Supplementary table 1

Residue		Δδ/ΔT	CSD	Hydrogen bond prediction: H exchange	Δδ/ΔT	H-bond acceptor
G	1	-	-	-	-	-
V	2	-5.78	0.86			
Y	3	-2.06	0.76	○	●	92
H	4	-3.67	0.85		●	
R	5	-2.62	0.46	●	●	90
E	6	-	-		-	6s
A	7	-4.79	0.65			10
R	8	-6.30	0.72			
S	9	-3.95	-0.81		○	
G	10	-2.09	-0.92		●	7
K	11	-6.24	-0.19			
Y	12	-5.12	1.88	●		89s
K	13	-	-	●	-	88
L	14	-4.11	1.18	●	●	88
T	15	-6.04	0.71	●		18s
Y	16	5.58	-0.82		●	84
A	17	-5.76	0.35			
E	18	-3.57	-1.06	●	●	15s
A	19	-3.50	0.48	●	●	15
K	20	-	-	●	-	16
A	21	-4.45	-0.82	●	●	17
V	22	0.00	0.11	●	●	18
C	23	-2.72	-0.59	●	●	19
E	24	-0.50	-0.29	●	●	20
F	25	-3.39	0.71	●	●	21
E	26	-4.65	-0.99			22/23
G	27	0.13	-0.67		●	23/24
G	28	-2.31	-0.56		●	23
H	29	-1.41	-0.06	●	●	93
L	30	-7.42	1.17			
A	31	-5.28	1.15	●		91
T	32	-1.15	0.36	○	●	35s
Y	33	-3.62	0.50		○	
K	34	-	-		-	
Q	35	-4.16	-0.53	●	●	32s
L	36	-5.28	0.31	●		32
E	37	-3.83	0.12	●	●	33
A	38	-2.91	-0.46	●	●	34
A	39	-	-	●	-	35
R	40	-2.81	0.56	○	●	36
K	41	-	-	●	-	37
I	42	-1.24	-0.86		●	39
G	43	-1.53	-0.54	○	●	40
F	44	-2.63	-0.24	○	●	39
H	45	-5.96	-1.06			43
V	46	-5.28	-0.02			60
C	47	-6.05	0.05			
A	48	-0.55	-1.78		○	
A	49	-4.28	0.26		●	47
G	50	-2.96	0.38	●	●	58

Residue		Δδ/ΔT	CSD	Hydrogen bond prediction: H exchange	Δδ/ΔT	H-bond acceptor
W	51	-2.08	0.54	●	●	89
M	52	-1.75	0.80	●	●	56
A	53	-0.79	0.32		●	31
K	54	-8.07	0.71			
G	55	-1.73	-0.07		●	52
R	56	-1.35	-1.49		●	52/53
V	57	1.30	-1.07		●	
G	58	-1.60	-0.28		○	50
Y	59	-0.47	-0.37		●	76
P	60	-	-	-	-	-
I	61	-	-		-	74
V	62	-	-		-	
K	63	-2.54	-1.00		○	
P	64	-	-	-	-	-
G	65	-9.34	0.14			
P	66	-	-	-	-	-
N	67	-	-		-	
C	68	2.35	-0.90		●	65
G	69	-	-		-	65
F	70	-3.06	-0.27		○	
G	71	-0.11	-0.18		●	
K	72	-	-		-	
T	73	-7.68	-0.17			
G	74	-3.44	-0.33		●	61
I	75	-	-		-	
I	76	-3.64	0.57		●	59
D	77	-7.34	-0.15			75
Y	78	-4.14	1.26		●	57
G	79	-2.75	0.58		●	77s
I	80	-	-		-	
R	81	-1.25	0.08		●	
L	82	-2.32	0.10		○	
N	83	-5.03	0.23			81
R	84	-8.72	0.43			
S	85	-2.24	0.28		●	83
E	86	0.14	-1.21		●	83
R	87	-5.46	-0.89			
W	88	-3.34	0.72	●	●	14
D	89	-	-	●	-	49
A	90	-2.45	0.20	●	●	5
Y	91	-3.74	0.24		●	51
C	92	-1.17	0.09	●	●	3
Y	93	-2.54	1.27	●	●	29
N	94	-1.96	-0.63		●	1
P	95	-	-	-	-	-
H	96	-	-		-	94s
A	97	-3.16	-1.31		●	94
K	98	-8.29	-0.25			96

Supplementary table 1. Temperature coefficients and chemical shift deviations for Link_TSG6 (columns 1-3).

