Supporting Information

Mannige and Brooks 10.1073/pnas.0811517106

SI Text

To show that canonical intrapentameric dihedral angles interact at ≈138.19°: Hexamers and pentamers within a canonical capsid (those capsids representable as "monohedral tilings" that display few holes, few overlaps and structural invariability; please see ref. 1 for a more rigorous description) may be treated as a 6- and 5-coordinated set of plates, respectively (Fig. S2 *A–C*).

Statement. *Any canonical subunit that possesses the ability to form both pentamer and hexamer must possess intrapentamer dihedral angles of ≈138.19°* (i.e., in Fig. S2*D*, $\phi \approx 138.19°$).

From the canonical capsid definitions (1), we find that (*i*) subunits can form both flat hexamers (Fig. S2*B*) and "curved" pentamers (Fig. S2*C*) from the same interface and (*ii*) all angles within a pentamer are identical [which is a reasonable assumption given that (*i*) these pentameric angles are formed from identical interfaces and not quasiequivalent ones and (*ii*) a 5-fold rotational symmetry element (axis) falls perpendicular to the center of pentamer in the crystal structure].

Proof. Specifically, from the right triangle $b'o''a$ in Fig. S2*D*, we can obtain a relationship for the intrapentamer dihedral angle (Φ) and edge lengths:

$$\sin(\phi/2) = \frac{|o''a|}{|ab'|} \quad \textbf{[S1]}$$

We now assume that the edge of the equilateral triangular faces is 1 with no loss of generality. Given that right triangle $ab'o$ is a 30–60–90 triangle and that $|oa| = 1$, we get

$$|ab'| = \sqrt{3}/2 \quad \textbf{[S2]}$$

Substituting Eq. **S2** in Eq. **S1** and rearranging, we get

$$\sin(\phi/2) = \frac{2}{\sqrt{3}}|o''a| \quad \textbf{[S3]}$$

Theta (θ) is the angle between the adjacent radiating edges once projected to a plane that contains a,b,c,d,e (there must be such a plane because all dihedral angles are set to the same value). From Fig. S2*D*, we get

$$|o''a| = |o'a|\sin(\theta) \quad \textbf{[S4]}$$

Substituting Eq. **S4** into Eq. **S3**, we get

$$\sin(\phi/2) = \frac{2}{\sqrt{3}}|o'a|\sin(\theta) \quad \textbf{[S5]}$$

Also, from the 30–60–90 triangle $o'aa'$ in Fig. S2*C*, because $|aa'| = ½$, we obtain

$$|o'a| = \frac{|a'a|}{\sin(\theta/2)} = \frac{1}{2\sin(\theta/2)}. \quad \textbf{[S6]}$$

Substituting Eq. **S6** in Eq. **S5** yields

$$\sin(\phi/2) = \frac{\sin(\theta)}{\sqrt{3}\sin(\theta/2)} \quad \text{or} \quad \phi = 2\cdot asin\left(\frac{\sin(\theta)}{\sqrt{3}\sin(\theta/2)}\right). \quad \textbf{[S6']}$$

If all of the dihedral angles within the pentamer are alike, then $\theta = 2\pi/5$ (this generalizes to $\theta = 2\pi/i$ if the pentamer is actually an i-mer), and

$$\phi = 2\cdot asin\left(\frac{\sin(2\pi/5)}{\sqrt{3}\sin(\pi/5)}\right) \approx 138.19°.$$

This will be true for any set of canonical capsid subunits that assemble into pentamers, and is also seen in true icosahedra (20-faced deltahedra) that describe $T = 1$ capsids, which, we claim, allows for $T > 1$ to $T = 1$ transformations (see main text).

1. Mannige RV, Brooks CL, III (2008) Tilable nature of virus capsids and the role of topological constraints in natural capsid design. *Phys Rev E* 77:051902.27.

