Structural analysis of a complex between small ubiquitin-like modifier 1 (SUMO1) and the ZZ domain of CREB-binding protein (CBP/p300) reveals a new interaction surface on SUMO

Carl Diehl, Mikael Akke, Simon Bekker-Jensen, Niels Mailand, Werner Streicher, and Mats Wikström

SUPPLEMENTAL TABLE 1. Parameters from the fitting of the ^{15}N CPMG relaxation dispersion curves of apo-SUMO1, SIMPX-SUMO1, and ZZ domain-SUMO1 respectively. The fitted parameters shown are the exchange rate k_{ex}, the population of the major state p_M, the difference in chemical shift between major and minor state $\Delta\Omega_{15N}$, $R_{2,0}$ in the absence of exchange at 60.8 and 80.1 MHz and the F-test probability p for distinguishing between the models in Equation 1.

apo-SUMO1

Residue	k_{ex} (s^{-1})	± std	p_M	± std	$\Delta\Omega_{15N}$ (ppm)	± std	$R_{2,0}$ 60MHz (s^{-1})	± std	$R_{2,0}$ 80MHz (s^{-1})	± std	p
2	49725.8	2225.0	0.998	0.002	2.288	1.617	21.88	0.12	24.78	0.19	0.98
3	11459.5	9090.6	0.991	0.006	1.251	0.365	8.33	0.22	10.38	0.36	0.77
4	12689.1	6618.7	0.989	0.005	1.306	0.400	6.74	0.28	9.14	0.40	0.8
5	9124.5	4868.6	0.988	0.007	0.881	0.229	5.93	0.26	8.14	0.30	0.62
6	1772.6	23698.5	0.999	0.003	0.314	0.407	5.76	0.09	7.75	0.14	0.95
7	1216.6	3447.6	0.992	0.022	0.401	0.239	6.32	0.24	8.30	0.37	0.0083
9	16261.7	11769.8	0.991	0.009	1.097	0.498	12.05	0.32	15.19	0.47	1.0
10	10327.0	8380.4	0.991	0.007	1.094	0.436	14.57	0.41	18.24	0.60	0.91
11	11713.8	1259.2	0.995	0.001	0.849	0.125	2.40	0.03	2.45	0.04	0.96
13	2029.6	6188.2	0.993	0.014	0.821	0.480	9.74	0.18	12.20	0.44	1.6E-5
14	8857.9	3827.1	0.990	0.003	1.540	0.248	9.24	0.26	11.78	0.41	0.031
15	4014.2	9200.7	0.989	0.016	1.022	0.691	13.55	0.28	17.04	0.73	0.0027
16	1384.1	2648.0	0.987	0.026	1.235	0.498	18.08	0.81	24.76	1.48	5.1E-13
18	1877.3	4957.3	0.995	0.011	1.120	0.626	15.26	0.29	18.51	0.52	3.6E-6
19	3948.0	7469.4	0.991	0.010	1.427	0.703	16.57	0.35	19.68	0.79	0.002
20	612.9	981.3	0.991	0.011	0.696	0.326	19.91	0.24	21.49	0.41	7.4E-6
21	2906.5	5790.4	0.993	0.006	2.852	1.557	22.97	0.98	27.56	1.94	1.6E-9
22	11771.9	7066.8	0.955	0.013	4.149	0.526	18.95	2.50	16.56	4.38	3.1E-8
23	8095.4	6465.0	0.994	0.003	4.970	1.065	22.58	0.91	24.48	1.53	0.0033
24	977.6	2340.4	0.994	0.004	2.415	1.239	25.09	0.76	28.75	1.24	4.7E-6

