

Supplementary Information

Evaluation of All-Atom Force Fields on Viral Capsid Simulations and Properties

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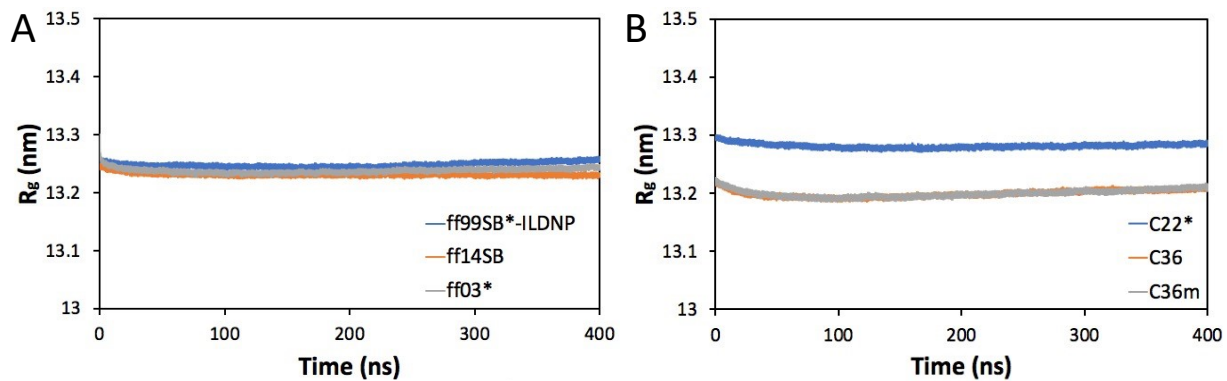


Fig. S1 Radius of gyration R_g (nm) of the EV-D68 capsid versus time (ns) for the AMBER and CHARMM force fields.

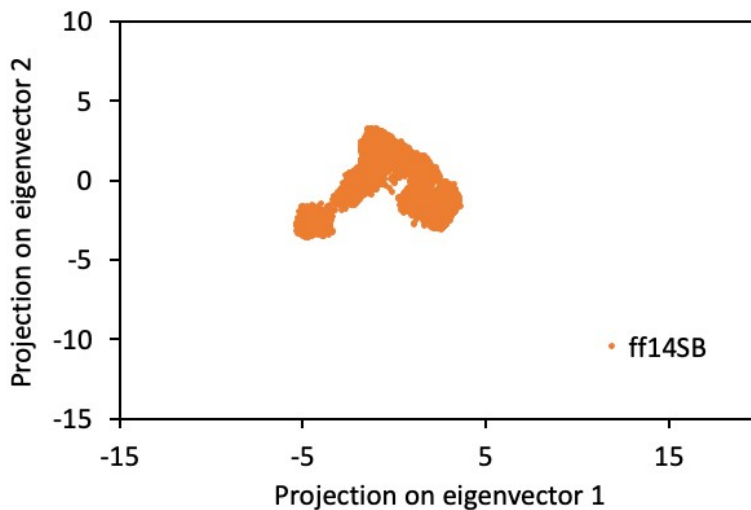


Fig. S2 Projection of the coordinates from the 400 ns MD simulation on the top two eigenvectors (principal components) for ff14SB.

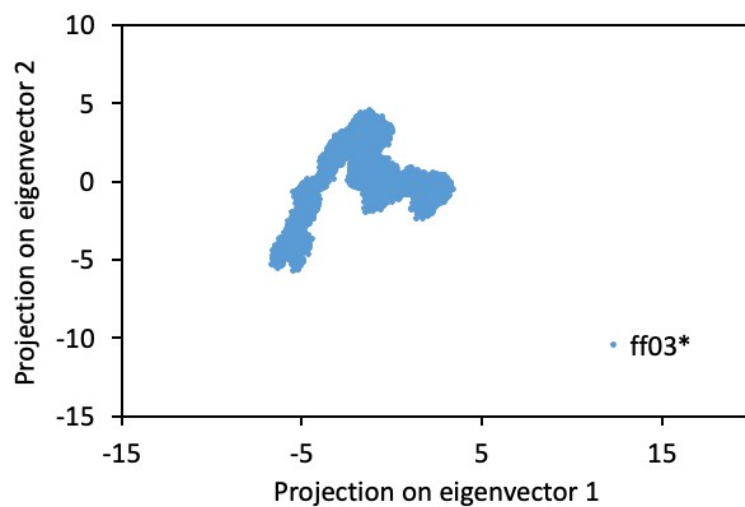


Fig. S3 Projection of the coordinates from the 400 ns MD simulation on the top two eigenvectors (principal components) for ff03*.

