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Molecular dynamics simulations reveal distinct differences in conformational dynamics and thermodynamics between the unliganded and CD4-bound states of HIV-1 gp120

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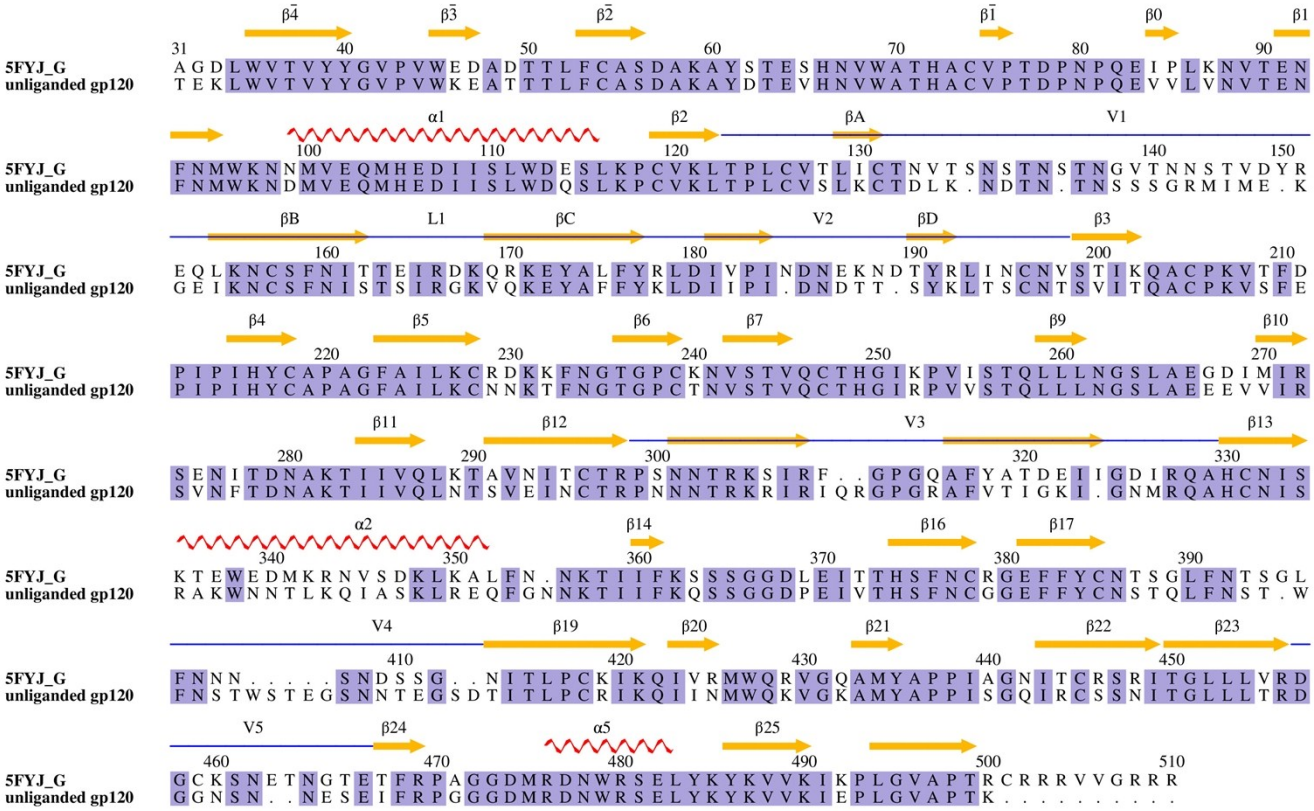
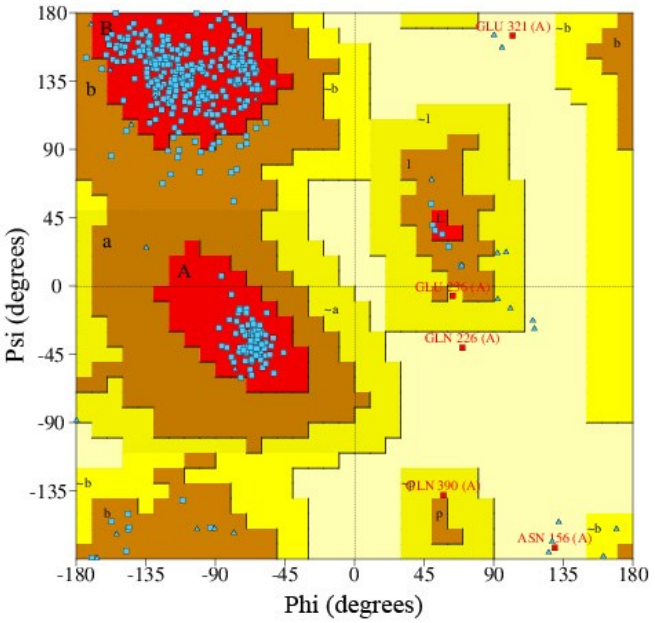


Fig. S1 Sequence alignment for building the structural model of the unliganded gp120. "5FYJ_G" represents the sequence of the template extracted from the crystal structure with PDB ID 5FYJ (chain G),[1] and "unliganded gp120" represents the target sequence. Conserved residues are shaded in light blue. Regular secondary structural elements are numbered according to the crystal structures with PDB IDs 3J70[2] and 3JWD[3] from the HIV-1 HXBc2 isolate, with spirals (red) and arrows (orange) denoting the α-helix and β-strand, respectively. The four blue line segments drawn above the alignment indicate the variable regions V1/V2, V3, V4, and V5, respectively. In the V1/V2 region, the four β-strands are labelled βA to βD, respectively, and the three connecting loops, i.e., the loop V1 (between βA and βB), L1 (between βB and βC), and V2 (between βC and βD), are also labelled.



		No. of residues	%=tage
Most favored regions	[A,B,L]	373	91.0%
Additional allowed regions	[a,b,l,p]	32	7.8%
Generously allowed regions	[~a,~b,~l,~p]	2	0.5%
Disallowed regions	[XX]	3	0.7%
Total number of residues		462	

Fig. S2 Ramachandran plot of the constructed structural model of the unliganded gp120.

Table S1 Cosine contents of the first three eigenvectors (Eigs. 1 to 3) for the unliganded and CD4-complexed gp120s calculated from the equilibrated portions of the 10 independent replicas (10-100 ns; replicas 1-10) and the 900-ns joined equilibrium trajectories.

	Unliganded			CD4-complexed		
	Eig. 1	Eig. 2	Eig. 3	Eig. 1	Eig. 2	Eig. 3
Replica 1	0.5796	0.3210	0.0408	0.6624	0.2412	0.3600
Replica 2	0.6543	0.0561	0.0024	0.0234	0.2040	0.0327
Replica 3	0.3368	0.1697	0.0179	0.5688	0.0642	0.1059
Replica 4	0.7652	0.2472	0.0024	0.0506	0.6243	0.3437
Replica 5	0.0440	0.0816	0.0000	0.4934	0.0016	0.0807
Replica 6	0.2240	0.0404	0.3412	0.5208	0.0222	0.0107
Replica 7	0.8223	0.0963	0.0033	0.3998	0.3055	0.0016
Replica 8	0.8381	0.3207	0.0703	0.6430	0.6253	0.4043
Replica 9	0.4874	0.0274	0.0025	0.5999	0.3918	0.1189
Replica 10	0.0862	0.0130	0.2126	0.7029	0.2496	0.0298
Joined	0.1296	0.0266	0.0067	0.0137	0.0748	0.0070

References

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