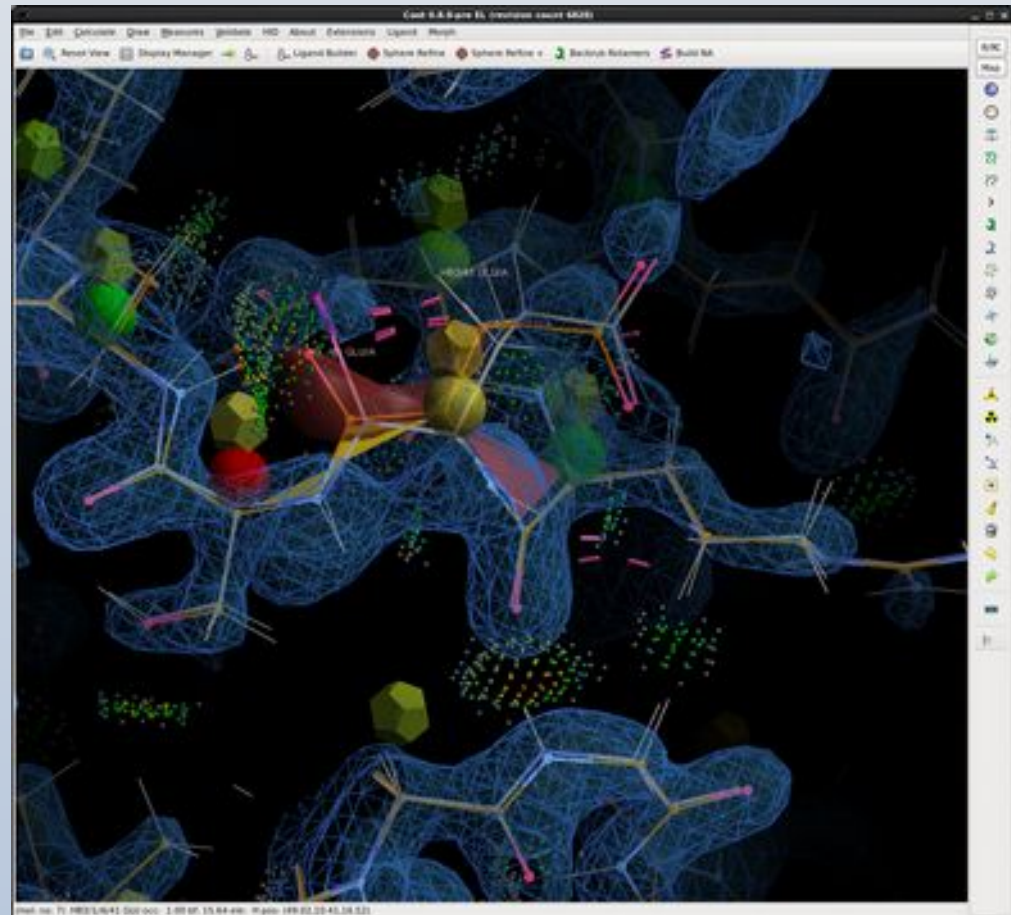


A Coot for Cryo-EM: 0.9 (pre-release)

- ~1500 revisions ahead of the master branch
- This new branch is actively developed
- Considerations for the CootVR interface
- Uses C++11
- Less stable
- More interesting
- Limited binary distribution from the Coot web site
 - in the “experimental” directory
 - Or from CCP-EM

Multi-threaded Modules in 0.9-prerelease

- Refinement
 - Target function and derivative evaluation, model and map all happen simultaneously now
 - Which means: more atoms, smoother updates and/or closer to the minimum
 - Refinement and Graphics updates/display are not separate threads
 - Thread starvation?
- Jiggle-Fit
- All-atom contact dots
- Ramachandran Score
- Rotamer Score
- Add Terminal Residue
 - ϕ, ψ hypothesis scoring



Cryo-EM Refinement: Using “ProSMART-like” Restraints

- Instead of using a reference model, more often I use “Self” restraints
 - which can be calculated internally
 - the starting model is the “reference” from which the ideal distances are calculated
 - message to the refinement:
 - “keep the local environments similar to how they were when you started”
- The minimizer in *Coot* is a 1st order (derivative) based method
 - “Jelly body” stabilizer cannot work

Coot Futures

- 0.8.9.3: Bug Fixes
 - Alt conf and insertion code refinement fixes
 - Patterson processing
- Beyond that...
- Further integration of the RDKit
 - RDKit representation → mmdb representation with dictionary
- extending the python interface
 - gemmi & mrcmap → mmdb & clipper → idiomatic pythonic refinement
- Integration of shiftfield B-factor refinement
- Carbohydrates for Cryo-EM
- CUDA-based refinement
- Stream-line EM fitting
- Ligand Validation

However...

