S²C² CCP-EM Workshop

Hosted online by the Stanford-SLAC Cryo-EM Center
10–13 November 2020

Computing setup instructions

Normally at our CCP-EM training workshops, participants use computers that we have set up in advance with the required software and tutorial data. Since we are running this workshop remotely, all of you will need to install the software yourselves on your own computers. Please do this well in advance so if there are any problems, we can help you solve them in plenty of time before the workshop. If you do run into any difficulties, please contact us at ccpem@stfc.ac.uk and we'll help you sort things out.

Required software

Linux or Mac operating system.

Note for Windows users: CCP-EM is not available for Windows. Please try to work on a Linux or Mac computer if possible (can you connect remotely to a computer at your lab?). If that's not possible, you could consider running Linux inside a virtual machine on Windows, for example by following these instructions: https://itsfoss.com/install-linux-in-virtualbox/. Everything should still run correctly in a virtual machine and you will be able to participate fully in the workshop, but programs will be slower and this can make highly interactive software (such as Coot and Chimera) harder to work with.

Please install the following software for the workshop:
- **CCP-EM** v1.5.0
  - Installation instructions and downloads on https://www.ccpem.ac.uk/download.php
- **CCP4** v7.1.007
  - Download from https://www.ccp4.ac.uk/download/
  - You can choose to install SHELX, ARP/wARP and other optional packages as part of the CCP4 installation. You won't need any of them for this workshop, but you can install them anyway if you might want to use them in future.
- **UCSF Chimera** v1.13 or later
  - Download from https://www.cgl.ucsf.edu/chimera/download.html. On Linux, please allow the Chimera installation script to put a symbolic link on your path, so CCP-EM can find it
- **Modeller**
  - On Linux, Modeller is included in the CCP-EM package, but you will still need to

register for a license key (free for academic use) at
https://salilab.org/modeller/registration.html. After you have your license key, go
to your `ccpem-1.5.0` directory and run `./install_modeller.sh`
- On Mac, you will need to install Modeller separately. Register and download
from https://salilab.org/modeller/. Please install it in the default installation
location so CCP-EM can find it.
- On Mac only: you will need to install **XQuartz** 2.7.11 from https://www.xquartz.org/

Required knowledge

For this workshop you'll need to be comfortable with simple operations on the Linux or Mac
command line (also sometimes called the shell, console or terminal). It will be helpful if you
are familiar with the following:
- Navigating the file system (`pwd`, `ls` and `cd` commands)
- Moving / copying files (`cp`, `mv` and `mkdir`)
- Extracting tar.gz files (`tar -xf file.tar.gz`)
- Running scripts in the current directory (`./script.sh`)
- Getting help on commands (`man command`, or try `command --help`)
- Viewing text files (`cat` or `less`)
- Simple job control (`bg`, `fg`, `jobs` and `ps` commands, and launching commands in the
background with `&`)

There are various tutorials online where you can learn about these. These two are useful for
covering most of the commands above:
- https://www.hostinger.com/tutorials/linux-commands
- https://www.digitalocean.com/community/tutorials/how-to-use-bash-s-job-control-to-manage-foreground-and-background-processes

but do note that the second of those goes into a bit more detail than we need. Please don't
be put off if this is new to you and it all seems too complicated! You won't need to do too
much on the command line, but since the workshop is running remotely and we have a large
number of participants, we won't be able to provide much individual help. It'll be very helpful if
you're familiar with the basics so you can sort out any simple problems yourself. It will be a
useful skill for working with many other scientific software packages, too.

We will also be using UCSF Chimera in the workshop, but we will not have time to teach you
how to use it. Chimera is a powerful program with many capabilities and features. We will
only use it in a very basic way in this workshop, to view and examine cryo-EM maps and
models. There are many tutorials and a Getting Started guide available on the Chimera
website (https://www.cgl.ucsf.edu/chimera/) but if you're not familiar with Chimera I suggest
you just have a look at the GroEL tutorial
(https://www.rbvi.ucsf.edu/chimera/data/tutorials/groel/groel.html) to learn how to open maps
and models, move the view around and make simple changes to the way objects are
displayed.

Checking everything is working

Please run through these instructions to check your software is installed and working correctly. (Lines written in `source code` font are commands to be typed into your terminal window.)

