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Validation of metal binding sites in virus structures

Metal ions play an important role in the virus life cycle. They not only are essential in maintaining the stability of viral structures, but also are involved in an array of phathogenesis processes such as catalysis and activation mechanisms, reverse transcription, and RNA maturation. Zinc, Calcium, Magnesium and Manganese are commonly observed from viral-containing structures in the Protein Data Bank (PDB). However, suboptimal modeling of metal binding environment or even incorrect characterization of metal ions are not uncommon in these structures containing viral components. Herein we use a novel algorithm to systematically validate experimetal-determined virus structures from the PDB and yield a benchmark dataset of high-quality metal binding sites in virus structures. Our dataset provides a reliable resource to futher investigate the metal-dependent mechanism of pathogenesis in virus and serves as a structural basis for the development of therapeutic agents targeting such mechanism against virus infection.

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