CD4-binding obstacles in conformational transitions and allosteric communications of HIV gp120

Supplementary data

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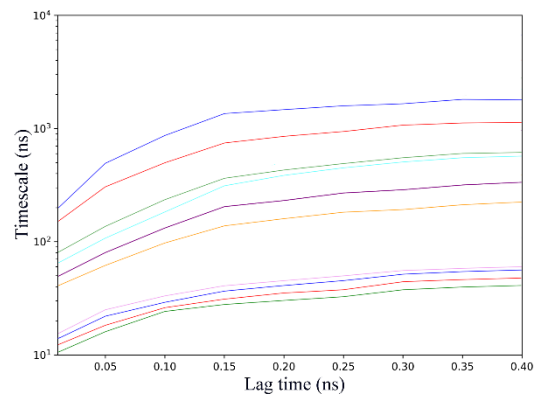* Co-correspondence: ylqbioinfo@gmail.com (L.Q.Y.).

Fig. S1 Relaxation timescales. Different lag time were test to estimate the relaxation timescale.
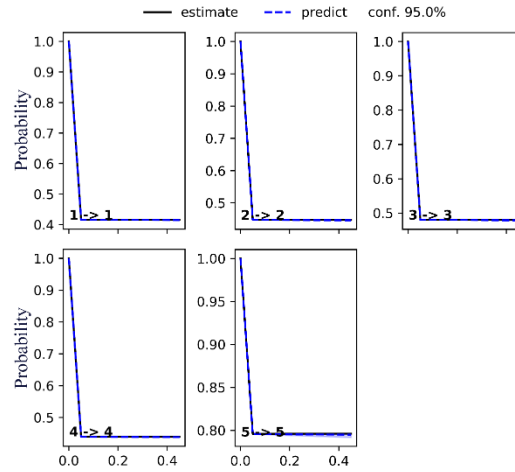
Fig. S2 A Chapman-Kolmogorov test of the Markov state model. Each graph shows the evolution of the population of a given metastable state (1-5, corresponding to A to E in the main text Fig. 4).
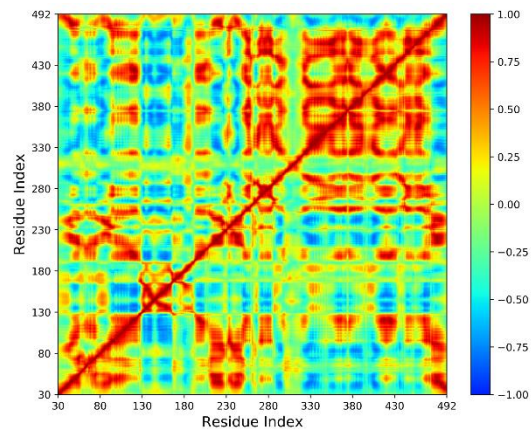
Fig. S3 Dynamic cross-correlation map (DCCM). The correlation coefficient values of C_α motions of the ligand-free and CD4-bound gp120 during simulations showed in the upper and lower triangle of DCCM, respectively.
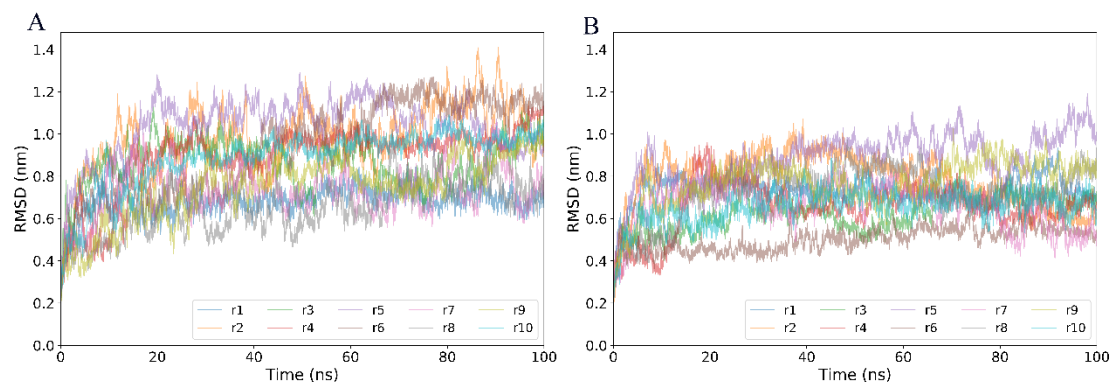
Fig. S4 Molecular dynamics of gp120. Time evolution of backbone root-mean-square deviation (RMSD) values of gp120 with respect to the starting structure calculated from ten replicas (r1-10) in ligand-free (A) and CD4-bound (B) systems.

Table S1 Cosine content values of the first three eigenvectors calculated from replicas and joined equilibrium trajectories.

	ligand-free system			CD4-bound system		
	Eigenvector 1	Eigenvector 2	Eigenvector 3	Eigenvector 1	Eigenvector 2	Eigenvector 3
Replica 1	0.0390	0.0796	0.0518	0.6624	0.2412	0.3600
Replica 2	0.2944	0.0954	0.2729	0.0234	0.2040	0.0327
Replica 3	0.6562	0.3313	0.0495	0.5688	0.0642	0.1059
Replica 4	0.8122	0.7335	0.6163	0.0506	0.6243	0.3437
Replica 5	0.4338	0.0868	0.1488	0.4934	0.0016	0.0807
Replica 6	0.6938	0.0505	0.0041	0.5208	0.0222	0.0107
Replica 7	0.1069	0.0981	0.0018	0.3998	0.3055	0.0016
Replica 8	0.7286	0.3991	0.0264	0.6430	0.6253	0.4043
Replica 9	0.3194	0.0215	0.0068	0.5999	0.3918	0.1189
Replica 10	0.7268	0.3253	0.0431	0.7029	0.2496	0.0298
Joined	0.0164	0.0044	0.0093	0.0137	0.0748	0.0070