



Supplementary Figure 1. Pulse scheme for backbone assignment and determination of protein substructures using $^{13}\text{C}^\alpha$ chemical shift, $^{13}\text{C}^\alpha$ - $\{^1\text{H}^\alpha\}$ splittings and $^{13}\text{C}^\alpha$ CSA. Narrow and wide pulses correspond to flip angles of 90° and 180° , respectively, with phase x unless indicated. Spectral overlap is minimized by an IPAP selection element (open pulses)¹. Pulses following the cpd ^1H -decoupling yield gradient-enhanced $^{15}\text{N} \rightarrow ^1\text{H}^\text{N}$ magnetization transfer². $^{13}\text{C}^\alpha$ pulses are applied with a RF strength of 10.5 kHz. Shaped $^{13}\text{C}'$ pulses have the shape of the center lobe of a $(\sin x)/x$ function, and a duration of 150 μs at 151 MHz ^{13}C frequency. Delay durations: $\epsilon \approx 1.4$ ms; $\Delta = 1.7$ ms; $T = 14$ ms; $\gamma = 7$ ms; $\kappa = 5.35$ ms; $\tau = 2.67$ ms. Phase cycling: $\phi_1 = y, -y$; $\phi_2 = x$; $\phi_3 = 2(x), 2(-x)$; $\phi_{\text{rec}} = x, 2(-x), x$. Quadrature detection in t_1 and t_2 is obtained by States-TPPI on ϕ_2 and by Rance-Kay alternation² on gradient(G_7)/phase(ϕ_4), respectively. All gradients are sine-bell shaped, with 25 G/cm (15 G/cm for G_3 ; 10 G/cm for $G_{7,10,11}$) at their center. Durations: $G_{1,2,3,4,5,6,7,8,9,10,11} = 1.5, 1.1, 0.75, 1.5, 1.1, 2.0, 2.075, 1.2, 1.1, 0.2, 0.075$ ms, with respective gradient axes: $xyz, z, xyz, xyz, xz, yz, z, x, y, z, z$. The sensitivity of this experiment is comparable to that of a 3D (HA)CA(CO)NH that is traditionally used for measurement of $^{13}\text{C}^\alpha$ - $\{^1\text{H}^\alpha\}$ rdc's and it is applicable for proteins up to 25 kDa³.

- (1) Yang, D. W.; Nagayama, K. *J. Magn. Reson. Ser. A* **1996**, *118*, 117-121. Ottiger, M.; Delaglio, F.; Bax, A. *J. Magn. Reson.* **1998**, *131*, 373-378.
- (2) Kay, L. E.; Keifer, P.; Saarinen, T. *J. Am. Chem. Soc.* **1992**, *114*, 10663-10665.
- (3) Kontaxis, G.; Clore, G. M.; Bax, A. *J. Magn. Reson.* **2000**, *143*, 184-196.

