

Advances in Structural Biology Encompassing Viruses, Infections, and Further Developments

Review Article

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Author Details

*Victor Padilla Sanchez***President, Washington Metropolitan University, USA****Corresponding author**

Victor Padilla Sanchez, President Washington Metropolitan University, Washington, DC 20002, USA

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Abstract

Since the initial characterization of bacteriophages as viruses that infect bacteria in 1917, substantial progress has been made in the field of molecular biology. X-ray crystallography has played a crucial role in elucidating the structures of proteins and nucleic acids that cannot be observed using optical or electron microscopy. X-ray crystallography provides high-resolution structures that offer details at the atomic level, enabling the study of proteins and other molecules through computer-based modeling. Furthermore, other techniques, such as cryo-electron microscopy, Nuclear Magnetic Resonance (NMR), and others, have been developed to provide structures for molecules like lipids, carbohydrates, drugs, and inorganic compounds, all of which can be analyzed at the atomic level.

These advancements have significantly enhanced our understanding of biology in numerous ways. This review presents the latest structures that have been built specifically for viruses, showcasing not only the first complete organisms at atomic detail but also providing insights into infection processes and beyond. These structures of organisms like viruses represent a significant leap from the first electron microscopy images that showed viruses and can now be analyzed in detail, including their movement with molecular dynamics software. Advances in all areas of science are made possible through the use of structural analysis in computers.

Introduction

During the 1940s, Max Delbruck identified seven T (type) bacteriophages, including t4, t5, and t7, and four others that displayed remarkable similarity to these. These viruses have served as model organisms for a number of significant experiments over several decades. As of 2024, we have obtained the structures of these organisms at approximately 95% completeness, as depicted in Figures 1-4 [1-8]. Additionally, structures of infection processes have been constructed, which have expanded the range of applications to the cellular level, such as bacteriophage t4 infection and bacteriophage t7 infection. Figures 5,6.

The construction of various viral structures, including P22, phi29, SPP1, Mycobacteriophage ZeeJ, Lambda bacteriophage, SF6 bacteriophage, adenoviruses, herpes viruses, cyanophages, bacteriophage Andhra, halomonas phage, SARS-CoV-2 virus, HIV virus, Nipah virus, crass virus, bacteriophage SU10, has been achieved. Moreover, the infection processes of coronavirus and hiv-1 have been investigated [9-11]. See other figures.

Structures are essential for conducting structure-function analysis at atomic resolution using computer software such as UCSF Chimera and for performing molecular dynamics analysis with NAMD/VMD. For more information about the aforementioned structures, you may visit the website: <https://www.drivictorpadillasanchez.com/> or contact me at the email address provided. Please note that due to space constraints, not all structures are depicted in this review [12-15].

The coronavirus pandemic that is ongoing has necessitated the examination of the structures of the SARS-CoV-2 virus in order to elucidate the atomic-level interactions between the spike proteins of various variants and the cellular receptor ACE2. This analysis has been conducted through molecular dynamics, with the aim of predicting the need for developing different vaccines to combat different variants. Although complete spike structures were not yet available, these findings have proven to be invaluable in guiding vaccine production efforts.

The examination of structures and molecular dynamics can enhance the efficiency of discovering new therapeutic agents for diseases, engineering antibodies to combat infections, and elucidating the intri-



cacies of protein-protein interactions at the level of individual amino acids, while considering the distinct properties of each amino acid. These methods are particularly suited to the 21st century research world, as they were previously very difficult to investigate, if not im-

possible, before the advent of computers. The scientific community should take advantage of these advanced methods to advance their research (Figures 7-14).

