Moorhen

Web-Based Interactive Model Building

This is a coot

This is a moorhen

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CCP4/DLS Workshop

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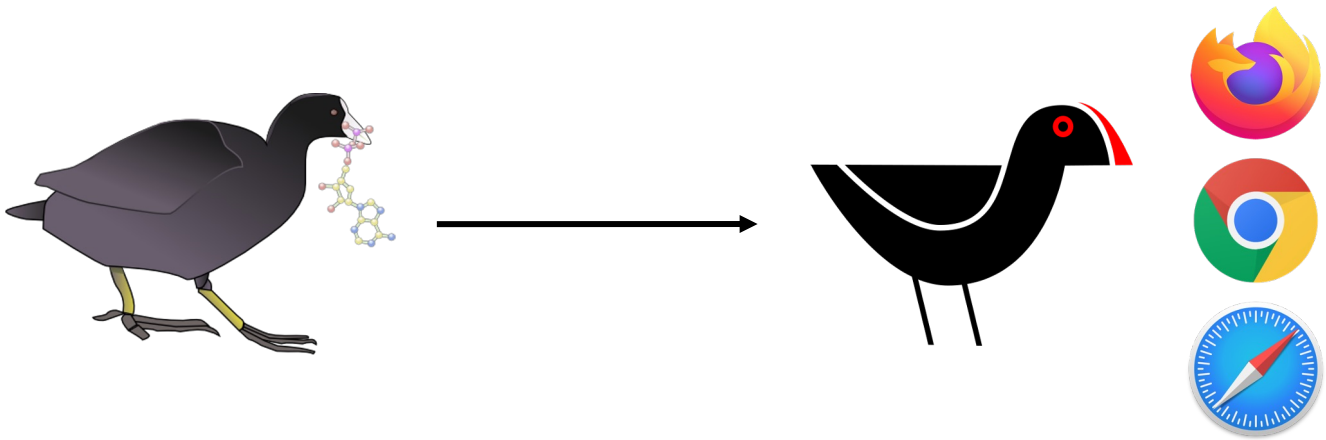
What is Moorhen?

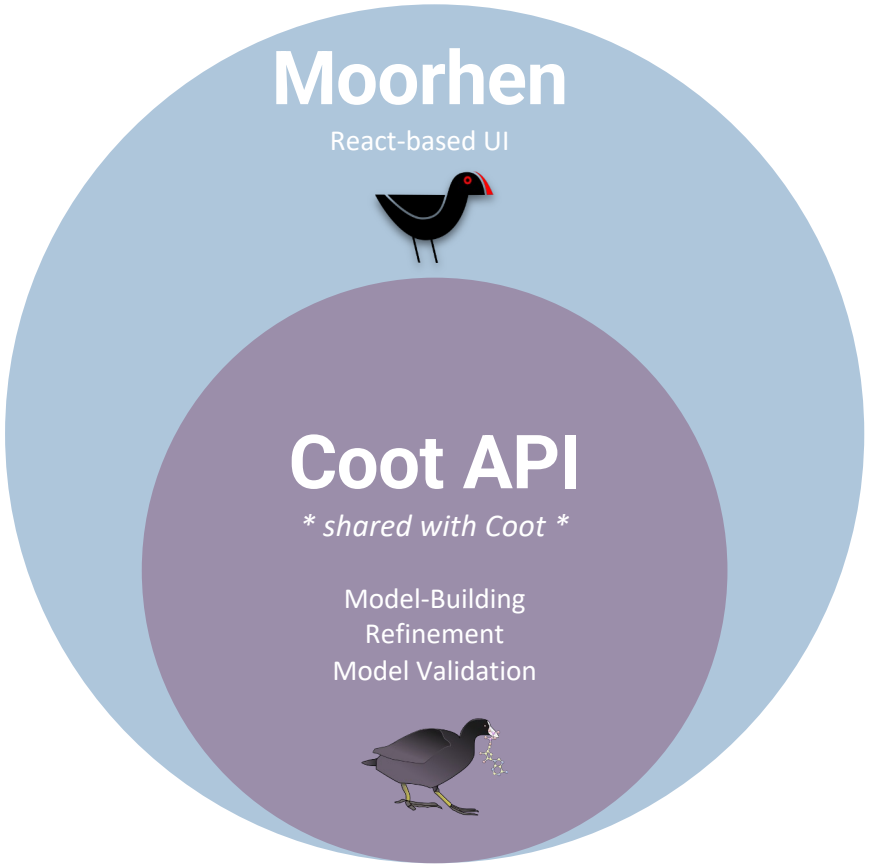
- Moorhen is a next-generation web-based application for the visualisation and manipulation of molecules in structure determination and analysis

  ➔ In short, Coot on the web browser



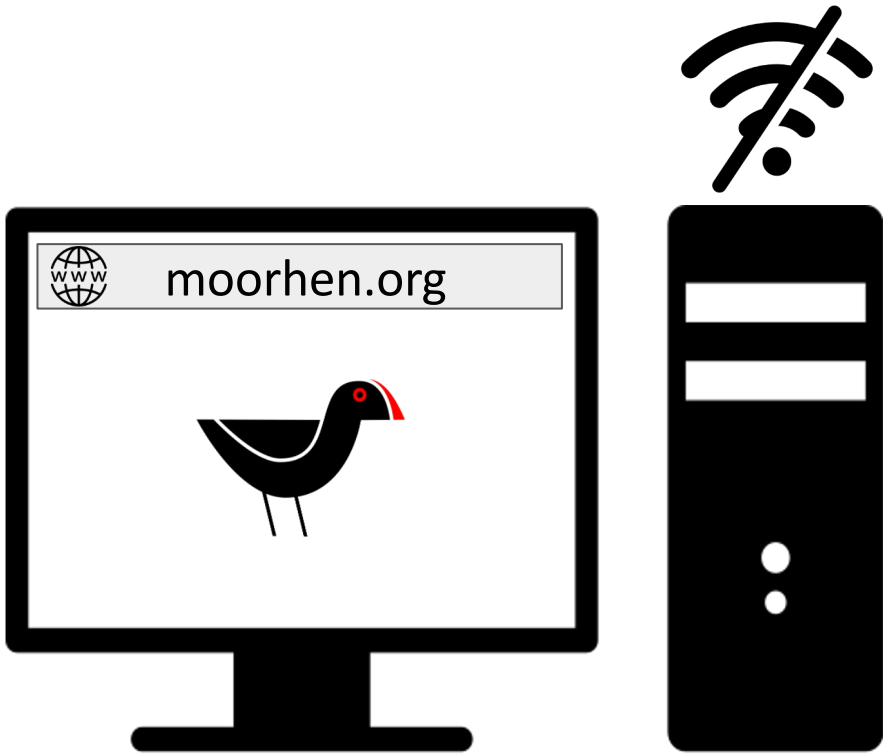
What is Moorhen?