Hydrogen bond predictions are shown for a variety of data (columns 4-6): (4) hydrogen exchange data; filled circles indicate slow-exchanging amide protons, outlined circles indicate amide hydrogen atom that were not found to be in slow exchange, but were considered to be involved in hydrogen bonds and were included in the NMR structure due to NOESY data. (5) Temperature coefficients; filled circles indicate groups with temperature coefficients more positive than -4.6 $\Delta\delta/\Delta K$, outlined circles indicate groups with temperature coefficients more positive than -4.6 $\Delta\delta/\Delta K$ but for which there is no other evidence for a hydrogen bond and upon inclusion of the chemical shift deviation fall above Anderson's line (see Methods), i.e., are not likely to be involved in a hydrogen bond.

Column (6) shows hydrogen bond acceptors listed as indicated by the NMR structure; the acceptor is the backbone carbonyl atom of the residue indicated, except where an 's' shows it to be a side chain oxygen.

	Experiment		Simulation	
Residue #	Order parameter	Err	N-H	N-Calpha
2	0.831	0.021	0.837	0.958
3	0.837	0.011	0.895	0.974
4	0.884	0.004	0.884	0.972
5	0.869	0.011	0.866	0.971
6			0.833	0.948
7	0.918	0.011	0.810	0.933
8			0.707	0.909
9			0.679	0.866
10	0.850	0.011	0.330	0.833
11	0.762	0.006	0.657	0.914
12	0.924	0.007	0.820	0.934
13			0.811	0.953
14	0.902	0.014	0.884	0.967
15	0.832	0.004	0.891	0.971
16	0.906	0.004	0.899	0.970
17	0.834	0.015	0.897	0.962
18	0.838	0.013	0.885	0.967
19	0.807	0.006	0.915	0.970
20			0.917	0.967
21	0.828	0.007	0.894	0.968
22	0.834	0.016	0.910	0.970
23	0.798	0.010	0.907	0.972
24			0.901	0.966
25	0.855	0.007	0.877	0.956
26	0.823	0.005	0.872	0.960
27	0.857	0.005	0.767	0.929
28	0.871	0.008	0.775	0.887
29	0.825	0.010	0.870	0.957
30	0.814	0.012	0.888	0.972
31	0.857	0.005	0.904	0.973
32	0.816	0.011	0.888	0.974
33			0.893	0.972
34			0.897	0.966
35	0.820	0.007	0.907	0.971
36	0.885	0.006	0.913	0.975
37	0.837	0.004	0.918	0.970
38	0.830	0.006	0.912	0.965
39			0.900	0.965
40	0.907	0.007	0.914	0.968
41			0.890	0.954
42	0.786	0.006	0.862	0.943
43	0.780	0.007	0.830	0.913
44	0.831	0.006	0.515	0.941
45	0.866	0.010	0.751	0.930
46	0.848	0.009	0.712	0.938
47			0.825	0.958
48	0.739	0.005	0.802	0.949
49	0.821	0.012	0.806	0.952
50	0.897	0.007	0.858	0.955
51	0.810	0.005	0.917	0.976
52	0.865	0.005	0.906	0.971
53	0.864	0.006	0.889	0.931
54	0.870	0.013	0.808	0.922

