Supplementary Material for

A maximum entropy approach to the study of residue-specific backbone angle distributions in α-synuclein, an intrinsically disordered protein

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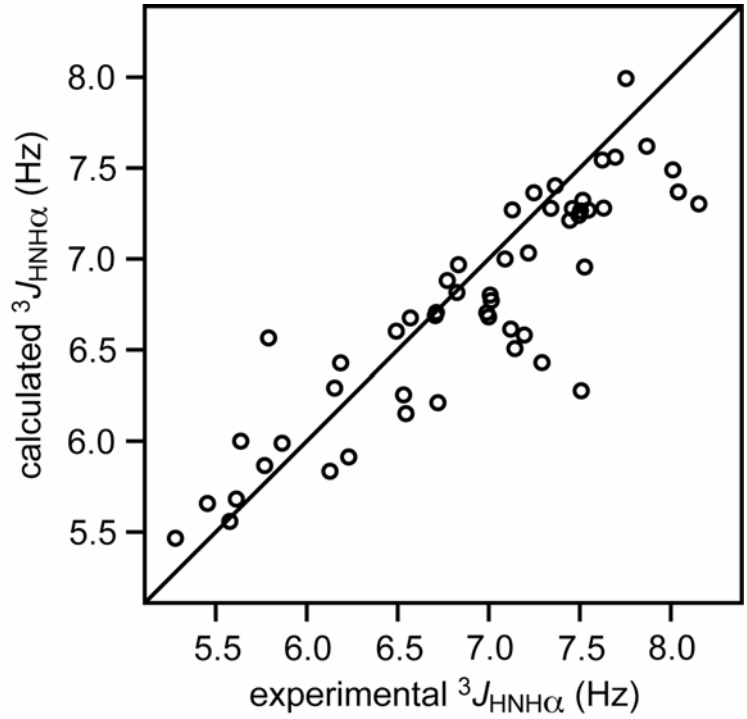
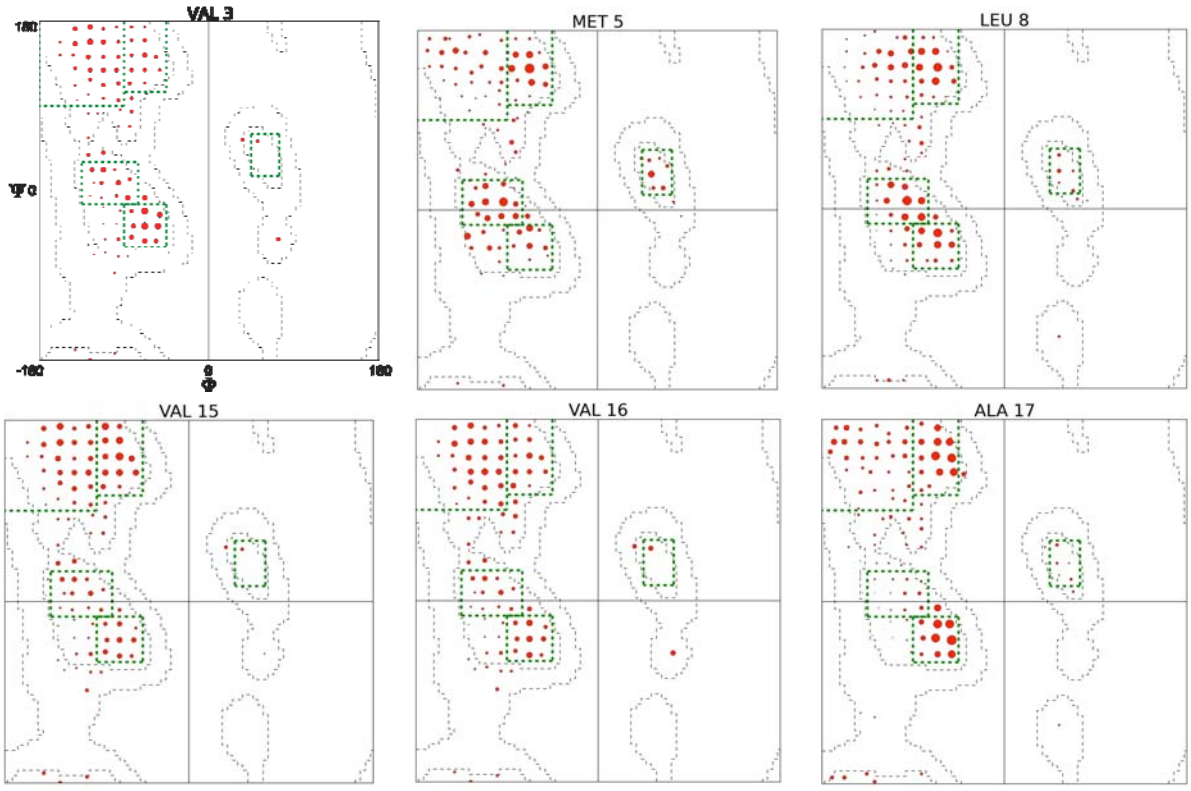
Cross validation of ϕ/ψ distributions

Cross validation of the residue-specific ϕ/ψ distributions is difficult due to the relatively modest departures from the statistical coil library obtained for aS. As a result, predicted deviations from random coil values are relatively small, and the difficulty is compounded by the substantial uncertainty in the relation between the predicted parameter and the structural variables ϕ and ψ. The most unambiguous parameter in this respect is the $^{3}J_{HNH\alpha}$ coupling, which has been shown to fit a Karplus equation of an RDC-refined structure to better than 0.4 Hz rmsd. However, omitting the $^{3}J_{HNH\alpha}$ couplings from the input parameters when optimizing eq 2, main text, removes one of the most important parameters from the input restraints. Cross validation that removes $^{3}J_{HNH\alpha}$ couplings from the input parameters therefore underestimates the true accuracy of the predictions. Bearing this in mind, with an rmsd between observed and calculated values of 0.38 Hz, results shown in Figure S5 indicate a good correlation between experimental and predicted values. In part, however, this correlation is biased by the different ϕ/ψ distributions present in the statistical coil library for different residue types, resulting in smaller $^{3}J_{HNH\alpha}$ values for e.g. Ala compared to the β-branched residues.[1] However, even when restricting the analysis to residues of a given type, where this consideration does not play a role, the correlation remains good, ranging from a Pearson's correlation coefficient, R_P = 0.53 for Ala residues (N=9; rmsd = 0.32 Hz) to R_P = 0.98 for Thr (N=7; rmsd = 0.21 Hz).



