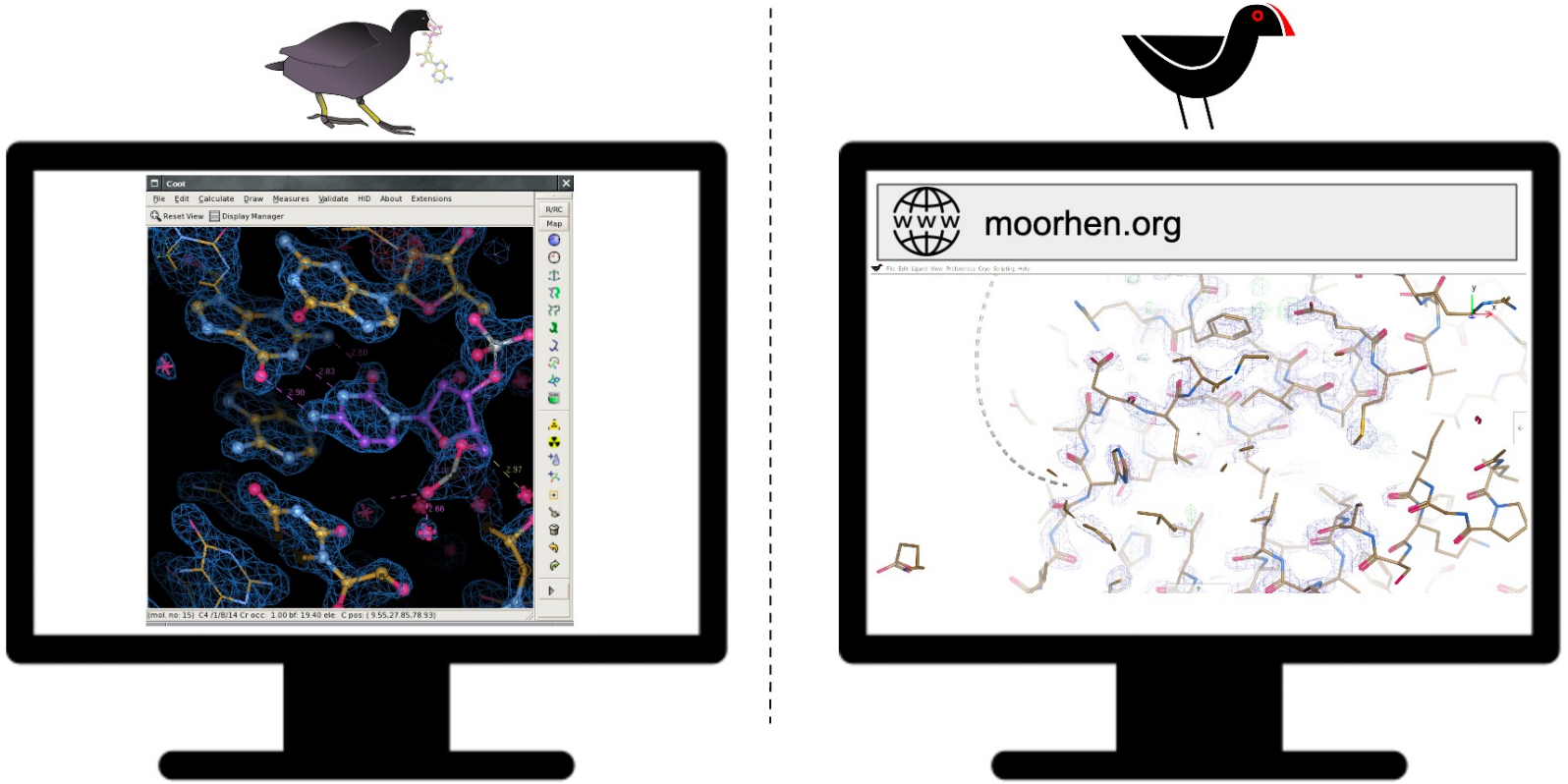
# Coot and Moorhen

## Model building, Real-space refinement & Graphics




**Lucrezia Catapano**

CCP-EM Icknield Workshop

6th November 2024

# Model-building with Coot

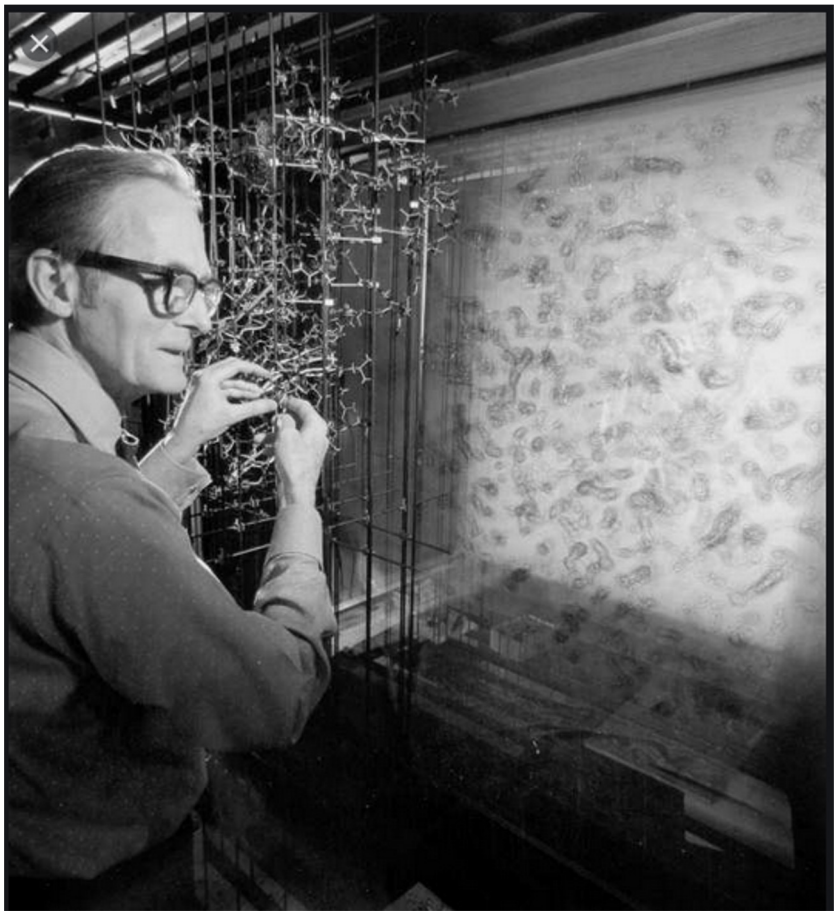
**Tools to help improve the quality of the macromolecular model:**

- Mutations
- Addition/Deletions/Merging
- Refinement tools
- Tools for ligand analysis and presentation
- Tools for Cryo-EM fitting

This is a coot

# On “Manual Model Building”

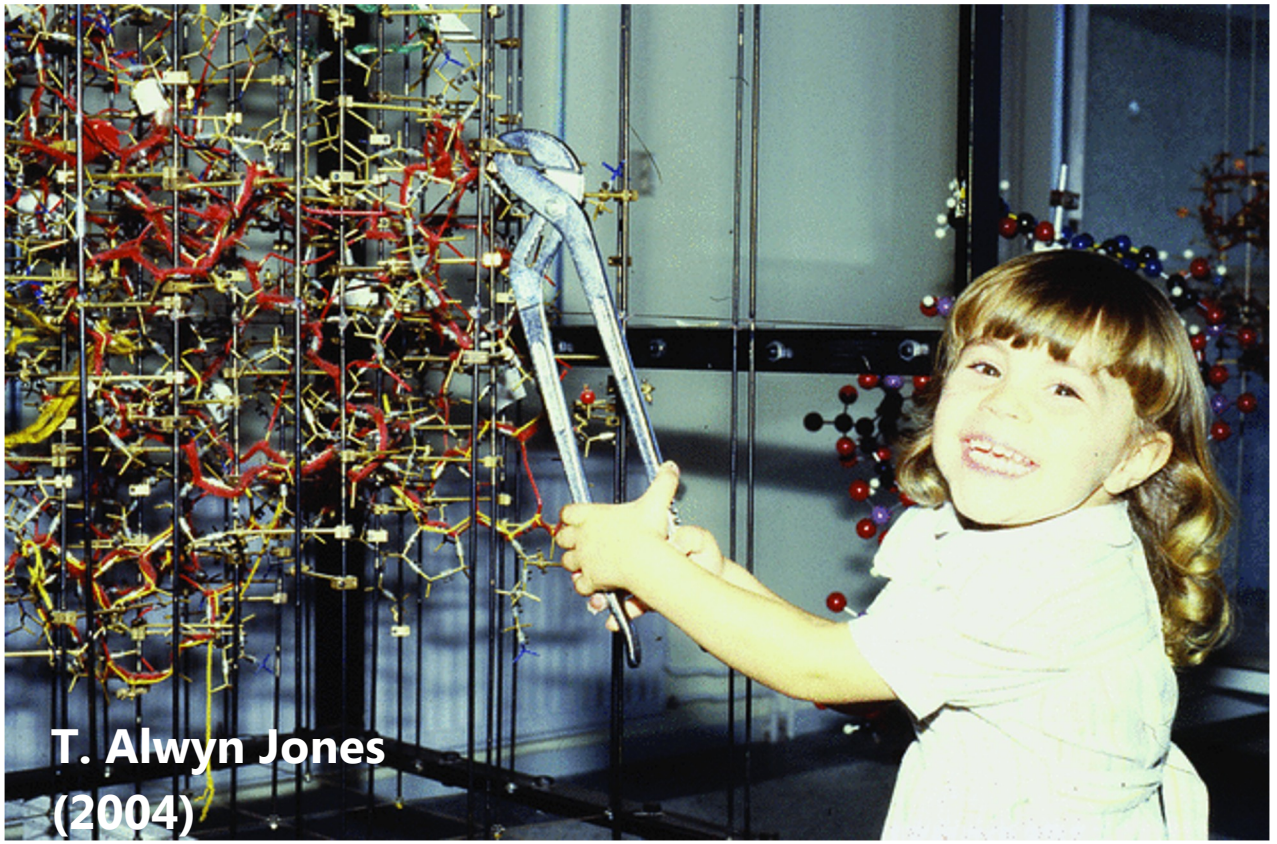
DCH building the first insulin model



William Lipscomb, model of carboxipeptidase

*This is “Manual Model-Building”*
*“twisting physical brass models held together by screws”*

Kendrew wire model of alcohol dehydrogenase that is about to undergo a round of rebuilding by Maelle Cambillau




"Manual" implies that you are deciding where the atoms go – in fact you aren't… Coot is.

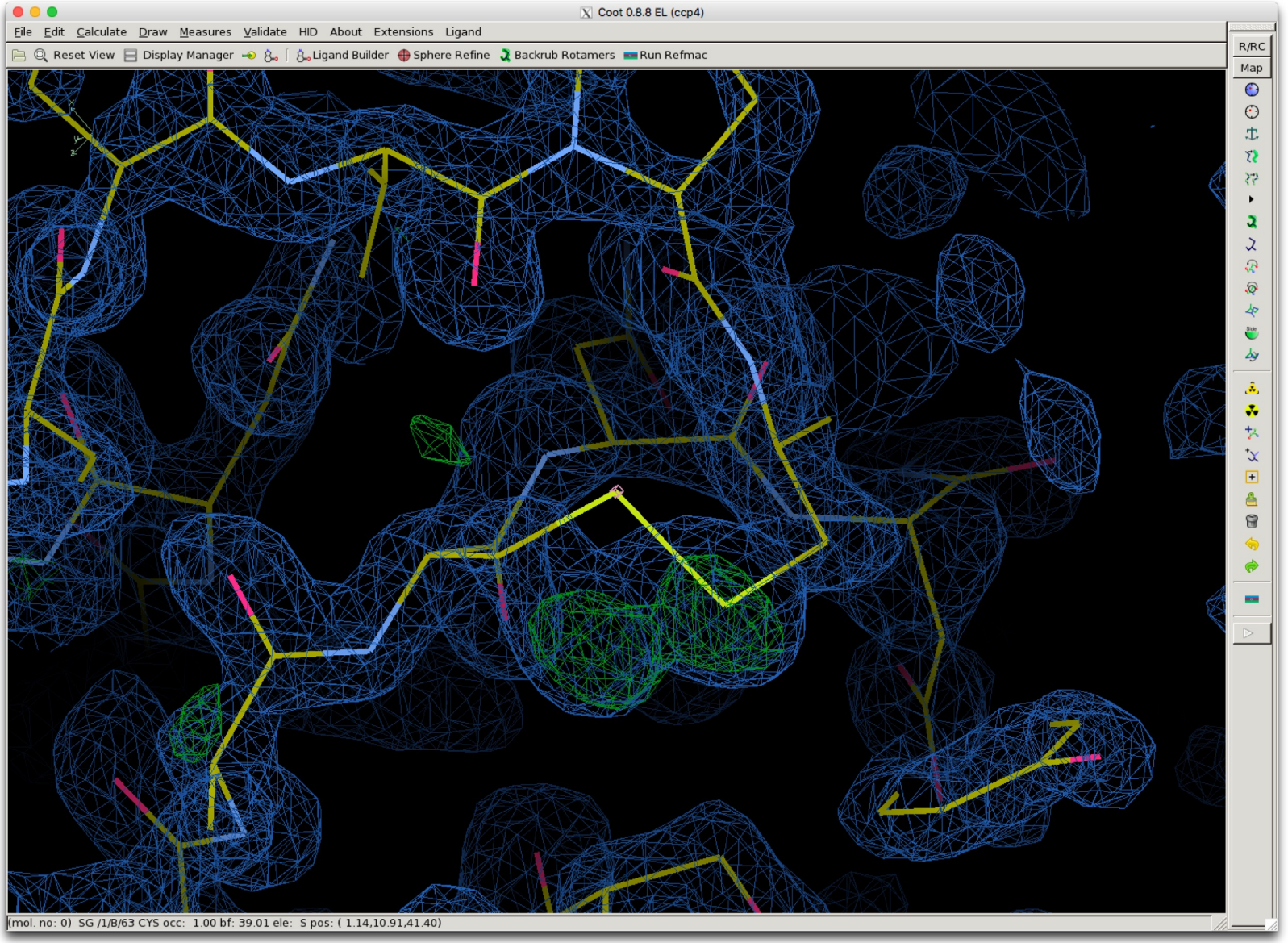
**Using *Coot* is not like this:**
***Coot* fitting tools are fast and automated**

Coot is (typically) local, automated and interactive.

# Coot

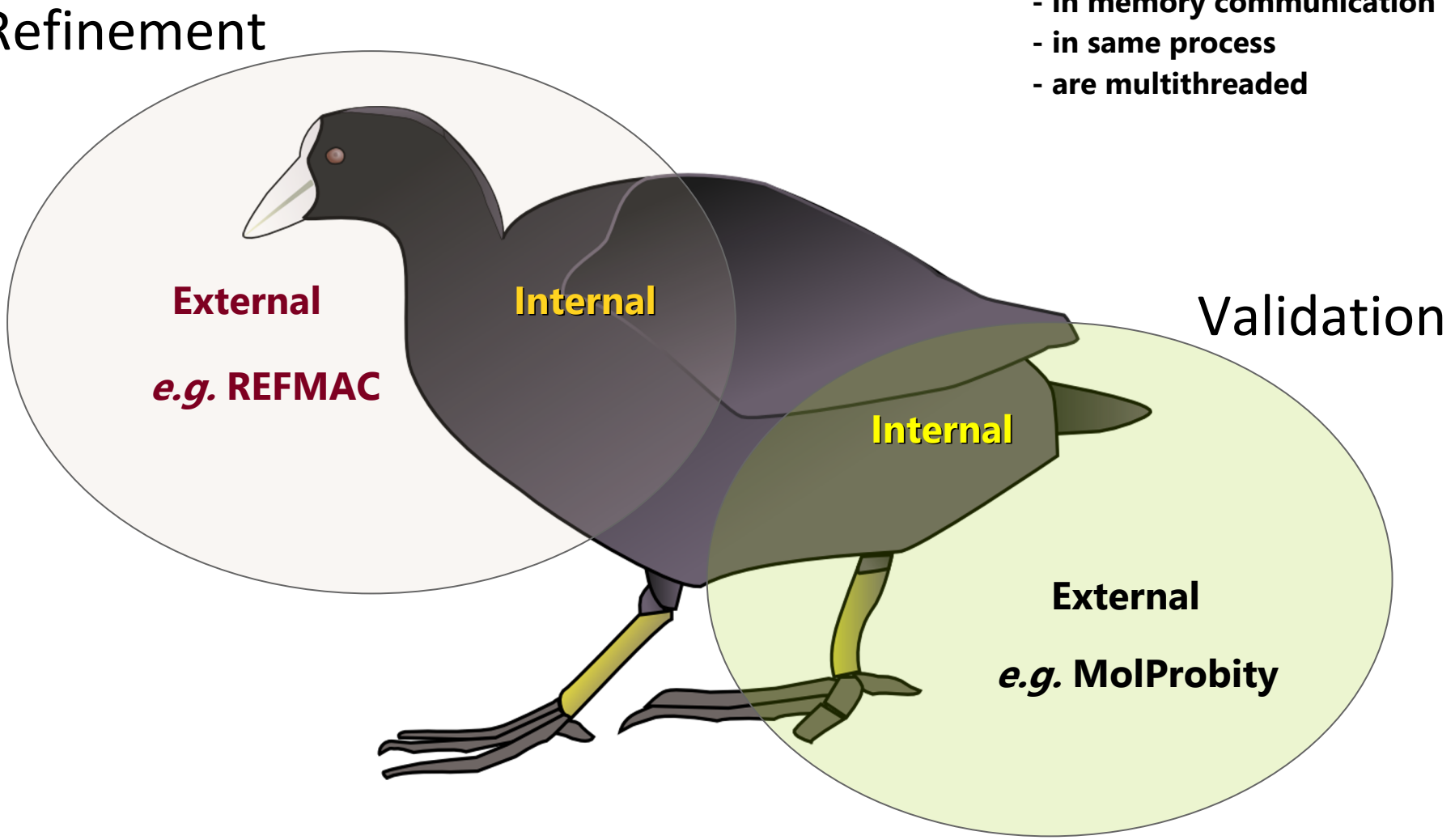
- Molecular Graphics application
- Protein Crystallographic **model-building** tools
- Designed to “fill the gap” where automatic methods fail
- (generally, we don't use molecular graphics programs to do what non-interactive methods can do)
- Interface to other programs: SHELXL, Refmac, Libcheck, Probe&Reduce (Molprobity), EBI, EDS, Povray... and others

# Fixing what auto-building doesn't get right



# Feature Integration

**Internal Tools:**
- **in memory communication**
- **in same process**
- **are multithreaded**




**Validation, Model Building and Refinement should be used together**

**Rapid Updates of Model, Maps and Validation considerably expediates the process**

# Real Space Refinement

Diamond, R. (1971). *Acta Cryst.* A 27, 436–452.

**Major Feature of Coot**

- Gradient-based minimiser (BFGS derivative)
- Geometry library is the standard CIF-based **CCP4 Monomer Library**
- Minimise deviations in bond length, angles, torsions, planes, chiral volume, non-bonded contacts
- Including links and modifications
- Provides “interactive” refinement
- Subject to substantial extension

# What prior geometric information do we have?

- We know chemistry….
- We know **bond lengths** and uncertainties
- We know **bond angles** and uncertainties
- We know the **chiral centres**
- We know which atoms should lie in a **plane**
- We know (more or less) about **torsions**
- We combine the gradients from the data with those from molecular mechanics in the minimisation

# CCP4 Monomer Library

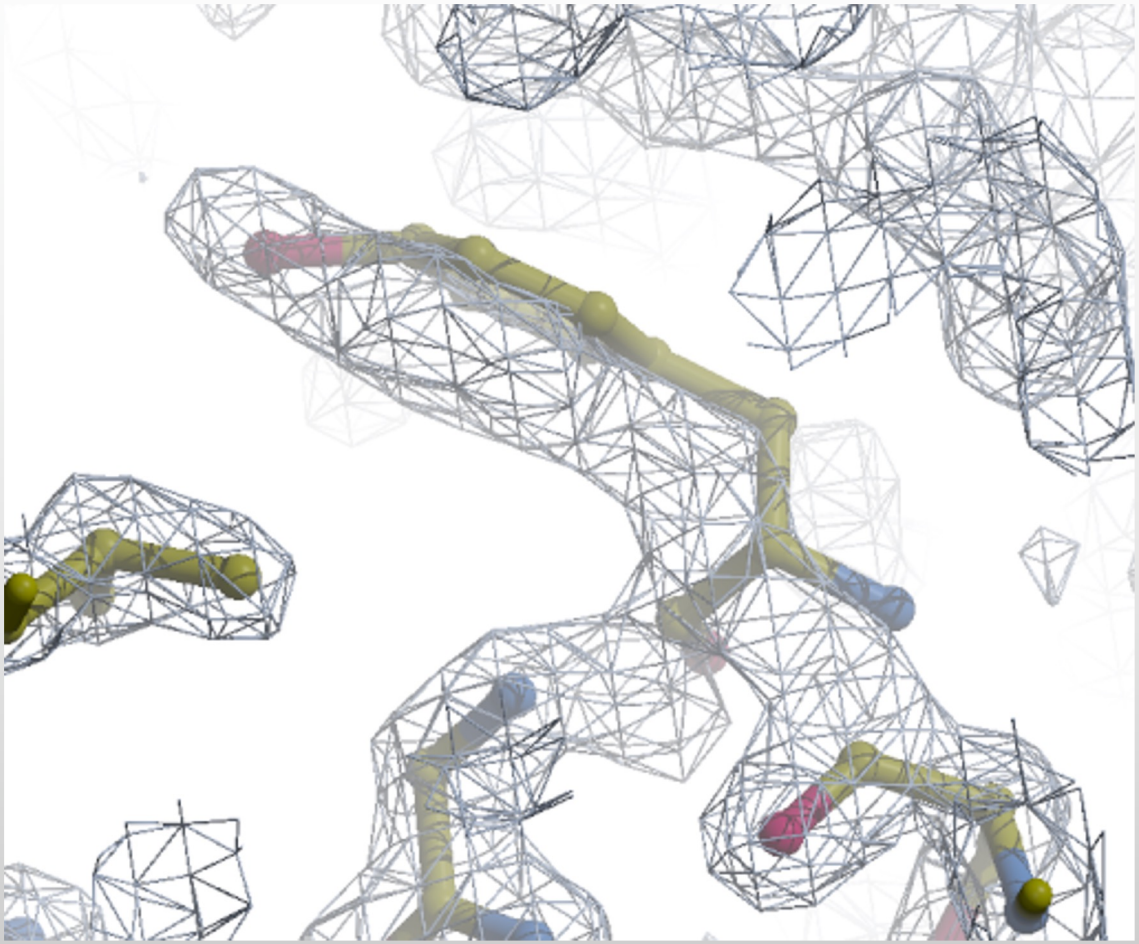
## chem_comp_bond

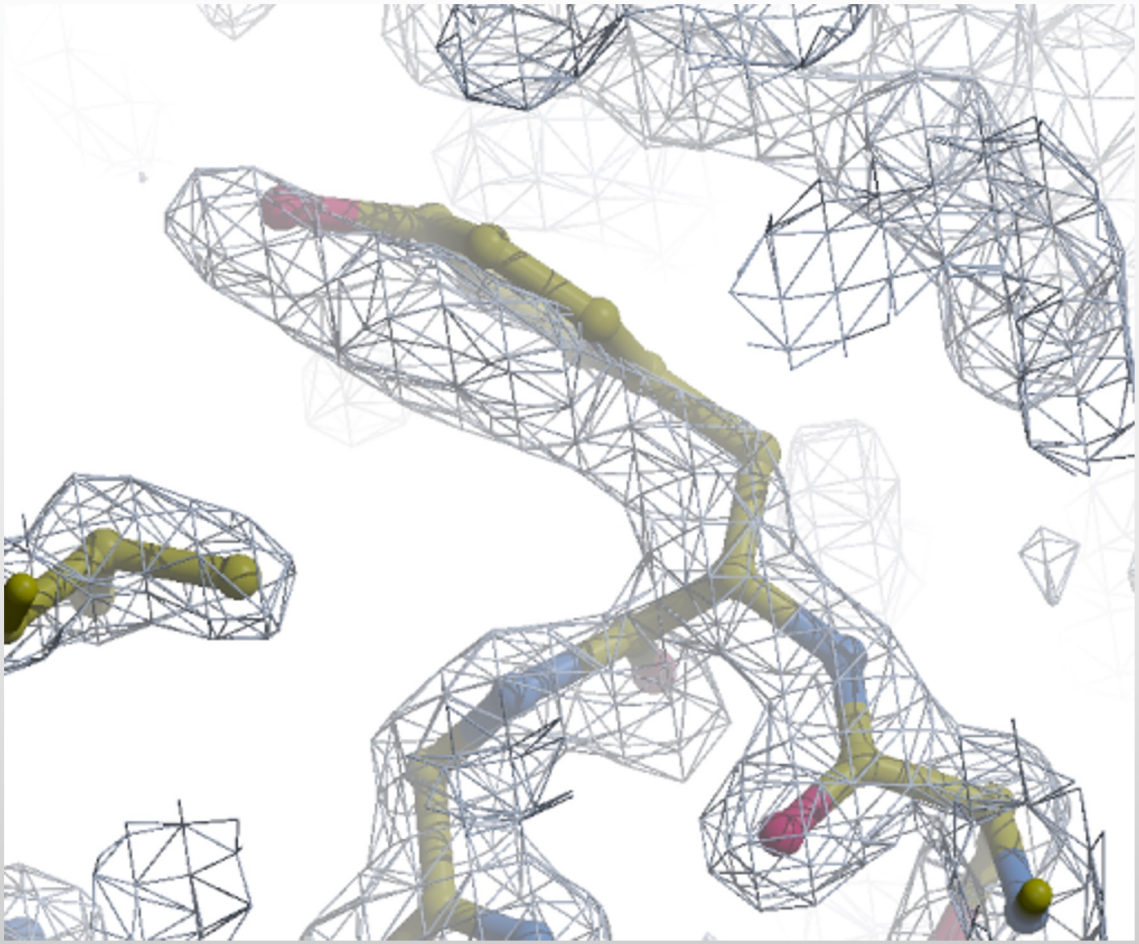
```
data_comp_list
loop_
_chem_comp.id
_chem_comp.three_letter_code
_chem_comp.name
_chem_comp.group
_chem_comp.number_atoms_all
_chem_comp.number_atoms_nh
_chem_comp.desc_level
ATP     ATP      "ADENOSINE-5'-TRIPHOSPHATE"     NON-POLYMER     43     31     .
loop_
_chem_comp_bond.comp_id
_chem_comp_bond.atom_id_1
_chem_comp_bond.atom_id_2
_chem_comp_bond.type
_chem_comp_bond.aromatic
_chem_comp_bond.value_dist_nucleus
_chem_comp_bond.value_dist_nucleus_esd
_chem_comp_bond.value_dist
_chem_comp_bond.value_dist_esd
ATP       "C5'"      "H5'1"      SINGLE       n     1.087  0.0100     0.989  0.0200
ATP       "C5'"      "H5'2"      SINGLE       n     1.087  0.0100     0.989  0.0200
ATP       "C4'"       "H4'"      SINGLE       n     1.087  0.0100     0.981  0.0200
ATP       "C3'"       "H3'"      SINGLE       n     1.087  0.0100     0.992  0.0200
ATP       "O3'"      "HO3'"      SINGLE       n     0.969  0.0180     0.849  0.0200
ATP       "C2'"       "H2'"      SINGLE       n     1.087  0.0100     0.994  0.0200
ATP       "O2'"      "HO2'"      SINGLE       n     0.969  0.0180     0.849  0.0200
ATP       "C1'"       "H1'"      SINGLE       n     1.087  0.0100     0.984  0.0200
ATP          C8          H8      SINGLE       n     1.083  0.0150     0.942  0.0170
ATP          N6        HN61      SINGLE       n     1.014  0.0120     0.877  0.0200
ATP          N6        HN62      SINGLE       n     1.014  0.0120     0.877  0.0200
ATP          C2          H2      SINGLE       n     1.083  0.0150     0.945  0.0200
```

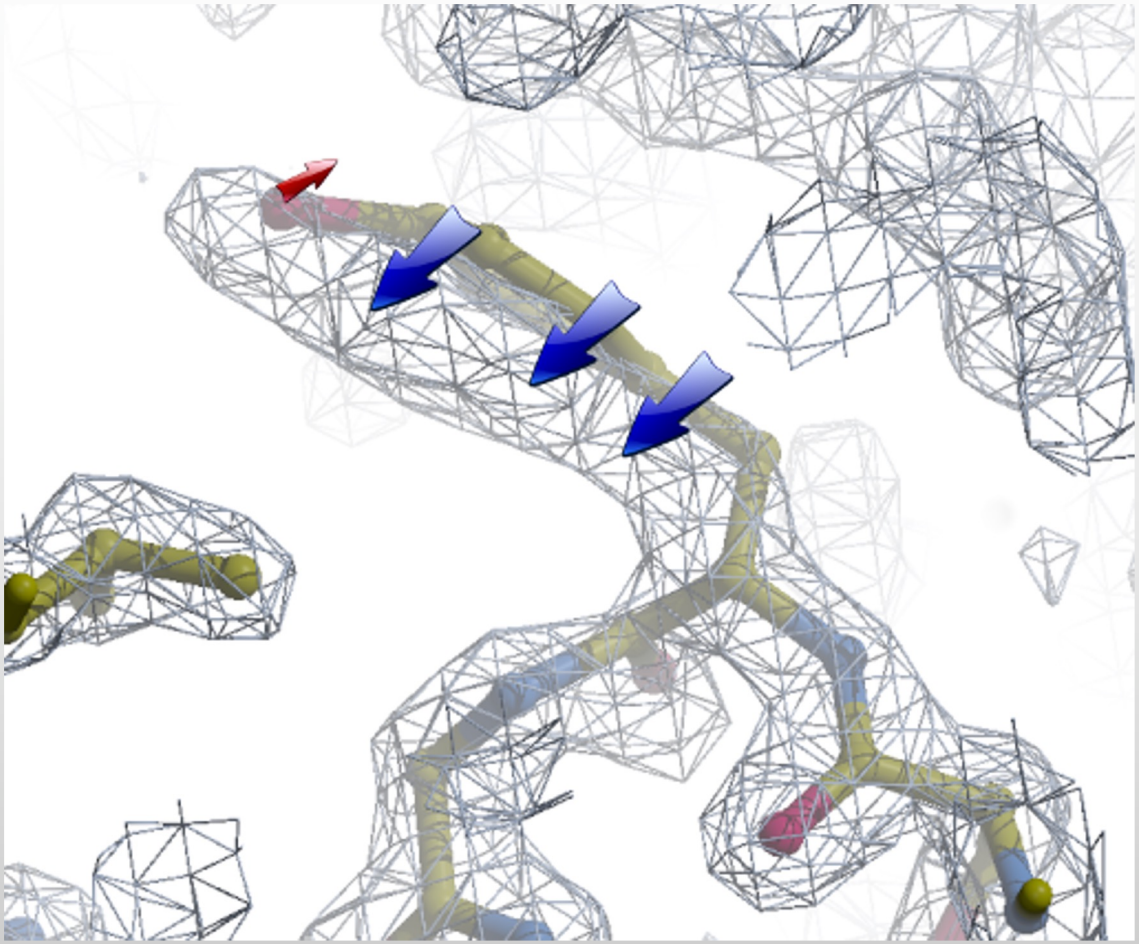
## APPENDIX *A*
## Regularization and refinement derivatives

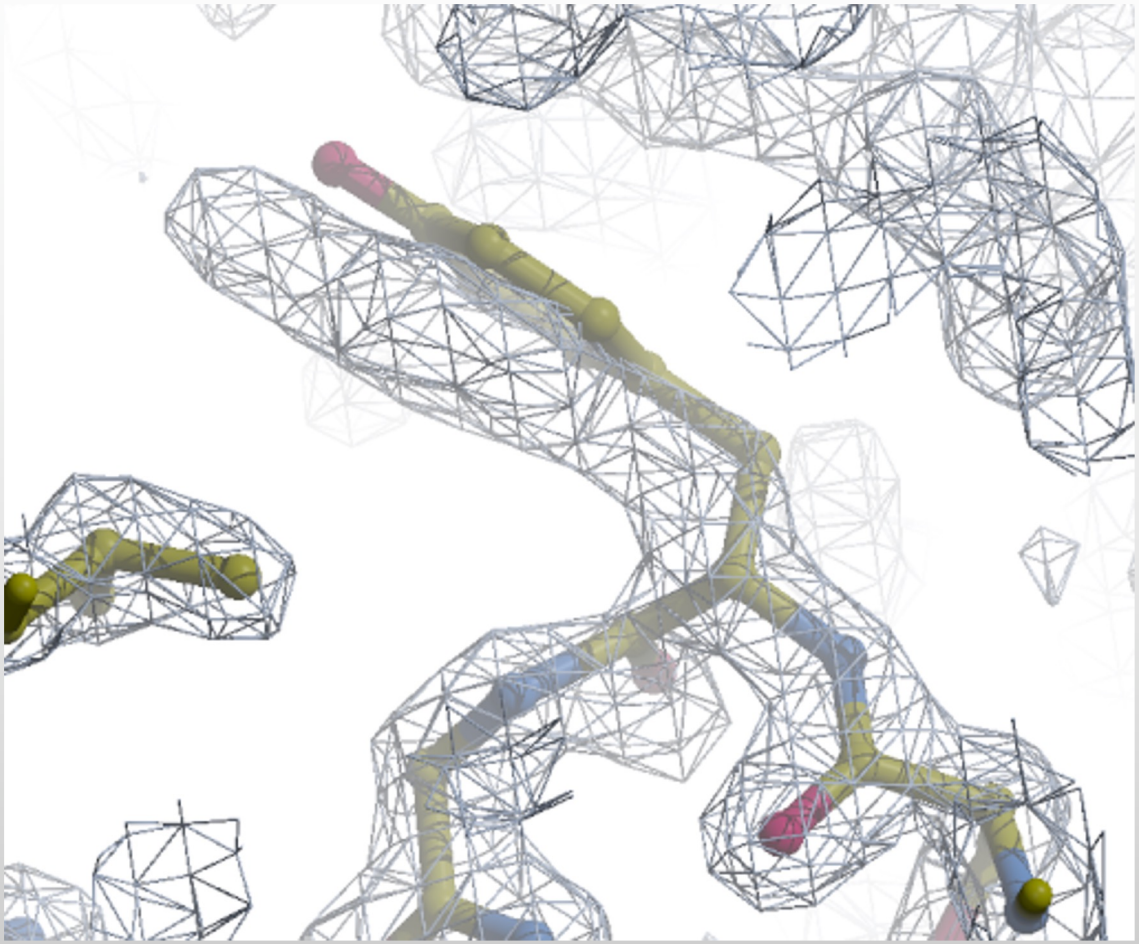
The function that we are trying to minimize is $S$, where

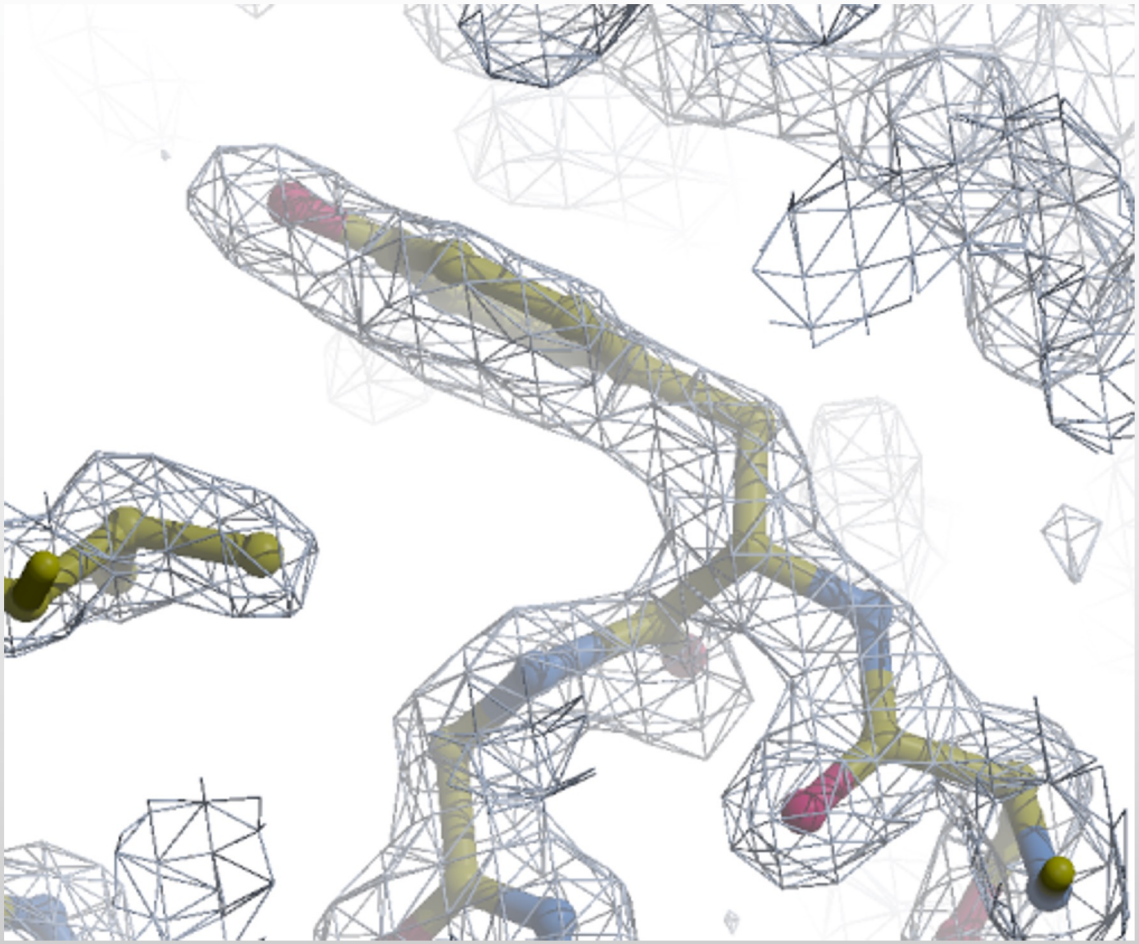
$$S = S_{\text{bond}} + S_{\text{angle}} + S_{\text{torsion}} + S_{\text{plane}} \quad - S_{\text{density}}$$