1. Open a Terminal window
2. Go to your CCP-EM installation directory. For example, if you unpacked CCP-EM in a directory called "software" in your user home directory:
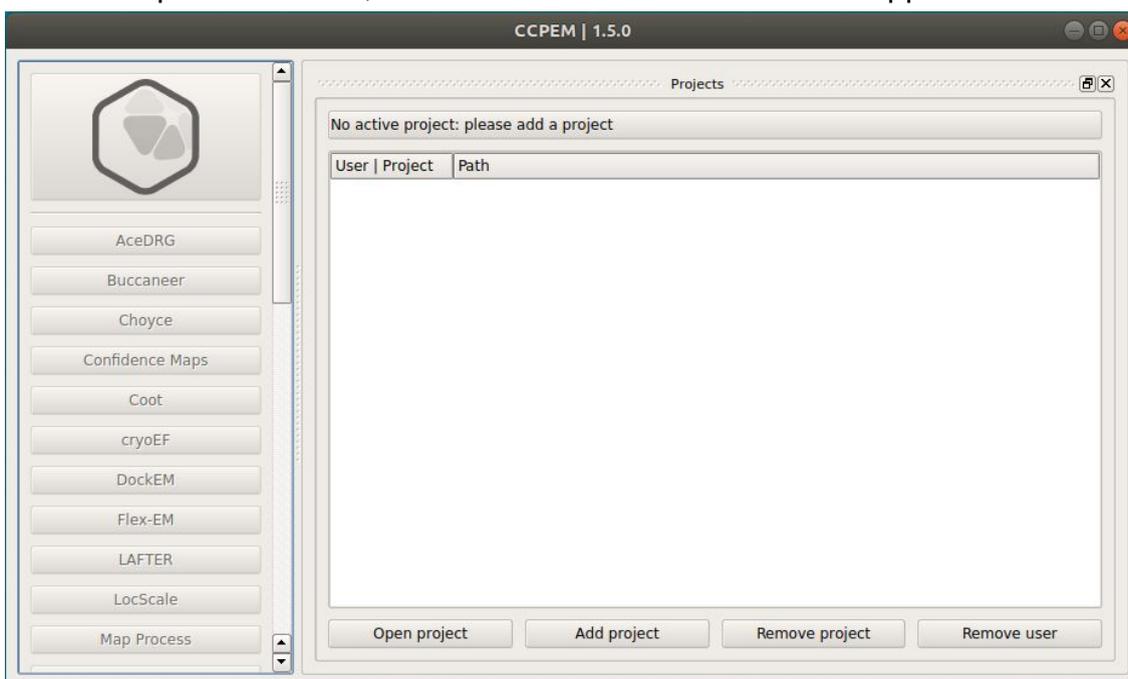   ```
   cd ~/software/ccpem-1.5.0/
   ```
3. Activate CCP-EM:
   ```
   source setup_ccpem.sh
   ```
4. Run CCP-EM:
   ```
   ccpem &
   ```
5. After a couple of seconds, the main CCP-EM window should appear:



6. CCP-EM uses projects to help you keep track of your work. All CCP-EM programs must be run in the context of a project, so when you open it for the first time, the task buttons on the left-hand side of the window are all greyed out. A message at the top of the main