

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)

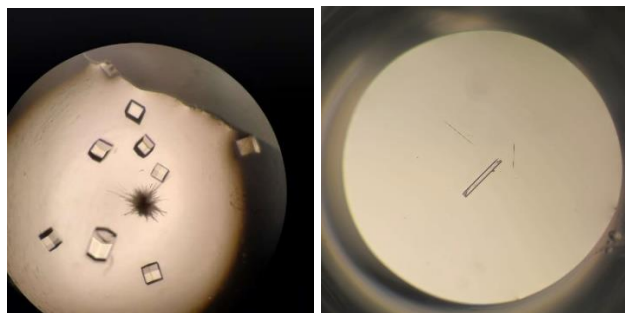


Figure 2. Left photo: lysozyme crystals grown for a STARS experiment (week 7, set up on March 14, 2024 by Susanna). Right photo: DNA crystals (CGCGCG) grown for an outside project (set up on 7/5/2024 and checked on 8/5/2024 by Susanna).

3. Crystal harvesting and diffraction of crystals

- 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

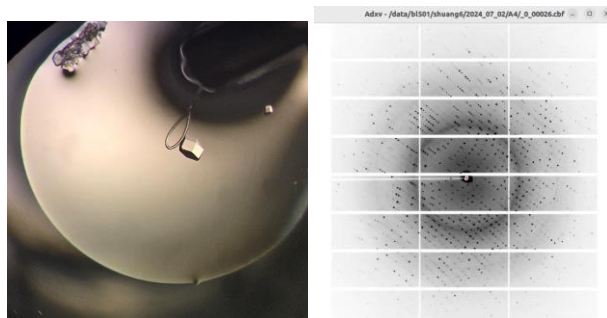


Figure 3. Left photo: a lysozyme crystal being harvested onto a loop. Right photo: An example of good lysozyme diffraction data (one snap) from a different lysozyme crystal. (photo credit: Susanna Huang with the support of LBNL)

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

- 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

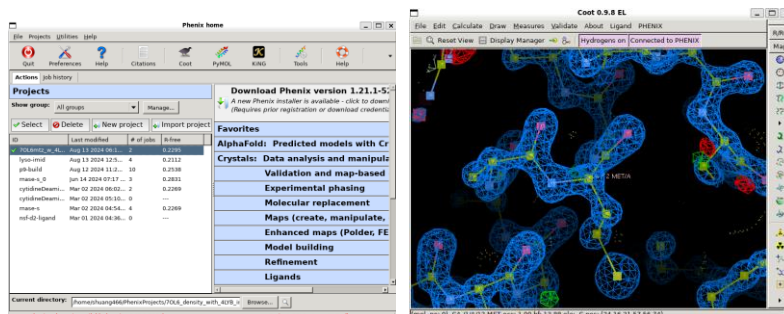


Figure 4. Left photo: Example of PHENIX GUI interface. Right photo: Example of Coot GUI interface, specifically for a 12-position methionine residue on lysozyme. (Susanna Huang)

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 SIGNIFICANCE

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:

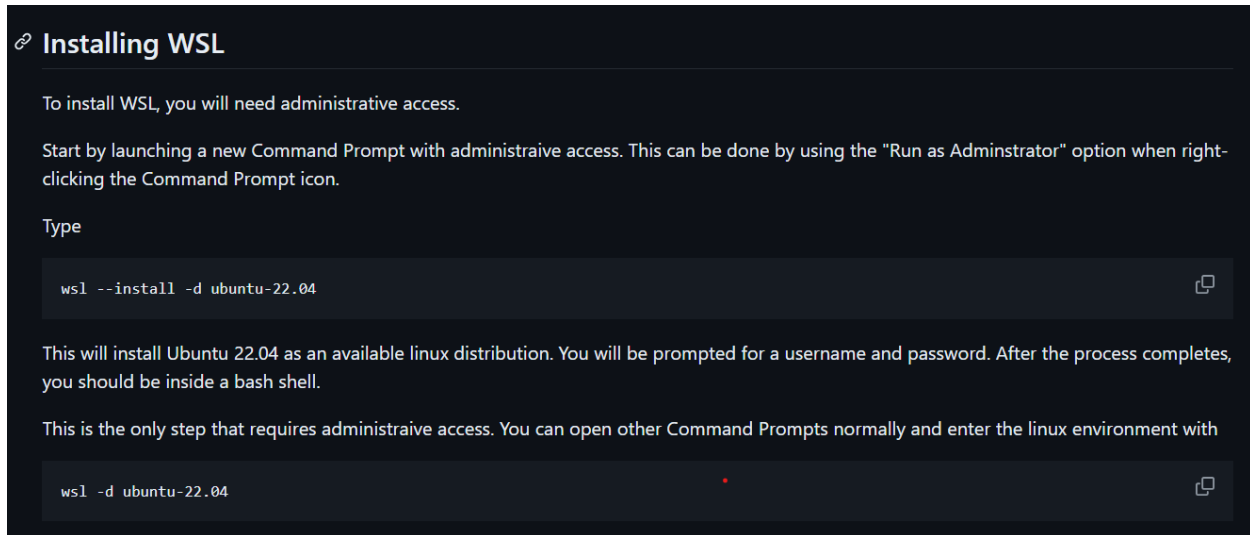
[Phenix Documentation \(phenix-online.org\)](https://phenix-online.org/)

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):



Installing WSL

To install WSL, you will need administrative access.

Start by launching a new Command Prompt with administrative access. This can be done by using the "Run as Administrator" option when right-clicking the Command Prompt icon.

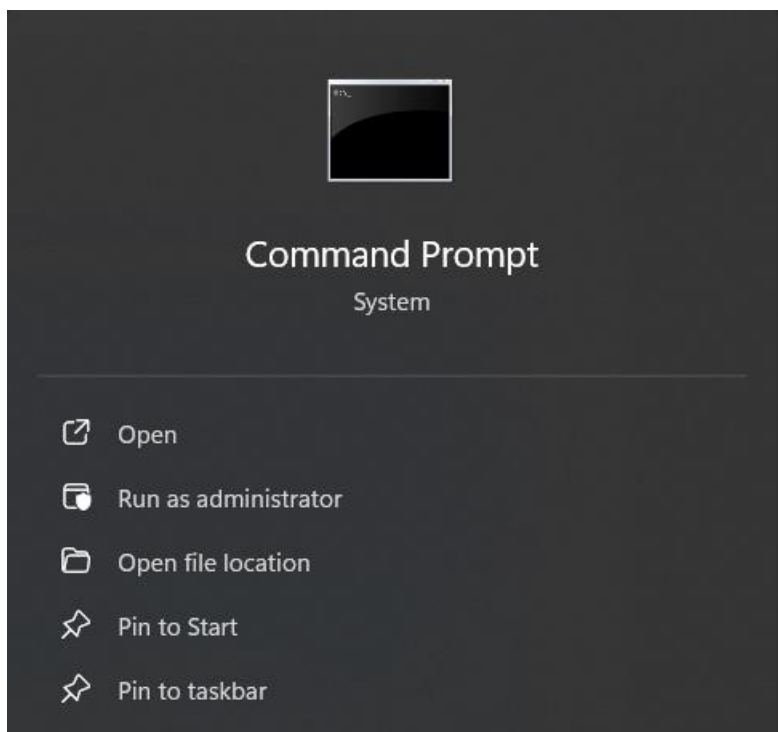
Type

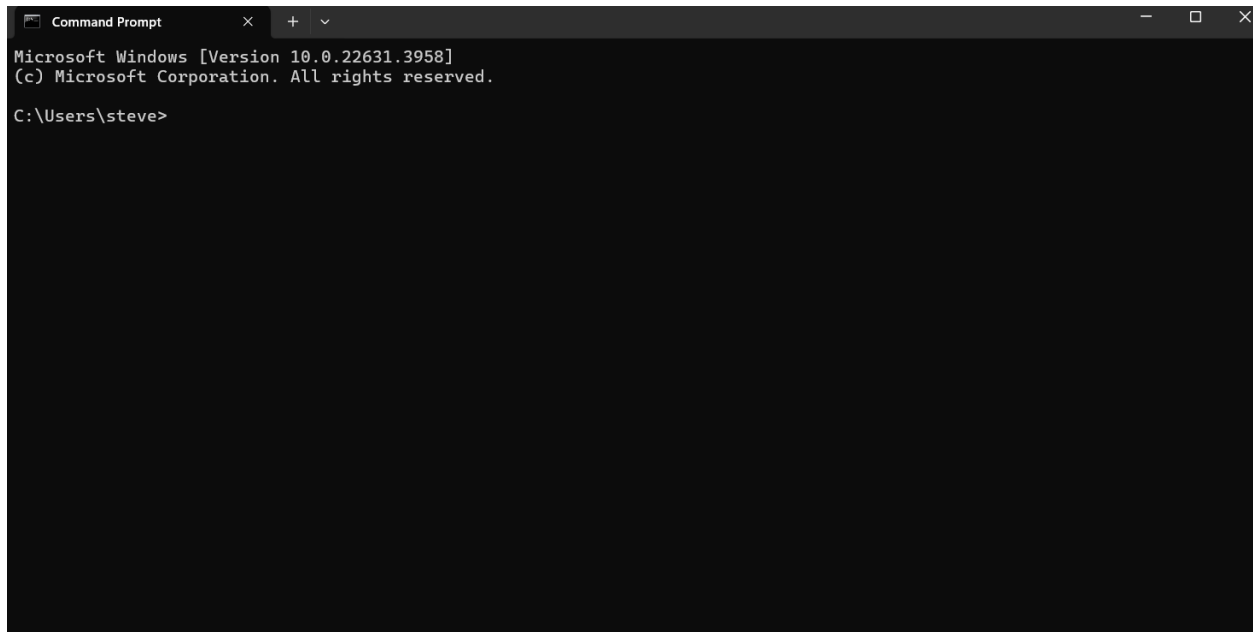
```
ws1 --install -d ubuntu-22.04
```

This will install Ubuntu 22.04 as an available linux distribution. You will be prompted for a username and password. After the process completes, you should be inside a bash shell.

This is the only step that requires administrative access. You can open other Command Prompts normally and enter the linux environment with

```
ws1 -d ubuntu-22.04
```

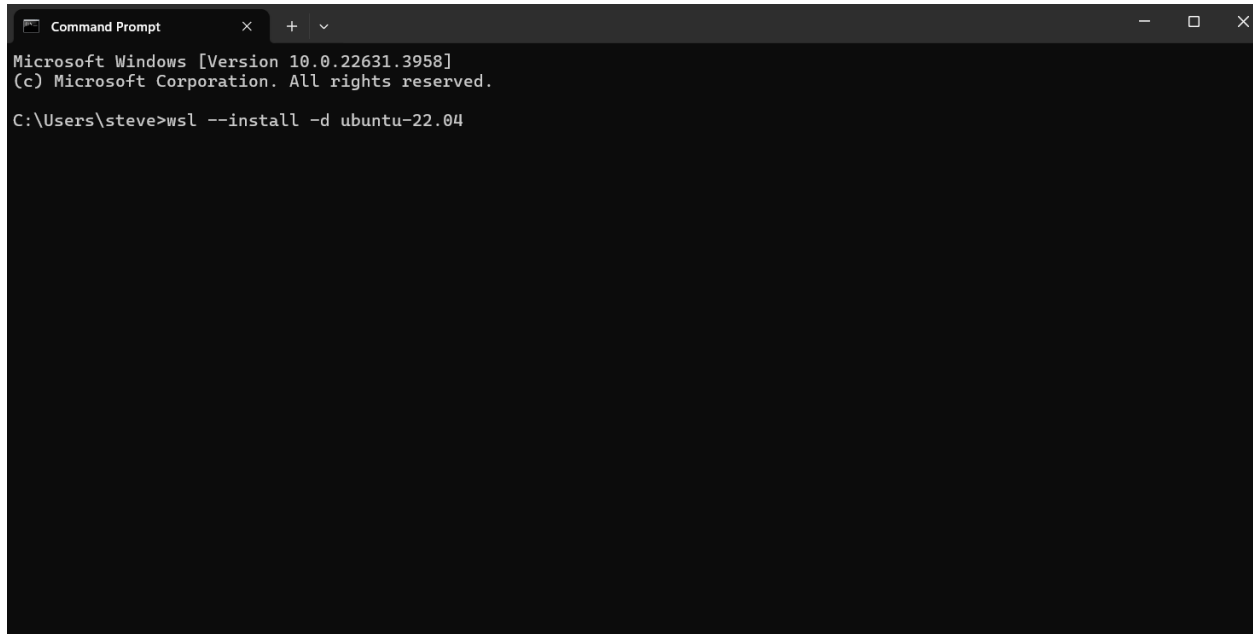




```
Command Prompt
Microsoft Windows [Version 10.0.22631.3958]
(c) Microsoft Corporation. All rights reserved.

C:\Users\steve>
```

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



```
Command Prompt
Microsoft Windows [Version 10.0.22631.3958]
(c) Microsoft Corporation. All rights reserved.

C:\Users\steve>wsl --install -d ubuntu-22.04
```

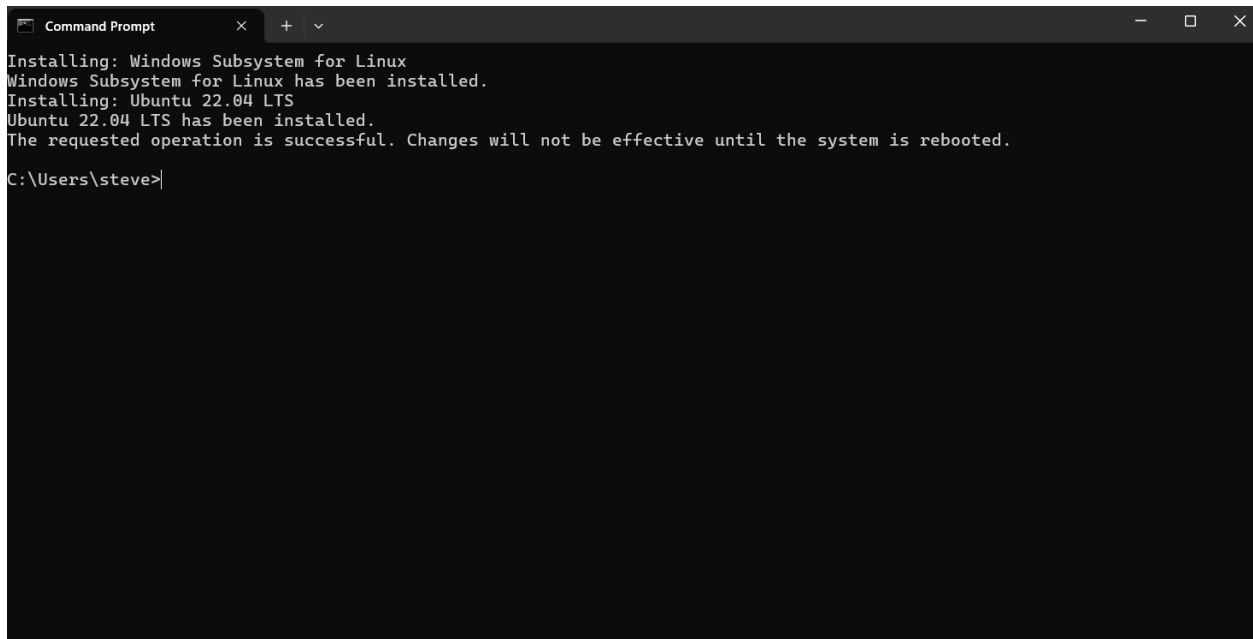
This will be Windows Subsystem for Linux, as the host process for Linux service on Windows.

```
C:\Windows\system32\wsl.exe x + v
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 x + v
Microsoft Windows [Version 10.0.22631.3958]
(c) Microsoft Corporation. All rights reserved.

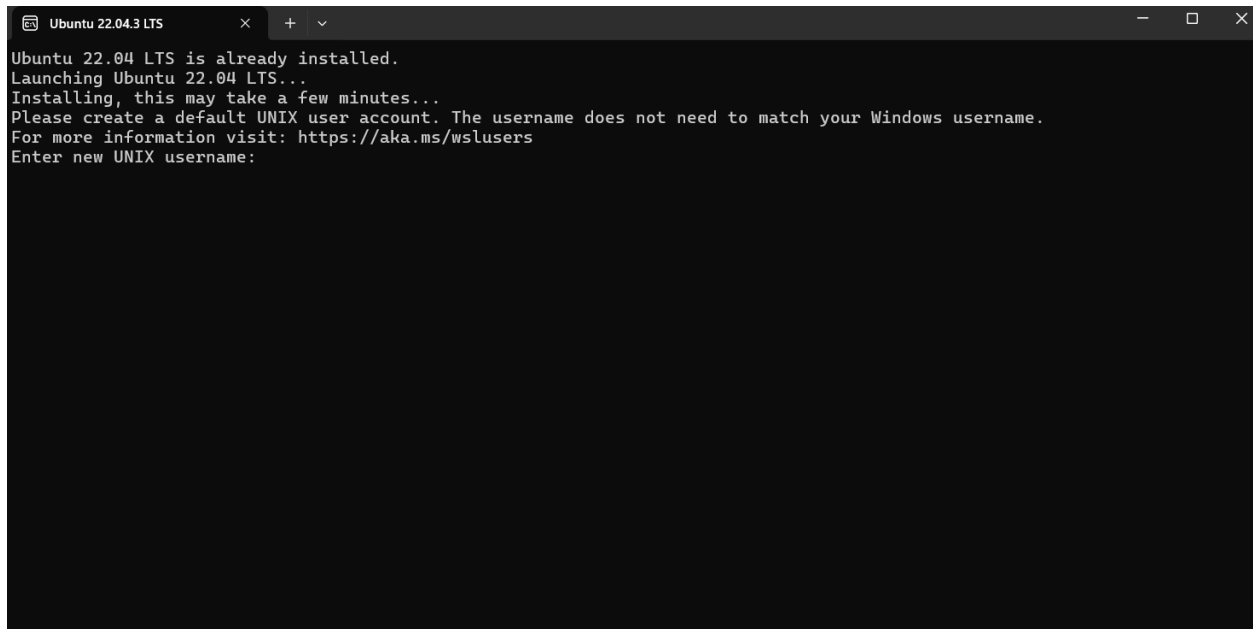
C:\Users\steve>wsl --install -d ubuntu-22.04
The requested operation requires elevation.
Installing: Windows Subsystem for Linux
Windows Subsystem for Linux has been installed.
Installing: Ubuntu 22.04 LTS
[=====56.0%] ]
```

```
Command Prompt
Installing: Windows Subsystem for Linux
Windows Subsystem for Linux has been installed.
Installing: Ubuntu 22.04 LTS
Ubuntu 22.04 LTS has been installed.
The requested operation is successful. Changes will not be effective until the system is rebooted.

C:\Users\steve>
```

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).



```
Ubuntu 22.04.3 LTS
Ubuntu 22.04 LTS is already installed.
Launching Ubuntu 22.04 LTS...
Installing, this may take a few minutes...
Please create a default UNIX user account. The username does not need to match your Windows username.
For more information visit: https://aka.ms/wslusers
Enter new UNIX username:
```

```
Ubuntu 22.04.3 LTS
Ubuntu 22.04 LTS is already installed.
Launching Ubuntu 22.04 LTS...
Installing, this may take a few minutes...
Please create a default UNIX user account. The username does not need to match your Windows username.
For more information visit: https://aka.ms/wslusers
Enter new UNIX username: Steve
```

Click enter

Lower case letters only

```
Ubuntu 22.04.3 LTS
Ubuntu 22.04 LTS is already installed.
Launching Ubuntu 22.04 LTS...
Installing, this may take a few minutes...
Please create a default UNIX user account. The username does not need to match your Windows username.
For more information visit: https://aka.ms/wslusers
Enter new UNIX username: Steve
adduser: Please enter a username matching the regular expression configured
via the NAME_REGEX[_SYSTEM] configuration variable. Use the '--force-badname'
option to relax this check or reconfigure NAME_REGEX.
Enter new UNIX username: steve
```

Click enter

```
Ubuntu 22.04.3 LTS
Ubuntu 22.04 LTS is already installed.
Launching Ubuntu 22.04 LTS...
Installing, this may take a few minutes...
Please create a default UNIX user account. The username does not need to match your Windows username.
For more information visit: https://aka.ms/wslusers
Enter new UNIX username: Steve
adduser: Please enter a username matching the regular expression configured
via the NAME_REGEX[_SYSTEM] configuration variable. Use the '--force-badname'
option to relax this check or reconfigure NAME_REGEX.
Enter new UNIX username: steve
New password: |
```

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:

```
Ubuntu 22.04.3 LTS
Ubuntu 22.04 LTS is already installed.
Launching Ubuntu 22.04 LTS...
Installing, this may take a few minutes...
Please create a default UNIX user account. The username does not need to match your Windows username.
For more information visit: https://aka.ms/wslusers
Enter new UNIX username: Steve
adduser: Please enter a username matching the regular expression configured
via the NAME_REGEX[_SYSTEM] configuration variable. Use the '--force-badname'
option to relax this check or reconfigure NAME_REGEX.
Enter new UNIX username: steve
New password:
Retype new password: |
```

```
Ubuntu 22.04.3 LTS
Ubuntu 22.04 LTS is already installed.
Launching Ubuntu 22.04 LTS...
Installing, this may take a few minutes...
Please create a default UNIX user account. The username does not need to match your Windows username.
For more information visit: https://aka.ms/wslusers
Enter new UNIX username: Steve
adduser: Please enter a username matching the regular expression configured
via the NAME_REGEX[_SYSTEM] configuration variable. Use the '--force-badname'
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!
```

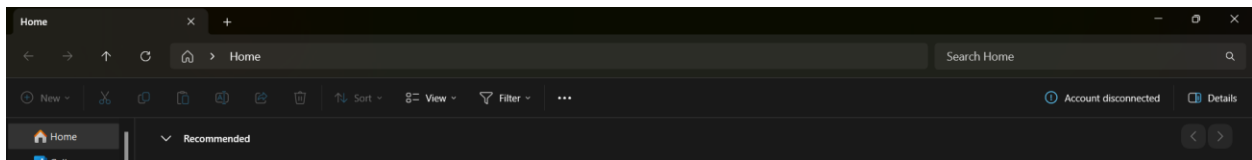
```
steve@StevenH: ~
Ubuntu 22.04 LTS is already installed.
Launching Ubuntu 22.04 LTS...
Installing, this may take a few minutes...
Please create a default UNIX user account. The username does not need to match your Windows username.
For more information visit: https://aka.ms/wslusers
Enter new UNIX username: Steve
adduser: Please enter a username matching the regular expression configured
via the NAME_REGEX[_SYSTEM] configuration variable. Use the '--force-badname'
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.

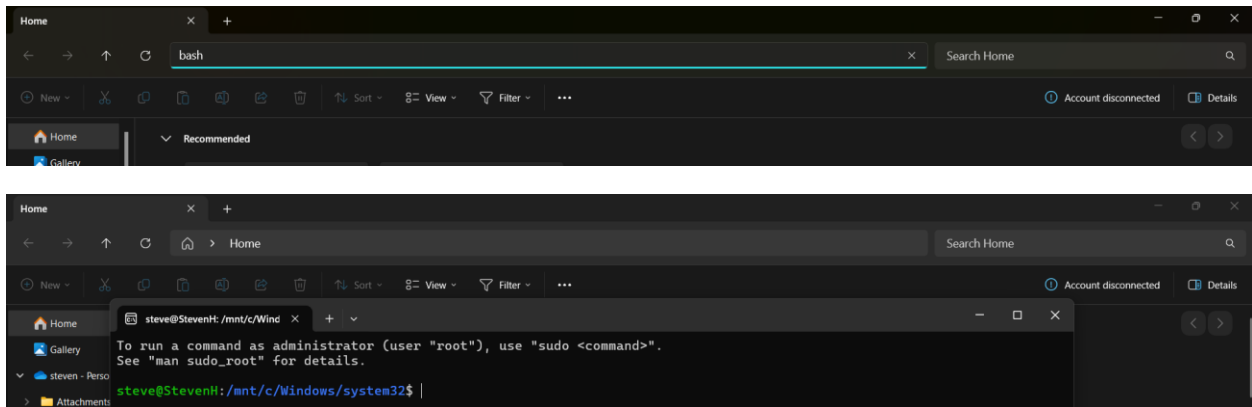
Welcome to Ubuntu 22.04.3 LTS (GNU/Linux 5.15.153.1-microsoft-standard-WSL2 x86_64)

 * Documentation:  https://help.ubuntu.com
 * Management:    https://landscape.canonical.com
 * Support:        https://ubuntu.com/advantage

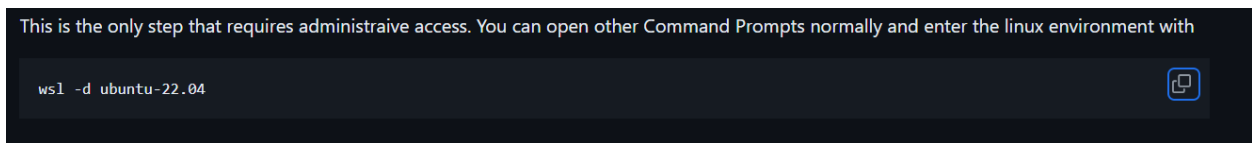
This message is shown once a day. To disable it please create the
/home/steve/.hushlogin file.
steve@StevenH:~$ |
```

