Supplementary Information

Graphene-extracted Membrane Lipids Facilitate the Activation of Integrin $\alpha_v\beta_8$

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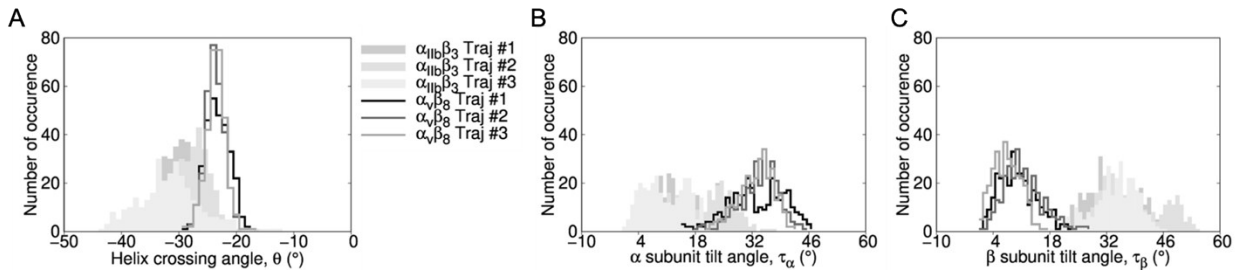

Figure S1. Comparison of the helix crossing angle, the tilt angles of the α and β subunits between the TM domains of integrins $\alpha_v\beta_8$ and $\alpha_{IIb}\beta_3$. We compared the distributions of (A) the helix crossing angle (θ), (B) the tilt angle of the α subunit (τ_α), and (C) the tilt angle of the β subunit (τ_β) in 300 ns simulations. Note that for the $\alpha_v\beta_8$ system (black/dark gray traces), only the first 300 ns out of the total 1.5-μs trajectories were used for the comparison. The ${}^{\tau_{\alpha_v}}$ and ${}^{\tau_{\beta_8}}$ became 32.8° ± 5.5° and 9.1° ± 4.5° after equilibration, respectively. Data from the $\alpha_{IIb}\beta_3$ system are shown in light gray in boxes.

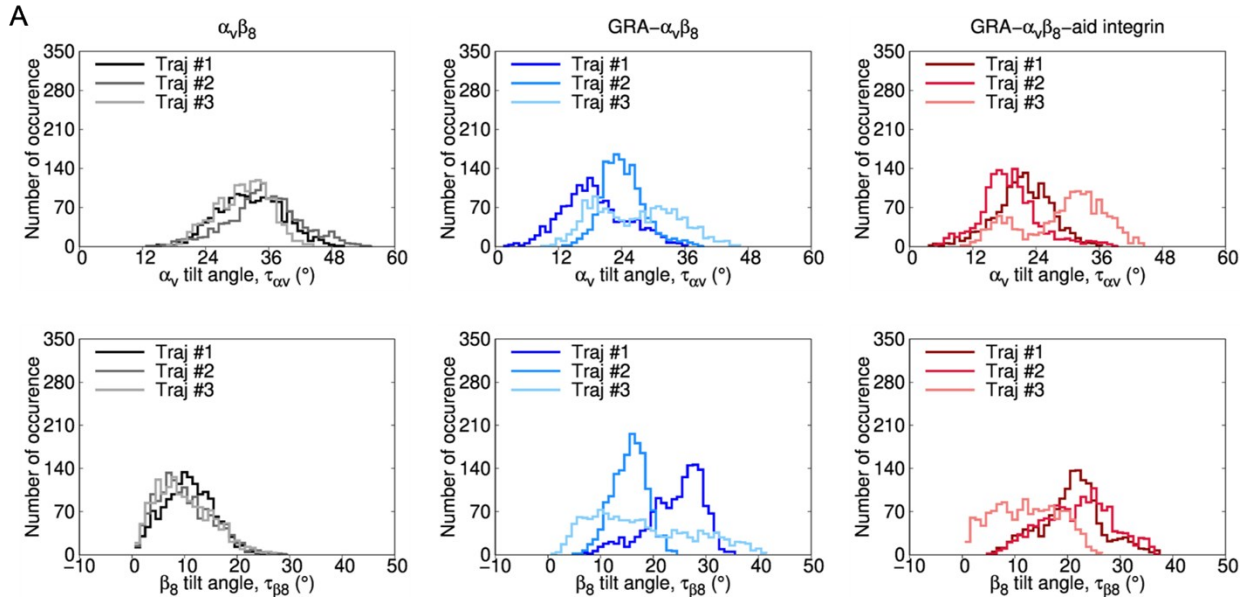

Figure S2. The tilt angles of the TM domains of the α_v and β_8 subunits in the three independent trajectories with and without a graphene nanosheet. The distributions of the α_v tilt angle (${}^{\tau_{\alpha_v}}$, top) and the β_8 tilt angle (${}^{\tau_{\beta_8}}$, bottom) during the 1.5-μs simulations for (A) the $\alpha_v\beta_8$

system, (B) the GRA-$\alpha_v\beta_8$ system, and (C) the GRA-$\alpha_v\beta_8$-aid integrin system. The color code is the same as that in Figure 2.

