Supporting information

Table1S Observed relaxation rates at 9.39T, corresponding to 400 MHz proton resonance frequency.

Residue #	R_1 / s^{-1}	ΔR_1 / s^{-1}	R_2 / s^{-1}	ΔR_2 / s^{-1}	NOE	η_z / s^{-1}	$\Delta\eta_z$ / s^{-1}	η_{xy} / s^{-1}	$\Delta\eta_{xy}$ / s^{-1}
2	2.88	0.04	6.14	0.07	0.55	1.53	0.05	3.40	0.09
3	2.98	0.05	6.31	0.15	0.58	1.57	0.07	3.10	0.09
4	3.05	0.05	6.31	0.11	0.59	1.54	0.03	3.06	0.08
5	2.94	0.03	6.08	0.13	0.58	1.46	0.07	3.04	0.10
6	3.05	0.03	6.45	0.11	0.58	1.64	0.04	3.39	0.08
7	2.99	0.05	5.93	0.10	0.55	1.54	0.05	3.23	0.10
8	2.83	0.04	5.49	0.08	0.47	1.27	0.04	2.60	0.13
9	2.81	0.04	5.63	0.13	0.44	1.26	0.05	2.73	0.17
10	2.68	0.04	4.99	0.07	0.43	1.46	0.05	2.73	0.08
11	2.46	0.03	4.91	0.24	0.41	1.50	0.06	2.96	0.10
12	2.78	0.04	5.53	0.11	0.51	1.30	0.06	2.70	0.08
13	2.95	0.04	6.14	0.12	0.55	1.53	0.04	3.15	0.10
14	2.85	0.03	6.00	0.14	0.58	1.44	0.04	3.07	0.08
15	3.01	0.03	6.23	0.10	0.56	1.53	0.05	3.17	0.09
16	2.81	0.02	5.83	0.06	0.58	1.20	0.04	2.95	0.22
17	3.02	0.04	6.20	0.06	0.58	1.56	0.03	3.31	0.12
18	2.92	0.09	6.10	0.13	0.60	1.24	0.04	2.67	0.17
20	2.92	0.05	6.37	0.15	0.57	1.51	0.03	3.01	0.10
21	3.15	0.04	6.53	0.09	0.59	1.68	0.06	3.44	0.23
22	3.00	0.03	6.10	0.07	0.58	1.52	0.05	3.16	0.17
23	3.15	0.06	6.87	0.08	0.58	1.69	0.07	3.55	0.10
25	3.08	0.04	7.61	0.07	0.60	1.58	0.05	3.10	0.18
26	3.03	0.05	6.23	0.12	0.57	1.46	0.04	3.13	0.19
27	3.11	0.05	6.32	0.14	0.59	1.61	0.05	3.27	0.05
28	3.06	0.03	6.58	0.07	0.59	1.72	0.03	3.57	0.12
29	3.02	0.03	6.27	0.10	0.58	1.59	0.03	3.20	0.11
30	3.07	0.04	6.33	0.08	0.57	1.59	0.06	3.11	0.11
31	3.01	0.06	6.18	0.08	0.59	1.34	0.04	2.99	0.33
32	3.02	0.04	6.25	0.07	0.58	1.57	0.06	3.19	0.08
33	2.91	0.04	5.96	0.07	0.56	1.46	0.03	3.09	0.11
34	2.97	0.07	6.08	0.07	0.56	1.36	0.04	2.64	0.08
35	2.99	0.05	6.70	0.06	0.60	1.39	0.06	3.19	0.14
36	2.60	0.03	5.82	0.14	0.61	1.49	0.03	3.30	0.06
39	2.94	0.05	5.95	0.16	0.57	1.56	0.03	3.01	0.10
40	2.98	0.05	6.21	0.07	0.58	1.45	0.03	3.07	0.12
41	2.99	0.04	6.06	0.07	0.55	1.41	0.06	3.24	0.15
42	2.99	0.05	6.18	0.08	0.58	1.36	0.03	3.07	0.21
43	2.93	0.03	6.24	0.07	0.58	1.33	0.04	3.09	0.12
44	3.04	0.04	6.15	0.07	0.58	1.54	0.07	3.01	0.08
45	3.07	0.05	6.47	0.06	0.58	1.58	0.04	3.63	0.15
46	3.09	0.06	6.52	0.10	0.55	1.64	0.04	3.14	0.14
47	2.84	0.03	6.01	0.12	0.56	1.30	0.04	2.75	0.11
48	2.84	0.03	6.05	0.14	0.59	1.62	0.07	3.58	0.14
49	2.75	0.03	5.57	0.06	0.52	1.41	0.06	2.93	0.09

