

Moorhen

Web-Based Interactive Model Building

This is a coot



This is a moorhen

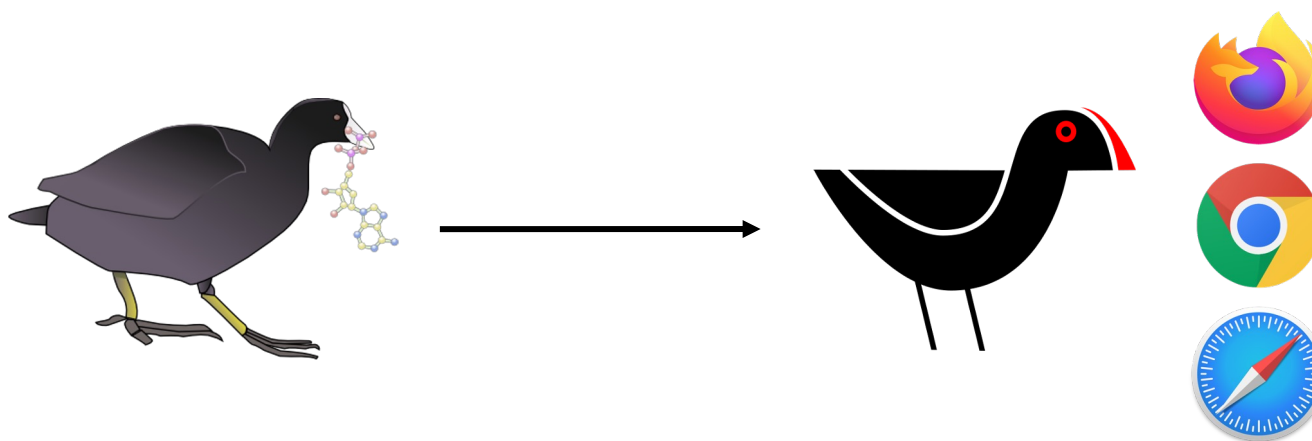


Lucrezia Catapano

CCP4/DLS Workshop
28th November 2024

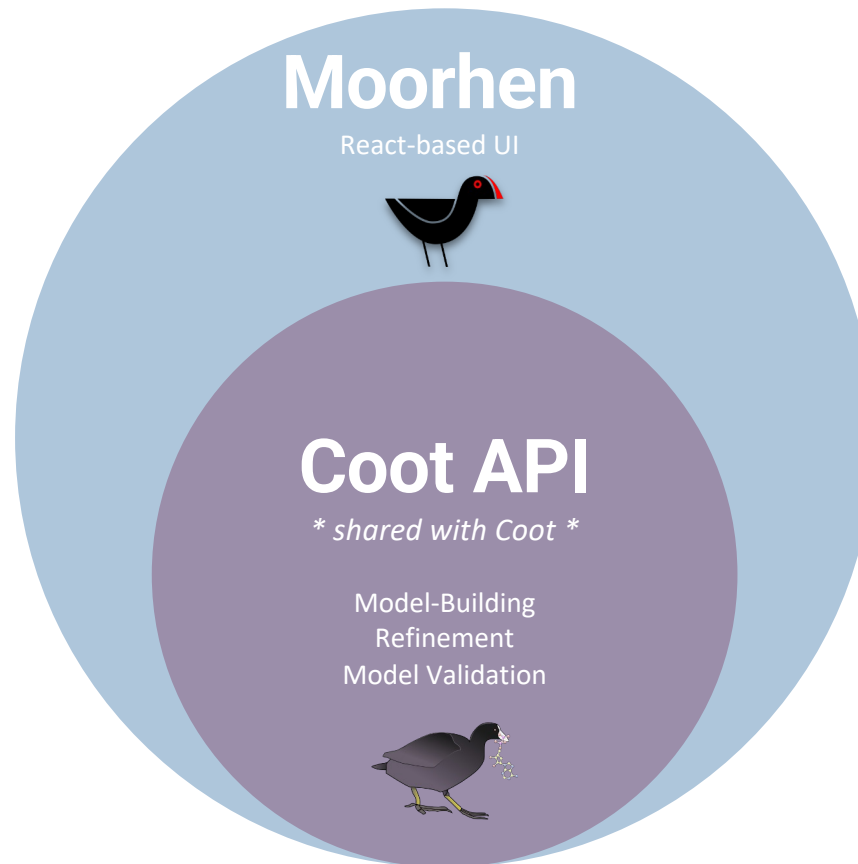
What is Moorhen?

- 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



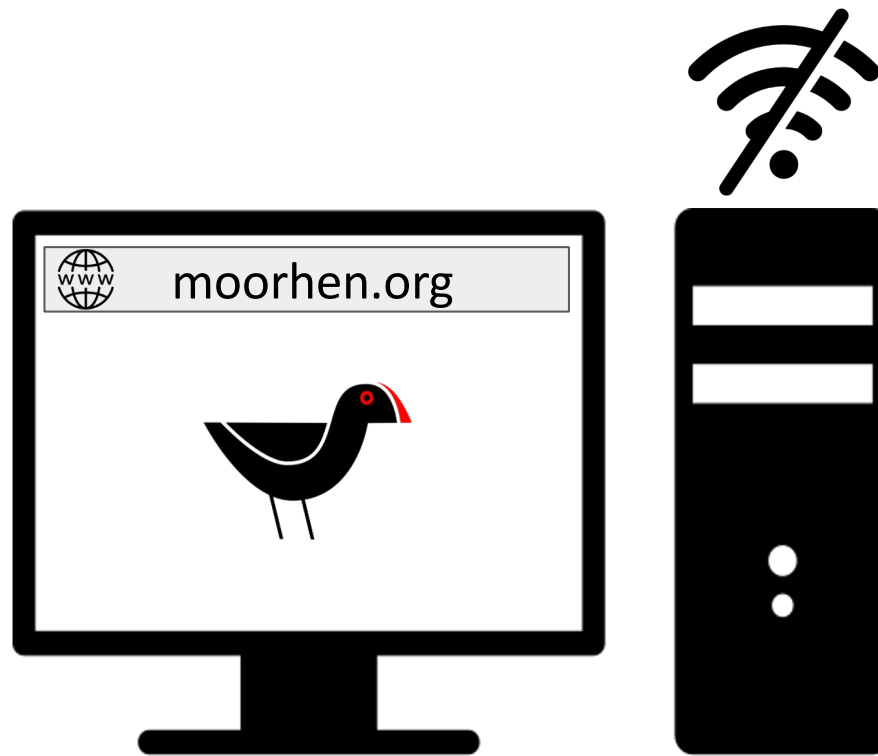
What is Moorhen?

