The measurement of binding affinities by NMR chemical shift perturbation

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Supplementary Information

The SI consists of plots of fitted K_d values for barnase and SH3b, before and after filtering of the data, corresponding to the data shown for HisJ in Figs. 4 and 5. In separate Excel files we provide the raw chemical shift data from the titrations together with fitted values, including residues considered to have K_d values significantly larger or smaller than the mean for each protein.

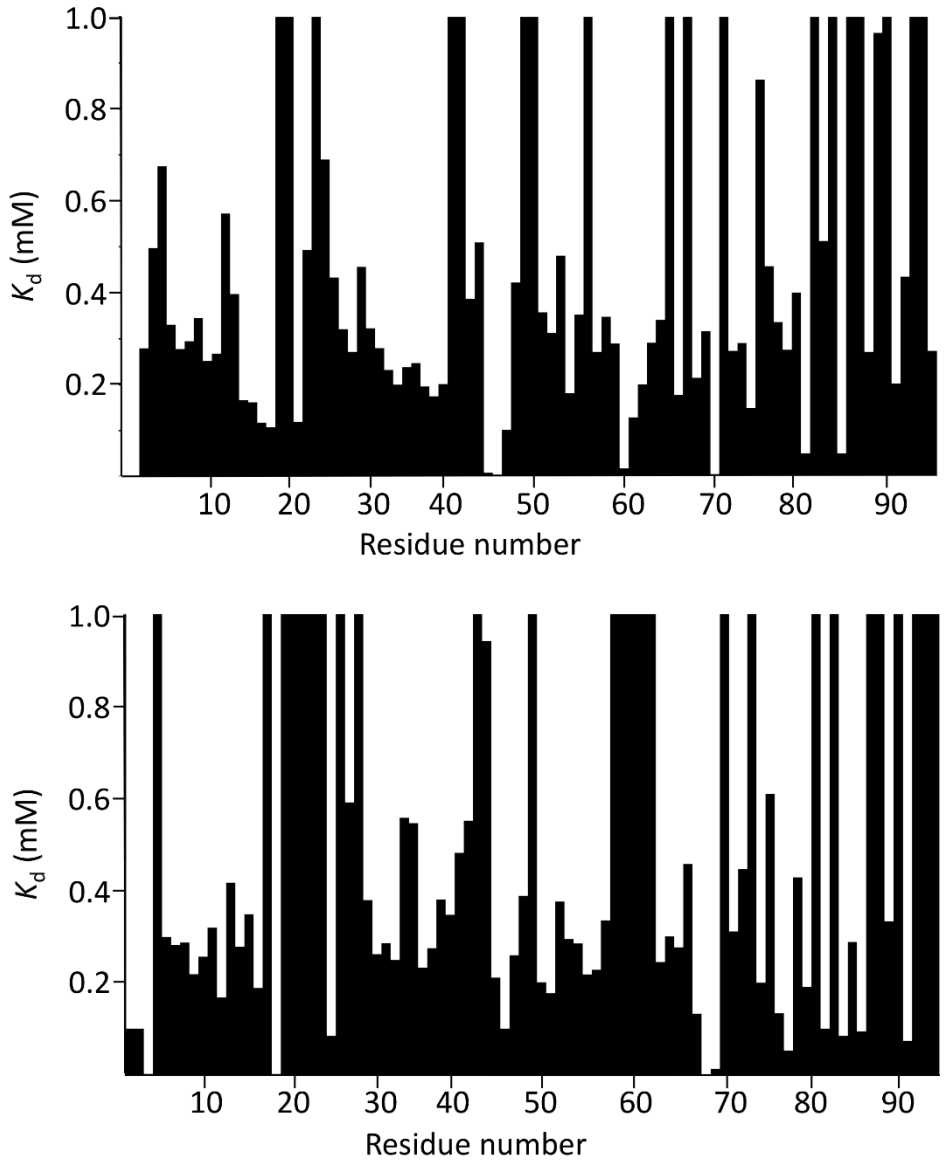

Fig. S1 K_d values fitted for SH3b binding to YG_5, for (top) ^1H (bottom) ^{15}N. Data are shown for all residues that could be fitted. A small number are not shown, mainly because of overlap or because they are prolines. Note that the K_d values are truncated at 1.0 mM: many are much larger than this.

