

Table S1. Multiple solutions for each residue of GB1 at the best RSDC determined alignment tensors. Two parameters are reported for each minimum, the RMSD between the experimental RDCs and the fitted one, and the angular deviation from the X-ray coordinates (1PGB).

Residue	Solution 1		Solution 2	
	RMSD	Angular Deviation	RMSD	Angular Deviation
3	0.449	3.42	2.954	35.86
5	0.906	6.94	8.138	46.9
8	0.253	4.63	4.016	51.19
9	0.166	19.68		
10	0.295	7.38		
11	0.044	37.82	2.31	4.47
12	1.175	6.03	8.176	77.25
13	0.132	18.73	5.586	46.3
14	0.076	15.8	3.664	17.34
15	0.301	1.78	3.085	27.43
16	0.213	9.86	1.315	21.83
17	0.274	13.96	1.033	7.8
18	0.149	4.33	11.99	28.57
19	0.305	5.63		
21	0.137	14.41	2.51	82.83
24	0.06	10.31	8.319	44.54
26	0.197	4.09	11.606	88.66
28	0.037	11.53		
29	0.024	13.46	10.284	46.18
32	0.104	1.77		
34	0.499	2.04	9.171	72.04
35	0.066	5.1	5.152	33.85
36	0.288	19.15		
37	0.036	8.43	9.848	78.31
38	0.136	5.68		
39	0.325	15.53	6.761	59.45
40	0.531	18.07	1.658	18.54
41	0.383	19.02	5.208	45.92
43	0.219	14.98	8.369	74.31
44	0.365	2.13	5	39.86
46	0.113	1.66	1.461	22.07
48	0.483	14.65	10.297	72.53
49	0.052	29.05	1.197	14.71
50	0.635	4.49	1.85	31.04
51	0.281	4.94	0.779	10.27
52	0.003	10.05	21.128	49.34
53	0.713	2.59	6.666	63.72
54	0.309	1.94	6.852	61.85
56	0.568	8.37	8.937	46.78

Table S2. Multiple solutions for each residue of ubiquitin at the best RSDC determined alignment tensors. Two parameters are reported for each minimum, the RMSD between the experimental RDCs and the fitted one, and the angular deviation from the X-ray coordinates (IUBQ).

Residue	Solution 1		Solution 2		Solution 3	
	RMSD	Angular Deviation	RMSD	Angular Deviation	RMSD	Angular Deviation
2	0.253	2.86				
3	0.02	3.44	0.1	86.58	1.72	65
4	0.067	3.64	1.838	62.26		
5	0.19	1.85	3.343	46.48		
6	0.17	11.21				
7	0.063	5.14	2.478	58.13		
8	0.626	41.85	0.852	10.06	1.099	50.12
11	0.314	8.44	1.192	63.12		
12	0.69	13.63	1.193	42.47		
13	0.109	6.06	3.304	52.78	3.309	48.58
14	0.272	9.34	1.221	37.71		
15	0.442	2.79	0.958	88.7		
17	0.281	6.61	3.084	85.75	7.404	85.87
18	0.151	8.77	0.554	29.51		
20	0.294	4.8	3.781	79.06	6.905	47.13
21	0.008	5.43	0.886	60.16	2.302	64.85
23	0.018	3.52				
25	0.04	64.09	0.176	1.44		
27	0.22	16.52	0.496	1.86		
28	0.196	28.83	0.304	58.81	0.482	2.67
29	0.141	4.48	0.589	24.91	0.964	49.47
30	0.014	0.15				
32	0.108	17.98	0.142	57.06	0.233	10.06
33	0.394	12.82	0.977	30.06	1.024	13.24
34	0.056	17.79	0.314	8.43	0.62	38.79
35	0.26	4.45	3.371	48.79	8.602	66.21
36	0.154	11.53				
40	0.228	4.1	4.095	74.79	7.763	69.34
41	0.014	6.42	0.817	17.07		
42	0.077	3.79	0.889	77.1	1.1	23.84
43	0.109	8.46	1.952	86.16		
44	0.174	2.98	0.312	14.99		
45	0.311	6.18	2.714	60.52		
47	0.219	8.23				
48	0.047	11.05	3.007	65.96		
49	0.077	5.82	4.198	68.72	5.233	63.32
50	0.171	5.74	0.371	31.82	0.509	25.57
51	0.039	7.95	0.25	53.71		
52	0.456	19.18	1.706	14.72		
54	0.096	17.62	4.407	61.46	4.696	78.08
55	0.221	2.72	0.592	24.72	0.988	53.22
56	0.015	7.01	2.97	66.68		
58	0.042	3.88	0.56	89.14	1.54	55.68
59	0.053	11.39	3.681	84.4		
60	0.037	0.88	1.02	32.46		
61	0.017	7.52	1.679	29.87		
62	0.036	14.93	2.287	19.1		
63	0.379	4	3.952	51.76	4.284	68.86
64	0.035	1.83	0.441	47.09		
65	0.205	2.44			3.658	49.39
66	0.113	7.43				
67	0.24	8.34				
68	0.19	6.05				