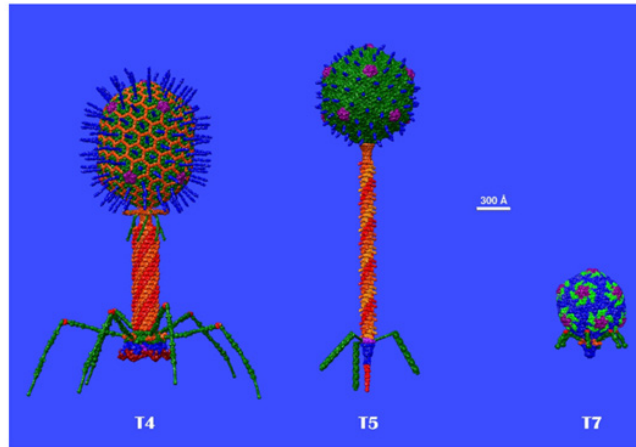


Figure 1: Bacteriophages T4, T5 and T7.

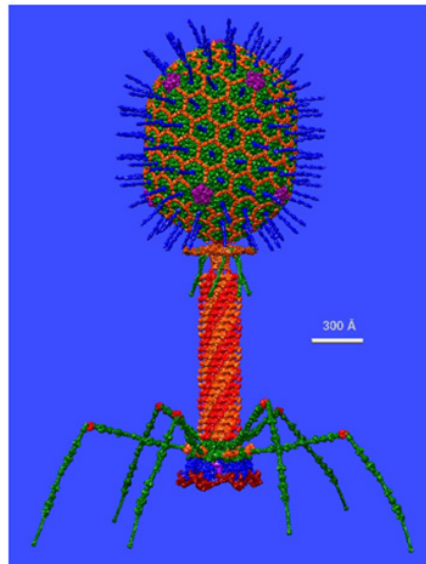


Figure 2: Bacteriophage T4 (2024).

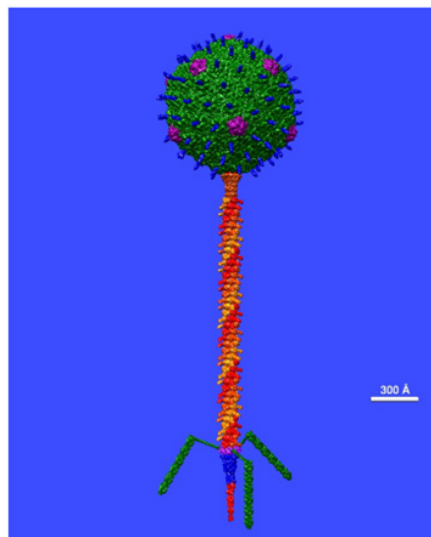


Figure 3: Bacteriophage T5.



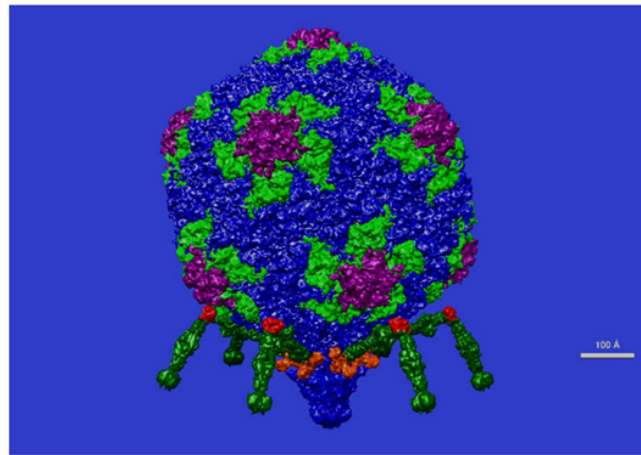


Figure 4: Bacteriophage T7.