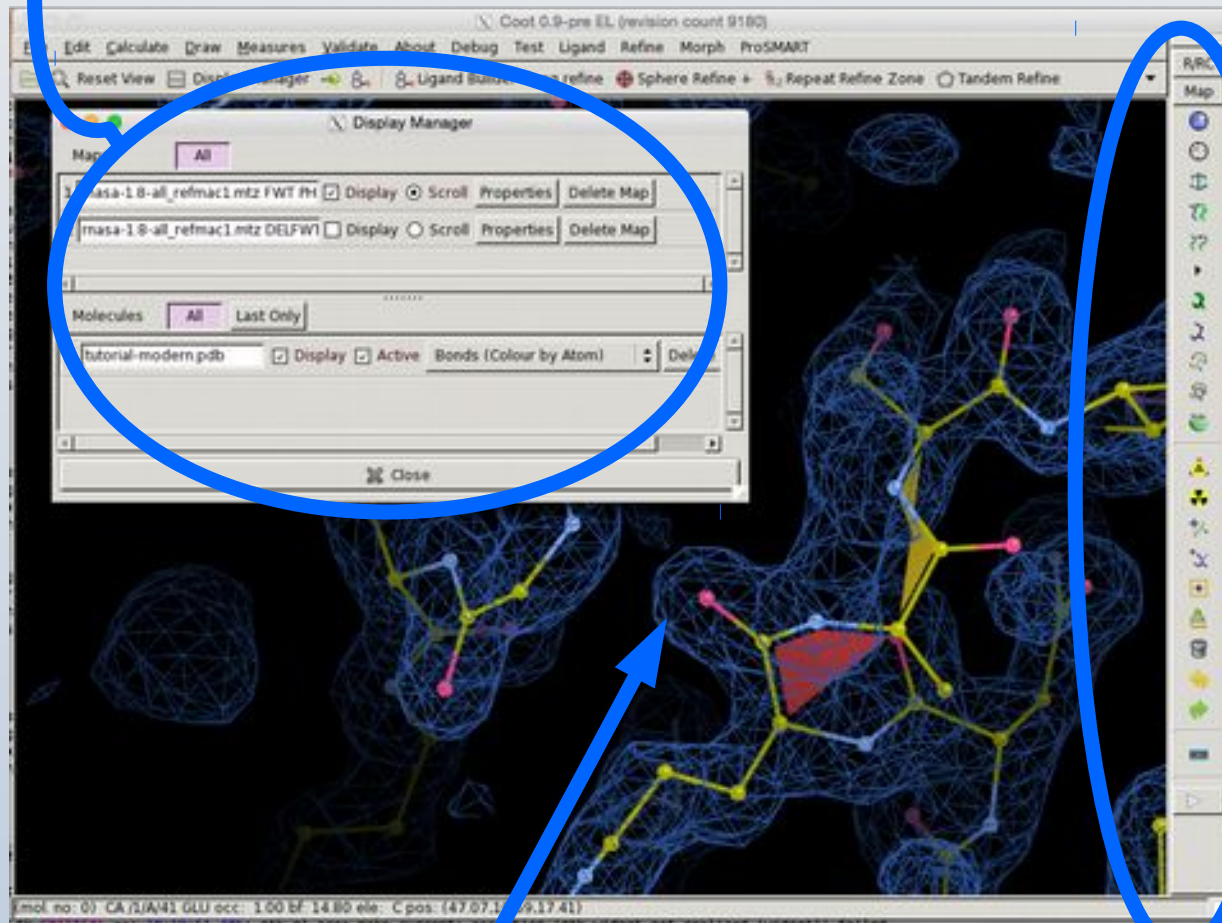
- Python 3...

The “Python 3” Roadmap (1)

- Python 2 is expiring at the end of the year
- *Coot* should move with the times
 - I've been avoiding doing so for years
- But...
 - Python 3 means PyGObject
 - PyGObject means GObject
 - GObject means Gtk+3
 - Gtk+3 means modern OpenGL (version 3+)
 - Gtk+3 means guile-gnome
 - guile-gnome means guile 2

“Graphics” / “GUI”

GUI (Gtk+)



GUI

Graphics (OpenGL)

The “Python 3” Roadmap (2)

- First step: Create a stripped-back Coot
 - Compile with GTK+3
 - Many fudges and deprecation warnings
- Working my way through re-writing the now-deleted widgets
 - ~50,000 line patch to bring Coot to GTK+3
- OpenGL v3 is different to the OpenGL I had used in 2003
 - The drawing of “every pixel” needs to be rewritten
- Maps and molecules are currently done with coloured lines
- This can be converted when the glue has been written
 - with a limitation that the line-width is 1 pixel
 - (depends on the graphics card/driver)
- Hopefully Coot+Python3+Gtk+3+OpenGLv3 will be ready
 - for the 2020 CCP4 Dev Meeting



