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S1

Supporting Table 1. Dipolar couplings measured with the uncharged bicelles ^a

	N-H ^N	C ^α -H ^α	C ^α -C'	C'-N	C'-H ^N
M1	-	-16.54	-2.42	-	-
Q2	-8.17	5.60	0.61	0.82	1.61
I3	8.27	8.98	-1.05	-2.11	-2.93
F4	10.49	24.27	-2.47	0.14	2.07
V5	9.87	21.73	-0.28	-0.80	1.34
K6	9.15	16.15	-3.13	0.48	2.68
T7	3.70	14.73	0.16	-0.11	1.73
L8	6.46	11.34		-2.03	-1.13
T9		-10.52	-1.59		
G10		-	-0.89		
K11	-7.53	7.01		0.96	1.06
T12	7.38	10.66	1.53	-1.76	-1.49
I13	6.95	17.52	-2.61	0.73	1.93
T14	9.71	22.82	1.77	-0.48	1.48
L15	9.85	21.36	-3.14	0.53	1.87
E16	1.91	7.30	1.10	0.76	3.20
V17	0.04	14.85	-2.14	0.70	0.90
E18	-10.51	-	-	0.81	0.44
P19	-	-6.28	0.52	-	-
S20	-4.07	18.73	-2.20	1.03	0.78
D21	2.12	20.50	-0.73	0.52	2.08
T22	11.81	19.76	-0.60		
I23	9.10	6.16		-0.26	2.23
E24		-24.93	0.77		
N25	2.95	12.46	1.41	-2.52	-3.88
V26	8.89	-6.23	-2.46	1.16	3.72
K27	8.22	13.61	2.49	-1.15	0.43

S2

A28	1.50	-31.98	0.45	0.21	-0.28
K29	7.18	22.49	-0.27	-1.02	-0.81
I30	8.71	2.98	-0.69	0.13	2.36
Q31	4.28	-19.74	1.36	0.58	2.89
D32	1.26	3.71	1.30	-2.01	-3.77
K33	8.26	13.61	-2.42	1.12	2.72
E34	6.53	15.26	-2.35	-0.40	1.99
G35	-12.50	-	-0.23	0.87	0.43
I36	-13.88	-	-	0.92	-1.02
P37	-	-	-	-	-
P38	-	1.63	-0.59	-	-
D39	10.70	7.86	0.71	-1.43	-0.01
Q40	1.94	-11.42	-0.37	0.79	1.97
Q41	7.87	11.35		-1.90	-2.03
R42	5.72	11.65	-1.94	1.15	2.81
L43	7.68	14.69	2.25	-1.39	-0.11
I44	7.98	15.59		0.75	2.55
F45	4.24	14.51	2.34	0.17	2.33
A46	7.05	14.12	-1.57	0.89	1.55
G47	9.05	-	1.17	-1.57	-0.45
K48	-10.83	-13.59	2.00	-0.01	-2.25
Q49	3.50	16.01	-0.73	-0.97	-1.94
L50	5.86	3.78	0.67	0.77	2.44
E51	-6.79	-31.42	1.17	0.38	-0.64
D52	-16.98			-0.09	-3.45
G53		-	-2.01		
R54	-6.30	-2.08		0.96	1.36
T55	6.76	13.24	1.87	-1.95	-2.76
L56	11.02	-18.95	-0.23	0.31	2.31
S57	10.86	6.95	1.11	-0.80	-0.28
D58	7.86	-5.99	1.19	-1.21	-0.97

S3

Y59	10.40	15.12	-0.94	0.62	3.00
N60	7.36	-18.30	1.58	-2.02	-2.14
I61	6.91	15.86	-2.47	0.68	2.00
Q62	2.51	4.39		0.44	2.42
K63	-11.05	5.45	0.80	-1.37	-5.05
E64	10.72	7.92	-0.92	-0.04	1.91
S65	4.03	21.17	-1.88	0.30	2.37
T66	11.32	24.43	-1.14	-0.65	1.78
L67	9.85	22.45	-1.87	0.39	2.90
H68	8.74	14.87	-0.14	-1.19	0.28
L69	6.35	14.38	-3.07	0.26	1.59
V70	4.55	13.92	0.40	-0.38	1.26
L71	6.23	1.91	-0.75	-1.43	-2.42
R72	3.34	15.94	-1.43	0.65	2.60
L73	8.33	14.31	-0.12	-0.82	0.57
R74	5.46	6.96	-0.26	0.34	1.35
G75	2.11	-	0.15	-0.39	10.41
G76	1.12	-	-	-0.49	-0.77

^a Measurements were made in a 5% w/v bicelle solution, with [DMPC]:[DHPC] = 3:1. Dashes indicate that this coupling cannot be measured with the methods used or does not apply for this residue. All empty entries are due to resonance overlap or very weak resonance intensities, thereby prohibiting accurate measurement of dipolar couplings. Random errors in the measurement are 0.16 Hz (D_{NH}), 0.7 Hz ($D_{\text{C}\alpha\text{H}\alpha}$), 0.1 Hz ($D_{\text{C}\alpha\text{C}'}$), 0.07 Hz ($D_{\text{C}'\text{N}}$) and 0.32 Hz ($D_{\text{C}'\text{HN}}$).