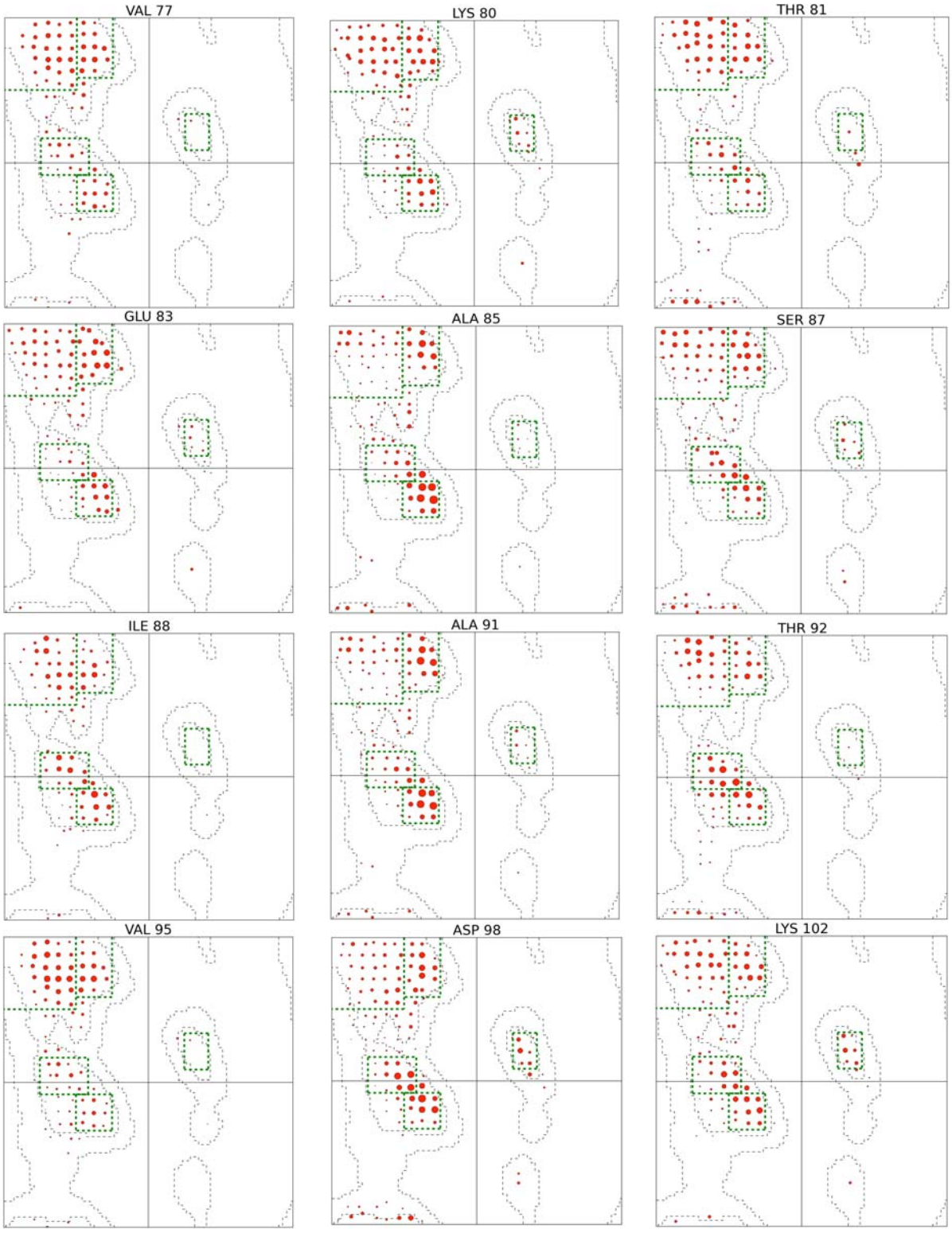
Supplementary Figure S1. Cross validation results for the $^3J_{HNH\alpha}$ values, obtained when deriving ϕ/ψ distributions in the same manner as described in the text, but omitting $^3J_{HNH\alpha}$ from the input restraints. Calculated $^3J_{HNH\alpha}$ values correspond to the weighted average of the conformers derived using the 9 remaining input parameters, and a θ value of 0.8. The Pearson's correlation coefficient equals 0.88, and the rmsd between observed and predicted $^3J_{HNH\alpha}$ values is 0.38 Hz.

Supplementary Figure S2. Distribution fits of the backbone angles to 10 independent experimental parameters for all non-Gly/Pro residues with complete sets of 10 NMR parameters. The value of θ which shows a modest increase (the larger of 0.25 or 25% of the χ^2 value obtained for θ=0.4) is selected to define the ensemble that best describes the experimental data. The following θ were selected: V3, 0.8; M5, 0.4; L8, 0.4; V15, 0.8; V16, 0.8; A17, 0.8; A19, 0.8; E20, 0.8; K21, 0.8; T22, 1.6; V26, 0.8; A27, 0.8; K32, 0.8; T33, 1.6; V37, 0.8; V40, 0.8; S42, 1.6; K43, 0.4; A53, 0.8; A56, 0.8; E57, 1.6; K58, 0.8; T64, 0.4; N65, 0.4; V66, 0.4; V70, 1.6; V71, 0.8; T72, 0.8; T75, 0.8; A76, 0.4; V77, 0.8; K80, 1.6; T81, 0.8; E83, 1.6; A85, 0.8; S87, 0.8; I88, 0.8; A91, 0.8; T92, 0.4; V95, 1.6; D98, 0.4; K102, 0.8; N103, 0.4; I112, 0.4; D121, 0.4; N122, 0.4; E123, 0.8; A124, 0.8; Y125, 0.8; Y133, 0.8; Q134, 0.8; E139, 0.8.