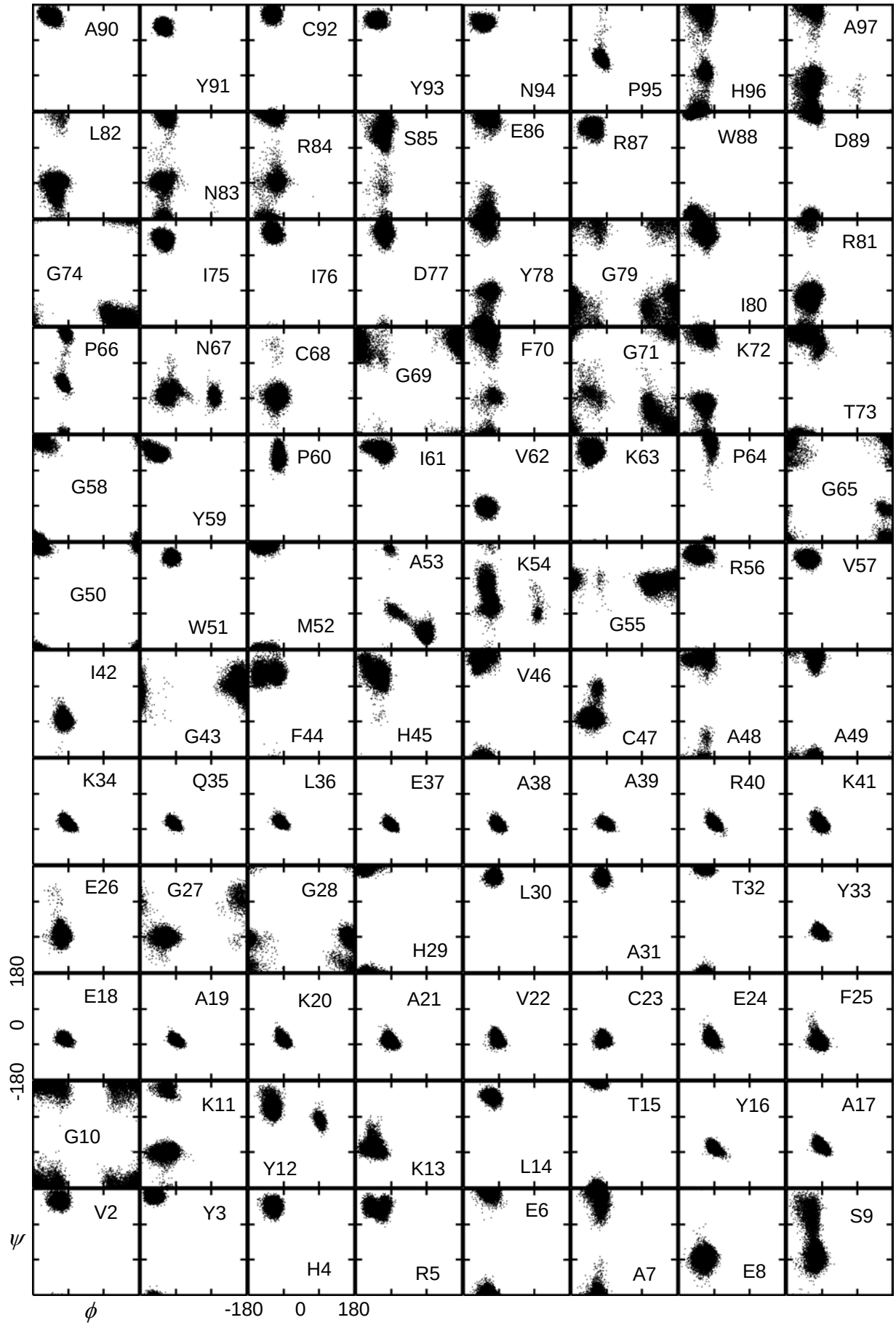
55	0.904	0.007	0.463	0.939
56	0.875	0.014	0.820	0.960
57	0.916	0.004	0.847	0.970
58	0.868	0.005	0.897	0.957
59	0.898	0.005	0.883	0.968
60				0.963
61			0.807	0.968
62			0.867	0.942
63	0.787	0.007	0.783	0.921
64				0.924
65			0.773	0.891
66				0.891
67			0.739	0.893
68	0.900	0.010	0.752	0.904
69			0.751	0.911
70	0.910	0.014	0.710	0.886
71	0.926	0.046	0.654	0.877
72			0.646	0.860
73	0.882	0.018	0.628	0.906
74	0.862	0.016	0.680	0.921
75			0.840	0.960
76	0.853	0.004	0.876	0.970
77	0.771	0.004	0.853	0.961
78	0.814	0.007	0.827	0.944
79	0.887	0.005	0.602	0.879
80			0.693	0.888
81	0.851	0.007	0.733	0.867
82			0.711	0.873
83	0.931	0.014	0.689	0.831
84	0.879	0.022	0.636	0.816
85			0.650	0.852
86	0.898	0.007	0.653	0.864
87	0.784	0.010	0.786	0.948
88	0.865	0.007	0.832	0.971
89			0.859	0.976
90	0.841	0.006	0.887	0.970
91	0.800	0.008	0.897	0.977
92	0.840	0.005	0.883	0.978
93	0.823	0.005	0.896	0.976
94	0.847	0.017	0.873	0.957
95				0.912
96			0.777	0.860
97	0.627	0.190	0.512	0.729
98	0.376	0.008	0.194	0.556

Supplementary table 2. Experimental order paramters and those calculated from the simulation using two different methods (correlation of the N-H vector and the N-Cα vector).