Supplementary Table 1. NMR constraints for ubiquitin obtained from IPAP-(HA)CANH and ϕ/ψ angles from MFR homology search

Res	$\delta(^1\text{H}^N)$ (ppm)	$\delta(^{15}\text{N})$ (ppm)	$\delta(^{13}\text{C}^\alpha)$ (ppm)	$^{13}\text{C}^\alpha$ $\sigma_{\text{orth}}-\sigma_{\text{par}}$ (ppm)	$^1\text{J}(\text{C}^\alpha-\text{H}^\alpha)$ (Hz)	$\Delta_{1\text{J}(\text{Ca-Ha})}$ (Hz)	Φ	Ψ
1	-	-	54.045	30.6	146.5	0.2		
2	9.013	122.984	54.72	30.0	145.2	0.1	-86	132
3	8.370	115.226	59.231	41.5	139.3	0.2	-127	147
4	8.671	118.718	54.705	38.3	144.3	0.2	-120	139
5	9.357	121.395	59.993	34.7	142.3	0.2	-127	143
6	9.025	128.096	54.237	38.4	142.5	0.2	-115	126
7	8.807	115.594	60.148	38.8	138.4	0.1	-104	141
8	9.187	121.393	57.091	13.5	145.3	0.1	-62	-25
9	7.698	106.022	61.026	30.9	141.7	0.1	-89	6
10	7.894	109.378	46.383	-66.8	282.7	0.1	a	a
11	7.330	122.041	55.902	23.1	143.1	0.1	-97	143
12	8.705	120.735	61.947	37.0	143.3	0.1	-106	128
13	9.617	127.789	59.615	36.8	141.4	0.2	-122	143
14	8.800	121.729	61.652	25.3	143.7	0.1	-117	131
15	8.805	125.304	52.372	45.5	141.1	0.1	-114	133
16	8.186	122.633	54.514	34.6	142.9	0.2	-114	133
17	9.003	117.679	58.048	44.8	140.7	0.1	-136	163
18	8.721	119.465	52.350	47.7	141.5	0.1	-96	142
19	-	-	64.861	29.5	149.9	0.4	-63	-22
20	7.091	103.567	56.981	27.3	141.8	0.1	-95	-2
21	8.115	124.054	55.465	16.9	144.6	0.1	-75	144
22	7.948	109.159	59.276	28.8	140.3	0.1	-83	163
23	8.580	121.360	61.984	12.2	144.6	0.2	-62	-39
24	10.166	121.380	60.364	29.0	145.7	4.5	-64	-41
25	7.993	121.609	55.590	6.1	149.1	0.1	-66	-40
26	8.173	122.299	67.244	0.8	145.9	0.1	-65	-41
27	8.623	119.089	58.769	5.7	150.3	0.1	-66	-40
28	8.038	123.599	54.972	4.5	147.5	0.1	-65	-37
29	7.924	120.362	59.357	10.5	148.0	0.1	-66	-40
30	8.350	121.476	65.702	7.9	145.6	0.1	-64	-42
31	8.619	123.715	59.629	0.9	148.7	0.1	-62	-42
32	8.080	119.862	57.016	-0.3	150.0	0.1	-67	-41
33	7.488	115.585	57.755	15.8	146.5	0.1	-76	-34
34	8.790	114.505	54.937	36.0	143.3	0.1	-91	-19
35	8.569	109.041	47.065	-64.2	285.1	0.1	a	a
36	6.217	120.429	57.388	41.0	143.1	0.1	-94	128
37	-	-	-	-	-	-	-62	126
38	-	-	65.718	23.8	148.3	0.4	-63	-23
39	8.593	113.783	55.375	15.9	145.0	0.1	-73	-17
40	7.883	117.009	55.212	33.1	140.7	0.1	-101	-4
41	7.549	118.222	56.272	30.3	142.1	0.1	-111	134
42	8.565	123.238	54.754	38.2	141.2	0.2	-119	135
43	8.890	124.597	52.627	30.8	142.2	0.2	-116	137
44	9.184	122.465	58.528	38.6	143.1	0.2	-114	132

45	8.916	125.112	56.071	31.4	142.8	0.2	-128	127