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

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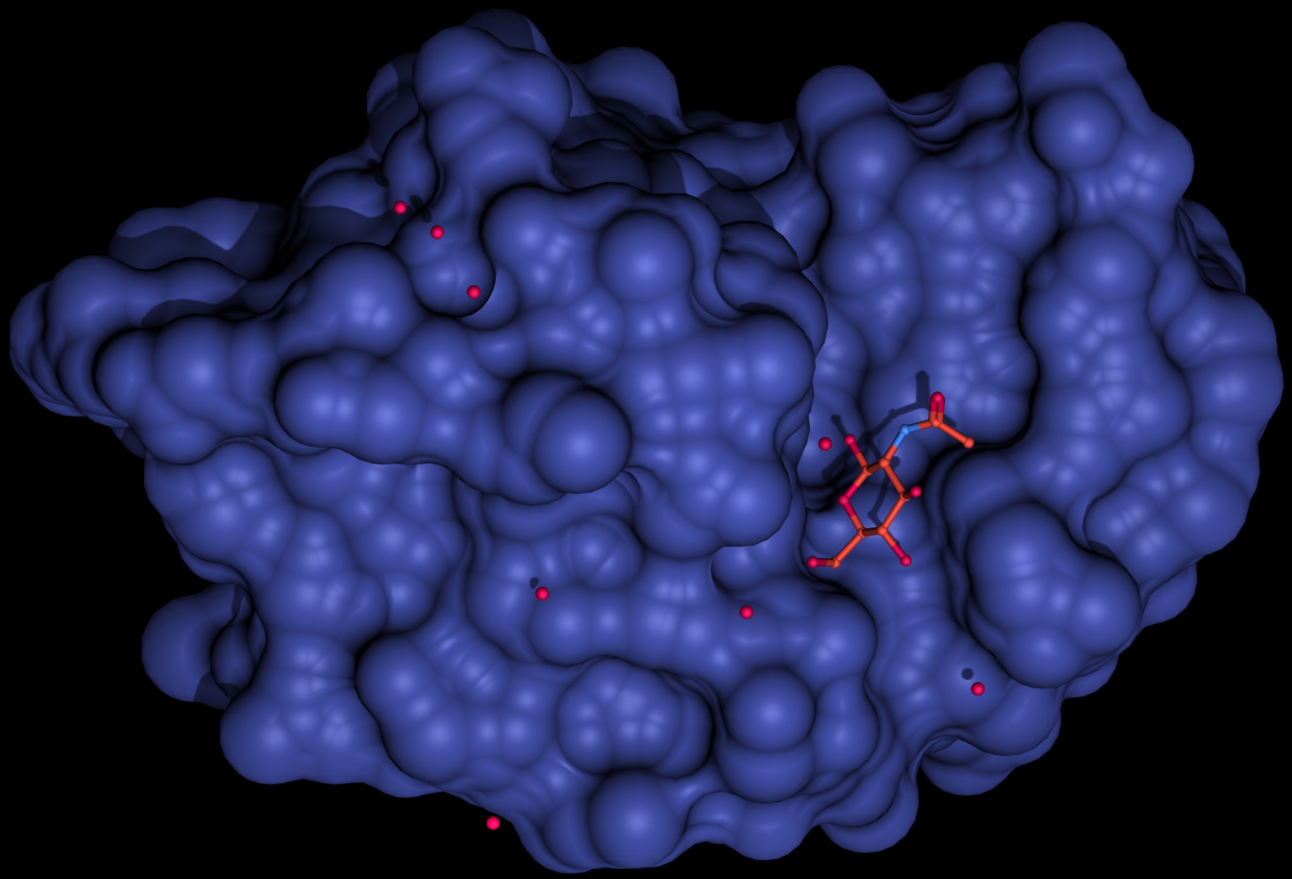
