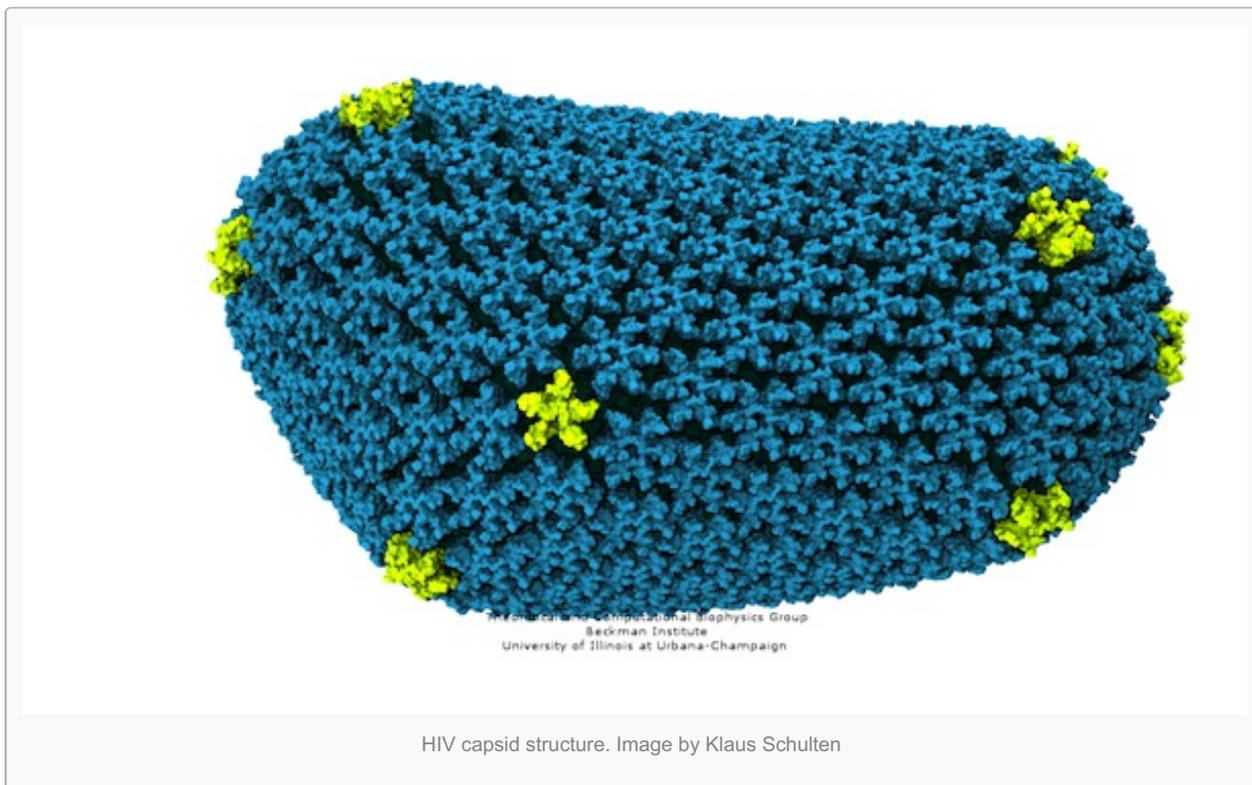


HIV Structure

by A&U

Small Protein, Big Picture



In order for HIV to replicate, the virus needs to carry its genetic material into new cells and then, once inside, to release it. This process is made possible in part by a protein shell: the HIV capsid, which functions to both protect the genetic material and then, at the right time, make it accessible. This makes the capsid an ideal antiviral target.

One of the keys of disrupting this function is knowing the precise chemical structure of the HIV-1 capsid, and researchers, as reported in the journal *Nature*, have done just that.

Up till now, scientists have been able to glimpse individual parts of the capsid but never a detailed molecular map of its whole, whose cone-shaped structure is formed by a polymorphic assemblage of more than 1,300 identical proteins. A dynamic view of the entire structure in atomic-level detail—namely, the interactions of 64 million atoms—was made possible with the use of the supercomputer Blue Waters at the National Center for Supercomputing Applications at the University of Illinois.

Thanks to the largest computer simulation ever run, the digital model was created by researchers Klaus Schulten and Juan Perilla at the University of Illinois, who built on previous research and their own simulations of how the building blocks of the proteins—hexagons and pentagons, arranged in ever-changing patterns—interacted and fit together, and in what numbers. The researchers discovered that the HIV capsid contained 216 protein hexagons and 12 protein pentagons, which were all joined together at varied angles. Next steps for the researchers include figuring out how the identical protein can achieve this malleability within the same capsid.

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