46	9.065	133.106	52.146	33.1	135.1	0.3	60	40
47	8.163	102.592	46.362	-66.6	282.1	0.1	a	a
48	8.042	122.193	54.210	36.1	141.6	0.1	-102	140
49	8.711	123.291	55.519	17.5	143.2	0.1	-95	124
50	8.626	125.857	53.813	26.2	141.6	0.2	-92	140
51	8.448	123.256	55.501	28.7	141.3	0.2	-88	136
52	8.224	120.502	56.159	1.6	146.5	0.2	-66	-23
53			46.173	-72.7	283.3	0.5	-90	-6
54	7.524	119.464	53.864	49.8	141.0	0.1	-89	145
55	8.899	109.003	59.309	36.6	138.5	0.2	-81	157
56	8.216	118.176	58.254	7.9	146.3	0.1	-63	-36
57	8.549	113.667	60.705	6.6	146.4	0.1	-65	-37
58	8.001	124.660	57.000	10.5	149.6	0.1	-67	-29
59	7.322	115.924	57.859	37.3	141.4	0.1	-94	4
60	8.219	116.134	53.773	46.0	135.8	0.1	61	38
61	7.307	119.036	62.047	25.9	141.6	0.1	a	a
62	7.681	125.084	53.216	49.7	139.6	0.1	-103	155
63	8.562	120.751	57.470	5.7	142.8	0.1	-65	133
64	9.385	114.751	58.033	42.9	132.5	0.2	68	18
65	7.728	115.081	60.521	28.6	144.6	0.1	-97	147
66	8.779	117.590	62.093	29.9	143.3	0.2	-108	132
67	9.475	127.929	53.397	45.8	141.8	0.2	-120	142
68	9.288	119.687	55.815	36.3	142.2	0.2	-107	135
69	8.338	123.939	53.381	35.5	143.0	0.2	-109	135
70	9.239	126.710	60.172	31.9	139.4	0.1	-125	143
71	8.166	123.166	53.619	35.3	143.5	0.1	-108	138
72	8.659	123.926	55.300	21.9	141.9	0.1	-126	141
73	8.419	124.708	54.401	20.3	141.7	0.1	-103	129
74	8.510	122.167	56.208	8.5	142.2	0.1	-105	123
75	8.564	111.254	46.241	-19.0	281.4	0.0		
76	8.016	115.218	47.030	-9.4	278.4	0.0		

Dashes indicate that the chemical shift, coupling, CSA or dihedral angle cannot be measured with the methods used or does not apply for this residue. All empty entries are due to resonance overlap, very weak resonance intensities or high flexibility, thereby prohibiting accurate determination of the corresponding values. The uncertainty in the CSA values is mainly caused by slightly different transfer efficiencies for the up- and downfield component and the approximated, average value for the spectral density for dipolar-CSA cross correlation. 'a' indicates residues for which the results of the MFR homology search were ambiguous.

Supplementary Table 2. NMR constraints for calmodulin obtained from IPAP-(HA)CANH and ϕ/ψ angles from MFR homology search

Res	$\delta(^1\text{H}^N)$ (ppm)	$\delta(^{15}\text{N})$ (ppm)	$\delta(^{13}\text{C}^\alpha)$ (ppm)	$^{13}\text{C}_{\text{iso}}^\alpha$ σ_{orth}^- σ_{par} (ppm)	$^{13}\text{C}_{\text{dc}}^\alpha$ σ_{orth}^- σ_{par} (ppm)	^1J ($\text{C}^\alpha\text{-H}^\alpha$) (Hz)	$\Delta_{1\text{J}(\text{Ca-Ha})}$ (Hz)	$^1\text{J+D}$ ($\text{C}^\alpha\text{-H}^\alpha$) (Hz)	$\Delta_{1\text{J+D}(\text{Ca-Ha})}$ (Hz)	Φ	Ψ
