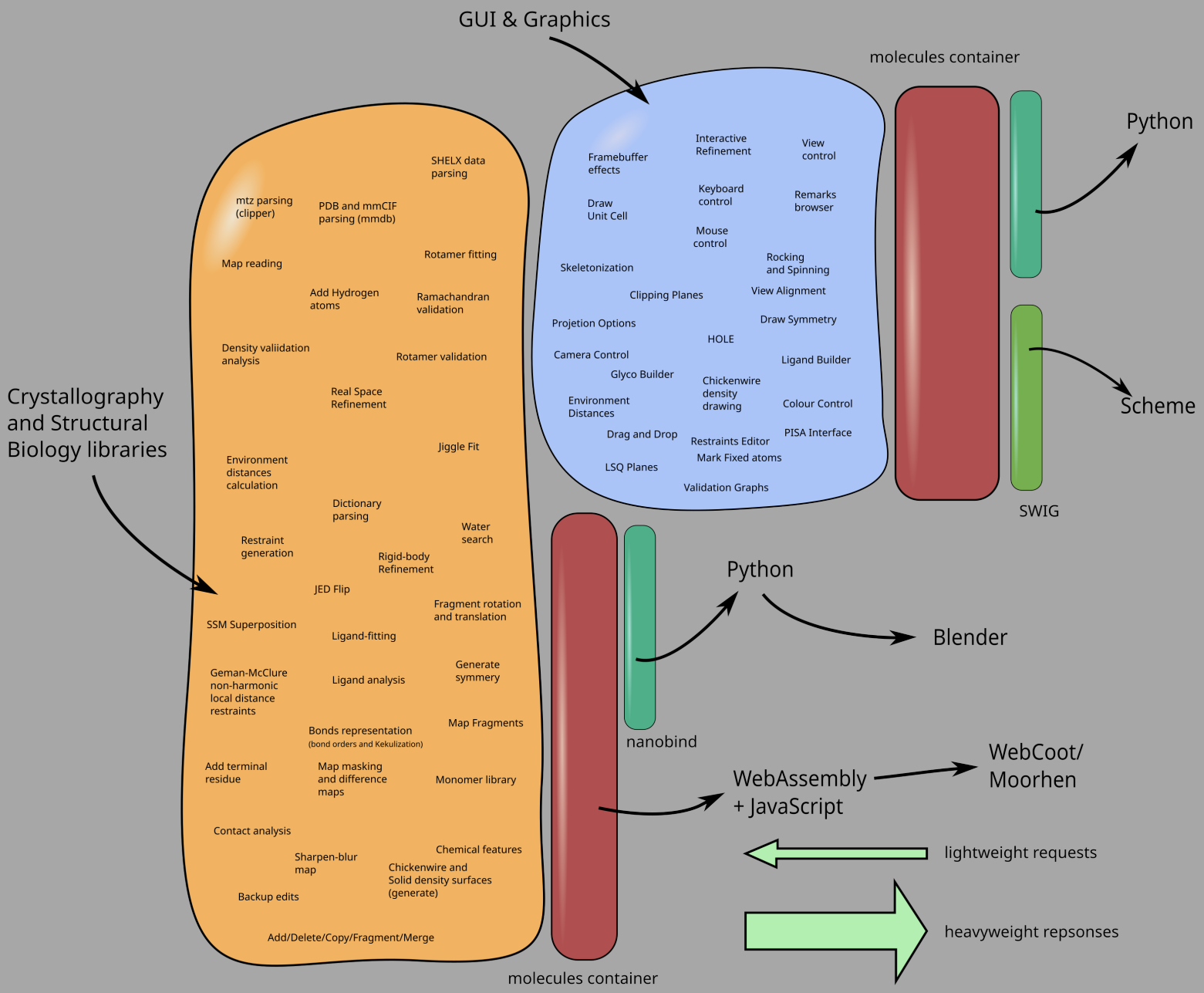
What's New in The Land Of Coot?

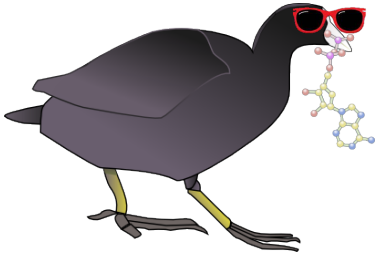
Lucrezia Catapano

CCP4 Study Weekend 2025

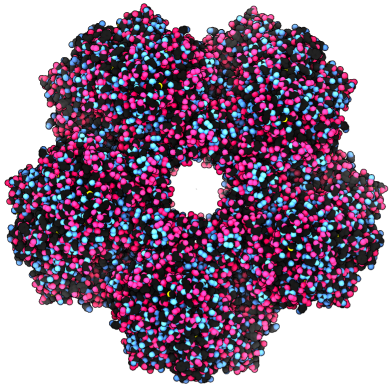
Coot infrastructure



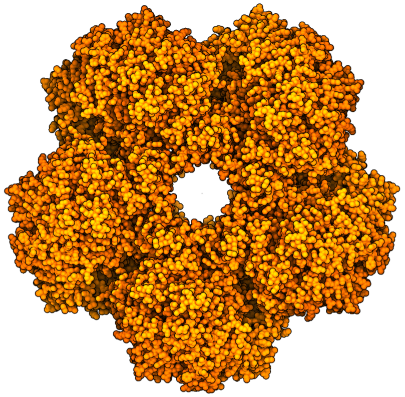
What's new in Coot 1.1?



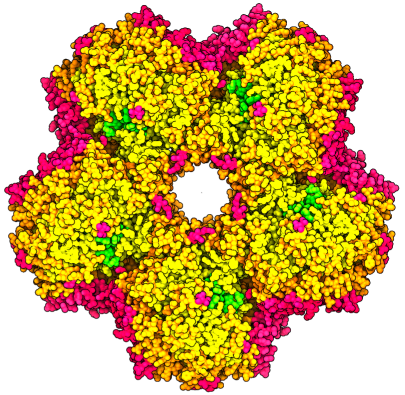
Attractive graphics



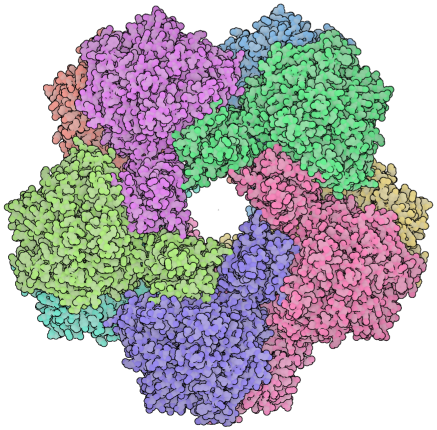
colour by atoms



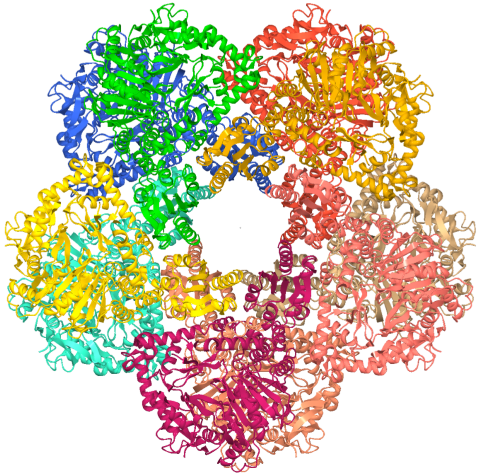
colour by molecule



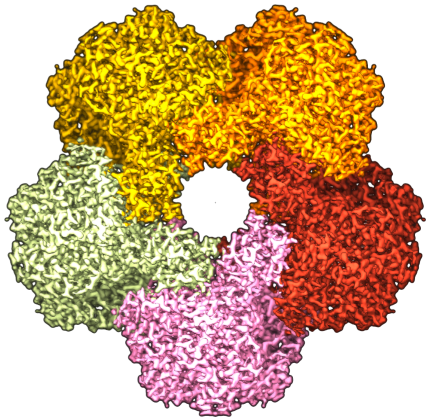
colour by B factors



Goodsell colours

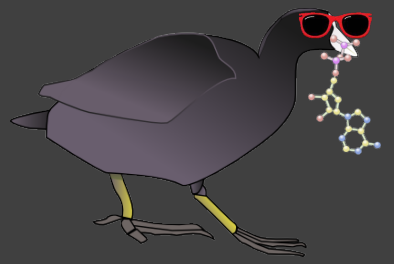


ribbons

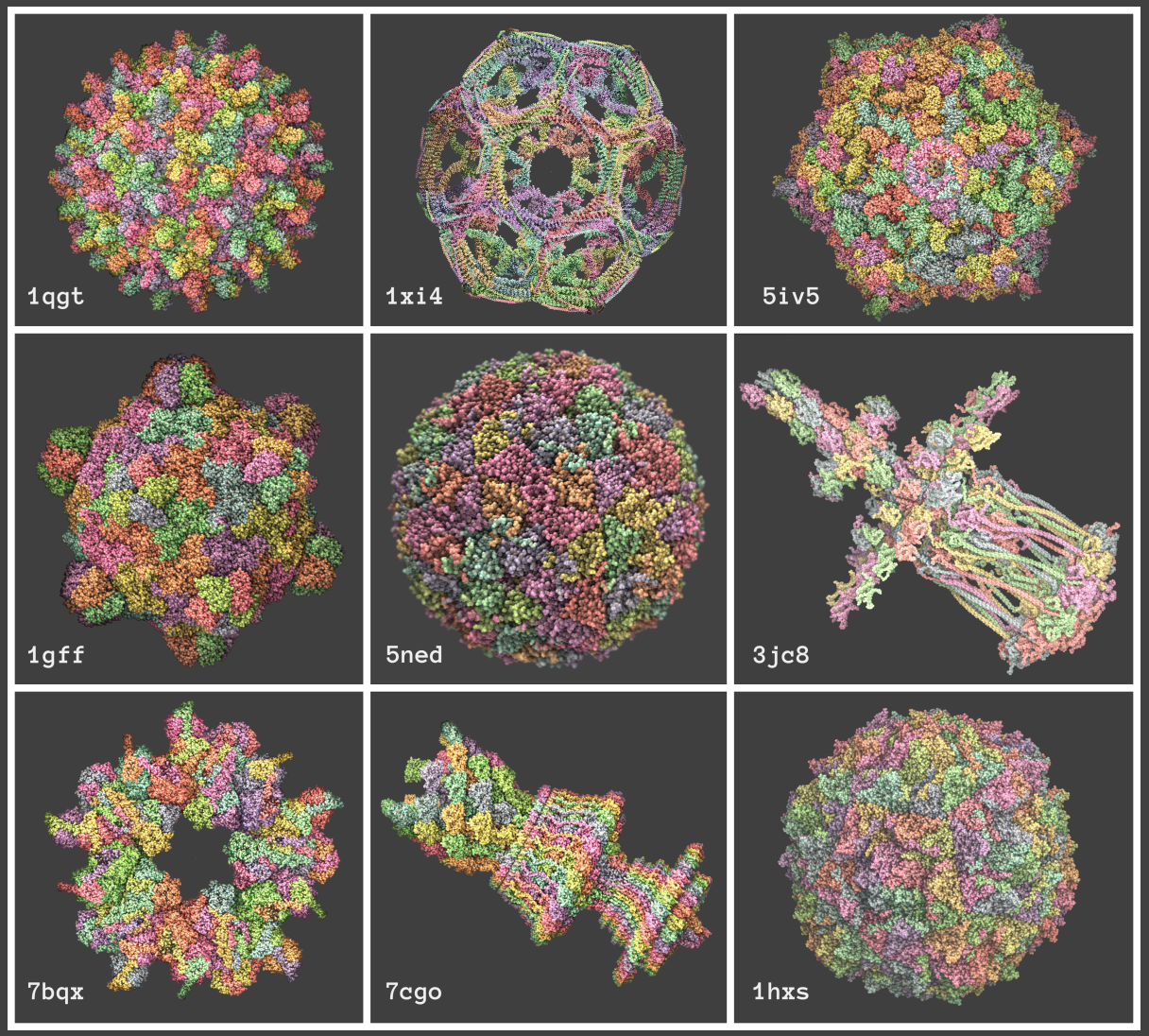


masked map

What's new in Coot 1.1?



Attractive graphics



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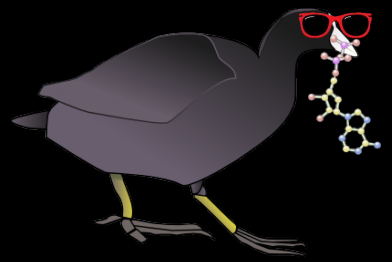
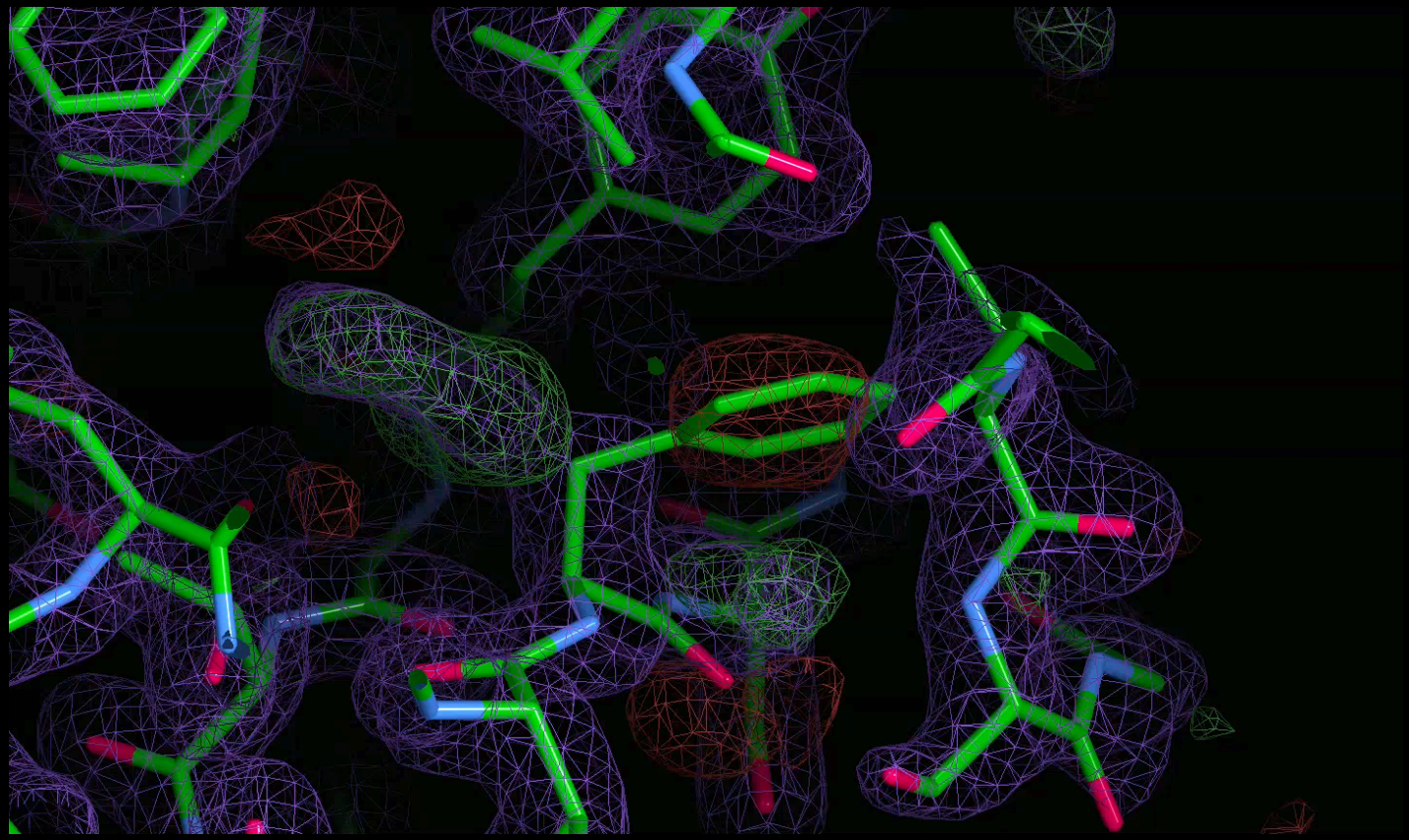


