.mtz', 'working_best.log_eval', 'working_best_placed.pdb',
'cycle_best_3.mtz', 'cycle_best_3.log_eval', 'refinement_PHX.mtz_xtriage.log.pkl',
'cycle_best_3.log_refine', 'AutoBuild_Facts.dat', 'cycle_best_3.log', 'refinement_PHX.mtz',
'cycle_best_1.log_eval', 'cycle_best_1.log', 'working_best.pdb', 'cycle_best_3.log_denmod',
'AutoBuild.inp', 'seq_from_file.dat', 'cycle_best_refine_map_coeffs_1.mtz', 'cycle_best_3.pdb',
'AutoBuild_summary.dat', 'exptl_fobs_phases_freeR_flags.mtz', 'cycle_best_1.pdb',
'working_best_denmod_map_coeffs.mtz', 'AutoBuild_warnings.dat', 'refinement_PHX.mtz_xtriage.log']) to
AutoBuild_run_1_/working_files
Done cleaning up ...
Pause Abort View log
Idle
Project: p9-build_0



If you would like to, you can try phenix.refine as well (to test Coot further)

As we can see though, there were those errors that happened when clicking in PHENIX, but no errors when we were running coot:



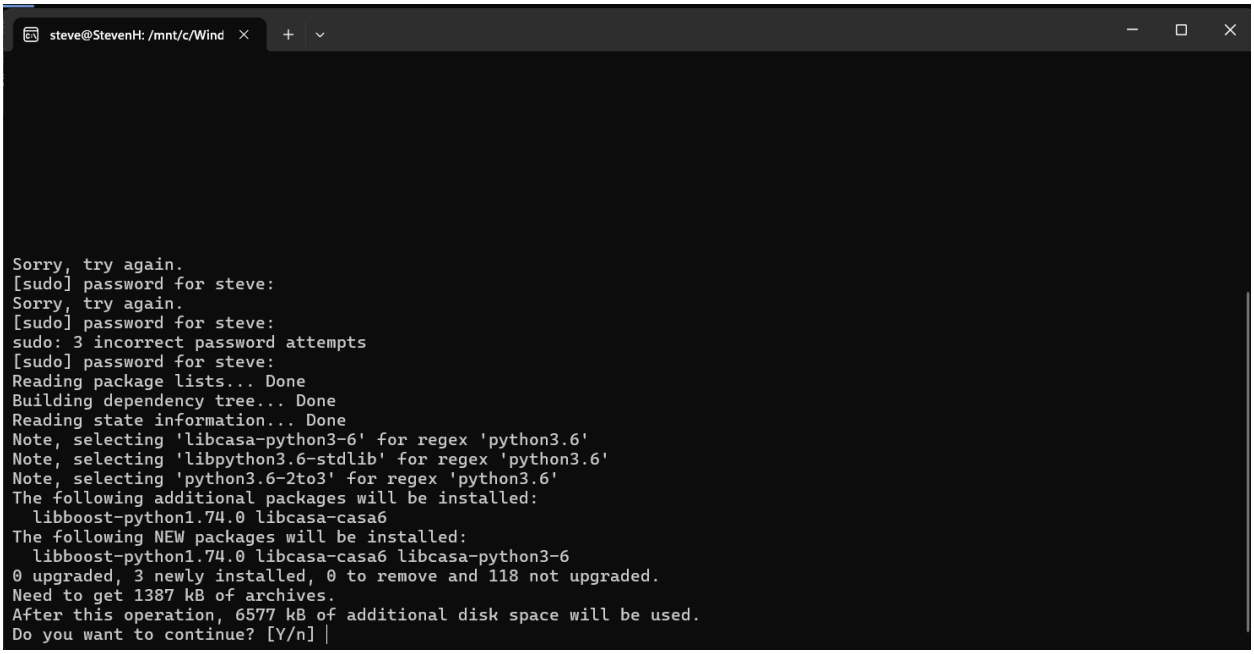
So, to fix this, let us see if downloading python3 will fix the PHENIX errors (also at this point **nano** already works)

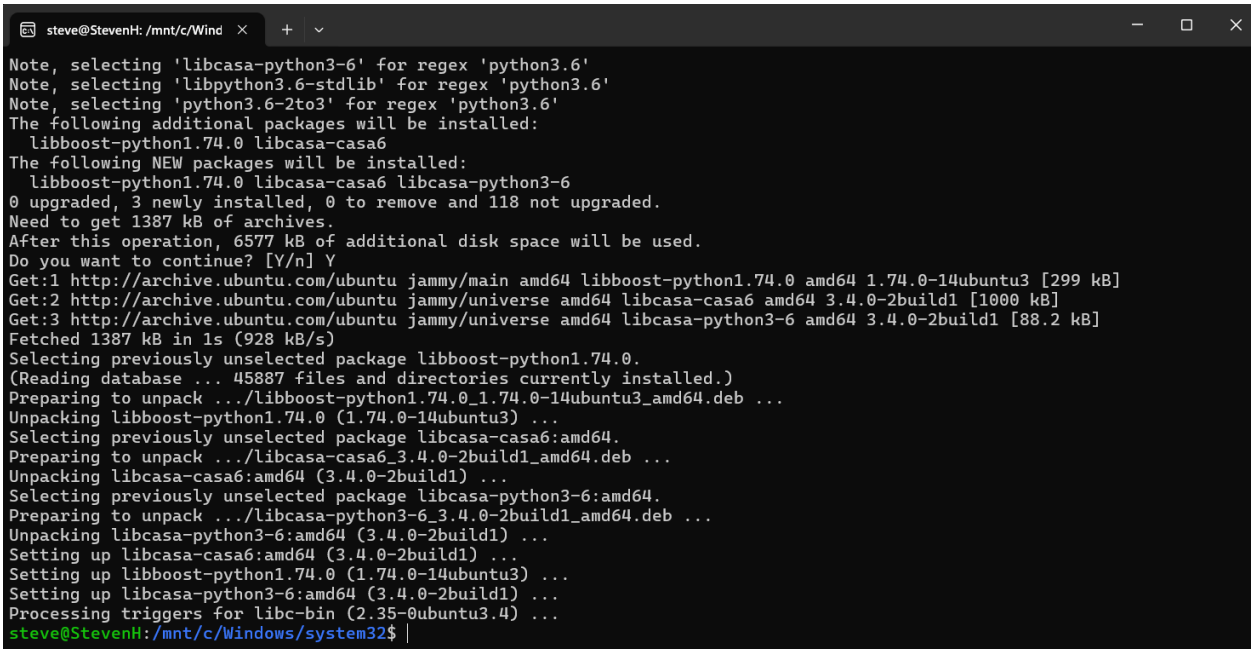
https://docs.python-guide.org/starting/install3/linux/