25	2400.6	4719.1	0.992	0.008	2.159	1.138	24.52	0.74	27.34	1.41	6.0E-09
26	10721.4	6408.8	0.986	0.005	4.112	0.754	22.32	1.09	23.66	1.78	0.0011
27	5453.4	6073.7	0.994	0.005	2.634	0.901	26.07	0.58	29.85	1.09	0.19
28	2273.1	4477.5	0.993	0.009	1.874	0.927	23.30	0.60	27.28	1.32	0.0099
29	2035.0	5691.6	0.990	0.021	1.081	0.623	23.49	0.43	28.74	0.97	0.0042
30	7412.1	5961.2	0.990	0.005	3.626	0.816	19.42	0.88	22.67	1.60	7.5E-5
31	8485.2	6743.9	0.984	0.007	2.585	0.628	19.06	0.73	22.31	1.22	0.0017
32	6362.7	8650.8	0.985	0.013	2.343	1.018	20.14	0.91	24.87	2.03	2.1E-6
33	7562.6	6285.5	0.981	0.010	2.278	0.635	19.86	0.85	23.91	1.56	0.0019
34	5161.5	6406.4	0.985	0.011	2.179	0.839	22.61	0.78	25.83	1.64	3.8E-7
35	1379.5	3017.3	0.993	0.007	2.331	1.247	24.49	0.99	29.45	1.66	8.6E-9
36	696.7	829.9	0.988	0.006	2.315	1.079	23.52	1.14	26.69	1.83	4.8E-16
37	776.9	1351.9	0.991	0.006	2.099	1.013	22.57	0.90	26.53	1.39	7.1E-10
38	859.9	1118.9	0.987	0.007	2.690	1.233	23.96	1.54	27.77	2.45	1.3E-15
40	1638.9	3322.0	0.995	0.006	2.200	1.065	26.51	0.66	30.99	1.26	8.8E-10
41	2062.3	3527.4	0.995	0.004	2.176	1.003	23.56	0.53	26.64	1.02	0.048
42	851.7	2106.3	0.994	0.006	2.034	1.025	23.08	0.77	27.91	1.24	1.8E-8
43	1018.6	3353.9	0.998	0.003	1.661	0.919	23.38	0.40	26.59	0.59	0.39
44	11976.9	6714.7	0.984	0.006	4.375	0.715	24.38	1.08	25.83	1.95	0.24
45	626.0	1165.5	0.987	0.011	1.608	0.773	26.01	0.83	29.57	1.46	7.4E-10
46	1001.4	2195.0	0.996	0.005	1.687	0.884	24.52	0.50	27.99	0.84	0.0045
47	1264.1	2099.9	0.990	0.008	2.505	1.279	24.69	1.37	29.21	2.28	1.5E-8
48	9362.1	7343.5	0.989	0.005	3.025	0.742	26.75	0.75	29.97	1.06	0.55
49	2072.1	4225.0	0.994	0.008	1.935	0.977	25.72	0.58	30.10	1.17	3.4E-6
50	5760.0	6387.2	0.991	0.006	3.043	1.087	22.00	0.92	24.54	1.69	1.9E-5
54	6663.0	6584.2	0.988	0.008	2.507	0.790	21.69	0.69	24.71	1.36	0.0014
55	6218.0	5753.0	0.987	0.008	2.913	0.841	21.72	0.94	23.89	1.68	9.5E-5
56	9301.2	6502.7	0.984	0.007	3.223	0.588	22.62	0.95	24.60	1.65	0.012
57	4002.6	6708.6	0.986	0.012	2.404	1.012	20.63	1.35	22.67	2.61	0.035
60	4778.5	6066.2	0.991	0.008	1.970	0.778	25.17	0.54	29.71	1.11	0.04
61	1784.4	3846.7	0.990	0.018	1.235	0.542	23.58	0.54	28.56	1.07	0.00039
62	7303.9	5723.1	0.992	0.004	2.662	0.718	22.73	0.52	25.98	0.95	0.16