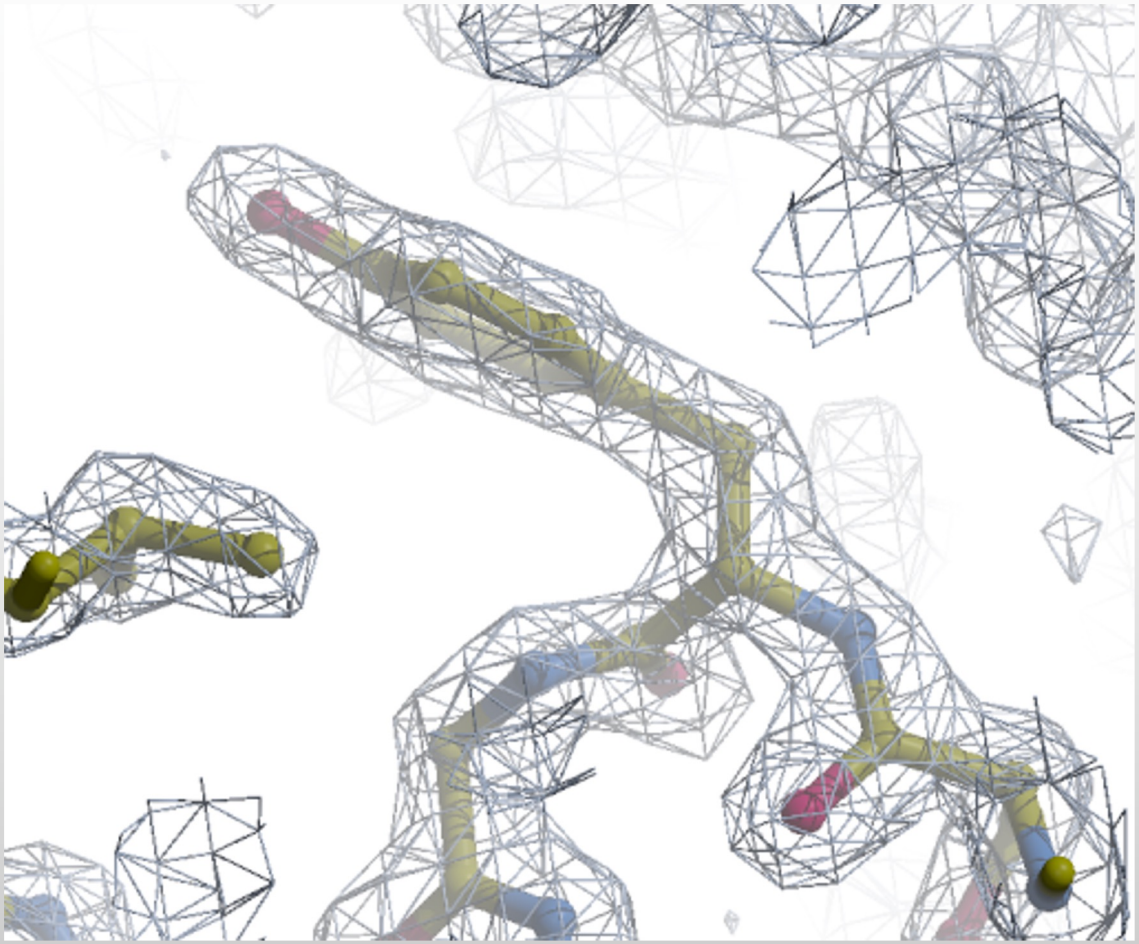












# Representation of Results:

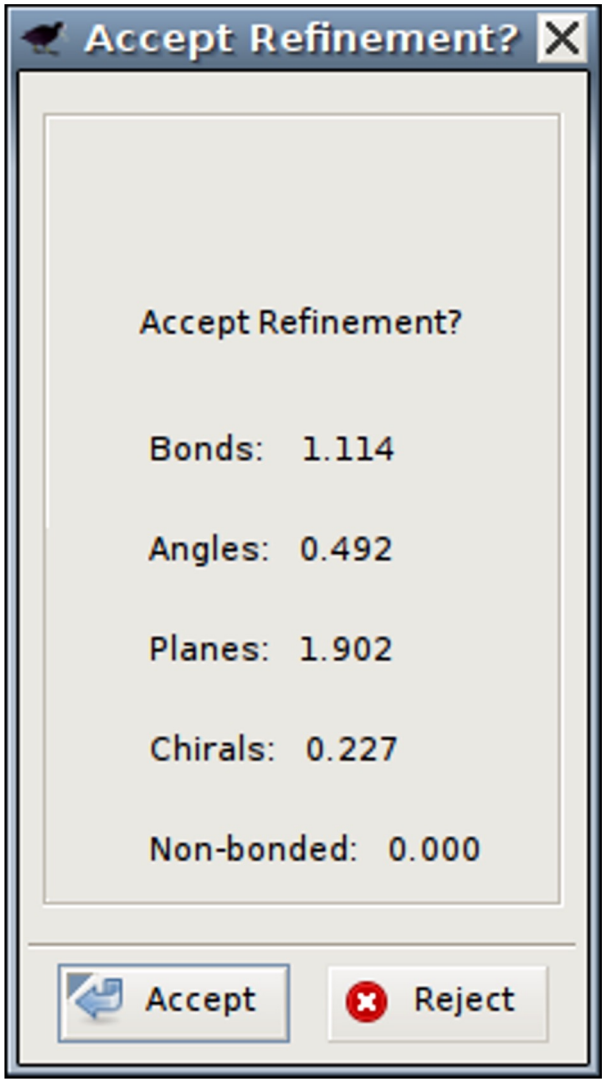
```
File  Edit  View  Terminal  Help
created 32 bond       restraints
created 38 angle      restraints
created 1 plane      restraints
created 5 chiral vol restraints
created 76 restraints

   INFO:: [spec: "A" 45 ""] [spec: "A" 46 ""] link_type :TRANS:
   INFO:: [spec: "A" 45 ""] [spec: "A" 44 ""] link_type :TRANS:
Link restraints:
   2 bond    links
   6 angle   links
   4 plane   links
Flanking residue restraints:
   4 bond    links
   12 angle   links
   8 plane   links
INFO:: made 668 non-bonded restraints
initial distortion_score: -16033.2
    Initial Chi Squareds
bonds:      1.15701
angles:     0.847832
torsions:   N/A
planes:     1.6176
non-bonded: 0
chiral vol: 0.705728
rama plot:  N/A
Minimum found (iteration number 67) at -16275.9
    Final Estimated RMS Z Scores:
bonds:      1.19412
angles:     0.713337
torsions:   N/A
planes:     1.05134
non-bonded: 0
chiral vol: 0.522415
rama plot:  N/A
 SUCCESS
 TIME:: (dragged refinement): 332.657
```

The first attempt

Student Reaction:

“Oh, I don't look at that window...”
(I maximise the window immediately)

# Representation of Results:




Second attempt…

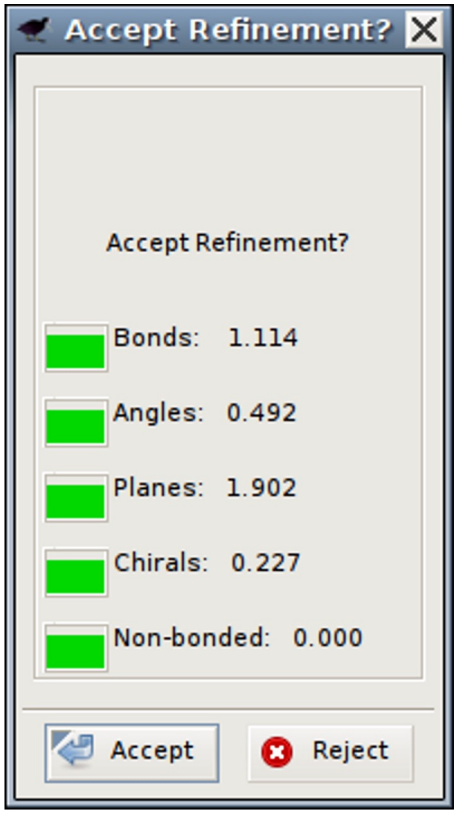
Student Reaction:

“Oh, box of meaningless numbers.

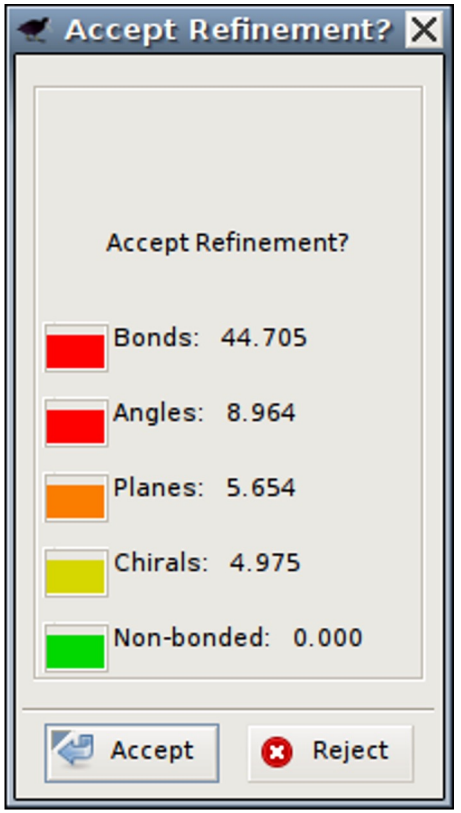
Go away”

# Representation of Results: “Traffic Lights”

“Traffic Lights” represent the RMSd values for each of the refined geometry types

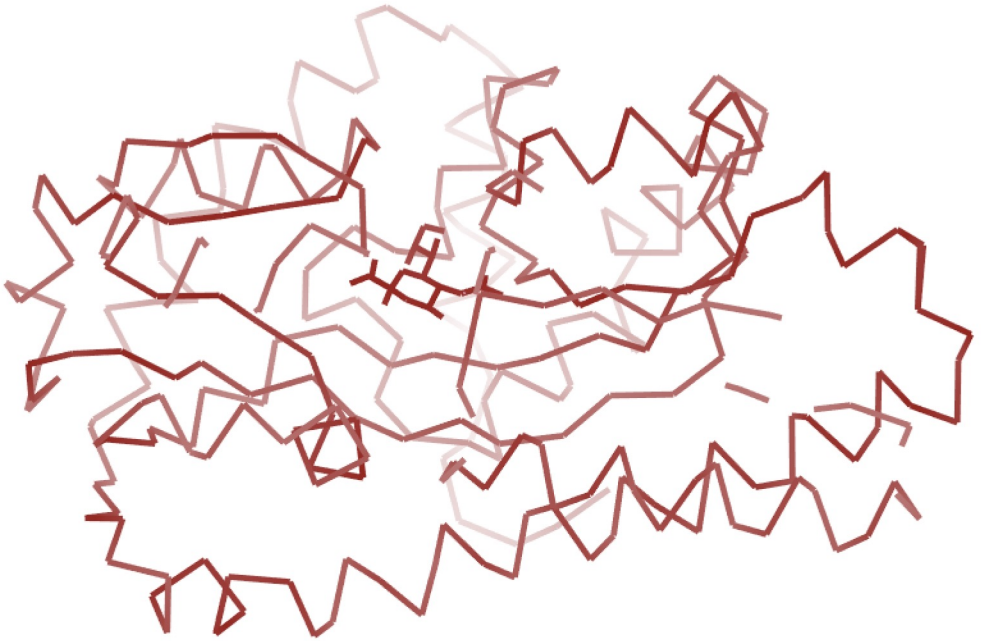



Good refinement




Bad refinement

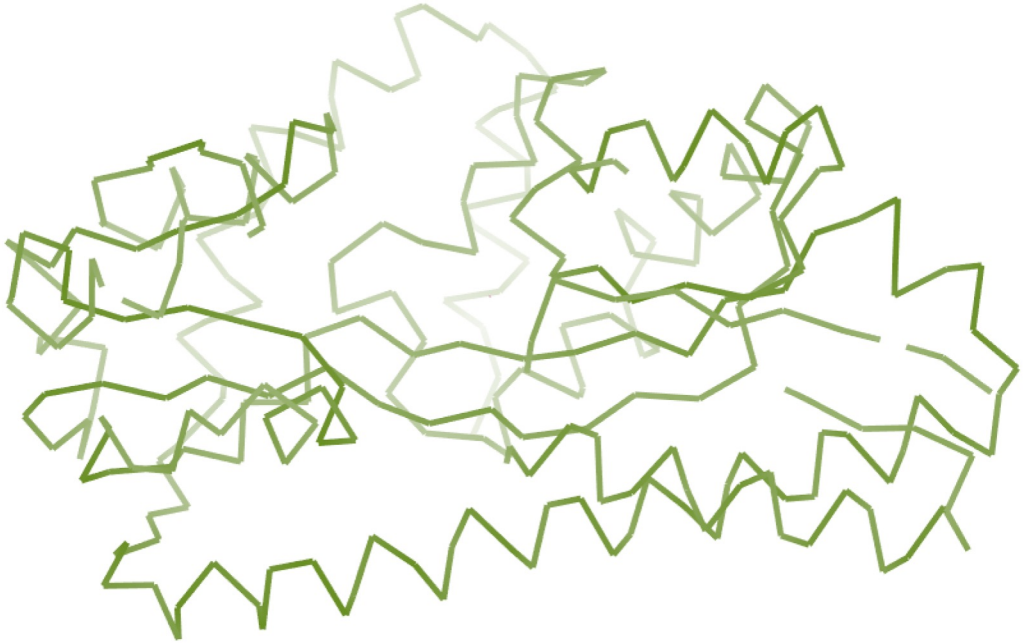
# Local Distance Restraints: Prior Structure



Model for High Resolution data

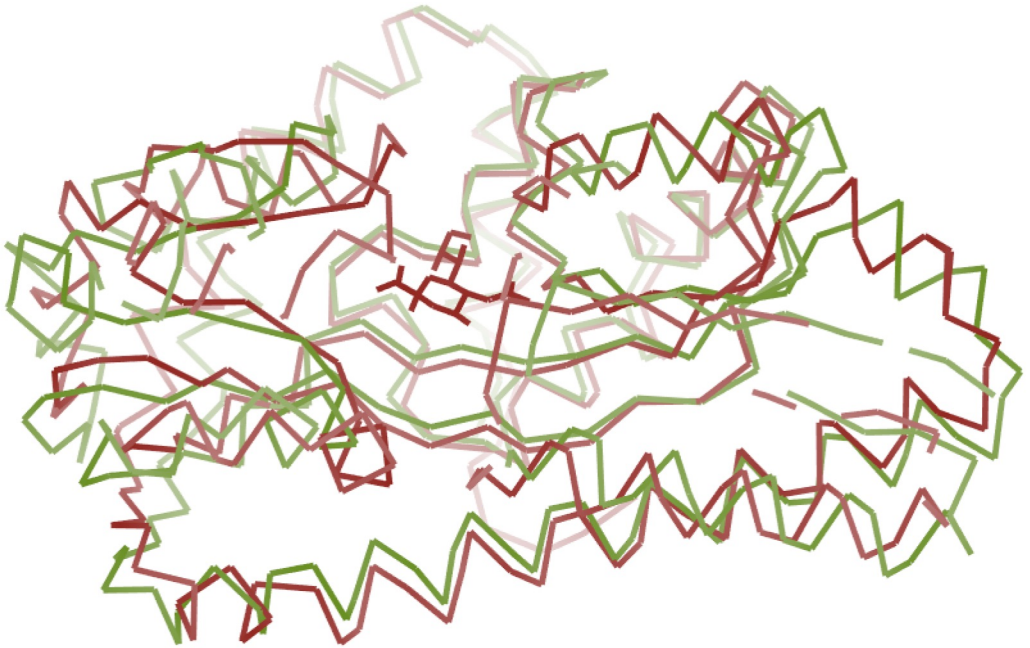
PDB code: 3b50, 1.4 Å

# Local Distance Restraints: Today's Structure



Model for Low Resolution data

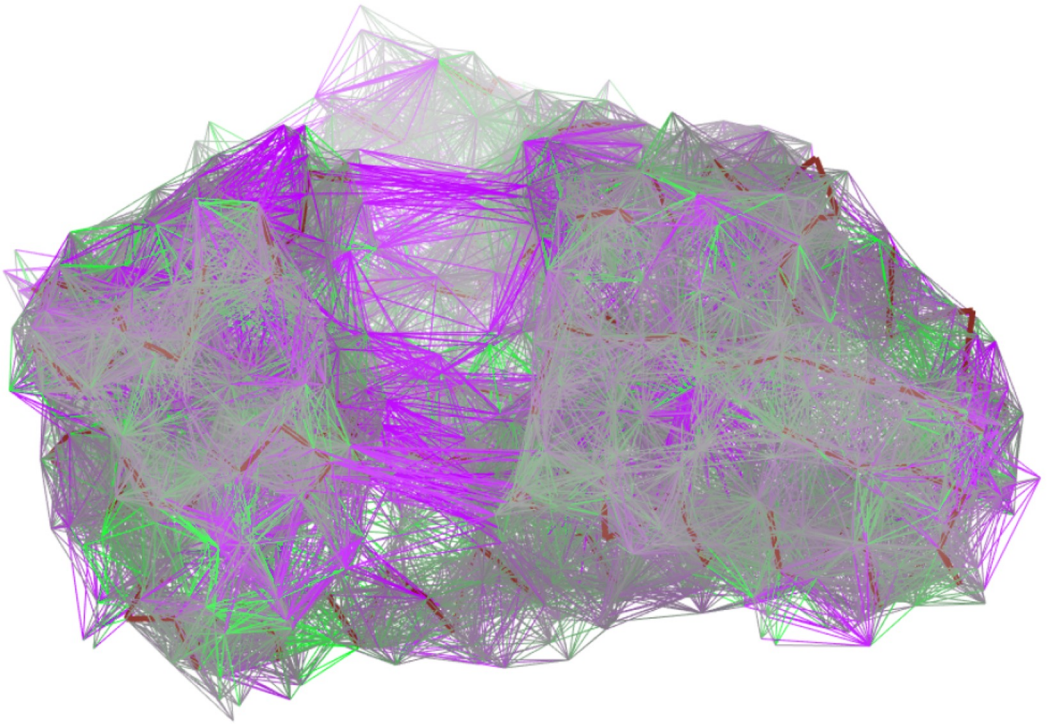
# Local Distance Restraints: Structure Comparison



Model for High Resolution data

Model for Low Resolution data

# Local Distance Restraints:
## ProSMART/Geman McClure Restraints



Longer than in prior

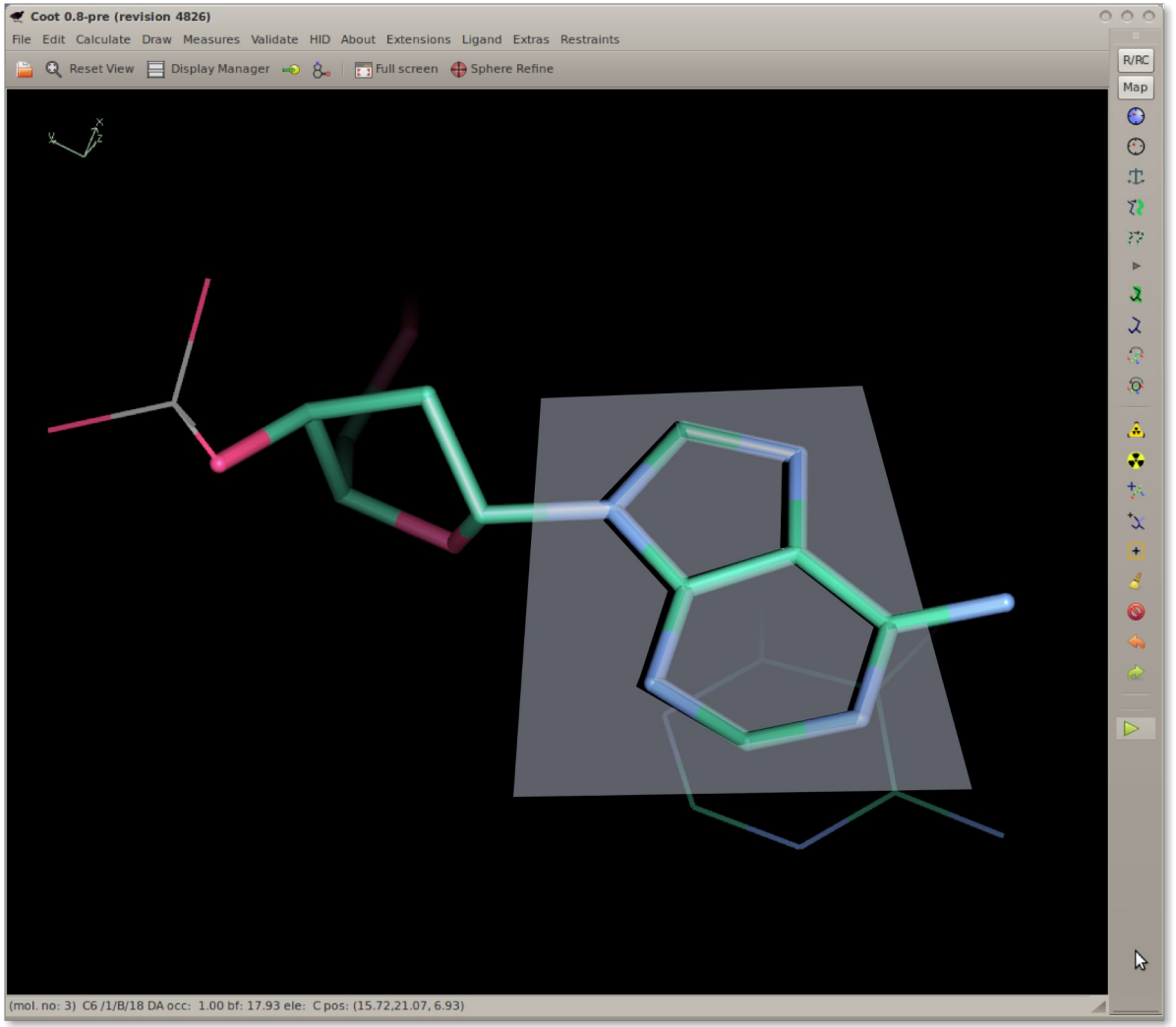
Shorter than prior

# ProSMART integration

**ProSMART** generates distance restraints from homologous structures

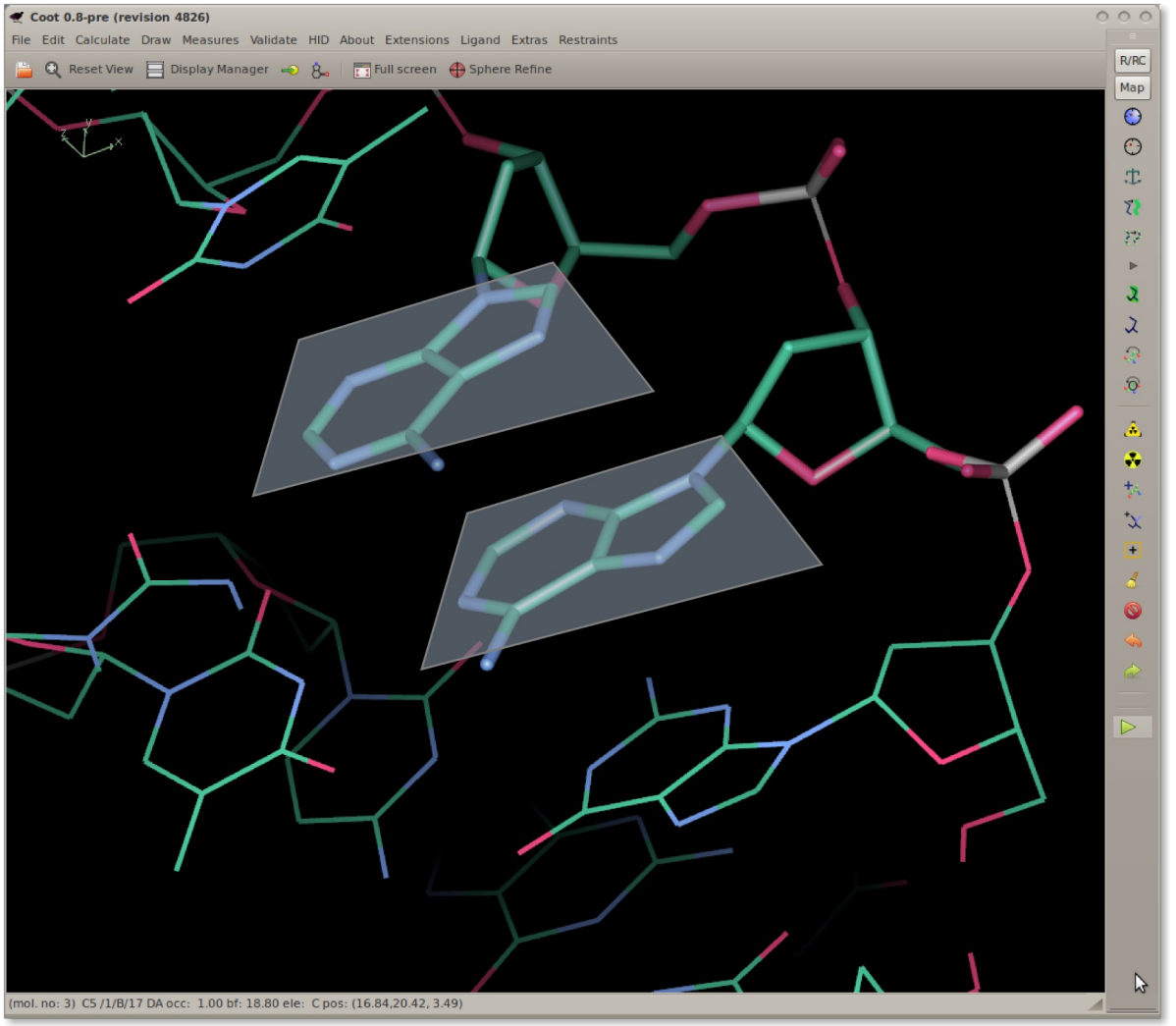
- to be applied to current model for refinement
- now available in Coot

# Nucleic acid: Plane Restraints




Derivativaties are an eigenvector scaled by out-of-plane distance

# Parallel Planes Restraints




$$S = (a_1 - a_2)^2 + (b_1 - b_2)^2 + (c_1 - c_2)^2$$

Used in Refmac,
analogous used in Coot

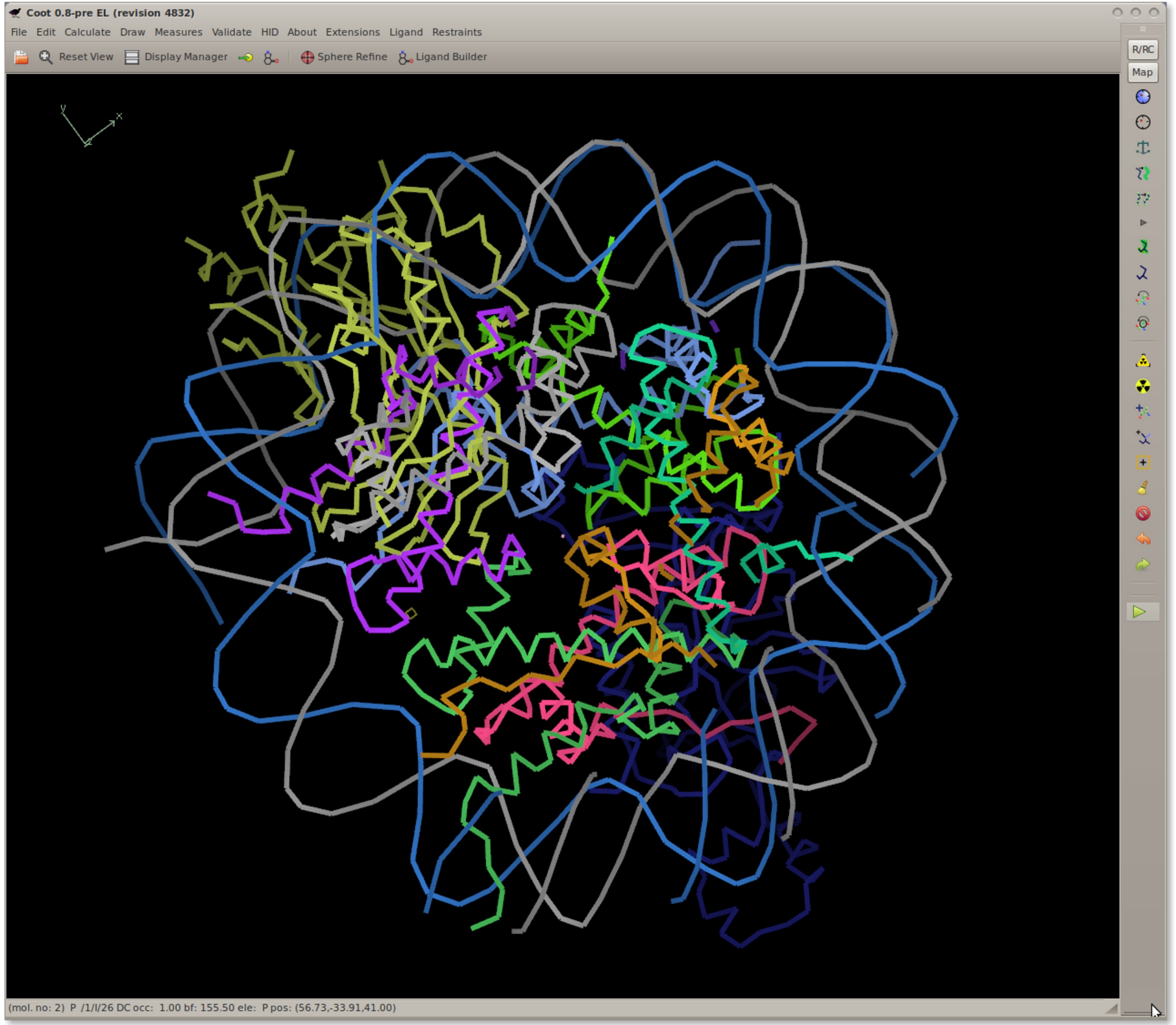
# Automatic Generation of Base Pairing and Stacking Restraints

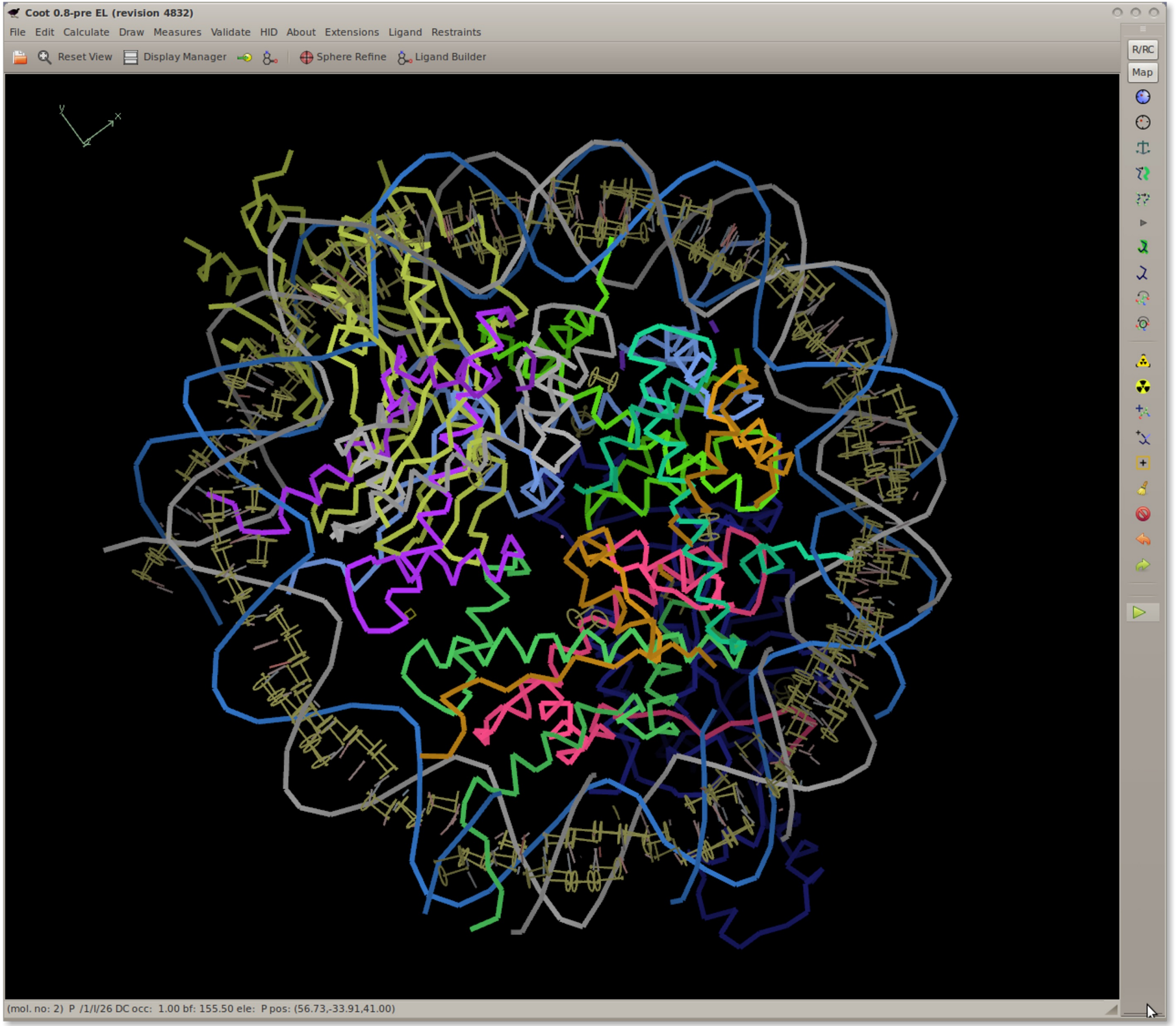
Fei Long's **LIBG**

Provide it with a model and it writes out Refmac restraint descriptions

... which Coot can also read

Coot can also create user-define base-paring and stacking restraints


Coot 0.8-pre EL (revision 4832)
File Edit Calculate Draw Measures Validate HID About Extensions Ligand Restraints
Reset View
Display Manager
Sphere Refine
Ligand Builder
R/RC
Map
(mol. no: 2) P /1/I/26 DC occ: 1.00 bf: 155.50 ele: P pos: (56.73,-33.91,41.00)


Coot 0.8-pre EL (revision 4832)
File Edit Calculate Draw Measures Validate HID About Extensions Ligand Restraints
Reset View
Display Manager
Sphere Refine
Ligand Builder
R/RC
Map
(mol. no: 2) P /1/I/26 DC occ: 1.00 bf: 155.50 ele: P pos: (56.73,-33.91,41.00)

# cis-Peptides

A number of papers have been published some time ago highlighting the unusually large number of cis-peptides in some structures:

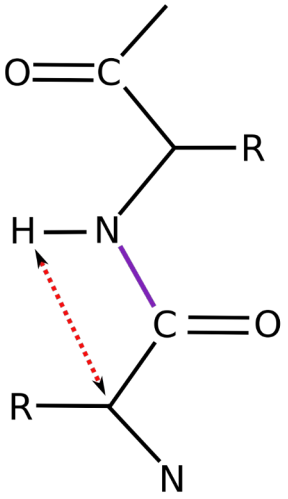
**Croll**: The rate of cis-trans conformation errors is increasing in low-resolution crystal structures Acta Cryst. (2015). D71, 706-709

**Touw et al**.: Detection of trans–cis flips and peptide-plane flips in protein structures Acta Cryst. (2015). D71, 1604-71614

