Rosetta Tips

- Always try Googling the error message
- Need to be aware of relative paths
- To extract need to have enough space for both the archive and expanded folder, then for compiled files
- Run bin files from source folder
  - `./bin/AbinitoRelax`
- Add `&` to end of command to run in the background
- Take advantage of Tab complete and arrows
main/source – Main folder to put files
main/source/bin – Executables to run
main/database – Chemical properties
demos/tutorials – Useful tutorials
tools – Handy automation scripts
-ln-
  -file-
    -fasta input_nanobody/nanobody.fasta-
    -frag3 input_nanobody/aat000_03_05.200_v1_3-
    -frag9 input_nanobody/aat000_09_05.200_v1_3-
  -abinitio-
    -relax-
    -increase_cycles 10-
    -rg_reweight 0.5-
    -rsd_wt_helix 0.5-
    -rsd_wt_loop 0.5-
  -relax-
    -fast-
  -out-
    -pdb-
    -nstruct 300-
    -file-
      -scorefile score.sc-
    -overwrite-
Linux terminal text editor
Run with ‘vim file.txt’
Modal text editor
  ○ To type text, press ‘i’ first
  ○ To get back to default mode, press ESC
Useful for editing files for Rosetta
See my Vim slides for more details
Use vimtutor to learn through doing
:w – Save file

:wq – Save and Quit

:sort – Sort selected lines

:set ff=unix – Use Unix line endings
Linux Tricks

- Use /mnt/c/ to access Windows from Linux subsystem
  - `mv /mnt/c/Downloads/rosetta ~`
  - `C:\Users\NAME\AppData\Local\Packages\DISTRO_FOLDER\LocalState\rootfs`

- Install things with
  - `sudo apt install PROGRAM`
  - Use ‘search’ to find program
  - Tab complete program
PyMOL

- Different from PyRosetta

- **Left click** Pan/Rotate
- **Right click** Zoom in/out
- **Middle click** Move
- **Scroll** Change visual depth
- Align all structures with one structure
  - align S_000X, all