Noughties Physics has been re-introduced

Standard physics of atom movement



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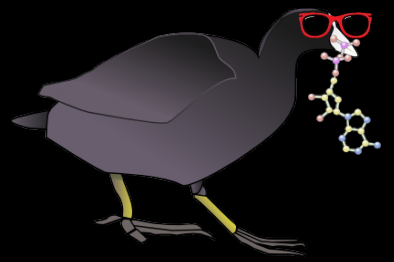
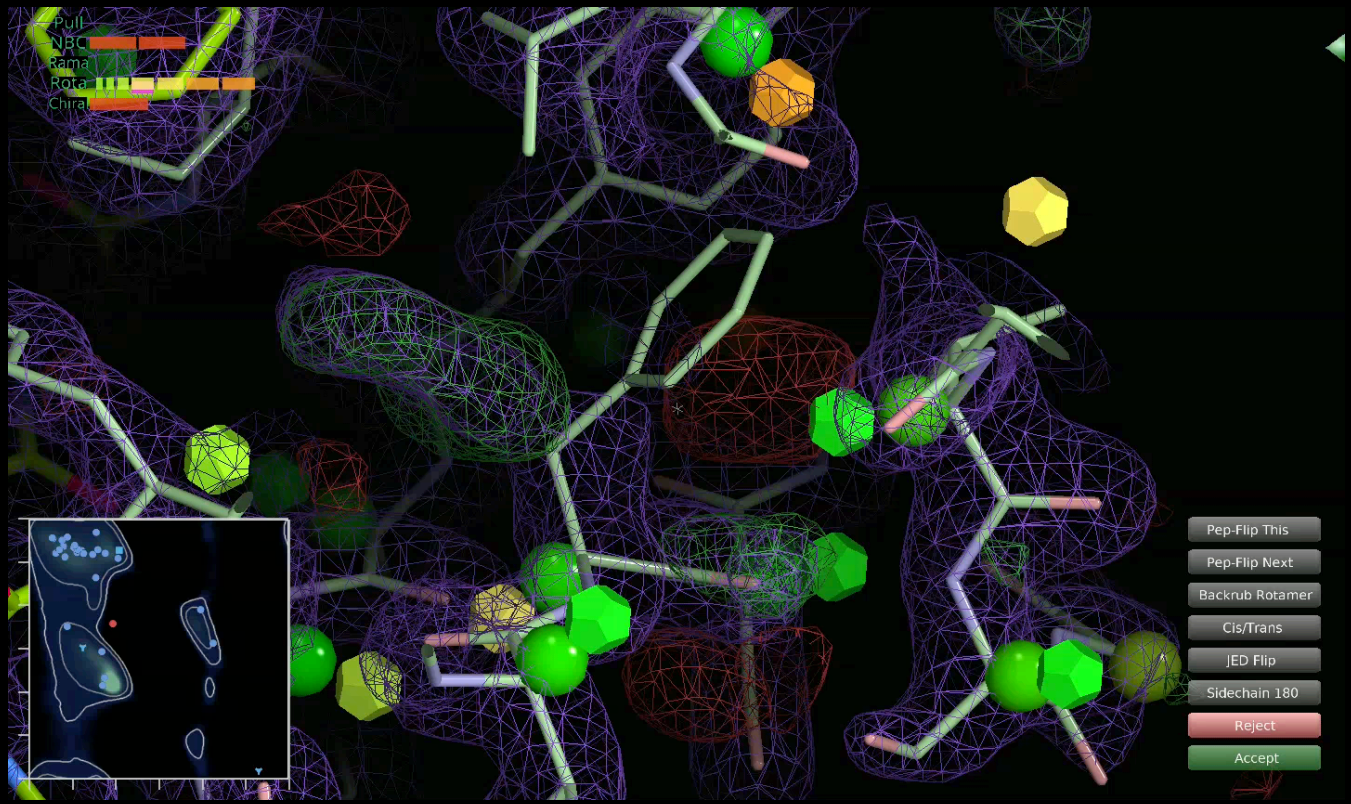


Noughties Physics has been re-introduced

- We restore noughties physics (from coot 0.8)
- elastic deformation of the atom positions as the picked atom is dragged without refinement (it doesn't care about bond distorsions until you release the mouse)



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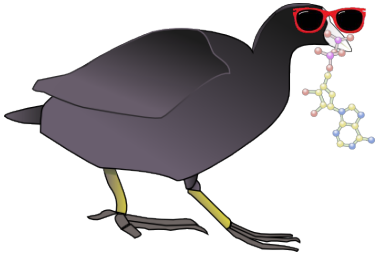
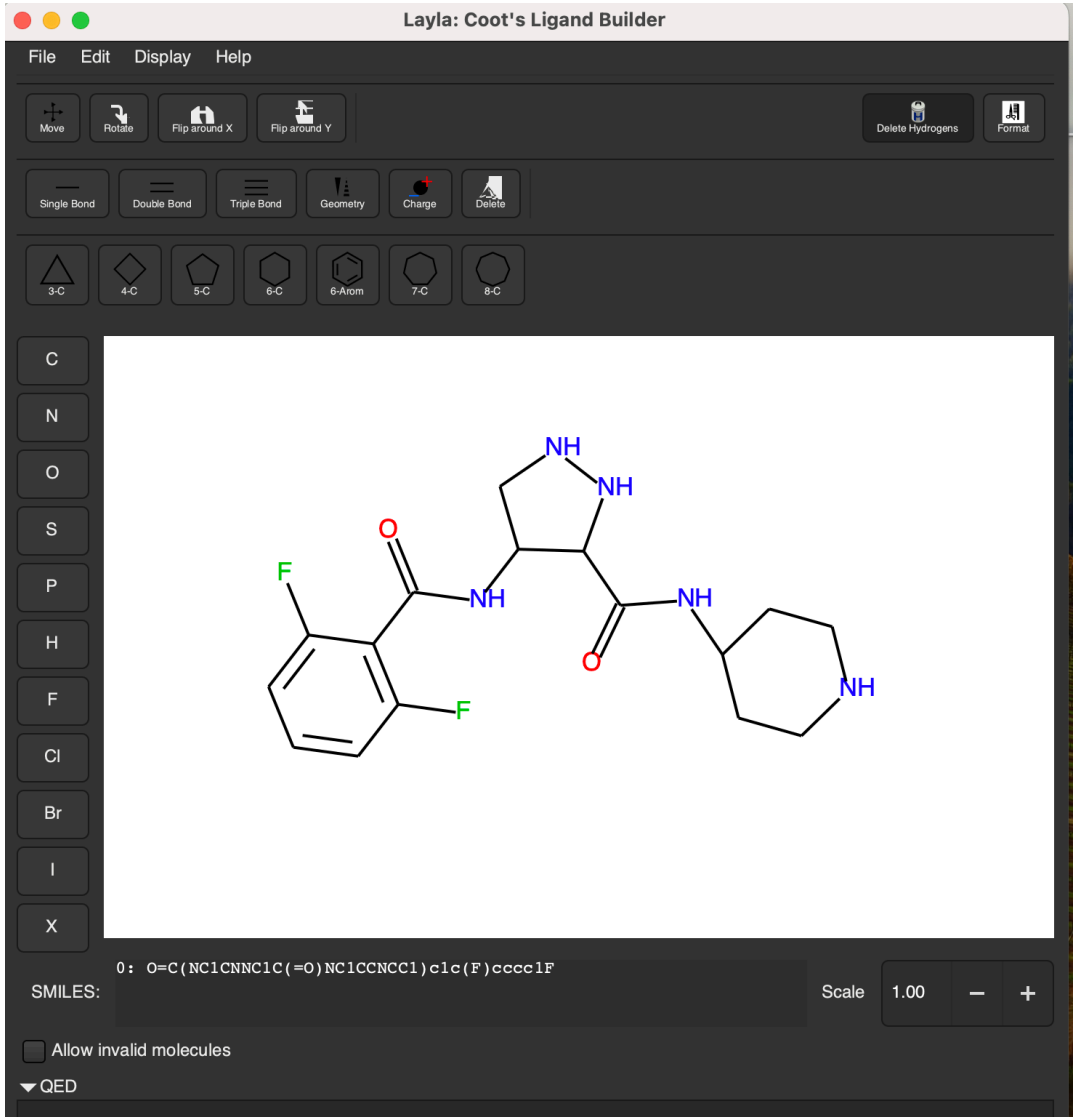
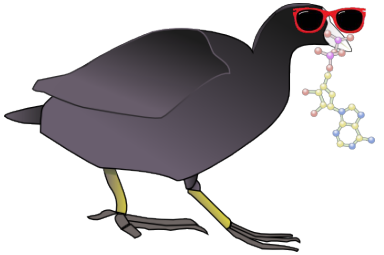


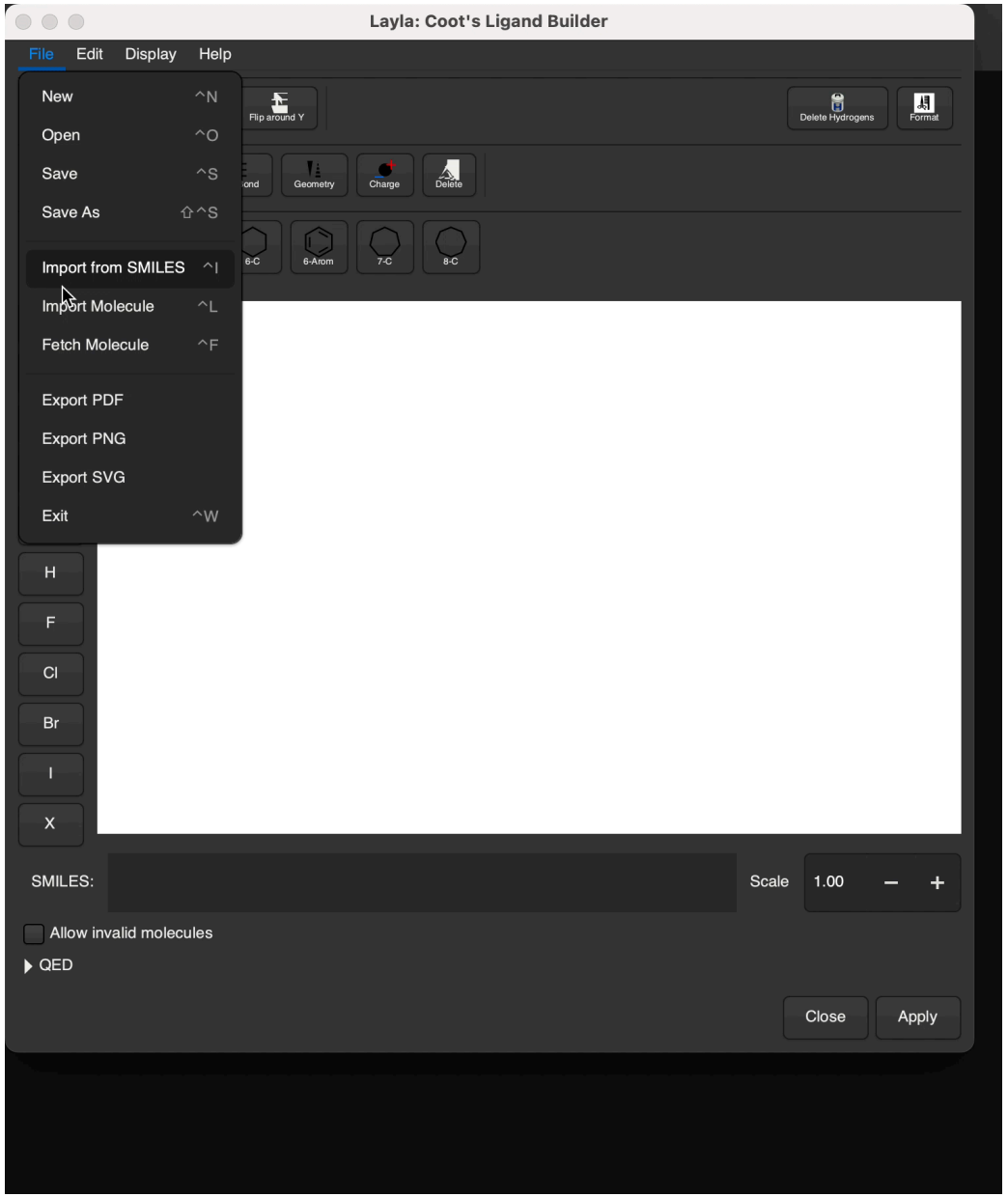


Ligand Builder and QED

Bickerton, G., Paolini, G., Besnard, J. *et al.* Quantifying the chemical beauty of drugs. *Nature Chem* **4**, 90–98 (2012).

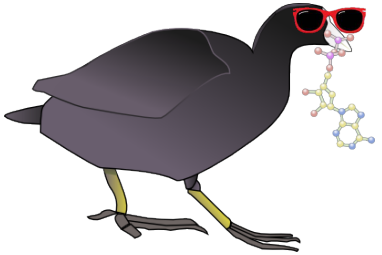
What's new in Coot 1.1?





Ligand Builder and QED

What's new in Coot 1.1?



Availability

1. **CCP4 9.0** (not installed by default)
2. **Homebrew**
3. **Flatpak**
4. **Debian**
5. **Arch Linux**

CCP4

Homebrew
The Missing Package Manager for macOS (or Linux)

Flatpak

archlinux

debian
The universal operating system

Moorhen

Web-Based Interactive Model Building

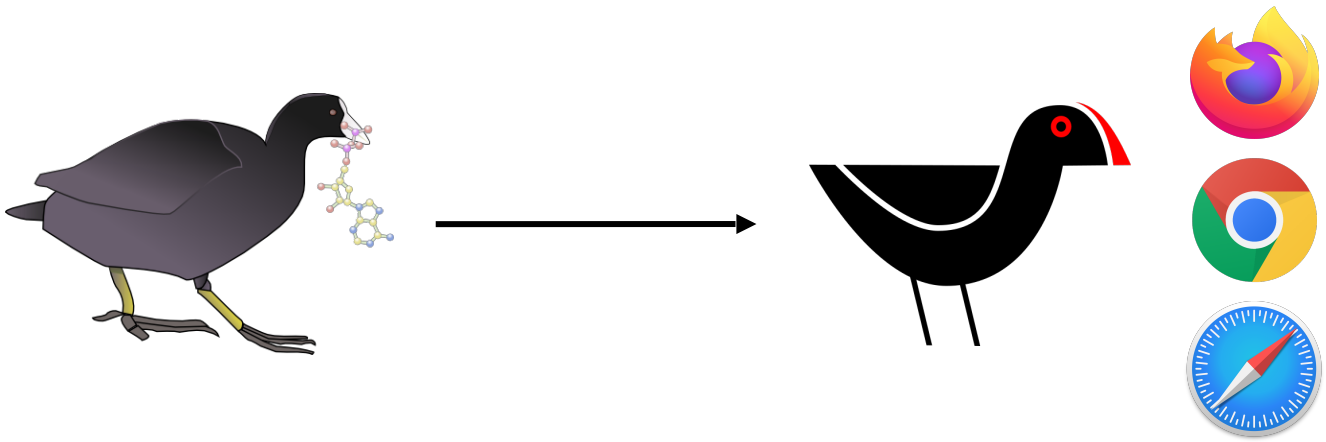
This is a coot

This is a moorhen

What is Moorhen?

