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Supporting Information

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N–H Spin–Spin Couplings: Probing Hydrogen Bonds in Proteins**

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Supporting Information

Supporting Experimental Section

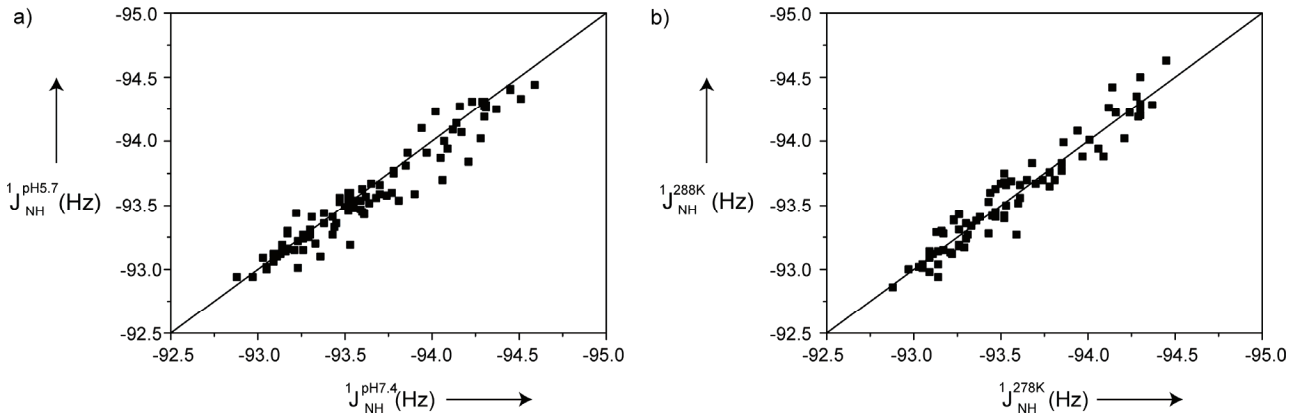
Sample preparation The 441-residue isoform of human Tau, hTau40, the 130-residue Tau fragment K18 (residues Gln244-Glu372 plus initial Met243), α-synuclein and ubiquitin were expressed and purified in ^{15}N-labelled form as described previously.[1-3] Sample conditions were: 0.7 mM ^{15}N-labelled hTau40 in 57 mM Na-phosphate buffer, pH 6.0, 42 mM NaCl; 0.35 mM ^{15}N-labelled K18 in 50 mM Na-phosphate buffer, pH 6.8, 100 mM NaCl; 0.25 mM ^{15}N-labelled α-synuclein in 50 mM Na-phosphate buffer, 100 mM NaCl, at pH values of 5.7, 6.0, 6.5 and 7.4; 0.5 mM ^{15}N-labelled ubiquitin in 50 mM HEPES buffer, pH 7.0, 300 mM NaCl. $^{1}J_{NH}$ values in hTau40 and K18 were measured at 278K, those in α-synuclein at 278K, 288K and 298K, and in ubiquitin at 298K.

NMR spectroscopy Protein G $^{1}J_{NH}$ couplings at 500 MHz and 750 MHz were taken from [4], which were obtained in 25 mM sodium phosphate, 50 mM NaCl, pH 6.5. DFS was calculated according to [5]. After DFS correction, the influence of the anisotropic magnetic susceptibility of the protein was removed by taking the difference between $^{1}J_{NH}$ at different magnetic fields.

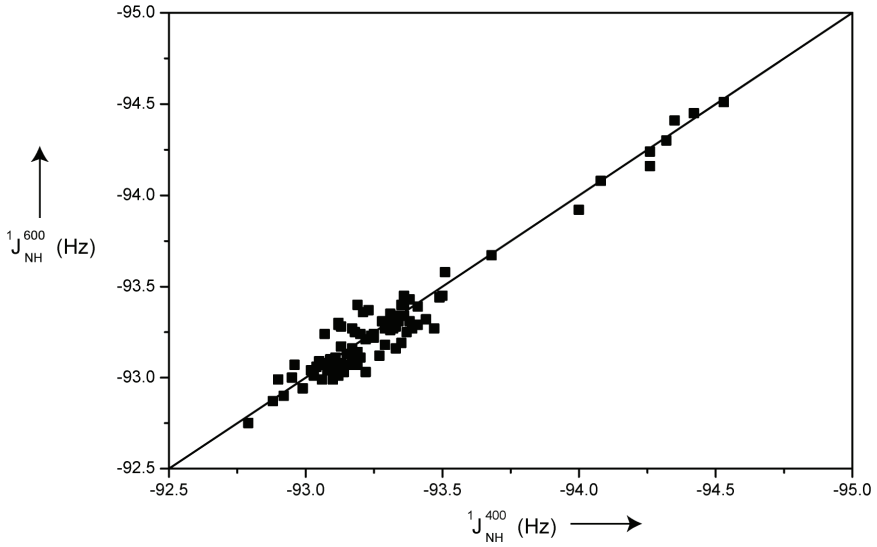
$^{1}J_{NH}$ in α-synuclein at pH 5.7, ph 6.5 and pH 7.4 were measured using a conventional IPAP-HSQC pulse program,[6] in which long-range proton-nitrogen couplings are effective. The experimental error of the conventional IPAP HSQC is ~0.2 Hz, as derived from repeat measurements. Experiments were carried on a Bruker Avance 700 MHz spectrometer with a z-axis gradient, triple resonance, room temperature probe. In-phase and anti-phase spectra were recorded interleaved with 256(^{15}N)*512(^{1}H) complex points. $^{1}J_{NH}$ in Dini (at pH 7.0, 298K) had previously been measured on a Bruker DRX 600 MHz spectrometer using a conventional IPAP-HSQC.[7]

