

Supplementary information

Insights into molecular mechanism underlying CD4 dependency and neutralization sensitivity of HIV-1: A comparative molecular dynamics study on gp120s from isolates with different phenotypes

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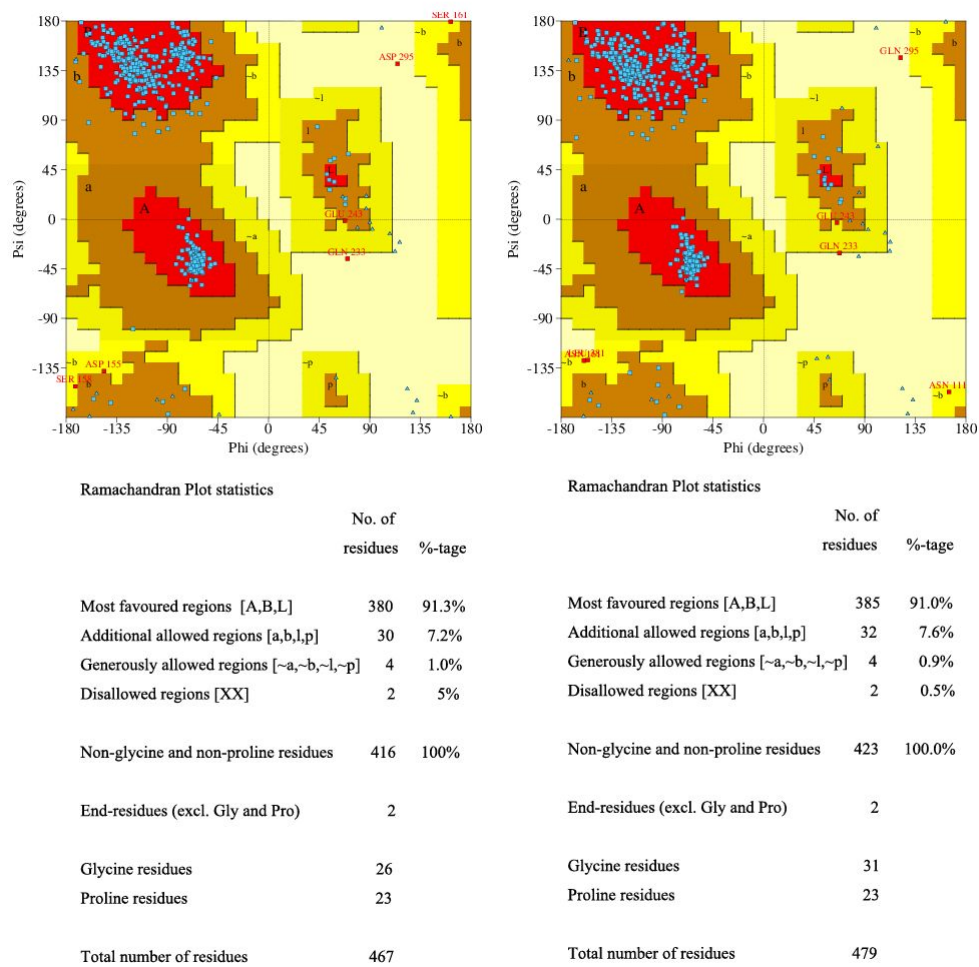


Fig. S1 Ramachandran plots of the constructed structural models of H061.14- (left) and R2-gp120 (right).

Table S1. Validation results of the constructed gp120 structural models (H061.14- and R2-gp120) and template (PDB ID: 5FYJ, chain G).

Structure or model	PROVE ^a	VERIFY3D ^b
5FYJ, chain G	74 (5%)	85.26%
H061.14-gp120	93 (6.1%)	79.66%
R2-gp120	101 (6.5%)	84.76%

^aThe total number of buried outlier protein atoms (percentage is in parentheses).

^bPercent of the residues had an averaged 3D-1D score ≥ 0.2 .