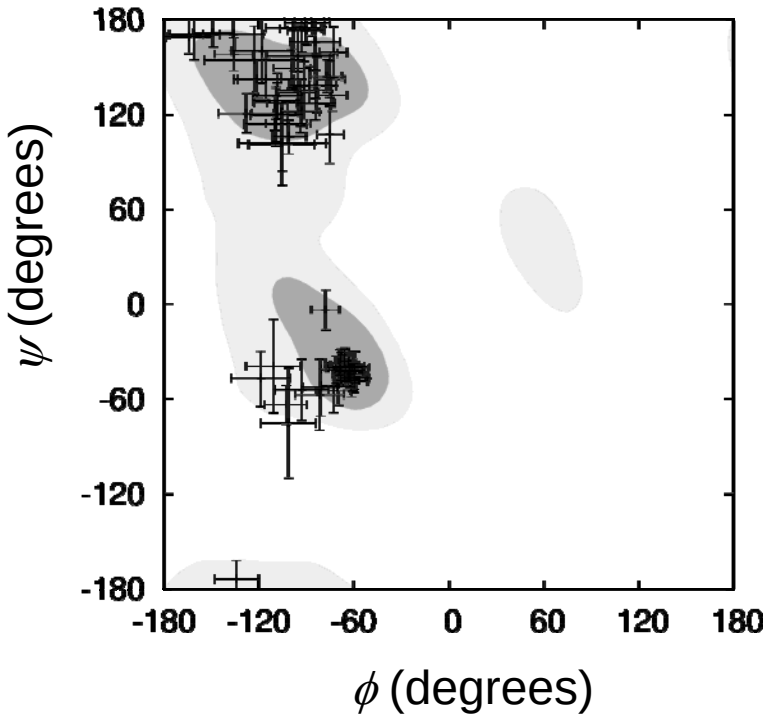
	Experimental data				Aligned CA		Aligned NCA	
Residue #	T1	Err	NOE	Err	T1	NOE	T1	NOE
2	2.503	0.056	0.726	0.011	2.446	0.717	2.552	0.754
3	2.513	0.036	0.768	0.019	2.612	0.722	2.593	0.759
4	2.655	0.005	0.783	0.023	2.578	0.724	2.587	0.757
5	2.611	0.030	0.776	0.022	2.535	0.707	2.587	0.755
6	2.444	0.016			2.469	0.663	2.546	0.723
7	2.757	0.029	0.758	0.019	2.413	0.642	2.508	0.717
8	3.050	0.017	0.759	0.018	2.132	0.591	2.454	0.702
9	3.141	0.047	0.722	0.015	2.072	0.552	2.357	0.672
10	2.557	0.036	0.754	0.010	1.143	0.096	2.288	0.636
11	2.347	0.016	0.610	0.010	2.002	0.553	2.464	0.709
12	2.778	0.016	0.766	0.028	2.426	0.665	2.510	0.722
13			0.762	0.020	2.400	0.668	2.547	0.742
14	2.713	0.045	0.806	0.024	2.586	0.710	2.577	0.751
15	2.501	0.009	0.784	0.022	2.605	0.714	2.586	0.755
16	2.721	0.005	0.806	0.034	2.621	0.724	2.585	0.753
17	2.504	0.046	0.705	0.013	2.617	0.721	2.561	0.755
18	2.515	0.034	0.795	0.013	2.580	0.725	2.576	0.755
19	2.423	0.014	0.781	0.014	2.664	0.728	2.581	0.757
20			0.771	0.012	2.671	0.726	2.578	0.753
21	2.485	0.020	0.786	0.015	2.609	0.720	2.576	0.758
22	2.507	0.042	0.757	0.013	2.655	0.722	2.584	0.756
23	2.401	0.027	0.792	0.013	2.646	0.723	2.587	0.757
24	2.423	0.014			2.634	0.715	2.574	0.751
25	2.568	0.017	0.784	0.017	2.566	0.709	2.553	0.744
26	2.471	0.009	0.760	0.018	2.557	0.701	2.565	0.743
27	2.573	0.009	0.799	0.015	2.266	0.674	2.501	0.715
28	2.616	0.023	0.762	0.014	2.335	0.602	2.430	0.651
29	2.479	0.029	0.764	0.018	2.551	0.702	2.553	0.749
30	2.451	0.035	0.744	0.017	2.596	0.715	2.590	0.754
31	2.572	0.009	0.767	0.019	2.635	0.727	2.588	0.761
32	2.450	0.029	0.759	0.020	2.588	0.725	2.591	0.761
33	3.261	0.035	0.750	0.023	2.601	0.729	2.587	0.758
34					2.613	0.727	2.574	0.755
35	2.463	0.017	0.746	0.019	2.642	0.727	2.585	0.757
36	2.658	0.013	0.727	0.011	2.658	0.730	2.594	0.758
37	2.512	0.006	0.760	0.018	2.673	0.729	2.583	0.757
38	2.492	0.014	0.751	0.015	2.655	0.730	2.570	0.756
39			0.722	0.009	2.621	0.727	2.570	0.755
40	2.720	0.017	0.760	0.017	2.664	0.725	2.578	0.755
41			0.674	0.013	2.598	0.719	2.545	0.746
42	2.363	0.017	0.750	0.017	2.517	0.716	2.518	0.745
43	2.345	0.017	0.740	0.019	2.431	0.708	2.441	0.739
44	2.507	0.011	0.709	0.017	1.595	0.498	2.515	0.741
45	2.599	0.031	0.784	0.042	2.238	0.644	2.497	0.723
46	2.565	0.018	0.699	0.036	2.134	0.617	2.525	0.717
47	2.801	0.074			2.434	0.678	2.557	0.746
48	2.219	0.010	0.733	0.019	2.382	0.657	2.537	0.739
49	2.465	0.037	0.764	0.022	2.405	0.637	2.547	0.736
50	2.693	0.018	0.775	0.028	2.513	0.705	2.545	0.753
51	2.434	0.010	0.769	0.019	2.671	0.728	2.595	0.761
52	2.597	0.010	0.770	0.024	2.639	0.728	2.585	0.757
53	2.594	0.012	0.749	0.014	2.617	0.689	2.514	0.704
54	2.609	0.038	0.760	0.030	2.406	0.646	2.488	0.704
55	2.718	0.020	0.743	0.019	1.586	0.173	2.506	0.746