NMR data were processed and analyzed using NMRPipe [8] and Sparky 3 (University of California, San Francisco). Backbone H-bonds were determined using the Whatif program.[9] The location of secondary structure elements were taken from the deposited 3D structures. Residues were labelled as being close to an aromatic ring when its amide or amide proton was less than 6 Å away from the center of an aromatic ring in the 3D structure.

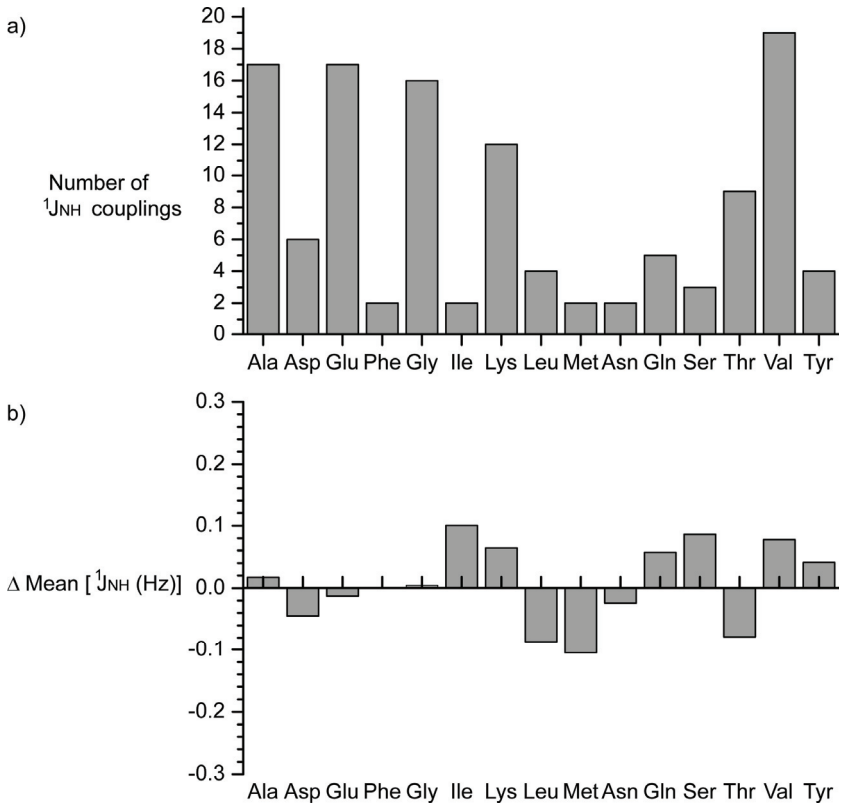
Supporting Figures



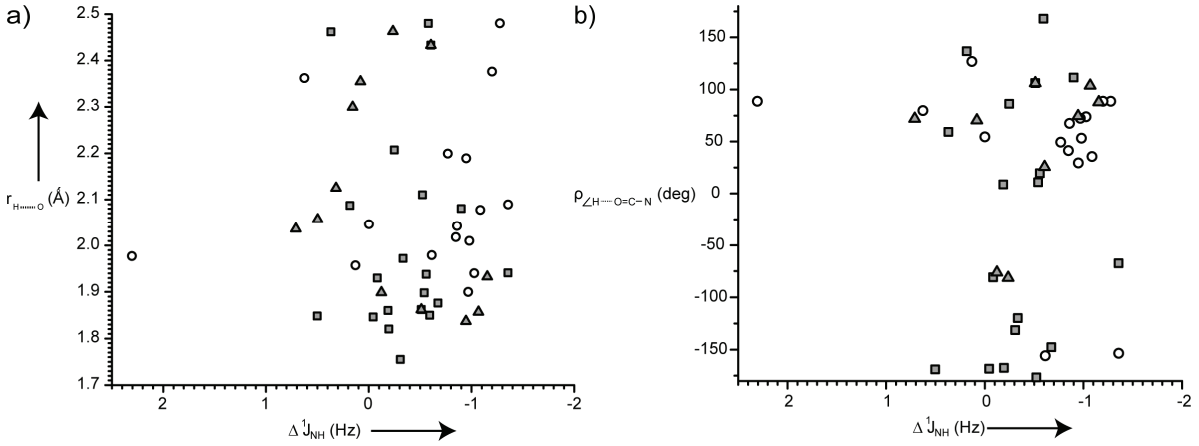
Supporting Figure S1. Influence of pH and temperature on $^1J_{NH}$ in the intrinsically disordered protein α-synuclein. a) Correlation between $^1J_{NH}$ in α-synuclein at pH 7.4 and pH 5.7, 278K. b) Correlation between $^1J_{NH}$ in α-synuclein at 278K and 288K, pH 7.4. Values in a) and b) were measured using a conventional IPAP-HSQC pulse program, in which long range couplings are not refocused.



