Supporting Information

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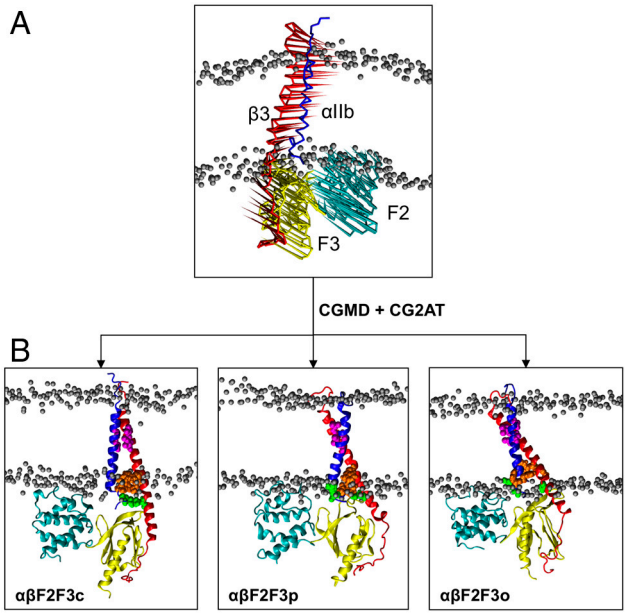

Fig. S1. Simulations of the αIIbβ3 transmembrane (TM) helix dimer in complex with talin F2-F3. (*A*) Relative movements of the β, F2, and F3 domains in the αβ-F2F3-CG simulation. The displacements of F2 (cyan), F3 (yellow), and the β TM helix (red) over the course of the simulation are shown as arrows mapped, the lengths of which represent the displacements. For this calculation, the αIIb TM coordinates were superimposed. (*B*) Initial configurations of the atomistic simulations of αβ-F2F3c-AT ("closed"; see Table 1 for details and nomenclature used for simulations), αβ-F2F3p-AT ("partial"), and αβ-F2F3o-AT ("open"); these configurations were obtained by clustering the coarse-grained–molecular dynamics simulations and converting them to AT resolution. The color scheme is outer membrane clasp (magenta), inner membrane clasp (orange and green), F2 (cyan), F3 (yellow), β TM (red), and αIIb TM (blue).

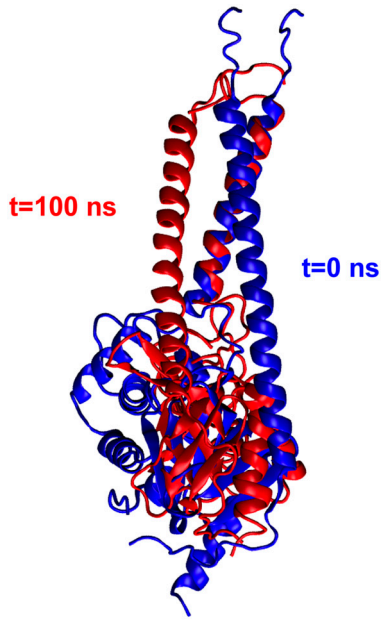

Fig. S2. Alignment of the αIIb subunit from the initial F2-F3 + αIIbβ_3 model (blue) and at the end of the αβ-F2F3o-AT (red) simulation, demonstrating the rotation of the β subunit perpendicular to the bilayer normal.

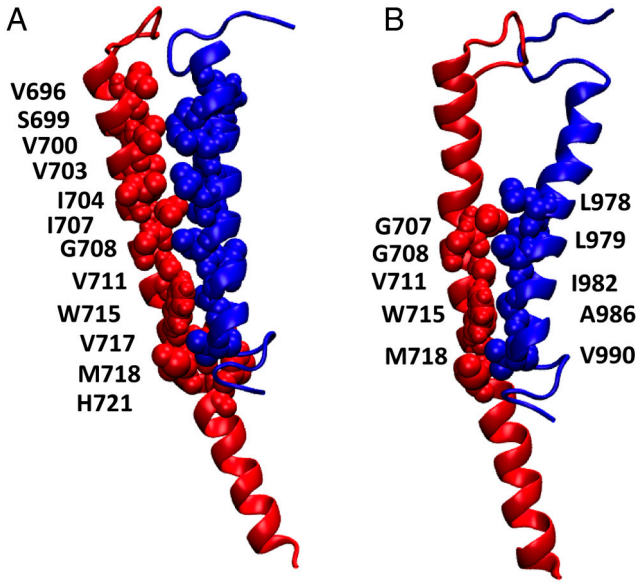

Fig. S3. Interface between the αIIb (blue) and the β3 (red) TM domains at (*A*) the beginning and (*B*) the end of the αβ-F2F3o-AT (open) simulation. The residues that make up the interaction surface in both subunits are shown in van der Waals format. The F2-F3 domains are omitted for clarity.

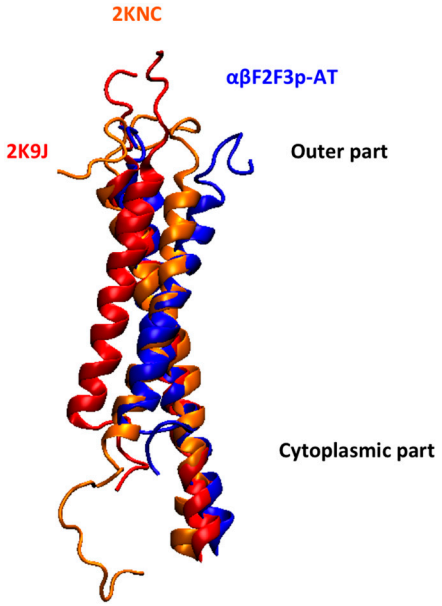

Fig. S4. Superposition of the β TM region (residues 697–726) from the αβ-F2F3p-AT simulation (blue) with the αIIβ/β3 (2KNC,orange) and the αIIβ/β3 (2K9J, red) structures. The alignment shows that the αIIβ/β3 (2KNC) structure is similar to the partial disrupted state (the αβ-F2F3p-AT simulation) and could therefore correspond to an intermediate state. The F2-F3 domain is omitted for clarity.

Other Supporting Information Files

Dataset S1 (TXT)

Dataset S2 (TXT)