50	2.98	0.04	6.17	0.06	0.54	1.53	0.04	3.33	0.10
51	2.86	0.04	6.05	0.10	0.57	1.47	0.07	3.41	0.32
52	2.73	0.05	5.90	0.09	0.58	1.22	0.05	3.06	0.12
54	2.88	0.04	6.08	0.14	0.60	1.51	0.07	3.45	0.13
55	2.97	0.04	6.52	0.07	0.59	1.51	0.03	2.95	0.08
56	3.13	0.04	6.14	0.10	0.58	1.50	0.04	3.58	0.25
57	3.02	0.08	6.06	0.09	0.56	1.44	0.03	2.57	0.27
58	3.08	0.03	6.42	0.06	0.61	1.65	0.04	3.22	0.08
59	2.98	0.04	6.03	0.07	0.56	1.38	0.05	2.97	0.08
60	2.99	0.05	6.27	0.10	0.59	1.73	0.06	3.62	0.16
61	3.01	0.05	6.08	0.09	0.60	1.50	0.07	3.06	0.08
62	2.59	0.02	5.28	0.13	0.45	1.30	0.04	2.72	0.07
63	2.79	0.09	6.24	0.08	0.58	1.40	0.03	3.43	0.30
64	3.09	0.06	6.20	0.09	0.57	1.50	0.03	3.12	0.14
65	2.92	0.04	6.25	0.16	0.58	1.60	0.08	3.40	0.19
66	2.96	0.04	5.87	0.10	0.58	1.39	0.06	3.05	0.10
67	3.01	0.03	6.15	0.15	0.55	1.58	0.03	3.27	0.18
68	3.01	0.05	6.09	0.16	0.60	1.46	0.03	2.95	0.10
69	2.72	0.05	4.29	0.15	0.55	1.35	0.03	2.81	0.27
70	3.04	0.05	6.70	0.11	0.58	1.64	0.04	3.37	0.08
71	2.84	0.03	5.69	0.09	0.55	1.21	0.05	2.78	0.12
72	2.80	0.04	5.36	0.15	0.47	1.38	0.04	2.72	0.06
73	2.27	0.03	3.94	0.09	0.10	1.08	0.04	1.80	0.06
74	1.92	0.02	3.55	0.15	-0.22	0.68	0.04	1.93	0.33
75	1.50	0.02	2.27	0.07	-0.83	0.33	0.03	0.63	0.06
76	0.85	0.01	1.26	0.11	-1.40	0.26	0.02	0.37	0.05

Table 2S Observed relaxation rates at 11.74T, corresponding to 500 MHz proton resonance frequency.

Residue #	R_1 / s^{-1}	ΔR_1 / s^{-1}	R_2 / s^{-1}	ΔR_2 / s^{-1}	NOE	η_z / s^{-1}	$\Delta\eta_z$ / s^{-1}	η_{xy} / s^{-1}	$\Delta\eta_{xy}$ / s^{-1}
2	2.34	0.03	6.40	0.14	0.66	1.50	0.09	4.20	0.07
3	2.45	0.03	6.39	0.13	0.65	1.46	0.02	3.86	0.08
4	2.55	0.03	6.68	0.17	0.71	1.53	0.04	3.38	0.11
5	2.43	0.03	6.20	0.16	0.72	1.40	0.07	3.40	0.06
6	2.50	0.03	6.14	0.18	0.73	1.63	0.06	4.19	0.14
7	2.48	0.03	6.60	0.15	0.69	1.48	0.04	4.01	0.15
8	2.40	0.03	5.76	0.13	0.57	1.35	0.04	2.87	0.07
9	2.27	0.04	5.10	0.35	0.59	1.16	0.03	3.39	0.05
10	2.29	0.03	5.56	0.17	0.54	1.32	0.02	3.35	0.07
11	2.14	0.03	5.53	0.15	0.56	1.44	0.05	3.77	0.04
12	2.32	0.03	6.02	0.16	0.56	1.38	0.04	3.44	0.07
13	2.43	0.03	6.03	0.15	0.66	1.51	0.08	3.83	0.11
14	2.37	0.03	6.33	0.16	0.67	1.60	0.12	3.50	0.13
15	2.51	0.03	6.15	0.14	0.70	1.59	0.14	4.01	0.20
16	2.29	0.04	6.18	0.17	0.67	1.53	0.02	4.32	0.06
17	2.50	0.03	6.79	0.18	0.70	1.52	0.03	4.35	0.10
18	2.39	0.03	6.66	0.18	0.76	1.17	0.13	3.53	0.06
20	2.37	0.03	6.40	0.44	0.65	1.40	0.02	4.04	0.05
21	2.63	0.04	6.59	0.17	0.72	1.59	0.12	4.29	0.23
22	2.49	0.03	5.90	0.16	0.65	1.51	0.03	3.85	0.11
23	2.65	0.03	7.69	0.14	0.72	1.61	0.05	3.99	0.12
25	2.55	0.04	8.76	0.16	0.71	1.54	0.03	3.73	0.14
26	2.45	0.04	6.46	0.14	0.70	1.24	0.10	3.75	0.09
27	2.60	0.03	7.09	0.22	0.72	1.63	0.09	3.86	0.20
28	2.60	0.03	6.35	0.20	0.77	1.65	0.15	4.45	0.08
29	2.53	0.03	6.57	0.15	0.69	1.59	0.07	3.91	0.04
30	2.56	0.03	6.50	0.11	0.68	1.64	0.02	3.69	0.06
31	2.56	0.03	6.23	0.17	0.65	1.50	0.10	4.28	0.11
32	2.50	0.03	6.72	0.17	0.80	1.64	0.02	4.43	0.08
33	2.40	0.03	6.21	0.16	0.66	1.52	0.03	3.77	0.05
34	2.43	0.03	6.21	0.12	0.69	1.34	0.02	3.26	0.20
35	2.49	0.04	6.22	0.18	0.74	1.43	0.03	3.92	0.09
36	2.14	0.03	5.94	0.23	0.74	1.49	0.02	4.17	0.07
39	2.49	0.03	6.30	0.14	0.71	1.62	0.04	4.10	0.06
40	2.51	0.03	6.38	0.13	0.67	1.50	0.04	3.68	0.12
41	2.50	0.03	6.38	0.16	0.67	1.68	0.09	3.51	0.11
42	2.54	0.03	6.30	0.10	0.69	1.61	0.02	4.07	0.06
43	2.40	0.04	6.32	0.22	0.72	1.43	0.08	3.80	0.04
44	2.50	0.03	6.33	0.17	0.69	1.49	0.11	3.46	0.08
45	2.50	0.03	6.36	0.17	0.74	1.70	0.07	4.64	0.20
46	2.50	0.04	6.75	0.55	0.69	1.52	0.08	3.97	0.09
47	2.39	0.03	6.88	0.63	0.67	0.92	0.09	3.48	0.04
48	2.40	0.03	6.58	0.15	0.72	1.51	0.12	4.55	0.05
49	2.28	0.03	5.73	0.14	0.55	1.42	0.09	4.11	0.07
50	2.47	0.03	6.02	0.14	0.69	1.68	0.08	4.19	0.22
51	2.35	0.03	5.97	0.15	0.73	1.47	0.05	3.81	0.08

