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Supplementary Table 1. Relaxation values in human ubiquitin at 600 MHz, 27 °C, and derived generalized order parameters (S^2) and correlation times for fast internal motion (τ_e).

	$T_{1,1}$[a]	$T_{1,2}$[a]	$T_{2,1}$	$T_{2,2}$	NOE_1	NOE_2	S^2_{iso}	S^2_{aniso}	$\tau_{e,iso}$	$\tau_{e,aniso}$
	(ms)								(ps)	
Q2	0.480	0.477	0.167	0.168	0.732	0.704	0.844	0.837	28	30
I3	0.453	0.453	0.162	0.165	0.755	0.773	0.880	0.883	5	3
F4	0.449	0.439	0.158	0.165	0.764	0.757	0.893	0.898	9	7
V5	0.473	0.471	0.175	0.179	0.754	0.748	0.823	0.830	10	8
K6	0.456	0.462	0.170	0.167	0.723	0.740	0.855	0.860	24	23
T7	0.465	0.460	0.167	0.167	0.716	0.705	0.856	0.859	38	37
L8	0.476	0.476	0.196	0.198	0.661	0.638	0.771	0.772	46	46
T9	0.517	0.510	0.195	0.196	0.570	0.569	0.731	0.731	63	63
G10	0.496	0.495	0.203	0.205	0.600	0.577	0.735	0.736	59	58
K11	0.524	0.525	0.201	0.205	0.557	0.572	0.711	0.709	58	58
T12	0.500	0.502	0.196	0.196	0.679	0.670	0.755	0.756	33	32
I13	0.470	0.467	0.169	0.171	0.686	0.672	0.840	0.845	52	53
T14	0.483	0.482	0.174	0.174	0.738	0.725	0.825	0.830	19	17
L15	0.457	0.457	0.183	0.178	0.744	0.736	0.820	0.822	16	15
E16	0.504	0.506	0.184	0.186	0.720	0.711	0.778	0.777	20	20
V17	0.461	0.456	0.164	0.163	0.724	0.718	0.876	0.876	36	36
E18	0.488	0.484	0.164	0.162	0.728	0.717	0.856	0.847	27	28
S20	0.475	0.471	0.165	0.168	0.664	0.663	0.844	0.842	64	63
D21	0.442	0.437	0.163	0.162	0.796	0.789	0.899	0.900	0	1
T22	0.457	0.457	0.172	0.174	0.757	0.743	0.846	0.852	13	11
I23	0.432	0.437	0.145	0.146	0.759	0.765				
N25	0.447	0.448	0.121	0.121	0.768	0.753				

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V26	0.446	0.453	0.170	0.175	0.739	0.749	0.853	0.858	17	16
K27	0.444	0.438	0.157	0.159	0.767	0.763	0.911	0.917	5	2
A28	0.435	0.438	0.160	0.162	0.727	0.720	0.898	0.897	44	44
K29	0.456	0.455	0.161	0.161	0.745	0.752	0.888	0.890	17	16
I30	0.450	0.445	0.164	0.167	0.756	0.756	0.879	0.887	11	9
D32	0.451	0.448	0.160	0.161	0.794	0.770	0.894	0.895	0	1
K33	0.469	0.466	0.170	0.169	0.760	0.742	0.851	0.855	11	9
E34	0.468	0.467	0.171	0.171	0.744	0.744	0.845	0.851	15	13
G35	0.469	0.469	0.164	0.165	0.770	0.757	0.867	0.855	3	7
I36	0.537	0.530	0.176	0.174	0.798	0.774	0.791	0.783	0	1
D39	0.461	0.457	0.172	0.174	0.763	0.750	0.850	0.852	9	7
Q40	0.460	0.456	0.165	0.168	0.749	0.730	0.864	0.865	20	19
Q41	0.465	0.458	0.171	0.171	0.743	0.726	0.847	0.853	22	20
R42	0.467	0.469	0.177	0.177	0.760	0.743	0.827	0.832	10	8
L43	0.474	0.468	0.176	0.178	0.732	0.725	0.822	0.828	21	20
I44	0.457	0.460	0.175	0.178	0.751	0.750	0.832	0.838	11	10
F45	0.460	0.458	0.164	0.167	0.759	0.748	0.868	0.872	11	9
A46	0.470	0.465	0.174	0.173	0.727	0.730	0.834	0.840	23	22
G47	0.481	0.478	0.179	0.178	0.744	0.733	0.817	0.821	16	14
K48	0.476	0.477	0.168	0.168	0.739	0.745	0.845	0.843	15	16
Q49	0.506	0.502	0.195	0.196	0.653	0.647	0.751	0.752	40	40
L50	0.462	0.456	0.177	0.176	0.723	0.729	0.833	0.836	24	24
E51	0.492	0.493	0.177	0.179	0.719	0.732	0.806	0.796	19	21
D52	0.514	0.513	0.173	0.175	0.710	0.701	0.797	0.788	25	27
R54	0.482	0.479	0.163	0.164	0.777	0.755	0.867	0.856	0	4
T55	0.465	0.468	0.164	0.166	0.741	0.729	0.866	0.868	23	23

