

Table S1. X-ray data collection and refinement statistics for the full-length N74D HIV-1 CA apo and PF74 complex crystal structures.

	<u>N74D CA apo</u>	<u>N74D CA/PF74</u>
	PDB ID: 7MN0	PDB ID: 7MKC
<u>Data collection</u>	Beamline ALS 4.2.2	Beamline APS 23-ID-D
Wavelength (Å)	1.000030	1.03317
Resolution (Å)	2.90 (2.90-3.08) ^a	2.65 (2.65-2.81) ^a
Space group	P6	P6
Cell dimensions		
a, c (Å)	91.7, 57.2	90.4, 55.7
Observed reflections	69,089	41,748
Unique reflections	6,190	7,562
Redundancy	11.1 (10.6)	5.5 (5.3)
Completeness (%)	99.8 (99.4)	98.3 (96.9)
R _{meas} ^b	0.129 (1.22)	0.100 (0.82)
CC _{1/2}	99.9 (71.5)	99.8 (68.8)
Avg I/σ	16.3 (2.0)	11.4 (2.0)
<u>Refinement statistics</u>		
Resolution (Å)	45.87-2.90	45.38-2.65
No. of reflections (working)	5,866	7,190
No. of reflections (test)	323	366
R _{work} ^c	0.219	0.183
R _{free} ^d	0.274	0.242
Overall B value (Å ²)	84.0	67.0
Wilson B value (Å ²)	70.1	60.0
Ramachandran plot (%) ^e		
Favored	93.4	94.5
Allowed	6.6	5.5
Disallowed	0	0
All-atom clashscore	4	3
RMSD Bond length (Å)	0.019	0.019
RMSD Angle (°)	1.904	1.960

^a Values in parentheses are for the outer resolution shell.

$$^b R_{\text{meas}} = \frac{\sum_{hkl} \sqrt{\frac{n}{n-1}} \sum_{j=1}^n |I_{hkl,j} - \langle I_{hkl} \rangle|}{\sum_{hkl} \sum_j I_{hkl,j}}$$

$$^c R_{\text{work}} = \frac{\sum_{hkl} |F_{\text{obs}} - F_{\text{calc}}|}{\sum_{hkl} |F_{\text{obs}}|}$$

^d R_{free} = R_{work}, except 5% of the data excluded from the refinement.

^e Evaluated by MolProbity (Chen *et al.*, *Acta Cryst.* D66, 2010, 12-21).

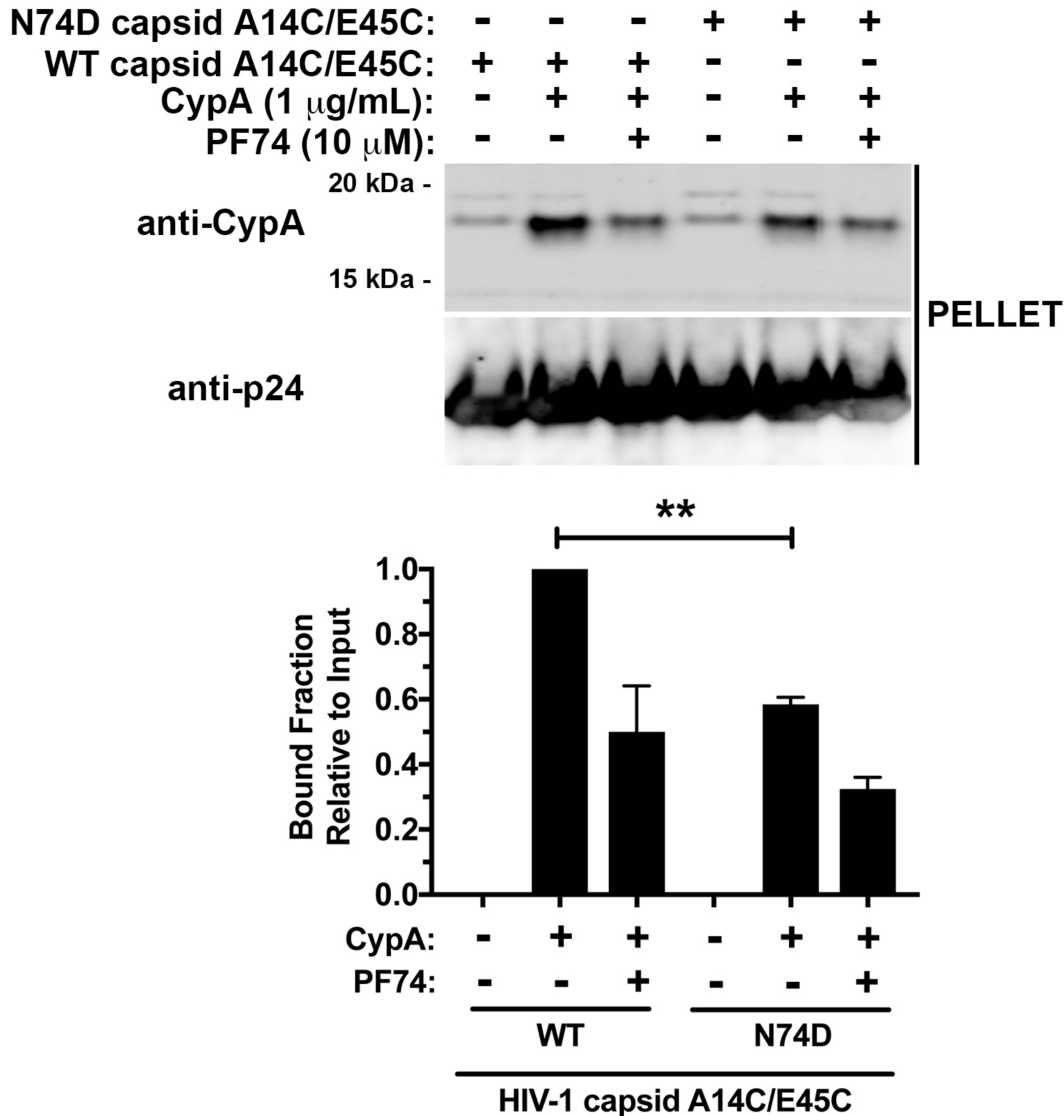


Figure S1. Recombinant CypA binds with decrease affinity to N74D-stabilized capsid tubes. Recombinant CypA protein was diluted in capsid binding buffer (CBB) to a final concentration of 1 μ g/mL. 40 μ L of this mixture were mixed with Laemmli buffer and used as INPUT (not shown). 300 μ L of this mixture were mixed with 10 μ L of either stabilized wild-type, or N74D capsid tubes (5 mg/ml) in presence of PF74 (10 μ M) or DMSO. Mixtures were incubated for 1 h at room temperature. Stabilized HIV-1 capsid tubes were collected by centrifugation and washed twice using CBB. Pellets were resuspended in 1 \times Laemmli buffer (BOUND) and then analyzed by western blotting using anti-Cyp A and anti-p24 antibodies. Experiments were repeated three times, and a representative experimental result is shown. The BOUND fraction relative to the INPUT fraction for three independent experiments (with standard deviation) is shown. ** indicates P-value < 0.001 as determined by using the unpaired t-test.