

Coot and Moorhen: evolving interactive model building from desktop to web

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Coot [1] is a powerful and widely used program for atomic model building, refinement, and validation of macromolecular structures derived from X-ray crystallography and cryo-EM data [2].

Recent developments include a redesigned, more user-friendly graphical user interface. The introduction of *Layla*, a ligand-building tool that supports SMILES editing and provides a QED (Quantitative Estimate of Drug-likeness) [3] score, and a complete rewrite of the graphics engine. New molecular representation styles have been introduced, such as ribbon diagrams and chemistry-aware bond rendering, along with advanced lighting effects including screen-space ambient occlusion, shadows, and improved shader-based lighting for high-quality visualisations.

In parallel, *Coot's* core algorithms have been modularised into clean, accessible libraries: *libcoot*. These are now available via both a Python API and as a JavaScript/WebAssembly module. This separation of computational logic from the graphical interface enables broader integration, scripting, and automation, and lays the foundation for modern, platform-independent applications.

One such application is *Moorhen* (moorhen.org), a fully web-based, client-side tool that leverages the *libcoot* API. Built with React, *Moorhen* offers an interactive interface for model building, refinement, and validation, all executed within the web browser, with no need for installation or server-side processing. This architecture makes *Moorhen* both private and portable, allowing users to access powerful structural biology tools from any modern device. *Moorhen* includes comprehensive validation features such as rotamer scores, Ramachandran, and density-fit analysis. It also provides tools particularly useful for cryo-EM workflows, including molecular placement via jiggle-fit and real-space refinement through model morphing with local distance restraints. Advanced molecular graphics support surfaces and ribbons complemented by high-end rendering techniques for publication-quality figures. It can also integrate with external tools such as *Slice'N'Dice* [4], or be embedded within other applications like the *Privateer* web app [5].

Moorhen is available as a standalone web application and is also integrated into the *CCP4 Cloud* [6] and *CCPEM* [7] interfaces. Its ease of access and powerful capabilities support a wide range of workflows, from research to teaching, helping to democratise structural biology tools for broader scientific and educational communities.

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