

Molecular art born from molecular science

By David Goodsell

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Presenting molecules as physical objects with a cartoon rendering

Ever wondered what a molecule looks like? We can use the methods of art and illustration to answer this question. When I started my training in structural biology in the 1980's, there was already a rich toolbox of methods for creating pictures of molecules, using visual metaphors to capture different aspects of atomic structures. These methods and metaphors were developed largely by scientists to present their work to colleagues and occasionally to the general public. Building on these tools, I have worked to develop a method for rendering molecules, be it in a virtual environment or in cells, that is intuitive and appealing.

My first goal was to simulate a picture that presents molecules as physical objects, with defined sizes, shapes and form that are essential for their particular functions. For this reason, I chose a space filling metaphor that represents each atom as a sphere that encloses all of its electrons. [Linus Pauling](#) developed this representation as a way to explore how molecules interact and fit together, which is perfect for what I'm trying to accomplish.

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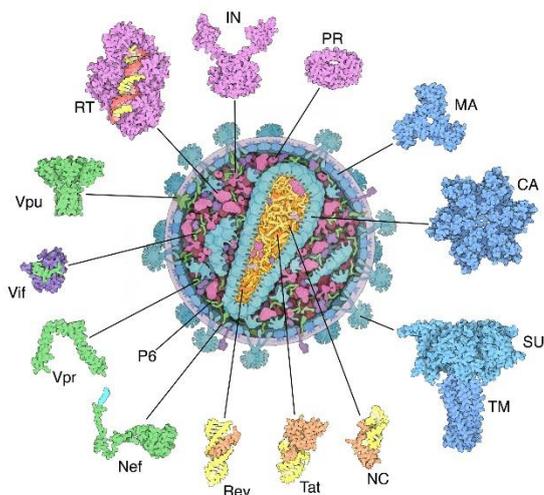


Figure 1 Proteins encoded in the HIV genome

Once that decision was made, I turned to rendering styles. Again, there is a rich history of scientific and artistic illustration to build upon. These provide many tools for creating pictures that enhance the understanding of the form and physical nature of the subjects being depicted. At the time I started, computer graphics were just becoming widely available, and a highly-rendered, shiny plastic style was very popular. I found, however, that the many highlights on these glossy renderings made images of large molecules quite confusing, especially when many molecules are included in the same image.

I turned instead to less photorealistic methods. And I chose a cartoony approach that highlights the shapes of molecules without getting caught up in all the tiny details. This approach uses an image processing technique to draw gestural outlines that have all the look and feel of a hand-drawn illustration, capturing the major features of form and shape. Combined with subtle shadows and a graphic

approach to color, the images turn out as quite simple and comprehensible.

I have used these types of illustrations for many years in a column at the [RCSB Protein Data Bank](http://www.rcsb.org), which presents a different molecule each month and explores the relationship between its structure and function. I find that these simplified illustrations are an effective way to provide an introduction to the molecule. They then may be combined with more detailed interactive graphics after the basic concepts are presented. This creates a world of colours and organic shapes that helps us better understand what molecules of all shapes and sizes look like and how they fit together in great scheme of life.

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Illustration credit: David Goodsell.

The image at the top shows a collection of proteins interacting with DNA, and the embedded image shows the proteins encoded in the HIV genome, surrounding a painting of the virus based on these structures.