52	2.20	0.03	6.41	0.15	0.65	1.44	0.02	3.86	0.16
54	2.36	0.03	6.54	0.13	0.68	1.50	0.10	4.56	0.09
55	2.42	0.03	6.16	0.19	0.72	1.52	0.02	3.71	0.05
56	2.63	0.03	6.89	0.21	0.72	1.50	0.06	2.86	0.33
57	2.53	0.03	6.29	0.16	0.73	1.37	0.12	3.89	0.07
58	2.59	0.03	6.40	0.16	0.70	1.67	0.05	4.39	0.15
59	2.47	0.03	6.12	0.11	0.70	1.38	0.05	3.24	0.12
60	2.53	0.04	6.56	0.12	0.70	1.72	0.02	4.07	0.20
61	2.53	0.03	6.40	0.19	0.73	1.46	0.07	4.02	0.08
62	2.14	0.03	5.26	0.21	0.60	1.36	0.07	3.51	0.10
63	2.33	0.03	6.62	0.17	0.70	1.33	0.06	4.21	0.11
64	2.55	0.03	6.40	0.12	0.70	1.52	0.05	3.68	0.08
65	2.46	0.03	6.31	0.16	0.72	1.53	0.02	3.83	0.11
66	2.45	0.04	6.33	0.14	0.71	1.52	0.04	4.09	0.19
67	2.48	0.03	5.93	0.16	0.68	1.57	0.05	3.57	0.06
68	2.47	0.03	6.35	0.17	0.72	1.54	0.03	3.56	0.10
69	2.49	0.03	5.63	0.14	0.57	1.50	0.05	3.36	0.17
70	2.52	0.03	6.77	0.26	0.73	1.62	0.03	4.27	0.05
71	2.44	0.04	5.60	0.21	0.66	1.49	0.20	3.97	0.05
72	2.34	0.03	5.52	0.17	0.56	1.52	0.07	3.55	0.05
73	2.02	0.03	4.11	0.19	0.29	1.17	0.03	2.27	0.04
74	1.73	0.02	3.43	0.15	0.08	0.98	0.02	1.74	0.10
75	1.33	0.05	2.18	0.15	-0.49	0.52	0.03	0.75	0.05
76	0.82	0.02	1.62	0.16	-1.16	0.36	0.02	0.58	0.09

Table 3S Observed relaxation rates at 14.09T, corresponding to 600 MHz proton resonance frequency.