Comparing Coots

0.8 series

- Crystallography & Ligands
- Stable
- “Bug fix” mode
- “Rubber-band” refinement
- C++-11 Conditionally compiled
 - will work with non-modern compiler
- Gtk+ 2.x (still has Gtk+1 code)
- Python 2.x
- Guile 1.8.x
- PyGtk
- OpenGL v1, GtkGLExt

0.9 → 1.x series

- + Cryo-EM
- Much more dangerous and crashy code
- Actively developed
- “Atom Pull” Refinement
- C++-11 dependent
- Multi-threaded
- Boost dependent
- Python 2 → Python 3, PyGObject
- Gtk+2 → Gtk+3 → Gtk4
- Guile 2 → Guile 3, guile-gnome
- OpenGL v3,v4 → Vulkan
- CUDA conditionally compiled
- Coot Version 1 won't work on Mac OS X
- May work on Windows with much work

Comparing Coots

The Past

0.8 series

- Gtk+2
- Python 2
- PyGtk
- OpenGLv1

Deprecated

Linux ✓

Mac OS X ✓

Windows ✓

Today

0.9 series

- Gtk+2
- Python 2
- PyGtk
- OpenGLv1
- C++-11
- Boost

**Mostly
Deprecated**

Linux ✓

Mac OS X ✓

Windows ✓?

The Future

1.x series

- Gtk+3
- Python 3
- PyGObject
- OpenGLv3
- C++-11
- Boost

The Future

Linux ✓

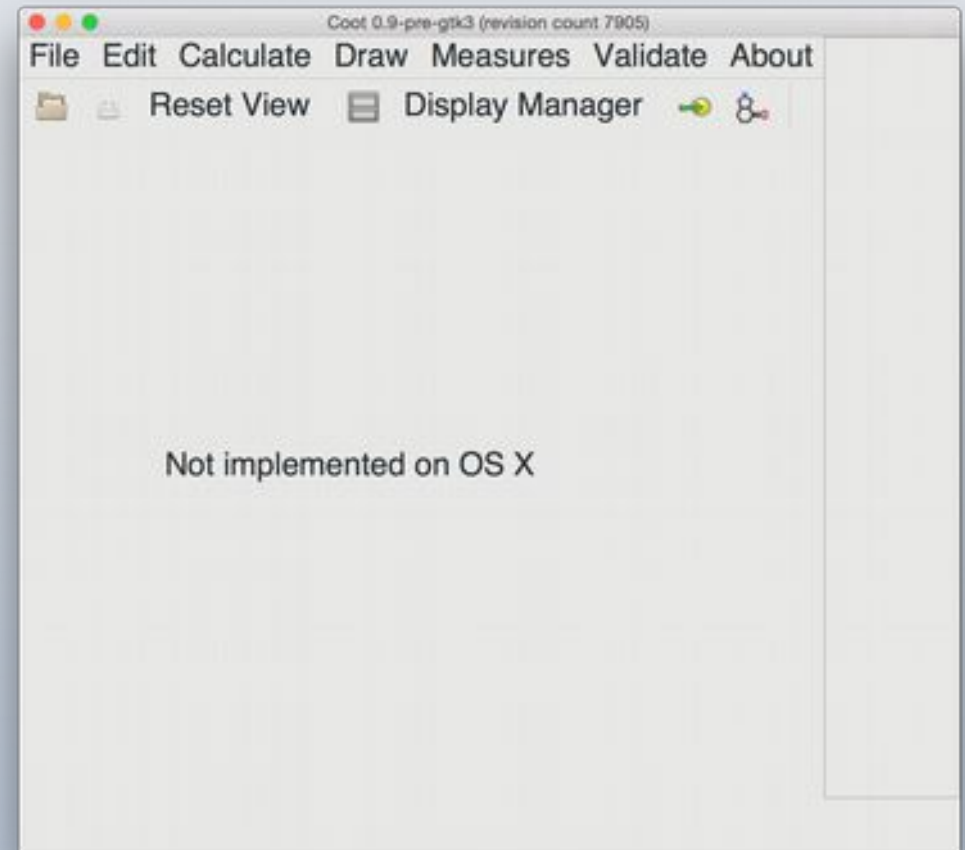
Mac OS X ✗

Windows ✗

Mac OS X ~~x~~

Windows ~~x~~

- It's not *impossible* that *Coot* will work on these platforms
 - but it won't work “out of the box”
- Ignore it
 - new *Coot* on Mac OS X and Windows doesn't matter
- Hope it goes away
 - someone else will do it for us
- Pay someone to do it



Coot 2 will use Vulkan