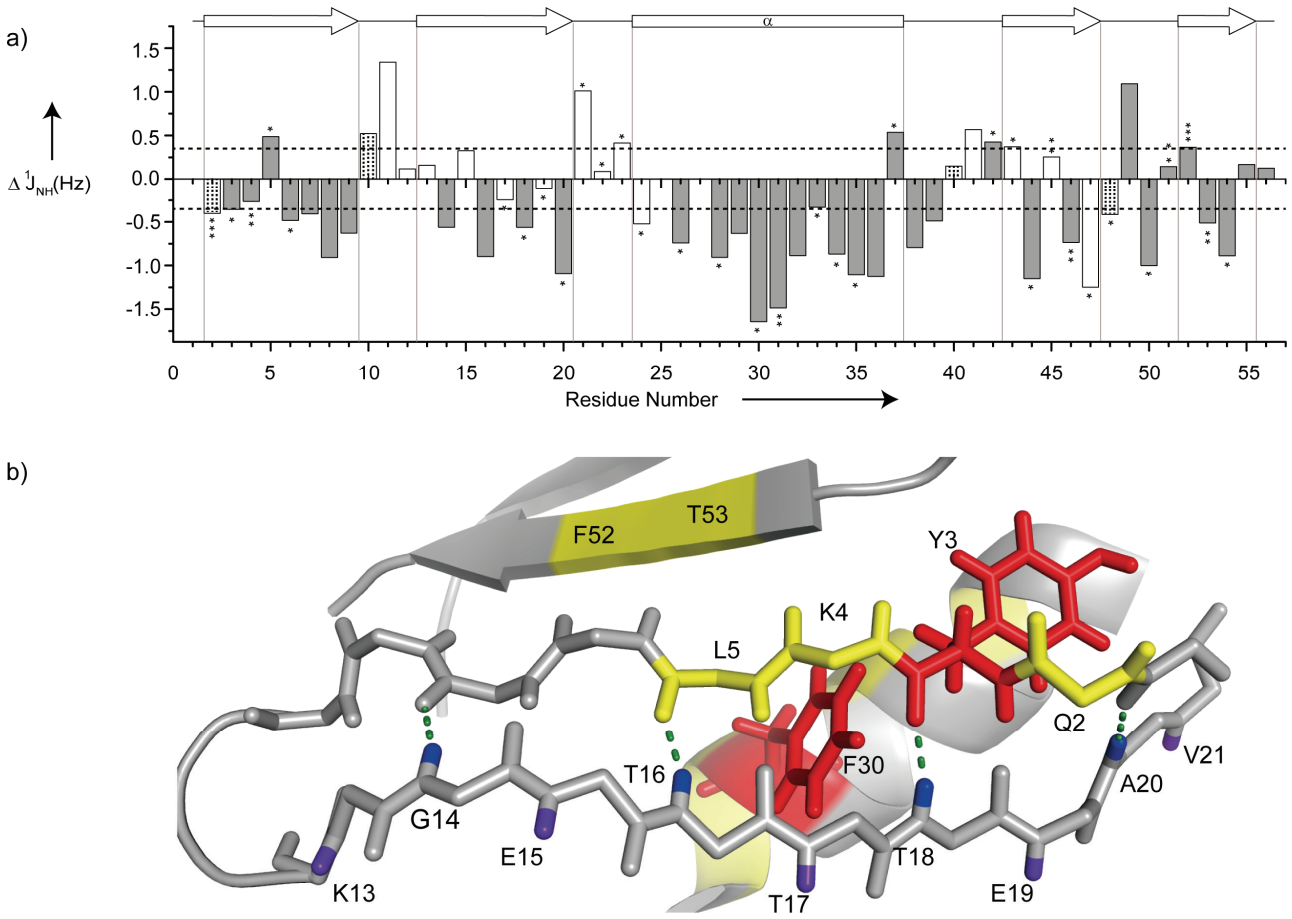
Supporting Figure S2. Correlation between $^1J_{NH}$ observed in K18 at 600 MHz and 400 MHz field strengths. $^1J_{NH}$ values were determined using BSD-IPAP-HSQC experiments.