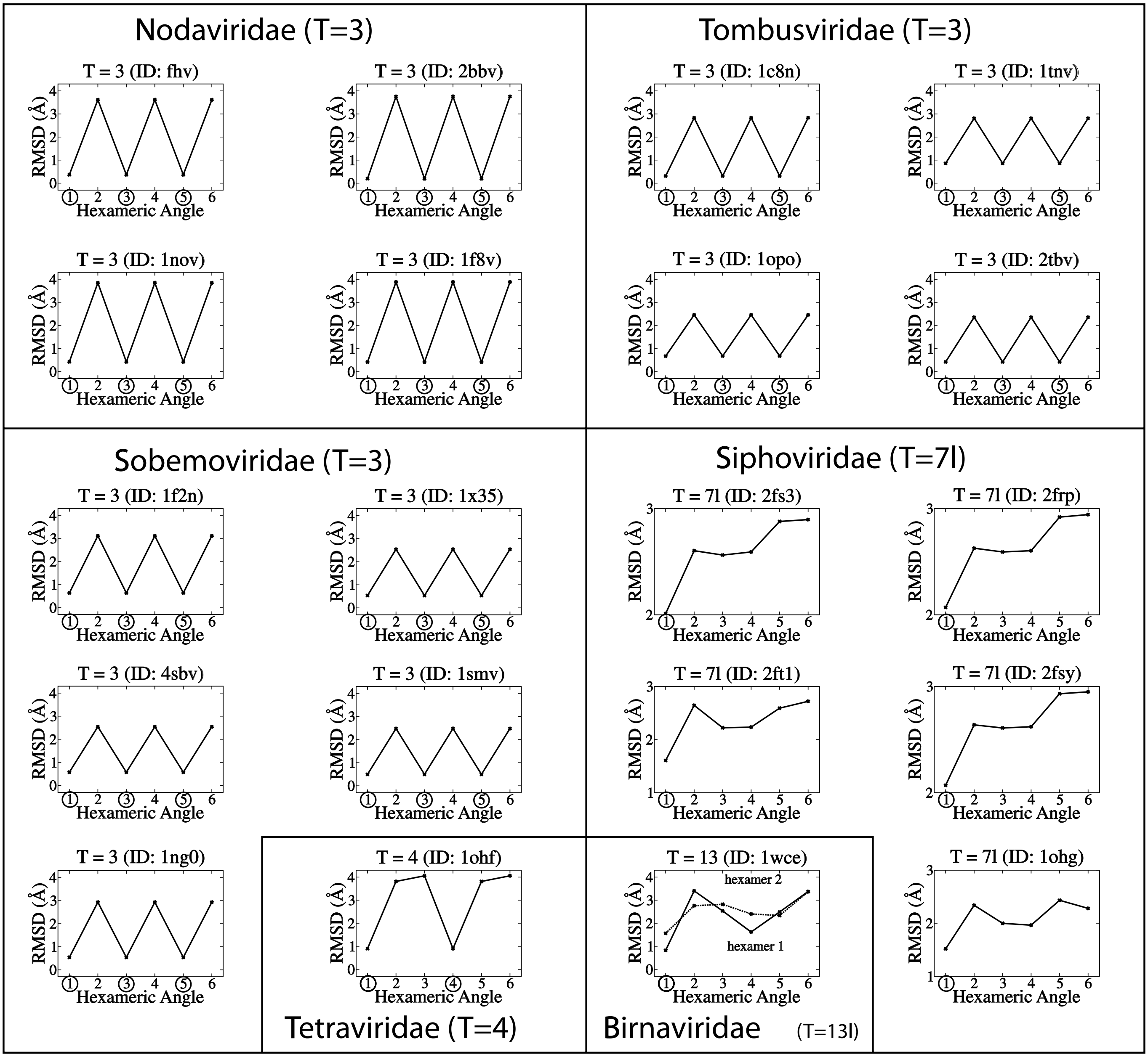

Fig. S1. Angle profiles of hexamers in unique environments when compared to a pentameric endo angle of the same capsid (low RMSD values indicate more pentamer-like angles) shown for individual capsids (indicated by their PDB ID or ID). This graph is an expanded version of Fig. 2*A*.