1	-	-									
2			54.457	7.5	3.9	141.6	1.1	152.7	0.8	-112	137
3	8.261	118.643	54.969	16.9	5.0	141.7	0.5	129.0	0.5	-83	132
4	8.371	122.090	53.945	15.9	9.5	143.4	1.0	129.6	1.2	-87	156
5	8.842	113.131	59.977	14.4	31.1	141.5	1.5	199.8	3.8	-80	159
6	9.095	120.431	59.572	-8.4	-15.5	148.6	1.2	118.1	3.2	-60	-39
7	7.794	120.704	59.793	15.4	67.1	145.4	5.4	117.7	2.3	-65	-42
8	7.795	120.726	58.235	4.1	6.3	148.3	1.4	193.9	3.0	-67	-40
9	8.308	118.651	66.387	6.0	1.3	150.2	1.8	142.1	3.0	-64	-43
10	7.856	120.465	54.947	10.1	1.1	145.5	6.7	113.0	2.6	-62	-42
11	8.793	120.473	59.035	28.2		139.8	7.8			-64	-43
12	8.795	120.543	57.942	21.3	7.6	146.0	2.0	185.1	3.5	-65	-41
13	9.331	122.102	59.311	-7.6	-10.3	149.7	1.8	129.2	3.9	-63	-40
14	7.787	121.290	59.043	9.3		156.2	5.6			-63	-43
15	7.796	121.313	54.842	-1.9	15.8	147.1	1.5	188.0	5.2	-64	-43
16	8.639	117.943	61.919	-6.3	9.0	151.8	1.5	157.4	3.2	-65	-44
17	8.530	111.462	61.483	5.9	3.9	144.9	1.8	116.5	2.8	-64	-35
18	7.669	121.832	56.844	15.8	17.2	149.8	1.2	119.8	1.9	-67	-30
19	7.348	114.517	59.117	27.5	21.0	143.4	1.8	197.0	4.1	-95	3
20	7.675	122.112	51.985	20.0	13.9	142.5	1.6	129.6	4.3	-106	128
21	8.004	122.867	58.380	6.5	13.4	144.6	1.0	136.8	2.0	a	a
22	8.668	114.026	53.006	24.6	17.9	141.9	1.4	141.0	2.4	a	a
23	7.659	109.369	48.222	-43.9	-35.3	282.6	1.2	229.5	8.0	a	a
24	8.518	120.061	53.628	21.4	26.1	140.4	1.3	120.6	1.5	a	a
25	10.433	112.796	46.485	-55.6	-52.4	281.1	1.3	301.9	2.7	a	a
26	8.110	109.992	59.548	32.0	42.2	140.5	1.9	152.8	2.9	-115	137
27	8.881	116.635	59.372	43.4	36.0	141.5	5.4	146.9	6.5	-100	138
28	8.703	111.141	60.050	27.0	23.8	139.8	2.0	146.5	3.2	-82	150
29	8.381	111.787	64.826	8.3	13.1	146.7	2.0	166.4	4.3	-61	-35
30	7.594	119.157	57.808	24.4	11.1	145.6	2.0	109.3	3.1	-67	-34
31	7.686	117.218	56.062	20.6	21.0	146.4	1.5	182.5	2.3	-77	-37
32	7.428	120.323	58.377	3.0	14.7	144.3	1.6	152.3	2.3	-62	-42
33	8.892	106.010	49.280	-30.0	-32.0	283.8	1.8	319.0	2.2	-65	-37
34	7.658	117.777	65.786	13.5	0.5	146.2	4.0	137.8	1.4	-67	-39
35	7.909	122.847	65.806	1.7	4.2	147.1	1.4	134.7	2.6	-66	-41
36	8.469	118.611	59.680	-1.4	5.6	144.0	2.1	183.3	6.0	-64	-40
37	8.469	119.554	58.784	-8.8	2.4	152.0	2.7	116.5	4.5	-64	-42
38	8.113	119.275	61.382	-12.5	-10.5	144.7	1.2	166.1	2.3	-67	-39
39	7.392	121.216	54.116	39.4	39.3	142.7	1.7	124.1	2.7	-76	-13