Supporting Figure S3. Differences in amino-acid specific values of $^{1}J_{NH}$ between α-synuclein and hTau40. a) Number of experimental $^{1}J_{NH}$ values for the most common residue types in α-synuclein. b) Differences between mean values of amino-acid specific $^{1}J_{NH}$ constants in α-synuclein and hTau40, both at pH 6.0, 278K. $^{1}J_{NH}$ values in α-synuclein were measured at 700 MHz, in htau40 at 900 MHz.



Supporting Figure S4. a) Comparison of secondary $^1J_{NH}$ values, Δ^1J_{NH}, with H-bond lengths, $r_{H...O}$, in ubiquitin for residues in β-strands (■), loops (▲) and the α-helix (○). b**)** Comparison of secondary $^1J_{NH}$ values, Δ^1J_{NH}, in ubiquitin with the dihedral angle ρ= <H•••O=C-N (which to a large extent distinguishes α-helix from β-sheet) for residues in β-strands (■), loops (▲) and the α-helix (○).



Supporting Figure S5. $^{1}J_{NH}$ spin-spin coupling constants in protein G. a) Deviation of $^{1}J_{NH}$ spin-spin coupling constants observed in protein G from their amino-acid specific random coil values as a function of residue number. Filled and hatched bars mark amide protons involved in an H-bond to the backbone or a side chain, respectively. Stars indicate spatial proximity (< 6 Å) to aromatic rings. Two or three stars indicate that two or three aromatic rings are within 6 Å of either the amide or amide proton. Secondary structure elements identified by DSSP [10] in the 3D structure (PDB code: 2oed) are shown above. b) Expanded region of the 3D structure of protein G to highlight the pattern of H-bonds in β-strand 2. H-bonds are in green. Amide protons which are involved in H-bonds are colour coded in blue while those not in H-bonds are in purple. Residues which are in spatial proximity (< 6 Å) to the aromatic rings of Tyr3 and Phe30 (red) are shown in yellow.

Supporting Table S1. NMR. $^{1}J_{NH}$ values of Tau protein pH 6.0, 278K, at 900MHz.

Residue	$^{1}J_{NH}$(Hz)	Residue	$^{1}J_{NH}$(Hz)	Residue	$^{1}J_{NH}$(Hz)
E3	-93.23	E53	-92.86	A103	-93.38
R5	-93.10	D54	-93.11	E104	-92.99
Q6	-92.92	G55	-94.33	E105	-93.06
E7	-92.73	S56	-93.26	A106	-93.24
E9	-92.95	E57	-92.96	G107	-94.25
V10	-92.89	E58	-93.10	I108	-92.78
M11	-93.20	G60	-94.11	G109	-94.44
E12	-92.89	S61	-93.15	D110	-93.08
D13	-93.26	E62	-93.01	T111	-93.37
H14	-93.09	T63	-93.19	S113	-93.17
G16	-94.26	S64	-93.28	L114	-93.03
T17	-92.85	D65	-93.34	E115	-93.03
Y18	-93.25	A66	-93.51	D116	-93.14
G19	-94.14	K67	-93.06	E117	-93.10
L20	-92.80	S68	-93.26	A118	-93.39
G21	-94.34	T69	-93.45	A119	-93.26
D22	-93.15	T71	-93.17	G120	-94.28
R23	-93.19	A72	-93.35	H121	-93.16
K24	-92.95	E73	-92.88	V122	-92.95
D25	-93.12	D74	-93.21	T123	-93.39
Q26	-92.78	V75	-92.83	Q124	-93.07
G27	-94.24	T76	-93.31	A125	-93.25
G28	-94.18	A77	-93.71	R126	-93.05
Y29	-92.92	L79	-93.05	M127	-93.06
T30	-93.20	V80	-92.90	V128	-92.90
M31	-93.26	D81	-93.41	S129	-93.51
Q33	-93.02	E82	-92.98	K130	-93.03
D34	-93.15	G83	-94.21	S131	-93.45
Q35	-92.88	A84	-93.57	K132	-92.83
E36	-92.95	G86	-94.25	D133	-93.19
G37	-94.24	K87	-92.99	G134	-94.40
D38	-93.18	Q88	-93.20	T135	-92.96
T39	-93.17	A89	-93.47	G136	-94.43
D40	-93.37	A90	-93.37	S137	-93.17
A41	-93.29	A91	-93.30	D139	-93.33
G42	-94.43	Q92	-93.20	K140	-93.16
L43	-93.05	H94	-93.08	K141	-93.15
K44	-92.88	T95	-93.25	A142	-93.40
E45	-93.10	E96	-93.02	K143	-92.94
S46	-93.49	I97	-93.28	G144	-94.38
L48	-93.10	E99	-92.96	A145	-93.14
Q49	-92.98	G100	-94.17	G147	-94.47
T50	-93.38	T101	-93.03	K148	-93.03
T52	-93.20	T102	-93.35	T149	-93.28

