Supporting Information

Invariant polymorphism in virus capsid assembly

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Movie S1: The final conformation of a T=3 oblate capsule which contains 216 subunits organized as 12 pentamers (blue), 24 hexamers (green, red) and 2 hexameric dislocations of A-subunits (blue), obtained from a coarse-grained molecular dynamics simulation of 1800 protein subunits (43200 pseudo-atoms) at 86.5μM and 308K.

Movie S2: The final conformation of a T=3 angular capsule containing 234 subunits organized as 12 pentamers (blue), 26 hexamers (green, red) and 3 hexameric dislocations (blue), obtained from a coarse-grained molecular dynamics simulation of 1800 protein subunits (43200 pseudo-atoms) at 86.5μM and 308K.

Movie S3: The final conformation of a T=3 twisted capsule containing 252 subunits organized in 12 pentamers (blue), 28 hexamers (green, red) and 4 hexameric dislocations (blue), obtained from a coarse-grained molecular dynamics simulation of 1800 protein subunits (43200 pseudo-atoms) at 86.5μM and 308K.

Movie S4: The final conformation of a T=3 tubular capsule containing 270 subunits organized in 12 pentamers (blue), 30 hexamers (green, red) and 5 hexameric dislocations (blue), obtained from a coarse-grained molecular dynamics simulation of 1800 protein subunits (43200 pseudo-atoms) at 86.5μM and 308K.

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Complete T=1 and T=3 capsids are characterized as icosahedral structures

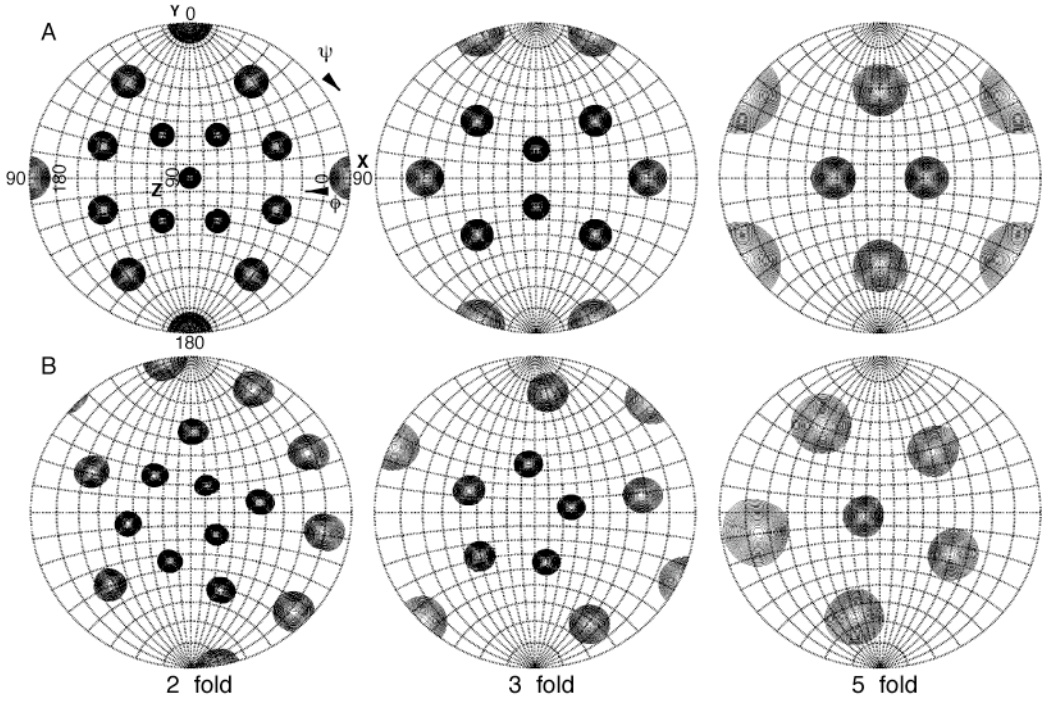

Figure S7: Stereographic projection of the rotation function showing twofold, threefold and fivefold rotation axes for assembled (A) T=1 capsids and (B) T=3 capsids. The relative positions of 15 twofold, 10 threefold and 5 fivefold rotation axes show that T=1 and T=3 capsids obtained from our simulations well conform to icosahedral symmetry.

