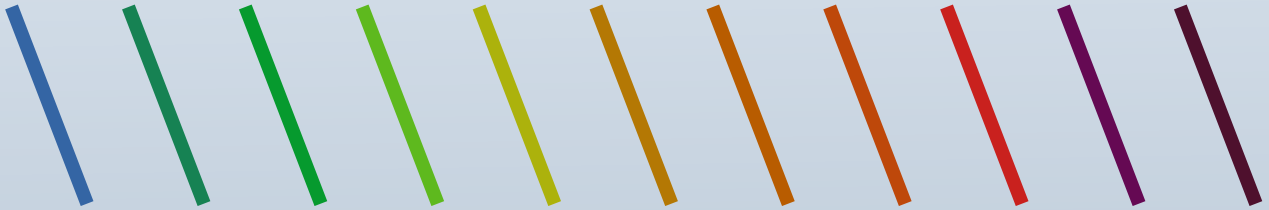


Beyond Coloured Lines

Progress in Representation in *Coot:*
A Program for Macromolecular
Model-Building, Refinement and Validation

Paul Emsley

Oct 2020

About this presentation

- Kelly has this presentation
- Available on cluster:
  - ~pemsley/2020-oct-presentation
- No videos in this presentation because internet is too slow/choppy
  - But screenshots are a poor replacement for a 60 FPS application
- A build for Scientific Linux 7.6 is available
- Scientific “back-end” remains the same,
  - this presentation will be about the interface
  - waters, ligands, metals and out-of-register errors (a different presentation)
- A discussion of representation updates, then some screenshots
  - there are no equations
- Aside: A slide on Real Space Refinement

Aside: RSR & Threading

- Following a discussion on CCP4BB, it seems to me that *Coot* refinement doesn't work for others as it works for me
  - Stall, "No Progress"? bad NBC?
  - Please let me know

- "Proportional Editing" in 0.9.1
  - see the video
  - Ctrl <middle-mouse> scroll

“Coloured Lines”

- “3D sticks in space” is the way in which *Coot* 0.0-0.9.1 has represented models and maps
- 1990s graphics system with no use of lighting
  - 2 months to learn and implement and little has changed since 2004
  - some improvement on the fringes:
    - Ligand Validation
    - Channels
    - Generic Objects

Things are Changing: Why/Why Now?

- I've known for 10 years that I need to make the shift, but there was always something more important to be done
  - this is more software engineering than science
  - but it must be done
    - CCP4 is moving/has moved to Python 3
    - Python 2 is dead

Coot 1.0

- *Coot* 1.0 will (and *Coot* 0.9.9 does) use "modern" graphics to represent, models, maps and validation information
  - much code has to be written/rewritten/edited
- We are in a state of flux
  - "the clay is wet"

An Opportunity for Feedback

- Sitting with Ester and Ana clarified my thinking
  - Many/most reconstructions will be at resolutions at which the sequence assignment is not obvious
- Open to other ideas about what needs to be done
  - So let me know

- "I don't know what I want but I'll know it when I see it"
  - Implement some ideas and "see what sticks"

What's *Coot* for?

- Interactive model-building, refinement and validation
- (Fast) automation over interaction
- Functionality over speed
- Speed over beauty
- Beauty over ugly (as long as it doesn't cost too much time)

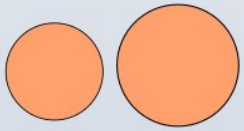
- *Coot* is a carthorse not a show pony
  - Optimised for the world of chicken-wire

Depth

- Flat/Ambient shading makes it difficult to perceive depth
- Failure to perceive depth (using *Coot*) is probably the main reason why stereo is needed/requested
- Modern hardware make depth perception easier
- Let's look at
  - how depth is represented in 3D applications
  - problems with the current representation
  - Screenshots: how New *Coot* is an improvement on Old *Coot*

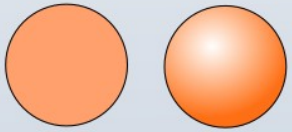
Visual Cues for Depth

Relative Size



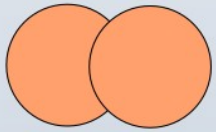
Old Coot:×
New Coot:✓

Shading



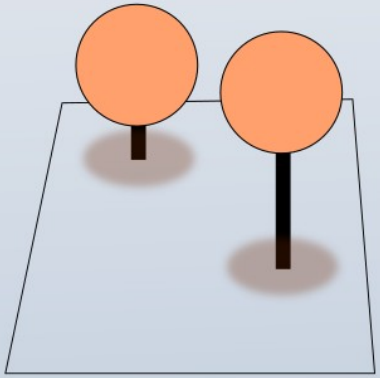
Old Coot:×
New Coot:✓

Occlusion



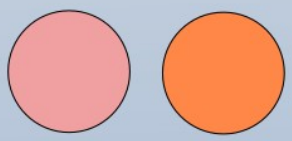
Old Coot:×
New Coot:✓

Shadows



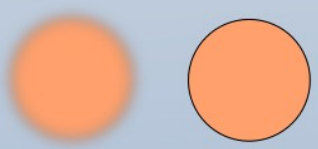
Old Coot:×
New Coot:×

Colour



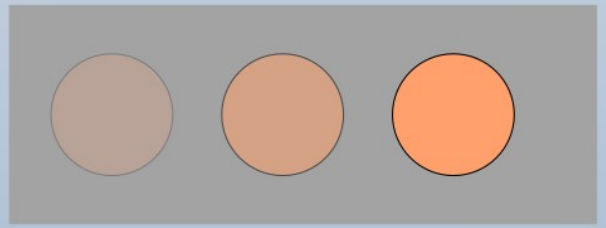
Old Coot:×
New Coot:✓

Focus/Blur



Old Coot:×
New Coot:✓

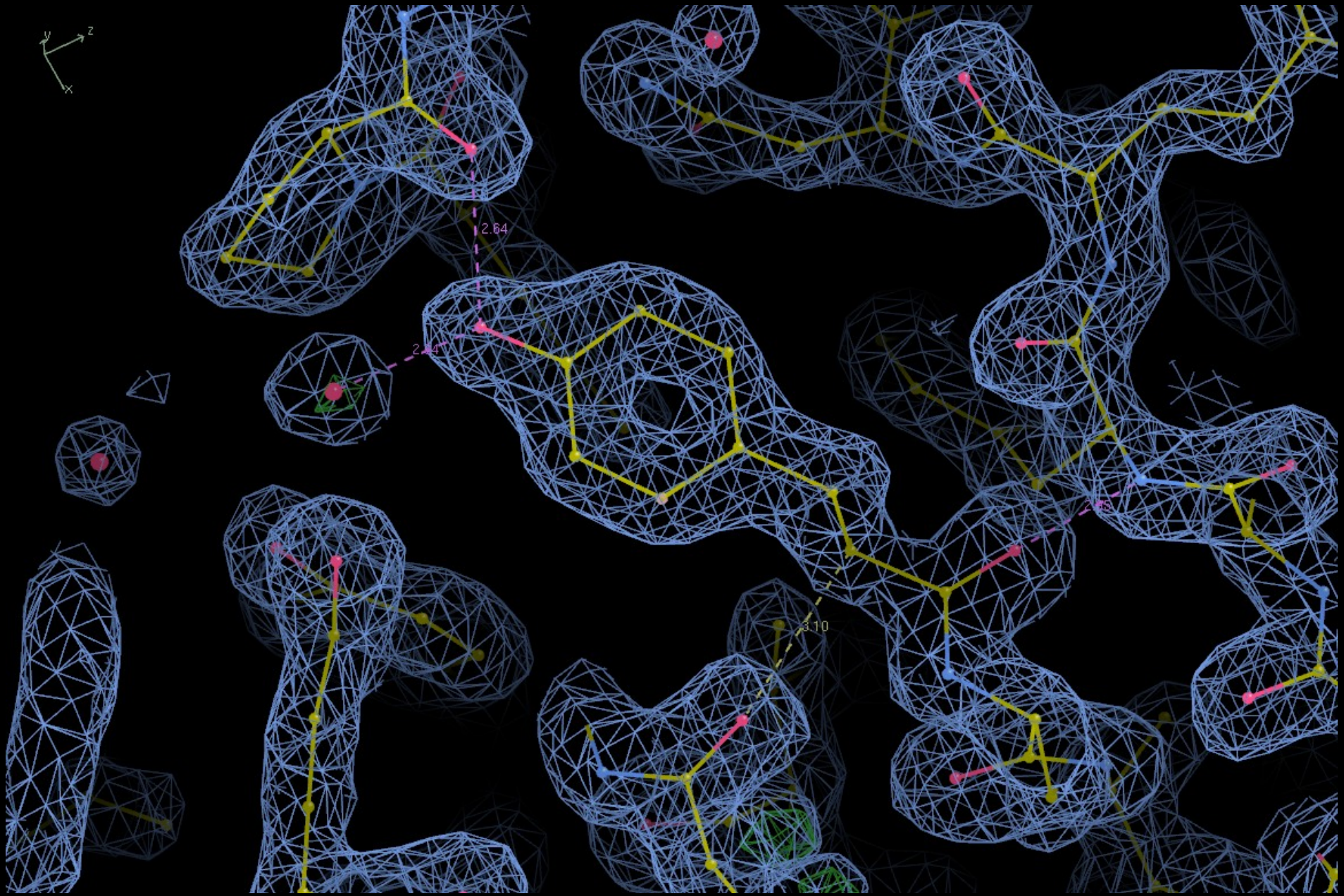
Fog Depth



Old Coot:✓
New Coot:✓

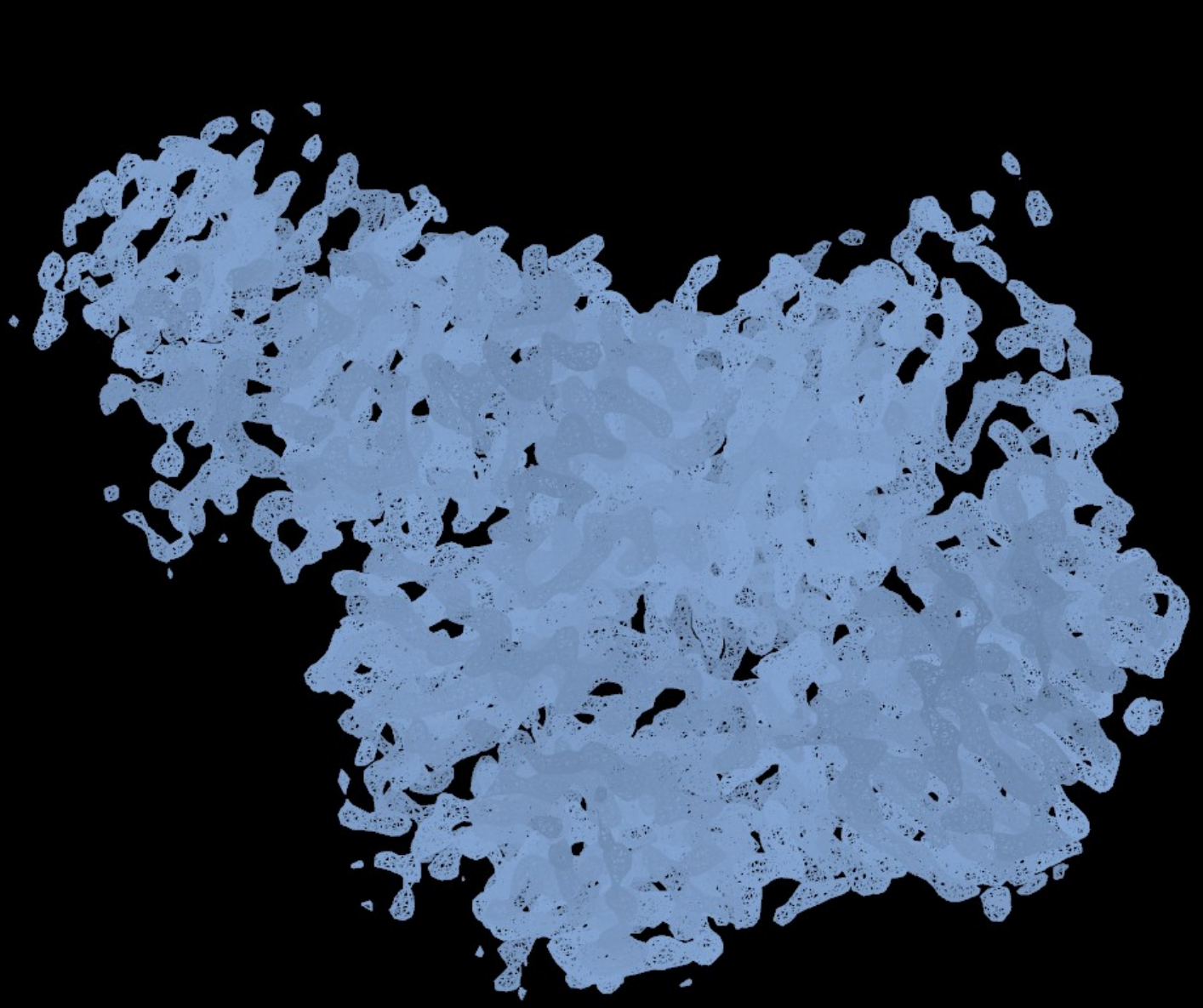
Old *Coot:* Lack of Depth

- When Zoomed in:

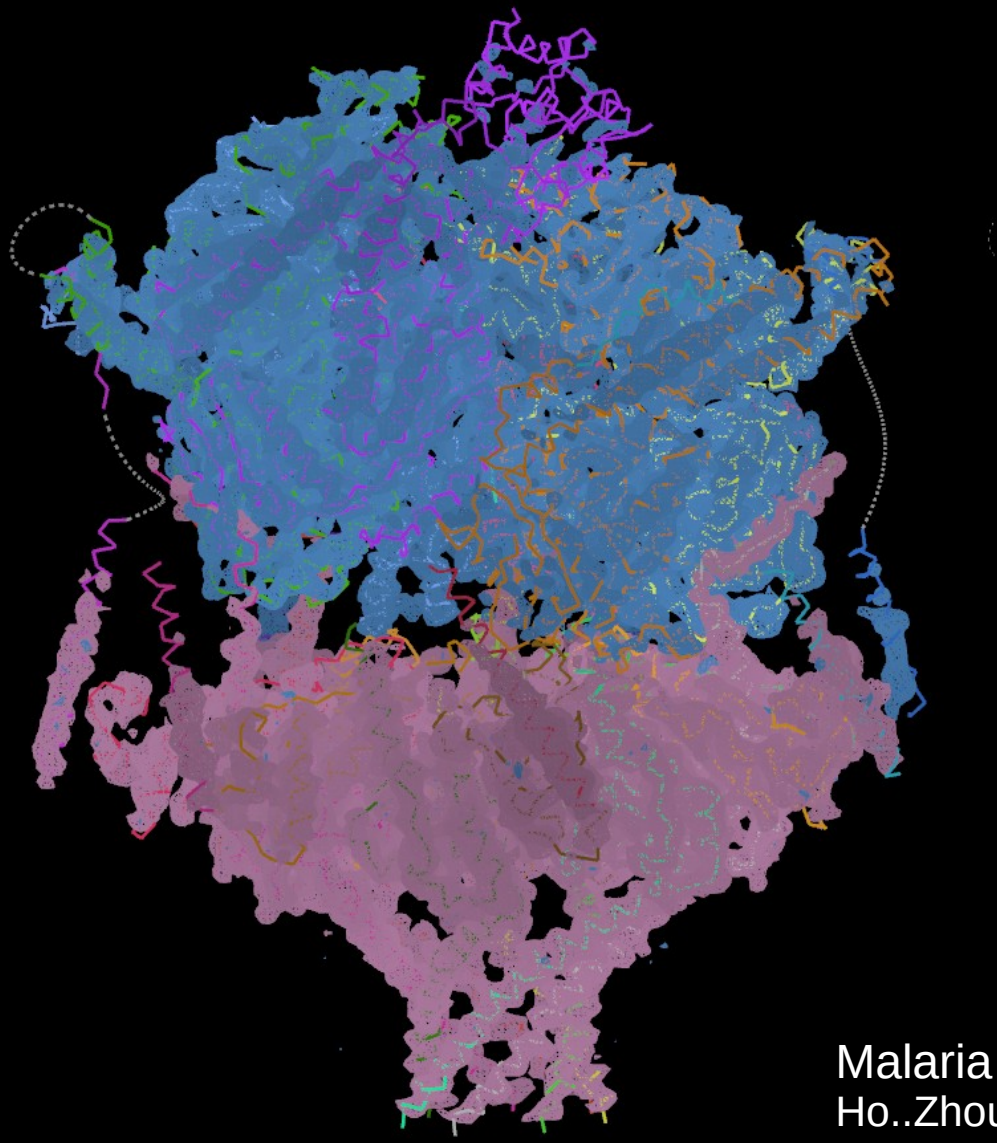


Old *Coot:* Lack of Depth

- When Zoomed out:



Old *Coot*



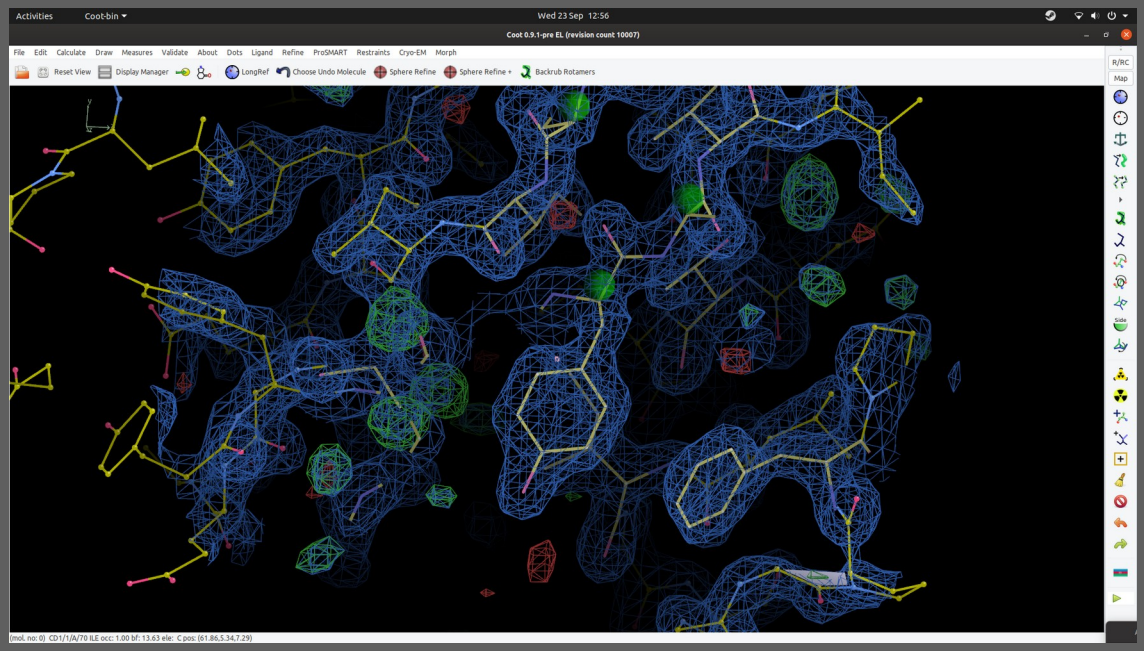
Malaria Parasite Translocon
Ho..Zhou (2018) *Nature*

Teaching *Coot* to Modern *Coot* Users

- Instead of
  - multiple windows/dialogs
- prefer
  - full screen, mini-map, HUD & revealers
- + Particles, instancing, texturing and lighting
- These are familiar idioms for the new generation
  - and by adopting them *Coot* can be made more accessible/easy to use/intuitive, rapid and productive

“Lay it out like this:”

“Not like this:”



Teaching *Coot* to Modern *Coot* Users

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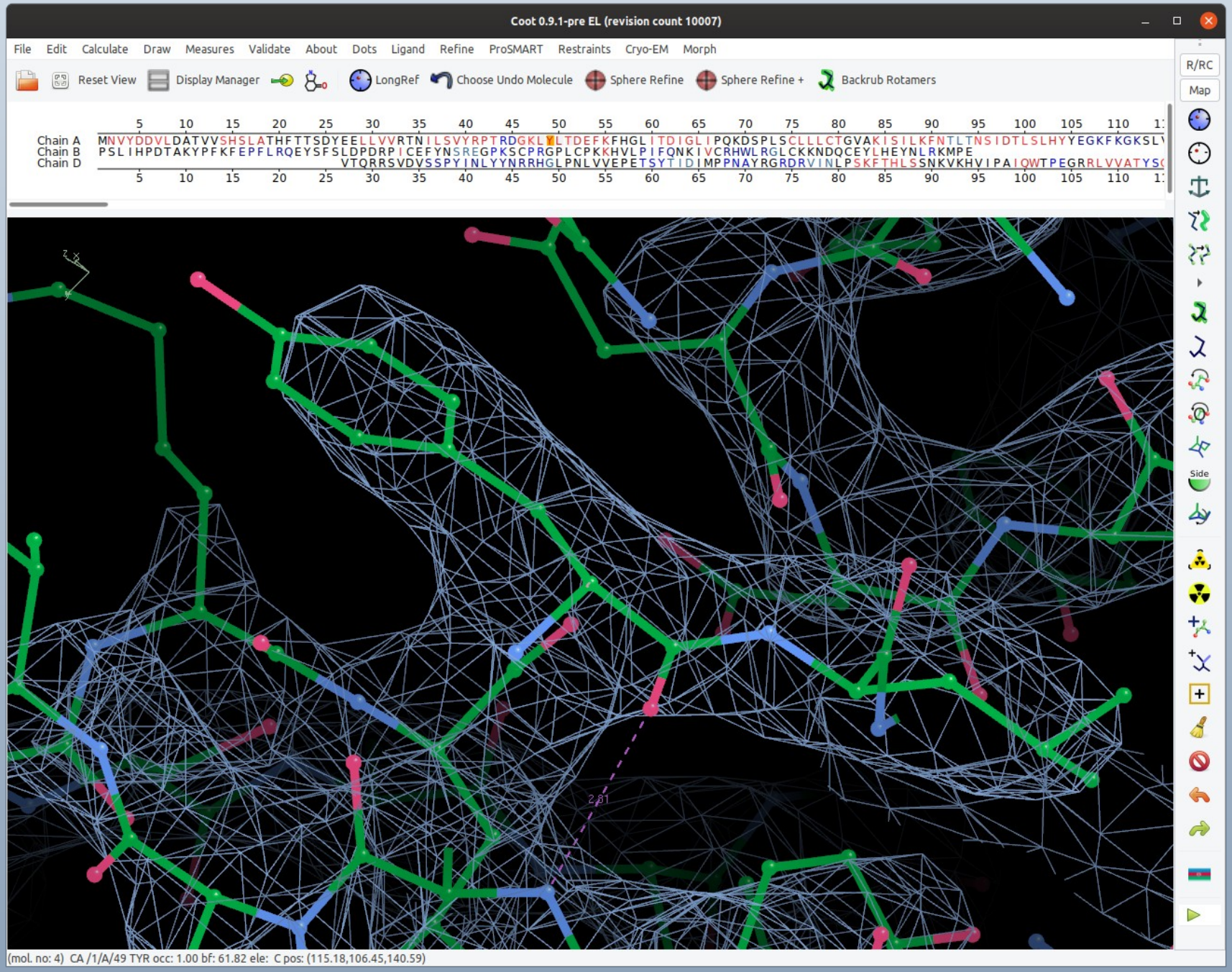
  - and by adopting them *Coot* can be made more accessible/easy to use/intuitive,
  - consequently more rapid and productive

“Sequence View” is Now Embedded



A Note on Hardware

- Targetted to a “Workstation”
  - 4+ threads
  - Nvidia GTX 1080 graphics
  - I don’t know how it will work on a Mac
  - “Make it *work* before making it *work fast*”
  - or “work fast enough for Mac users”

16.6ms

- Improvements in visualization are of little value if they cost too much FPS
- Fortunately (using modern hardware) they do not
- 1ms is spend searching and sorting the restraints
  - detailed, interactive representation of “high energy”

Colour-blindness Considerations

- Red ⟶ Green (Bad ⟶ Good) is useless for most colour-blind people
- One way to improve this is to add blue to the red side, so the colour range becomes Purple ⟶ Green
- Another cue could be texture:
  - Rough/Dull ⟶ Smooth/Shiny
    - (but Metallic Shiny means reflections (not easy))

But What about the Pretty?

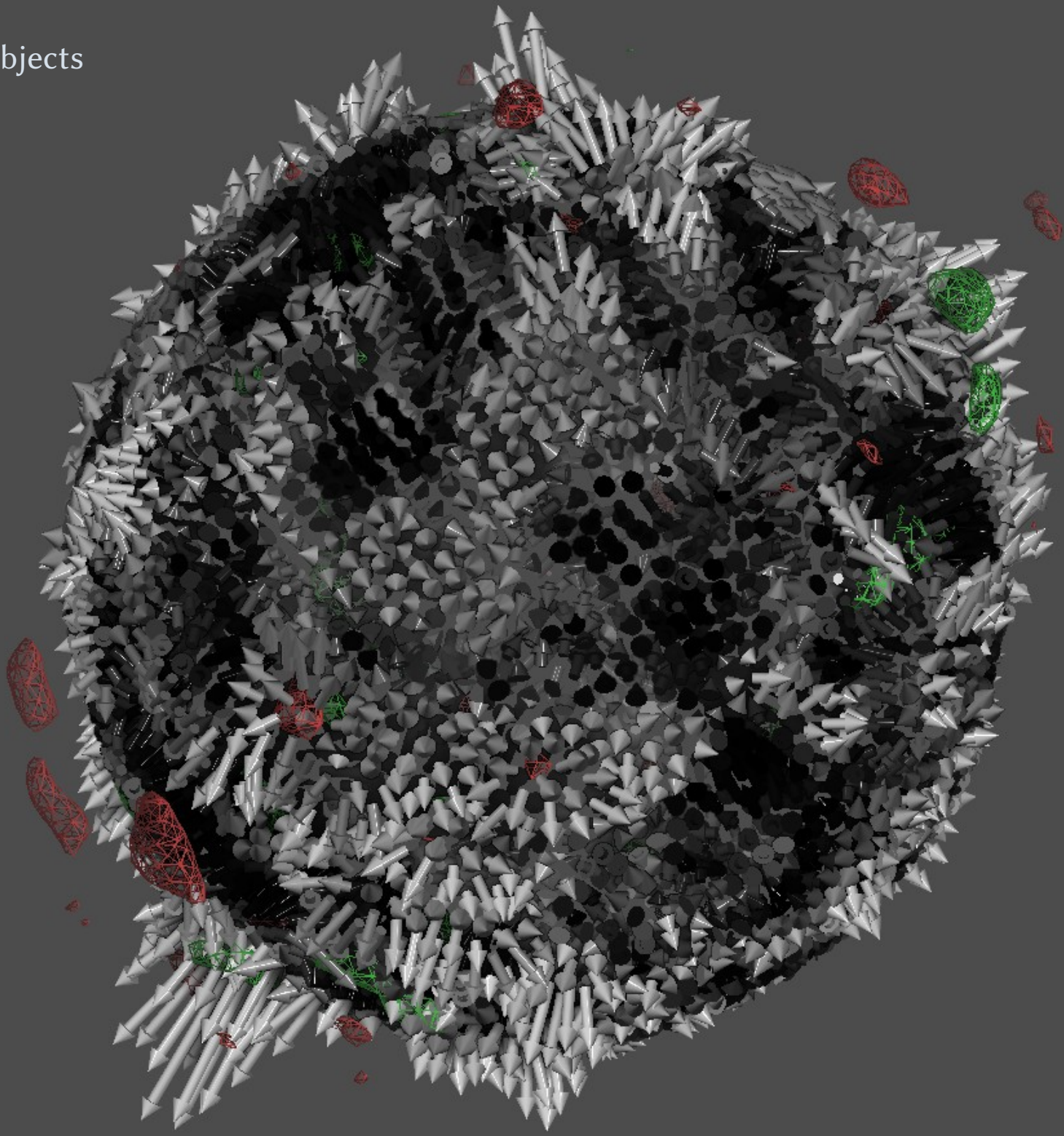
- “MoleculesToTriangles” from Martin Noble