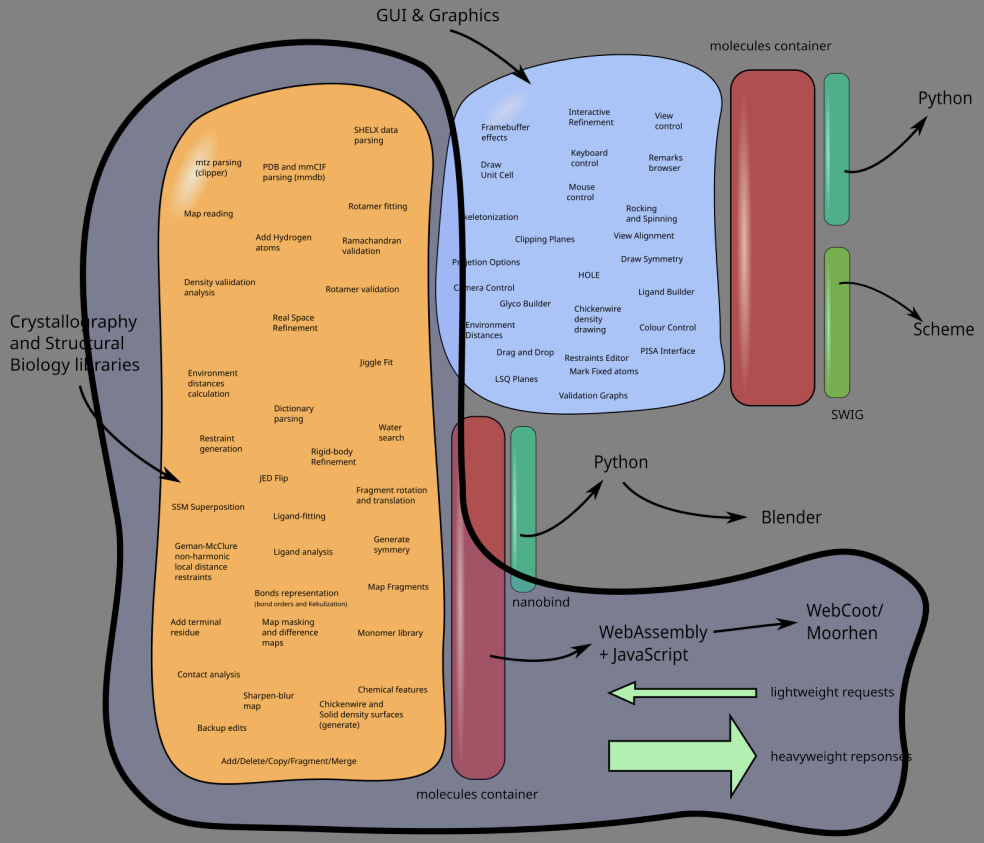
- Moorhen is a next-generation web-based application for the visualisation and manipulation of molecules in structure determination and analysis

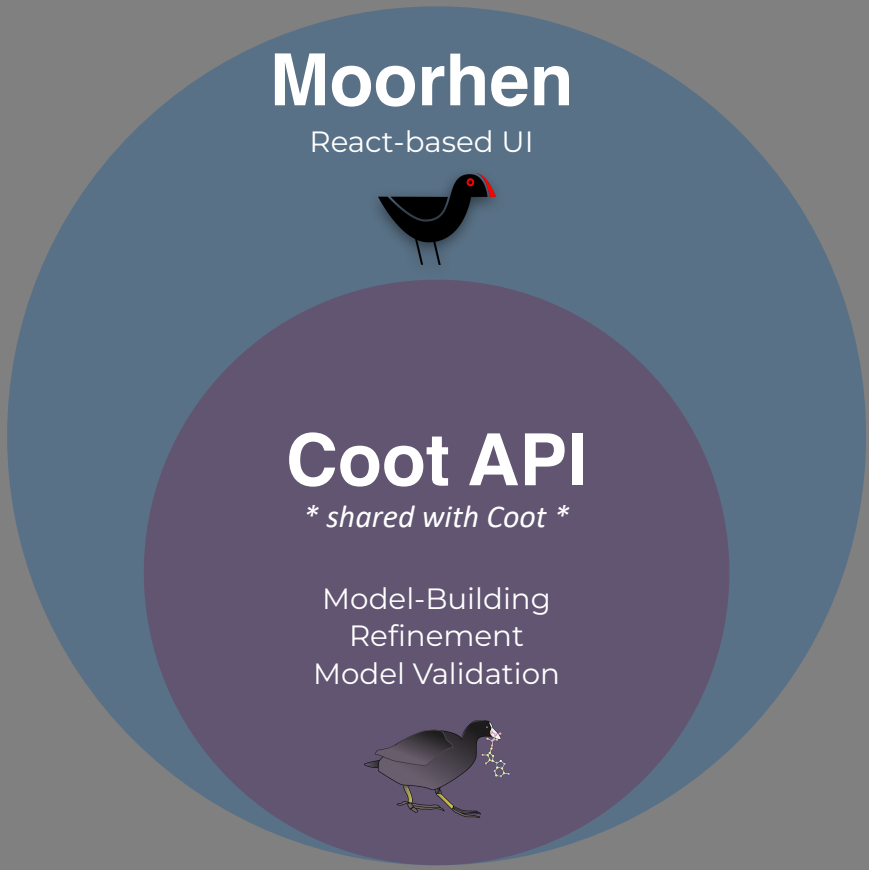
  ➔ In short, Coot on the web browser



What is Moorhen?

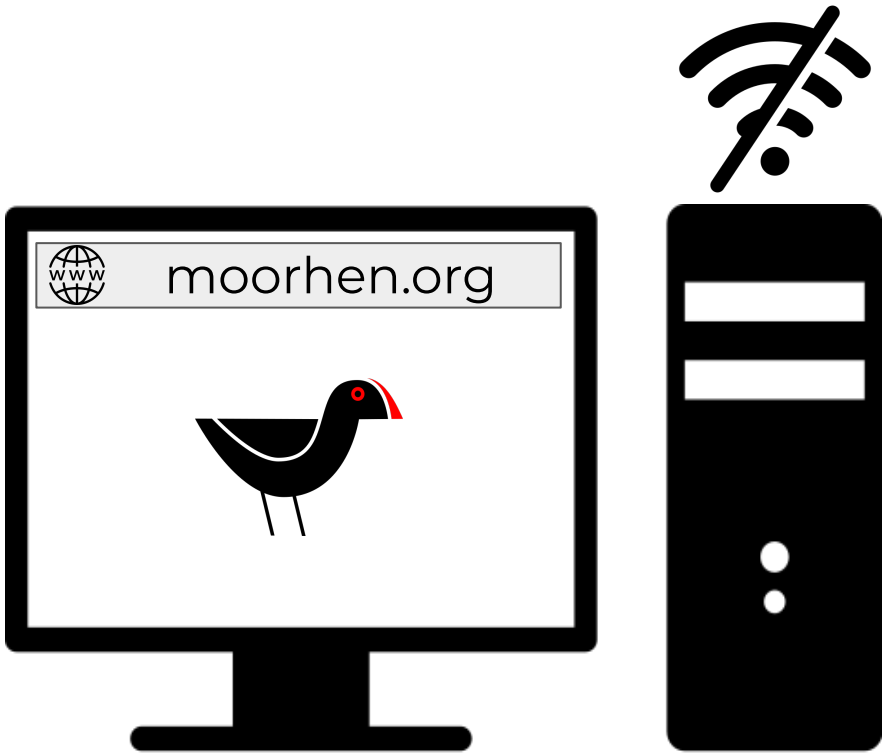
➔ Moorhen extends libcoot API with a web-based React GUI.





What is Moorhen?

➔ Moorhen is a client-side-only app.
This means **there is no server-side computation**



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

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

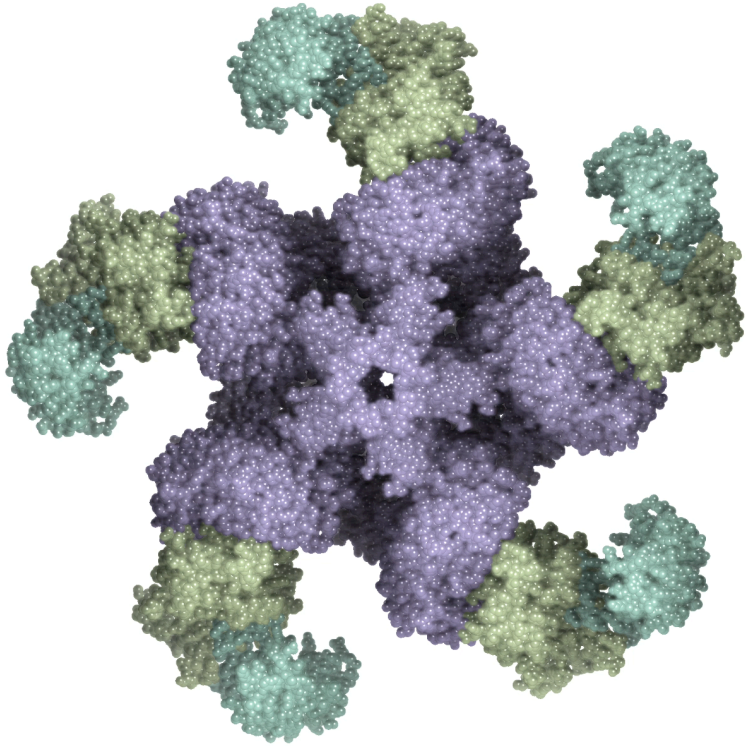
Figure-Making Features

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

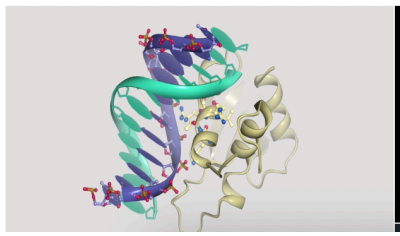
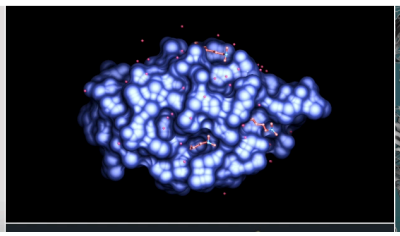
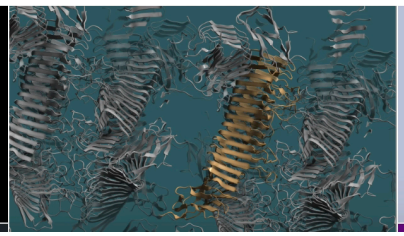
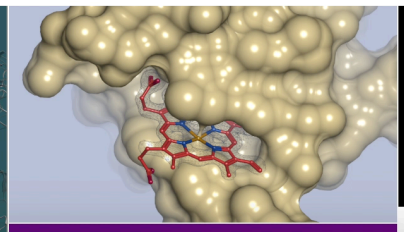
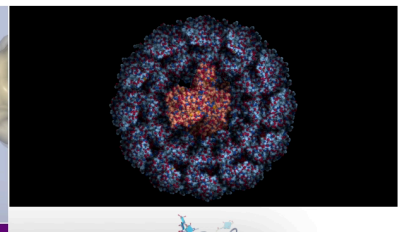
Moorhen

