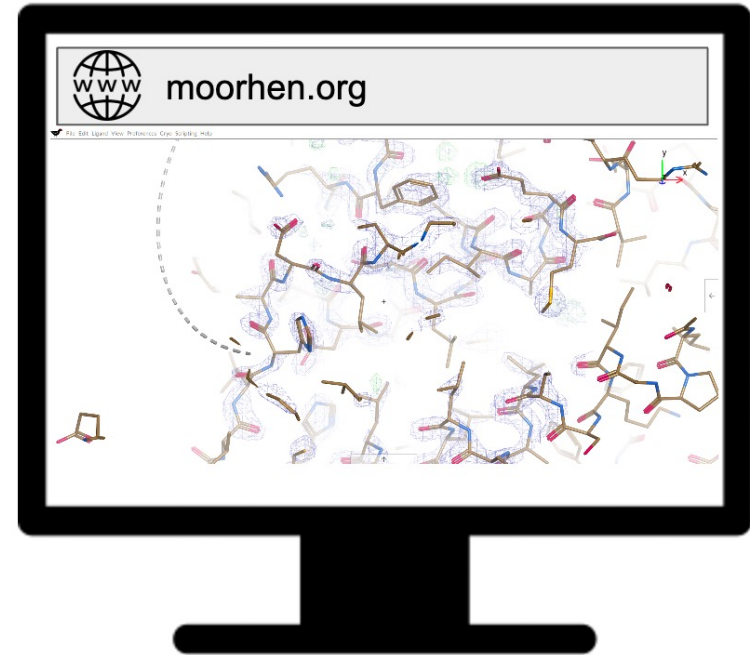
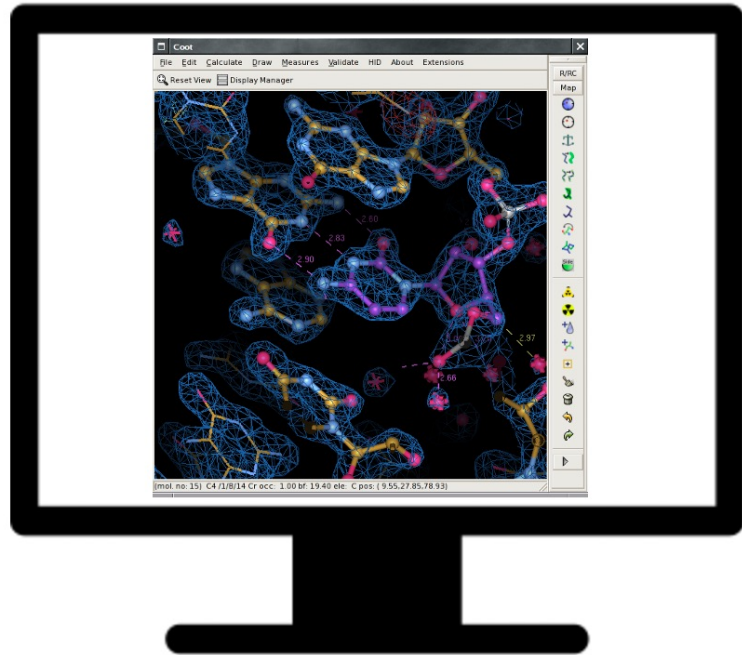


Coot and Moorhen

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”



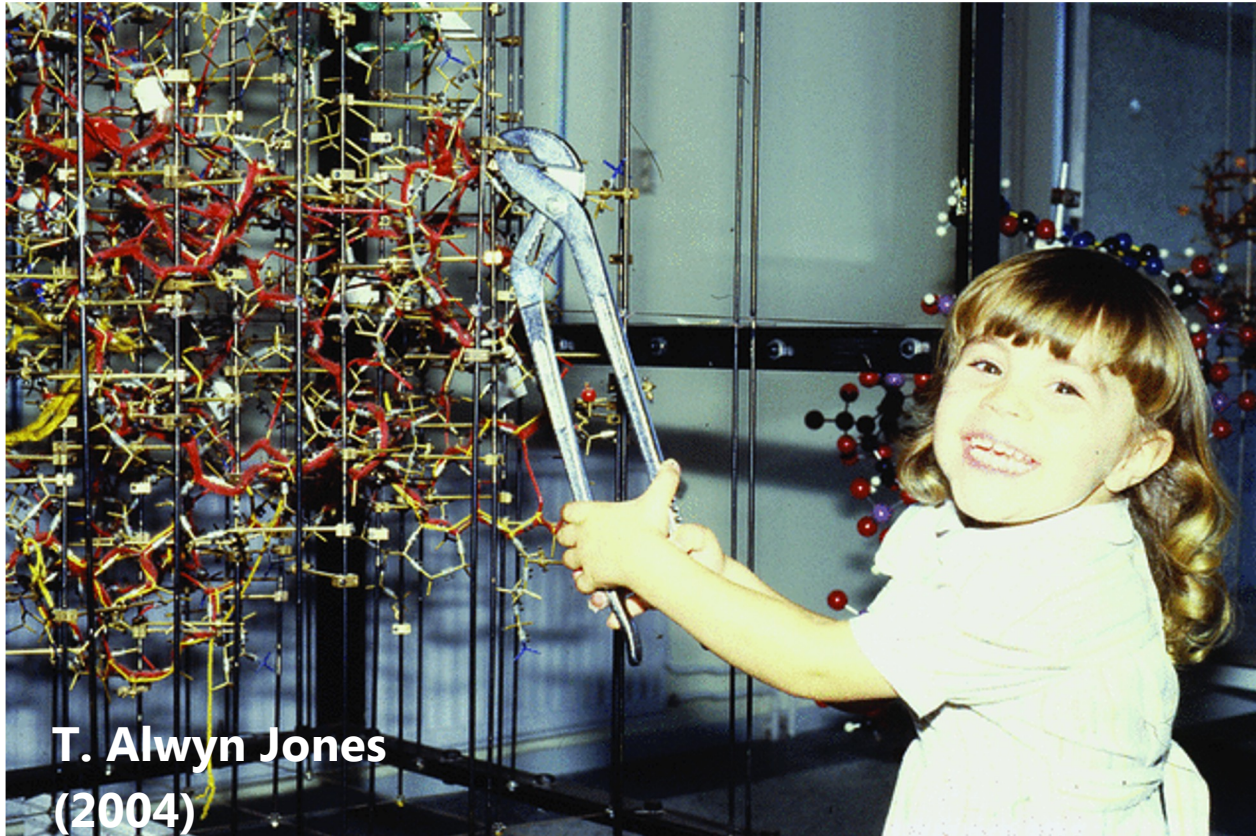
DCH building the first insulin model



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.

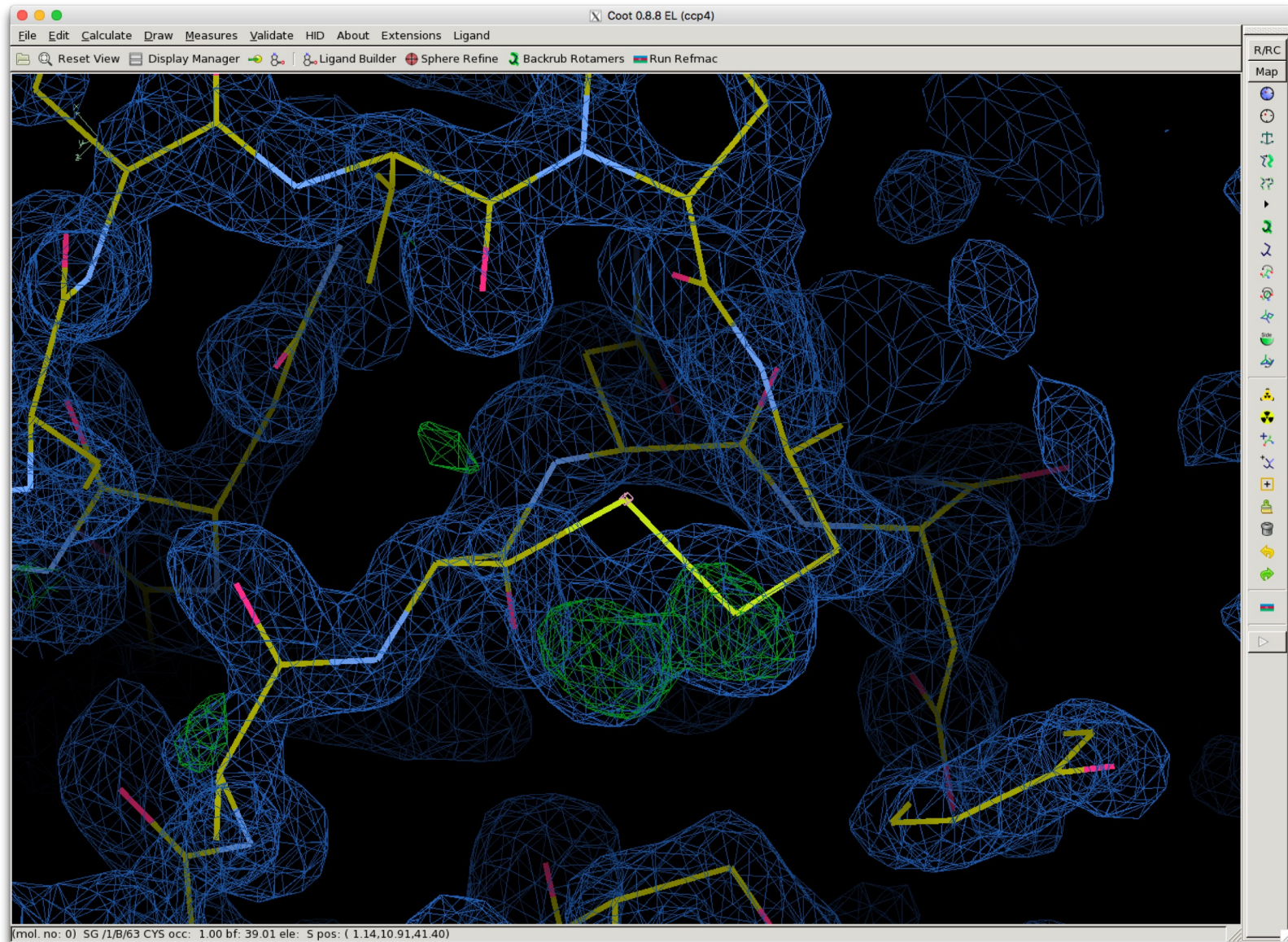
**Using Coot is not like this:
Coot fitting tools are fast and automated**

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 (Molprobability), EBI, EDS, Povray... and others

Fixing what auto-building doesn't get right

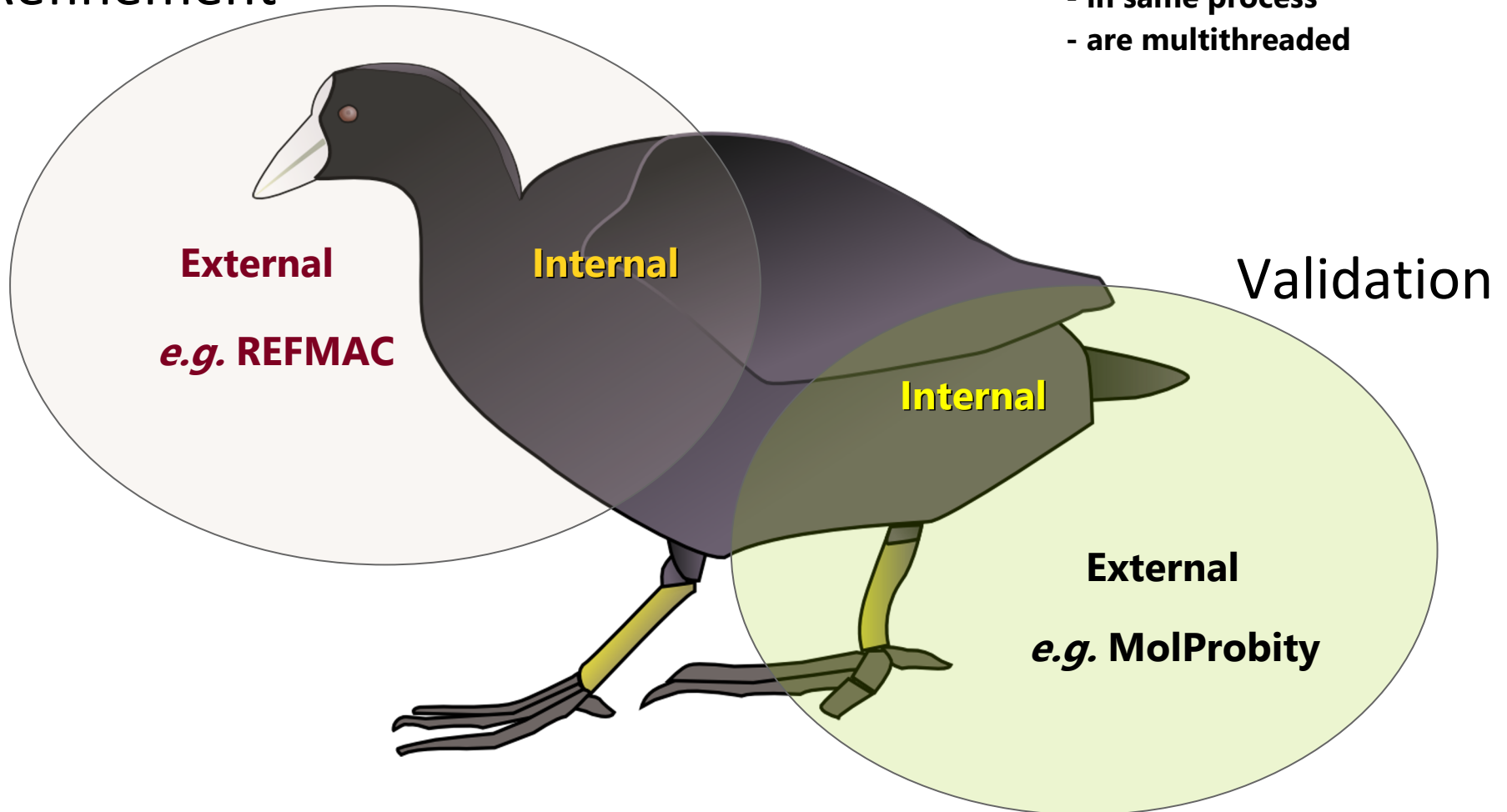


Feature Integration

Refinement

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 expedites 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

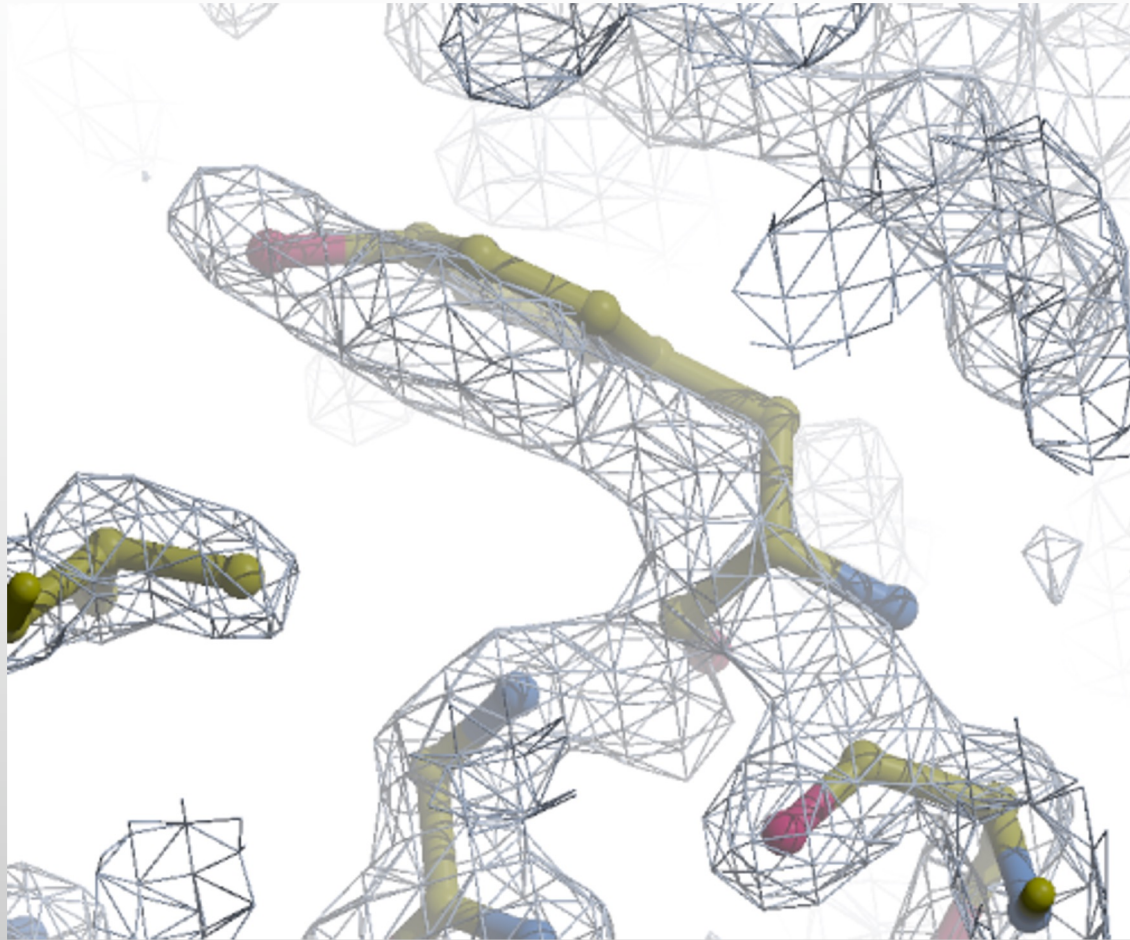
```
data_comp_list
loop_
  _chem_comp.id
  _chem_comp.three_letter_code
  _chem_comp.name
  _chem_comp.group
  _chem_comp.number_atoms_all
  _chem_comp.number_atoms_nh
  _chem_comp.desc_level
ATP      ATP      "ADENOSINE-5'-TRIPHOSPHATE"      NON-POLYMER      43      31      .
loop_
  _chem_comp_bond.comp_id
  _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'"      "H03'"      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'"      "H02'"      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
```

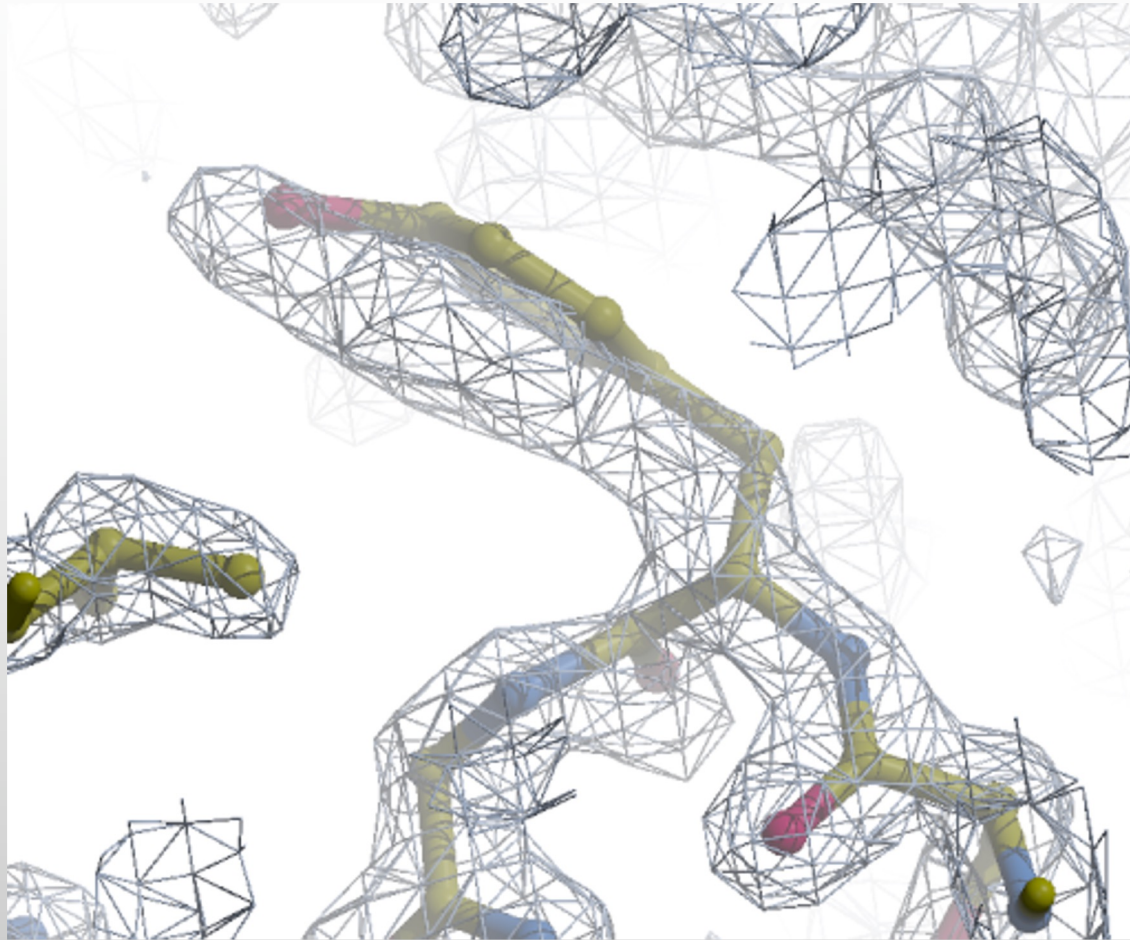
APPENDIX A

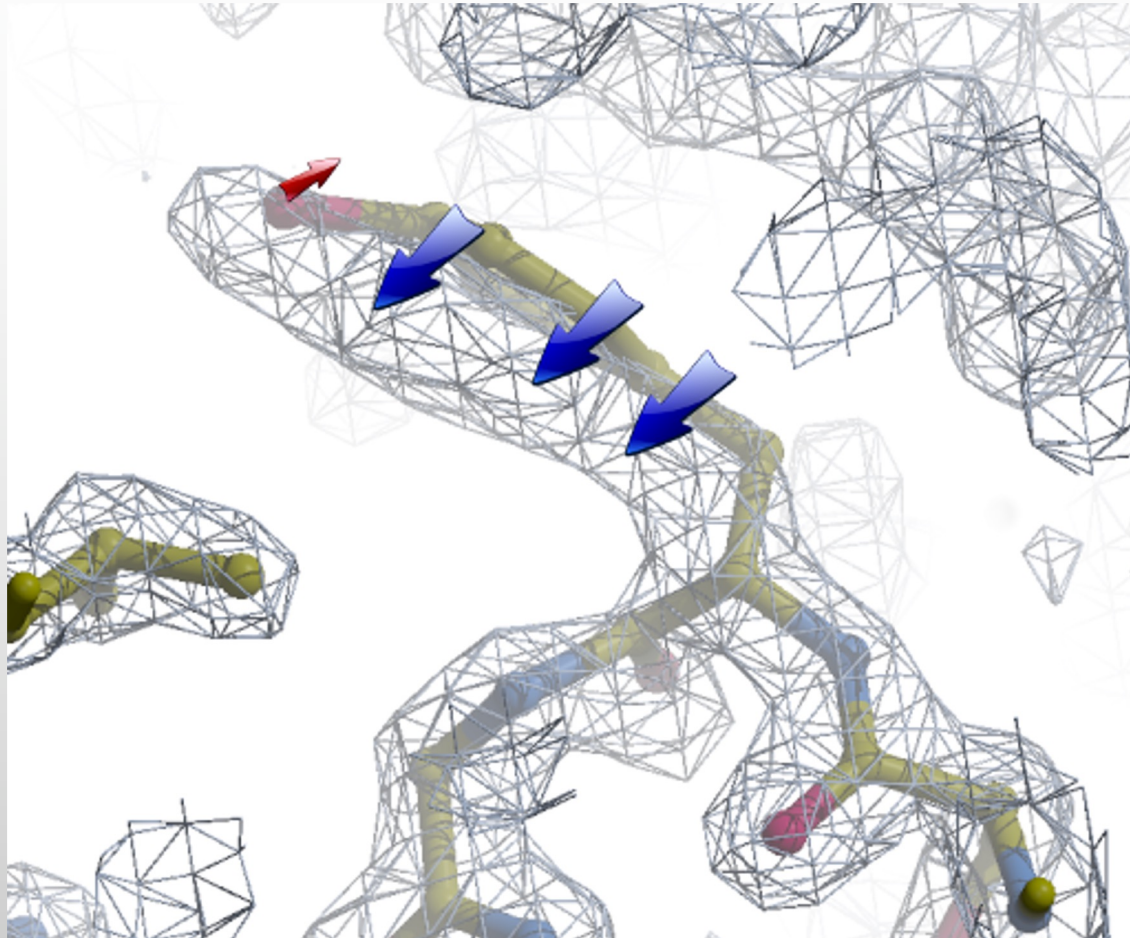
Regularization and refinement derivatives

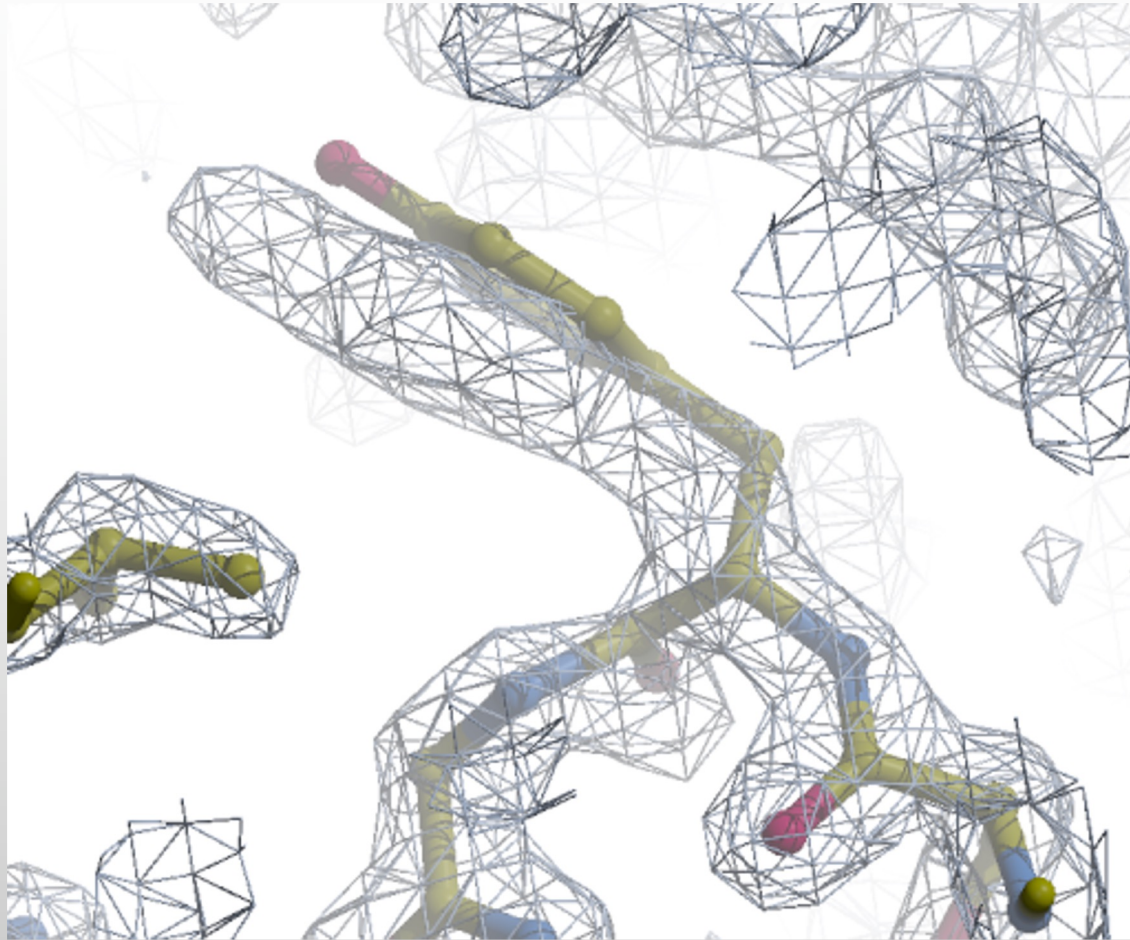
The function that we are trying to minimize is S , where