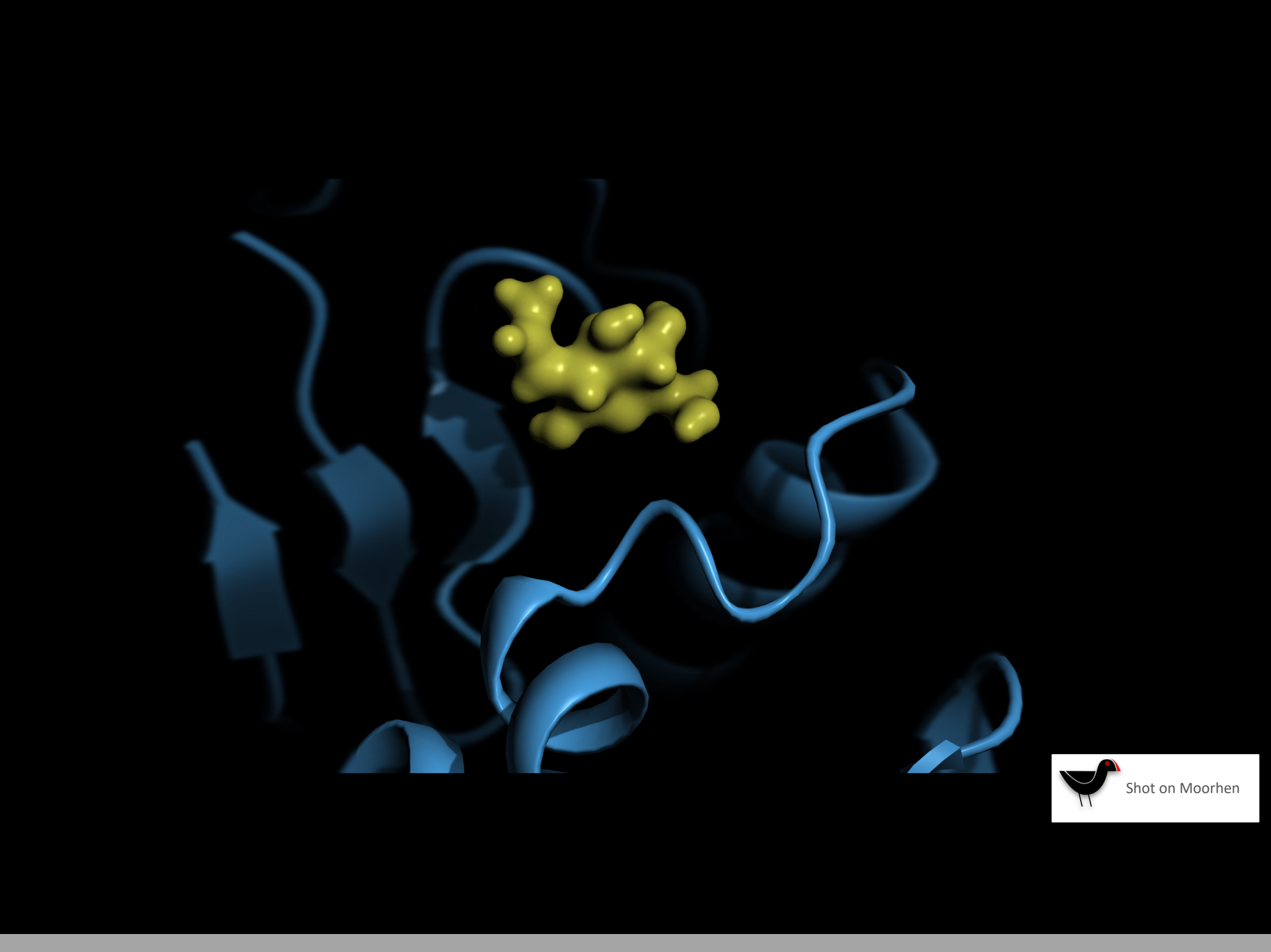
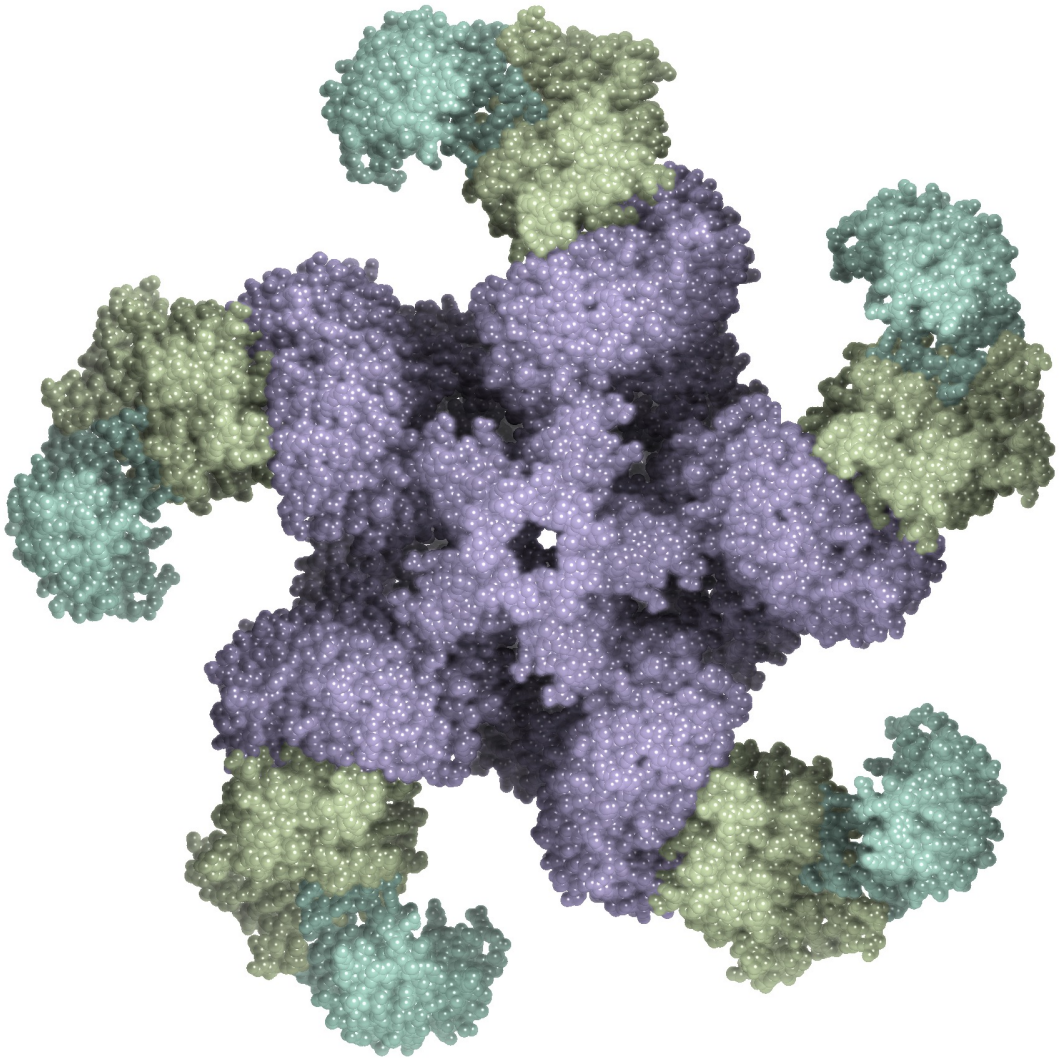
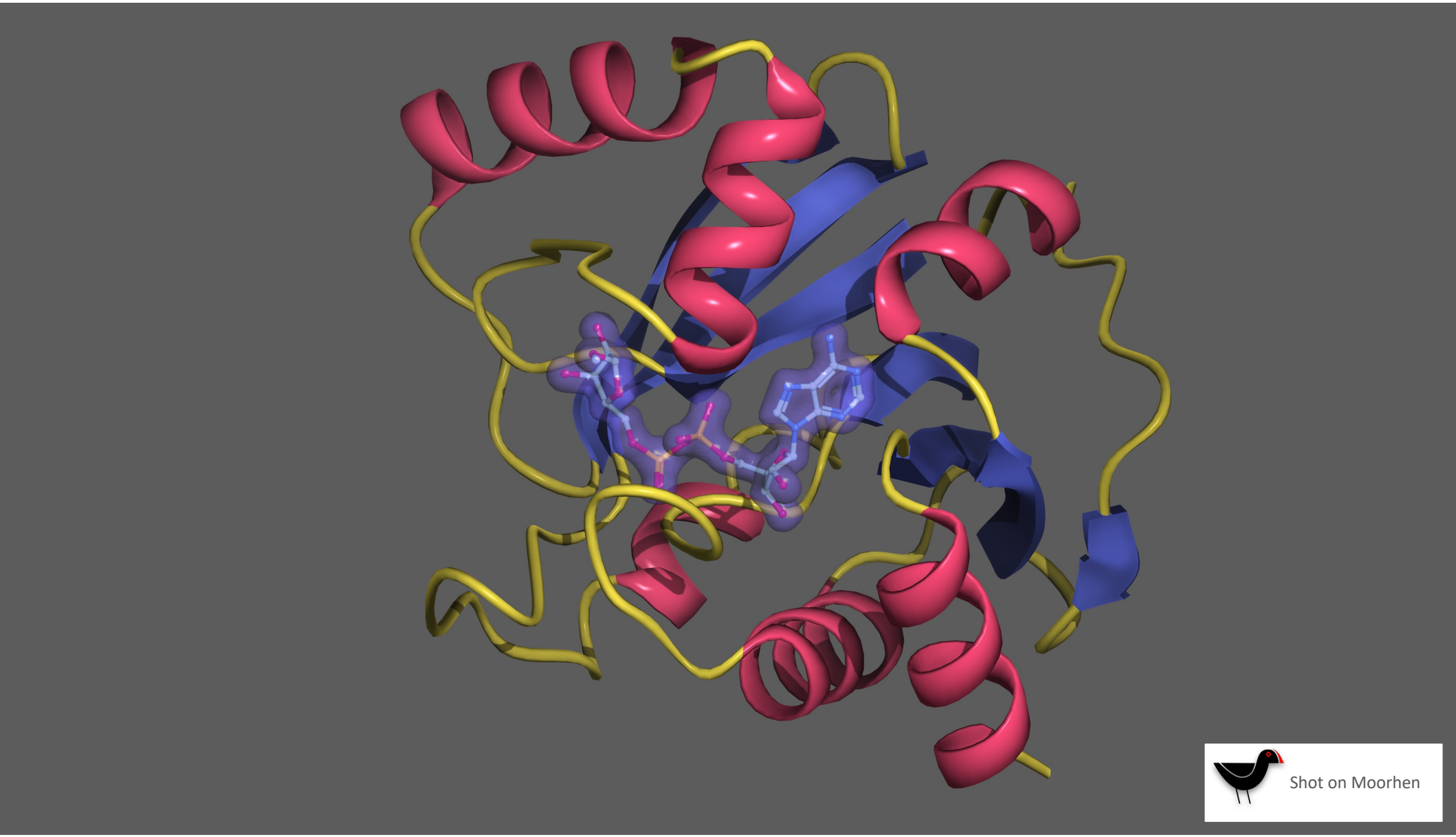
Figure-Making Features