- There is no antialiasing (at the moment)
  - There is framebuffer scaling (*e.g.* *x*8 ⟶ 8000 pixel image)

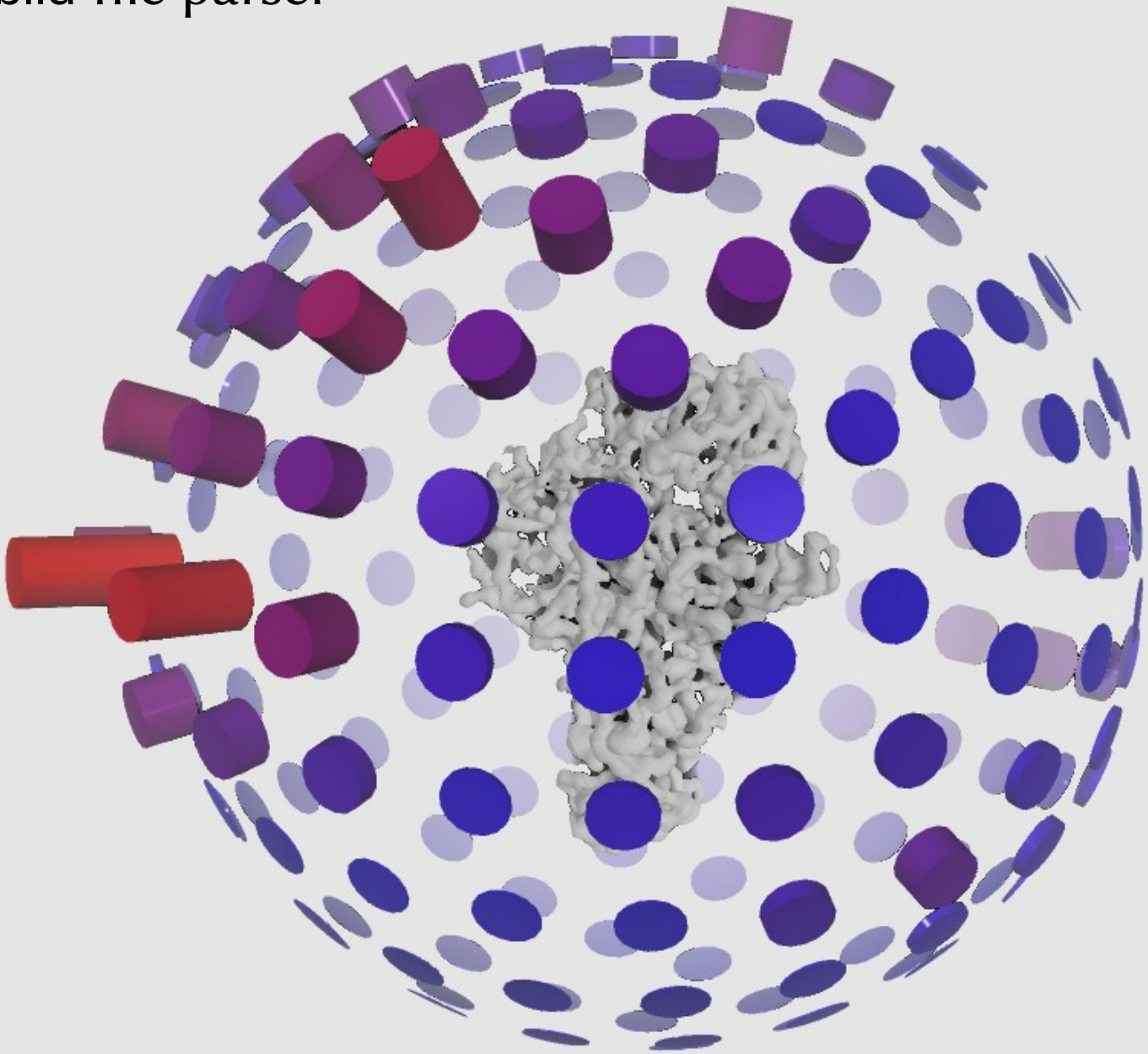
Lighting & Ray Tracing

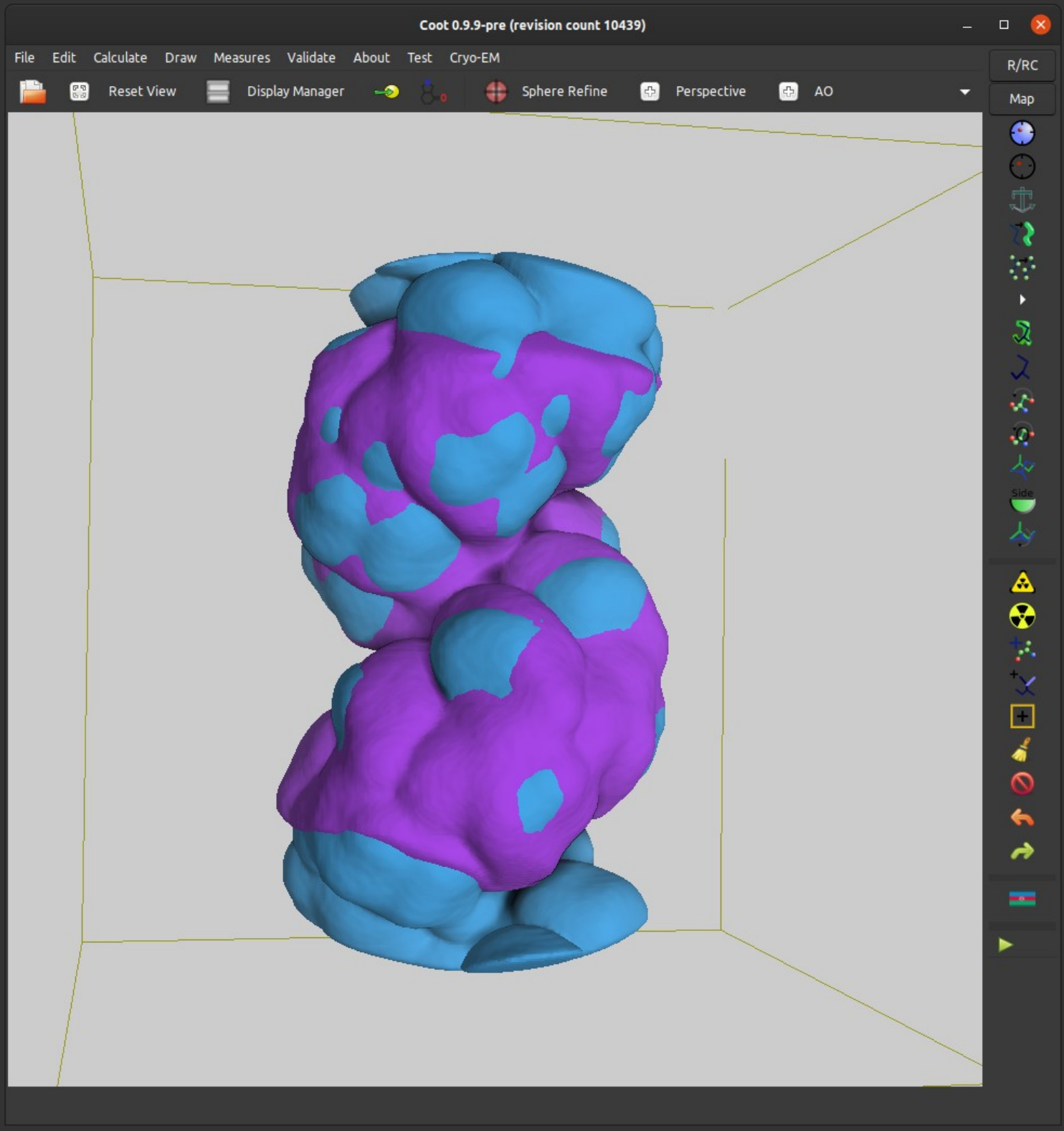
- Old Lighting Model:
  - Ambient
- New Lighting Model:
  - Ambient, Diffuse, Specular, Fresnel, Ambient Occlusion
  - Not yet: Shadows & Reflections
- The lighting model in *Coot* is improved but doesn't match a ray-traced representation
- So how do we use a ray-tracer?
  - Export the map and model into Wavefront obj format
  - Materials, shading, lighting, camera, animation
  - Blender (or C4D – used by Visual Aids)