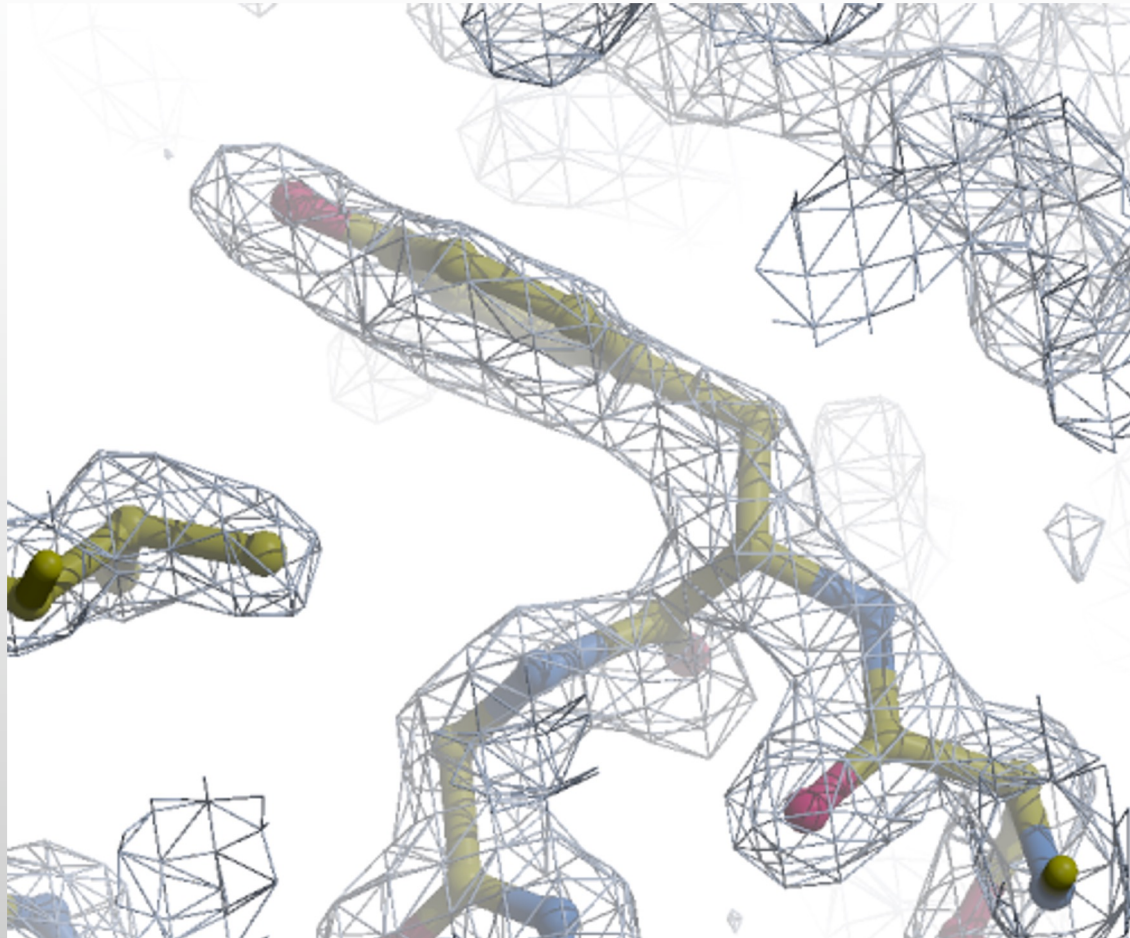
$$S = S_{\text{bond}} + S_{\text{angle}} + S_{\text{torsion}} + S_{\text{plane}} - S_{\text{density}}$$

