A Chiral Pentagonal Polyhedral Framework for Characterizing Virus Capsid Structures

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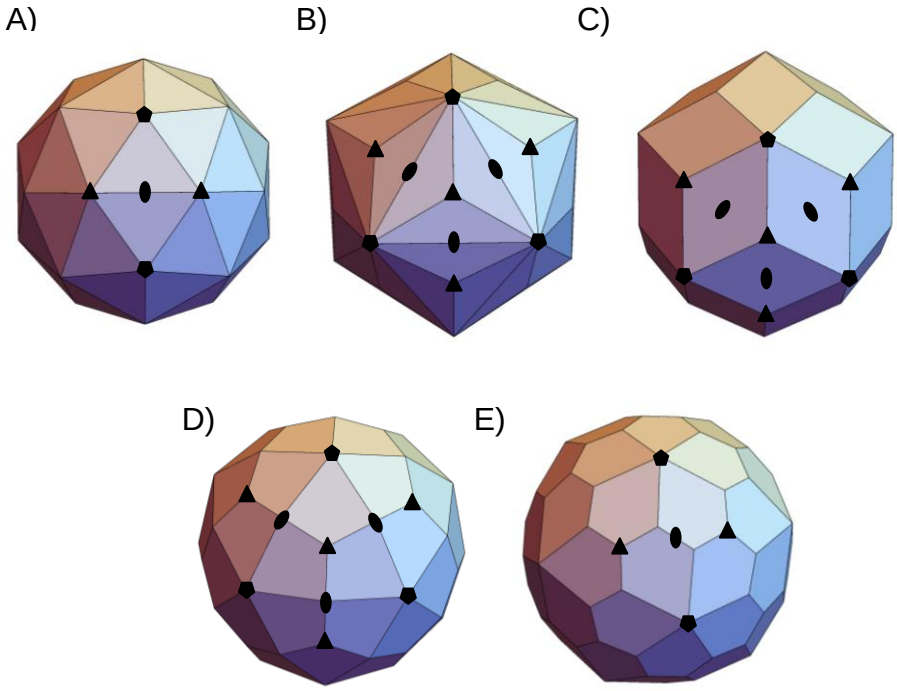


Figure S1. Catalan polyhedra. *a) pentakis dodecahedron b) triakis icosahedron c) rhombic triacontahedron d) deltoidal hexecontahedron e) pentagonal hexecontahedron. Five-fold, three-fold, and two-fold symmetry axes are labeled with pentagons, triangles, and ovals respectively.*