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

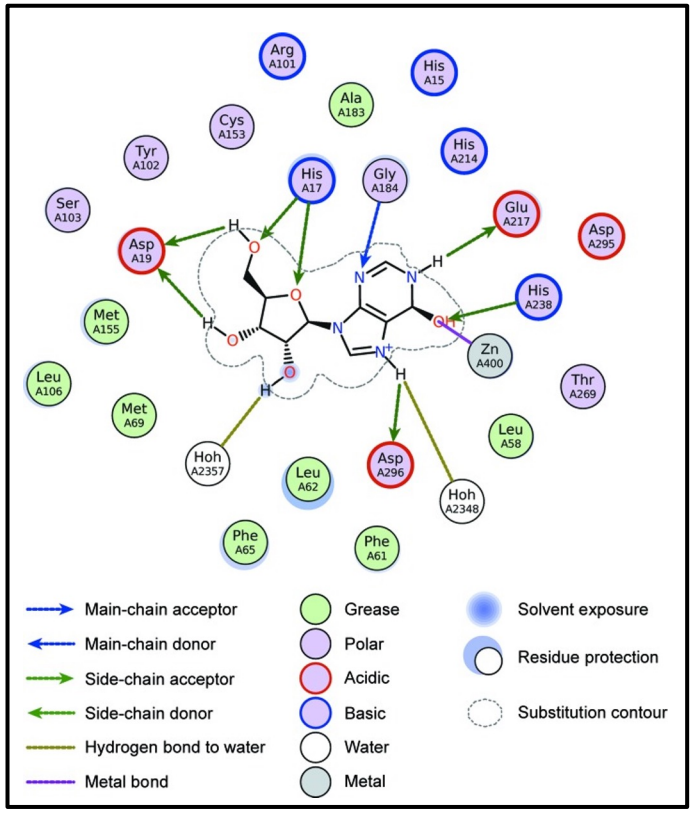



Shot on Moorhen



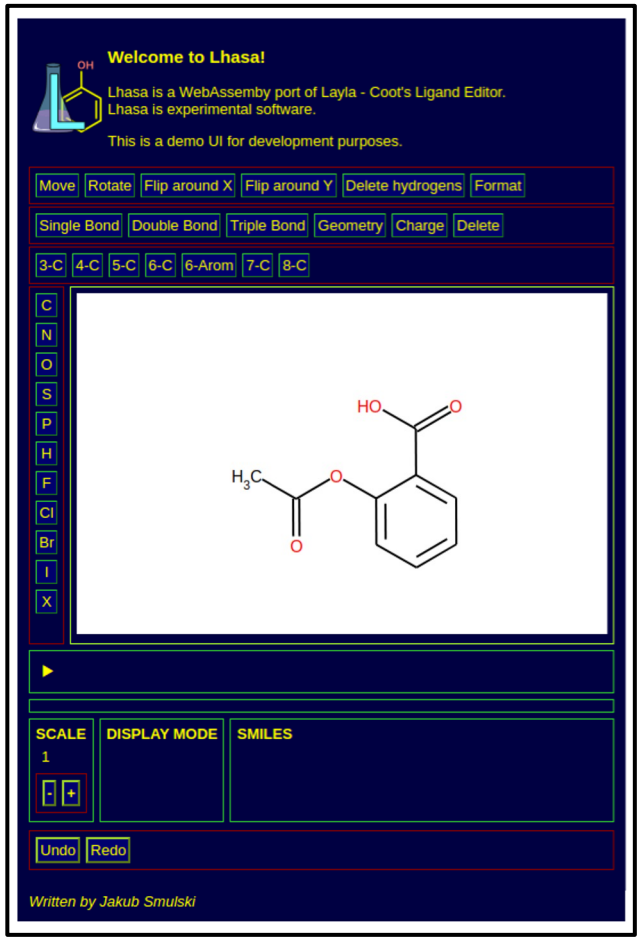

Shot on Moorhen

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



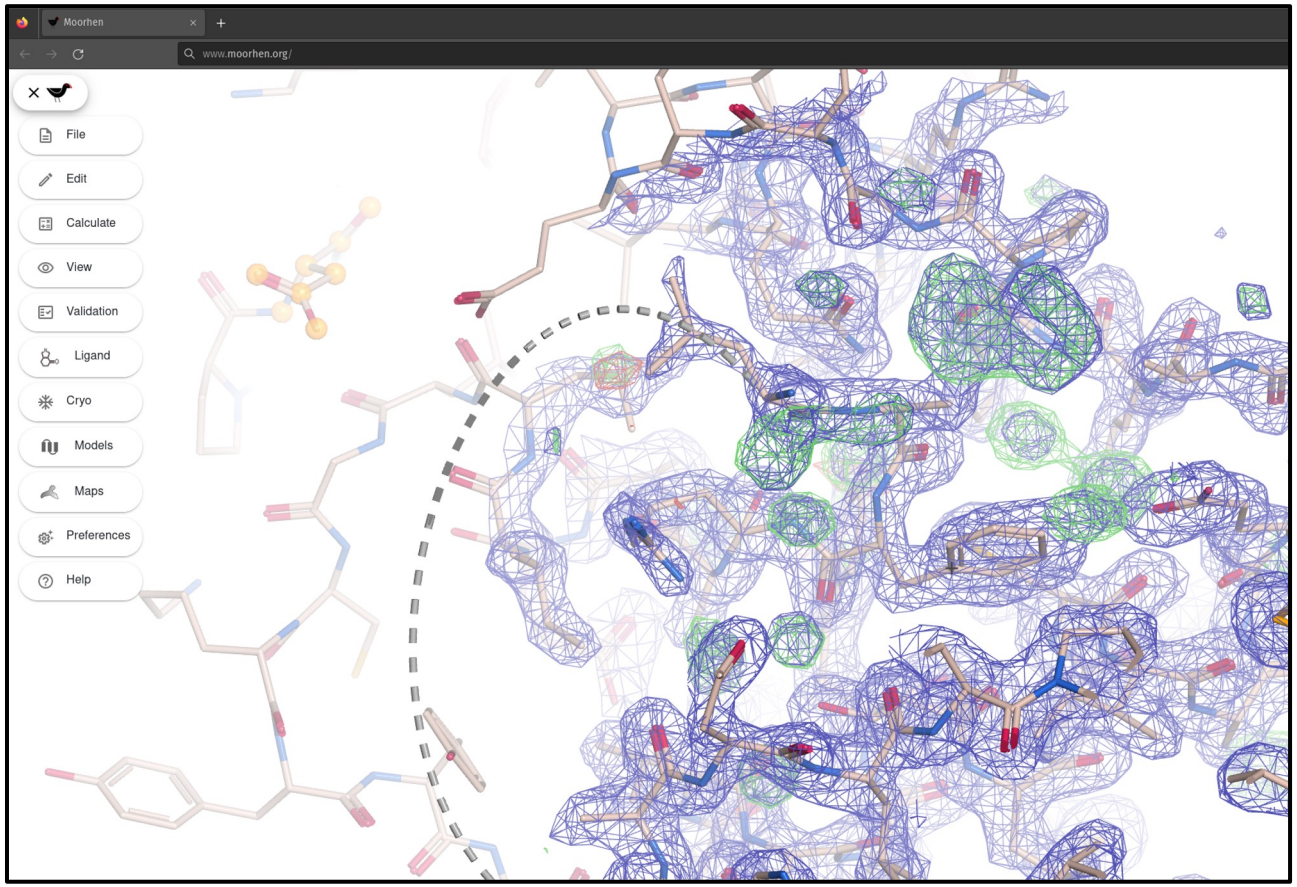
Source: Jakub Smulski

Provide input for dictionary generators:

- elBOW
- AceDRG
- Grade 2

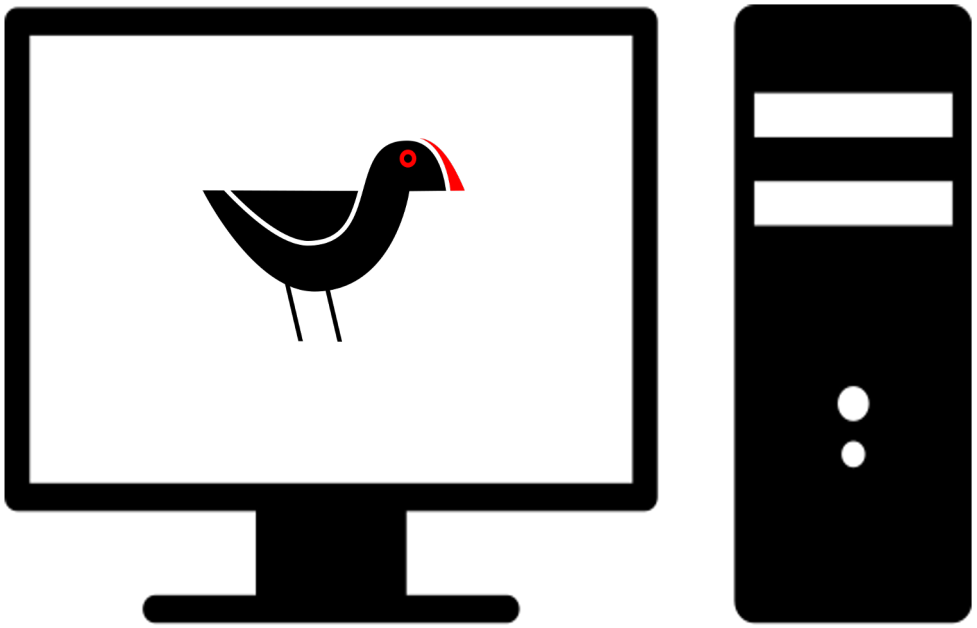
Where is Moorhen available?

