

A new service for preparing enhanced figures in IUCr journals

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Visualization of data is one of the most powerful tools available to a scientist. In the biological structural sciences, the visual representation of three-dimensional molecular models often provides insights into biological function. Indeed, different representations (space-filling, trace or cartoon abstractions; colouration by atom species, amino-acid group or secondary structure, *etc.*) help the understanding of different aspects of the structure, its interactions and biological function.

In our field we are particularly fortunate to have at our disposal a vast range of visualization software. The available programs allow us to create alternative representations of molecular structures, to switch easily between different renderings, to rotate the molecule or view it as a stereoscopic image in a virtual three-dimensional world, to interrogate the visual representation for information about individual atom or bond properties, *etc.* For crystal structures, we can isolate individual molecules or view their packing arrangements and interactions in the solid state.

We are pleased to introduce with this issue a new service, unique to IUCr journals, that allows authors to create enhanced illustrations of molecular structures that will be published as intrinsic components of their articles (and not simply as supplementary files). The first illustration prepared in this way appears in the article of Mueller-Dieckmann *et al.* [*Acta Cryst.* (2008), **F64**, 156–162] on the crystal structure of mouse ADP-ribosylhydrolase 3. We thank the authors for being early adopters in showcasing the benefits of this new service.

This illustration will appear to readers with modern browsers using Java and JavaScript as a rotating view of a cartoon structure embedded in a translucent space-filling envelope. (Readers with older browsers, or who have disabled active content, will see instead a static image.) However, the illustration is not simply an animation. It is a view rendered within an interactive *Jmol* applet (*Jmol: an open-source Java viewer for chemical structures in 3D*, <http://www.jmol.org/>). Readers may use their mouse to easily change the orientation and size of the view. Further, by right-clicking within the illustration, they have access to the full repertoire of menu options provided by *Jmol*, with which they can select different representations, orientations, colourings; or they can make measurements of distances and angles within the model, generate a stereoview, or carry out many more manipulations.

The toolkit used to create this illustration is now available to authors, and forms an integral part of the journal's submission and review systems. It can be accessed from the author services page of the journal web site (<http://journals.iucr.org/t/services/authorservices.html>).

In addition to creating complex and instructive views of the model, authors may add buttons and menus linked to scripts that will demonstrate specific views or representations of the model of their own choosing.

In every case, the initial view is also saved as a static image that will appear in the PDF version of the article, or in browsers that do not show active content. In this way, we are aiming to retain for posterity the essence of the figure in an archival format. It is well known that new technologies are volatile, and many exciting visualization tools of a few years ago are already unusable, as operating systems, computing languages and graphics libraries have moved on. Nevertheless, we have hopes that a program such as *Jmol* will enjoy greater longevity. As a Java application, it runs on all the current major computing platforms. It implements its own graphics engine, and is actively supported as open-source software by an enthusiastic and vigorous community of scientists, who include active biochemists, crystallographers and bioinformaticists. It supports the stable CIF/mmCIF data format (among others).

Jmol is already well established as a standard tool for those who wish to visualize structures. It is a very powerful application, but it has a steep learning curve. By making our new toolkit available for authors, we are hoping to provide a gentle introduction to *Jmol* for inexperienced users. At the same time, the toolkit does support advanced scripting by experienced users. We expect that as our authors become more experienced in its use, so will the quality and power of their illustrations and animations grow. And so, in consequence, will the information content of their articles, and the power to improve the reader's total comprehension of the structure they describe.

The toolkit appears now as a 'beta' release. Its functionality in providing active illustrations for publication in IUCr journals will not change. However, we hope to improve the presentation of options and tools within the editing palettes, in the light of experience and the specific requirements of our authors. We therefore invite our authors to try out the new toolkit, to create value-added

illustrations for some of their articles, and to report back to us (jtki@iucr.org) with their experiences, suggestions and criticisms. We are pleased to recognize the work of the Editorial Staff in Chester in making this service available.

We look forward to the appearance in the journal of an increasing number of enhanced illustrations that will not only be works of beauty in their own right, but that will add immensely to the reader's understanding and enjoyment of the science being presented.