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Supplementary Table 1. ${}^3J_{C',C'}$ coupling constants in human ubiquitin and backbone ϕ angles calculated from the X-ray structure.

	${}^3J_{C',C'}$ (Hz)	ϕ (degree)
Q2 ^a	0.730	-91.0
I3	1.919	-131.1
F4	1.183	-116.0
V5	1.767	-118.0
K6	0.929	-95.2
T7	0.682	-99.6
L8	0.416	-73.4
T9	0.574	-101.4
G10	0.655	77.4
K11	0.617	-96.3
T12	1.112	-119.9
I13	1.139	-109.5
T14	0.753	-101.4
L15	1.577	-126.4
E16	0.853	-111.8
V17	2.283	-139.0
E18	1.213	-120.0
D21	0.600	-71.0
T22	0.434	-83.7
N25	0.484	-65.5
V26	0.529	-58.4
K27	0.437	-60.8
A28	0.467	-66.1
I30	0.586	-70.0
Q31	0.582	-62.1
D32	0.451	-53.4
K33	0.649	-93.6
G35	0.391	81.2
I36	0.627	-79.7
D39	0.398	-68.2
Q40	0.729	-95.8
Q41	0.610	-84.8
R42	1.622	-121.2
L43	0.974	-103.6
I44	1.681	-122.1
F45	2.033	-144.3
A46	0.757	48.2
G47	0.393	61.7
K48	1.240	-115.1
Q49	0.461	-85.8
L50	0.594	-79.6
E51	0.818	-101.8
R54	0.787	-85.4

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T55	0.741	-104.5
L56	0.416	-61.2
S57	0.433	-63.9
D58	0.453	-55.6
Y59	0.720	-91.0
N60	0.505	57.9
I61	0.465	-88.7
Q62	1.061	-103.4
S65	0.515	-71.1
T66	1.125	-119.2
L67	0.822	-103.1
H68	1.038	-105.6
L69	0.793	-107.0
V70	1.666	-108.1
L71	0.699	-96.0
R72	0.963	-117.6
L73	0.769	-83.7
R74	0.947	-97.7
G75	0.836	120.4
G76	1.217	174.2

^aJ_{C',C'} couplings between C' of residue i-1 and residue i.

Supplementary Figure 1. Reproducibility plot of measured ${}^3J_{C'C'}$ couplings in human ubiquitin, measured in a 4-scan (12 h) and a 16-scan-per-FID (48 h) experiment, both recorded at 600 MHz ${}^1\text{H}$ frequency. The pairwise root-mean-square difference is 0.06 Hz.