→ Moorhen extends libccoot 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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 - 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**

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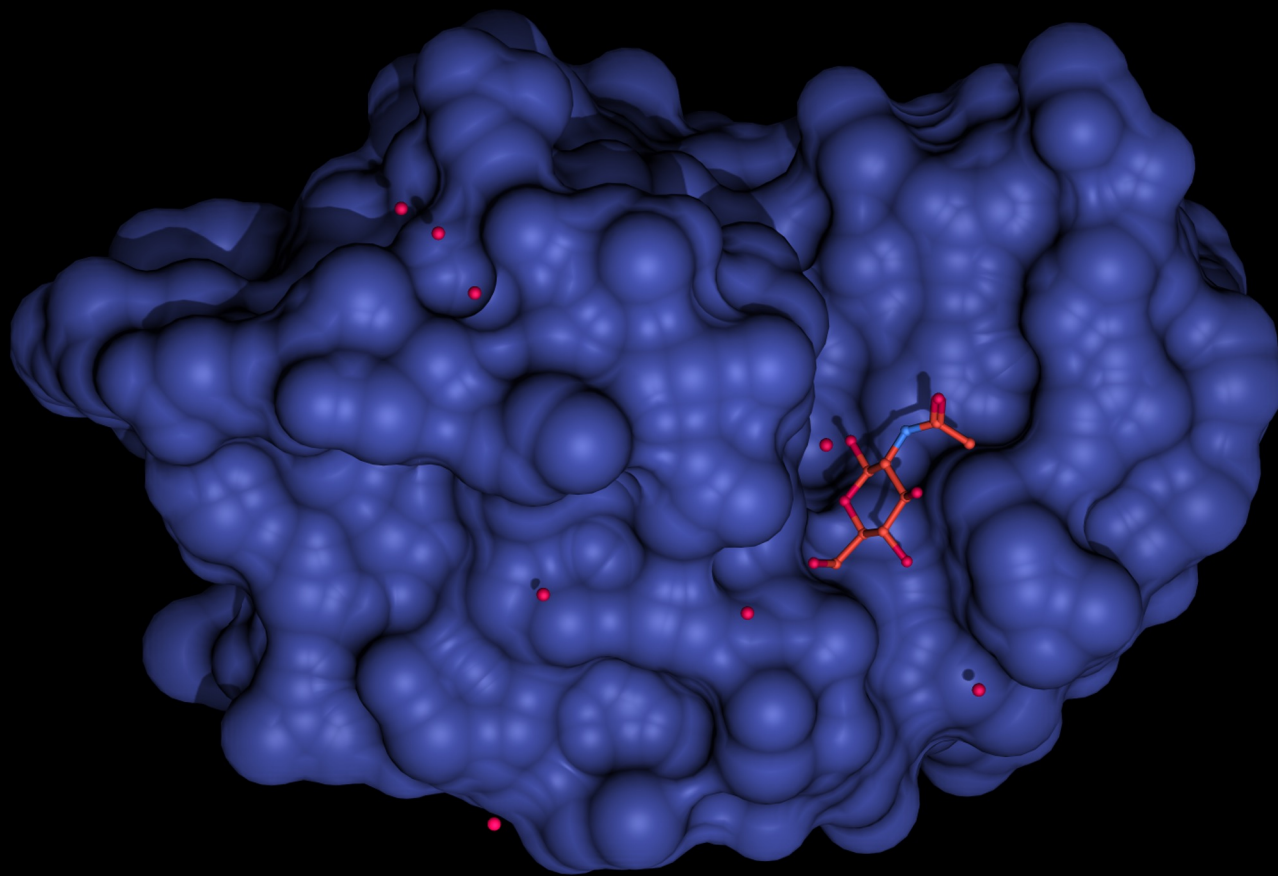
Env. Distances