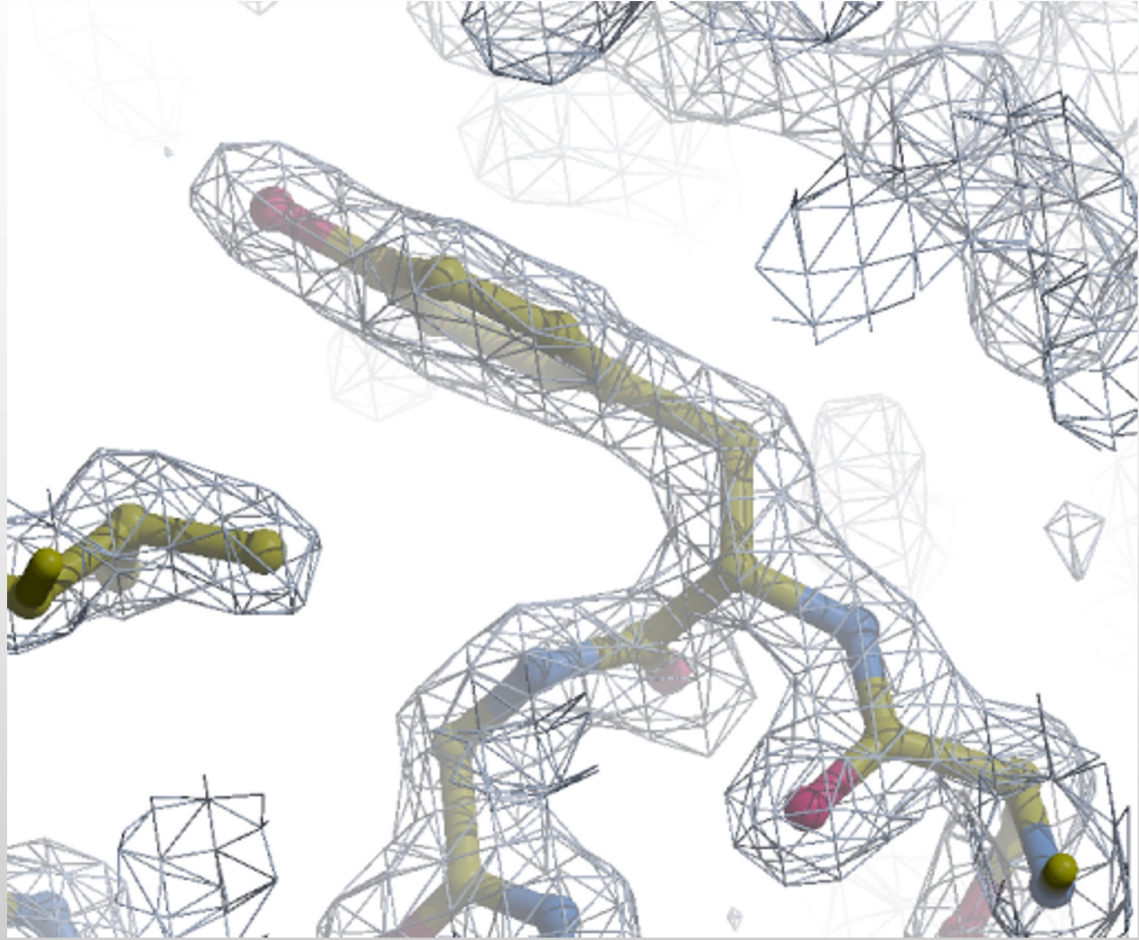












Representation of Results:

```
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

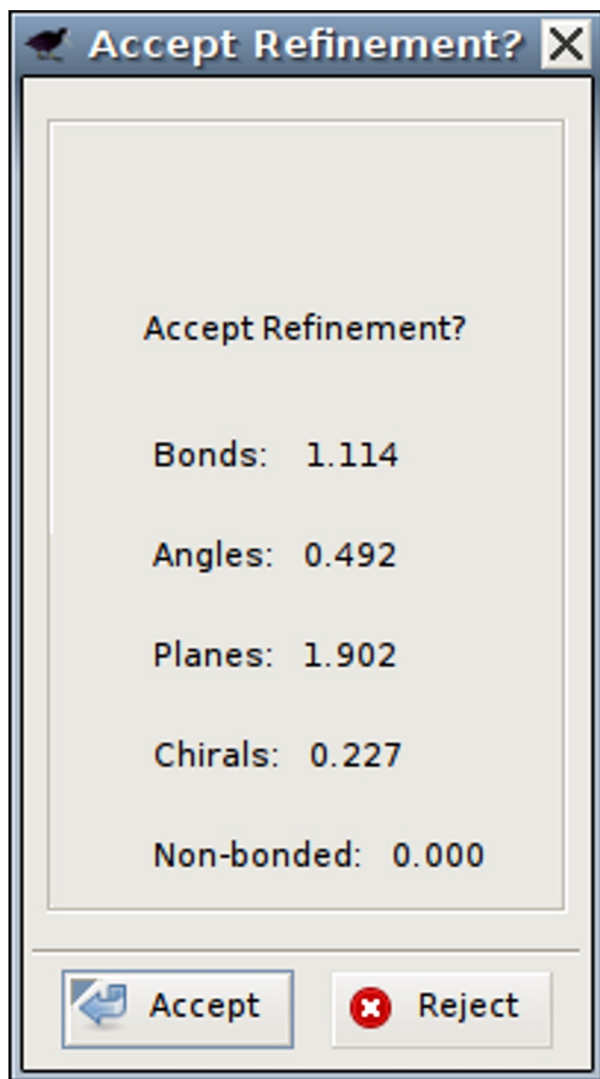
      INFO:: [spec: "A" 45 "" ] [spec: "A" 46 "" ] link_type :TRANS:
      INFO:: [spec: "A" 45 "" ] [spec: "A" 44 "" ] link_type :TRANS:
Link restraints:
  2 bond    links
  6 angle   links
  4 plane   links
Flanking residue restraints:
  4 bond    links
 12 angle   links
  8 plane   links
INFO:: made 668 non-bonded restraints
initial distortion score: -16033.2
      Initial Chi Squares
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...

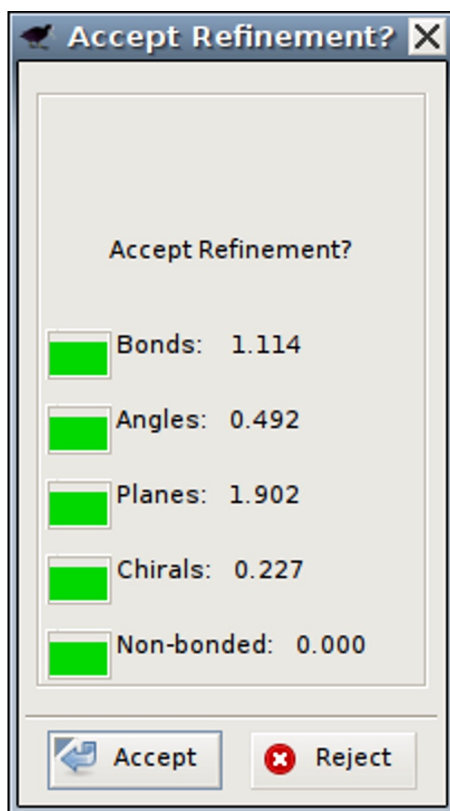
Student Reaction:

"Oh, box of meaningless numbers.

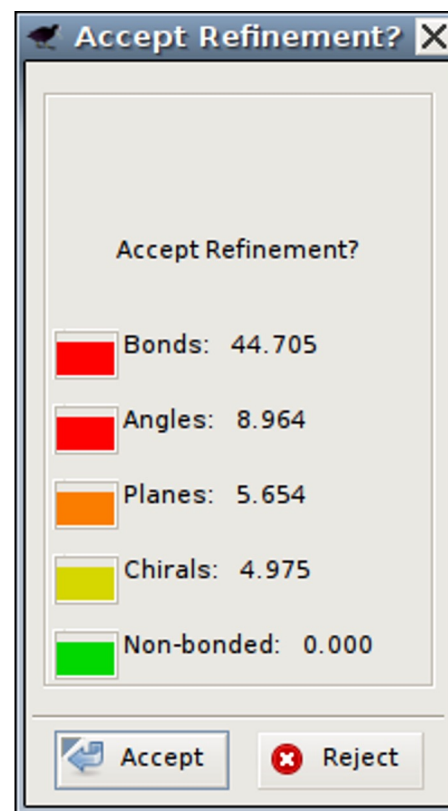
Go away"

Representation of Results: “Traffic Lights”

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

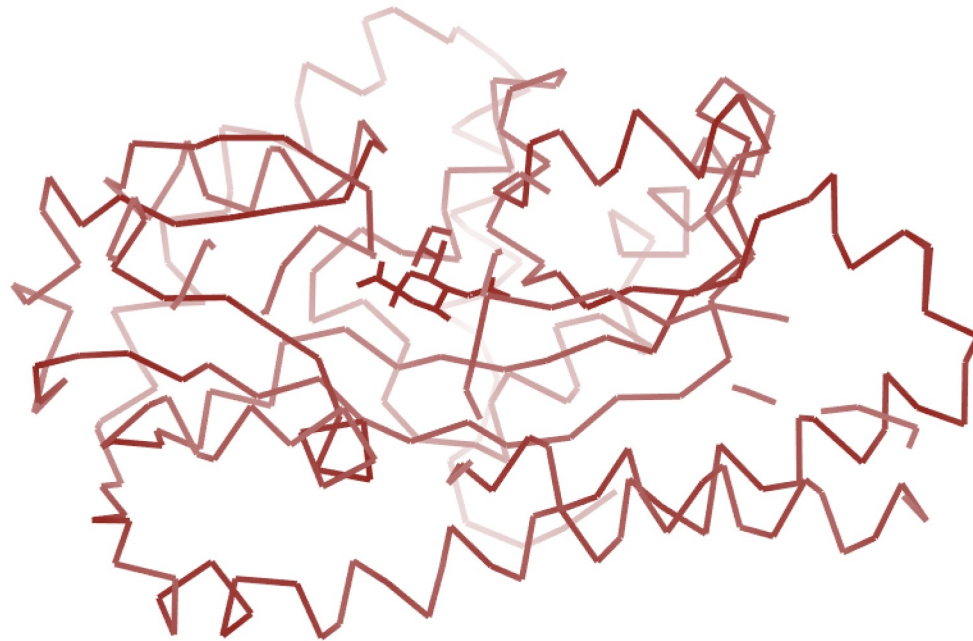


Good refinement



Bad refinement

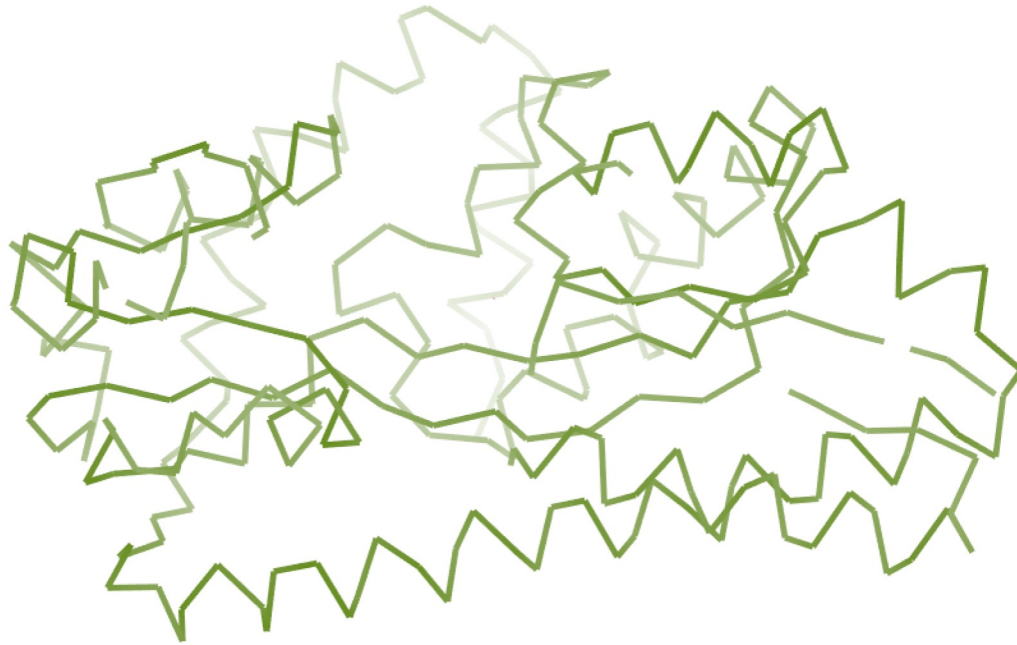
Local Distance Restraints: Prior Structure



■ Model for High Resolution data

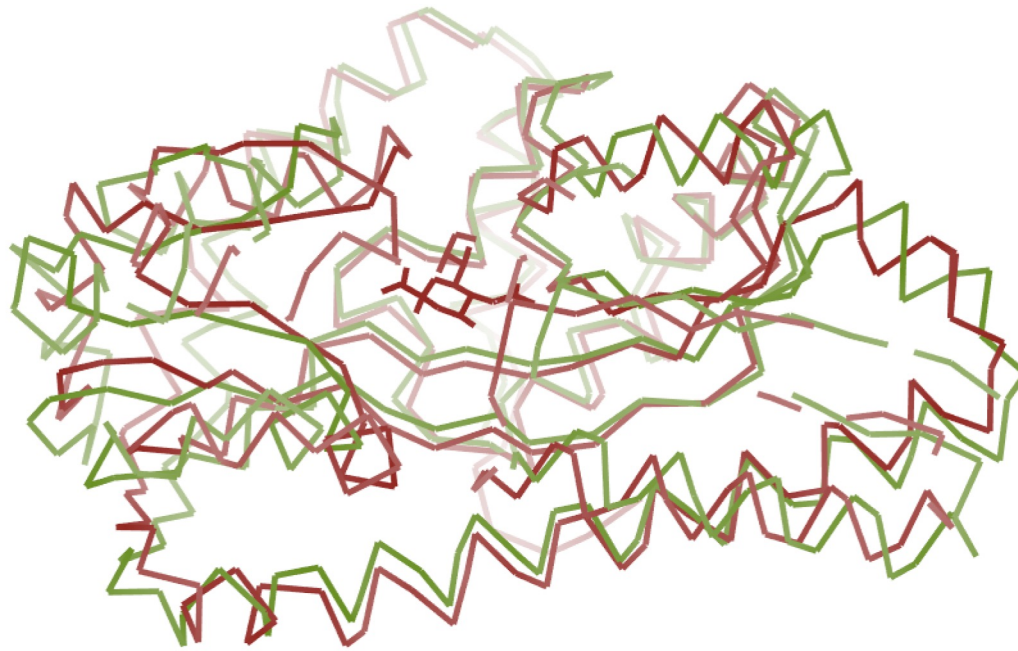
PDB code: 3b50, 1.4 Å

Local Distance Restraints: Today's Structure



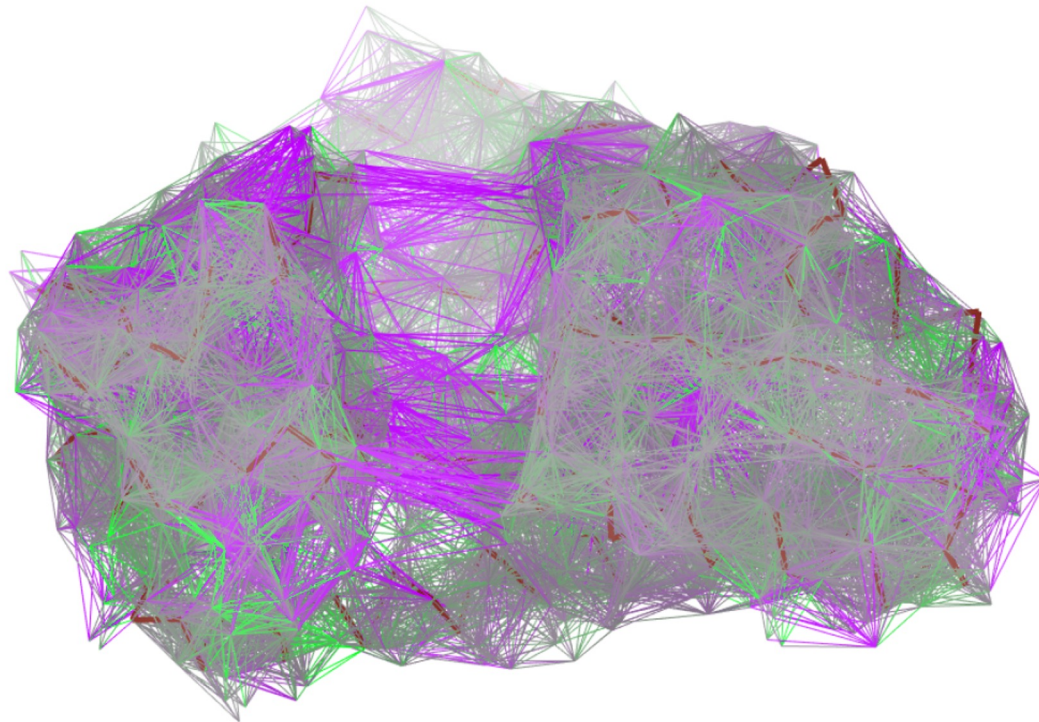
 Model for Low Resolution data

Local Distance Restraints: Structure Comparison



- Model for High Resolution data
- Model for Low Resolution data

Local Distance Restraints: ProSMART/Geman McClure Restraints



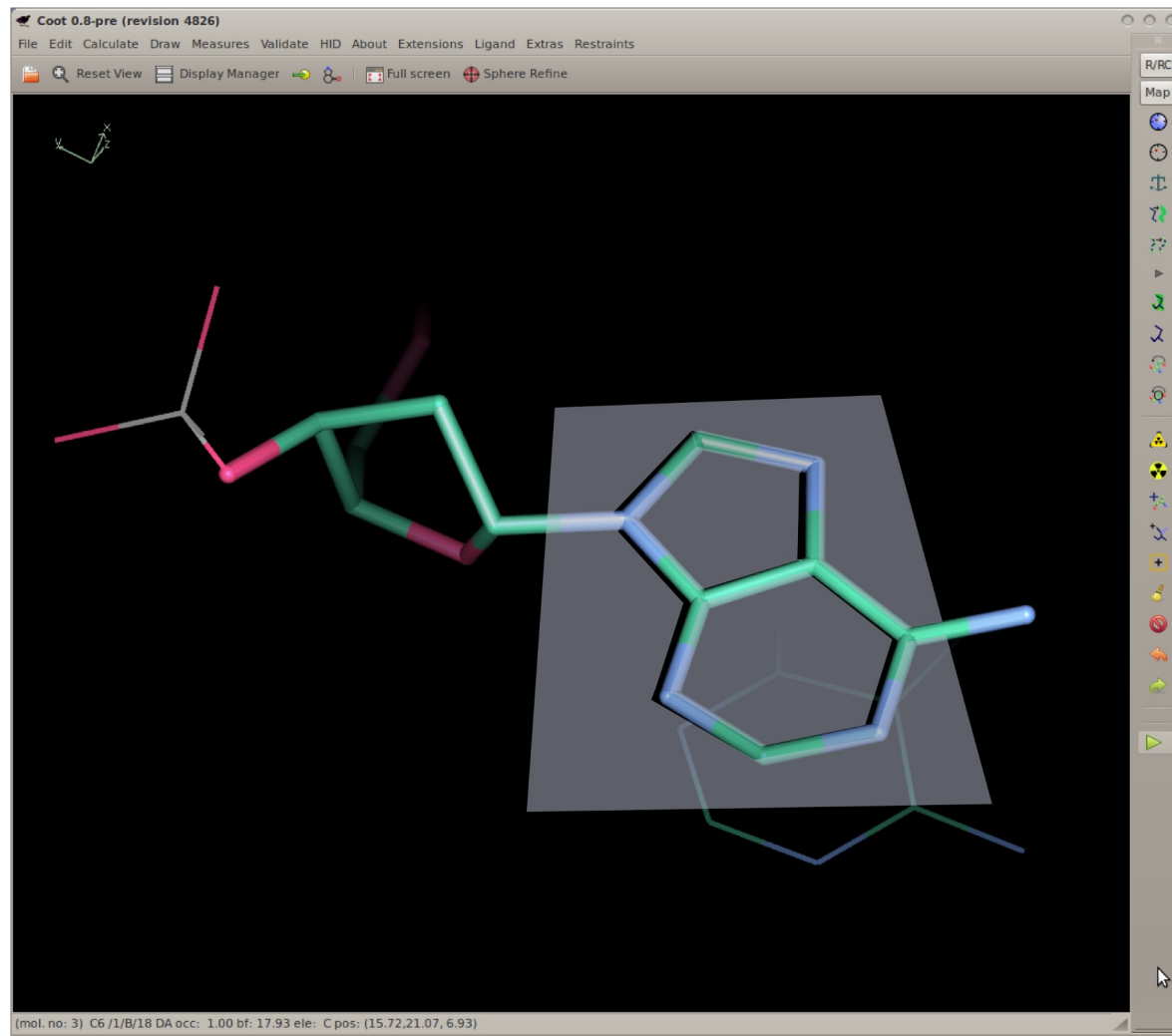
- Longer than in prior
- Shorter than prior

ProSMART integration

ProSMART generates distance restraints from homologous structures

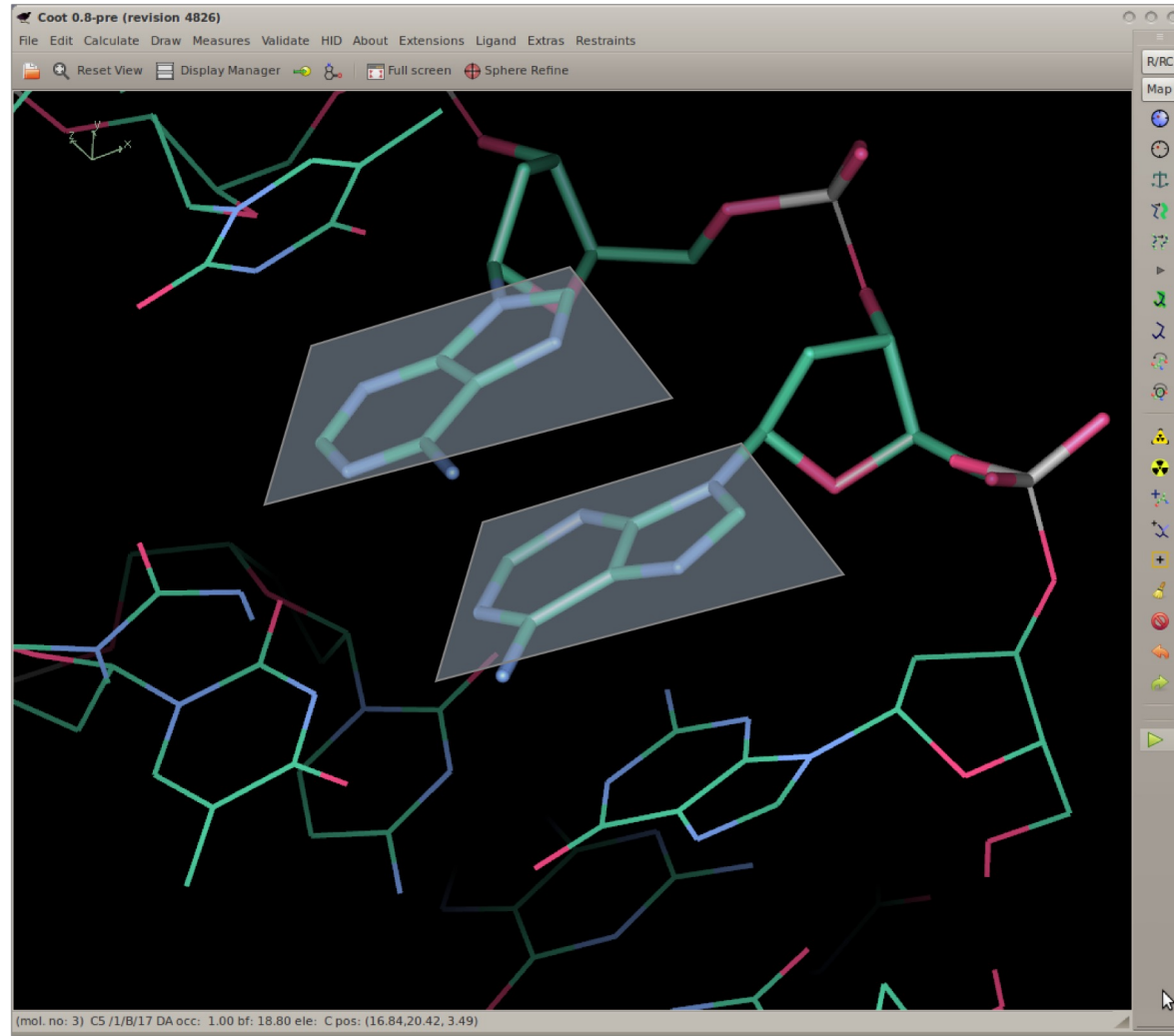
- to be applied to current model for refinement
- now available in Coot

Nucleic acid: Plane Restraints



Derivatives
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

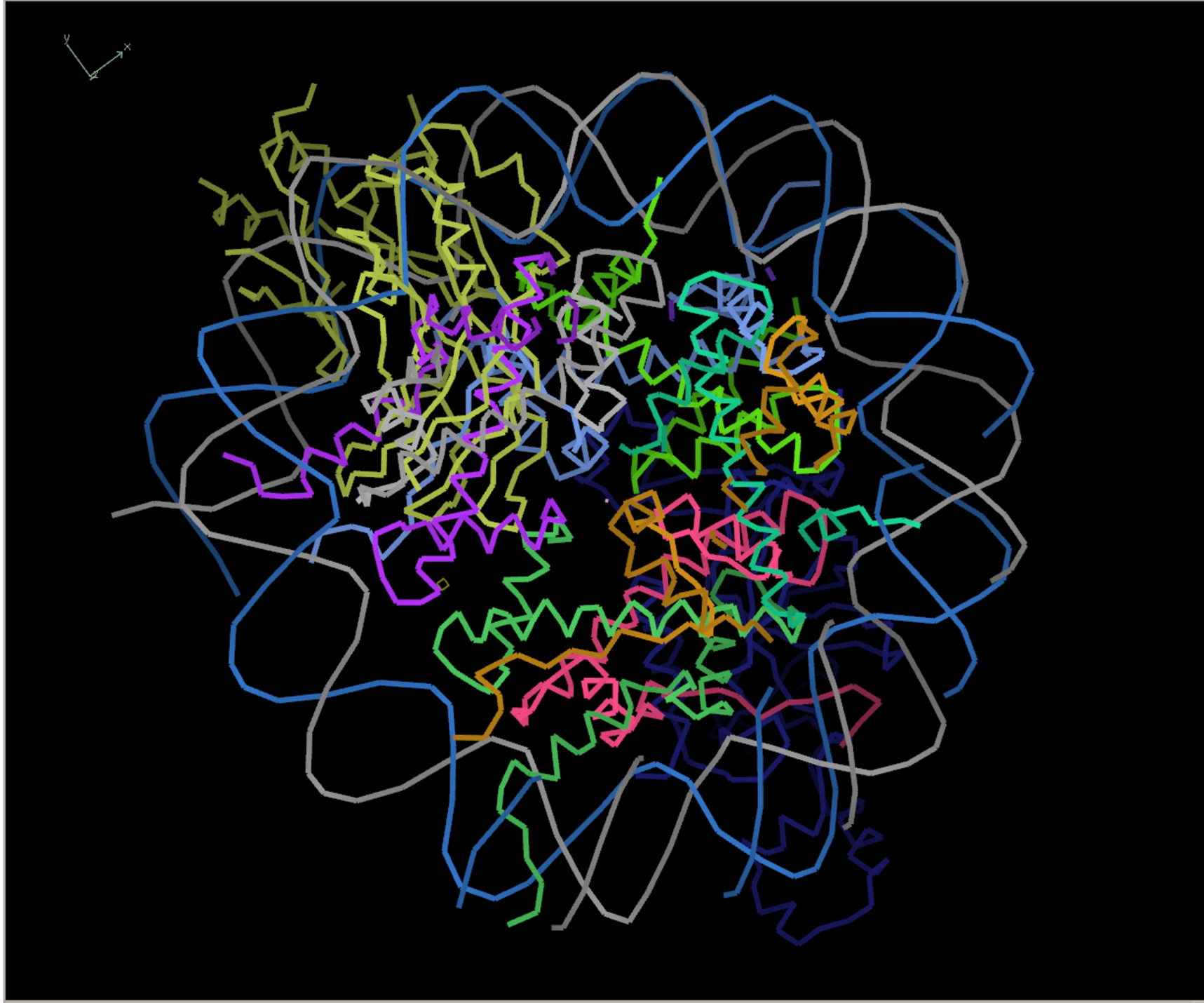
Automatic Generation of Base Pairing and Stacking Restraints

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-pairing and stacking restraints



- Navigation icons: Home, Back, Forward, Search, etc.
- Display Manager icon
- Map icon
- 3D coordinate system icon
- Zoom in/out icons
- Rotation icons
- Selection icons
- Other tool icons for model manipulation

cis-Peptides

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

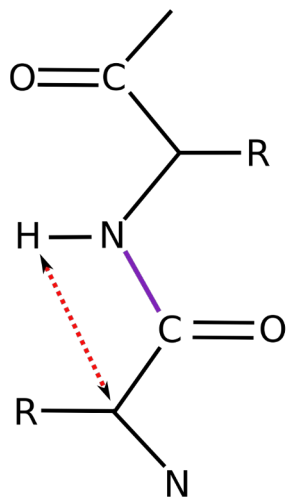
Croll: The rate of cis-trans conformation errors is increasing in low-resolution crystal structures *Acta Cryst.* (2015). D71, 706-709

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

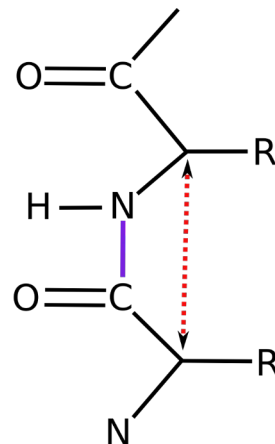
cis-Peptides

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

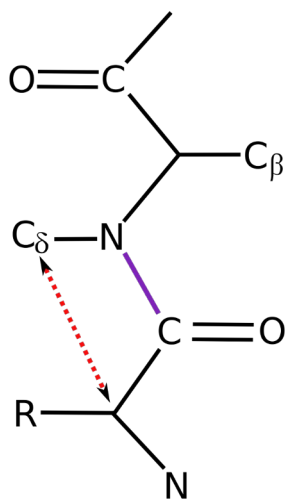
cis-Peptides



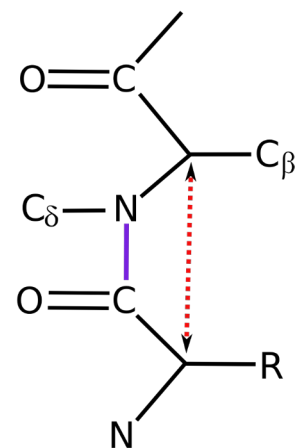
trans-peptide



cis-peptide

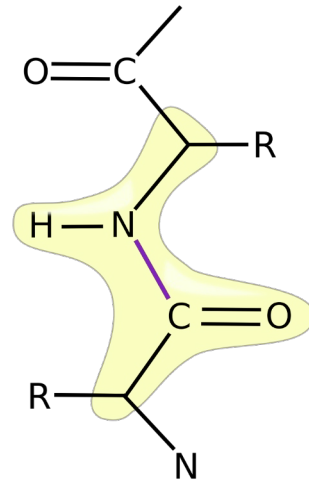


PRO trans-peptide

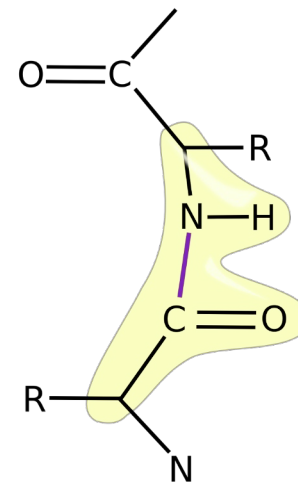


PRO cis-peptide

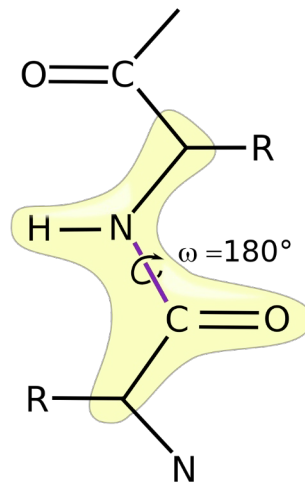
cis-Peptides



trans-peptide
with plane restraints

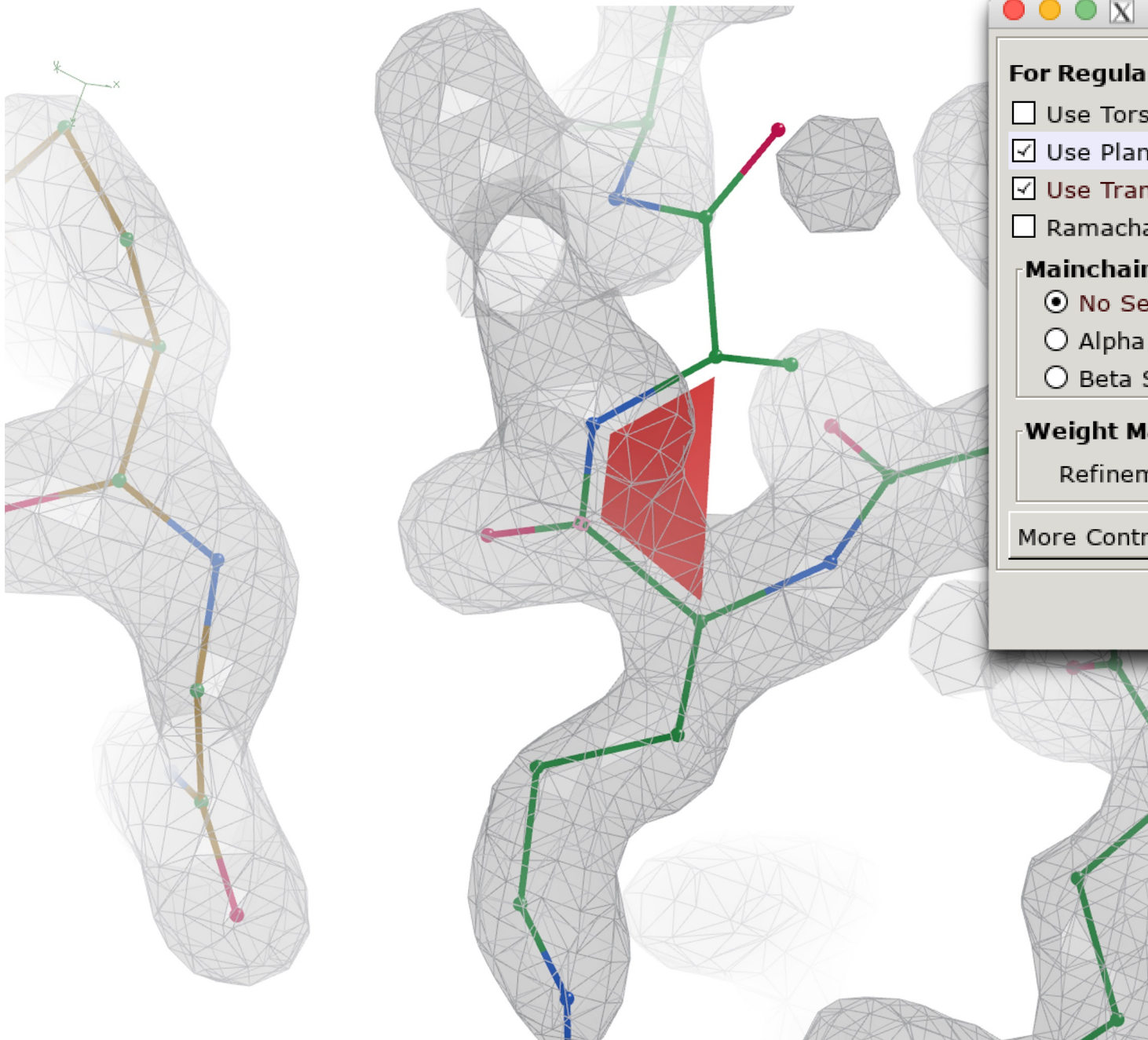


cis-peptide
with plane restraints



trans-peptide
with plane and trans restraints

cis-Peptide Representation



Refinement and Regularization...

For Regularization and Refinement:

- Use Torsion Restraints
- Use Planar Peptide Restraints
- Use Trans Peptide Restraints
- Ramachandran Restraints

Mainchain Restraints

- No Secondary Structure Restraints
- Alpha Helix Restraints
- Beta Strand Restraints

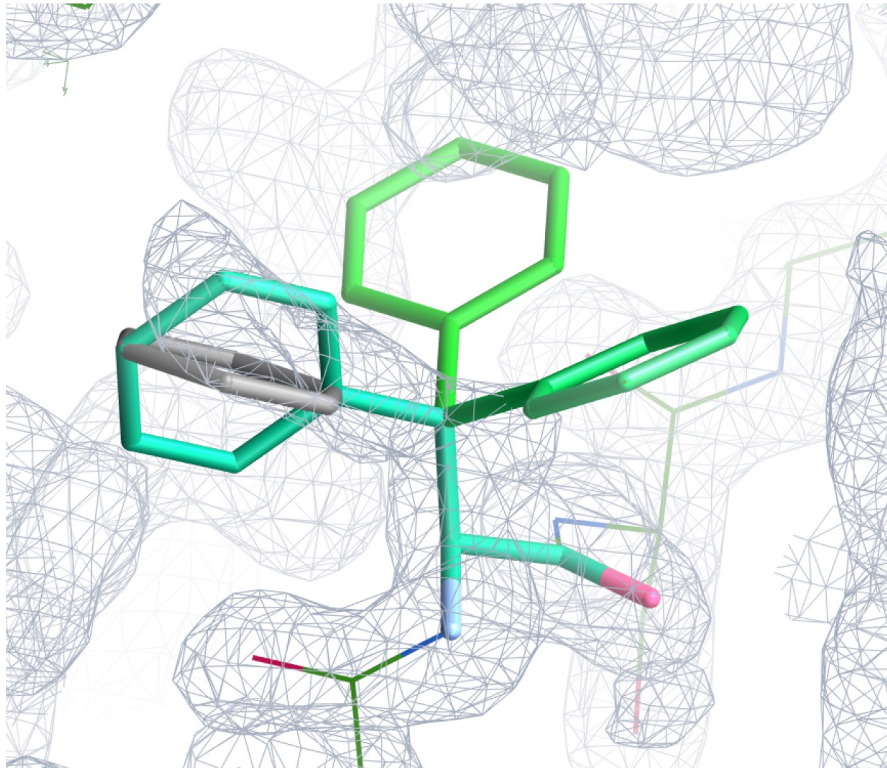
Weight Matrix

Refinement Weight

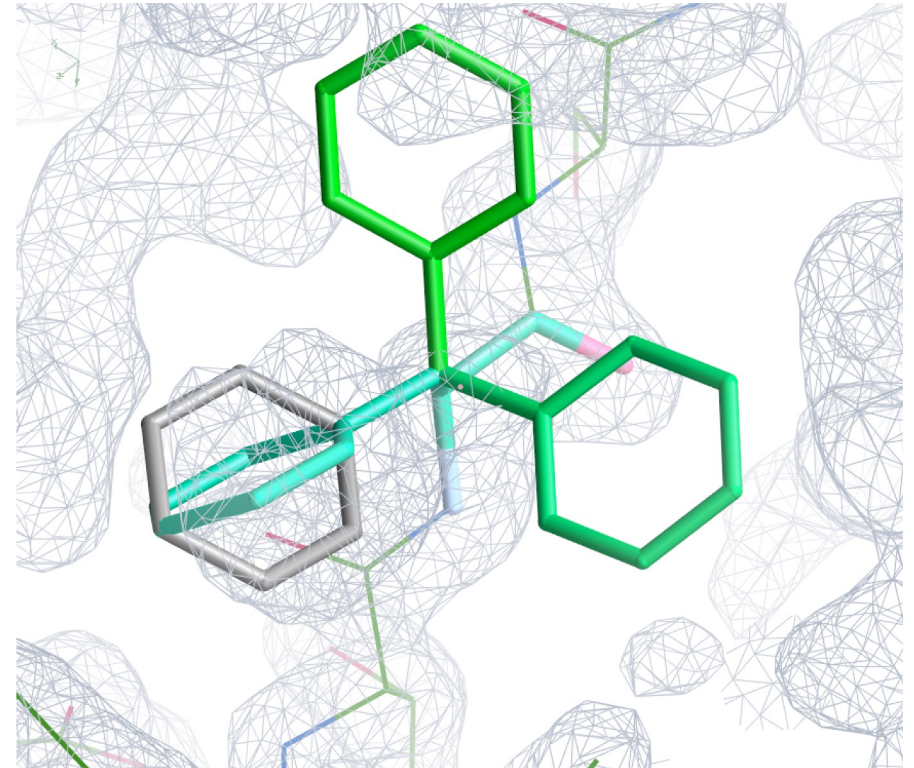
Rotamers

- 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

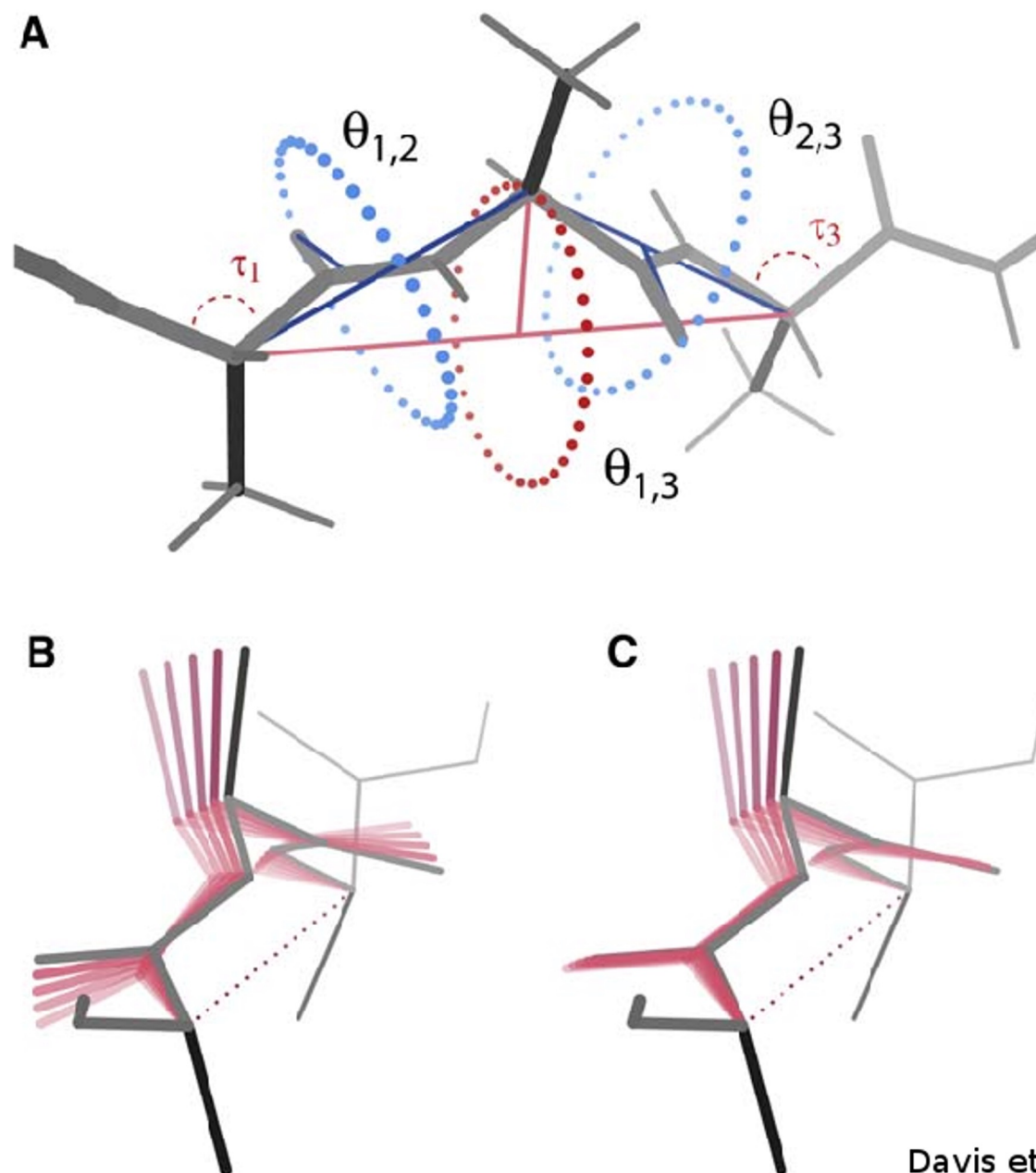


Side view



Top view

Backrub rotamer algo



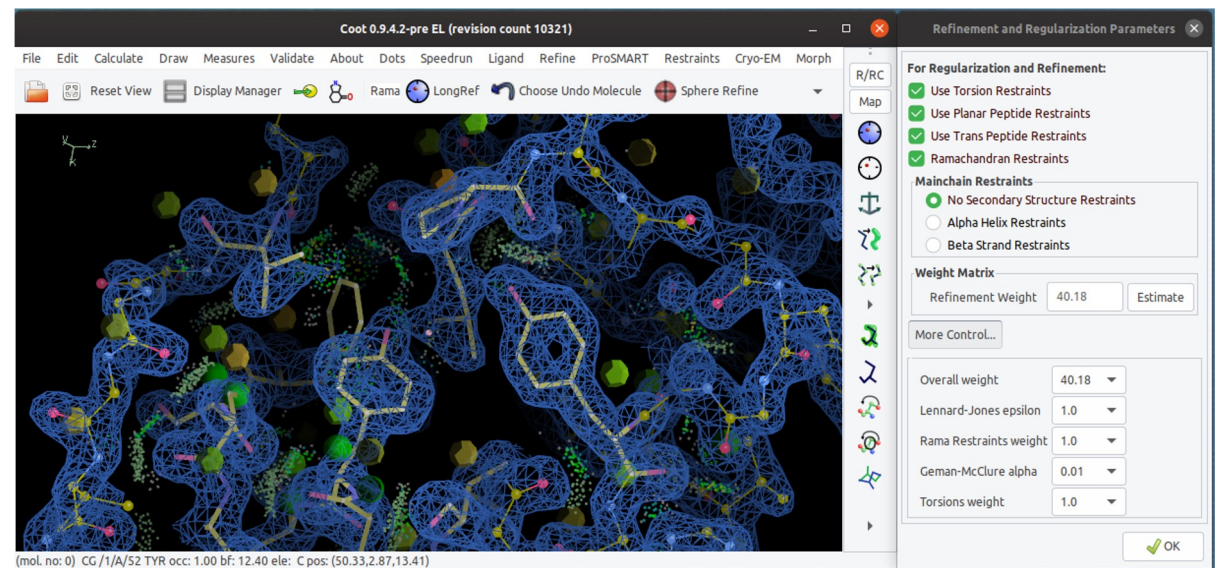
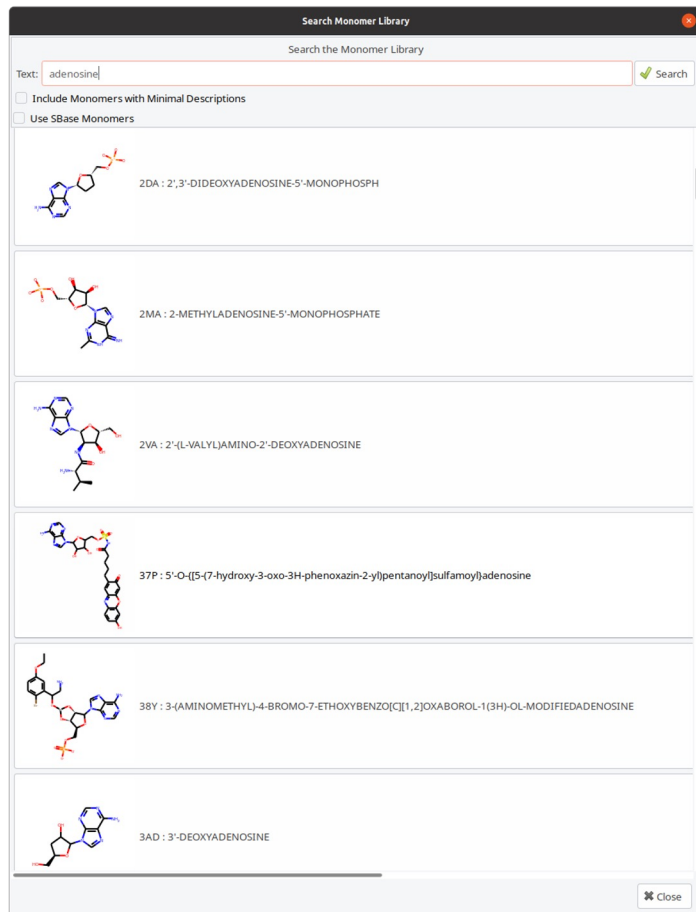
Coot 0.9.x and 1.1

coot-ligand-validation

API torsion restraint weights

Dynamic Weights

Parses Nuclear Hydrogen Atom Positions



Interactive Validation

The screenshot displays the Coot 0.9.5.1-pre EL software interface. The main window shows a 3D molecular model with atoms represented by colored spheres and bonds by sticks, overlaid on a blue mesh representing the electron density. A validation panel is open on the right, listing 17 interesting/outliers/problems. The panel includes a list of validation items, an 'Update' button, and a 'Close' button. The status bar at the bottom indicates that coordinates were successfully read from a file.

File Edit Calculate Draw Measures Validate About Ligand

Reset View Display Manager Sphere Refine Repeat Refine Zone Tandem Refine Backrub Rotamers

Coot 0.9.5.1-pre EL (revision count 10567)

Coot Interesting/Outliers/Problems: 17

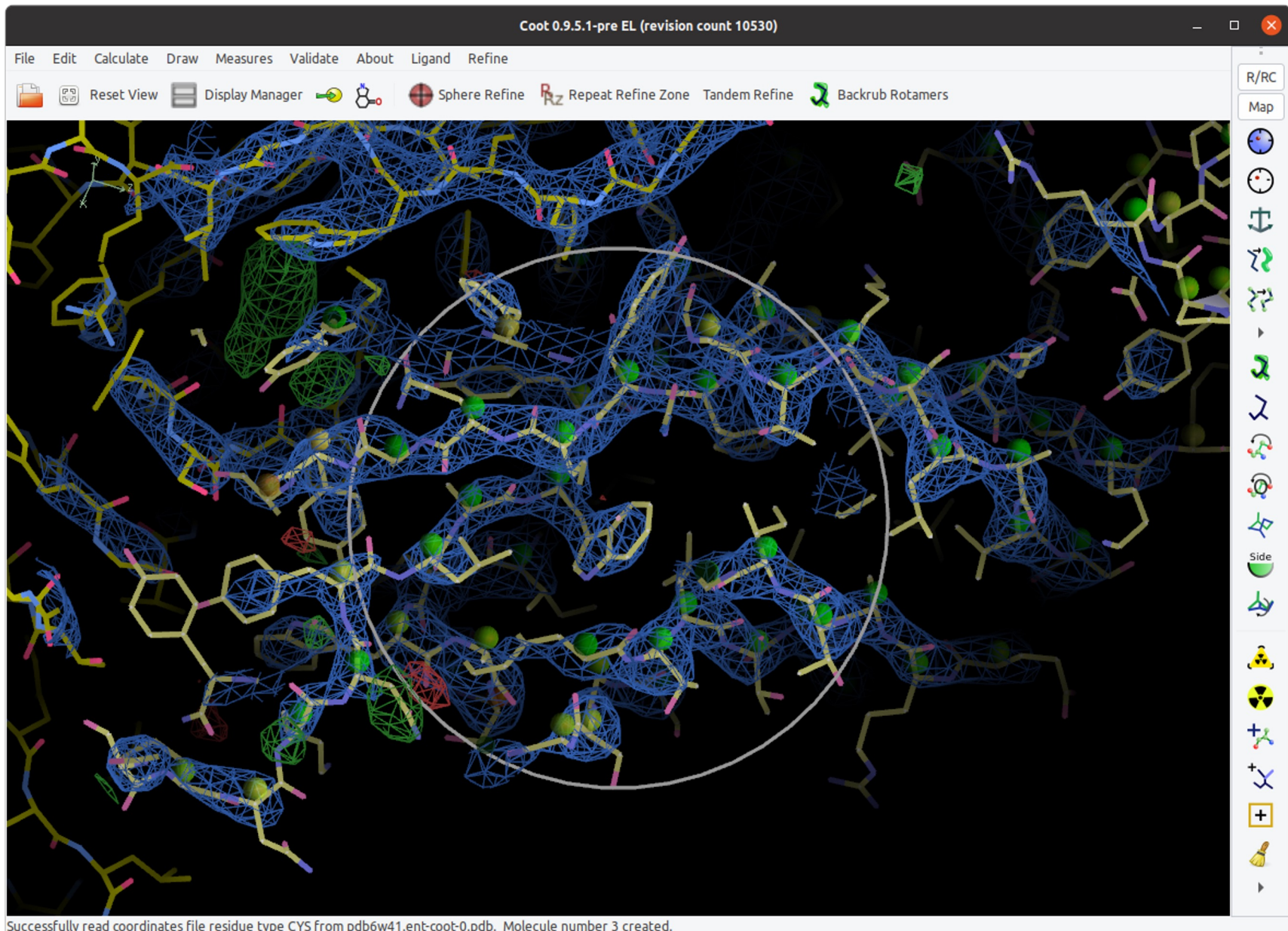
- Atom Overlap A 2 CG2 on A 89 CZ OV: 3.412
- Atom Overlap A 2 CG1 on A 89 CZ OV: 3.651
- Atom Overlap A 2 CA on A 89 CE2 OV: 3.711
- Atom Overlap A 2 CG1 on A 89 CE1 OV: 4.785
- Atom Overlap A 2 CB on A 89 CZ OV: 6.395
- Atom Overlap A 2 CA on A 89 CZ OV: 7.450
- Rotamer Outlier A 32 GLN 0.010 %
- Non-PRO cis-peptide A 40 - A 41
- Atom Overlap A 41 O on A 43 N OV: 2.071
- C-beta deviant A 41 GLU 2.28 Å
- Twisted trans-peptide A 41 - A 42
- Ramachandran A 41 GLU 0.004 %
- Chiral Volume Error A 41 CA
- Ramachandran A 42 SER 0.002 %
- Missing Sidechain A 72 CYS none

Update

Close

Successfully read coordinates file /Users/pemsley/autobuild/build-refinement-pre-release-gtk2-python/share/cool/data/tutorial-modern.pdb. Molecule number 0 ...

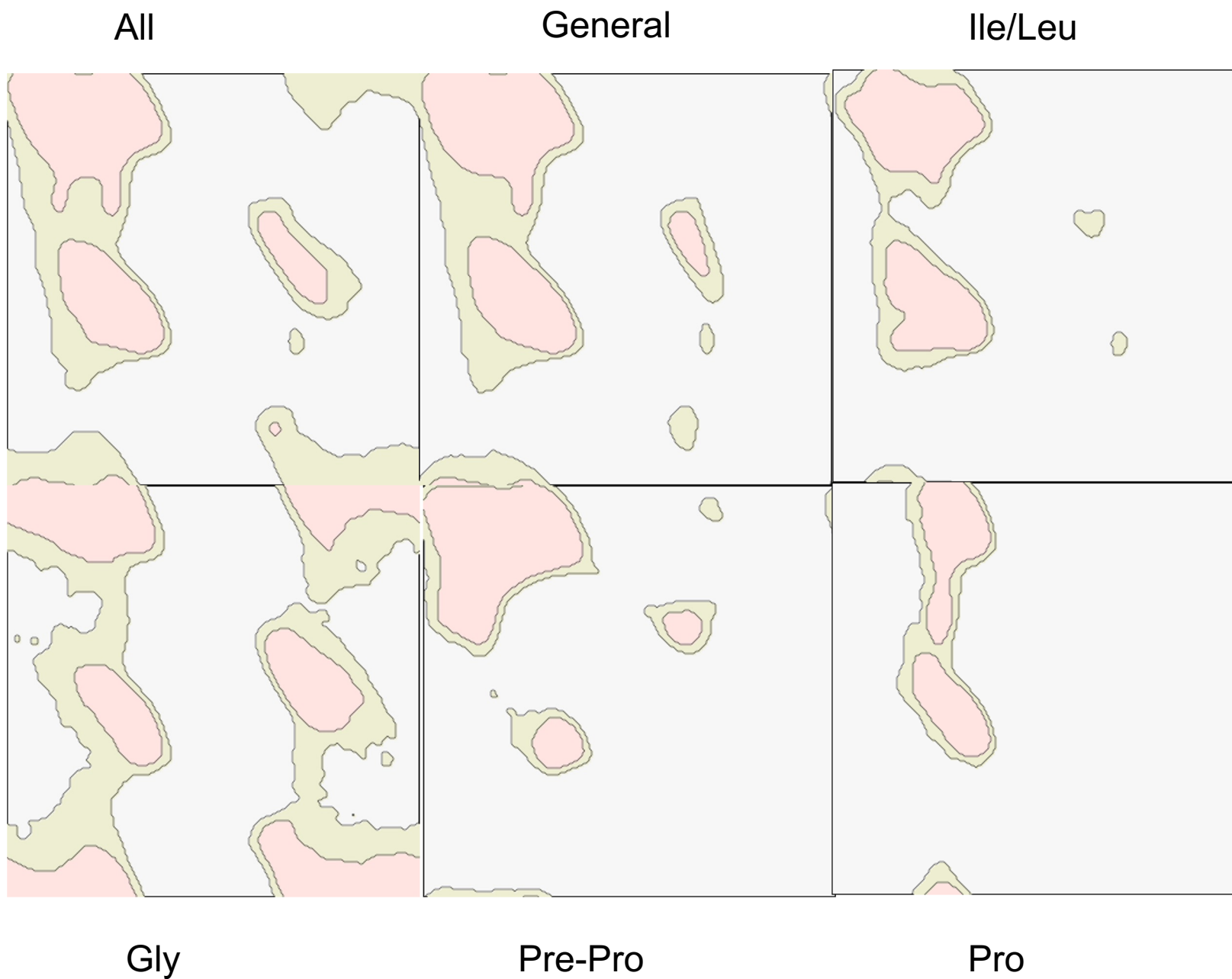
Real-Space Refinement Proportional Editing



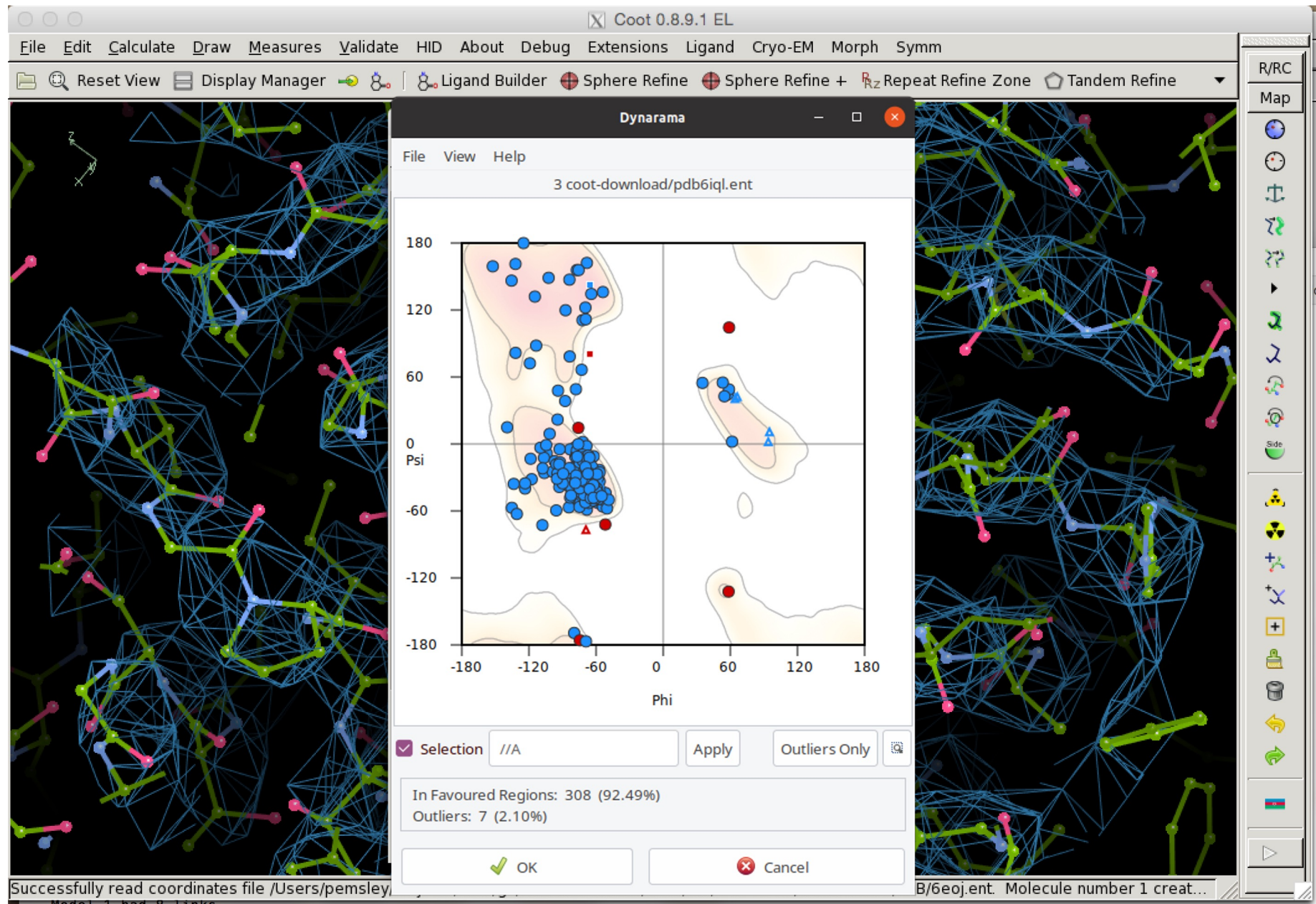
Activate/Change with Ctrl Middle-mouse scroll

Improved Ramachandran Plot(s)

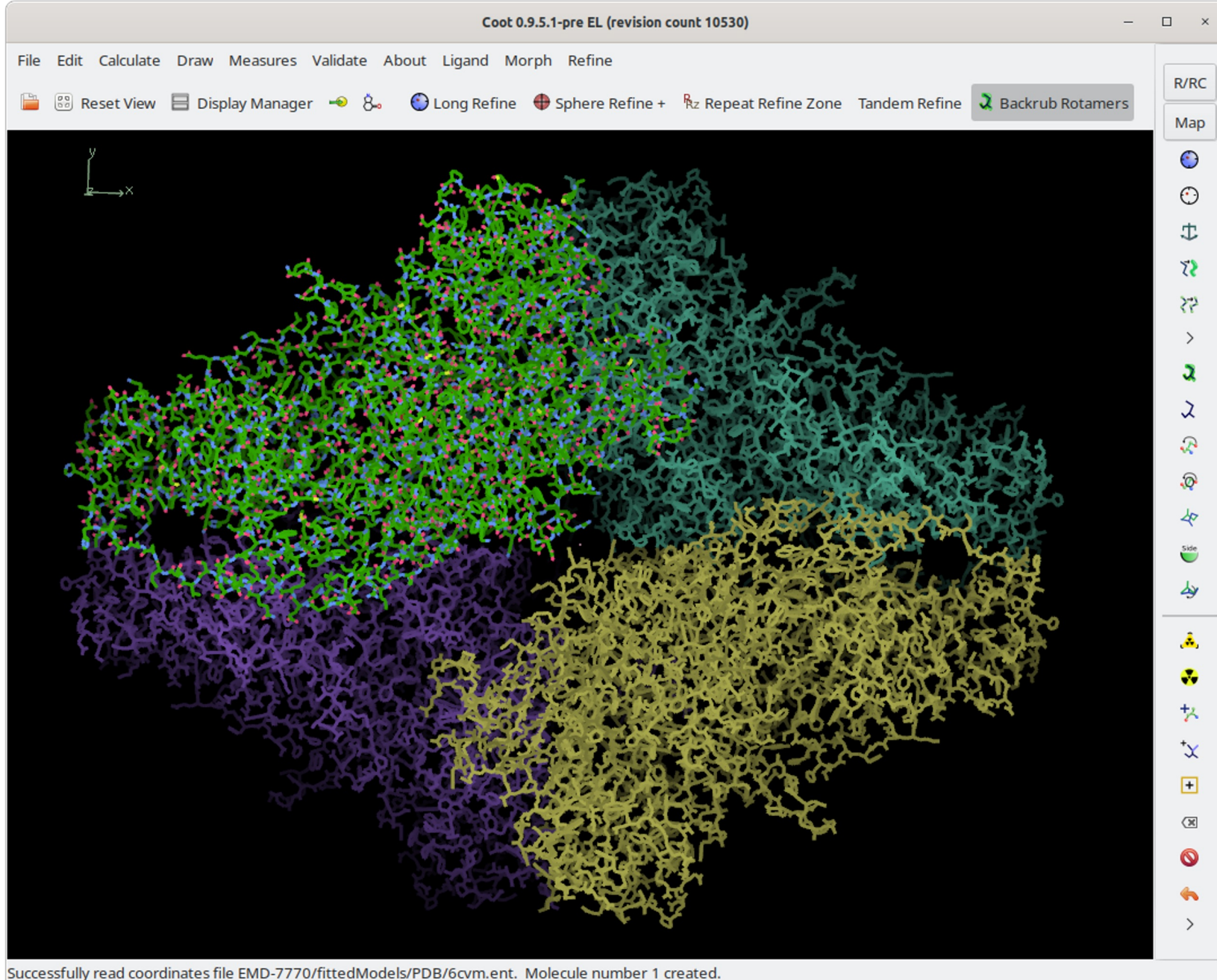
A. Thorn
B. Lohkamp



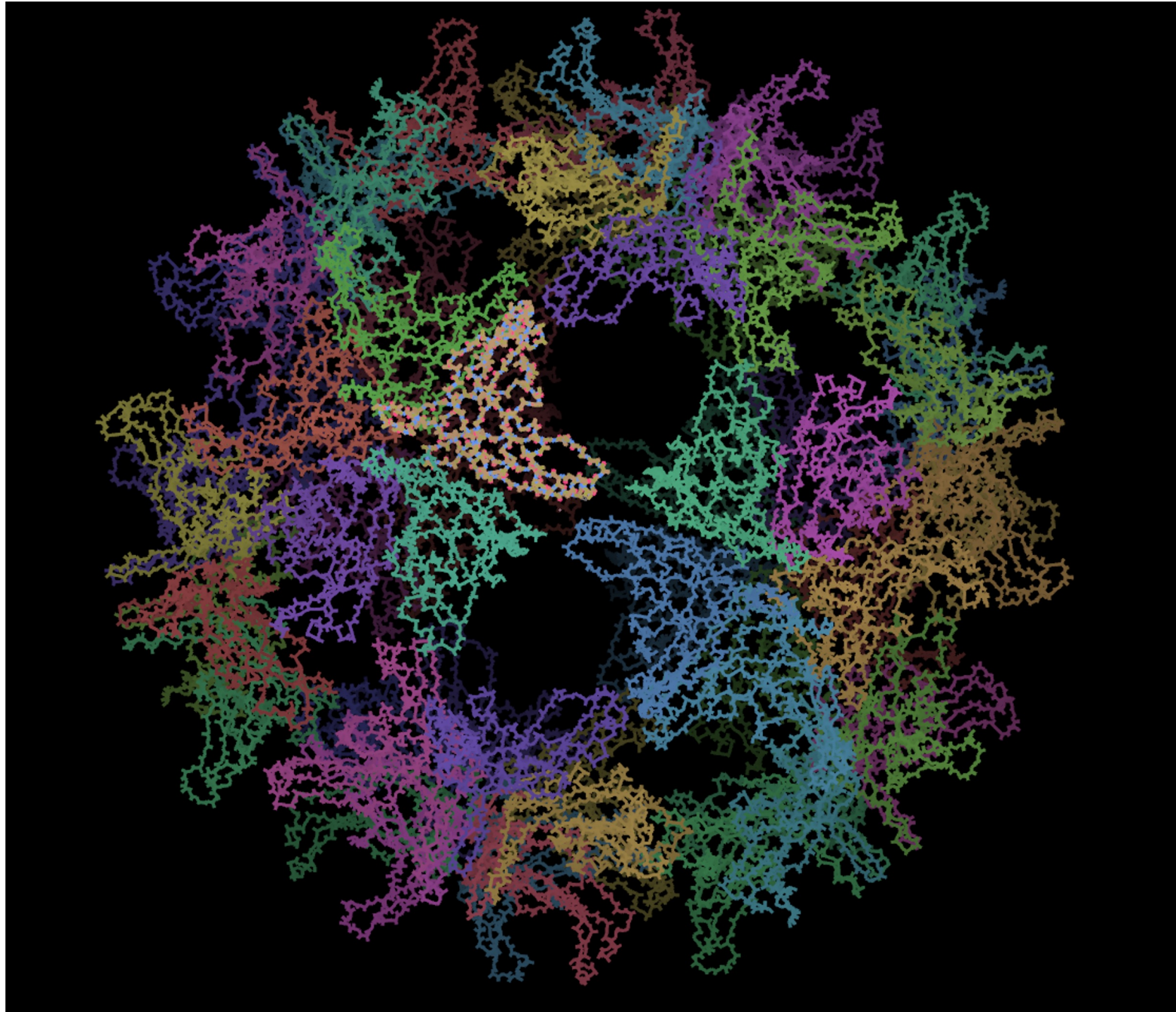
The New Ramachandran Plot



Molecular Symmetry



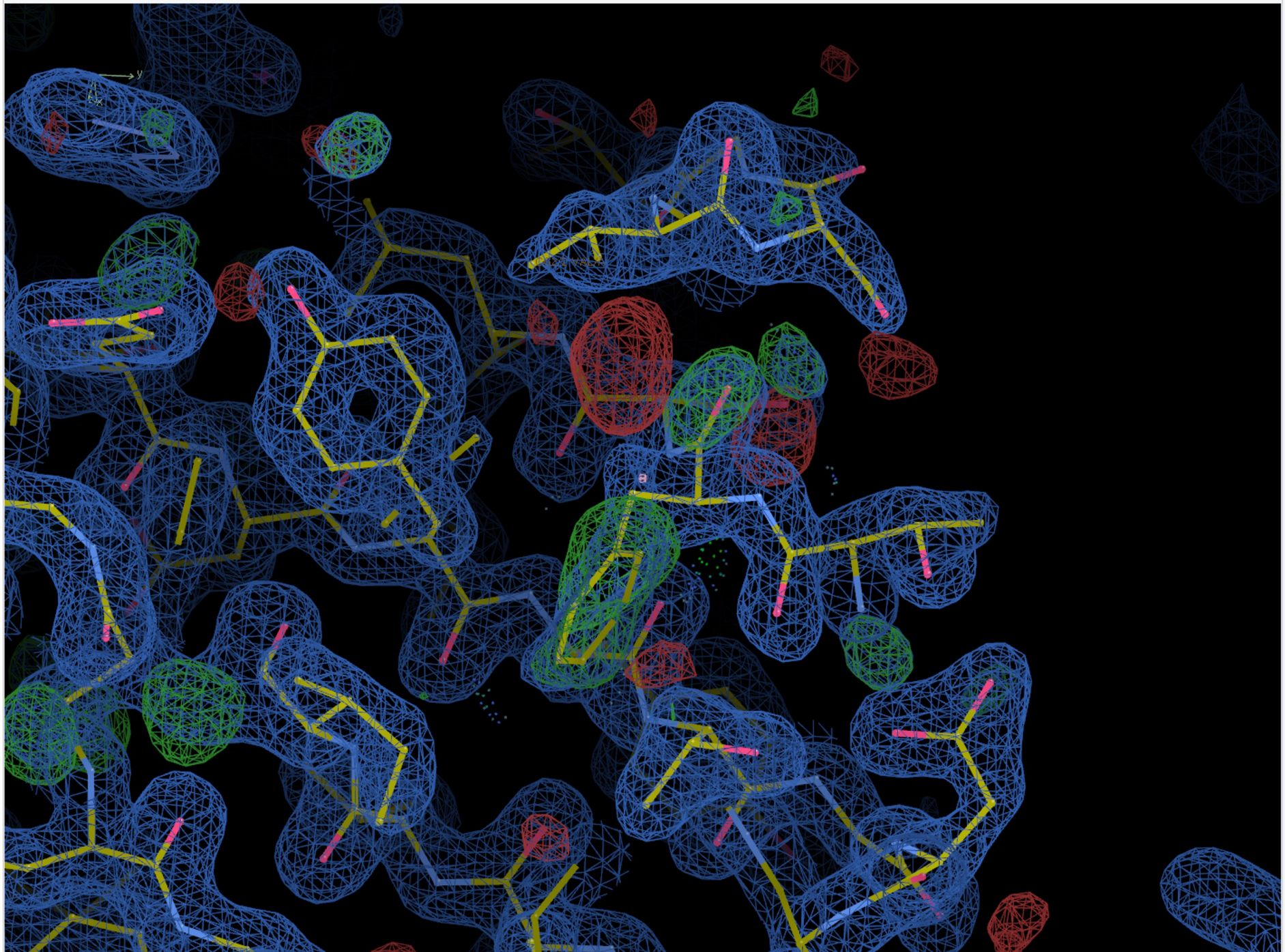
Molecular Symmetry

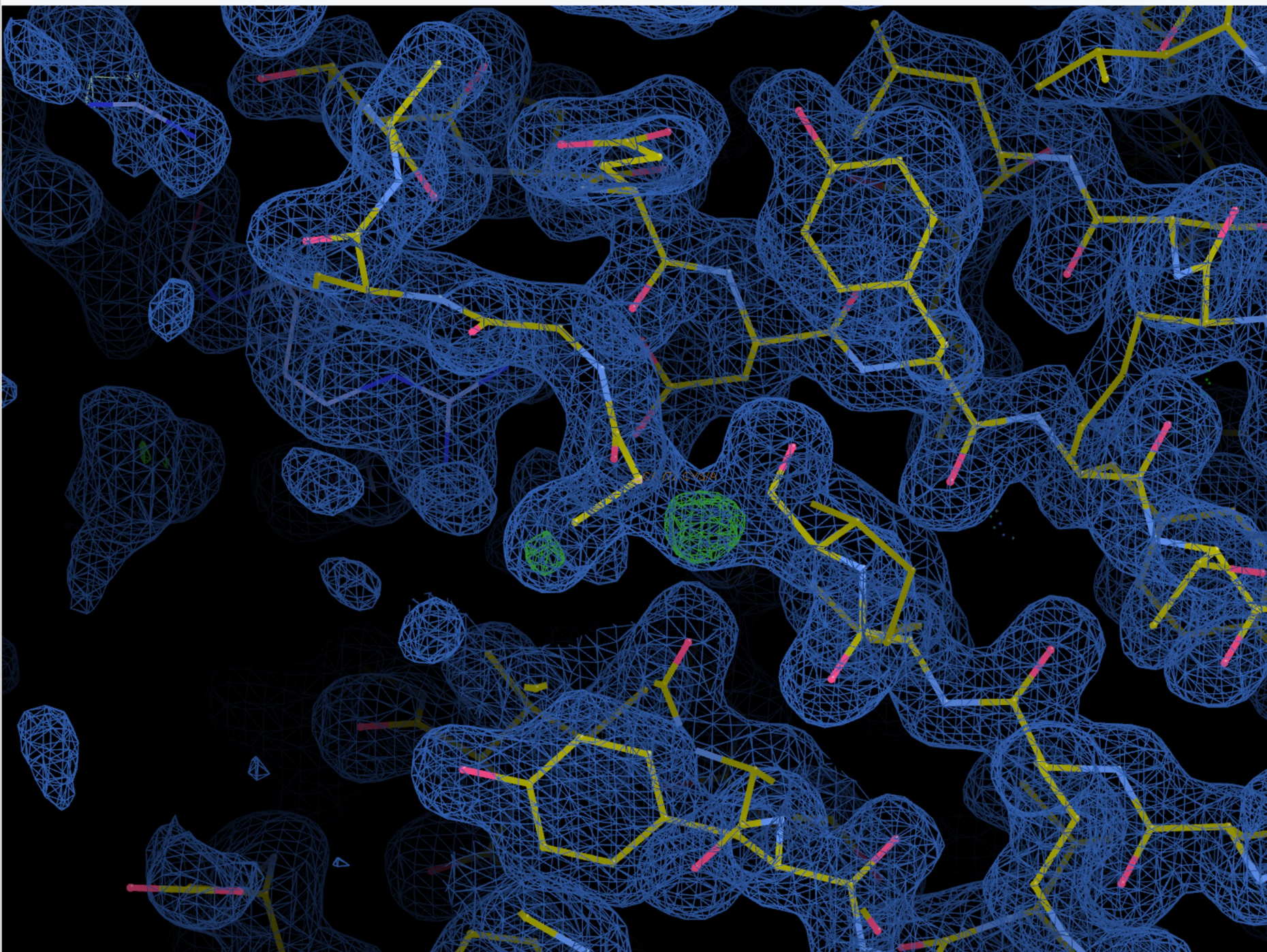


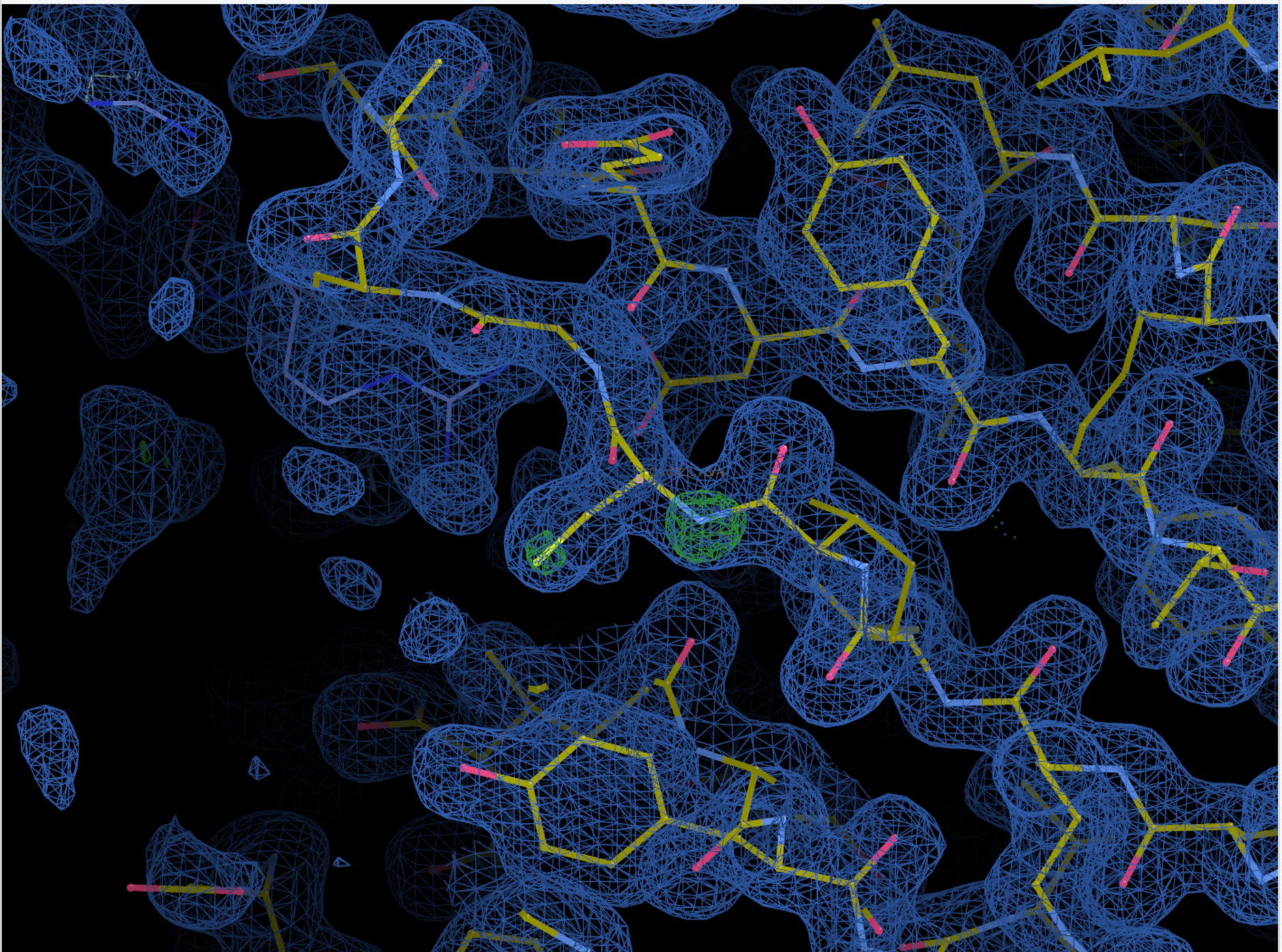
Updating Maps

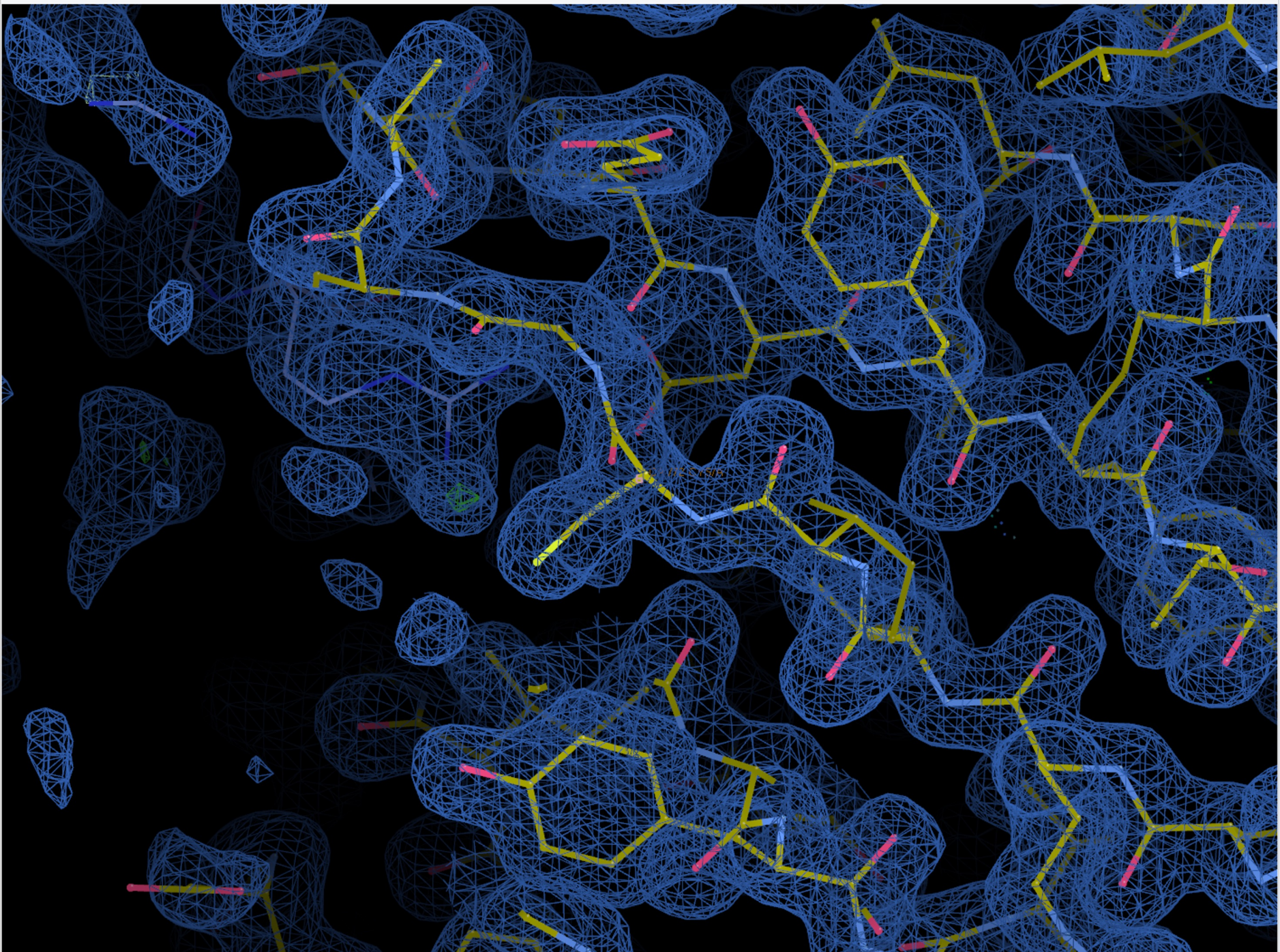
Thanks to **Tristan Croll** who implemented this in Isolde and inspired Paul to add it to Coot.
Thanks to **Kathryn Cowtan** for help in doing so

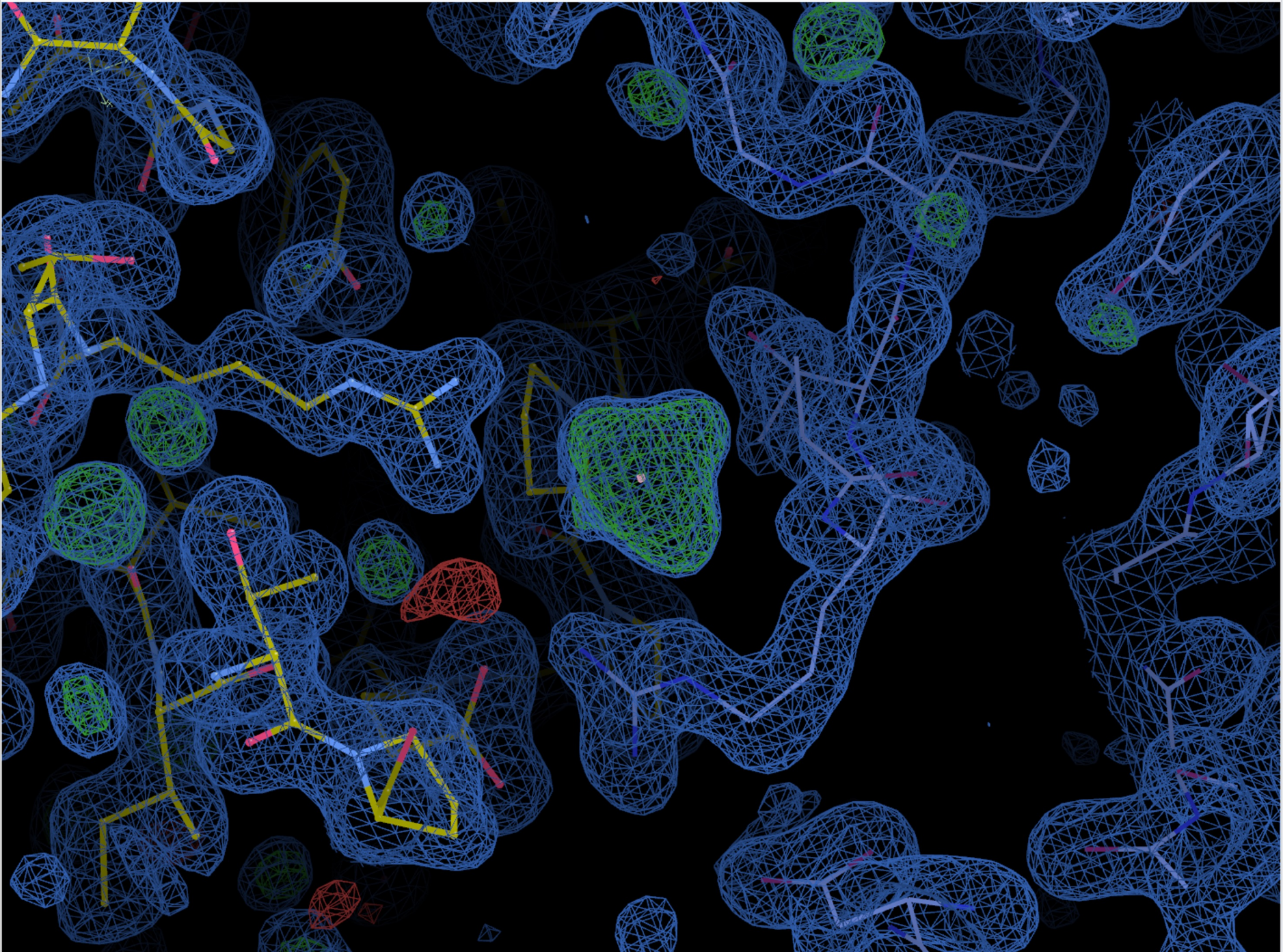
Note: updating maps takes ~ 0.7 s for 200 AA and 1.8Å data

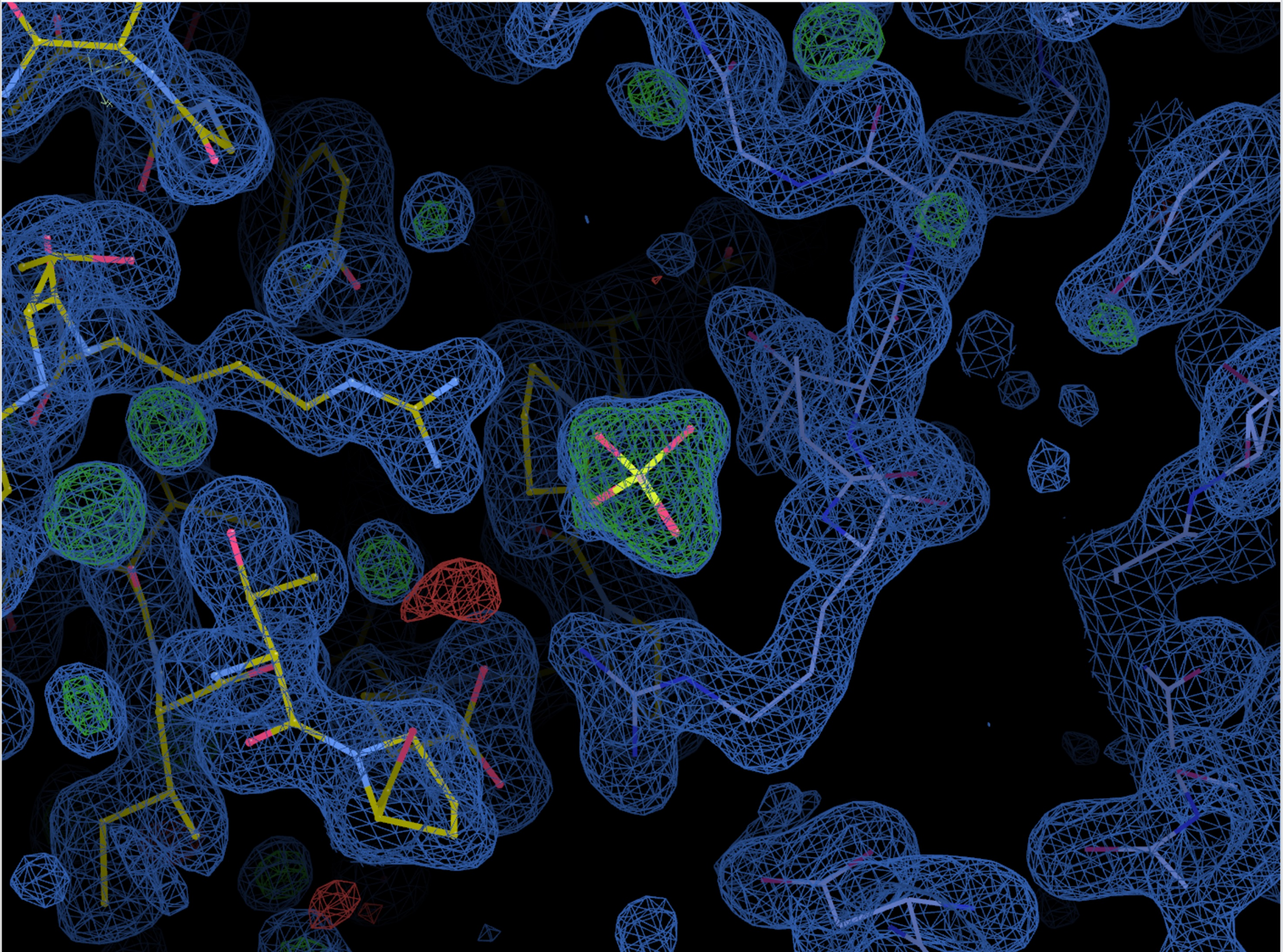




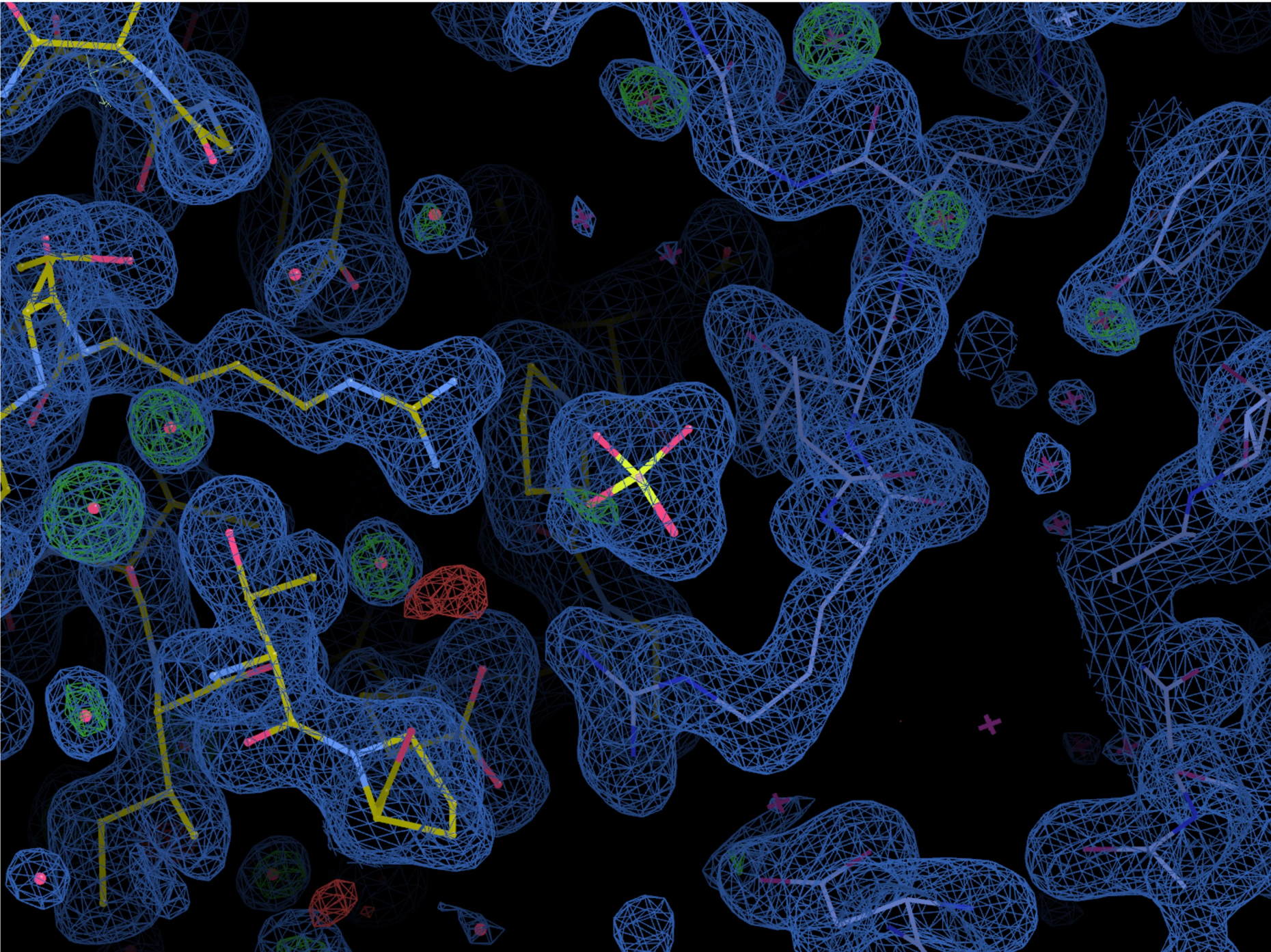




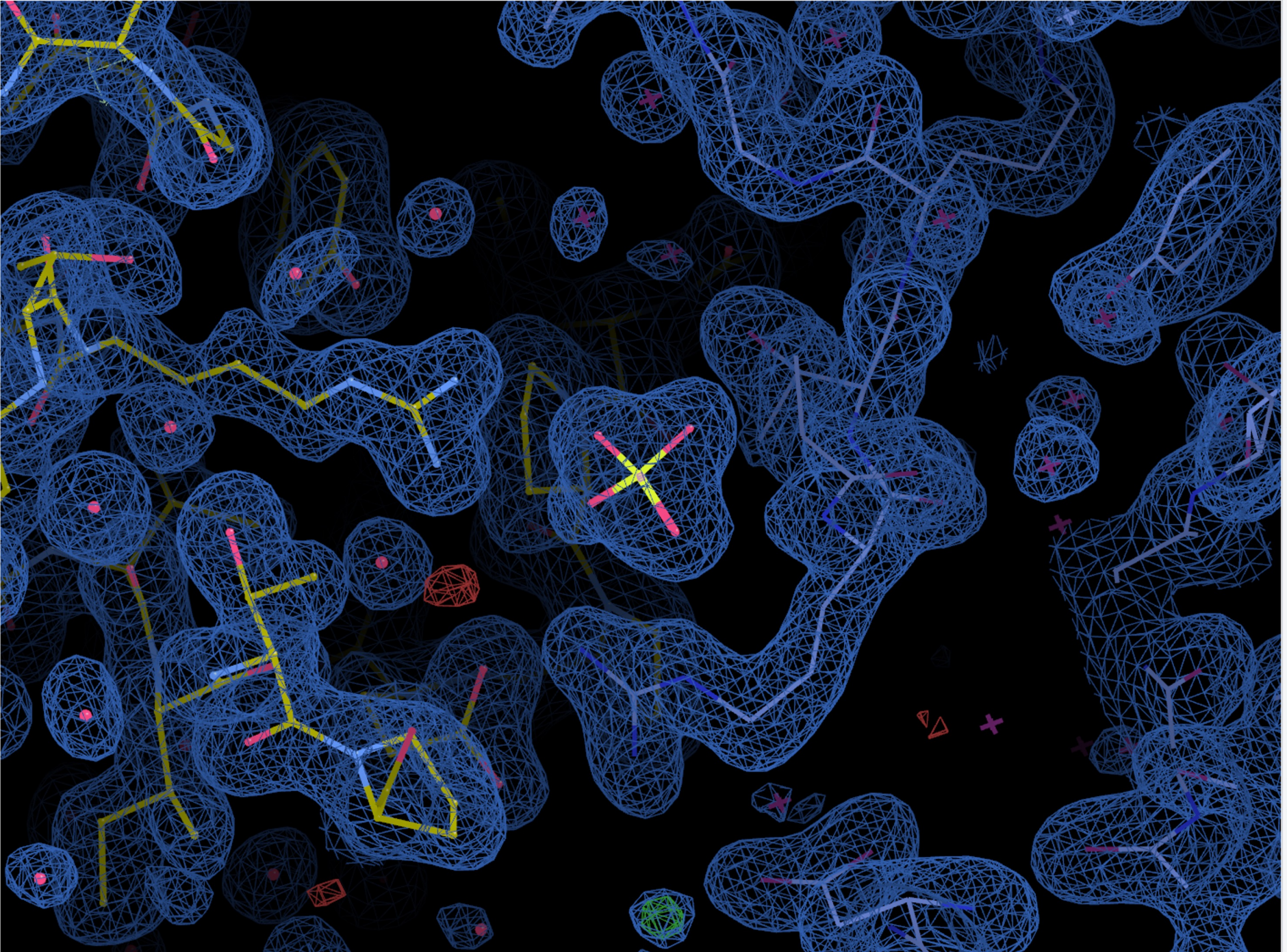