Screenshots

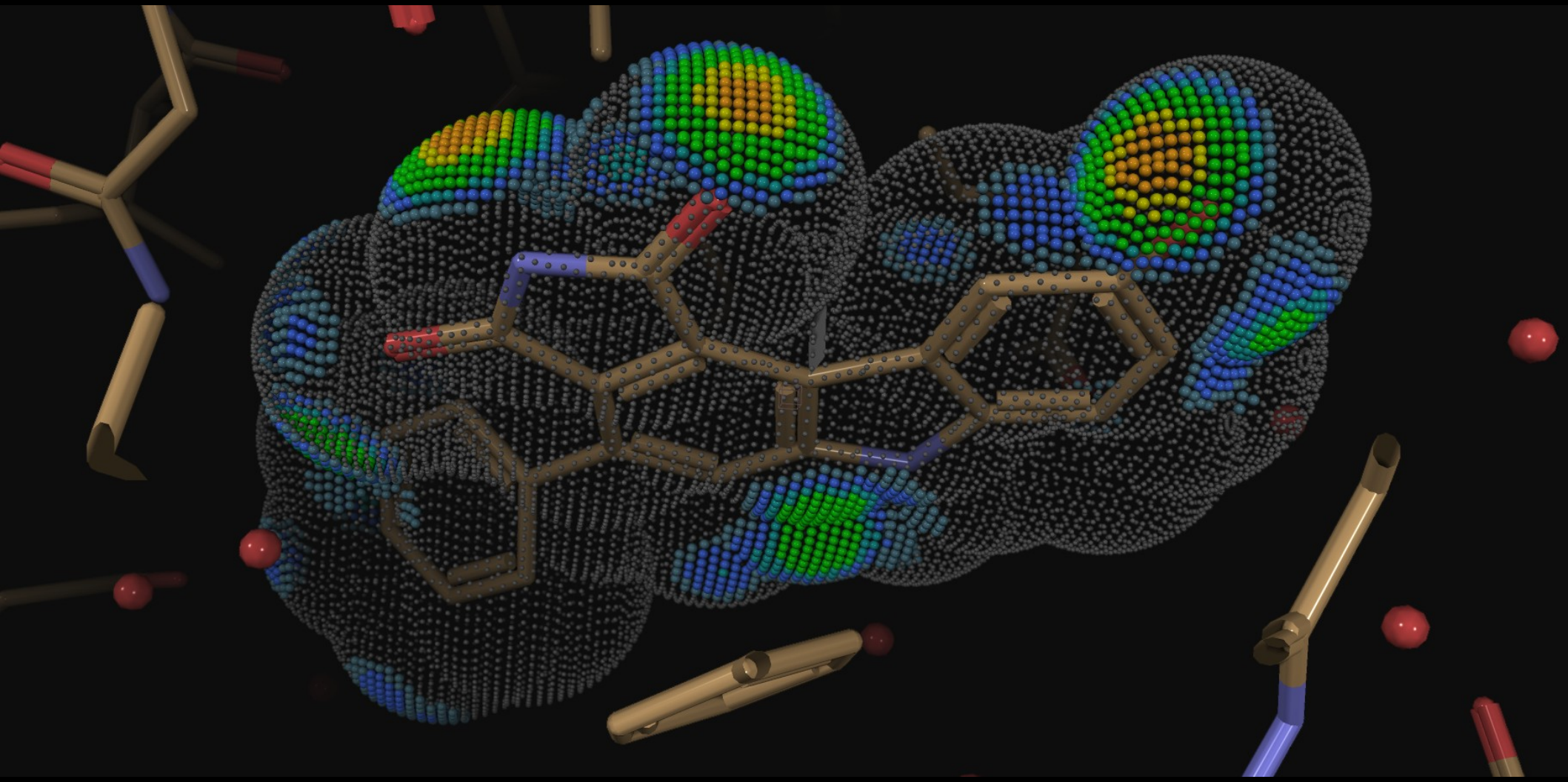


.bild file parser

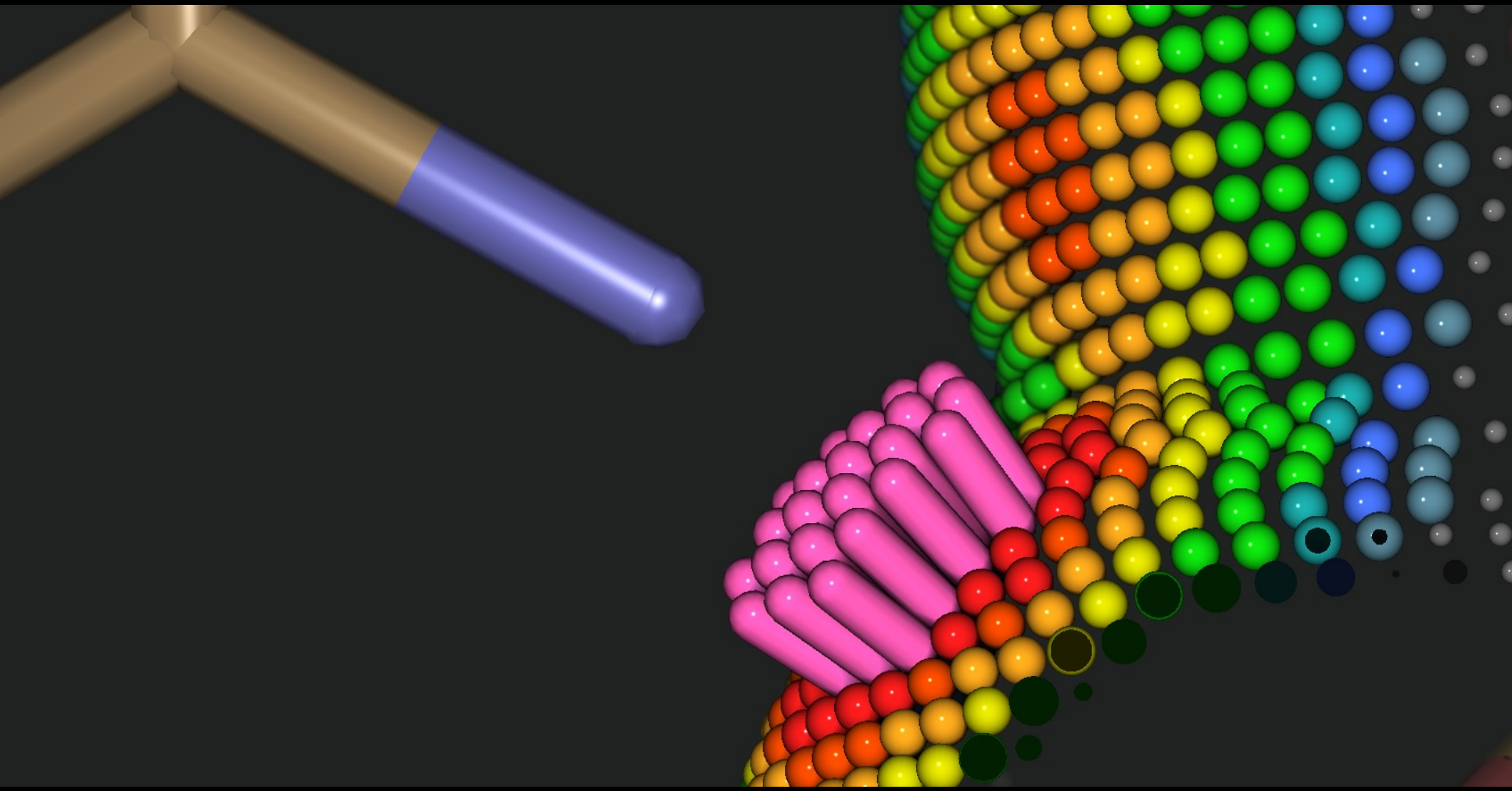



Coot 0.9.9-pre (revision count 10439)
File
Edit
Calculate
Draw
Measures
Validate
About
Test
Cryo-EM
Reset View
Display Manager
Sphere Refine
Perspective
AO
R/RC
Map
Side