Validation Features

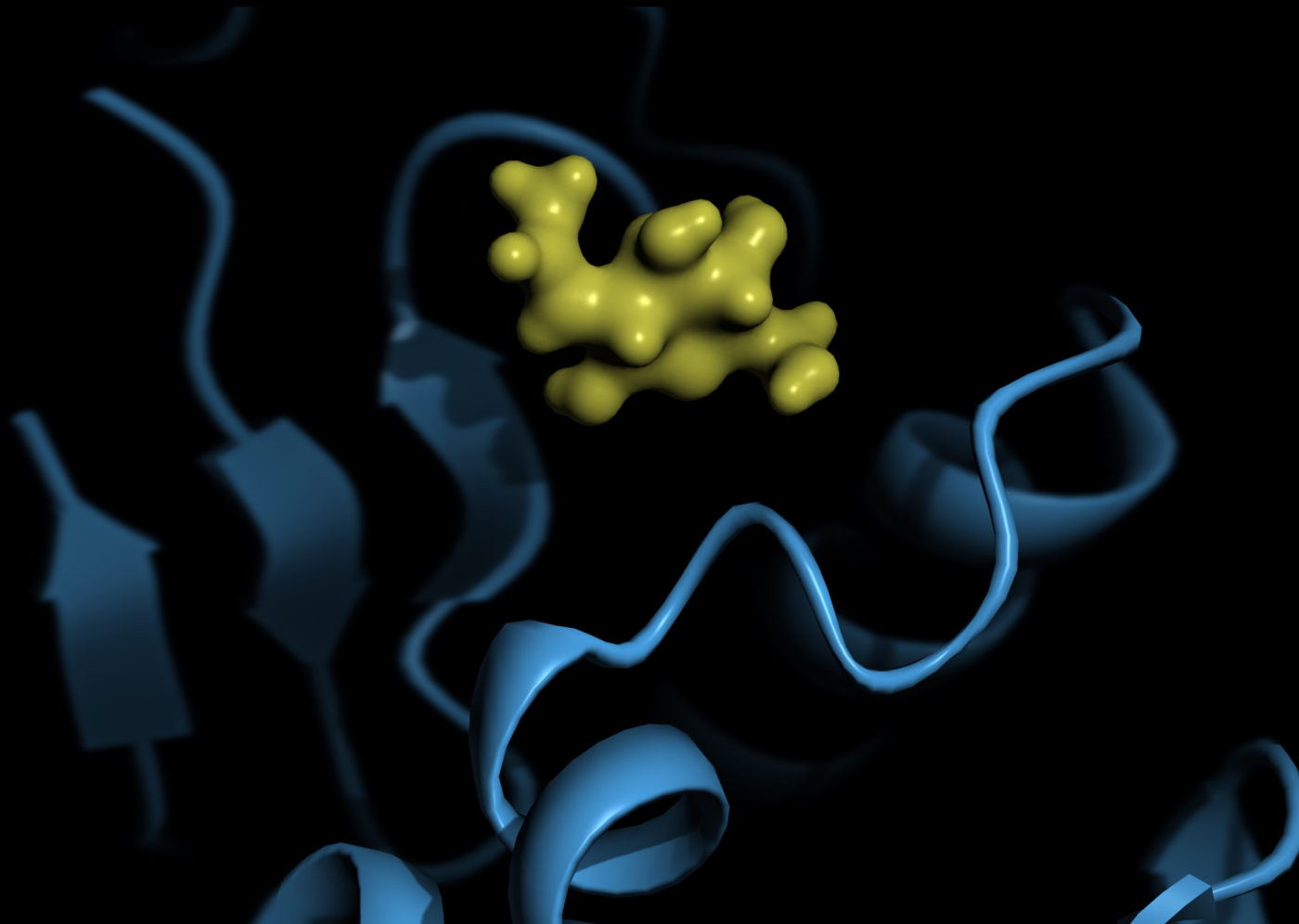
| | |
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Figure-Making Features

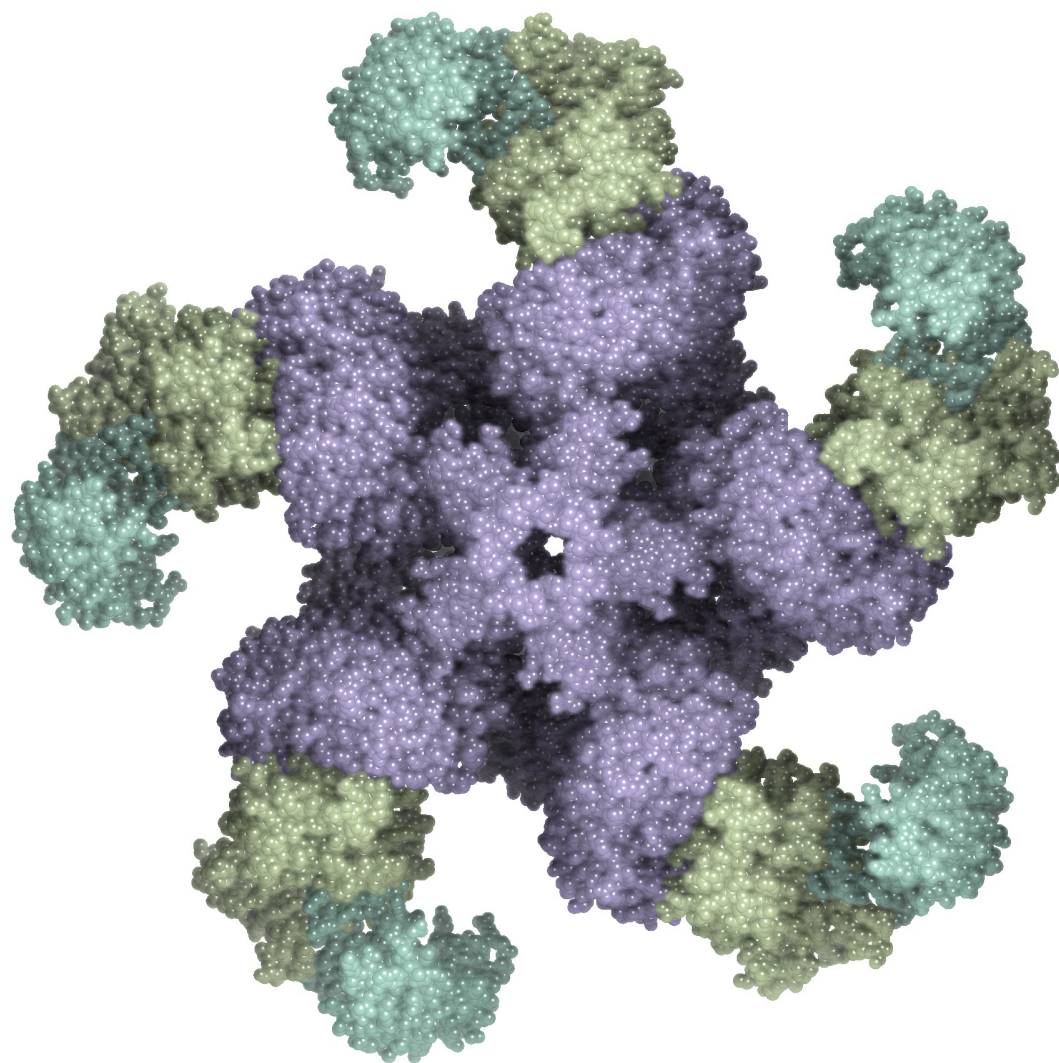
| | | |
|--------------------------------------|--------------------------|------------------------|
| Multiple Model Representation Styles | Arbitrary Colour schemes | Basic Movie Making |
| Shadows | Depth Blur | Perspective Projection |
| Clipping/Fogging | Ambient Occlusion | Screenshots |