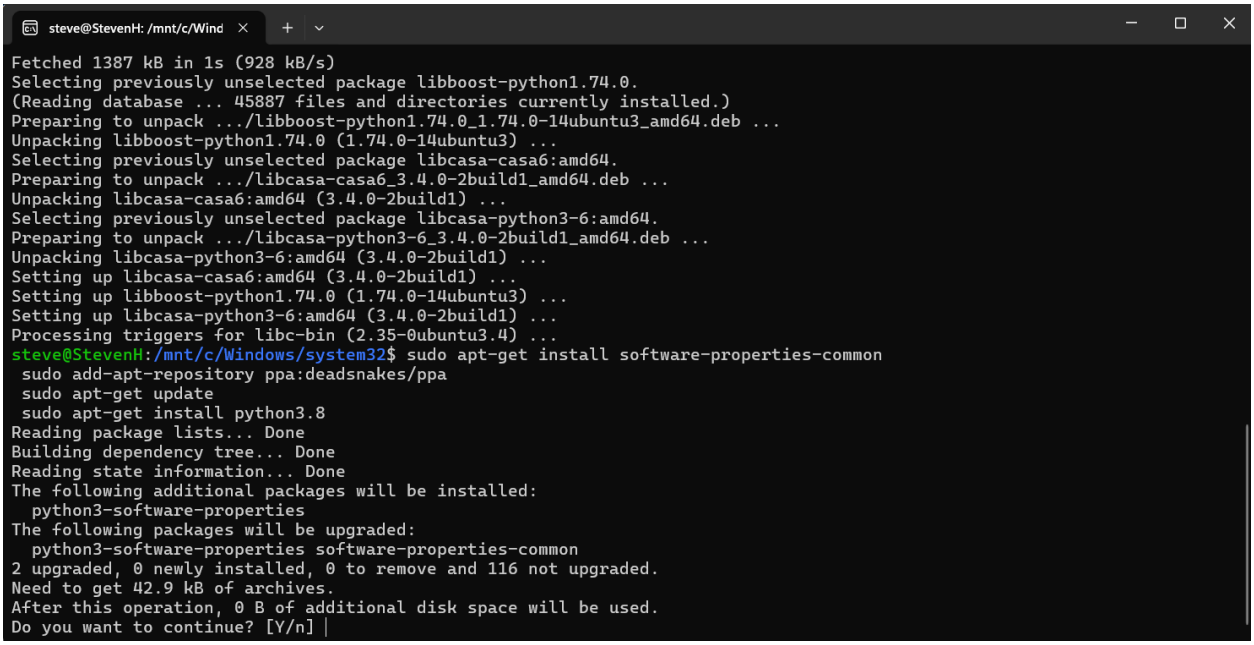
as you can see, it already has python3

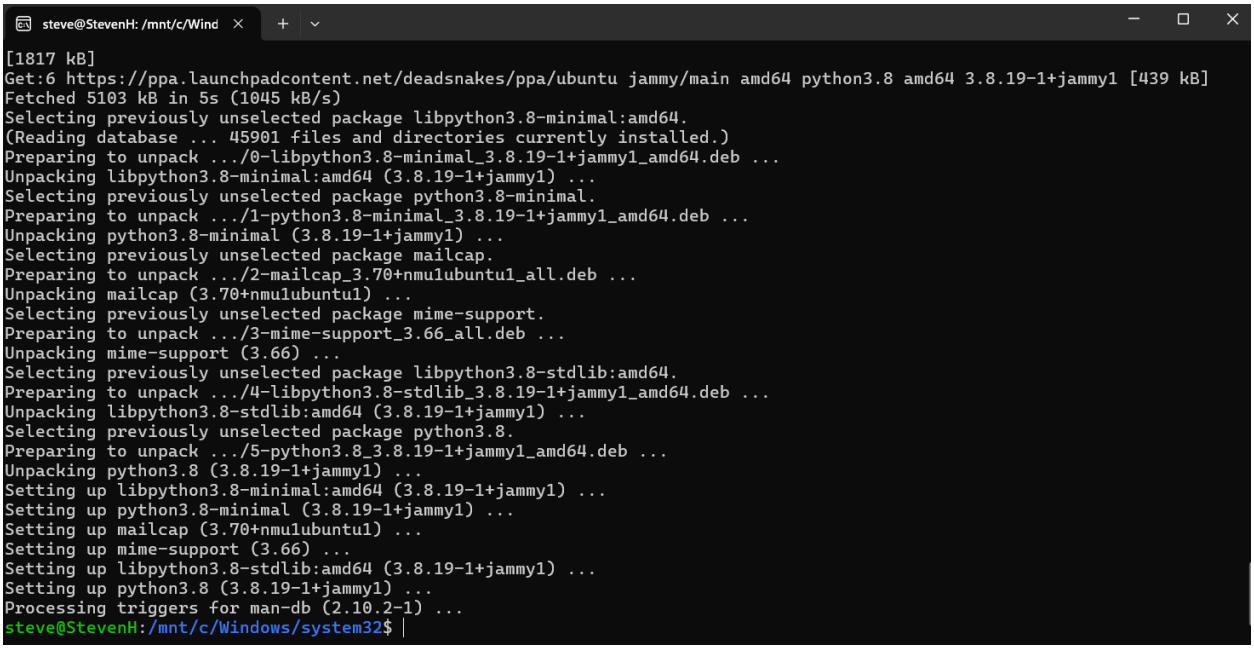
$ sudo apt-get update

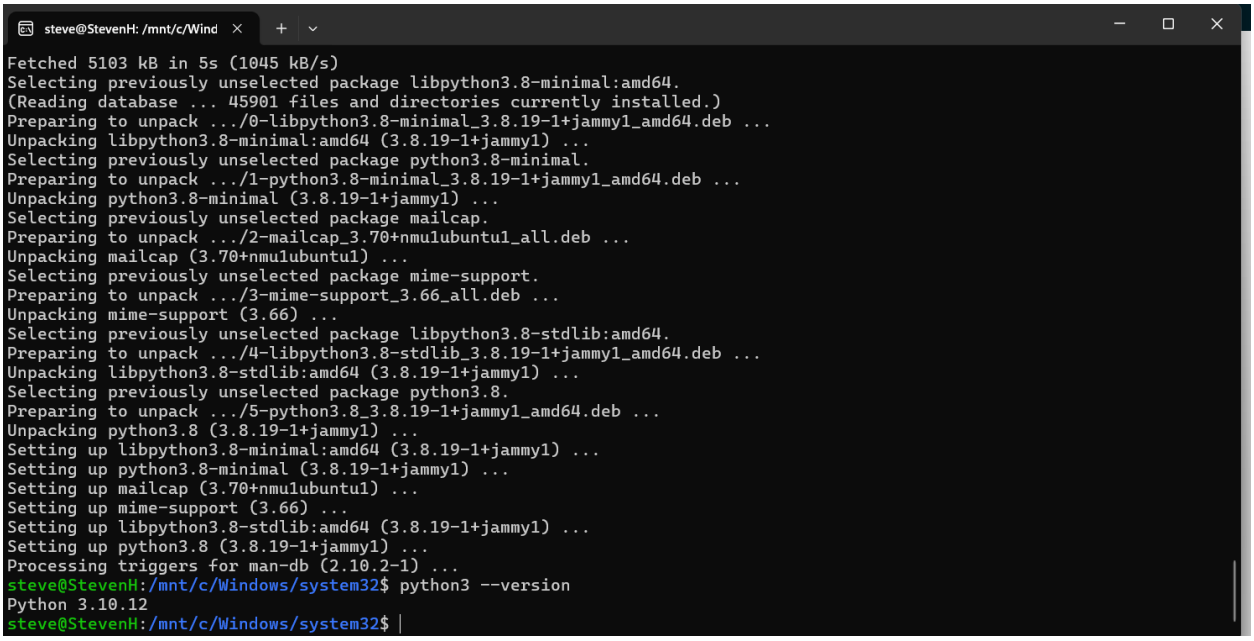
$ sudo apt-get install python3.6


steve@StevenH: /mnt/c/Wind
Sorry, try again.
[sudo] password for steve:
Sorry, try again.
[sudo] password for steve:
sudo: 3 incorrect password attempts
[sudo] password for steve:
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
Note, selecting 'libcasa-python3-6' for regex 'python3.6'
Note, selecting 'libpython3.6-stdlib' for regex 'python3.6'
Note, selecting 'python3.6-2to3' for regex 'python3.6'
The following additional packages will be installed:
libboost-python1.74.0 libcasa-casa6
The following NEW packages will be installed:
libboost-python1.74.0 libcasa-casa6 libcasa-python3-6
0 upgraded, 3 newly installed, 0 to remove and 118 not upgraded.
Need to get 1387 kB of archives.
After this operation, 6577 kB of additional disk space will be used.
Do you want to continue? [Y/n]

