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Supporting Material

Primary changes of the mechanical properties of Southern Bean Mosaic Virus upon calcium removal

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Primary changes of the mechanical properties
of Southern Bean Mosaic Virus upon calcium
removal – SUPPORTING MATERIAL

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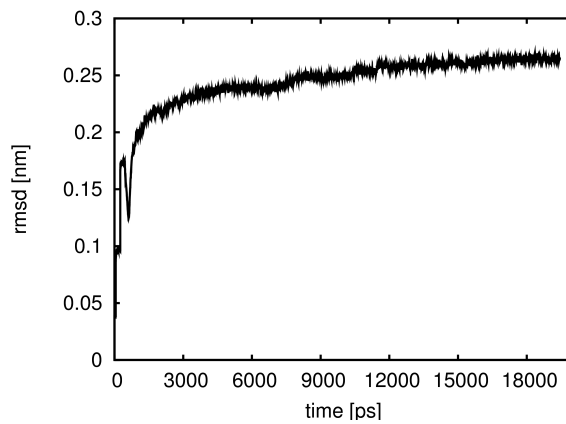


Figure 1: Root mean square deviation (rmsd) of the viral shell heavy atoms with respect to the initial structure after 300 steepest decent steps for the 19.5 ns equilibration phase. After 12 ns, the rmsd remained at 2.62 \AA and seams sufficiently converged. The simulation was started with a temperature set to 10 K. Pressure coupling was switched on after 250 ps, resulting in a drop of the simulation box size, which caused a slight compression of the capsid reflected in the rmsd. During heating, the capsid radius relaxed and the protein atoms approached their original positions, causing a dip in the rmsd plot at 450 ps, followed by a slight further expansion.

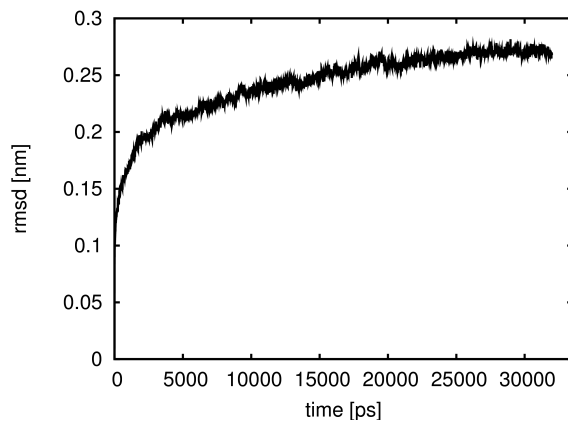


Figure 2: Rmsd of viral shell heavy atoms during equilibration, fitted on the starting structure after calcium removal.