64	6624.3	6963.6	0.990	0.007	2.382	0.769	23.61	0.61	28.57	1.20	0.35
65	7540.9	6286.7	0.985	0.008	2.973	0.666	22.05	0.83	23.45	1.47	0.00047
66	10309.3	7208.1	0.983	0.009	2.586	0.615	23.62	0.67	25.91	1.37	0.076
67	6840.6	6698.8	0.991	0.005	3.165	0.946	21.64	0.81	23.72	1.37	0.0037
68	7752.0	5519.4	0.988	0.005	2.479	0.586	20.35	0.52	22.26	0.92	0.053
69	5330.7	6374.2	0.987	0.011	2.530	0.913	21.63	1.06	24.34	1.98	1.9E-9
70	7491.7	5814.5	0.989	0.006	2.988	0.722	21.14	0.77	24.03	1.50	0.00055
71	10661.6	7848.3	0.986	0.006	3.204	0.683	26.22	0.69	28.64	1.37	0.49
72	7625.8	6129.6	0.989	0.006	2.928	0.798	23.67	0.68	26.43	1.26	0.047
73	4325.8	7026.0	0.991	0.008	1.556	0.746	27.01	0.41	31.78	0.89	0.33
74	7996.9	5282.4	0.992	0.003	4.516	0.941	22.76	0.96	25.29	1.58	0.0048
75	3485.2	7365.0	0.993	0.008	2.494	1.289	23.98	0.87	28.36	1.76	0.0032
76	6411.2	6089.4	0.987	0.008	2.425	0.735	22.27	0.70	24.51	1.36	0.0035
78	740.7	2041.7	0.996	0.004	1.462	0.758	24.96	0.51	29.21	0.83	0.024
80	8630.4	5326.9	0.990	0.005	3.334	0.652	23.61	0.82	25.78	1.45	0.066
81	6500.7	6212.4	0.990	0.006	2.705	0.845	22.35	0.67	24.71	1.32	0.018
82	7485.0	7016.4	0.991	0.005	4.104	0.912	23.32	0.89	24.91	1.58	0.00021
83	2440.1	5967.1	0.982	0.024	1.441	0.776	26.51	0.91	29.29	1.83	0.00053
84	507.6	1195.3	0.997	0.005	1.227	0.620	26.45	0.38	29.22	0.68	0.1
85	8465.1	5455.9	0.991	0.004	5.172	0.878	23.23	0.98	24.59	1.89	0.1
87	3921.1	6067.5	0.991	0.008	2.525	1.089	24.64	0.95	27.64	1.68	0.00082
88	6839.1	6375.5	0.992	0.005	3.735	1.130	27.18	0.91	30.90	1.87	0.055
89	3705.7	7321.4	0.994	0.006	2.133	1.075	24.79	0.57	27.97	1.17	0.18
90	5561.5	6342.8	0.983	0.010	2.242	0.743	20.54	0.86	22.78	1.63	1.6E-8
92	1739.9	3954.8	0.994	0.011	1.333	0.571	21.68	0.37	25.18	0.70	0.0009
94	9099.1	5688.2	0.978	0.009	2.089	0.432	16.39	0.51	18.74	0.96	5.3E-5
95	17681.1	6582.7	1.005	0.005	1.867	0.778	16.77	0.31	20.38	0.61	0.99
96	24870.7	3501.5	1.009	0.012	0.996	0.501	17.07	0.29	20.22	0.43	1.0
97	24694.1	6669.5	0.997	0.004	1.695	0.843	14.82	0.24	17.70	0.28	0.98
99	9351.1	15332.5	0.997	0.010	0.930	0.890	13.15	0.31	16.15	0.42	1.0
100	816.8	2357.6	0.992	0.015	0.710	0.340	12.07	0.65	16.89	0.90	3.2E-7
101	987.5	3166.6	0.993	0.018	0.610	0.326	12.17	0.56	16.59	0.74	0.004