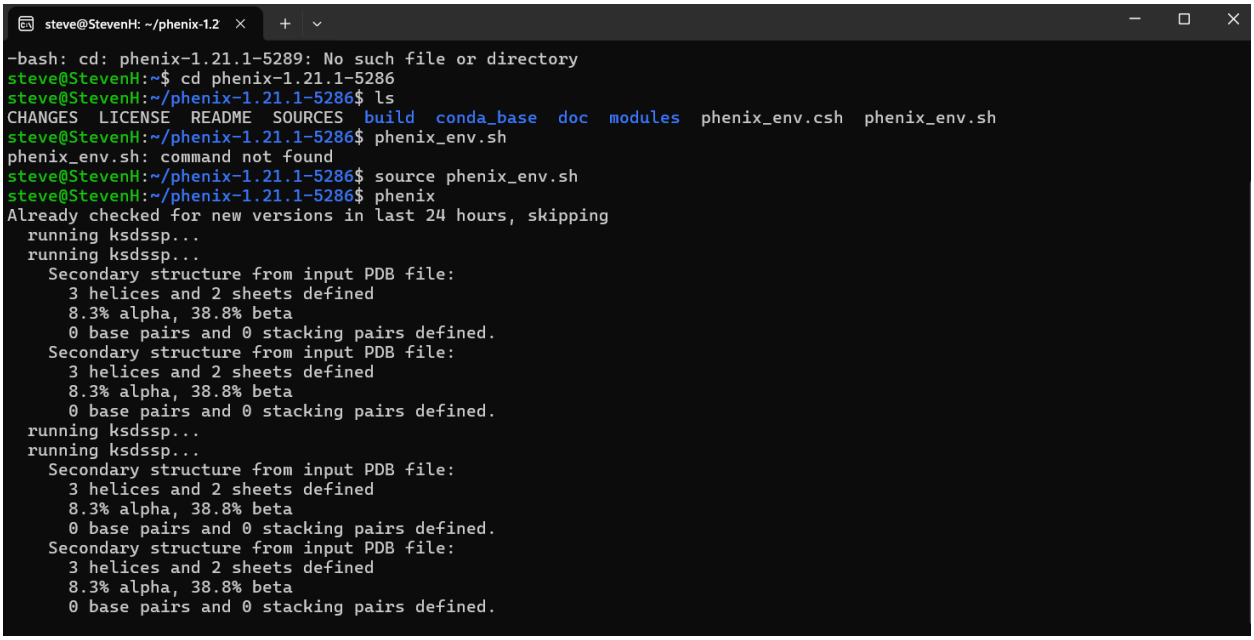

steve@StevenH: /mnt/c/Wind
Note, selecting 'libcasa-python3-6' for regex 'python3.6'
Note, selecting 'libpython3.6-stdlib' for regex 'python3.6'
Note, selecting 'python3.6-2to3' for regex 'python3.6'
The following additional packages will be installed:
libboost-python1.74.0 libcasa-casa6
The following NEW packages will be installed:
libboost-python1.74.0 libcasa-casa6 libcasa-python3-6
0 upgraded, 3 newly installed, 0 to remove and 118 not upgraded.
Need to get 1387 kB of archives.
After this operation, 6577 kB of additional disk space will be used.
Do you want to continue? [Y/n] Y
Get:1 http://archive.ubuntu.com/ubuntu jammy/main amd64 libboost-python1.74.0 amd64 1.74.0-14ubuntu3 [299 kB]
Get:2 http://archive.ubuntu.com/ubuntu jammy/universe amd64 libcasa-casa6 amd64 3.4.0-2build1 [1000 kB]
Get:3 http://archive.ubuntu.com/ubuntu jammy/universe amd64 libcasa-python3-6 amd64 3.4.0-2build1 [88.2 kB]
Fetched 1387 kB in 1s (928 kB/s)
Selecting previously unselected package libboost-python1.74.0.
(Reading database ... 45887 files and directories currently installed.)
Preparing to unpack .../libboost-python1.74.0_1.74.0-14ubuntu3_amd64.deb ...
Unpacking libboost-python1.74.0 (1.74.0-14ubuntu3) ...
Selecting previously unselected package libcasa-casa6:amd64.
Preparing to unpack .../libcasa-casa6_3.4.0-2build1_amd64.deb ...
Unpacking libcasa-casa6:amd64 (3.4.0-2build1) ...
Selecting previously unselected package libcasa-python3-6:amd64.
Preparing to unpack .../libcasa-python3-6_3.4.0-2build1_amd64.deb ...
Unpacking libcasa-python3-6:amd64 (3.4.0-2build1) ...
Setting up libcasa-casa6:amd64 (3.4.0-2build1) ...
Setting up libboost-python1.74.0 (1.74.0-14ubuntu3) ...
Setting up libcasa-python3-6:amd64 (3.4.0-2build1) ...
Processing triggers for libc-bin (2.35-0ubuntu3.4) ...
steve@StevenH:/mnt/c/Windows/system32$


steve@StevenH: /mnt/c/Wind
Fetched 1387 kB in 1s (928 kB/s)
Selecting previously unselected package libboost-python1.74.0.
(Reading database ... 45887 files and directories currently installed.)
Preparing to unpack .../libboost-python1.74.0_1.74.0-14ubuntu3_amd64.deb ...
Unpacking libboost-python1.74.0 (1.74.0-14ubuntu3) ...
Selecting previously unselected package libcasa-casa6:amd64.
Preparing to unpack .../libcasa-casa6_3.4.0-2build1_amd64.deb ...
Unpacking libcasa-casa6:amd64 (3.4.0-2build1) ...
Selecting previously unselected package libcasa-python3-6:amd64.
Preparing to unpack .../libcasa-python3-6_3.4.0-2build1_amd64.deb ...
Unpacking libcasa-python3-6:amd64 (3.4.0-2build1) ...
Setting up libcasa-casa6:amd64 (3.4.0-2build1) ...
Setting up libboost-python1.74.0 (1.74.0-14ubuntu3) ...
Setting up libcasa-python3-6:amd64 (3.4.0-2build1) ...
Processing triggers for libc-bin (2.35-0ubuntu3.4) ...
steve@StevenH:/mnt/c/Windows/system32$ sudo apt-get install software-properties-common
sudo add-apt-repository ppa:deadsnakes/ppa
sudo apt-get update
sudo apt-get install python3.8
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
The following additional packages will be installed:
python3-software-properties
The following packages will be upgraded:
python3-software-properties software-properties-common
2 upgraded, 0 newly installed, 0 to remove and 116 not upgraded.
Need to get 42.9 kB of archives.
After this operation, 0 B of additional disk space will be used.
Do you want to continue? [Y/n]