www.moorhen.org



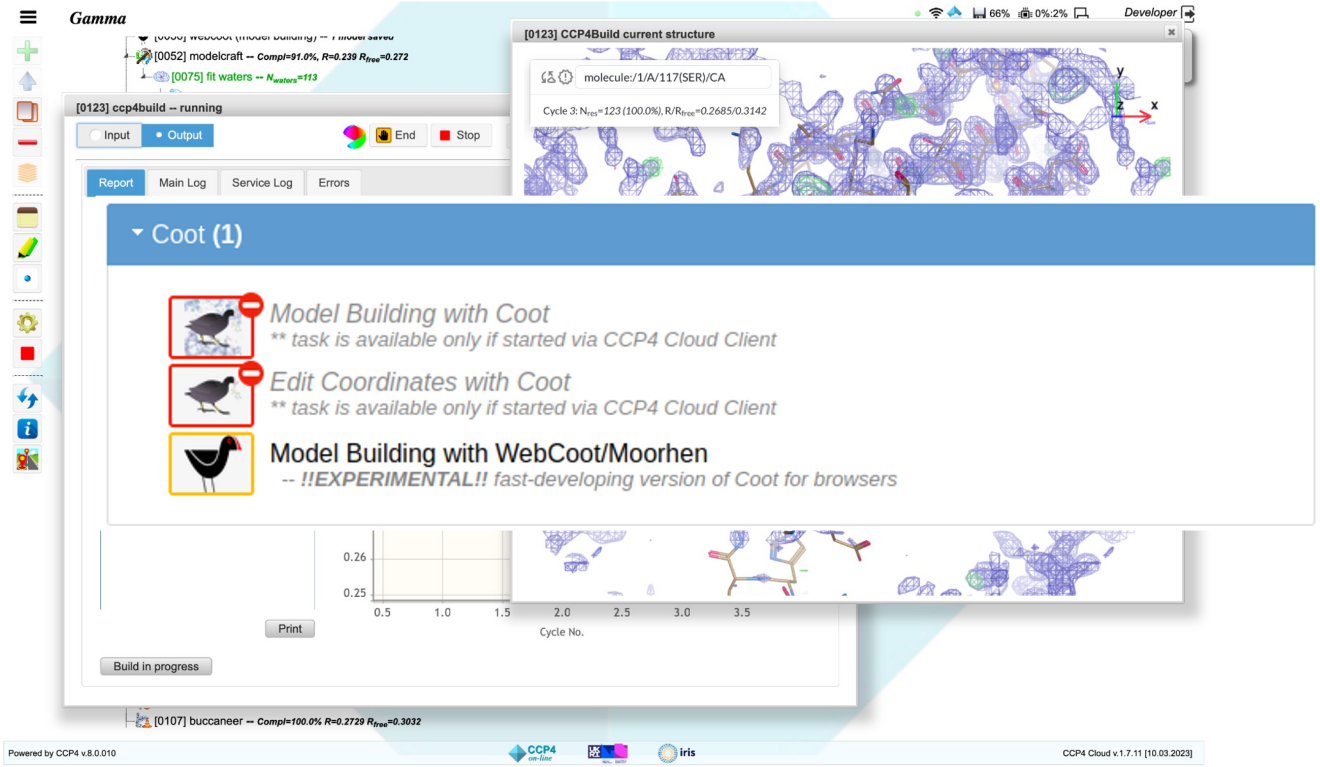
Where is Moorhen available?

Electron Desktop App



Where is Moorhen available?