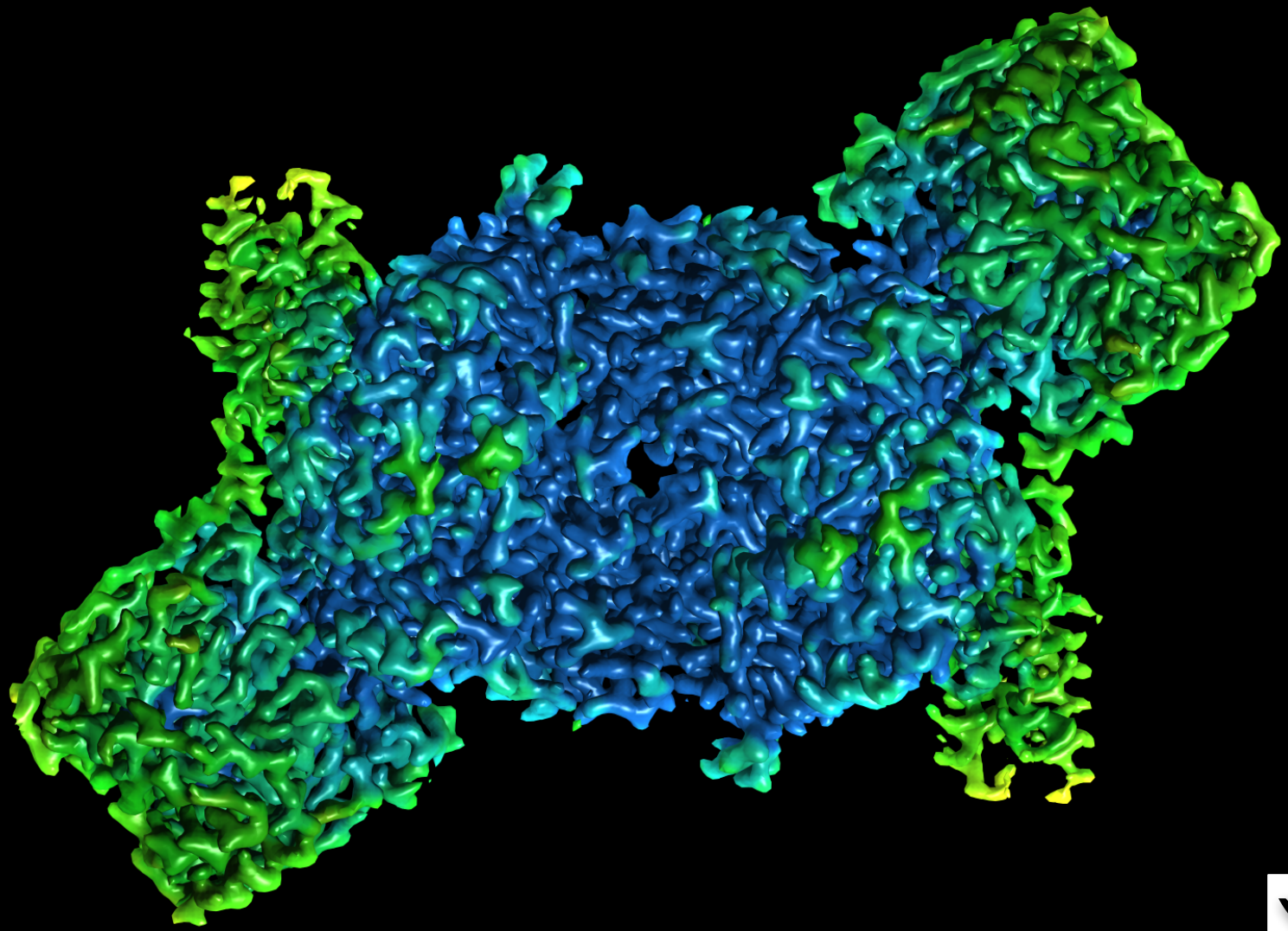
localhost:5173/gallery

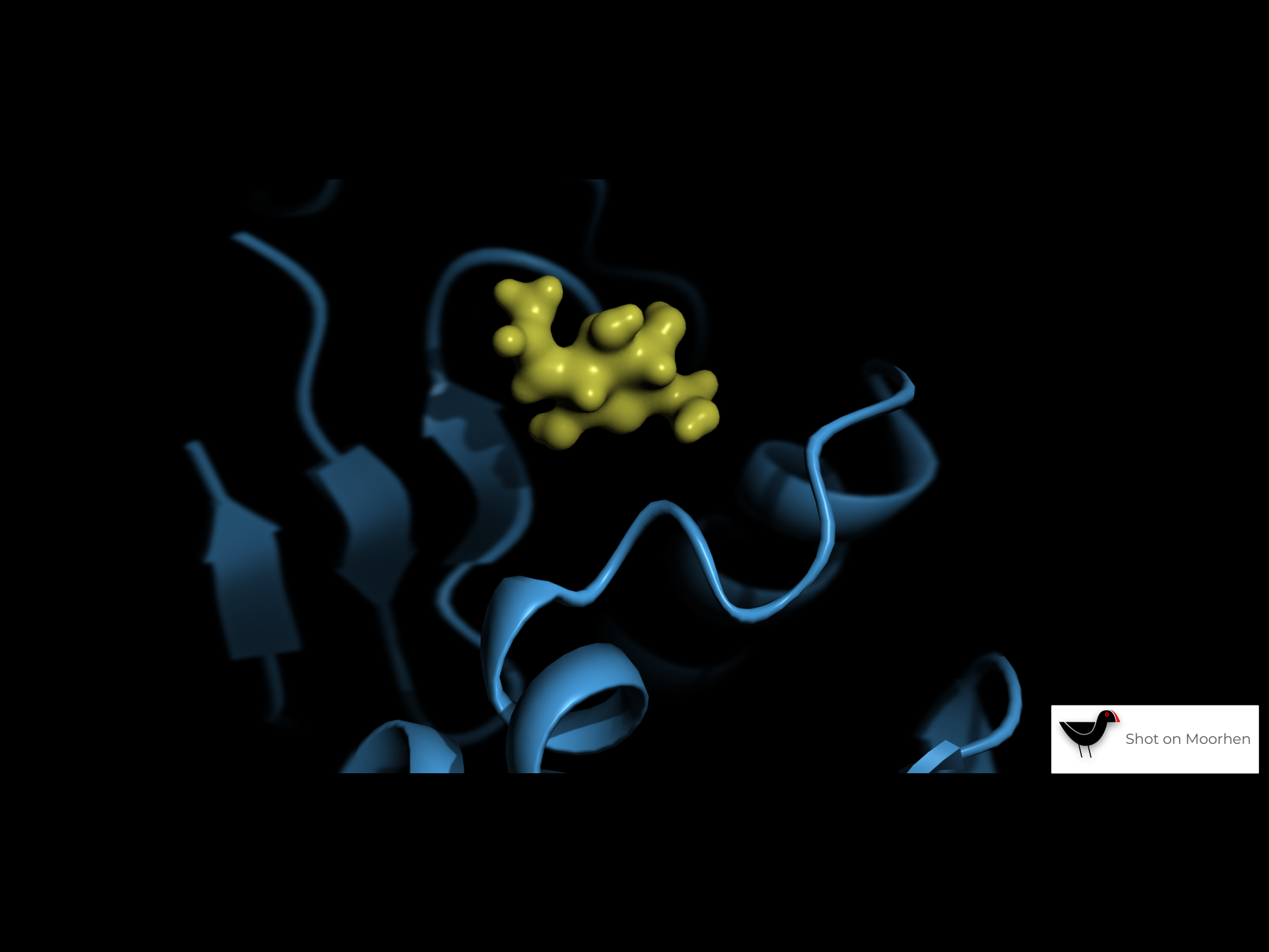
Moorhen Gallery

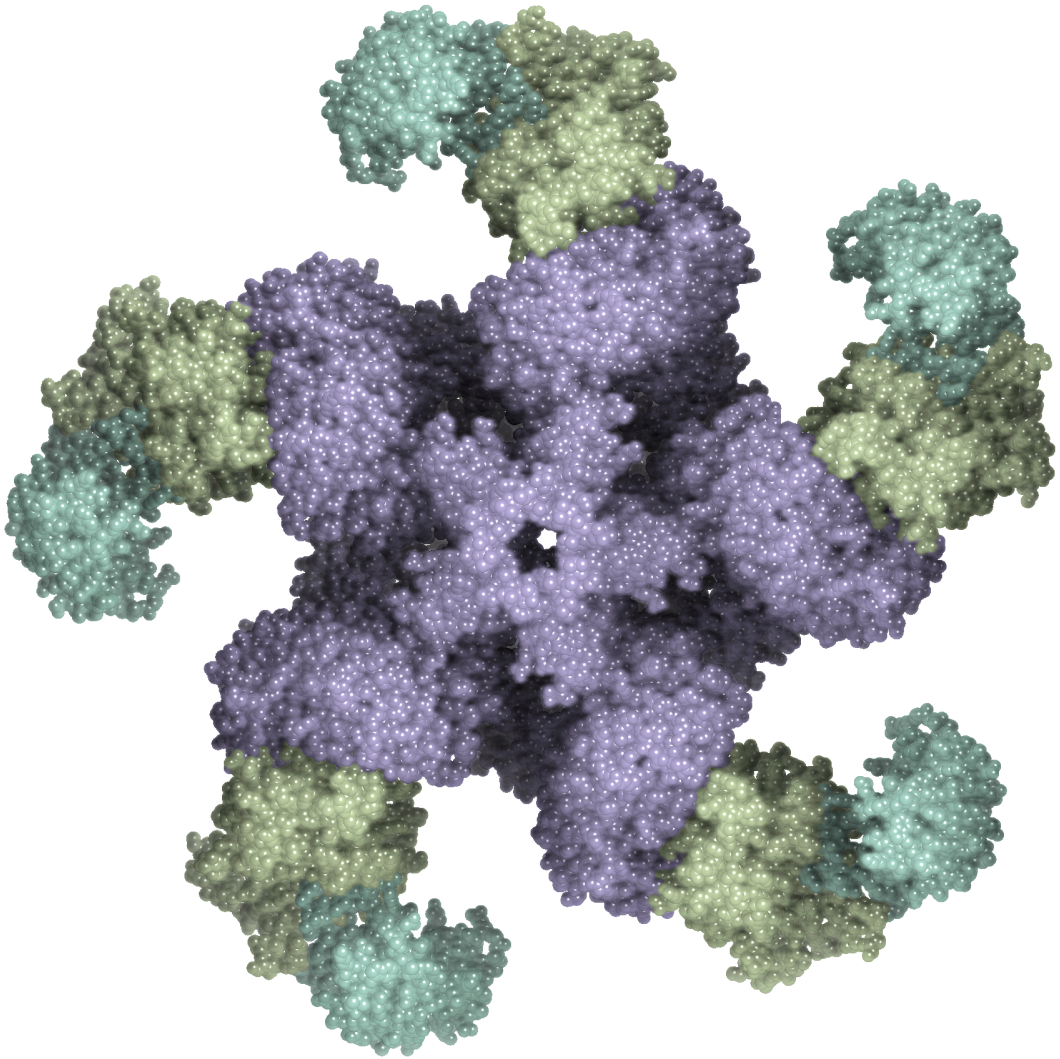


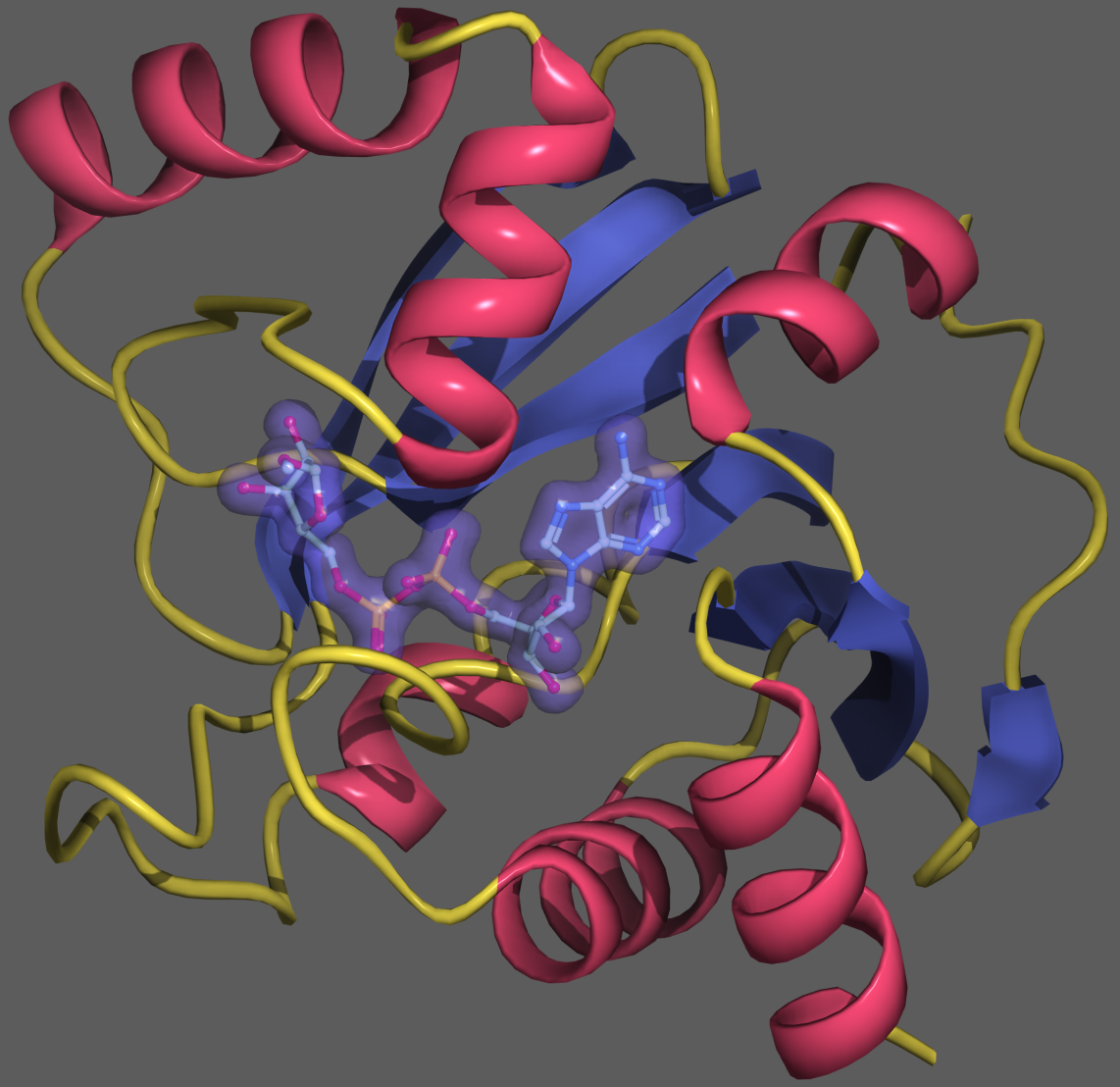
Screenshots and Animations provided by moorhen.org



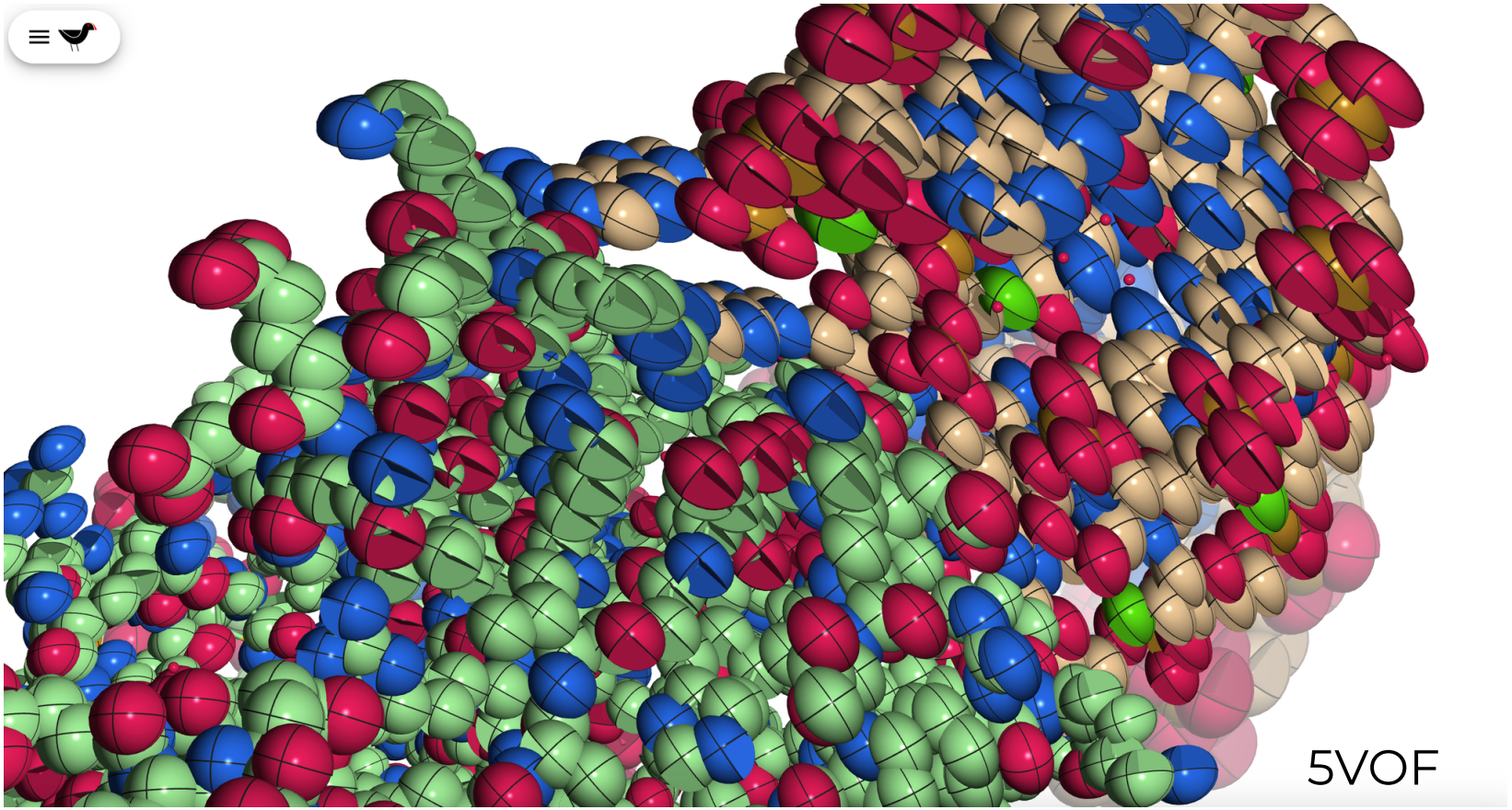

Shot on Moorhen





What's new in Moorhen?

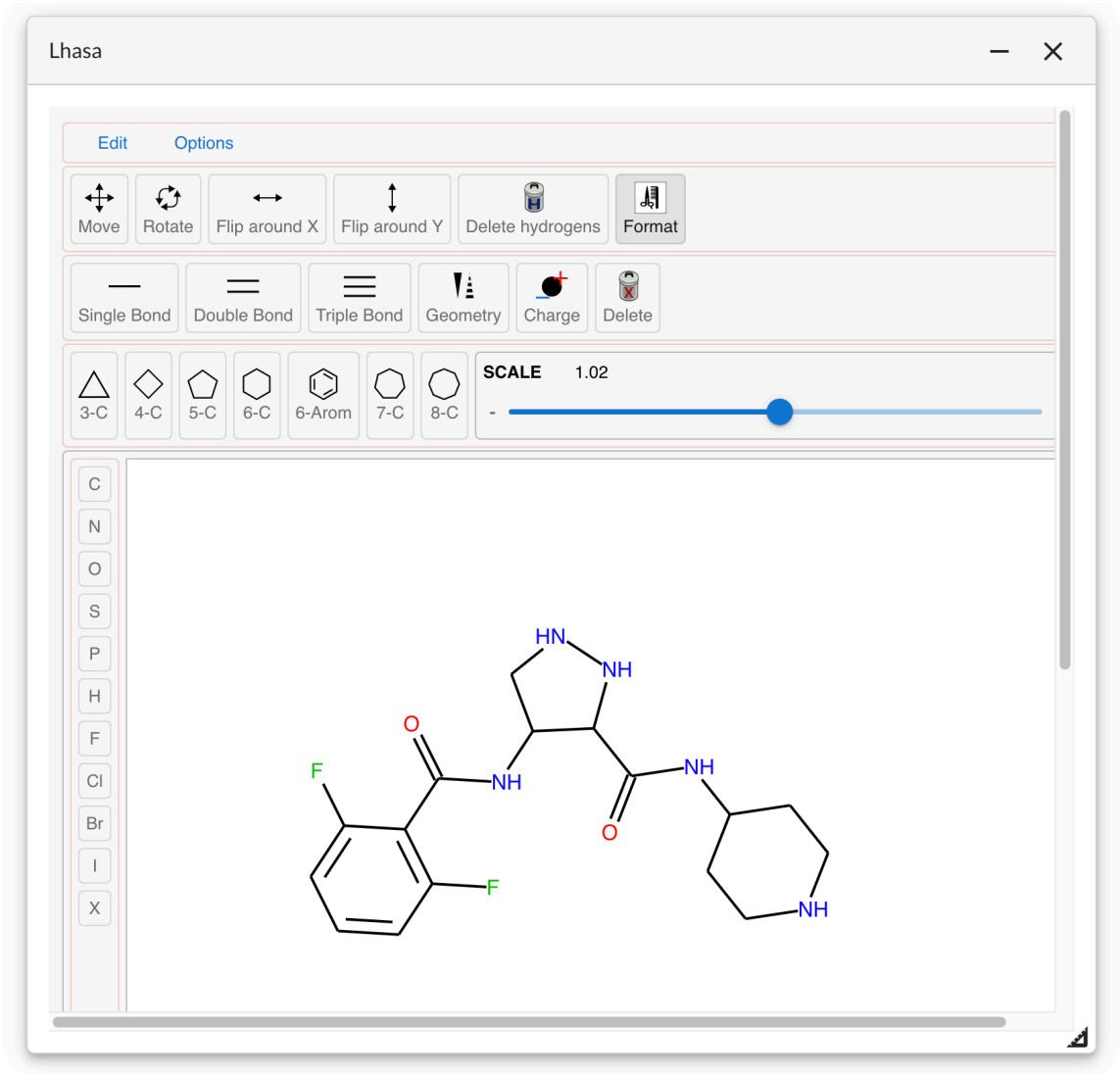
Anisotropic atoms representation



Thanks to Global Phasing

What's new in Moorhen?