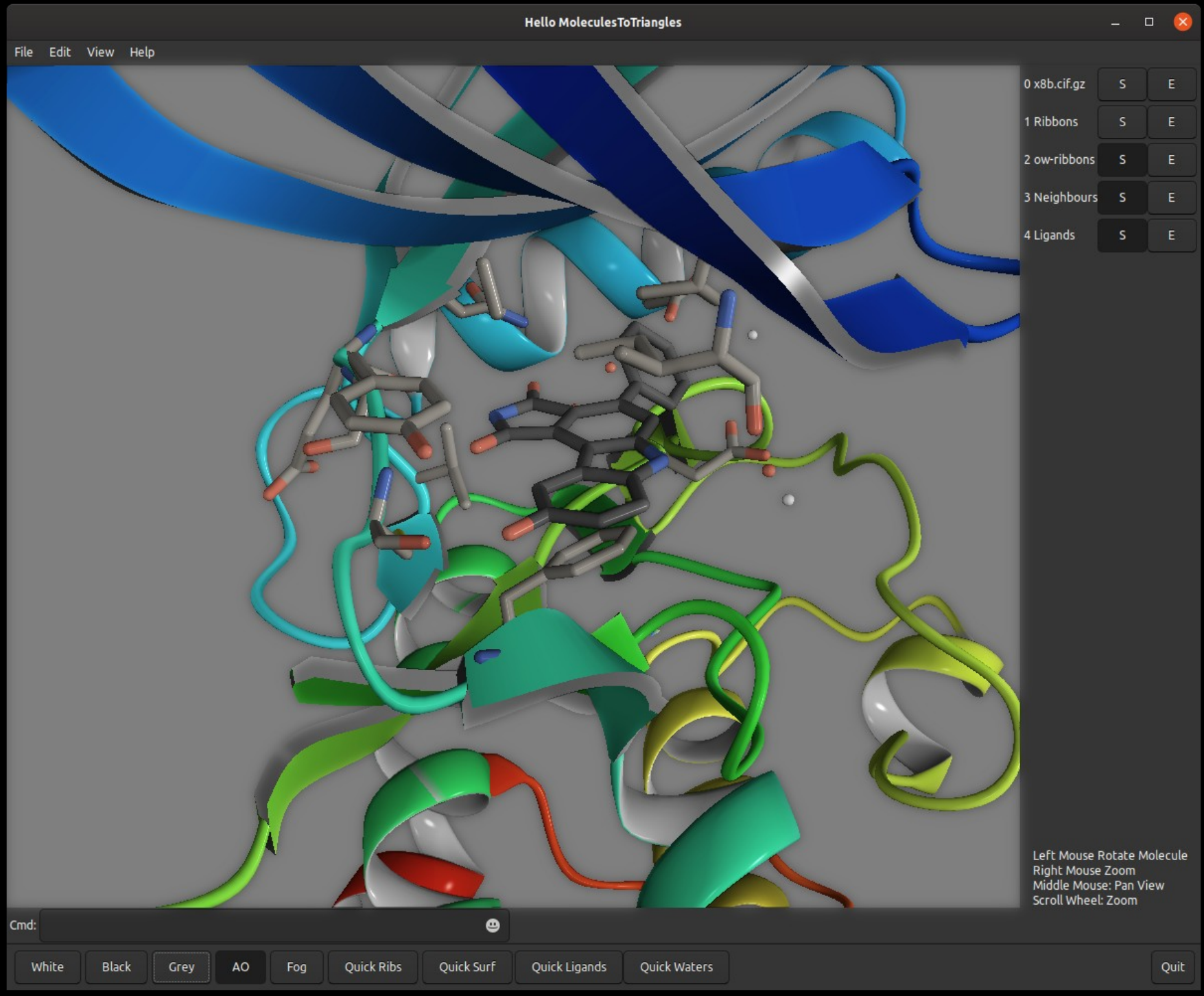
Ligand Interactions



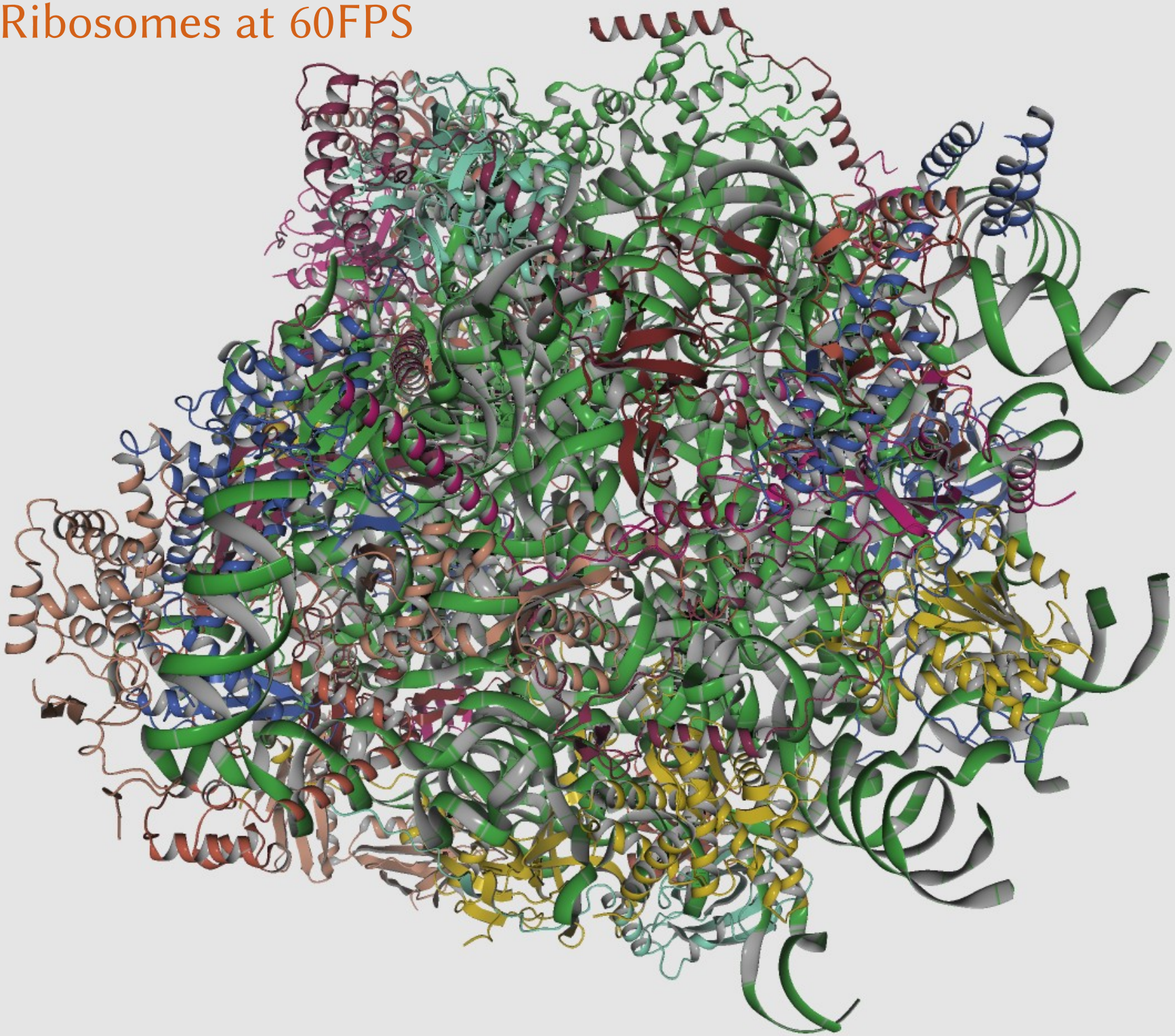
Atoms Clashing

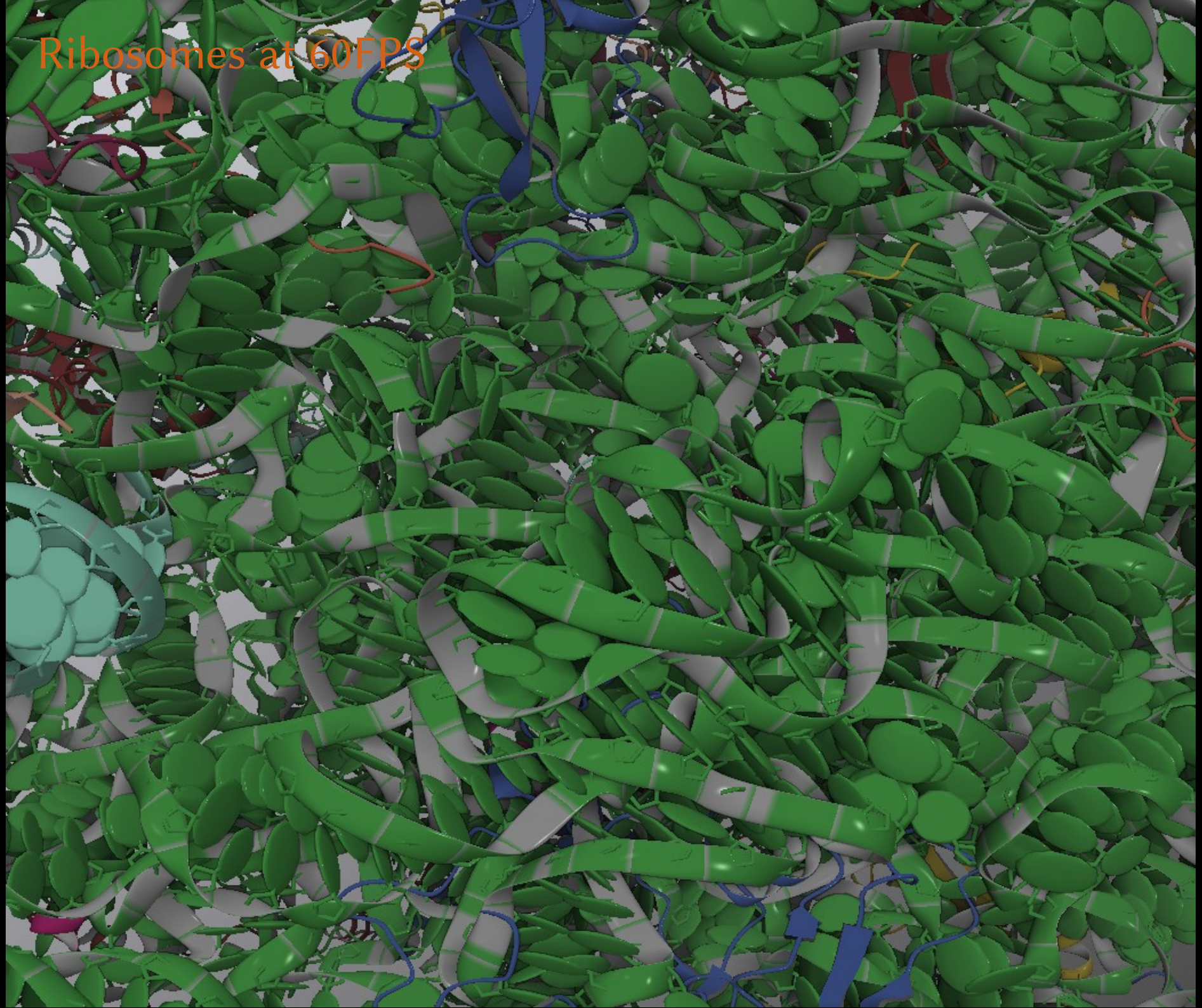


Test-bed/Hello World



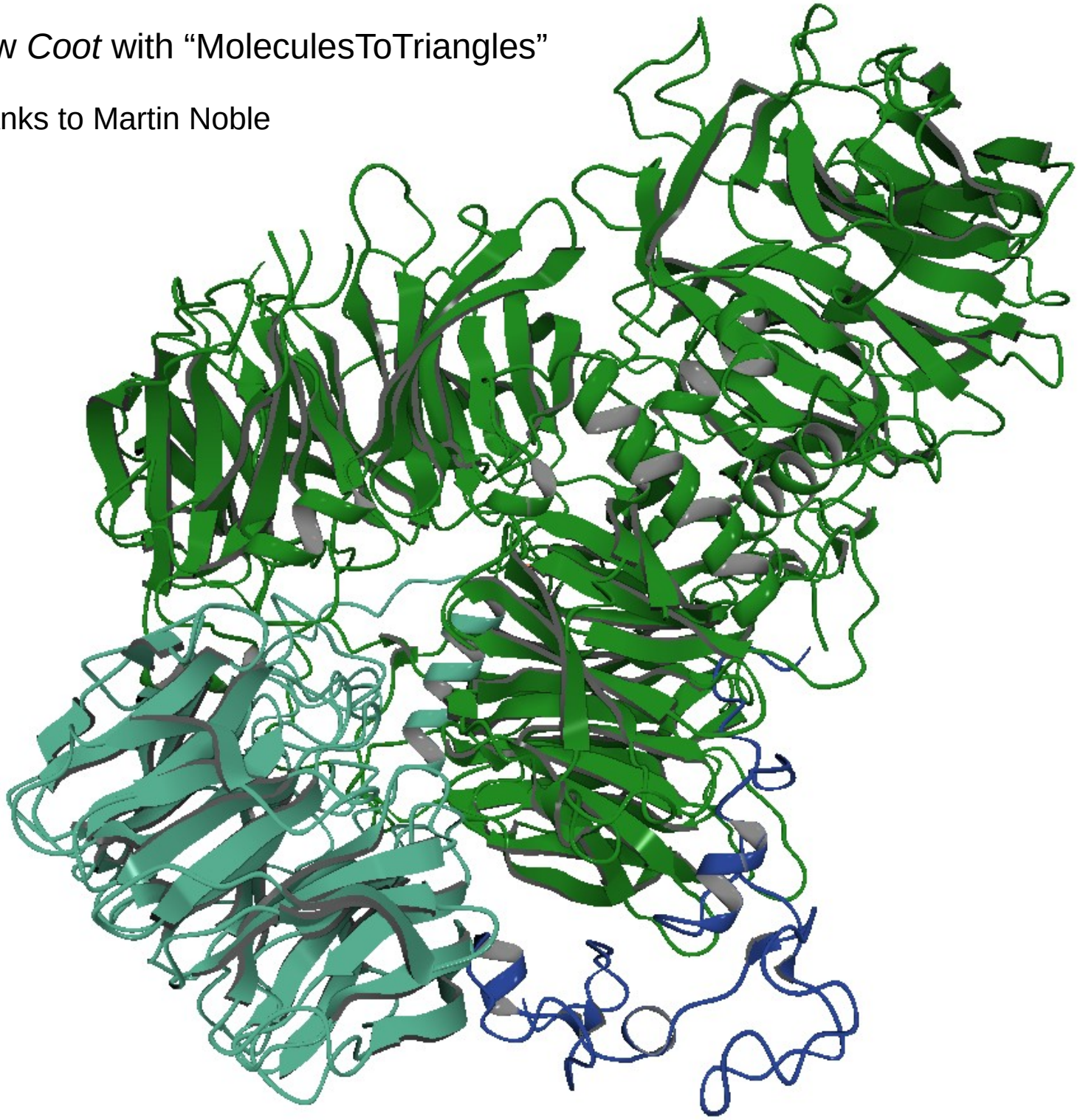
Ribosomes at 60FPS




Ribosomes at 60FPS

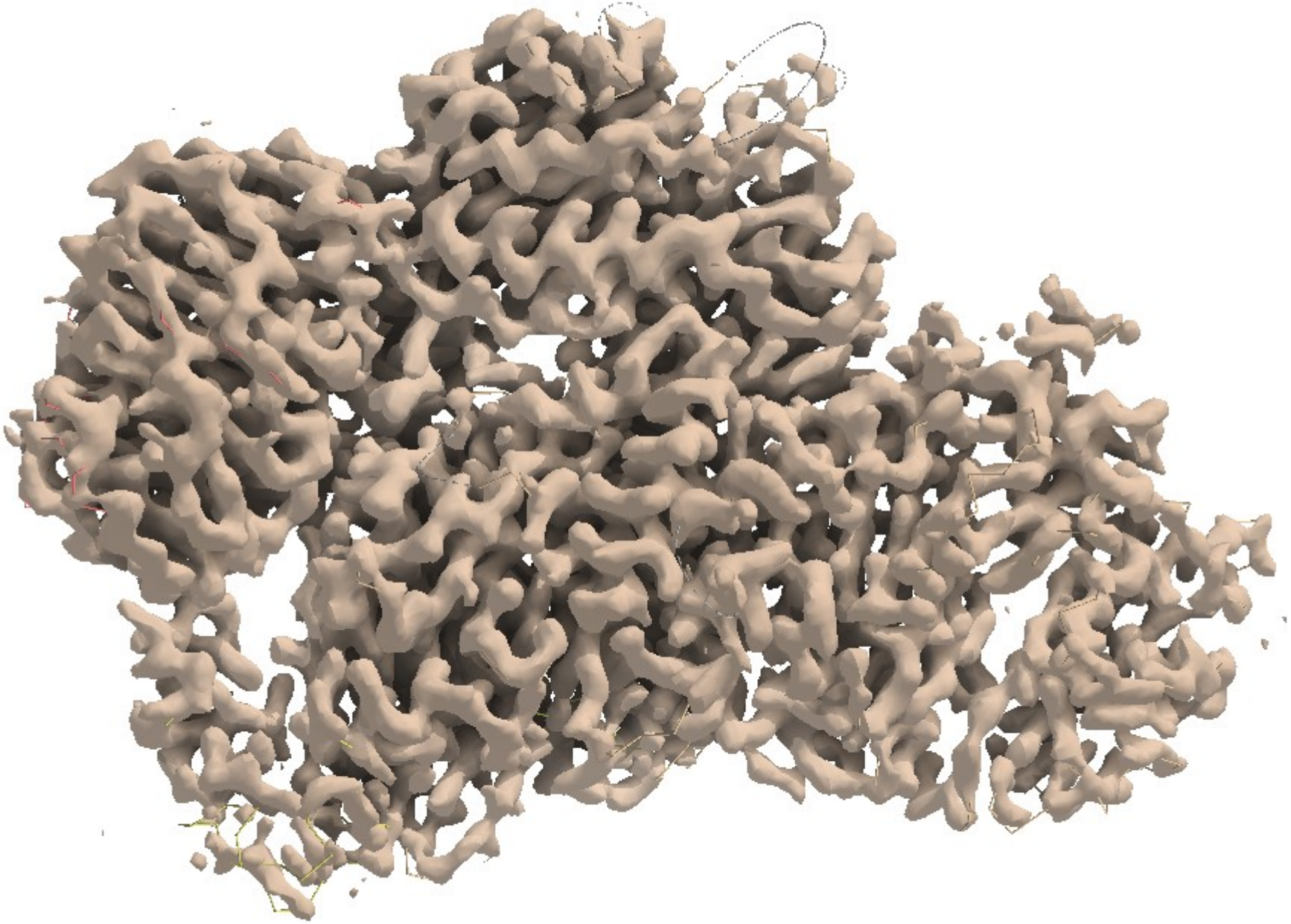
New *Coot* with “MoleculesToTriangles”

Thanks to Martin Noble

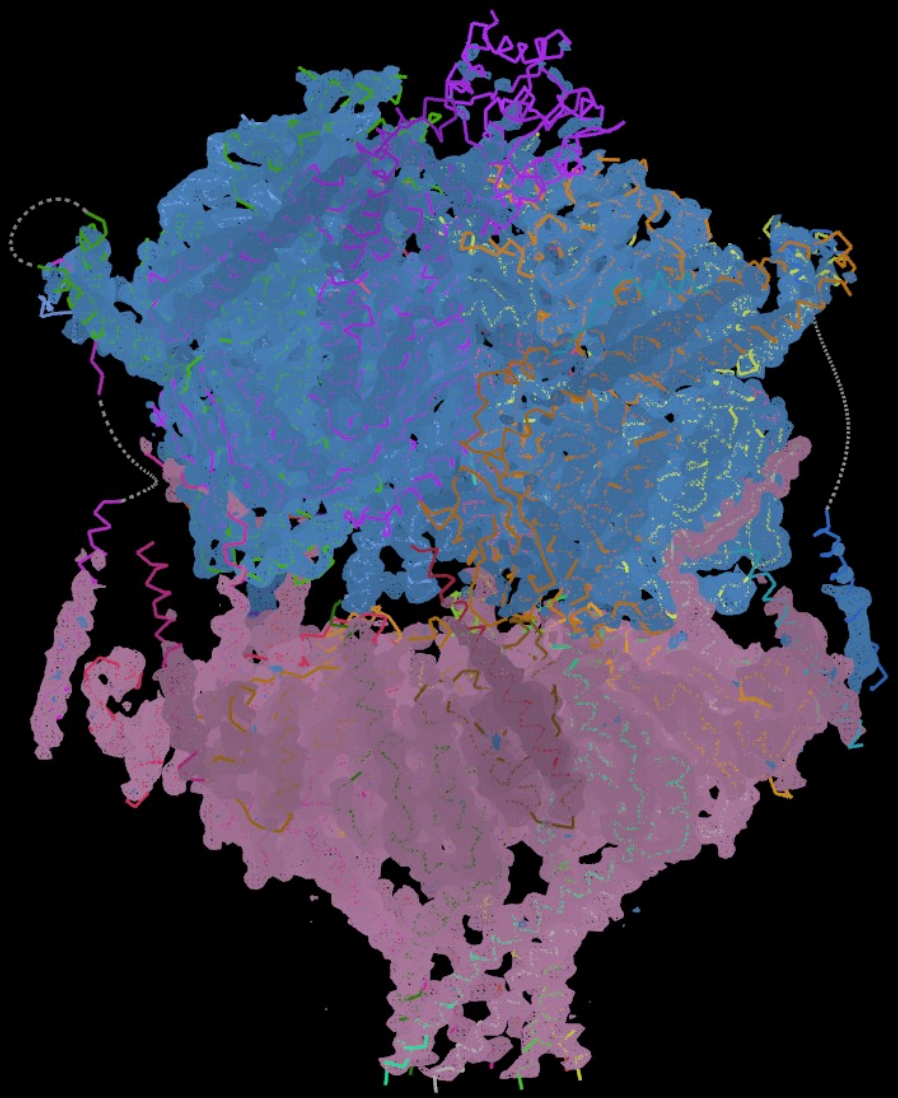


Old *Coot:* Cleavage and Polyadenylation Factor (CPF)

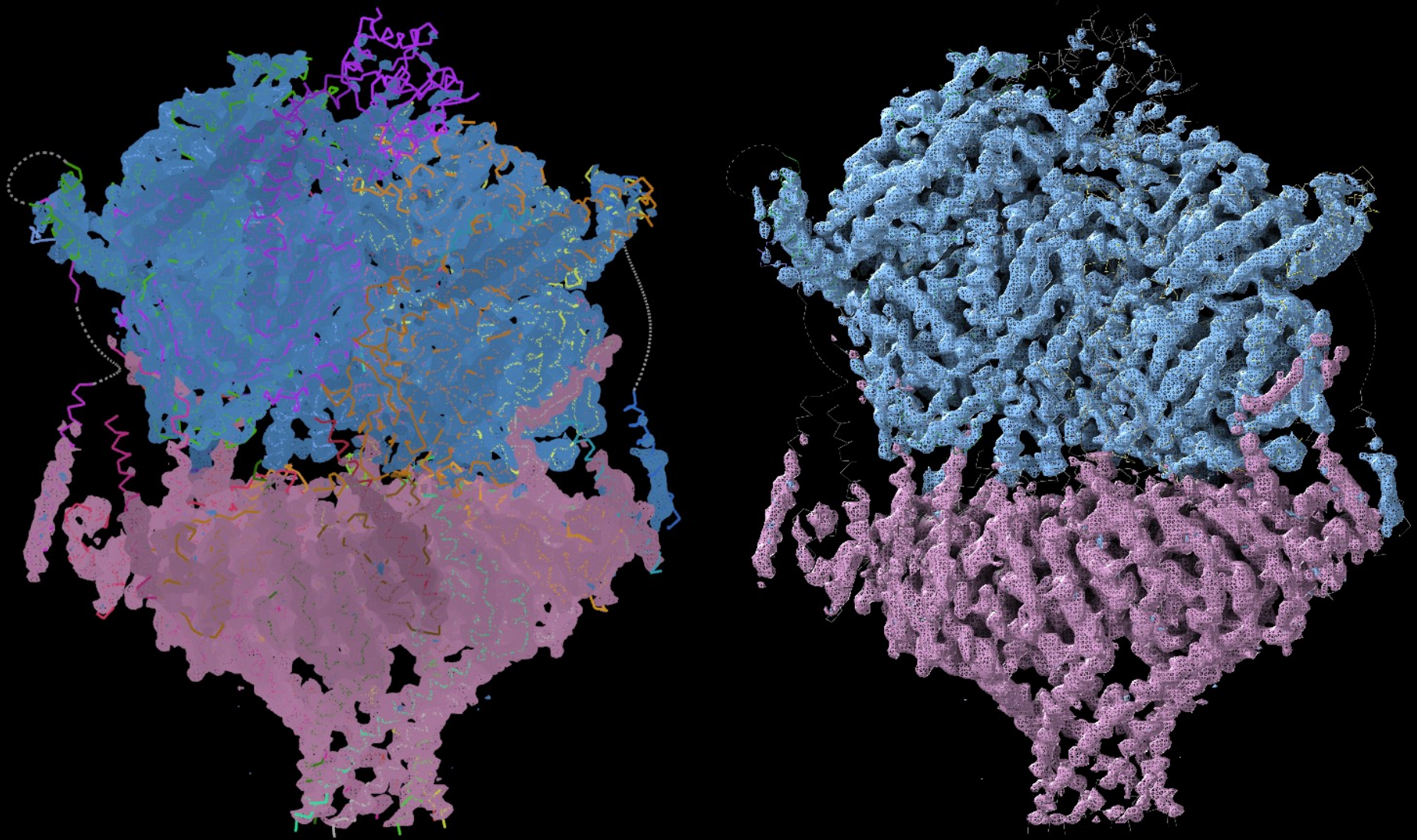
New *Coot:* Cleavage and Polyadenylation Factor (CPF)