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

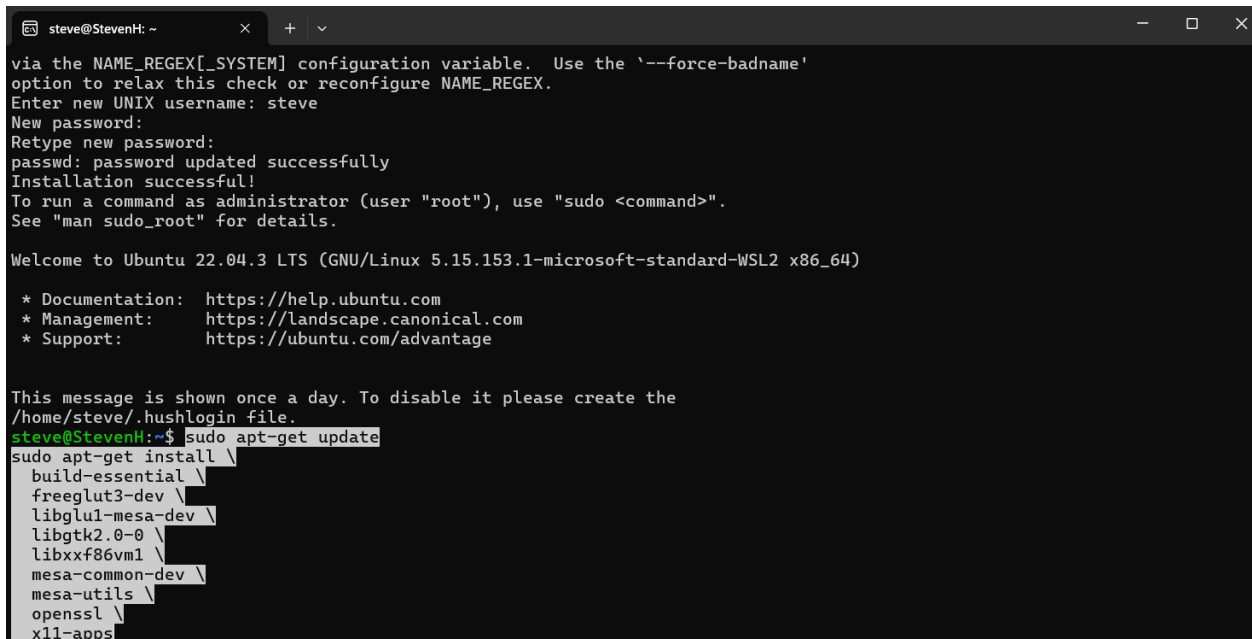




You can also enter by going into the command prompt this way:



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]
Get:10 http://security.ubuntu.com/ubuntu jammy-security/restricted Translation-en [387 kB]
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%]
```

```

steve@StevenH: ~
librsvg2-bin lm-sensors libsm-doc libstdc++-11-doc libx11-doc libxcb-doc libxext-doc libxt-doc make-doc
Recommended packages:
libnss-nis libnss-nisplus
The following NEW packages will be installed:
adwaita-icon-theme build-essential bzip2 cpp cpp-11 dpkg-dev fakeroot fontconfig fontconfig-config fonts-dejavu-core
freeglut3 freeglut3-dev g++ g++-11 gcc gcc-11 gcc-11-base gtk-update-icon-cache hicolor-icon-theme
humanity-icon-theme libalgorithm-diff-perl libalgorithm-diff-xs-perl libalgorithm-merge-perl libasan6 libatk1.0-0
libatk1.0-data libatomic1 libavahi-client3 libavahi-common-data libavahi-common3 libc-dev-bin libc-devtools
libc6-dev libcairo-gobject2 libcairo2 libcc1-0 libcrypt-dev libcups2 libdatrie1 libdeflate0 libdpkg-perl
libdrm-amdgpu1 libdrm-dev libdrm-intel1 libdrm-nouveau2 libdrm-radeon1 libegl-dev libegl-mesa0 libegl1 libfakeroot
libfile-fcntllock-perl libfontconfig1 libfonttype6 libgail-common libgail18 libgbm1 libgcc-11-dev libgd3
libgdk-pixbuf-2.0-0 libgdk-pixbuf2.0-bin libgdk-pixbuf2.0-common libgl-dev libgl1 libgl1-amber-dri libgl1-mesa-dev
libgl1-mesa-dri libglapi-mesa libgles-dev libgles1 libgles2 libglul-mesa libglul-mesa-dev libglvnd-core-dev
libglvnd-dev libglvnd0 libglx-dev libglx-mesa0 libglx0 libgomp1 libgraphite2-3 libgtk2.0-0 libgtk2.0-bin
libgtk2.0-common libharfbuzz0b libice-dev libice6 libisl23 libitm1 libjbig0 libjpeg-turbo8 libjpeg8 libllvm15
liblsan0 libmpc3 libnsl-dev libopengl-dev libopenl0 libpango-1.0-0 libpangocairo-1.0-0 libpangoft2-1.0-0
libpciaccess-dev libpciaccess0 libpixman-1-0 libpthread-stubs0-dev libquadmath0 librsvg2-2 librsvg2-common
libsensors-config libsensors5 libsm-dev libsm6 libstdc++-11-dev libthai-data libthai0 libtiff5 libtirpc-dev libtsan0
libubsan1 libwayland-client0 libwayland-egl1 libwayland-server0 libwebp7 libx11-dev libx11-xcb1 libxau-dev libxaw7
libxcb-dri2-0 libxcb-dri3-0 libxcb-glx0 libxcb-present0 libxcb-randr0 libxcb-render0 libxcb-shm0 libxcb-sync1
libxcb-xfixes0 libxcb1-dev libxcomposite1 libxcursor1 libxdamage1 libxdmcp-dev libxext-dev libxfixes3 libxft2 libxi6
libxinerama1 libxkbfile1 libxmu6 libxpm4 libxrandr2 libxrender1 libxshmfence1 libxt-dev libxt6 libxxf86vm1
linux-libc-dev lto-disabled-list make manpages-dev mesa-common-dev mesa-utils mesa-utils-bin rpcsvc-proto
ubuntu-mono x11-apps x11-common x11proto-dev xbitmaps xorg-sgml-doctools xtrans-dev
The following packages will be upgraded:
libc6 openssl
2 upgraded, 169 newly installed, 0 to remove and 118 not upgraded.
Need to get 129 MB of archives.
After this operation, 462 MB of additional disk space will be used.
Do you want to continue? [Y/n] |

```

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

```

steve@StevenH: ~
librsvg2-bin lm-sensors libsm-doc libstdc++-11-doc libx11-doc libxcb-doc libxext-doc libxt-doc make-doc
Recommended packages:
libnss-nis libnss-nisplus
The following NEW packages will be installed:
adwaita-icon-theme build-essential bzip2 cpp cpp-11 dpkg-dev fakeroot fontconfig fontconfig-config fonts-dejavu-core
freeglut3 freeglut3-dev g++ g++-11 gcc gcc-11 gcc-11-base gtk-update-icon-cache hicolor-icon-theme
humanity-icon-theme libalgorithm-diff-perl libalgorithm-diff-xs-perl libalgorithm-merge-perl libasan6 libatk1.0-0
libatk1.0-data libatomic1 libavahi-client3 libavahi-common-data libavahi-common3 libc-dev-bin libc-devtools
libc6-dev libcairo-gobject2 libcairo2 libcc1-0 libcrypt-dev libcups2 libdatrie1 libdeflate0 libdpkg-perl
libdrm-amdgpu1 libdrm-dev libdrm-intel1 libdrm-nouveau2 libdrm-radeon1 libegl-dev libegl-mesa0 libegl1 libfakeroot
libfile-fcntllock-perl libfontconfig1 libfonttype6 libgail-common libgail18 libgbm1 libgcc-11-dev libgd3
libgdk-pixbuf-2.0-0 libgdk-pixbuf2.0-bin libgdk-pixbuf2.0-common libgl-dev libgl1 libgl1-amber-dri libgl1-mesa-dev
libgl1-mesa-dri libglapi-mesa libgles-dev libgles1 libgles2 libglul-mesa libglul-mesa-dev libglvnd-core-dev
libglvnd-dev libglvnd0 libglx-dev libglx-mesa0 libglx0 libgomp1 libgraphite2-3 libgtk2.0-0 libgtk2.0-bin
libgtk2.0-common libharfbuzz0b libice-dev libice6 libisl23 libitm1 libjbig0 libjpeg-turbo8 libjpeg8 libllvm15
liblsan0 libmpc3 libnsl-dev libopenl0 libopenl0 libpango-1.0-0 libpangocairo-1.0-0 libpangoft2-1.0-0
libpciaccess-dev libpciaccess0 libpixman-1-0 libpthread-stubs0-dev libquadmath0 librsvg2-2 librsvg2-common
libsensors-config libsensors5 libsm-dev libsm6 libstdc++-11-dev libthai-data libthai0 libtiff5 libtirpc-dev libtsan0
libubsan1 libwayland-client0 libwayland-egl1 libwayland-server0 libwebp7 libx11-dev libx11-xcb1 libxau-dev libxaw7
libxcb-dri2-0 libxcb-dri3-0 libxcb-glx0 libxcb-present0 libxcb-randr0 libxcb-render0 libxcb-shm0 libxcb-sync1
libxcb-xfixes0 libxcb1-dev libxcomposite1 libxcursor1 libxdamage1 libxdmcp-dev libxext-dev libxfixes3 libxft2 libxi6
libxinerama1 libxkbfile1 libxmu6 libxpm4 libxrandr2 libxrender1 libxshmfence1 libxt-dev libxt6 libxxf86vm1
linux-libc-dev lto-disabled-list make manpages-dev mesa-common-dev mesa-utils mesa-utils-bin rpcsvc-proto
ubuntu-mono x11-apps x11-common x11proto-dev xbitmaps xorg-sgml-doctools xtrans-dev
The following packages will be upgraded:
libc6 openssl
2 upgraded, 169 newly installed, 0 to remove and 118 not upgraded.
Need to get 129 MB of archives.
After this operation, 462 MB of additional disk space will be used.
Do you want to continue? [Y/n] Y

```

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  
steve@StevenH:~$ sudo apt-get update  
steve@StevenH:~$ sudo apt-get install libssl1.1  
steve@StevenH:~$ sudo rm /etc/apt/sources.list.d/focal-security.list  
steve@StevenH:~$ 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
```

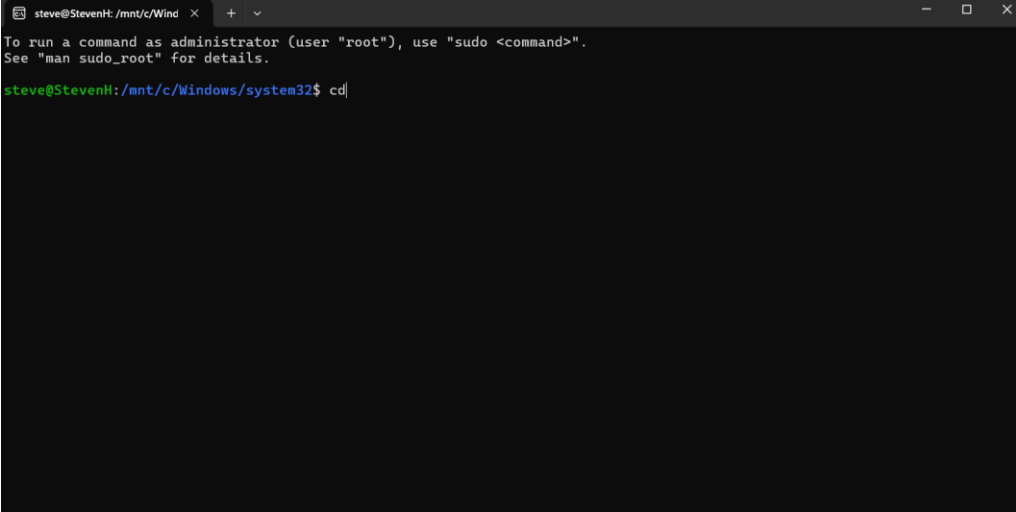
```
steve@StevenH: ~  
Fetched 3731 kB in 3s (1077 kB/s)  
Reading package lists... Done  
Reading package lists... Done  
Building dependency tree... Done  
Reading state information... Done  
The following NEW packages will be installed:  
  libssl1.1  
0 upgraded, 1 newly installed, 0 to remove and 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  
Generating locales (this might take a while)...  
  en_GB.UTF-8... done  
  en_US.UTF-8... done  
Generation complete.  
steve@StevenH:~$
```

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”:

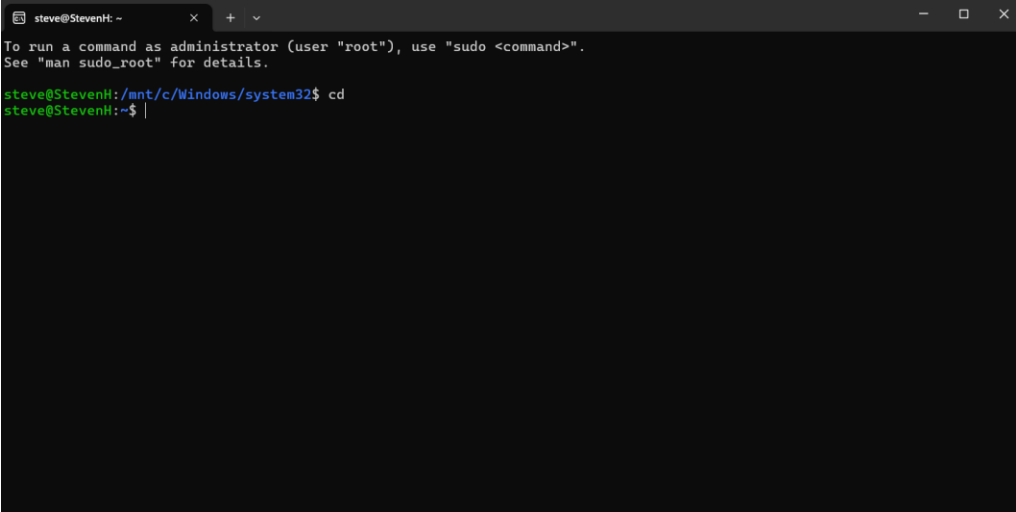
```
steve@StevenH:/mnt/c/Windows/system32$  
To run a command as administrator (user "root"), use "sudo <command>".  
See "man sudo_root" for details.  
steve@StevenH:/mnt/c/Windows/system32$
```

i.



```
steve@StevenH: /mnt/c/Wind x + v
To run a command as administrator (user "root"), use "sudo <command>".
See "man sudo_root" for details.
steve@StevenH: /mnt/c/Windows/system32$ cd|
```

- ii.
- iii. “cd” means change directory, it will bring you to the root directory



```
steve@StevenH: ~ x + v
To run a command as administrator (user "root"), use "sudo <command>".
See "man sudo_root" for details.
steve@StevenH: /mnt/c/Windows/system32$ cd
steve@StevenH: ~$ |
```

- 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:

```
steve@StevenH: ~  
To run a command as administrator (user "root"), use "sudo <command>".  
See "man sudo_root" for details.  
steve@StevenH:~/mnt/c/Windows/system32$ cd  
steve@StevenH:~$ ls
```

i.

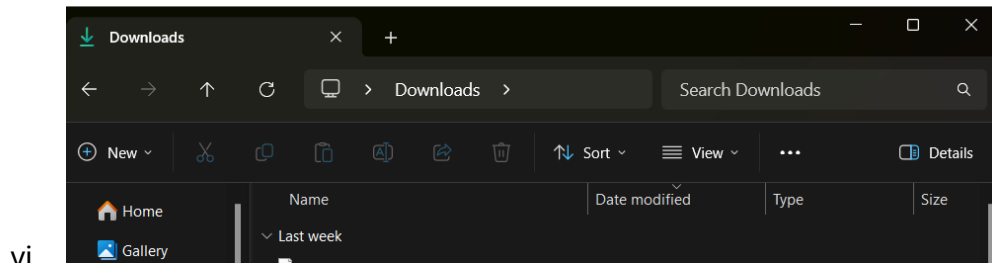
```
steve@StevenH: ~  
To run a command as administrator (user "root"), use "sudo <command>".  
See "man sudo_root" for details.  
steve@StevenH:~/mnt/c/Windows/system32$ cd  
steve@StevenH:~$ ls  
steve@StevenH:~$ |
```

ii.

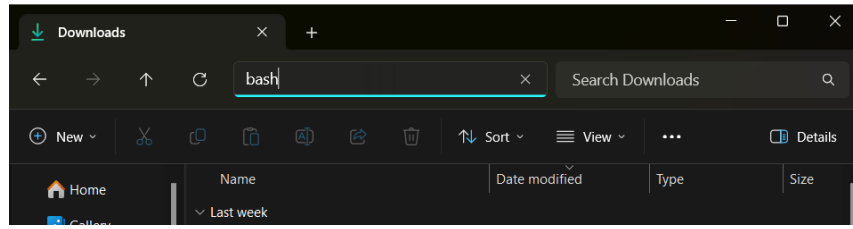
iii. There is nothing in the Linux subsystem folder just yet, which is why nothing is there.

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

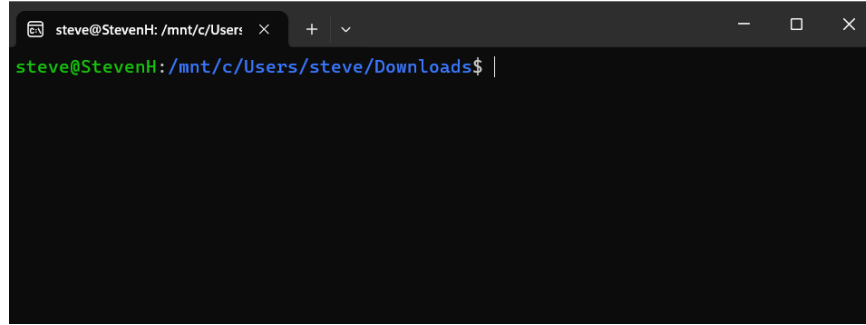
v. Open the downloads folder in Windows, type bash at the top, **cd ..** on folder below, like so:



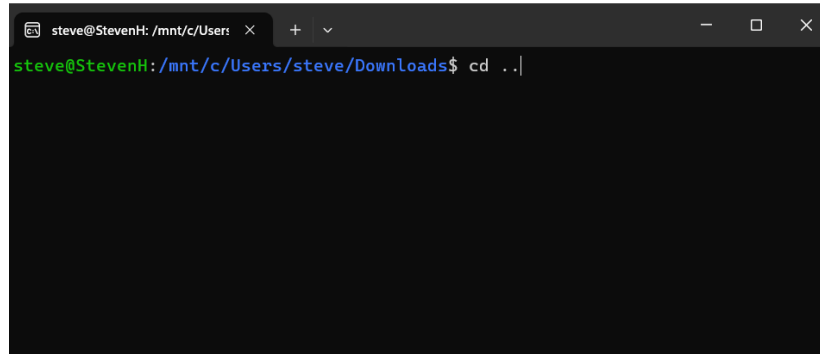
vii.



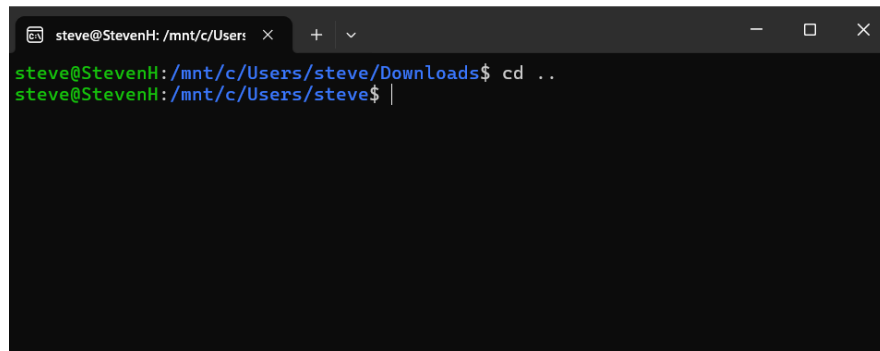
viii.



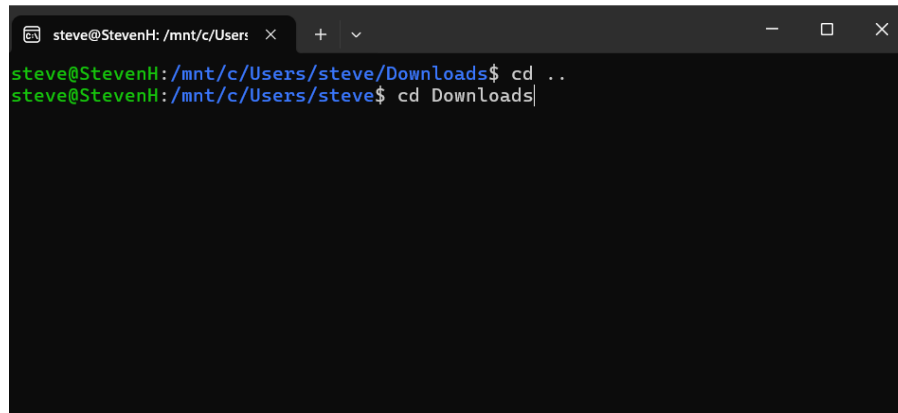
ix.



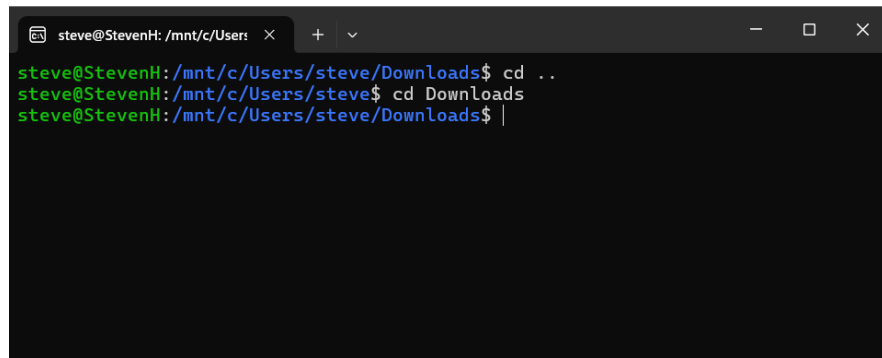
x.



xi.

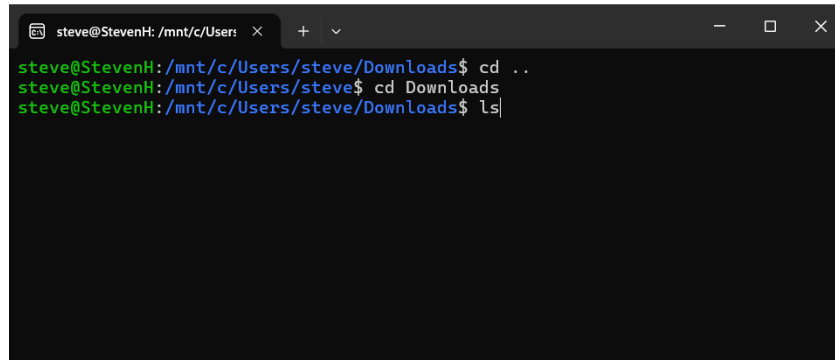


xii.