Lhasa - Ligand Builder

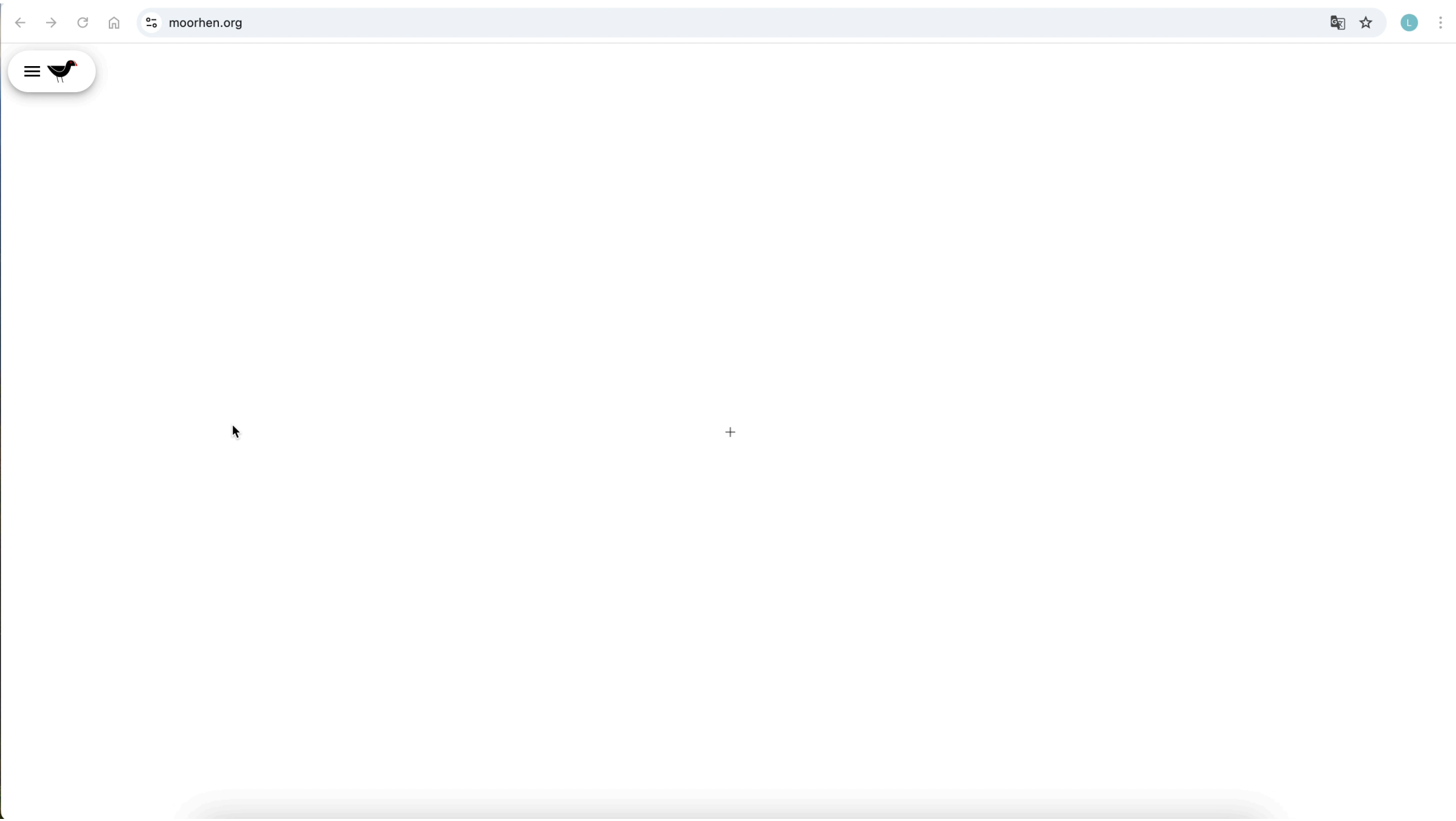


Will provide input for dictionary generators:

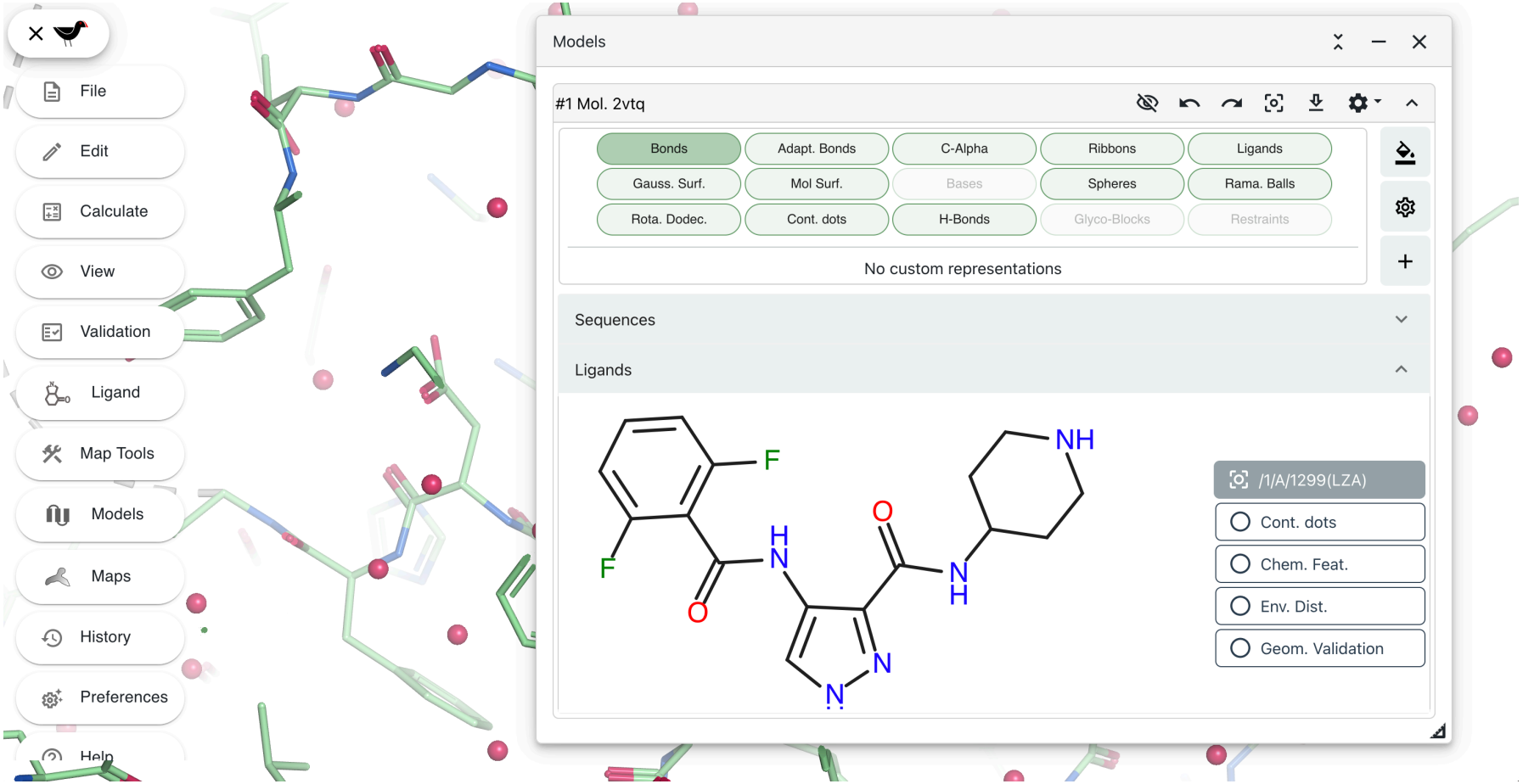
- AceDRG
- Grade 2
- elBOW

Jakub Smulski

Moorhen – Ligand fitting

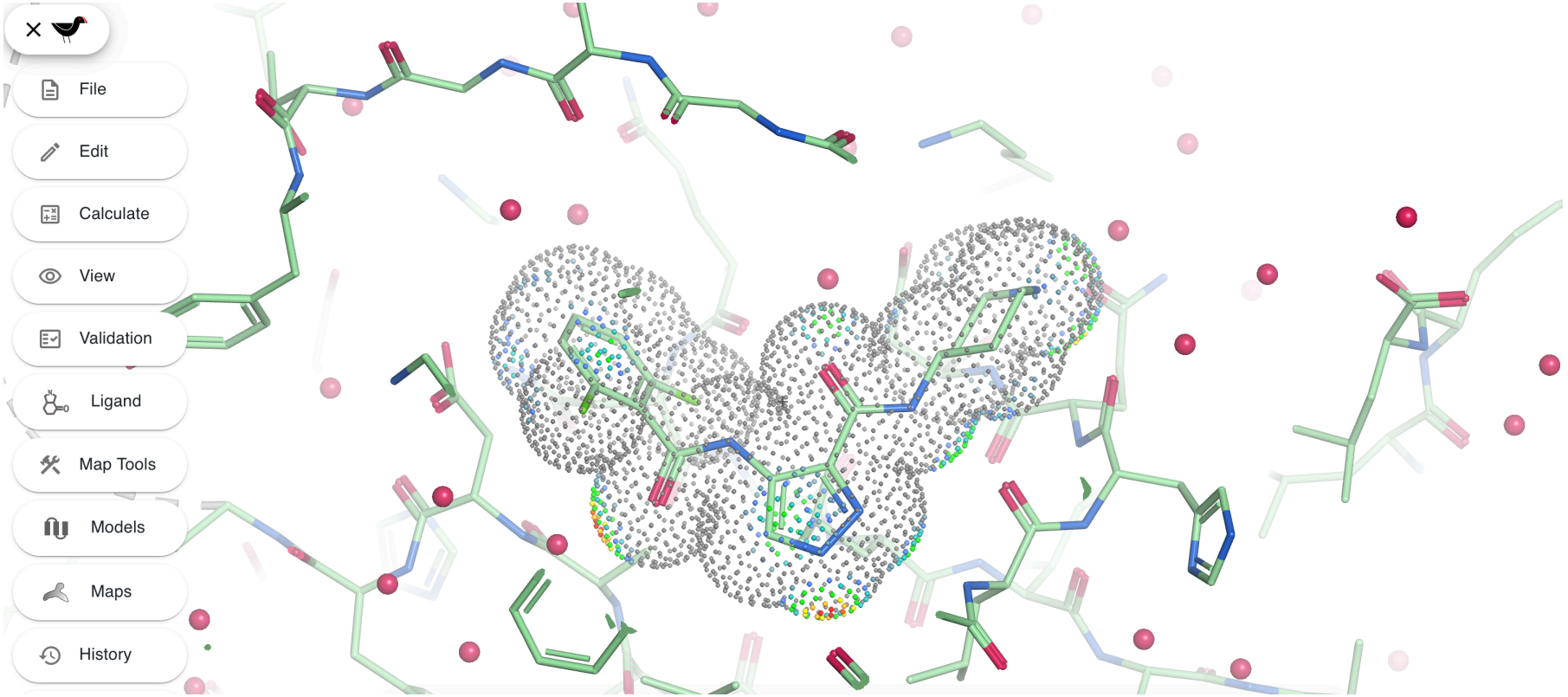


Moorhen – Ligand validation



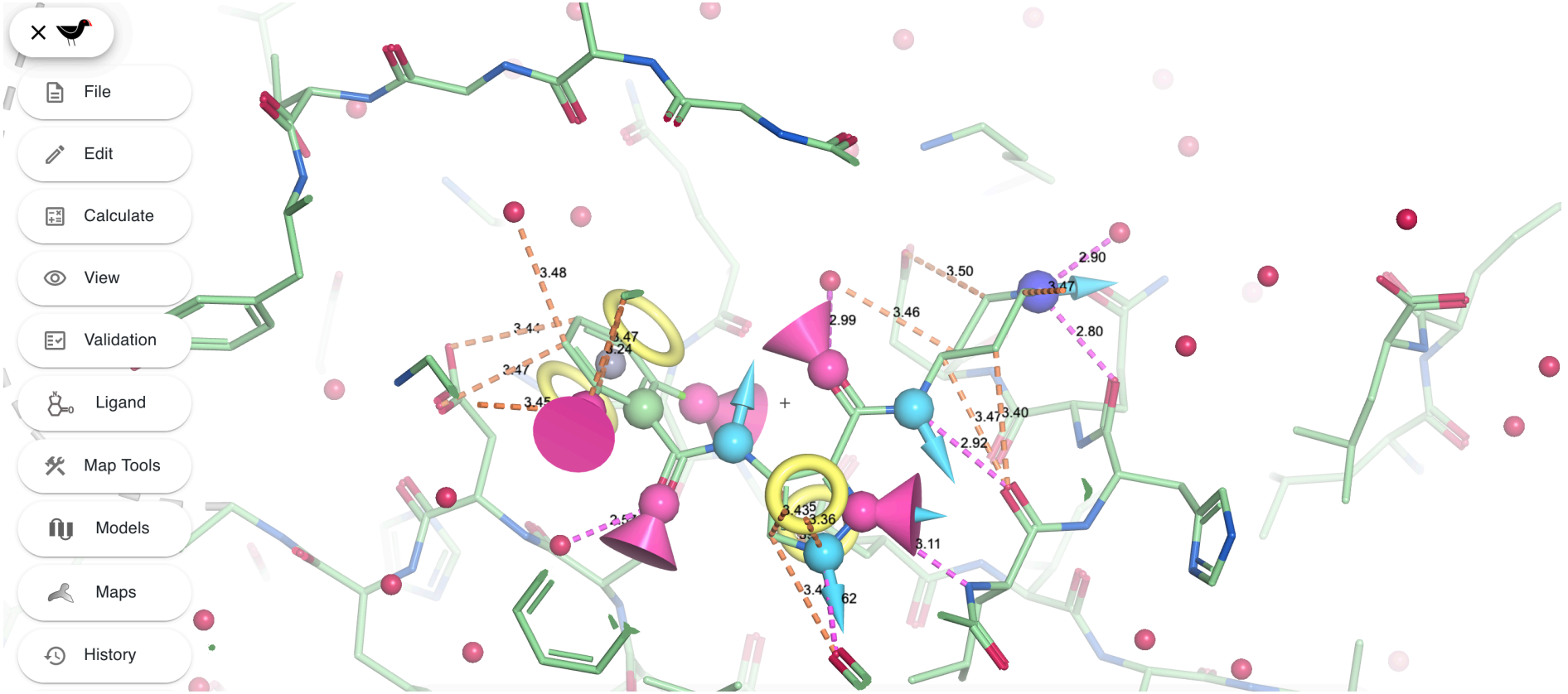
Moorhen – Ligand validation

Contact dots



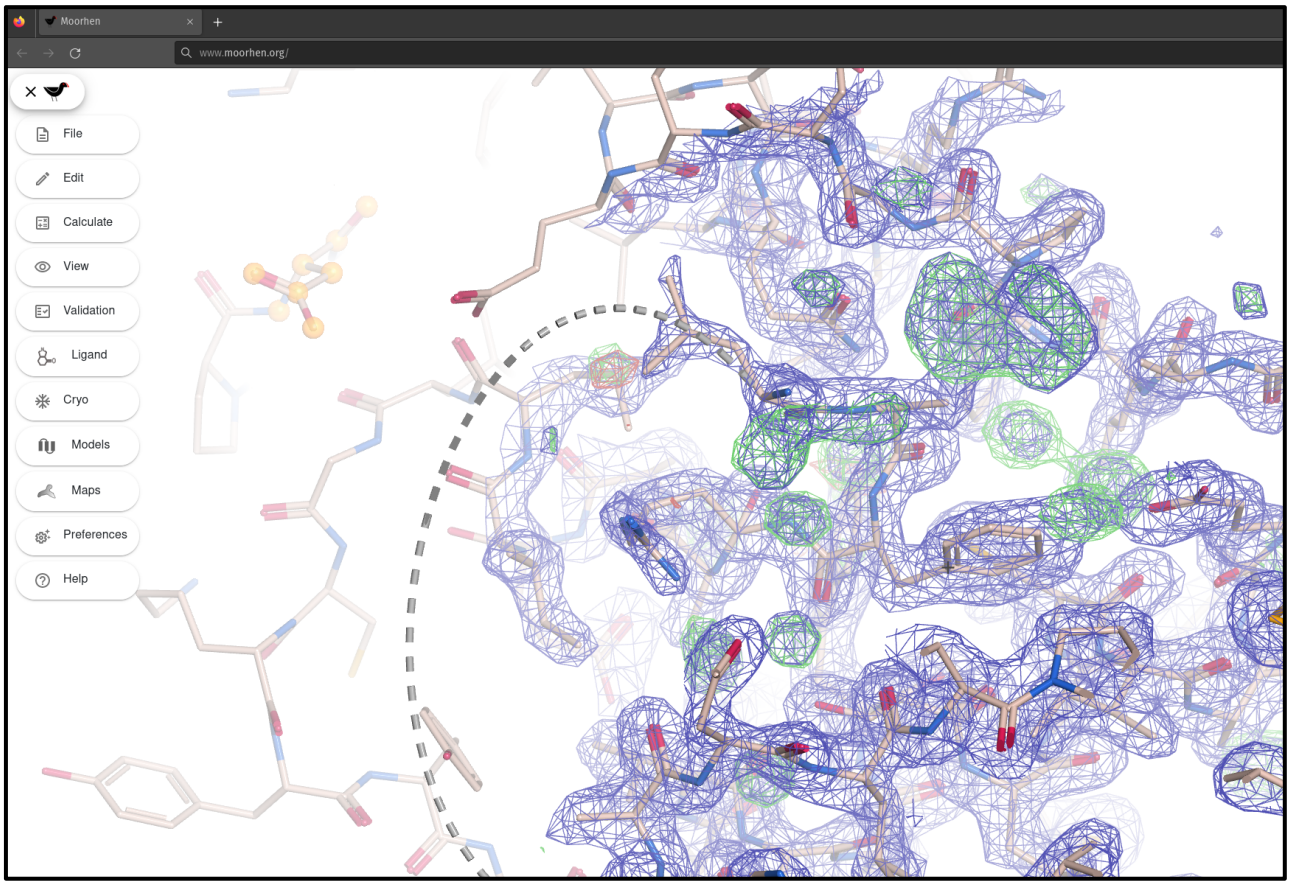
Moorhen – Ligand validation

Chemical features



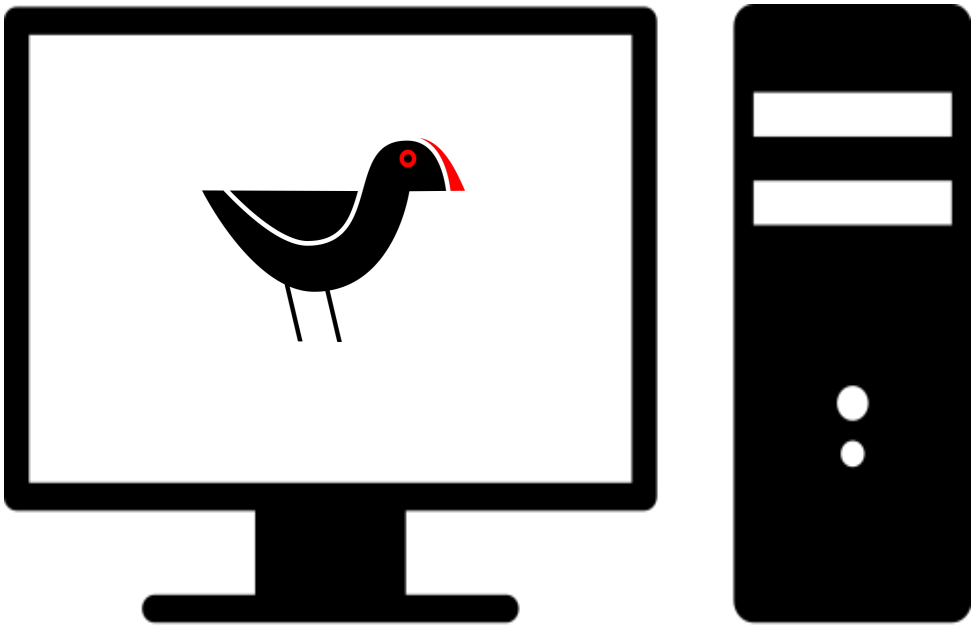
Where is Moorhen available?

www.moorhen.org



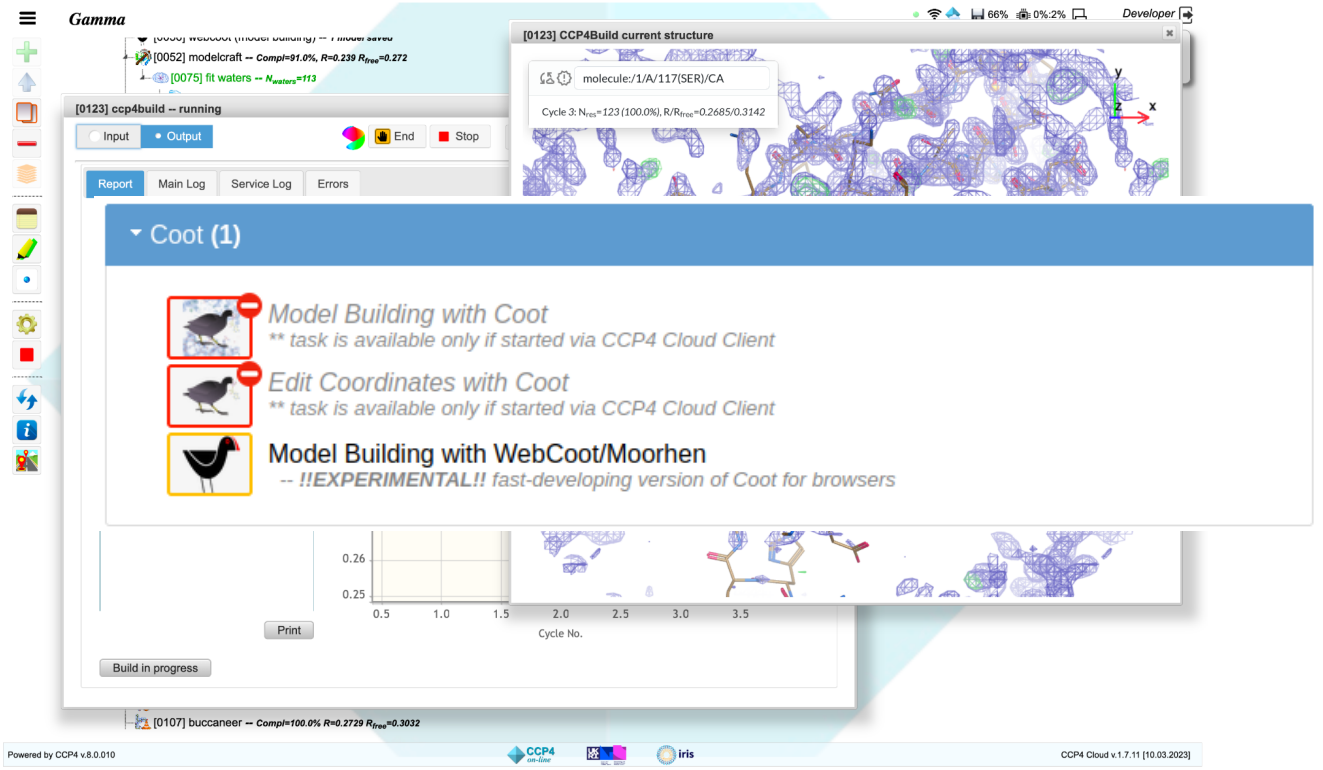
Where is Moorhen available?

Electron
Desktop App



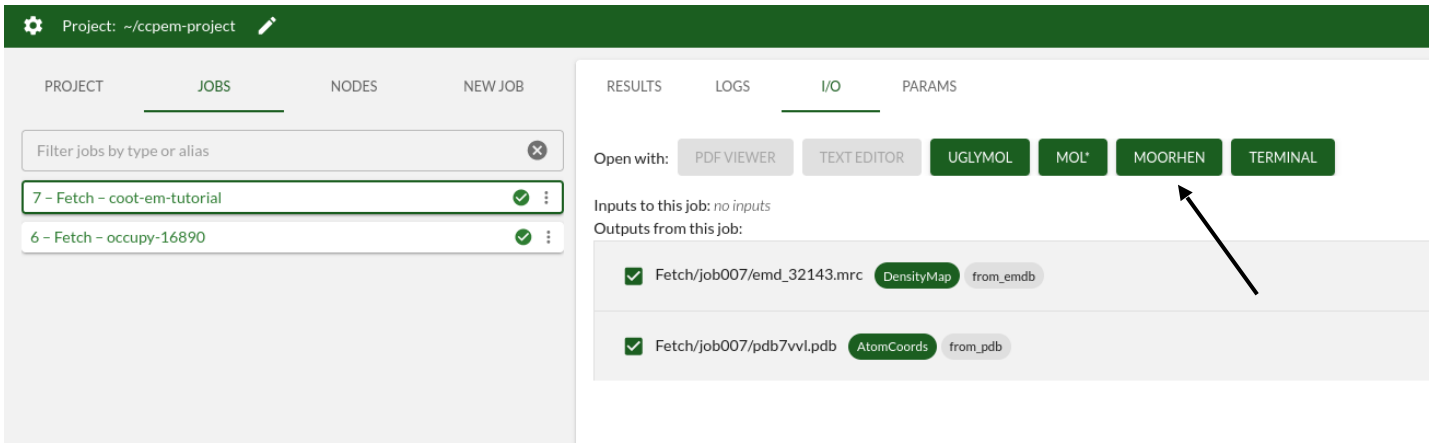
Where is Moorhen available?

CCP4 Cloud



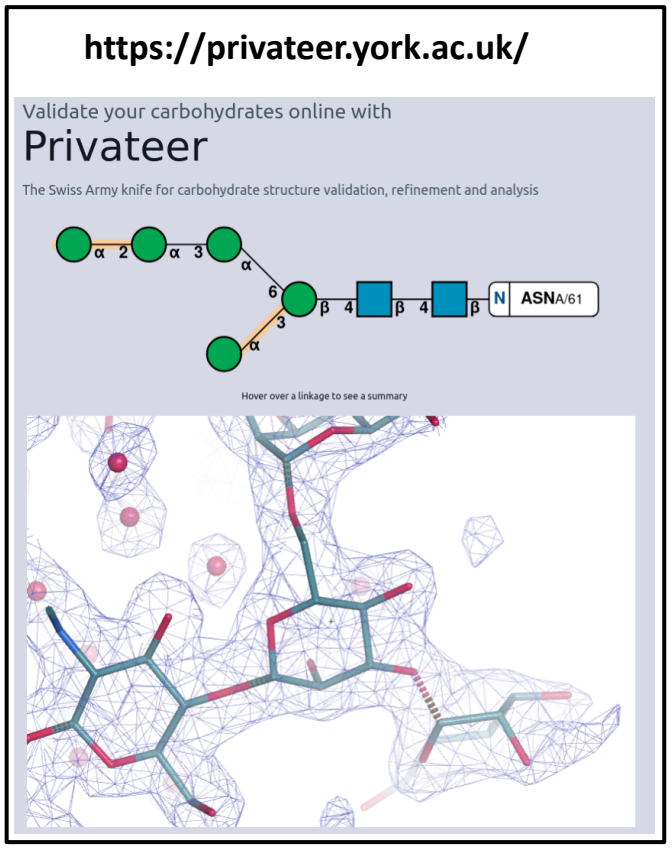
Where is Moorhen available?

CCP-EM



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

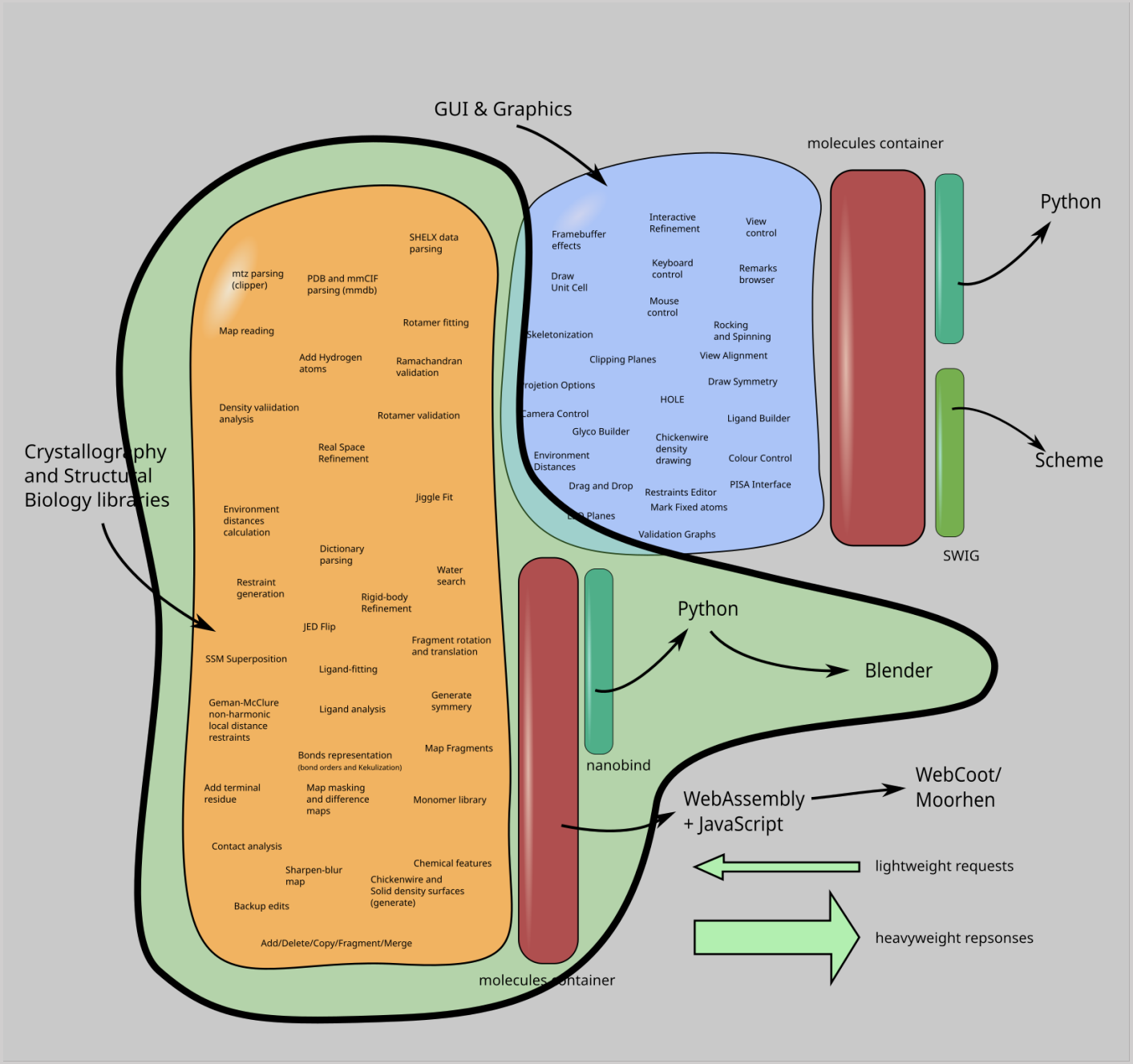
Jul 6, 2023
Using Moorhen in a react app

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

Moorhen mailing list:

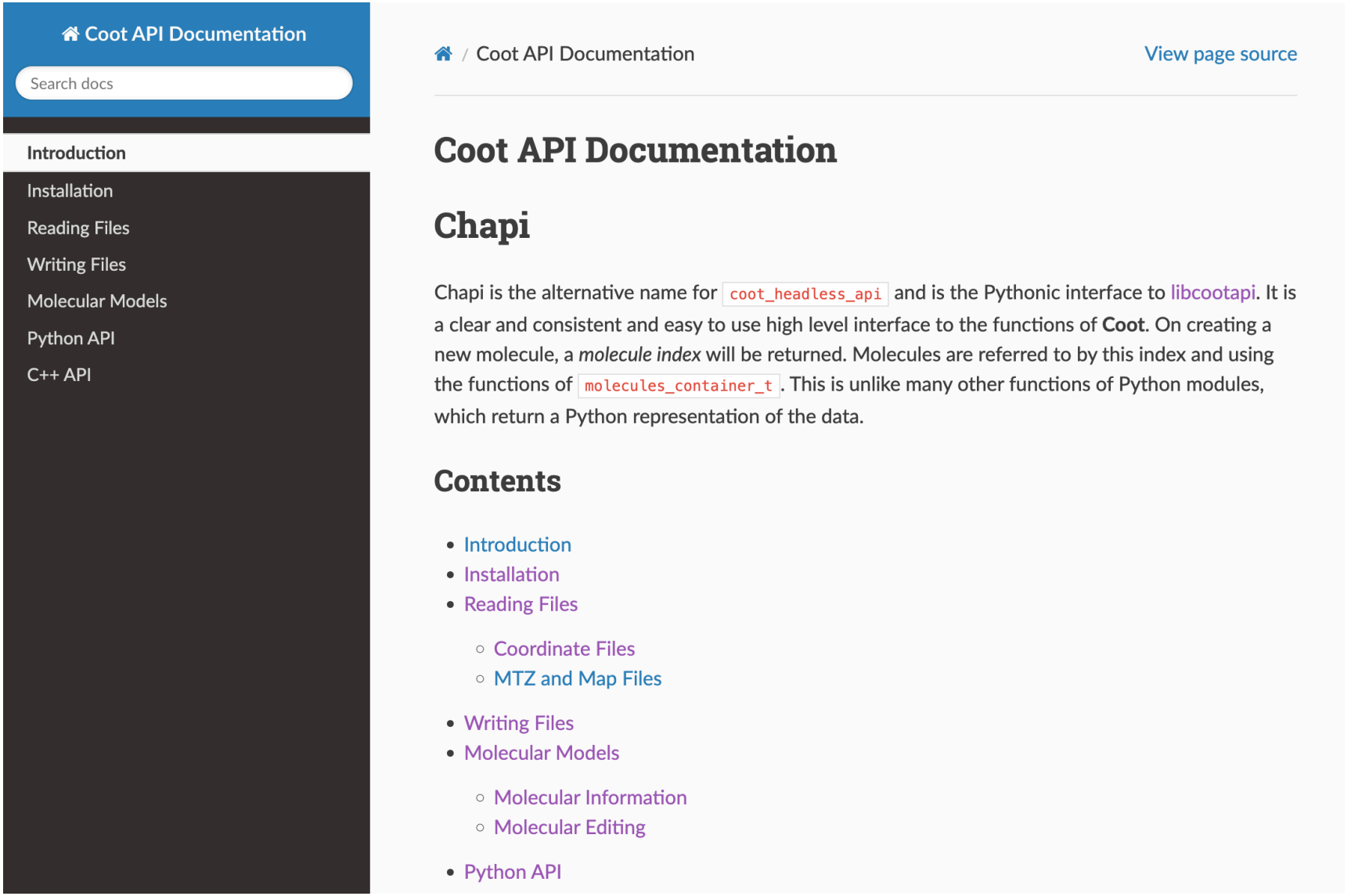
https://groups.google.com/a/york.ac.uk/g/moorhen-group

Programming with Coot



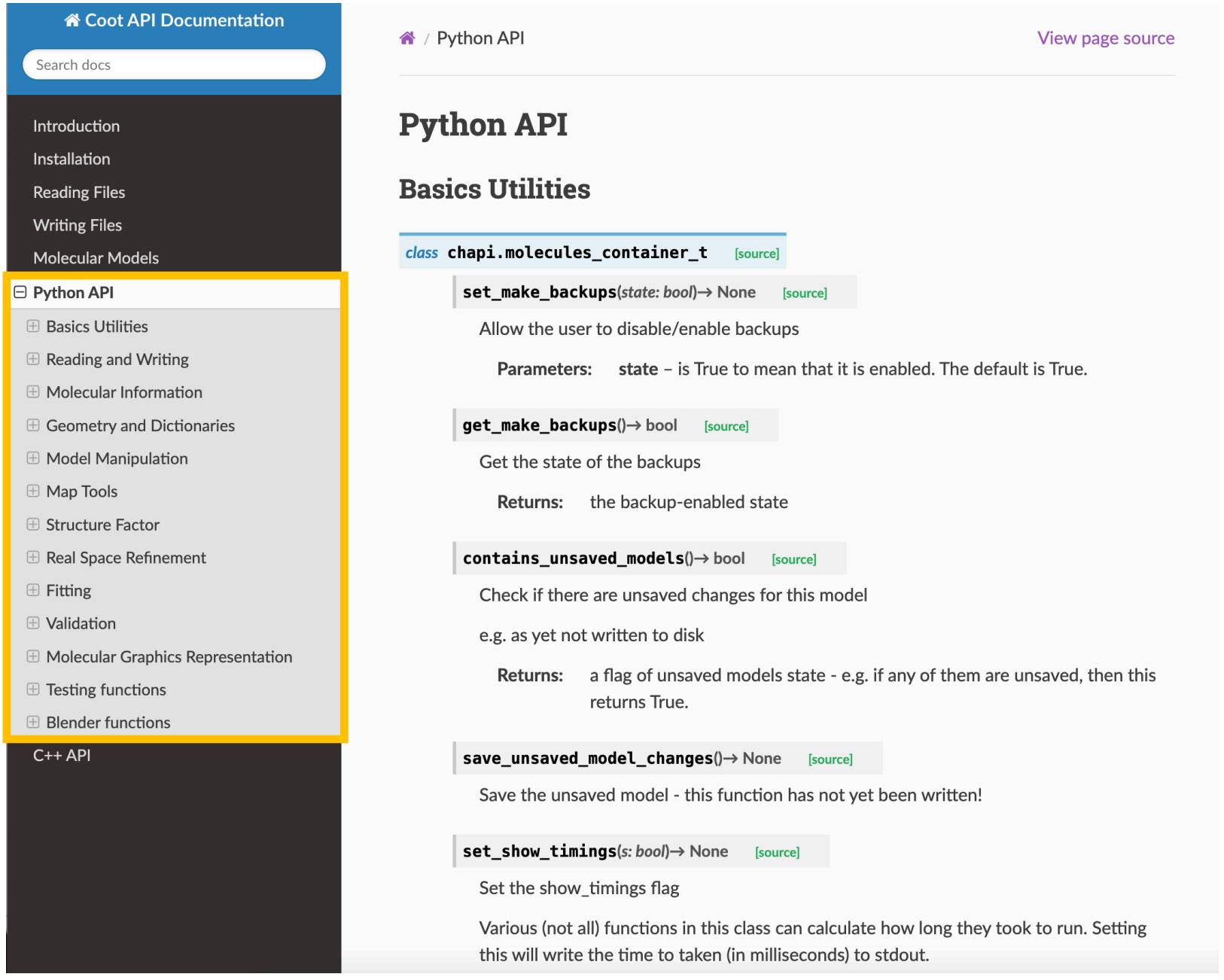
Chapi documentation

https://www.mrc-lmb.cam.ac.uk/lucrezia/libcootapi-documentation/



Chapi documentation

Detailed Python Reference API



Chapi documentation

Python script examples

Example #1: adding water molecules

```
import chapi

mc = chapi.molecules_container_t(True)

# read coordinates and map
imol = mc.read_pdb('tutorial-modern.pdb')
imol_mtz = mc.read_mtz("rnasa-1.8-all_refmac1.mtz", "FWT", "PHWT", "W", False, False)

# set the parameters for waters addition (the default values are given as arguments)
mc.set_add_waters_water_to_protein_distance_lim_min(2.4)
mc.set_add_waters_water_to_protein_distance_lim_max(3.4)
mc.set_add_waters_variance_limit(0.1)
mc.set_add_waters_sigma_cutoff(1.75)

# add waters
mc.add_waters(imol, imol_mtz)
```

https://www.mrc-lmb.cam.ac.uk/lucrezia/libcootapi-documentation/

Chapi documentation

Python script examples

Example #2 : deleting water molecules outliers

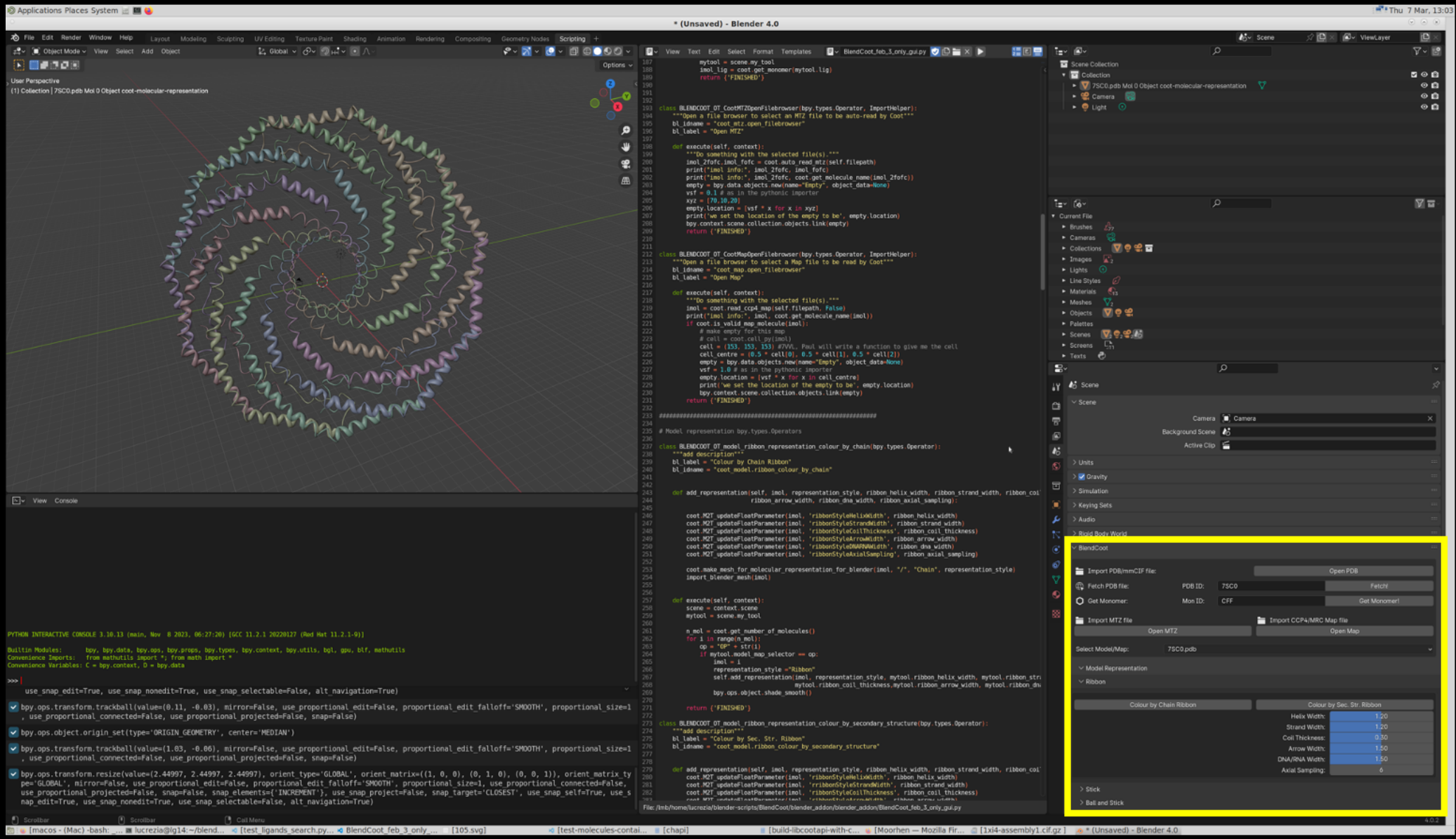
```
# read coordinates and map
imol = mc.read_pdb('tutorial-modern.pdb')
imol_mtz = mc.read_mtz("rnasa-1.8-all_refmac1.mtz", "FWT", "PHWT", "W", False, False)

# delete water "outliers" - e.g., those with a distance to the protein less than 2.5
# or more than 3.5
min_dist = 2.5
max_dist = 3.5
median_temperature_factor = mc.get_median_temperature_factor(imol)
b_factor_limit = 2.0 * median_temperature_factor
outlier_map_rmsd_level = 1.0
ignore_part_occ_contact_flag = False
ignore_zero_occ_flag = False
water_outliers = mc.find_water_baddies(imol,
                                       imol_mtz,
                                       b_factor_limit,
                                       outlier_map_rmsd_level,
                                       min_dist,
                                       max_dist,
                                       ignore_part_occ_contact_flag,
                                       ignore_zero_occ_flag)
for res in water_outliers:
    cid = '//' + res.chain_id + '/' + str(res.res_no)
    print("Deleting water", cid)
    mc.delete_atom_using_cid(imol, cid)
```

https://www.mrc-lmb.cam.ac.uk/lucrezia/libcootapi-documentation/

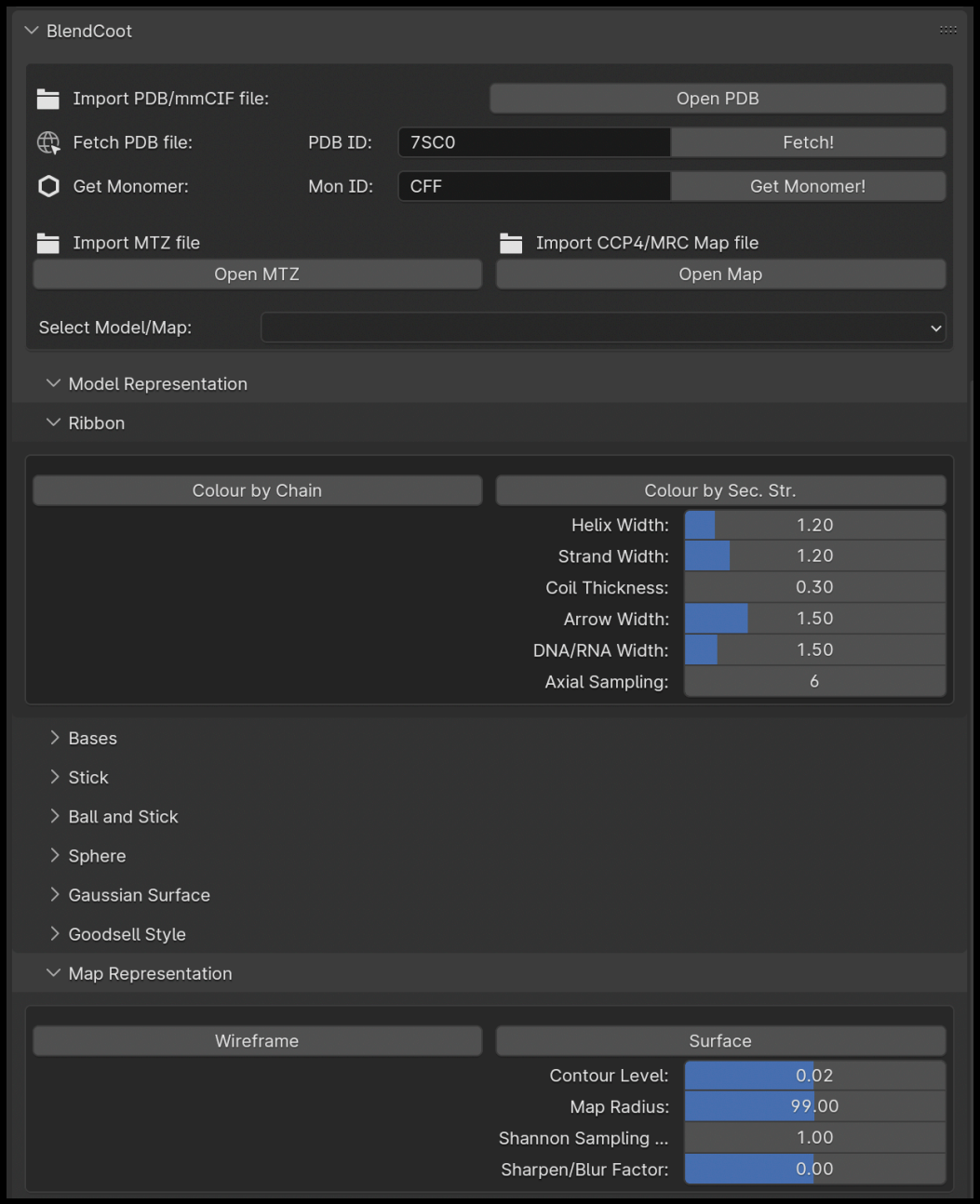
BlendCoot

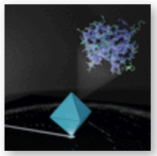
- **Blender** is 3D modelling software for graphics & ray-tracing
- **BlendCoot** is an interface between Coot and Blender
- BlendCoot builds on the Pythonic non-graphical interface **chapi**
- We have added a blender-based GUI to chapi to provide an easy means to import molecules, ligands and maps into Blender