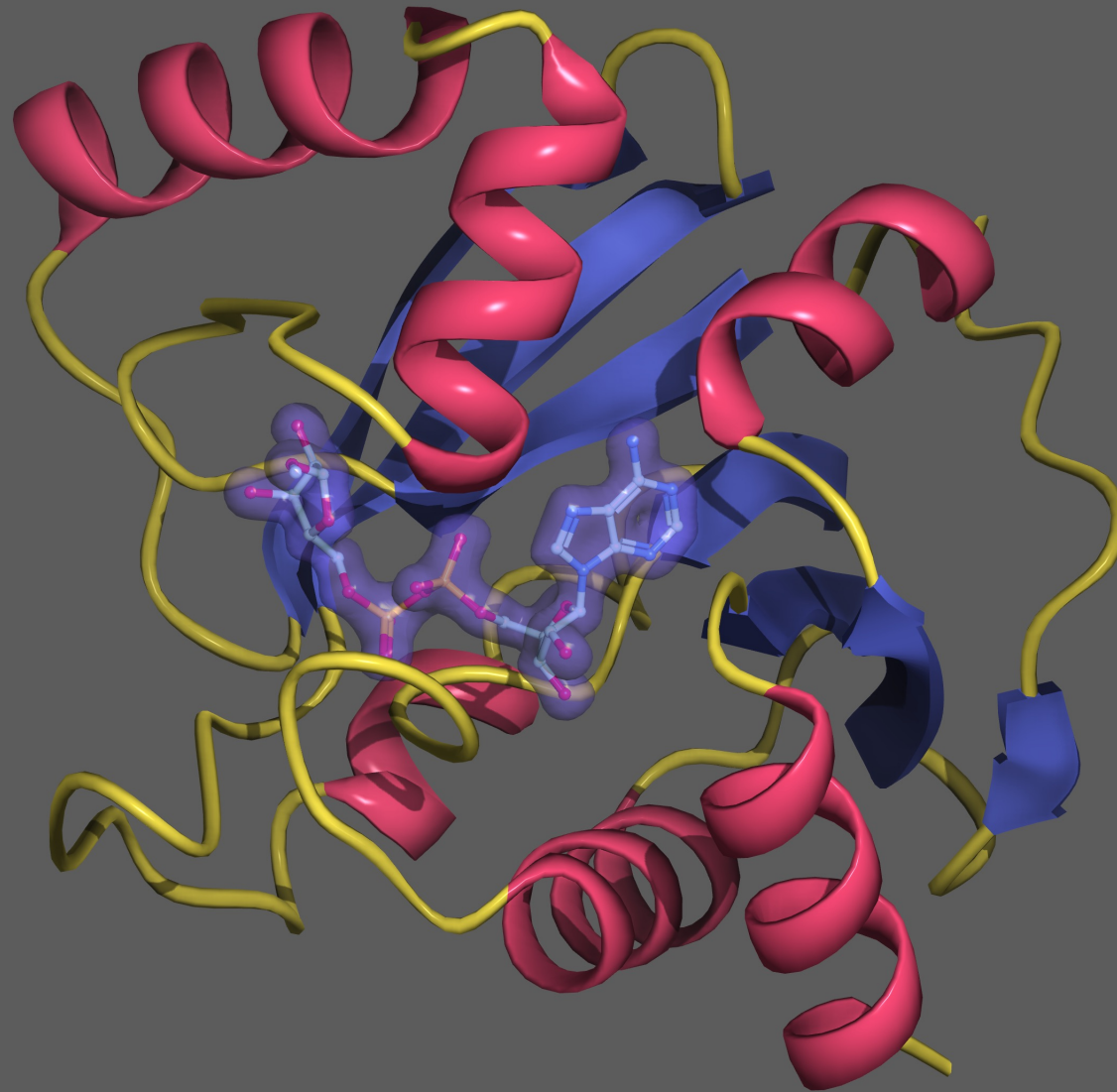
Shot on Moorhen



Shot on Moorhen

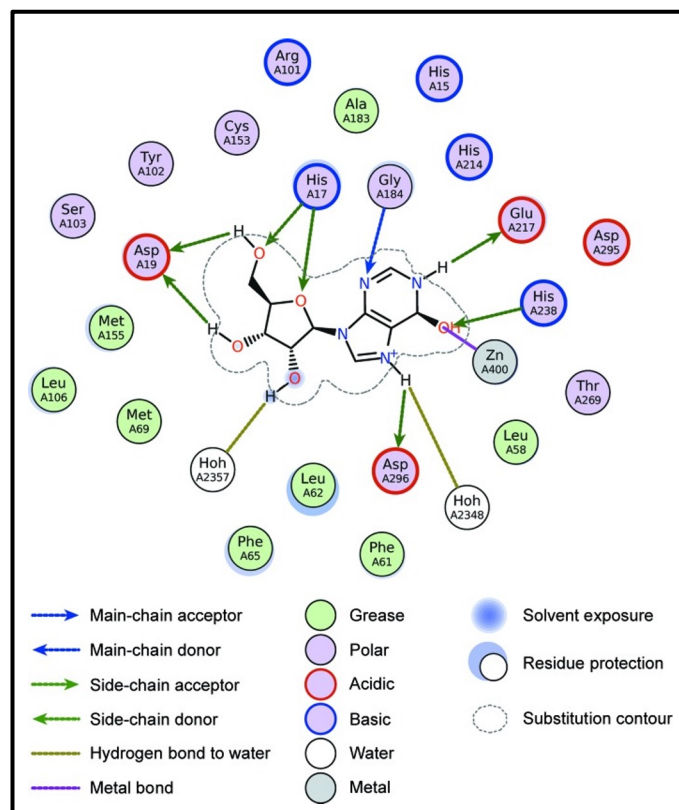


Shot on Moorhen



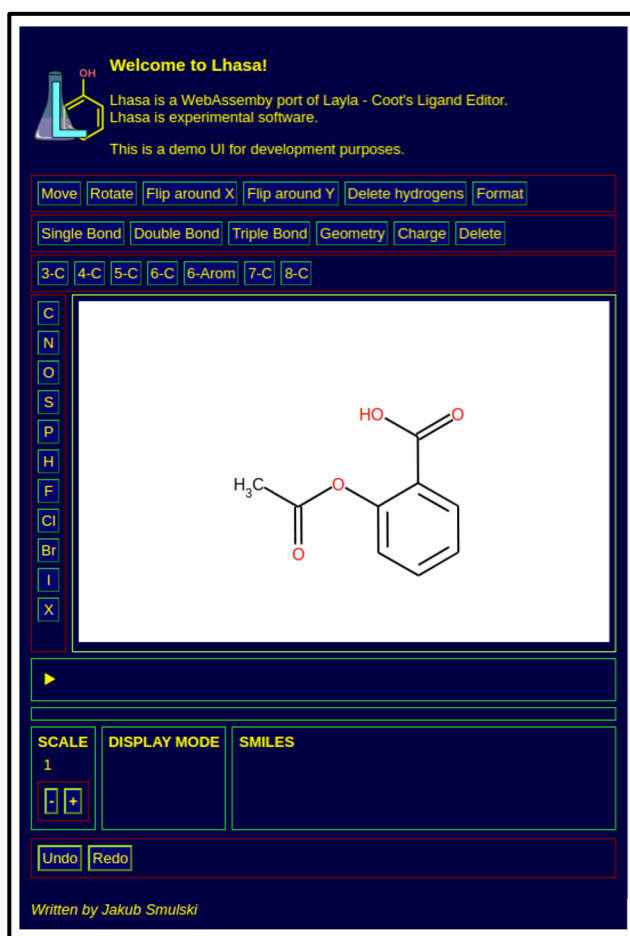
Shot on Moorhen