residue #	R_1 / s^{-1}	ΔR_1 / s^{-1}	NOE	η_z / s^{-1}	$\Delta\eta_z$ / s^{-1}
2	1.89	0.08	0.66	1.32	0.05
3	2.19	0.06	0.70	1.55	0.06
4	2.21	0.03	0.71	1.45	0.03
5	2.08	0.03	0.69	1.46	0.02
6	2.19	0.04	0.68	1.62	0.03
7	2.12	0.05	0.64	1.48	0.05
8	2.09	0.03	0.58	1.36	0.04
9	1.97	0.06	0.53	1.35	0.13
10	1.99	0.04	0.53	1.28	0.05
11	1.87	0.04	0.53	1.40	0.04
12	1.98	0.02	0.62	1.36	0.02
13	2.10	0.04	0.67	1.53	0.03
14	1.96	0.06	0.66	1.38	0.04
15	2.14	0.04	0.68	1.57	0.03
16	1.89	0.08	0.64	1.32	0.04
17	2.14	0.04	0.68	1.49	0.04
18	1.96	0.03	0.64	1.24	0.02
20	2.09	0.03	0.63	1.40	0.03
21	2.25	0.02	0.77	1.60	0.02
22	2.11	0.04	0.70	1.36	0.03
23	2.24	0.02	0.71	1.61	0.02
25	2.20	0.02	0.71	1.56	0.02
26	2.26	0.06	0.66	1.58	0.05
27	2.26	0.03	0.71	1.56	0.03
28	2.24	0.03	0.67	1.69	0.03
29	2.19	0.03	0.69	1.53	0.03
30	2.18	0.05	0.70	1.53	0.05
31	2.29	0.04	0.76	1.60	0.04
32	2.18	0.03	0.71	1.49	0.03
33	2.12	0.03	0.68	1.47	0.03
34	2.11	0.04	0.68	1.36	0.04
35	2.11	0.05	0.71	1.41	0.05
36	1.85	0.03	0.72	1.37	0.03
39	2.13	0.02	0.69	1.42	0.02
40	2.14	0.05	0.68	1.42	0.05
41	2.13	0.03	0.67	1.55	0.03
42	2.14	0.02	0.70	1.52	0.02
43	2.08	0.04	0.67	1.46	0.04
44	2.15	0.04	0.69	1.44	0.03
45	2.15	0.03	0.69	1.58	0.02
46	2.15	0.05	0.69	1.54	0.09
47	2.07	0.03	0.62	1.31	0.03
48	1.97	0.04	0.69	1.42	0.03
49	1.98	0.03	0.61	1.38	0.03
50	2.12	0.03	0.66	1.52	0.02
51	2.00	0.04	0.67	1.37	0.04

52	1.90	0.03	0.65	1.26	0.02
54	2.04	0.03	0.70	1.51	0.02
55	2.15	0.03	0.68	1.46	0.03
56	2.24	0.04	0.70	1.60	0.03
57	2.22	0.04	0.71	1.51	0.04
58	2.22	0.05	0.72	1.61	0.06
59	2.16	0.03	0.70	1.44	0.03
60	2.18	0.04	0.70	1.63	0.04
61	2.21	0.04	0.69	1.50	0.04
62	1.85	0.04	0.55	1.23	0.04
63	1.80	0.09	0.64	1.18	0.07
64	2.23	0.02	0.68	1.51	0.02
65	2.14	0.04	0.71	1.47	0.04
66	2.06	0.04	0.67	1.44	0.04
67	2.13	0.05	0.71	1.51	0.04
68	2.13	0.02	0.71	1.43	0.02
69	2.08	0.03	0.74	1.49	0.04
70	2.18	0.03	0.70	1.55	0.03
71	2.01	0.04	0.61	1.39	0.03
72	1.94	0.03	0.70	1.37	0.02
73	1.76	0.04	0.29	1.16	0.04
74	1.52	0.06	-0.04	0.91	0.05
75	1.22	0.03	-0.50	0.58	0.06
76	0.72	0.05	-1.20	0.35	0.03

Table 4S Observed relaxation rates at 18.78, corresponding to 800 MHz proton resonance frequency.