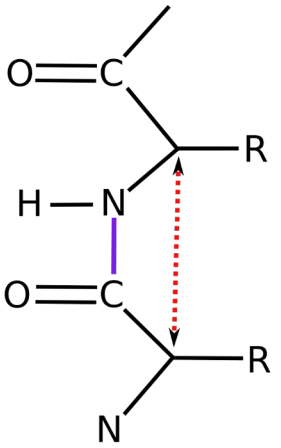
# cis-Peptides

- What is a cis-peptide?
- Peptide restraints in Coot 2004-2015

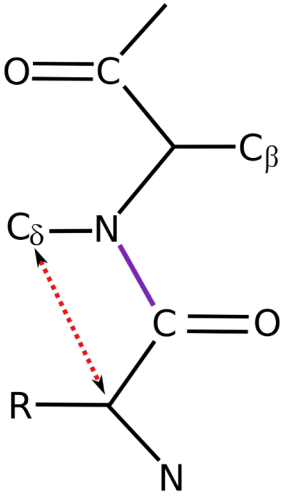
# cis-Peptides



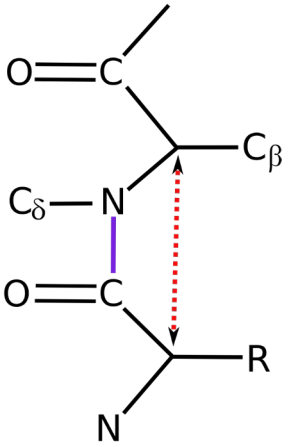

*trans-peptide*




*cis-peptide*

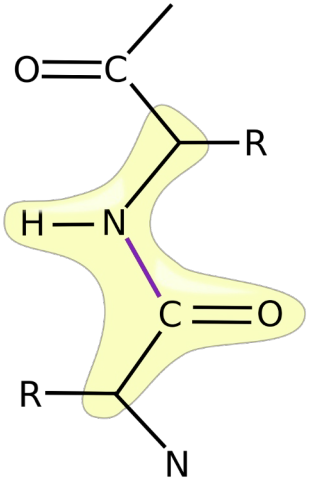



PRO *trans-peptide*

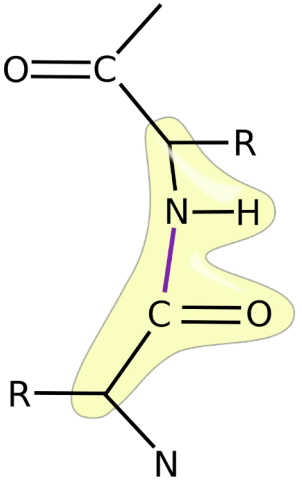



PRO *cis-peptide*

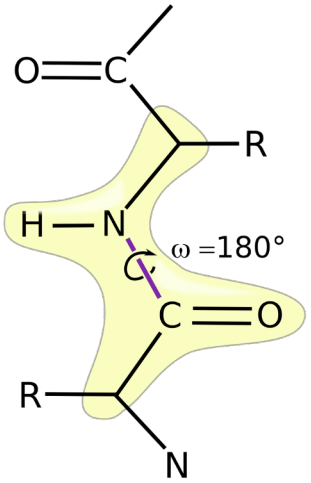
# cis-Peptides




*trans-peptide*
with plane restraints

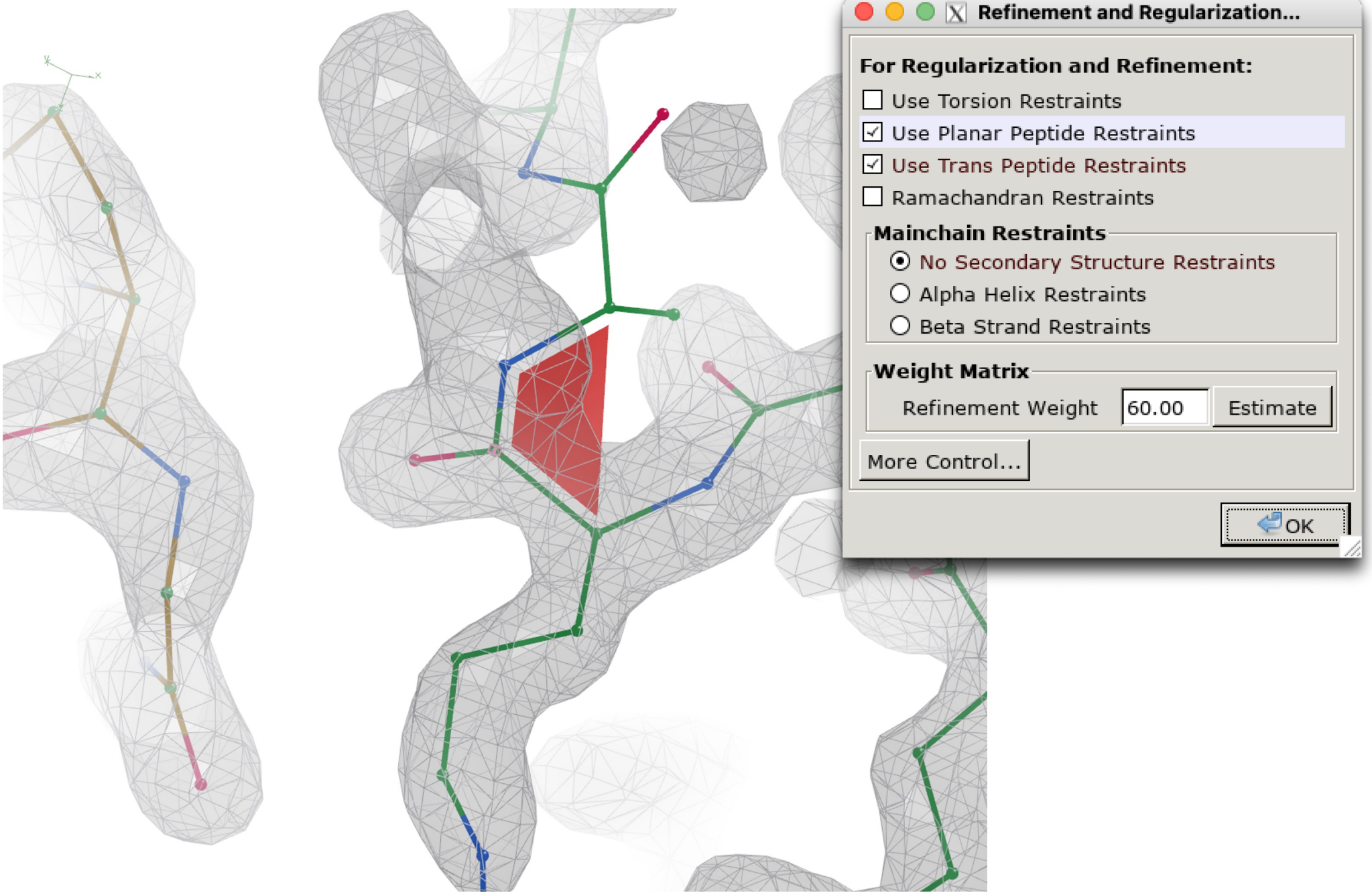



*cis-peptide*
with plane restraints




*trans-peptide*
with plane and trans restraints

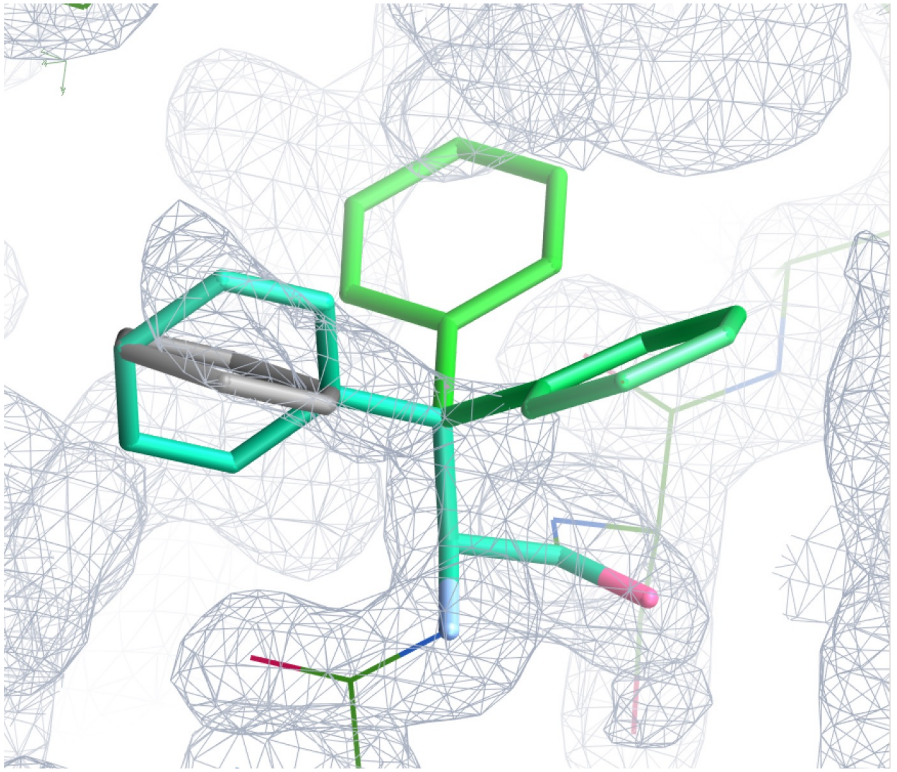
# cis-Peptide Representation



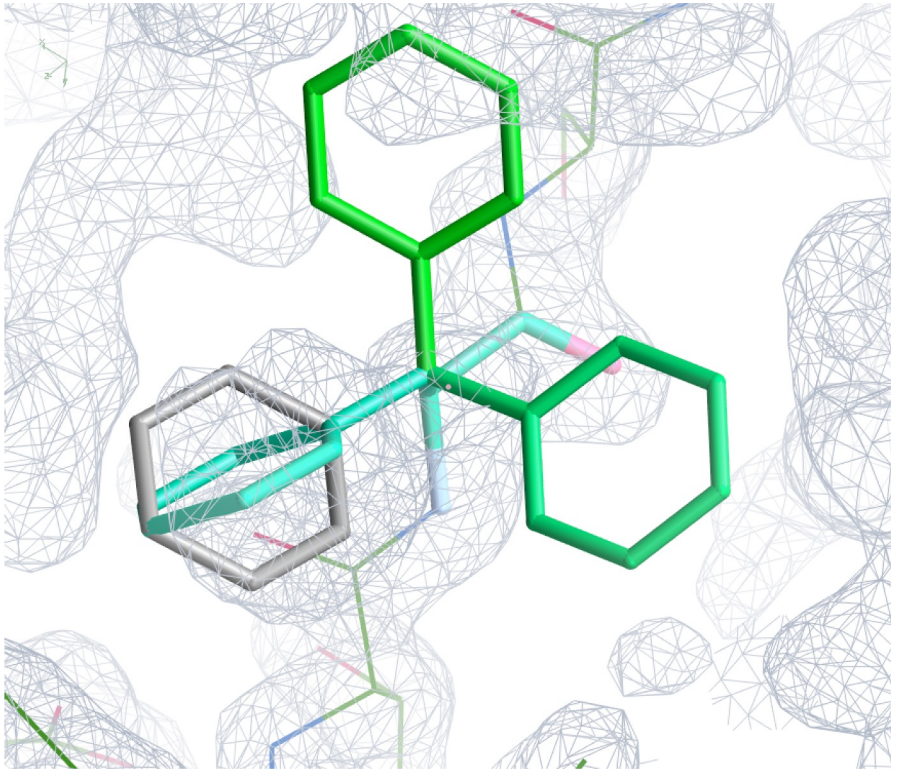
# Rotamers

- Rotamers are preferred configurations of a **side-chains rotatable bonds**
- where “preferred” means these configurations occur more frequently in a set of reference protein structures
- “preferred” because they are low-energy conformations
- Several Rotamer “databases” exist
- (Son of) Penultimate Rotamer Library

# 4 PHE Rotamers

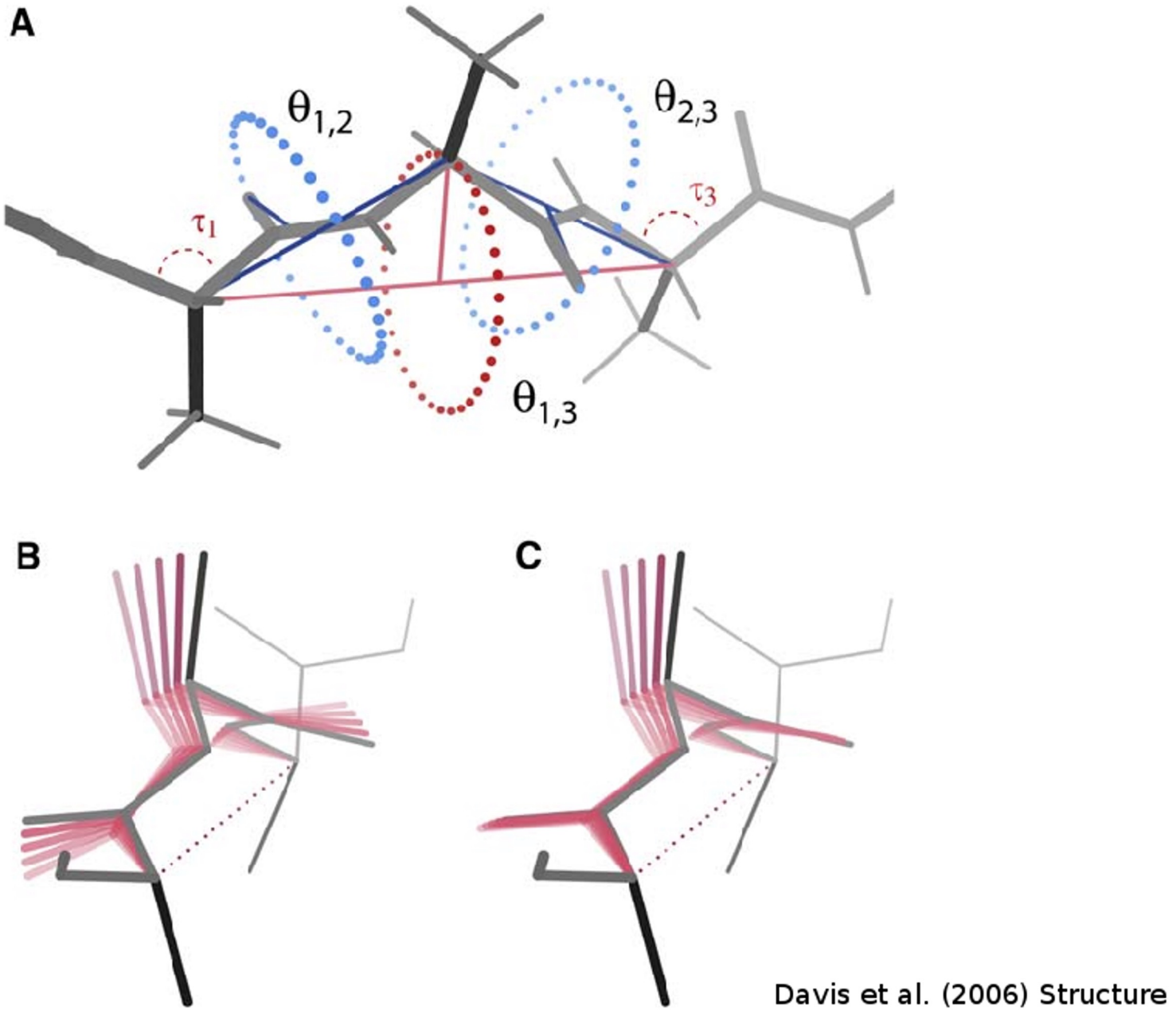


Side view



Top view

# Backrub rotamer algo




Davis et al. (2006) Structure

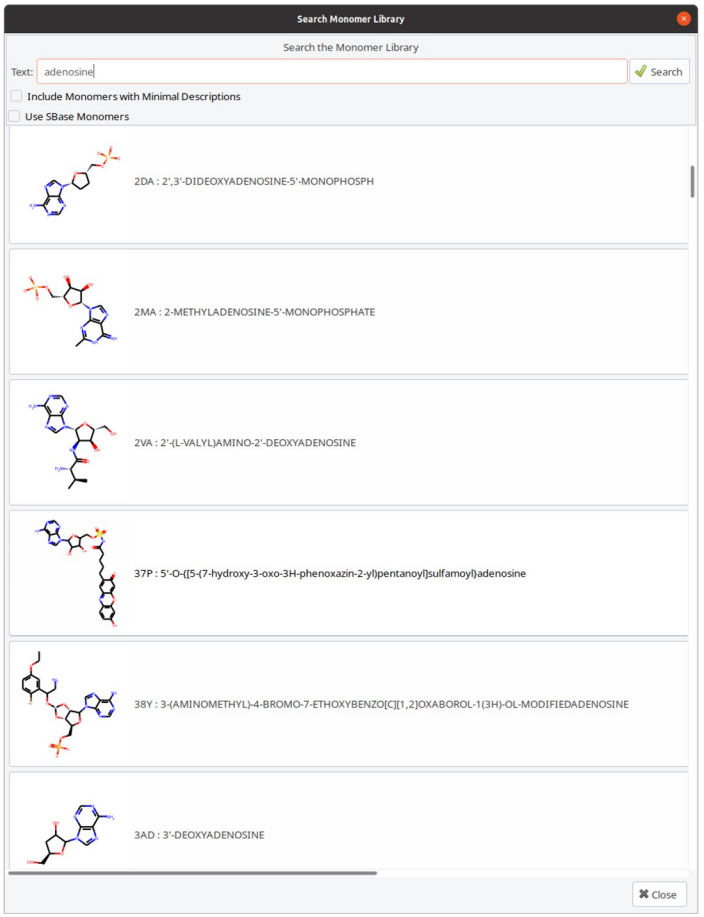
# Coot 0.9.x and 1.1

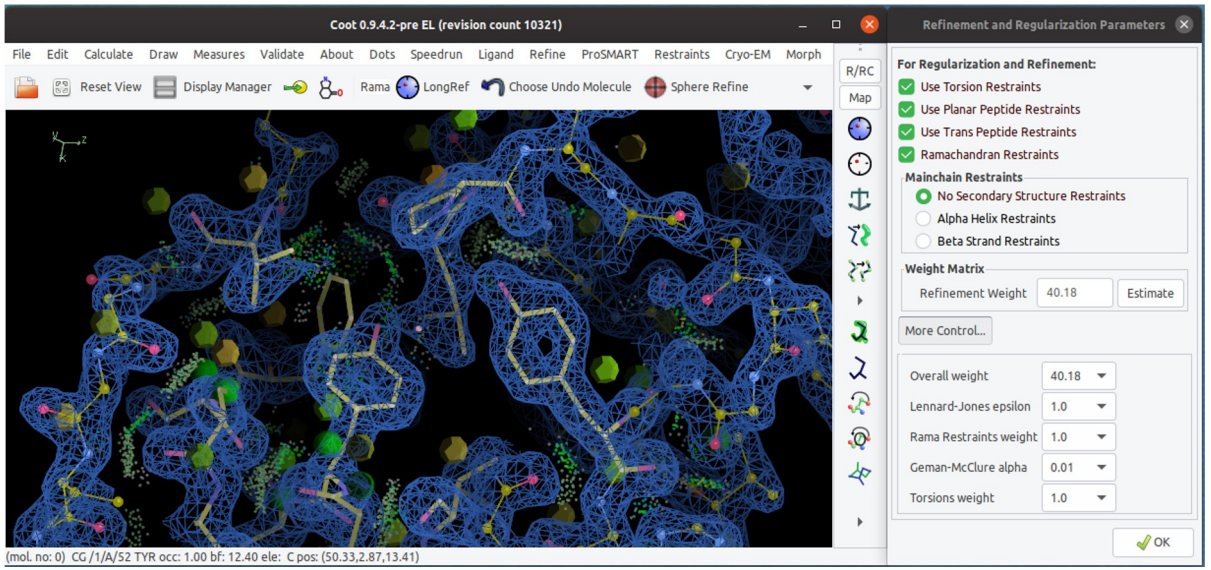
coot-ligand-validation

API torsion restraint weights

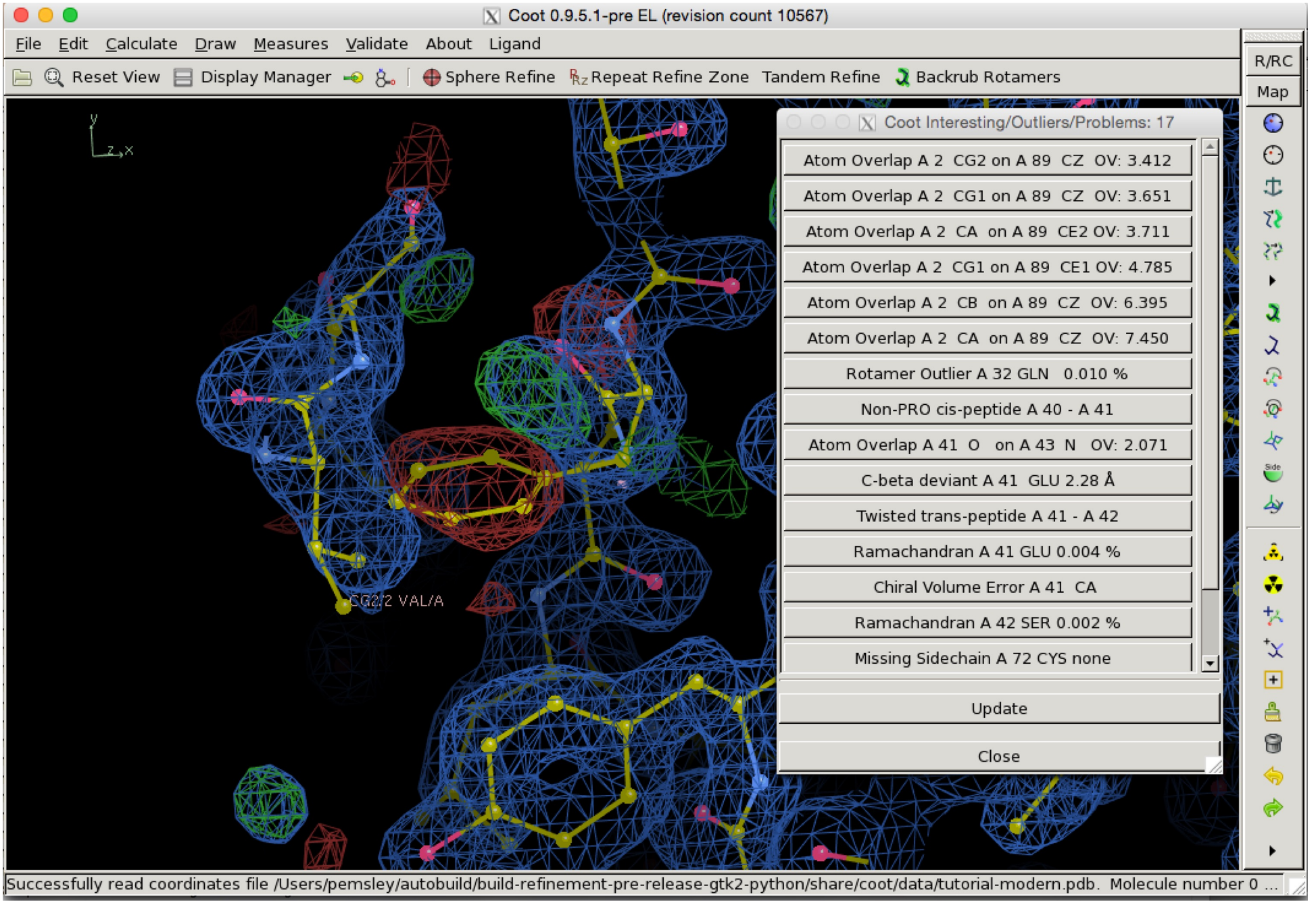
Dynamic Weights

Parses Nuclear Hydrogen Atom Positions

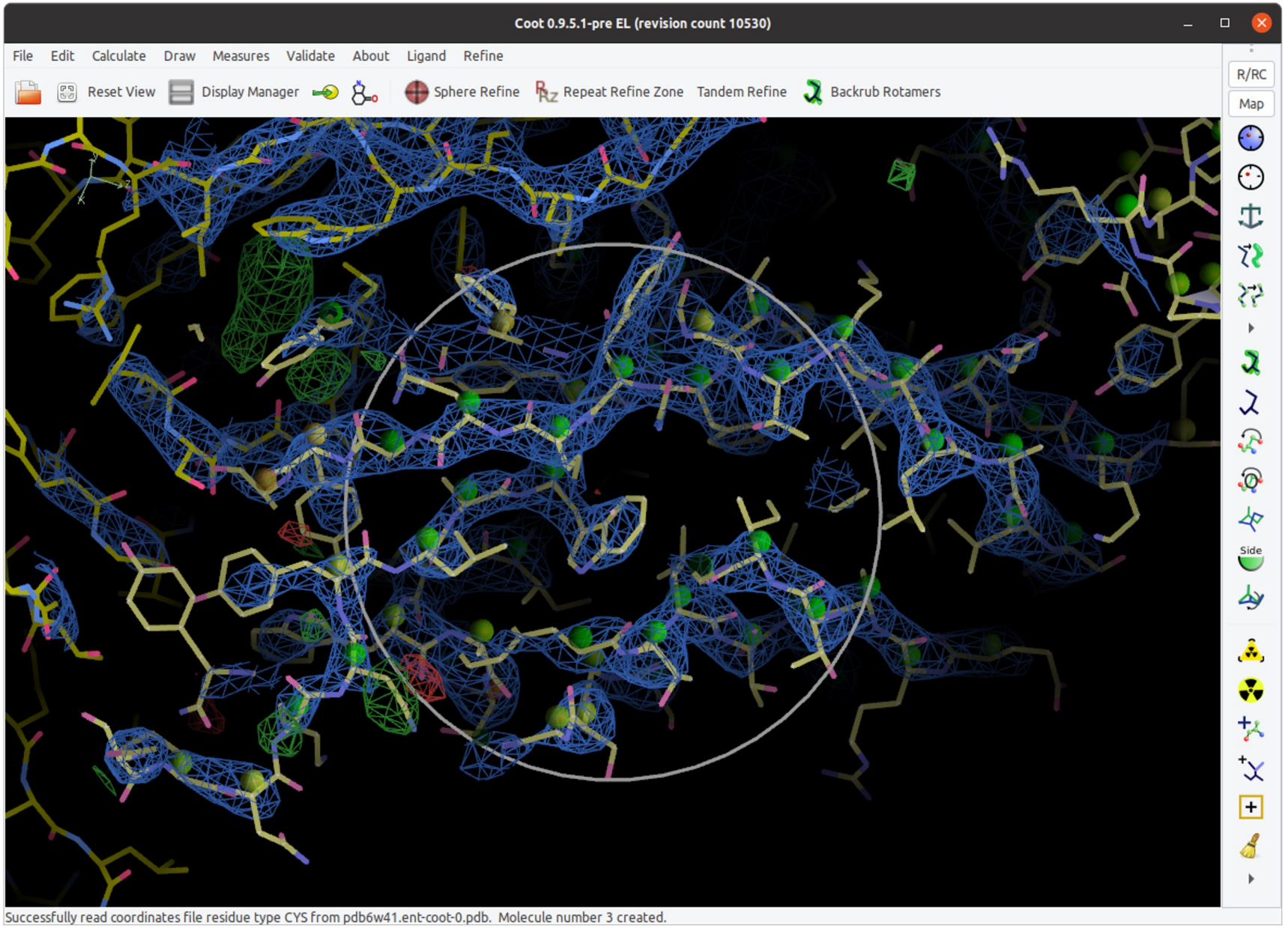


# Interactive Validation



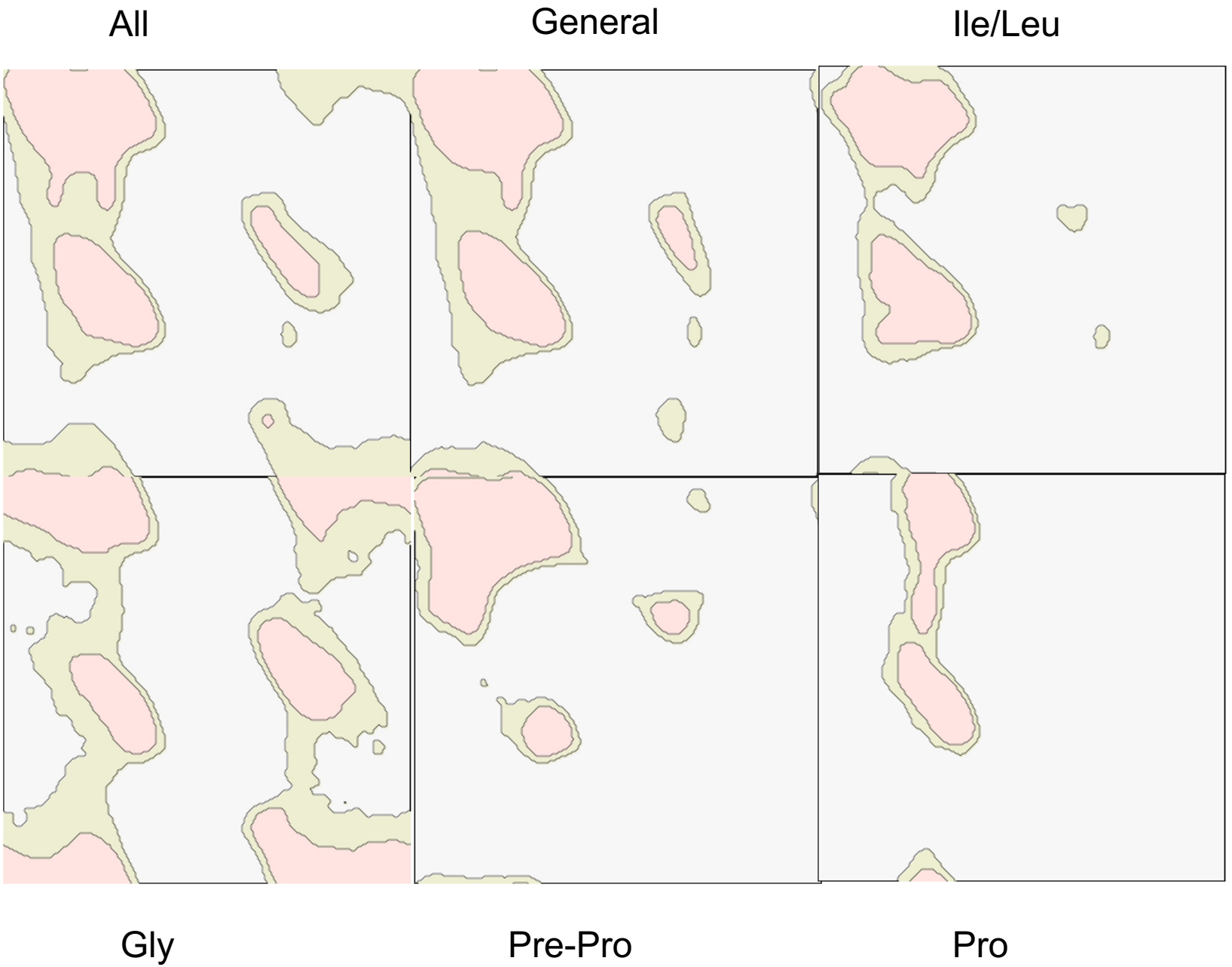
# Real-Space Refinement Proportional Editing



