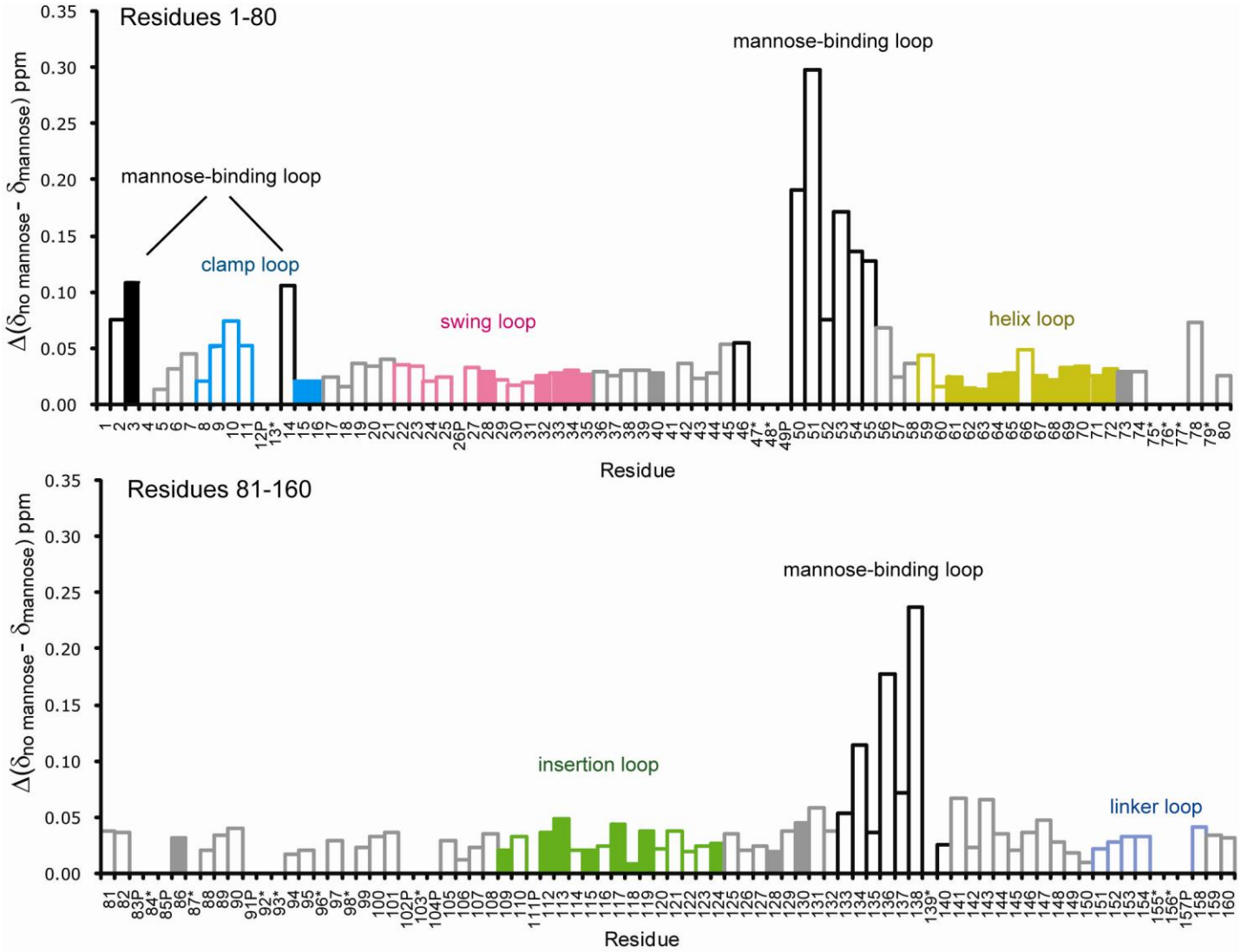

Figure S1: NMR shift differences of residues and structural regions, related to Figure 3. The chemical shift differences between the mannose-free and mannose-bound forms, $\Delta(\delta_{\text{no mannose}} - \delta_{\text{mannose}})$ ppm versus residue number are shown in this bar graph. Δ ppm was computed from the absolute, weighted average of backbone amide proton and nitrogen chemical shift differences as follows: $(((\Delta\delta_H)^2 + (\Delta\delta_N/5)^2)/2)^{1/2}$. Amino acids in the clamp loop, swing loop, helix loop, insertion loop, and linker loop are colored according to the color scheme used in Figure 1, while those in the mannose-binding loops (1-3, 12-14, 46-55, and 133-140) are colored black, and the remainder gray. The main and split sheets are not colored purple and orange in this figure. Residues marked with an asterisk indicate unassigned residues and those marked with a P indicate prolines, with no data available for either of these sets. The solid bars indicate residues that have NH atoms that form state-dependent backbone hydrogen bonds (backbone hydrogen bonds that are found in one crystal structure state but not the other). Note that residues in the mannose-binding loops exhibit chemical shift differences significantly above the mean, which is expected since the difference between the two experiments is the presence of mannose. In contrast, residues in the five loops that change between the crystal structure states, including those involved in state-dependent backbone hydrogen bonds, experience below-average chemical shift perturbations. The only exception is residue 3, which is also in a mannose-binding loop. Even the largest shift perturbations observed in this comparative experiment are not large enough to be due to a state-dependent backbone hydrogen bond. It can therefore be concluded that the conformational changes observed in the comparison of the two crystal structures are not observed in solution by NMR with the addition or removal of mannose from the isolated lectin domain.

Supplemental Movie 1: The *Escherichia coli* fimbrial adhesive protein, FimH, mediates shear-dependent binding to mannosylated surfaces via force-enhanced allosteric catch bonds. This video shows the underlying structural changes causing this behavior. When force is applied and the autoinhibitory pilin domain is pulled away, the mannose-binding lectin domain switches from a twisted compressed conformation to an untwisted elongated conformation, much like a finger trap toy. The initial conformation shown here is the lectin domain, or the first 158 amino acids, of the X-ray structure of FimH in the low affinity compressed state (chain H in PDB code 3JWN). The final conformation contains the lectin domain in the high affinity state (chain A in PDB code 1UWF). This 'morph movie' is made with the morph server (Krebs and Gerstein, 2000) using a combination of interpolation and minimization. The atomic coordinates of the morph are freely available through the morph server web site.

Krebs, W. G., and Gerstein, M. (2000). The morph server: a standardized system for analyzing and visualizing macromolecular motions in a database framework. Nucleic Acids Res *28*, 1665-1675.