residue #	R_1 / s^{-1}	ΔR_1 / s^{-1}	R_2 / s^{-1}	ΔR_2 / s^{-1}	NOE	η_z / s^{-1}	$\Delta\eta_z$ / s^{-1}	η_{xy} / s^{-1}	$\Delta\eta_{xy}$ / s^{-1}
2	1.56	0.03	7.24	0.13	0.75	1.27	0.03	5.62	0.07
3	1.66	0.03	7.04	0.19	0.78	1.27	0.03	5.00	0.04
4	1.72	0.02	7.50	0.10	0.79	1.31	0.05	5.32	0.06
5	1.59	0.02	6.57	0.10	0.76	1.26	0.06	5.09	0.13
6	1.67	0.02	7.01	0.14	0.77	1.30	0.04	5.67	0.12
7	1.67	0.03	7.05	0.17	0.74	1.32	0.04	5.27	0.07
8	1.78	0.07	6.26	0.12	0.66	1.21	0.08	4.57	0.16
9	1.66	0.06	7.25	0.24	0.65	0.94	0.31	4.55	0.18
10	1.59	0.04	5.95	0.24	0.66	1.23	0.06	4.86	0.28
11	1.52	0.04	6.08	0.06	0.61	1.27	0.02	5.10	0.12
12	1.60	0.03	6.29	0.11	0.67	1.16	0.05	4.63	0.11
13	1.66	0.02	7.18	0.23	0.76	1.28	0.02	5.24	0.05
14	1.59	0.04	7.02	0.10	0.74	1.22	0.02	5.24	0.13
15	1.69	0.03	6.81	0.16	0.79	1.27	0.04	5.22	0.19
16	1.47	0.03	6.18	0.18	0.68	1.15	0.06	5.26	0.09
17	1.67	0.02	7.14	0.12	0.78	1.20	0.03	5.34	0.26
18	1.53	0.03	7.19	0.17	0.80	1.04	0.04	5.18	0.13
20	1.61	0.02	8.05	0.09	0.80	1.17	0.02	5.48	0.17
21	1.74	0.03	7.43	0.11	0.78	1.35	0.04	6.00	0.11
22	1.68	0.02	7.51	0.06	0.77	1.26	0.04	5.10	0.18
23	1.73	0.03	9.35	0.13	0.80	1.45	0.06	6.11	0.17
25	1.70	0.03	11.51	0.14	0.81	1.32	0.05	5.61	0.24
26	1.66	0.04	6.26	0.45	0.75	1.33	0.05	5.53	0.09
27	1.72	0.03	7.57	0.12	0.82	1.24	0.04	5.52	0.08
28	1.75	0.03	7.59	0.08	0.78	1.45	0.03	6.15	0.09
29	1.68	0.02	7.07	0.11	0.79	1.24	0.03	5.40	0.14
30	1.70	0.05	6.98	0.11	0.81	1.30	0.04	5.52	0.13
31	1.72	0.04	7.06	0.12	0.79	1.23	0.05	5.47	0.09
32	1.72	0.03	7.13	0.11	0.78	1.29	0.04	5.38	0.12
33	1.63	0.02	7.03	0.15	0.79	1.21	0.03	5.02	0.05
34	1.60	0.02	6.75	0.13	0.78	1.07	0.03	4.76	0.12
35	1.60	0.03	7.88	0.17	0.82	1.05	0.04	5.69	0.15
36	1.44	0.02	6.81	0.12	0.80	1.18	0.03	5.59	0.10
39	1.74	0.03	7.21	0.09	0.78	1.28	0.03	4.90	0.06
40	1.67	0.02	7.03	0.10	0.78	1.15	0.04	5.20	0.12
41	1.66	0.02	6.85	0.07	0.79	1.17	0.03	5.17	0.12
42	1.73	0.04	6.92	0.11	0.79	1.23	0.04	5.47	0.07
43	1.57	0.03	7.05	0.13	0.75	1.22	0.03	5.15	0.25
44	1.63	0.05	6.69	0.11	0.78	1.27	0.04	5.18	0.11
45	1.68	0.03	7.30	0.14	0.82	1.35	0.04	5.86	0.12
46	1.65	0.07	7.49	0.36	0.74	1.22	0.29	5.30	0.35
47	1.61	0.03	7.41	0.16	0.73	1.10	0.05	4.34	0.11
48	1.59	0.03	7.14	0.07	0.72	1.22	0.04	5.83	0.11
49	1.56	0.03	6.32	0.08	0.63	1.27	0.06	4.67	0.19
50	1.68	0.03	6.94	0.13	0.72	1.23	0.06	5.41	0.11
51	1.51	0.04	6.65	0.10	0.85	1.15	0.05	5.38	0.20

52	1.43	0.02	6.67	0.10	0.72	1.09	0.03	4.98	0.10
54	1.58	0.02	7.27	0.07	0.73	1.16	0.04	5.89	0.06
55	1.66	0.02	8.52	0.26	0.82	1.17	0.05	5.07	0.13
56	1.78	0.04	6.81	0.17	0.80	1.30	0.07	4.99	0.35
57	1.70	0.04	7.18	0.31	0.83	1.23	0.02	4.99	0.07
58	1.77	0.03	7.22	0.11	0.80	1.40	0.03	5.83	0.13
59	1.62	0.02	6.33	0.22	0.77	1.14	0.03	4.95	0.10
60	1.70	0.02	7.06	0.14	0.76	1.38	0.04	5.72	0.16
61	1.67	0.02	7.00	0.10	0.73	1.20	0.03	5.25	0.08
62	1.45	0.02	5.91	0.08	0.64	1.14	0.04	4.61	0.07
63	1.54	0.09	6.89	0.08	0.71	1.10	0.10	4.24	1.78
64	1.73	0.02	7.14	0.12	0.76	1.23	0.03	5.02	0.07
65	1.67	0.03	7.41	0.10	0.81	1.22	0.05	5.42	0.03
66	1.59	0.03	6.64	0.09	0.73	1.10	0.04	4.88	0.28
67	1.64	0.02	6.94	0.20	0.78	1.28	0.02	5.44	0.07
68	1.61	0.02	6.97	0.14	0.82	1.13	0.02	5.01	0.08
69	1.63	0.03	5.94	0.13	0.79	1.33	0.05	4.58	0.19
70	1.69	0.02	8.20	0.20	0.79	1.32	0.04	5.63	0.10
71	1.59	0.03	6.37	0.08	0.69	1.29	0.05	4.64	0.25
72	1.65	0.03	6.17	0.10	0.65	1.42	0.08	4.57	0.14
73	1.58	0.06	4.44	0.08	0.46	1.27	0.03	3.03	0.70
74	1.46	0.08	3.41	0.07	0.29	1.06	0.03	1.61	0.36
75	1.25	0.04	2.51	0.14	0.02	0.61	0.23	0.79	1.29
76	0.66	0.10	1.41	0.12	-0.44	0.34	0.13	0.61	0.17

