UglyMol: a WebGL macromolecular viewer focused on the electron density

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Summary

UglyMol (Wojdyr 2016) is a macromolecular viewer specialized in presenting macromolecular models together with the electron density. It uses web technologies (JavaScript and WebGL) and is suitable for embedding in web applications. The project was started as a fork of xtal.js (Echols 2015).

Three-dimensional structural models of macromolecules are used to gain insights into biological processes. Most of the macromolecular structures are determined using X-ray crystallography, which provides information about electron density in a crystal. The electron density map is used to build a model and can be later used to check the local quality of the model.

UglyMol is aimed at crystallographers who inspect electron density at various stages of structure solution and model completion. It can be also used by researchers who before using a model from the Protein Data Bank want to check how well the model is supported by the experimental data.

To make UglyMol easy to use by its audience, the user interface is closely resembling Coot (Emsley et al. 2010), a desktop program popular among crystallographers.

Originally, UglyMol was developed to present results from the refinement pipeline Dimple (Wojdyr and others 2016). Currently, it has also other uses. It is included in at least five web applications:

- SynchWeb (Fisher et al. 2015) in Diamond Light Source,
- EXI (Maria Antolinos and others 2016) in European Synchrotron Radiation Facility,
- CCP4 web services (Krissinel et al. submitted),
- molstack (Minor Lab 2017)
- and ContaMiner (Hungler et al. 2016).

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