40	7.989	107.385	46.775	-37.7	-53.1	281.3	1.2	331.5	4.8	a	a
41	7.843	118.205	53.713	35.0	17.3	142.5	3.1	113.7	3.7	-113	135
42	8.738	116.976	50.730	27.0	21.7	135.9	4.5	125.7	7.4	-117	107

43	-	-	61.939	19.9	17.9	147.2	6.3	139.9	9.8	-53	73
44	8.831	113.441	60.384	20.9	36.9	145.2	1.6	181.8	3.7	-110	141
45	8.936	120.728	59.599	6.1	-3.2	149.0	1.5	115.8	2.1	-65	-39
46	7.811	119.202	54.615	0.4	14.5	148.3	4.5	123.4	12.3	-64	-43
47	7.812	119.270	58.428	12.8	3.4	151.0	1.3	175.1	2.1	-66	-41
48	8.501	120.472	57.584	5.4	13.0	144.4	1.3	167.0	3.3	-65	-42
49	8.135	117.866	58.268	-3.8	-2.1	149.4	1.3	109.2	2.2	-64	-40
50	7.891	119.264	57.099	-0.8	-2.4	152.4	0.8	132.7	1.1	-67	-40
51	8.114	119.463	59.376	12.1	2.1	147.0	1.9	200.3	4.3	-64	-42
52	8.529	120.099	65.426	3.8	-3.2	142.8	2.0	129.9	3.9	-66	-41
53	8.324	117.495	54.954	15.0	9.8	145.8	1.2	121.5	1.5	-62	-39
54	7.593	117.432	58.081	16.4	-0.4	144.9	1.1	146.2	1.3	-70	-31
55	8.101	114.708	62.548	22.3	11.9	142.3	1.9	202.1	8.0	-87	-22
56	8.573	122.688	52.927	25.8	22.8	139.4	1.7	125.6	2.3	-76	140
57	7.797	124.998	54.422	20.1	20.8	144.9	1.4	147.3	1.6	-70	-31
58	8.439	113.906	54.019	26.1	16.5	144.5	1.0	141.9	1.2	-83	-22
59	7.877	108.311	47.753	-40.2	-64.0	286.4	1.3	256.1	2.4	a	a
60	8.763	119.060	53.186	13.7	35.7	143.5	1.8	136.2	2.9	a	a
61	10.041	111.203	47.055	-44.0	-65.7	280.8	1.8	280.3	2.5	a	a
62	7.802	111.162	59.284	27.2	29.5	140.3	1.2	158.9	1.6	-108	129
63	9.142	120.161	59.392	24.3	6.7	141.6	2.7	163.6	5.4	-103	130
64	8.584	124.895	51.596	35.8	33.6	135.3	2.4	157.3	3.6	-91	171
65	8.770	118.203	62.658	9.3	-6.1	144.8	3.1	157.7	5.8	-61	-39
66	-	-	66.194	11.5	20.2	145.2	8.6	138.7	9.8	-64	-41
67	8.387	117.355	58.664	7.2	2.3	149.5	2.0	182.8	4.5	-66	-40
68	8.577	122.703	61.038	14.6	-8.8	151.9	2.2	142.9	2.8	-65	-39
69	8.628	119.034	57.356	8.8	1.9	149.5	1.7	137.8	2.3	-63	-44
70	7.834	115.468	66.224	-2.9	1.2	146.3	1.4	175.1	2.0	-66	-40
71	7.710	121.305	49.473	-24.7	11.4	150.0	6.9	135.6	2.7	-62	-44
72	8.050	118.043	56.119	24.8	17.1	144.3	2.2	161.7	4.2	-68	-39
73	8.439	121.536	54.435	13.3	6.8	145.7	6.9	122.4	5.8	-65	-38
74	7.512	117.027	58.166	22.3	13.0	149.9	1.9	188.7	2.8	-70	-39
75	7.841	118.652	56.312	9.9	22.6	147.5	1.5	122.4	1.9	-71	-27
76	8.050	118.043	56.119	24.8	34.4	144.3	2.2	167.4	1.8		
77	7.801	120.766	56.602	17.4	7.3	146.5	1.3	149.4	0.8		
78	8.339	121.845	54.428	16.4	18.4	142.7	0.9	160.6	1.1		
79	8.201	115.062	62.177	7.1	13.7	141.7	0.7	152.7	0.6		