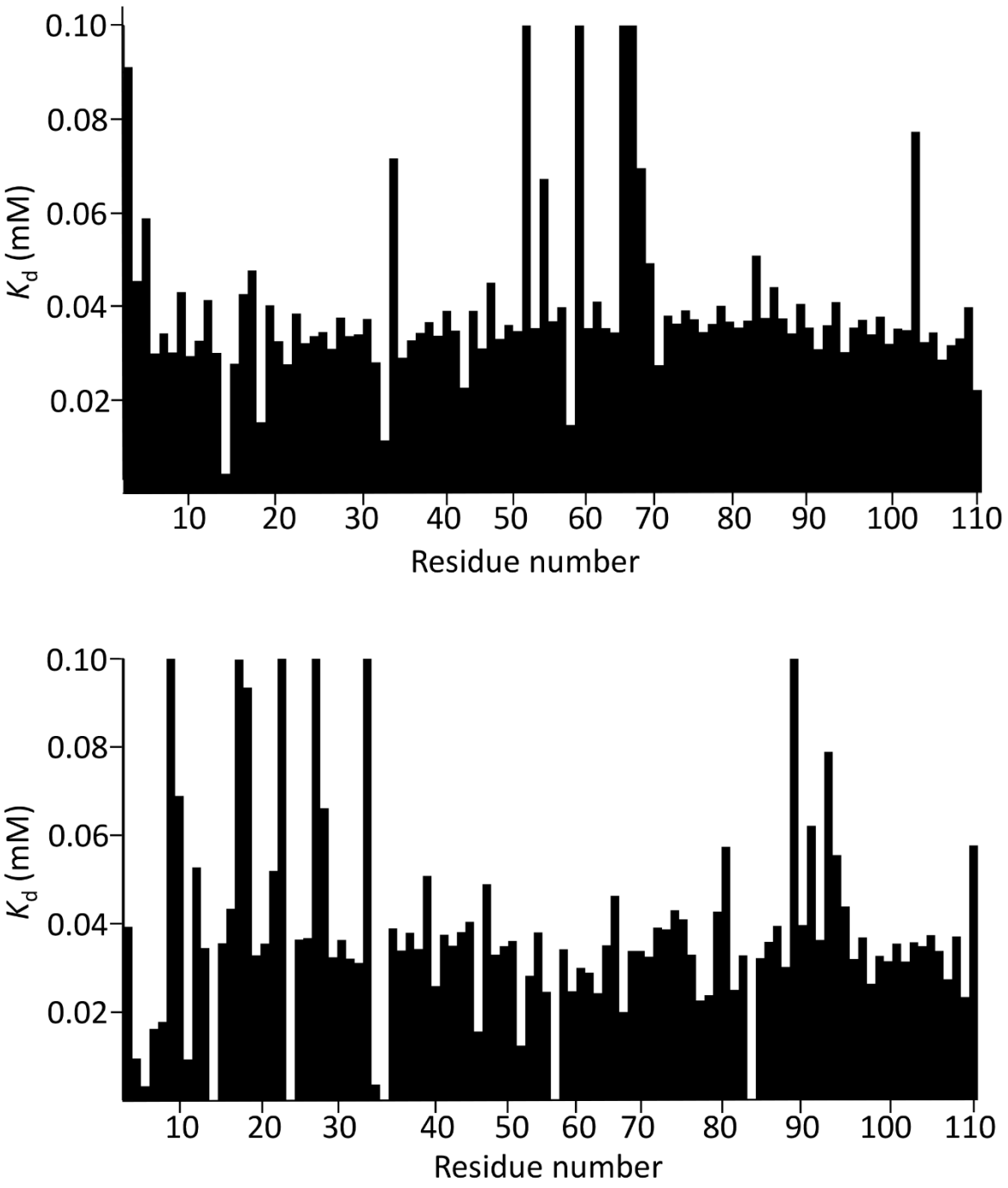

Fig. S2 K_d values fitted for barnase binding to d(CGAC), for (top) ^{1}H (bottom) ^{15}N. Data are shown for all residues that could be fitted. A small number are not shown, mainly because of overlap. Note that the K_d values are truncated at 0.1 mM: many are much larger than this.