Residue	$^1J_{NH}$(Hz)	Residue	$^1J_{NH}$(Hz)	Residue	$^1J_{NH}$(Hz)
K150	-93.23	T212	-93.17	Q269	-93.03
I151	-93.09	S214	-93.17	G271	-94.03
A152	-93.58	L215	-93.01	G273	-94.19
T153	-93.41	T217	-93.42	K274	-93.05
G156	-94.30	T220	-93.12	V275	-93.09
A157	-93.25	R221	-93.00	Q276	-93.28
A158	-93.60	E222	-93.32	I277	-93.06
G161	-94.25	K224	-93.10	I278	-93.17
Q162	-92.98	K225	-93.09	N279	-93.42
K163	-93.13	V226	-93.11	K280	-93.18
G164	-94.40	A227	-93.62	K281	-93.06
E165	-92.99	V228	-92.90	L282	-93.16
A166	-93.48	V229	-93.13	D283	-93.01
N167	-93.29	R230	-93.26	L284	-92.89
A168	-93.36	K234	-93.09	S285	-93.22
T169	-93.22	S235	-93.56	N286	-93.17
I171	-93.28	S237	-93.27	V287	-92.96
A173	-93.33	S238	-93.41	Q288	-93.36
K174	-92.88	A239	-93.53	S289	-93.31
A178	-93.61	K240	-93.04	K290	-93.03
K180	-92.92	S241	-93.39	C291	-92.88
T181	-93.32	R242	-93.07	G292	-94.37
S184	-93.17	L243	-93.28	S293	-93.17
S185	-93.18	Q244	-92.98	K294	-93.13
G186	-94.30	T245	-93.14	D295	-93.21
E187	-93.27	A246	-93.71	N296	-93.19
S191	-93.25	V248	-93.04	I297	-92.94
G192	-94.21	M250	-93.18	K298	-93.28
D193	-93.23	D252	-93.05	H299	-93.09
R194	-92.96	L253	-93.10	V300	-93.28
S195	-93.25	K254	-93.13	S305	-93.11
G196	-94.25	N255	-93.27	V306	-92.90
Y197	-93.03	V256	-92.94	Q307	-92.77
S198	-93.30	K257	-93.30	V313	-92.99
S199	-93.59	S258	-93.36	D314	-93.32
G201	-94.21	K259	-93.03	L315	-93.39
S202	-93.53	I260	-93.13	K317	-92.89
G204	-94.29	G261	-94.42	V318	-93.01
T205	-93.39	S262	-93.17	T319	-92.92
G207	-94.22	T263	-93.20	S320	-93.54
S208	-93.33	E264	-93.09	K321	-93.08
R209	-93.06	N265	-93.27	C322	-92.88
S210	-93.33	L266	-93.22	S324	-93.17
R211	-93.26	K267	-93.14	L325	-93.01

Residue	$^1J_{NH}$(Hz)
G326	-94.22
N327	-93.33
I328	-92.92
H329	-93.05
H330	-93.32
K331	-93.41
G333	-93.95
Q336	-92.98
V337	-92.95
K338	-93.24
V339	-93.01
K340	-93.33
S341	-93.27
E342	-92.89
K343	-92.99
L344	-93.29
D345	-93.07
F346	-93.14
K347	-93.27
D348	-93.16
R349	-93.03
V350	-93.02
Q351	-93.15
S352	-93.35
K353	-92.96
I354	-93.11
G355	-94.34
S356	-93.18
L357	-93.18
D358	-93.13
I360	-92.92
H362	-93.37
V363	-93.19
G365	-94.00
N368	-93.27
K369	-93.30
K370	-93.26
I371	-93.03
E372	-93.20
T373	-93.17
H374	-93.26
K375	-93.04
L376	-93.15
T377	-93.16

Residue	$^1J_{NH}$(Hz)
F378	-93.04
R379	-93.24
E380	-93.06
N381	-93.35
A382	-93.36
K383	-93.18
A384	-93.53
K385	-93.00
T386	-93.06
D387	-93.25
H388	-93.26
G389	-94.49
A390	-93.16
E391	-93.05
I392	-92.96
V393	-93.13
Y394	-93.36
K395	-93.06
V398	-92.90
V399	-93.34
S400	-93.46
G401	-94.20
D402	-93.30
T403	-93.12
S404	-93.71
R406	-93.10
H407	-93.12
L408	-93.05
S409	-93.23
N410	-93.29
V411	-92.95
S412	-93.48
S413	-93.26
T414	-93.15
G415	-94.38
S416	-93.26
I417	-92.89
D418	-93.38
M419	-93.05
V420	-92.95
D421	-93.26
S422	-93.34
Q424	-92.92
L425	-93.05

Residue	$^1J_{NH}$(Hz)
A426	-93.34
T427	-93.01
L428	-93.12
A429	-93.41
D430	-93.29
E431	-92.95
V432	-92.97
S433	-93.54
A434	-93.54
S435	-93.35
L436	-93.28
A437	-93.55
K438	-93.10
Q439	-93.33
G440	-94.19

Supporting Table S2. NMR. Amino-acid specific random coil values of $^{1}J_{NH}$ spin-spin coupling constants.

