Supplementary online materials for:

The interplay between transient α-helix formation and side chain rotamer distributions in disordered proteins probed by methyl chemical shifts

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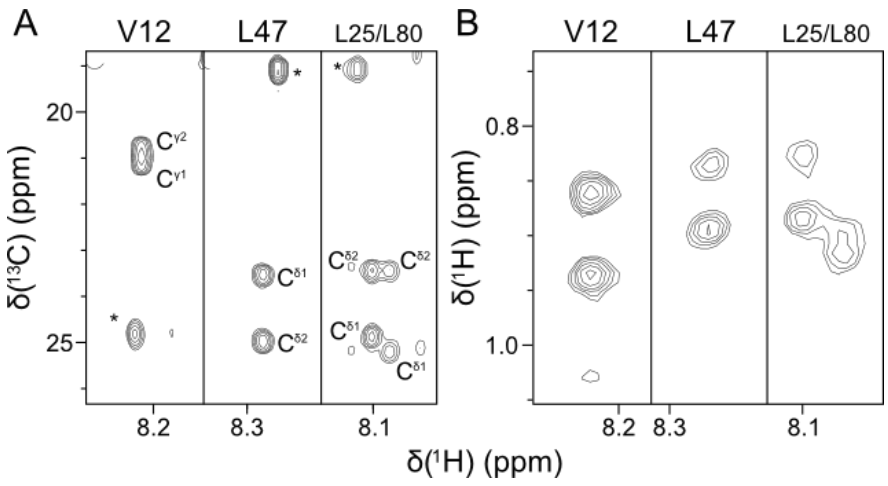
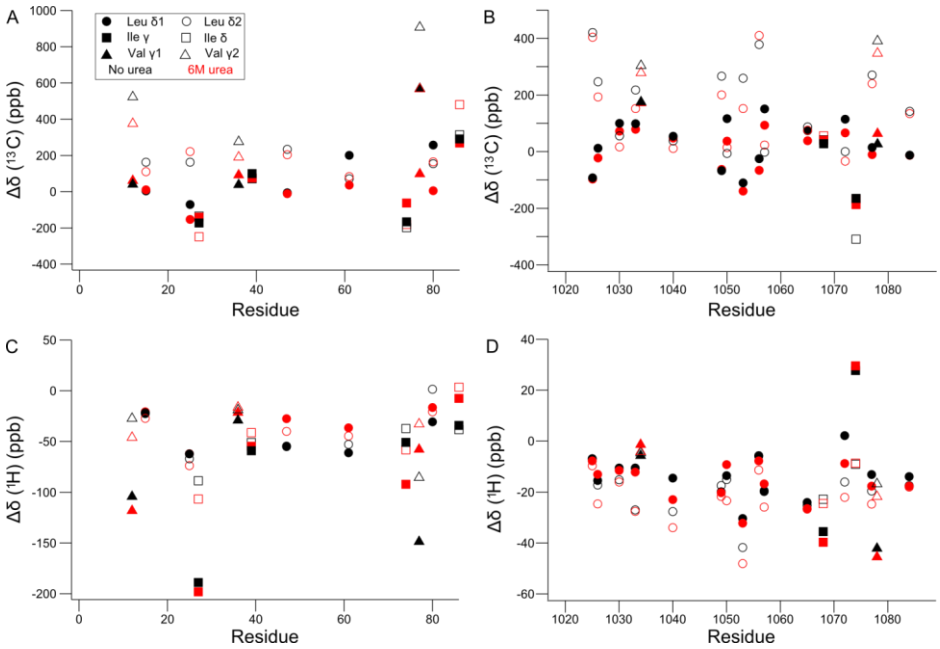
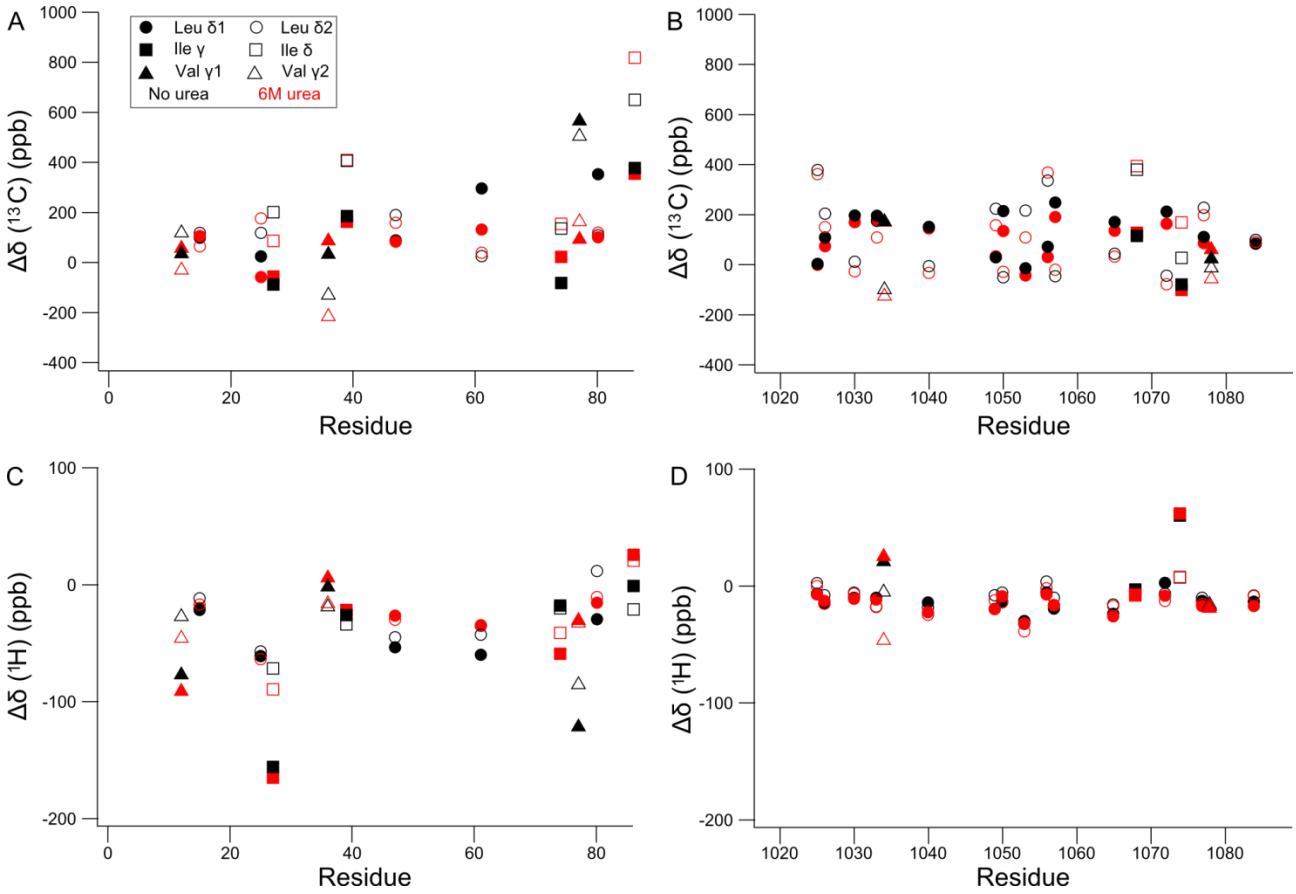