panel asks you to "please add a project". Click the "Add project" button at the bottom and then choose a project name, a directory where the project will be stored, and a user name. For example:
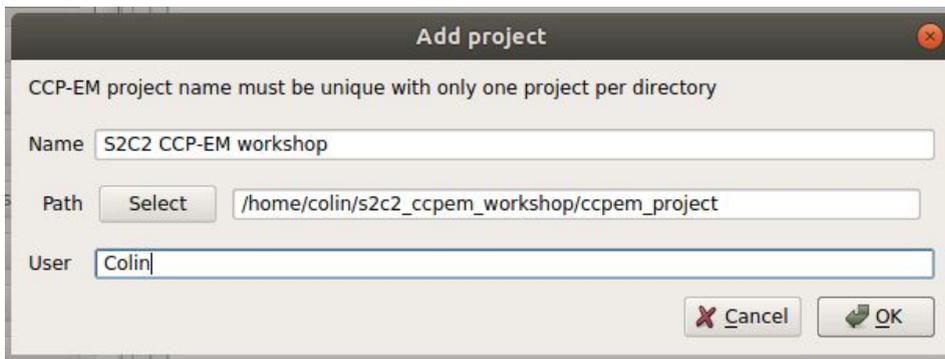
7. When you click OK, CCP-EM will create and open your new project and show you the (empty) list of jobs. Notice that the task buttons on the left-hand side are now active, and your current project details are shown at the bottom of the window:
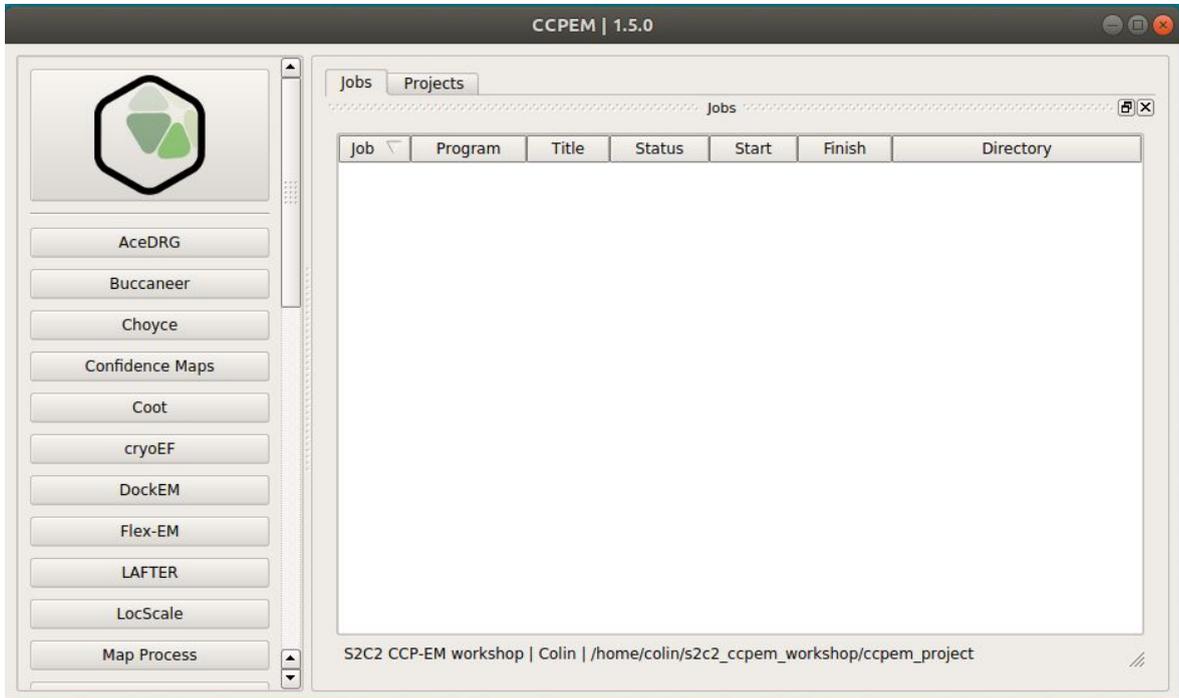


8. All CCP-EM jobs can be tested automatically to check they are working properly. Scroll down the task list to the bottom, and click the "Test mode" button:
