

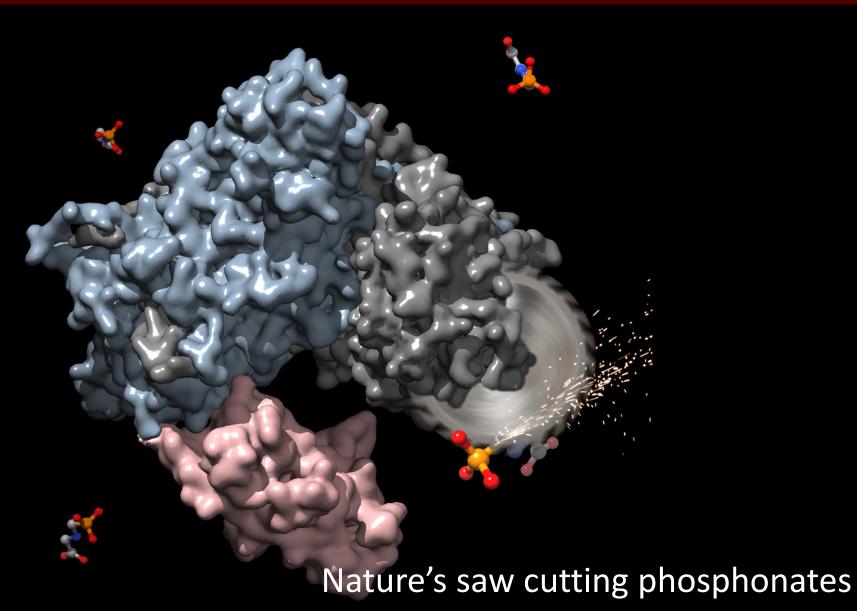
Spotlights: Research Expedited by HPC

Carbon-Phosphorus Lyase **Complex Structures Reveal** the Binding Mode of the NBD-like PhnK Junjie Zhang, et al.



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Published in *Structure*, 2016.





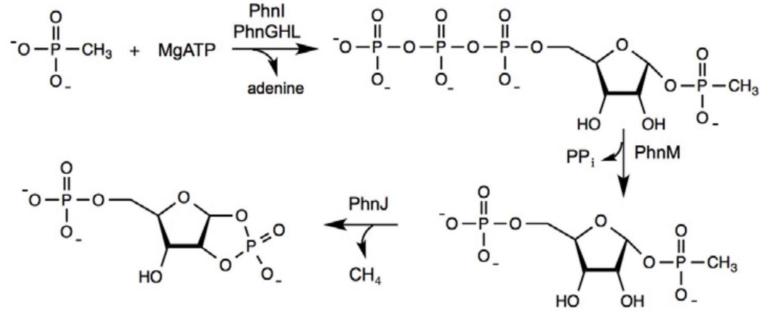


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Background

- The carbon-phosphorus (C-P) lyase complex, which is encoded by the 7 essential genes (phnGHIJKLM) within the phn operon, is essential for the metabolism of unactivated phosphonates to phosphate in bacteria.
- PhnK is homologous to the nucleotide-binding domain (NBD) of ATP-binding cassette (ABC) transporters. PhnK has all the NBD motifs.





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Problems to be solved

- Why is there only one copy of PhnK bound to a dimeric $phnG_2H_2I_2J_2$ core complex?
- How does PhnK bind to the core complex?
- What is the effect on the core complex after PhnK binds?



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Data processing details

- Software: EMAN2, Relion1.4, Unblur, PRIME, B-soft
- Cluster: Ada
- Typical job size: 140 hours
- 200 cores with a total of 1 million SUs.





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Conclusion

- PhnJ subunits in PhnG₂H₂I₂J₂ provide two identical binding sites for PhnK. Only one PhnK binds to PhnG₂H₂I₂J₂ due to steric hindrance.
- The NBD-like PhnK binds to a cytoplasmic protein, distinct from NBD-TMD interaction
- Binding of PhnK exposes the active site residue, Gly32 of PhnJ, located near the interface between PhnJ and PhnH.



Asymmetric cryo-EM structure of the canonical Allolevivirus QB reveals a single maturation protein and the genomic ssRNA in situ – Junjie Zhang, et al.