Table 5S Fitted CSA parameters

Residue #	$\Delta\sigma_{eff}$	$\Delta\Delta\sigma_{eff}$	f_{orient}	Δf_{orient}	Asymptotic Correlation Coefficient, ρ*
2	172	7	-0.829	0.014	0.987
3	162	8	-0.799	0.018	0.991
4	170	10	-0.751	0.019	0.985
5	158	13	-0.835	0.033	0.994
6	174	8	-0.835	0.016	0.989
7	175	13	-0.775	0.023	0.987
8	161	21	-0.820	0.052	0.994
9	207	27	-0.701	0.024	0.971
10	163	27	-0.871	0.068	0.991
11	182	10	-0.871	0.019	0.979
12	154	13	-0.852	0.036	0.994
13	173	14	-0.792	0.026	0.986
14	161	7	-0.814	0.016	0.992
15	158	13	-0.881	0.036	0.994
16	149	16	-0.883	0.050	0.995
17	185	8	-0.762	0.011	0.984
18	161	12	-0.762	0.026	0.995
20	185	10	-0.761	0.015	0.974
21	179	35	-0.844	0.063	0.990
22	184	18	-0.758	0.027	0.985
23	167	17	-0.825	0.039	0.975
25	162	5	-0.825	0.012	0.986
26	143	16	-0.934	0.058	0.996
27	176	6	-0.777	0.010	0.985
28	168	12	-0.850	0.027	0.986
29	173	11	-0.770	0.022	0.985
30	157	11	-0.835	0.029	0.994
31	160	20	-0.823	0.051	0.962
32	185	15	-0.754	0.023	0.980
33	190	14	-0.736	0.019	0.967
34	161	8	-0.751	0.017	0.992
35	175	19	-0.797	0.035	0.991
36	181	8	-0.833	0.015	0.982
39	185	12	-0.745	0.017	0.978
40	177	11	-0.759	0.019	0.986
41	176	17	-0.787	0.031	0.989
42	149	15	-0.851	0.046	0.995
43	155	12	-0.853	0.034	0.993
44	144	12	-0.871	0.041	0.995
45	163	14	-0.868	0.033	0.993
46	138	12	-0.953	0.047	0.998
47	168	23	-0.710	0.043	0.993
48	182	12	-0.838	0.021	0.986
49	168	15	-0.850	0.034	0.991
50	178	20	-0.843	0.037	0.988
51	158	14	-0.846	0.035	0.995
52	166	12	-0.787	0.029	0.961
54	157	17	-0.848	0.044	0.992

55	192	18	-0.716	0.023	0.979
56	152	13	-0.843	0.038	0.996
57	182	7	-0.758	0.011	0.983
58	168	10	-0.818	0.022	0.988
59	170	17	-0.735	0.032	0.989
60	179	16	-0.811	0.028	0.987
61	165	7	-0.804	0.014	0.990
62	162	12	-0.853	0.030	0.988
63	181	6	-0.753	0.010	0.988
64	175	5	-0.766	0.010	0.988
65	196	11	-0.779	0.013	0.968
66	179	14	-0.756	0.022	0.990
67	166	12	-0.825	0.027	0.986
68	179	19	-0.728	0.030	0.982
69	153	16	-0.864	0.047	0.974
70	174	17	-0.785	0.031	0.988
71	164	20	-0.830	0.046	0.994
72	154	17	-0.856	0.050	0.982
73	149	15	-0.880	0.048	0.990
74	151	37	-0.873	0.112	0.993
75	109	95	-1.038	0.658	0.999
76	113	58	-0.958	0.353	0.997

* The Asymptotic Correlation Coefficient, ρ, indicates the covariance between the errors in $\Delta\sigma_{eff}$ and f_{orient}.