56	2.629	0.039	0.755	0.017	2.403	0.702	2.564	0.745
57	2.752	0.002	0.763	0.026	2.482	0.704	2.582	0.757
58	2.606	0.011	0.768	0.022	2.615	0.722	2.546	0.757
59	2.698	0.008	0.774	0.023	2.579	0.720	2.581	0.750
60							2.567	0.750
61					2.384	0.670	2.580	0.751
62					2.549	0.690	2.528	0.726
63	2.371	0.013	0.723	0.029	2.321	0.662	2.470	0.727
64							2.485	0.716
65	2.402	0.024			2.315	0.623	2.408	0.698
66							2.410	0.695
67			0.706	0.022	2.225	0.602	2.412	0.701
68	2.713	0.029	0.710	0.021	2.235	0.649	2.439	0.706
69					2.235	0.645	2.452	0.715
70	2.804	0.031	0.620	0.019	2.145	0.590	2.412	0.670
71	2.920	0.115	0.596	0.017	2.007	0.530	2.382	0.678
72			0.722	0.009	1.971	0.548	2.349	0.659
73	2.707	0.054	0.637	0.016	2.008	0.389	2.453	0.691
74	2.605	0.045	0.699	0.021	2.114	0.492	2.481	0.713
75			0.699	0.016	2.460	0.707	2.561	0.750
76	2.561	0.005	0.779	0.033	2.560	0.718	2.582	0.755
77	2.322	0.008	0.714	0.020	2.490	0.717	2.562	0.750
78	2.451	0.019	0.732	0.024	2.430	0.692	2.528	0.731
79	2.666	0.007	0.773	0.020	1.890	0.454	2.395	0.667
80			0.753	0.013	2.116	0.555	2.424	0.659
81	2.557	0.018	0.774	0.027	2.267	0.509	2.412	0.596
82	1.443	0.003			2.187	0.526	2.402	0.631
83	2.800	0.038	0.764	0.017	2.148	0.477	2.326	0.572
84	2.645	0.059	0.763	0.022	2.044	0.371	2.304	0.539
85	3.227	0.082	0.767	0.017	2.100	0.358	2.367	0.597
86	2.704	0.017	0.781	0.023	2.060	0.441	2.407	0.589
87	2.353	0.025	0.796	0.016	2.349	0.635	2.542	0.729
88	2.597	0.018	0.772	0.027	2.438	0.704	2.584	0.757
89			0.771	0.026	2.513	0.712	2.595	0.760
90	2.530	0.018	0.716	0.019	2.591	0.717	2.581	0.756
91	2.417	0.019	0.697	0.023	2.612	0.729	2.598	0.762
92	2.526	0.011	0.727	0.018	2.573	0.727	2.599	0.761
93	2.472	0.011	0.790	0.019	2.611	0.726	2.596	0.761
94	2.549	0.048	0.737	0.017	2.546	0.721	2.551	0.753
95							2.444	0.730
96			0.609	0.013	2.298	0.662	2.329	0.685
97	2.341	0.390	0.294	0.007	1.640	0.363	2.052	0.532
98	1.469	0.031	-0.273	0.007	0.842	-0.625	1.695	0.252