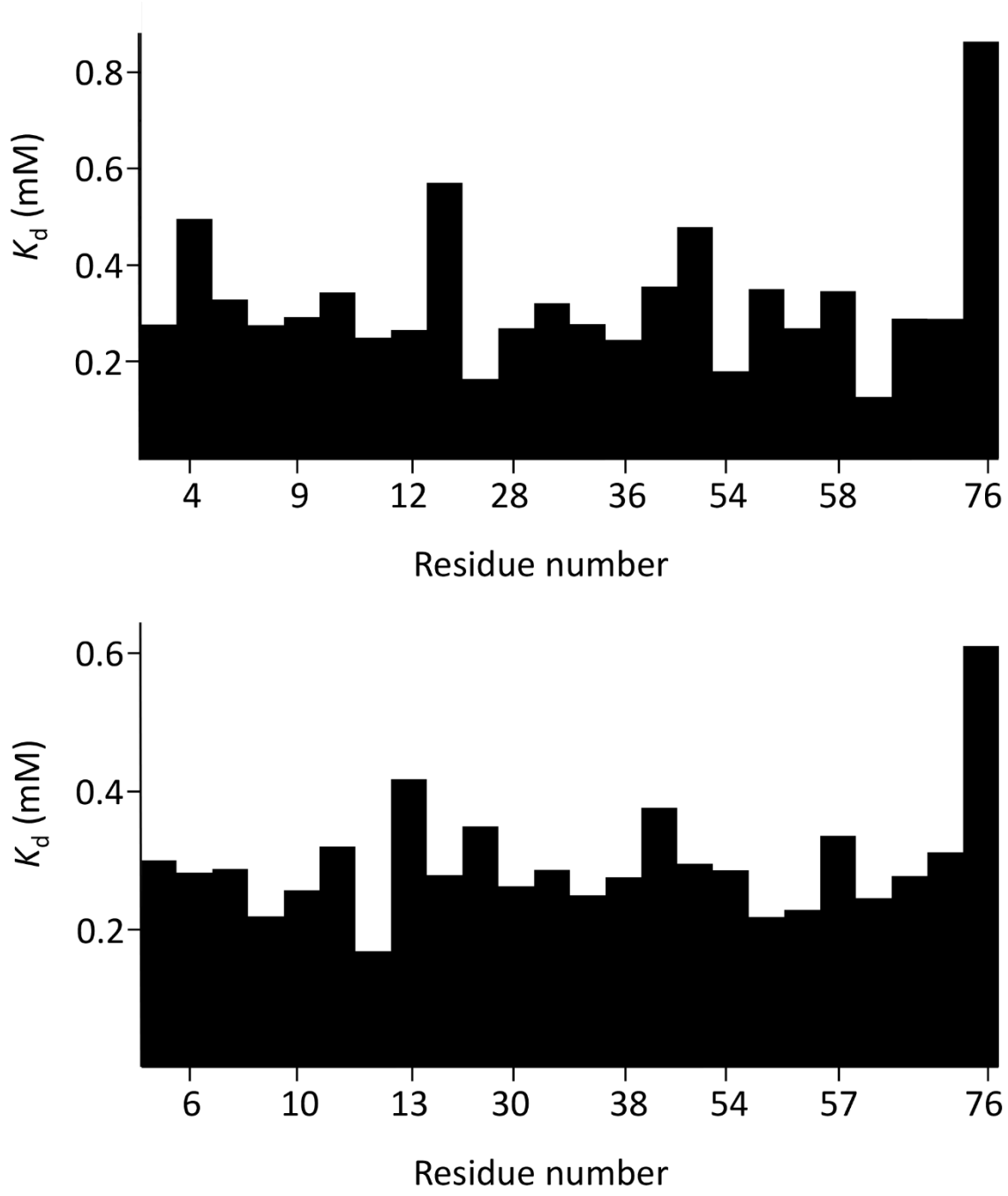

Fig. S3 K_d values fitted for SH3b binding to YG_5, after filtering out unreliable values, for (top) ^{1}H (bottom) ^{15}N. Nuclei were removed if they had a fitted K_d of > 1 mM, total ^{1}H shift changes of < 0.03 ppm, and total ^{15}N changes of < 0.15 ppm.

