SUPPLEMENTARY FIGURE LEGENDS

Supplementary Figure 1. K_d measurements. Dissociation constant for the ubiquitin-STAM I UIM interaction was determined from the changes in chemical shift of the amides of Ala 46, Gly 47 and Ile 13. The data was fitted to eq. 1 to obtain the K_d value. A dotted line represents the ligand concentration used in the backbone relaxation experiments and hydrogen bond experiments.

Supplementary Figure 2. Comparison of the chemical shift changes in ubiquitin upon UIM interaction. a) Superimposed graphs for the chemical shift changes in $\Delta\delta$HN (o), $\Delta\delta C_\alpha$ (o) and $\Delta\delta$CO (o) chemical shifts for all the residues in ubiquitin upon UIM binding. b) A ribbon representation displaying one ubiquitin molecule bound to a UIM, highlighting residues (colored red) that show changes in $\Delta\delta$HN and $\Delta\delta$CO chemical shifts only and not $\Delta\delta C_\alpha$.

Supplementary Figure 3. Predicted *vs*. experimental C_α and C_β chemical shift changes. The predicted differences for a) C_α chemical shifts and b) C_β chemical shifts plotted as a function of experimentally observed chemical shift changes. Chemical shifts were predicted using Sparta+[52] based on the PDB entry 1UBQ (free ubiquitin) and 2D3G (ubiquitin complexed to UIM). The closed and open symbols represent the two ubiquitin molecules, A and B, respectively, both complexed to the same UIM in the entry 2D3G.

Supplementary Figure 4. Backbone hydrogen bonds in the crystal structures. Hydrogen bonds in the 66 ubiquitin molecules, present in 29 PDB entries of ubiquitin complexes (1P3Q, 1S1Q, 1UZX, 1WR6, 1WRD, 2C7M, 2C7N, 2D3G, 2FIF, 2G45, 2GMI, 2HD5, 2IBI, 2OOB, 2QHO, 2QHE, 2ZNV, 3A9J, 3A9K, 3BY4, 3C0R, 3DVG, 3I3T, 3K9O, 3LDZ, 3NHE, 3PRM, 3PRP, 3OJ3) with a resolution 2.6 Å or better. The graphs have been arranged in the order of degree

of perturbation, with the ones displaying least perturbations appearing first. The value displayed at the top right indicates standard deviation for the hydrogen bond in all 69 molecules. Hydrogen bond distances were measured using Chimera[53].

Supplementary Figure 5. Backbone conformational changes in the entry 2ZNV. Changes in the backbone in the four ubiquitin molecules present in the entry 2ZNV are shown, in blue, cyan, magenta and green. The molecule colored cyan displays changes in backbone not only in the β_1-β_2 loop, but also β_3 strand, β_4 strand as well as β_3-α_2 loop.