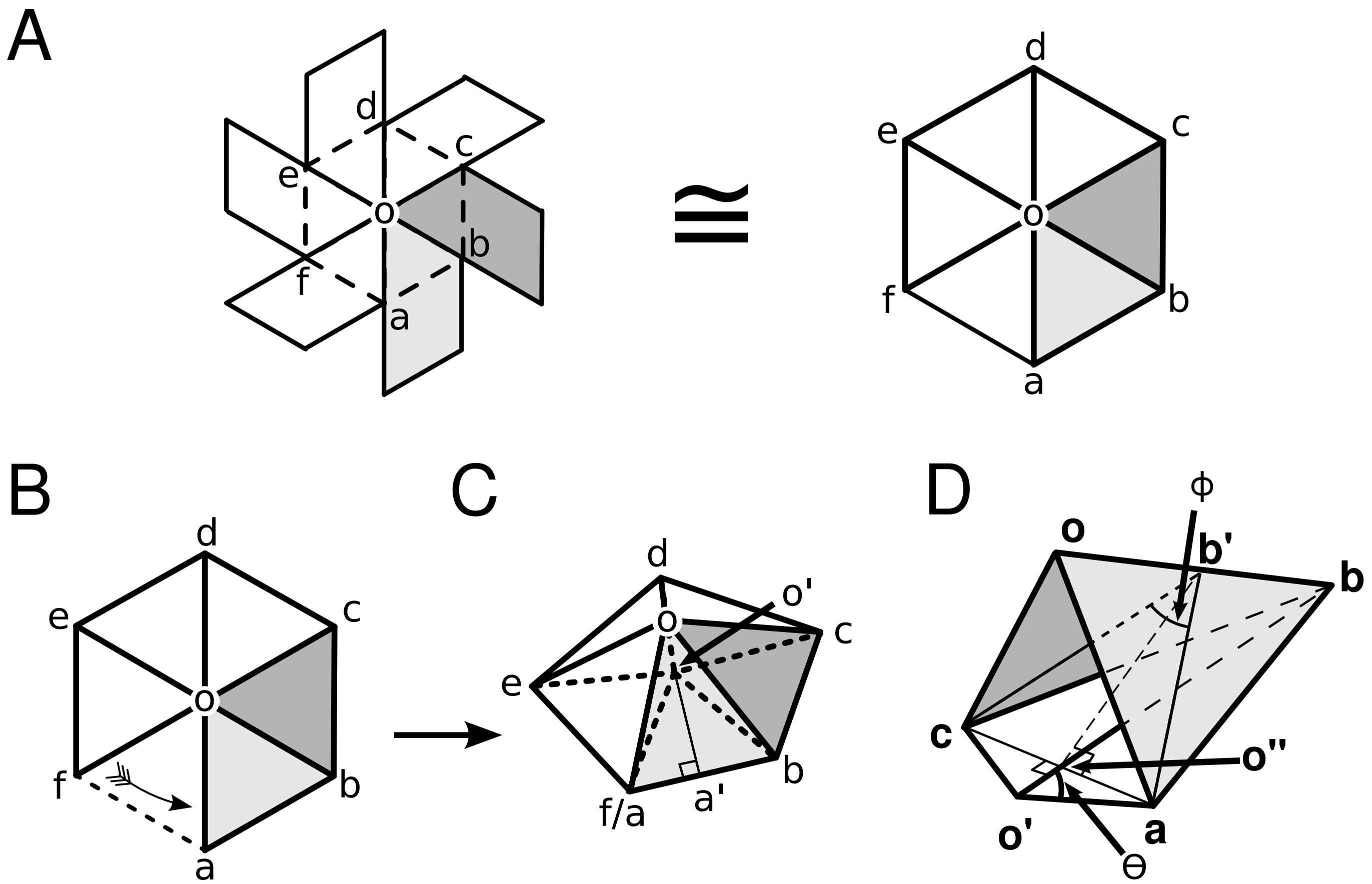

Fig. S2. Showing that $\Phi = \approx 138.19°$. (*A*) Indicates that *n*-valent clusters formed from trapezoids (shown in the diagram for hexamers) may be reduced/simplified to clusters of equilateral triangles for the purpose of analyzing dihedral angle properties. (*B* and *C*) Hexamers (*B*) and pentamers (*C*) in canonical capsids are formed from the same subunit interface that interact at varying dihedral angles. (*D*) A pair of adjacent subunits is shaded in the pentamer (*C*) and isolated environment (*D*), which will be used to obtain a relationship for the dihedral angle (Φ).