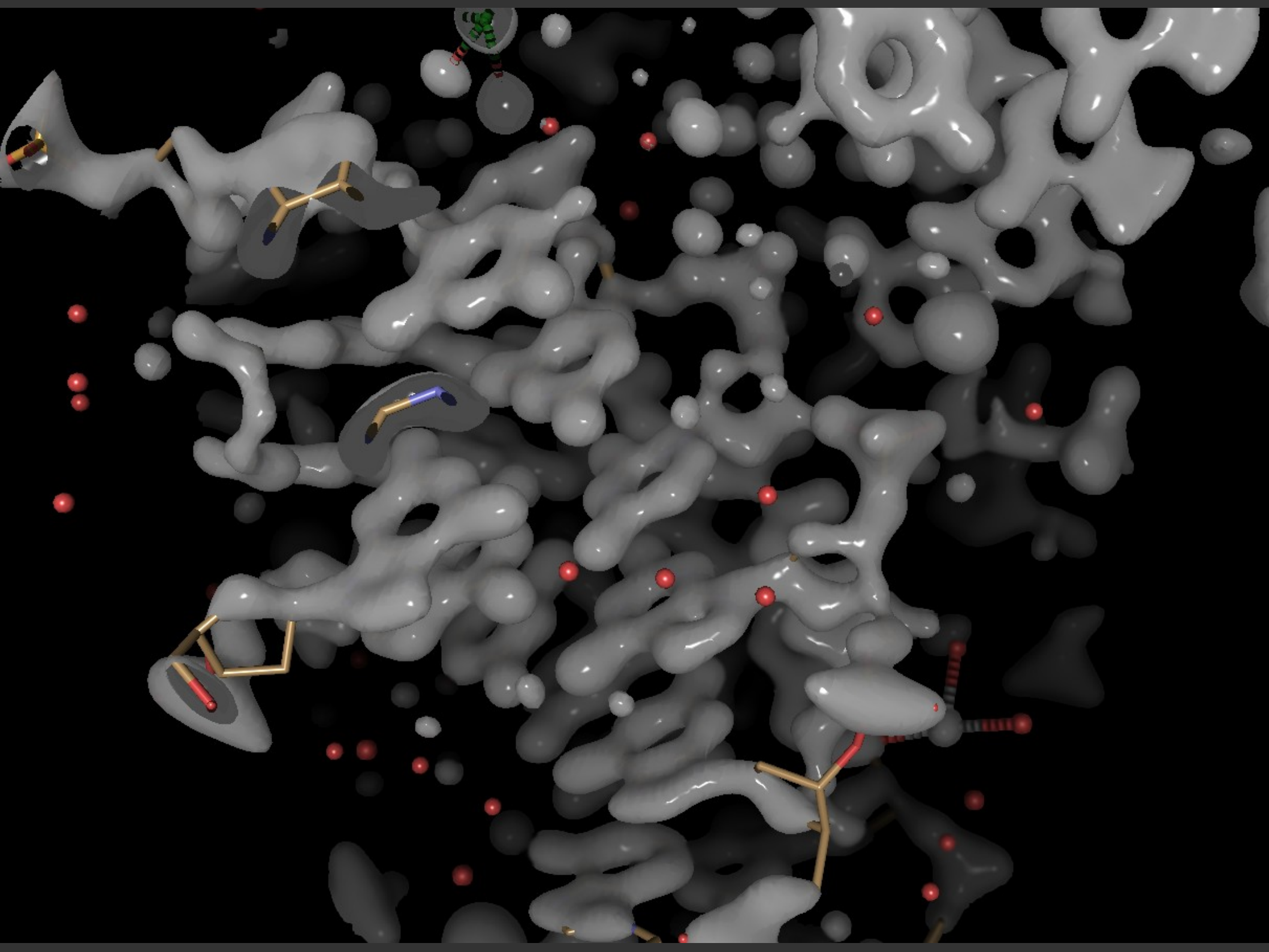
Old *Coot vs.* New *Coot*



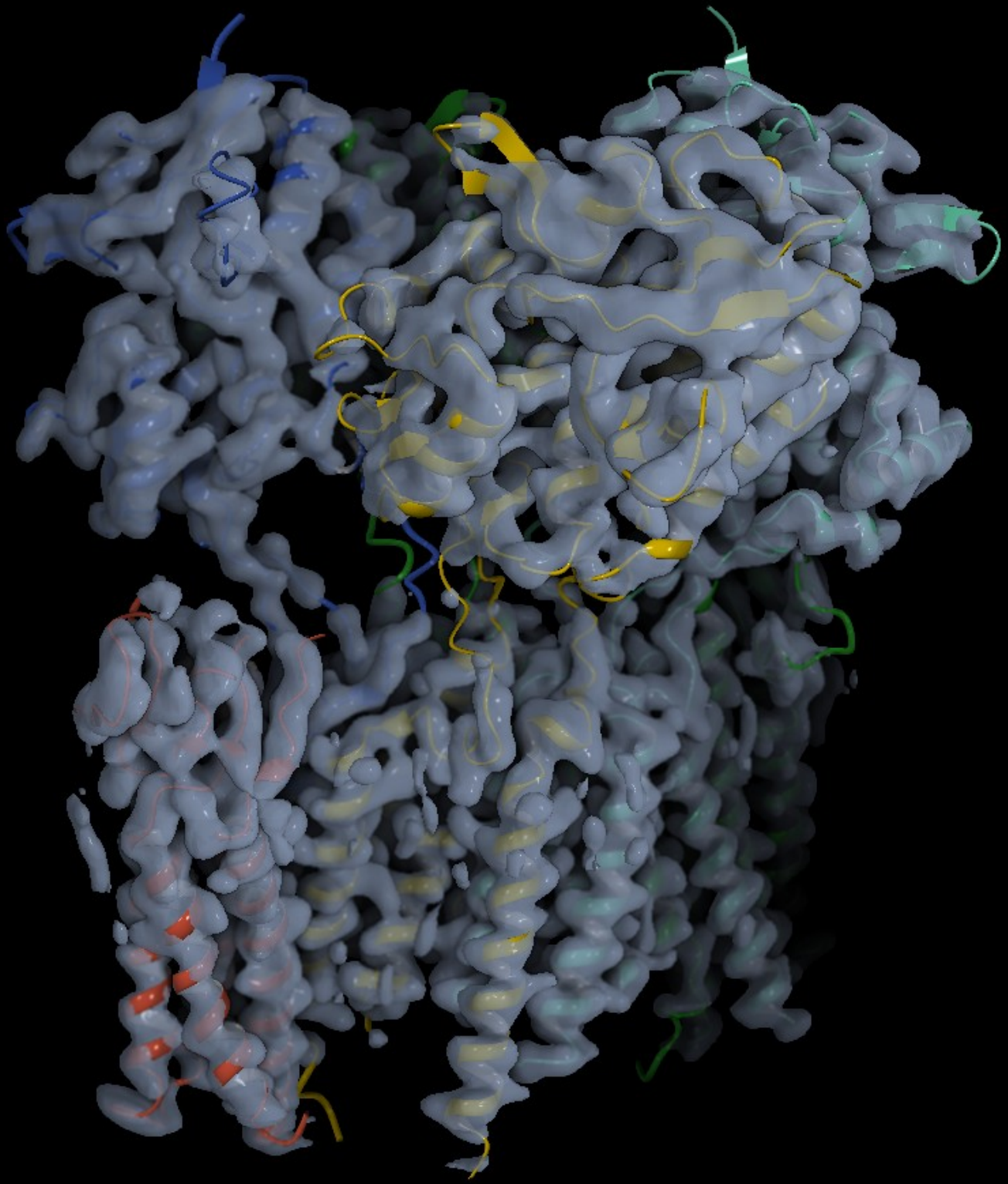
Old *Coot* *vs.* New *Coot*



"Chicken-wire"