R/R/C
Map
[Icons for various tools: zoom, pan, rotate, etc.]
Side
[Icons for various tools: zoom, pan, rotate, etc.]



R/R/C
Map
[Icons for map management and navigation]



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

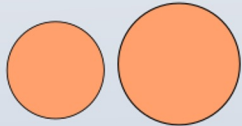
Ambient Occlusion

Approximation, so artefacts

Textures (something other than shiny plastic)

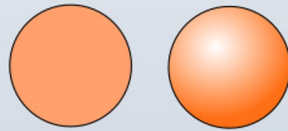
Visual Cues for Depth

Relative Size



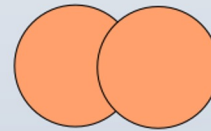
Old Coot: ✗
New Coot: ✓

Shading



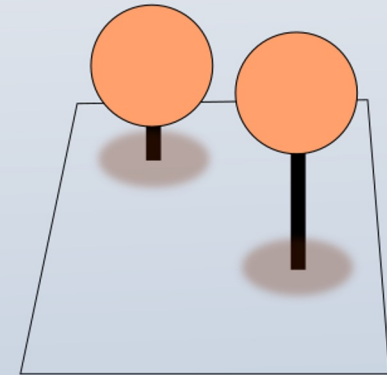
Old Coot: ✗
New Coot: ✓

Occlusion



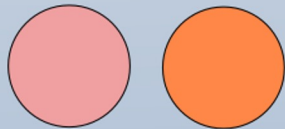
Old Coot: ✗
New Coot: ✓

Shadows



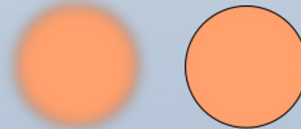
Old Coot: ✗
New Coot: ✓

Colour



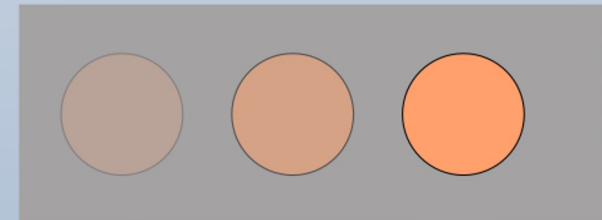
Old Coot: ✗
New Coot: ✓

Focus/Blur



Old Coot: ✗
New Coot: ✓

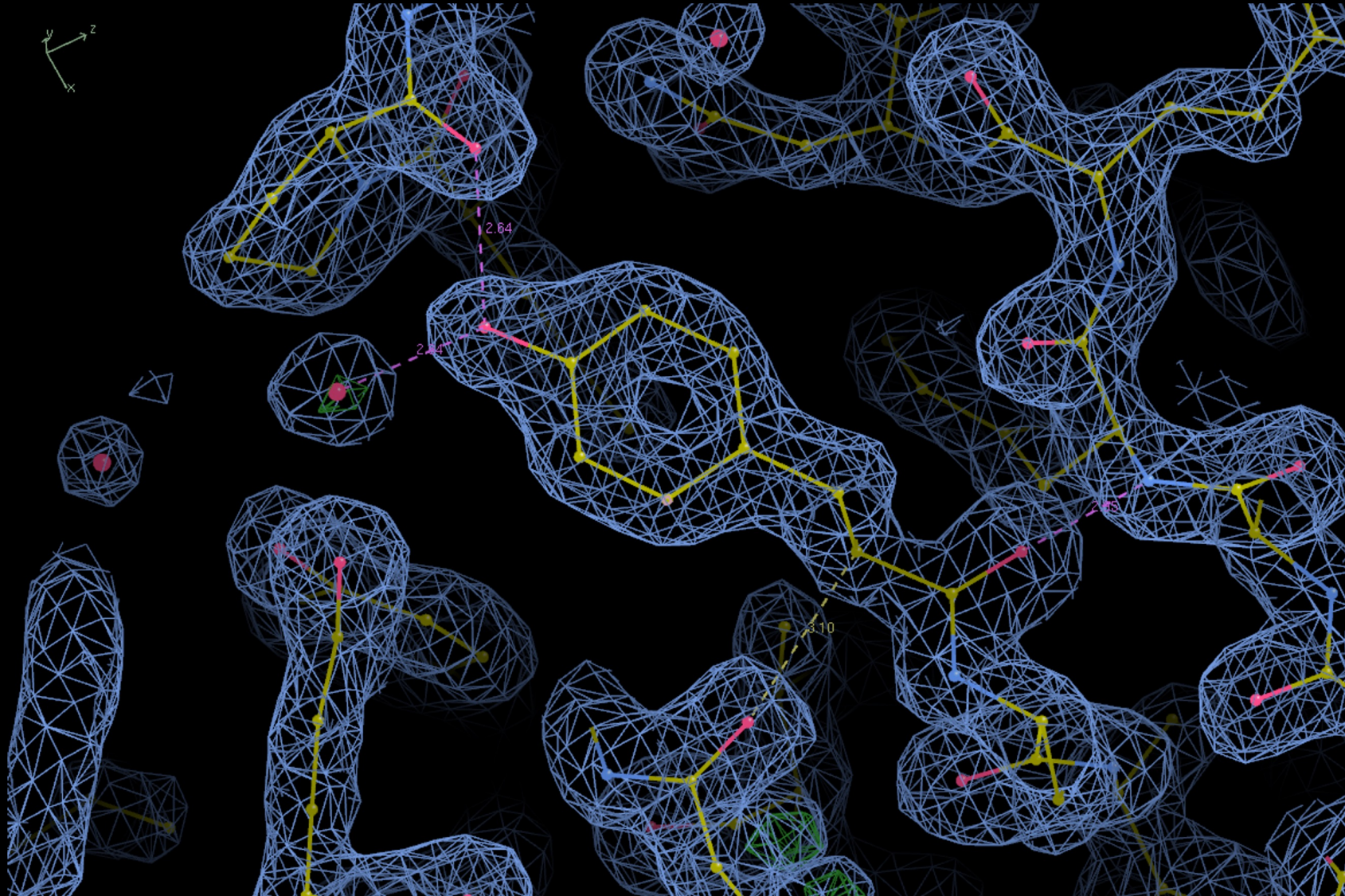
Fog Depth



Old Coot: ✓
New Coot: ✓

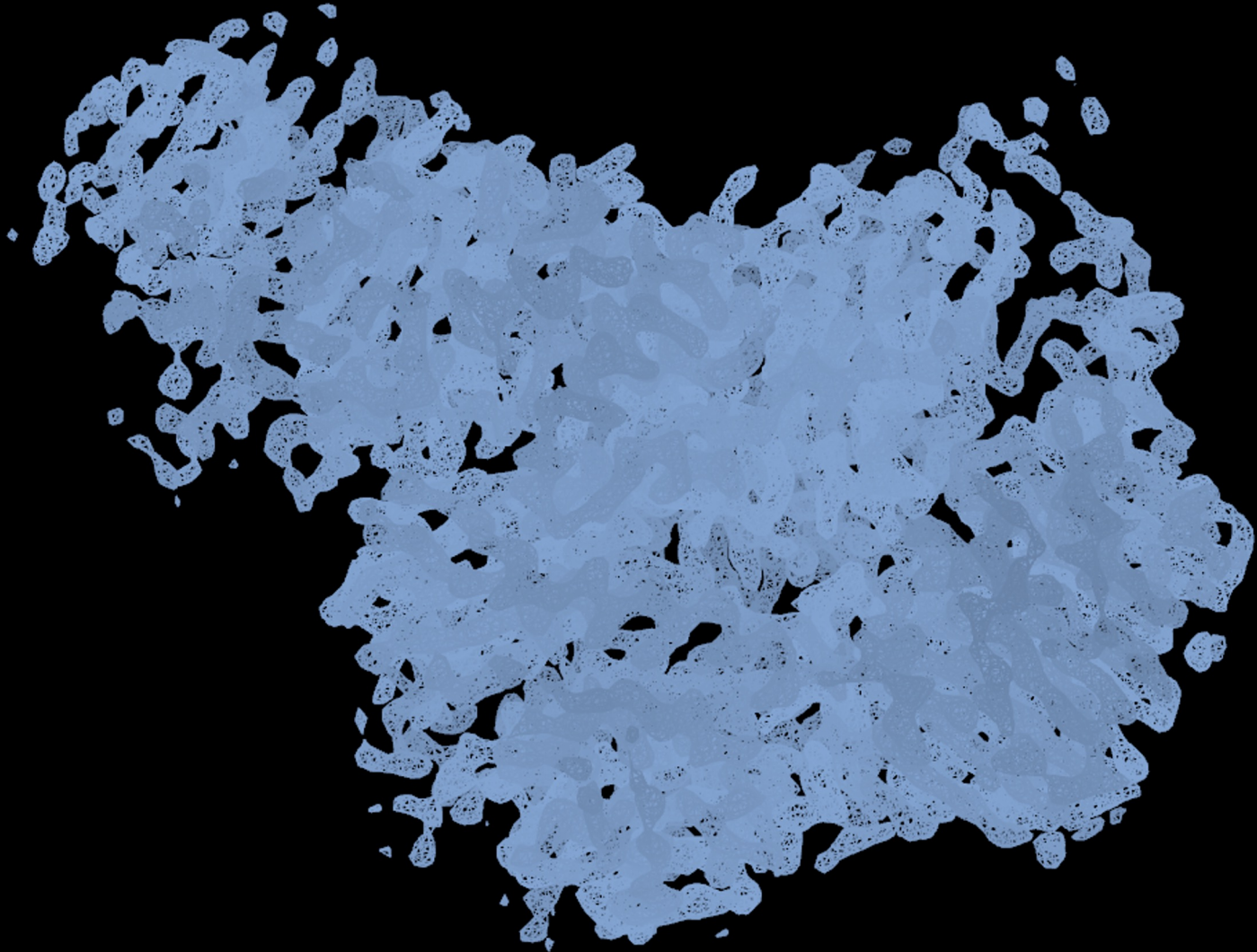
Old Coot: Lack of Depth

When Zoomed in:



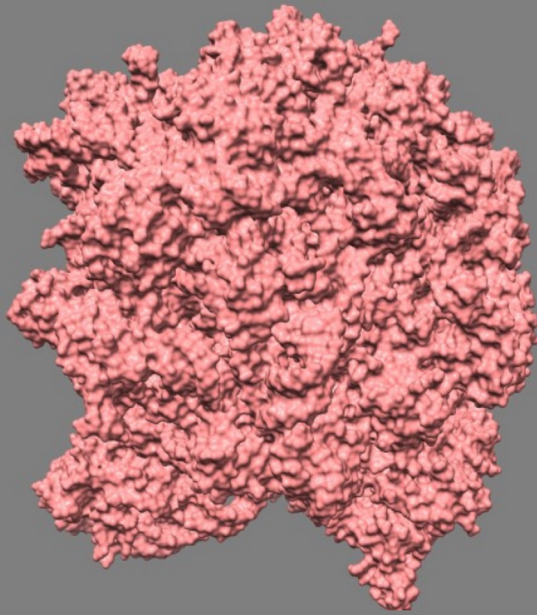
Old Coot: Lack of Depth

When Zoomed out:

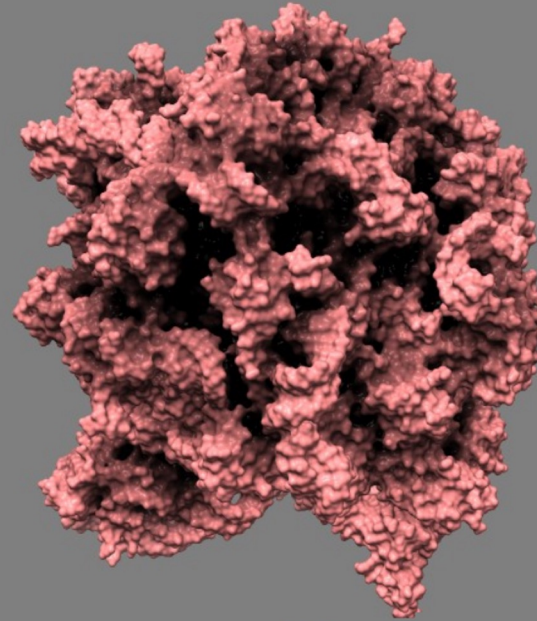


Ambient Occlusion and Shadows in ChimeraX

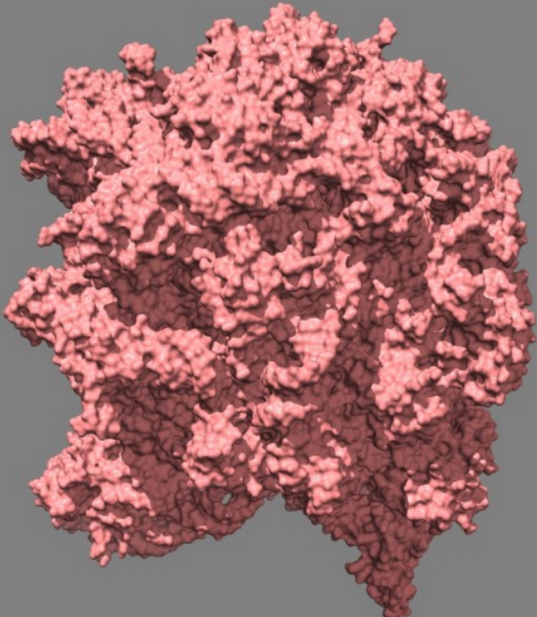
Basic Lighting



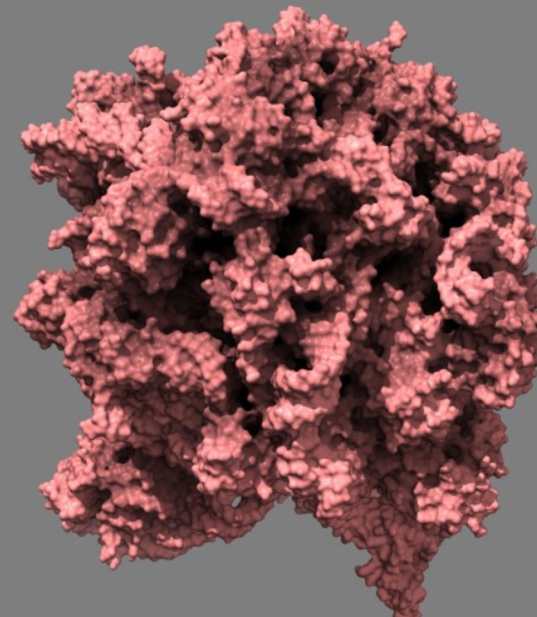
Ambient Occlusion



Shadows



Ambient Occlusion & Shadows



Molecular surface, not cry-EM reconstruction



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



Quit

Blur depth 0.60 SSAO radius 0.00

Blur Strength 0.00 SSAO bias 0.05

Rotation Centre Height 2.35 SSAO N-kernel points 64



Quit

Blur depth 0.58

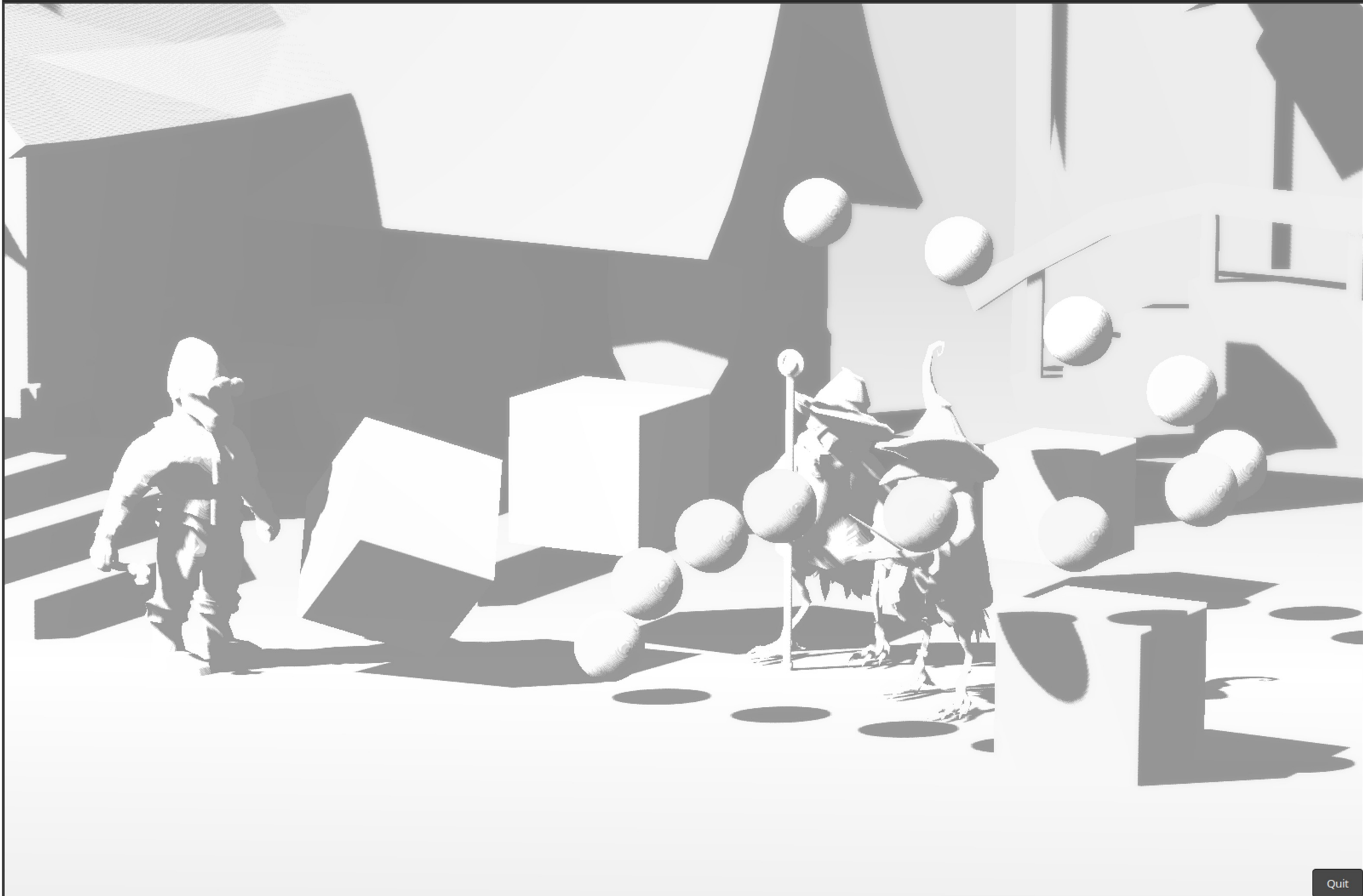
Blur Strength 1.72

Rotation Centre Height 2.35

SSAO radius 0.00

SSAO bias 0.05

SSAO N-kernel points 64



Quit

Blur depth 0.58

Blur Strength 1.72

Rotation Centre Height 2.35

SSAO radius 0.00

SSAO bias 0.05

SSAO N-kernel points 64



Quit

Blur depth 0.58

Blur Strength 1.72

Rotation Centre Height 2.35

SSAO radius 0.07

SSAO bias 0.05

SSAO N-kernel points 138



Quit

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



Quit

Blur depth 0.58

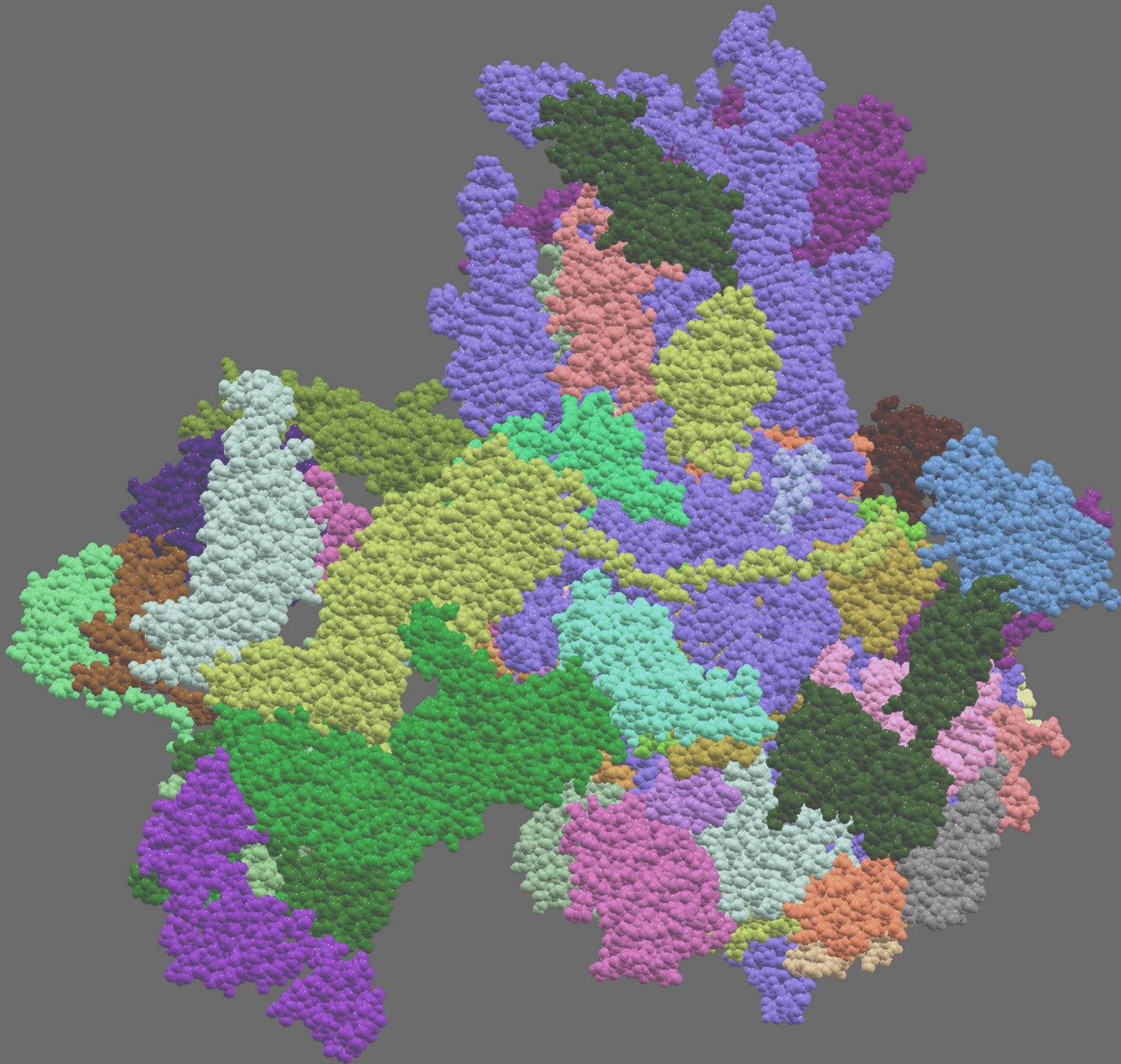
Blur Strength 3.65

Rotation Centre Height 2.35

SSAO radius 0.00

SSAO bias 0.05

SSAO N-kernel points 138



Quit

Blur depth 0.44

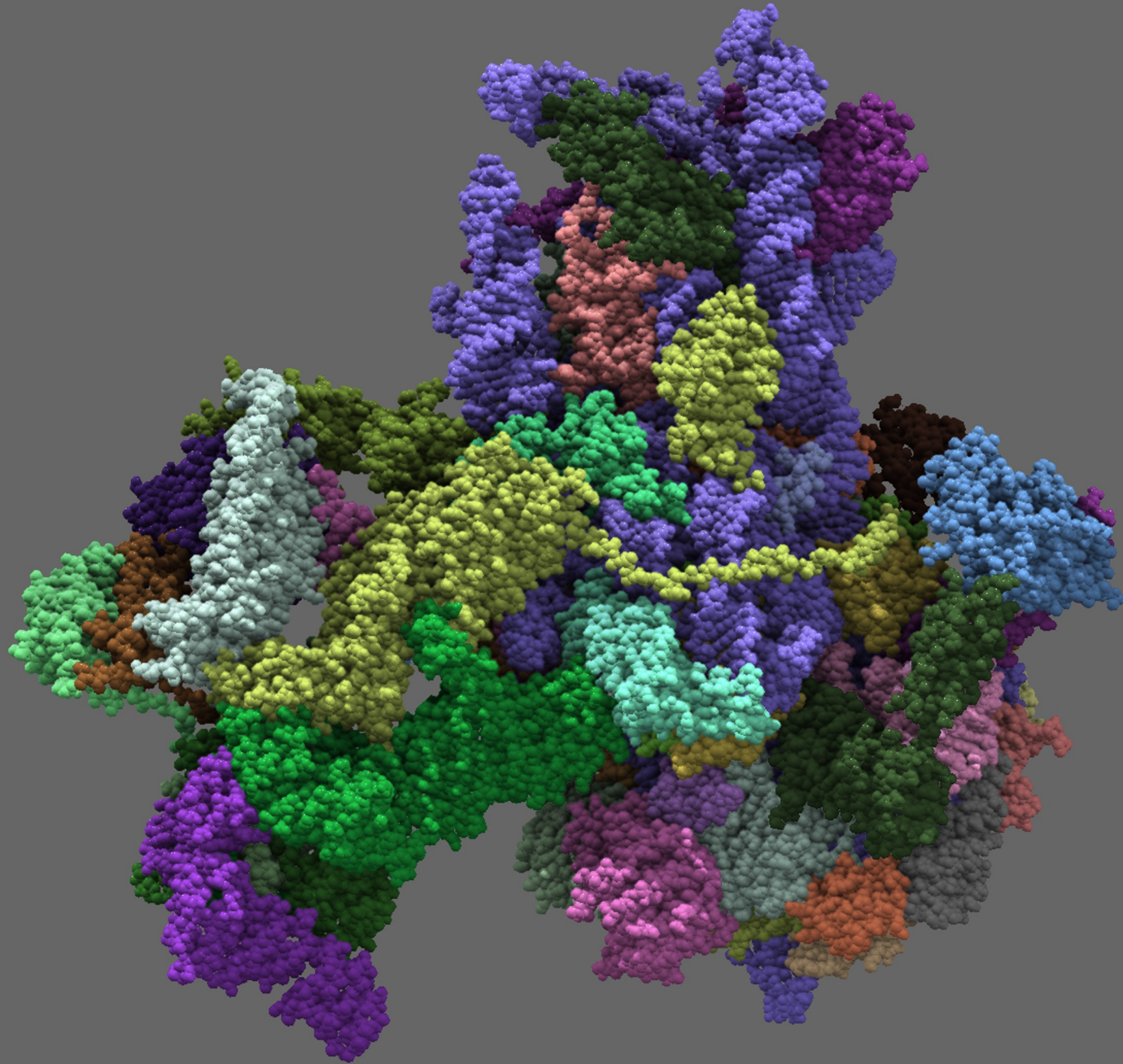
Blur Strength 0.00

Rotation Centre Height 3.13

SSAO radius 0.00

SSAO bias 0.01

SSAO N-kernel points 319



Quit

Blur depth 0.44

SSAO radius 1.77

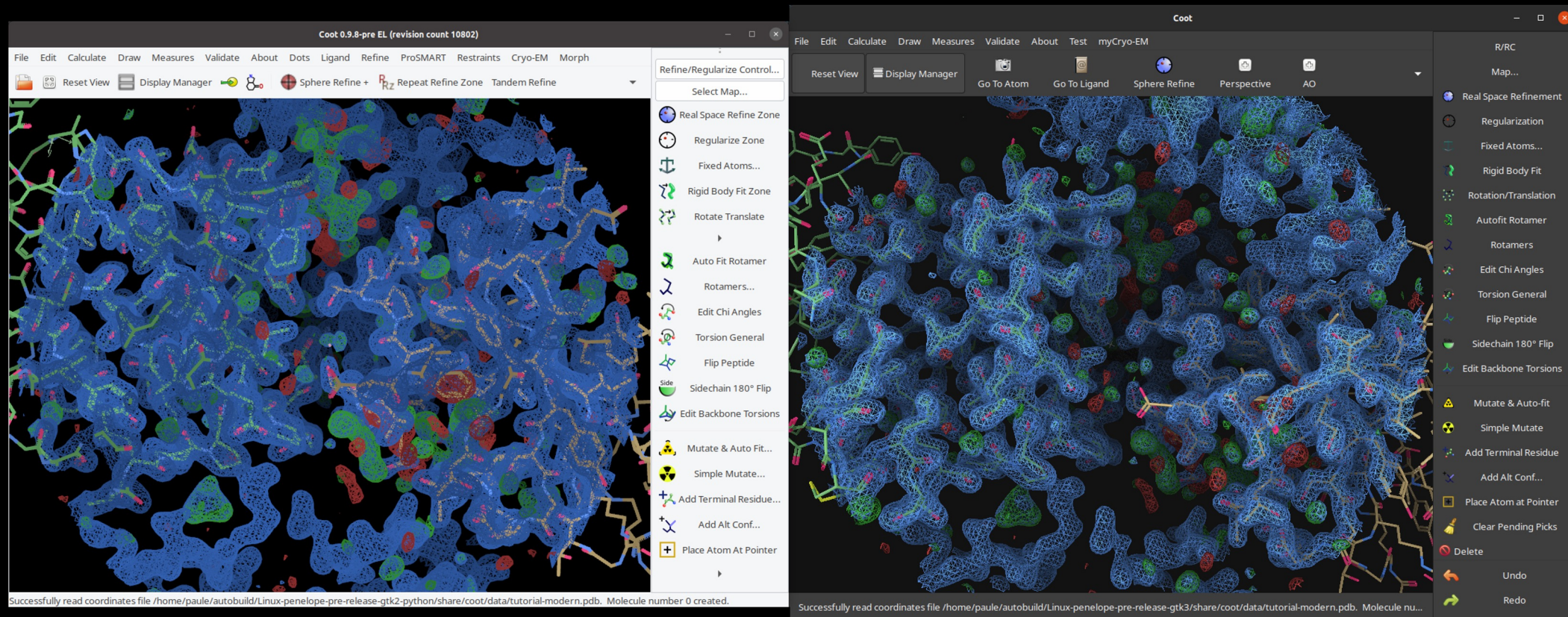
Blur Strength 0.00

SSAO bias 0.04

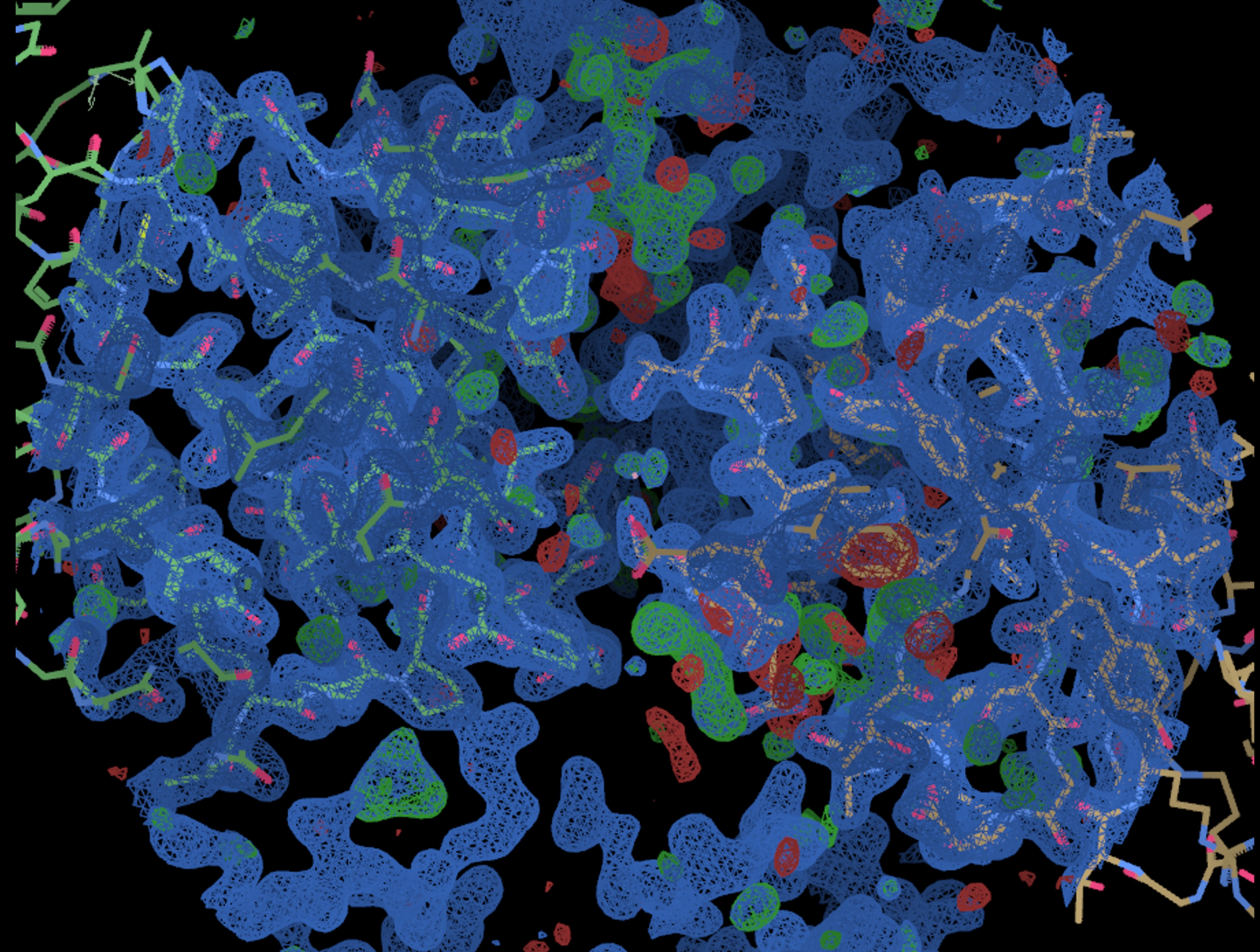
Rotation Centre Height 3.13

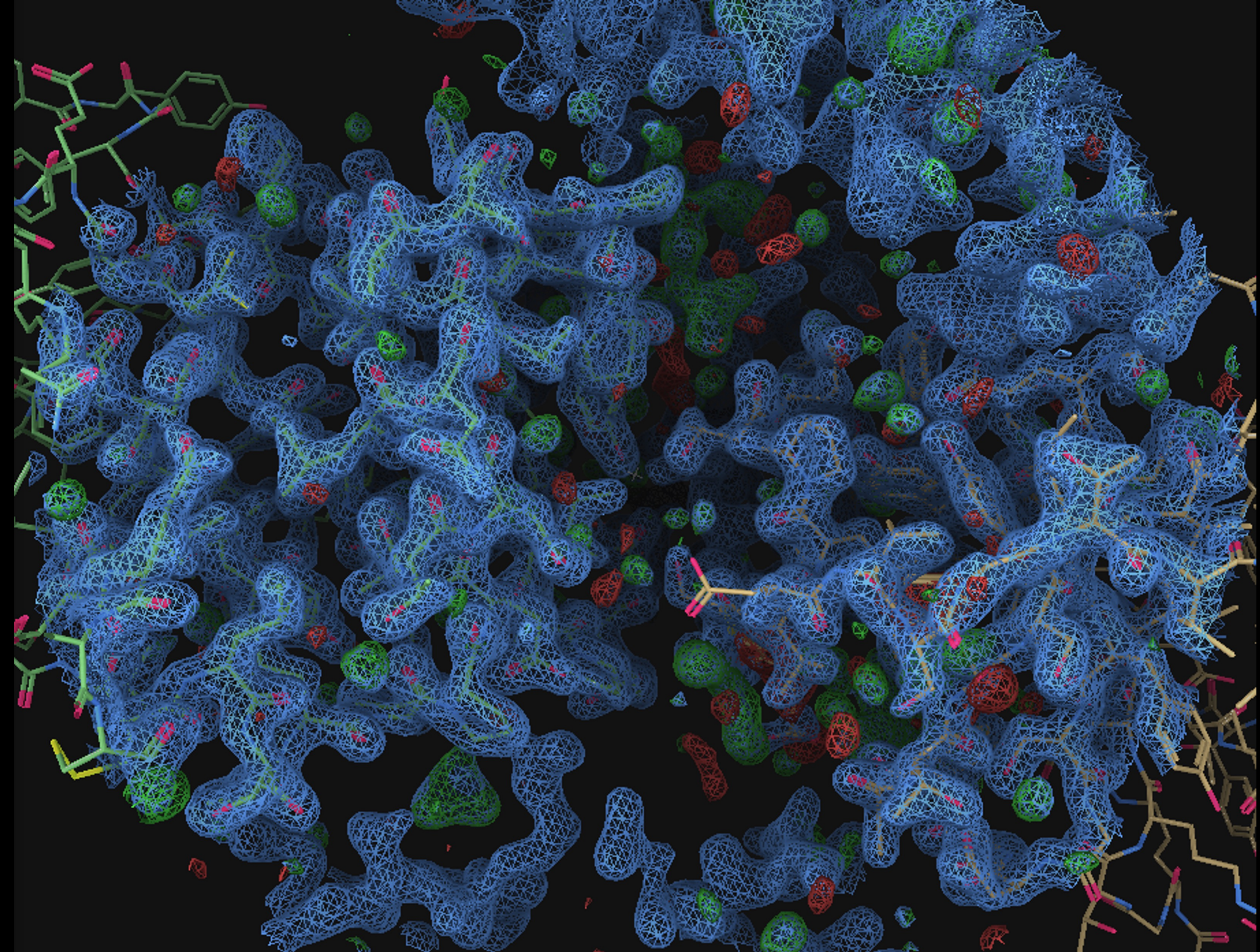
SSAO N-kernel points 319

Old Coot and New Coot



Dark-mode enabled by default



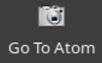


How Real-Space Refinement Has Improved

- By the addition of **interactive validation**
- By **updating the map**
structure factor calculation,
sigmaA calculation

Reset View

Display Manager



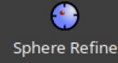
Go To Atom



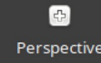
Go To Ligand

Clear Atom Pull Restraints

Auto-clear Atom Pull Restraints



Sphere Refine



Perspective