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

```
steve@StevenH: /mnt/c/Users/steve/Downloads$ ls
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$
```

xiv.

```

steve@StevenH: /mnt/c/Users/steve$ ls
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
Application Data
Cookies
Documents
Downloads
Favorites
Links
Local Settings
My Documents
NTUSER.DAT
NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TM.blf
NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TMContainer0000000000000000
00001.regtrans-ms
NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TMContainer0000000000000000
00002.regtrans-ms
NetHood
PrintHood
Recent
Saved Games
Searches
SendTo
Start Menu
Templates
ntuser.dat.LOG1
ntuser.dat.LOG2
ntuser.ini
steve@StevenH: /mnt/c/Users/steve$

```

- 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.


```
steve@StevenH: /mnt/c/Users/steve/Downloads$ ls
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}.TMContainer0000000000000000
00001.regtrans-ms
  NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TMContainer0000000000000000
00002.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"
```

xvii.

```
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}.TMContainer0000000000000000
00001.regtrans-ms
NTUSER.DAT{2319190f-30cc-11ee-af11-d03957a3b70c}.TMContainer0000000000000000
00002.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"
steve@StevenH: /mnt/c/Users/steve/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

```

steve@StevenH: /mnt/c/Users
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"
steve@StevenH:/mnt/c/Users/steve/Local Settings$ ls
ASP.NET
'Application Data'
Avast Software
Avira
AviraSpeedup
AviraWebView2Cache
BSTCache
Backup
Bluestacks
Bytedance
CEI
CapCut
Comms
ConnectedDevicesPlatform
CrashDumps
D3DSCache
Discord
ElevatedDiagnostics
Enlistea
GUT
Gaijin
Google
HD-Player
HP
HPE
History
'NetHistory'
IconCache.db
Lenovo
Microsoft
NVIDIA Corporation
OneDrive
Opera Software
PlaceholderFileLogoFolder
Programs
Publishers
Roblox
SquirrelTemp
Temp
'Temporary Internet Files'
Tencent
ToastNotificationManagerCompat
VEDetector
VirtualStore
WarThunder
Zoom
bluestacks-services-updates
cache
packages
speech
xxi. steve@StevenH:/mnt/c/Users/steve/Local Settings$ |

```

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

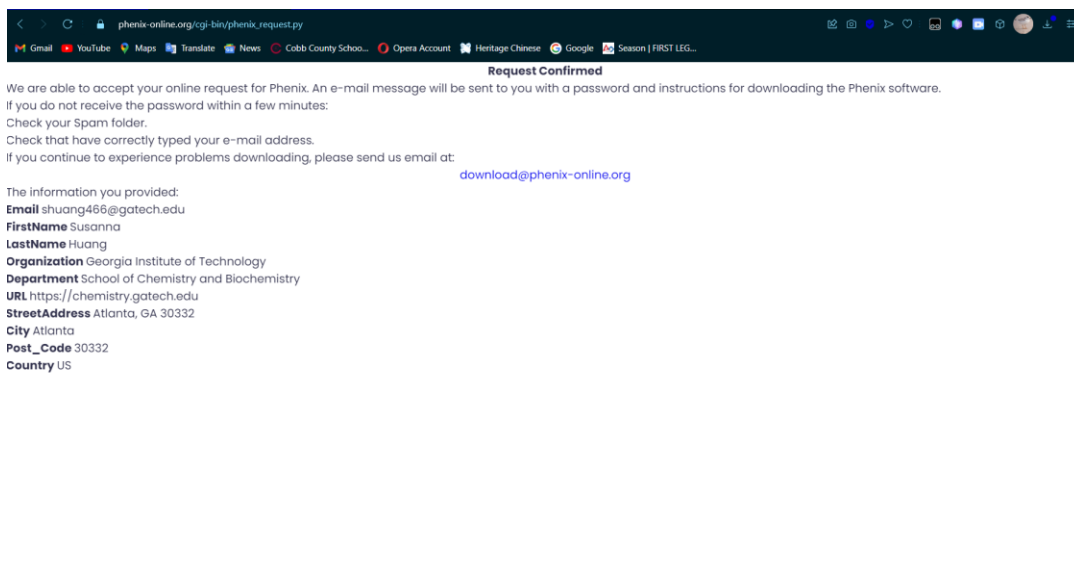
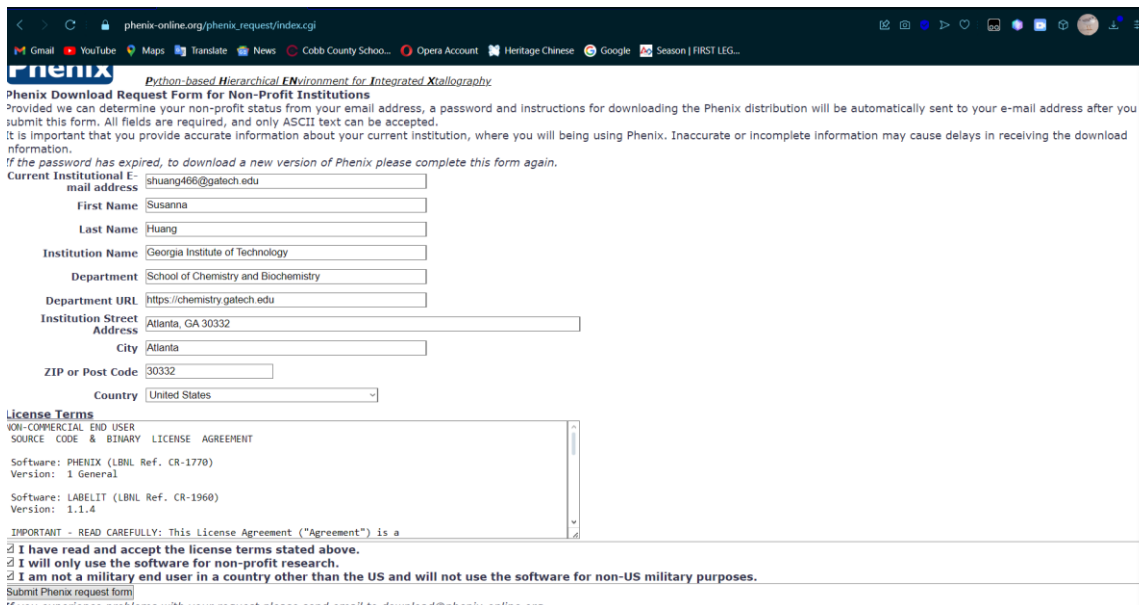
- **cd**
 - o goes to the home directory
- **ls**
 - o list out the items in the folder
- **cp**
 - o the copy file or directory function
 - o a file:
 - `cd <file name> <copy-to-folder directory>`
 - o an entire directory
 - `cd -r <file directory name> <copy-to-folder directory>`
- **pwd**
 - o print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

- **mkdir**

- makes a new directory or folder
- **Ex: mkdir 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.,

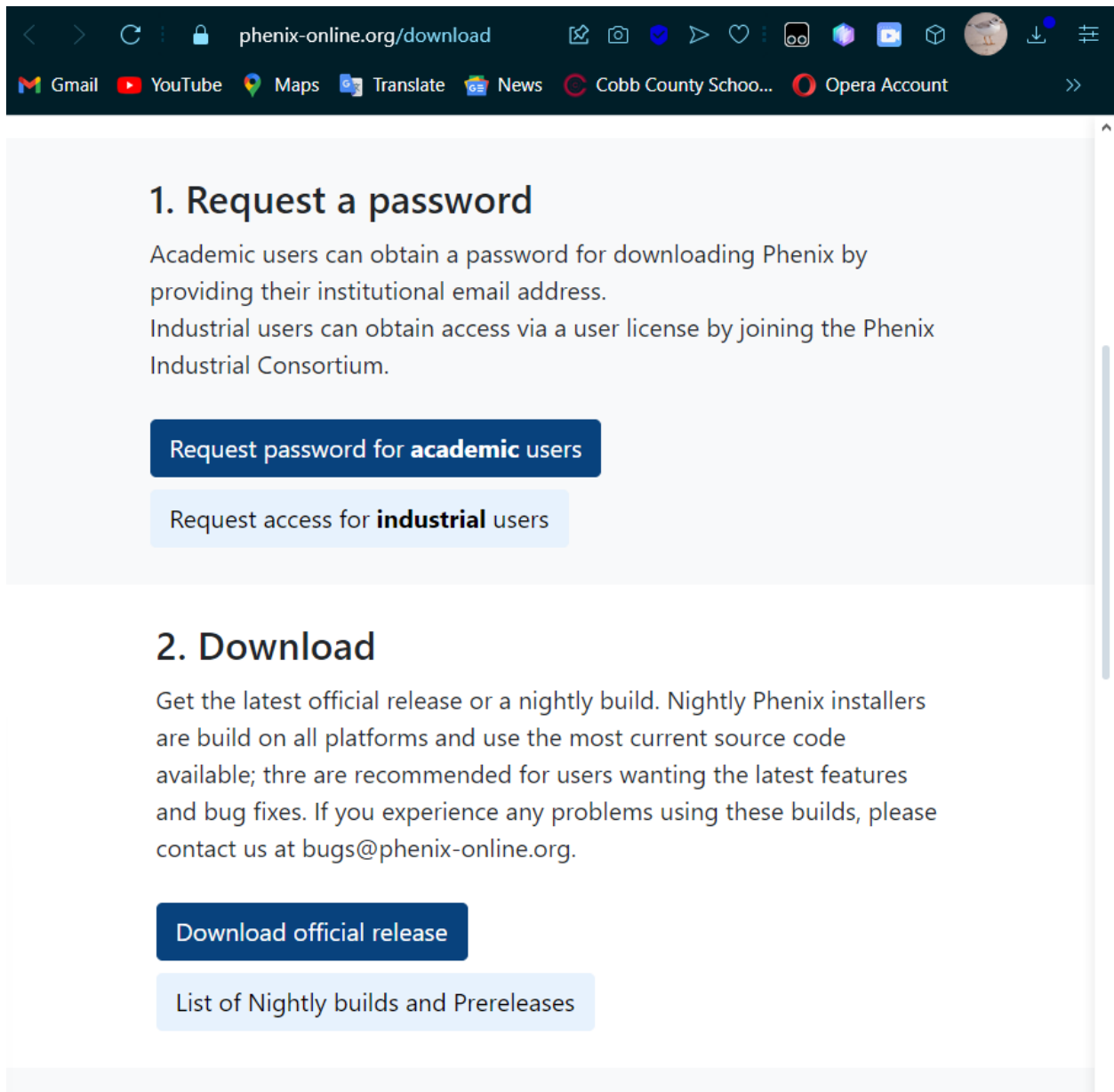
Terwilliger T.C., Urzhumtsev A.G., Videau L.L., Williams C.J., and Adams P.D.

Acta Cryst. D75, 861-877 (2019).

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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



phenix-online.org/download

Gmail YouTube Maps Translate News Cobb County Schoo... Opera Account

1. Request a password

Academic users can obtain a password for downloading Phenix by providing their institutional email address.
Industrial users can obtain access via a user license by joining the Phenix Industrial Consortium.

[Request password for **academic** users](#)

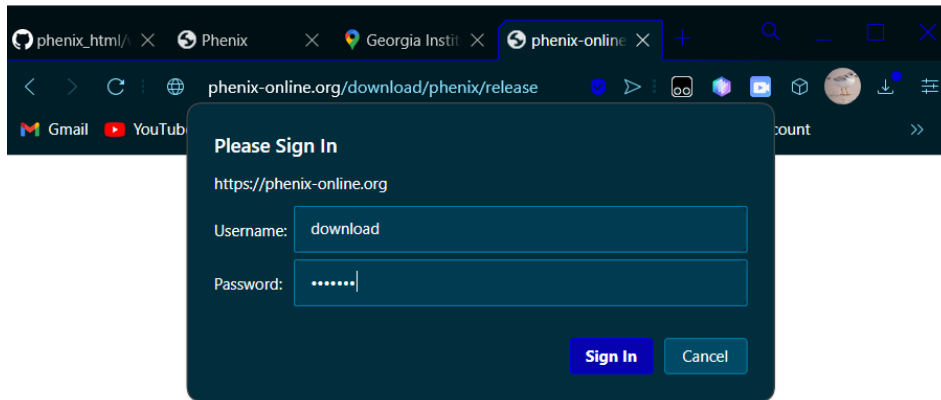
[Request access for **industrial** users](#)

2. Download

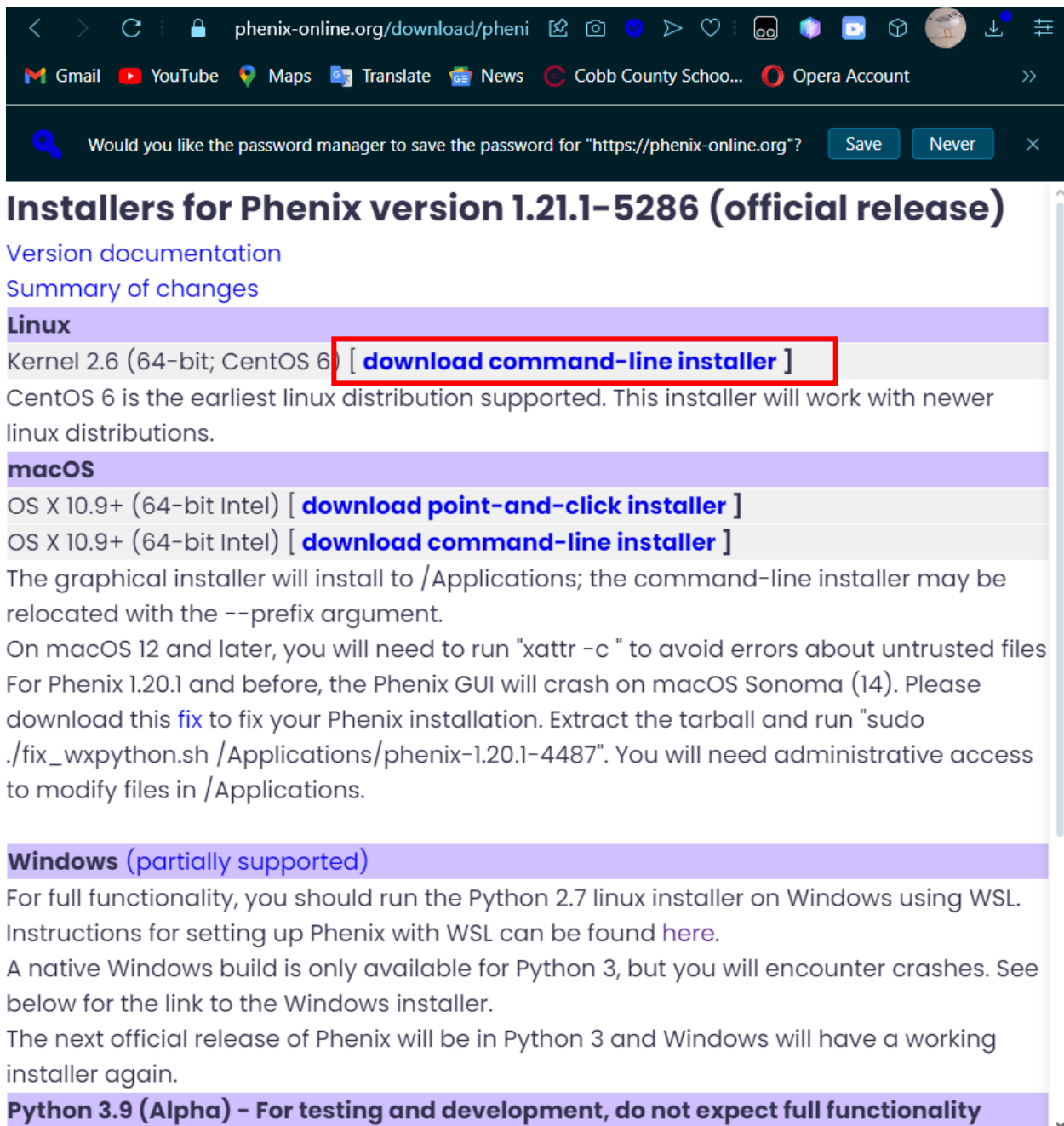
Get the latest official release or a nightly build. Nightly Phenix installers are build on all platforms and use the most current source code available; there are recommended for users wanting the latest features and bug fixes. If you experience any problems using these builds, please contact us at bugs@phenix-online.org.

[Download official release](#)

[List of Nightly builds and Prereleases](#)



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



phenix-online.org/download/pheni

Would you like the password manager to save the password for "https://phenix-online.org"? Save Never

Installers for Phenix version 1.21.1-5286 (official release)

[Version documentation](#)
[Summary of changes](#)

Linux

Kernel 2.6 (64-bit; CentOS 6) [[download command-line installer](#)]

CentOS 6 is the earliest linux distribution supported. This installer will work with newer linux distributions.

macOS

OS X 10.9+ (64-bit Intel) [[download point-and-click installer](#)]
OS X 10.9+ (64-bit Intel) [[download command-line installer](#)]

The graphical installer will install to /Applications; the command-line installer may be relocated with the --prefix argument.

On macOS 12 and later, you will need to run "xattr -c " to avoid errors about untrusted files. For Phenix 1.20.1 and before, the Phenix GUI will crash on macOS Sonoma (14). Please download this [fix](#) to fix your Phenix installation. Extract the tarball and run "sudo ./fix_wxpython.sh /Applications/phenix-1.20.1-4487". You will need administrative access to modify files in /Applications.

Windows (partially supported)

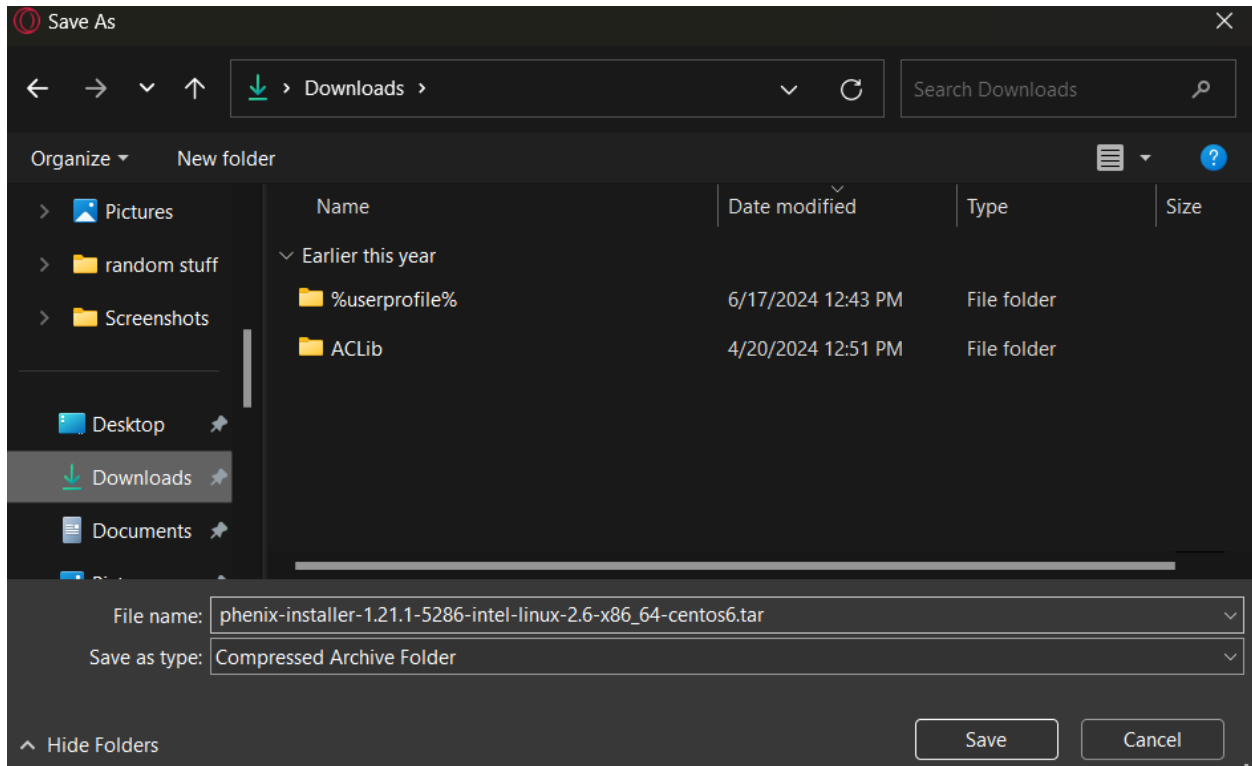
For full functionality, you should run the Python 2.7 linux installer on Windows using WSL. Instructions for setting up Phenix with WSL can be found [here](#).

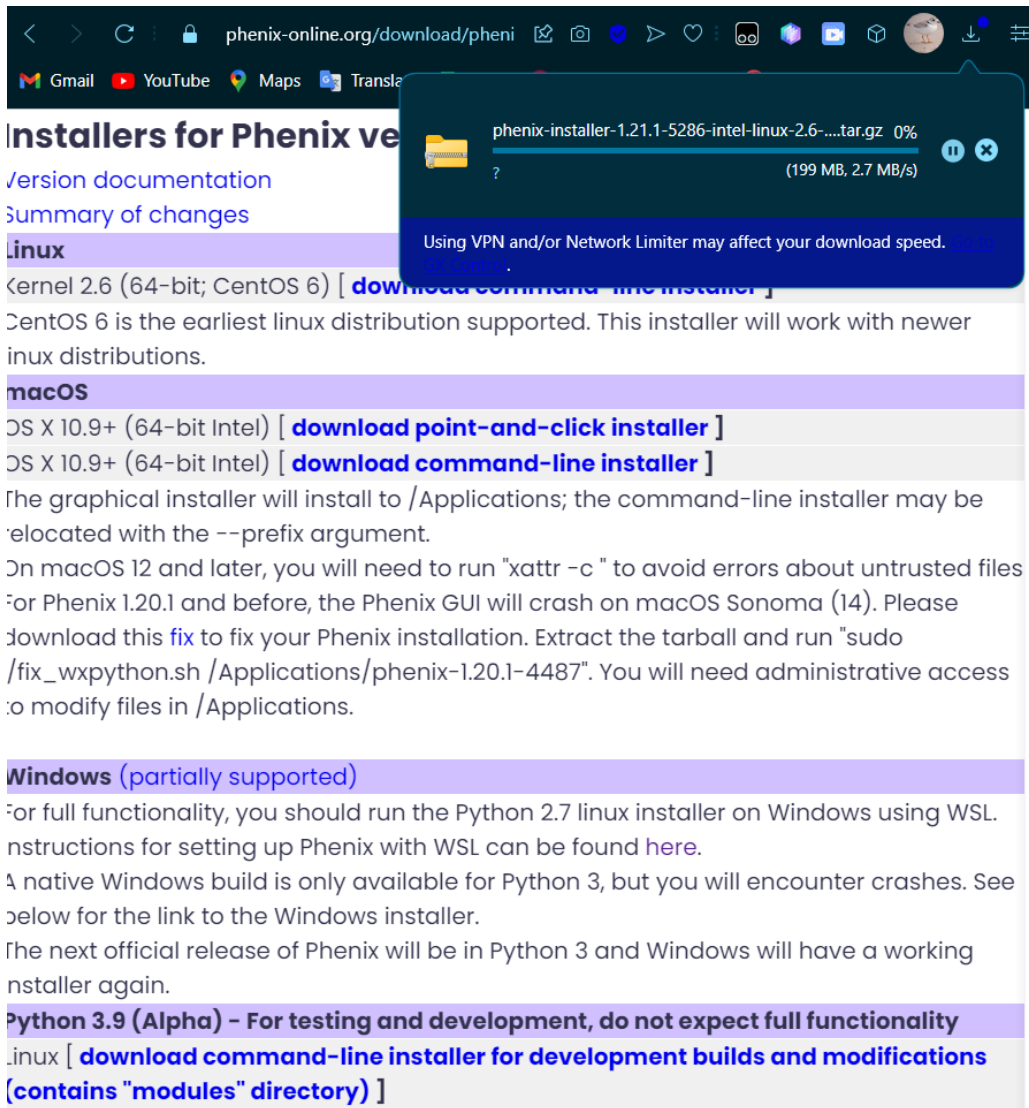
A native Windows build is only available for Python 3, but you will encounter crashes. See below for the link to the Windows installer.

The next official release of Phenix will be in Python 3 and Windows will have a working installer again.

Python 3.9 (Alpha) - For testing and development, do not expect full functionality

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





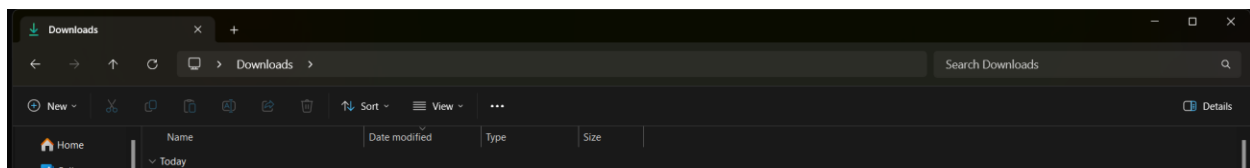
The screenshot shows a web browser window with the URL `phenix-online.org/download/phenix`. The page title is "Installers for Phenix version 1.20.1". The page content includes links for "Version documentation" and "Summary of changes". The "Linux" section is highlighted, showing instructions for CentOS 6, macOS (OS X 10.9+), and Windows (partially supported). A download progress bar is overlaid on the page, showing the file `phenix-installer-1.21.1-5286-intel-linux-2.6-....tar.gz` at 0% completion, with a size of 199 MB and a download speed of 2.7 MB/s. A notification message states: "Using VPN and/or Network Limiter may affect your download speed."

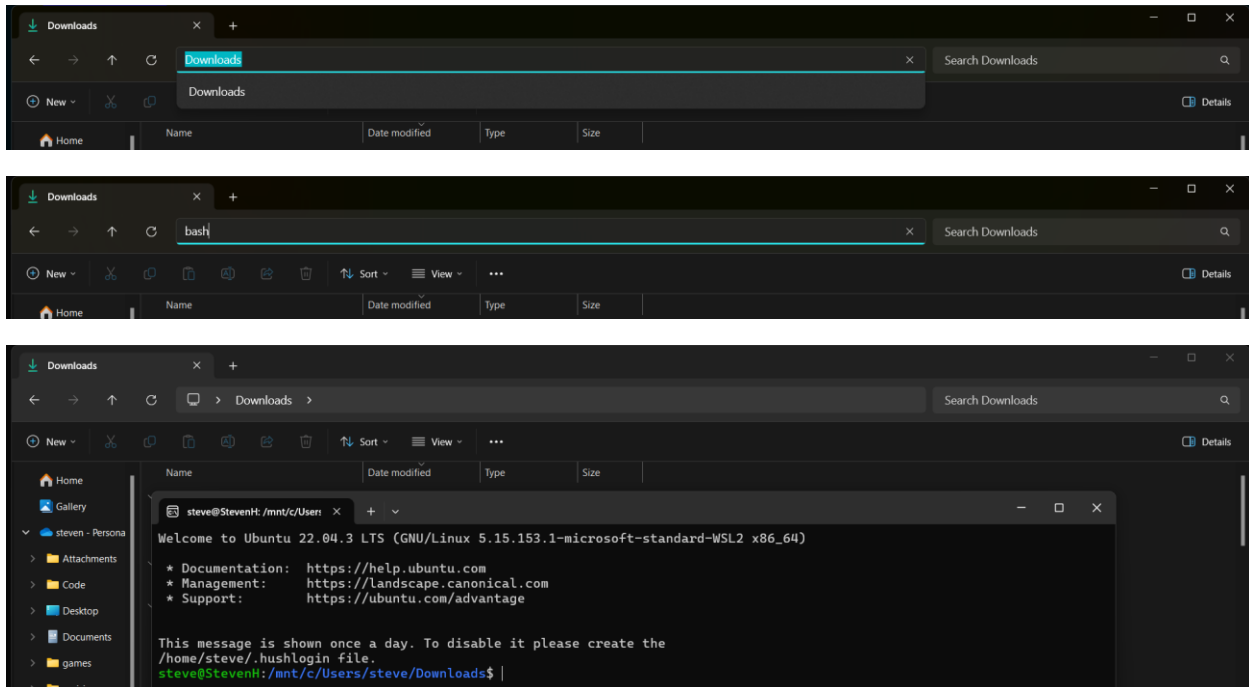
Meanwhile, while we get the phenix thing working, we can go ahead and download Coot:

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.

