

Xiong et al., <http://www.jcb.org/cgi/content/full/jcb.200905085/DC1>

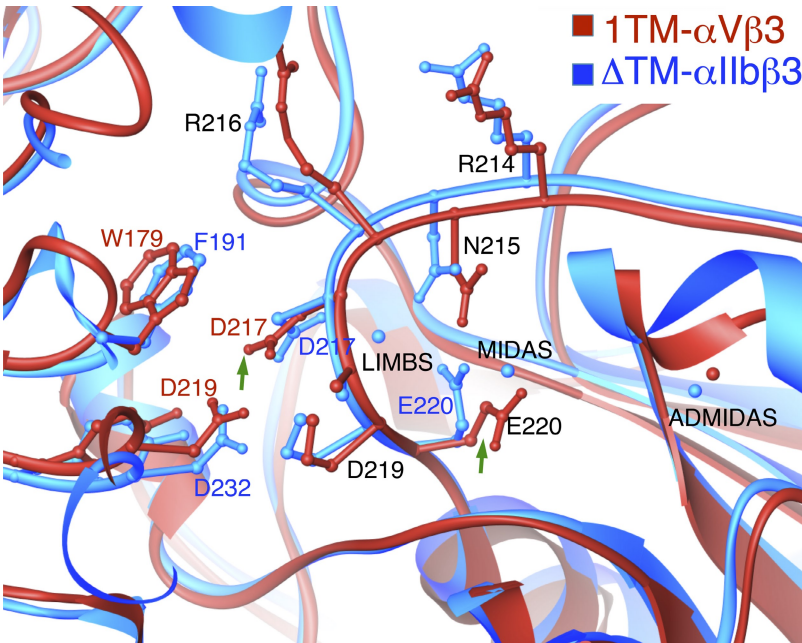


Figure S1. **Ribbon diagram of the MIDAS face in the 1TM- α V β 3 and Δ TM- α IIb β 3 structures.** The main chains of the corresponding β A structures from 1TM- α V β 3 and Δ TM- α IIb β 3 were superposed using Matchmaker in Chimera. ADMIDAS (adjacent to MIDAS) metal is present in both, but LIMBS and MIDAS metals are lacking in 1TM- α V β 3. The side chains of residues in the MIDAS region are superposable except for D217 and E220 (green arrows), which have moved inwards in Δ TM- α IIb β 3. In unliganded 1TM- α V β 3, the side chain of D217 points outward (away from LIMBS) into a polar pocket composed of Y164, W179, D219, and Y221 of α V. In the unliganded Δ TM- α IIb β 3 structure, α V's W179 (which is invariant in all other α subunits except α IIb) is replaced with the hydrophobic residue F191, likely forcing the D217 side chain to point away (and toward LIMBS) to avoid a clash.

Table S1. **Elution characteristics of 1TM- α V β 3 and its complex with intact plasma FN**

Divalent cations present	Preparation	Elution volume \pm SD	Elution coefficient \pm SD	Stokes radius \pm SD	<i>n</i>
		<i>ml</i>		<i>nm</i>	
Mn	1TM	11.58 \pm 0.061	0.229 \pm 0.004	6.08 \pm 0.23	9
Mn	FN	9.98 \pm 0.013	0.127 \pm 0.001	8.19 \pm 0.13	5
Mn	1TM-FN ^a	9.02 \pm 0.009	0.066 \pm 0.001	10.12 \pm 0.07	5
Ca/Mg	1TM	12.06 \pm 0.030	0.261 \pm 0.002	5.60 \pm 0.260	9
Ca/Mg	FN	9.99 \pm 0.020	0.129 \pm 0.001	8.35 \pm 0.121	4
Ca/Mg	1TM-FN	9.91 \pm 0.070	0.123 \pm 0.002	8.18 \pm 0.127	5

A molar excess of 1TM- α V β 3 (1TM) was incubated with human plasma FN in physiological buffered saline containing 0.2 mM Mn²⁺ (Mn) or 1 mM Ca²⁺ + 1 mM Mg²⁺ (Ca/Mg) before resolution by molecular sieve chromatography. The proteins eluted as discrete well-resolved peaks and were the only proteins detected on the chromatograms. The Stokes radii of the eluted proteins were calculated by comparison with defined standards.

^aThe 1TM-FN complex was larger than thyroglobulin, the largest standard available (Stokes radius, 8.5 nm), and the radius has been estimated by interpolating the standard curve. Differences between 1TM Mn versus 1TM Ca/Mg, FN versus 1TM-FN, and 1TM-FN Mn versus 1TM-FN Ca/Mg were significant ($P < 0.0001$ in each pair); differences between FN Mn versus FN Ca/Mg were not significant.