SUPPLEMENTARY MATERIAL: Highly conserved glycine 86 and arginine 87 residues contribute differently to the structure and activity of the mature HIV-1 protease.

Rieko Ishima[a,*], Qinguo Gong[a], Yunfeng Tie[b], Irene T. Weber[b], John M. Louis[c]

[a] Department of Structural Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA 15260
[b] Department of Biology, Molecular Basis of Disease Program, Georgia State University, Atlanta, GA 30303
[c] Laboratory of Chemical Physics, National Institute of Diabetes, Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD 20892

[*] Corresponding author: Rieko Ishima (Email: ishima@pitt.edu)

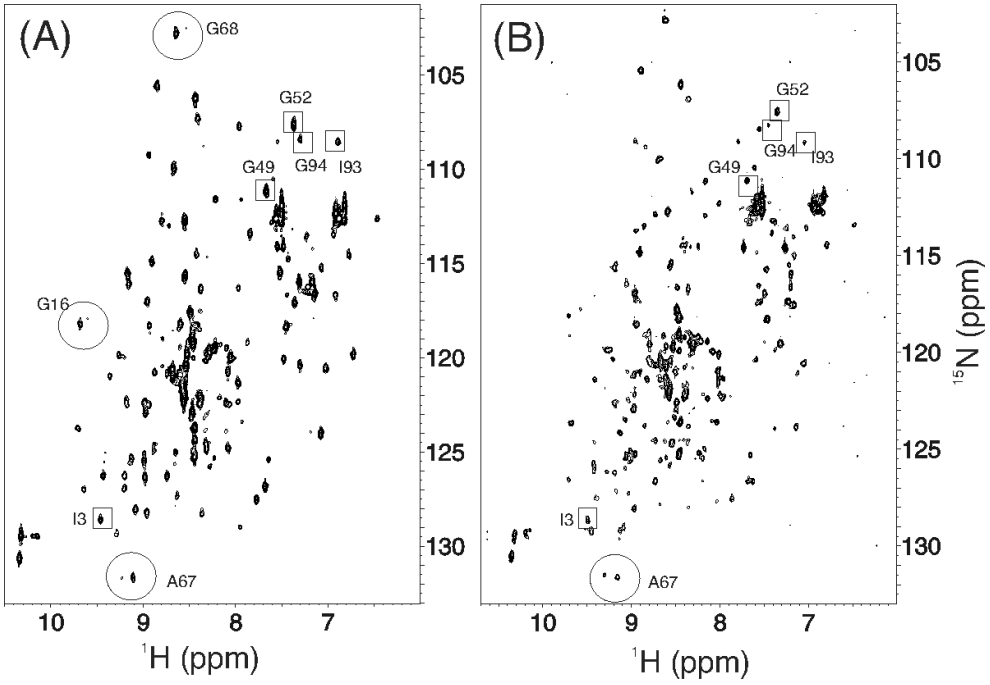

Figure S1. ^{15}N-^{1}H HSQC spectra of (A) PR_{G86A} at 7 μM and (B) PR_{G86S} at 4 μM concentration (calculated as a dimer). Characteristic peaks for dimers are shown by squares. Peaks used to estimate the dimer-dissociation constants are marked by circles, in which two peaks are observed, a major peak for dimer and a minor peak for monomer. The assignments shown in these figures are tentative based on the similarity of the signals to PR. Sensitivity and resolution of the data were limited by the life-time of the samples (< overnight).

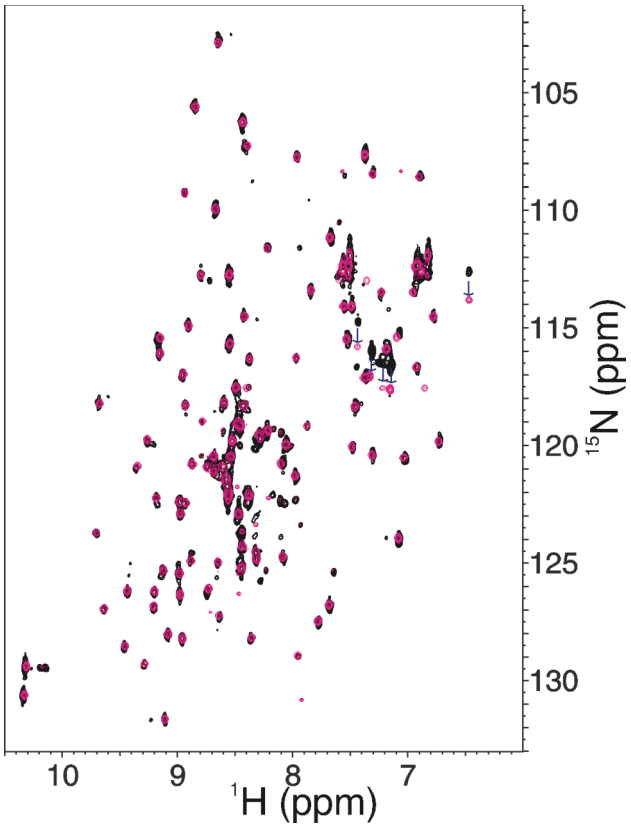

Figure S2. Overlay of the ^{15}N-^{1}H HSQC spectra of PR_{G86A} in the absence (black) and the presence (pink) of the 20 fold excess substrate IV. The spectra were recorded at 15-20 μM dimer concentrations. Systematic shifts of the peaks due to different spectral widths are shown by arrows. There were no significant changes in the peak positions upon substrate titration.