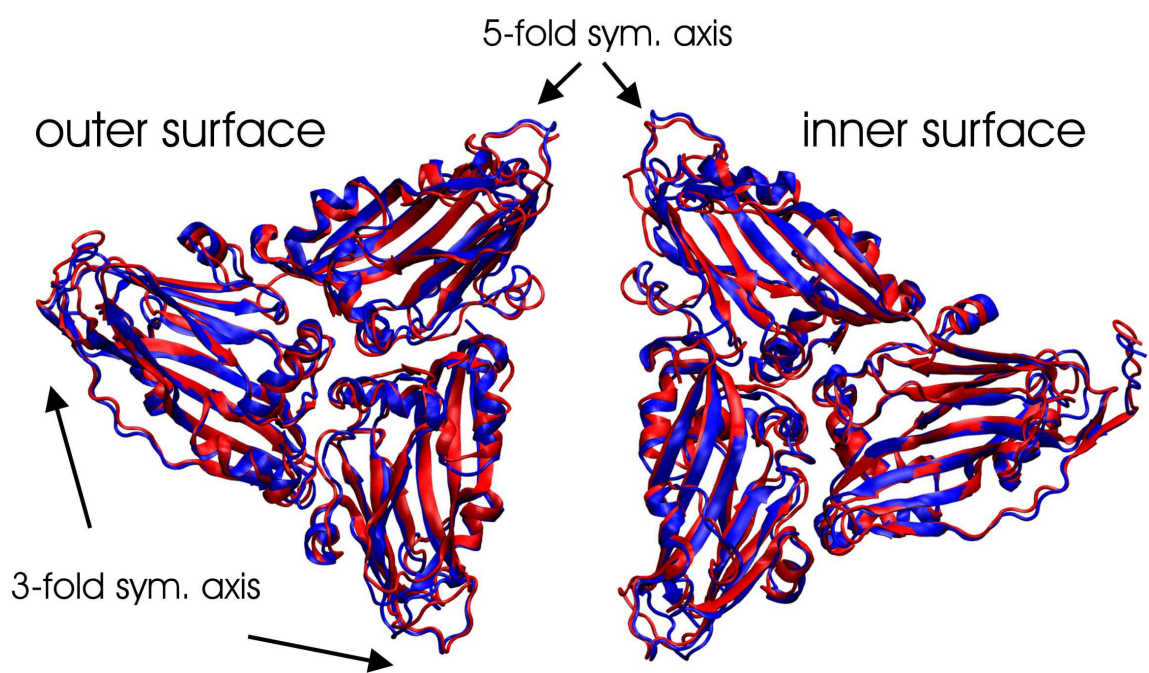


Figure 3: Cartoon representation of subunit 12 on the inner and outer surface. Both structure with calcium ions (red) and without ions (blue) were extracted after the respective equilibration simulations.

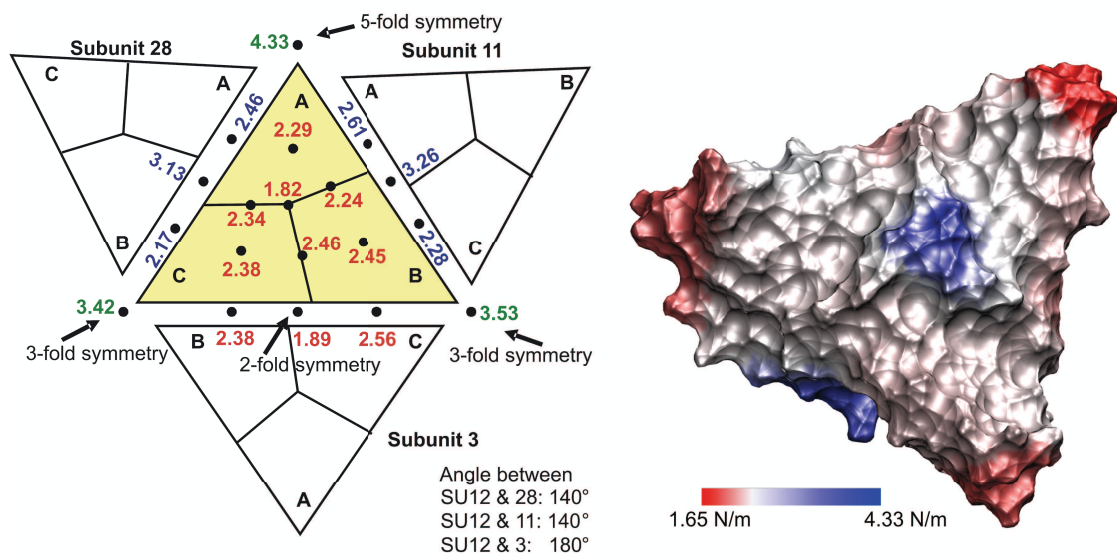


Figure 4: **Elastic constants** from the simulations in with the tip-sphere was pushed against the **outer** surface of the calcium-bound SBMV capsid.

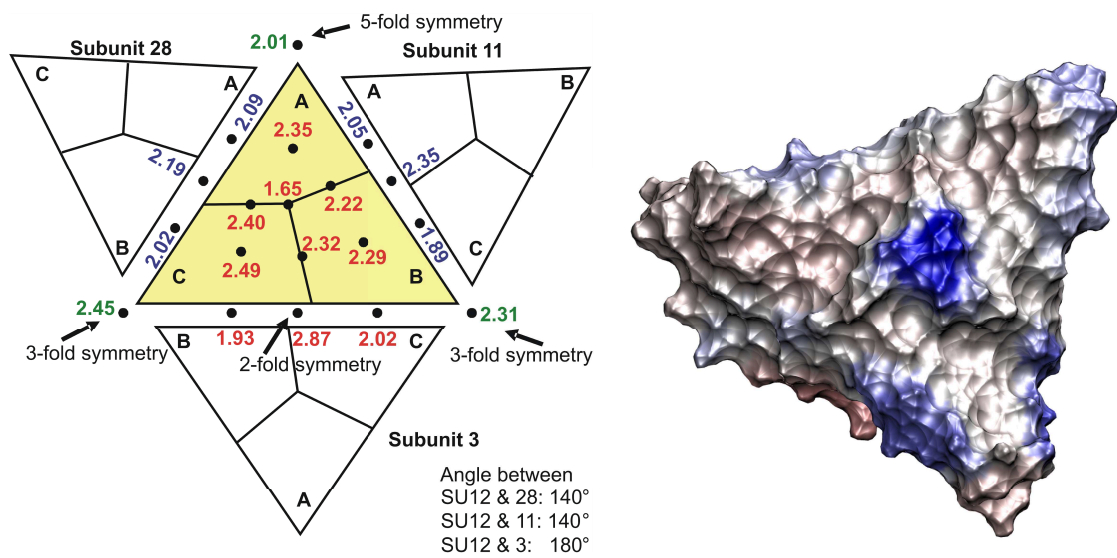


Figure 5: **Elastic constants** from the simulations in with the tip-sphere was pushed against the **inner** surface of the calcium-bound SBMV capsid.