AO



Depth Blur



Fog

Pull
NBC|||||
Rama
Rotal

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

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

Pep-Flip This

Pep-Flip Next

Backrub Rotamer

Cis/Trans

JED Flip

Sidechain 180

Cancel

OK

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

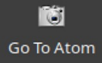
The screenshot displays the Coot software interface for real-space refinement. The main 3D view shows a protein structure with a semi-transparent higher-level contoured map. Colored bonds represent the fixed original structure, while grey bonds represent the refined atoms after real space refinement. The interface includes several key features:

- Dynamic Interactive Restraint Analysis:** A panel on the left showing restraint weights for Pull, NBC, Rama, and Rotal.
- Dynamic Active Residue Marker:** A marker highlighting the residue being refined.
- Rotamer Probability:** A tool for selecting the most probable rotamer conformation for a residue.
- Ramachandran Probability:** A tool for selecting the most probable Ramachandran conformation for a residue.
- Dynamic Rama Plot:** A 2D plot showing the distribution of Ramachandran angles for the residue.
- Semi-transparent higher level contoured map:** A map showing the density of the electron density.
- HUD Weight Tools:** A panel on the right showing the weights for various restraints (Torsion, Planar Peptide, Trans-peptide, Ramachandran, Secondary Structure, Alpha Helix, Beta Strand) and their overall weight.
- HUD Modelling Tools:** A panel on the right showing tools for peptide flipping, backbone rotamer selection, cis/trans isomerism, JED flip, and sidechain 180-degree rotation.

The status bar at the bottom indicates the current model parameters: (mol. no: 2) O /1/D/213 HOH occ: 1.00 bf: 30.00 ele: O pos: (41.79,17.12,20.78)

Reset View

Display Manager



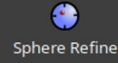
Go To Atom



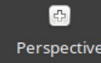
Go To Ligand

Clear Atom Pull Restraints

Auto-clear Atom Pull Restraints



Sphere Refine



Perspective



AO



Depth Blur



Fog

Pull
NBC|||||
Rama
Rotal

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

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

Pep-Flip This

Pep-Flip Next

Backrub Rotamer

Cis/Trans

JED Flip

Sidechain 180

Cancel

OK

Coot

File Edit Calculate Draw Measures Validate About Test 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 II
Rama
RotaII

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

German-McClure alpha: 0.01

Lennard-Jones epsilon: 1.0

Rama Restraints Weight: 1.0

Torsion Weight: 1.0

Close

R/R/C

Map...

- Real Space Refinement
- Regularization
- Fixed Atoms...
- Rigid Body Fit
- Rotation/Translation
- Autofit Rotamer
- Rotamers
- Edit Chi Angles
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- 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)

Reset View Display Manager

Go To Atom

Go To Ligand

Clear Atom Pull Restraints

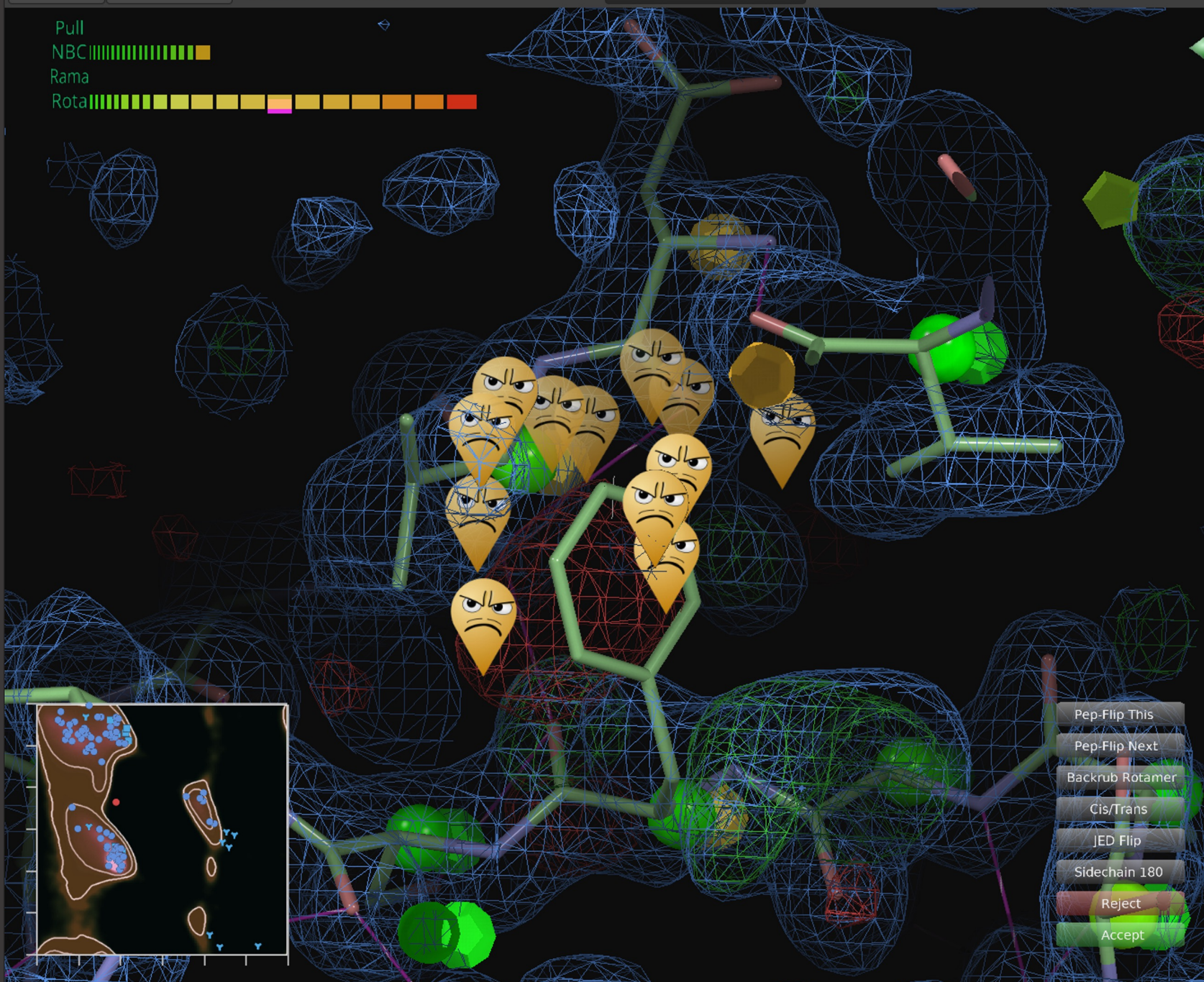
Auto-clear Atom Pull Restraints

Sphere Refine

Perspective

Fog

Long5



- 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