```
steve@StevenH:/mnt/c/Users/ X + v
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:/mnt/c/Users/steve/Downloads$ pwd
/mnt/c/Users/steve/Downloads
steve@StevenH:/mnt/c/Users/steve/Downloads$ |
```

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.

```
steve@StevenH: ~
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: /mnt/c/Users/steve/Downloads$ pwd
/mnt/c/Users/steve/Downloads
steve@StevenH: /mnt/c/Users/steve/Downloads$ cd
steve@StevenH: ~$ |
```

There most likely is nothing in it right now:

```
steve@StevenH: ~
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: /mnt/c/Users/steve/Downloads$ pwd
/mnt/c/Users/steve/Downloads
steve@StevenH: /mnt/c/Users/steve/Downloads$ cd
steve@StevenH: ~$ ls
steve@StevenH: ~$ |
```

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”:

```

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

```

```

steve@StevenH: /mnt/c/Users/
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
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz
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$ |

```

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

```
steve@StevenH: ~  
'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  
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz  
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$ cd  
steve@StevenH:~$
```

```
steve@StevenH: ~  
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  
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz  
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$ cd  
steve@StevenH:~$ pwd  
/home/steve  
steve@StevenH:~$
```

Now type in your command

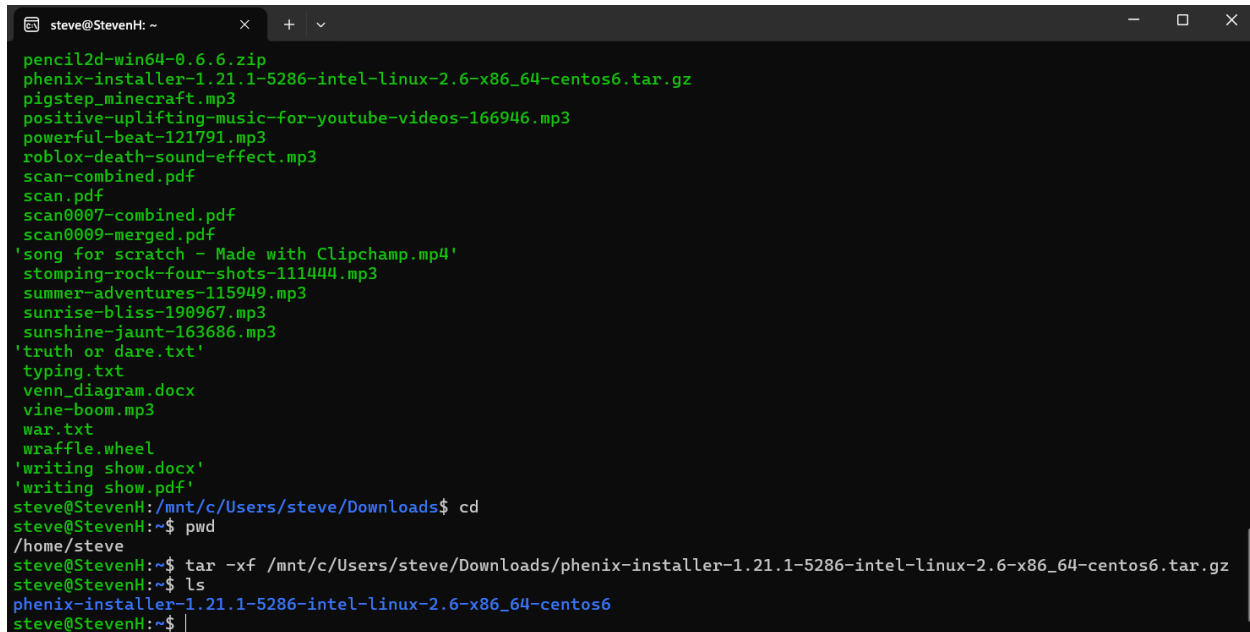
```
steve@StevenH: ~  
pct_free_installer_20240709.1-17205423117937b14590.exe  
'pencil2d-win64-0.6.6 (1).zip'  
pencil2d-win64-0.6.6.zip  
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz  
pigstep_minecraft.mp3  
positive-uplifting-music-for-youtube-videos-166946.mp3  
powerful-beat-121791.mp3  
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$ cd  
steve@StevenH:~$ pwd  
/home/steve  
steve@StevenH:~$ tar -xvf /mnt/c/Users/steve/Downloads/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz
```

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:

```
steve@StevenH: ~  
pct_free_installer_20240709.1-17205423117937b14590.exe  
'pencil2d-win64-0.6.6 (1).zip'  
pencil2d-win64-0.6.6.zip  
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz  
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$ cd  
steve@StevenH:~$ pwd  
/home/steve  
steve@StevenH:~$ tar -xvf /mnt/c/Users/steve/Downloads/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz  
steve@StevenH:~$
```

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

A terminal window titled 'steve@StevenH: ~' showing a list of files in the Downloads directory. The files include various audio files (mp3), PDFs, a zip file, a docx, and a wheel. The user then navigates to the directory containing the 'phenix-installer' tar.gz file and lists its contents.

```
steve@StevenH: ~  
pencil2d-win64-0.6.6.zip  
phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6.tar.gz  
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  
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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:~$
```

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.


```

steve@StevenH: ~/phenix-ins  ×  +  ▾
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$ ./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
  args ['--build_dir=/home/steve/phenix-1.21.1-5286/build', '--base_dir=/home/steve/phenix-1.21.1-5286/conda_base', '--s
uffix=phenix', '--gtk_version=2.10.0', '--quiet', '--use_conda', '--ignore_missing_dirs']
  prologue export PHENIX="/home/steve/phenix-1.21.1-5286"
export PHENIX_VERSION=1.21.1-5286
export PHENIX_ENVIRONMENT=1
export PHENIX_MTYPE=intel-linux-2.6-x86_64
  epilogue if [ ! -z "$QB_PYTHONPATH" ]; then
    export PYTHONPATH=$PYTHONPATH:$QB_PYTHONPATH
  fi
if [ ! -z "$QB_LD_LIBRARY_PATH" ]; then
  export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$QB_LD_LIBRARY_PATH
fi
if [ ! -z "$QB_DYLD_LIBRARY_PATH" ]; then
  export DYLD_LIBRARY_PATH=$DYLD_LIBRARY_PATH:$QB_DYLD_LIBRARY_PATH
fi
if [ "$PHENIX_MTYPE" != "mac-ppc-osx" ] && \
  [ "$PHENIX_MTYPE" != "mac-intel-osx" ] && \
  [ "$PHENIX_MTYPE" != "mac-intel-osx-x86_64" ]; then
  export PYMOL_PATH=$PHENIX/pymol
fi
Configuring Phenix components...
Precompiling .py files...

```

```
steve@StevenH: ~/phenix-ins x + v
Configuring Phenix components...
Precompiling .py files...
Generating SOLVE/RESOLVE license file...
Rebuilding HTML documentation...
Creating rotamer/Ramachandran database files... ok
Checking for monomer library files... ok
PyMOL not available!

=====

                PHENIX installation complete
                -----

You can begin using PHENIX now by setting your environment with the
'source' command:

  csh users:
    source /home/steve/phenix-1.21.1-5286/phenix_env.csh

  bash users:
    source /home/steve/phenix-1.21.1-5286/phenix_env.sh

To use PHENIX, go to a work directory and type:

  phenix

You may wish to put the source statement in your .cshrc or .bashrc
file.
```

```
steve@StevenH: ~/phenix-ins x + v
PyMOL not available!

=====

                PHENIX installation complete
                -----

You can begin using PHENIX now by setting your environment with the
'source' command:

  csh users:
    source /home/steve/phenix-1.21.1-5286/phenix_env.csh

  bash users:
    source /home/steve/phenix-1.21.1-5286/phenix_env.sh

To use PHENIX, go to a work directory and type:

  phenix

You may wish to put the source statement in your .cshrc or .bashrc
file.

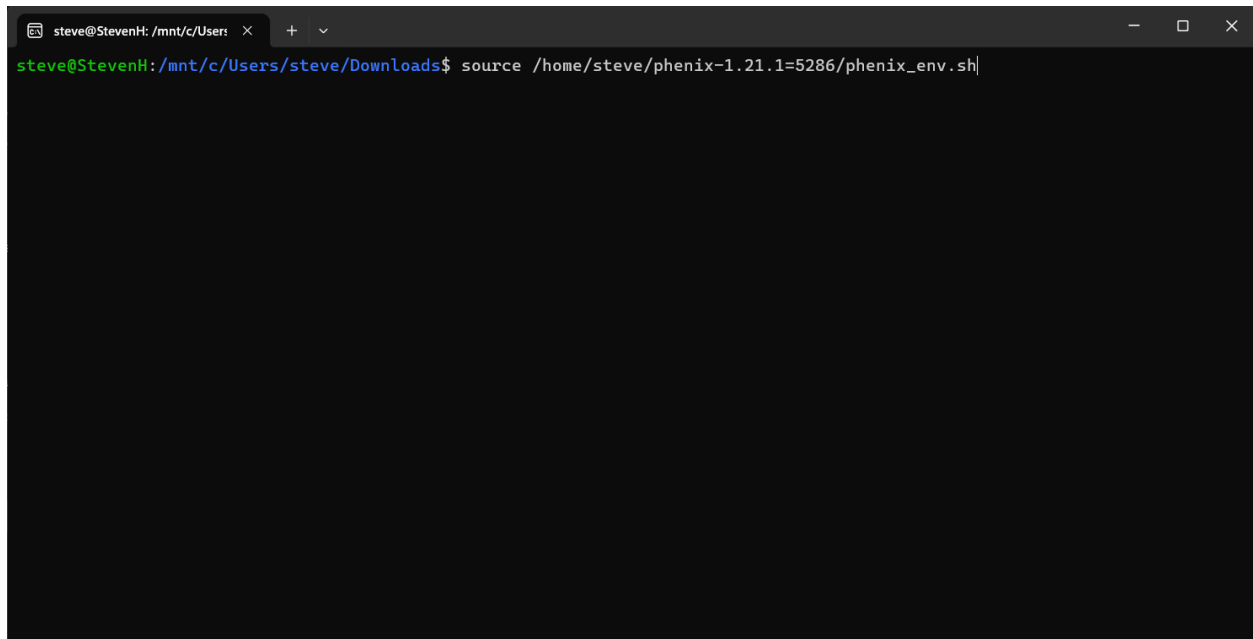
*****
* Installation complete! *
*****

steve@StevenH:~/phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6$ |
```

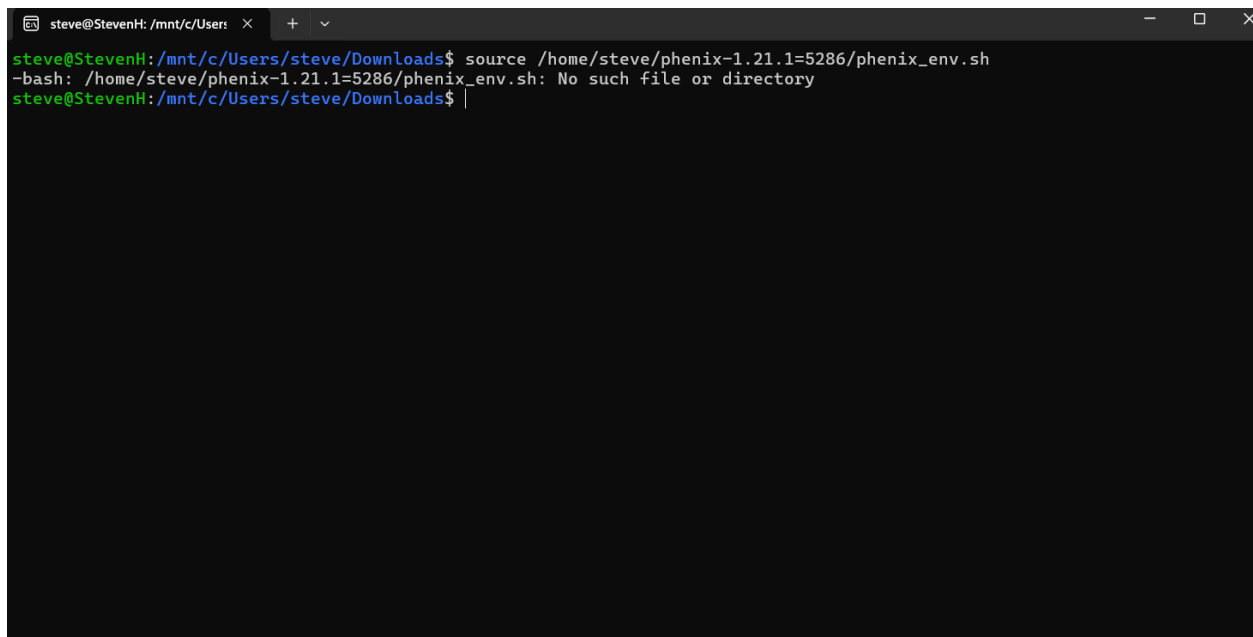
So, now if you want to open PHENIX, you just bash into any folder, for this example, type:

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

Then type **phenix**

A terminal window with a dark background. The title bar shows 'steve@StevenH: /mnt/c/Users/steve/Downloads'. The prompt is 'steve@StevenH: /mnt/c/Users/steve/Downloads\$'. The command 'source /home/steve/phenix-1.21.1=5286/phenix_env.sh' has been entered and executed. The prompt returns to the same state, indicating the command was successful.

```
steve@StevenH: /mnt/c/Users/steve/Downloads$ source /home/steve/phenix-1.21.1=5286/phenix_env.sh
```

A terminal window with a dark background. The title bar shows 'steve@StevenH: /mnt/c/Users/steve/Downloads'. The prompt is 'steve@StevenH: /mnt/c/Users/steve/Downloads\$'. The command 'source /home/steve/phenix-1.21.1=5286/phenix_env.sh' has been entered and executed. The output is '-bash: /home/steve/phenix-1.21.1=5286/phenix_env.sh: No such file or directory'. The prompt returns to the same state.

```
steve@StevenH: /mnt/c/Users/steve/Downloads$ source /home/steve/phenix-1.21.1=5286/phenix_env.sh
-bash: /home/steve/phenix-1.21.1=5286/phenix_env.sh: No such file or directory
steve@StevenH: /mnt/c/Users/steve/Downloads$
```

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.

```
steve@StevenH: /mnt/c/Users/steve/Downloads$ source /home/steve/phenix-1.21.1=5286/phenix_env.sh
-bash: /home/steve/phenix-1.21.1=5286/phenix_env.sh: No such file or directory
steve@StevenH: /mnt/c/Users/steve/Downloads$ |
```

It seems that it is here:

```
steve@StevenH: ~/phenix-1.2$ source /home/steve/phenix-1.21.1=5286/phenix_env.sh
-bash: /home/steve/phenix-1.21.1=5286/phenix_env.sh: No such file or directory
steve@StevenH: /mnt/c/Users/steve/Downloads$ cd
steve@StevenH: ~$ ls
phenix-1.21.1-5286  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH: ~$ cd
steve@StevenH: ~$ cd ..
steve@StevenH: /home$ ls
steve
steve@StevenH: /home$ cd
steve@StevenH: ~$ ls
phenix-1.21.1-5286  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH: ~$ cd
steve@StevenH: ~$ cd
steve@StevenH: ~$ cd
steve@StevenH: ~$ cd ^C
steve@StevenH: ~$ cd ^C
steve@StevenH: ~$ cd phenix-1.21.1-5286
steve@StevenH: ~/phenix-1.21.1-5286$ ls
CHANGES LICENSE README SOURCES build conda_base doc modules phenix_env.csh phenix_env.sh
steve@StevenH: ~/phenix-1.21.1-5286$ |
```

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:

```

steve@StevenH: ~/phenix-1.2
+
-
x
steve@StevenH:~/mnt/c/Users/steve/Downloads$ source /home/steve/phenix-1.21.1=5286/phenix_env.sh
-bash: /home/steve/phenix-1.21.1=5286/phenix_env.sh: No such file or directory
steve@StevenH:~/mnt/c/Users/steve/Downloads$ cd
steve@StevenH:~$ ls
phenix-1.21.1-5286  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd
steve@StevenH:~$ cd ..
steve@StevenH:/home$ ls
steve
steve@StevenH:/home$ cd
steve@StevenH:~$ ls
phenix-1.21.1-5286  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd
steve@StevenH:~$ cd
steve@StevenH:~$ cd
steve@StevenH:~$ cd ^C
steve@StevenH:~$ ^C
steve@StevenH:~$ cd phenix-1.21.1-5286
steve@StevenH:~/phenix-1.21.1-5286$ ls
CHANGES LICENSE README SOURCES build conda_base doc modules phenix_env.csh phenix_env.sh
steve@StevenH:~/phenix-1.21.1-5286$ ^C
steve@StevenH:~/phenix-1.21.1-5286$ source /home/steve/phenix-1.21.1-5286/phenix_env.sh

steve@StevenH:~/phenix-1.21.1-5286$
steve@StevenH:~/phenix-1.21.1-5286$ |

```

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

```
steve@StevenH: /mnt/c/Users/steve/Downloads$ cd
tar -xvf /mnt/c/Users/steve/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz
```

```
steve@StevenH: ~
1841steve@StevenH: /mnt/c/Users/steve/Downloads$ cd
tar -xvf /mnt/c/Users/steve/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz
steve@StevenH: ~$
```

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


```

steve@StevenH: ~
1841steve@StevenH:~/mnt/c/Users/steve/Download$ cd
tar -xf /mnt/c/Users/steve/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz
steve@StevenH:~$ bash
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ |

```

Coot is extracted now.

```

steve@StevenH: ~
1841steve@StevenH:~/mnt/c/Users/steve/Download$ cd
tar -xf /mnt/c/Users/steve/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz
steve@StevenH:~$ bash
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 <Phenix directory>/conda_base/lib/libstdc++.so.6

```

```

steve@StevenH: ~
1841steve@StevenH:~/mnt/c/Users/steve/Download$ cd
tar -xf /mnt/c/Users/steve/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz
steve@StevenH:~$ bash
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 <Phenix directory>/conda_base/lib/libstdc++.so.6
bash: /conda_base/lib/libstdc++.so.6: No such file or directory
steve@StevenH:~$ |

```

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

```

steve@StevenH: ~/Phenix
1841steve@StevenH:~/mnt/c/Users/steve/Downloads$ cd
tar -xvf /mnt/c/Users/steve/Downloads/coot-0.9.8-binary-Linux-x86_64-ubuntu-20.04.4-python-gtk2.tar.gz
steve@StevenH:~$ bash
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 <Phenix directory>/conda_base/lib/libstdc++.so.6
bash: /conda_base/lib/libstdc++.so.6: No such file or directory
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd Phenix
steve@StevenH:~/Phenix$ pwd
/home/steve/Phenix
steve@StevenH:~/Phenix$ |

```

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

```

steve@StevenH: ~
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 <Phenix directory>/conda_base/lib/libstdc++.so.6
bash: /conda_base/lib/libstdc++.so.6: No such file or directory
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd Phenix
steve@StevenH:~/Phenix$ pwd
/home/steve/Phenix
steve@StevenH:~/Phenix$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 /home/steve/Phenix/conda_base/lib/libstdc++.so.6
ln: failed to create symbolic link '/home/steve/Phenix/conda_base/lib/libstdc++.so.6': No such file or directory
steve@StevenH:~/Phenix$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 /home/steve/Phenix/conda_base/lib/libstdc++.so.6
ln: failed to create symbolic link '/home/steve/Phenix/conda_base/lib/libstdc++.so.6': No such file or directory
steve@StevenH:~/Phenix$ ls
LOCK  prefs.params  project_db.phil  tmp
steve@StevenH:~/Phenix$ cd
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd phenix-1.21.1-5286/
steve@StevenH:~/phenix-1.21.1-5286$ pwd
/home/steve/phenix-1.21.1-5286
steve@StevenH:~/phenix-1.21.1-5286$ ^C
steve@StevenH:~/phenix-1.21.1-5286$ ^C
steve@StevenH:~/phenix-1.21.1-5286$ cd
steve@StevenH:~$ 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.