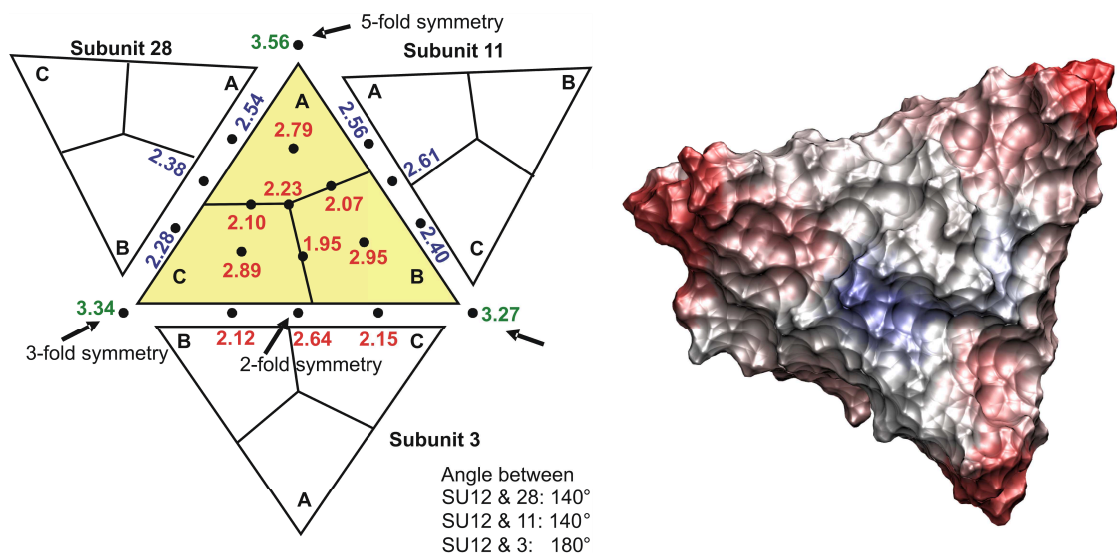


Figure 6: **Elastic constants** from the simulations in with the tip-sphere was pushed against the **outer surface of calcium-free SBMV**.

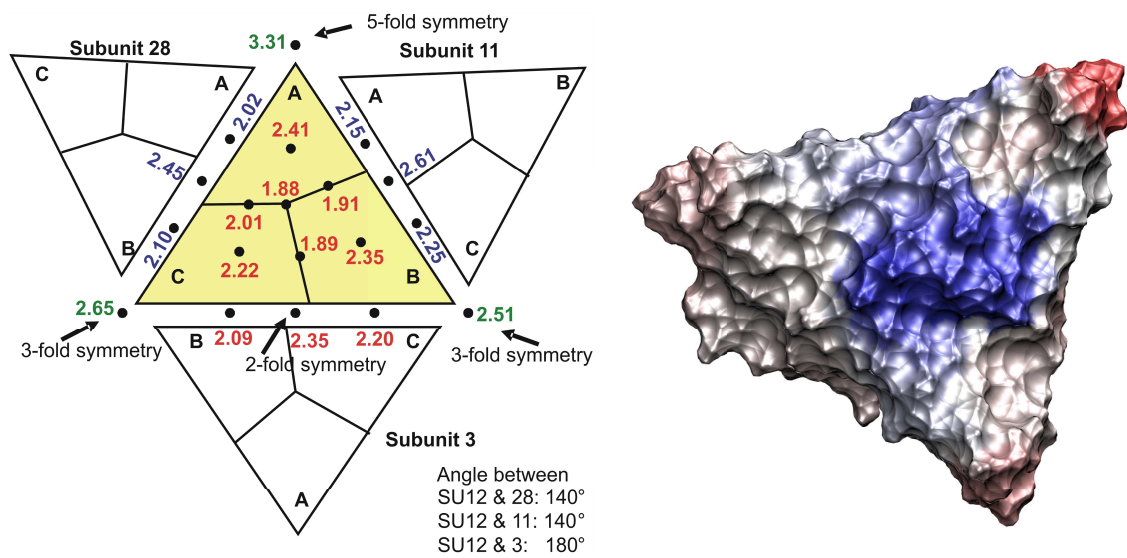


Figure 7: **Elastic constants** from the simulations in with the tip-sphere was pushed against the **inner surface** of **calcium-free SBMV**.