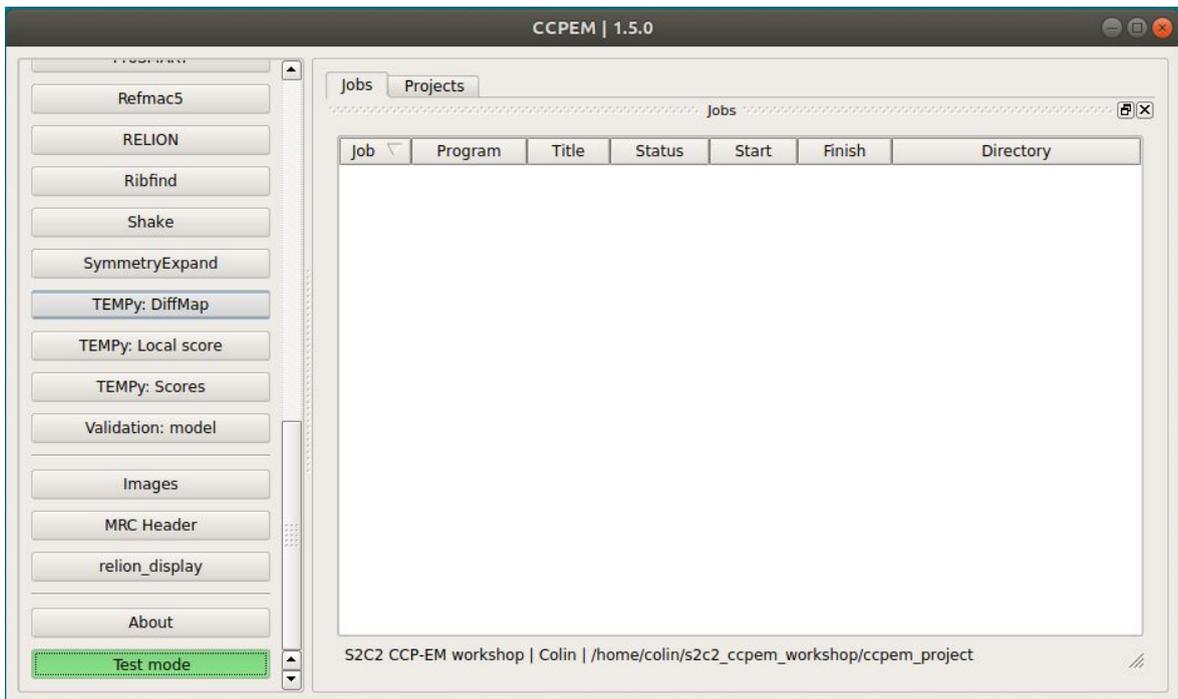
9. Then, any job you click on will load with pre-populated options, ready to run immediately. (If you forget about this later and you're surprised to find new jobs already have their options filled in, remember to check if you've left test mode on by mistake!) To make sure everything's working for this workshop, check the "Test mode" button is selected, then scroll back up the task list and click the Buccaneer button to open the Buccaneer task window:
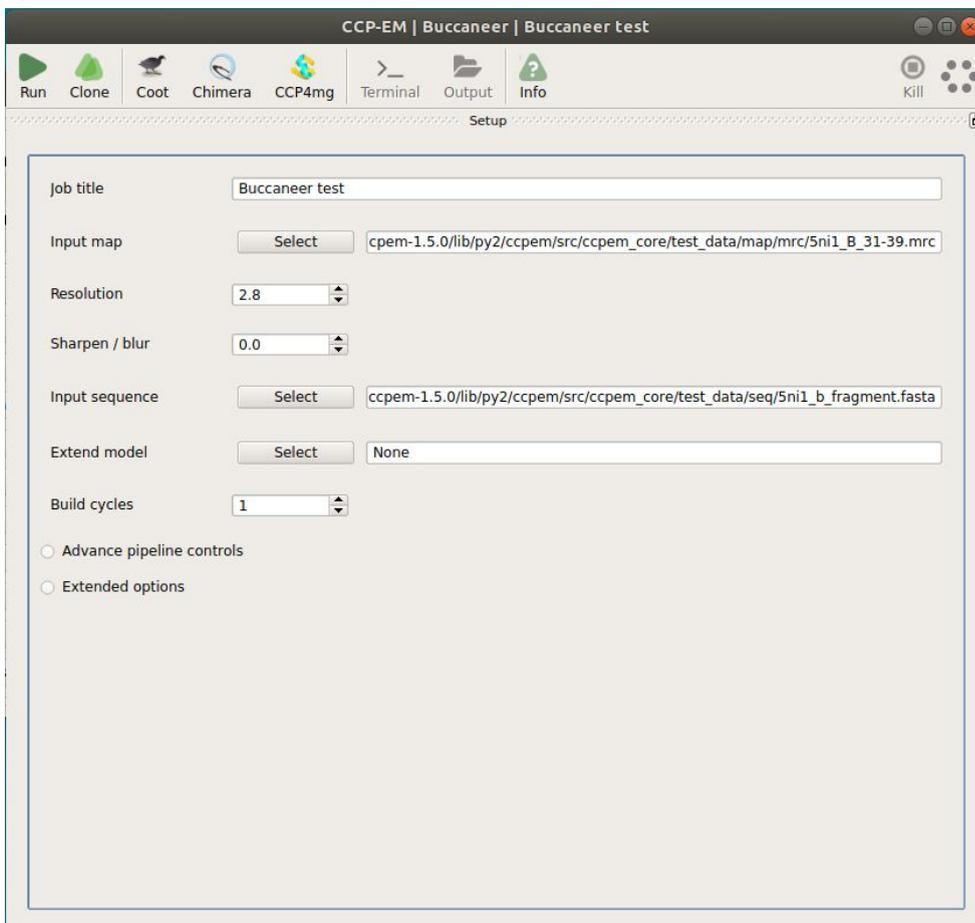
10. Click the "Run" button at the top left to run the Buccaneer test job. The window will switch to the Pipeline tab to show you the output from each stage