S4

Supporting Information Table 2. Dipolar couplings measured with the charged bicelles ^a

	N-H ^N	C ^α -H ^α	C ^α -C'	C'-N	C'-H ^N
M1	-	-38.32	-3.35	-	-
Q2	-15.52	11.55	0.82	2.65	3.99
I3	10.52	19.19	-1.84	-3.77	-5.65
F4	9.65	27.01		1.46	
V5	6.08	15.64	0.91	-1.73	0.83
K6	3.85	2.81	-5.58	1.35	3.26
T7	-3.40	15.22	2.13	-0.70	1.02
L8	15.05	11.06		-3.21	-4.04
T9	17.76	3.58	-3.26	1.21	3.81
G10		-	-1.18		
K11	-16.94	1.18		2.32	2.51
T12	2.50	-5.97	4.33	-3.15	-5.69
I13	0.70	4.40	-3.99	1.83	1.61
T14	6.43	23.88	5.02	-0.86	1.46
L15	14.20	23.95	-5.03	0.28	1.18
E16	0.08	13.46	1.23	2.77	7.24
V17	1.96	34.38	-3.81	0.16	-0.06
E18	-20.11	-	-	1.25	0.49
P19	-	15.56	0.20	-	-
S20	-12.09	12.74	-4.48	3.19	3.42
D21	4.58	56.78	-2.23	0.71	3.74
T22	23.73	18.68	-0.02	-1.47	2.44
I23	3.83	1.37		-0.35	-0.19
E24		-25.22	-0.68		
N25	-2.55	18.61	3.47	-3.66	-6.73
V26	3.17	-26.48		2.69	3.86
K27	5.07	46.25	3.38	-2.63	

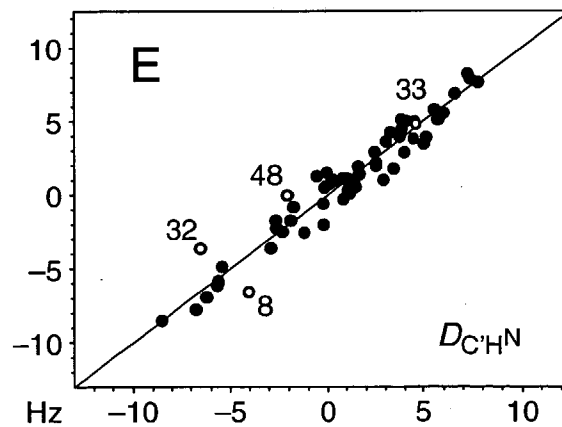
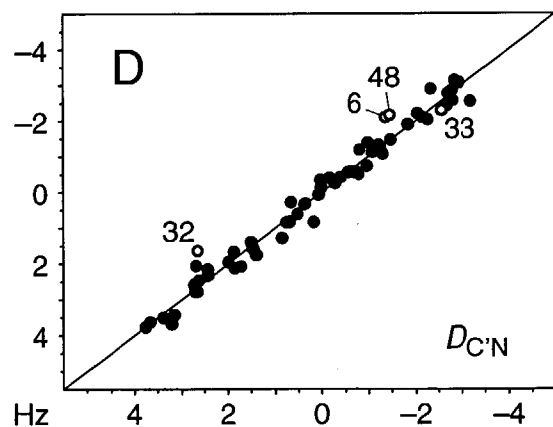
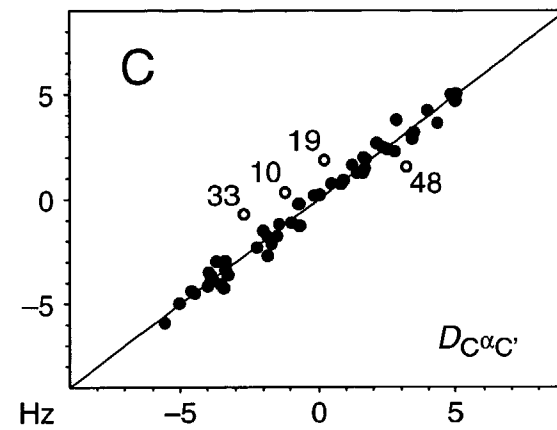
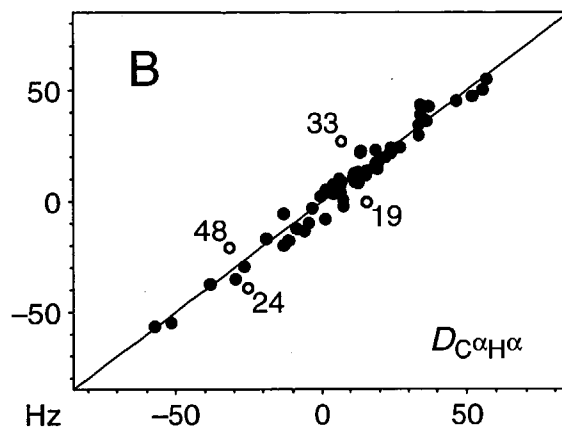
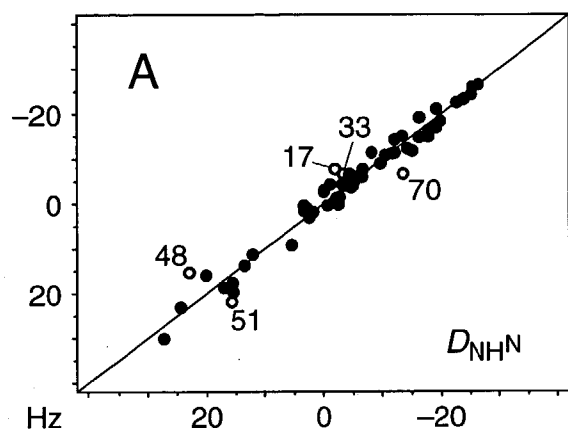
S5