Amino acid	# of exp. values in Tau	Random coil value of $^{1}J_{NH}$(Hz)
Alanine	32	-93.40
Arginine	12	-93.12
Asparagine	10	-93.27
Aspartate	29	-93.20
Cysteine	2	-92.88
Glutamine	18	-93.05
Glutamate	27	-93.01
Glycine	41	-94.23
Histidine	10	-93.17
Isoleucine	14	-93.03
Leucine	19	-93.08
Lysine	43	-93.08
Methionine	5	-93.13
Phenylalanine	3	-93.08
Serine	43	-93.30
Threonine	33	-93.20
Tyrosine	4	-93.13
Valine	27	-93.00

Supporting Table S3. NMR. $^{1}J_{NH}$ values of α-synclein at different pH and temperatures, measured at 700MHz. The missing data due to signal overlapping and broadening are labeled as "N.A."

Residues	$^{1}J_{NH}$(Hz)					
	278K			288K		298K
	pH 5.7	pH 6.5	pH 7.4	pH 5.7	pH 7.4	pH 5.7
V3	-92.9	-93.0	-93.0	-92.9	-93.0	-92.9
F4	-93.2	-93.5	-93.9	-93.5	-93.8	-93.4
M5	-93.5	-93.7	-93.6	-93.5	N.A.	-93.8
G7	-94.1	-94.3	N.A.	-94.3	N.A.	-94.1
L8	-93.3	-93.3	N.A.	-93.4	N.A.	-93.2
S9	-93.6	-93.6	N.A.	-93.6	N.A.	-93.6
K12	-93.3	-93.2	-93.2	-93.4	N.A.	-93.3
E13	-93.1	-93.4	N.A.	-93.3	N.A.	-93.2
G14	-94.3	-94.4	-94.2	-94.2	-94.2	-94.2
V15	-93.0	-92.9	-93.2	-93.0	-93.4	-93.0
A17	-94.1	-93.6	-94.1	-94.0	-94.3	-94.0
A18	-93.7	-93.6	-94.1	-93.6	-93.9	-93.7
A19	-93.8	-93.9	-94.2	-93.8	-94.0	-93.7
E20	-93.6	-93.6	-93.6	-93.4	N.A.	-93.3
K21	-93.1	-93.2	-93.1	-93.5	-93.3	-93.4
T22	-93.4	-93.4	-93.3	-93.4	-93.3	-93.4
G25	-94.3	-94.3	-94.3	-94.2	N.A.	-94.2
V26	-93.4	-93.2	-93.2	-93.2	-93.1	-93.2
A27	-94.1	N.A.	N.A.	-94.0	-94.2	-94.0
E28	-93.6	-93.6	-93.7	-93.2	-93.8	-93.5
A29	-94.1	-93.8	-93.9	N.A.	-94.1	-93.3
G31	-94.3	-94.3	-94.3	-94.3	-94.3	-94.3
K32	-93.4	-93.5	N.A.	-93.3	N.A.	-93.4
T33	-93.6	-93.5	-93.5	-93.4	N.A.	-93.4
V37	-93.0	-93.2	-93.1	-93.0	-93.0	-92.9
L38	-93.8	-93.5	-93.9	-93.7	-93.8	-93.7
Y39	-93.5	-93.3	N.A.	-93.4	-93.4	-93.3
V40	-93.1	-93.1	-93.1	-93.1	-93.1	-93.0
G41	-94.4	-94.5	-94.6	-94.4	N.A.	-94.4
T44	-93.5	-93.5	-93.5	-93.5	-93.4	-93.5
V48	-93.0	-93.0	-93.1	-92.9	-93.0	-92.9
V49	N.A.	-93.1	-93.1	-93.1	-93.1	-93.2
H50	-93.6	N.A.	-93.8	-93.6	N.A.	-93.9
G51	-94.3	-94.2	-94.5	-94.4	N.A.	-94.3
V52	-93.1	N.A.	-93.1	-93.0	-93.0	N.A.
A53	-94.0	-94.1	-94.3	-94.0	N.A.	-94.0
V55	-93.3	-93.3	-93.3	-93.1	-93.2	N.A.
A56	N.A.	-94.1	N.A.	-93.9	N.A.	-93.8
E57	-93.4	-93.4	-93.6	-93.4	-93.6	-93.2