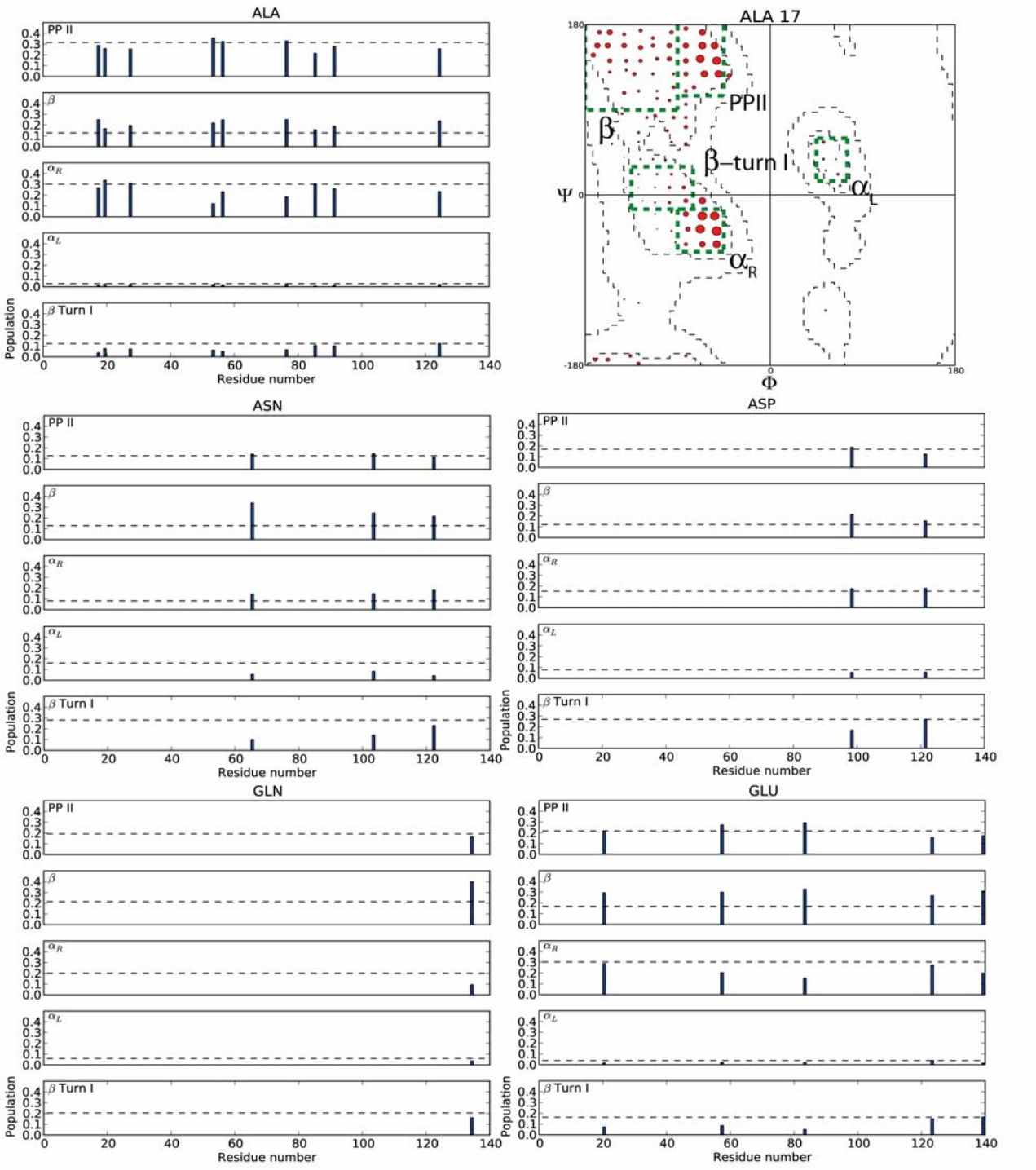



ALA 19
GLU 20
LYS 21
THR 22
VAL 26
ALA 27
LYS 32
THR 33
VAL 37
VAL 40
SER 42
LYS 43

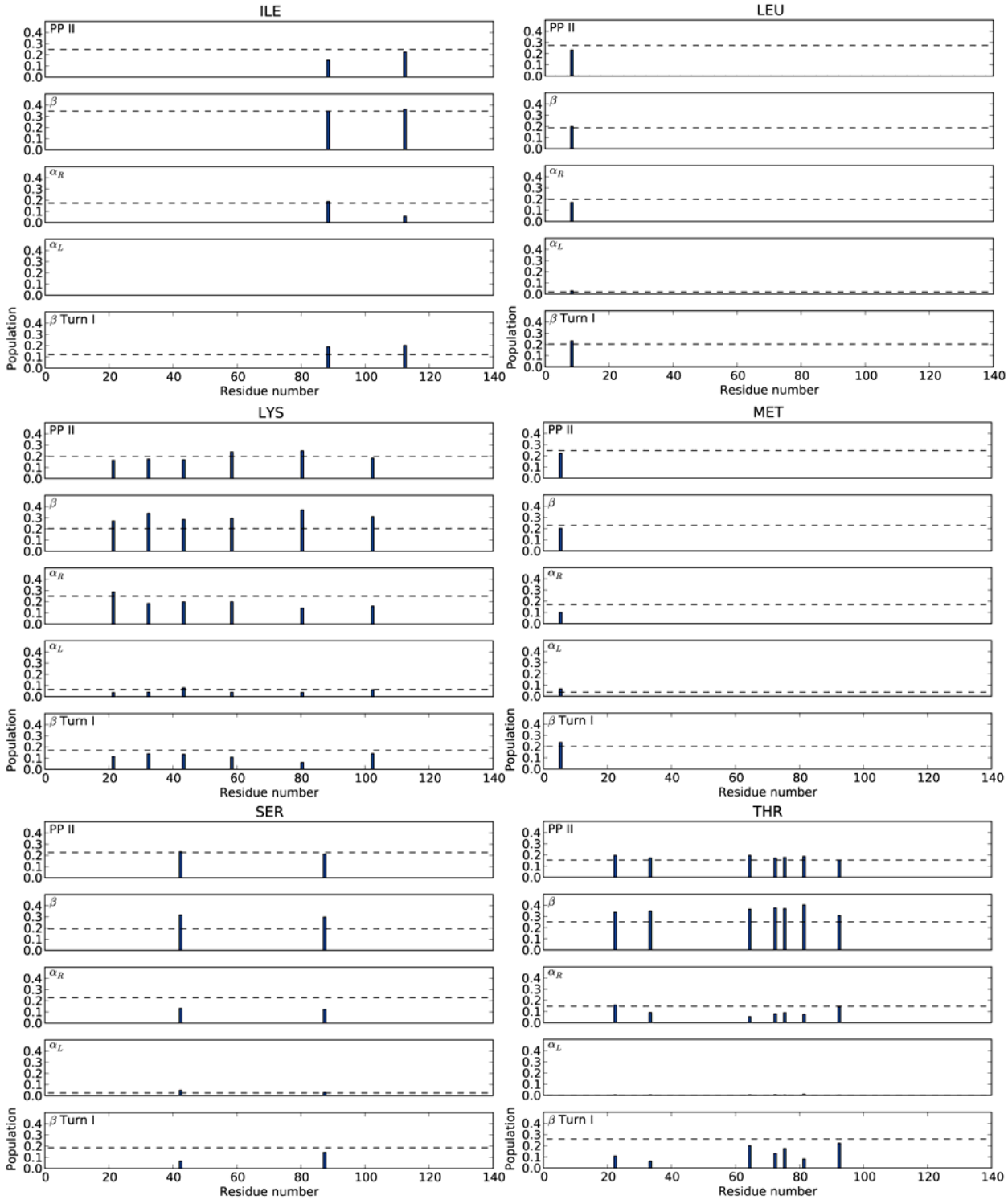

ALA 53
ALA 56
GLU 57
LYS 58
THR 64
ASN 65
VAL 66
VAL 70
VAL 71
THR 72
THR 75
ALA 76


VAL 77
LYS 80
THR 81
GLU 83
ALA 85
SER 87
ILE 88
ALA 91
THR 92
VAL 95
ASP 98
LYS 102

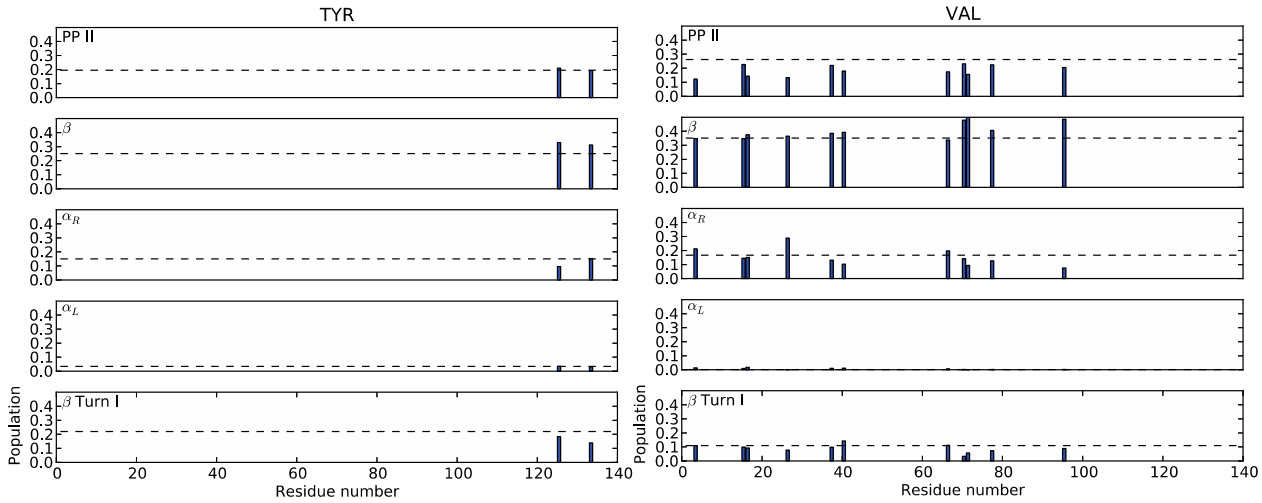
End of Supplementary Figure S2.



Supplementary Figure S3. Populations of the five main regions in the Ramachandran map for all non-Pro/Gly residues in aS for which a full set of 10 parameters was available. Regions are marked in the top right panel for A17. The dashed line for each residue type corresponds to the population of the region in the coil database.



Supplementary Figure S3, continued



Supplementary Figure S3, continued

Supplementary Table S1. *J* couplings and ^{1}H-^{1}H cross relaxation rates measured in ^{1}H/^{15}N-aS (for ^{1}H-^{1}H cross relaxation rates and $^{3}J_{HNH\alpha}$), in ^{1}H/^{15}N/^{13}C-aS (for $^{1}J_{H\alpha C\alpha}$), and in ^{2}H/^{15}N/^{13}C-aS (for $^{1}J_{NC\alpha}$; $^{2}J_{NC\alpha}$), at 15 °C, pH 6. Experimental uncertainties for $^{1}J_{H\alpha C\alpha}$, $^{2}J_{NC\alpha}$ and $^{2}J_{NC\alpha}$ are 0.1 Hz, and 0.03 Hz for $^{3}J_{HNH\alpha}$. Uncertainties in the ^{1}H-^{1}H cross relaxation rates are <~10%.