of the job as it runs. While the job is running, the hexagon at the top right will spin around to show you it's working. This test job should only take a minute or two. At the end the window will switch to the Launcher tab, showing you the input and output files from the job:
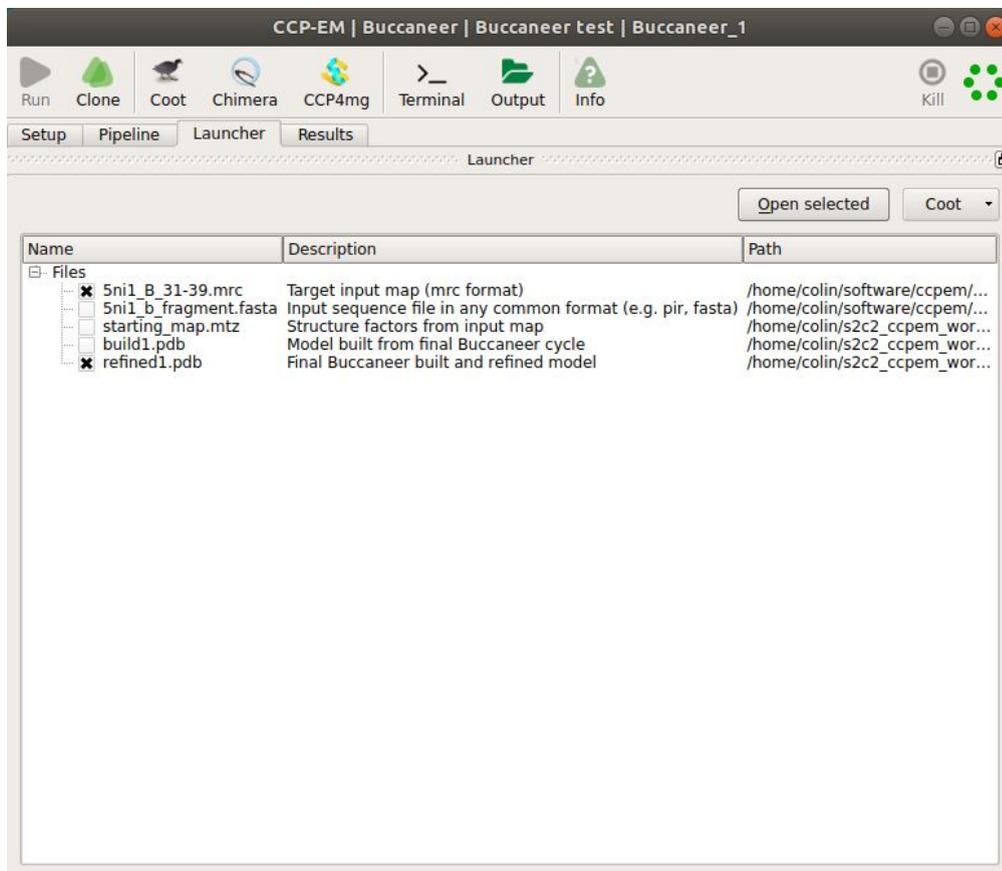


11. You'll see that the hexagon at the top right is green to show the job ran successfully (unless there's a problem and the job failed - then the hexagon will be red.) Also notice there is now a Results tab, which shows a summary and plots of some statistics from the job.