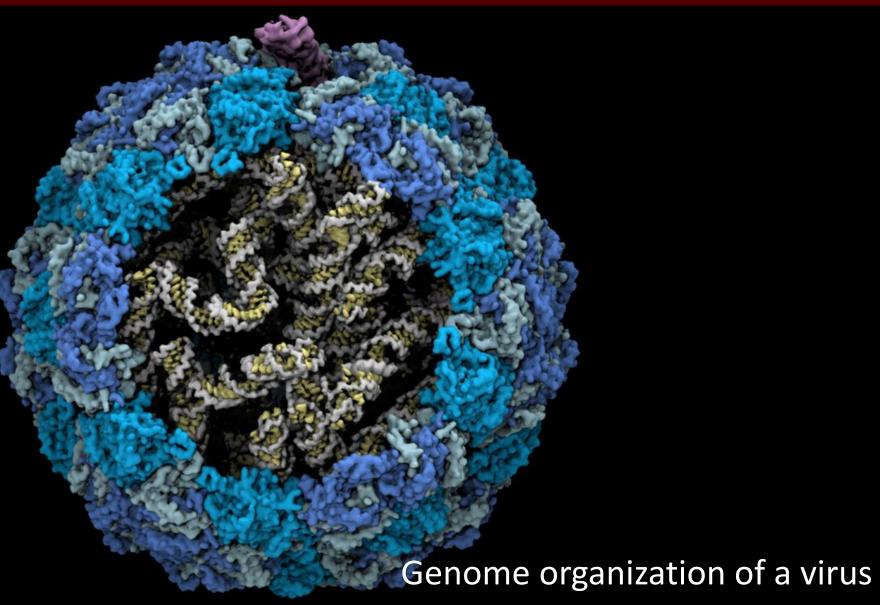
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Published in PNAS, 2016.







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Background and Results

Single-stranded (ss) RNA viruses have ribonucleic acid as their genetic material and infect animals, plants and bacteria. Here we used cryoelectron microscopy to reveal, for the first time, the genomic RNA (gRNA) of the ssRNA virus Qβ. The asymmetric gRNA adopts a single dominant structure in all virions and binds the capsid of QB at each coat protein. At the same time, we determined the structure of the maturation protein, A2, which functions both as the virion's "tail" and its lysis protein. We see the gRNA is more ordered when interacting with A2. These results provide new structural insights into gRNA packaging and host infection in ssRNA viruses.

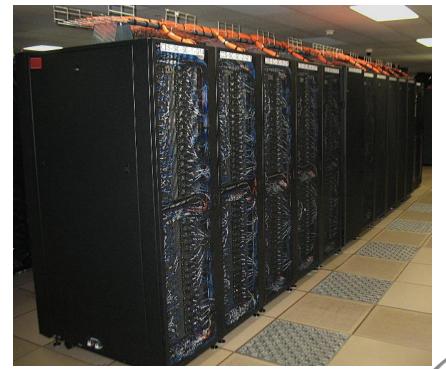


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Data processing details

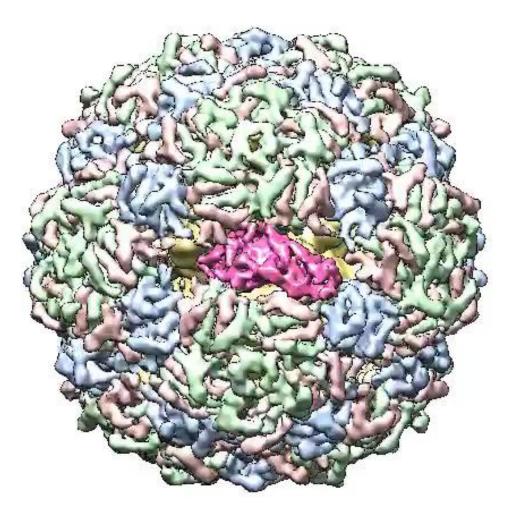
- Software: EMAN2, Relion1.4, Unblur, B-soft
- Cluster: Ada
- Typical job size:
 - 200 Cores with each core of 10GB memory
 - ~1M SUs on Ada.





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Asymmetric structure of Q β . Coat proteins are in salmon (conformer A), green (conformer B), and blue (conformer C), respectively. A₂ is in hot pink. RNA is in yellow and low-pass–filtered to 10-Å resolution.





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