	$^{1}J_{H\alpha C\alpha}$ [Hz]	$^{1}J_{NC\alpha}$ [Hz]	$^{2}J_{C\alpha iNi+1}$ [Hz]	$^{3}J_{HNH\alpha}$ [Hz]	R_{cross} [1/s]		
					H^{N}_{i}-H^{α}_{i}	H^{α}_{i} - H^{N}_{i+1}	H^{N}_{i}-H^{N}_{i+1}
D2	143.5		8.54			0.412	
V3	142.0	10.48	7.26	7.25	0.114	0.414	0.098
F4	144.0	10.73	7.70	7.13	0.136	0.456	0.108
M5	142.1	10.63	7.95	7.13	0.198	0.473	0.297
K6		10.65	8.06	6.11	0.178		0.080
G7		11.65	8.17				
L8	142.2	10.84	7.79	7.01	0.167	0.504	0.135
S9	143.2	11.52	7.69	6.53	0.195		0.047
K10	142.2	10.71	7.62			0.485	0.071
A11	144.2	11.04	8.35	5.30	0.167		0.070
K12		10.68	7.81	6.64			0.105
E13	143.1		8.34	6.18		0.701	0.070
G14		11.63	8.32				
V15	142.3	10.85	8.33	7.37	0.171	0.765	0.123
V16	142.0	10.10	7.72	7.63	0.213	0.750	0.122
A17	144.2	10.80	8.31	5.45	0.193	0.643	0.084
A18	144.1	10.74	7.95	5.22	0.174	0.522	
A19	144.7	10.74	7.86	5.28	0.206	0.559	0.120
E20	143.8	10.69	7.90	6.13	0.209	0.734	0.111
K21	143.2	10.40	7.77	6.53	0.227	0.624	0.156
T22	142.0	11.51	7.54	6.99	0.250	0.890	0.108
K23		10.65		6.65	0.195		0.072
Q24	141.9		8.35	6.69			0.075
G25		11.75	8.39				
V26	141.8	10.77	7.40	7.12	0.183	0.554	0.128
A27	144.6	10.71	8.03	5.58	0.190	0.512	0.110
E28	143.6	10.60	7.67	6.08	0.178		0.088
A29	143.8	10.62	8.06				0.053
A30	143.7		8.15			0.473	0.134
G31		11.65	7.95				
K32	142.5	10.91	8.01	7.01	0.174	0.653	0.111
T33	141.5	11.70	7.72	7.22	0.188	0.583	0.061
K34	142.4		7.73		0.212		
E35		11.00	8.21	6.30			
G36		11.66	8.29				
V37	141.6	10.87	7.65	7.50	0.209	1.016	0.119

L38	142.3	10.54		7.04	0.205	1.026	0.125
Y39	143.0	10.88	7.94	7.47	0.243	1.019	0.106
V40	141.2	10.40	7.74	8.01	0.225	0.953	0.148
G41		11.93					
S42	142.3	11.64	7.64	6.49	0.275	0.926	0.076
K43	142.3	10.59	7.77	7.00	0.262	0.689	0.185
T44	141.5	11.69	7.69	7.26	0.225		0.093
K45		10.55	7.76	6.65			0.113
E46		11.09	8.26	6.37			
G47		11.70					
V48	142.4		8.29	7.58	0.156		0.078
V49	141.4	10.13	8.17			1.407	0.126
H50	140.5	11.15	8.67	7.59	0.321		
G51		11.83	8.72				
V52	141.5	10.90	7.73			0.813	0.080
A53	143.7	10.94	8.61	5.79	0.148	0.819	0.081
T54	141.5	11.62		7.56	0.165		0.098
V55	142.2		7.68			0.885	0.103
A56	144.0	10.82	8.32	5.61	0.195	0.790	0.090
E57	143.6	10.90	8.13	6.15	0.178	1.018	0.110
K58	143.3	10.59	8.06	6.57	0.204	0.829	0.135
T59	142.9	11.59	7.67	7.01	0.237		0.105
K60	142.9	10.69	7.81				
E61				6.17			
Q62	142.9			7.01		0.784	0.129
V63	141.3		7.90	7.70	0.174	0.872	
T64	141.5	11.43	7.77	7.87	0.173	0.800	0.227
N65	142.7	10.91	8.26	7.51	0.245	0.331	0.066
V66	141.8	10.31	7.58	7.34	0.108	0.439	0.095
G67		11.52	8.56				
G68		11.96	8.35				
A69	143.6	11.19	8.29	5.83	0.077	0.439	0.036
V70	141.5	10.85	8.03	7.53	0.101	0.722	0.054
V71	141.4	10.32	7.98	8.15	0.085	0.667	0.054
T72	141.0	11.50	7.91	7.70	0.123	0.520	0.071
G73		11.73	8.51				
V74	142.1	10.76	7.80			0.638	0.000
T75	141.1	11.44	7.62	7.62	0.120	0.641	0.096
A76	143.7	10.87	8.39	5.87	0.131	0.674	0.078
V77	142.0	10.63	7.70	7.45	0.120	0.793	0.073
A78	143.7	10.96	8.43	5.62	0.155		0.065
Q79	142.9	10.96	8.31	6.79		0.813	0.077
K80	143.2	10.79	8.28	6.71	0.166	0.792	0.065
T81	*141.5*	11.61	*7.87*	*7.52*	0.240	0.811	0.064
V82	141.7		7.73	7.65	0.111	0.594	0.080
E83	142.9	10.83	8.41	6.19	0.132	0.578	0.046

G84		11.69	8.21				
A85	143.7	10.77	7.95	5.64	0.093	0.216	0.062
G86		11.72	8.36				
S87	142.5	11.58	7.59	6.82	0.109	0.441	0.068
I88	141.9	10.37	7.28	7.46	0.099	0.474	0.097
A89	144.1	10.78	8.09	5.57	0.118		0.068
A90	144.0	10.91	8.01	5.62		0.433	
A91	144.0	10.75	8.15	5.77	0.114	0.398	0.089
T92		11.44	7.45	7.50	0.127	0.451	0.146
G93		11.63	8.29				
F94	143.8	11.27	7.97	6.92	0.140	0.764	0.075
V95	141.8	10.68	7.98	8.04	0.139	1.016	0.085
K96	142.1	10.78	8.39	6.51	0.186		
K97	141.6		7.85			0.667	0.092
D98	142.8	10.94	7.91	6.72	0.237	0.532	0.119
Q99	142.4	10.59	7.60	7.23	0.184		0.152
L100	142.3		7.91	6.80		0.489	0.137
G101		11.76	8.43				
K102	142.1	10.95	7.97	6.83	0.173	0.524	0.093
N103	142.5	11.02	8.02	7.20	0.219	0.383	0.097
E104	142.5	10.64	7.66	6.79	0.156		
E105	142.4	10.66	7.99	6.39		0.476	0.094
G106		11.70	8.16				
A107		11.54		5.92	0.122		
P108	148.2		9.05			0.789	
Q109	142.6	10.72	8.08	6.94	0.155		0.082
E110	142.8	10.86	8.34	6.52		0.728	0.078
G111		11.72	8.44				
I112	141.2	10.84	7.75	7.75	0.146	1.039	0.103
L113	141.8	10.54	8.02	7.16	0.181		0.105
E114	142.5	10.83	8.07	6.72		0.884	0.109
D115	143.1	10.88		6.85	0.245	0.895	0.165
M116				7.17	0.201		
P117						1.657	
V118	141.5		7.88	7.68	0.210		0.140
D119		10.89		6.79			
P120	149.2		7.66			0.701	
D121	143.5	10.56	7.54	7.14	0.338	0.537	
N122	143.1	10.95	7.71	7.29	0.326	0.525	0.259
E123	143.1	10.53	7.54	6.55	0.264	0.650	0.178
A124	143.5	10.66	7.95	6.23	0.222	0.803	0.172
Y125	143.8	11.13	7.95	7.09	0.216	1.228	0.170
E126	142.4	10.85		7.29	0.243	0.993	
M127				6.62	0.180		
P128	148.2		9.06				
S129	142.7	11.63	7.85	6.65		0.925	