SIMPX-SUMO1

Residue	k_{ex} (s^{-1})	± std	p_M	± std	$\Delta\Omega_{15N}$ (ppm)	± std	$R_{2,0}$ 60MHz (s^{-1})	± std	$R_{2,0}$ 80MHz (s^{-1})	± std	p
2	14753.9	9942.4	0.992	0.005	1.717	0.514	9.60	0.39	12.52	0.42	0.98
3	32423.8	15889.2	0.996	0.006	1.615	0.662	4.73	0.29	7.99	0.29	1.0
4	23945.5	2047.3	0.991	0.003	1.801	0.232	4.33	0.19	5.59	0.14	1.0
5	16543.0	10260.3	0.990	0.005	1.829	0.483	4.38	0.26	6.18	0.29	1.0
6	11040.0	6992.8	0.992	0.007	0.923	0.313	3.87	0.19	5.61	0.24	0.99
7	2384.6	3946.1	0.993	0.004	1.083	0.402	4.68	0.16	4.93	0.29	0.056
9	786.3	2183.0	0.997	0.006	0.645	0.387	6.09	0.23	7.89	0.30	0.18
10	124.7	159.2	0.991	0.006	0.867	0.603	6.76	0.32	9.35	0.38	6.8E-7
11	1933.0	14366.9	1.000	0.002	0.408	0.475	2.39	0.04	2.38	0.05	0.98
13	11850.2	4171.7	0.982	0.005	1.760	0.230	5.62	0.24	6.20	0.41	0.19
14	6495.6	5941.6	0.988	0.007	1.162	0.338	5.94	0.28	7.57	0.40	0.39
15	5403.9	6001.1	0.982	0.013	1.524	0.534	6.52	0.56	8.97	0.96	0.00054
17	834.3	1157.9	0.986	0.013	1.444	0.640	7.37	0.98	9.62	1.84	3.3E-6
18	1062.6	1511.4	0.991	0.010	0.869	0.440	11.02	0.31	12.88	0.44	1.0E-05
19	7668.1	4433.6	0.985	0.005	2.074	0.380	11.31	0.45	13.06	0.66	0.086
20	538.4	983.5	0.959	0.051	0.800	0.381	16.89	0.69	16.55	1.27	9.5E-19
23	1911.2	2428.8	0.977	0.020	1.802	0.677	25.22	2.20	31.14	4.08	0.00011
26	1129.4	1401.2	0.988	0.010	2.275	1.038	26.16	1.37	29.88	2.50	1.2E-5
27	1478.9	1990.1	0.992	0.006	2.020	0.857	27.04	0.99	30.89	1.43	0.065
28	5242.6	6017.1	0.974	0.013	2.494	0.736	22.88	1.62	21.30	2.87	0.003
30	13872.3	7185.9	0.988	0.004	3.553	0.721	20.41	0.79	25.33	1.37	0.85
31	18952.9	6232.4	0.988	0.003	3.619	0.495	19.51	0.60	22.20	0.86	0.92
32	8036.8	6564.5	0.982	0.007	3.154	0.670	19.46	1.05	23.36	1.82	0.022
33	44634.6	9174.2	0.981	0.003	8.278	0.589	11.09	1.33	14.43	2.09	0.92
34	6973.0	6025.1	0.987	0.005	3.147	0.830	23.72	1.04	26.16	1.79	0.21
35	64393.8	6819.7	0.990	0.001	12.218	0.570	20.73	1.66	19.16	1.32	0.95
38	7640.8	12009.9	0.987	0.014	5.221	2.666	25.66	5.92	23.37	9.28	0.087
41	3703.8	5728.1	0.993	0.007	1.821	0.861	25.79	0.85	28.27	1.04	0.74
42	17066.8	16749.0	1.013	0.019	2.098	0.626	32.89	2.75	40.83	1.77	0.0047
43	441.5	426.9	0.985	0.012	1.622	0.851	26.02	0.83	26.80	1.37	3.1E-5