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



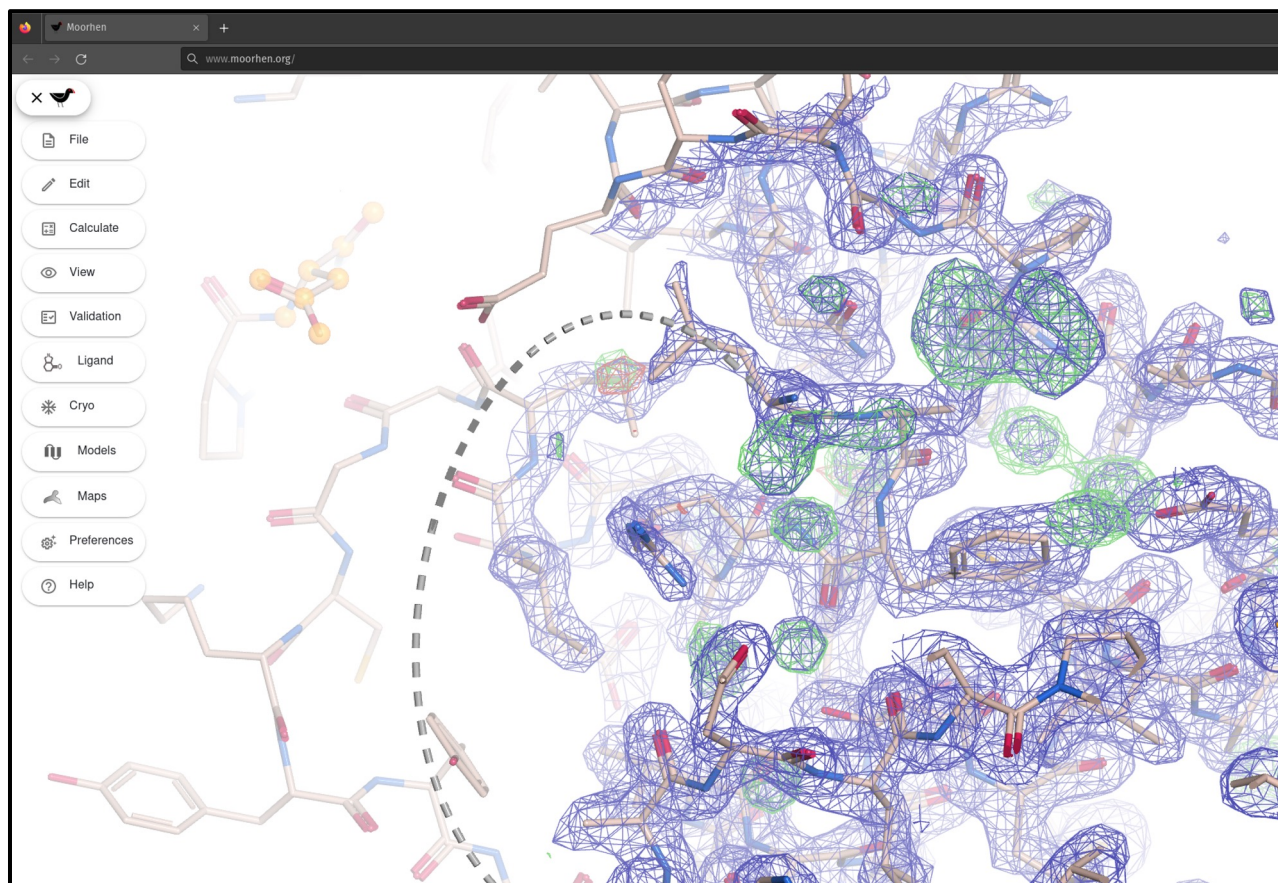
Provide input for dictionary generators:

- eLBOW
- AceDRG
- Grade 2

Source: Jakub Smulski

Where is Moorhen available?