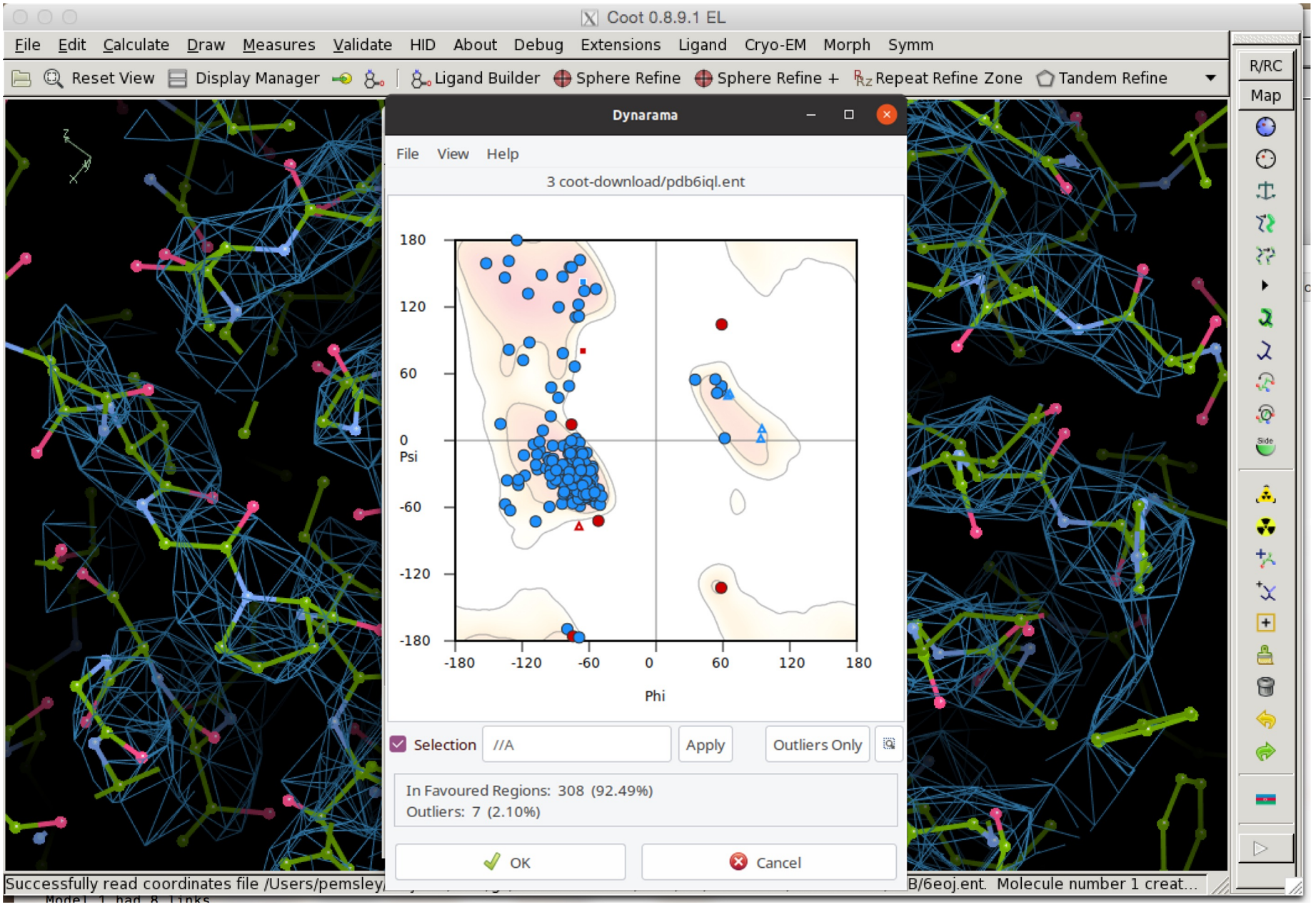

**Activate/Change with Ctrl Middle-mouse scroll**

# Improved Ramachandran Plot(s)

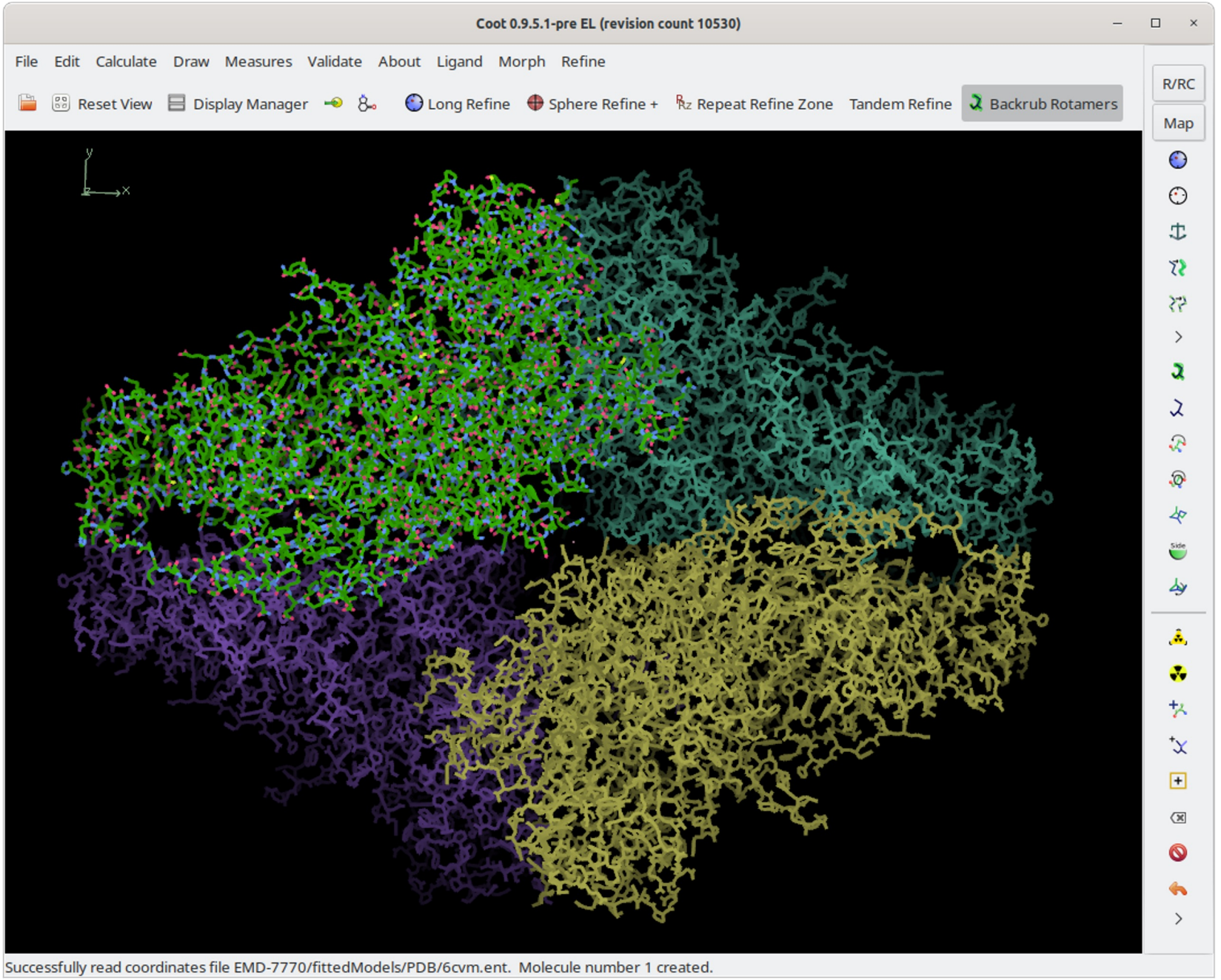
A. Thorn
B. Lohkamp



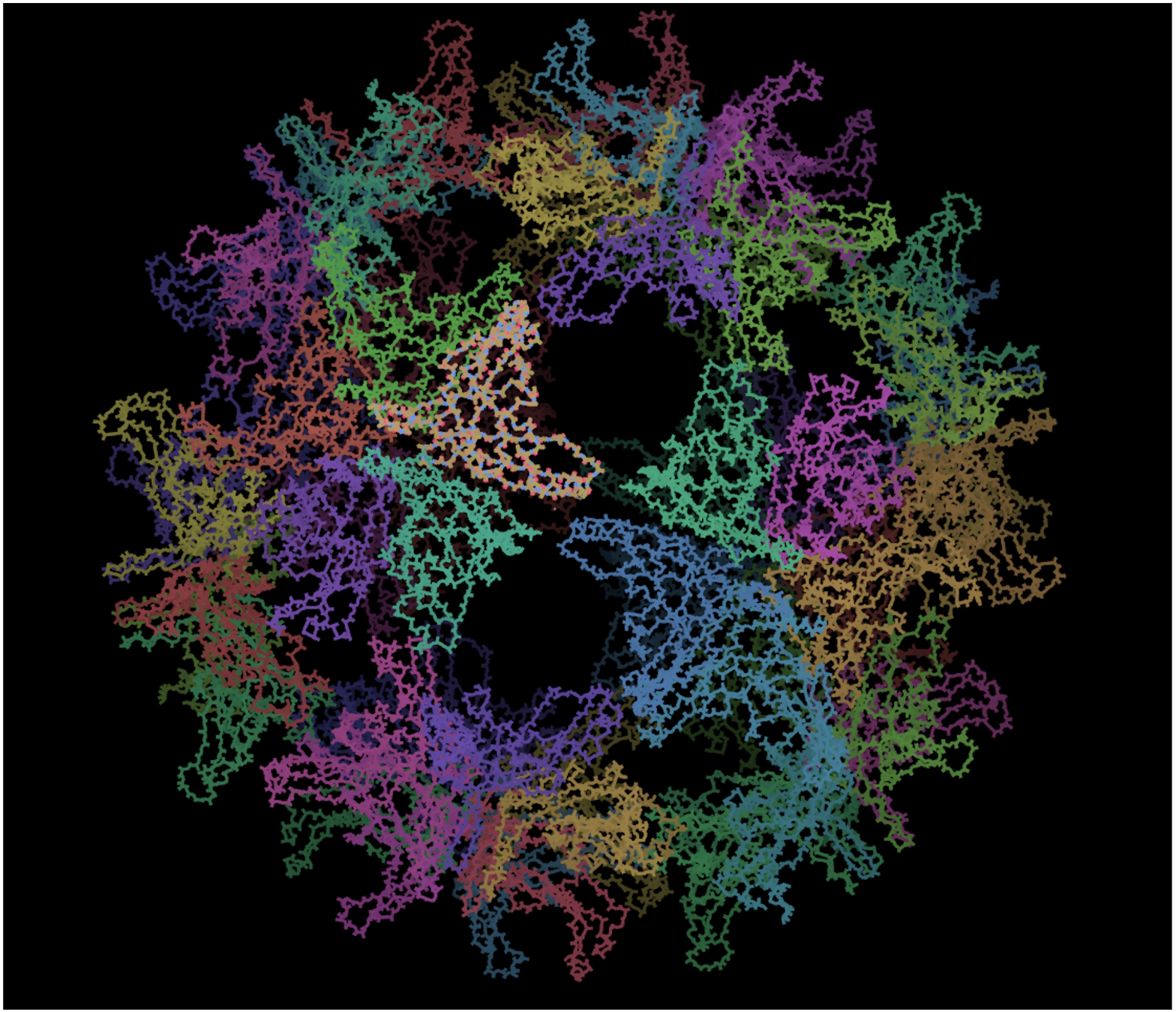
# The New Ramachandran Plot



# Molecular Symmetry



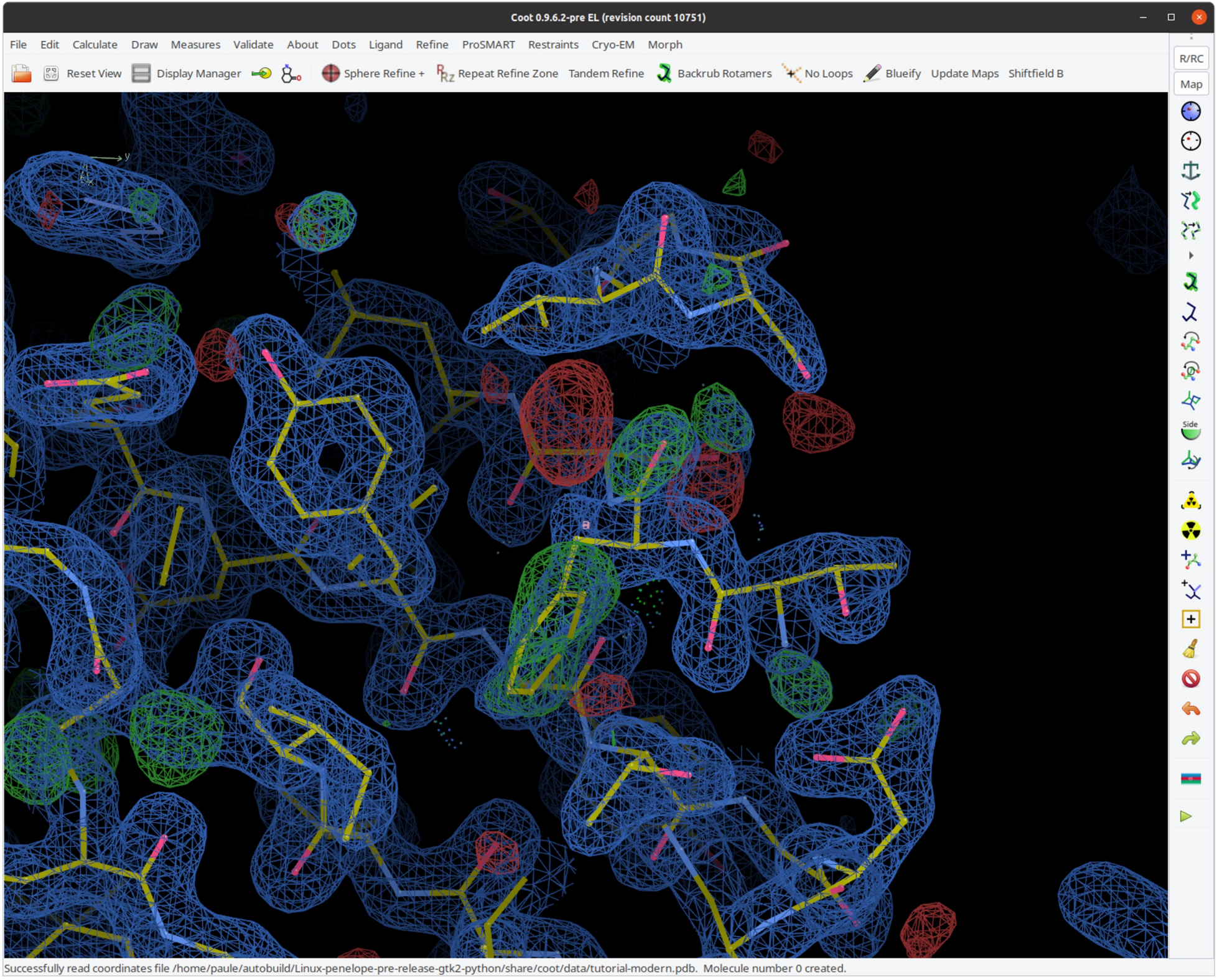
# Molecular Symmetry



# Updating Maps

Thanks to **Tristan Croll** who implemented this in Isolde and inspired Paul to add it to Coot. Thanks to **Kathryn Cowtan** for help in doing so

Note: updating maps takes ~0.7s for 200 AA and 1.8A data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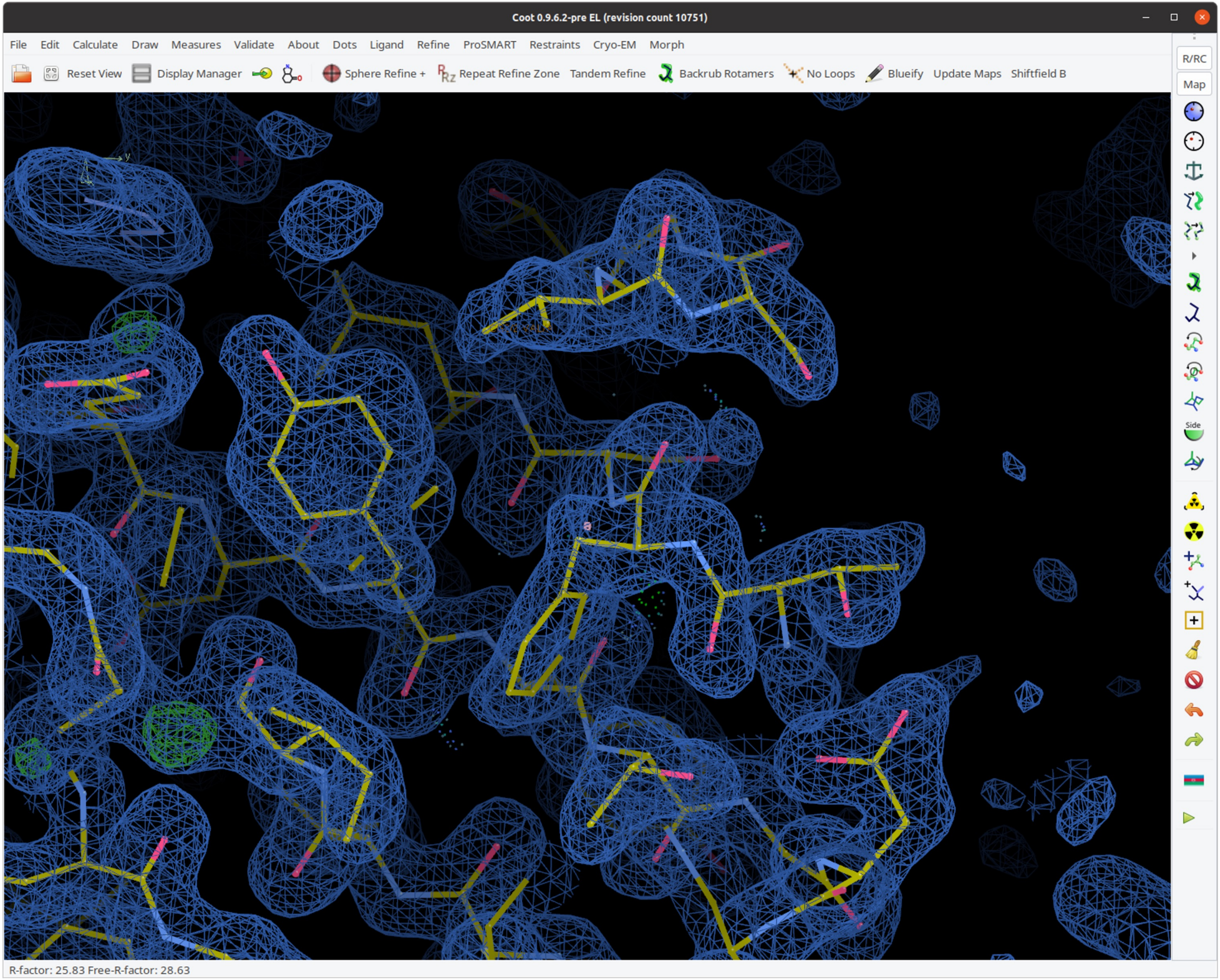
File
Edit
Calculate
Draw
Measures
Validate
About
Dots
Ligand
Refine
ProSMART
Restraints
Cryo-EM
Morph
Reset View
Display Manager
Sphere Refine +
Repeat Refine Zone
Tandem Refine
Backrub Rotamers
No Loops
Blueify
Update Maps
Shiftfield B
R/RC
Map
Side
Successfully read coordinates file /home/paule/autobuild/Linux-penelope-pre-release-gtk2-python/share/coot/data/tutorial-modern.pdb. Molecule number 0 created.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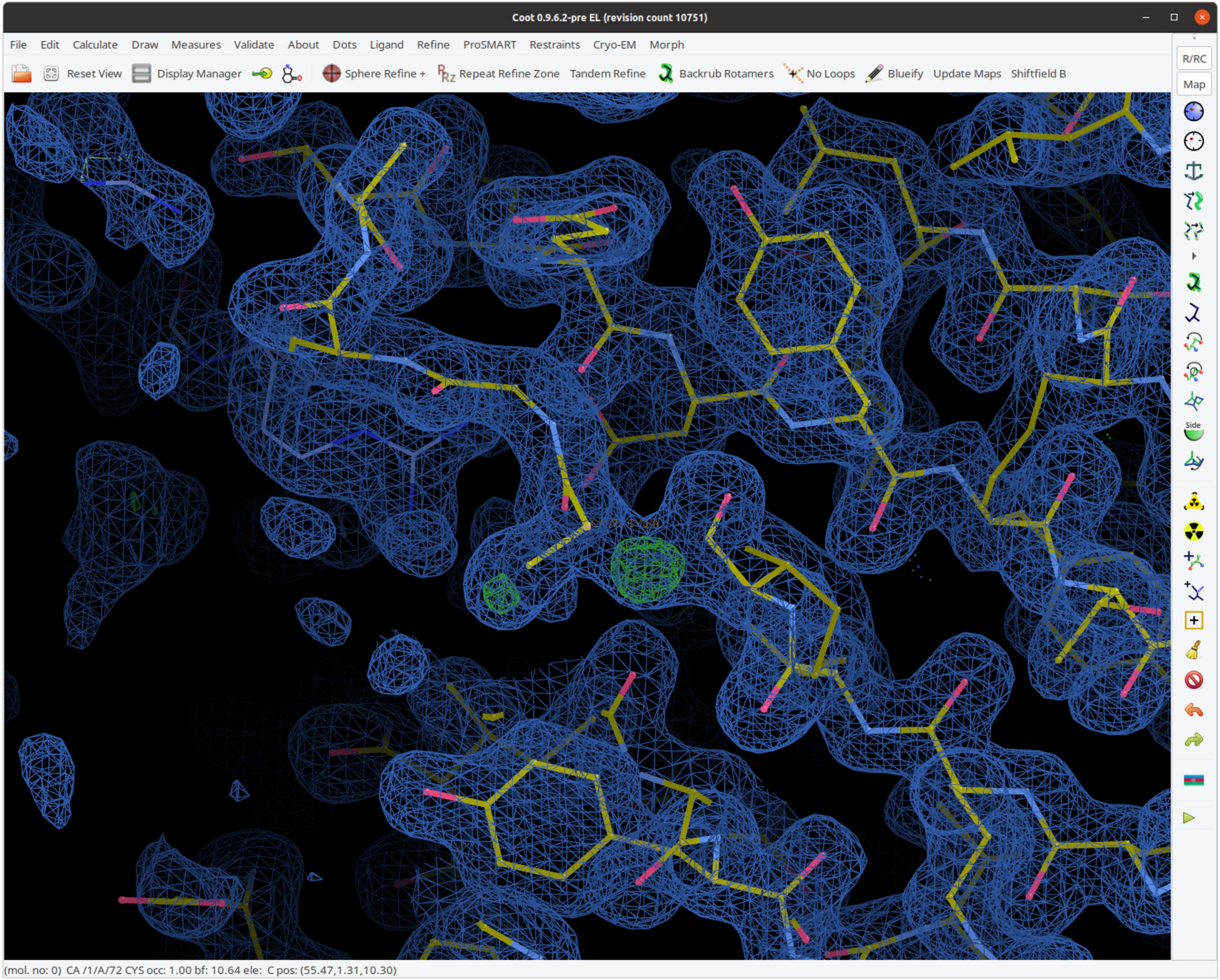
Refine
ProSMART
Restraints
Cryo-EM
Morph
Reset View
Display Manager
Sphere Refine +
Repeat Refine Zone
Tandem Refine
Backrub Rotamers
No Loops
Blueify
Update Maps
Shiftfield B
R/RC
Map
Side
R-factor: 25.83 Free-R-factor: 28.63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Repeat Refine Zone
Tandem Refine
Backrub Rotamers
No Loops
Blueify
Update Maps
Shiftfield B
R/RC
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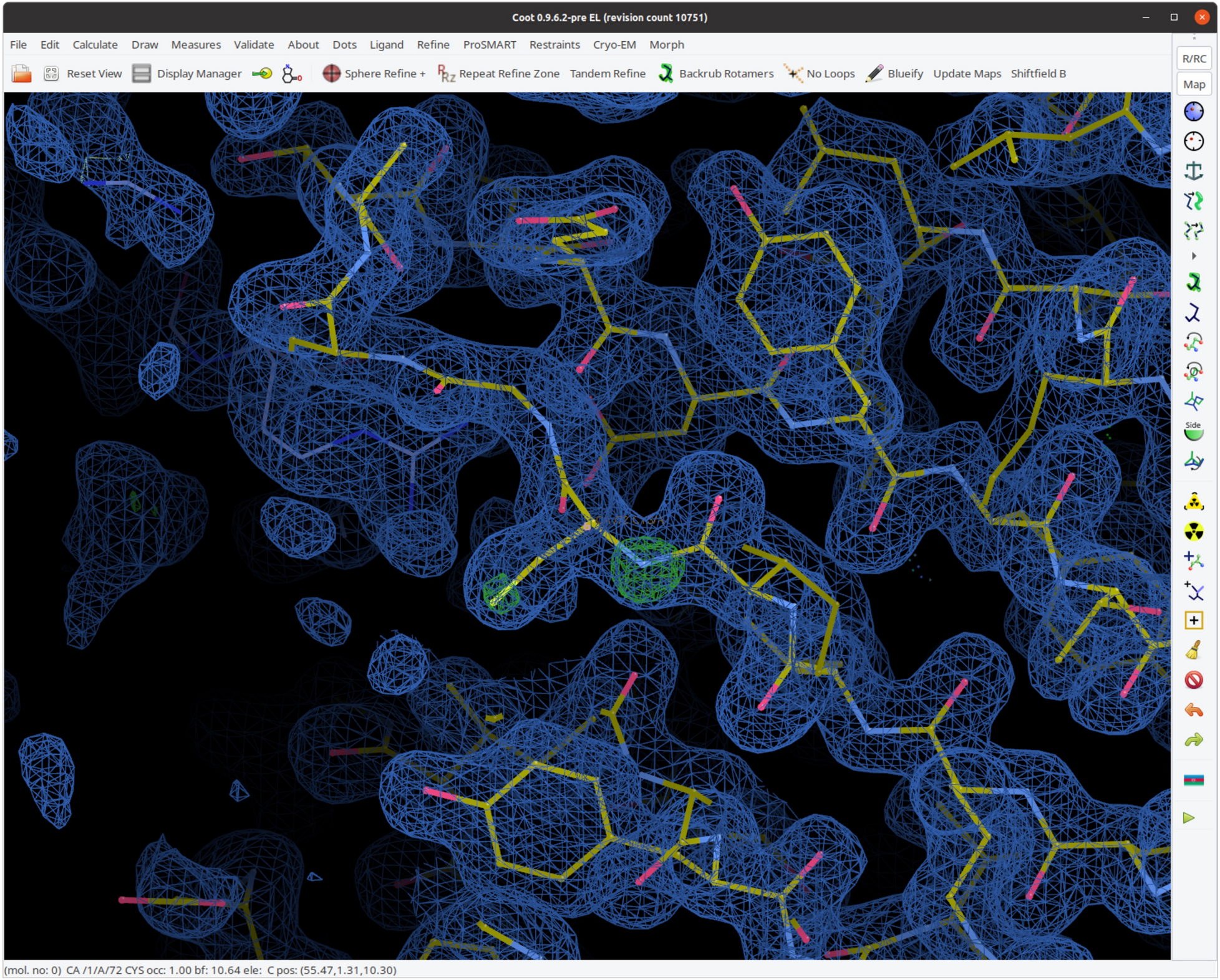
Side
(mol. no: 0) CA /1/A/72 CYS occ: 1.00 bf: 10.64 ele: C pos: (55.47,1.31,10.30)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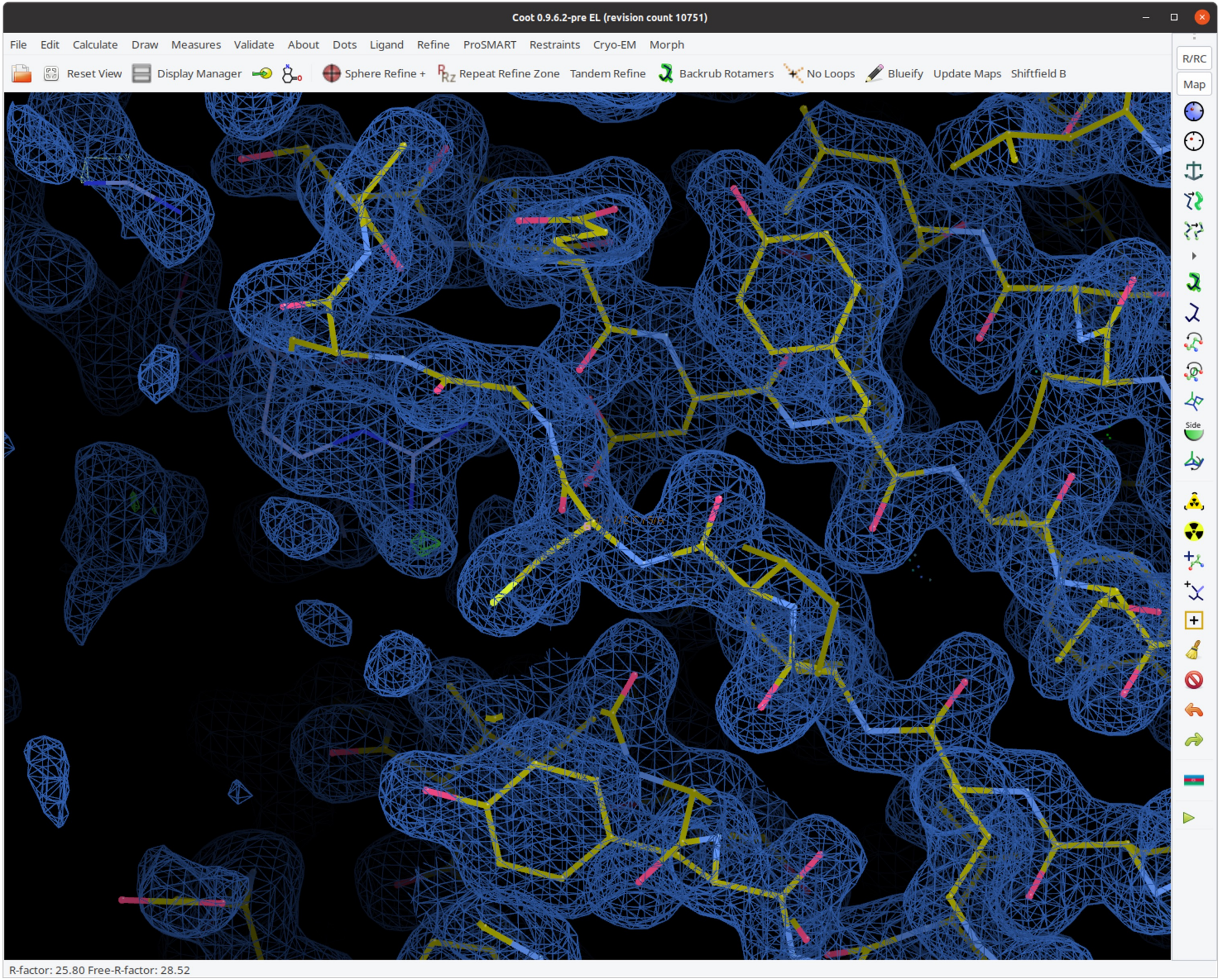
Backrub Rotamers
No Loops
Blueify
Update Maps
Shiftfield B
R/RC
Map
Side
(mol. no: 0) CA /1/A/72 CYS occ: 1.00 bf: 10.64 ele: C pos: (55.47,1.31,10.30)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No Loops
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Update Maps
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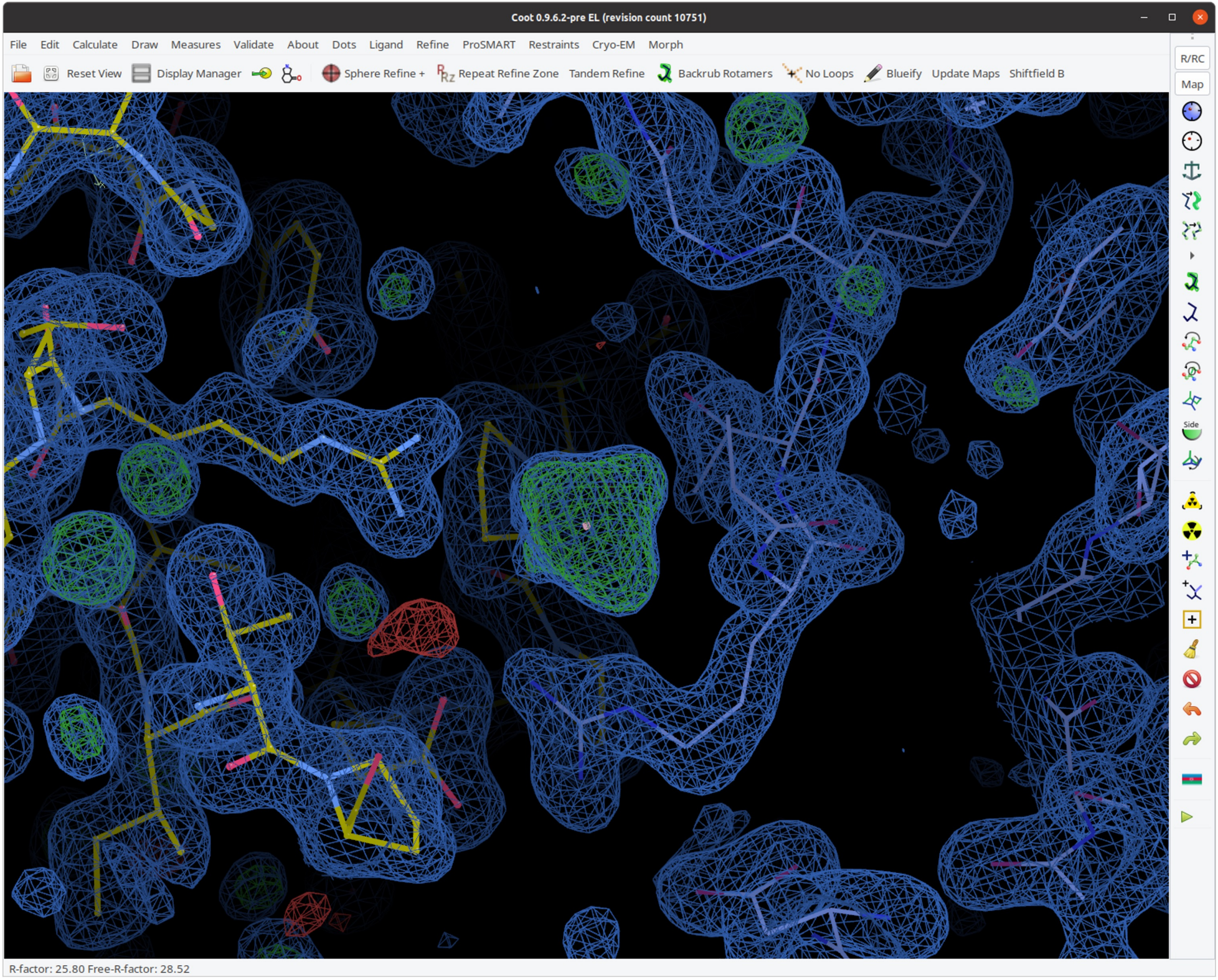
R/RC
Map
Side
R-factor: 25.80 Free-R-factor: 28.52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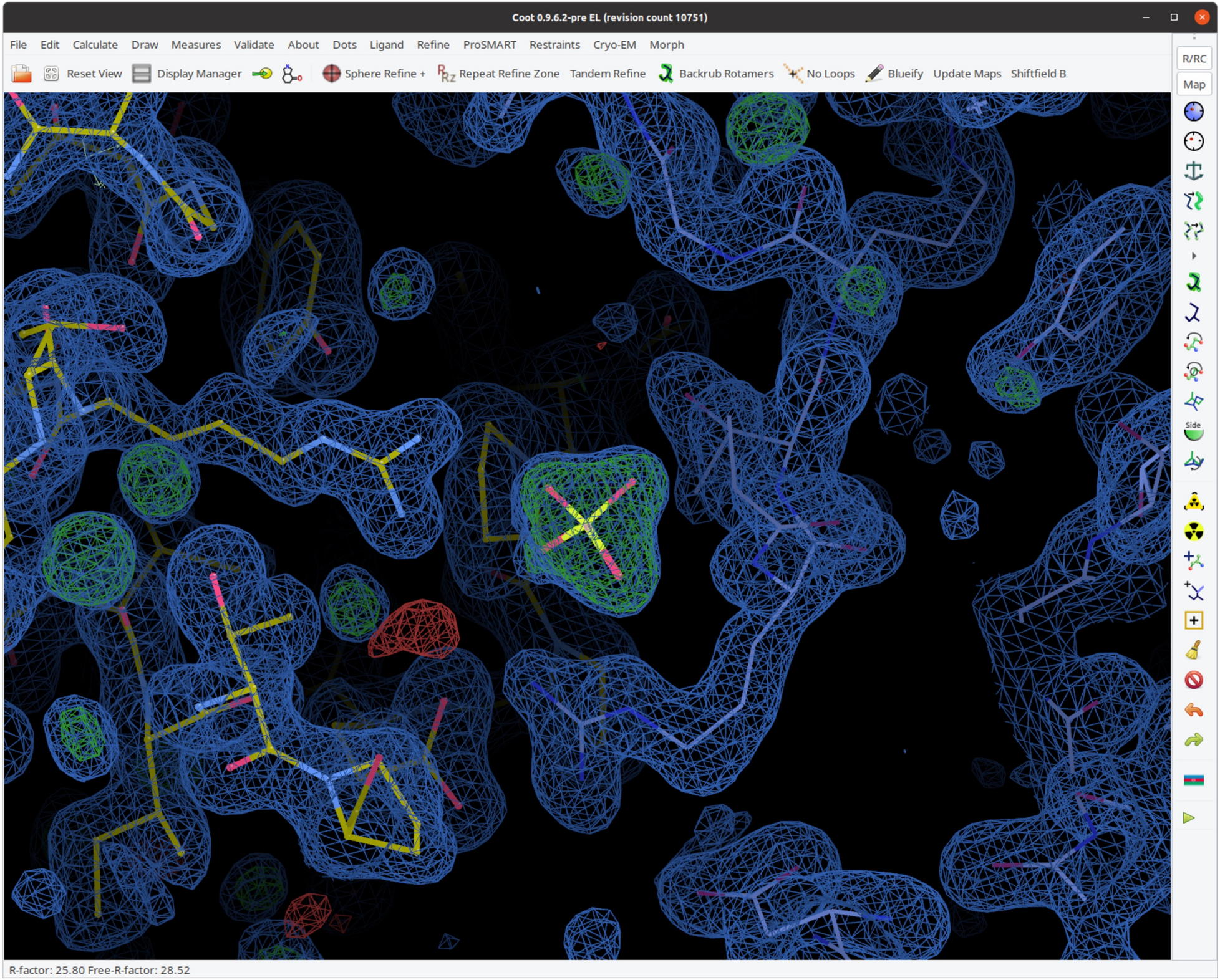
R-factor: 25.80 Free-R-factor: 28.52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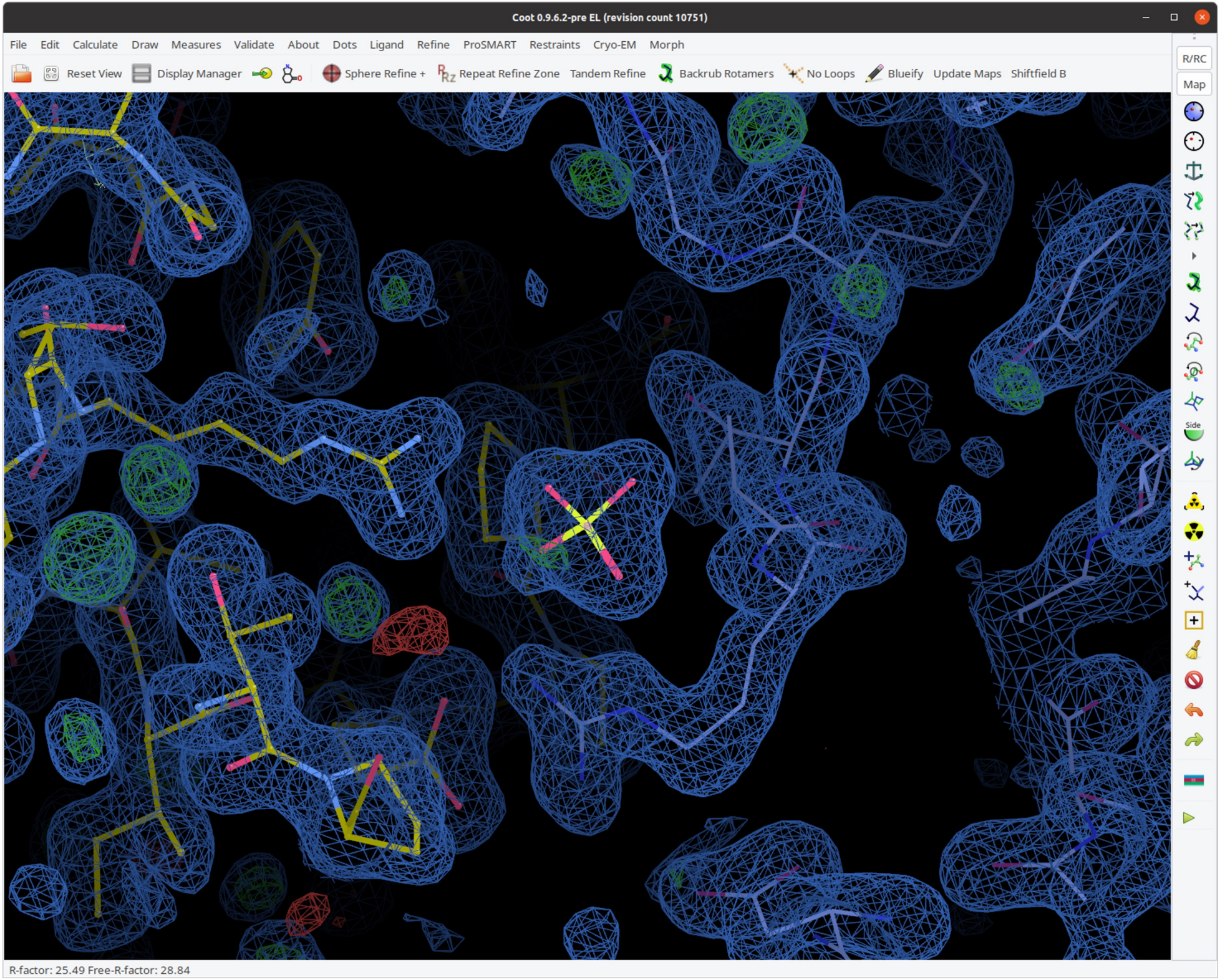
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Repeat Refine Zone
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R/RC
Map
Side
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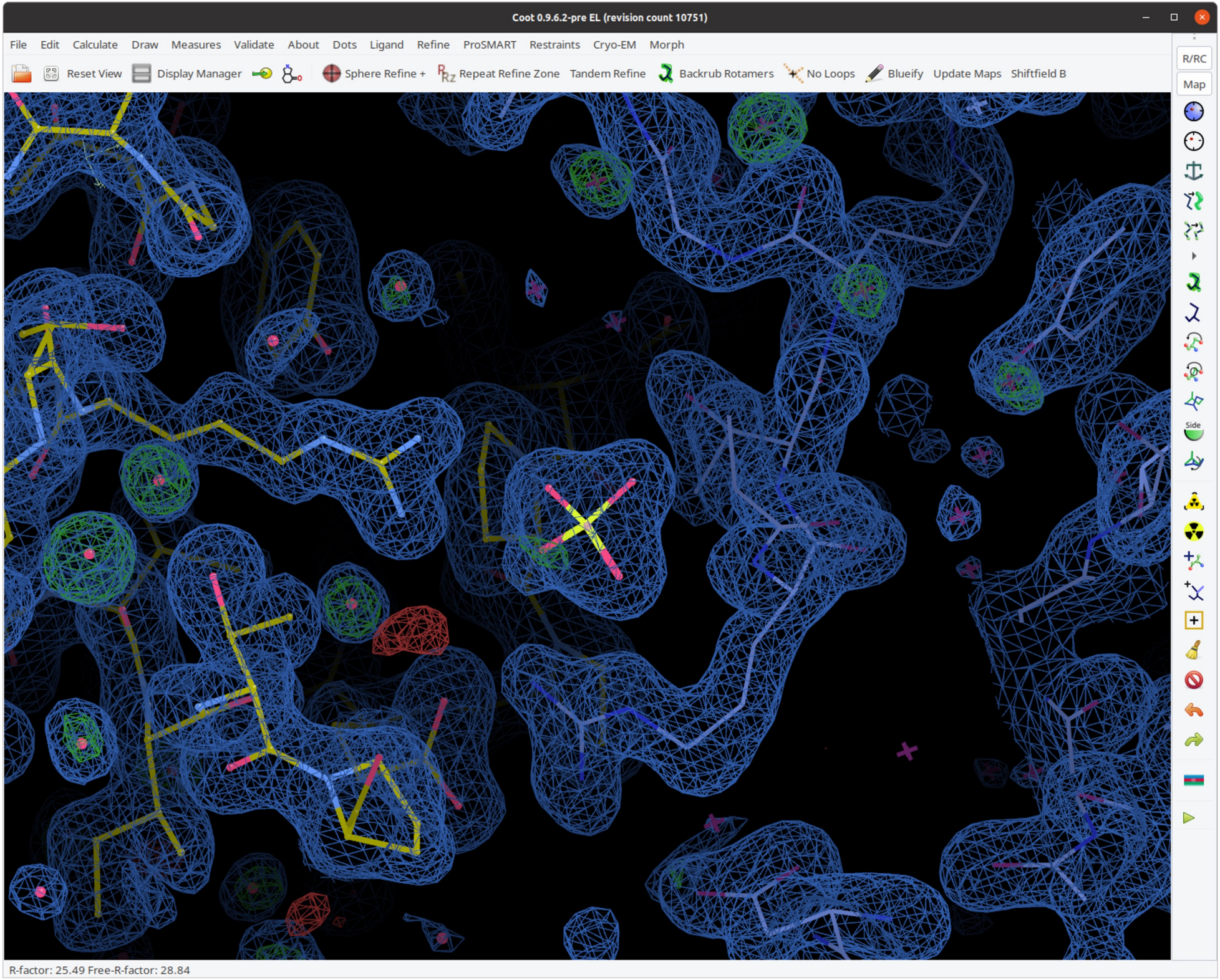
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R/RC
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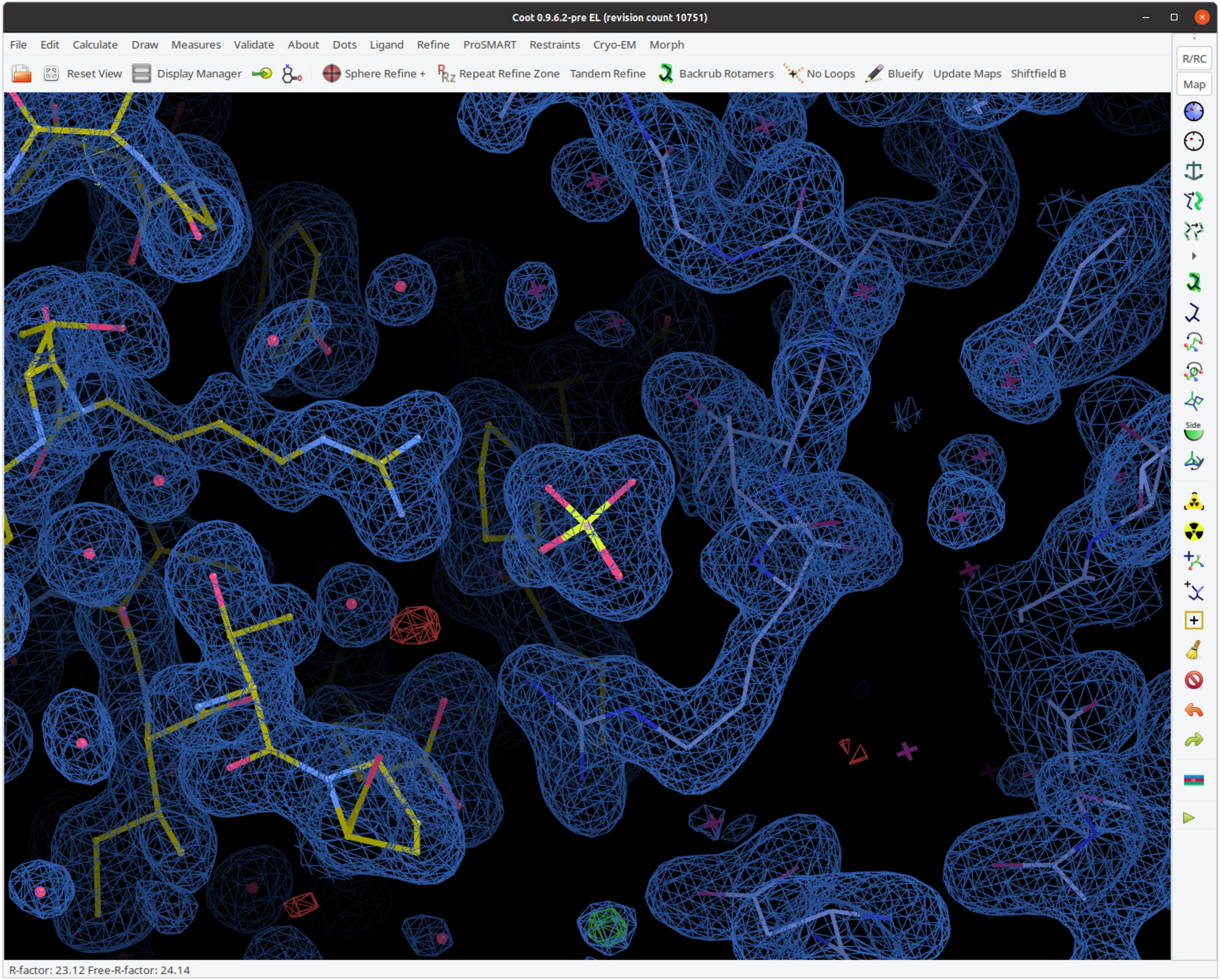
R-factor: 25.49 Free-R-factor: 28.84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Morph
Reset View
Display Manager
Sphere Refine +
Repeat Refine Zone
Tandem Refine
Backrub Rotamers
No Loops
Blueify
Update Maps
Shiftfield B
R/RC
Map
Side
R-factor: 23.12 Free-R-factor: 24.14

