Table S1. Related to Figures 2 and 6. Data collection and refinement statistics

	589-B35(HIV)	55-B35(HIV)	55-B35(Pep20)
Wavelength	0.9795	1	0.9795
Resolution range	39.1 - 3.35 (3.47 - 3.35)	45.15 - 1.898 (1.966 - 1.898)	46.82 - 1.75 (1.813 - 1.75)
Space group	C 1 2 1	C 1 2 1	C 1 2 1
Unit cell	156.48 59.28 123.57 90 110.77 90	199.996 61.414 92.064 90 105.628 90	194.492 61.698 92.145 90 104.872 90
Total reflections	50510 (4562)	287500 (25914)	299246 (26653)
Unique reflections	15094 (1439)	83485 (7910)	103605 (10087)
Multiplicity	3.3 (3.2)	3.4 (3.3)	2.9 (2.6)
Completeness (%)	97.03 (94.02)	97.79 (92.69)	97.14 (94.81)
Mean I/sigma(I)	8.96 (1.60)	4.67 (0.70)	10.84 (2.34)
Wilson B-factor	102.67	34.9	19.44
R-merge	0.1116 (0.7365)	0.1382 (1.313)	0.06306 (0.4594)
R-meas	0.1333 (0.889)	0.1628 (1.563)	0.07631 (0.5622)
R-pim	0.07175 (0.489)	0.08533 (0.8382)	0.04226 (0.3183)
CC1/2	0.995 (0.795)	0.985 (0.406)	0.988 (0.696)
CC*	0.999 (0.941)	0.996 (0.76)	0.997 (0.906)
Reflections used in refinement	15082 (1431)	83453 (7885)	103600 (10087)
Reflections used for R-free	708 (66)	2000 (190)	1856 (180)
R-work	0.2451 (0.3388)	0.1876 (0.3569)	0.1585 (0.2261)
R-free	0.2745 (0.3637)	0.2160 (0.3988)	0.1834 (0.2512)
CC(work)	0.936 (0.762)	0.962 (0.676)	0.965 (0.873)
CC(free)	0.939 (0.716)	0.945 (0.566)	0.960 (0.803)
Number of non-hydrogen atoms	6445	7022	7447
macromolecules	6399	6621	6648
ligands	45	37	182
solvent	1	364	617
Protein residues	825	826	822
RMS(bonds)	0.002	0.003	0.009
RMS(angles)	0.56	0.6	0.98
Ramachandran favored (%)	95.66	98.28	98.4
Ramachandran allowed (%)	4.21	1.72	1.6
Ramachandran outliers (%)	0.12	0	0
Rotamer outliers (%)	2.1	1.12	0.55
Clashscore	7.37	1.86	2.25
Average B-factor	121.22	45.99	27.26
macromolecules	120.9	45.98	26.1
ligands	167.48	80.16	42.29
solvent	120.15	42.76	35.32
Number of TLS groups	8	22	30

Statistics for the highest-resolution shell are shown in parentheses.