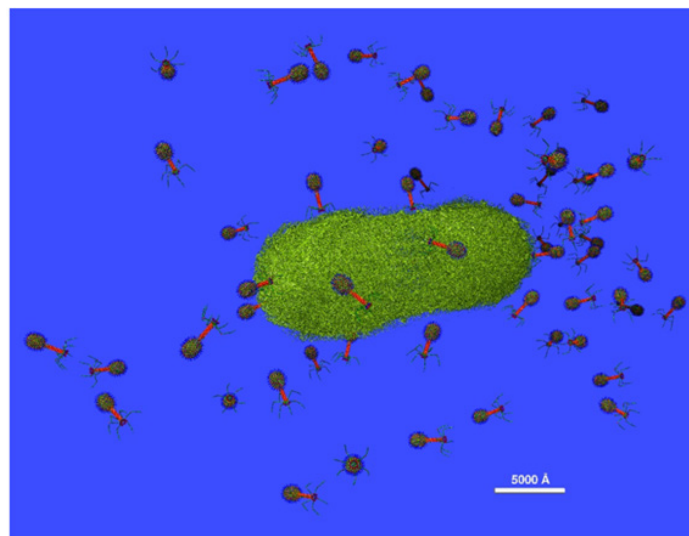


Figure 5: Bacteriophage T4 Infection of Escherichia coli cell. The image includes 64 viruses.

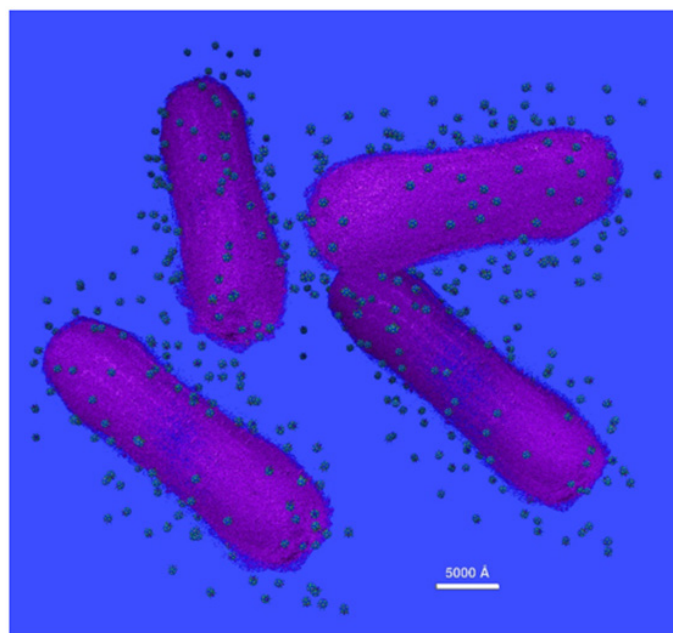


Figure 6: Bacteriophage T7 Infection of Escherichia coli cells. The image includes 512 viruses.

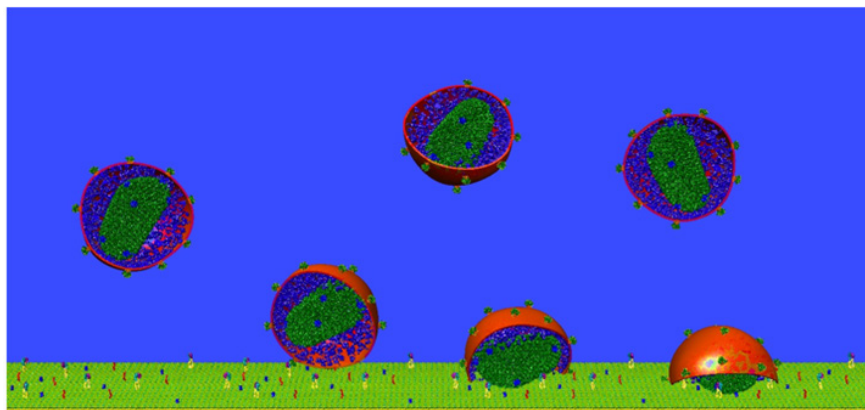


Figure 7: HIV-1 viruses approaching the cell membrane including $\alpha 4\beta 7$ integrin, CD4 (red) and CCR5 (blue) receptors [16].

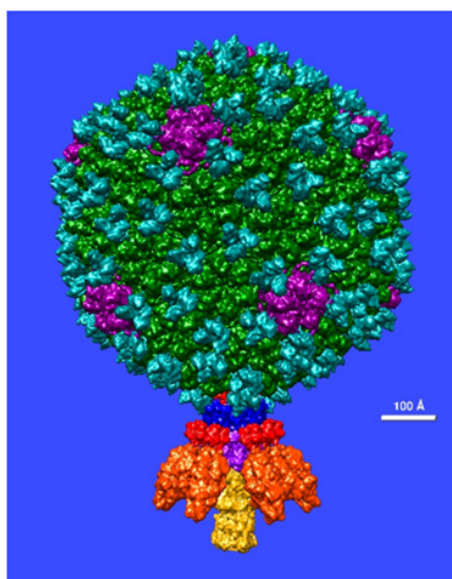


Figure 8: Cyanophage Pam1 [17].