# Coot 1.1

## Refinement and Representation

# Moving to Python 3

2017:

“Python 2 is going to die, let’s build Coot using Python 3”

Moving to Python 3 meant:

Moving to GTK 3 which meant

Moving to OpenGL 3.3

# Major Changes

“Single Panel View”

Sequence view

Ramachandran plot

Geometry analysis

Chimera → ChimeraX underwent a similar transformation some years ago

Lighting/Representation improvements

Real Space Refinement

Improved analysis and navigation

# More Sophisticated Lighting in Coot

**Old Lighting Model:**

Ambient

**New lighting:**

Ambient, Diffuse, Specular, Key and Fill lights (Basic)

Depth of Field

Shadows

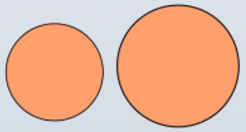
Ambient Occlusion

Approximation, so artefacts

Textures (something other than shiny plastic)

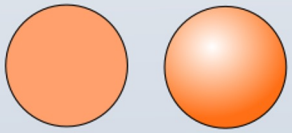
# Visual Cues for Depth

Relative Size



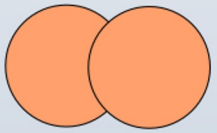
Old Coot:×
New Coot:✓

Shading



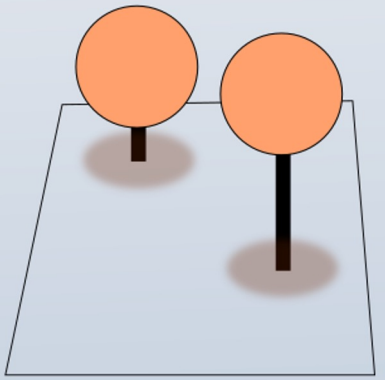
Old Coot:×
New Coot:✓

Occlusion



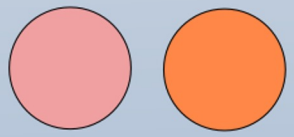
Old Coot:×
New Coot:✓

Shadows



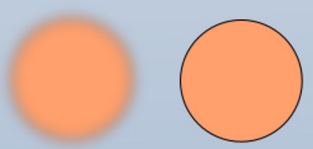
Old Coot:×
New Coot:✓

Colour



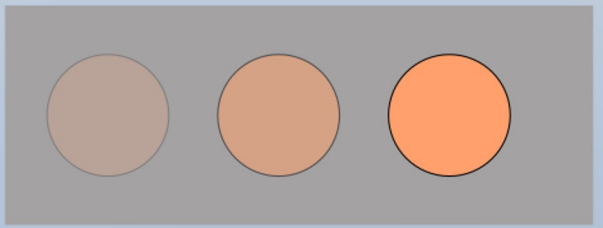
Old Coot:×
New Coot:✓

Focus/Blur



Old Coot:×
New Coot:✓

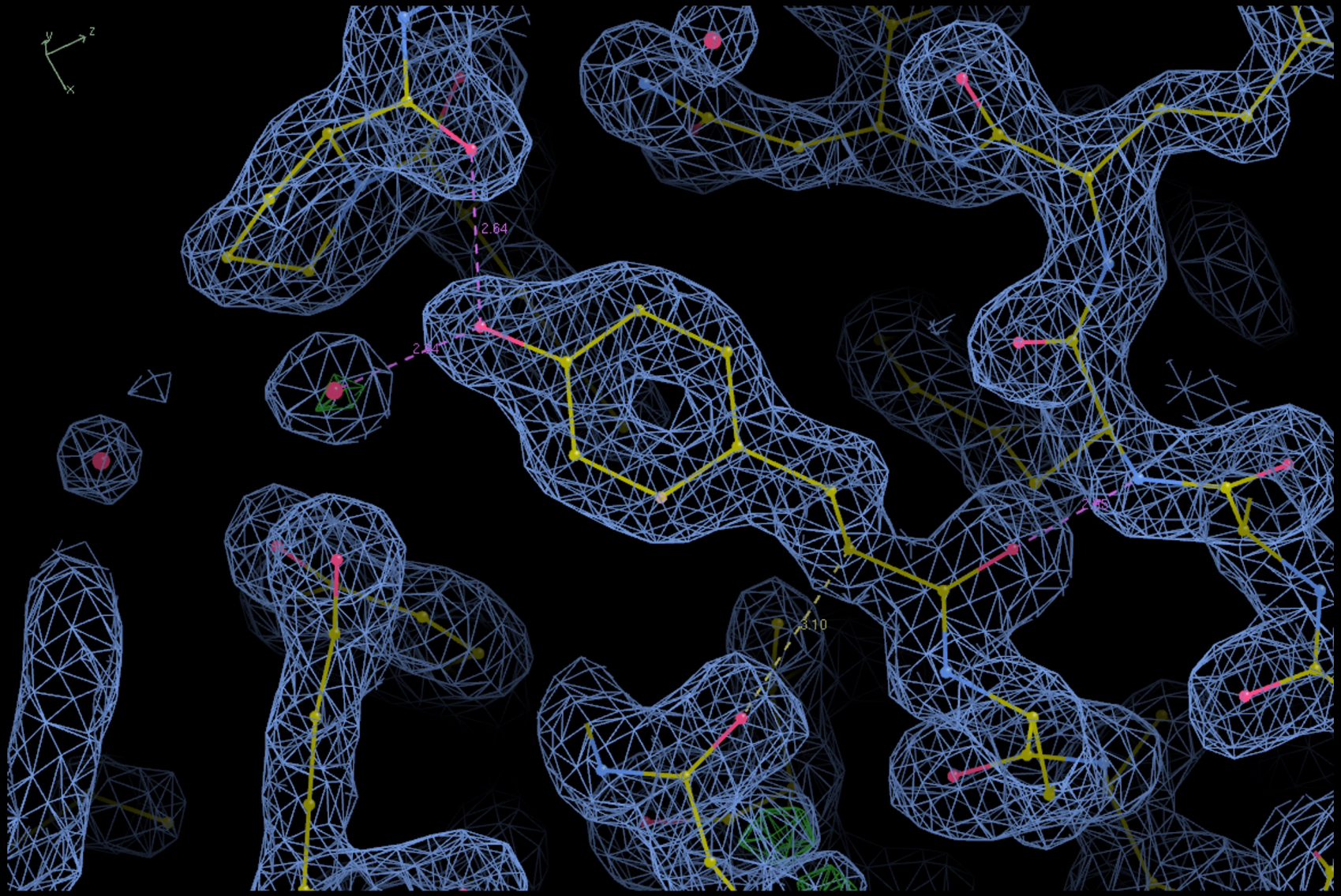
Fog Depth



Old Coot:✓
New Coot:✓

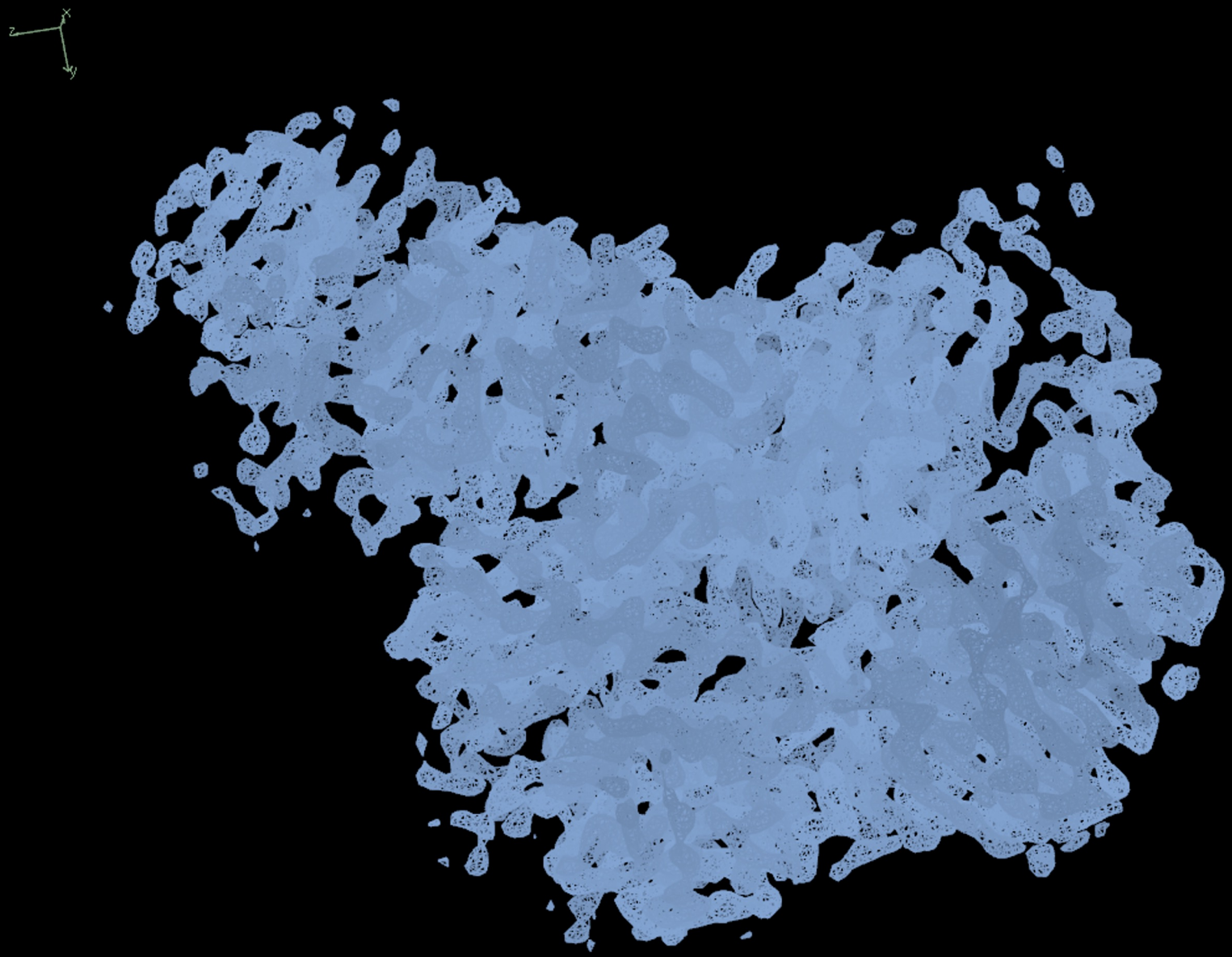
# Old Coot: Lack of Depth

When Zoomed in:



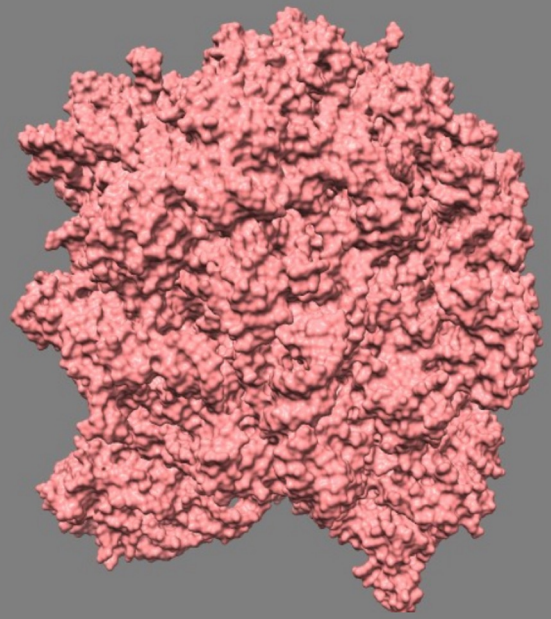
# Old Coot: Lack of Depth

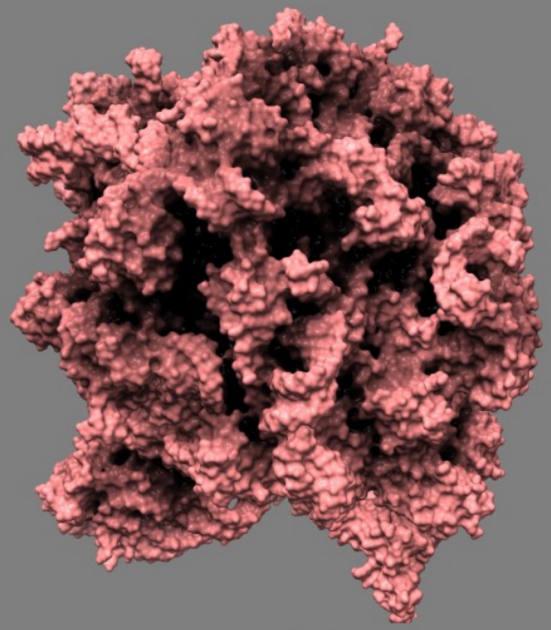
When Zoomed out:



# Ambient Occlusion and Shadows in ChimeraX

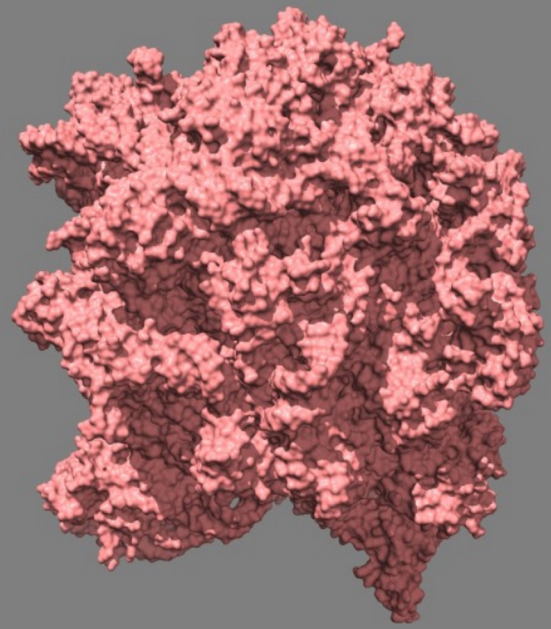
Basic Lighting

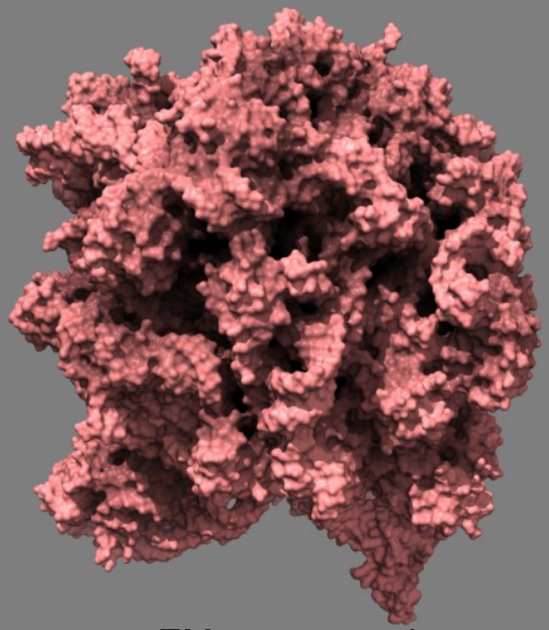




Ambient Occlusion

Shadows

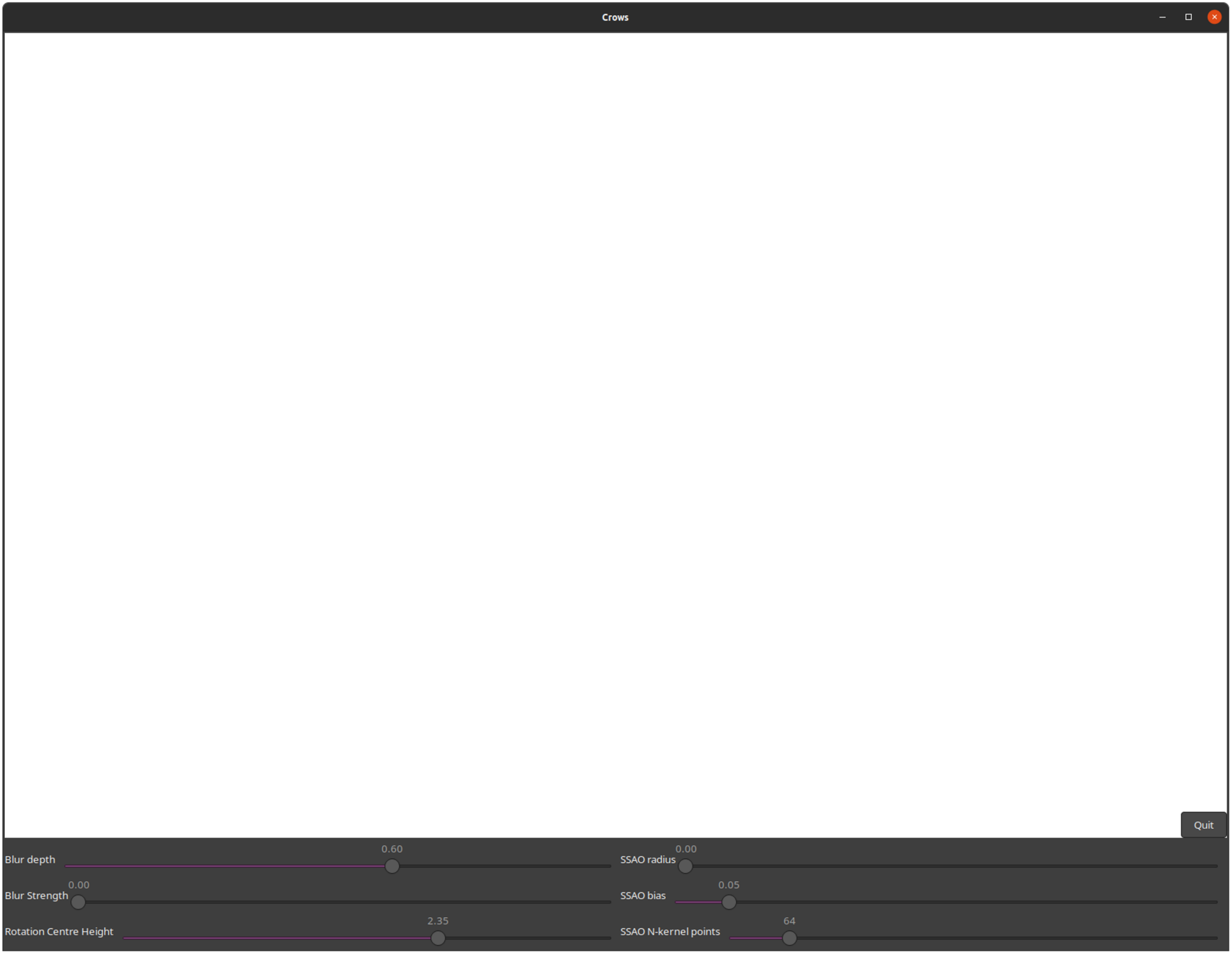




Ambient Occlusion & Shadows

Molecular surface, not cryo-EM reconstruction


Crows
Quit
Blur depth
0.58
Blur Strength
0.00
Rotation Centre Height
2.35
SSAO radius
0.00
SSAO bias
0.05
SSAO N-kernel points
138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SSAO N-kernel points
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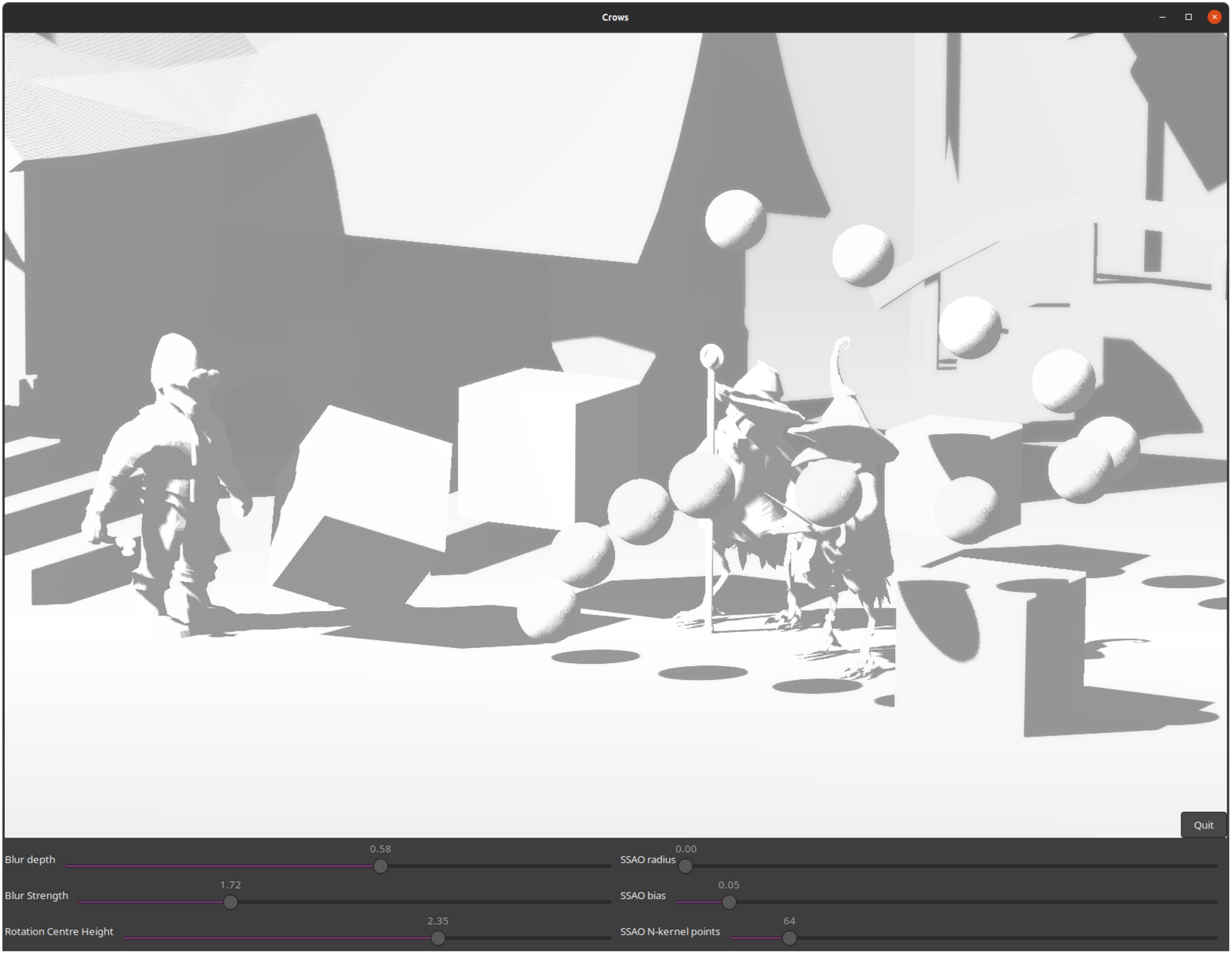
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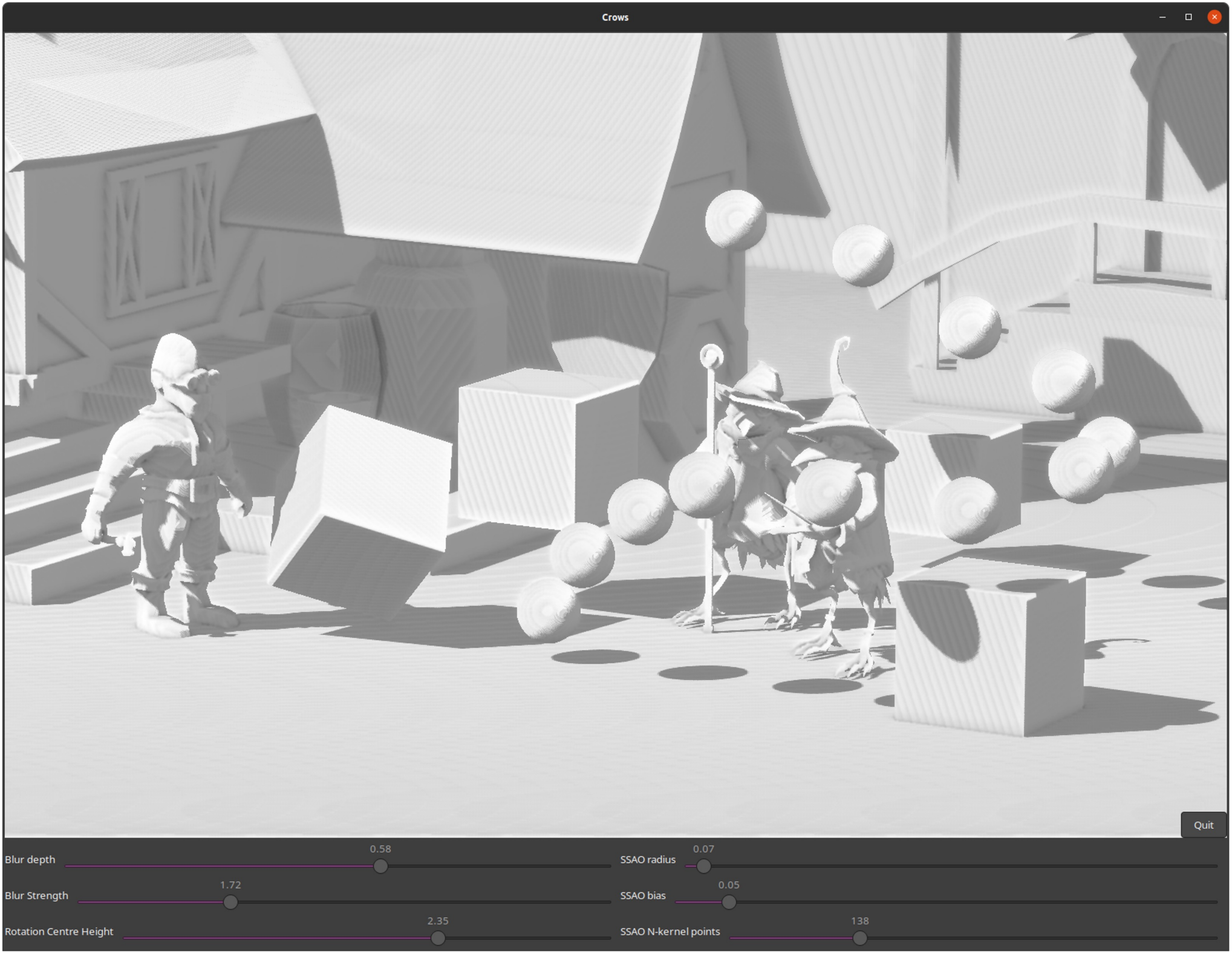
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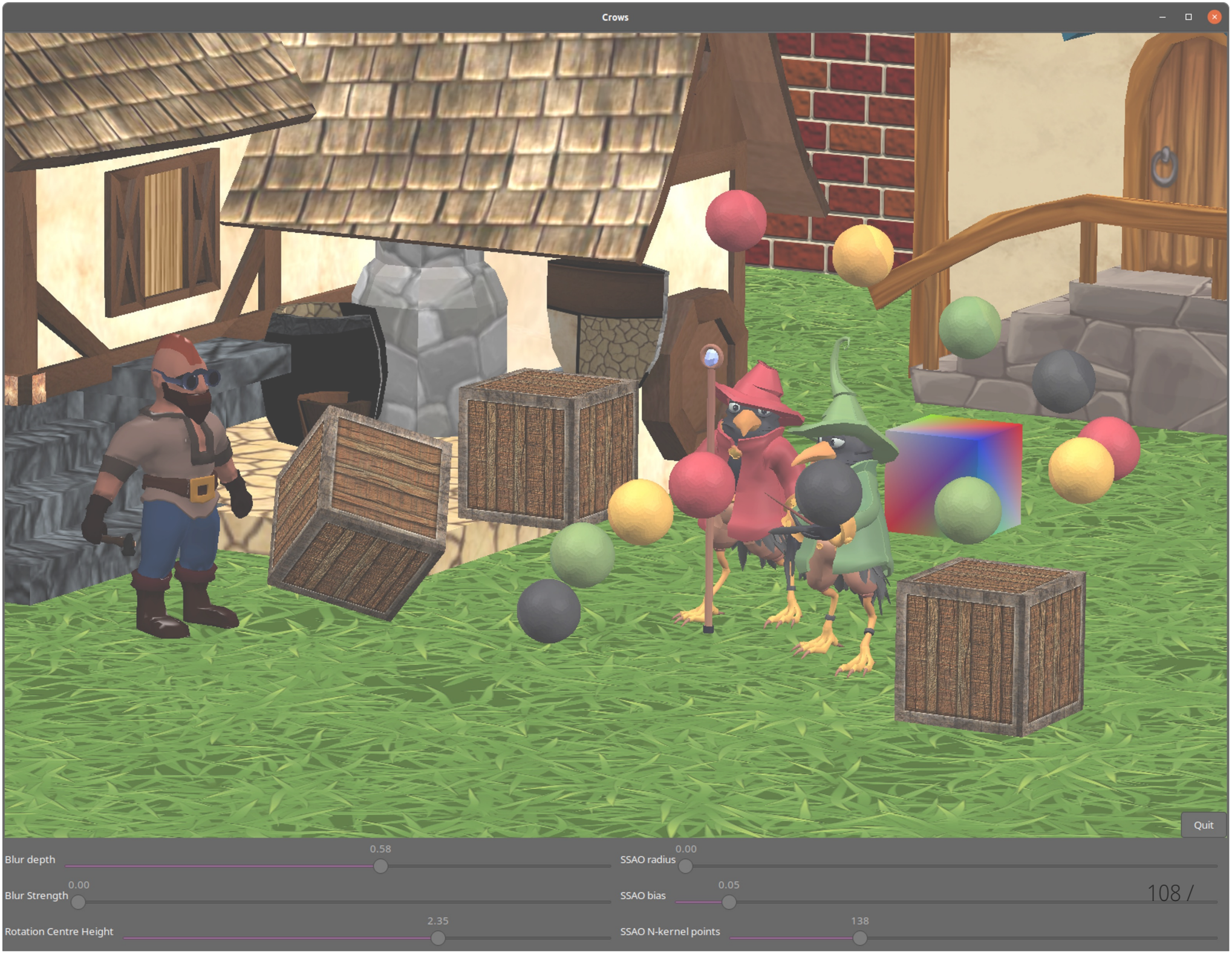
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SSAO N-kernel points
138
108 /