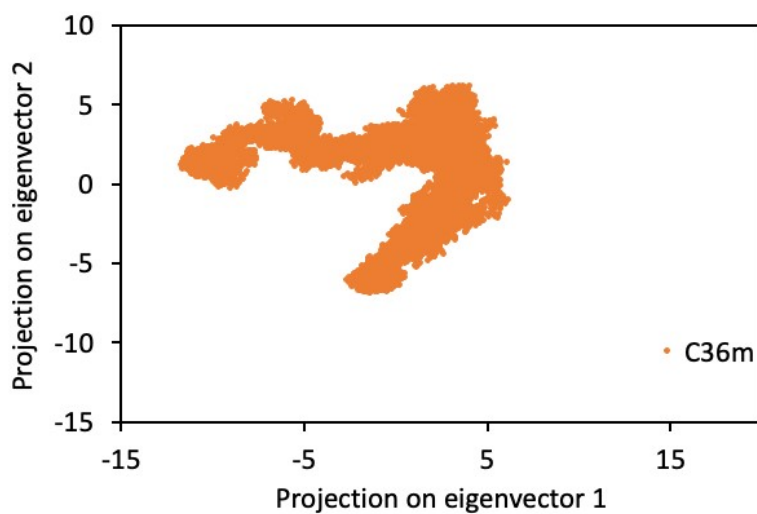


Fig. S4 Projection of the coordinates from the 400 ns MD simulation on the top two eigenvectors (principal components) for C36m.

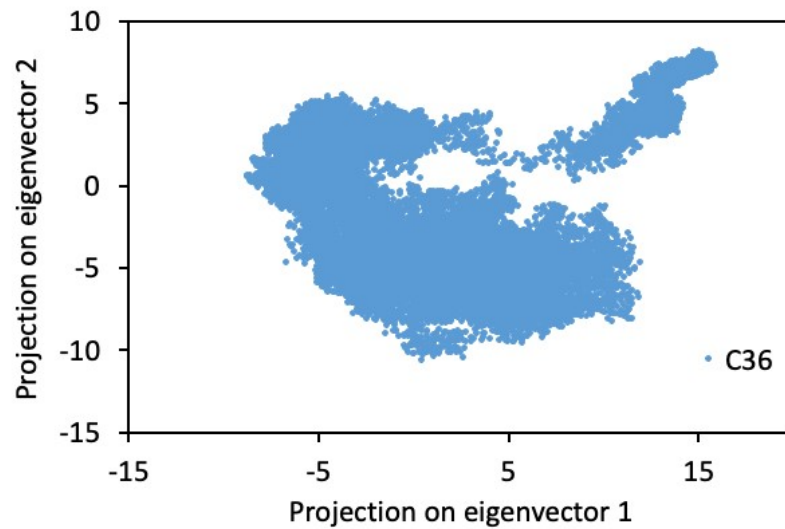


Fig. S5 Projection of the coordinates from the 400 ns MD simulation on the top two eigenvectors (principal components) for C36.

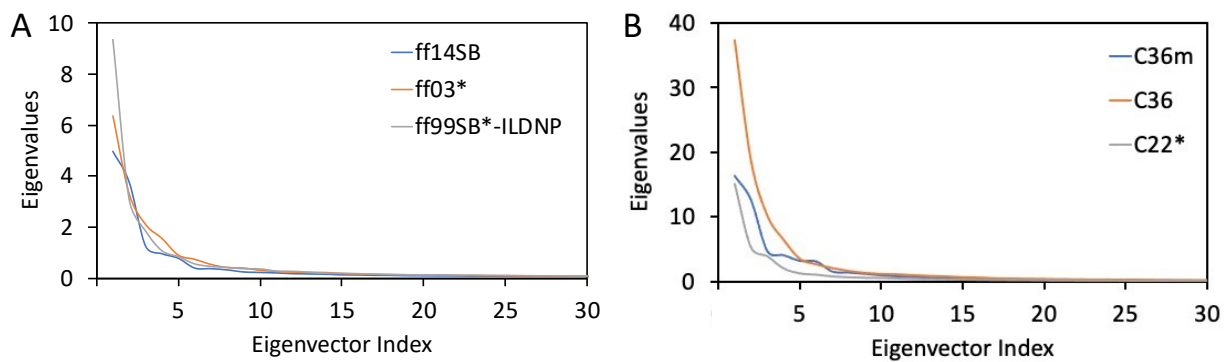


Fig. S6 Eigenvalues of the covariance matrix of the atomic coordinates from MD trajectories obtained with the a) AMBER and b) CHARMM force field.