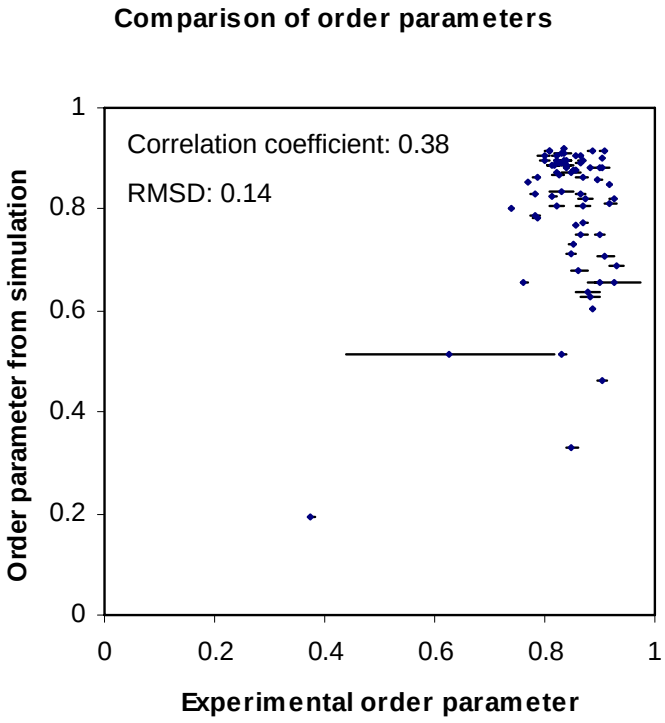
Supplementary table 3. Comparison between experimental and theoretical relaxation measurements calculated using two different methods (correlation of the N-H vector and the N-Cα vector).

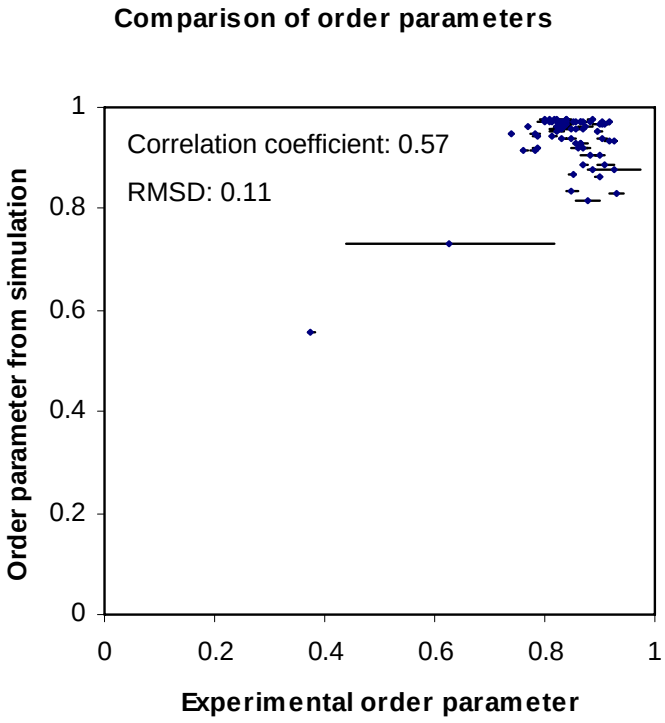


Supplementary figure 1. Scatter plots for each of the (ϕ,ψ)-angles from a 0.25μs molecular dynamics simulation of Link_TSG6 with explicit water and ions.