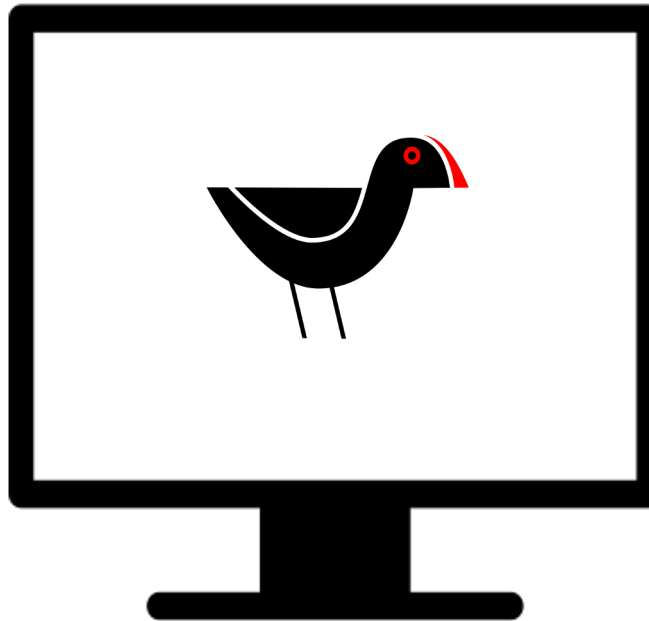
www.moorhen.org



Where is Moorhen available?



Electron Desktop
App



Where is Moorhen available?



CCP4 Cloud

Gamma

[0052] modelcraft -- Compl=91.0%, R=0.239 R_{free}=0.272

[0075] fit waters -- N_{waters}=113

[0123] ccp4build -- running

Input Output End Stop




Report Main Log Service Log Errors

[0123] CCP4Build current structure

molecule/1/A/117(SER)/CA

Cycle 3: N_{res}=123 (100.0%), R/R_{free}=0.2685/0.3142

▼ Coot (1)

-  **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

0.26
0.25
0.5 1.0 1.5 2.0 2.5 3.0 3.5
Cycle No.

