

Supporting Information Table 1. List of $^1J_{C\alpha C\beta}$ values measured in human ubiquitin.

Residue	$^1J_{C\alpha C\beta}$ (Hz)
M1	32.48
Q2	34.82
I3	34.19
F4	32.98
V5	35.34
K6	34.87
T7	37.68
L8	33.67
T9	39.24
K11	33.94
T12	38.08
I13	34.45
T14	38.04
L15	32.49
E16	36.13
V17	33.04
P19	31.68
S20	37.82
D21	36.33
T22	37.18
E24	33.30
N25	35.41
V26	33.35
K27	33.31
A28	33.50
K29	33.35
I30	33.17
Q31	33.36
D32	34.95
K33	33.07
E34	34.46
P38	31.36
D39	35.28
Q40	36.21
Q41	34.69
R42	35.42
L43	35.35
I44	33.70
F45	34.31
A46	38.46
K48	33.90

Q49	35.54
L50	34.51
E51	33.92
R54	34.21
T55	37.21
L56	33.22
S57	37.79
D58	35.44
Y59	35.47
N60	41.23
I61	35.53
Q62	34.18
K63	33.18
E64	37.83
S65	35.65
T66	38.03
L67	34.60
H68	34.78
L69	35.16
V70	34.06
L71	34.16
R72	35.29
L73	34.10
R74	34.77

Supporting Information Table 2. Experimental $\Delta^1J_{C\alpha C\beta}$ (Hz) values and backbone torsion angles in human ubiquitin.

$\Delta^1J_{C\alpha C\beta}$ (Hz)	ϕ (degree)	ψ (degree)	Res. #
0.46	-91	138	Q2
0.46	-131	163	I3
-0.52	-116	140	F4
1.66	-118	114	V5
0.51	-95	128	K6
0.41	-100	171	T7
-0.55	-73	-7	L8
1.97	-101	15	T9
-0.35	-96	138	K11
0.82	-120	132	T12
0.80	-109	142	I13
0.76	-101	140	T14
-0.01	-126	154	L15
1.81	-112	121	E16
-0.56	-139	171	V17
-1.38	-55	-25	P19
0.47	-80	-8	S20
-0.20	-71	148	D21
-0.10	-84	160	T22
-0.99	-58	-40	E24
-0.88	-65	-44	N25
-0.17	-58	-46	V26
-0.87	-61	-38	K27
-1.44	-66	-38	A28
-0.98	-64	-37	K29
-0.49	-70	-40	I30
-0.93	-62	-49	Q31
-1.61	-53	-42	D32
-1.07	-94	-24	K33
0.30	-124	-6	E34
-1.55	-57	-32	P38
-1.21	-68	-16	D39
1.79	-96	-10	Q40
0.40	-85	130	Q41
1.25	-121	116	R42
1.00	-104	130	L43
0.00	-122	132	I44

1.02	-144	130	F45
4.14	48	46	A46
-0.33	-115	143	K48
1.09	-86	130	Q49
0.23	-80	138	L50
-0.40	-102	140	E51
-0.19	-85	165	R54
-0.04	-105	165	T55
-0.79	-61	-36	L56
-0.12	-64	-30	S57
-1.03	-56	-39	D58
1.83	-91	5	Y59
4.85	58	45	N60
1.93	-89	116	I61
-0.22	-103	170	Q62
-1.06	-55	143	K63
3.45	67	19	E64
-1.82	-71	160	S65
0.46	-119	127	T66
0.26	-103	155	L67
0.68	-106	136	H68
0.88	-107	116	L69
0.66	-108	140	V70
-0.15	-96	139	L71