Table 6S The averages of the q(13T)-values for each residue type (except PRO).

residue type	⟨q(13T)⟩	standard deviation	number of observations
ALA	1.36	0.03	11
LEU	1.37	0.06	18
LYS	1.40	0.07	10
TYR	1.40	0.12	5
CYS	1.40	not determined	1
GLN	1.40	0.05	9
ARG	1.41	0.05	11
VAL	1.41	0.04	8
PHE	1.41	0.10	3
TRP	1.42	not determined	1
ASN	1.42	0.03	6
ASP	1.42	0.07	9
ILE	1.44	0.05	11
GLU	1.44	0.07	11
THR	1.45	0.04	13
MET	1.45	0.08	3
SER	1.46	0.07	6
HIS	1.46	0.06	3
GLY	1.51	0.12	12

Consistency testing:

Under the assumption of equal uncertainty for all sites and an underlying normal distribution the sample variance, s^2, of the q_{long} values observed at a particular field is expected to depend on the squared true variability, Λ^2, and the squared uncertainty, Δ^2, as:

$$s^2\left(q_{long}(B_0)\right) = \Lambda^2\left(q(B_0)\right) + \Delta^2\left(q_{long}(B_0)\right) \qquad \text{(S1)}$$

The corresponding expression for q_{trans} is:

$$s^2\left(q_{trans}(B_0)\right) = \Lambda^2\left(q(B_0)\right) + \Delta^2\left(q_{trans}(B_0)\right) \qquad \text{(S2)}$$

The expected sample variance of the averages of q_{long} and q_{trans} is given by the expression:

$$s^2\left(q_{average}(B_0)\right) = \Lambda^2\left(q(B_0)\right) + 0.25\,\Delta^2\left(q_{long}(B_0)\right) + 0.25\,\Delta^2\left(q_{trans}(B_0)\right) \qquad \text{8S3)}$$

The three equations (S1-S3) constitute an equation system that can be solved for Λ and $\Delta(q_{long})$ and $\Delta(q_{trans})$. The sites that are affected by conformational exchange broadening (D23 and N25) and the data with increased uncertainty due to hydrogen exchange with water (L8, T9, G10, N25, A46, D58, S65, R74, G75), slow relaxation (R74, G75, G76) or if data are missing in any of the data sets derived from refs 1S or 2S (D21, A28, Q31, L69, R72) are excluded from the analysis. Another estimate of the average uncertainty in q_{long} or q_{trans} can be calculated as the average of the uncertainties derived by propagating the uncertainties in the relaxation rates for the same sites, here denoted $\langle s(q_{long})\rangle$ or $\langle s(q_{trans})\rangle$. The error propagation formula was used for propagating the errors. The ratio $\Delta(q_{long})/\langle s(q_{long})\rangle$ was used to scale the uncertainties in all the q_{long} at a particular field. Likewise the uncertainties in q_{trans} were scaled by the ratio $\Delta(q_{trans})/\ \langle s(q_{trans})\rangle$. The q_{trans} at 14.09 T evaluated from ref 1S where compared to the q_{long} values at 14.09 T from the present study. From 11.74 T five different datasets are available. Each of them was matched against the average of the other four. The q_{trans} at 8.45T evaluated from ref1S was matched against the average of the q-values determined at 9.39T, rescaled to correspond to 8.45T according to the best fitting line obtained from the fit to the twelve averages of B_0 q.