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- Add Terminal Residue
- Add Alt Conf...
- Place Atom at Pointer
- Clear Pending Picks
- Delete
- Refmac
- Undo
- Redo

- Pep-Flip This
- Pep-Flip Next
- Backrub Rotamer
- Cis/Trans
- JED Flip
- Sidechain 180
- Reject
- Accept

Reset View Display Manager

Go To Atom

Go To Ligand

Clear Atom Pull Restraints

Auto-clear Atom Pull Restraints

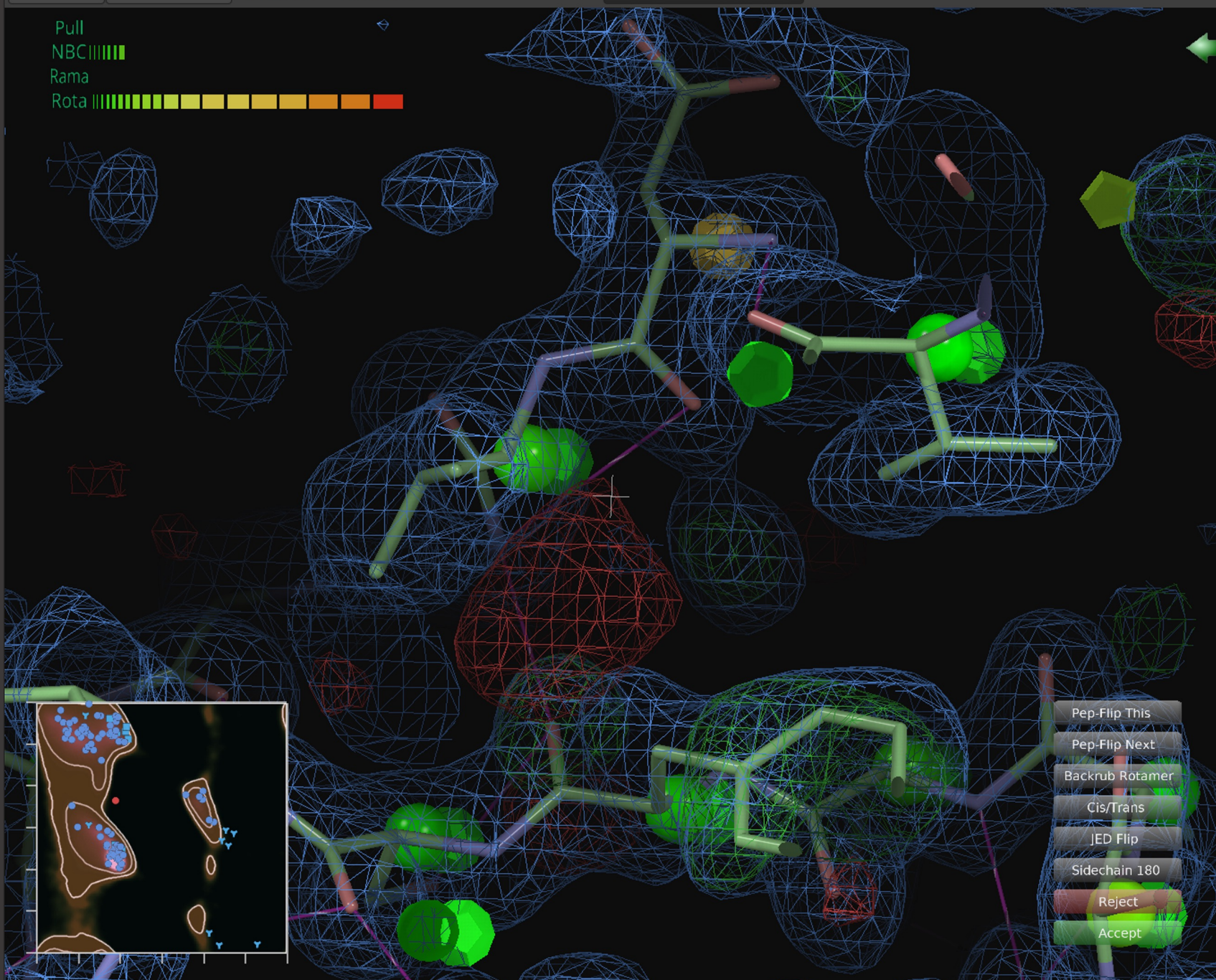
Sphere Refine

Perspective

Fog

Long5

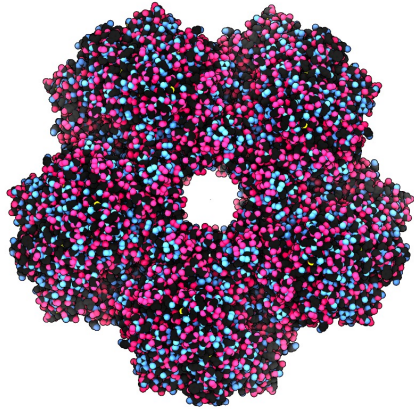
Pull
NBCI |||||
Rama
Rota |||||



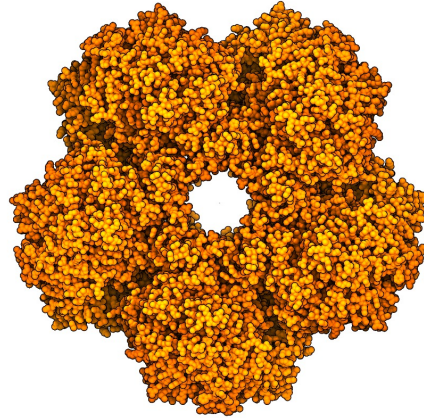
- Pep-Flip This
- Pep-Flip Next
- Backrub Rotamer
- Cis/Trans
- JED Flip
- Sidechain 180
- Reject
- Accept

- R/RC
- Map...
- Real Space Refinement
- Fixed Atoms...
- Rigid Body Fit
- Rotate/Translate
- Autofit Rotamer
- Rotamers
- Edit Chi Angles
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- Simple Mutate
- Add Terminal Residue
- Add Alt Conf...
- Place Atom at Pointer
- Clear Pending Picks
- Delete
- Refmac
- Undo
- Redo

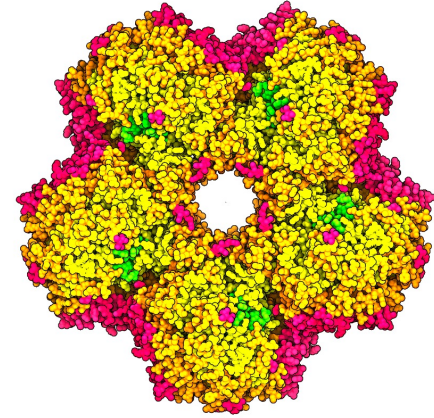
New Coot Graphics



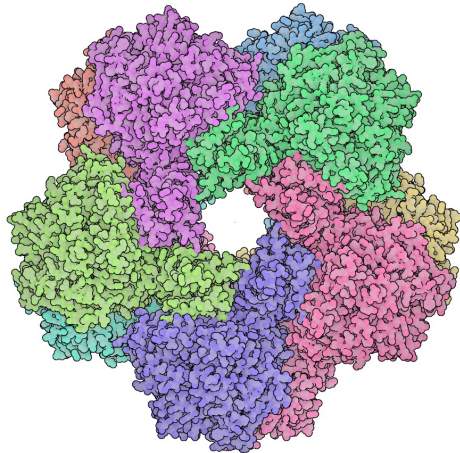
colour by atoms



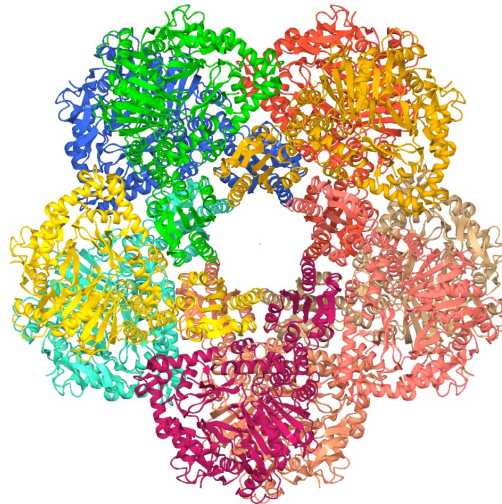
colour by molecule



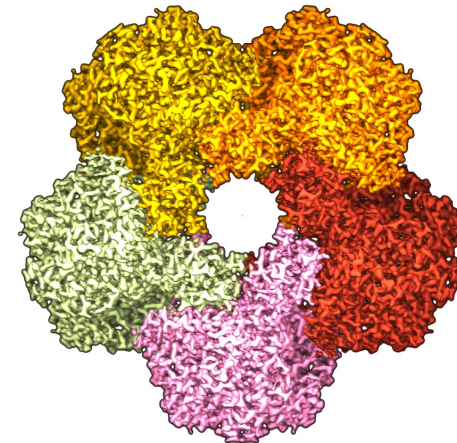
colour by B factors



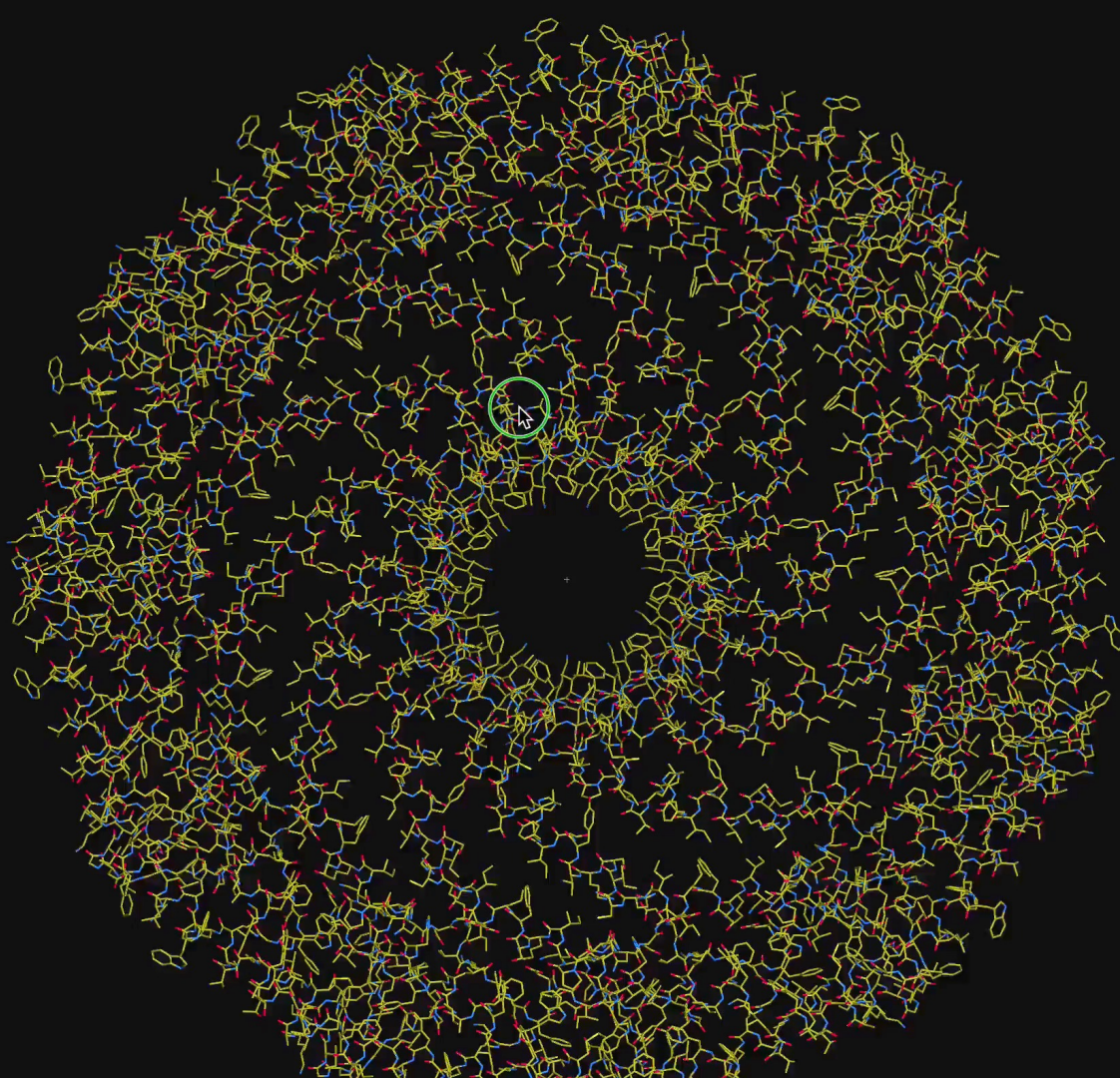
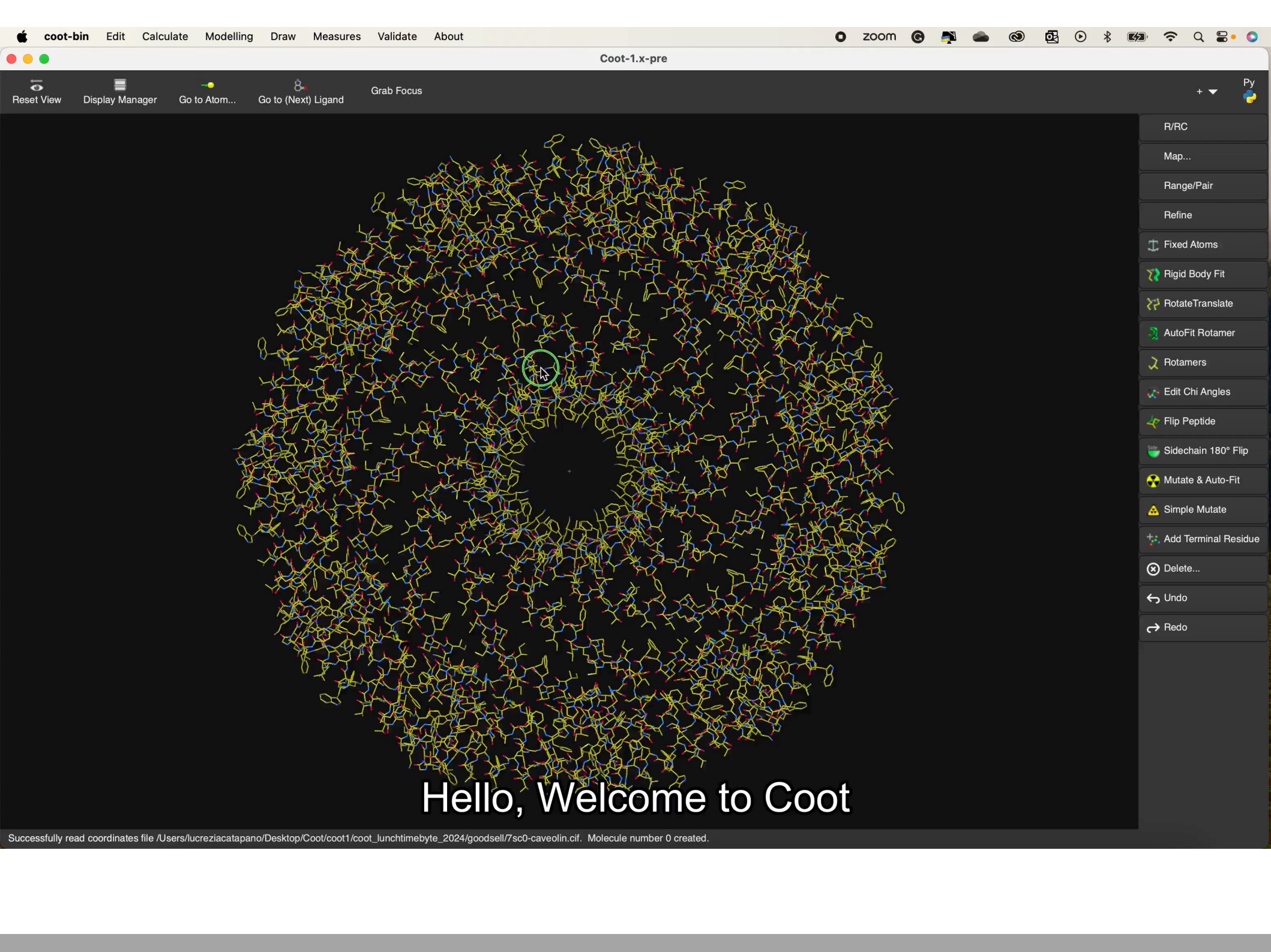
Goodsell colours



ribbons



masked map



- R/RC
- Map...
- Range/Pair
- Refine
- Fixed Atoms
- Rigid Body Fit
- Rotate/Translate
- 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

Moorhen

Web-Based Interactive Model Building

This is a coot

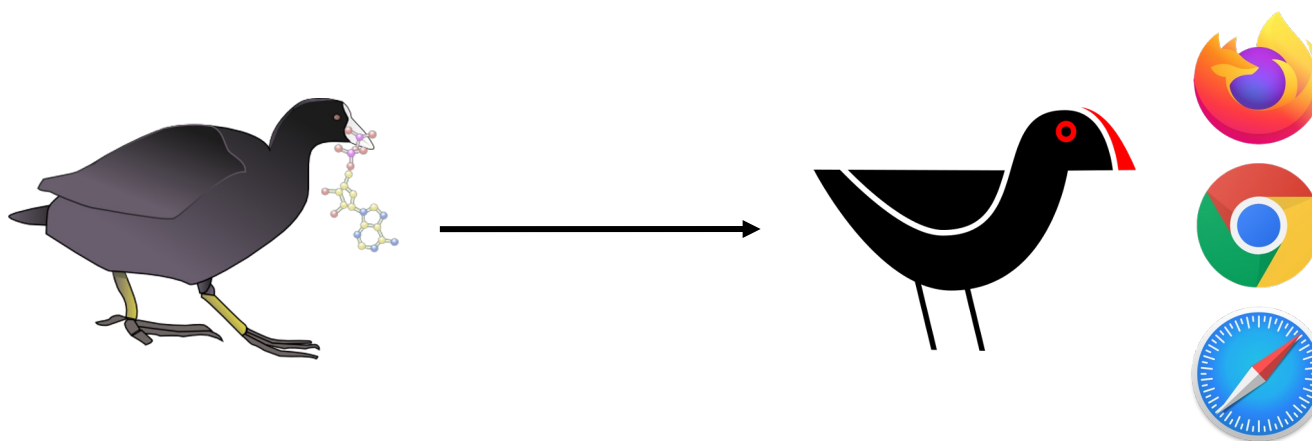


This is a moorhen



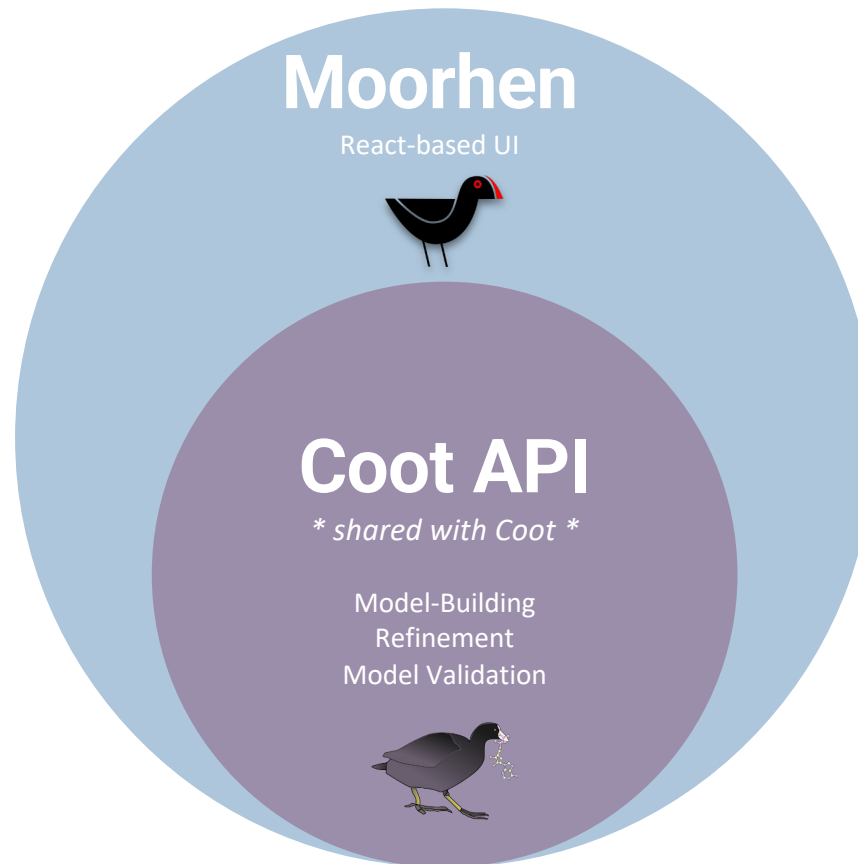
What is Moorhen?

- 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



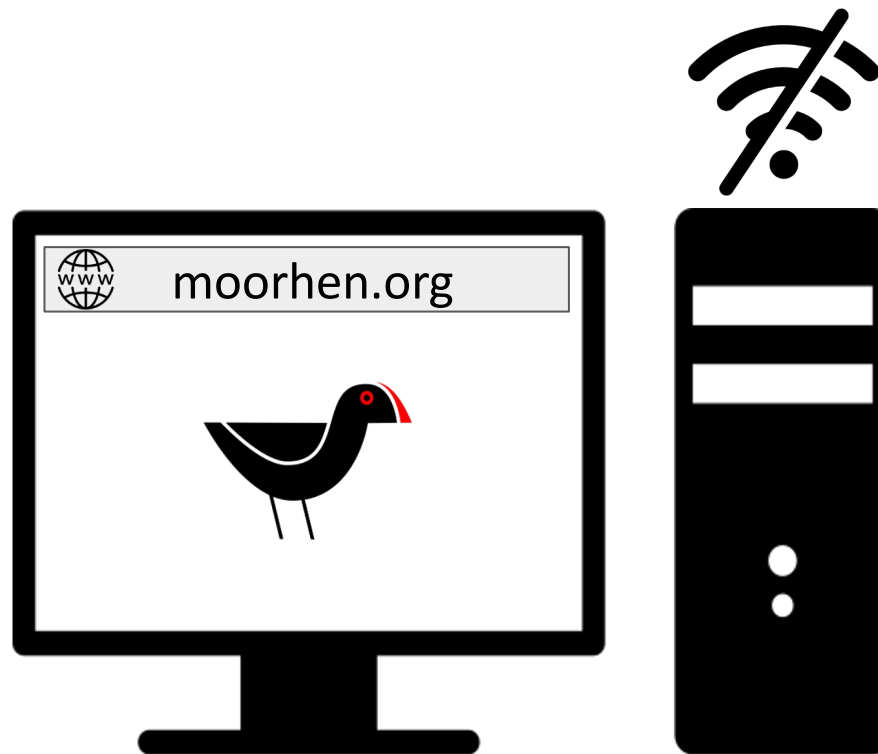
What is Moorhen?

→ 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	

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, 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

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

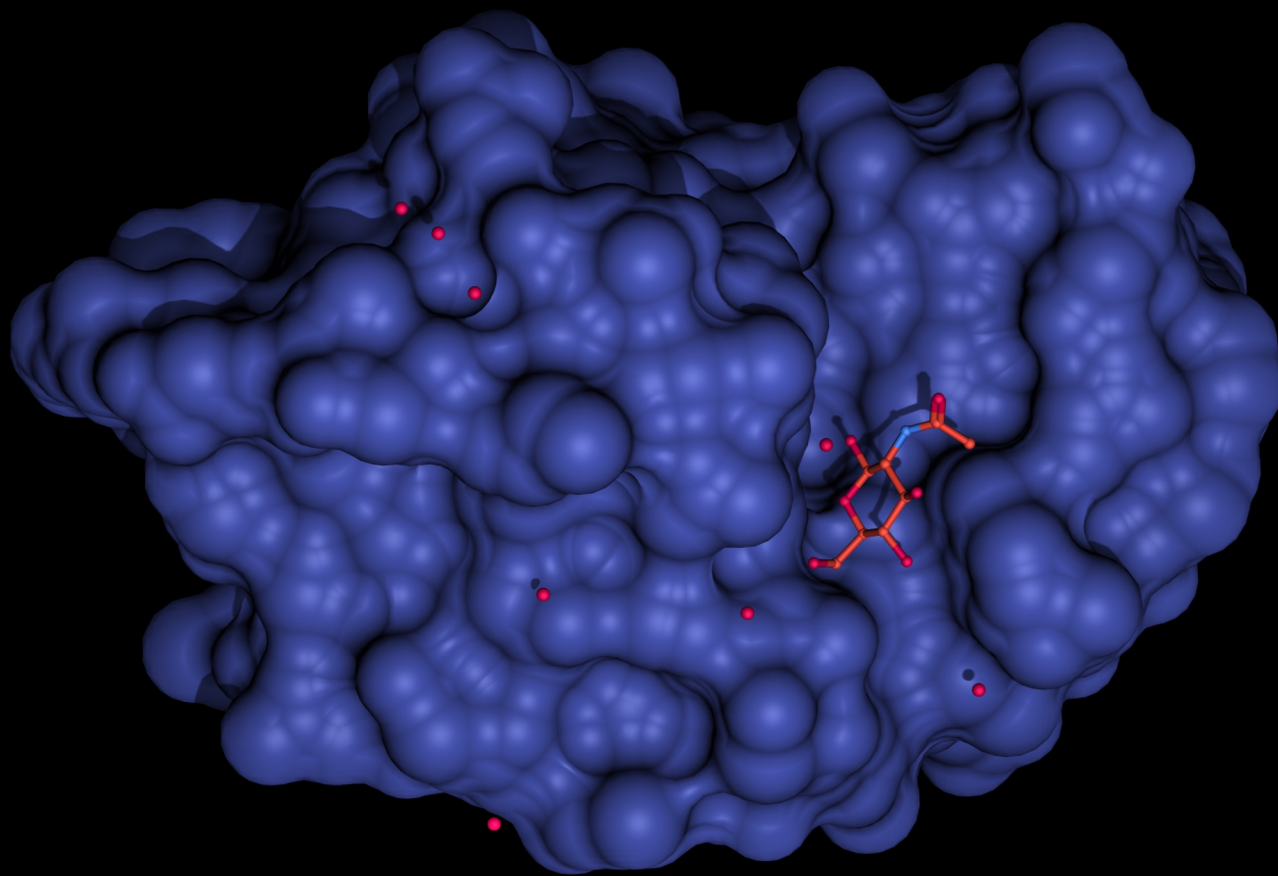
Env. Distances

Validation Features

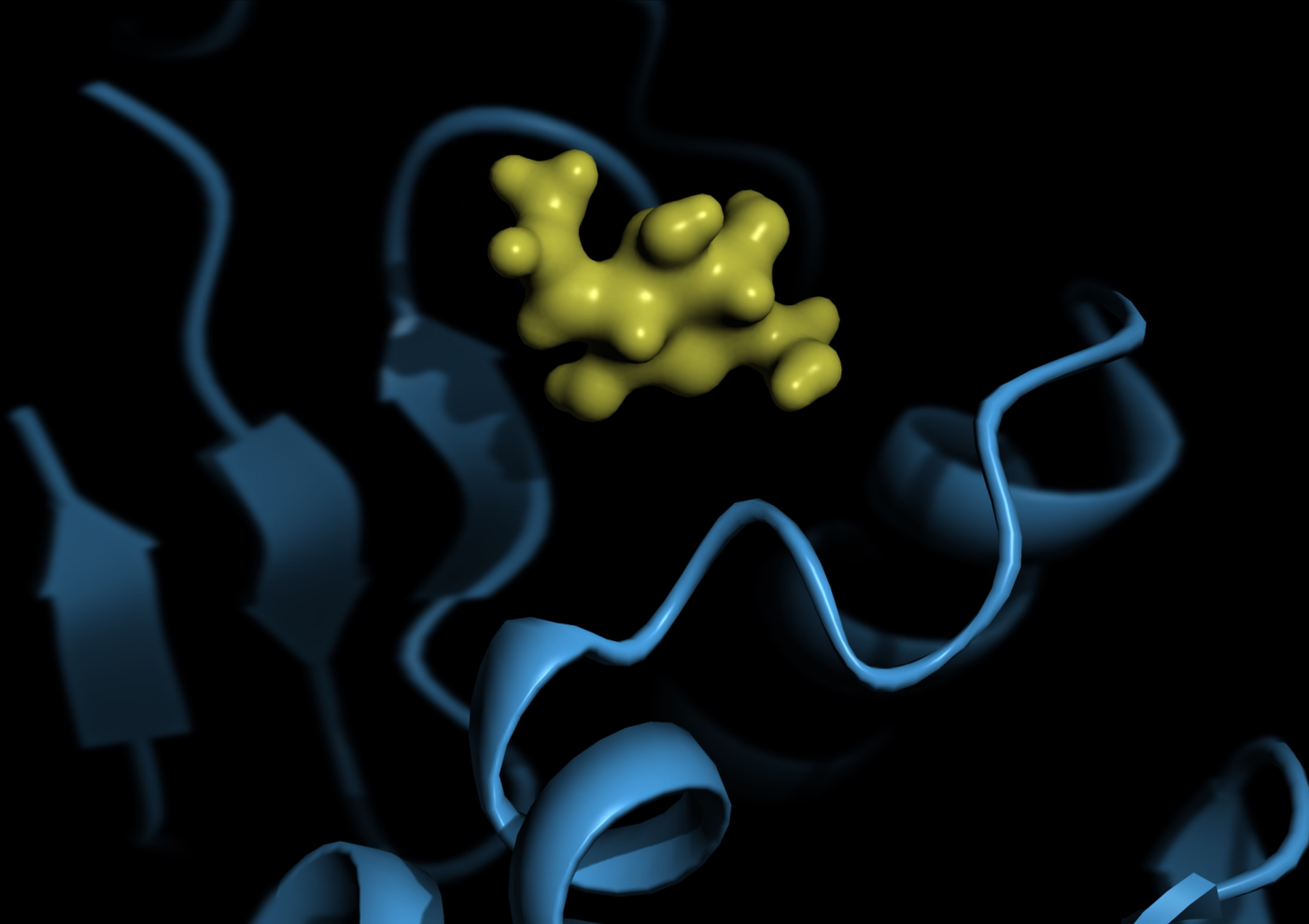
Rama. Plot	Unmodeled Blobs
Density Fit	Diff. Map Peaks
Geom. Analysis	Combined Validation Plot
Rotamers	

Figure-Making Features

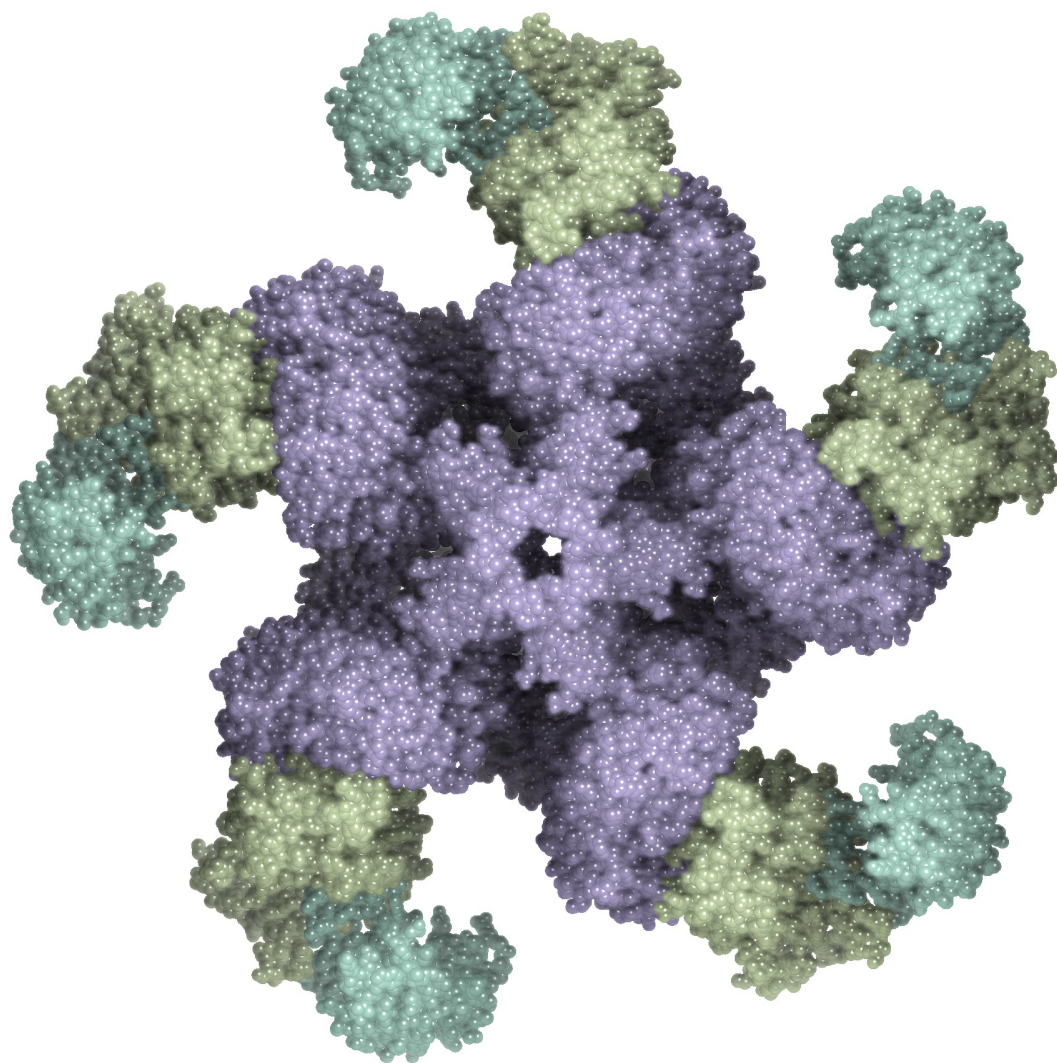
Multiple Model Representation Styles	Arbitrary Colour schemes	Basic Movie Making
Shadows	Depth Blur	Perspective Projection
Clipping/Fogging	Ambient Occlusion	Screenshots



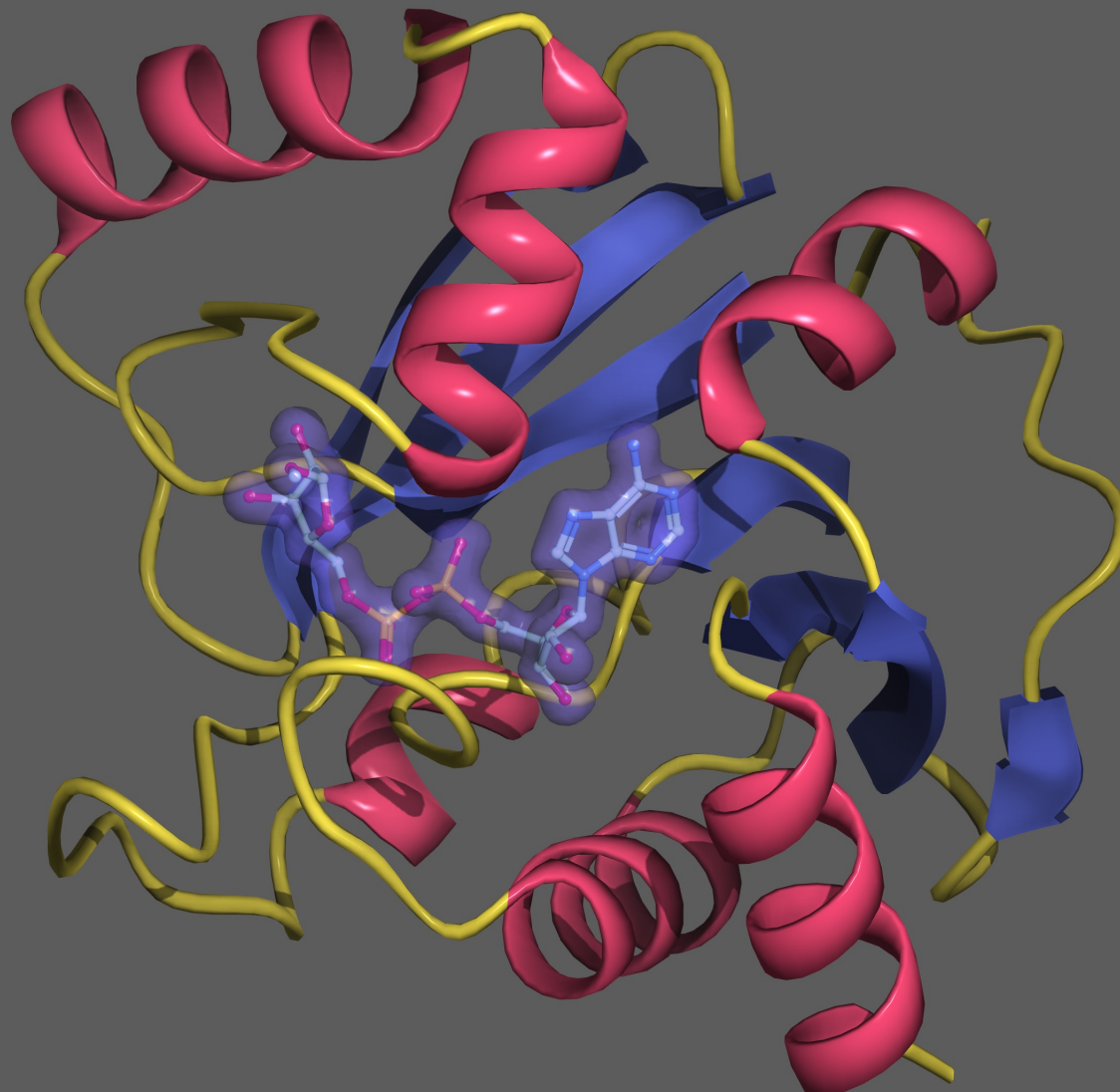
Shot on Moorhen



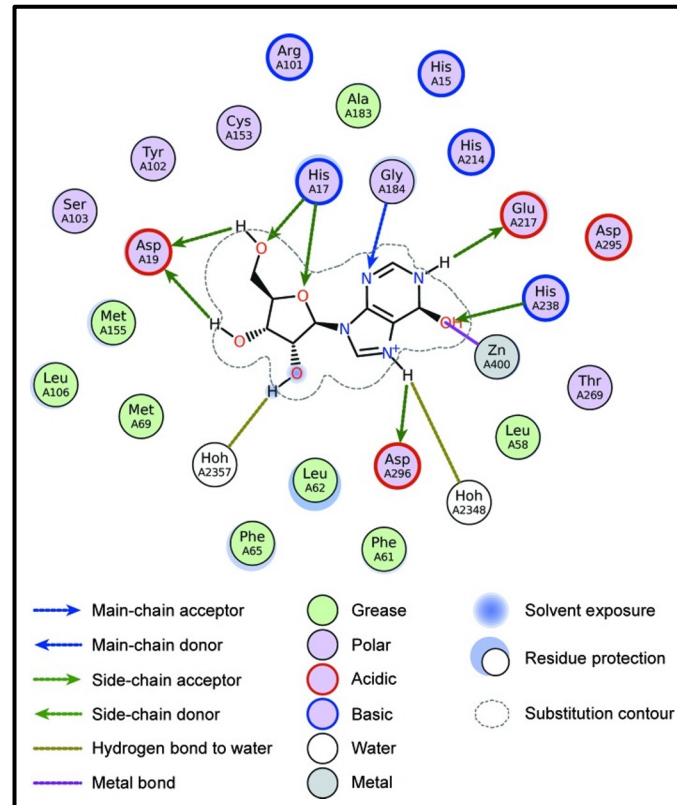
Shot on Moorhen



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

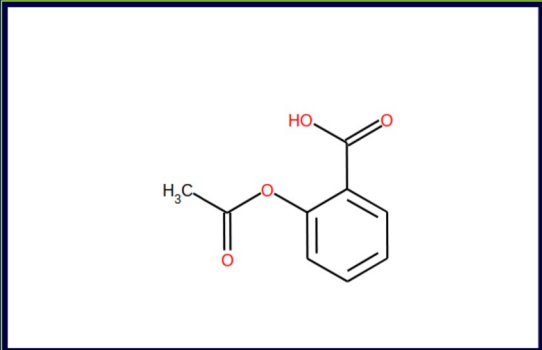
Welcome to Lhasa!
Lhasa is a WebAssembly port of Layla - Coot's Ligand Editor.
Lhasa is experimental software.
This is a demo UI for development purposes.

Move Rotate Flip around X Flip around Y Delete hydrogens Format

Single Bond Double Bond Triple Bond Geometry Charge Delete

3-C 4-C 5-C 6-C 6-Arom 7-C 8-C

C
N
O
S
P
H
F
Cl
Br
I
X



▶

SCALE 1
[-] [+]

DISPLAY MODE

SMILES

Undo Redo

Written by Jakub Smulski

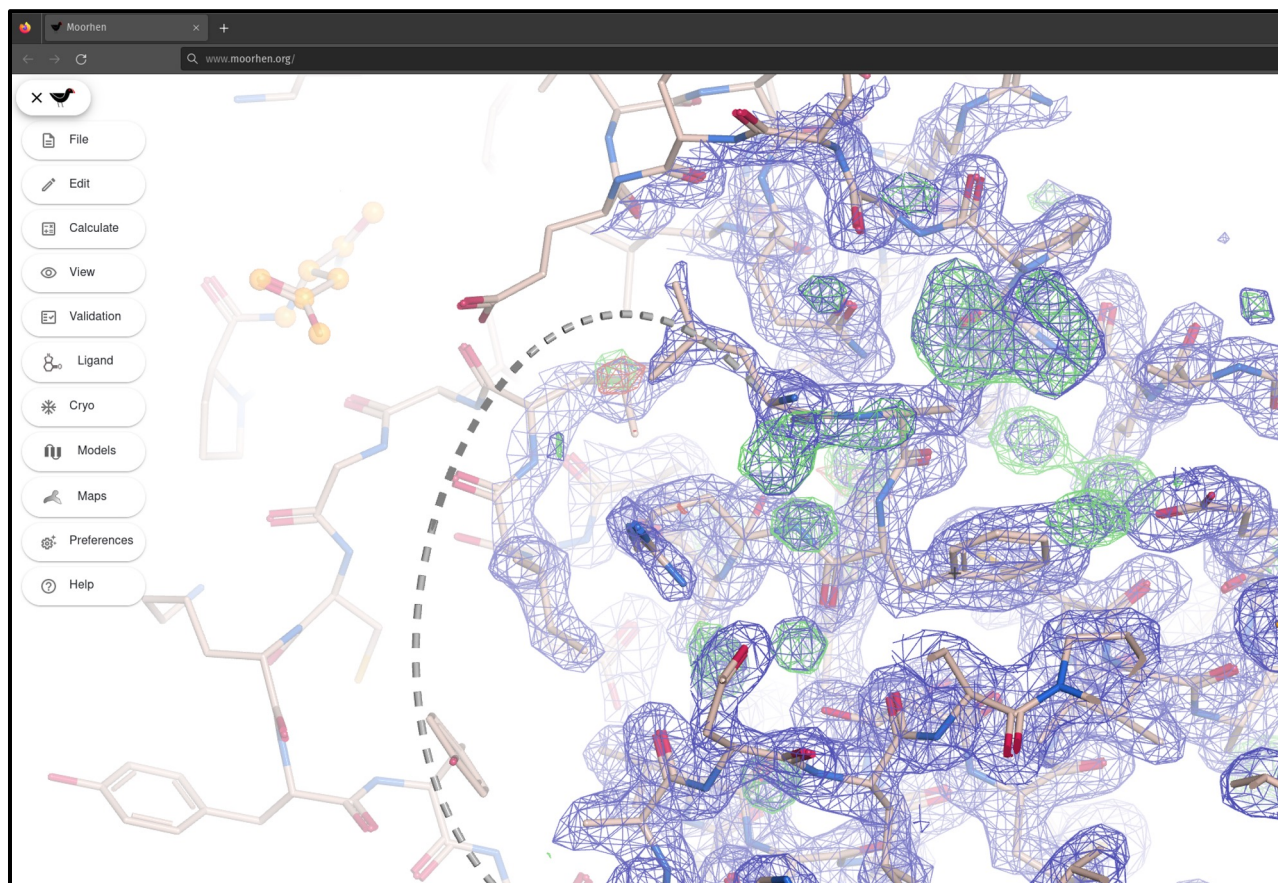
Provide input for dictionary generators:

- eIBOW
- AceDRG
- Grade 2

Source: Jakub Smulski

Where is Moorhen available?

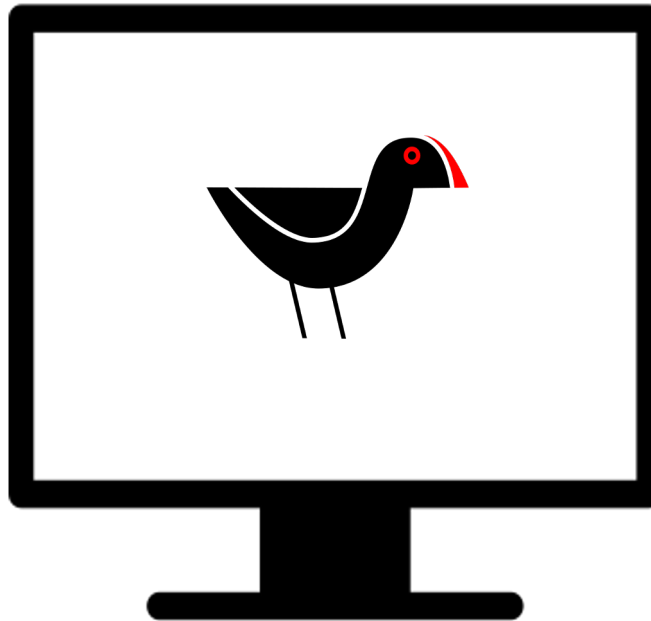
www.moorhen.org



Where is Moorhen available?



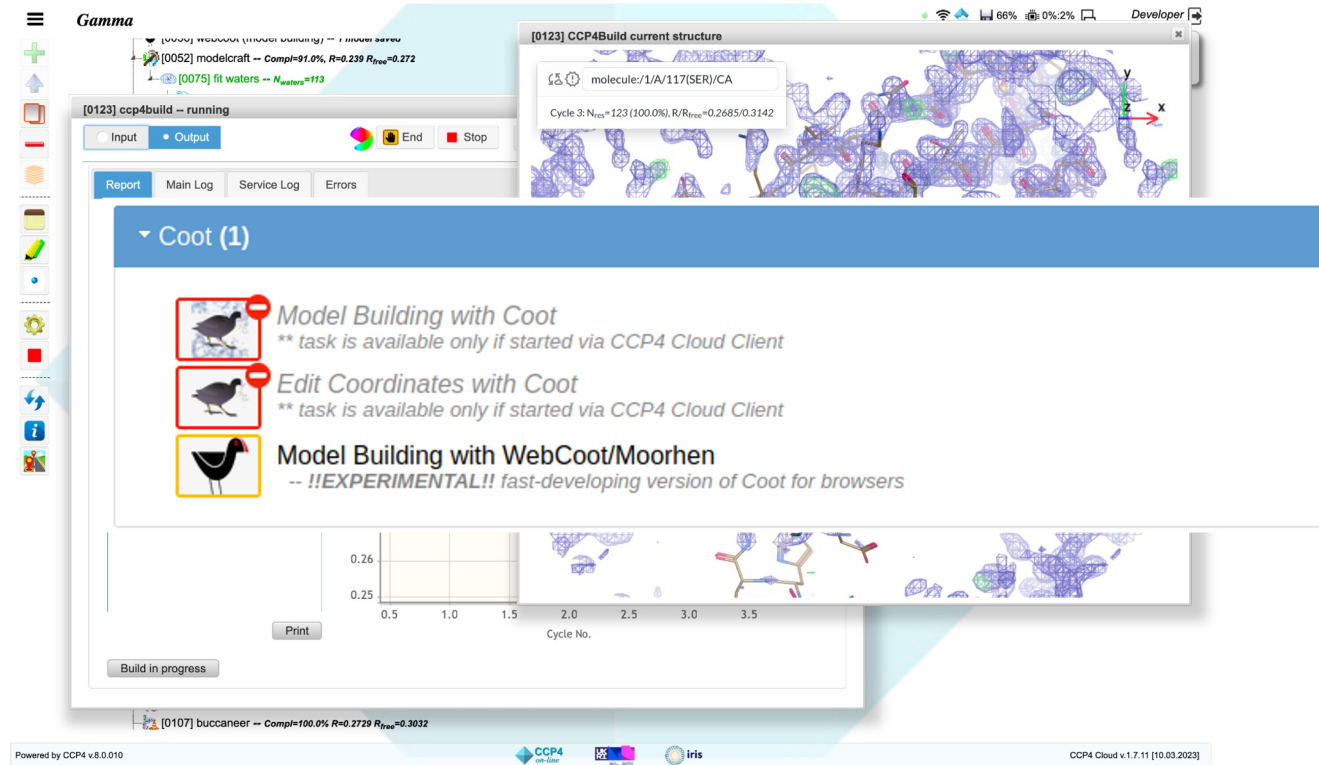
Electron Desktop
App






Where is Moorhen available?



CCP4 Cloud



The screenshot displays the CCP4 Cloud interface. At the top, there are several task windows: '[0052] modelcraft -- Compl=91.0%, R=0.239 R_{free}=0.272', '[0075] fit waters -- N_{waters}=113', and '[0123] ccp4build -- running'. A 'Coot (1)' window is open, showing a list of tasks:

-  **Model Building with Coot**
** task is available only if started via CCP4 Cloud Client
-  **Edit Coordinates with Coot**
** task is available only if started via CCP4 Cloud Client
-  **Model Building with WebCoot/Moorhen**
-- **!!EXPERIMENTAL!!** fast-developing version of Coot for browsers

Below the task list, there is a graph showing 'Cycle No.' on the x-axis (0.5 to 3.5) and a y-axis with values 0.25 and 0.26. A 'Print' button is located below the graph. At the bottom of the interface, there is a status bar with the text 'Powered by CCP4 v.8.0.010', the CCP4 logo, the Iris logo, and 'CCP4 Cloud v.1.7.11 [10.03.2023]'.

Where is Moorhen available?



Project: ~/ccpem-project

PROJECT JOBS NODES NEW JOB

Filter jobs by type or alias

- 7 - Fetch - coot-em-tutorial
- 6 - Fetch - occupy-16890

RESULTS LOGS I/O PARAMS

Open with: PDF VIEWER TEXT EDITOR UGLYMOL MOL' MOORHEN TERMINAL

Inputs to this job: no inputs

Outputs from this job:

- Fetch/job007/emd_32143.mrc DensityMap from_emdb
- Fetch/job007/pdb7vv1.pdb AtomCoords from_pdb

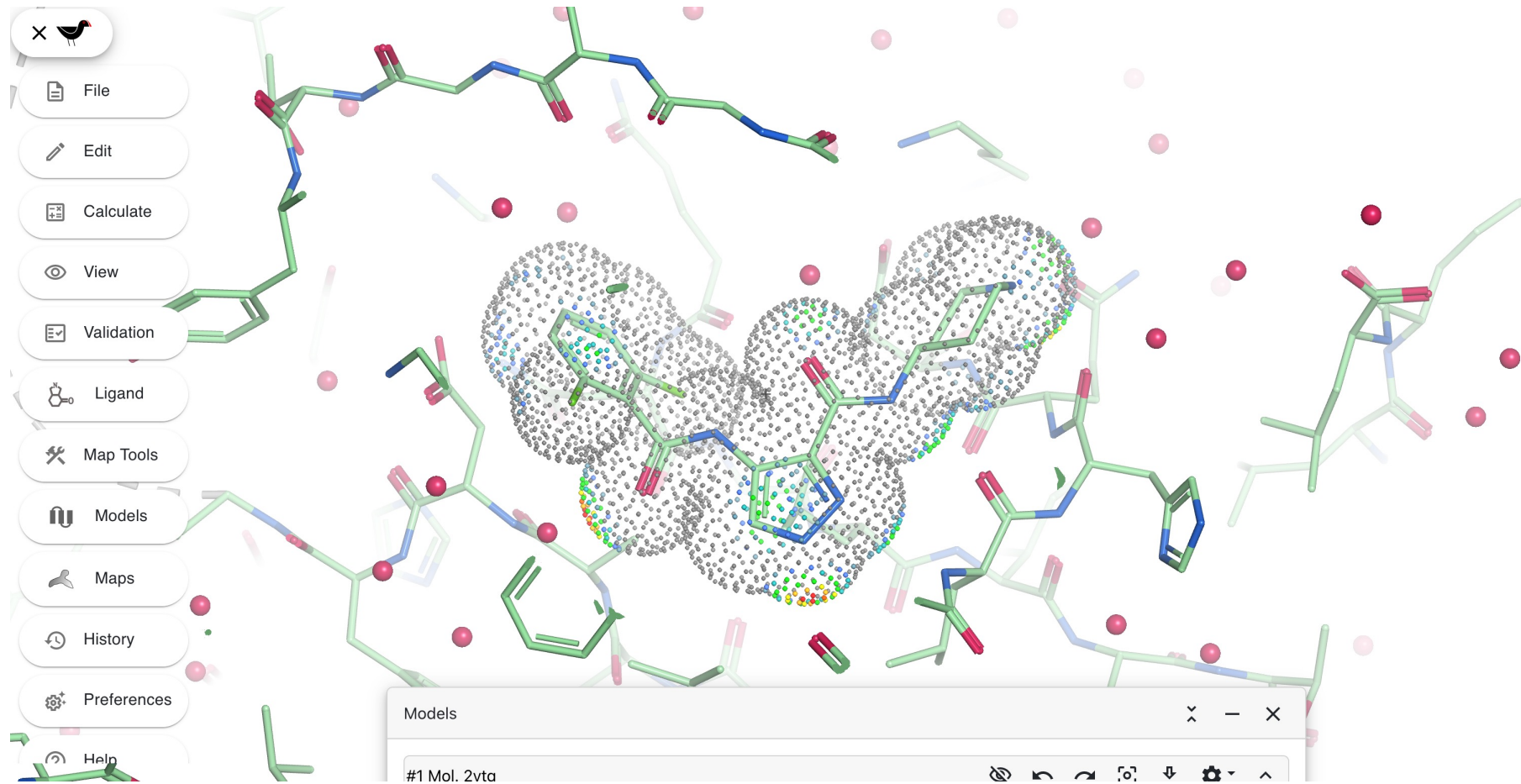
A black arrow points from the bottom right towards the "MOORHEN" button in the "Open with:" section.

Moorhen - Ligand validation

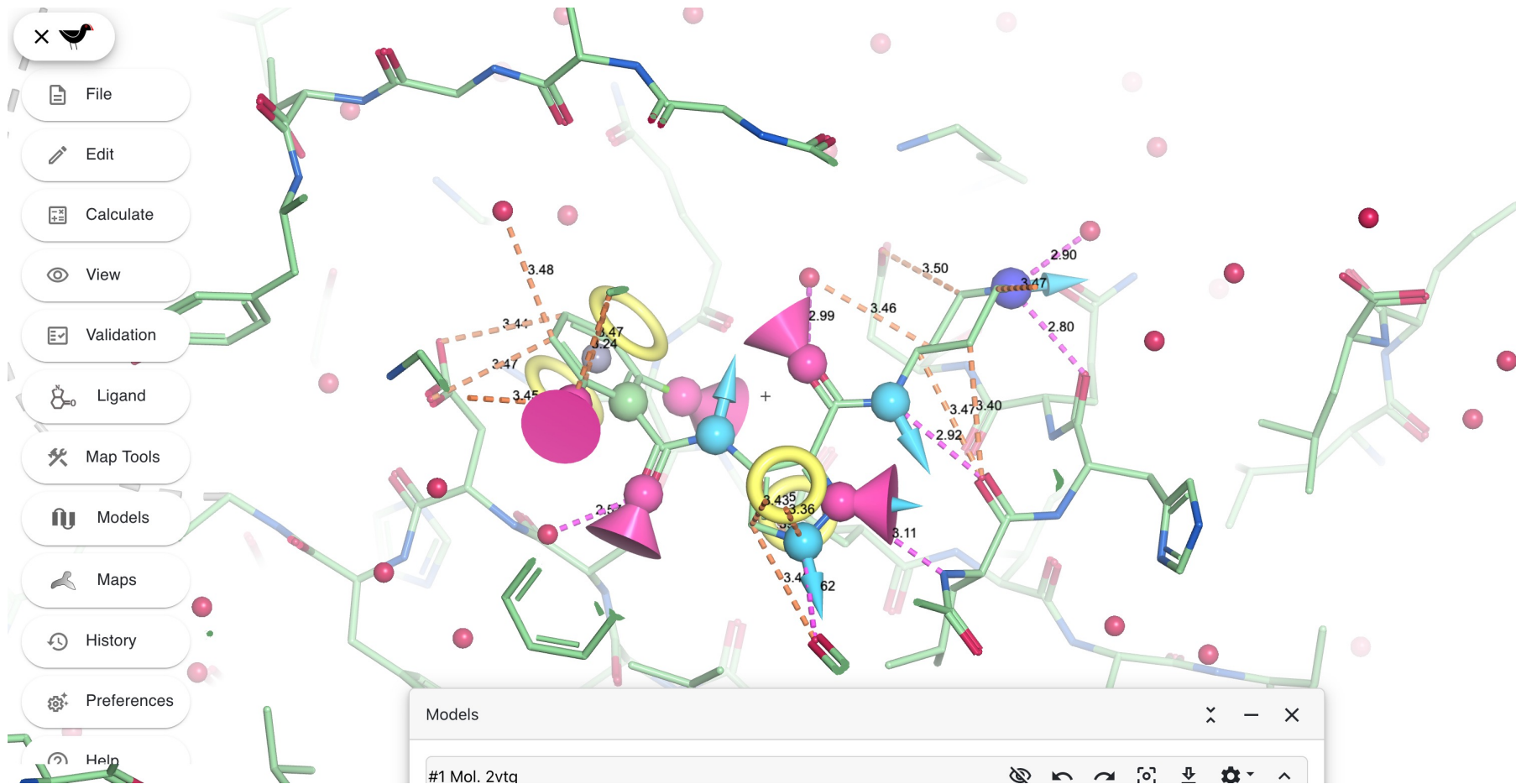
The image displays the Moorhen software interface for ligand validation. On the left, a vertical toolbar contains icons and labels for: File, Edit, Calculate, View, Validation, Ligand, Map Tools, Models, Maps, History, Preferences, and Help. The main window shows a 3D molecular model of a protein-ligand complex. A 'Models' panel is open, displaying the following information:

- Model ID: #1 Mol. 2vtq
- Representation options: Bonds (selected), Adapt. Bonds, C-Alpha, Ribbons, Ligands, Gauss. Surf., Mol Surf., Bases, Spheres, Rama. Balls, Rota. Dodec., Cont. dots, H-Bonds, Glyco-Blocks, Restraints.
- Sequences: (collapsed)
- Ligands: (expanded) showing a chemical structure of a ligand with a benzene ring substituted with two fluorine atoms (F), an imidazole ring, and a piperidine ring.
- Validation options: /1/A/1299(LZA) (selected), Cont. dots, Chem. Feat., Env. Dist., and Geom. Validation.

Moorhen - Ligand validation

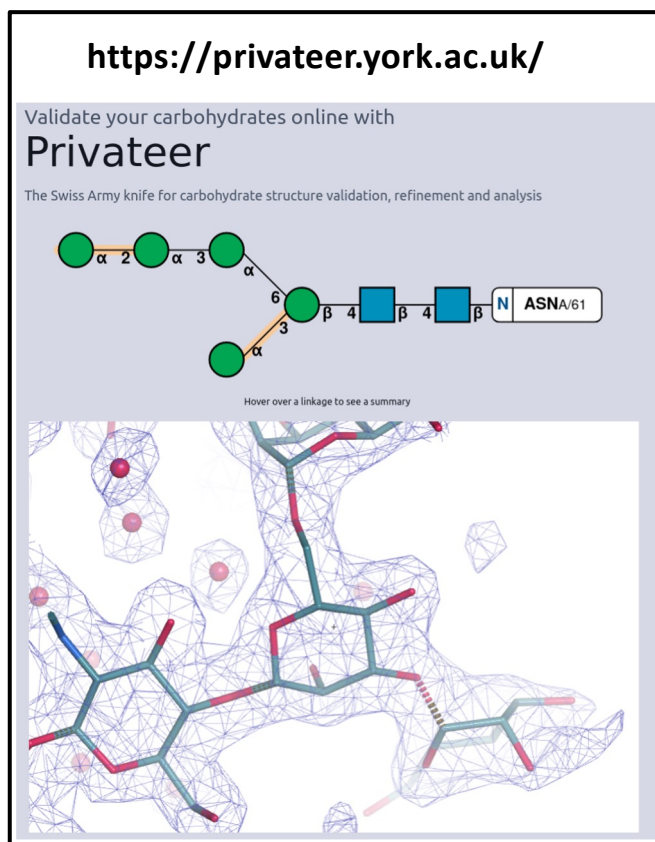


Moorhen - Ligand validation



Moorhen as a React component

→ Moorhen can be easily integrated to any other website to extend 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



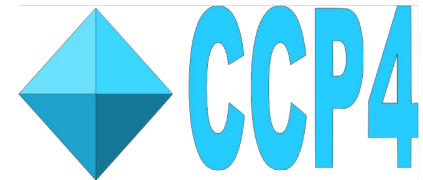
Eugene
Krissinel



Jakub
Smulski




Martin
Noble



... And everyone who has contributed to CCP4

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