44	5618.4	5114.6	0.990	0.005	3.986	1.066	28.44	1.75	29.54	2.71	0.26
46	13339.7	6766.2	0.990	0.003	4.355	0.618	11.62	0.95	15.92	1.63	0.85
48	1578.0	2871.5	0.986	0.012	2.761	1.443	29.85	3.56	33.86	4.97	0.00045
52	18282.4	7725.3	0.990	0.005	2.902	0.710	21.21	0.63	24.31	0.55	1.0
53	23264.1	13117.5	0.993	0.008	2.238	1.085	17.57	0.63	23.03	0.70	0.95
54	19182.9	8057.9	0.986	0.004	3.943	0.529	23.58	0.72	26.04	1.25	0.86
55	938.0	972.6	0.990	0.008	2.364	1.158	24.23	1.41	29.32	2.14	0.0013
56	6910.2	5993.7	0.980	0.010	2.666	0.699	24.66	1.26	27.62	2.24	0.12
57	310.0	1284.9	0.852	0.195	0.297	0.103	14.28	0.43	16.08	0.71	1.6E-6
60	5364.9	5670.4	0.989	0.007	2.136	0.724	21.54	0.68	25.05	1.15	0.22
61	739.2	1302.2	0.994	0.005	1.734	0.844	24.96	0.85	30.97	1.16	0.0036
62	1194.9	1607.1	0.983	0.020	1.213	0.541	24.28	0.91	28.08	1.35	0.00084
63	3131.9	3267.1	0.997	0.001	3.541	1.584	25.05	0.66	27.22	0.75	0.52
64	1500.2	6259.7	0.998	0.002	2.600	2.164	24.43	0.73	32.17	1.15	0.42
65	34722.2	6549.0	0.993	0.003	4.311	0.745	24.70	0.51	26.53	0.57	0.99
66	4032.7	4163.9	0.996	0.002	2.794	1.043	26.84	0.66	29.44	0.95	0.71
67	4051.0	5242.3	0.984	0.012	1.881	0.661	22.93	0.96	24.34	1.82	0.17
68	2579.9	4234.9	0.993	0.006	1.663	0.883	22.02	0.59	23.92	1.04	0.4
69	8780.5	6162.5	0.980	0.008	2.561	0.501	22.50	0.71	23.98	1.21	0.055
70	1748.4	2406.8	0.987	0.013	1.678	0.808	22.04	1.09	26.50	1.95	5.2E-6
71	40.8	49.0	1.004	0.008	3.363	17.589	28.73	0.67	31.36	0.60	0.97
72	7876.8	6583.9	0.991	0.005	4.798	1.171	23.07	1.34	26.52	2.63	0.42
74	700.0	993.7	0.987	0.010	1.853	0.913	25.40	1.12	29.55	1.78	0.002
75	7653.8	5286.8	0.991	0.004	4.378	0.937	24.01	1.30	27.29	2.10	0.12
76	11956.2	7749.9	0.993	0.003	7.159	0.982	18.23	2.34	20.59	2.73	0.7
80	937.9	1270.8	0.969	0.030	1.185	0.519	26.19	1.33	28.51	2.44	8.9E-7
81	1194.4	1830.1	0.979	0.026	1.363	0.626	24.40	1.07	27.05	1.94	5.9E-6
82	1746.9	2193.9	0.994	0.003	2.049	0.887	26.38	0.87	28.71	1.26	0.3
83	3919.2	6802.6	0.983	0.014	1.838	0.835	29.14	1.73	32.44	2.09	0.46
84	1565.7	5056.2	1.002	0.002	1.904	1.161	28.59	0.55	32.24	0.58	0.9
87	2647.3	3820.3	0.985	0.010	2.527	0.980	25.48	1.74	29.29	2.85	0.0032
88	2284.8	2989.8	0.991	0.008	2.027	0.816	25.46	1.06	30.40	1.67	0.064

