

Supporting Material to

"All-atom Multiscale Simulation of CCMV Capsid Swelling" by
Yinglong Miao, John Johnson, and Peter Ortoleva

Figures

Fig. S1 Time courses of the CCMV capsid diameter as simulated at pH 7.0 (sim2), pH5.0 (sim4), and pH 5.0 with 0.05M MgCl₂ (sim5).

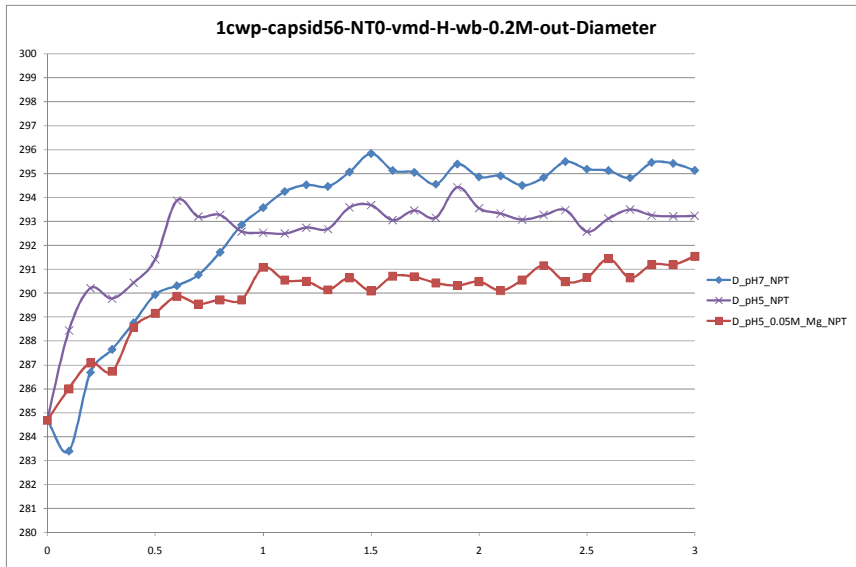


Fig. S2 Time courses of the CCMV capsid outer radius as simulated at pH 7.0 (sim2), pH5.0 (sim4), and pH 5.0 with 0.05M MgCl₂ (sim5).

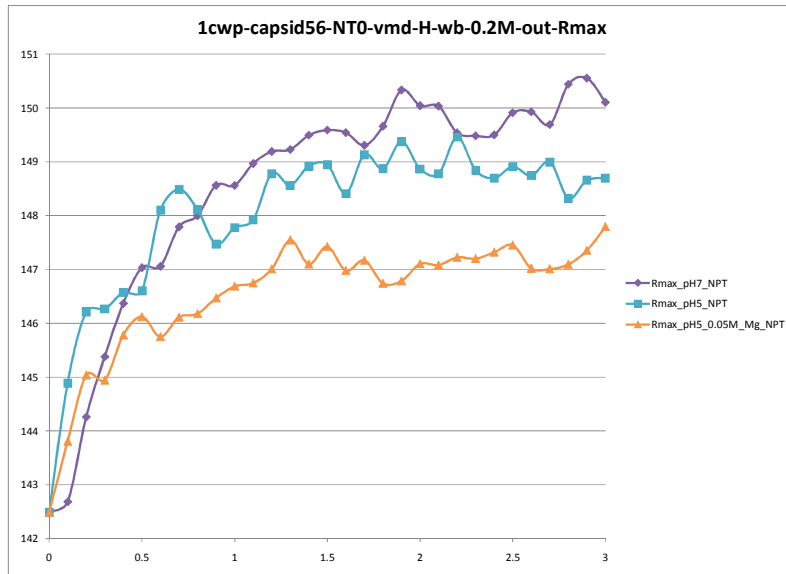


Fig. S3 Time courses of the CCMV capsid average radius as simulated at pH 7.0 (sim2), pH5.0 (sim4), and pH 5.0 with 0.05M MgCl₂ (sim5).

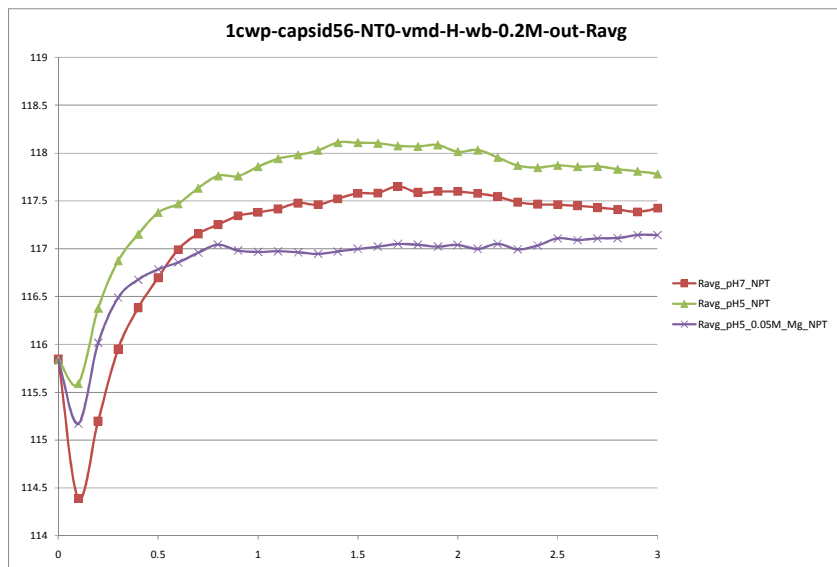


Fig. S4 The number of Mg^{2+} ions that diffuse into CCMV capsid during the simulation at pH 5.0 with 0.05M $MgCl_2$ (sim5).