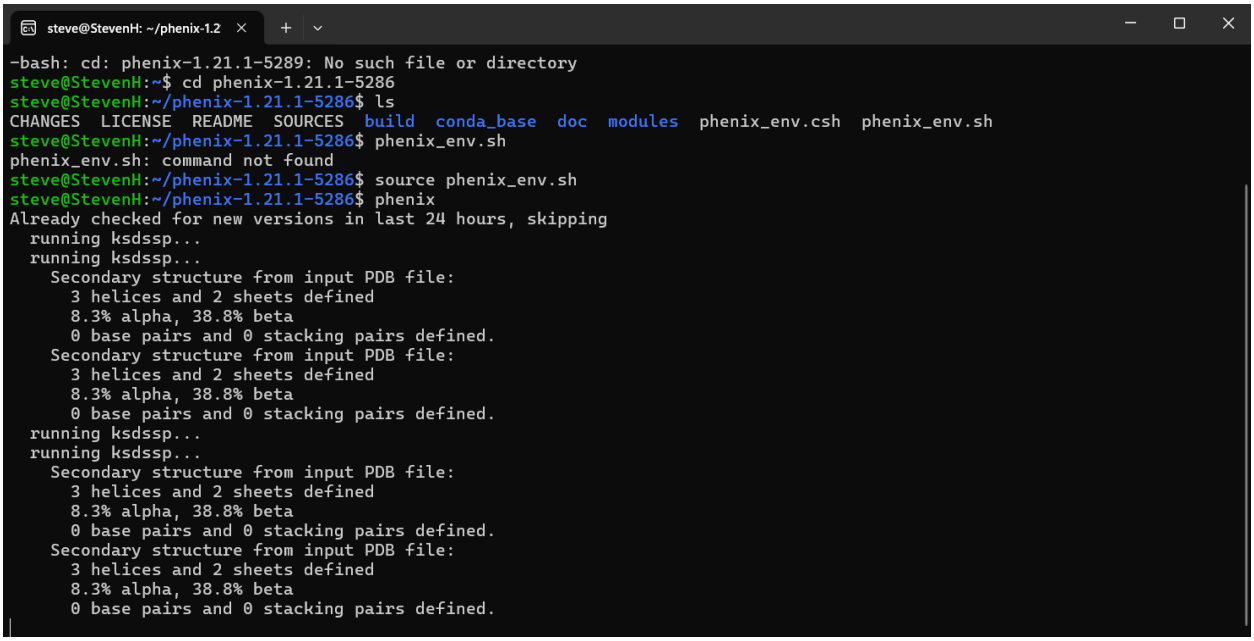

steve@StevenH: /mnt/c/Wind
[1817 kB]
Get:6 https://ppa.launchpadcontent.net/deadsnakes/ppa/ubuntu jammy/main amd64 python3.8 amd64 3.8.19-1+jammy1 [439 kB]
Fetched 5103 kB in 5s (1045 kB/s)
Selecting previously unselected package libpython3.8-minimal:amd64.
(Reading database ... 45901 files and directories currently installed.)
Preparing to unpack .../0-libpython3.8-minimal_3.8.19-1+jammy1_amd64.deb ...
Unpacking libpython3.8-minimal:amd64 (3.8.19-1+jammy1) ...
Selecting previously unselected package python3.8-minimal.
Preparing to unpack .../1-python3.8-minimal_3.8.19-1+jammy1_amd64.deb ...
Unpacking python3.8-minimal (3.8.19-1+jammy1) ...
Selecting previously unselected package mailcap.
Preparing to unpack .../2-mailcap_3.70+nmu1ubuntu1_all.deb ...
Unpacking mailcap (3.70+nmu1ubuntu1) ...
Selecting previously unselected package mime-support.
Preparing to unpack .../3-mime-support_3.66_all.deb ...
Unpacking mime-support (3.66) ...
Selecting previously unselected package libpython3.8-stdlib:amd64.
Preparing to unpack .../4-libpython3.8-stdlib_3.8.19-1+jammy1_amd64.deb ...
Unpacking libpython3.8-stdlib:amd64 (3.8.19-1+jammy1) ...
Selecting previously unselected package python3.8.
Preparing to unpack .../5-python3.8_3.8.19-1+jammy1_amd64.deb ...
Unpacking python3.8 (3.8.19-1+jammy1) ...
Setting up libpython3.8-minimal:amd64 (3.8.19-1+jammy1) ...
Setting up python3.8-minimal (3.8.19-1+jammy1) ...
Setting up mailcap (3.70+nmu1ubuntu1) ...
Setting up mime-support (3.66) ...
Setting up libpython3.8-stdlib:amd64 (3.8.19-1+jammy1) ...
Setting up python3.8 (3.8.19-1+jammy1) ...
Processing triggers for man-db (2.10.2-1) ...
steve@StevenH:/mnt/c/Windows/system32$



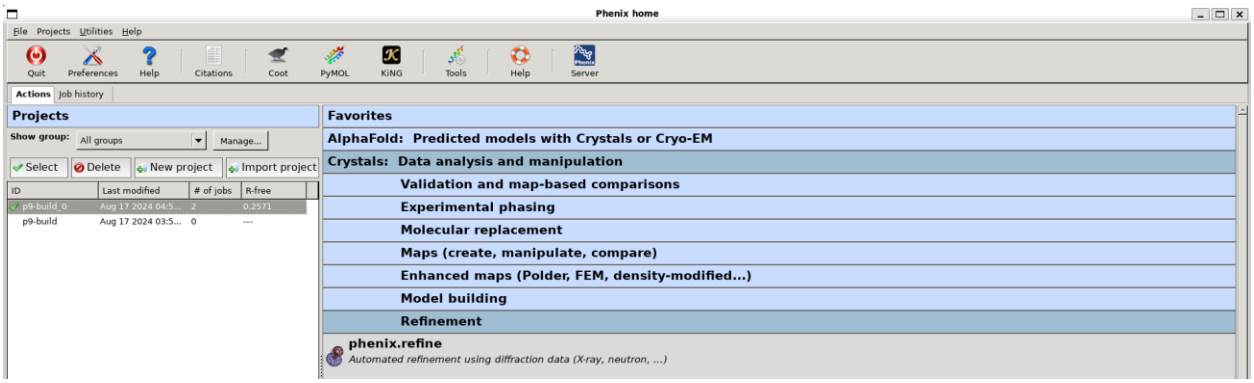
So now let us try doing the same p9 and see if the errors are still there:

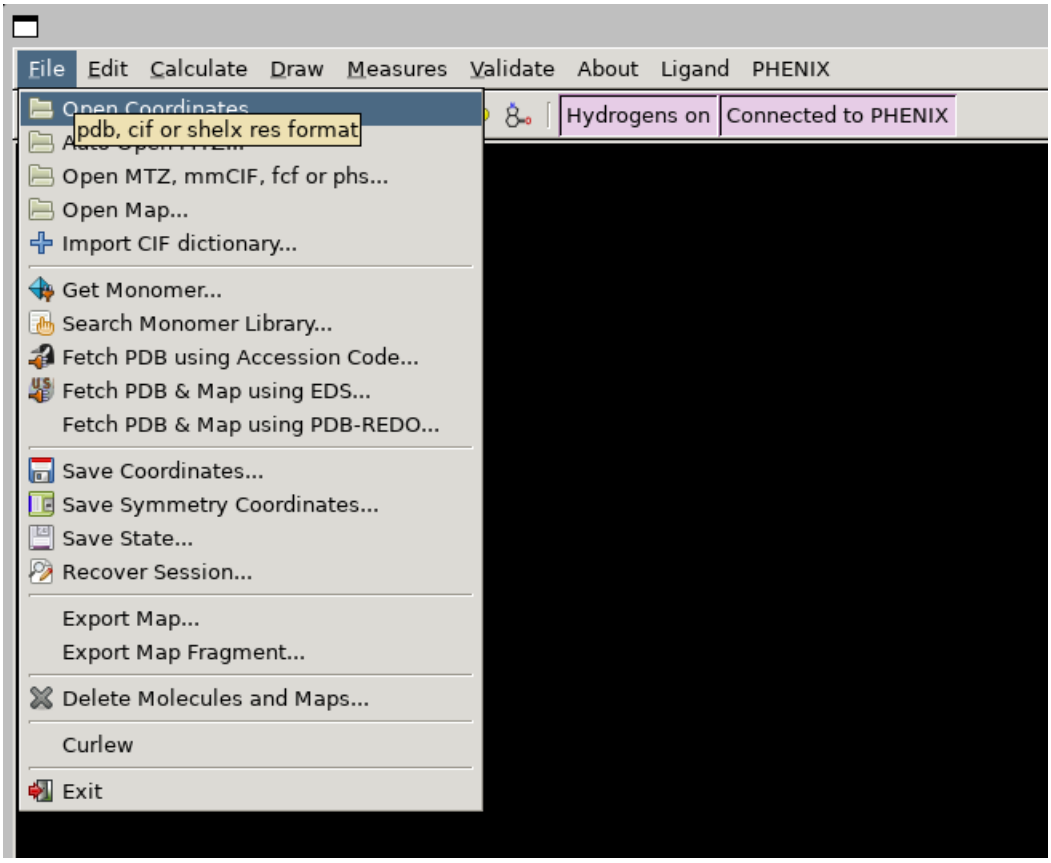


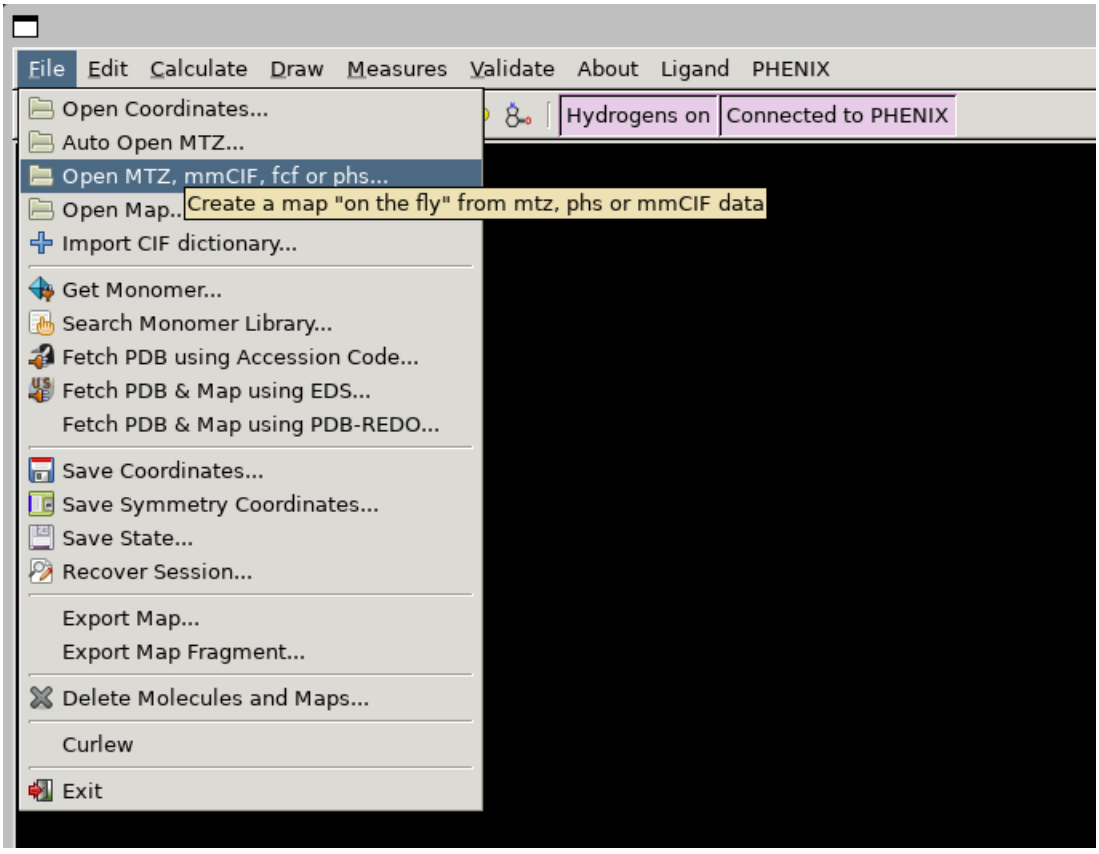
Now there are no more errors!!