CCP4 Cloud



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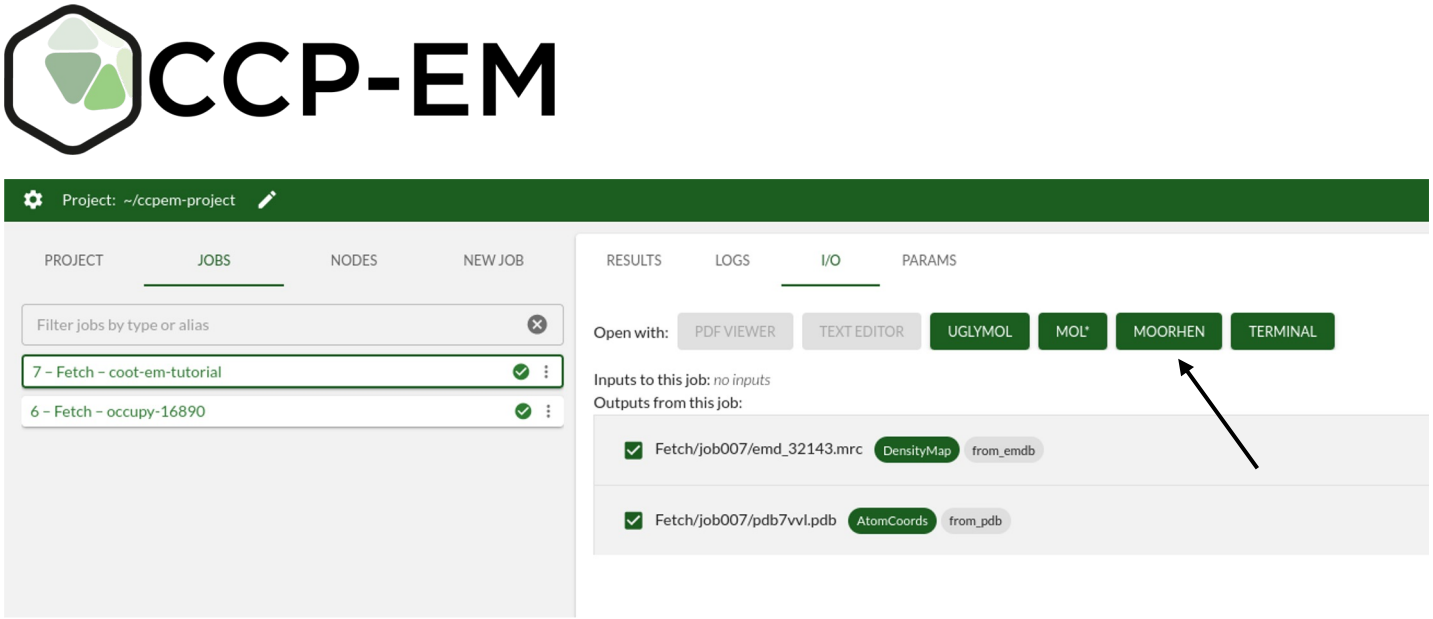
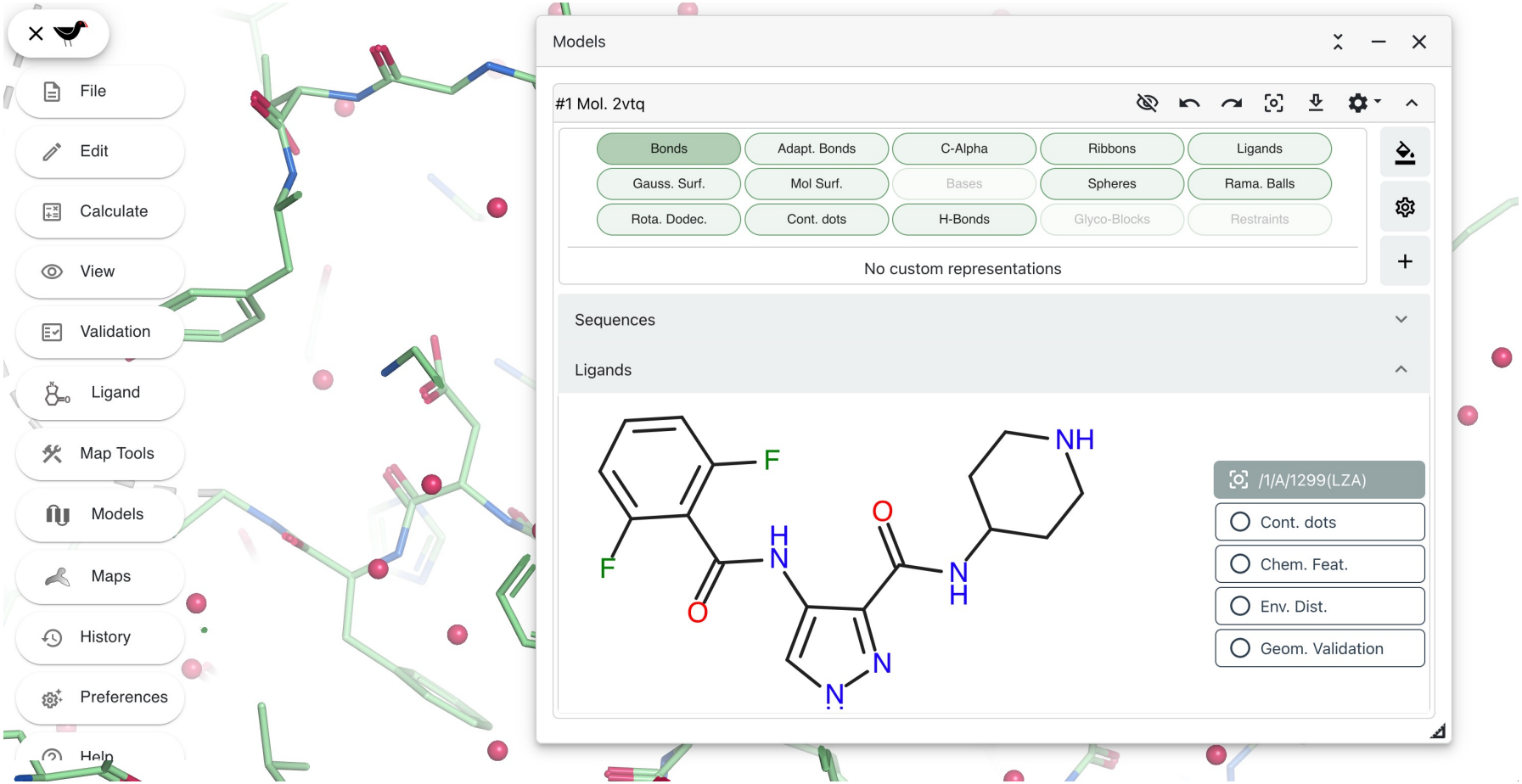