Print

Build in progress

[0107] buccaneer -- Compl=100.0% R=0.2729 R_{free}=0.3032

Powered by CCP4 v.8.0.010

CCP4

Iris

CCP4 Cloud v1.7.11 [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

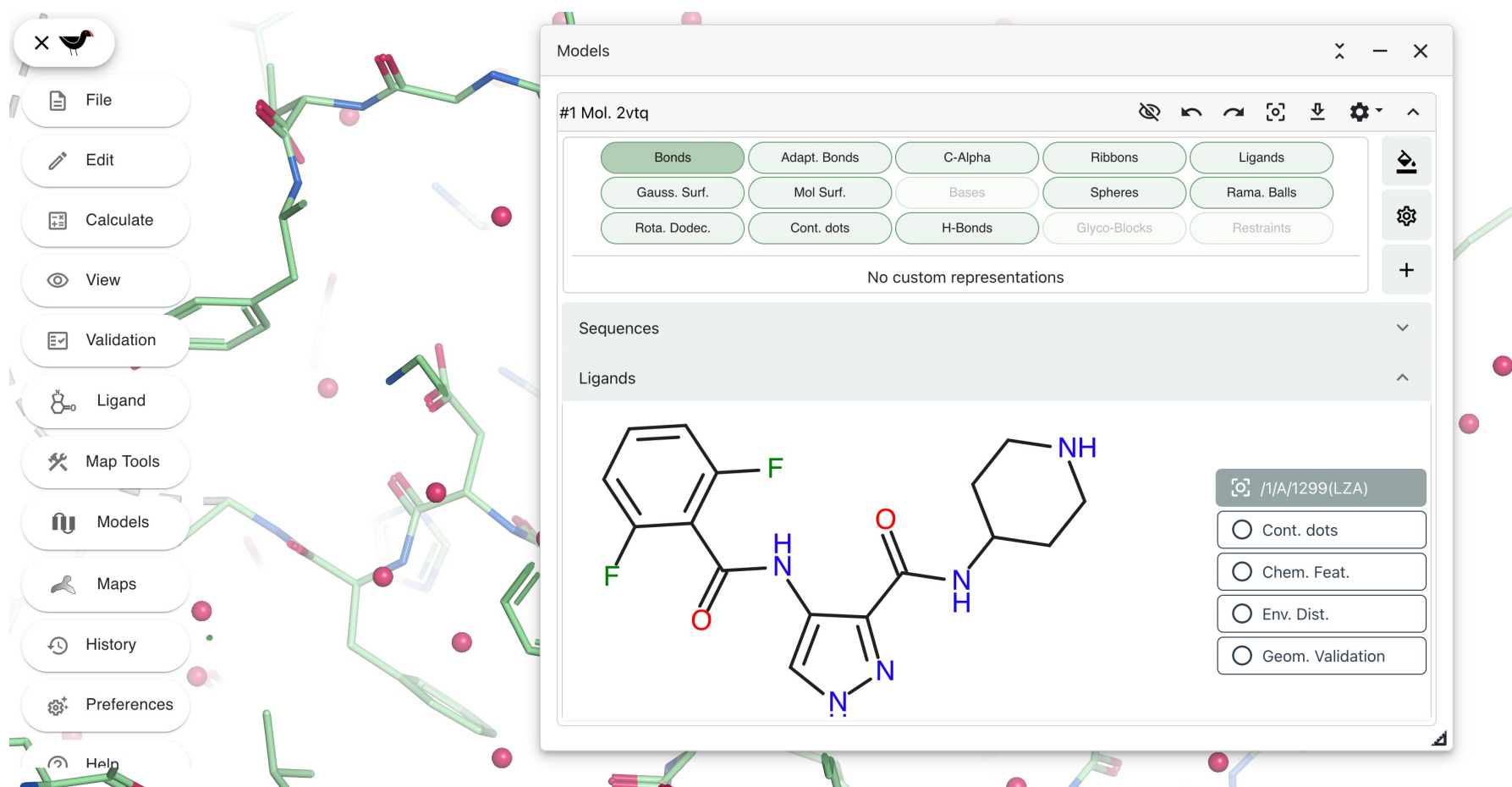
Inputs to this job: no inputs

Outputs from this job:

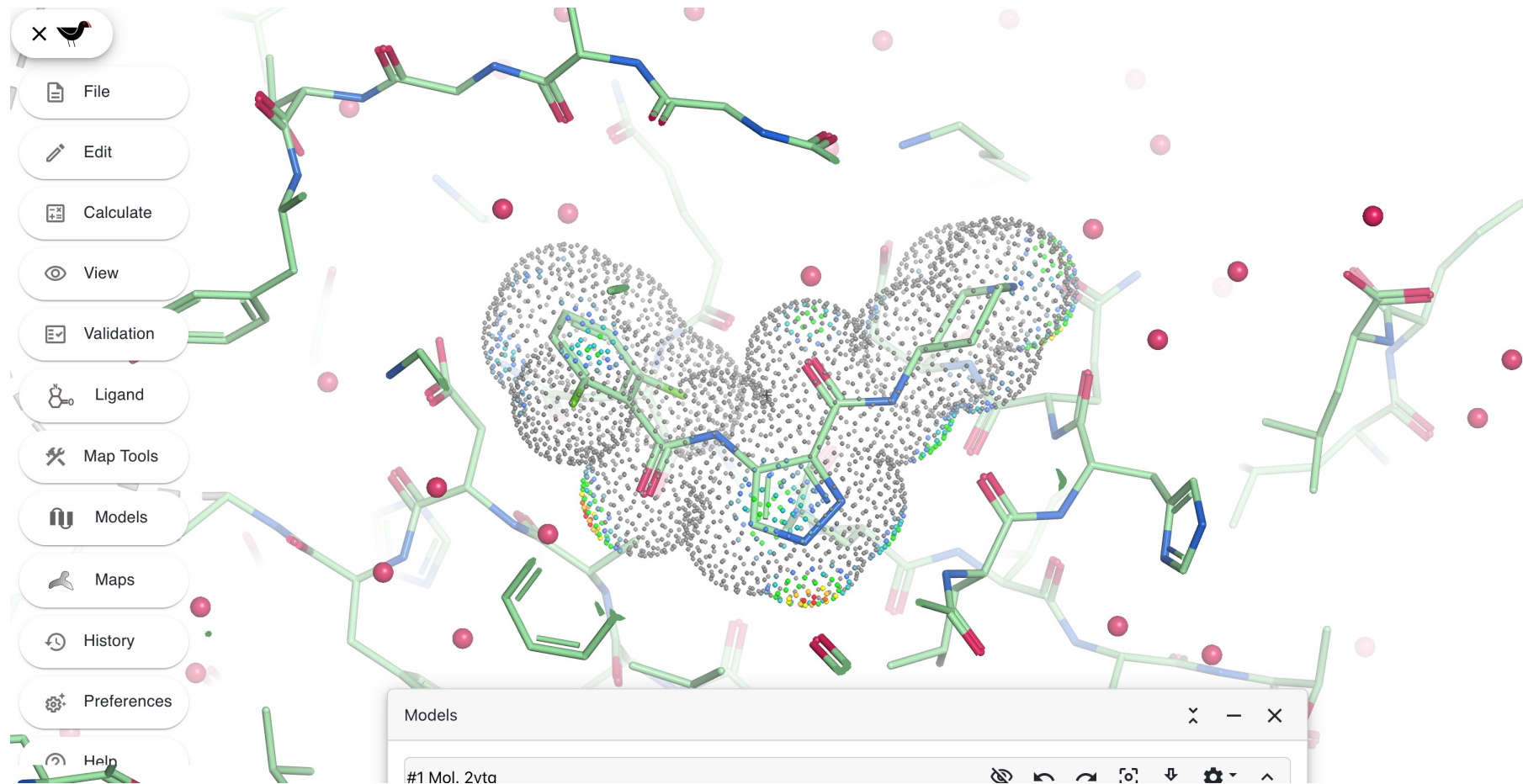
- Fetch/job007/emd_32143.mrc DensityMap from_emdb
- Fetch/job007/pdb7vv1.pdb AtomCoords from_pdb

An arrow points to the MOORHEN button in the 'Open with:' section.

