

Supporting information for N. R. Skrynnikov, F. W. Dahlquist, and L. E. Kay, "Reconstructing NMR spectra of 'invisible' excited protein states using HSQC and HMQC experiments"

Table S1: Signed values of $\Delta\tilde{\omega}_N$ for 52 residues in the L99A cavity mutant of T4 lysozyme. The absolute values, $|\Delta\tilde{\omega}_N|$, have been determined from analyses of the relaxation dispersion profiles [19], and the sign was obtained from the H(S/M)QC experiment as described in the text. The uncertainty in $|\Delta\tilde{\omega}_N|$ obtained from Monte-Carlo simulations based on repeat CPMG measurements (likely to be underestimated) is 0.5 ppm for Gly 110 and <0.25 ppm for all other residues.

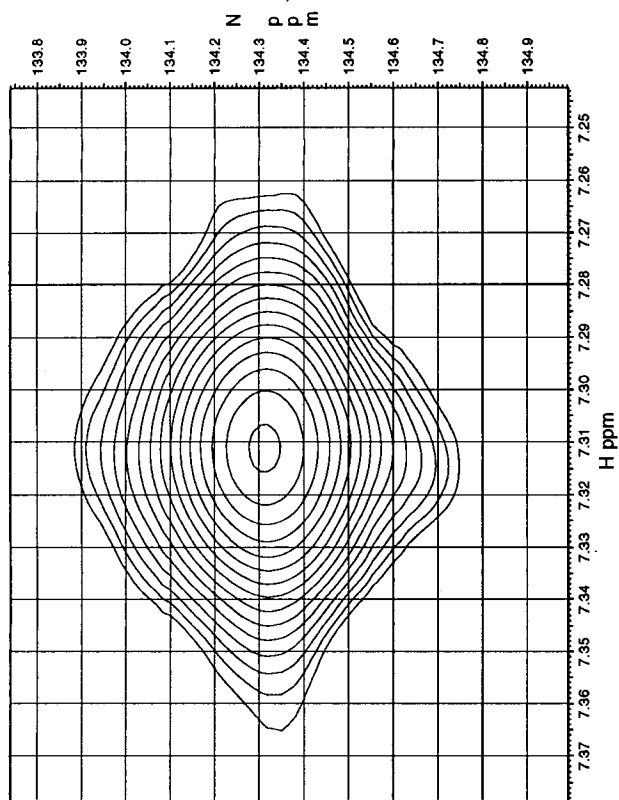
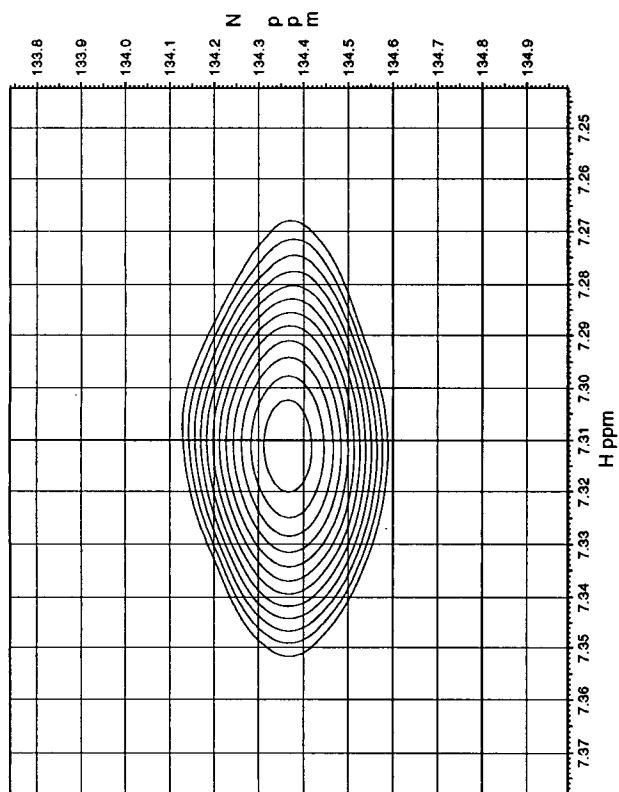
Table 1:

Residue number	$\Delta\tilde{\omega}_N$ [ppm]	Residue number	$\Delta\tilde{\omega}_N$ [ppm]
3	-0.74	98	-0.20
4	-1.27	100	-2.25
7	-2.27	101	-2.75
9	1.28	104	2.83
14	-0.60	105	2.76
26	-0.35	106	3.85
27	-0.37	107	-2.94
28	-0.42	108	2.82
29	3.80	110	5.33
30	-1.37	111	-1.61
31	-1.36	113	3.54
32	-0.29	114	-0.77
65	0.85	117	-3.42
68	-0.74	118	0.80
69	-0.87	119	-1.11
74	-0.77	120	-1.05
78	-2.00	126	0.51
80	-1.68	133	-1.14
81	-1.11	135	-3.00
82	-1.03	137	-0.53
84	0.79	139	0.95
85	-1.45	141	-0.92
87	0.75	142	4.69
91	1.59	144	0.14
96	-0.57	150	0.87
97	-0.33	153	0.37

HSQC

HMQC

Gly 113



Gly 51

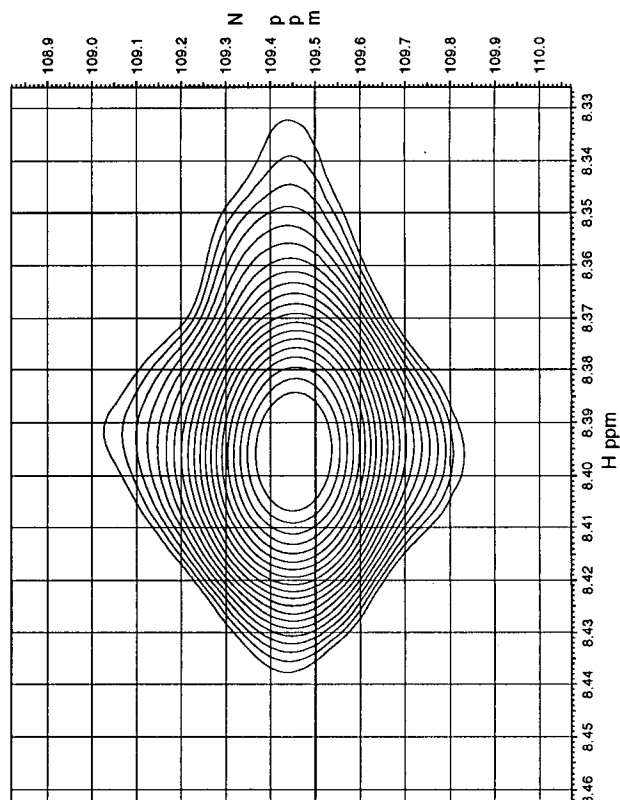
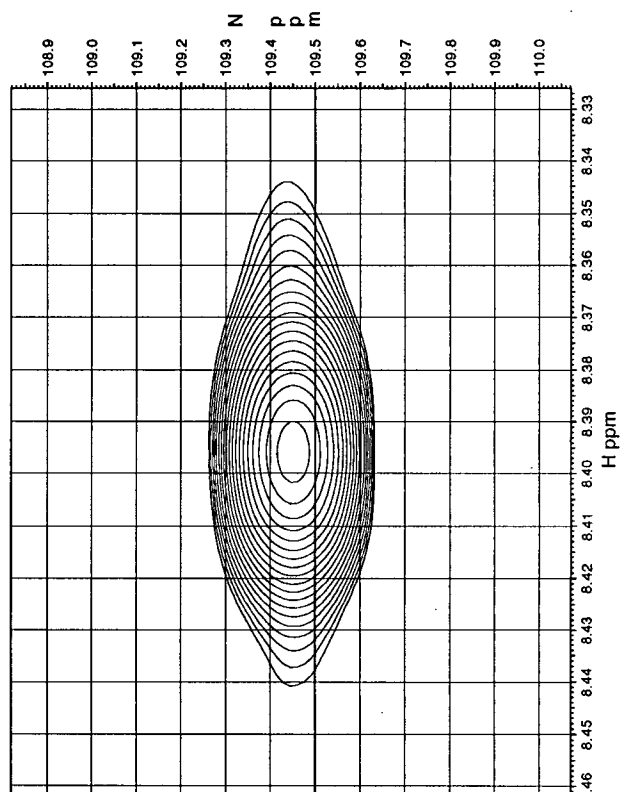


Figure S1