Moorhen – Ligand validation



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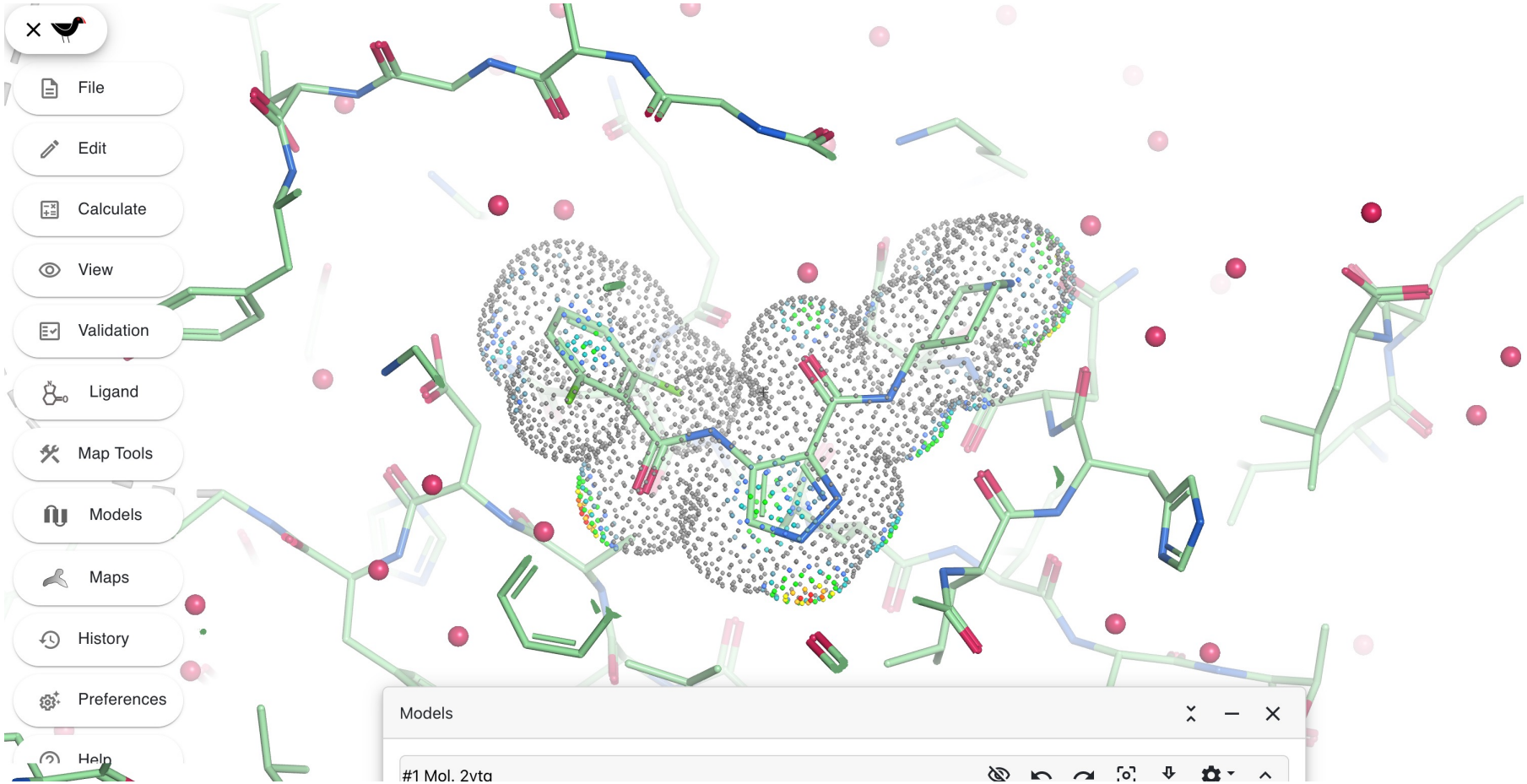