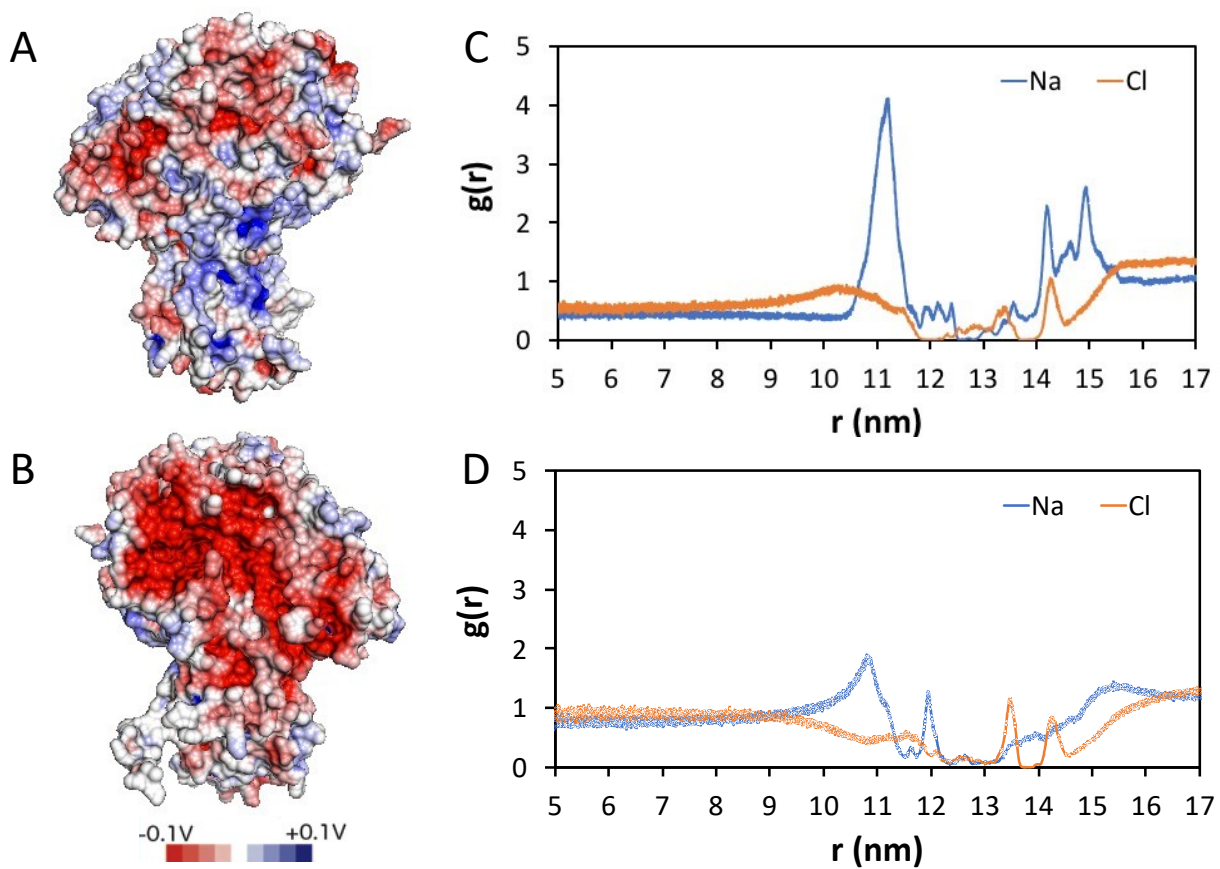


Fig. S7 Electrostatic potential maps of the a) outer and b) inner surface of the viral capsomer, and the radial distribution function of the Na and Cl ions with respect to the center of mass obtained from the last 50 ns of the MD simulation using c) ff14SB and d) C36m.

