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Supplemental information

Pressure, motion, and conformational entropy in molecular recognition

by proteins

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Supplementary Material

Pressure, motion and conformational entropy in molecular recognition by proteins

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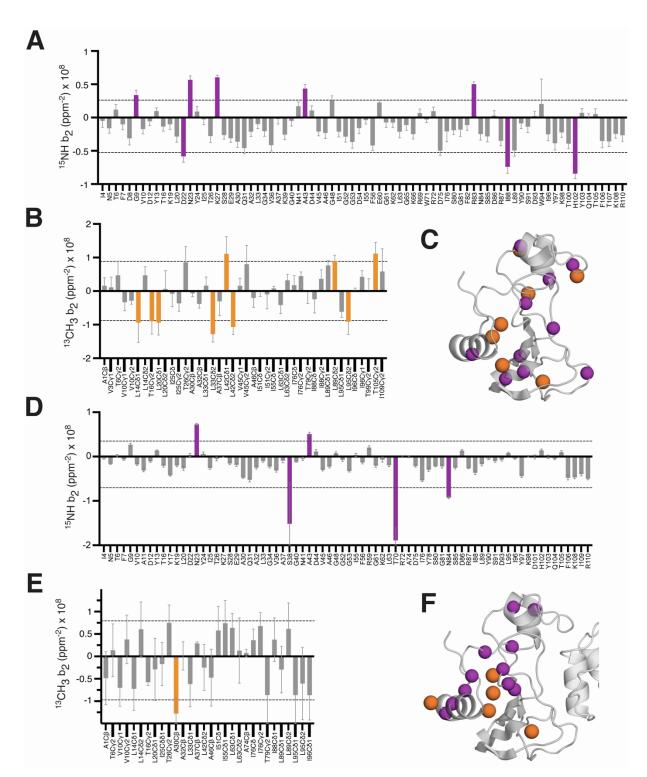


FIGURE S1 Pressure sensitivity of the ¹⁵N amide NH and ¹³C methyl CH₃ chemical shifts in free and complexed barnase. Fitted quadratic coefficients (b₂) of the pressure dependence of the gyromagnetic weighted chemical shifts of (A) amide NH crosspeaks in ¹⁵N-HSQC and (B) methyl crosspeaks in ¹³C-spectra of free barnase as a function of pressure. Error bars represent one standard deviation as derived from the fitting. Sites having quadratic coefficients greater than 1.5 standard deviations from the mean are highlighted on a ribbon representation of the ambient pressure structure (C). Amide and methyl groups are indicated as purple and orange spheres respectively. The pressure sensitivity of amide and methyl chemical shifts of barnase in complex with barstar is similarly shown (D, E, F).

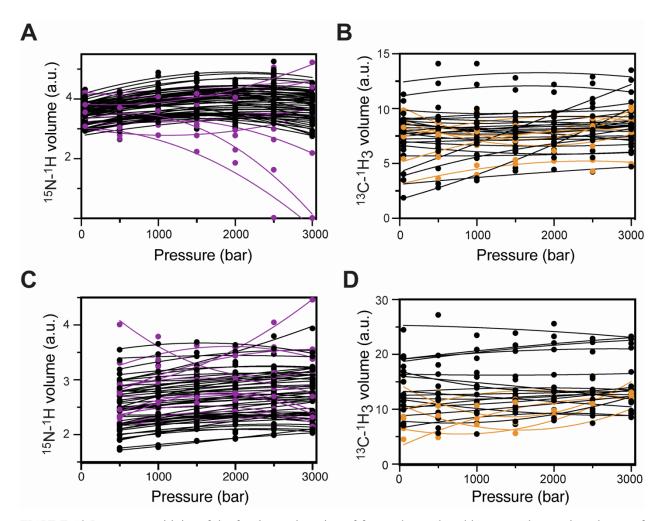


FIGURE S2 Pressure sensitivity of the fast internal motion of free and complexed barnase. Changes in volumes of (A) amide NH crosspeaks in ¹⁵N-HSQC and (B) methyl crosspeaks in ¹³C-spectra of free barnase and (C) amide NH crosspeaks in ¹⁵N-HSQC and (D) methyl crosspeaks in ¹³C-spectra of barnase in complex with barstar as a function of pressure. Lines fitted to a second order Taylor expansion are shown. Sites having b₂ coefficients greater than 1.5 standard deviations from the mean are indicated as purple and orange lines for amide and methyl crosspeaks, respectively. Fitted second order coefficients (b₂) are summarized in Fig. 3 of the main text.