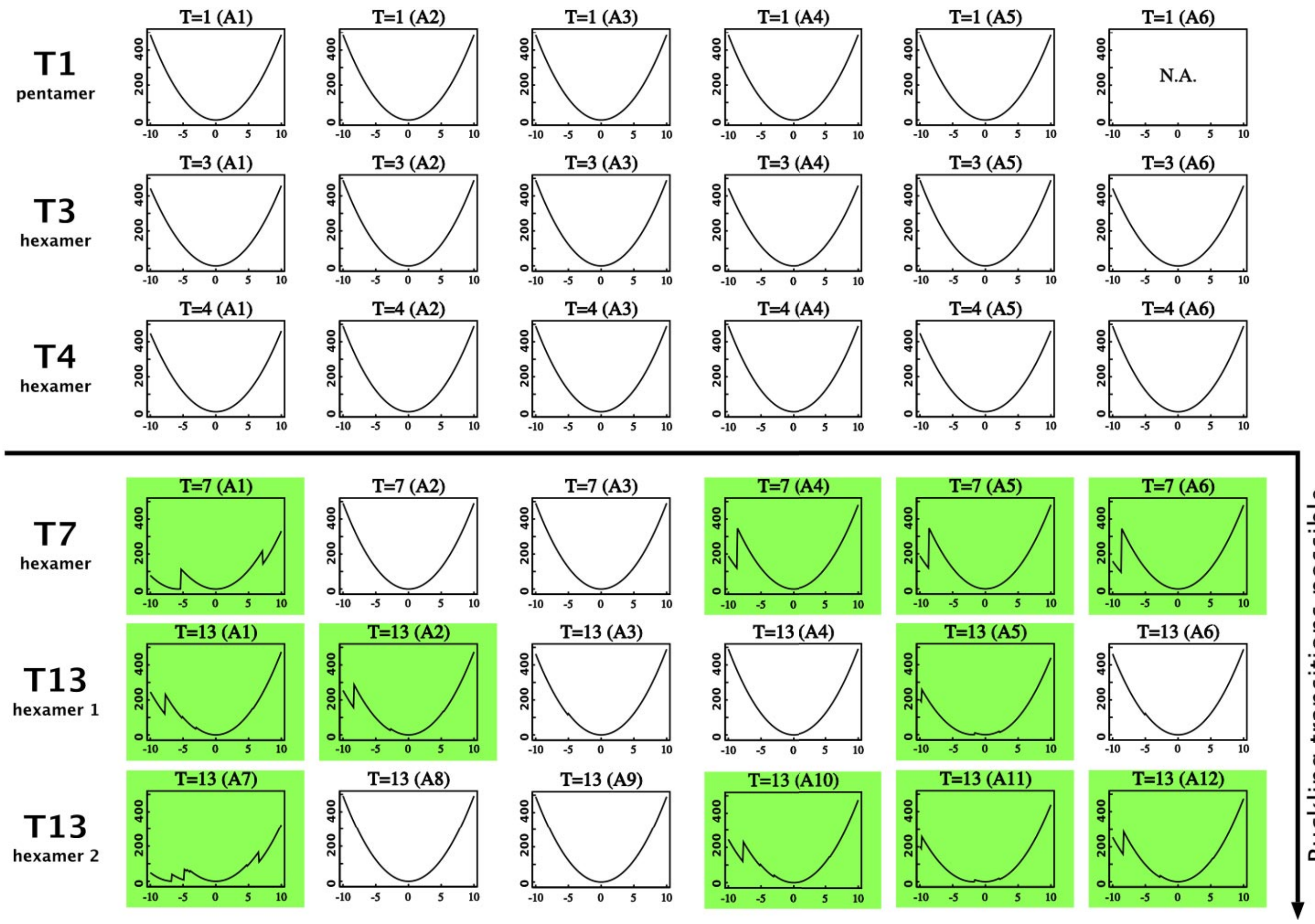

Fig. S3. Energy (*y* axis) vs. angle constraint disequilibrium (r_0-r'; *x* axis) profiles for individual angles (labeled A1–A6 for a unique hexamer and an additional A7–A12 for the second hexamer) within hexamers for capsids with $T = 3$, 4, 7, and13. $T = 1$ pentameric angle profiles are included to give a sense for rigid angle profiles. Only $T > 4$ canonical capsids hexamer angles (whose profiles are highlighted green) appear to sample multiple conformations upon application of small forces, indicating that buckling transitions are possible for only $T > 4$ canonical capsids. This figure is an expansion of Fig. 4*B* in the main text.