Supporting Information

Molecular Determinants of Human T-cell Leukemia Virus Type 1 Gag Targeting to the Plasma Membrane for Assembly

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Running Title**:** Determinants of HTLV-1 Gag-membrane interactions

Table S1. Statistics for the HADDOCK clusters of HTLV-1 myr(–)MA$_{99}$ docked to IP$_3$

Cluster	1
Number of structures in cluster	175
HADDOCK score	-126.6 ± 2.5
RMSD from the overall lowest-energy structure	0.3 ± 0.2
Van der Waals energy	18.3 ± 5.9
Electrostatic energy	-781 ± 22
Restraints violation energy	0
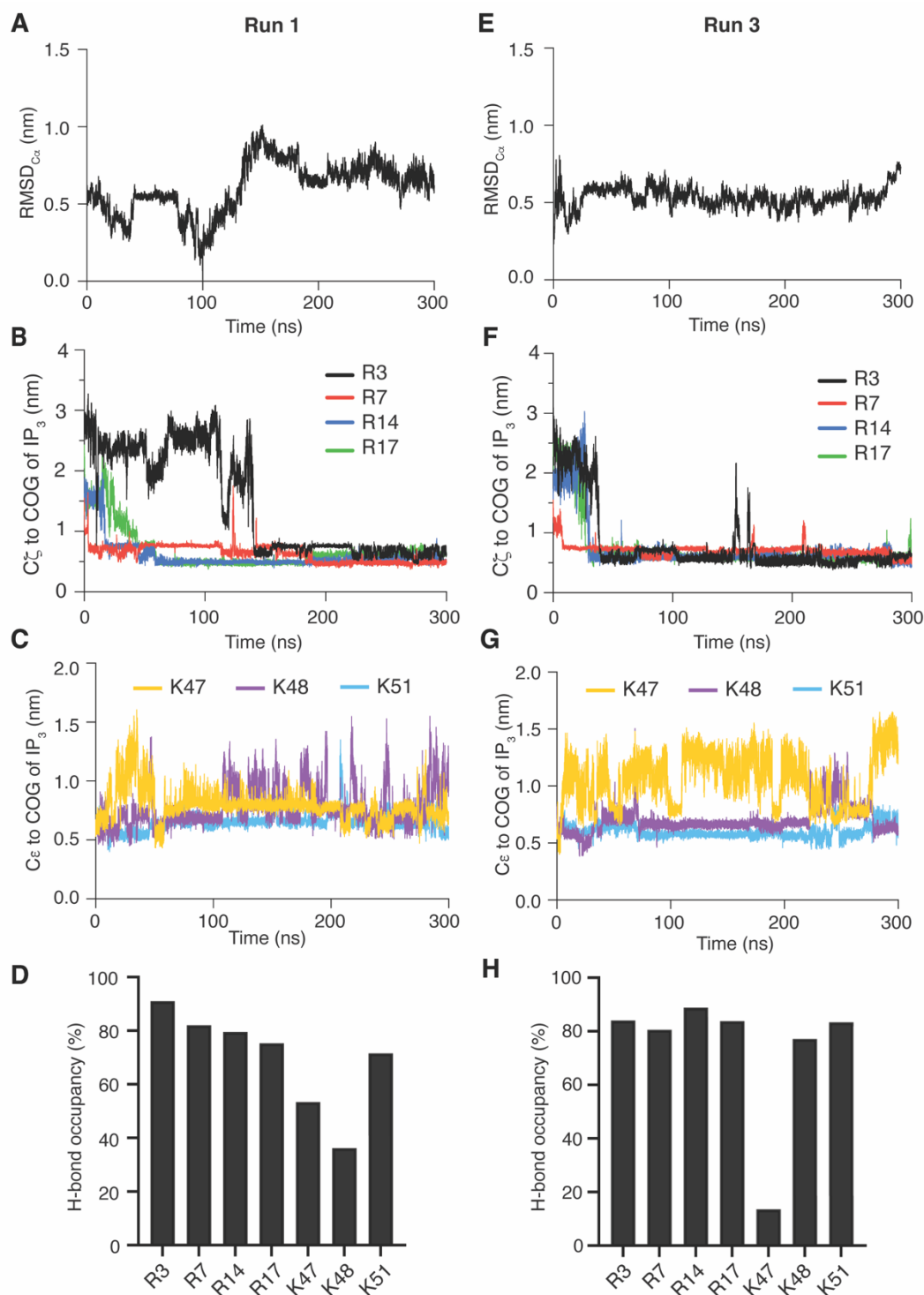
Figure S1. **MD simulations of myr(–)MA$_{99}$ bound to IP$_3$**. (A-D) Analysis of run 1 and (E-F) analysis of run 3 of simulations with identical starting parameters. (A and D) RMSD values of Cα carbons of myr(–)MA$_{99}$ over time. (B and F) Distance of arginine side-chain Cζ carbons to the center of geometry (COG) of IP$_3$ over time. (C and G) Distance of Cε lysine side-chain carbons to the COG of IP$_3$. (D and H) H-bond occupancy of the equilibrated state (distance of all arginines to IP$_3$ < 1nm), analyzed using VMD.