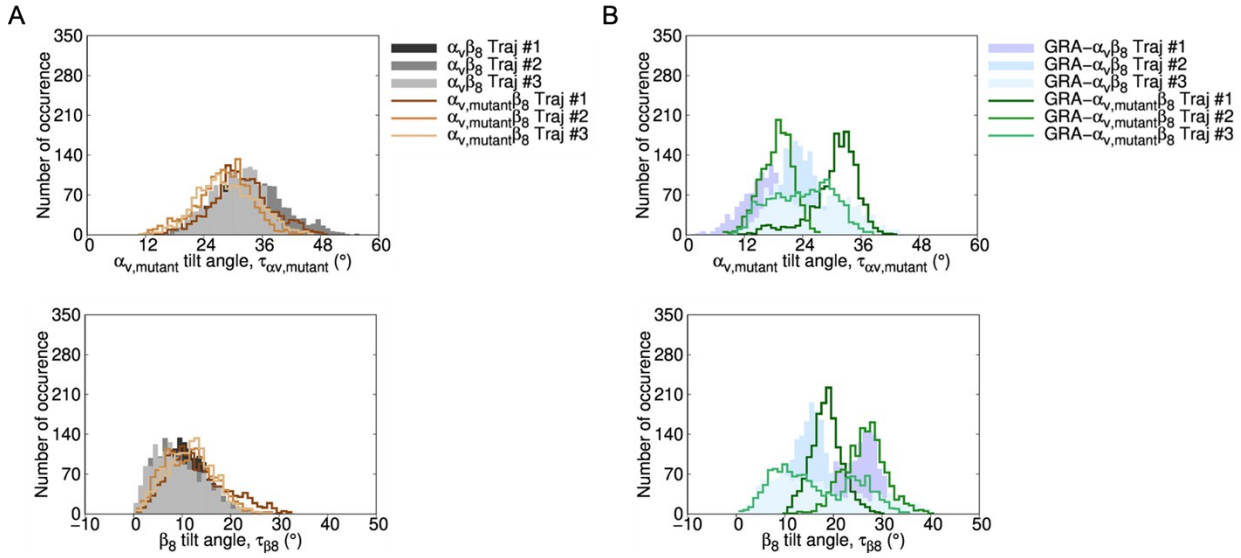

Figure S3. The tilt angles of the TM domains of the $\alpha_{v,mutant}$ and β_8 subunits in the three independent trajectories with and without a graphene nanosheet. The distributions of the $\alpha_{v,mutant}$ tilt angle ($\tau_{\alpha_{v,,mutant}}$, top) and the β_8 tilt angle (τ_{β_8}, bottom) during the 1.5-μs simulations for (A) the $\alpha_{v,mutant}\beta_8$ system and (B) the GRA-$\alpha_{v,mutant}\beta_8$ system. The color code is the same as that in Figure 7. Data from the $\alpha_v\beta_8$ system (gray boxes) and the GRA-$\alpha_v\beta_8$ system (blue boxes) are shown for reference.

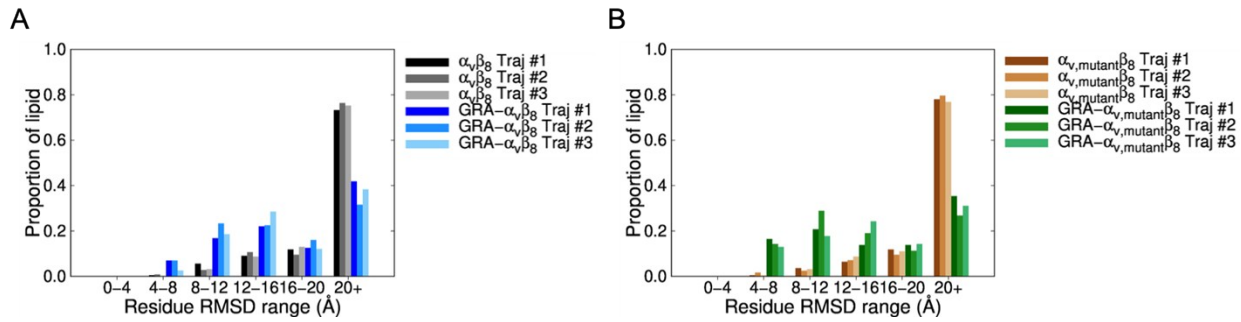

Figure S4. Mobility of the lipids in the wild-type and mutant integrin-membrane complexes with and without a graphene nanosheet. We calculated the residue RMSD of each lipid in (A) the

wild-type systems ($\alpha_v\beta_8$ and GRA-$\alpha_v\beta_8$) and (B) the mutant systems ($\alpha_{v,mutant}\beta_8$ and GRA-$\alpha_{v,mutant}\beta_8$). The total number of lipids in each trajectory was normalized to 1.