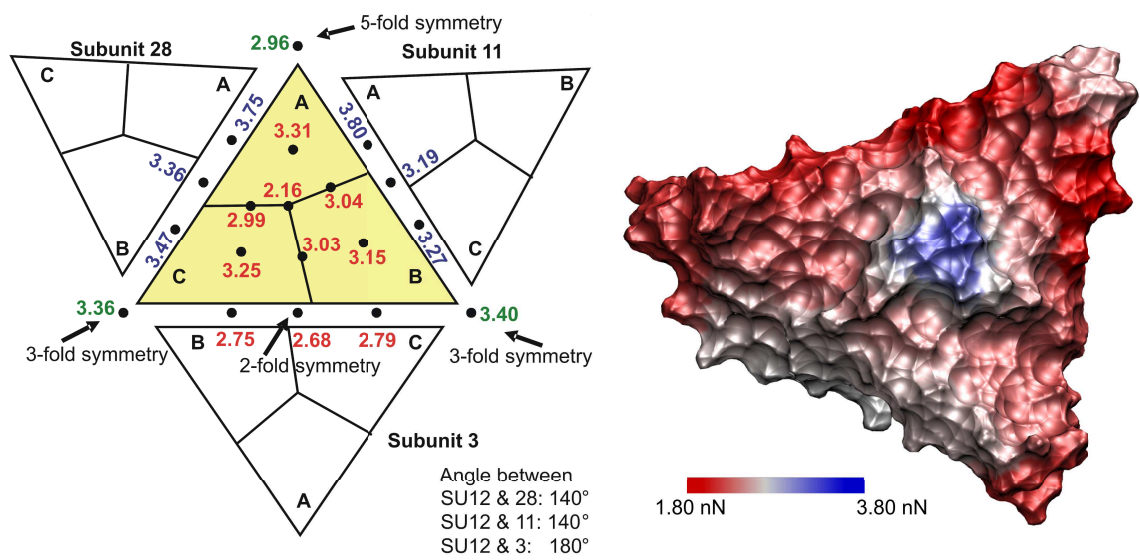


Figure 8: **Yielding forces** from the simulations in with the tip-sphere was pushed against the **outer** surface of the calcium-bound SBMV capsid.

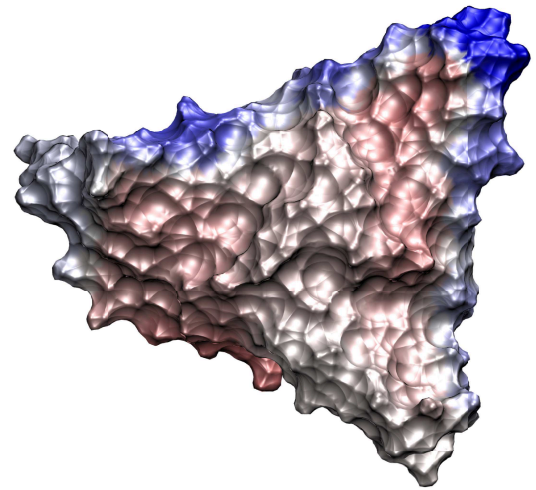
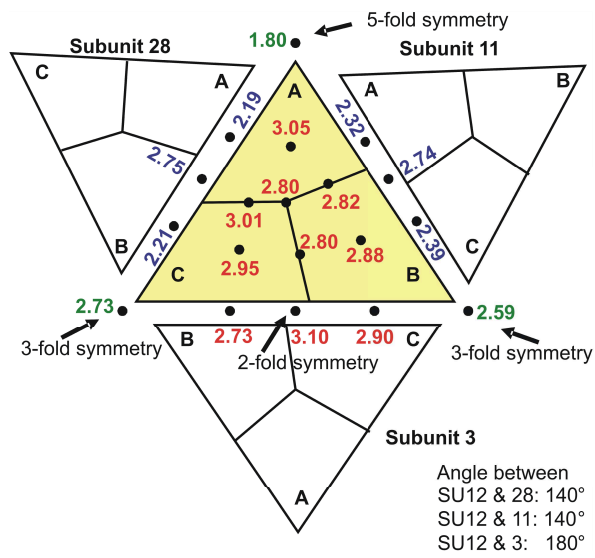


Figure 9: **Yielding forces** from the simulations in with the tip-sphere was pushed against the **inner** surface of the calcium-bound SBMV capsid.