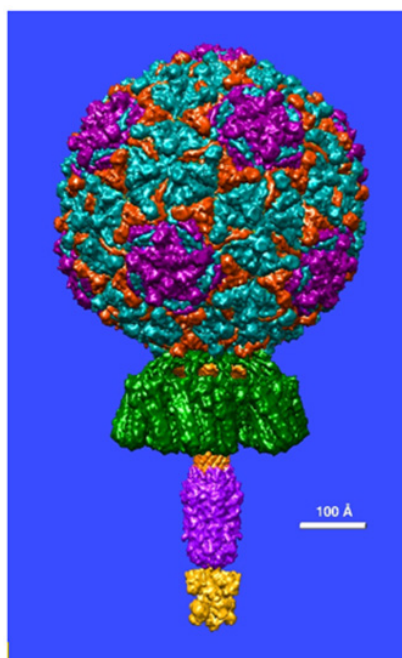


Figure 9: Bacteriophage Andhra [18].

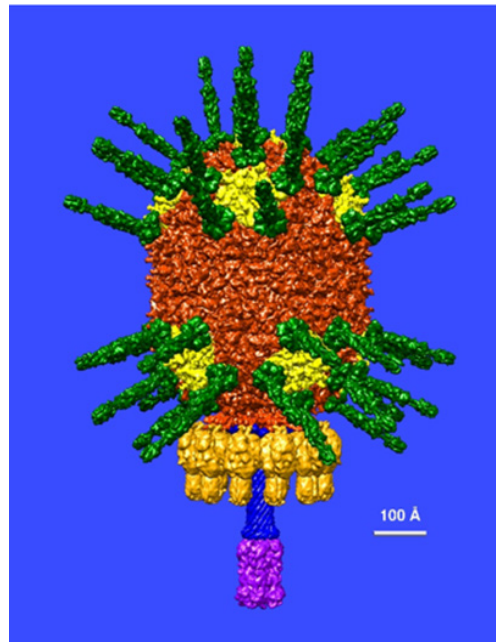


Figure 10: Bacteriophage phi29 [19].

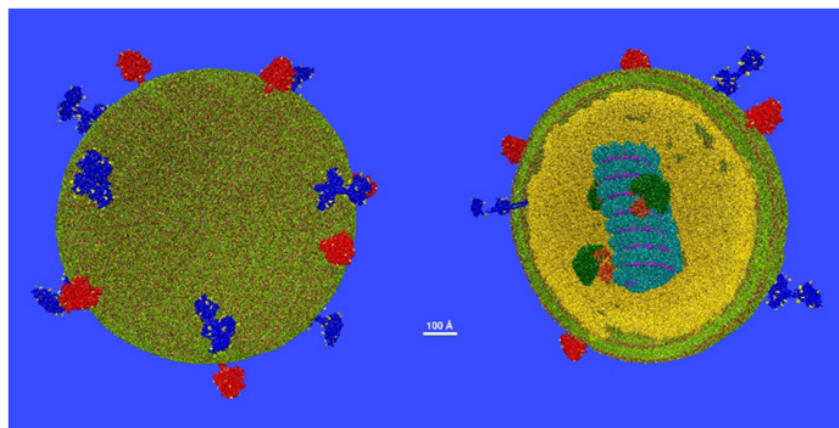


Figure 11: Nipah Virus [20].