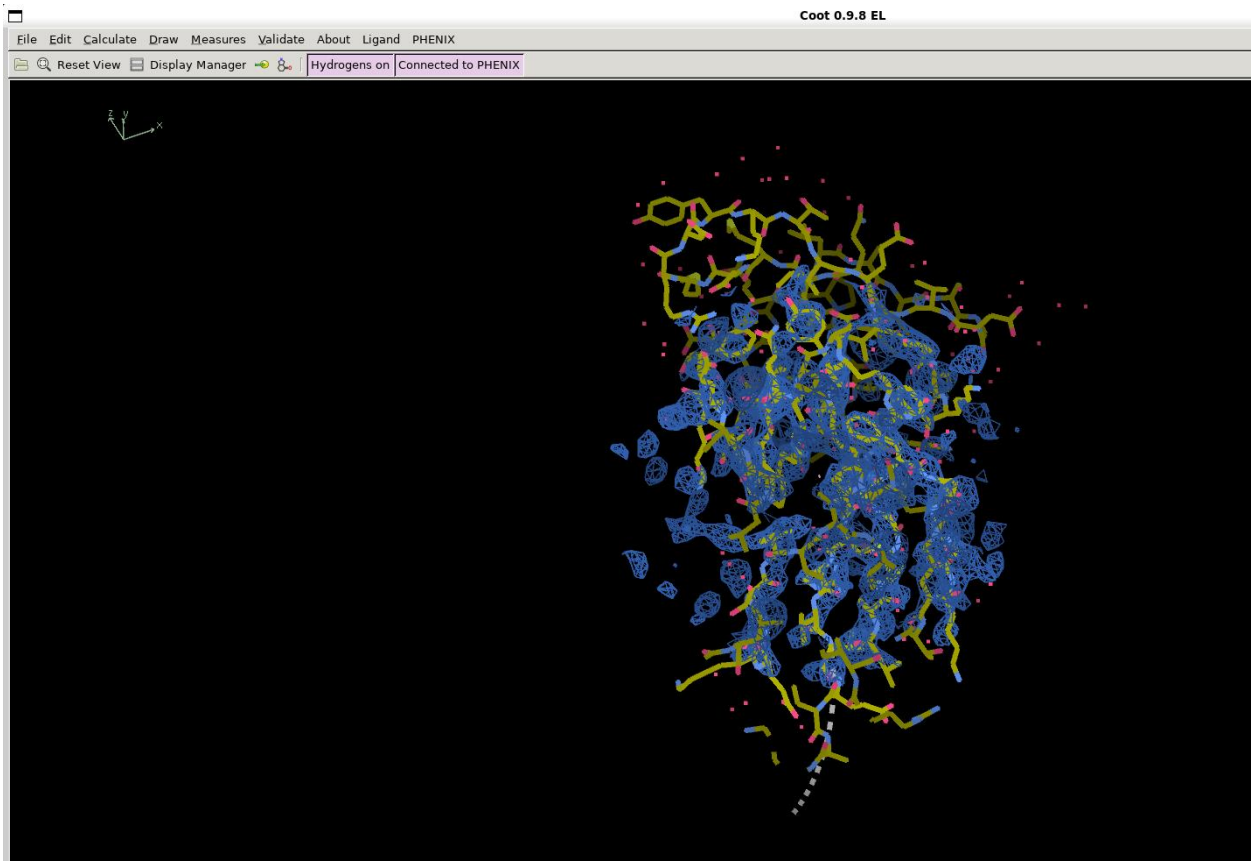


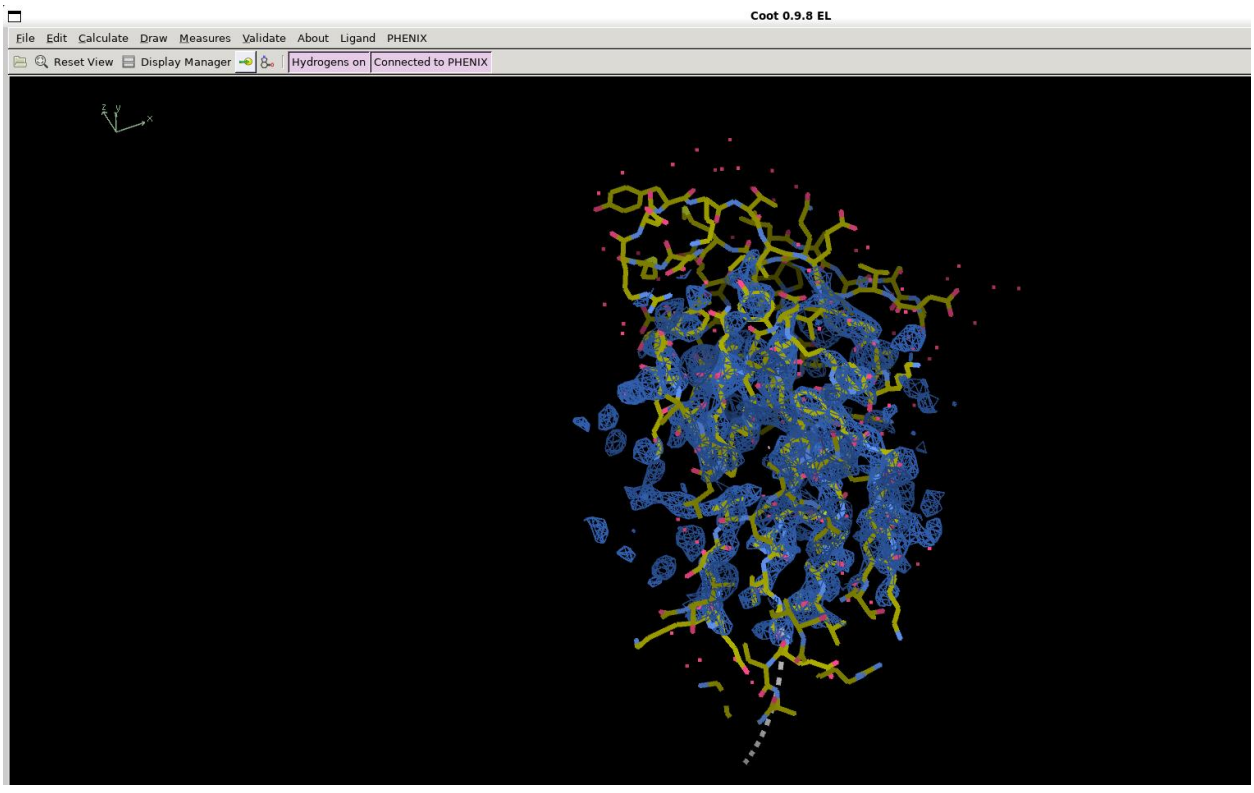
To check if Coot is running fine, you can take the p9 build and run .refine:

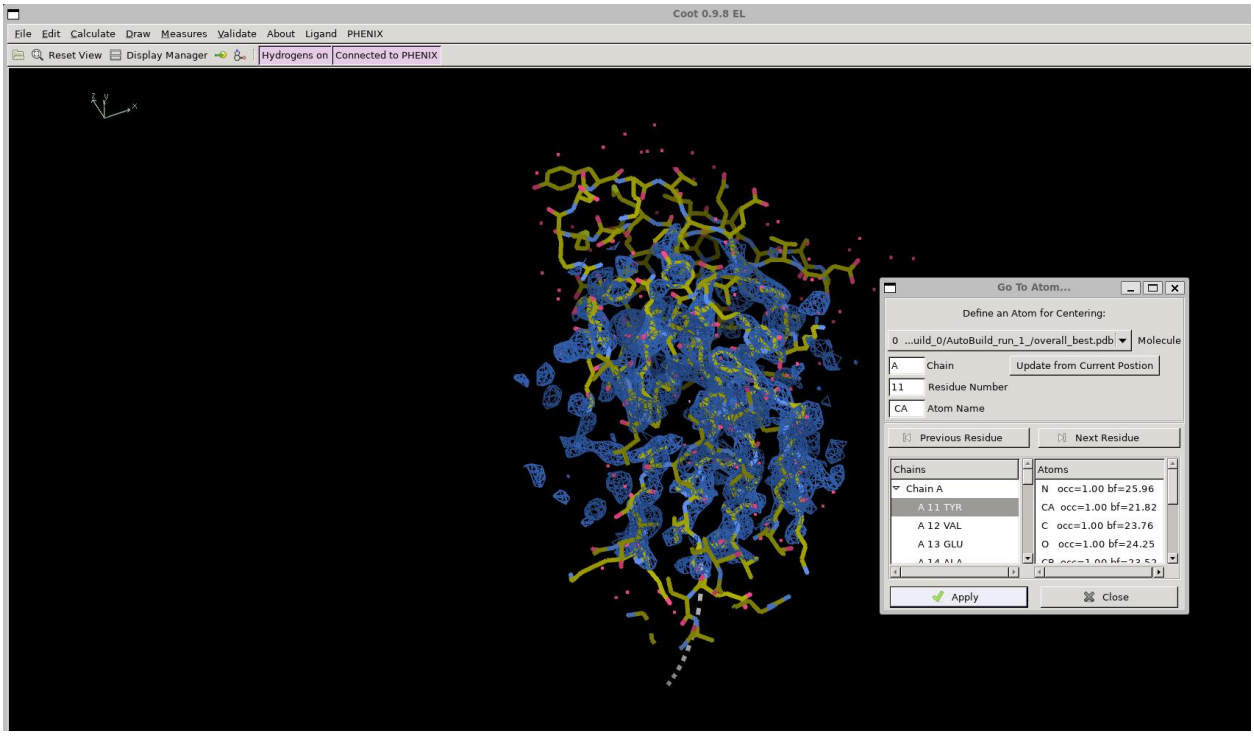



File Edit Calculate Draw Measures Validate About Ligand PHENIX
Open Coordinates
pdb, cif or shelx res format
Open MTZ, mmCIF, fcf or phs...
Open Map...
Import CIF dictionary...
Get Monomer...
Search Monomer Library...
Fetch PDB using Accession Code...
Fetch PDB & Map using EDS...
Fetch PDB & Map using PDB-REDO...
Save Coordinates...
Save Symmetry Coordinates...
Save State...
Recover Session...
Export Map...
Export Map Fragment...
Delete Molecules and Maps...
Curlew
Exit
Hydrogens on
Connected to PHENIX


File Edit Calculate Draw Measures Validate About Ligand PHENIX
Open Coordinates...
Auto Open MTZ...
Open MTZ, mmCIF, fcf or phs...
Open Map...
Create a map "on the fly" from mtz, phs or mmCIF data
Import CIF dictionary...
Get Monomer...
Search Monomer Library...
Fetch PDB using Accession Code...
Fetch PDB & Map using EDS...
Fetch PDB & Map using PDB-REDO...
Save Coordinates...
Save Symmetry Coordinates...
Save State...
Recover Session...
Export Map...
Export Map Fragment...
Delete Molecules and Maps...
Curlew
Exit
Hydrogens on
Connected to PHENIX


Coot 0.9.8 EL
File Edit Calculate Draw Measures Validate About Ligand PHENIX
Reset View
Display Manager
Hydrogens on
Connected to PHENIX


Coot 0.9.8 EL
File Edit Calculate Draw Measures Validate About Ligand PHENIX
Reset View
Display Manager
Hydrogens on
Connected to PHENIX



If you press space and you can go from amino acid to amino acid, then that means Coot is successfully working!

And no more errors in the terminal for PHENIX!!

```
steve@StevenH: ~/phenix-1.2
phenix_env.sh: command not found
steve@StevenH:~/phenix-1.21.1-5286$ source phenix_env.sh
steve@StevenH:~/phenix-1.21.1-5286$ phenix
Already checked for new versions in last 24 hours, skipping
  running ksdssp...
  running ksdssp...
    Secondary structure from input PDB file:
      3 helices and 2 sheets defined
      8.3% alpha, 38.8% beta
      0 base pairs and 0 stacking pairs defined.
    Secondary structure from input PDB file:
      3 helices and 2 sheets defined
      8.3% alpha, 38.8% beta
      0 base pairs and 0 stacking pairs defined.
  running ksdssp...
  running ksdssp...
    Secondary structure from input PDB file:
      3 helices and 2 sheets defined
      8.3% alpha, 38.8% beta
      0 base pairs and 0 stacking pairs defined.
    Secondary structure from input PDB file:
      3 helices and 2 sheets defined
      8.3% alpha, 38.8% beta
      0 base pairs and 0 stacking pairs defined.
There are 143 data in /home/steve/coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python/share/coot/lib/data/monomers/list/mon_lib
_list.cif
There are 2 data in /home/steve/coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python/share/coot/lib/data/monomers/a/ALA.cif
There are 2 data in /home/steve/coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python/share/coot/lib/data/monomers/a/ASP.cif
There are 2 data in /home/steve/coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python/share/coot/lib/data/monomers/a/ASN.cif
There are 2 data in /home/steve/coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python/share/coot/lib/data/monomers/c/CYS.cif
```

Congratulations you have successfully download PHENIX and Coot!!!!