BlendCoot


* (Unsaved) - Blender 4.0
BlendCoot
Import PDB/mmCIF file:
Open PDB
Fetch PDB file:
PDB ID:
7SC0
Fetch!
Get Monomer:
Mon ID:
CFF
Get Monomer!
Import MTZ file
Open MTZ
Import CCP4/MRC Map file
Open Map
Select Model/Map:
7SC0.pdb
Model Representation
Ribbon
Colour by Chain Ribbon
Colour by Sec. Str. Ribbon
Helix Width:
Strand Width:
Coil Thickness:
Arrow Width:
DNA/RNA Width:
Axial Sampling:
Stick
Ball and Stick

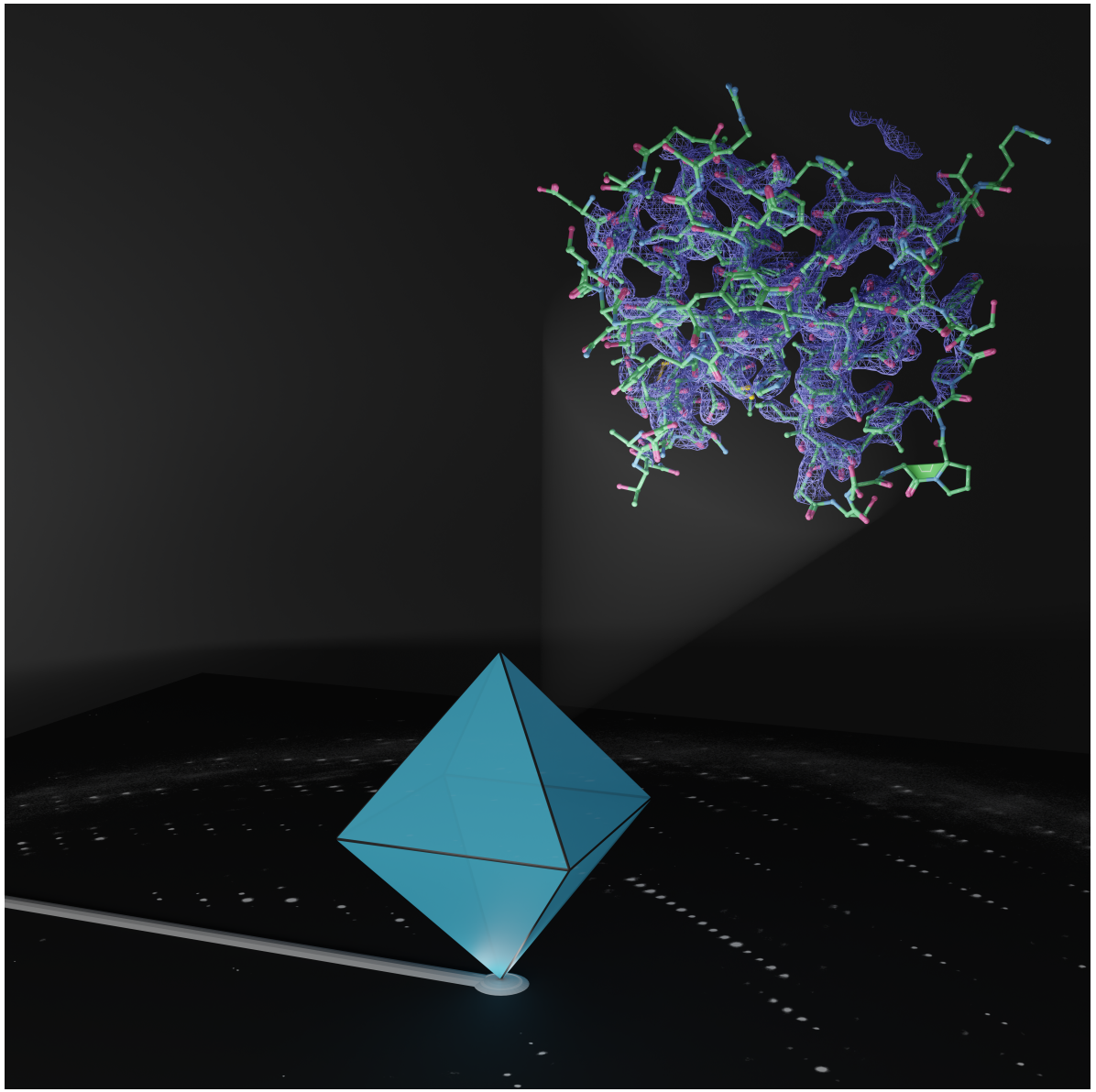
BlendCoot


BlendCoot
Import PDB/mmCIF file:
Open PDB
Fetch PDB file:
PDB ID:
7SC0
Fetch!
Get Monomer:
Mon ID:
CFF
Get Monomer!
Import MTZ file
Open MTZ
Import CCP4/MRC Map file
Open Map
Select Model/Map:
Model Representation
Ribbon
Colour by Chain
Colour by Sec. Str.
Helix Width:
1.20
Strand Width:
1.20
Coil Thickness:
0.30
Arrow Width:
1.50
DNA/RNA Width:
1.50
Axial Sampling:
6
Bases
Stick
Ball and Stick
Sphere
Gaussian Surface
Goodsell Style
Map Representation
Wireframe
Surface
Contour Level:
0.02
Map Radius:
99.00
Shannon Sampling ...
1.00
Sharpen/Blur Factor:
0.00

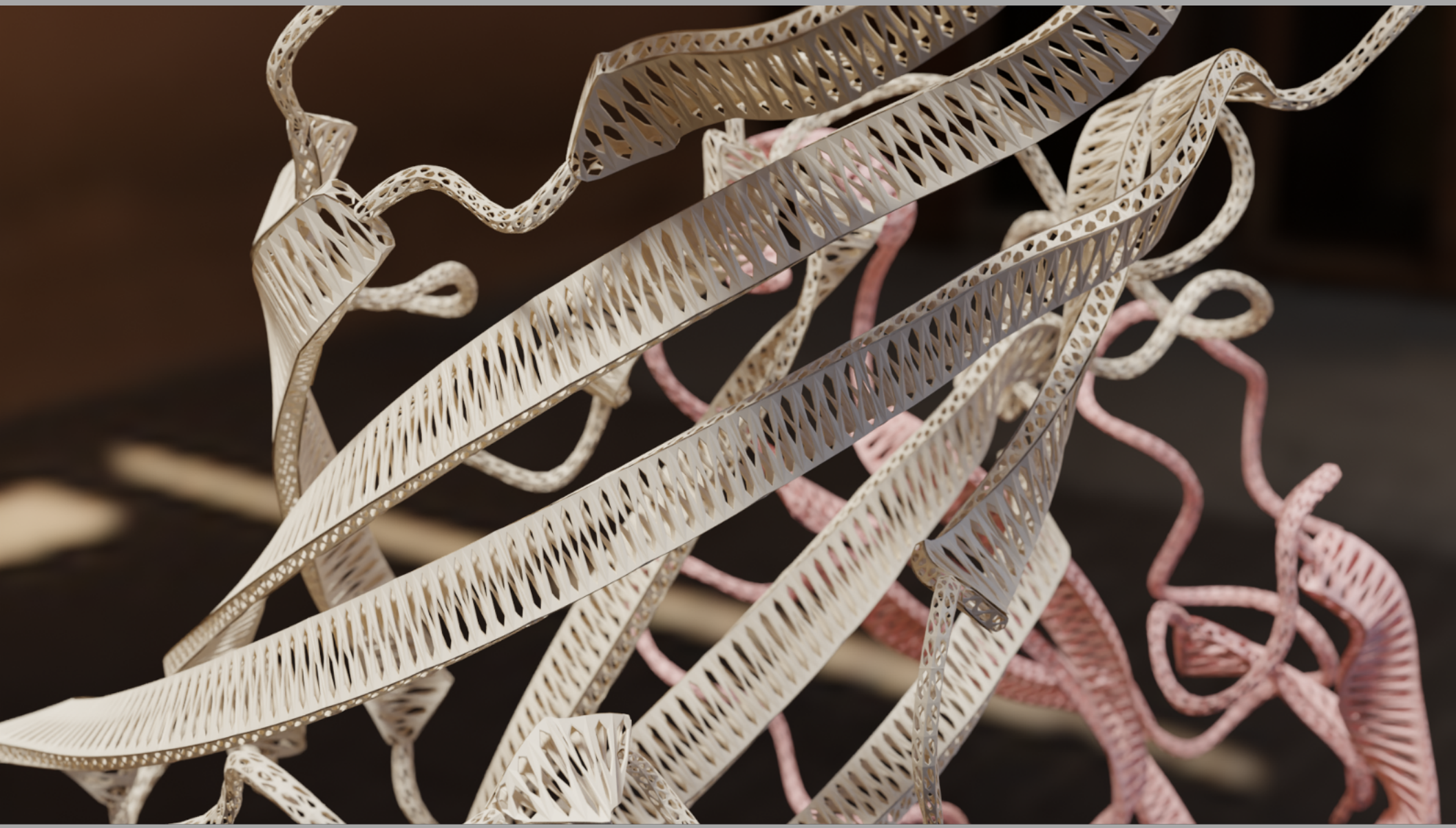


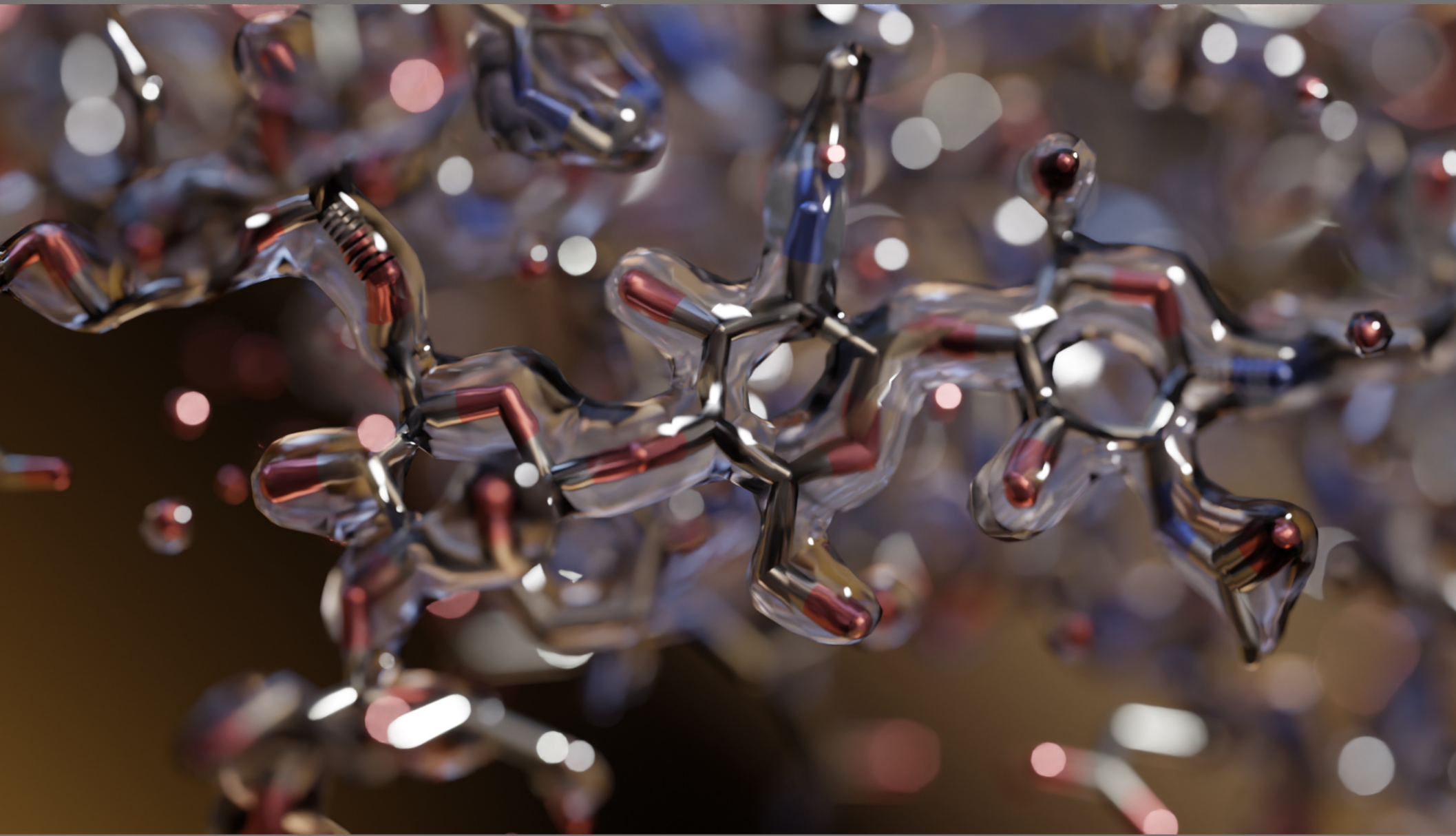
The *CCP*4 suite: integrative software for macromolecular crystallography

J. Agirre, M. Atanasova, H. Bagdonas, C. B. Ballard, A. Baslé, J. Beilsten-Edmands, R. J. Borges, D. G. Brown, J. J. Burgos-Mármol, J. M. Berrisford, P. S. Bond, I. Caballero, L. Catapano, G. Chojnowski, A. G. Cook, K. D. Cowtan, T. I. Croll, J. É. Debreczeni, N. E. Devenish, E. J. Dodson, T. R. Drevon, P. Emsley, G. Evans, P. R. Evans, M. Fando, J. Foadi, L. Fuentes-Montero, E. F. Garman, M. Gerstel, R. J. Gildea, K. Hatti, M. L. Hekkelman, P. Heuser, S. W. Hoh, M. A. Hough, H. T. Jenkins, E. Jiménez, R. P. Joosten, R. M. Keegan, N. Keep, E. B. Krissinel, P. Kolenko, O. Kovalevskiy, V. S. Lamzin, D. M. Lawson, A. A. Lebedev, A. G. W. Leslie, B. Lohkamp, F. Long, M. Malý, A. J. McCoy, S. J. McNicholas, A. Medina, C. Millán, J. W. Murray, G. N. Murshudov, R. A. Nicholls, M. E. M. Noble, R. Oeffner, N. S. Pannu, J. M. Parkhurst, N. Pearce, J. Pereira, A. Perrakis, H. R. Powell, R. J. Read, D. J. Rigden, W. Rochira, M. Sammito, F. Sánchez Rodríguez, G. M. Sheldrick, K. L. Shelley, F. Simkovic, A. J. Simpkin, P. Skubak, E. Sobolev, R. A. Steiner, K. Stevenson, I. Tews, J. M. H. Thomas, A. Thorn, J. T. Valls, V. Uski, I. Usón, A. Vagin, S. Velankar, M. Vollmar, H. Walden, D. Waterman, K. S. Wilson, M. D. Winn, G. Winter, M. Wojdyr and K. Yamashita



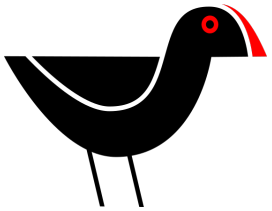
Cover:
Acta Cryst D
June 2023



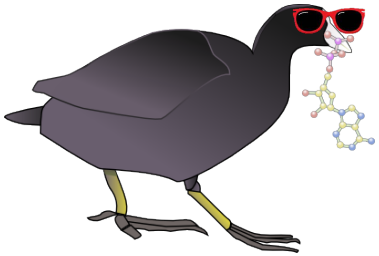


Lunchtime Byte

- **Moorhen**: Today at 1pm



- **Coot 1.1**: Tomorrow at 1pm



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