89	5717.4	6027.1	0.991	0.005	3.040	1.051	25.73	1.01	27.05	1.62	0.53
90	2614.2	4095.5	0.992	0.006	2.189	1.088	23.52	0.98	26.06	1.54	0.054
94	404.1	2766.1	0.999	0.002	1.306	1.274	15.55	0.52	20.16	0.53	1.0
95	6206.2	7221.2	0.992	0.007	1.455	0.673	10.90	0.37	14.61	0.44	0.57
96	18499.0	6941.1	0.994	0.004	1.373	0.526	10.32	0.24	13.20	0.29	1.0
97	9821.4	11617.3	0.996	0.004	1.767	0.791	8.61	0.43	12.55	0.59	0.98
99	17042.0	5449.6	0.990	0.005	2.045	0.489	6.81	0.38	10.37	0.58	1.0
100	357.5	1450.7	0.982	0.019	0.819	0.406	6.31	0.40	8.17	0.58	5.1E-16
101	483.8	1266.4	0.986	0.021	0.769	0.378	6.63	0.28	8.12	0.49	1.1E-15

ZZ domain-SUMO1

Residue	k_{ex} (s^{-1})	± std	p_M	± std	$\Delta\Omega_{15N}$ (ppm)	± std	$R_{2,0}$ 60MHz (s^{-1})	± std	$R_{2,0}$ 80MHz (s^{-1})	± std	p
2	2103.6	2734.2	0.992	0.006	3.126	1.582	19.50	1.51	23.33	2.32	6.4E-12
3	1838.9	2758.1	0.986	0.014	1.015	0.505	7.83	0.36	10.73	0.73	1.3E-10
4	1963.8	3139.0	0.992	0.007	2.500	1.181	7.28	1.09	10.34	1.63	3.1E-21
5	1808.2	2380.5	0.989	0.009	0.930	0.493	6.16	0.25	8.77	0.52	6.0E-12
6	6898.0	4968.5	0.984	0.010	1.144	0.367	5.74	0.24	7.77	0.40	0.032
7	2344.3	4089.7	0.990	0.011	0.715	0.504	6.17	0.18	8.58	0.40	6.3E-5
9	13101.9	15729.4	0.989	0.015	1.536	0.899	10.89	0.33	13.92	0.76	0.87
10	1394.0	3423.3	0.992	0.010	0.746	0.626	12.98	0.19	16.93	0.53	0.002
11	18293.1	1404.9	0.993	0.005	0.832	0.232	2.39	0.04	2.64	0.08	1.0
13	1733.9	2549.3	0.953	0.038	0.402	0.188	9.74	0.24	12.15	0.47	2.6E-5
14	348.4	4306.0	0.997	0.005	0.588	0.459	9.31	0.21	12.31	0.31	0.15
15	4198.4	5329.5	0.988	0.010	1.216	0.623	12.77	0.34	16.37	0.76	0.003
16	986.0	2678.2	0.956	0.090	0.599	0.368	17.37	0.52	24.82	1.29	1.6E-8
18	1927.2	3165.0	0.993	0.006	1.252	0.765	14.67	0.33	17.91	0.61	9.2E-8
19	10106.8	5766.1	0.965	0.014	1.869	0.339	15.20	0.62	17.91	1.16	0.0069
20	1068.7	1443.2	0.988	0.012	0.872	0.380	18.76	0.35	21.35	0.47	1.6E-5
21	1054.7	2936.5	0.990	0.015	1.100	0.699	24.72	0.49	30.71	1.02	0.0077
22	4083.9	4801.2	0.983	0.013	2.493	1.012	25.68	1.66	30.10	3.14	0.0059
23	2503.9	3976.6	0.996	0.003	3.124	1.580	25.40	0.78	29.31	1.24	0.033