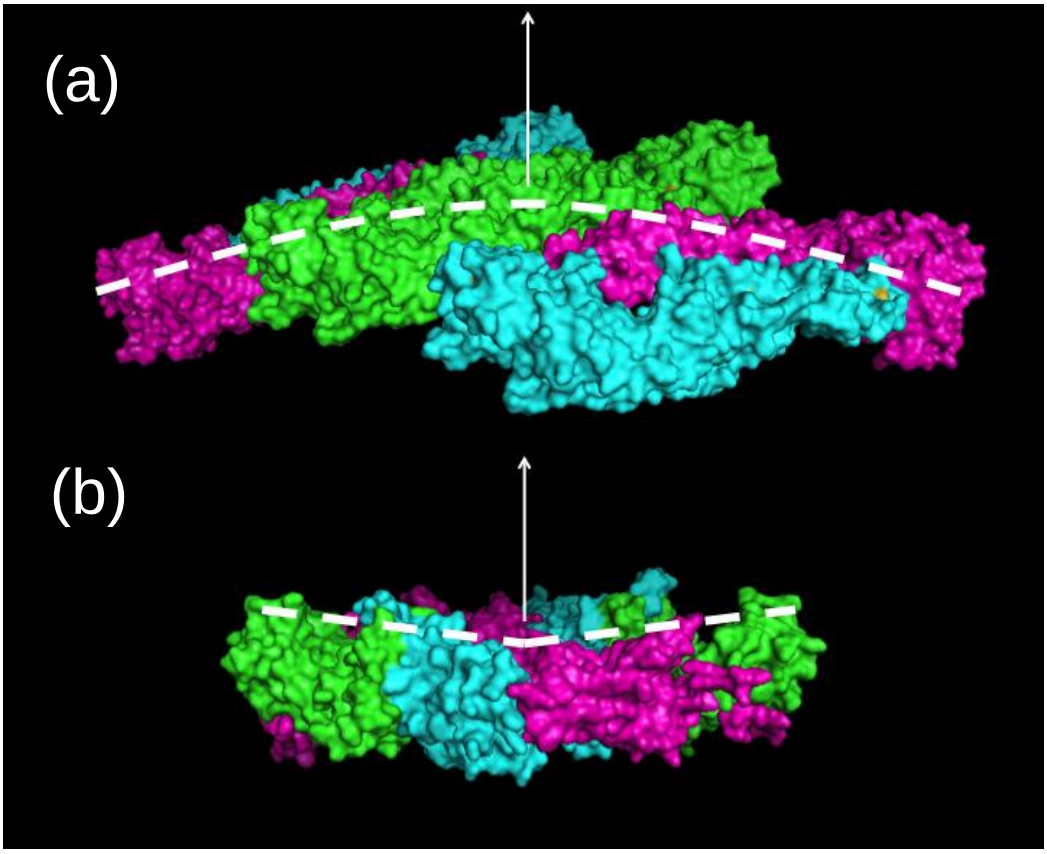


Figure S2. Viral Protein Subunit Interfaces. *This figure illustrates the differences in the viral protein subunit interfaces in two capsids that are both designated as pseudo T=3, a) dengue virus (PDB ID: 1K4R) and b) enterovirus 71 (PDB ID: 3VBU). The arrows lie along a two-fold symmetry axis in each case, pointing away from the inside of the capsid. In a), the geometry (indicated by the dashed white line) is flat and somewhat convex, while in b) the geometry is concave, kinked about the two-fold axis. In this way, two capsids characterized by the same triangulation number exhibit very different inter-protein interfaces.*

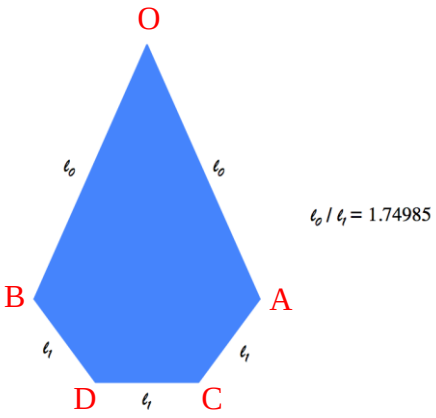


Figure S3. Building block of the pentagonal hexecontahedron. *This pentagon is symmetric, and possesses only two different lengths and angles.*

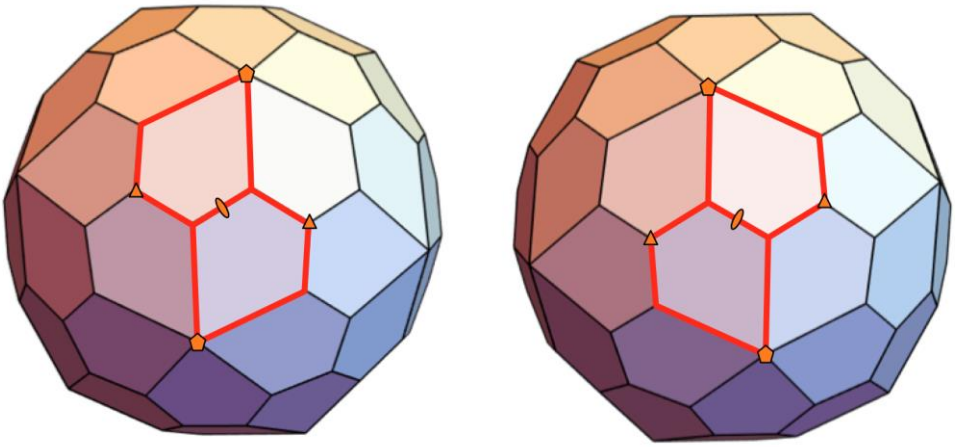


Figure S4. Pentagonal Hexecontahedron. *The pentagonal hexecontahedron in its two chiral forms, laevo shown on the left and dextro on the right. Two units related by two-fold symmetry are outlined in red, with the other symmetry axes notated with orange symbols: pentagons for five-fold axes, triangles for three-fold axes, and ovals for two-fold axes. Caspar & Klug [S1] include a figure that illustrates a similar pentagonal solid, although they do not refer to this polyhedron specifically. They use this figure solely to illustrate the geometric fact that units that have no individual symmetry can still be assembled in 3D to create a polyhedron that possesses overall icosahedral symmetry. They do not actually apply it to virus capsid structures, which is what we show in the main text.*

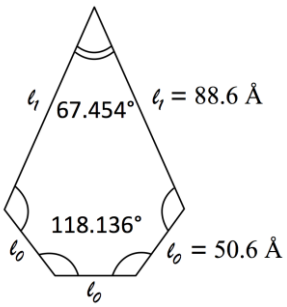


Figure S5. The L-A Virus Pentagon. *The dimensions of an appropriate pentagon (as calculated from the L-A virus atomic coordinates in PDB: 1M1C) that will tile in 3D to form a pentagonal hexecontahedron that describes the whole capsid.*