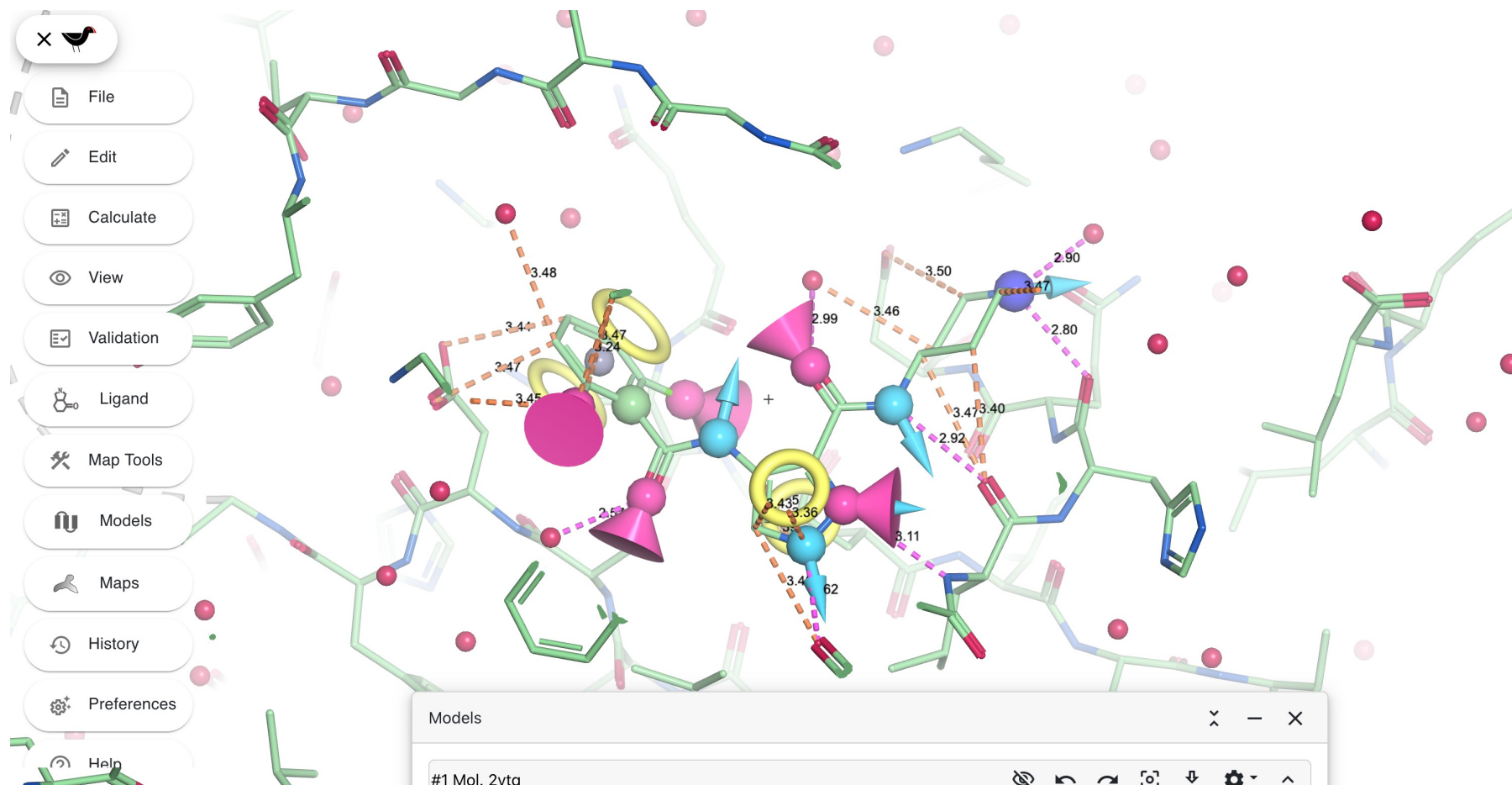
Moorhen – Ligand validation



Moorhen – Ligand validation

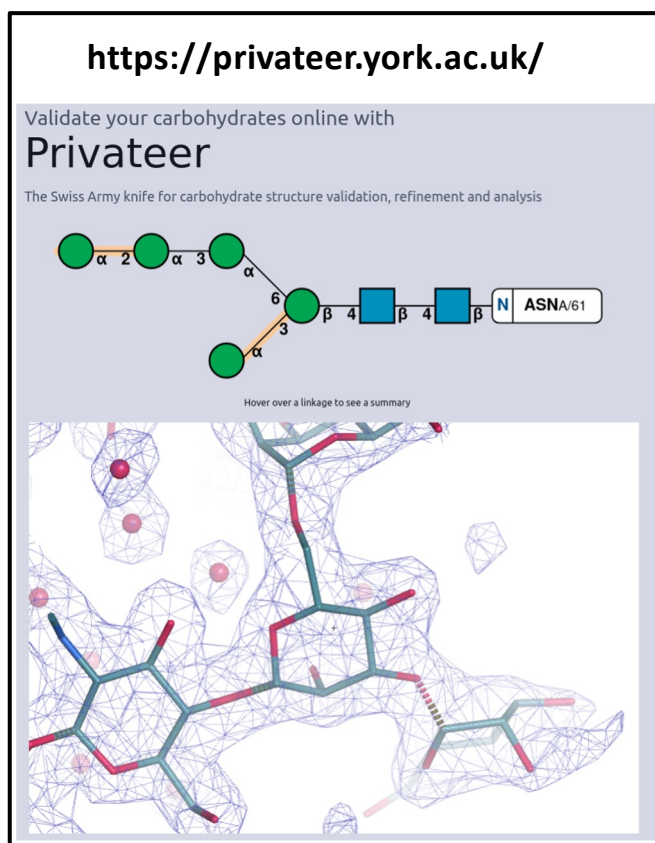


Moorhen – Ligand validation




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



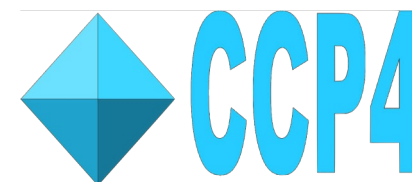
Eugene
Krissinel



Jakub
Smulski



Martin
Noble



... And everyone who has contributed to CCP4

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 @lulu_catapano