K58	-93.5	-93.5	-93.8	-93.4	-93.7	-93.4
T59	-93.5	-93.5	-93.6	-93.5	-93.3	-93.3
K60	-93.5	-93.4	-93.6	-93.7	N.A.	N.A.
E61	-93.4	-93.8	-93.6	-93.5	-93.7	N.A.
Q62	-93.6	-93.5	-93.5	N.A.	-93.8	-93.4
V63	-93.2	N.A.	N.A.	-93.1	-93.2	-93.0
T64	-93.5	-93.5	N.A.	-93.4	-93.3	-93.4
V66	-93.1	-93.2	-93.2	-93.1	-93.3	-93.0
G67	-94.4	-94.4	-94.5	-94.4	-94.6	-94.4
G68	-94.3	-94.3	-94.3	-94.3	-94.5	-94.3
A69	-93.9	-93.8	-94.1	-93.9	N.A.	-93.8
V70	-93.1	-93.1	-93.1	-93.1	-93.0	-93.0
V71	-93.3	-93.2	-93.3	-93.2	-93.2	-93.1
T72	-93.6	-93.4	-93.6	-93.5	-93.5	-93.5
G73	-94.3	-94.2	-94.2	-94.2	N.A.	-94.1
V74	-93.1	-93.0	-93.1	-92.9	-93.1	-92.8
T75	-93.6	-93.6	-93.5	-93.5	-93.7	-93.5
A76	-94.0	-94.0	-94.1	-93.8	N.A.	-93.9
V77	-93.2	-93.2	-93.2	-93.0	-93.1	-93.0
A78	-94.3	-94.3	-94.4	-94.1	-94.3	-94.0
Q79	-93.3	-93.4	-93.4	-93.4	N.A.	-93.5
K80	-93.6	-93.6	N.A.	-93.4	N.A.	-93.5
T81	-93.5	-93.5	-93.5	-93.4	-93.4	-93.3
V82	-93.2	-93.2	-93.2	-93.1	-93.2	-93.2
E83	-93.6	N.A.	-93.7	-93.6	-93.7	-93.5
G84	-94.3	-94.3	-94.3	-94.3	N.A.	-94.3
A85	-93.7	-93.9	-93.7	-93.6	N.A.	-93.9
G86	-94.4	-94.6	-94.5	-94.4	N.A.	-94.4
S87	-93.5	-93.5	-93.6	-93.5	N.A.	-93.4
I88	-93.3	-93.3	-93.2	-93.2	-93.3	-93.1
A89	-94.1	-94.0	N.A.	-94.0	N.A.	-93.9
A90	-94.0	-94.0	-94.1	-93.8	-93.9	-93.7
A91	-93.9	-94.0	N.A.	-93.7	N.A.	-93.9
T92	-93.2	-93.0	-93.2	-93.1	-93.4	-93.1
G93	-94.2	-94.4	-94.0	-94.2	N.A.	-94.3
F94	-93.4	N.A.	-93.4	-93.4	-93.4	-93.4
V95	-93.3	-93.2	-93.3	-93.2	-93.2	-93.1
K96	-93.9	-94.0	-93.9	-93.9	-94.0	-93.7
K97	N.A.	-93.1	-93.1	N.A.	-93.1	N.A.
D98	-93.7	-93.5	-93.7	-93.5	-93.7	-93.6
Q99	-93.2	-93.1	-93.5	-93.2	N.A.	N.A.
L100	-93.6	-93.6	-93.7	-93.5	-93.7	-93.4
G101	-94.3	-94.3	-94.3	-94.3	-94.2	-94.3
K102	-93.2	-93.5	N.A.	-93.2	-93.4	-93.3
N103	-93.6	-93.8	-93.9	-93.6	N.A.	-93.7

E104	-93.3	-93.4	-93.3	-93.3	-93.4	-93.2
E105	-93.1	-93.6	-93.4	-93.4	-93.6	N.A.
G106	-94.3	-94.2	-94.3	-94.3	-94.3	-94.2
A107	-94.1	-93.8	-94.1	-93.9	-94.4	-93.9
Q109	-93.2	-93.2	-93.3	-93.2	-93.3	-93.2
E110	-93.3	N.A.	-93.4	-93.2	-93.5	-93.2
G111	-94.2	-94.2	-94.3	-94.2	-94.2	-94.2
I112	-93.1	-93.1	-93.0	-93.0	-93.0	-93.0
E114	-93.1	N.A.	N.A.	-93.6	-93.3	-93.3
D115	-93.5	-93.3	-93.6	-93.4	-93.7	-93.4
M116	-93.8	-93.5	N.A.	-93.5	-93.7	-93.7
V118	-93.2	-93.2	-93.1	-93.0	-92.9	-92.9
D119	-93.9	-93.8	-94.0	-93.8	-93.9	-93.8
D121	-93.5	N.A.	-93.5	-93.5	-93.5	-93.5
N122	-93.6	-93.6	-93.5	-93.5	-93.7	-93.5
E123	-93.5	-93.6	-93.5	-93.4	-93.7	-93.4
A124	-93.8	-93.7	-93.8	N.A.	-93.7	-93.6
Y125	-93.1	-93.3	-93.4	-93.0	-93.4	-92.9
E126	-93.6	-93.5	-93.5	-93.4	-93.6	-93.4
S129	-93.4	-93.2	-93.4	-93.3	-93.3	-93.3
E130	-93.3	-93.4	-93.3	-93.3	-93.4	-93.3
G132	-94.3	-94.3	-94.3	-94.2	N.A.	-94.1
Y133	-93.4	N.A.	-93.4	-93.3	-93.4	-93.2
Q134	-93.9	N.A.	N.A.	-93.5	-93.7	N.A.
D135	-93.6	-93.6	-93.5	-93.6	-93.5	N.A.
Y136	-93.2	-93.3	-93.3	-93.2	-93.2	-93.2
E137	-93.8	-93.7	-93.8	-93.7	-93.8	-93.7
E139	-93.2	-93.1	-93.3	-93.1	-93.3	-93.0