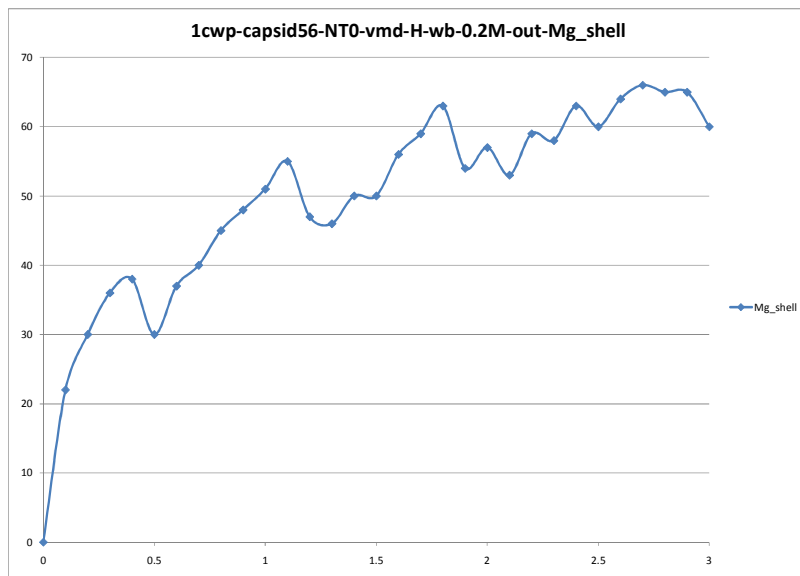
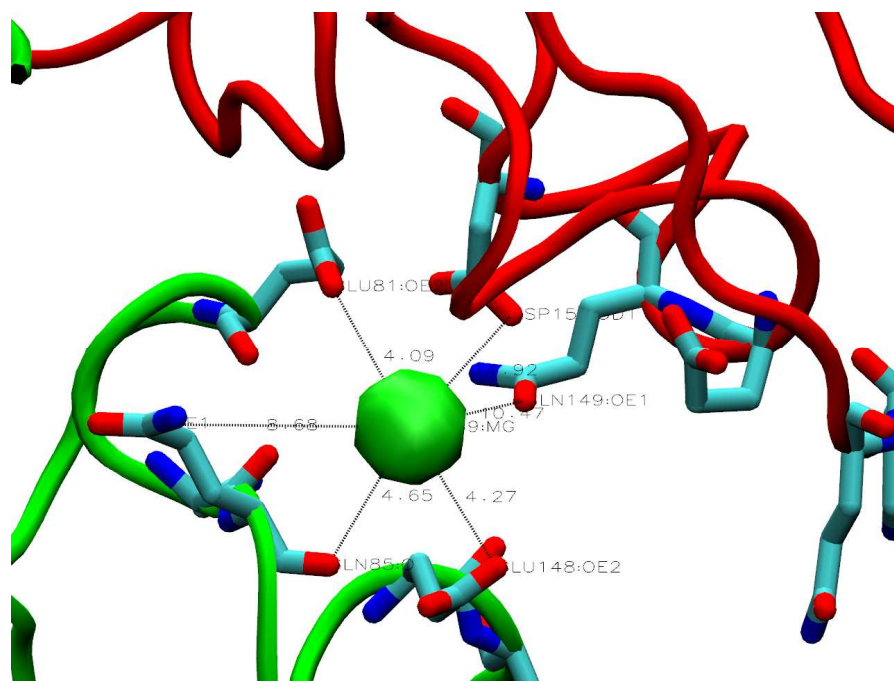
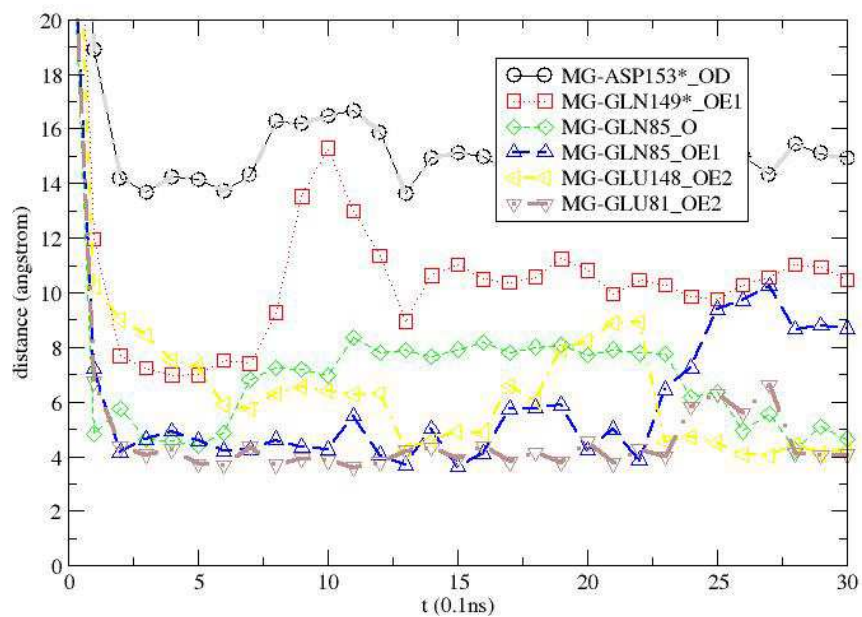


Fig. S5 (a) Schematic representation of a divalent cation inter-protein binding site in CCMV capsid, which are composed of residues Glu81, Gln85, Lys84 and Glu148 from a protein and Gln149* and Asp153* from its adjacent protein. (b) Time courses of the distances between Mg²⁺ ion in the center and its ligand atoms during the simulation at pH 5.0 with 0.05M MgCl₂ (sim5).



(a)
Mg binding



(b)