E130		10.66	7.67	6.86	0.190		0.143
E131		10.66	8.11	6.41		0.579	0.084
G132		11.67	8.38				
Y133	143.7	11.22	7.93	6.77	0.159	0.647	0.098
Q134	142.3	10.89	8.13	7.55	0.164	0.592	0.089
D135	142.7	10.84	7.95	6.97	0.183		0.109
Y136	143.2	11.27	7.97	7.17			
E137		10.81		7.63			
P138	147.4		8.86			0.425	
E139	142.5	10.73	7.57	6.71	0.077	0.196	0.098
A140		10.44		6.65	0.038		

Supplementary Table S2. ^{15}N relaxation rates measured in perdeuterated, ^{15}N-enriched aS (except for Met residues, which are $^{13}C^{\varepsilon}$–enriched, but natural abundance ^{15}N) at 500 and 900 MHz ^{1}H frequency for a 150 μM sample, 15 °C, pH 6.0.

	500 MHz			900 MHz	
	R_1 [1/s]	R_2 [1/s]	NOE	R_1 [1/s]	NOE
name	±0.006 [a]	±0.011 [a]	±0.009 [a]	±0.004 [a]	±0.007 [a]
D2					
V3	1.319	2.072	-0.841	1.296	0.088
F4	1.524	2.495	-0.613	1.510	0.253
M5					
K6	1.643	2.801	-0.331	1.545	0.365
G7	1.590	2.648	-0.320		
L8	1.640	2.810	-0.214	1.535	0.435
S9	1.521	2.626	-0.336	1.428	0.348
K10				1.530	0.395
A11	1.643	2.972	-0.211	1.508	0.388
K12	1.610	2.912	-0.238	1.432	0.374
E13	1.650	3.009	-0.216	1.450	0.363
G14	1.546	2.768	-0.275		
V15	1.537	2.973	-0.198	1.388	0.385
V16	1.537	3.137	-0.354	1.370	0.280
A17	1.539	3.286	-0.289	1.380	0.293
A18	1.480	3.149	-0.240	1.300	0.296
A19	1.511	3.164	-0.195	1.320	0.326
E20	1.565	3.261	-0.201	1.375	0.354
K21	1.667	3.398	-0.186	1.445	0.376
T22	1.653	3.328	-0.162	1.461	0.404
K23	1.679	3.425	-0.150	1.493	0.399
Q24				1.414	0.395
G25					
V26	1.531	3.090	-0.168	1.387	0.390
A27	1.573	3.156	-0.266	1.420	0.341
E28	1.547	2.972	-0.248	1.373	0.329
A29	1.573	3.024	-0.266	1.404	0.320
A30				1.336	0.285
G31	1.488	2.727	-0.248		
K32	1.601	2.954	-0.137	1.429	0.407
T33	1.614	3.028	-0.202	1.455	0.388
K34					
E35	1.701	3.240	-0.126	1.479	0.411
G36	1.642	3.070	-0.137		
V37	1.632	3.324	-0.035	1.424	0.469
L38	1.696	3.551	-0.122	1.469	0.422
Y39	1.711	3.593	-0.032	1.453	0.454
V40	1.680	3.592	-0.092	1.436	0.430
G41	1.682	3.368	-0.076		

S42	1.589	3.160	-0.054	1.411	0.445
K43	1.646	3.211	-0.155	1.458	0.419
T44	1.693	3.183	-0.104	1.489	0.427
K45	1.701	3.316	-0.145	1.503	0.431
E46	1.694	3.280	-0.134	1.456	0.430
G47	1.607	2.851	-0.190		
V48	1.574	2.950	-0.112	1.422	0.414
V49	1.606	3.079	-0.258	1.421	0.354
H50	1.590	3.078	-0.228	1.412	0.351
G51					
V52	1.469	2.863	-0.253	1.335	0.338
A53	1.484	2.869	-0.371	1.364	0.274
T54	1.457	2.709	-0.324	1.308	0.278
V55				1.376	0.328
A56	1.554	3.179	-0.255	1.387	0.306
E57	1.557	3.048	-0.230	1.356	0.348
K58	1.654	3.267	-0.186	1.444	0.375
T59	1.645	3.231	-0.150	1.454	0.384
K60				1.451	0.411
E61	1.685	3.201	-0.155	1.474	0.422
Q62				1.476	0.389
V63	1.569	2.834	-0.268	1.421	0.329
T64	1.575	2.788	-0.317	1.427	0.295
N65	1.565	2.565	-0.326	1.432	0.317
V66	1.439	2.220	-0.479	1.347	0.246
G67	1.500	2.222	-0.401		
G68	1.337	1.943	-0.488		
A69	1.343	1.981	-0.484	1.340	0.247
V70	1.349	2.065	-0.561	1.278	0.166
V71	1.488	2.310	-0.508	1.404	0.233
T72	1.507	2.365	-0.457	1.405	0.246
G73	1.435	2.256	-0.450		
V74	1.479	2.310	-0.318	1.398	0.337
T75	1.464	2.480	-0.458	1.381	0.222
A76	1.468	2.405	-0.413	1.410	0.256
V77	1.417	2.487	-0.431	1.298	0.221
A78	1.506	2.667	-0.407	1.398	0.269
Q79	1.473	2.531	-0.382	1.341	0.265
K80	1.553	2.699	-0.337	1.428	0.310
T81	1.560	2.619	-0.323	1.439	0.336
V82	1.557	2.593	-0.357	1.443	0.284
E83	1.599	2.573	-0.358	1.455	0.290
G84	1.466	2.234	-0.446		
A85	1.486	2.248	-0.345	1.423	0.334
G86	1.347	1.973	-0.529		
S87	1.400	2.113	-0.427	1.369	0.282