L56	0.445	0.439	0.162	0.162	0.790	0.741	0.895	0.902	4	1
S57	0.454	0.449	0.168	0.169	0.777	0.749	0.868	0.871	6	3
D58	0.447	0.443	0.163	0.162	0.781	0.760	0.890	0.892	1	1
Y59	0.465	0.466	0.168	0.168	0.778	0.759	0.860	0.866	1	1
N60	0.456	0.458	0.164	0.164	0.764	0.769	0.878	0.884	3	1
I61	0.455	0.453	0.171	0.171	0.732	0.734	0.852	0.857	23	22
Q62	0.530	0.531	0.208	0.207	0.602	0.594	0.701	0.703	46	46
K63	0.488	0.488	0.171	0.169	0.695	0.696	0.824	0.817	36	37
E64	0.444	0.439	0.168	0.165	0.734	0.724	0.872	0.878	31	30
S65	0.453	0.456	0.167	0.167	0.765	0.764	0.869	0.871	5	3
T66	0.480	0.475	0.172	0.171	0.739	0.748	0.835	0.841	14	12
L67	0.468	0.459	0.174	0.176	0.766	0.776	0.838	0.843	0	1
H68	0.472	0.465	0.165	0.165	0.758	0.761	0.866	0.873	6	3
L69	0.465	0.459	0.174	0.174	0.783	0.764	0.843	0.847	0	1
V70	0.448	0.456	0.156	0.157	0.779	0.743	0.907	0.910	7	5
L71	0.480	0.478	0.186	0.183	0.688	0.660	0.794	0.796	42	41
L73	0.557	0.553	0.301	0.303	0.348	0.325	0.565	0.565	71	71
R74	0.642	0.643	0.394	0.391	0.020	0.026				
G75	0.838	0.841	0.638	0.643	-0.408	-0.433				
G76	1.26	1.27	0.899	0.908	-1.280	-1.400				

[a] Data are obtained from two separate measurements. Derived values (S^2 and τ_e) are calculated from the T_1, T_2 and NOE values, averaged over the two data sets.

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Supplementary Table 2. Calculated hydrodynamic parameters of human ubiquitin[a]

	R=3.5Å			R=3.7Å			R=4.0Å		
	X-ray[b]	clip[c]	dyn[d]	X-ray[b]	clip[c]	dyn[d]	X-ray[b]	clip[c]	dyn[d]
$D_{//}/D_{\perp}$	1.44	1.13	1.23 ±0.013	1.40	1.18	1.24 ±0.011	1.41	1.17	1.24 ±0.017
τ_c (ns)	5.19	4.38	4.64 ±0.031	5.44	4.65	4.90 ±0.05	5.83	5.02	5.39 ±0.046
D_t (10^{-6} cm^2/s)[a]	1.28	1.34	1.32 ±0.004	1.26	1.32	1.29 ±0.005	1.23	1.28	1.26 ±0.005
D_1 (10^7 s^{-1})[a]	2.76	3.56	3.27 ±0.03	2.66	3.31	3.08 ±0.04	2.47	3.08	2.80 ±0.03
D_2 (10^7 s^{-1})[a]	2.85	3.74	3.40 ±0.03	2.74	3.45	3.21 ±0.05	2.56	3.20	2.94 ±0.04
D_3 (10^7 s^{-1})[a]	4.03	4.12	4.09 ±0.05	3.79	4.00	3.90 ±0.05	3.55	3.68	3.55 ±0.03
θ (°)[e]	43.7	46.2	48.8 ±1.0	45.4	45.6	49.5 ±0.7	45.9	45.6	50.6 ±1.0
ϕ (°)[e]	47.3	48.0	44.3 ±2.4	45.9	50.5	50.6 ±1.0	44.0	47.4	44.0 ±1.6
ψ (°)	-29.7	-22.1	-19.4 ±3.3	-35.6	-27.0	-21.8 ±3.4	-37.0	-12.7	-22.8 ±1.4

[a] Using bead models, at 20 °C. For obtaining values at 27 °C, values of the diffusion constants should be divided by 0.8314.

[b] Using X-ray coordinates

[c] Using X-ray coordinates, but excluding the three C-terminal residues

[d] Using X-ray coordinates, but assuming conformations of the C-terminal 6 residues which correspond to 8 equally spaced snapshots of a 2-ns Langevin dynamics simulation.

[e] Eigenvectors of the diffusion tensor in the X-ray coordinate frame, using spherical coordinates.