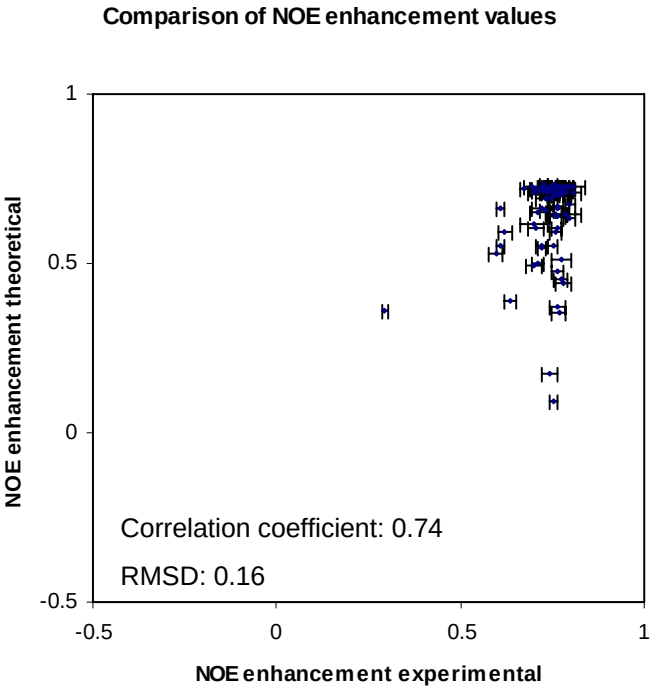


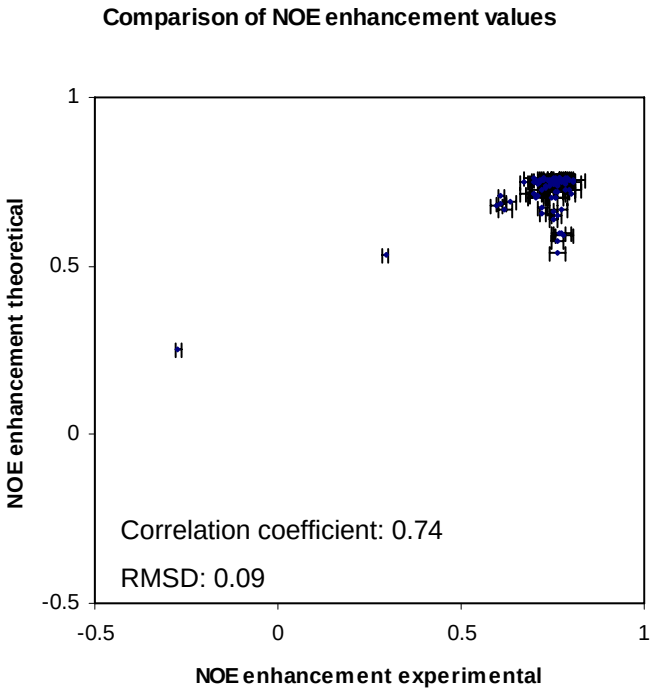
Supplementary figure 2. Average and standard deviation for (ϕ,ψ)-angles that had a monomodal distribution plotted on top of the preferred Ramachandran range of angles (shaded), from a 0.25μs molecular dynamics simulation of Link_TSG6.



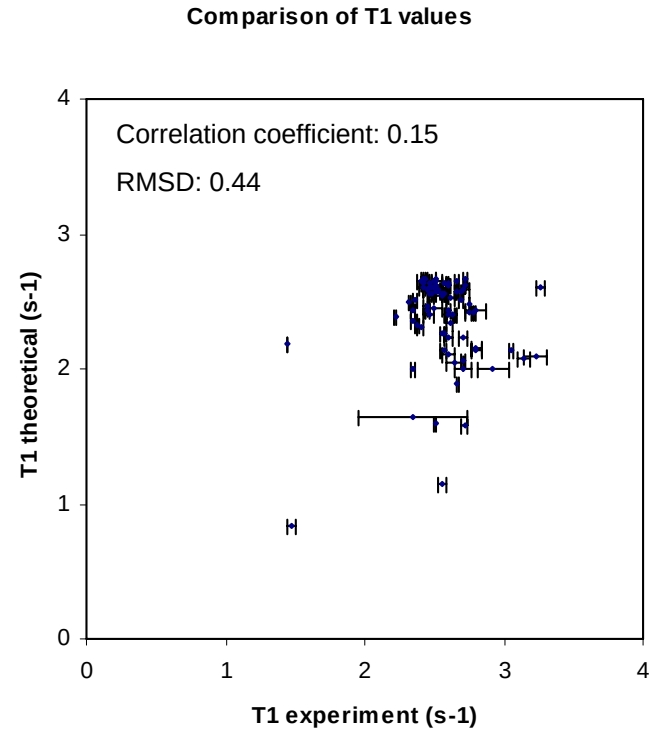


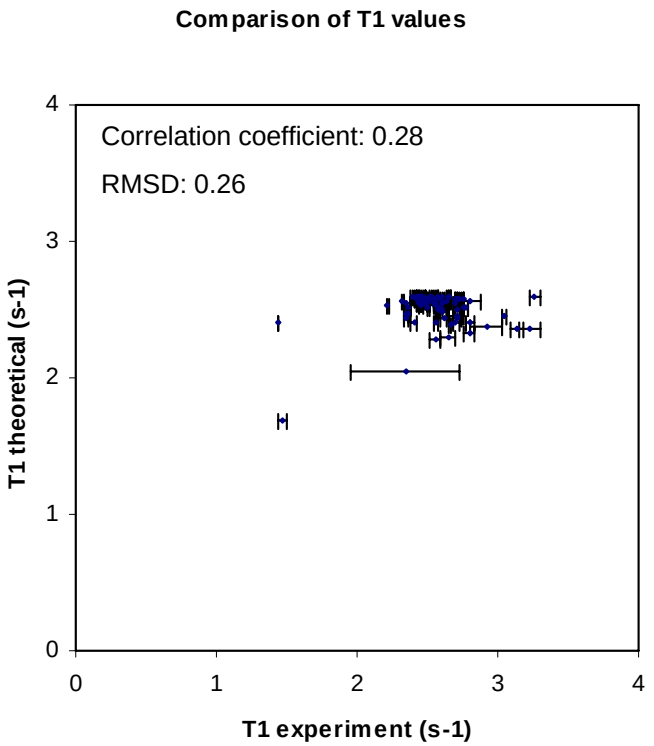
Supplementary figure 3. Comparison between experimental and theoretical Lipari-Szabo order parameters (S^2) based on correlations of the N-H vector (*top*) and the N-Cα vector (*bottom*).