Crows
Quit
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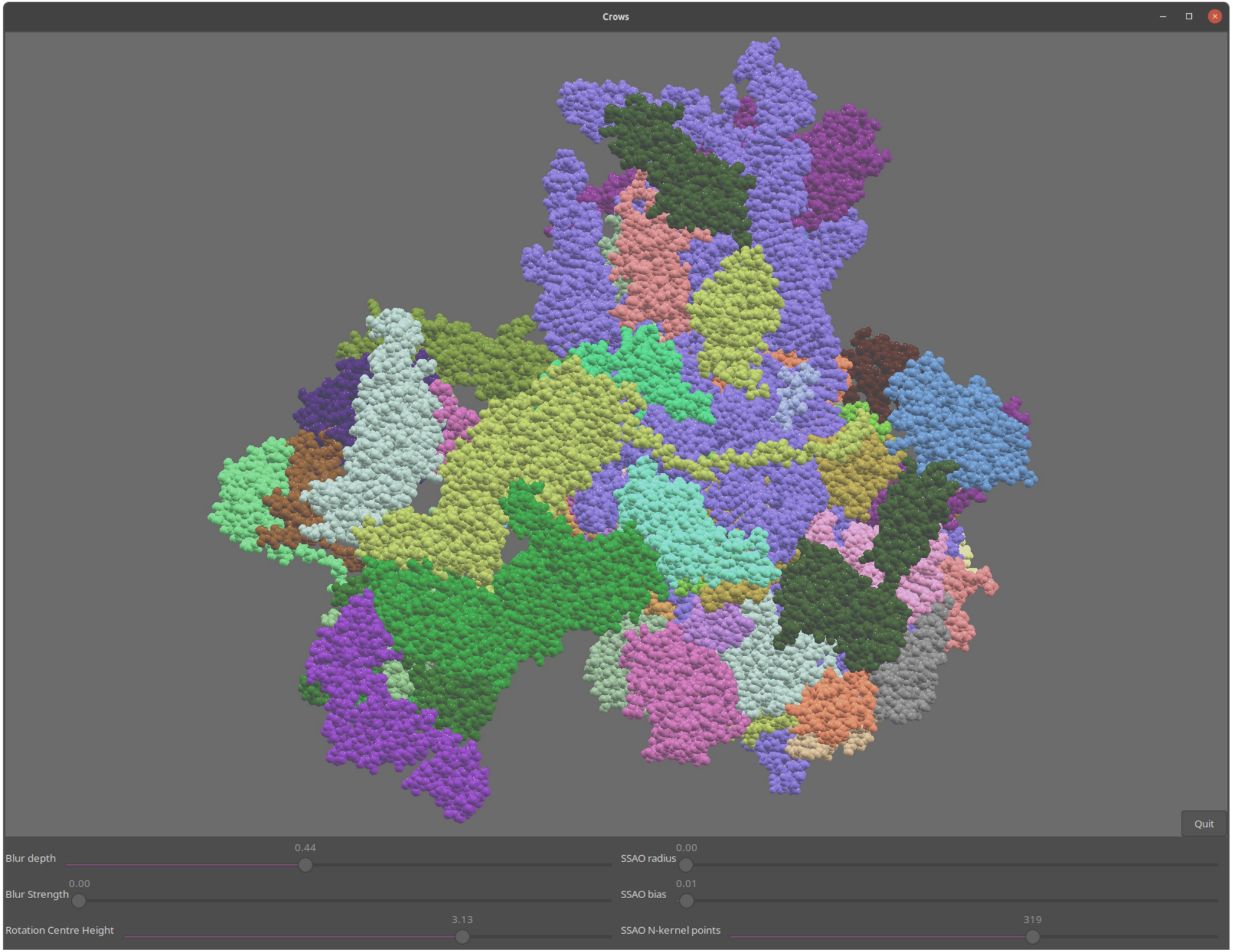
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SSAO N-kernel points
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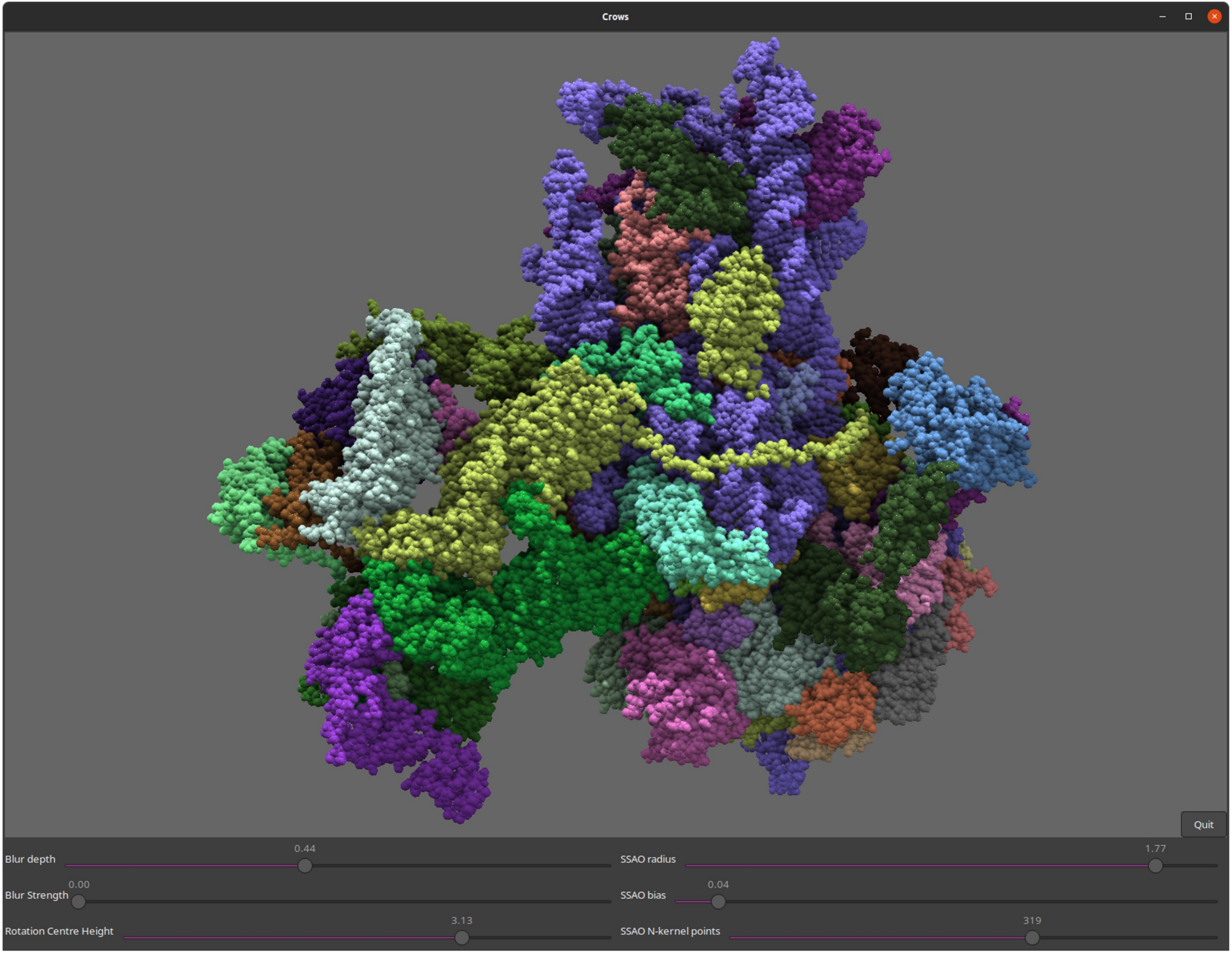
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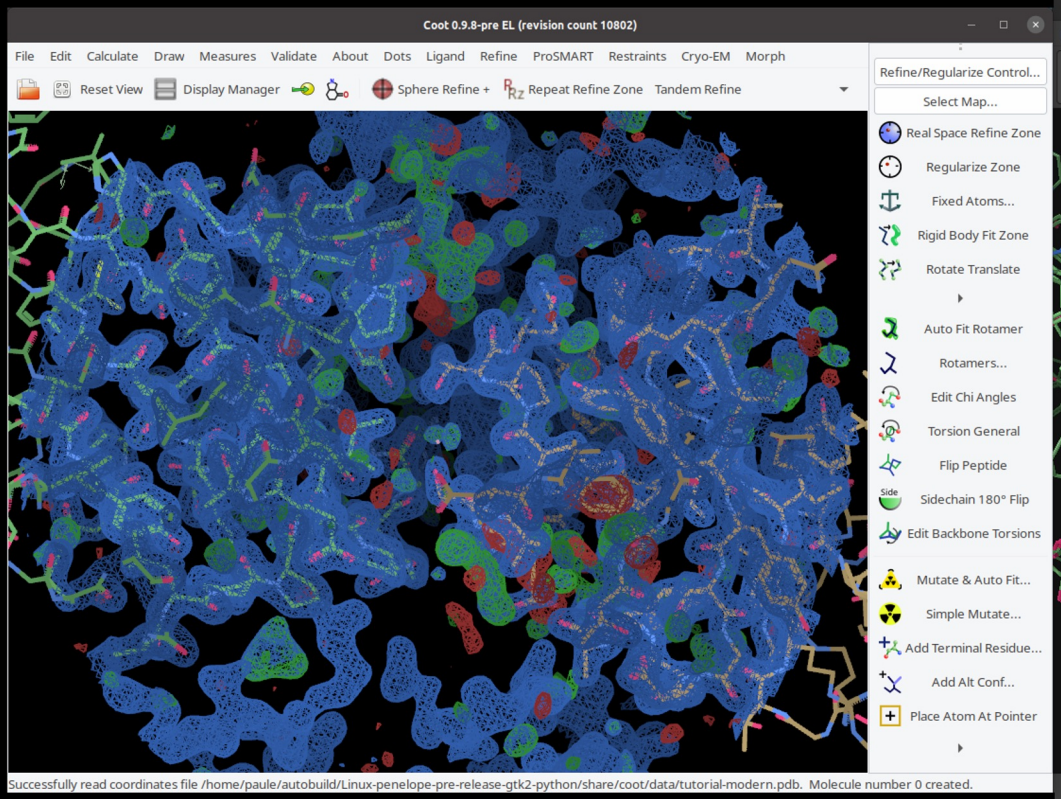
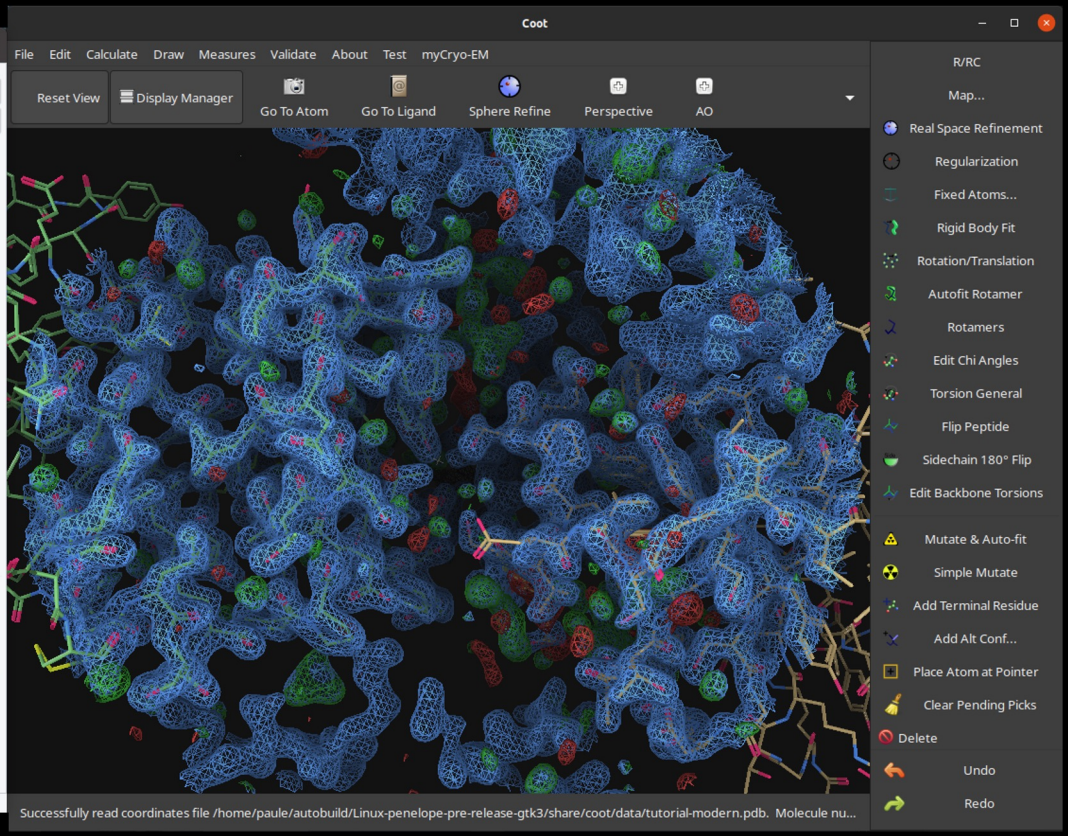
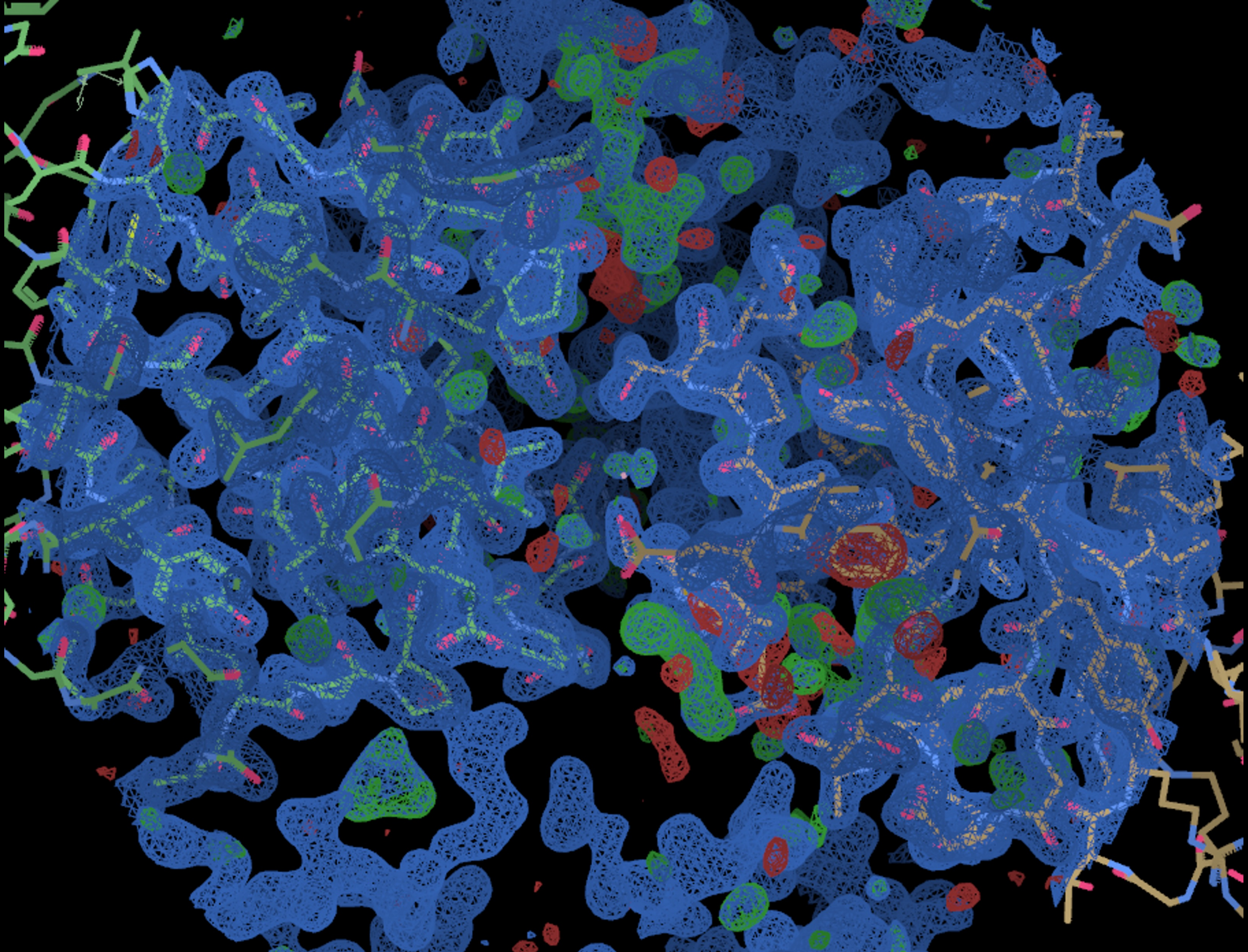
319

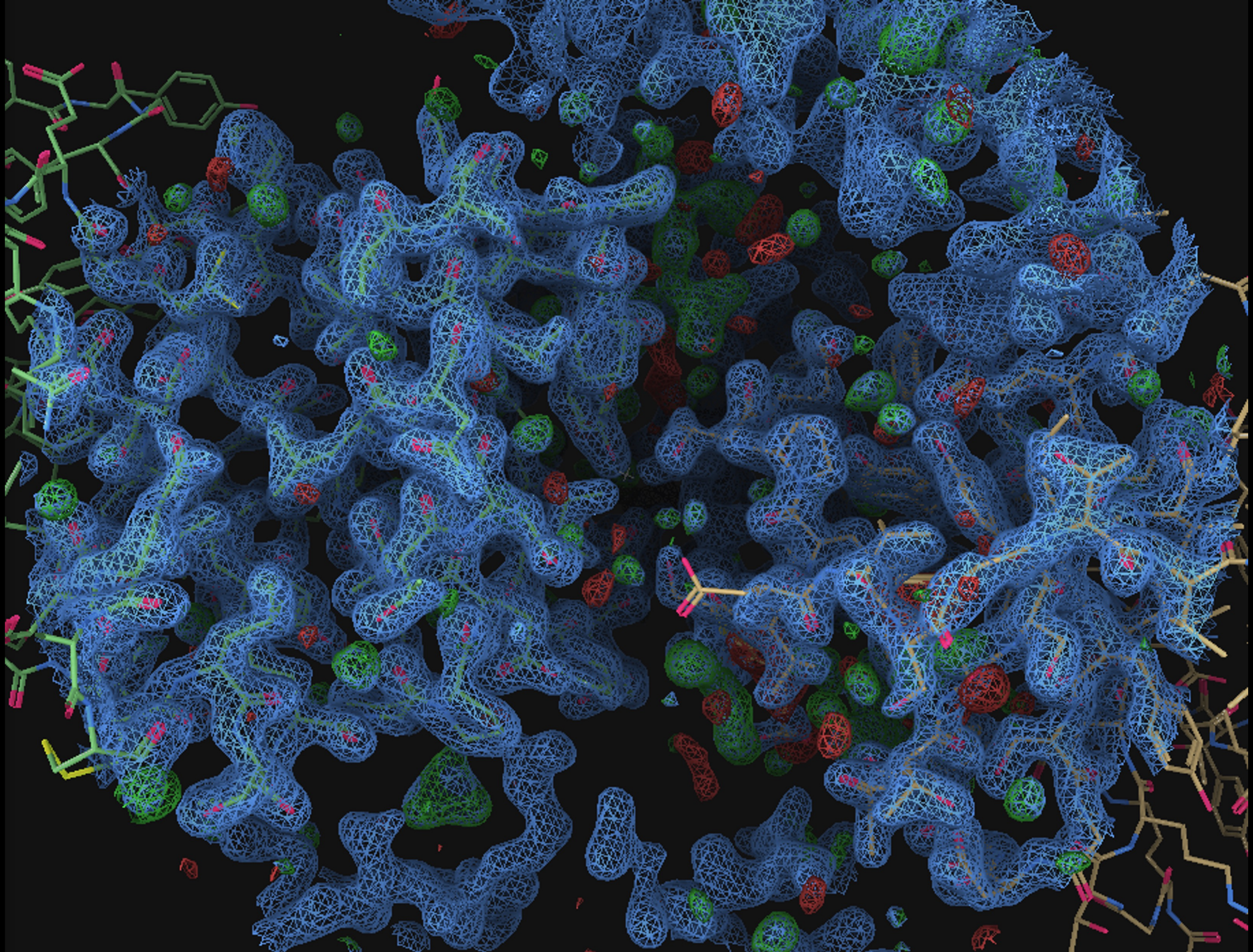
# Old Coot and New Coot




**Dark-mode enabled by default**



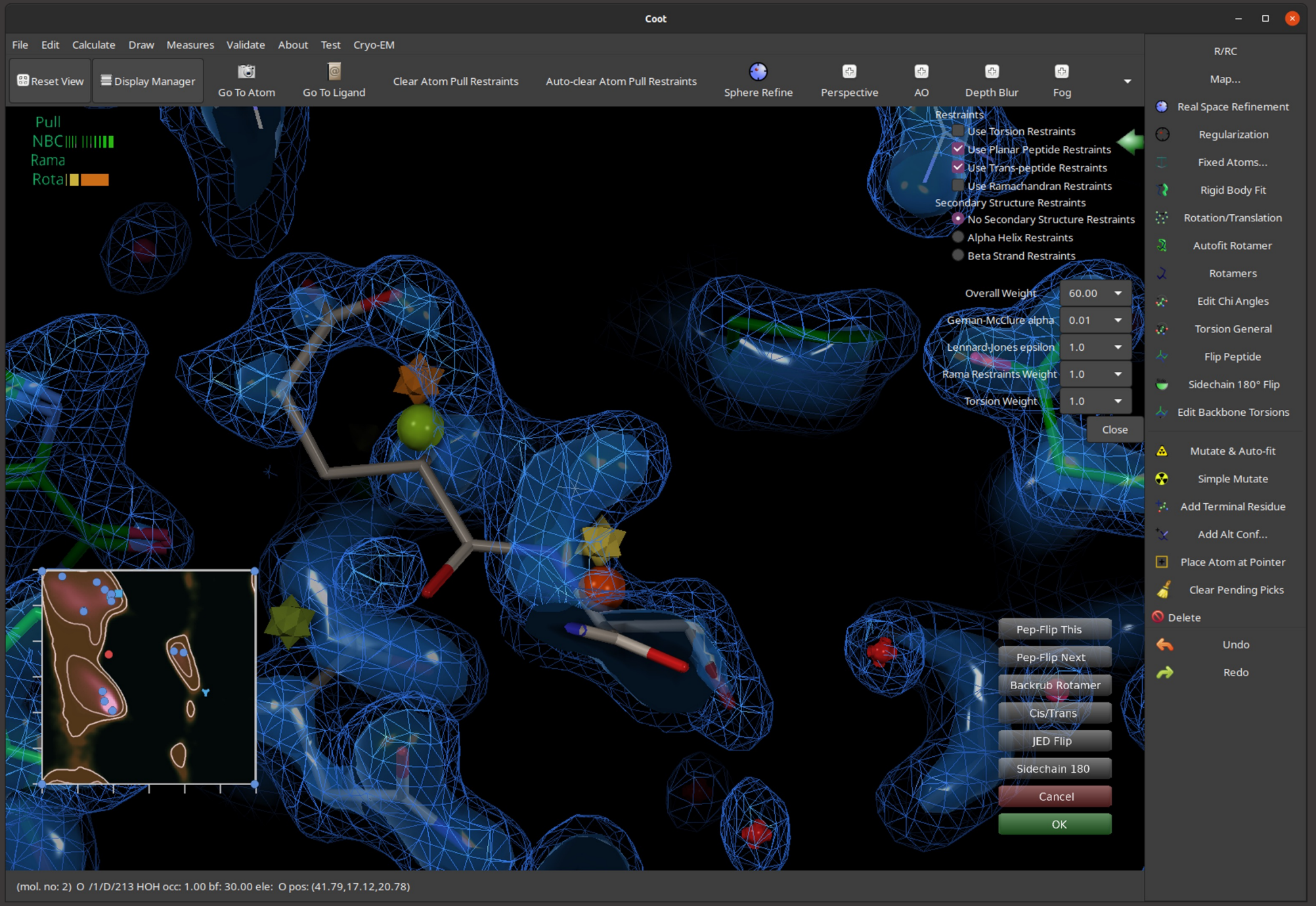


# How Real-Space Refinement Has Improved

- By the addition of **interactive validation**
- By **updating the map**

  structure factor calculation,

  sigmaA calculation


Coot
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Reset View
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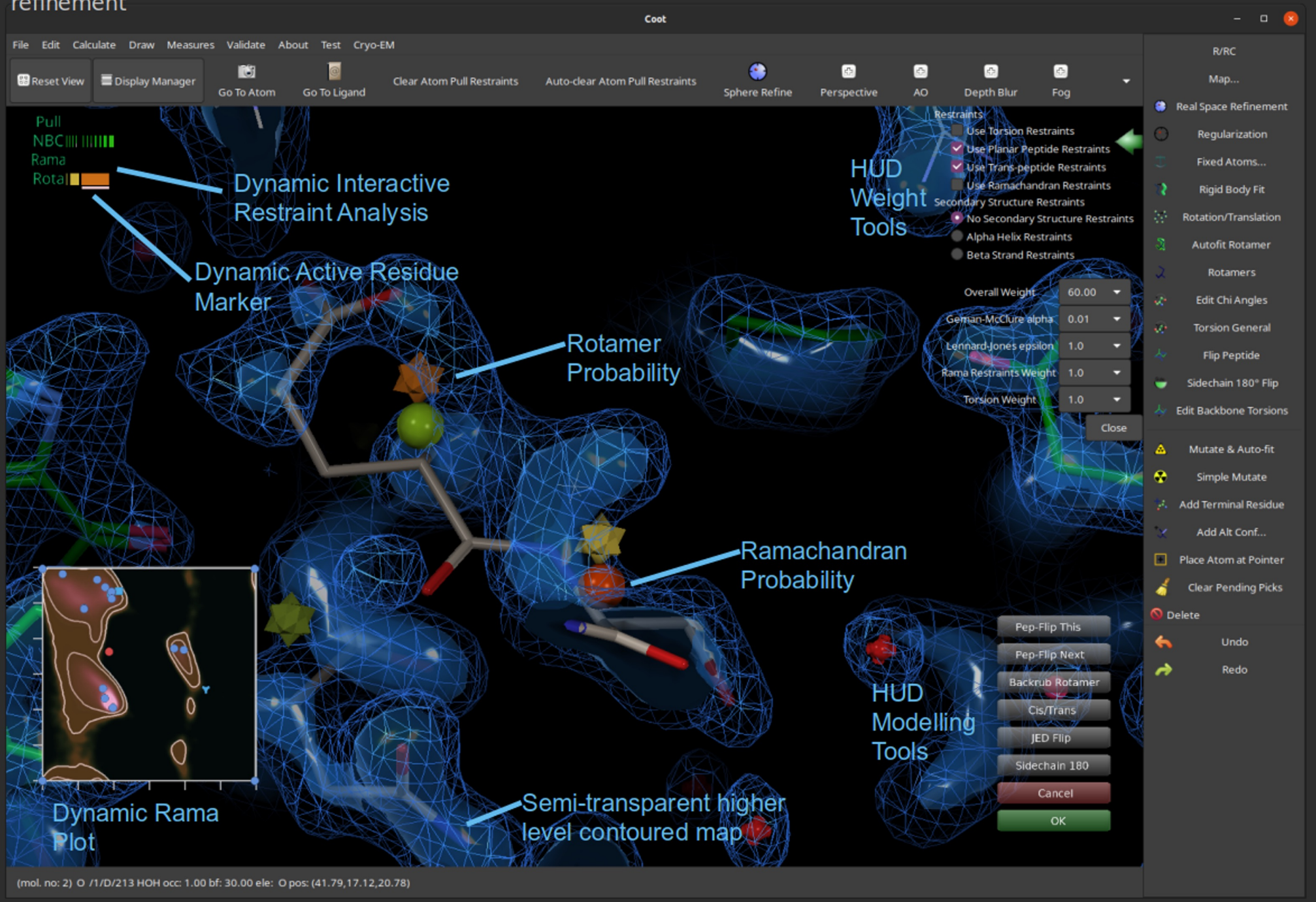
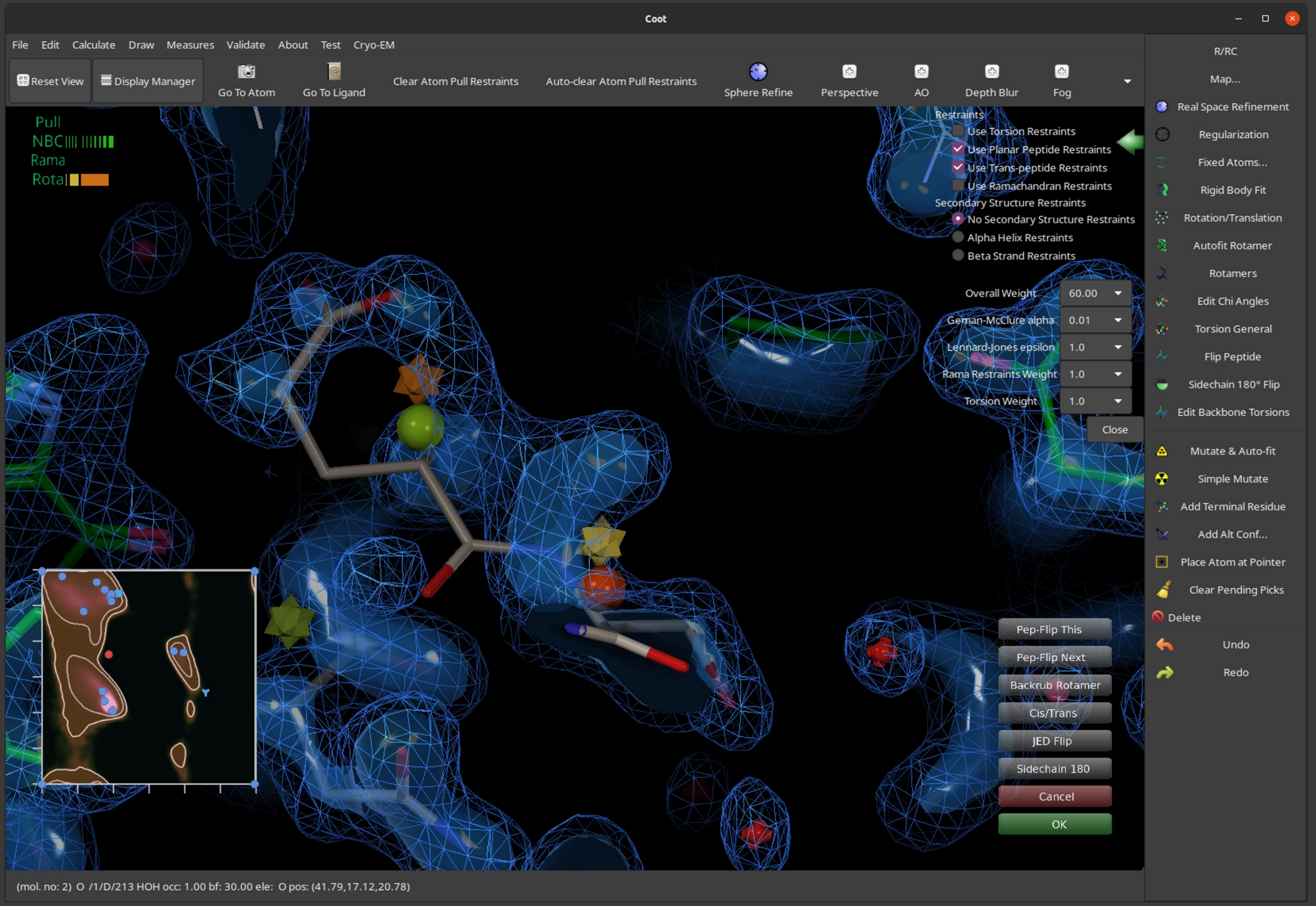
Auto-clear Atom Pull Restraints
Sphere Refine
Perspective
AO
Depth Blur
Fog
Pull
NBC
Rama
Rota
Restraints
Use Torsion Restraints
Use Planar Peptide Restraints
Use Trans-peptide Restraints
Use Ramachandran Restraints
Secondary Structure Restraints
No Secondary Structure Restraints
Alpha Helix Restraints
Beta Strand Restraints
Overall Weight
60.00
Geman-McClure alpha
0.01
Lennard-Jones epsilon
1.0
Rama Restraints Weight
1.0
Torsion Weight
1.0
Close
Pep-Flip This
Pep-Flip Next
Backrub Rotamer
Cis/Trans
JED Flip
Sidechain 180
Cancel
OK
R/RC
Map...
Real Space Refinement
Regularization
Fixed Atoms...
Rigid Body Fit
Rotation/Translation
Autofit Rotamer
Rotamers
Edit Chi Angles
Torsion General
Flip Peptide
Sidechain 180° Flip
Edit Backbone Torsions
Mutate & Auto-fit
Simple Mutate
Add Terminal Residue
Add Alt Conf...
Place Atom at Pointer
Clear Pending Picks
Delete
Undo
Redo
(mol. no: 2) O /1/D/213 HOH occ: 1.00 bf: 30.00 ele: O pos: (41.79,17.12,20.78)

# Real-Space Refinement of a mispositioned residue in modern Coot

The coloured bonds show the fixed original structure, the grey bonds show the refined atoms after real space refinement




