Supporting Information

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SI Methods

The highest-resolution structures available for both conformations of P-selectin (PDB ID codes 1G1Q and IG1S) and the bent conformation of E-selectin (PDB ID code IGIT) (1) were submitted to the MOLPROBITY server (2), which found them, after flips described below, of average structural quality for their resolution. All Asn, Gln, and His flips suggested by MOLPROBITY were accepted, and the resulting downloaded coordinate files were used for analysis and figure preparation. Flips were strongly preferred for Asn-21 in chain A, Asn-83 in chains A and B, and His-108 in chains A and B of IG1S. At typical resolution, crystallographic data cannot distinguish between 180° flipped orientations of the Asn and Gln amides and the His side chain. However, the correct orientation can be established stereochemically (2). The flip at Asn-83 removes a large, 0.8-Å clash and adds a strong 2.8-Å hydrogen bond between OD1 of Asn-83 and N of Glu-88 that is important for the hydrogen-bonding network around the Ca^{2+} binding site. There is also an Asn-82 residue, and to avoid confusion it should be noted that in Fig. 6*C* and in the text of ref. 1, Asn-82 is erroneously called Asn-83. Structures were viewed with COOT (3), with close contacts and hydrogen bonds represented by using the probe clashes plug-in of MOLPROBITY. Figures were prepared with PYMOL (Delano Scientific). Superposition and distance measurements were with the align and distance commands of PYMOL or MALIGN and MALIGN3D commands of MODELLER (4) followed by export of the log file to EXCEL.

For Fig. 7, because sialyl $Lewis^X$ soaked into bent E-selectin crystals binds similarly to the sialyl $Lewis^X$ component of PSGL-1 in extended P-selectin crystals (1), we modeled liganded, bent P-selectin by adding PSGL-1 to the bent conformation after superposition on the lectin domain of the extended conformation. Liganded bent and extended models were superimposed by using N and Cα atoms of P-selectin residue 157 and Cα atoms of PSGL-1 residues 17 and 18 to obtain the orientations shown in Fig. 7.

1. Somers WS, Tang J, Shaw GD, Camphausen RT (2000) Insights into the molecular basis of leukocyte tethering and rolling revealed by structures of P- and E-selectin bound to SLeX and PSGL-1. *Cell* 103:467–479.
2. Davis IW, *et al.* (2007) MolProbity: All-atom contacts and structure validation for proteins and nucleic acids. *Nucleic Acids Res* 35:W375–W383.
3. Emsley P, Cowtan K (2004) Coot: Model-building tools for molecular graphics. *Acta Crystallogr D* 60:2126–2132.
4. Eswar N, *et al.* (2003) Tools for comparative protein structure modeling and analysis. *Nucleic Acids Res* 31:3375–3380.