Supplemental Table I (Table SI). Distance measurements from prominent capsid features to the fitted (virus-Fab) and unfitted (virus) BC loop.*

	Average Distance (Å) from BC Loop* to							
	center of capsid		center of mesa		adjacent BC loop*		neighboring (non-adjacent) BC loop*	
Model	virus-Fab†	virus‡	virus-Fab	virus	virus-Fab	virus	virus-Fab	virus
160S	154.5	157.4	26.5	23.5	31.2	27.6	50.4	44.7
135S	162.3	164.4	27.6	24.5	32.4	28.8	52.5	46.6
Increase#	5.0 %	4.5 %	4.0 %	4.1 %	4.0 %	4.1 %	4.0 %	4.1 %

*The "BC loop" used here refers only to residues 97–103. The average position of the seven Cα atoms was computed and served as the reference point.

†"Virus-Fab" measurements made from the C3-Fab, peptide coordinates fitted into the 160S-C3 or 135S-C3 map. Original structure is from reference (12), Protein Data Bank entry 1FPT.

‡"Virus" measurements made from published structures. 160S structure from reference (2), Protein Data Bank entry 1ASJ. 135S structure from reference (13), Protein Data Bank entry 1XYR.

¶The center of the mesa lies along a fivefold symmetry axis. This point was determined by taking the average of the coordinates for five BC loops around a single fivefold vertex.

#For the 160S-to-135S transition.

Supplemental Table II (Table SII). The deviation of residues in the BC loop in 160S[1] and 135S[2] models from the modeled BC loop in 160S-C3 and 135S-C3 complexes (peptide bound to antigen-binding domain of C3 Fab[¶]) and data indicating flexibility in the BC loop.

		Absolute distance (in Å) of each Cα atom in 160S[1]/135S[2] from the corresponding peptide Cα in respective 160S-C3/135S-C3 fitting*								
Model	**Fitting**	**97 SER**	**98 THR**	**99 THR**	**100 ASN**	**101 LYS**	**102 ASP**	**103 LYS**	**Average**	**RMSD**
160S[1]	**160S-C3**	2.5	4.4	5.0	6.8	8.4	6.0	5.1	5.4 (± 1.9)	5.7
135S[2]	**135S-C3**	4.1	2.9	5.0	6.6	9.0	5.6	4.2	5.3 (± 2.0)	5.7
****B-Factor (Å²)**		49	58	63	67	59	42	24		

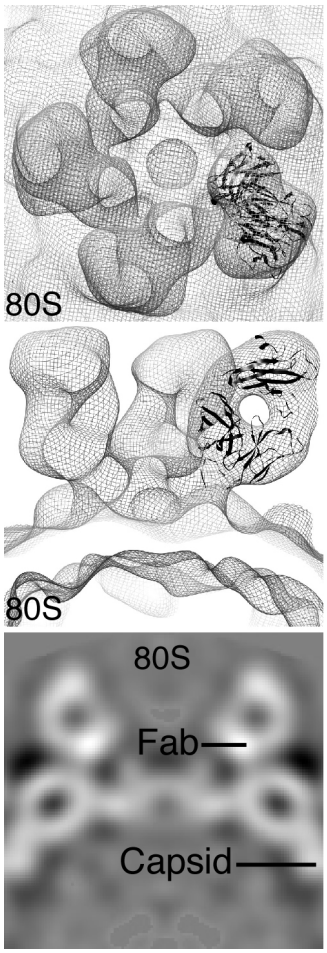
[1]160S structure from reference (2), Protein Data Bank entry 1ASJ.

[2]135S structure from reference (13), Protein Data Bank entry 1XYR.

[¶]Unfitted, original structure from reference (12), Protein Data Bank entry 1FPT.

*Only the distance between Cα coordinates was measured.

**Temperature (B) factors for the Cα atoms of the listed residues in the 160S poliovirus structure (2) (Protein Data Bank entry 1ASJ).



Supplemental Figure 1 (Fig. S1). C3 Fab bound to 80S particles. Close-up renderings viewed along fivefold symmetry axis (top) and perpendicular to a fivefold axis (middle) are shown. C3 Fab coordinates (12) were fitted into one mesa-bound Fab (black ribbon). Fine mesh is surface rendering of 3D reconstruction. 80S-C3 map was contoured at 0.5σ. Center slices from density maps of C3 complexed with 80S (bottom). Relative density estimates: a sphere of radius = 3 pixels was centered on the designated spots (bottom) and the average density computed. The density of C3 is almost the same as the density of the poliovirus capsid.

A relatively small number of 80S particles were found in the 135S-C3 sample (cf. (15)) (Fig. 2A). The 80S-C3 images were picked separately and used to reconstruct the 80S-C3 structure. Therefore, for the 80S-C3 data, sample preparation, microscopy, three-dimensional reconstruction, and fitting of C3 Fab coordinates were performed as described (see Materials and Methods), with three exceptions: 1) A 135S-C3 map was used to begin iterative model-based determination of orientations and origins. 2) In the final 80S-C3 map, the CTF was only corrected for phase-flipping effects (Table 1). The 80S-C3 map was calculated from 238 particles and had a resolution of 22 Å. 3) The full C3-Fab-peptide structure (12) was used as input for CHARMM fitting into the cryo-EM density map.

The 3D reconstruction of 80S-C3 showed that, as expected, C3 Fab binds to the tip of the mesa (cf. Video 3)—where the BC loop was modeled in the 80S particle state (30).

Although the C3 epitope (bound to C3 Fab) shifts outwards in radius by ~8 Å and twists through 13° in the 160S-to-135S transition, the epitope appears unchanged in the 135S-to-80S transition. In contrast to the large changes in the position of the BC loop in the 160S-to-135S transition, the fit of the C3 Fab coordinates into the 80S-C3 3D map showed a similar position and orientation of the Fab to that in the 135S-C3 map (cf. Fig. 2, Video 3), inferring a similar position of the C3 epitope in the two particle states. The lower resolution of the 80S-C3 map compared to the 160S-C3 and 135S-C3 maps made the fit of the C3 Fab coordinates less reliable. Hence, a detailed comparison was impractical. Assuming our fit of the antigen-binding domain of the C3 Fab is a reasonable approximation (top and middle), the 135S-to-80S transition causes little change in the position of the C3 antibody. This observation is consistent with the previous models of the 135S (13) and 80S (30) particles.

The binding affinities of C3 for 160S, 135S and 80S particles are similar (11), and we observed similar Fab:capsid density ratios in the 160S-C3, 135S-C3, and 80S-C3 3D maps (cf. Fig. 2C).

Video Captions

Video 1. Movie showing the shift of C3 Fab in 160S-C3 and 135S-C3 complexes. Coordinates from a model of the C3 Fab (12) were fitted into the Fab density in the 160S-C3 and 135S-C3 reconstructions. Four different views are shown, with antigen-binding domain (purple) and the bound antigenic peptide in the crystal structure (12) (green) fitted into 160S-C3 and 135S-C3 complexes (mesh).

Video 2. Movie showing the shift of C3 Fab in top and side views of C3 Fab on the capsid of 160S and 135S particles. Figures are surface renderings.

Video 3. Movie showing the shift of C3 Fab in top and side views of the C3 Fab on the capsid of 135S and 80S particles. Figures are surface renderings.

Video 4. Movie of shift of bound C3 antibody in 160S-C3 and 135S-C3 complexes (cf. Fig. 4A). The small Ab movement between 160S and 135S states suggests that such a transition might be accommodated by the Ab. Therefore, the actual transition from 160S to 135S state might involve a state significantly larger than the final 4% larger 135S state (see Fig. 4B).