24	928.0	1349.0	0.991	0.007	2.138	1.067	26.21	0.94	31.41	1.67	0.00014
25	2129.3	2750.9	0.994	0.004	2.566	1.246	26.09	0.84	30.42	1.29	0.0031
26	2190.4	2877.5	0.995	0.003	2.409	1.167	26.49	0.74	30.57	1.21	0.016
27	6475.1	4763.3	0.990	0.005	3.998	1.036	25.80	1.26	27.93	2.06	0.0094
28	678.4	621.6	0.994	0.003	2.508	1.231	24.56	0.68	30.22	0.79	8.7E-5
29	6803.0	4901.2	0.985	0.009	2.481	0.604	23.65	0.99	27.87	1.61	0.013
30	5094.1	3940.2	0.994	0.003	3.284	0.992	21.45	0.74	25.67	1.22	0.014
31	2886.6	3715.2	0.990	0.009	1.759	0.922	20.83	0.66	25.47	1.22	3.9E-5
32	3578.9	4420.9	0.990	0.007	2.433	1.153	21.22	0.99	27.25	1.79	1.9E-5
33	2425.7	3502.6	0.993	0.006	1.616	0.947	21.88	0.59	26.21	1.01	0.02
34	5286.9	4236.1	0.987	0.007	2.593	0.771	24.19	1.02	27.99	1.71	0.015
35	1899.8	2072.9	0.995	0.002	3.851	1.670	25.52	1.39	30.88	1.89	0.00064
36	1185.0	1339.6	0.988	0.008	2.541	1.130	25.40	1.49	30.65	2.35	4.3E-8
37	1314.7	1816.7	0.982	0.020	1.600	0.786	23.52	1.11	28.20	1.81	4.6E-9
38	2235.2	3041.3	0.980	0.022	1.878	0.821	25.51	1.61	31.07	3.06	0.00011
40	6660.1	4592.0	0.971	0.015	2.504	0.587	25.36	1.60	30.58	2.86	0.00035
41	7893.9	5651.5	0.989	0.005	3.666	0.728	24.05	1.01	27.28	1.65	0.39
42	8286.5	6137.0	0.978	0.009	3.866	0.699	21.58	1.59	25.71	2.79	0.00039
43	9018.2	5096.9	0.990	0.004	4.734	0.931	22.98	1.12	25.52	1.94	0.19
44	8938.0	6014.1	0.991	0.004	4.000	0.910	28.51	0.84	31.34	1.52	0.65
45	1116.1	1572.3	0.986	0.015	1.612	0.807	27.00	0.88	29.41	1.37	7.0E-07
46	992.3	1419.9	0.996	0.002	2.154	0.904	26.10	0.51	30.69	0.88	0.11
47	1333.8	1763.6	0.978	0.024	1.506	0.684	27.19	1.47	32.30	2.27	0.00059
48	7404.7	6171.8	0.985	0.008	2.621	0.680	29.13	0.94	32.77	1.76	0.59
49	1202.9	1722.9	0.990	0.010	1.494	0.665	28.20	0.61	32.09	1.02	0.00081
50	1683.5	2290.3	0.994	0.004	2.184	1.124	24.22	0.76	28.97	1.09	0.00033
52	27915.6	9564.6	0.993	0.003	3.525	0.776	29.47	0.43	29.79	0.55	0.96
53	15334.7	14622.8	0.993	0.006	2.609	1.024	22.58	0.33	24.69	0.72	1.0
54	10163.1	5024.0	0.987	0.004	3.731	0.677	22.45	0.87	25.91	1.57	0.044
55	2501.0	4104.6	0.978	0.022	1.307	0.704	23.94	0.97	28.38	1.90	0.046
56	21323.5	7138.0	0.971	0.006	5.742	0.535	21.17	1.57	21.46	2.60	0.28
57	2156.6	3936.1	0.997	0.002	2.862	1.453	22.30	0.78	25.62	1.19	0.42