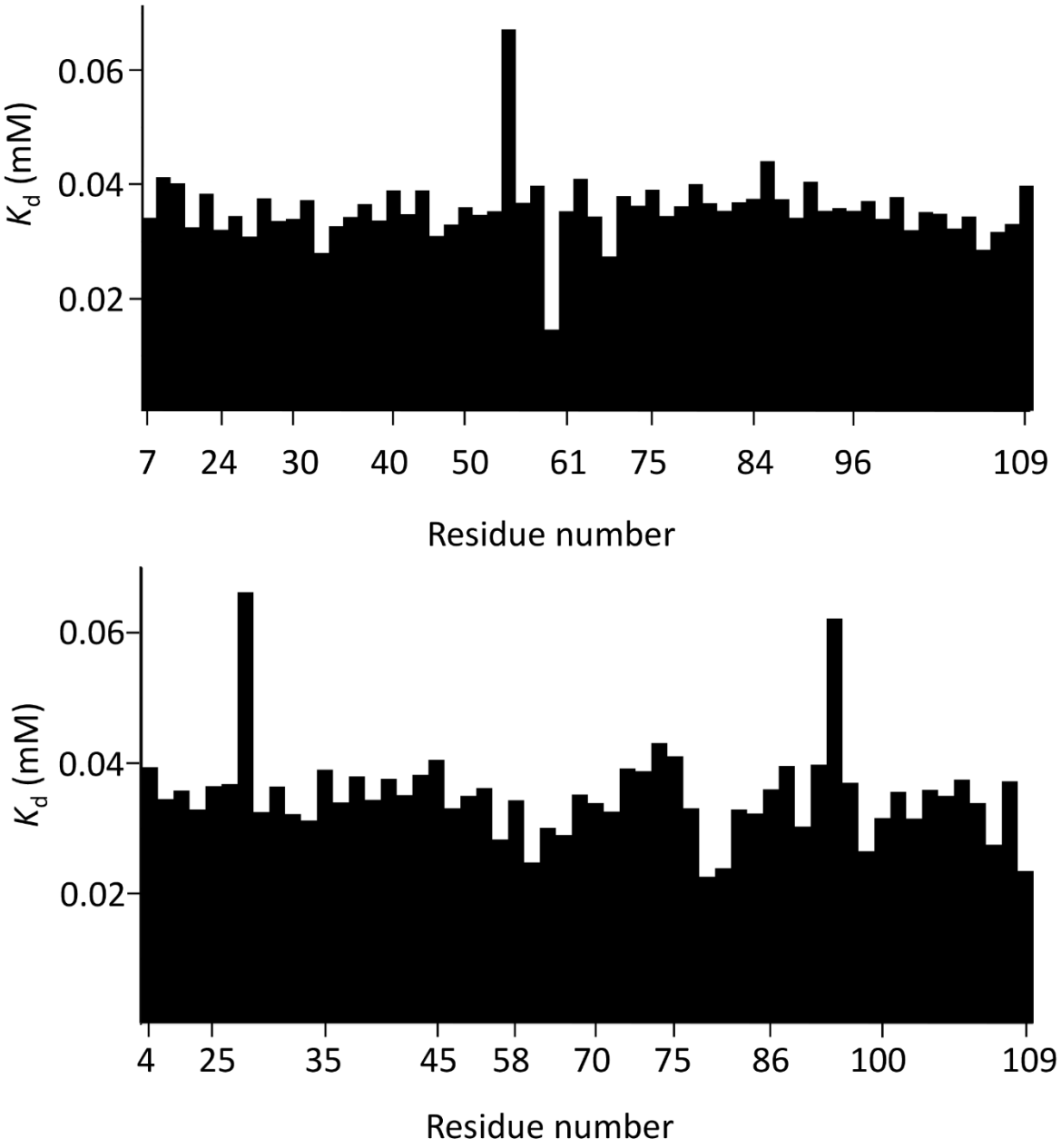

Fig. S4 K_d values fitted for barnase binding to d(CGAC), after filtering out unreliable values, for (top) ^{1}H (bottom) ^{15}N. Nuclei were removed if they had a fitted K_d of > 1 mM, total ^{1}H shift changes of < 0.025 ppm, and total ^{15}N changes of < 0.1 ppm.