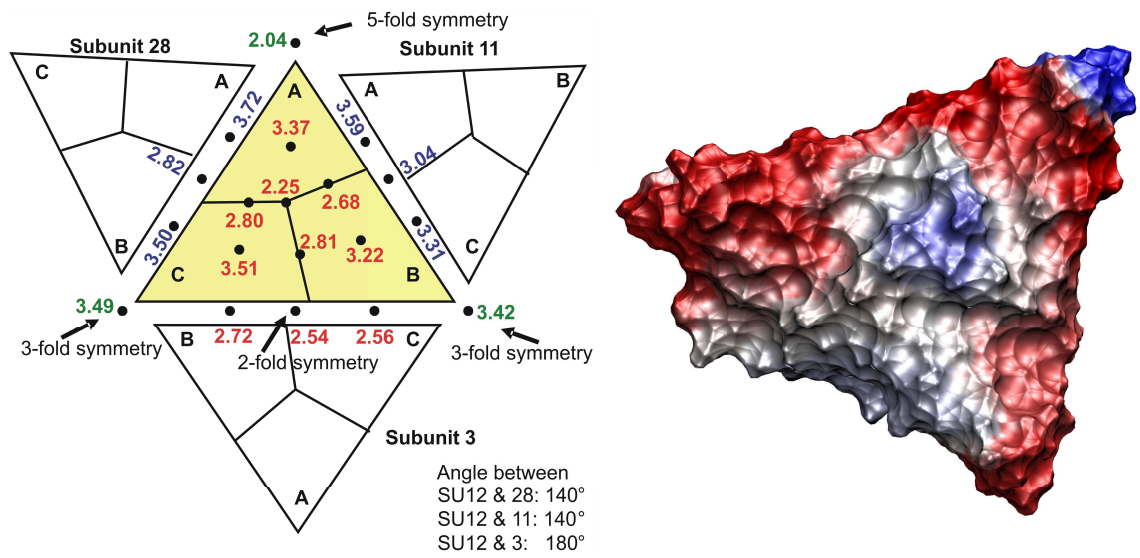


Figure 10: **Yielding forces** from the simulations in with the tip-sphere was pushed against the **outer surface of calcium-free SBMV**.

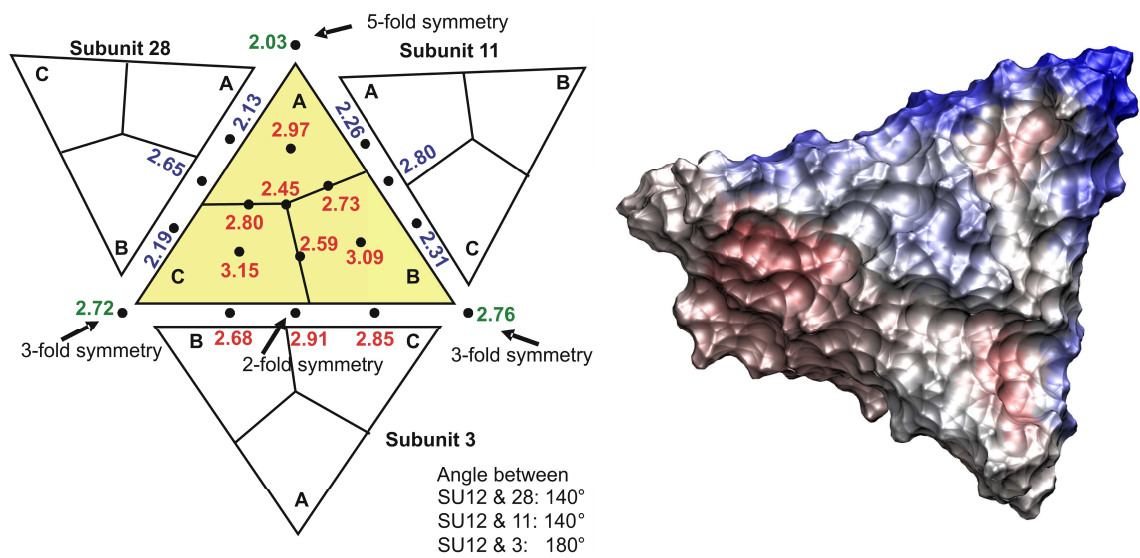


Figure 11: **Yielding forces** from the simulations in with the tip-sphere was pushed against the **inner surface of calcium-free SBMV**.