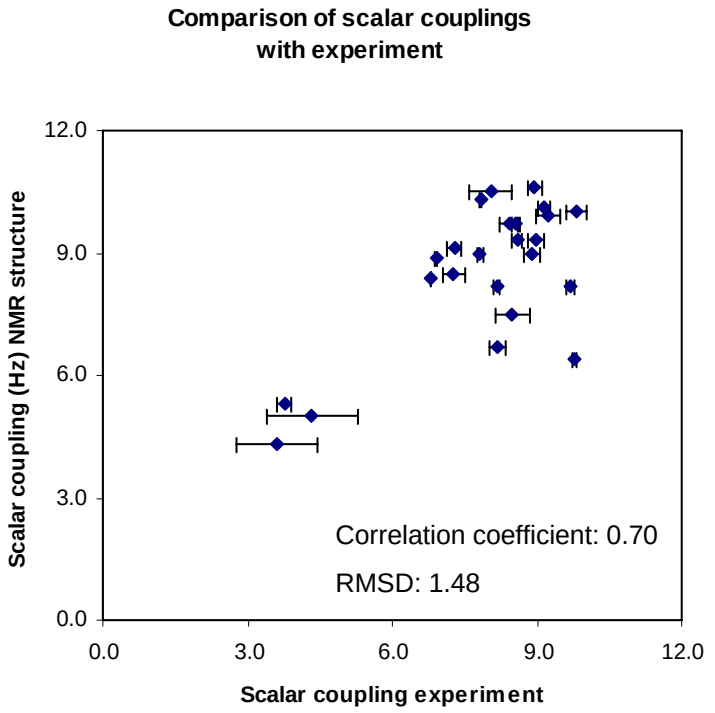


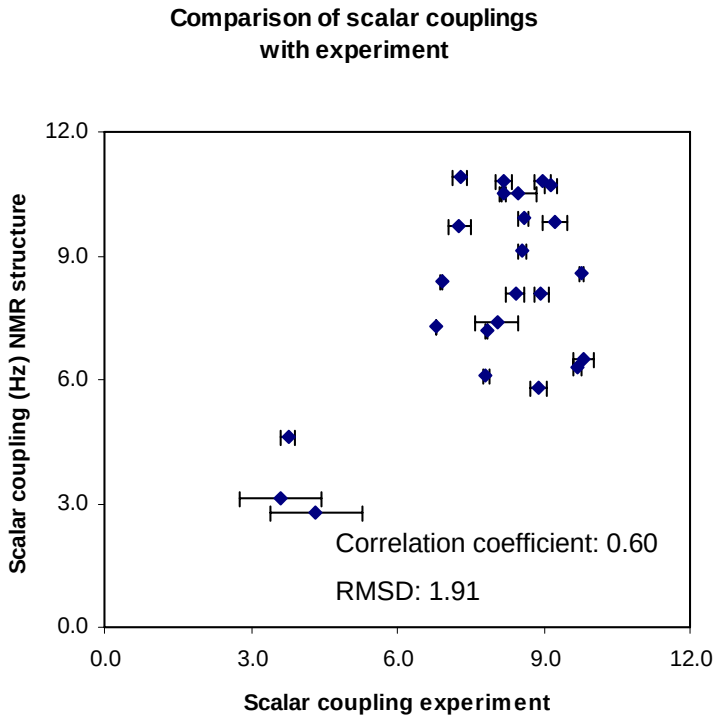
Supplementary figure 4. Comparison between experimental and theoretical ^{1}H-^{15}N NOE enhancement values based on correlations of the N-H vector (*top*) and the N-Cα vector (*bottom*).





Supplementary figure 5. Comparison between experimental and theoretical T1 values based on correlations of the N-H vector (*top*) and the N-Cα vector (*bottom*).





Supplementary figure 6. Comparison between experimental and theoretical scalar couplings (in Hz) based on the simulation (*top*) and the lowest-energy NMR structure (*bottom*).