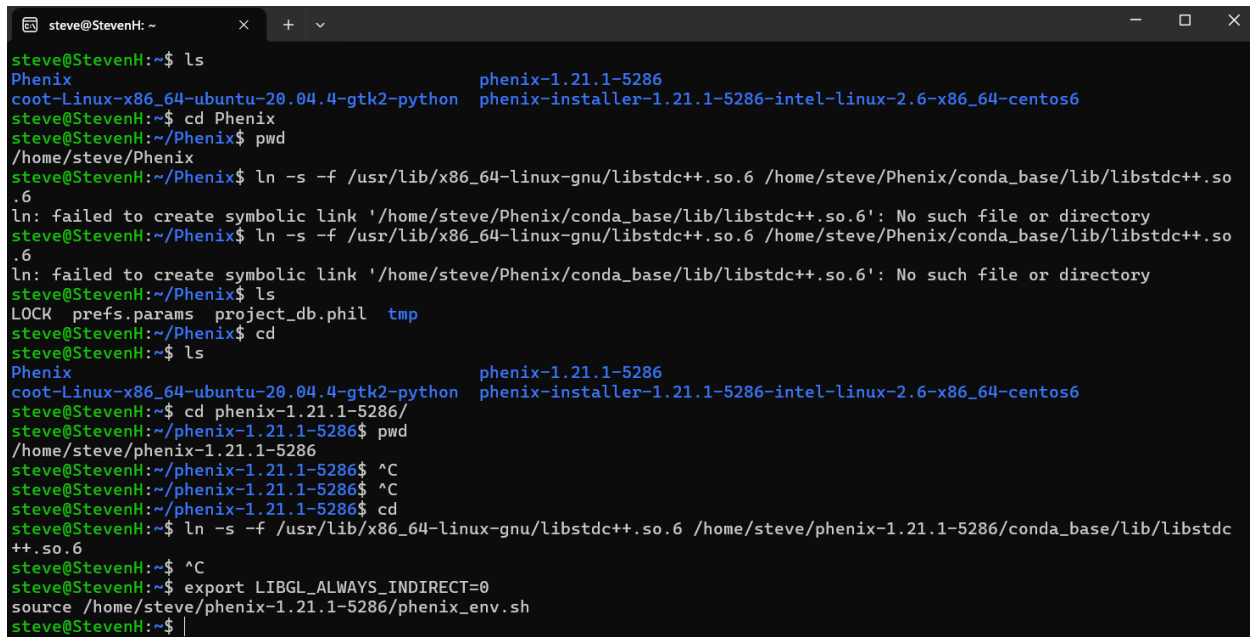
Then this part:

```
export LIBGL_ALWAYS_INDIRECT=0
```

```
source <Phenix directory>/phenix_env.sh
```

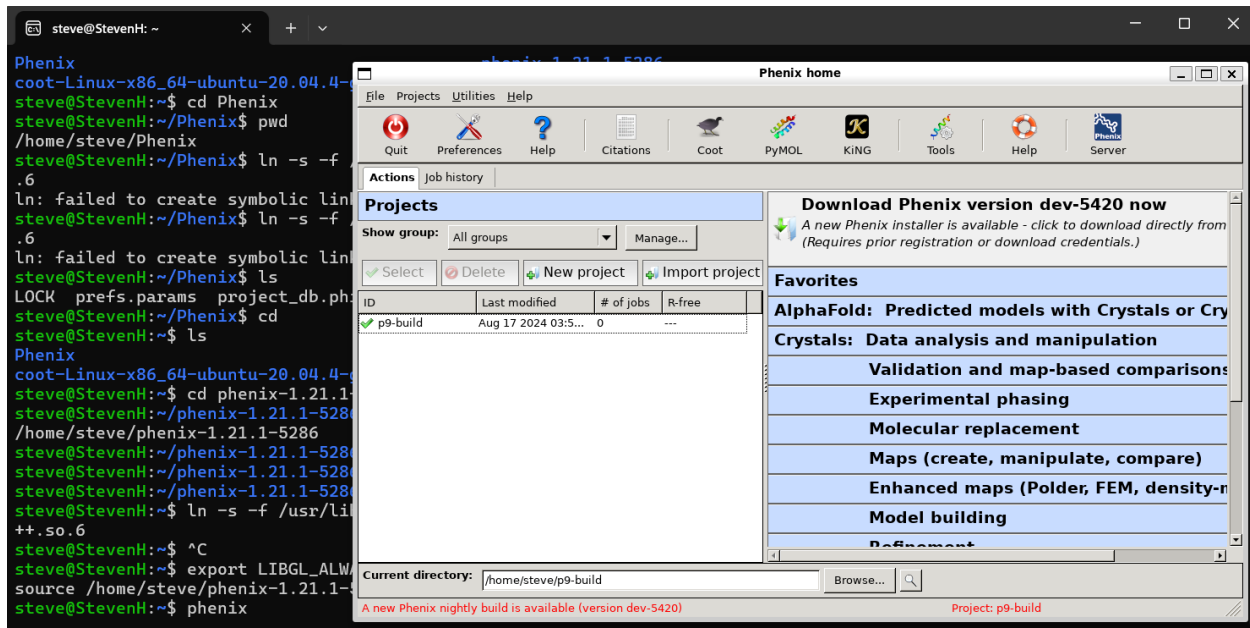
```
export LIBGL_ALWAYS_INDIRECT=0
```

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



```

steve@StevenH: ~
┌───┴───
└─┬───
   ├───
   └───
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd Phenix
steve@StevenH:~/Phenix$ pwd
/home/steve/Phenix
steve@StevenH:~/Phenix$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 /home/steve/Phenix/conda_base/lib/libstdc++.so.6
ln: failed to create symbolic link '/home/steve/Phenix/conda_base/lib/libstdc++.so.6': No such file or directory
steve@StevenH:~/Phenix$ ln -s -f /usr/lib/x86_64-linux-gnu/libstdc++.so.6 /home/steve/Phenix/conda_base/lib/libstdc++.so.6
ln: failed to create symbolic link '/home/steve/Phenix/conda_base/lib/libstdc++.so.6': No such file or directory
steve@StevenH:~/Phenix$ ls
LOCK  prefs.params  project_db.phil  tmp
steve@StevenH:~/Phenix$ cd
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd phenix-1.21.1-5286/
steve@StevenH:~/phenix-1.21.1-5286$ pwd
/home/steve/phenix-1.21.1-5286
steve@StevenH:~/phenix-1.21.1-5286$ ^C
steve@StevenH:~/phenix-1.21.1-5286$ ^C
steve@StevenH:~/phenix-1.21.1-5286$ cd
steve@StevenH:~$ 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
steve@StevenH:~$ ^C
steve@StevenH:~$ export LIBGL_ALWAYS_INDIRECT=0
steve@StevenH:~$ source /home/steve/phenix-1.21.1-5286/phenix_env.sh
steve@StevenH:~$ |
  
```

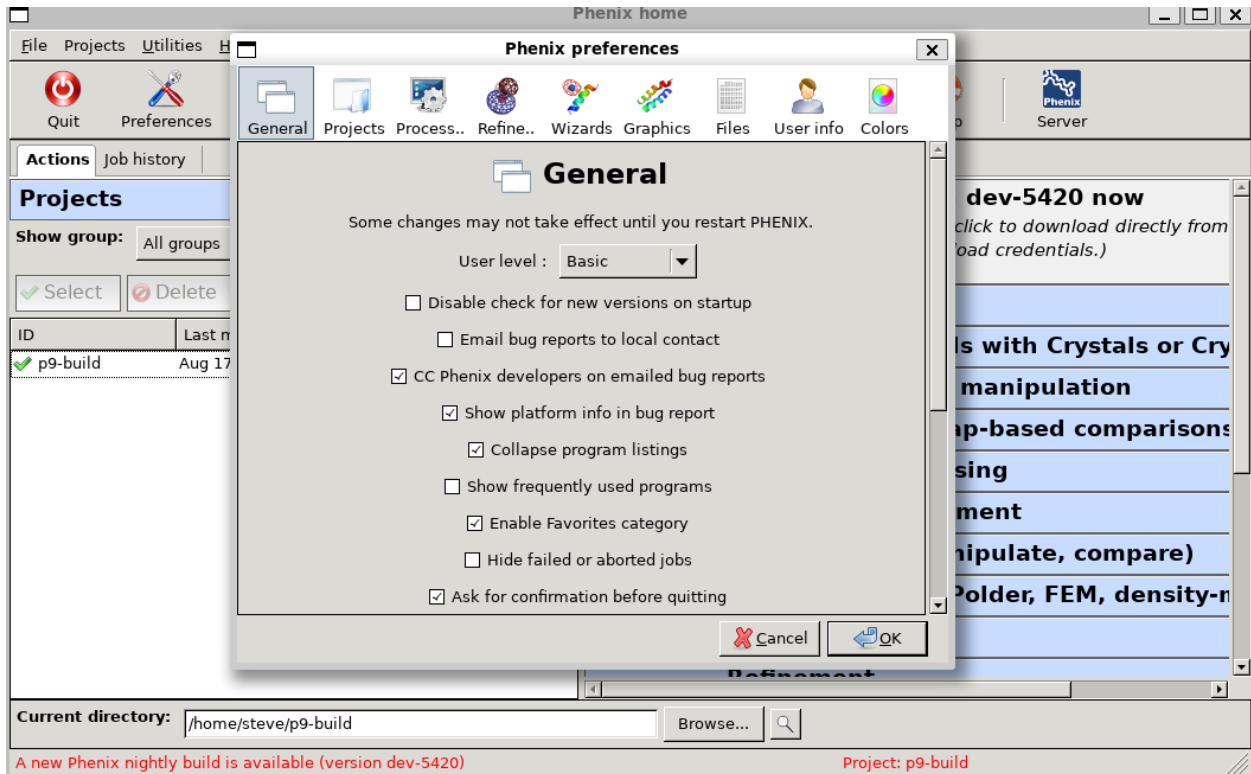


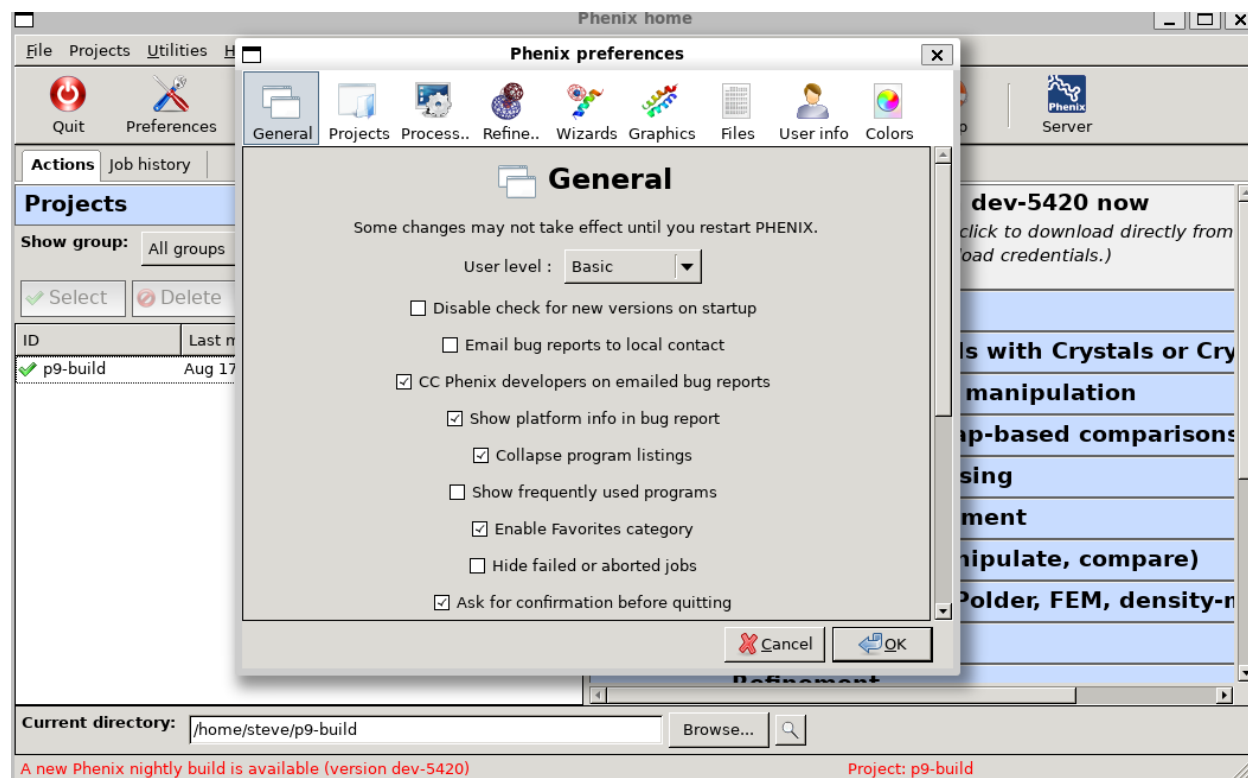
And you may have to set up tutorial data first before you can open the phenix window, but now the phenix window is working perfectly fine.

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.



Create project

Please choose a simple project ID (alphanumeric and underscore characters only) and project directory. The directory should not overlap with a previously defined project directory. Phenix will store settings and files specific to this project in a subdirectory named '.phenix'.

Project ID :

Project directory :

Sequence file :

Add to group :

Switch to this project

```
steve@StevenH: ~  
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd  
steve@StevenH:~$ ls  
Phenix                               phenix-1.21.1-5286  
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python  phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6  
p9-build  
steve@StevenH:~$ mkdir PhenixProjects
```

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

```

steve@StevenH: ~
LOCK prefs.params project_db.phil tmp
steve@StevenH:~/Phenix$ cd
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ cd phenix-1.21.1-5286/
steve@StevenH:~/phenix-1.21.1-5286$ pwd
/home/steve/phenix-1.21.1-5286
steve@StevenH:~/phenix-1.21.1-5286$ ^C
steve@StevenH:~/phenix-1.21.1-5286$ ^C
steve@StevenH:~/phenix-1.21.1-5286$ cd
steve@StevenH:~$ 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
steve@StevenH:~$ ^C
steve@StevenH:~$ export LIBGL_ALWAYS_INDIRECT=0
source /home/steve/phenix-1.21.1-5286/phenix_env.sh
steve@StevenH:~$ phenix

(main.py:2380): Gtk-WARNING **: 15:54:44.067: Attempting to store changes into `/home/steve/.local/share/recently-used.xbel', but failed: Failed to create file "/home/steve/.local/share/recently-used.xbel.VYLM52": No such file or directory

(main.py:2380): Gtk-WARNING **: 15:54:44.067: Attempting to set the permissions of `/home/steve/.local/share/recently-used.xbel', but failed: No such file or directory

(main.py:2380): Gtk-WARNING **: 15:56:08.042: Attempting to store changes into `/home/steve/.local/share/recently-used.xbel', but failed: Failed to create file "/home/steve/.local/share/recently-used.xbel.CGV0S2": No such file or directory

(main.py:2380): Gtk-WARNING **: 15:56:08.042: Attempting to set the permissions of `/home/steve/.local/share/recently-used.xbel', but failed: No such file or directory

```

```

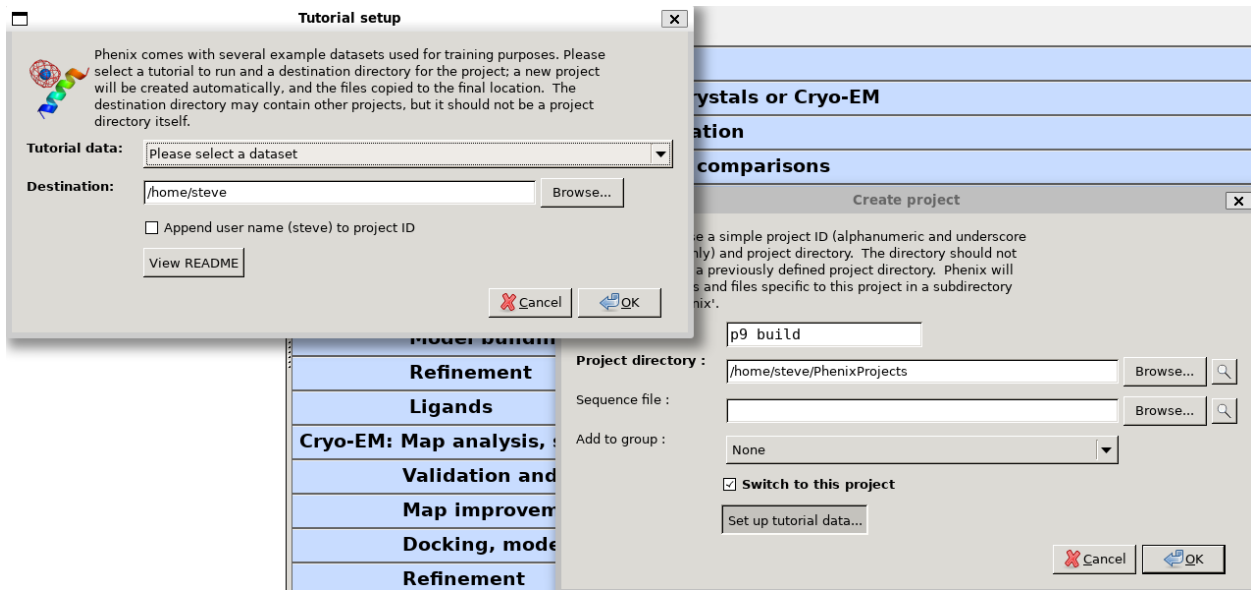
steve@StevenH: ~
steve@StevenH:/mnt/c/Users/steve/Downloads$ cd
steve@StevenH:~$ ls
Phenix                               phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
p9-build
steve@StevenH:~$ mkdir PhenixProjects
steve@StevenH:~$ ls
Phenix                               p9-build
PhenixProjects                       phenix-1.21.1-5286
coot-Linux-x86_64-ubuntu-20.04.4-gtk2-python phenix-installer-1.21.1-5286-intel-linux-2.6-x86_64-centos6
steve@StevenH:~$ |

```

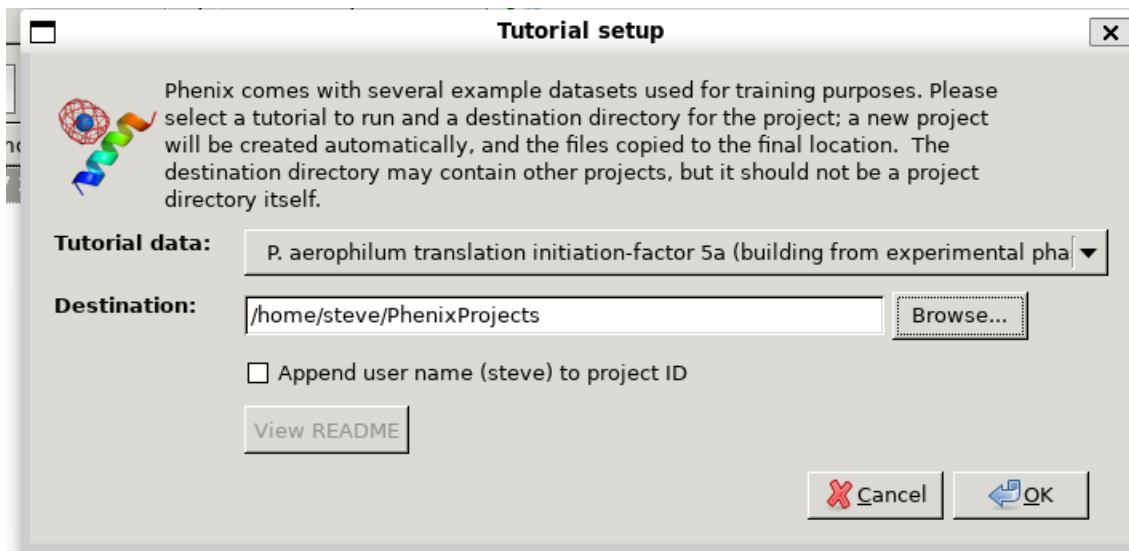
This PhenixProjects folder is where you will put your PHENIX projects into (because they cannot be out in the open in your root directory)

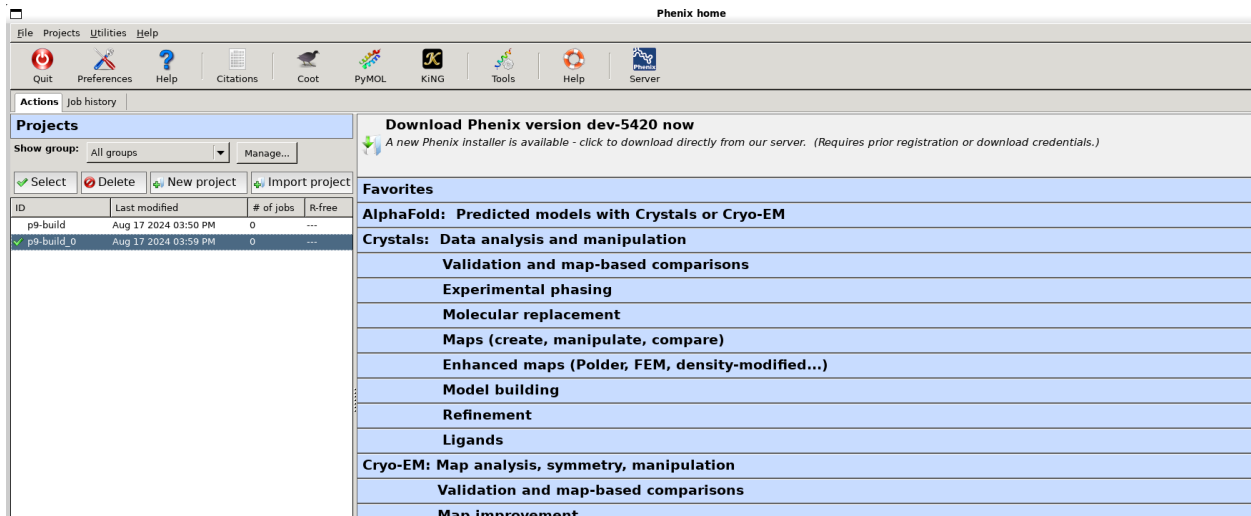
You can make a new directory in your root directory by typing: **mkdir PhenixProjects**

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



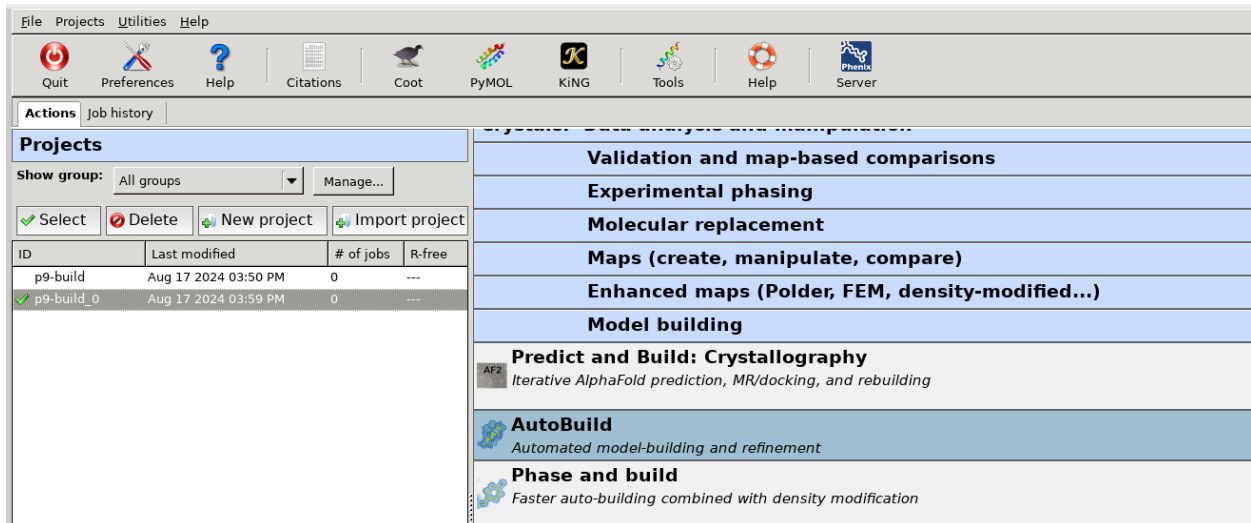
The only tutorial data under BUILDING:



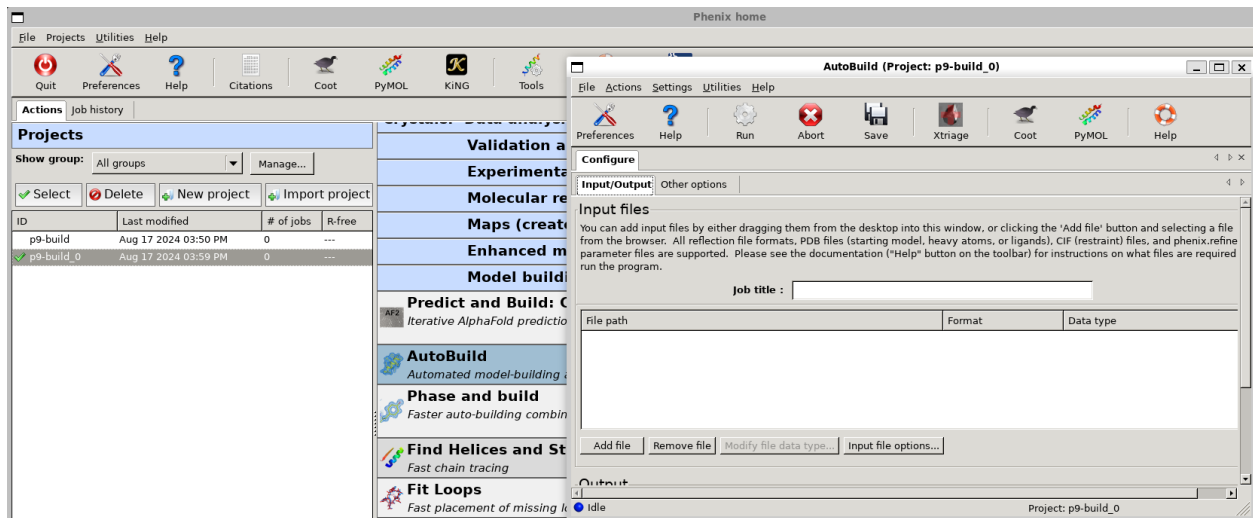


Now click ok and go to this one, double click.