Supplementary figure 1. Assignment of methyl groups by correlation to H^N(i+1) resonances. C(CO)NH (A) and HC(CO)NH (B) spectra of ACBP at pH 2.4 readily allow assignment of methyl resonances from crowded spectral regions by correlation to the well dispersed amide resonances. Strips are centered on the amide frequencies of K13, D48 and F26/K81. * indicates peaks from neighboring slides.



Supplementary figure 2 Methyl secondary chemical shifts of ACBP (A & C) and ACTR (B & D). The secondary chemical shifts are calculated by subtracting random coil chemical shifts determined in Ac-GGXGG-NH_2 peptides (Table 1) from the experimental chemical shifts. Black and red symbols correspond to no urea or 6 M urea, respectively.



Supplementary figure 3 Methyl secondary chemical shifts of ACBP (A & C) and ACTR (B & D). The secondary chemical shifts are calculated by subtracting random coil chemical shifts determined in Ac-QQXQQ-NH_2 peptides (Table 1) from the experimental chemical shifts. Black and red symbols correspond to no urea or 6 M urea, respectively.

Supplementary table 1: Leu, Val and Ile methyl chemical shift for ACTR

		0 M urea			6 M urea			Resolved in CT-HSQC
Residue	**Resonance**	**^{1}H (ppm)**	**^{13}C (ppm)**	**P_t (%)**	**^{1}H (ppm)**	**^{13}C (ppm)**	**P_t (%)**	
L1024	δ1	0.937	24.857	61.4	0.936	24.853	61.5	n
	δ2	0.885	23.720		0.882	23.704		n
L1025	δ1	0.929	24.962	64.2	0.931	24.927	64.3	n
	δ2	0.875	23.547		0.867	23.493		n
L1029	δ1	0.933	25.050	66.9	0.933	25.022	67.1	n
	δ2	0.877	23.355		0.876	23.317		n
L1032	δ1	0.933	25.049	65.3	0.932	25.029	65.8	n
	δ2	0.865	23.517		0.864	23.452		n
V1033	γ1	0.957	21.235	-	0.962	21.232	-	y
	γ2	0.955	20.584		0.956	20.558		y
L1039	δ1	0.930	25.004	66.7	0.921	24.998	66.9	n
	δ2	0.864	23.338		0.858	23.311		n
L1048	δ1	0.924	24.883	63.2	0.924	24.887	63.9	n
	δ2	0.875	23.566		0.870	23.500		n
L1049	δ1	0.930	25.067	67.7	0.935	24.987	66.7	n
	δ2	0.877	23.293		0.869	23.315		n
L1052	δ1	0.914	24.839	62.8	0.912	24.810	63.6	n
	δ2	0.850	23.559		0.844	23.452		n
L1055	δ1	0.938	24.925	62.5	0.936	24.884	61.7	n
	δ2	0.886	23.678		0.881	23.710		n
L1056	δ1	0.924	25.101	68.0	0.927	25.043	67.2	n
	δ2	0.873	23.298		0.866	23.323		n
L1064	δ1	0.920	25.024	66.4	0.918	24.988	66.1	n
	δ2	0.867	23.387		0.865	23.376		n
I1067	γ2	0.903	17.488	68.8	0.899	17.500	69.0	y
	δ1	0.865	13.082		0.864	13.096		y
L1071	δ1	0.946	25.064	67.6	0.935	25.016	67.5	n
	δ2	0.876	23.300		0.870	23.266		n
I1073	γ2	0.967	17.294	62.4	0.969	17.273	64.9	y
	δ1	0.879	12.731		0.879	12.872		y
L1076	δ1	0.931	24.964	63.9	0.926	24.940	64.0	n
	δ2	0.872	23.571		0.867	23.540		n
V1077	γ1	0.921	21.087	-	0.918	21.123	-	y
	γ2	0.943	20.671		0.938	20.627		y
L1083	δ1	0.930	24.938	65.0	0.926	24.937	65.0	n
	δ2	0.875	23.443		0.874	23.434		n

Supplementary table 2: Leu, Val and Ile methyl chemical shift for ACBP

		0M urea			6M urea			Resolved in CT-HSQC
Residue	**Resonance**	**^{1}H (ppm)**	**^{13}C (ppm)**	**P_t (%)**	**^{1}H (ppm)**	**^{13}C (ppm)**	**P_t (%)**	
V12	γ1	0.859	21.100	-	0.845	21.121	-	y
	γ2	0.933	20.803		0.914	20.655		y
L15	δ1	0.921	24.954	64.9	0.923	24.961	65.5	n
	δ2	0.870	23.463		0.865	23.410		n
L25	δ1	0.882	24.880	64.2	0.882	24.797	62.8	y
	δ2	0.825	23.463		0.818	23.521		y
I27	γ2	0.750	17.288	65.6	0.741	17.319	63.5	y
	δ1	0.799	12.906		0.781	12.791		y
V36	γ1	0.934	21.098	-	0.942	21.152	-	y
	γ2	0.941	20.556		0.944	20.470		y
I39	γ2	0.880	17.560	69.3	0.884	17.537	69.3	y
	δ1	0.837	13.111		0.847	13.114		y
L47	δ1	0.889	24.944	64.1	0.916	24.939	64.3	n
	δ2	0.837	23.534		0.852	23.504		n
L61	δ1	0.883	25.150	67.8	0.908	24.986	66.0	n
	δ2	0.839	23.371		0.847	23.384		n
I74	γ2	0.888	17.293	64.4	0.847	17.397	64.7	y
	δ1	0.851	12.841		0.830	12.859		y
V77	γ1	0.814	21.629	-	0.905	21.158	-	y
	γ2	0.874	21.188		0.927	20.847		y
L80	δ1	0.913	25.207	67.5	0.928	24.955	64.9	n
	δ2	0.894	23.454		0.871	23.465		n
I86	γ2	0.905	17.752	73.7	0.931	17.729	76.7	y
	δ1	0.850	13.353		0.892	13.521		y