Supplementary Information to article

"MS2 bacteriophage capsid studied using all-atom Molecular Dynamics"

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1. Reconstruction of the capsid model

To build the initial coordinates for simulations we, first, positioned 60 copies of the trimer block according to the icosahedral symmetry, which formed a closed structure. Then, the maturation protein and the adjacent deformed monomers were introduced by replacing 2 and 5 monomers, respectively.

Finally, the sequence containing residues 68-77 was copied from another monomer (denoted as chain A in PDB) and manually aligned to fill the gap. In order to fit it well and remove steric clashes, the whole monomer was energy minimised, where all atoms apart from the reconstructed sequence were frozen. Here and further, the steepest descent algorithm was employed and minimisation was carried until the largest residual force becomes less than 5000 kJ nm^{-1} that ensured the subsequent MD simulation would not crash. The resulting structure was copied into the capsid. This finishes the assembling process, Fig. 1. We did not perform the reconstruction of the missing sequences in the maturation protein because they are located far from the capsid wall and thus they do not affect the properties we investigate here.

Hydrogen atoms were added to the amino acids and protonation states were set using *gmx pdb2gmx* tool using default settings.

2. Preparation of the simulation box

Because the capsid is almost spherical, the rhombic dodecahedron shape of the simulation box was chosen in order to minimise its volume, Fig. S1. The edge length was set to 21.4 nm, which allows for 2×5.5 nm margin around the capsid, as periodic boundary conditions were applied. The water molecules were added to the box using *gmx solvate* utility.

The capsid divides the system into two parts, the inner cavity and the outer solution. The capsid carries high total charge (+192 e), which is distributed non-uniformly, its inner surface is charged positively, while the outer surface is negative. Therefore, when neutralising the total charge it should be done for each part separately. We followed the procedure that we used in our previous work on PCV2 [5-7]. The cumulative charge of the capsid atoms in a sphere of radius *r* centred at the capsid centre of mass (COM) was computed, Fig. 2. The obtained curve was smoothed via adjacent averaging with the 0.3 nm window to remove noise. Before these computations, energy minimisation of the structure in water was carried out.

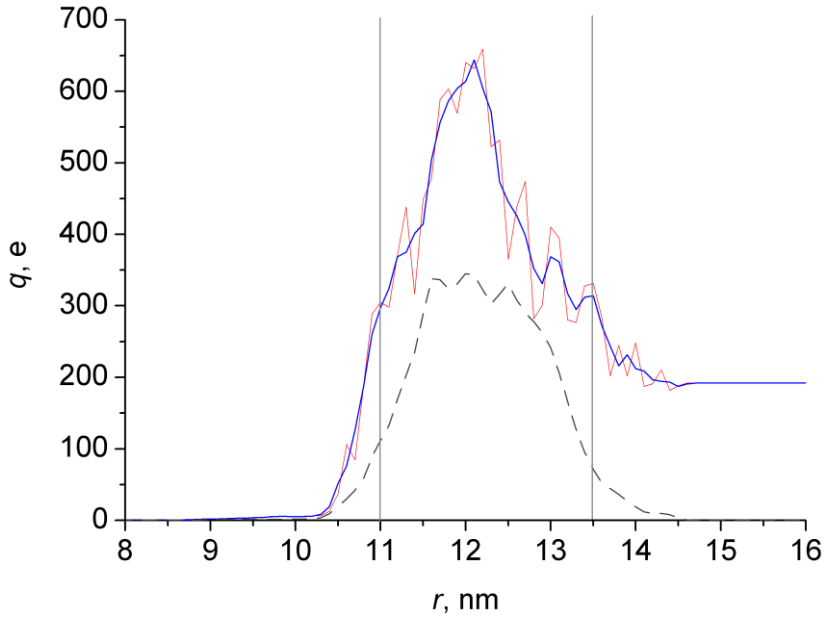

Figure S1. The cumulative charge of capsid atoms in a sphere of radius *r* centred at the capsid centre of mass (red curve). Blue curve is a smoothed original charge. Dashed gray curve shows radial distribution function of capsid atoms (scaled vertically for visual purposes). The vertical lines indicate the boundaries that include 90% of the capsid atoms.

The integral charge increases with distance up to +644e at 12.1 nm and then decreases to +192 e. The position of the maximum roughly corresponds to the middle of the capsid wall. These facts indicate that the capsid is highly polarised with the inner surface having the charge of +644 e, and the outer surface charged at –452 e. According to this information, 644 Cl^- ions were placed into the capsid cavity and 452 Na^+ ions were distributed in the outer solution. Home made scripts and *gmx genion* utility were used for this. Finally, background electrolyte in the amount of 2971 Na^+ and Cl^- ions was randomly distributed across the whole cell, which made the total salt concentration matching that of the physiological solution (0.9% wt. NaCl). The number was calculated from the total number of water molecules in the cell and the number ratio 1:358 between NaCl and water molecules in physiological solution.