Table 1. Crystallographic Statistics

Data Collection			
Stabilization method	Crosslink	Crosslink	Template
Beam line	APS 22-BM	SSRL BL7-1	SSRL BL7-1
Space group	P6	$P2_12_12_1$	C2
Cell dimensions, Å	*a* = 91.0	*a* = 136.1	*a* = 90.6
	b = 91.0	*b* = 136.7	*b* = 156.4
	c = 56.8	*c* = 208.4	*c* = 196.6
Resolution range, Å	50–1.90 (1.97–1.90)	50–2.70 (2.80–2.70)	50–7.0 (7.25–7.0)
R_{sym}, %	10.0 (52.0)	8.5 (45.3)	11.4 (32.3)
Mean I/σ <I>	21.1 (3.3)	14.1 (2.5)	8 (2.5)
Completeness, %	99.9 (100)	96.0 (92.4)	99.6 (98.5)
Average redundancy	10.5 (10.5)	4.2 (3.7)	7.5 (7.0)
Average mosaicity, °	0.46	0.57	0.60
Wilson B factor, Å^2	23.5	66.7	
Refinement			
Resolution range	27–1.90 (1.98–1.90)	35–2.70 (2.75–2.70)	50–7.0 (7.95–7.0)
Number of unique reflections	21,334 (2,489)	102,181 (4,871)	4,070 (1,105)
Reflections in free set	1,060 (149)	2,565 (171)	407 (128)
R_{work}, %	23.2 (24.1)	23.8 (31.3)	28.2 (31.2)
R_{free}, %	26.9 (30.7)	26.3 (33.4)	32.3 (35.9)
Number of nonhydrogen atoms			
Protein	1,553	19,082	10,218
Water	193		
Average B factor, Å^2			
Protein	25.85	56.43	
Water	30.88		
Coordinate deviations from ideal geometry			
Bond lengths, Å	0.005	0.007	
Bond angles, °	0.775	0.915	
PROCHECK/MOLPROBITY distribution of phi and psi angles, %			
Favored	95.2/99.5	95.1/98.3	
Allowed	4.8/0.5	4.5/1.7	
Disallowed	0/0	0.3/0	

Values in parentheses are for the highest resolution shell. $R_{sym} = \Sigma|I - \langle I \rangle| / \Sigma|\langle I \rangle|$, where I is the measured intensity of each reflection, and $\langle I \rangle$ is the intensity averaged from symmetry equivalents. $R_{work} = \Sigma||F_o| - |F_c|| / \Sigma|F_c|$, where F_o and F_c are observed and calculated structure factors, respectively. R_{free} is the cross-validation R factor calculated for reflections in the free set, which were not used in refinement.

and mutually validate the two oligomer-stabilizing strategies. The hexamers are also very similar to the cryoEM structure (Ganser-Pornillos et al., 2007) (Figure S4) and are consistent with other structural and biochemical data (Bartonova et al., 2008; Bowzard et al., 2001; Cardone et al., 2009; Gamble et al., 1997; Ganser-Pornillos et al., 2004, 2007; Lanman et al., 2003, 2004; Li et al., 2000; Mortuza et al., 2004; von Schwedler et al., 1998, 2003). As shown in Figure 2, the CA hexamer is composed of two concentric rings, with the NTD and CTD forming the inner and outer rings, respectively. Intramolecular interactions between the two domains of each protomer are minimal, but both pack against the neighboring NTD subunit. Indeed, the NTD-NTD and NTD-CTD interfaces essentially merge into one contiguous hexamerization interface (Figure 3), emphasizing the degree to which the NTD and CTD interactions cooperate to create the hexameric assembly.

Interactions between Hexamers

The CcmK4-templated crystal and the hexagonal crystal of crosslinked CA were composed of stacked sheets, with each sheet corresponding to a flattened version of the mature hexameric lattice (Figure 2C, Figures S1B and S2B), as also seen in the HIV-1 CA cryoEM structure (Ganser-Pornillos et al., 2007). These structures therefore recapitulate all three relevant CA-CA interfaces. Within each sheet, neighboring hexamers are connected exclusively by CTD contacts made through the CTD-CTD dimerization interface (Figure 2C). The crystallographically distinct dimer interactions appear to be very similar to each