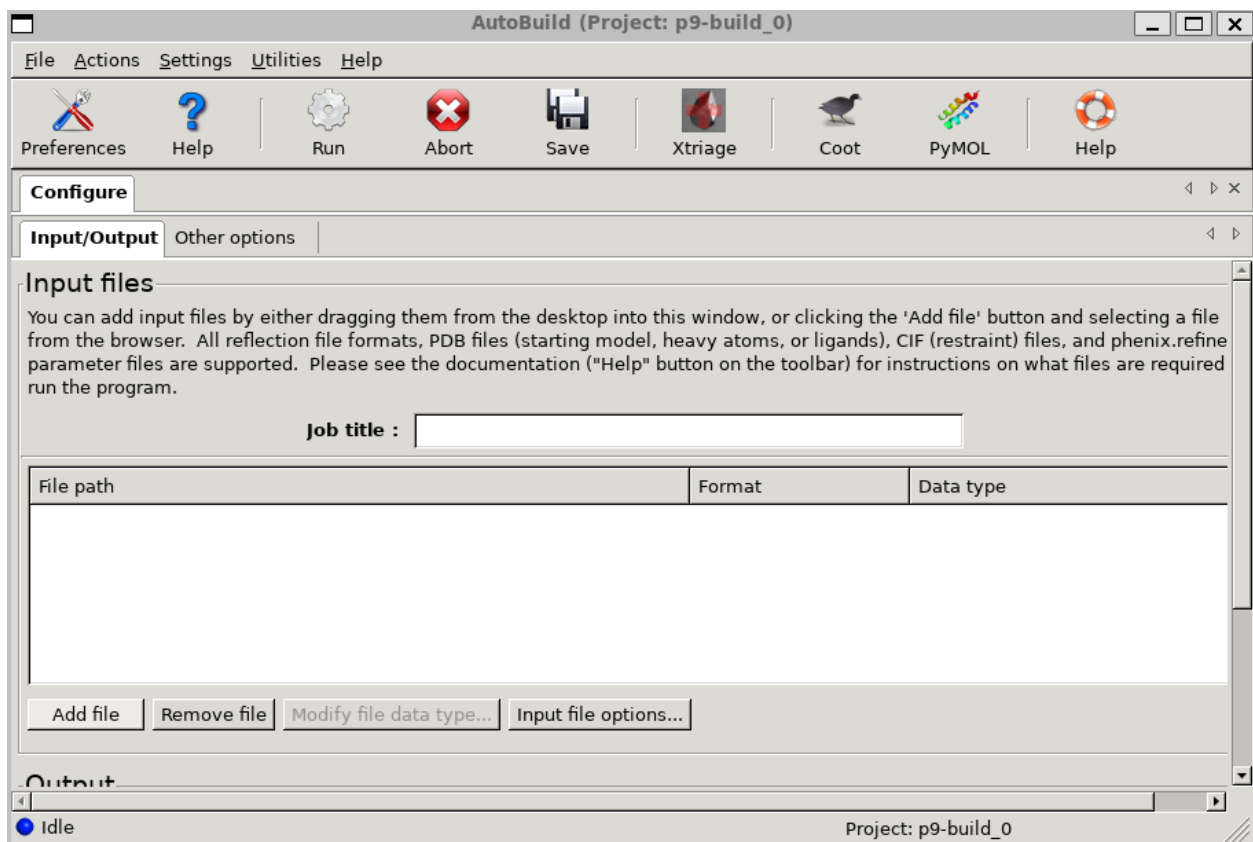
Then click Model Building and go to AutoBuild:

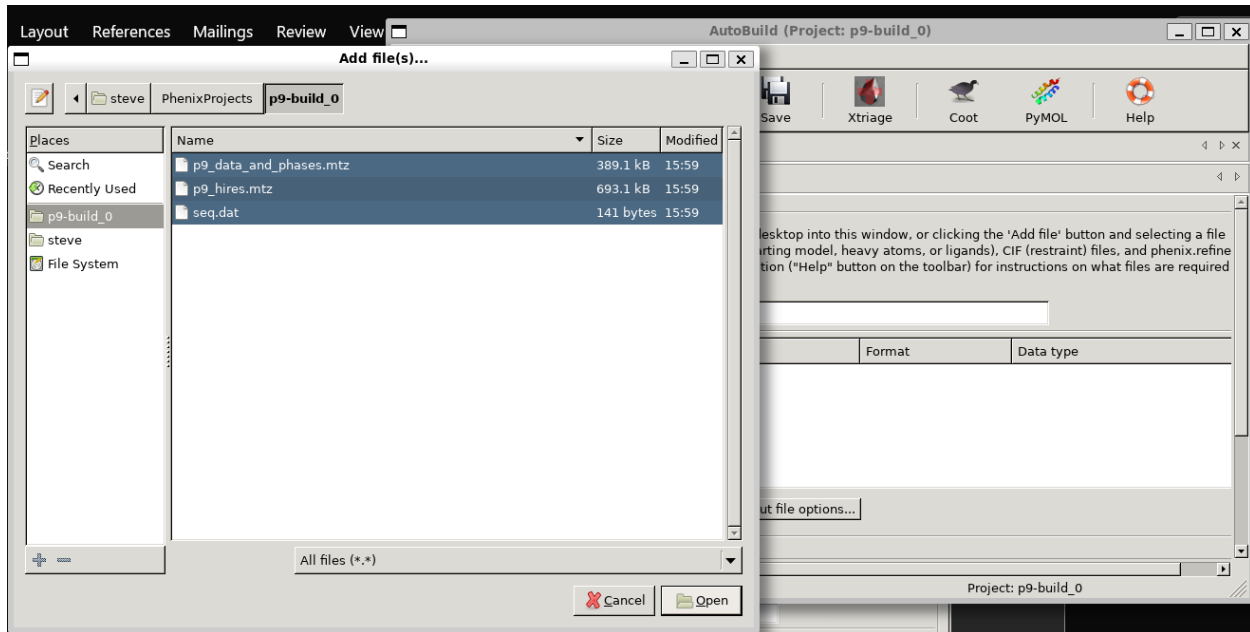


and click on it

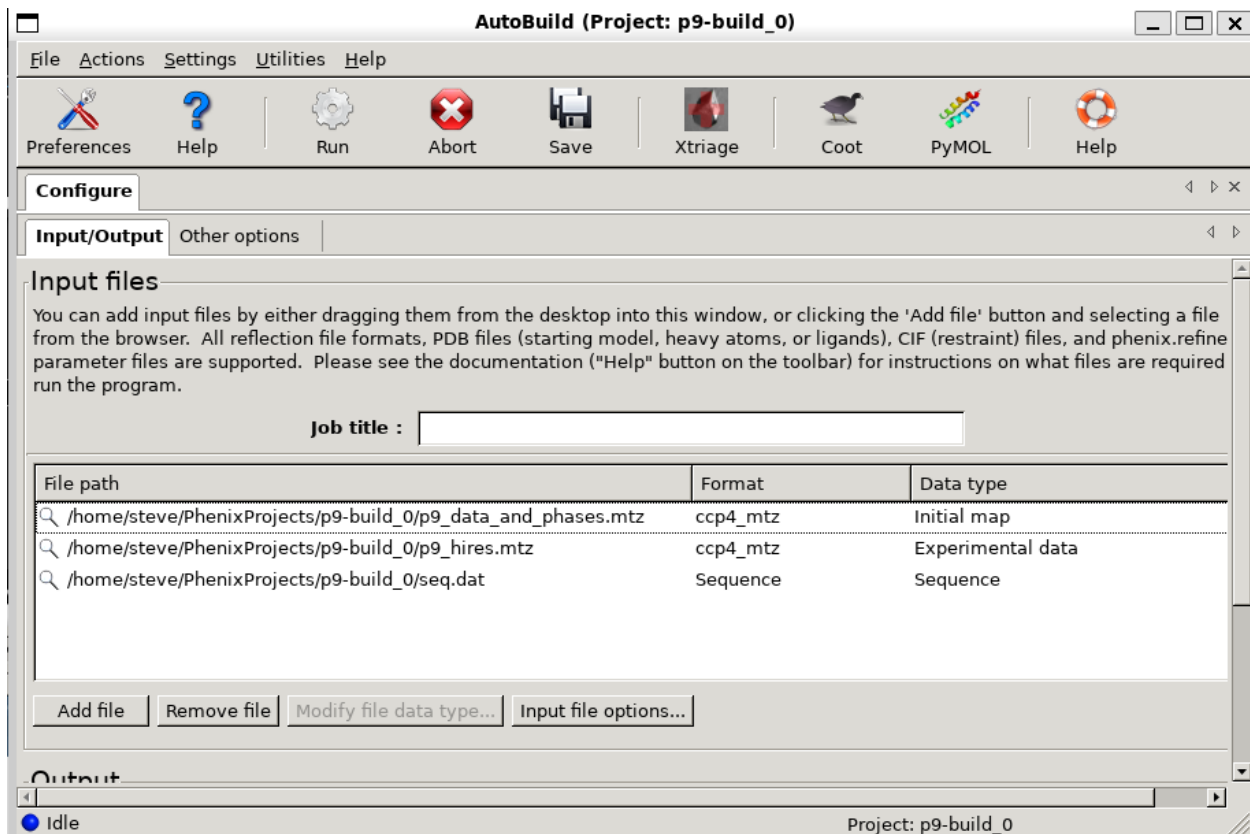


Follow the tutorial here: <https://youtu.be/og3TM9Cwve0?si=iqtepsk4G8bu0VZ1> or follow along on this document as well:



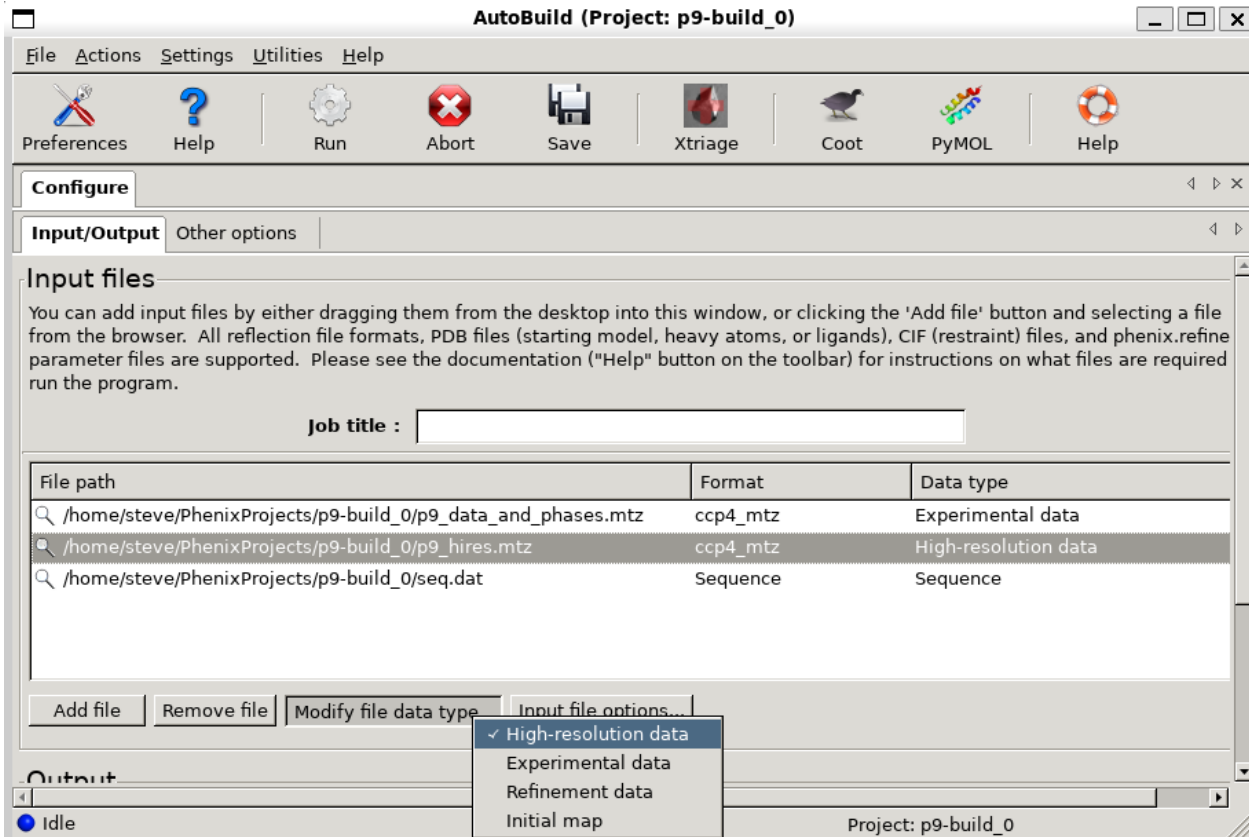


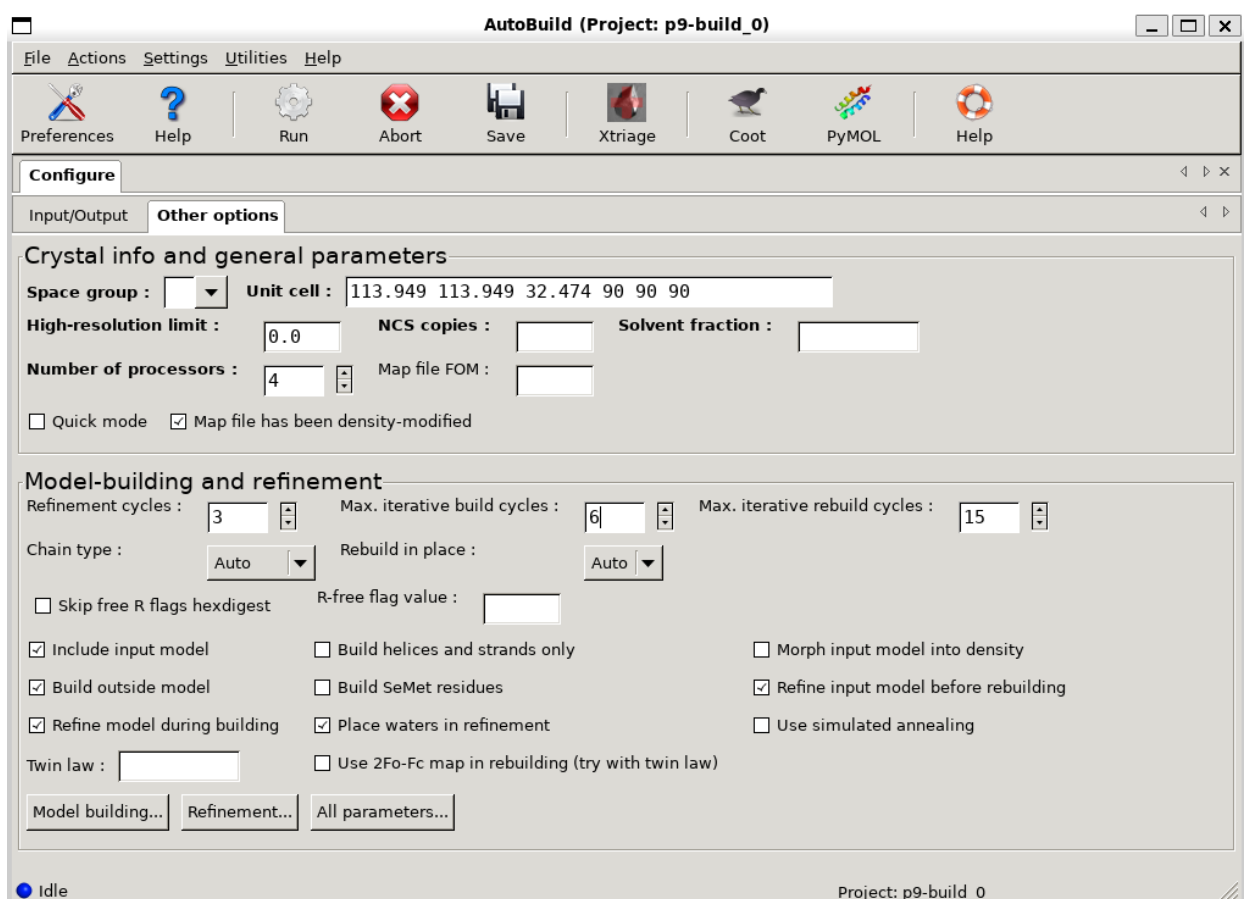
And click open



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:





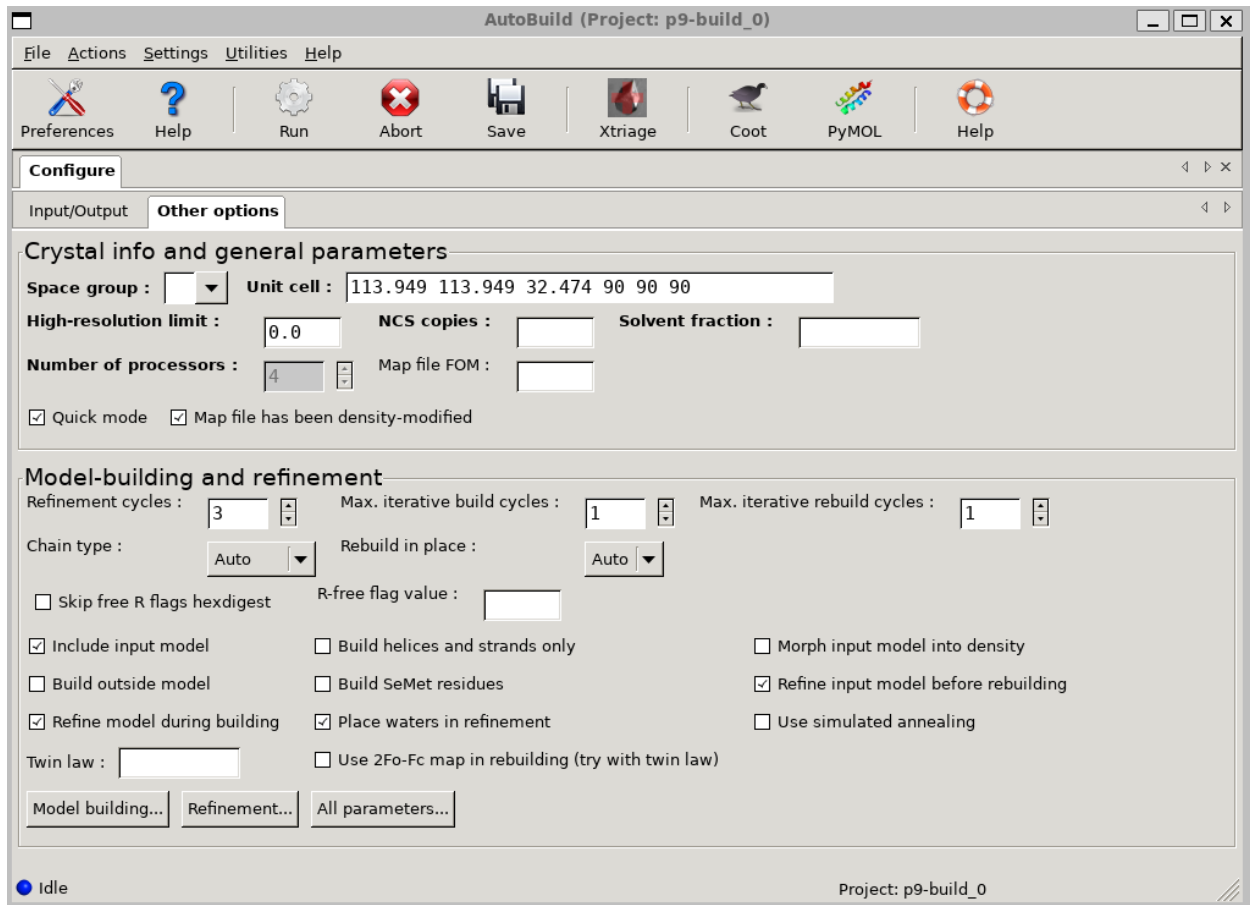
This is the original

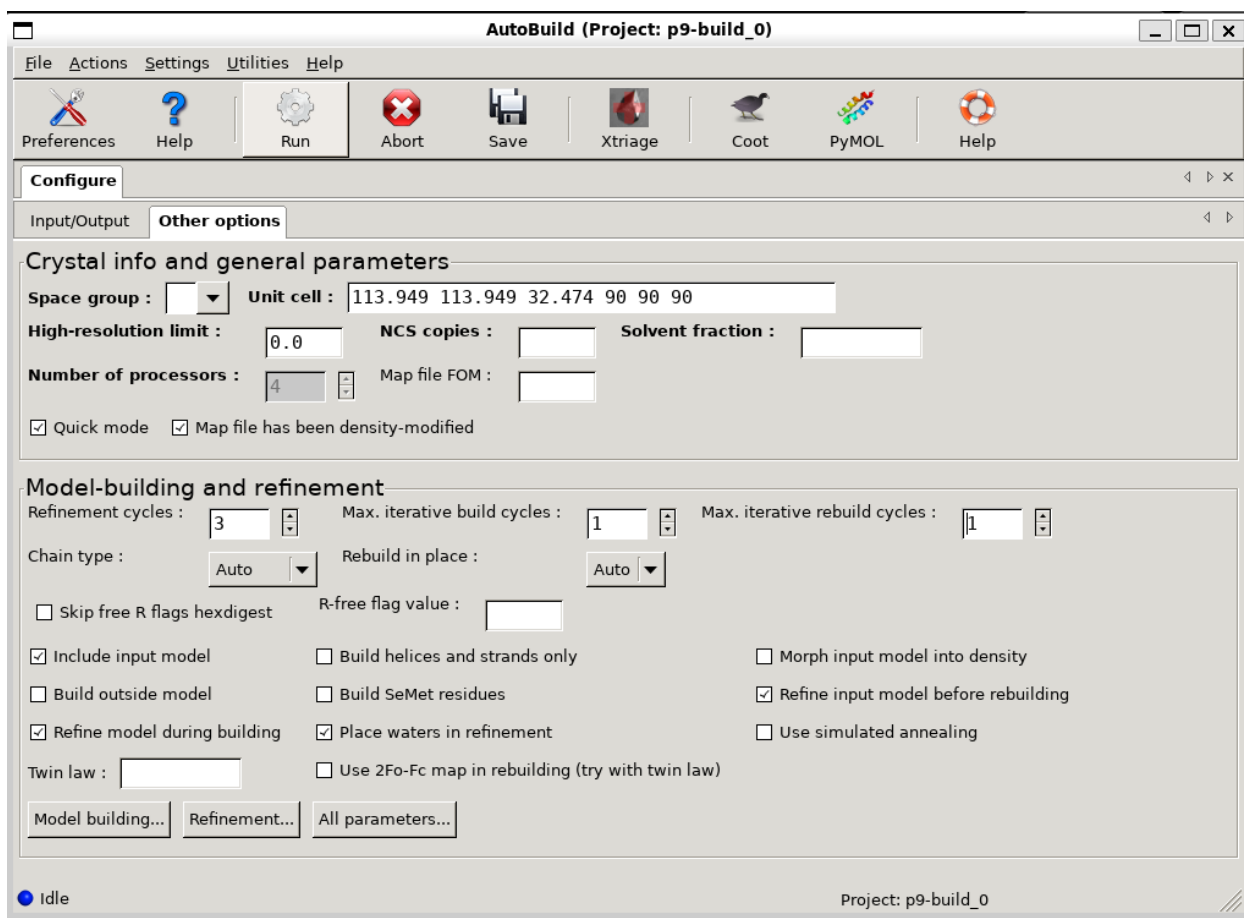
Just check “quick mode”