Coot
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Measures
Validate
About
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Cryo-EM
Reset View
Display Manager
Go To Atom
Go To Ligand
Clear Atom Pull Restraints
Auto-clear Atom Pull Restraints
Sphere Refine
Perspective
AO
Depth Blur
Fog
Pull
NBC
Rama
Rota
Restraints
Use Torsion Restraints
Use Planar Peptide Restraints
Use Trans-peptide Restraints
Use Ramachandran Restraints
Secondary Structure Restraints
No Secondary Structure Restraints
Alpha Helix Restraints
Beta Strand Restraints
Overall Weight
60.00
Geman-McClure alpha
0.01
Lennard-Jones epsilon
1.0
Rama Restraints Weight
1.0
Torsion Weight
1.0
Close
Pep-Flip This
Pep-Flip Next
Backrub Rotamer
Cis/Trans
JED Flip
Sidechain 180
Cancel
OK
R/RC
Map...
Real Space Refinement
Regularization
Fixed Atoms...
Rigid Body Fit
Rotation/Translation
Autofit Rotamer
Rotamers
Edit Chi Angles
Torsion General
Flip Peptide
Sidechain 180° Flip
Edit Backbone Torsions
Mutate & Auto-fit
Simple Mutate
Add Terminal Residue
Add Alt Conf...
Place Atom at Pointer
Clear Pending Picks
Delete
Undo
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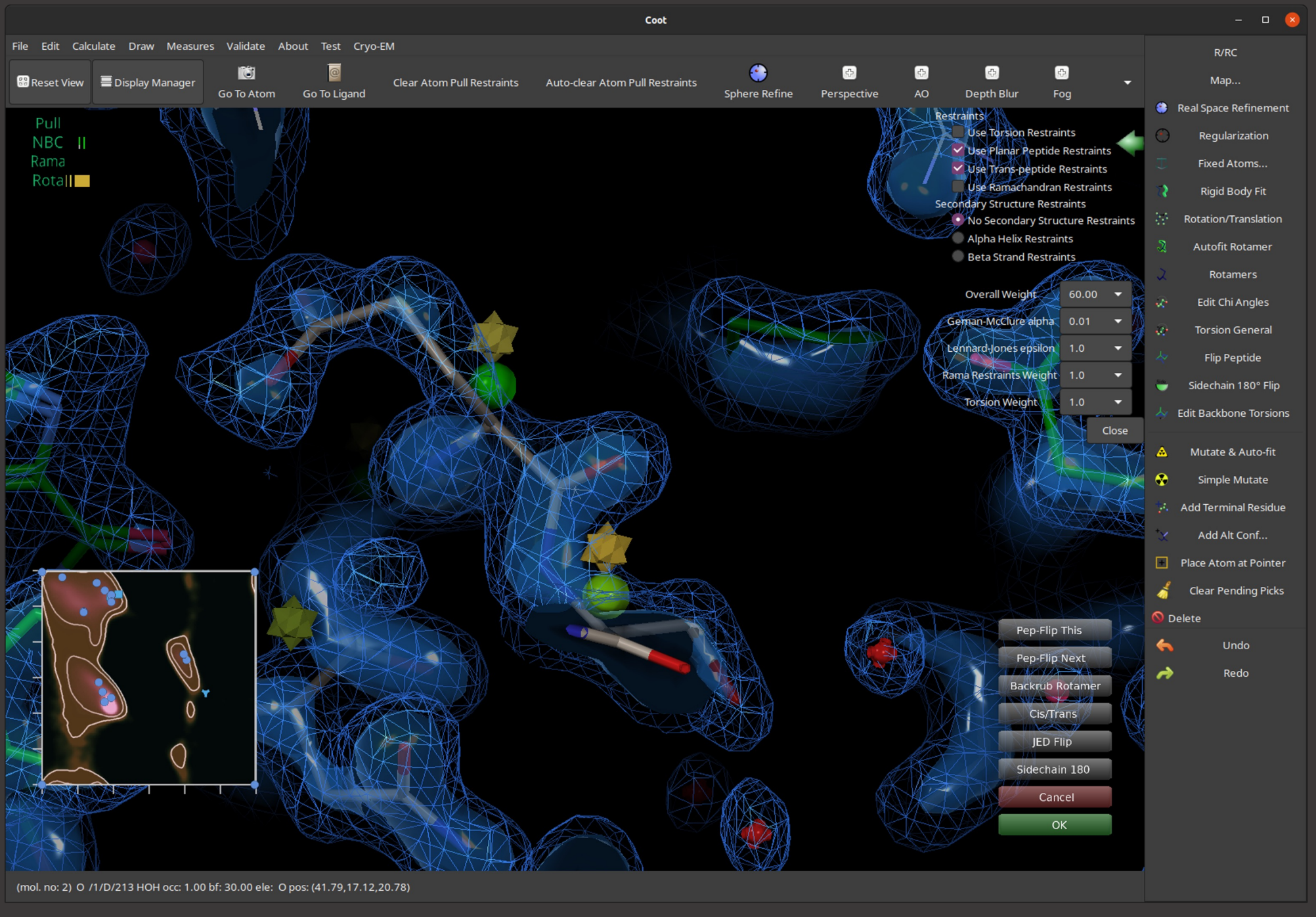
(mol. no: 2) O /1/D/213 HOH occ: 1.00 bf: 30.00 ele: O pos: (41.79,17.12,20.78)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Go To Atom
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Auto-clear Atom Pull Restraints
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Use Trans-peptide Restraints
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Secondary Structure Restraints
No Secondary Structure Restraints
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Overall Weight 60.00
Geman-McClure alpha 0.01
Lennard-Jones epsilon 1.0
Rama Restraints Weight 1.0
Torsion Weight 1.0
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Pep-Flip Next
Backrub Rotamer
Cis/Trans
JED Flip
Sidechain 180
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OK
R/RC
Map...
Real Space Refinement
Regularization
Fixed Atoms...
Rigid Body Fit
Rotation/Translation
Autofit Rotamer
Rotamers
Edit Chi Angles
Torsion General
Flip Peptide
Sidechain 180° Flip
Edit Backbone Torsions
Mutate & Auto-fit
Simple Mutate
Add Terminal Residue
Add Alt Conf...
Place Atom at Pointer
Clear Pending Picks
Delete
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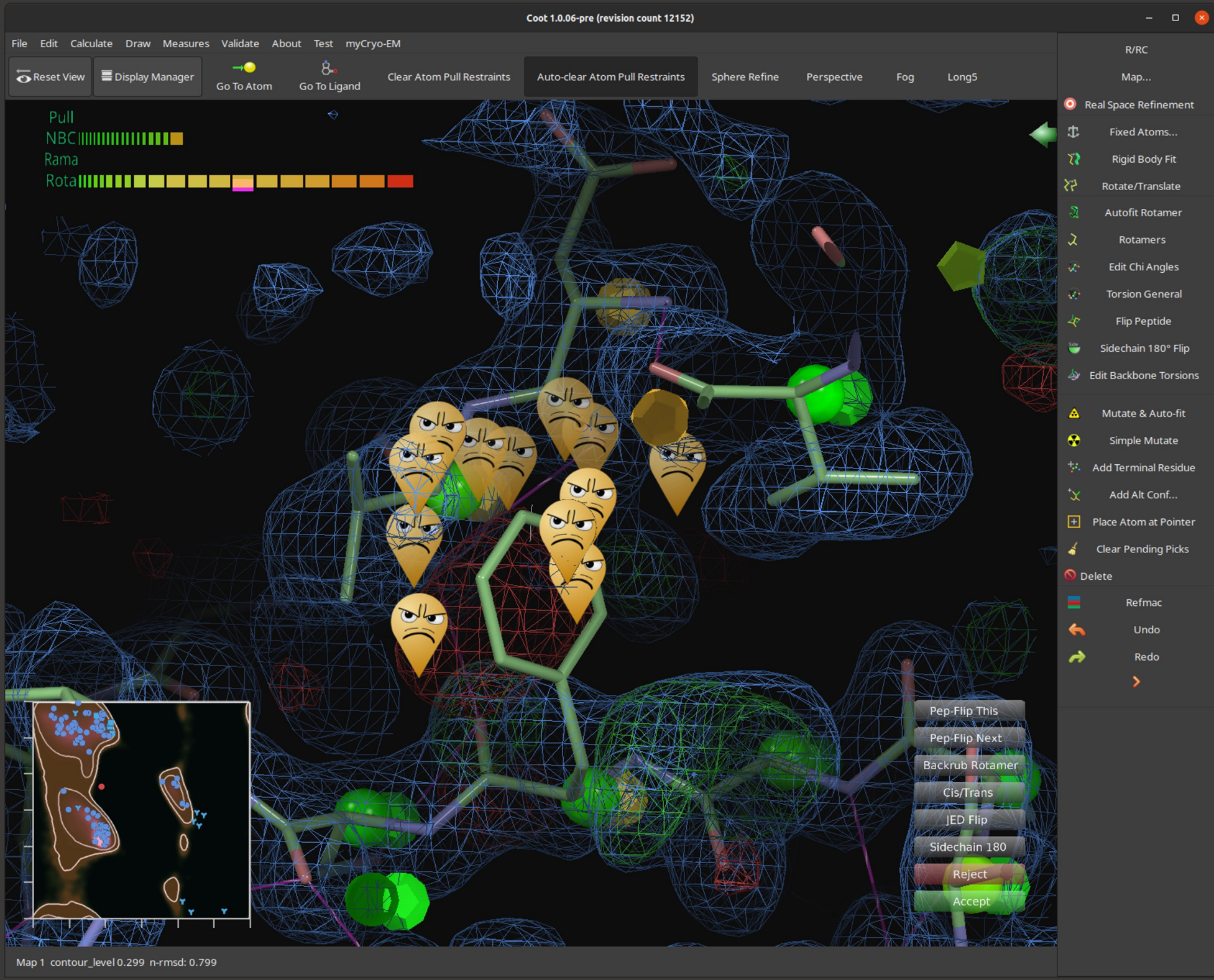
(mol. no: 2) O /1/D/213 HOH occ: 1.00 bf: 30.00 ele: O pos: (41.79,17.12,20.78)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myCryo-EM
Reset View
Display Manager
Go To Atom
Go To Ligand
Clear Atom Pull Restraints
Auto-clear Atom Pull Restraints
Sphere Refine
Perspective
Fog
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Rama
Rota
R/RC
Map...
Real Space Refinement
Fixed Atoms...
Rigid Body Fit
Rotate/Translate
Autofit Rotamer
Rotamers
Edit Chi Angles
Torsion General
Flip Peptide
Sidechain 180° Flip
Edit Backbone Torsions
Mutate & Auto-fit
Simple Mutate
Add Terminal Residue
Add Alt Conf...
Place Atom at Pointer
Clear Pending Picks
Delete
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Undo
Redo
Pep-Flip This
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JED Flip
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Accept
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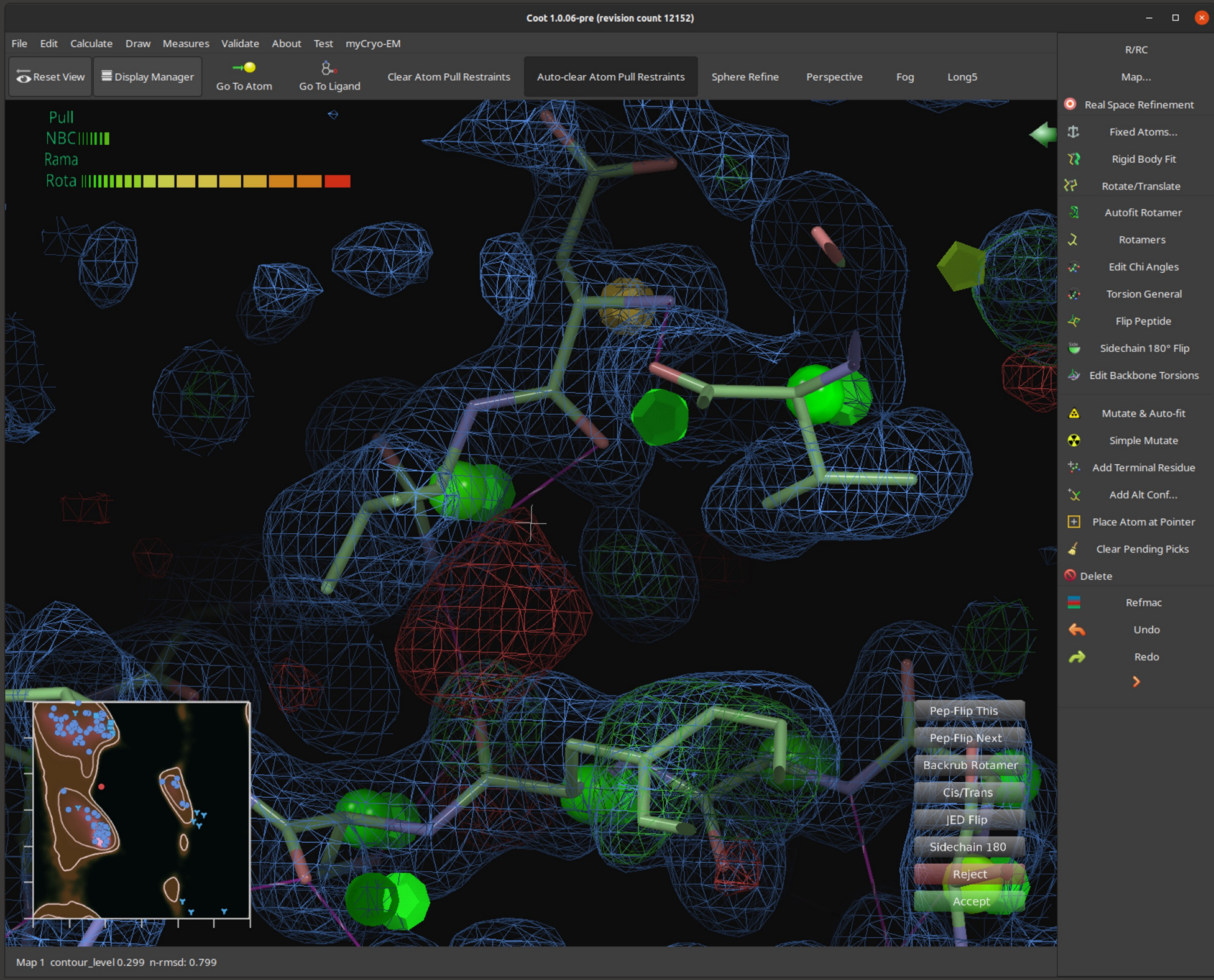
Coot 1.0.06-pre (revision count 12152)
File
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Measures
Validate
About
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myCryo-EM
Reset View
Display Manager
Go To Atom
Go To Ligand
Clear Atom Pull Restraints
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Perspective
Fog
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Rota
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Real Space Refinement
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Rigid Body Fit
Rotate/Translate
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Edit Chi Angles
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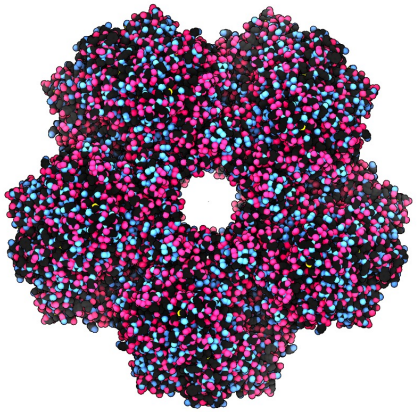
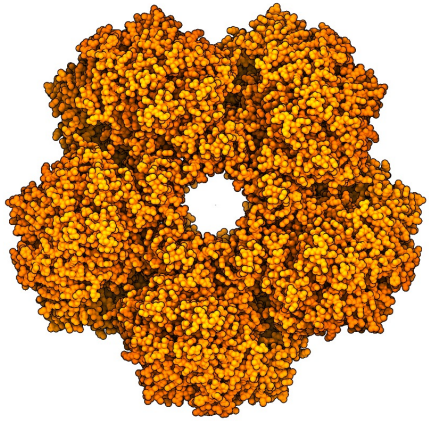
Pep-Flip Next
Backrub Rotamer
Cis/Trans
JED Flip
Sidechain 180
Reject
Accept
Map 1 contour_level 0.299 n-rmsd: 0.799

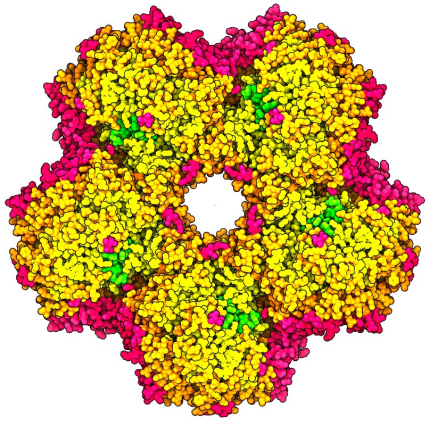
# New Coot Graphics



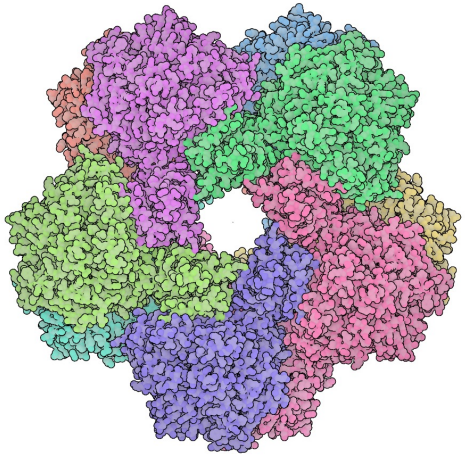
colour by atoms



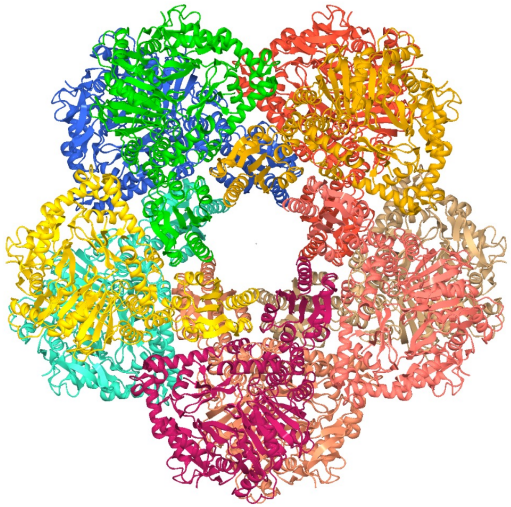
colour by molecule



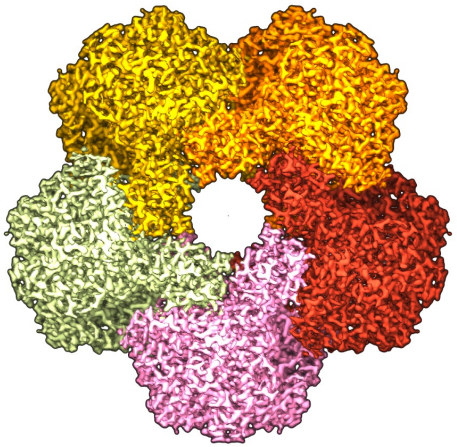
colour by B factors



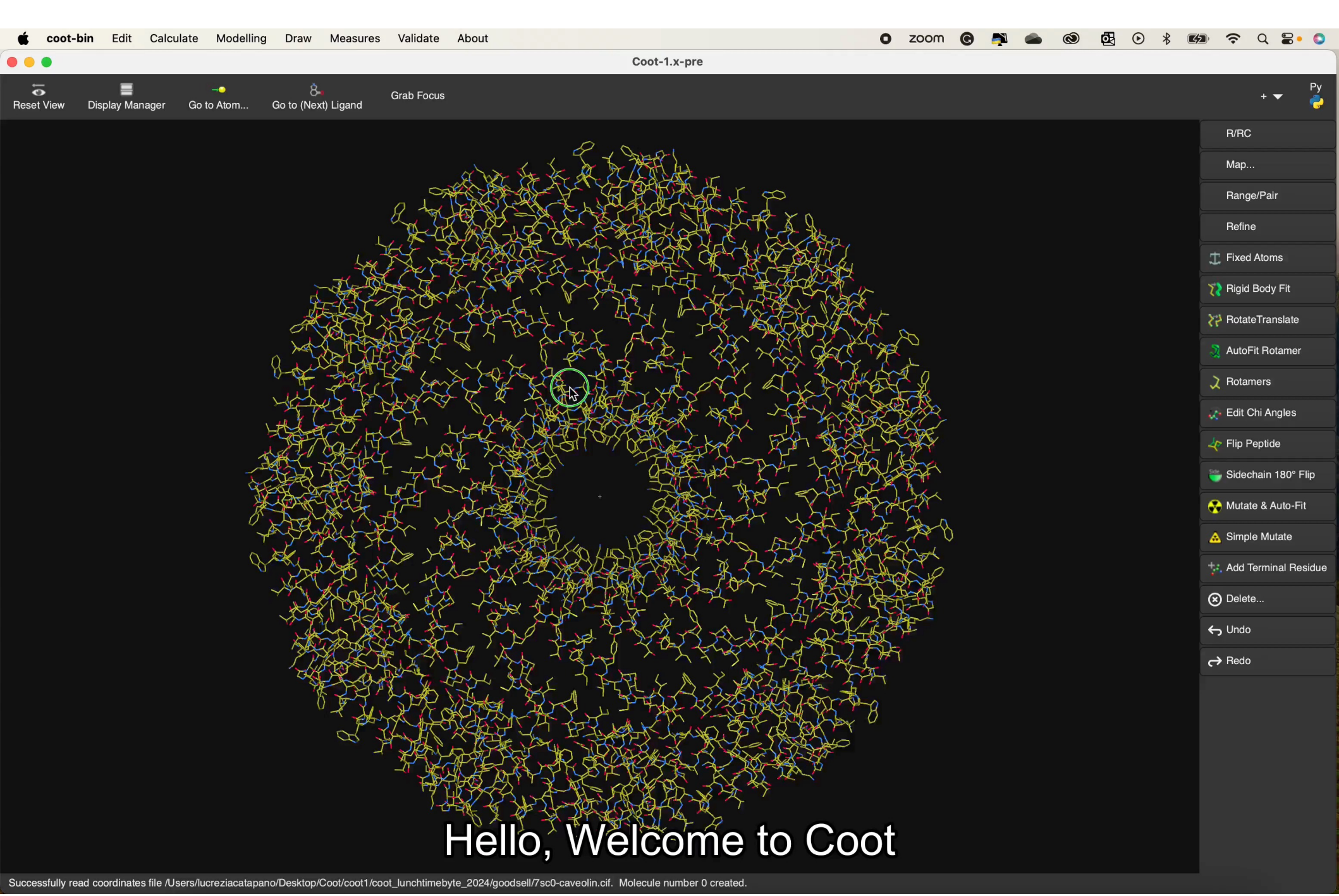
Goodsell colours



ribbons



masked map


coot-bin
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Calculate
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Measures
Validate
About
Coot-1.x-pre
Reset View
Display Manager
Go to Atom...
Go to (Next) Ligand
Grab Focus
Py
R/RC
Map...
Range/Pair
Refine
Fixed Atoms
Rigid Body Fit
RotateTranslate
AutoFit Rotamer
Rotamers
Edit Chi Angles
Flip Peptide
Sidechain 180° Flip
Mutate & Auto-Fit
Simple Mutate
Add Terminal Residue
Delete...
Undo
Redo
Hello, Welcome to Coot
Successfully read coordinates file /Users/lucreziacatapano/Desktop/Coot/coot1/coot_lunchtimebyte_2024/goodsell/7sc0-caveolin.cif. Molecule number 0 created.

# Moorhen

## Web-Based Interactive Model Building

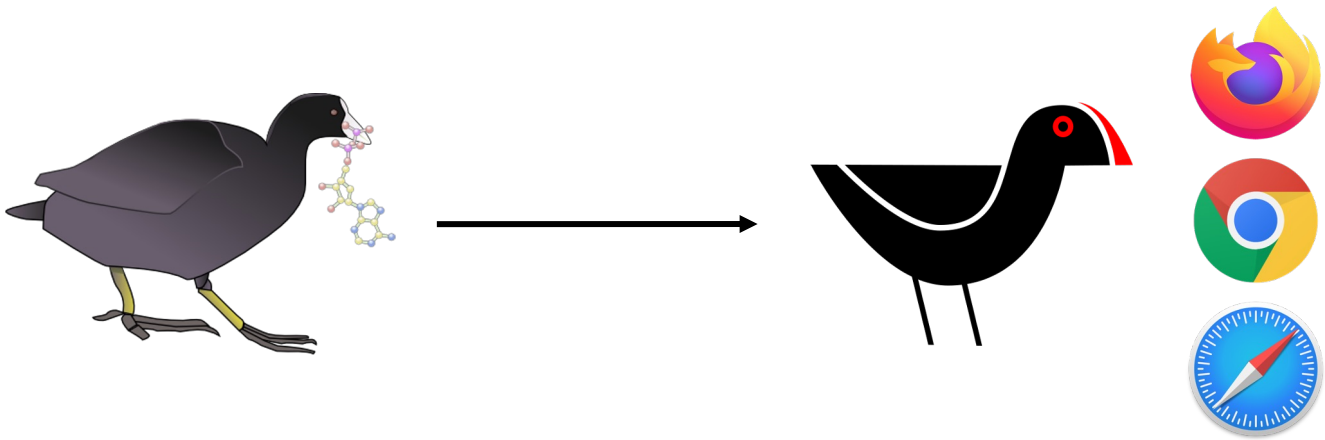
This is a coot

This is a moorhen

# What is Moorhen?

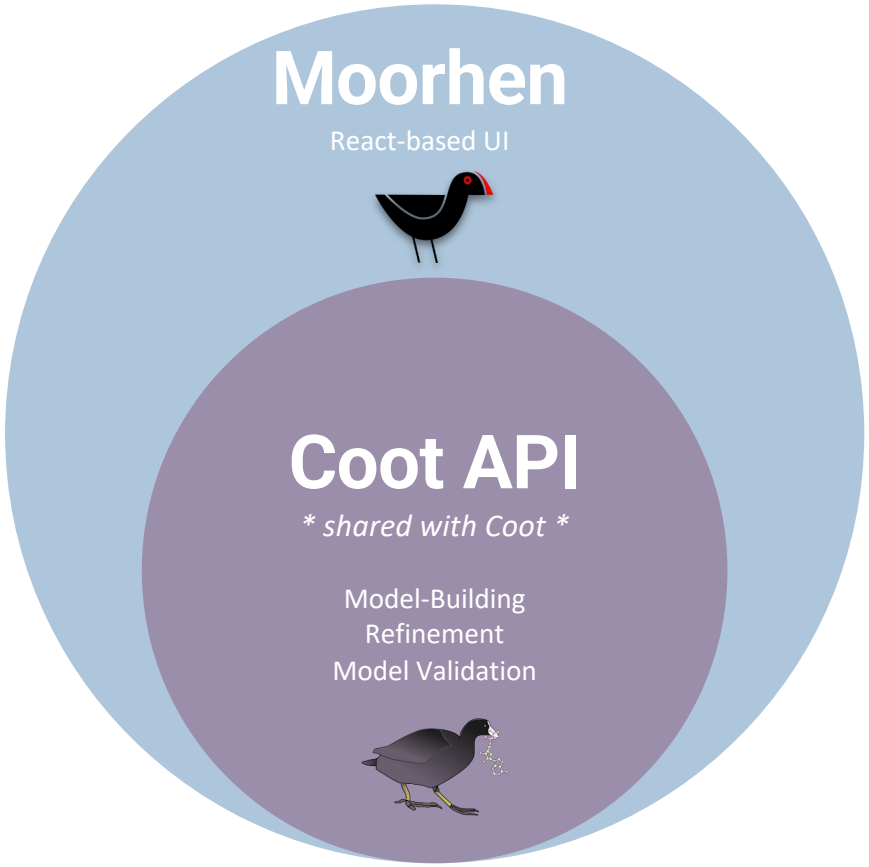
- Moorhen is a next-generation web-based application for the visualisation and manipulation of molecules in structure determination and analysis

  ➔ In short, Coot on the web browser



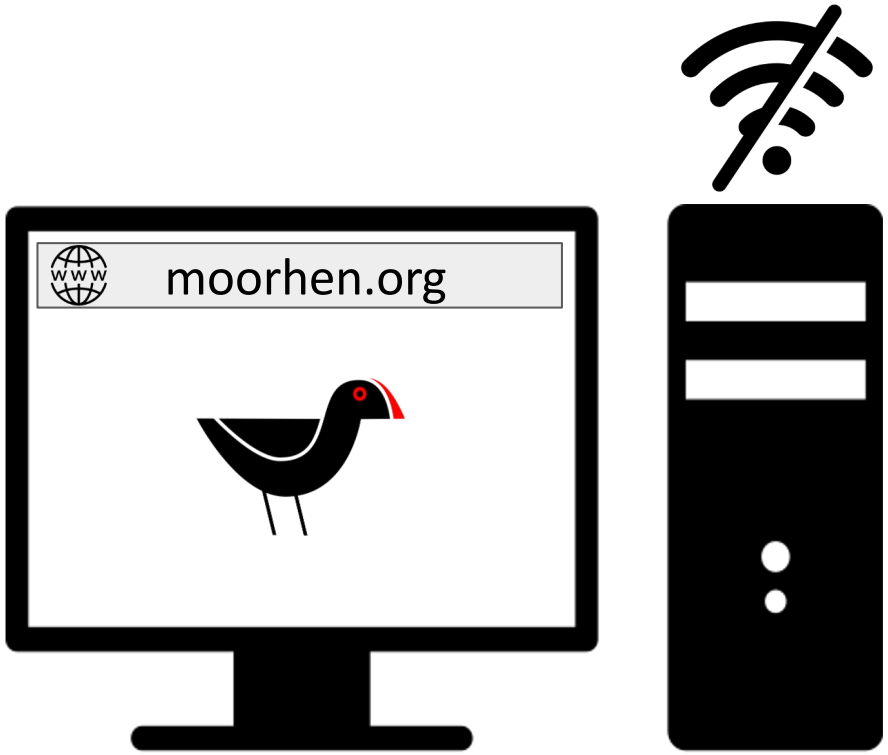
# What is Moorhen?

➔ Moorhen extends libcoot API with a web-based React GUI.



# What is Moorhen?

➔ Moorhen is a client-side-only app. This means **it is 100% private**.



# Current state of Moorhen

- The original motivation of the project was to offer Coot users the ability to use coot in any device at any time. Also having Coot available in CCP4 Cloud without having to have a local CCP4 installation.
- After one year of intense development, Moorhen is now routinely useful in common day-to-day tasks.
- **All “must-have” features set at the start of the project are now available in Moorhen.**

# Current state of Moorhen

## Model Editing Features

- Mutate Residue
- Peptide Flip
- Real Space Refinement
- Auto-fit Rotamer
- JED Flip
- Add Residue
- Check/Delete Waters
- Rotate/Translate Residue
- Delete Item
- Drag Atoms
- Edit Chi Angles
- Fill Sidechain

## Presentation Features

- SSM Superpose
- Map Contouring
- Map and Model colour change
- Env. Distances

## Validation Features

- Rama. Plot
- Unmodeled Blobs
- Density Fit
- Diff. Map Peaks
- Geom. Analysis
- Combined Validation Plot
- Rotamers

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- The original motivation of the project was to offer Coot users the ability to use coot in any device at any time. Also having Coot available in CCP4 Cloud without having to have a local CCP4 installation.
- After one year of intense development, the Moorhen is now routinely useful in common day-to-day tasks.
- All “must-have” features set at the start of the project are now available in Moorhen.

➔ **Moorhen is also intended to be a web-based replacement of CCP4MG**

## Model Editing Features

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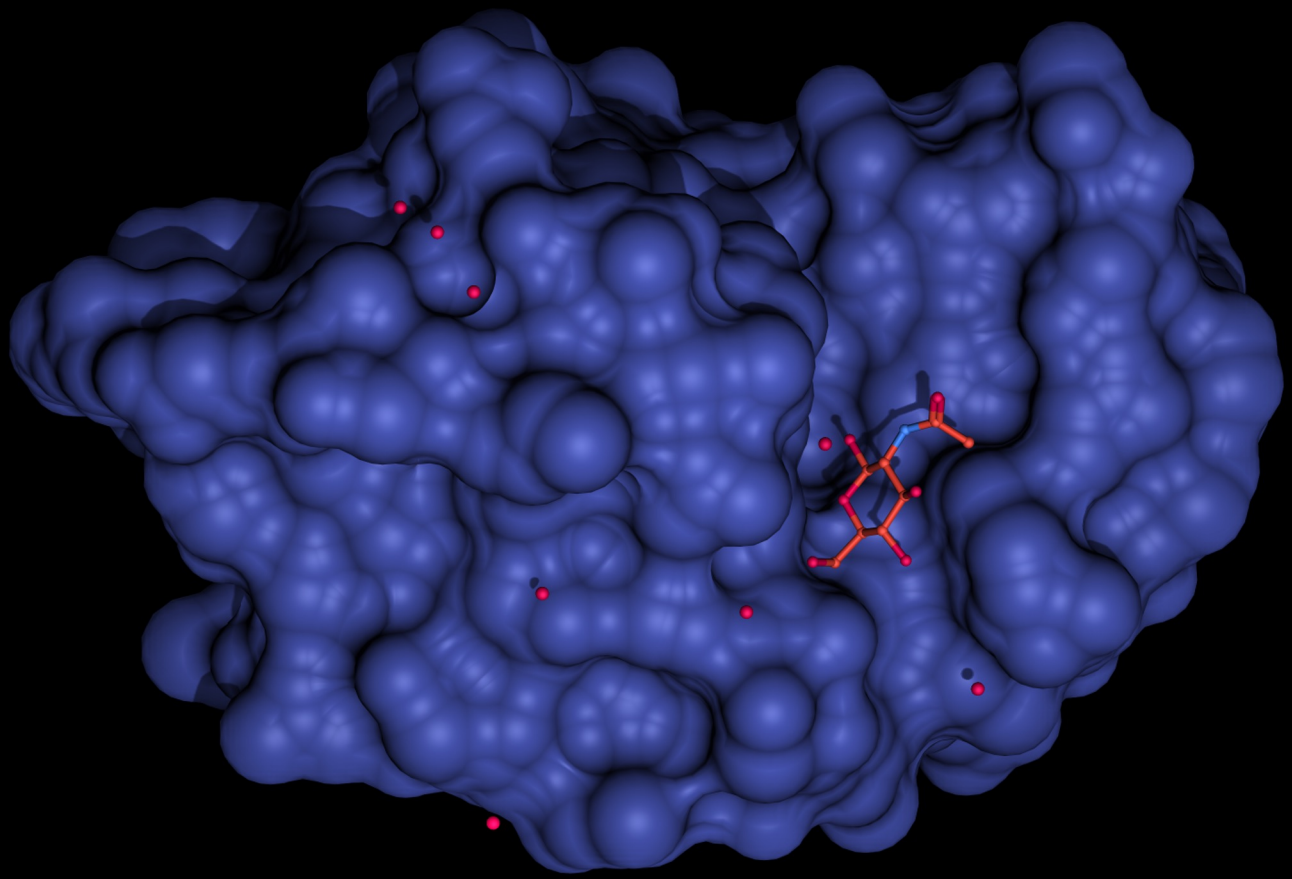
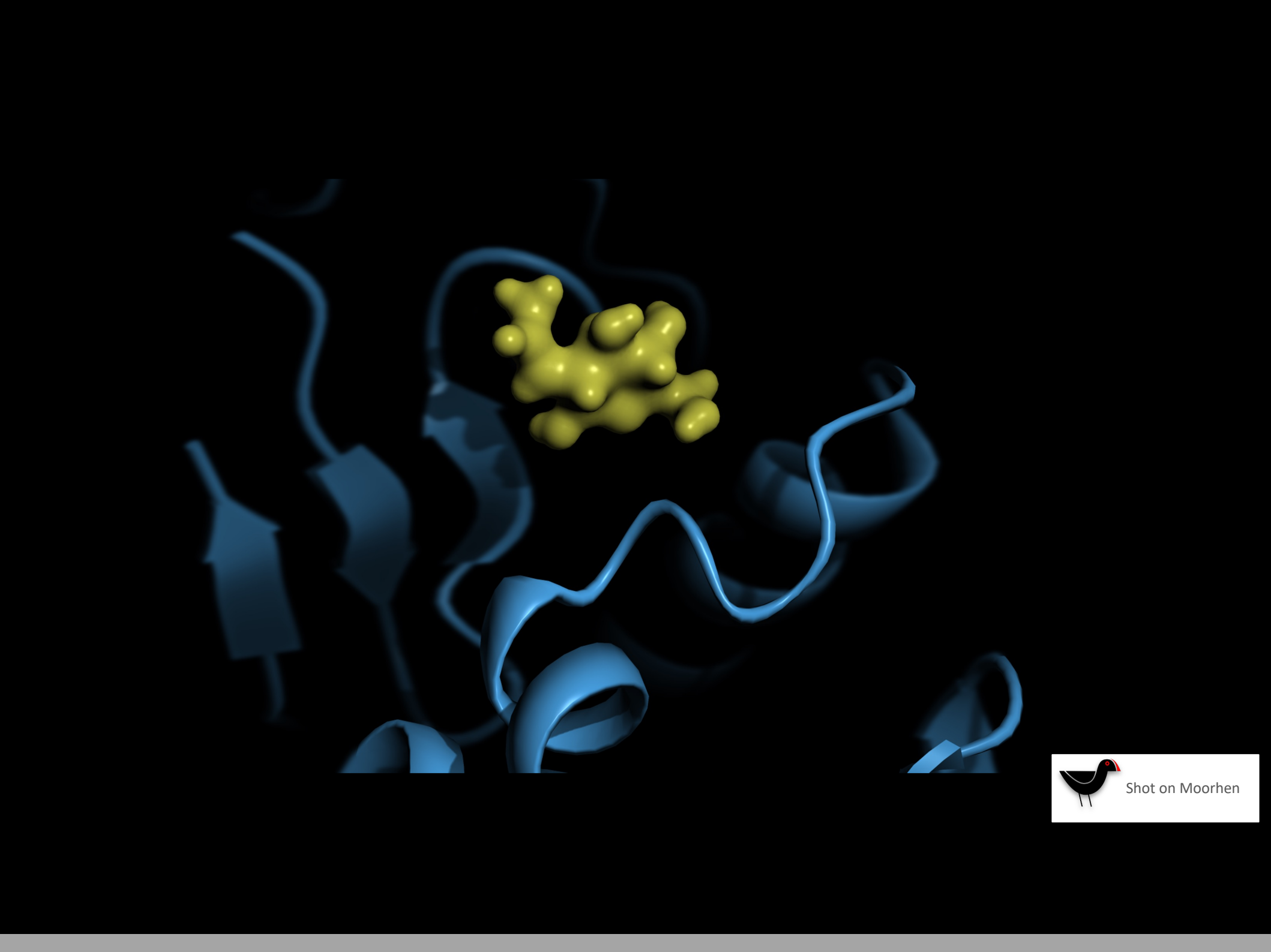
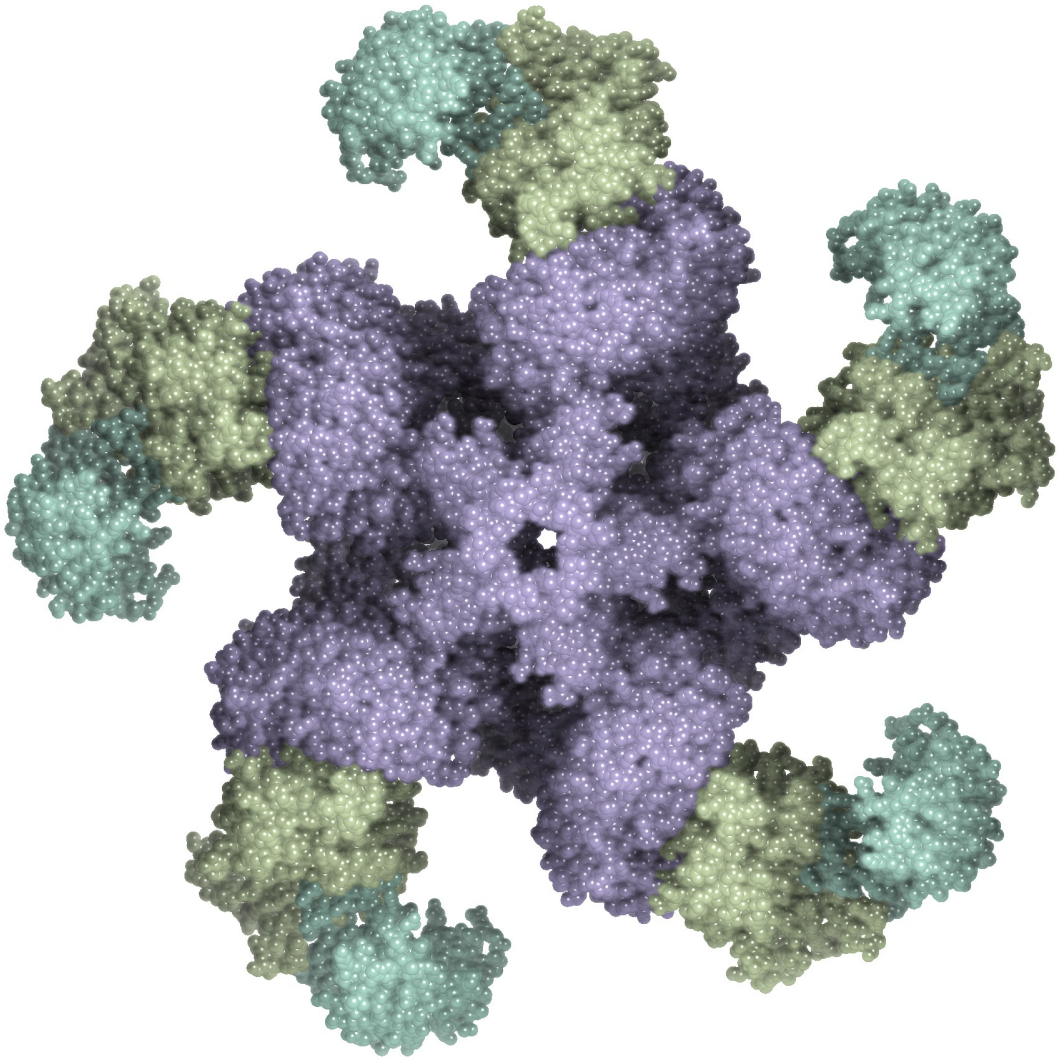
- Density Fit
- Diff. Map Peaks
- Geom. Analysis
- Combined Validation Plot
- Rotamers