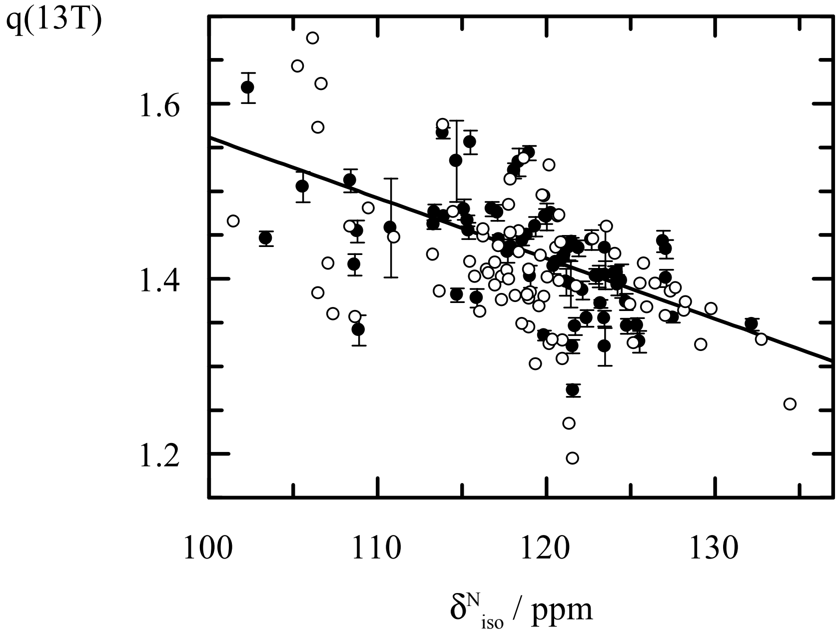

Figure 1S. The graph illustrates the tendency for nitrogen atoms with low isotropic chemical shifts to display large q(13T)-values. The filled circles with error bars represent the ubiquitin data. The error bars correspond to 68 % confidence intervals. The open circles represent the q-values for ribonuclease H evaluated from the data in ref 3S . The ribonuclease H data are generally associated with higher uncertainty, 0.05 according to the ANOVA-analysis, hence the error bars are left out for clarity. The straight line was obtained by weighted linear regression to the ubiquitin data. Apparently a similar trend is observed also for the ribonuclease H data.

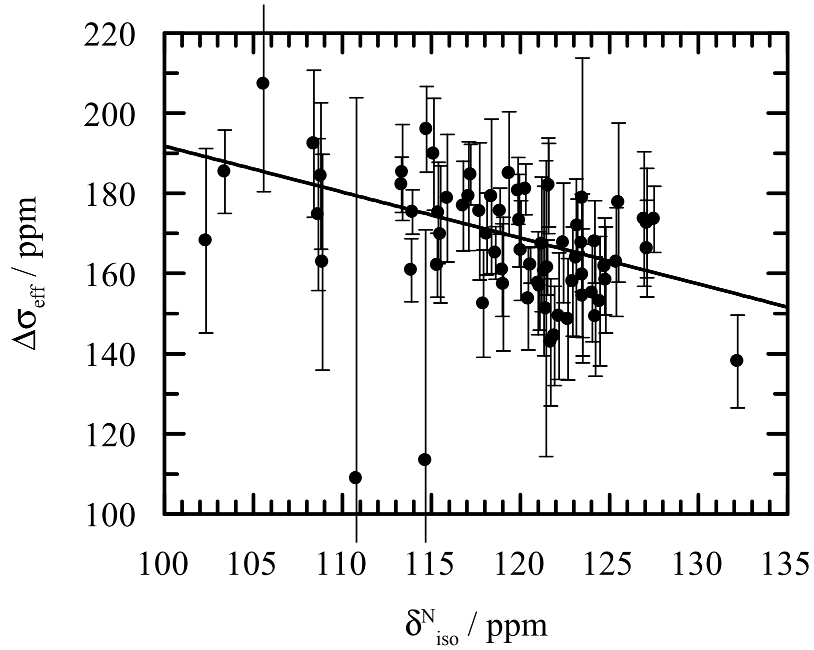

Figure 2S The graph illustrates the tendency for backbone nitrogen atom with a low isotropic chemical shift to display large $\Delta\sigma_{eff}$-values. The fitted slope of -1.15 and its associated uncertainty 0.26 are not compatible with a true slope of zero as seen by comparing their ratio to the t-distribution with 68 degrees of freedom (p-value for the hypothesis that the slope is zero is 3×10^{-5}).

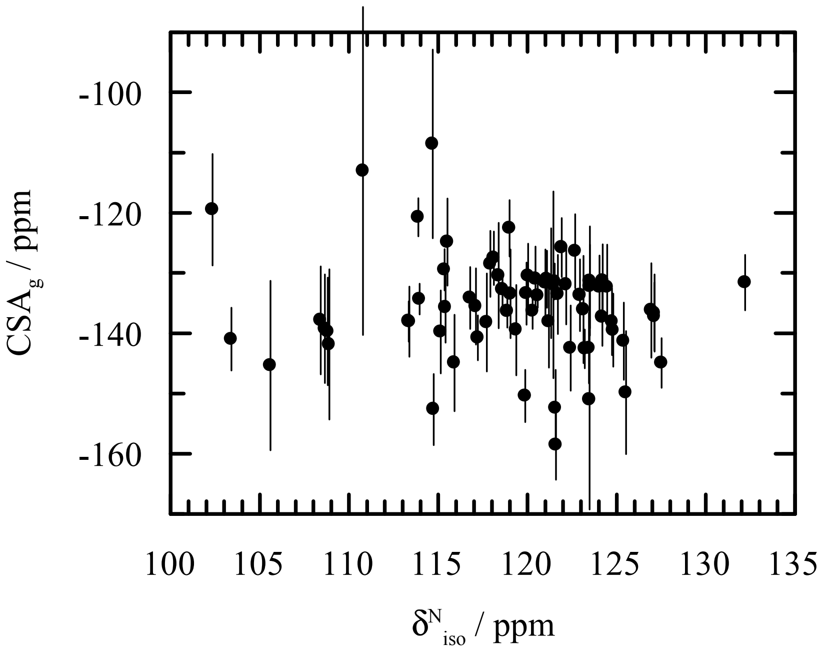

Figure 3S The graph illustrates the lack of apparent correlation between the isotropic chemical shift and the observed CSA_g.

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