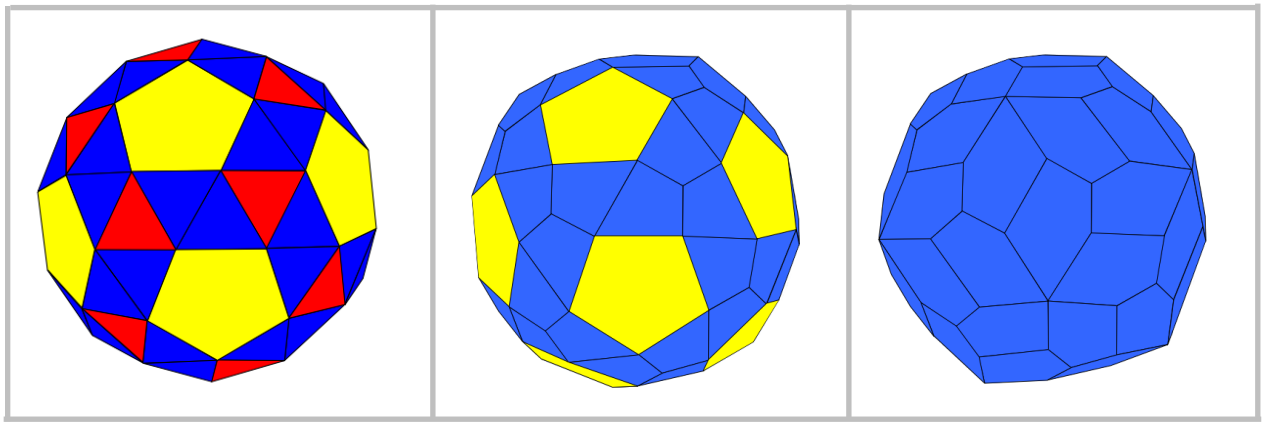


Figure S6. Asymmetric Pentagonal Hexecontahedron. *The creation of a right-handed asymmetric pentagonal hexecontahedron (right) starting from the snub dodecahedron (left). An intermediate solid is shown in the center, which shows the addition of a vertex on the three-fold axes above the red triangles in the snub dodecahedron. Note also that the snub dodecahedron is the dual of the pentagonal hexecontahedron (Figure S4).*

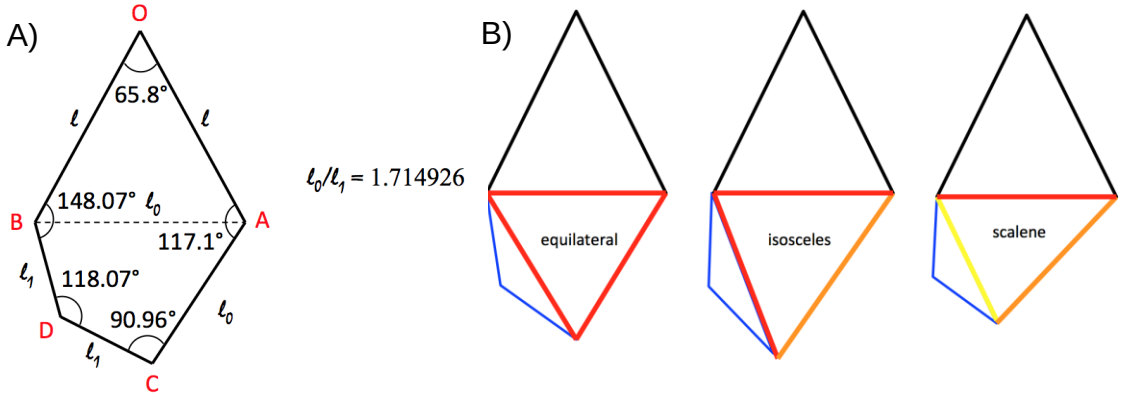
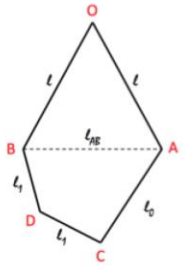


Figure S7. The Asymmetric Pentagonal Unit. *a) The asymmetric irregular pentagon derived explicitly from the snub dodecahedron. b) Three types of asymmetric irregular pentagons. All have two isosceles triangles (marked in black and blue), but the middle triangle can be of any type. The maximum number of unique distances between vertices O, A, B, and C is four, as illustrated by the different colored line segments in the scalene triangle case (black, red, orange, and yellow).*



	Polyomavirus	Papillomavirus	Simian Virus 40
O	66.147°	66.046°	66.171°
A	119.626°	114.575°	119.624°
B	140.063°	145.853°	139.642°
C	95.923°	95.501°	96.319°
D	118.240°	118.026°	118.244°
ℓ_{AB}	96.218 Å	114.635 Å	97.770 Å
ℓ_0	83.922 Å	107.565 Å	84.532 Å
ℓ_1	54.942 Å	62.535 Å	55.653 Å
ℓ	88.158 Å	105.175 Å	89.551 Å

Figure S8. Asymmetric Pentagon Dimensions. *Three asymmetric pentagons generated from crystal structure data of polyomavirus, papillomavirus, and SV40 (from left to right), using atomic coordinates deposited in PDB IDs: 1SIE, 3J6R, and 1SVA. These will tile in 3D to form an asymmetric pentagonal hexecontahedron that describes the whole capsid in each case.*

References

S1. Caspar, D.L.D. and Klug, A. (1962) Physical principles in the construction of regular viruses. *Cold Spring Harb. Symp. Quant. Biol.* 27, 1-24.