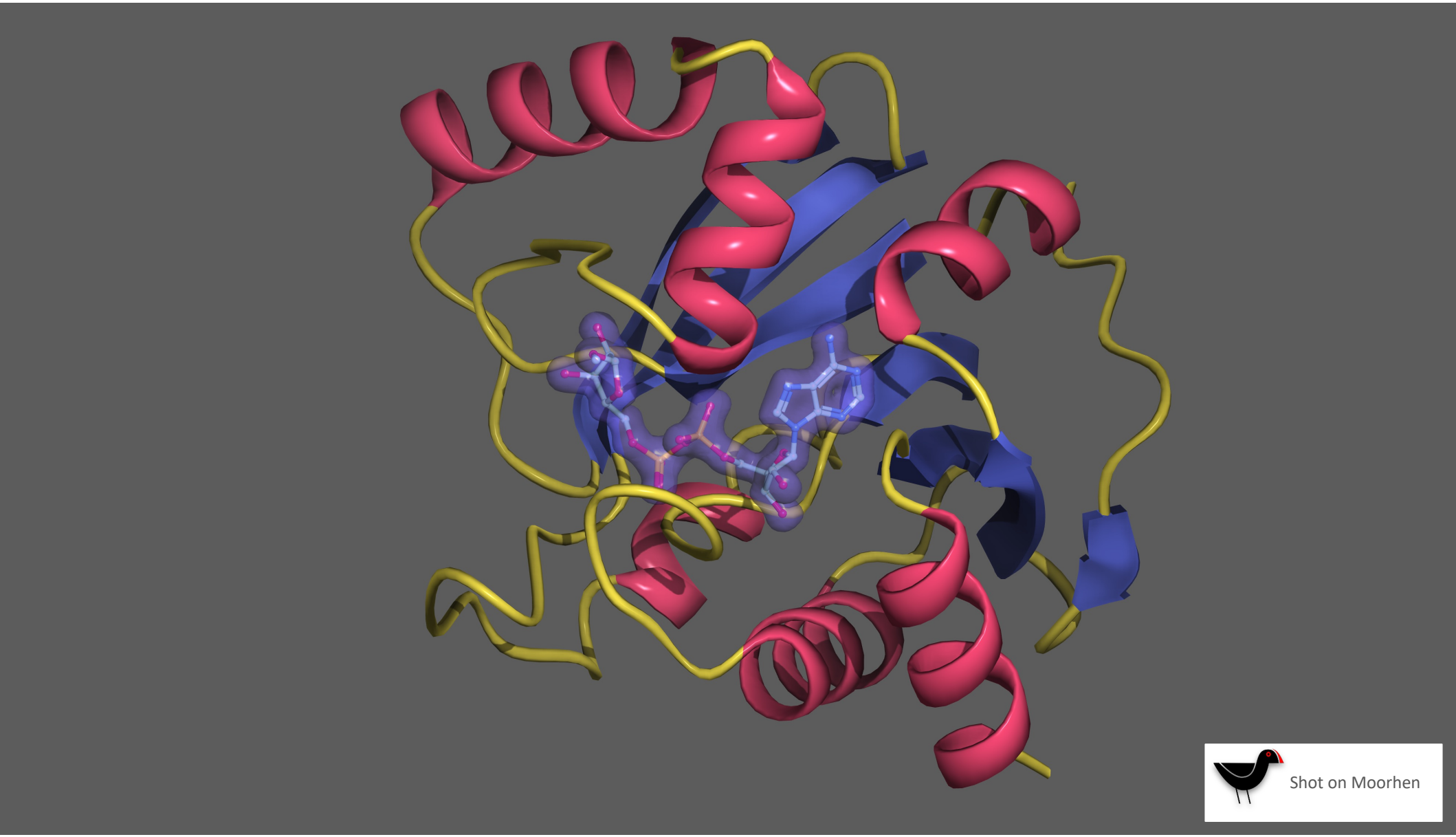
## Figure-Making Features

- Multiple Model Representation Styles
- Arbitrary Colour schemes
- Basic Movie Making
- Shadows
- Depth Blur
- Perspective Projection
- Clipping/Fogging
- Ambient Occlusion
- Screenshots

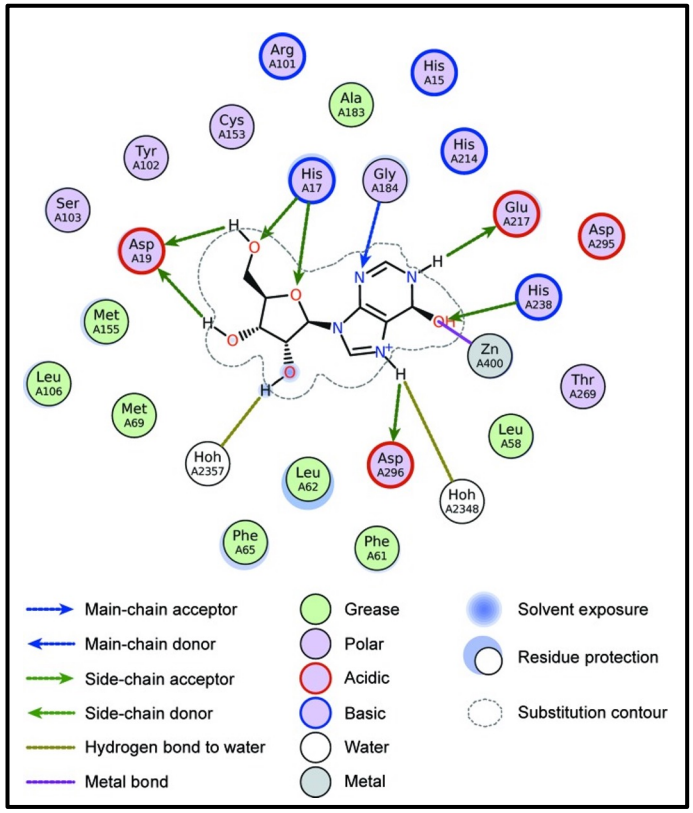



Shot on Moorhen



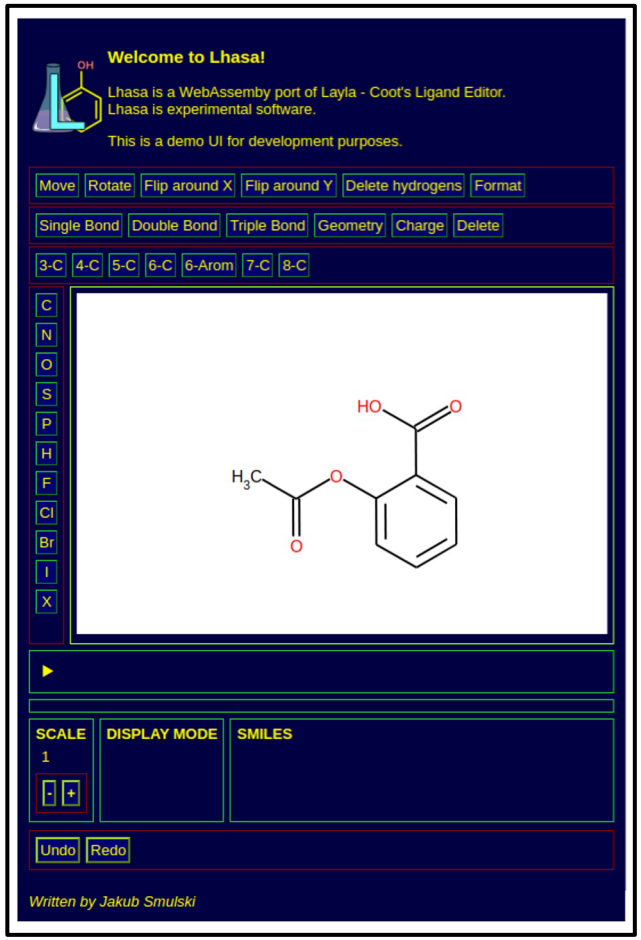

Shot on Moorhen

# Current state of Moorhen – Future work (FLEV)




Source: Emsley P. Tools for ligand validation in Coot. Acta Cryst. D (2017)

# Current state of Moorhen – Lhasa



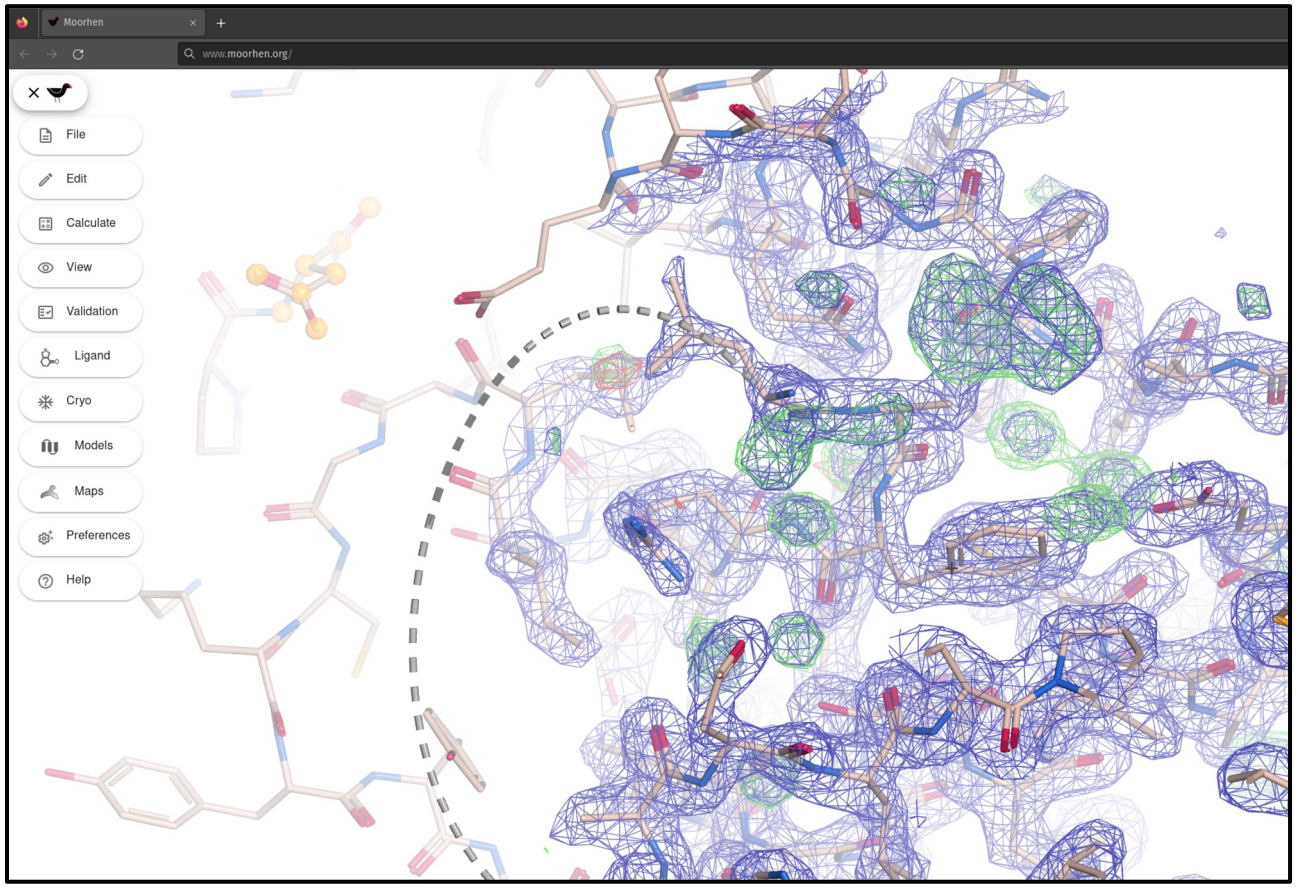

Source: Jakub Smulski

Provide input for dictionary generators:

- elBOW
- AceDRG
- Grade 2

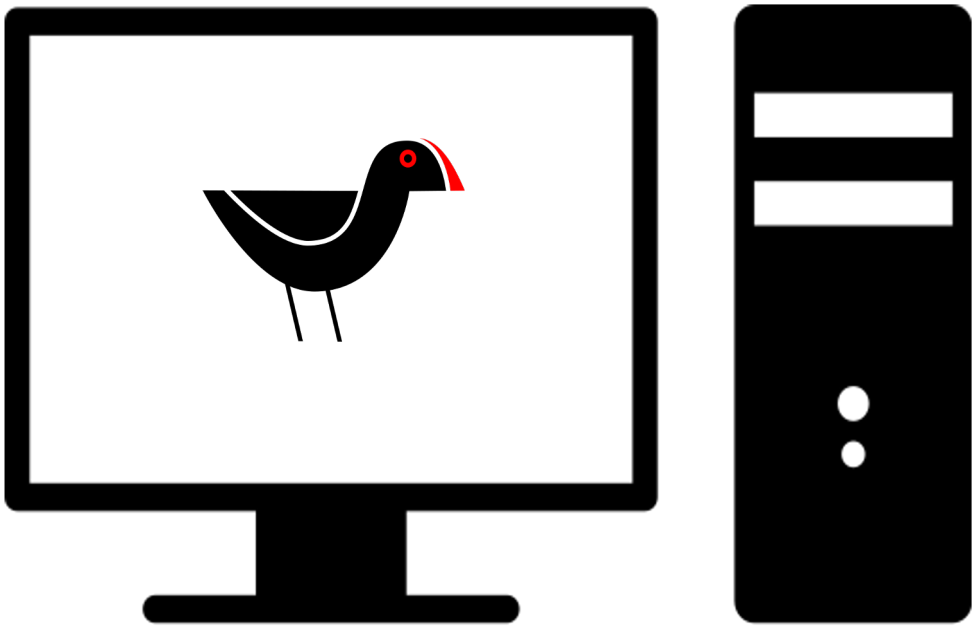
# Where is Moorhen available?

**www.moorhen.org**



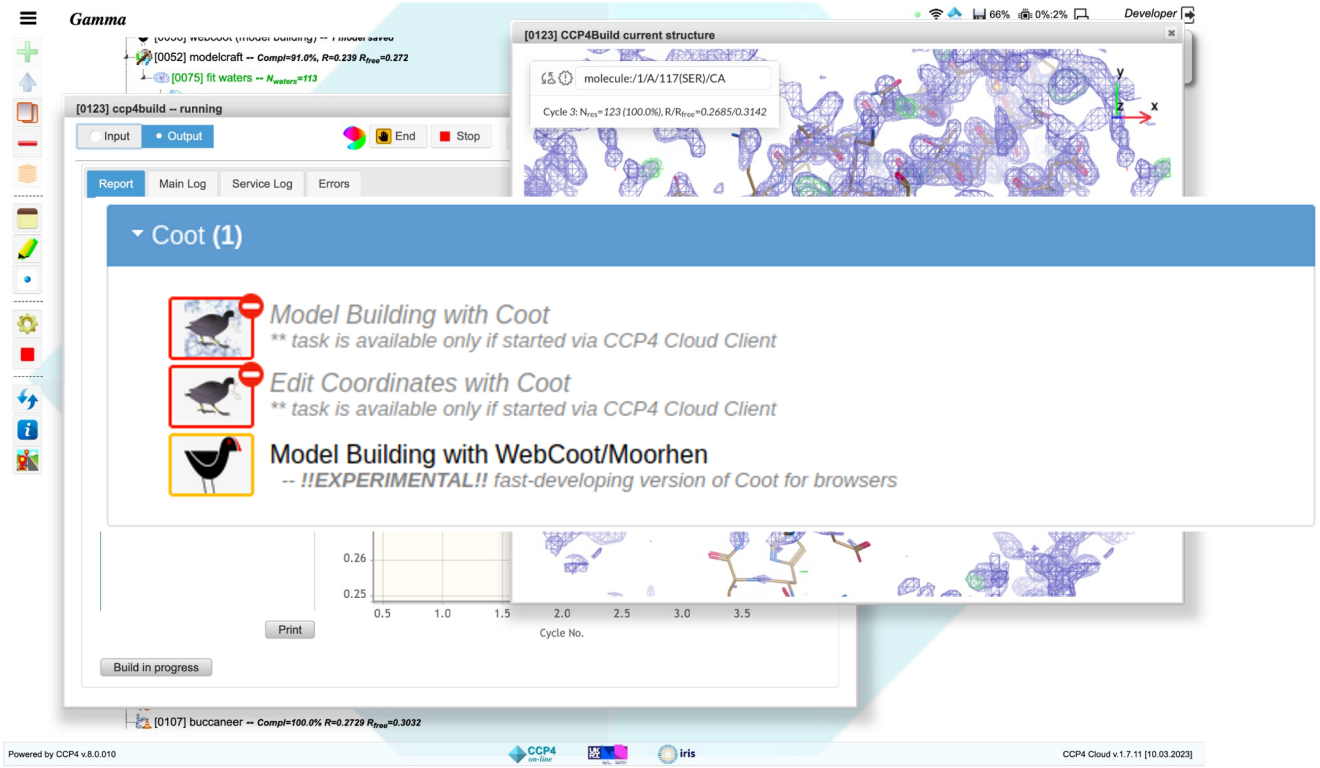
# Where is Moorhen available?

**Electron Desktop App**

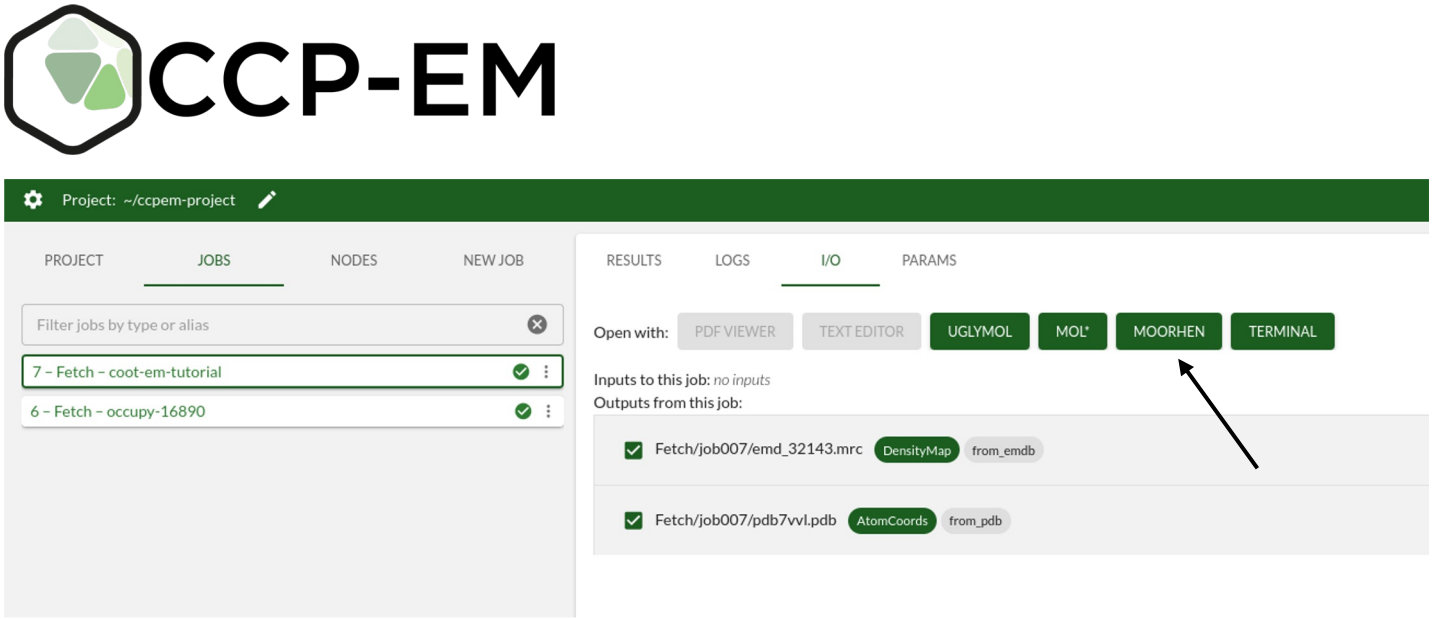


# Where is Moorhen available?

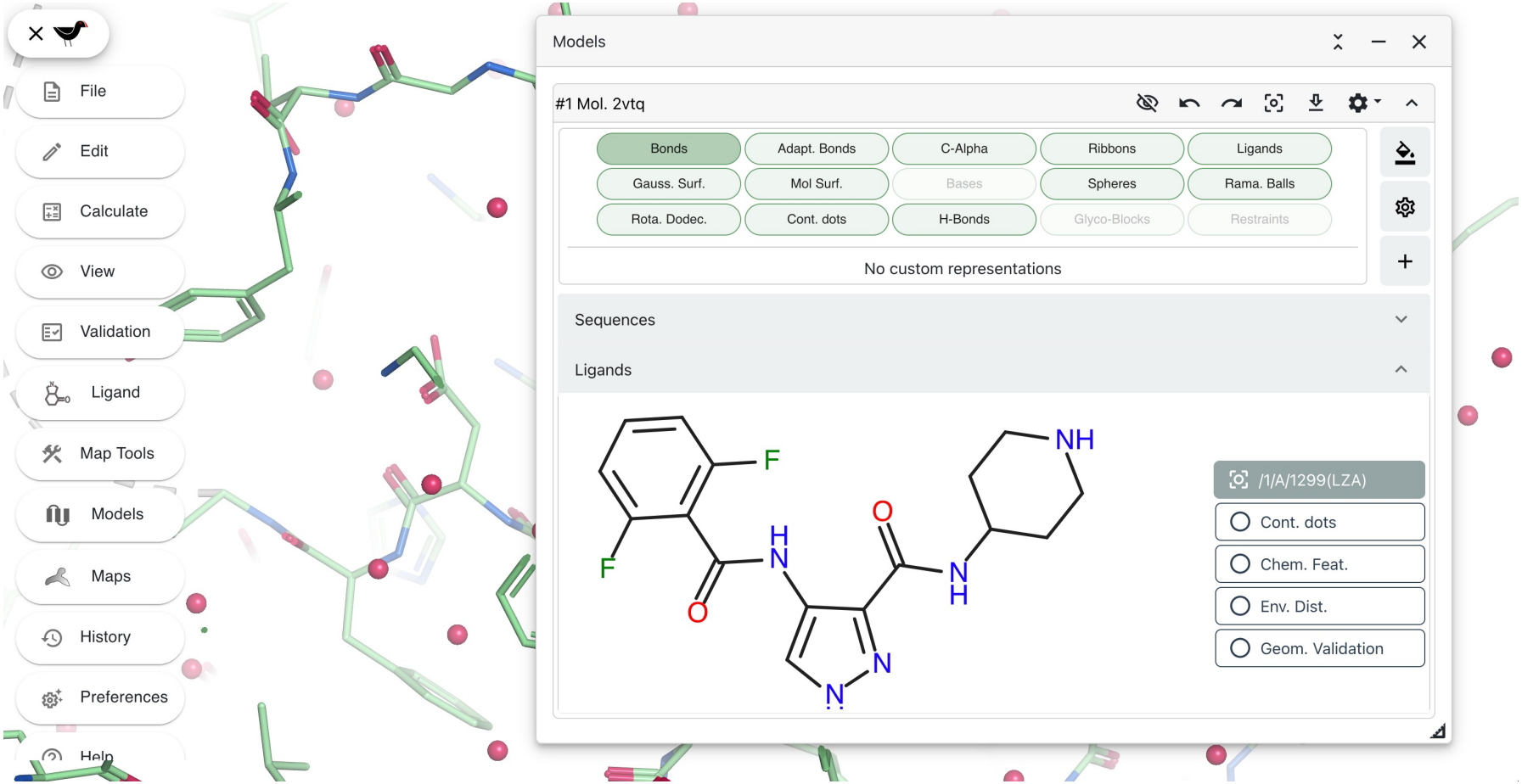
**CCP4 Cloud**



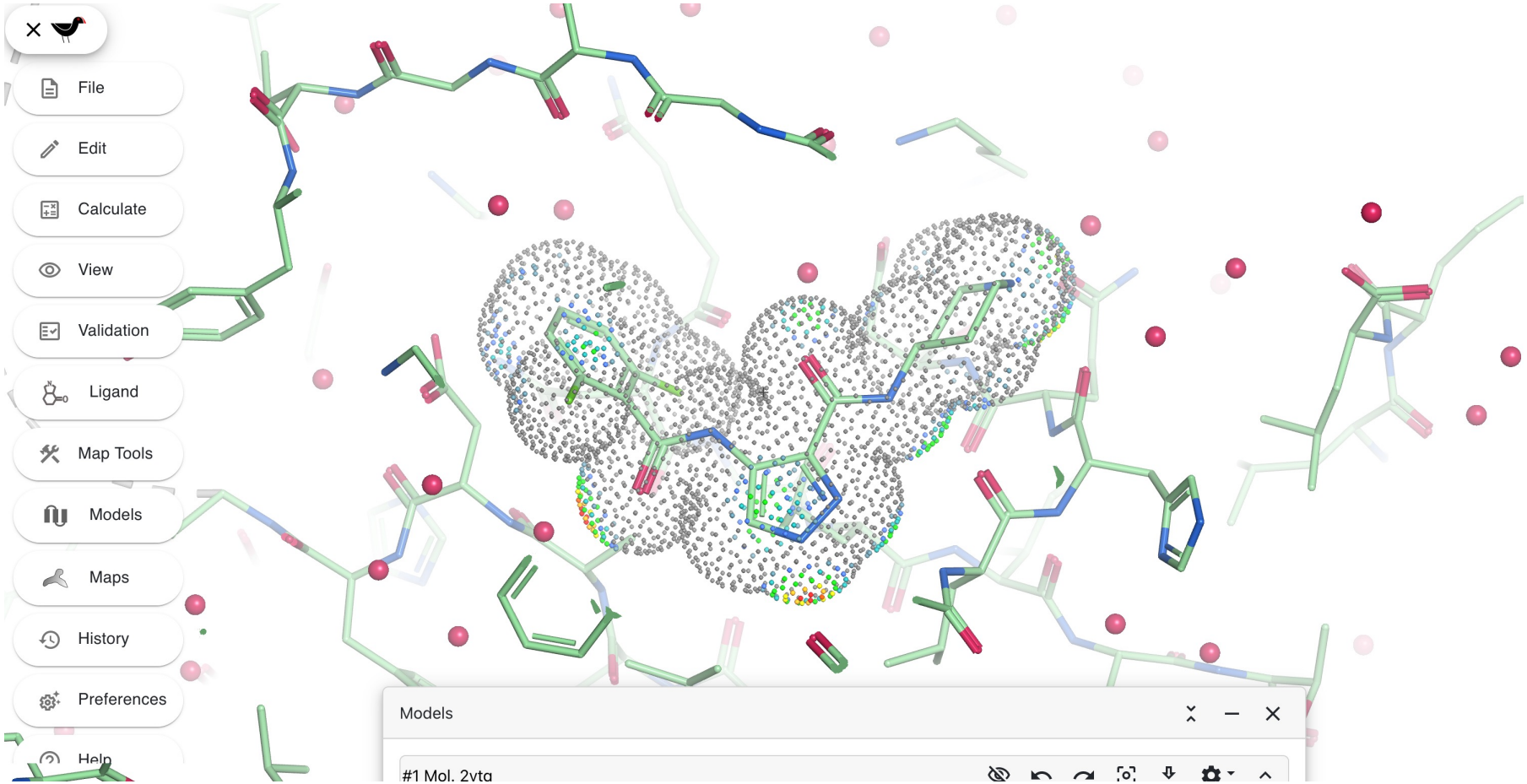
# Where is Moorhen available?



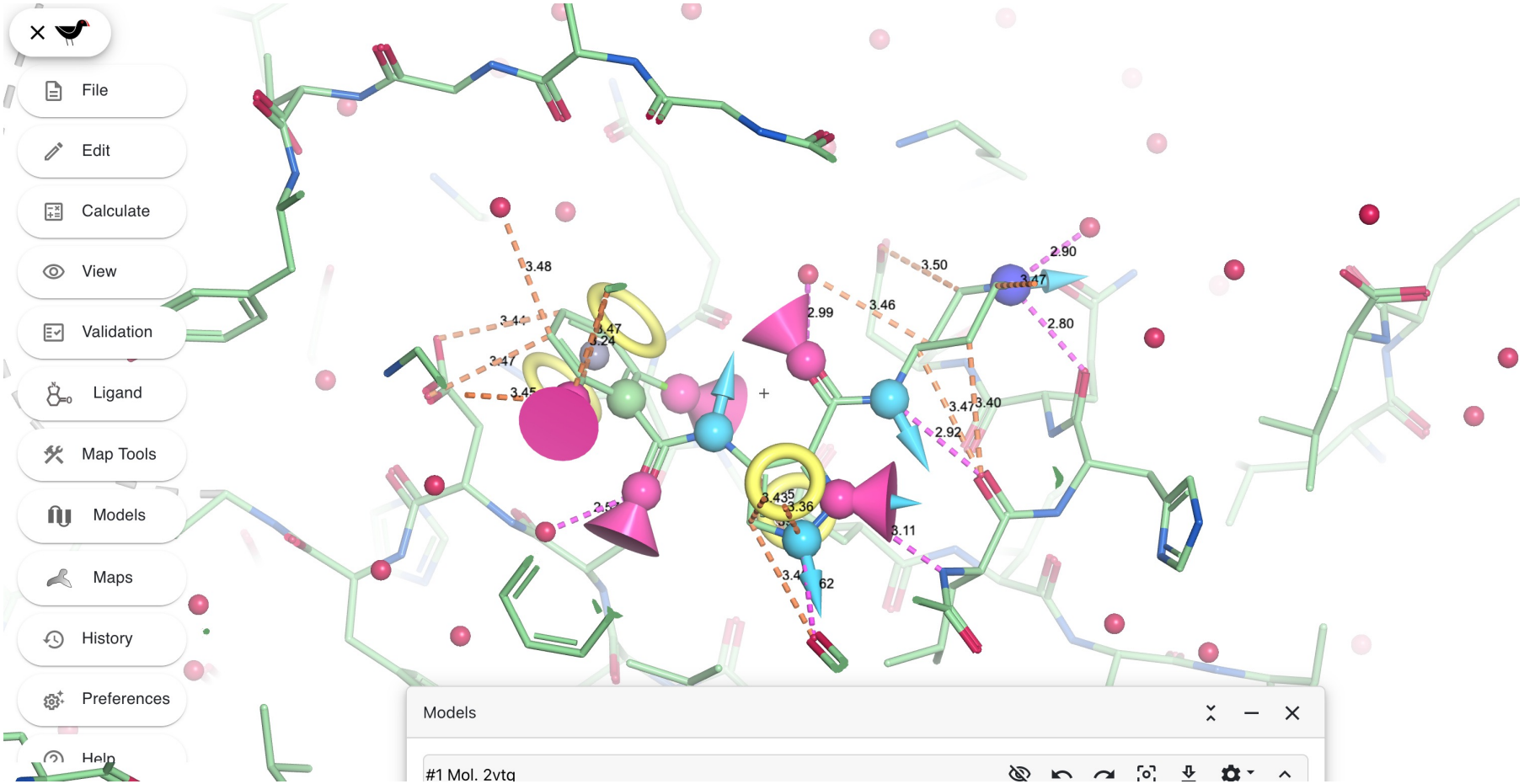
# Moorhen – Ligand validation



# Moorhen – Ligand validation

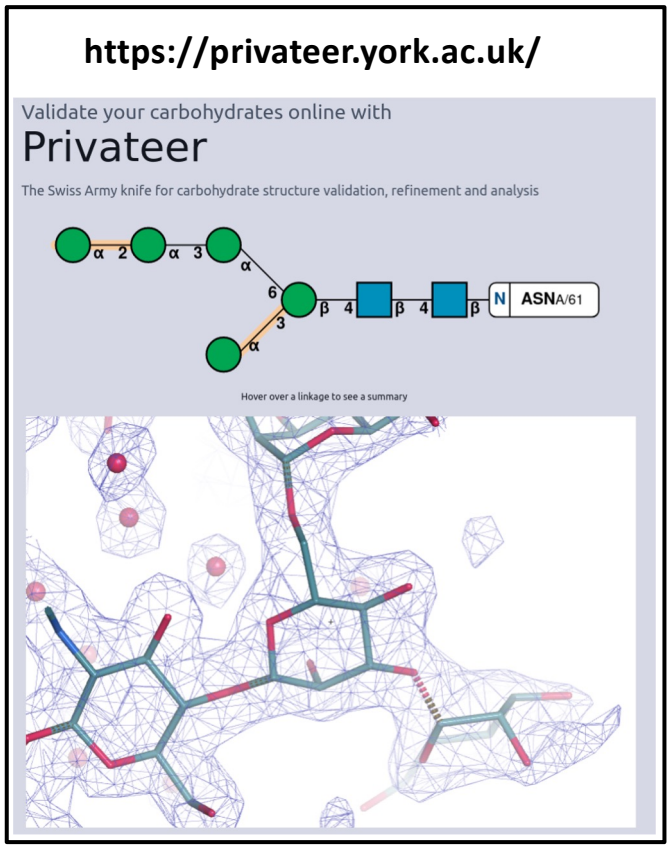


# Moorhen – Ligand validation



# Moorhen as a React component

➔ Moorhen can be easily integrated to any other website to extends its capabilities.




Source: Dialpuri J. et al., (2024). Online carbohydrate 3D structure validation with the Privateer web app. (Manuscript submitted for publication)

# GitHub

https://github.com/moorhen-coot/Moorhen

## Moorhen

npm package 0.8.5 | Nightly tests failing | Deploy moorhen.org passing | Dev docs passing | Wiki passing

Moorhen is a web browser molecular graphics program based on the Coot desktop program. It is developed by porting some CCP4 libraries and programs, Coot, FFTW2, Privateer and the Gnu Scientific Library to Web Assembly.

The emscripten suite of tools is required to do the compilation.

The sources of CCP4, Coot, Privateer, FFTW, and GSL are not included. They are downloaded and (possibly) patched by the running the `get_sources` script, which is part of the build process of this project.

The following libraries/programs are compiled to Web Assembly:

- libccp4 (8.0.0)
- clipper (20240123)
- ssm (1.4.0)
- mmdb2 (2.0.22)
- gemmi 0.6.4
- Coot 1.0 ('gtk3' git branch)
- fftw 2.1.5
- gsl 2.7.1
- Boost 1.83.0
- glm 0.9.9.8
- RDKit 2023_09_1

Moorhen is available to use at https://moorhen.org.

https://moorhen-coot.github.io/wiki/

Moorhen Wiki

### Posts

Nov 3, 2023
Creating Figures with Moorhen

Nov 2, 2023
Fetch data from Moorhen in your React app

Jul 6, 2023
Using Moorhen in a react app

Apr 16, 2023
Moorhen Tutorial 1: Fix up the Cyclin-Dependent Kinase

## Moorhen mailing list:

https://groups.google.com/a/york.ac.uk/g/moorhen-group

# Acknowledgements


Filo Sanchez

Stuart McNicholas

Paul Emsley

Eugene Krissinel

Jakub Smulski

Martin Noble

... And everyone who has contributed to CCP4



lucrezia@mrc-lmb.cam.ac.uk

@lulu_catapano