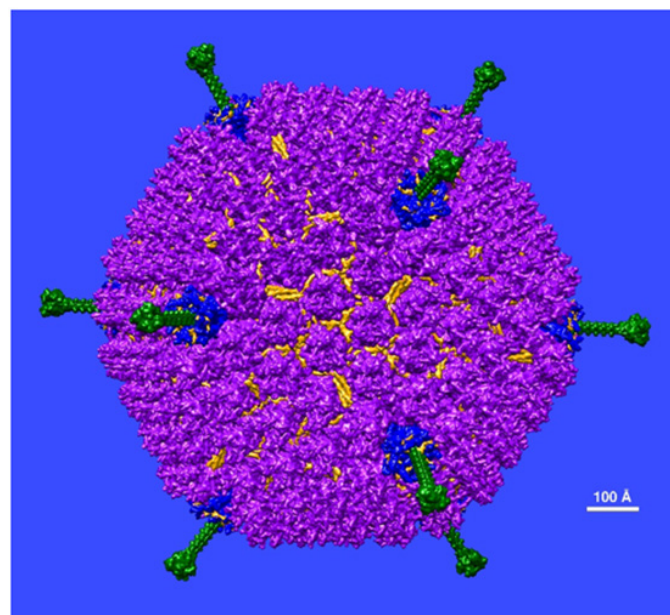


Figure 12: Adenovirus D26 [21].

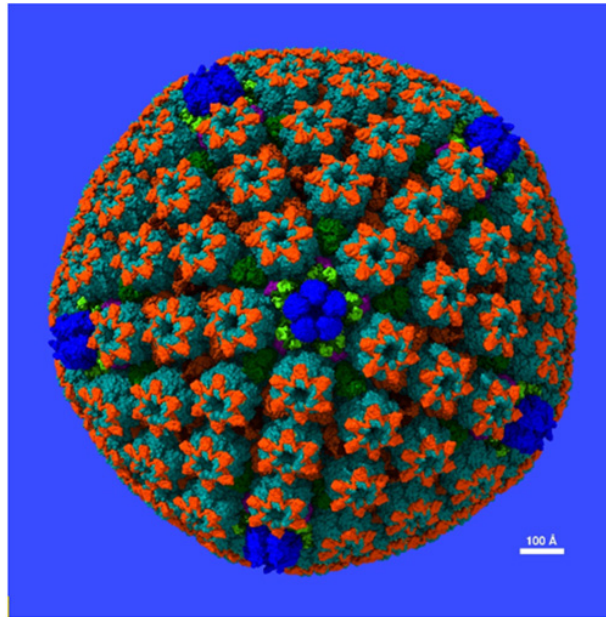


Figure 13: Herpes Virus 2 [22-25].

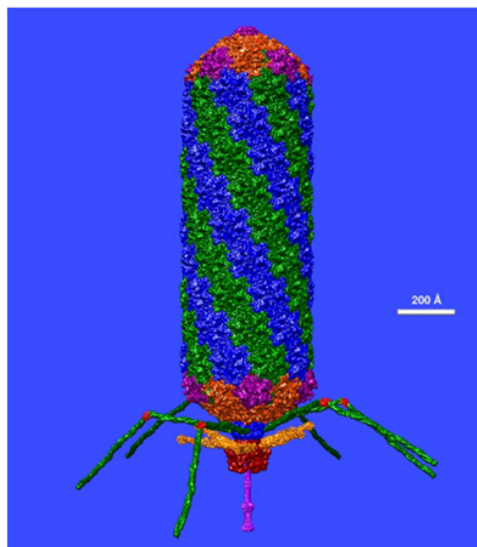


Figure 14: Bacteriophage SU10 [26].

Conclusion

The achievement of visualizing the atomic resolution structures of viruses, cellular organelles, and cells remains a future objective. It is only a matter of time before computational power, potentially enhanced by quantum computers, allows for the display of all proteins within a cell in a complete, analysable structure. In the interim, researchers must continue to push the boundaries of knowledge at the structural level of organisms, ranging from simple viruses to cells and tissues in both prokaryotic and eukaryotic organisms, animal and plant-based, to enhance understanding and facilitate advancements in various fields, such as environmental sustainability, healthier food production, medical applications for disease treatment and prevention, and overall improvements to human life.

Conflict of Interest

The author declares no potential conflict of interest.

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