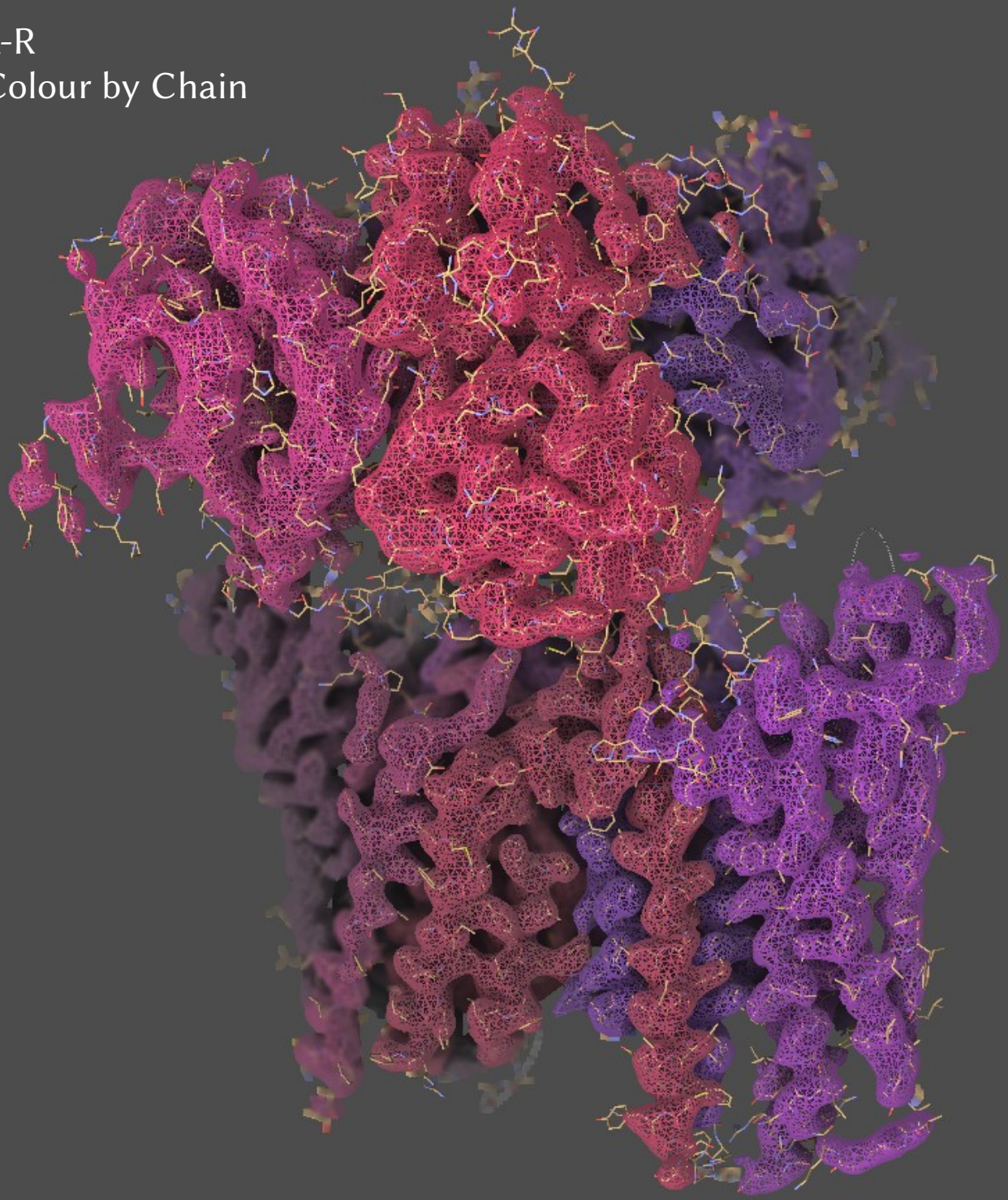


AMPA-R

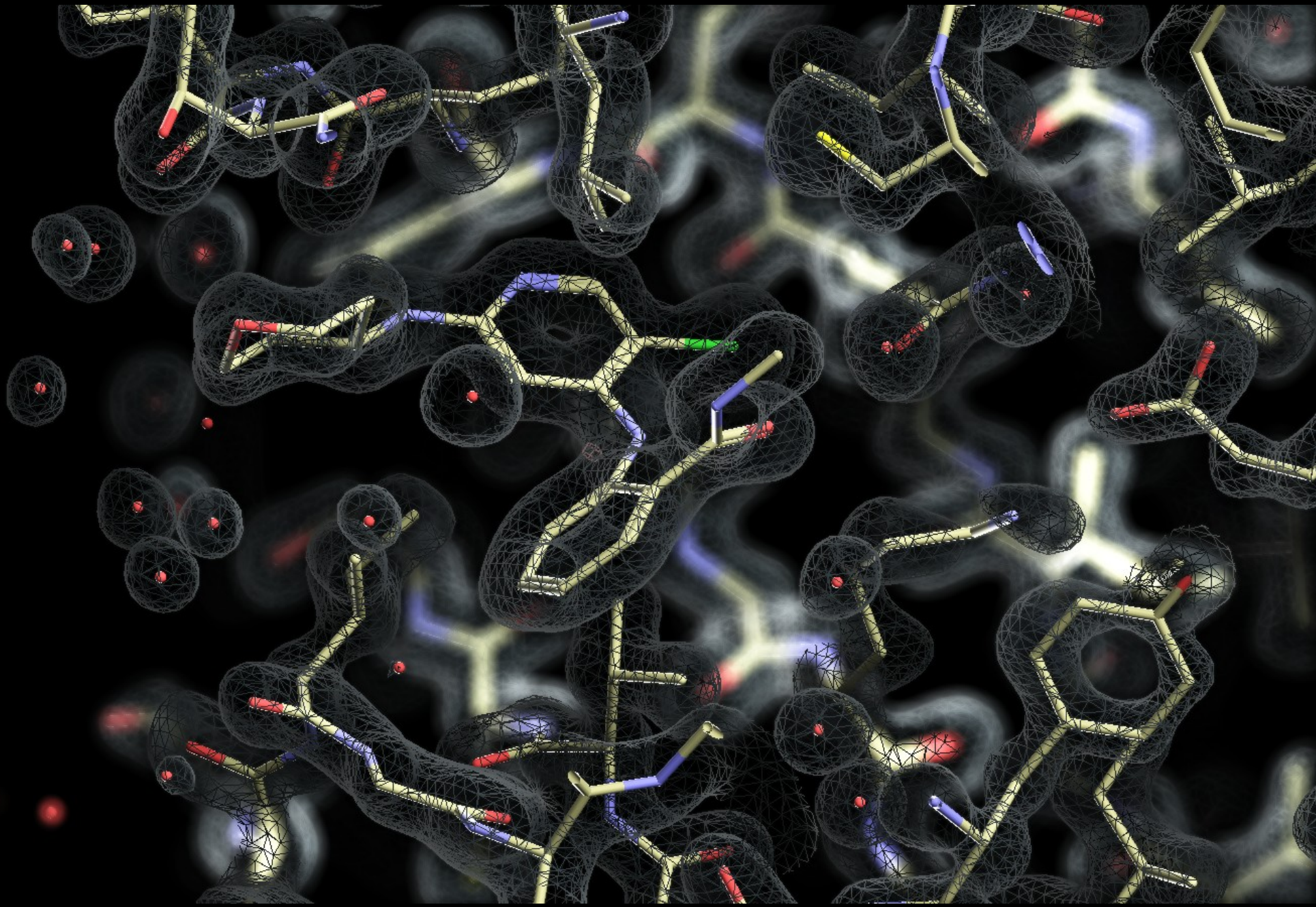


Welcome to Coot

AMPA-R
Map Colour by Chain

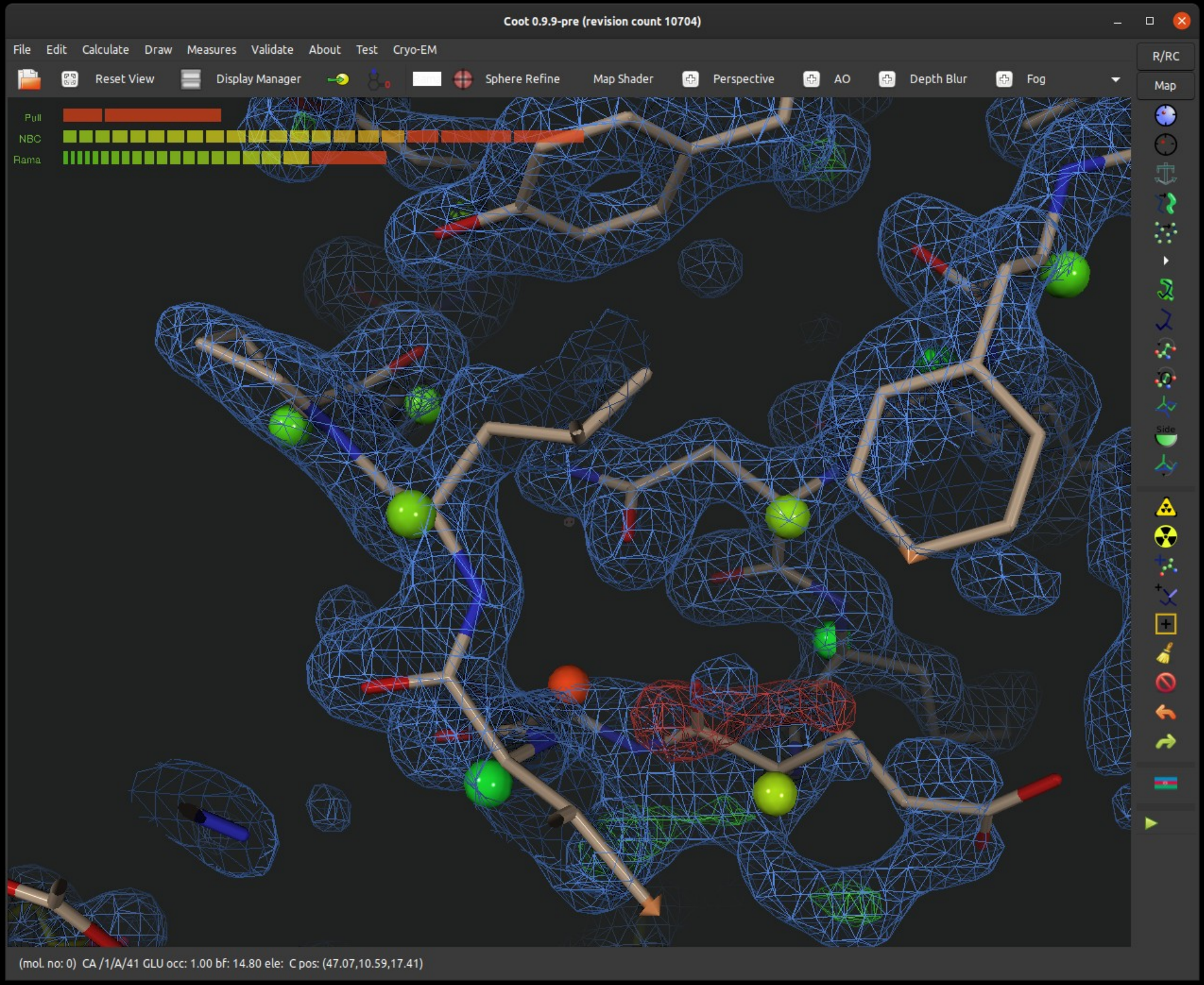


Fresnel Lighting



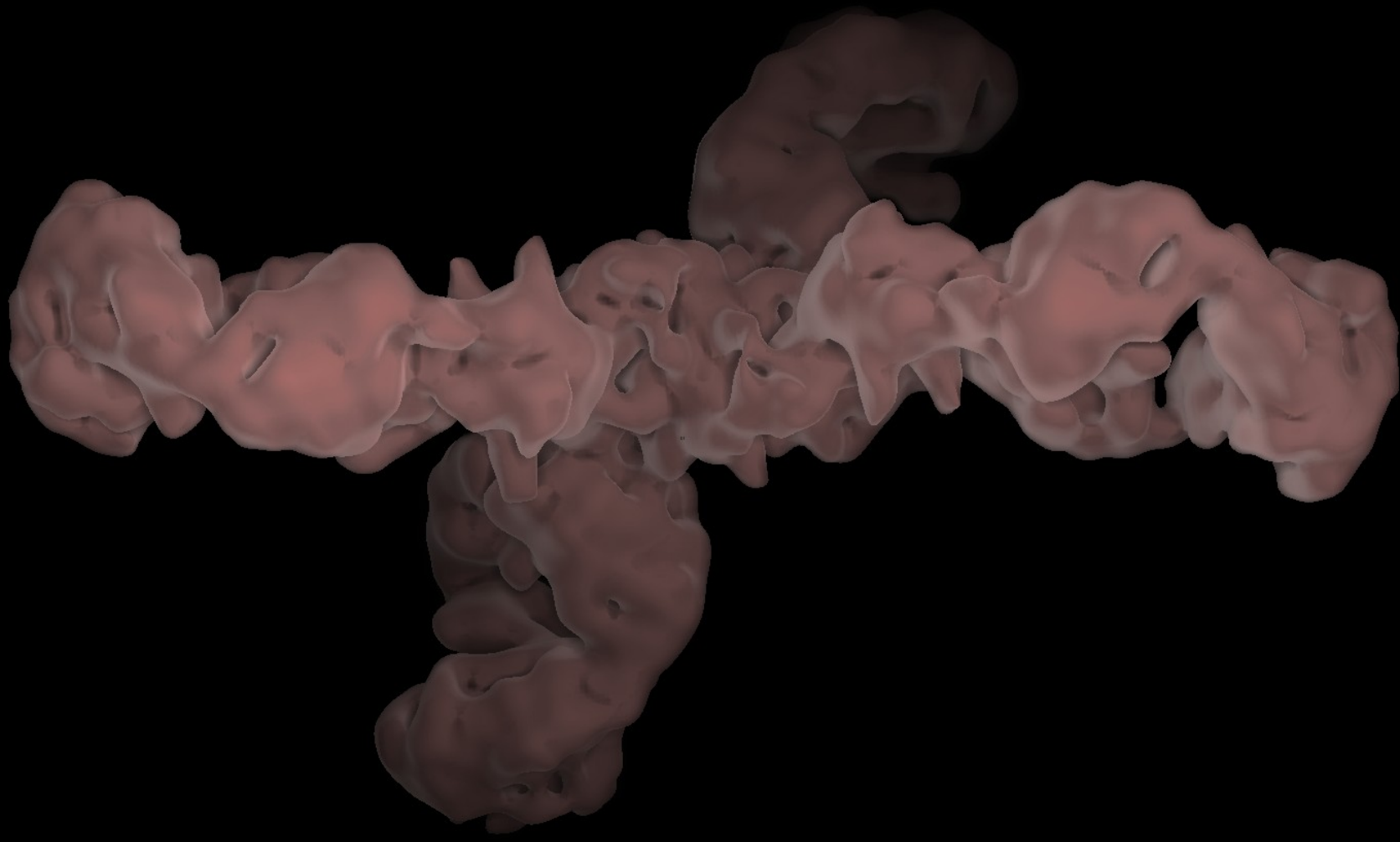
Real Space Refinement

- Change of feedback:
  - No more Accept/Reject dialog
  - More HUD information


Coot 0.9.9-pre (revision count 10704)
File
Edit
Calculate
Draw
Measures
Validate
About
Test
Cryo-EM
Reset View
Display Manager
Sphere Refine
Map Shader
Perspective
AO
Depth Blur
Fog
Pull
NBC
Rama
R/RC
Map
Side
(mol. no: 0) CA /1/A/41 GLU occ: 1.00 bf: 14.80 ele: C pos: (47.07,10.59,17.41)

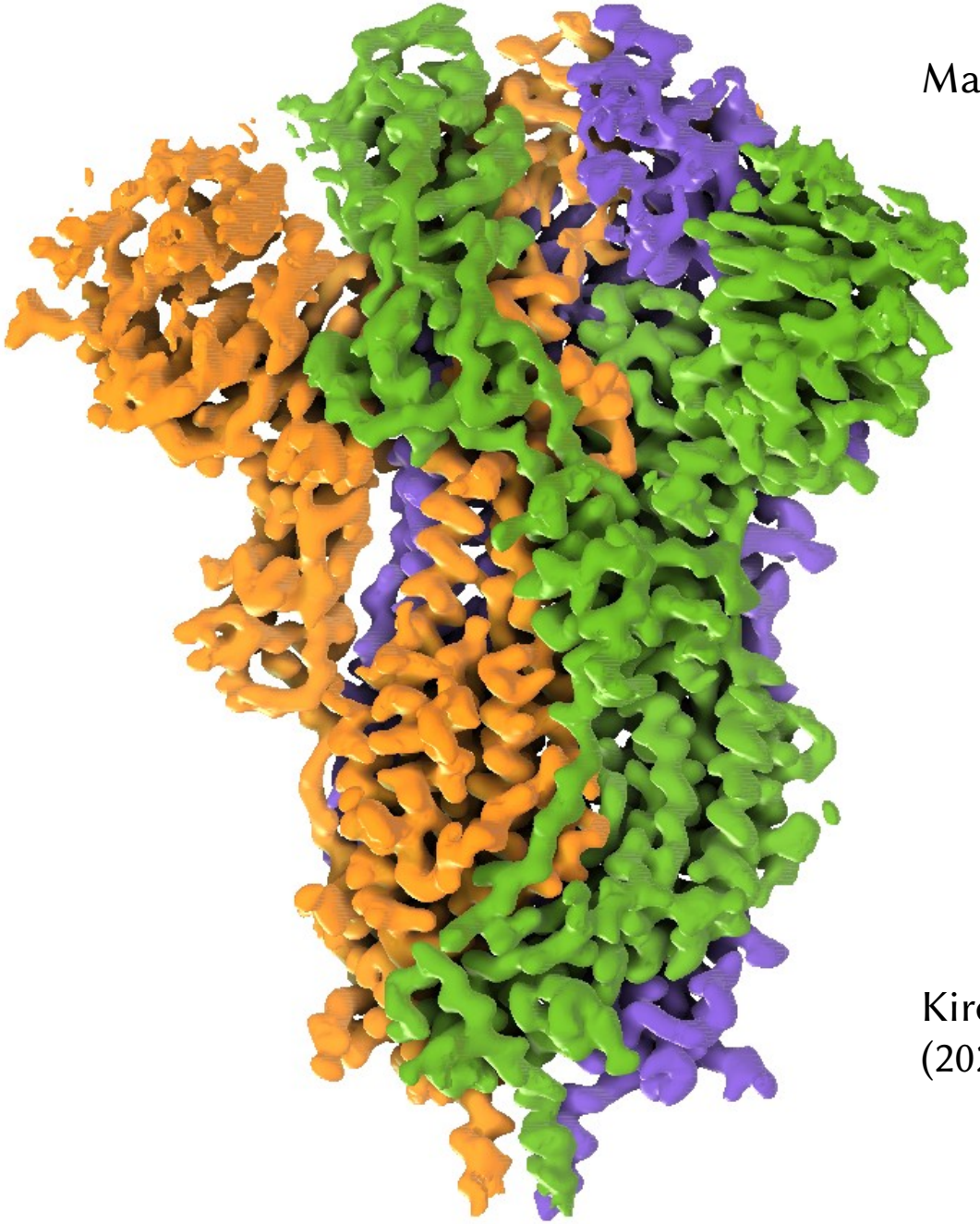
A Few Virus Screenshots

Ebola Virus Glycoprotein & Fabs



Saphire, Ward & co-workers (2018)