60	2329.3	3276.6	0.993	0.006	1.826	0.884	25.88	0.59	30.53	1.00	0.012
61	9744.7	5835.5	0.973	0.009	2.995	0.539	22.68	1.00	26.77	1.86	0.015
62	6527.3	5110.0	0.993	0.004	2.798	0.898	24.13	0.65	28.58	1.03	0.54
64	9284.8	6124.7	0.980	0.009	3.279	0.529	22.93	1.21	26.71	2.25	0.17
65	4623.0	4658.9	0.982	0.012	1.761	0.559	24.56	0.83	27.77	1.50	0.037
66	6247.8	5661.0	0.989	0.006	2.519	0.770	25.93	0.79	28.60	1.38	0.43
67	6711.6	5354.5	0.987	0.007	3.534	0.804	22.81	1.17	25.27	2.06	0.00019
68	5116.7	4475.9	0.990	0.006	2.031	0.638	22.43	0.64	24.69	1.12	0.12
70	2592.1	2873.0	0.994	0.004	2.181	0.952	23.66	0.60	27.07	0.97	0.0058
71	9314.6	7413.8	0.976	0.011	3.556	0.689	25.67	1.35	27.65	2.36	0.053
72	19707.5	5492.4	0.987	0.003	5.150	0.522	24.26	0.66	27.31	1.26	0.89
73	11259.3	5589.7	0.986	0.006	3.208	0.714	26.90	0.69	32.91	1.42	0.59
74	5854.0	4558.8	0.991	0.005	3.391	0.979	24.23	1.01	28.42	1.85	0.00052
75	1946.3	2627.4	0.996	0.003	1.780	0.778	26.77	0.53	31.85	0.65	0.42
76	4808.5	4410.2	0.991	0.004	3.218	1.080	24.22	1.06	25.68	1.74	0.045
78	4694.8	4155.2	0.995	0.002	4.072	1.188	25.74	0.90	29.60	1.11	0.044
80	12925.9	7062.8	0.990	0.005	2.960	0.656	26.19	0.68	29.48	0.96	0.86
81	6904.2	5637.7	0.979	0.010	2.651	0.659	22.75	1.13	24.72	1.91	0.01
82	9195.1	5890.7	0.985	0.006	3.704	0.644	24.03	0.97	26.24	1.80	0.012
83	10246.7	6316.1	0.990	0.004	4.525	0.873	26.43	1.19	29.88	2.30	0.67
84	2161.6	2769.9	0.997	0.002	2.299	1.143	27.20	0.48	29.02	0.91	0.36
85	6987.9	5746.9	0.991	0.005	3.458	0.896	26.25	0.93	28.86	1.61	0.61
87	7427.6	5034.5	0.990	0.005	2.940	0.644	25.94	0.82	28.86	1.26	0.62
88	5105.7	4484.9	0.989	0.007	2.703	0.873	28.50	0.98	32.60	1.83	0.14
89	7854.6	5046.2	0.973	0.012	2.397	0.455	24.76	1.00	27.94	1.79	0.048
90	3089.3	3869.4	0.995	0.004	2.938	1.247	22.75	0.87	26.01	1.35	0.0033
92	317.5	296.6	0.995	0.003	1.467	0.802	22.98	0.38	27.41	0.42	0.00037
94	9881.9	6312.0	0.978	0.011	2.315	0.606	15.68	0.69	18.48	1.25	3.8E-5
95	12051.4	17365.9	0.985	0.016	1.487	0.748	14.76	0.35	18.24	0.81	0.7
96	19823.3	6376.3	0.989	0.005	2.496	0.575	14.39	0.25	17.42	0.53	1.0
97	23617.5	2238.4	0.976	0.028	0.311	0.085	12.89	0.09	16.03	0.20	0.99
99	23389.2	9550.5	0.991	0.006	1.531	0.484	11.12	0.20	14.39	0.41	1.0

| 100 | 3107.7 | 4390.3 | 0.988 | 0.012 | 1.065 | 0.709 | 11.52 | 0.43 | 16.26 | 0.87 | 7.0E-5 |
| 101 | 457.0 | 3501.1 | 0.996 | 0.008 | 0.718 | 0.458 | 11.69 | 0.29 | 16.30 | 0.47 | 0.022 |