12. Finally, we'll use the buttons at the top of the window to check that Coot and Chimera are working properly. Click the "Coot" button and Coot should open to show you the input map and the model that Buccaneer has built into it:
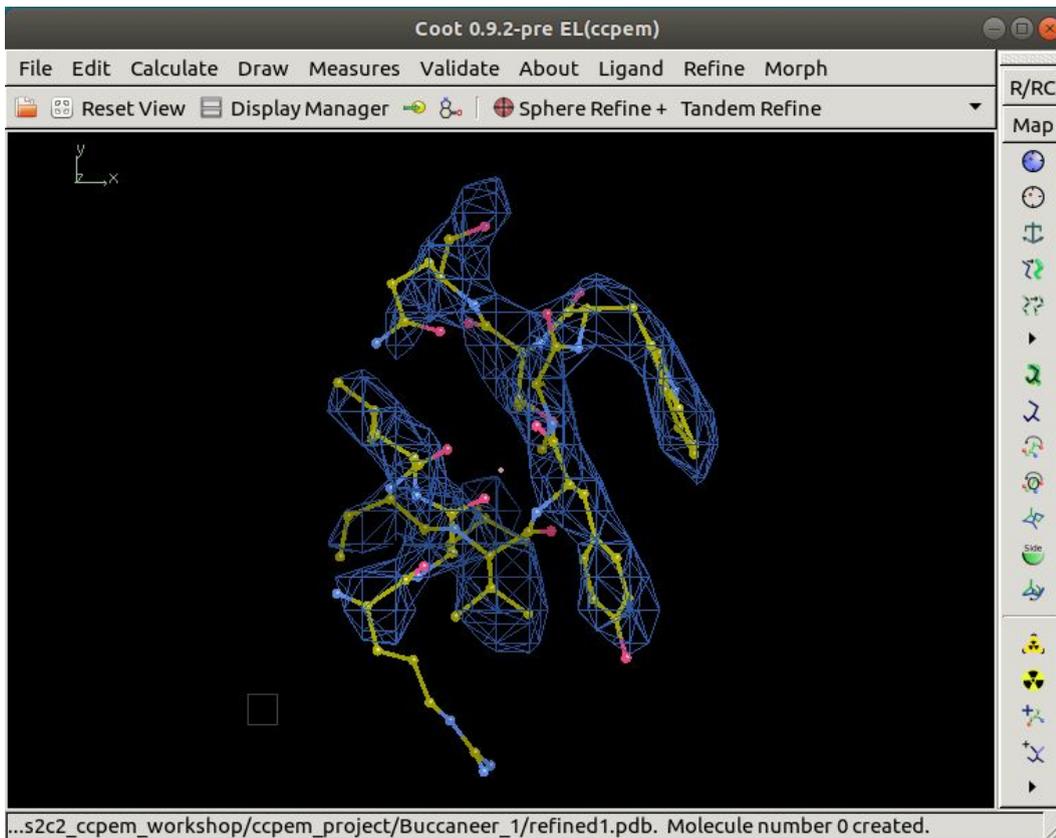
*(You might need to scroll down with your mouse or press "-" a few times to be able to see the map density)*

13. Close Coot and then click the "Chimera" button in the Buccaneer window. Chimera will open to show you the same map and model from the Buccaneer job:
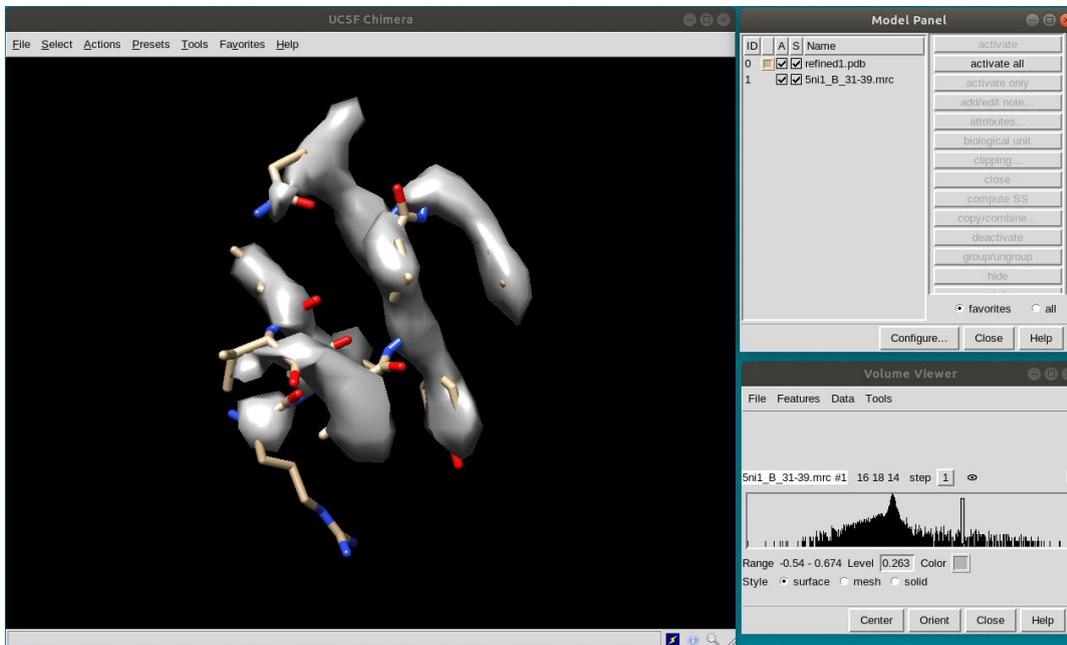


14. That's it! If everything worked up to this point, you're all ready for the workshop. If anything didn't work as described here, do contact us at ccpem@stfc.ac.uk and we'll help you get things working.