80	8.536	123.551	54.409	21.2	13.0	144.4	1.0	157.6	0.9		
81	8.557	117.630	59.297	6.2	5.9	143.2	0.9	164.2	1.2		
82	8.519	122.467	57.985	12.2	26.2	143.0	1.4	126.1	2.0		
83	8.318	120.063	59.062	3.2	-1.5	151.1	1.3	149.6	1.1	-64	-37
84	8.317	118.869	59.099	23.2	16.9	148.4	1.5	173.5	3.0	-66	-40
85	8.061	122.206	64.084	20.8	24.5	145.3	2.6	145.6	3.3	-66	-42
86	8.472	121.993	59.714	-2.7	10.0	150.0	2.1	113.6	2.7	-65	-40
87	8.242	118.877	58.515	0.6	0.4	148.2	1.5	169.7	1.3	-63	-41
88	8.023	122.260	54.733	-0.4	3.2	150.7	1.4	174.3	2.1	-65	-41
89	8.635	119.006	61.745	-0.2	7.8	146.7	2.0	120.9	2.3	-65	-41
90	7.761	115.899	58.539	15.6	7.0	148.9	1.7	138.0	1.8	-66	-35
91	7.651	118.514	65.316	-2.3	11.0	147.8	1.1	174.5	1.6	-70	-40

92	7.683	116.943	59.569	1.9	10.2	145.0	1.7	157.1	2.9	-74	-31
93	7.932	117.212	51.856	23.0		143.7	2.2			-83	83
94	7.790	126.039	58.689	10.1	1.6	149.2	1.3	114.0	1.4	-65	-35
95	8.251	114.075	52.642	21.1	23.9	137.4	0.8	158.6	1.0	-68	-35
96	7.866	109.415	48.185	-42.9	-31.9	283.2	0.7	287.9	1.1	a	a
97	8.385	119.594	52.347	25.3	30.3	137.5	1.1	139.2	1.4	a	a
98	10.727	113.160	46.178	-39.8	-42.7	283.5	1.2	267.8	1.6	a	a
99	7.676	115.866	55.667	16.0	19.1	147.0	1.0	171.7	2.3	-72	-32
100	10.209	127.357	59.801	23.6	23.3	145.8	2.9	166.7	5.1	-78	-29
101	9.015	123.876	55.479	23.9	14.3	140.4	1.5	154.1	2.6	-108	10
102	8.337	118.478	55.629	-20.5	-15.2	147.1	2.9	159.1	8.1	-60	-41
103	8.334	118.509	54.809	14.6	-0.9	145.1	1.2	142.7	1.1	-64	-40
104	7.941	119.756	58.862	10.7	10.8	145.6	1.7	172.3	3.8	-66	-41
105	8.700	121.353	57.824	7.3	1.0	143.6	1.7	110.4	1.9	-67	-40
106	8.633	117.690	59.425	-3.2	-3.0	144.8	1.4	164.6	1.8	-69	-32
107	7.930	118.806	48.740	-3.3	7.5	149.4	1.8	155.6	4.0	-73	-23
108	7.936	118.749	59.158	-0.9	-7.7	149.3	1.4	152.9	1.9	-68	-35
109	8.319	116.833	57.018	21.4	18.3	145.7	2.5	124.5	2.2	-71	-39
110	8.246	114.830	65.066	-4.3	0.3	150.2	1.8	152.9	1.5	-64	-40
111	8.031	122.132	55.227	11.5	6.7	144.5	1.5	161.9	1.9	-66	-34
112	8.008	119.447	55.037	17.0	7.0	141.7	1.5	112.9	1.2	-71	-35
113	7.962	107.126	46.502	-39.9	-43.2	281.1	0.6	288.1	0.8	a	a
114	7.968	120.354	54.984	15.0	19.5	142.3	0.8	153.9	0.9	-125	132
115	8.671	123.819	55.327	22.4	4.8	141.1	1.1	149.6	1.1	-102	123
116	8.165	124.609	53.804	20.9	28.7	142.1	0.9	160.4	1.0	-104	155
117	9.309	114.772	60.346	18.1	17.4	140.3	1.0	165.8	2.4	-82	169
118	8.981	121.202	57.620	5.4	5.5	151.2	0.9	126.2	1.4	-62	-41
119	8.780	119.295	59.662	9.5	12.4	145.8	0.7	153.2	0.9	-66	-40