I88	1.454	2.300	-0.476	1.387	0.234
A89	1.517	2.522	-0.452	1.432	0.241
A90	1.439	2.340	-0.420	1.341	0.242
A91	1.432	2.296	-0.412	1.347	0.252
T92	1.443	2.419	-0.380	1.323	0.263
G93	1.529	2.464	-0.315		
F94	1.584	2.674	-0.152	1.456	0.411
V95	1.598	2.865	-0.237	1.430	0.358
K96	1.703	3.008	-0.171	1.510	0.394
K97					
D98	1.750	3.129	-0.066	1.525	0.466
Q99	1.698	2.999	-0.089	1.481	0.419
L100	1.708	2.890	-0.133	1.518	0.431
G101	1.627	2.626	-0.191		
K102	1.668	2.796	-0.141	1.501	0.432
N103	1.654	2.695	-0.233	1.495	0.387
E104	1.651	2.700	-0.199	1.476	0.386
E105	1.653	2.711	-0.215	1.463	0.382
G106	1.527	2.403	-0.299		
A107	1.521	2.610	-0.181	1.398	0.407
P108					
Q109	1.550	2.672	-0.303	1.393	0.333
E110	1.581	2.753	-0.242	1.400	0.329
G111	1.505	2.554	-0.285		
I112	1.556	2.869	-0.172	1.400	0.385
L113	1.580	3.069	-0.295	1.430	0.337
E114	1.568	3.168	-0.249	1.357	0.351
D115	1.577	3.135	-0.225	1.372	0.341
M116					
P117					
V118	1.523	3.456	-0.199	1.322	0.343
D119	1.592	3.695	-0.156	1.367	0.375
P120					
D121	1.662	3.989	-0.028	1.390	0.409
N122	1.626	3.692	-0.068	1.355	0.407
E123	1.608	3.516	-0.126	1.364	0.380
A124	1.595	3.533	-0.145	1.375	0.405
Y125	1.545	3.330	-0.101	1.320	0.397
E126	1.637	3.593	-0.135	1.401	0.408
M127					
P128					
S129	1.520	3.171	-0.220	1.337	0.338
E130	1.570	3.069	-0.198	1.386	0.363
E131	1.614	3.027	-0.200	1.398	0.348
G132	1.554	2.669	-0.239		
Y133	1.620	2.885	-0.117	1.476	0.441

Q134	1.615	2.854	-0.241	1.465	0.379
D135	1.634	2.736	-0.250	1.483	0.403
Y136	1.556	2.583	-0.257	1.448	0.421
E137	1.578	2.508	-0.407	1.495	0.369
P138					
E139	1.370	1.942	-0.767	1.346	0.144
A140	1.006	1.342	-1.367	1.084	-0.235

[a] Reported errors correspond to the statistical uncertainties in the fits and do not include the unknown impact of potential systematic errors.

Supplementary Table S3. Spectral densities derived from the relaxation rates of Supplementary Table 2 using reduced spectral density mapping. Values reported for $J(2\omega_H)$ at 600 and 900 MHz are calculated from $J(0.87\omega_H)$ at 900 MHz assuming a Lorentzian distribution.

	$J(0)$ [ns/rad]	$J(\omega_N)$ 500 MHz [ns/rad]	$J(0.87\omega_H)$ 500 MHz [ps/rad]	$J(0.87\omega_H)$ 900 MHz [ps/rad]	$J(2\omega_H)$ 600 MHz [ps/rad]	$J(2\omega_H)$ 900 MHz [ps/rad]
D2						
V3	0.39	0.20	37.87	18.43	7.89	3.49
F4	0.49	0.24	38.34	17.59	7.53	3.33
M5						
K6	0.57	0.27	34.11	15.30	6.55	2.90
L8	0.57	0.28	31.05	13.53	5.79	2.56
S9	0.54	0.25	31.69	14.52	6.21	2.75
K10						
A11	0.62	0.28	31.03	14.39	6.16	2.72
K12	0.61	0.27	31.09	13.98	5.98	2.65
E13	0.63	0.28	31.29	14.41	6.16	2.73
V15	0.64	0.26	28.72	13.31	5.70	2.52
V16	0.69	0.25	32.46	15.38	6.58	2.91
A17	0.74	0.26	30.94	15.22	6.51	2.88
A18	0.71	0.25	28.62	14.27	6.11	2.70
A19	0.71	0.26	28.16	13.88	5.94	2.63
E20	0.73	0.27	29.31	13.85	5.93	2.62
K21	0.75	0.28	30.84	14.06	6.02	2.66
T22	0.73	0.28	29.96	13.58	5.81	2.57
K23	0.76	0.29	30.11	13.99	5.99	2.65
Q24						
V26	0.68	0.26	27.89	13.20	5.65	2.50
A27	0.69	0.26	31.06	14.59	6.25	2.76
E28	0.64	0.26	30.11	14.37	6.15	2.72
A29	0.65	0.26	31.06	14.89	6.37	2.82
A30						
K32	0.63	0.28	28.39	13.22	5.66	2.50
T33	0.65	0.27	30.26	13.89	5.94	2.63
K34						
E35	0.70	0.29	29.87	13.59	5.81	2.57
V37	0.74	0.29	26.34	11.79	5.05	2.23
L38	0.80	0.29	29.68	13.24	5.67	2.51
Y39	0.81	0.30	27.54	12.37	5.29	2.34
V40	0.81	0.29	28.61	12.77	5.46	2.42
S42	0.70	0.28	26.12	12.21	5.23	2.31