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

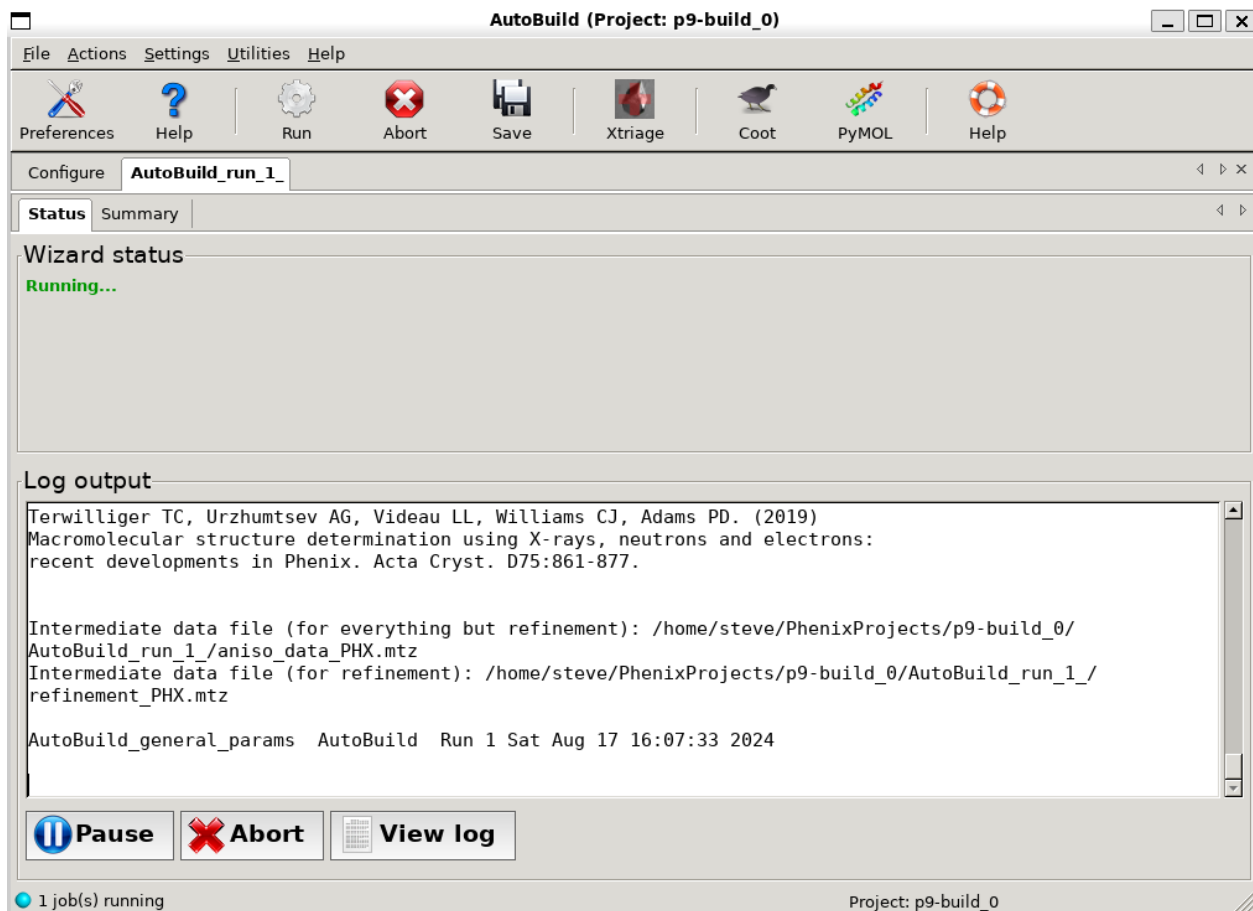
Change the “max iterative rebuild cycles” to 1 from 15

Un-check “build outside model”

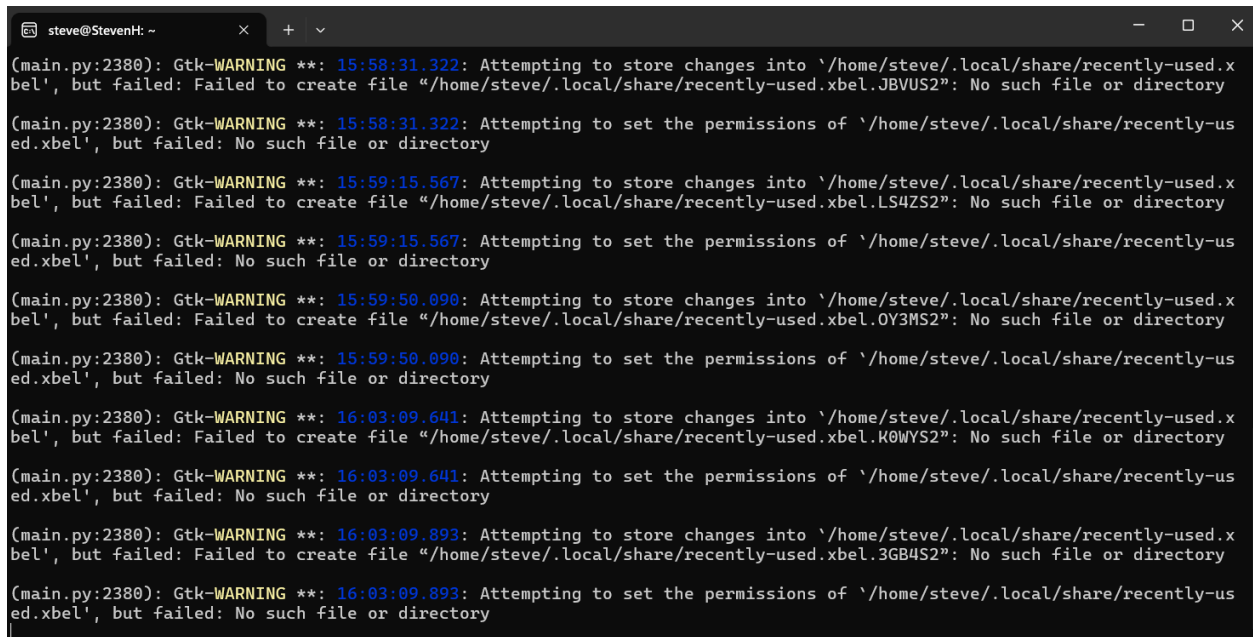




Now click run



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



The screenshot shows the AutoBuild software interface for project 'p9-build_0'. The window title is 'AutoBuild (Project: p9-build_0)'. The menu bar includes 'File', 'Actions', 'Settings', 'Utilities', and 'Help'. The toolbar contains icons for Preferences, Help, Run, Abort, Save, Xtrriage, Coot, PyMOL, and another Help icon. The 'Configure' tab is set to 'AutoBuild_run_1_'. The 'Status' tab is set to 'Summary'. The 'Output files' section shows a directory path: '/home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1_'. A table lists one file: 'AutoBuild_run_1_1.log' with contents 'AutoBuild log'. To the right of the table are buttons for 'Open in Coot' and 'Open in PyMOL'. The 'Data analysis' section states: 'AutoBuild has analyzed your X-ray data with Xtrriage. This will indicate whether you have any pathologies such as twinning or pseudosymmetry, as well as providing information on data quality and anomalous signal.' Below this text are buttons for 'Xtrriage log file' and 'Results and graphs'. At the bottom left, it says '1 job(s) running' and at the bottom right, 'Project: p9-build_0'.

AutoBuild (Project: p9-build_0)

File Actions Settings Utilities Help

Preferences Help Run Abort Save Xtrriage 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 Xtrriage. This will indicate whether you have any pathologies such as twinning or pseudosymmetry, as well as providing information on data quality and anomalous signal.

Xtrriage log file Results and graphs

1 job(s) running Project: p9-build_0

The screenshot shows the AutoBuild software interface for project 'p9-build_0'. The window title is 'AutoBuild (Project: p9-build_0)'. The menu bar includes 'File', 'Actions', 'Settings', 'Utilities', and 'Help'. The toolbar contains icons for Preferences, Help, Run, Abort, Save, Xtrriage, Coot, PyMOL, and Help. The 'Configure' dropdown is set to 'AutoBuild_run_1_'. The 'Status' bar shows 'Summary', 'Model-building', and 'Structure status'. The 'Output files' section displays a table with one entry: 'AutoBuild_run_1_1.log' with contents 'AutoBuild log'. To the right of the table are buttons for 'Open in Coot' and 'Open in PyMOL'. The 'Data analysis' section explains that Xtrriage has analyzed the X-ray data for pathologies like twinning or pseudosymmetry. It includes buttons for 'Xtrriage log file' and 'Results and graphs'. At the bottom left, a green dot indicates '1 job(s) running'. At the bottom right, it says 'Project: p9-build_0'.

AutoBuild (Project: p9-build_0)

File Actions Settings Utilities Help

Preferences Help Run Abort Save Xtrriage 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

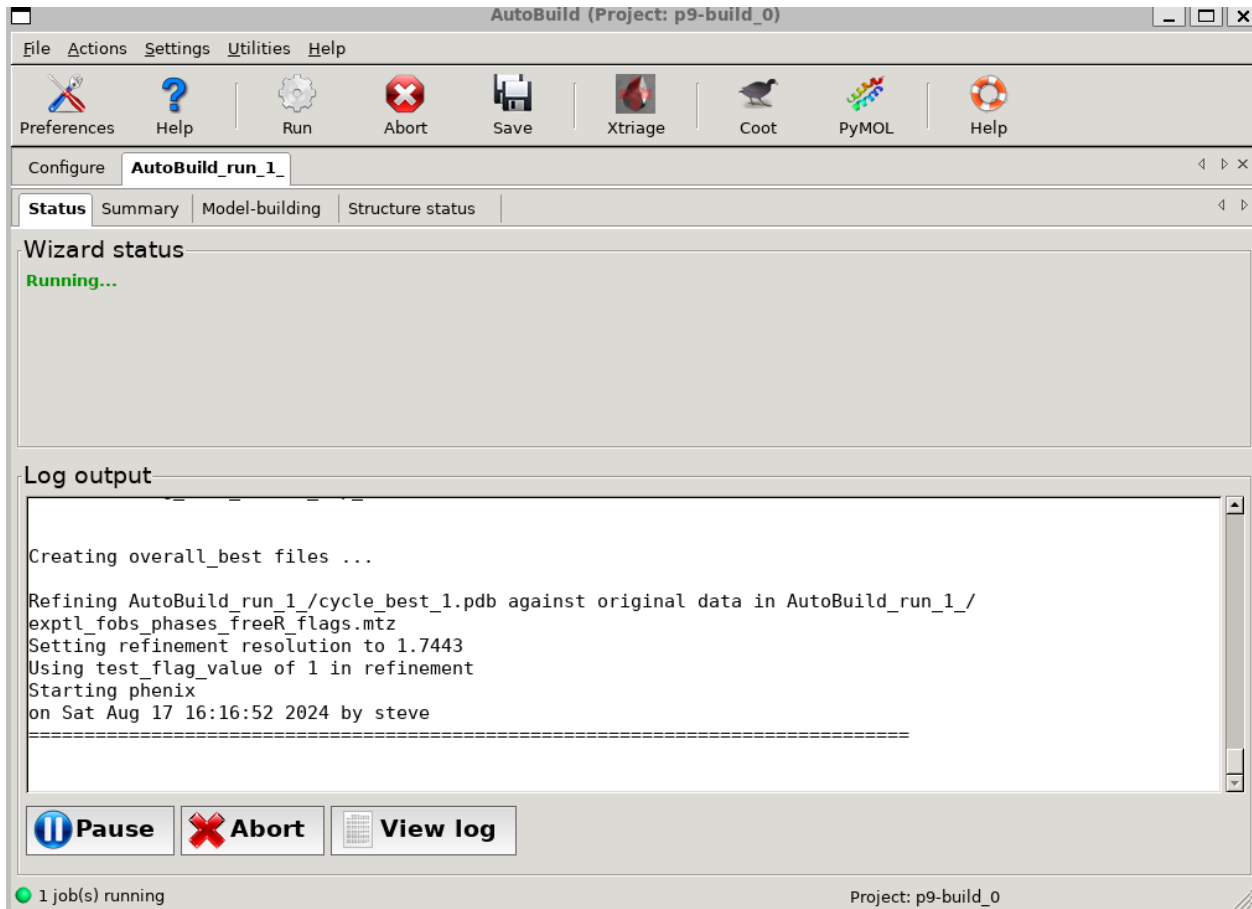
Open in PyMOL

Data analysis

AutoBuild has analyzed your X-ray data with Xtrriage. This will indicate whether you have any pathologies such as twinning or pseudosymmetry, as well as providing information on data quality and anomalous signal.

Xtrriage 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:

The screenshot shows the AutoBuild software interface for a project named 'p9-build_0'. The main window has a menu bar (File, Actions, Settings, Utilities, Help) and a toolbar with icons for Preferences, Help, Run, Abort, Save, Xtrriage, Coot, PyMOL, and another Help icon. Below the toolbar is a configuration bar for 'AutoBuild_run_1_'. The main area is divided into sections: 'Output files' and 'Data analysis'. The 'Output files' section shows a directory path and a table with one entry: 'AutoBuild_run_1_1.log' with contents 'AutoBuild log'. To the right of this table are buttons for 'Open in Coot' and 'Open in PyMOL'. The 'Data analysis' section contains text about Xtrriage analysis and buttons for 'Xtrriage log file' and 'Results and graph'. A 'Starting Coot' dialog box is overlaid on the interface, containing the text: 'Coot is being started with the Phenix extensions pre-loaded. Depending on computer speed, it may take several seconds for the program to open.' Below this text is a checkbox labeled 'Don't show this message again' and buttons for 'Cancel' and 'OK'. At the bottom left of the main window, it says '1 job(s) running' and at the bottom right, 'Project: p9-build_0'.

AutoBuild (Project: p9-build_0)

File Actions Settings Utilities Help

Preferences Help Run Abort Save Xtrriage 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 Xtrriage. This will indicate pseudosymmetry, as well as providing information on data quality a

Xtrriage log file Results and graph

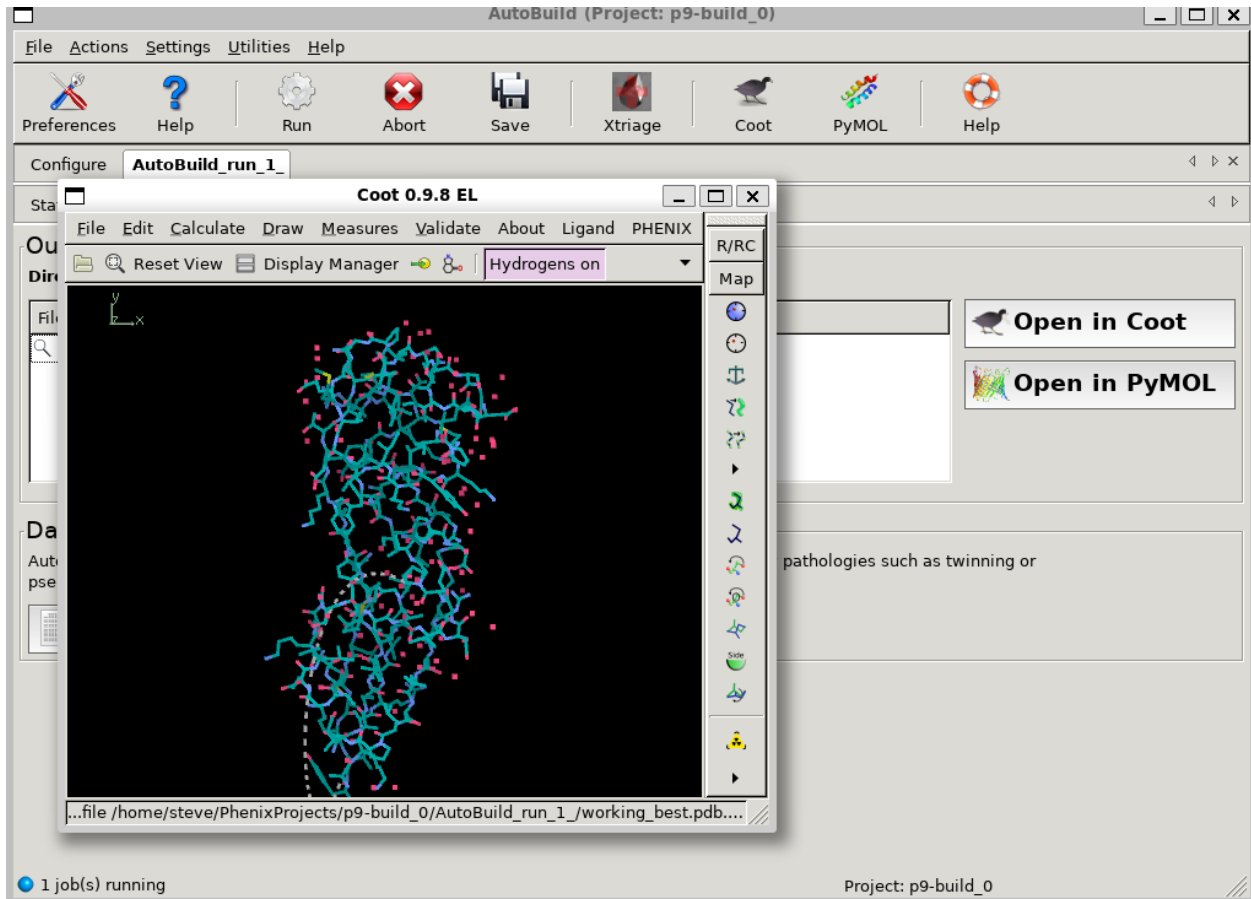
Starting Coot

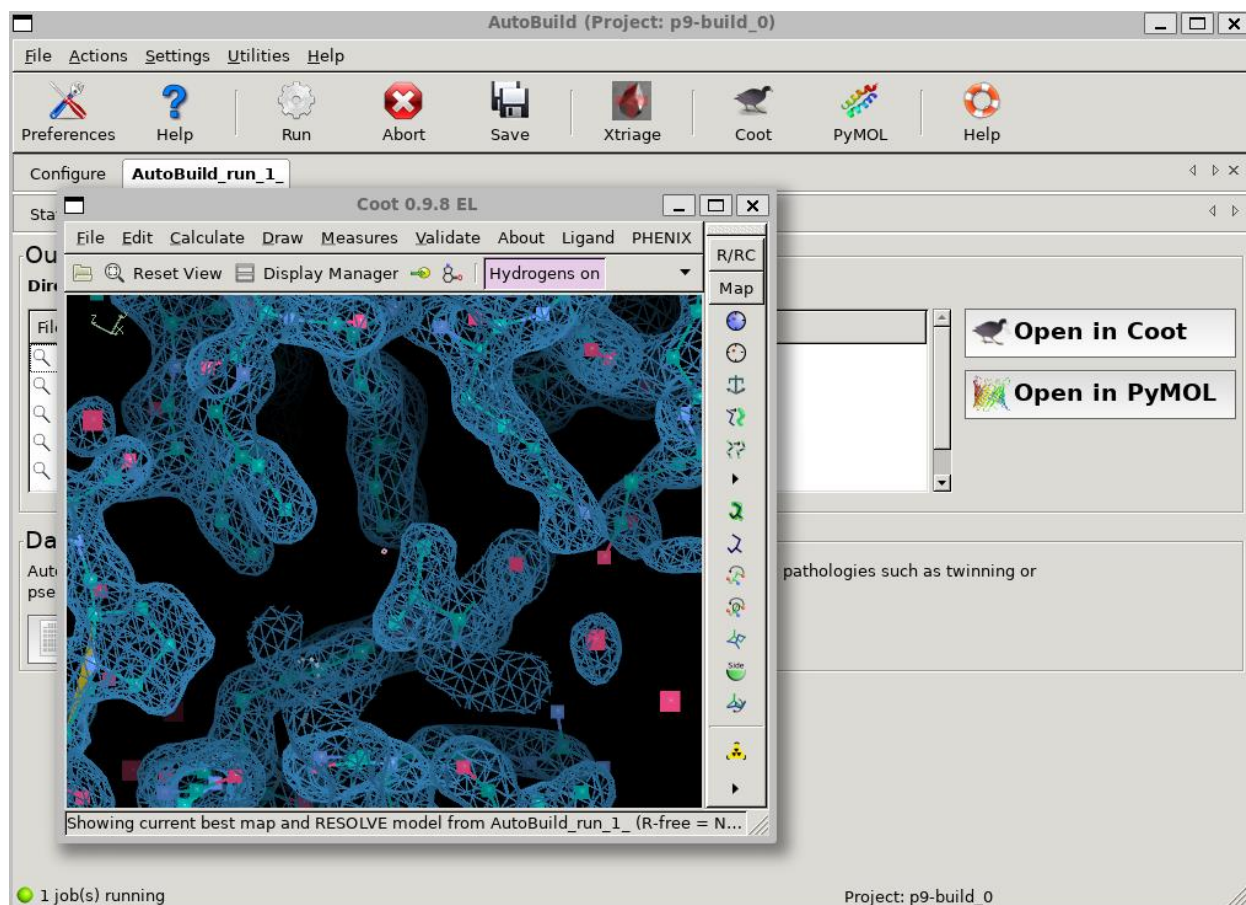
Coot is being started with the Phenix extensions pre-loaded. Depending on computer speed, it may take several seconds for the program to open.

Don't show this message again

Cancel OK

1 job(s) running Project: p9-build_0





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_coefs.mtz	Best refined maps (2Fo-Fc, Fo-Fc)
overall_best_denmod_map_coefs.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 Xtrriage 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	XXXXXXXXXXXXVEAGELKEGSYVVIDGEPXXXXXXXXXXXXAKARI	50
51	VAVGVFDGGKRTLSPVDAQVEVPIIEKFTAQILSVSGDVIQLMDMRDYK	100
101	TIEVPMKYVEEEAKGRLAPGAEVEVWQILDYKII	150

1 job(s) running Project: p9-build_0

The screenshot displays the AutoBuild software interface for a project named 'p9-build_0'. The window title is 'AutoBuild (Project: p9-build_0)'. The menu bar includes 'File', 'Actions', 'Settings', 'Utilities', and 'Help'. The toolbar contains icons for 'Preferences', 'Help', 'Run', 'Abort', 'Save', 'Xtrriage', 'Coot', 'PyMOL', and another 'Help' icon. Below the toolbar is a 'Configure' section with a dropdown menu set to 'AutoBuild_run_1_'. A tabbed interface shows 'Status' as the active tab, with other tabs for 'Summary', 'Model-building', and 'Structure status'. The 'Wizard status' section indicates the process is 'Running...'. The 'Log output' section contains the following text:

```
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)
```

At the bottom of the log output section, there are three buttons: 'Pause' (with a pause icon), 'Abort' (with a red 'X' icon), and 'View log' (with a document icon). The status bar at the bottom left shows '1 job(s) running' with a green dot, and the bottom right shows 'Project: p9-build_0'.

The screenshot displays the AutoBuild software interface for a project named 'p9-build_0'. The window title is 'AutoBuild (Project: p9-build_0)'. The menu bar includes 'File', 'Actions', 'Settings', 'Utilities', and 'Help'. The toolbar contains icons for 'Preferences', 'Help', 'Run', 'Abort', 'Save', 'Xtrriage', 'Coot', 'PyMOL', and another 'Help' icon. Below the toolbar, there are tabs for 'Configure' (selected), 'AutoBuild_run_1_', 'Status', 'Summary', 'Model-building', and 'Structure status'. The 'Status' tab is active, showing 'Wizard status' as 'Running...'. The 'Log output' section contains the following text:

```
'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 (2F0FCWT PH2F0FCWT)  
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)
```

At the bottom of the log output section, there are three buttons: 'Pause', 'Abort', and 'View log'. The status bar at the bottom left shows '1 job(s) running' and the bottom right shows 'Project: p9-build_0'.

The screenshot shows the AutoBuild software interface for a project named 'p9-build_0'. The window title is 'AutoBuild (Project: p9-build_0)'. The menu bar includes 'File', 'Actions', 'Settings', 'Utilities', and 'Help'. The toolbar contains icons for 'Preferences', 'Help', 'Run', 'Abort', 'Save', 'Xtrriage', 'Coot', 'PyMOL', and 'Help'. Below the toolbar is a 'Configure' section with a dropdown menu set to 'AutoBuild_run_1_'. The main area is divided into tabs: 'Status', 'Summary', 'Model-building', and 'Structure status'. The 'Status' tab is active, displaying 'Wizard status' as 'FINISHED'. Below this is a 'Log output' window showing a list of files and a message: 'Done cleaning up ...'. At the bottom of the window, there are three buttons: 'Pause', 'Abort', and 'View log'. The status bar at the bottom left shows 'Idle' and the bottom right shows 'Project: p9-build_0'.