Supporting Table S4. NMR. $^{1}J_{NH}$ values of native ubiquitin at 400MHz, 600MHz and 900MHz field strength, pH 7.0, 298K. I36 was not included because its amid proton chemical shift is close to the edge of the selective pulse excitation profile. T9 and G75 were excluded because of low sensitivity.

Residue	$^{1}J_{NH}$(Hz) 400M	$^{1}J_{NH}$(Hz) 600M	$^{1}J_{NH}$(Hz) 900M
Q2	-92.97	-92.99	-92.90
I3	-92.65	-92.64	-92.48
F4	-93.37	-93.22	-92.95
V5	-92.95	-92.71	-92.67
K6	-93.37	-93.43	-93.01
T7	-94.2	-94.09	-93.76
L8	-92.38	-92.48	-92.61
T9	N.A.	N.A.	N.A.
G10	-93.64	-93.49	-93.40
K11	-93.52	-93.43	-93.41
T12	-92.68	-92.49	-92.26
I13	-93.2	-93.03	-92.88
T14	-92.84	-92.76	-92.65
L15	-93.83	-93.72	-93.58
E16	-92.02	-91.93	-91.86
V17	-93.47	-93.41	-93.28
E18	-92.15	-92.07	-91.85
S20	91.95	91.95	-92.00
D21	-93.96	-93.87	-93.78
T22	-93.43	-93.38	-93.36
I23	-93.96	-93.87	-93.95
N25	-94.22	-94.11	-93.84
V26	-93.76	-93.67	-93.45
K27	-93.66	-93.55	-93.19
A28	-94.03	-93.85	-93.68
K29	-93.67	-93.61	-93.31
I30	-93.79	-93.68	-93.31
Q31	-93.9	-93.83	-93.90
D32	-93.9	-93.98	-93.55
K33	-92.87	-92.74	-92.54
E34	-90.54	-90.46	-90.14
G35	-93.98	-94.00	-94.03
I36	N.A.	N.A.	N.A.
D39	-93.4	-93.32	-93.16
Q40	-92.15	-92.15	-92.06
Q41	-93.22	-93.27	-93.44
R42	-93.35	-93.34	-93.57
L43	-92.92	-92.93	-93.03

Residue	$^{1}J_{NH}$(Hz) 400M	$^{1}J_{NH}$(Hz) 600M	$^{1}J_{NH}$(Hz) 900M
I44	-92.42	-92.34	-92.30
F45	-93.59	-93.51	-93.67
A46	-93.91	94.01	-94.01
G47	-93.28	-93.21	-93.00
K48	-93.03	-92.99	-92.97
Q49	-93.02	-93.04	-92.99
L50	-93.97	-93.85	-93.65
E51	-92.47	-92.38	-92.33
D52	-92.45	-92.39	-92.44
R54	-92.86	-92.91	-92.82
T55	-92.57	-92.45	-92.23
L56	-94.18	-94.13	-93.88
S57	-93.73	-93.75	-93.71
D58	-94.26	-94.09	-94.07
Y59	-92.32	-92.31	-92.13
N60	-94.15	-94.25	-94.19
I61	-93.07	-93.03	-92.99
Q62	-92.91	-92.93	-93.14
K63	-93.26	-93.28	-93.23
E64	-93.35	-93.29	-93.21
S65	-93.84	-93.84	-93.82
T66	91.85	91.76	91.58
L67	-93.08	-92.97	-92.87
H68	-93.08	-92.98	-92.74
L69	-93.10	-93.02	-93.06
V70	-93.45	-93.47	-93.62
L71	-92.97	-93.00	-93.14
R72	-93.12	-93.11	-93.24
L73	-92.86	-92.91	-92.87
R74	-92.99	-92.86	-92.88
G75	N.A.	N.A.	N.A.

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