Relative stability of icosahedral capsids and non-icosahedral capsules

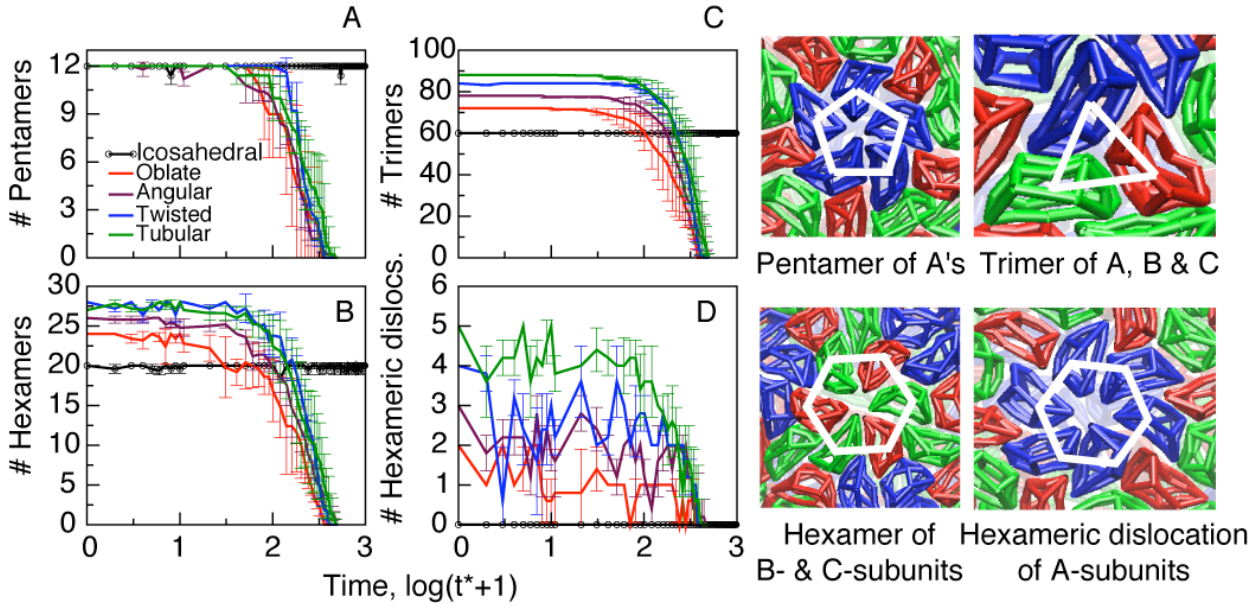

Figure S8: The number of (A) pentamers, (B) hexamers, (C) trimers and (D) hexameric dislocations as a function of time: averages from 10 simulations at 86.5μM and 381K for each system containing a structure originally obtained at 86.5μM and 308K.

Non-icosahedral capsules originally obtained at 86.5μM and 308K are slightly less stable than icosahedral capsids as demonstrated by heating simulations of each structure at 86.5μM and a wide variety of temperatures ranging from 318K to 400K. All non-icosahedral capsules and icosahedral capsids maintain their structural integrity up to 372K. However, at 381K the non-icosahedral capsules begin to lose structural integrity, as shown in **Fig. S8**. This indicates that the hexameric dislocations are unstable since they constantly break and reform. This fluctuation causes ruptures in surrounding hexamers of B- and C-subunits (in contrast to the constant stability of pentamers and trimers), and results in the gradual disassembly of the starting structure into free monomers. At 400K, icosahedral capsids and non-icosahedral capsules undergo rapid disassembly. Non-icosahedral capsules are slightly less stable than icosahedral capsids due to the presence of kinetically trapped, conformationally strained, hexameric dislocations, which are the weak points and thereby more susceptible to structural disruptions.

Shifting assembly conditions to the optimal region increases the population of icosahedral capsids and decreases the population of aberrant structures

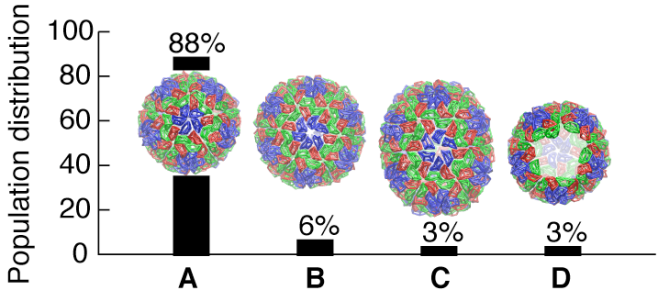

Figure S9: The population distribution obtained from 100 simulations for the T=3 system at 21.7μM and 290K. Four supramolecular structures are shown: (A) complete icosahedral capsid, (B) oblate capsule, (C) angular capsule and (D) partial capsid.

When assembly of the T=3 system is simulated at 21.7μM and 290K, the resultant population of supramolecular structures shifts to a higher population of icosahedral capsids and lower population of aberrant structures as compared to the population shown in **Fig. 2**.

Excess A-subunits decreases the population of icosahedral capsids and increases the population of aberrant structures

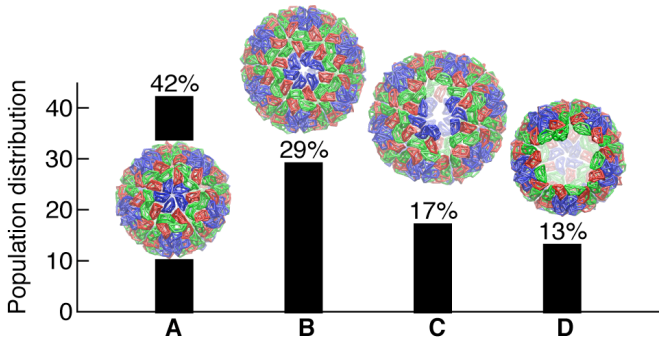

Figure S10: The population distribution for the T=3 system at 115.3μM and 308K obtained from 100 simulations. Four supramolecular structures are shown: (A) complete icosahedral capsid, (B) non-icosahedral yet highly symmetric enclosed oblate capsule, (C) open monster particle and (D) partial capsid.

Mimicking a shift in the pre-equilibrium population of the A-subunit by performing simulations of the T=3 system with twice the number of A-subunits than either B- or C-subunits (at a total concentration of 115.3μM) yields a population of supramolecular structures at 308K with a lower number of icosahedral capsids and higher number of aberrant structures, including the oblate capsules (as compared to the population shown in **Fig. 2**). One notable type of structure observed under these conditions is monster particles that resemble oblate and other non-icosahedral capsules; however, they are not completely enclosed due to the presence of too many A-subunits that grow on each side of the opening. In short, shifting the conformational equilibrium to pentameric conformations (A-subunits) increases the proclivity for five-to-six (and higher) symmetric dislocations.