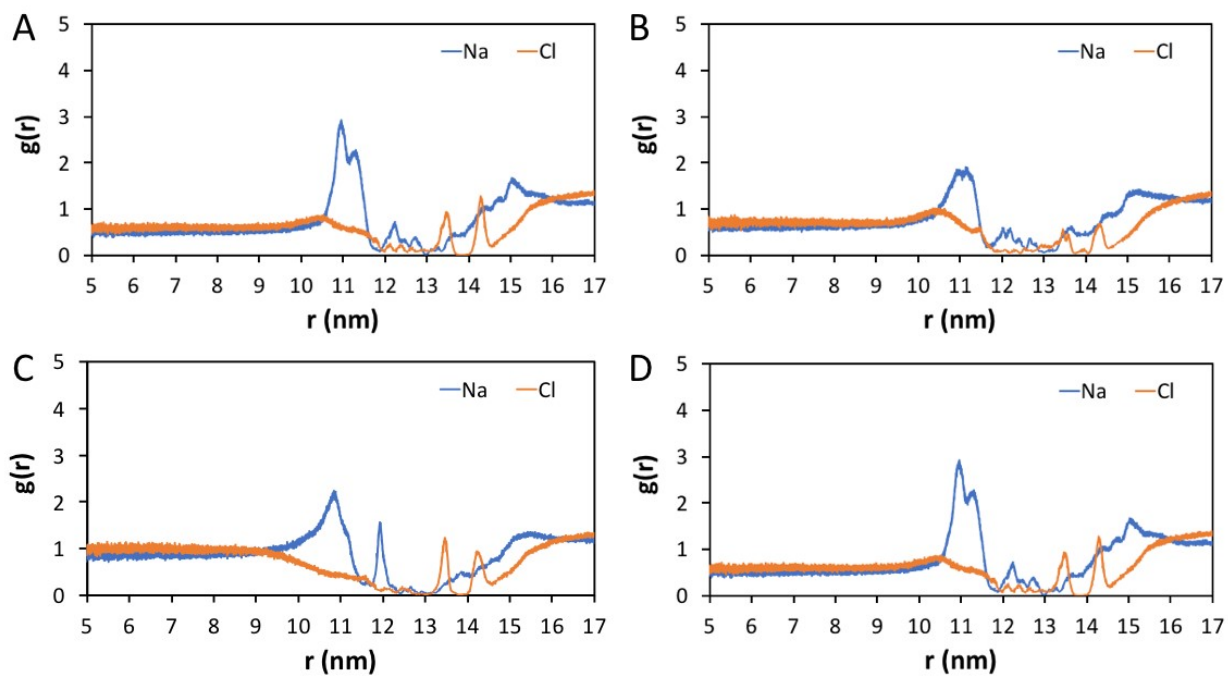


Fig. S8 Radial distribution function of the Na and Cl ions with respect to the center of mass obtained from the last 50 ns of the MD simulation using a) ff03*, b) ff99SB*-ILDNP, c) C36 and d) C22*.

Table S1. Number of clusters with an RMSD cutoff of 0.2 nm from MD snapshots sampled every 1 ns.

	ff14SB	ff03*	ff99SB*-ILDNP	C36m	C36	C22*
# of clusters	2	5	3	16	19	5

Table S2. Percentage and composition of the capsid secondary structure corresponding to the minima of Fig. 3a (ff14SB) and 3d (C36m).

	Coil	β -Sheet	β -Bridge	Bend	Turn	α -Helix	3_{10} -Helix
ff14SB	30.9	29.3	3.6	14.9	10.9	5.2	5.2
C36m	33.5	28.4	3.3	16.0	10.0	4.8	4.0

Table S3. Percentage and composition of the capsid secondary structure averaged across MD snapshots (sampled every 1 ns) generated using the six force fields.

	Coil	β -Sheet	β -Bridge	Bend	Turn	α -Helix	3_{10} -Helix
ff14SB	31.1	29.1	3.6	15.0	10.9	5.2	5.2
ff03*	31.5	29.0	3.4	16.4	10.0	5.1	4.5
ff99SB*-ILDNP	31.0	29.6	3.6	15.6	10.4	4.8	5.1
C36m	33.1	28.5	3.3	16.1	10.0	4.9	4.1
C36	33.2	28.5	3.3	16.0	10.1	4.9	4.0
C22*	32.5	28.9	3.3	15.5	10.2	5.1	4.4