AutoBuild (Project: p9-build_0)

File Actions Settings Utilities Help

Preferences Help Run Abort Save Xtrriage 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_xtrriage_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_xtrriage.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_xtrriage.log'}) to  
AutoBuild_run_1/working_files  
Done cleaning up ...
```

Pause Abort View log

Idle Project: p9-build_0

The screenshot shows the AutoBuild software interface for Project: p9-build_0. The main window displays the Summary tab, which provides a comprehensive overview of the current project's status and results.

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...

Data analysis
AutoBuild has analyzed your X-ray data with Xtrriage. This will indicate whether you have any pathologies such as twinning or pseudosymmetry, as well as providing information on data quality and anomalous signal.

Warnings
NOTE: Free R Flag (FreeR_flag) in input data file will not be used as a hires or refinement file is present

Final model

R-work:	0.2384	R-free:	0.2571	CC:	---
Residues:	121	Fragments:	3	Waters:	110
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:

```
Model 1 had 0 links
INFO:: NCS chain comparison 0/113
INFO:: in run_post_read_model_hook() pFunc 0x55dc521bdc80 is not callable
INFO:: in run_post_read_model_hook() pDict 0x7fe8f0110170
INFO:: in run_post_read_model_hook() pModule 0x7fe8f010f1d0
Molecule 2 read successfully
INFO:: Command: (set-molecule-bonds-colour-map-rotation 2 30.00)
coot_phenix_interface.load_ccp4_style_map(/home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1/overall_best_denmod_map
_coeffs.mtz)
INFO:: Command: (set-colour-map-rotation-for-map 0.00)
INFO:: Command: (make-and-draw-map "/home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1/overall_best_denmod_map_coeff
s.mtz" "/crystal/dataset/FWT" "/crystal/dataset/PHWT" "" 0 0)
INFO:: making map from mtz filename /home/steve/PhenixProjects/p9-build_0/AutoBuild_run_1/overall_best_denmod_map_coeff
s.mtz
INFO:: Number of observed reflections: 21369
INFO:: finding ASU unique map points with sampling rate 1.8
INFO:: grid sampling...Nuvw = ( 240, 240, 72)
Pre-filter Map statistics: mean: 1.667e-06 st.d: 0.1233
Pre-filter Map statistics: min: -0.3574 max: 2.943
INFO:: n grid points: 518472
INFO:: mean before filtering: 1.667e-06
INFO:: variance before filtering: 0.01521
INFO:: filter by ignoring 2135 of 518472 counts ( = 0.4118%) with values around -0.001768 bounds -0.001933 -0.001603 fro
m bin-number 1077 of 10000
Post-filter Map statistics: mean: 8.813e-06 st.d: 0.1236
Post-filter Map statistics: min: -0.3574 max: 2.943
Map extents: ..... 240 240 72
Map mean: ..... 8.813e-06
Map sigma: ..... 0.1236
Map maximum: ..... 2.943
```

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

```
steve@StevenH: /mnt/c/Wind x + v
steve@StevenH:/mnt/c/Windows/system32$ python3 --version
Python 3.10.12
steve@StevenH:/mnt/c/Windows/system32$ |
```

\$ sudo apt-get update

\$ sudo apt-get install python3.6

```
steve@StevenH: /mnt/c/Wind x + v
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 x + v
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 x + v
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] |

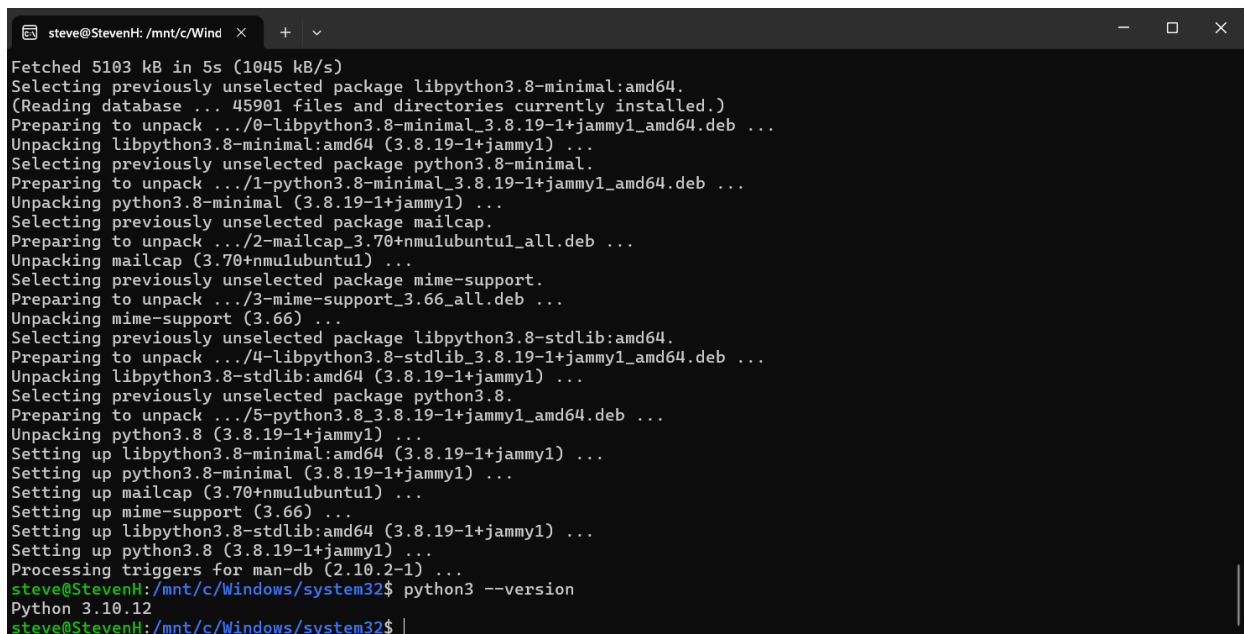
```

```

steve@StevenH: /mnt/c/Wind x + v
[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+nmulubuntu1_all.deb ...
Unpacking mailcap (3.70+nmulubuntu1) ...
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+nmulubuntu1) ...
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$ |

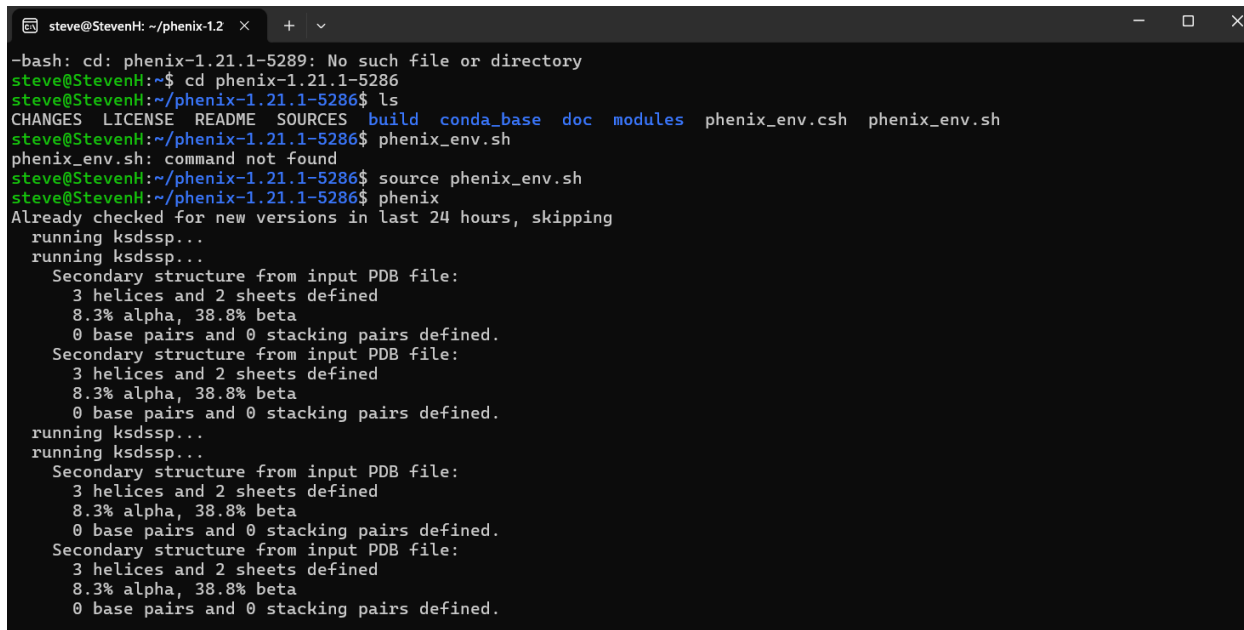
```

```
steve@StevenH: /mnt/c/Windows/system32$ python3 --version
Python 3.10.12
steve@StevenH: /mnt/c/Windows/system32$ |
```



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

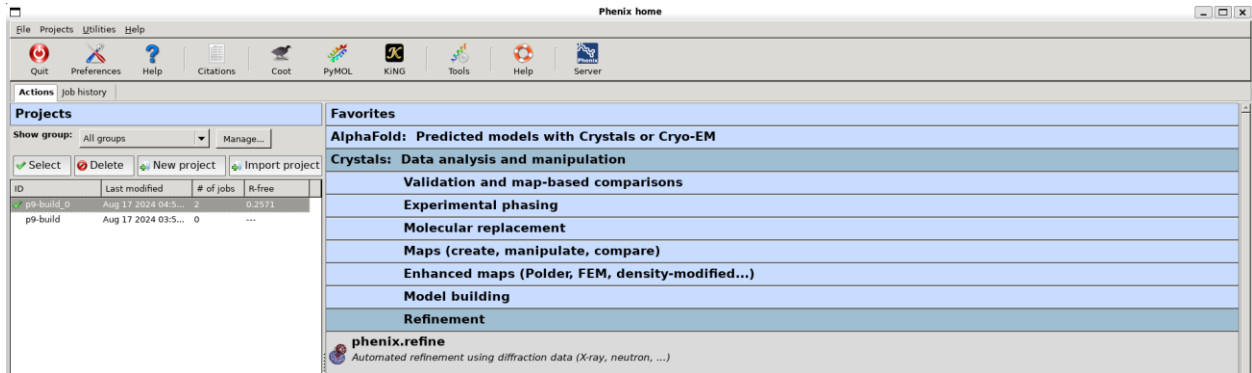
```
steve@StevenH: ~/phenix-1.21.1-5286$ ls
CHANGES LICENSE README SOURCES build conda_base doc modules phenix_env.csh phenix_env.sh
steve@StevenH: ~/phenix-1.21.1-5286$ phenix_env.sh
phenix_env.sh: command not found
steve@StevenH: ~/phenix-1.21.1-5286$ source phenix_env.sh
steve@StevenH: ~/phenix-1.21.1-5286$ 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.
```

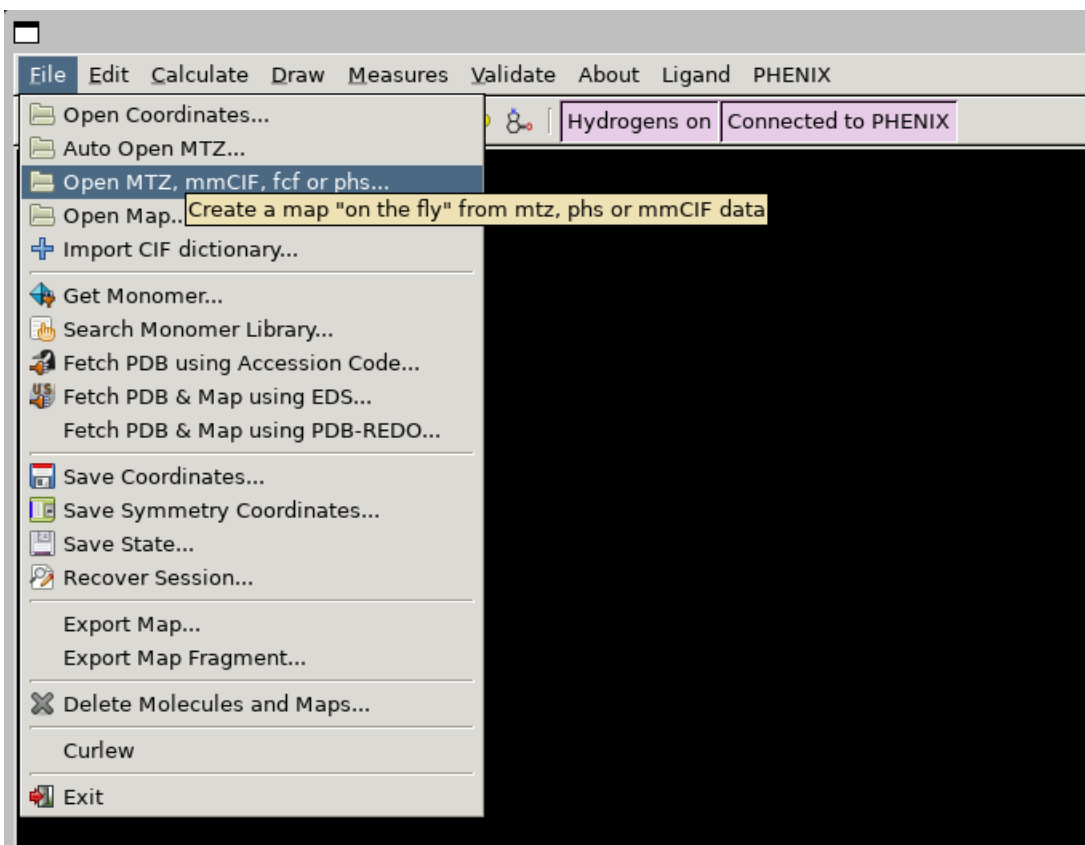
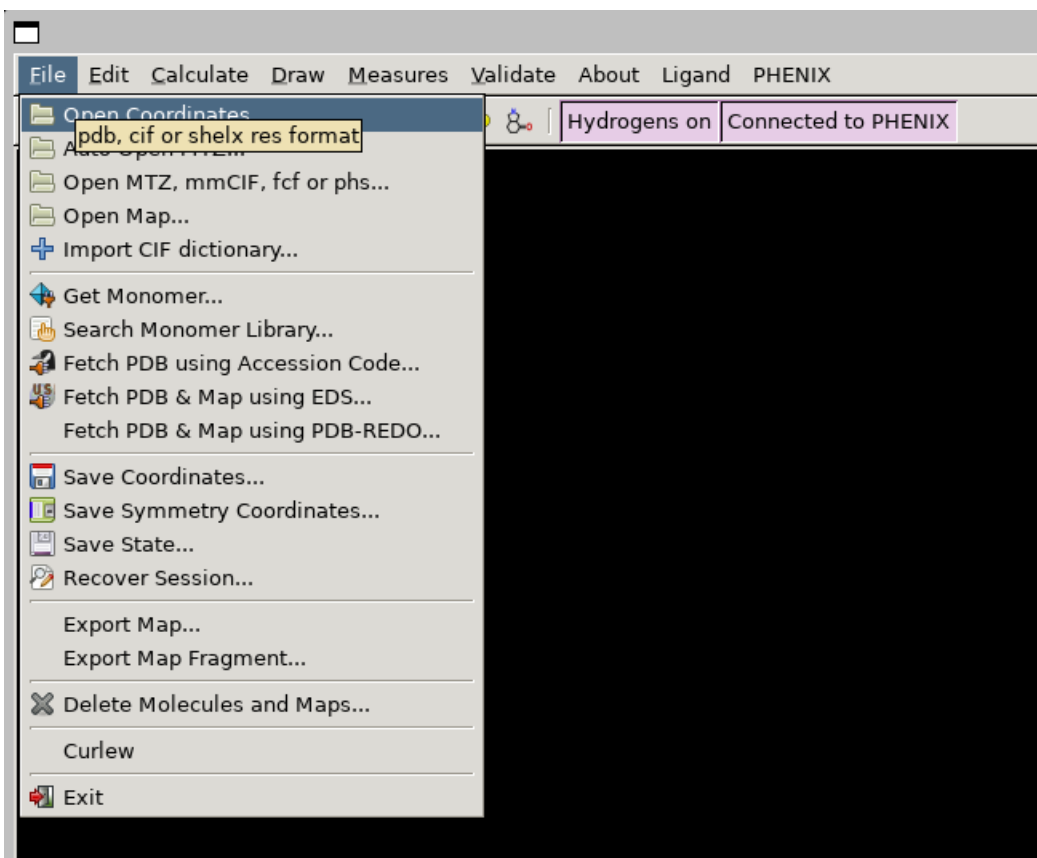


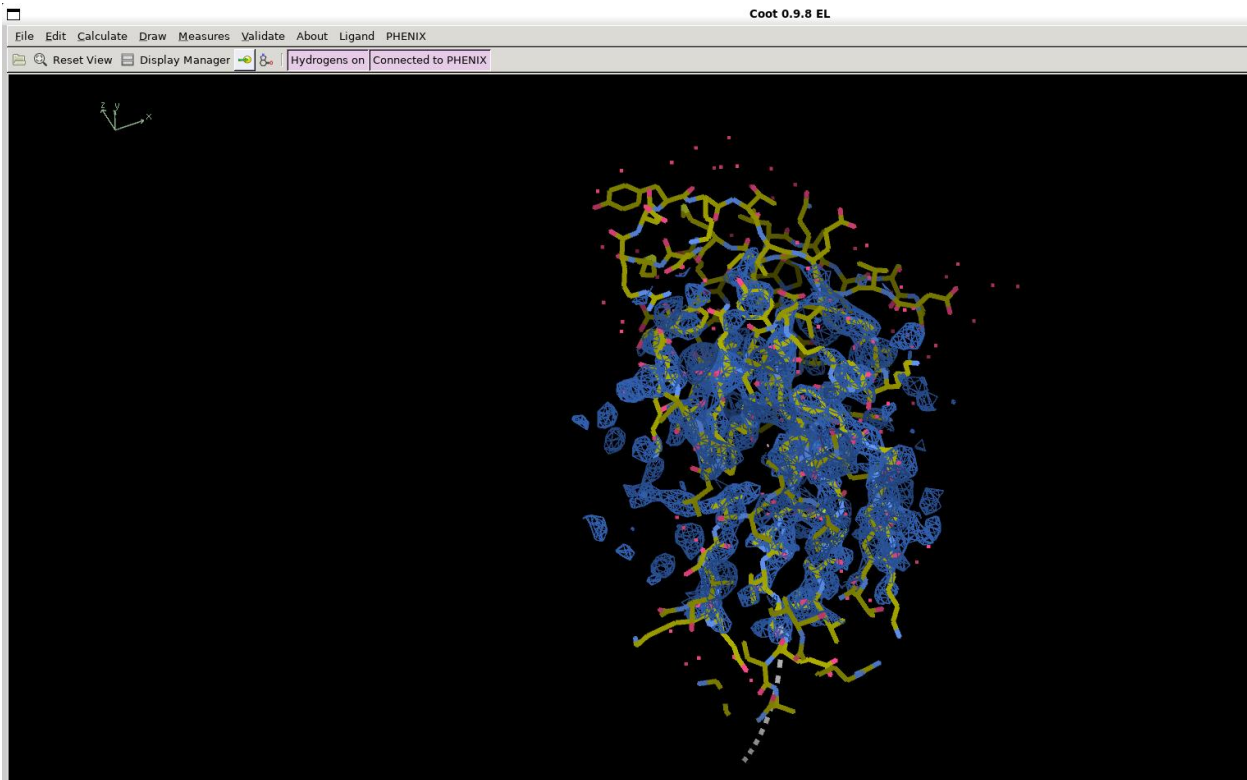
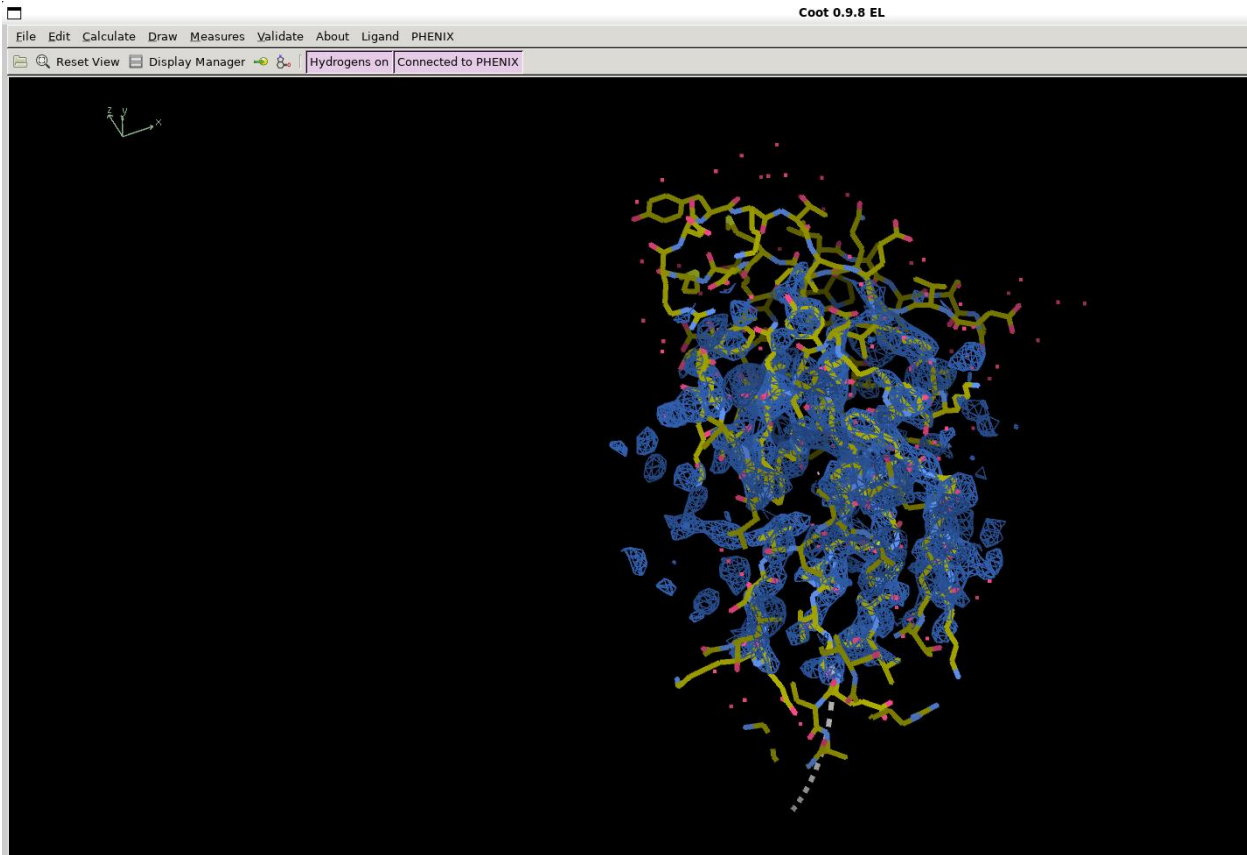
Now there are no more errors!!

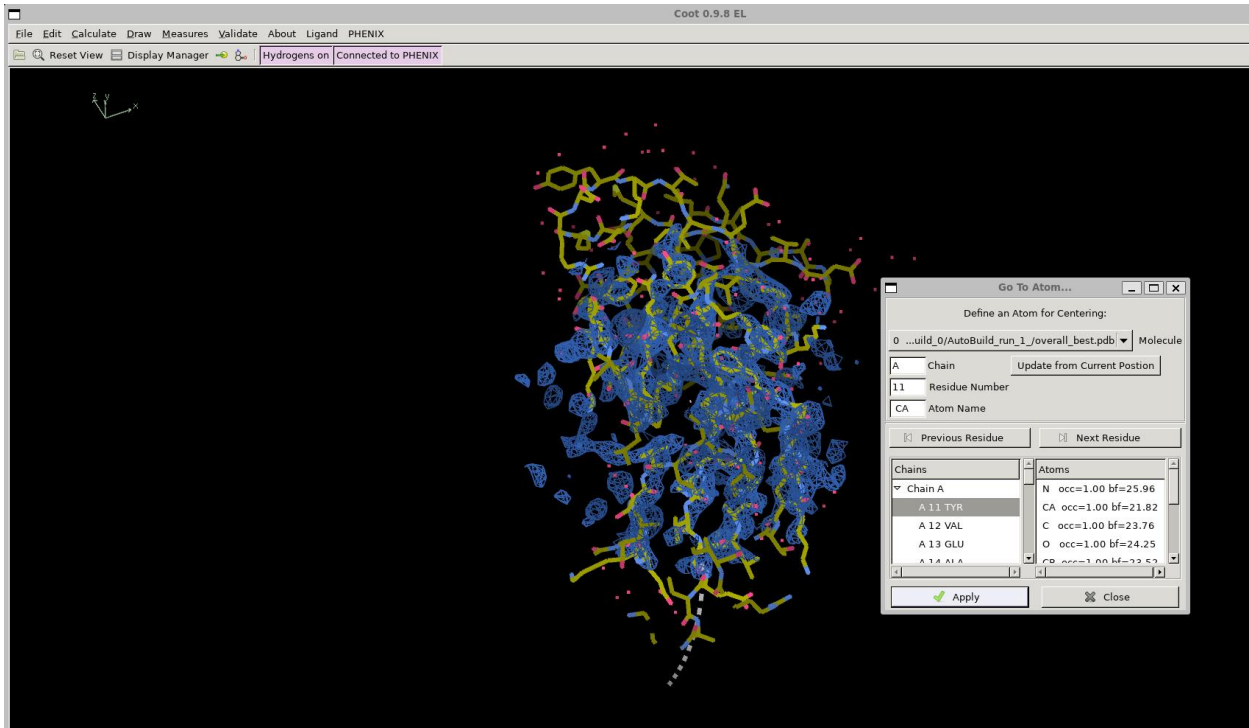

```
steve@StevenH: ~/phenix-1.2
-bash: cd: phenix-1.21.1-5289: No such file or directory
steve@StevenH:~$ cd phenix-1.21.1-5286
steve@StevenH:~/phenix-1.21.1-5286$ ls
CHANGES LICENSE README SOURCES build conda_base doc modules phenix_env.csh phenix_env.sh
steve@StevenH:~/phenix-1.21.1-5286$ phenix_env.sh
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.
```

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









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!!!!

