Inter-chain hydrophobic clustering promotes rigidity in HIV-1 protease flap dynamics: New insights from Molecular Dynamics

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Supplementary Materials

Figure S1: Box size dimension plot.

Ramachandran Plot

NOPOL-3

Figure S2: Ramachandran plot of the 1000 protein models obtained from the 20 ns trajectories of the NOPOL-3 simulation and computed with the PROCHECK program.

Figure S3: TriCa angle (Gly147-Gly148-Ile149) in chain -B for all POL & NOPOL simulations.

Figure S4(a): C_{α} RMSD values for the flap elbow residues of HIV-1 protease chain-A.

Figure S4(b): C_{α} RMSD values for the flap elbow residues of HIV-1 protease chain-B.

Table S1: Mean and standard deviation (SD) values for different angles calculated (in the flap tip region of HIV-pr) for all the five trajectories. All values are in Degree [°] unit.

		NOPOL-1		NOPOL-2		NOPOL-3		POL-1		POL-2	
		Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
Flap TriCa Angles	48-49-50	139.87	13.5	130.47	14.0	144.84	4.3	145.28	4.3	143.32	8.3
	49-50-51	98.30	8.0	104.13	9.3	96.43	3.0	95.45	3.0	96.21	5.3
	50-51-52	109.22	4.3	111.22	4.0	111.12	3.8	107.59	4.0	109.40	3.7
	51-52-53	148.60	4.7	147.30	4.6	149.36	4.9	151.28	3.9	149.88	4.6
	147-148-149	140.65	12.0	145.21	5.4	137.91	4.5	147.47	4.2	144.54	7.3
	148-149-150	97.23	7.4	97.74	6.0	111.29	3.6	95.28	3.5	101.14	9.4
	149-150-151	105.23	7.1	108.22	5.6	97.77	3.7	110.12	3.6	105.75	6.7
	150-151-152	149.40	5.0	151.72	4.6	149.07	6.1	151.59	3.5	151.33	4.4