120	8.182	121.463	58.888	14.5	-4.1	143.9	3.6	176.1	6.1	-65	-40
121	8.180	121.441	66.587	12.1	4.2	146.6	1.6	118.7	1.8	-67	-40
122	8.133	119.884	57.256	9.5	-7.5	151.4	0.8	154.1	0.8	-62	-45
123	8.059	119.780	58.739	15.8	16.3	145.1	1.1	152.6	1.1	-67	-37
124	7.885	119.766	59.033	-17.7	-23.1	146.8	1.0	171.1	4.0	-68	-40
125	8.026	118.535	63.477	1.3	14.2	144.7	1.5	114.5	1.7	-67	-38
126	8.221	118.562	59.408	1.7	0.0	145.2	1.0	157.4	1.1	-66	-39
127	8.036	116.033	58.137	1.5	7.7	148.8	0.7	158.2	1.1	-67	-42
128	7.425	118.952	51.734	8.2	38.9	146.4	1.0	148.8	2.6	-66	-33
129	7.933	117.609	53.578	12.7	30.6	145.6	1.4	128.3	1.9	-62	-40
130	8.425	127.793	62.958	6.3	19.7	144.6	1.3	147.3	2.0	-70	-44
131	8.365	116.636	53.416	28.5	26.9	138.4	0.9	161.6	1.2	-67	-35
132	7.654	108.668	48.566	-47.8	-43.5	284.6	0.7	286.2	1.5	a	a
133	8.408	120.893	53.293	26.3	42.0	137.9	0.9	110.9	1.6	-99	6
134	10.473	113.102	46.761	-36.0	-41.4	280.5	0.7	287.0	1.1	a	a
135	8.029	115.525	52.771	26.5	40.6	141.5	0.9	156.4	1.4	-123	143
136	9.211	125.446	61.337	28.5	22.5	145.1	2.6	171.9	5.4	-109	126
137	9.562	129.047	50.794	33.1	50.3	137.6	1.7	170.9	4.2	-102	168
138	8.563	118.523	62.451	-4.6	-9.0	150.5	1.6	162.0	3.9	-61	-39
139	8.202	118.470	60.075	0.9	-1.8	144.0	0.9	116.2	1.1	-64	-42
140	8.839	119.918	58.007	3.6	1.9	150.4	1.1	176.8	2.4	-66	-40

141	9.069	124.943	61.164	2.2	1.2	150.4	1.5	134.7	2.0	-66	-41
142	8.594	119.523	66.637	-9.0	8.4	150.0	1.3	146.5	2.3	-64	-40
143	7.405	118.007	58.376	3.6	11.2	145.1	1.3	141.1	1.9	-67	-40
144	8.040	119.795	58.005	0.7	10.3	151.5	0.9	151.2	1.6	-66	-34
145	7.920	114.825	54.793	35.3	31.6	145.0	2.3	148.2	2.5	-86	-14
146	7.645	112.407	62.423	14.7	18.6	140.5	0.7	125.0	0.6	-77	65
147	7.878	126.874	52.465	20.4	5.2	142.1	0.6	142.3	0.4		
148	7.802	125.793	57.171	8.8	5.1	140.9	0.2	137.9	0.1		

Dashes indicate that the chemical shift, coupling, CSA or dihedral angle cannot be measured with the methods used or does not apply for this residue. All empty entries are due to resonance overlap, very weak resonance intensities or high flexibility, thereby prohibiting accurate determination of the corresponding values. The uncertainty in the CSA values is mainly caused by slightly different transfer efficiencies for the up- and downfield component and the approximated, average value for the spectral density for dipolar-CSA cross correlation. 'a' indicates residues for which the results of the MFR homology search were ambiguous.