K43	0.70	0.28	29.65	13.21	5.65	2.50
T44	0.68	0.29	29.15	13.31	5.69	2.52
K45	0.72	0.29	30.38	13.34	5.71	2.52
E46	0.71	0.29	29.96	12.94	5.54	2.45
V48	0.63	0.27	27.30	13.00	5.56	2.46
V49	0.66	0.27	31.51	14.32	6.13	2.71
H50	0.67	0.27	30.45	14.29	6.12	2.70
V52	0.62	0.25	28.71	13.78	5.90	2.61
A53	0.62	0.25	31.73	15.44	6.61	2.92
T54	0.57	0.24	30.09	14.73	6.30	2.79
V55						
A56	0.70	0.26	30.42	15.01	6.42	2.84
E57	0.66	0.26	29.87	13.79	5.90	2.61
K58	0.71	0.28	30.59	14.08	6.02	2.66
T59	0.71	0.28	29.50	13.97	5.98	2.64
K60						
E61	0.69	0.29	30.35	13.29	5.69	2.51
Q62						
V63	0.59	0.26	31.03	14.87	6.36	2.81
T64	0.58	0.26	32.35	15.69	6.71	2.97
N65	0.51	0.26	32.37	15.25	6.53	2.89
V66	0.42	0.23	33.19	15.84	6.78	3.00
A69	0.37	0.22	31.08	15.74	6.73	2.98
V70	0.39	0.22	32.84	16.62	7.11	3.15
V71	0.44	0.24	35.00	16.80	7.19	3.18
T72	0.45	0.25	34.25	16.52	7.07	3.13
V74	0.45	0.25	30.40	14.46	6.19	2.74
T75	0.50	0.24	33.29	16.76	7.17	3.17
A76	0.48	0.24	32.35	16.36	7.00	3.10
V77	0.51	0.23	31.63	15.77	6.75	2.98
A78	0.55	0.25	33.05	15.94	6.82	3.02
Q79	0.51	0.24	31.75	15.37	6.58	2.91
K80	0.55	0.26	32.38	15.37	6.58	2.91
T81	0.53	0.26	32.19	14.90	6.38	2.82
V82	0.52	0.26	32.95	16.11	6.90	3.05
E83	0.51	0.26	33.87	16.11	6.89	3.05
A85	0.43	0.25	31.17	14.78	6.32	2.80
S87	0.40	0.23	31.16	15.33	6.56	2.90
I88	0.44	0.24	33.47	16.57	7.09	3.14
A89	0.50	0.25	34.35	16.95	7.25	3.21
A90	0.46	0.24	31.87	15.85	6.78	3.00
A91	0.45	0.23	31.54	15.71	6.72	2.97
T92	0.48	0.24	31.06	15.21	6.51	2.88

F94	0.54	0.27	28.46	13.38	5.72	2.53
V95	0.60	0.27	30.83	14.32	6.13	2.71
K96	0.63	0.29	31.10	14.27	6.11	2.70
K97						
D98	0.66	0.30	29.10	12.70	5.43	2.40
Q99	0.63	0.29	28.84	13.42	5.74	2.54
L100	0.59	0.29	30.18	13.47	5.76	2.55
K102	0.57	0.29	29.68	13.30	5.69	2.52
N103	0.54	0.28	31.81	14.29	6.12	2.70
E104	0.54	0.28	30.87	14.13	6.05	2.67
E105	0.54	0.28	31.32	14.10	6.03	2.67
A107	0.54	0.26	28.02	12.93	5.53	2.45
P108						
Q109	0.55	0.26	31.50	14.49	6.20	2.74
E110	0.57	0.27	30.63	14.65	6.27	2.77
I112	0.61	0.27	28.44	13.43	5.75	2.54
L113	0.66	0.26	31.91	14.79	6.33	2.80
E114	0.70	0.26	30.54	13.74	5.88	2.60
D115	0.69	0.27	30.13	14.10	6.03	2.67
M116						
P117						
V118	0.79	0.26	28.48	13.55	5.80	2.56
D119	0.86	0.27	28.70	13.33	5.70	2.52
P120						
D121	0.94	0.29	26.65	12.81	5.48	2.42
N122	0.85	0.28	27.08	12.53	5.36	2.37
E123	0.80	0.28	28.24	13.19	5.64	2.50
A124	0.81	0.27	28.48	12.76	5.46	2.41
Y125	0.76	0.27	26.53	12.41	5.31	2.35
E126	0.82	0.28	28.98	12.94	5.54	2.45
M127						
P128						
S129	0.71	0.26	28.92	13.80	5.91	2.61
E130	0.67	0.27	29.33	13.77	5.89	2.61
E131	0.65	0.27	30.21	14.22	6.08	2.69
Y133	0.60	0.28	28.22	12.87	5.51	2.44
Q134	0.59	0.27	31.26	14.19	6.07	2.68
D135	0.55	0.28	31.86	13.81	5.91	2.61
Y136	0.52	0.26	30.51	13.08	5.60	2.47
E137	0.49	0.26	34.63	14.71	6.30	2.78
P138						
E139	0.34	0.21	37.76	17.97	7.69	3.40
A140	0.21	0.14	37.14			

Supplementary Table S4. Number of conformers for each residue type in the coil data base after applying the selection criteria described in Material and Methods.

Residue type	**Ala**	**Asp**	**Asn**	**Arg**	**Gln**	**Glu**	**His**	**Ile**
Number of conformers	8564	9467	7423	5435	4136	7182	3107	4547
Residue type	**Leu**	**Lys**	**Met**	**Phe**	**Ser**	**Thr**	**Tyr**	**Val**
Number of conformers	7837	6738	1685	4356	8584	7017	3991	6013

References

1. Smith LJ, Bolin KA, Schwalbe H, MacArthur MW, Thornton JM, Dobson CM. (1996) Analysis of main chain torsion angles in proteins: Prediction of NMR coupling constants for native and random coil conformations. J Mol Biol 255:494-506.