SARS-CoV-2 Spike protein

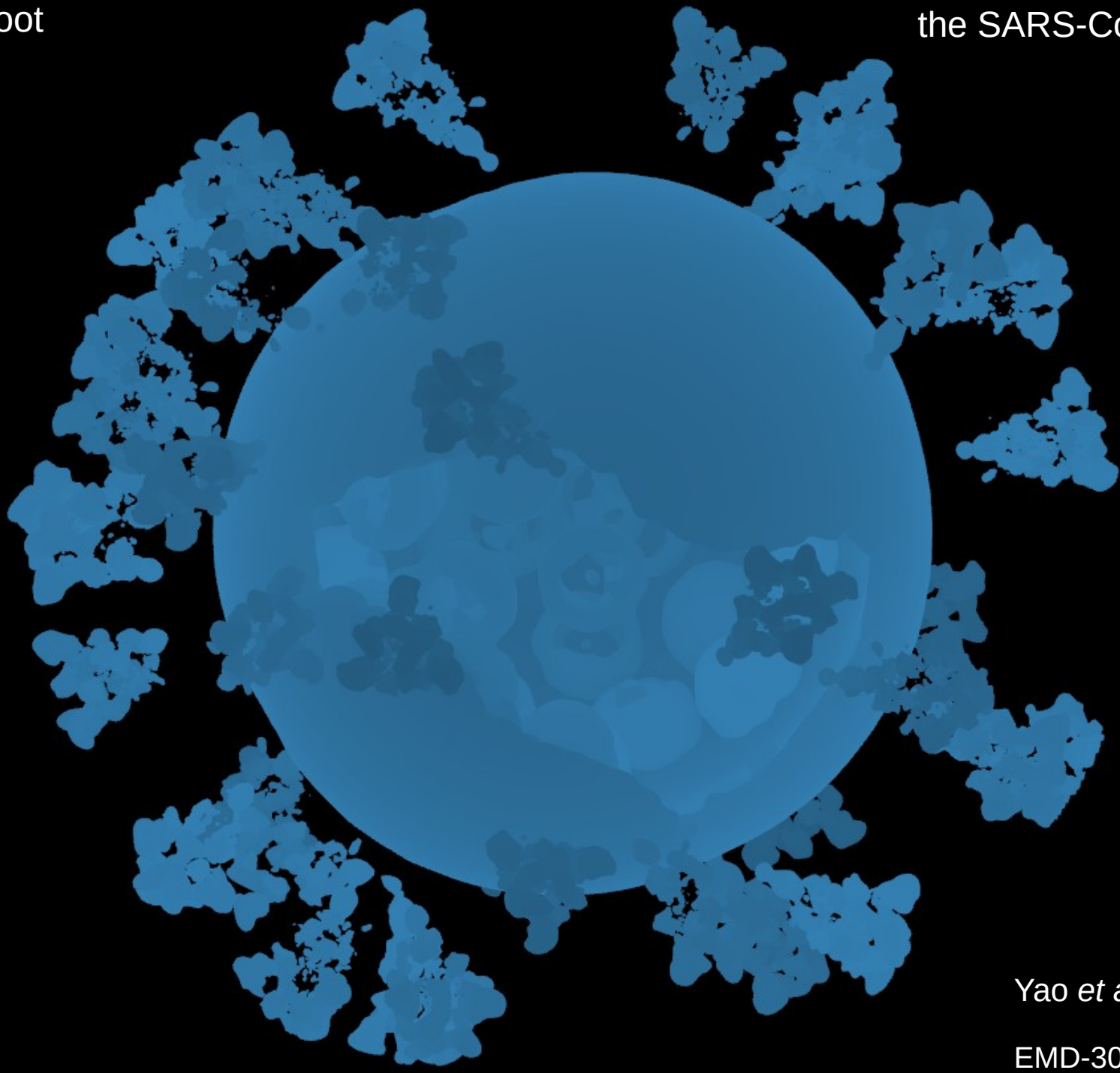


Map Colour by Chain mode

Kirchdoerfer, Ward & co-workers (2020)

Old Coot

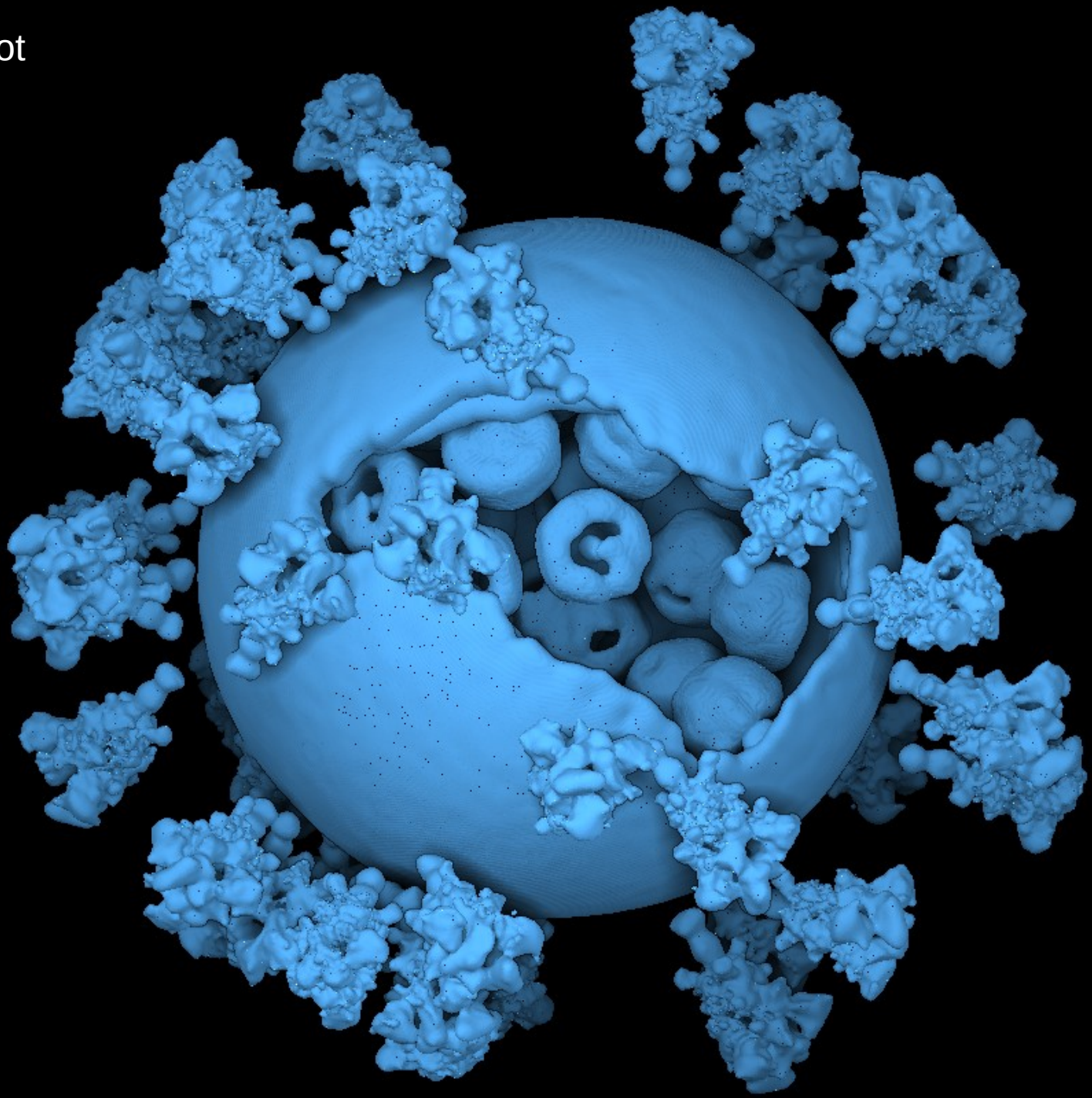
Molecular architecture of the SARS-CoV-2 virus



Yao *et al.*, Cell (2020)

EMD-30430

New Coot

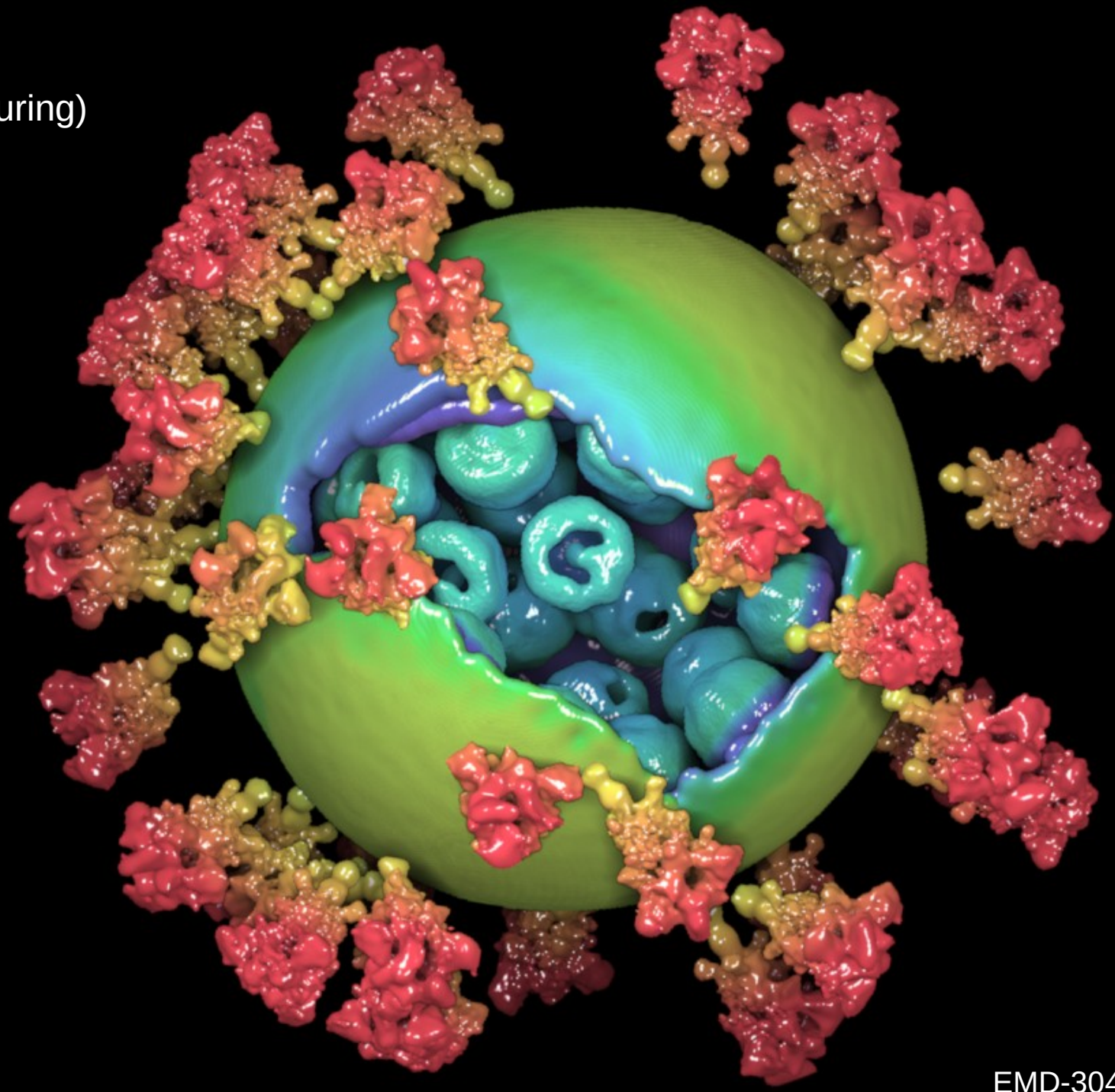


EMD-30430

New Coot

(radial colouring)

(video)



EMD-30430

Summary

- The graphics in *Coot* have been improved
  - Improved perception of depth
  - Improved FPS, bigger objects, more realism
  - Fold in ribbons, molecular surfaces representations
  - More sophisticated colour schemes for maps

- Interactive Interface (RSR):
  - Less dialogs, more HUD (on-going change)

- Videos available

Acknowledgements

- Martin Noble
- LMB members
  - Ana Casañal, Ester Vazquez Fernandez, Andrew Carter