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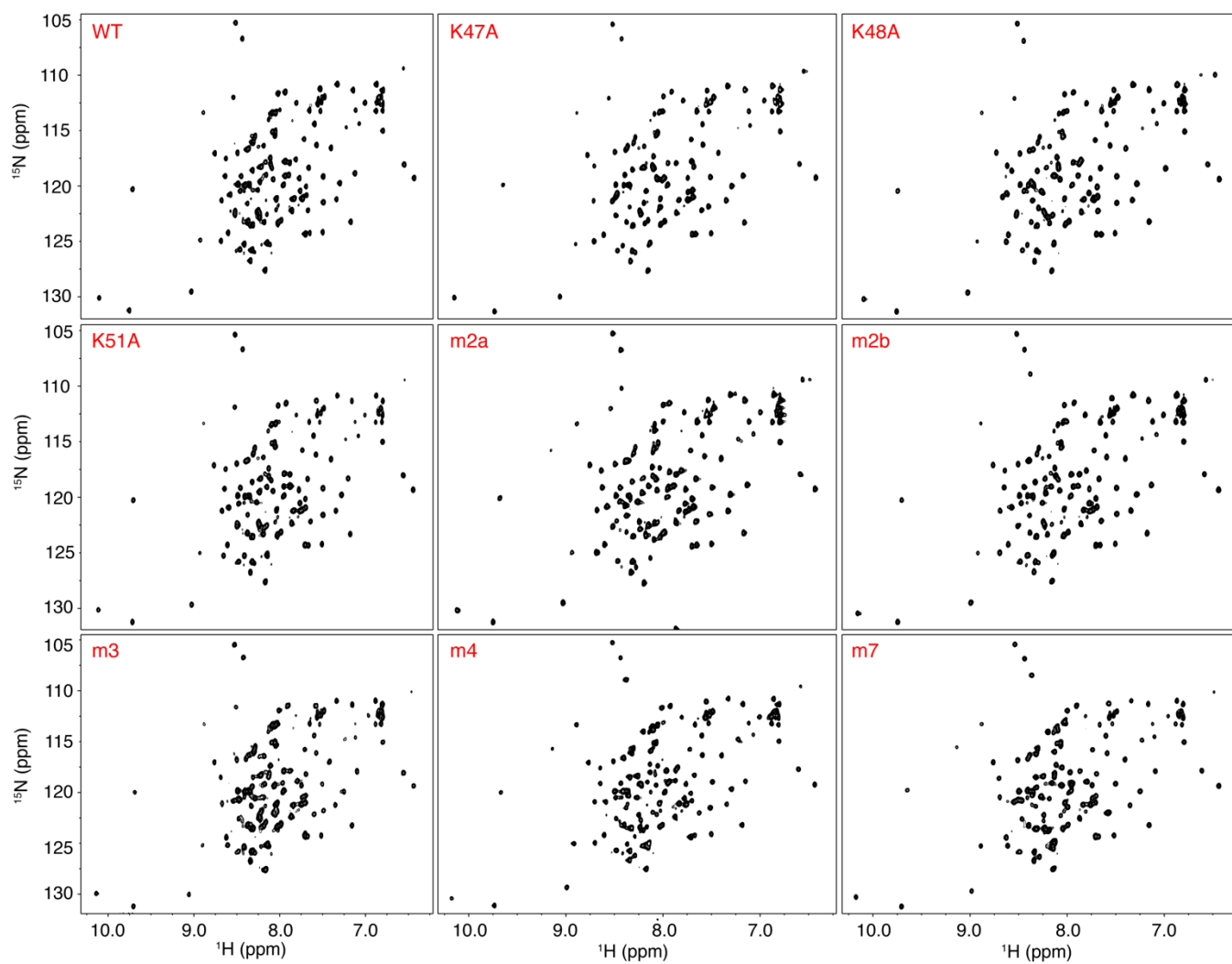
Figure S2. **NMR spectra of HTLV-1 myr(–)MA$_{130}$ mutants**. 2D ^{1}H-^{15}N HSQC spectra of WT and mutant HTLV-1 myr(–)MA$_{130}$ proteins confirming overall fold is maintained. Mutations are indicated in the top left corner of each spectrum.
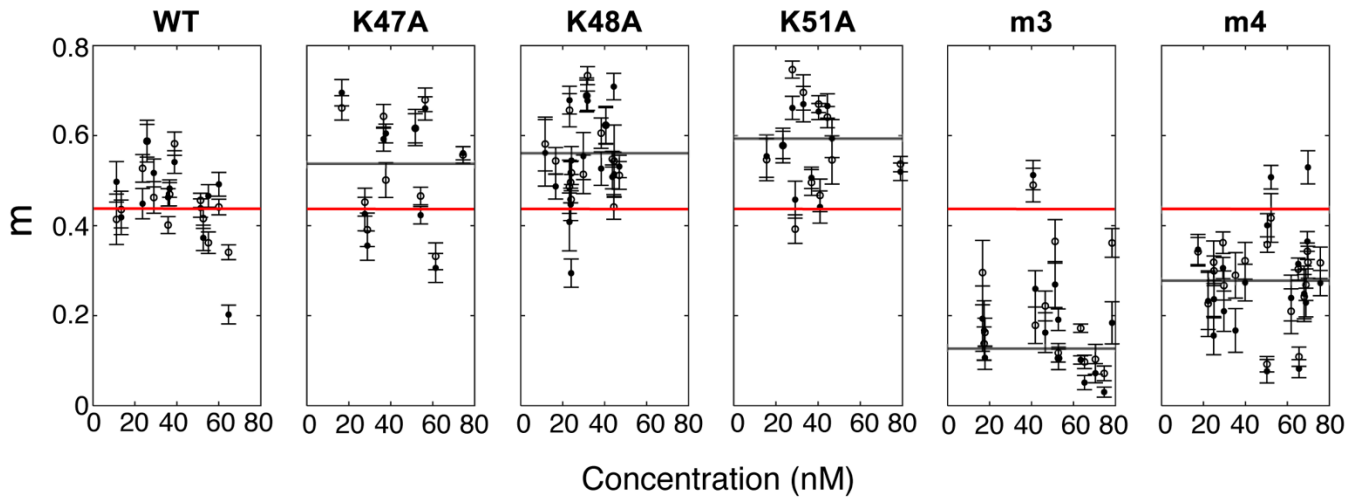
Figure S3. Membrane intensity fractions for WT and Gag mutants. Shown are the membrane intensity fractions (m) for WT and Gag mutants (filled= top PM, unfilled= bottom PM) vs. cytoplasmic Gag concentration. Lines indicate the weighted average m for WT Gag-EYFP (red) and Gag mutants (black). Error bars are the standard error derived from repeated z-scan traces.