Supporting Information

Title: Structural dynamics of V3 loop with different electrostatics: Implications on co-receptor recognition. A molecular dynamics study of HIV gp120.

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Table I

		A	B	C	D
Residue	Atom	%Occupancy	%Occupancy	%Occupancy	%Occupancy
E370	C β	100.0	91.1	100.0	98.4
E370	C γ	100.0	50.5	100.0	81.0
E370	C δ	99.9	4.3	61.3	34.8
N425	C β	99.9	99.9	74.4	97.7
N425	O	79.3	95.8	80.7	94.9
W427	C α	79.3	98.3	82.0	82.4
W427	C β	20.2	96.9	82.9	77.6
G473	C α	82.6	76.5	82.0	91.5

% Occurrence of inter-atomic contacts between the heavy atoms of CD4 Phe43 phenyl ring and gp120 residues within 4 Å for A) R5P3, B) R5P5, C) X4P3 and D) X4P5. The contact is considered only if the distance between the specific gp120 atom and the center of mass of phenyl ring is less than 5 Å.

Table II

A			B		
GP120	CD4	%Occupancy	GP120	CD4	%Occupancy
D368	R59	99.5	D368	R59	99.8
			D279	K29	76.5
			E102	K22	60.3
C			D		
GP120	CD4	%Occupancy	GP120	CD4	%Occupancy
D368	R59	100.0	D368	R59	100.0
D457	K35	91.5	D279	K29	97.2

% occurrence of inter-molecular salt-bridges between gp120 and CD4 residues for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems, occurring for at least 50% during the last 30 ns. A salt-bridge was considered to exist if the Oxygen-Nitrogen distance is less than 4.5 Å.

Table III

A					B				
Gp120	Atom	CD4	Atom	%Occupancy	Gp120	Atom	CD4	Atom	%Occupancy
Main chain					Main chain				
D368	N	L44	O	56.0	D368	N	L44	O	62
					G366	O	K46	N	59
Side chain					Side chain				
M426	O	S42	OG	76.0	N280	ND2	Q33	O	67
D268	OD1	R59	Nh2	76	D368	OD2	R59	Nh1	53
					D268	OD1	R59	Nh2	52
C					D				
Gp120	Atom	CD4	Atom	%Occupancy	Gp120	Atom	CD4	Atom	%Occupancy
Main chain					Main chain				
G366	O	K46	N	63.0	G366	O	K46	N	68
					D368	N	L44	O	55
Side chain					Side chain				
D368	OD2	R59	Nh2	98.0	D368	OD2	R59	Nh2	98
N280	ND2	Q33	O	83.0	N280	ND2	Q33	O	64
G128	O	Q64	Ne2	76.0	D368	OD1	R59	Nh1	62
D368	OD1	R59	Nh1	70.0					
G130	N	Q64	Oe1	58.0					

% occurrence of inter-molecular hydrogen bonds between gp120 and CD4 for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems, occurring for at least 50% during the last 30 ns. The analysis was done with acceptor-donor distance cutoff of 3Å and acceptor-hydrogen-donor angle cutoff of $180^\circ \pm 60^\circ$.

Figure S1

DCC maps of gp120 for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems. Residues having positive correlation range $0.25 \leq C_{ij} < 0.5$, $0.50 \leq C_{ij} < 0.75$, $0.75 \leq C_{ij} < 1.0$ are shown in green, yellow and red. Residues having negative correlation range $-0.75 \leq C_{ij} < -0.5$ and $-1.0 \leq C_{ij} < -0.75$ are shown in cyan and blue. The portion inside the dotted lines represents V3 loop.

Figure S2

DCC maps of gp120 for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems, calculated over the first 15 ns. Residues having positive correlation range $0.25 \leq C_{ij} < 0.5$, $0.50 \leq C_{ij} < 0.75$, $0.75 \leq C_{ij} < 1.0$ are shown in green, yellow and red. Residues having negative correlation range $-0.75 \leq C_{ij} < -0.5$ and $-1.0 \leq C_{ij} < -0.75$ are shown in cyan and blue.

Figure S3

3D mapping of the cross correlation values on the average structure of gp120 for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems, calculated over the first 15 ns. Each C_α pair having a correlation value of $C_{ij} > 0.70$ is connected by black lines.

Figure S4

DCC maps of gp120 for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems, calculated over the last 15 ns. Residues having positive correlation range $0.25 \leq C_{ij} < 0.5$, $0.50 \leq C_{ij} < 0.75$, $0.75 \leq C_{ij} < 1.0$ are shown in green, yellow and red. Residues having negative correlation range $-0.75 \leq C_{ij} < -0.5$ and $-1.0 \leq C_{ij} < -0.75$ are shown in cyan and blue.

Figure S5

3D mapping of the cross correlation values on the average structure of gp120 for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems, calculated over the last 15 ns. Each C_α pair having a correlation value of $C_{ij} > 0.70$ are connected by black lines.

Figure S6

Motion of the C_{α} atoms of gp120 residues along the first eigenvector vector, obtained by principal component analysis for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems. The arrows represent the magnitude and direction of the motion.

Figure S7

Evolution of the conformational clusters of gp120 structures from A) R5P3, B) R5P5, C) X4P3 and D) X4P5 simulations. The clusters are coloured on the basis of their population size black > red > green > blue > cyan.

Figure S8

Electrostatic surface for the representative conformers from the most populated cluster of A) R5P3, B) R5P5, C) X4P3 and D) X4P5 simulations, calculated omitting the V3 loop. The red and blue surfaces correspond to electrostatic potentials of -2.5 and + 2.5 KT/e, respectively.

Figure S9

Secondary structure evolution of the V3 loop residues as a function of simulation time for A) R5P3, B) R5P5, C) X4P3 and D) X4P5 systems. The grey shaded portion represents the crown region.

Figure S10

2D rmsd in Å (of C_α atoms) calculated for the crown region (residues 11 to 25) of V3 loop conformations extracted from A) R5P3, R5P5 and B) X4P3, X4P5 systems.