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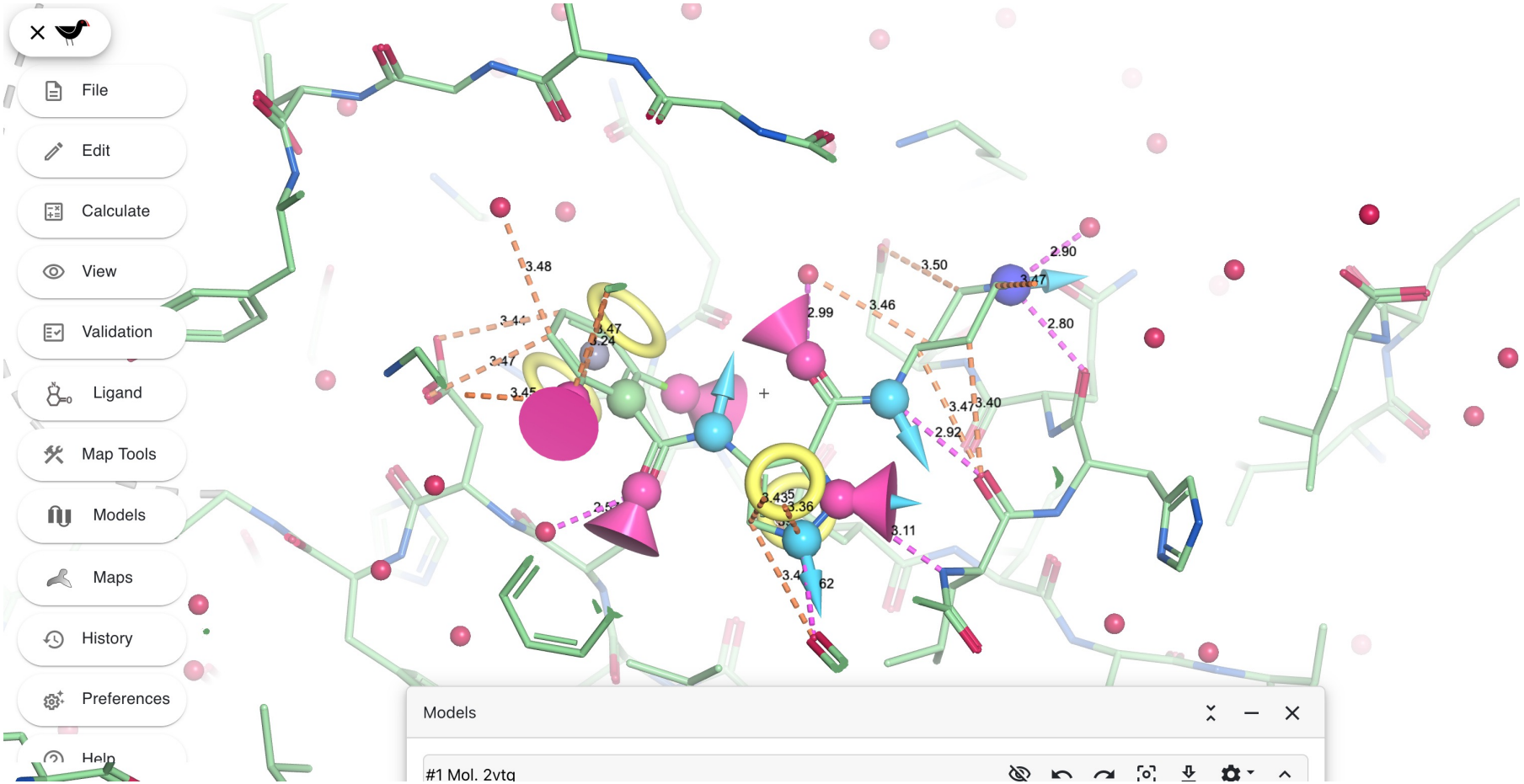
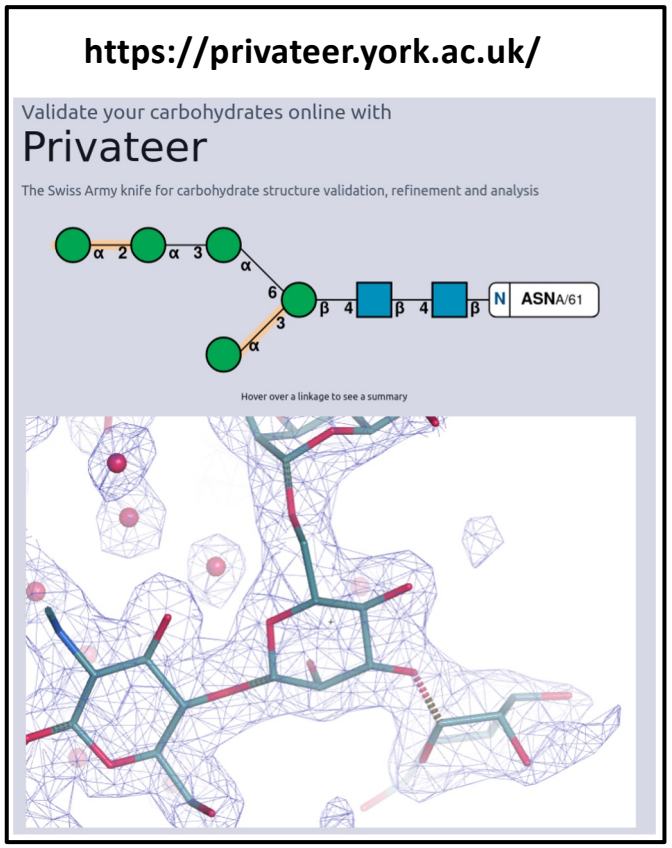


Moorhen as a React component

➔ 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

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Paul Emsley

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Jakub Smulski

Martin Noble

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