Supplemental Video 1. <http://www.prism.gatech.edu/~jl308/v01_pbent.mpg>
Stability of the closed-angle conformation of P-selectin. Comparison of the simulated structure (cyan) with the crystal structures of the closed-angle (mauve, PDB code 1G1R) and open-angle (blue, PDB code 1G1S) P-selectin (20) after deleting the PSGL-1. The lectin domains (residues 1-120) of the crystal structures and of the simulated structure in each frame were aligned through the backbone atoms, while the EGF domains were unconstrained. Over the 5 ns free dynamics simulation time, the simulated structure fluctuated about its starting structure - the closed-angle crystal structure. The golden sphere depicts the Ca^{2+} ion coordinated by the lectin domain. The movie was generated with VMD (25)

Supplemental Video 2. <http://www.prism.gatech.edu/~jl308/v02_pstraight.mpg>
Same as Supplemental Video 1 except that the starting structure for simulation was the open-angle crystal structure.

Supplemental Video 3. <http://www.prism.gatech.edu/~jl308/v03_slex.mpg>
SMD simulation of P-selectin lectin-EGF domain in complex with sLe^x. The O1 atom of sLe^x residue GlcNAc (ice-blue) was pulled through a spring (70 pN/Å) that moved at a constant speed (10 Å/ns) and the C_α atom of EGF Gly147 (orange) was constrained.

Supplemental Video 4. <http://www.prism.gatech.edu/~jl308/v04_LecEGF.mpg>
SMD simulation of P-selectin lectin-EGF domain in complex with N-terminal segment of PSGL-1. The C_α atom of PSGL-1 Pro18 (ice-blue) was pulled through a spring (70 pN/Å) that moved at a constant speed (10 Å/ns) and the C_α atom of EGF Gly147 (orange) was constrained.

Supplemental Video 5. <http://www.prism.gatech.edu/~jl308/v05_LecOnly.mpg>
SMD simulation of P-selectin lectin domain in complex with N-terminal segment of PSGL-1. The C_α atom of PSGL-1 Pro18 (ice-blue) was pulled through a spring (70 pN/Å) that moved at a constant speed (10 Å/ns) and the C_α atom of lectin Ala120 (orange) was constrained.