A28	-1.76	-57.38	-0.94	2.12	2.52
K29	2.72	35.88	1.62	-1.85	-2.90
I30	3.62	-4.63	-1.70	0.40	2.89
Q31	4.87	-13.05	0.47	1.29	5.15
D32	-3.47	4.14	2.74	-2.65	-6.52
K33	3.36	6.81	-2.71	2.55	4.61
E34	4.36	12.71		-1.40	-0.23
G35	-13.49	-	-2.01	2.78	4.55
I36	-24.37	-	-	0.98	-1.78
P37	-	-	-	-	-
P38	-	7.55		-	-
D39	17.72	-3.42	3.96	-2.71	-1.93
Q40	0.16	-29.49	-0.67	0.58	-0.24
Q41	26.40	36.54		-2.74	0.12
R42	11.61	33.81	-3.51	2.94	7.77
L43	13.33	22.01	2.50	-2.00	0.79
I44	4.37	11.38		2.03	4.48
F45	-3.00	13.59		-0.53	-0.58
A46	1.19	37.19	-3.96	2.25	3.02
G47	4.39	-	2.33	-2.65	-2.63
K48	-22.97	-31.66	3.18	1.45	-2.10
Q49	-2.83	6.08	1.64	-1.87	-5.45
L50	3.92	-8.75	1.70	0.72	1.66
E51	-15.69	-51.55	3.41	1.07	-1.24
D52	-27.26			-0.02	-6.23
G53	-	-	-3.88		
R54	-5.53	6.68		2.82	6.57
T55	2.25	6.56	4.99	-3.38	-5.62
L56	19.04	-13.09	-1.48	-0.67	1.06
S57	25.26	18.86	-0.16	-0.07	5.98
D58	12.08	-18.83	4.85	-2.43	-2.33

S6

Y59	12.03	7.06	-1.84	0.55	0.87
N60	25.03	-11.47	1.40	-2.72	-0.11
I61	19.07	55.38	-4.59	0.80	5.57
Q62	16.25	34.35		0.96	7.35
K63	-15.43	8.14	2.81	-2.69	-8.54
E64	22.60	-0.48	-1.41	-0.76	1.38
S65	19.75	51.90	-3.86	-0.01	5.74
T66	16.22	33.71	-3.36	-0.16	5.04
L67	8.13	19.62	-3.67	0.79	4.08
H68	4.57	3.86	0.03	-2.44	-2.66
L69	6.57	23.56	-3.41	-0.39	0.28
V70	13.50	24.28	1.73	-1.51	1.38
L71	21.30	28.08	-2.93	-2.43	-0.67
R72	12.55	29.96	-2.15	1.85	7.53
L73	12.06	18.11	-0.53	-0.87	1.54
R74	6.60	10.29	-0.92	-0.06	1.25
G75	3.90	-	0.10	0.06	0.87
G76	1.70	-	-	-0.67	-0.81

^a Measurements were made in a 5% w/v bicelle solution, with [DMPC]:[DHPC]:[CTAB] = 30:10:1. Dashes indicate that this coupling cannot be measured with the methods used or does not apply for this residue. All empty entries are due to resonance overlap or very weak resonance intensities, thereby prohibiting accurate measurement of dipolar couplings. Random errors in the measurement are 0.17 Hz (D_{NH}), 0.75 Hz ($D_{\text{C}\alpha\text{H}\alpha}$), 0.17 Hz ($D_{\text{C}\alpha\text{C}'}$), 0.07 Hz ($D_{\text{C}'\text{N}}$) and 0.67 Hz ($D_{\text{C}'\text{HN}}$).



Supplementary Figure 1. Plots of measured *versus* predicted residual dipolar couplings in ubiquitin, dissolved in the CTAB-charged liquid crystal sample. (A) $^1D_{NH}$, (B) $^1D_{C\alpha H\alpha}$, (C) $^1D_{C\alpha C'}$, (D) $^1D_{C'N}$ and (E) $^2D_{C'HN}$. The data represented by open circles are outliers which are due to structural differences between the solution and crystalline states, and they were not used for further analysis.