doi:10.1017/S1431927622004883
Microsc. Microanal. 28 (Suppl 1), 2022

Structure Of The Head-tail Interface Part Of Myoviridae Bacteriophage TaPaz Revealed by Cryo-EM

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Acinetobacter baumannii, a representative of non-fermenting Gram-negative aerobic bacteria, is one of the most significant nosocomial pathogens. In 2017, the World Health Organization included carbapenem-resistant *A.baumannii* strains in the list of bacteria that pose the greatest threat to human health and ranked them priority in the field of creating new antibacterial drugs [1]. The application of bacteriophages, viruses that specifically infect bacterial cells, as a possible alternative to the use of antibiotics to control multidrug-resistant *A. baumannii* strains, causes obvious and increasing interest around the world.

The portal complex is a specialized part of a viral particle, which provides the delivery of viral genomes to the host cell. The complexes are arranged as dodecameric rings being a structural part of phage capsids incorporated at a five-fold vertex [2].

We used single particle reconstruction in RELION [3] to obtain the reconstruction of phage TaPaz head-tail interface at 3.15 Å resolution. Totally about 1500 raw frame stacks were involved for processing the head-tail interface structure. Motion correction was performed with Relion implementation of MotionCor2. CTF was estimated with CTFFIND-4.1. The capsid parts were automatically picked with 800^3 pixels box size. Totally 5600 particles were selected for processing. The subsets were subjected to 2d classification in Relion. Then we performed 3D classification in Relion and symmetry expansion to I3, followed by masked classification on one of the pentamers. This approach allowed to locate the interface density. A new model was built without realigning the particles with the same box size as template. Perform 3d classification and 3D refinement in Relion with C6 symmetry. Then CTF refinement and Bayesian polishing were performed on the head-tail interface dataset. The final reconstruction yielded map (Fig. 1A) with 3.15 Å resolution according to FSC 0.143 criterion (Fig. 1B) [4].

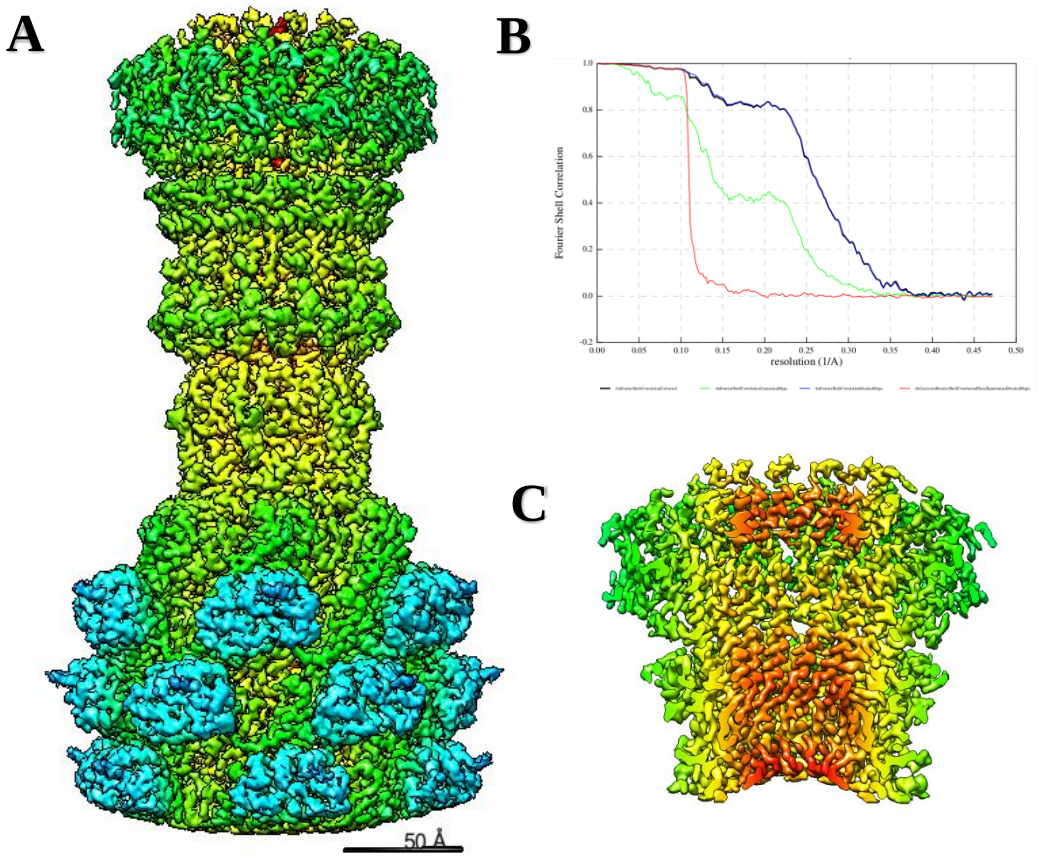

Figure 1.(A) Cryo-EM reconstruction of the TaPaz phage head-tail interface with C6 symmetry applied, Bar=50Å; (B) FSC curve indicates 3.1 Å resolution. Green – unmasked half-maps, blue – masked half-maps, red – phase randomized masked half-maps, black – corrected. (C) Inside view of portal protein part.

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[4] We would like to thank Dr. Liu and the Kobilka Cryo-Electron Microscopy Center, the Chinese University of Hong Kong, Shenzhen for help with cryo-electron microscopy. This work was carried out with support from the Innovation Committee of Science and Technology of Shenzhen, China (Grant No. 20200828172651001).

https://doi.org/10.1017/S1431927622004883 Published online by Cambridge University Press