Problem Data				Numerical Results			Timing	
#	name	p	n_0	lbd	ubd	rel-gap	iter	time(sec)
1	1AIE	26	34	-46.95892	-46.95892	1.04802e-15	200	0.10
2	2ERL	34	103	55.33285	55.33284	1.17985e-12	200	5.85
3	1CBN	37	112	-40.42751	-40.42751	1.68402e-14	300	7.77
4	1RB9	41	105	-76.96501	-76.96501	7.11964e-13	1000	26.39
5	1BX7	41	99	16.96026	16.96026	5.21525e-12	300	7.25
6	2FDN	42	51	-59.43091	-59.43092	3.71094e-14	200	0.04
7	1MOF	46	94	-79.05580	-79.05580	3.52629e-12	200	4.03
8	1CTF	47	74	-97.18893	-97.18893	4.64633e-13	200	2.81
9	1NKD	50	199	-51.78466	-51.78466	4.40639e-12	2680	192.65
10	2IGD	50	126	-78.50608	-78.50608	5.39611e-15	500	14.67
11	2SN3	53	112	-5.56818	-5.56818	6.73872e-13	700	16.77
12	1MSI	54	112	-87.46958	-87.46958	1.72043e-13	700	19.39
13	1AHO	54	140	24.66925	24.66925	4.19224e-14	1500	56.22
14	1COR	60	131	15.58314	15.58314	4.58637e-12	1000	32.31
15	1CTJ	61	258	-103.32705	-103.32705	1.64217e-12	1872	162.80
16	1RZL	65	121	17.26470	17.26470	1.22992e-11	2468	68.52
17	1TIF	66	614	-155.17859	-155.17859	4.69196e-14	1000	350.89
18	1BDO	69	221	-136.29933	-136.29933	8.93377e-15	1000	75.06
19	1OPD	70	112	-139.64632	-139.64632	1.18233e-13	300	5.98
20	1VQB	75	406	-96.94940	-96.94940	4.34568e-14	900	147.36
21	1IUZ	75	221	-150.88238	-150.88238	1.25791e-14	3200	227.45
22	1ABA	76	376	-137.59962	-137.59963	9.05546e-15	600	88.43
23	1FNA	76	131	-172.01313	-172.01313	3.64100e-14	800	23.32
24	1CYO	78	220	-75.36668	-75.36668	1.36739e-14	700	48.50
25	1FUS	79	302	-4.66627	-4.66627	1.11145e-12	3000	312.35
26	2MCM	80	123	-135.14024	-135.14024	8.30816e-13	400	10.30
27	1SVY	80	147	-141.92437	-141.92437	6.21219e-13	400	14.51
28	1A68	81	424	-178.12555	-178.12555	2.54581e-15	1500	249.80
29	1YCC	84	223	-79.21270	-79.21270	2.11079e-12	955	66.26
30	2ACY	84	580	-146.32254	-146.32254	1.06468e-14	7800	2175.04
31	1BM8	85	687	-119.54537	-119.54537	2.02428e-14	1300	509.88
32	1BKF	89	339	-170.80514	-170.80514	1.60935e-14	1000	117.73
33	3CYR	91	137	-144.06405	-144.06405	2.48290e-12	1900	52.09
34	3VUB	92	544	-229.38312	-229.38312	7.41813e-16	1400	349.67
35	1JER	96	462	-120.78401	-120.78400	1.15131e-12	3232	633.90
36	2HBG	97	275	-178.42210	-178.42210	2.70839e-13	500	42.98
37	1POA	97	470	278.08280	278.08280	2.02964e-12	5463	1099.55
38	1C52	99	256	-223.31096	-223.31096	2.41281e-15	2700	203.46
39	2A0B	99	642	-161.45228	-161.45228	1.75494e-16	5200	1800.90
40	2TGI	100	355	-14.03554	-14.03554	2.46249e-13	1300	153.95

Table A.1: Computational results on selected PDB instances up to 100 amino acids

Problem Data				Numerical Results			Timing	
#	name	p	n_0	lbd	ubd	rel-gap	iter	time(sec)
41	3NUL	101	285	-154.87542	-154.87542	1.28046e-15	2300	307.34
42	1WHI	101	298	-247.13457	-247.13457	6.94375e-14	1500	199.52
43	1PDO	104	453	-188.29848	-188.29848	9.10541e-12	5754	1456.33
44	3LZT	105	530	-48.81821	-48.81821	8.48591e-13	1100	300.50
45	1DHN	105	519	-133.77464	-133.77464	1.35468e-13	2000	535.83
46	1KUH	106	580	-155.56590	-155.56590	2.18536e-15	2296	743.57
47	1ECA	108	655	-169.74717	-169.74717	1.66944e-16	25200	12563.89
48	1BFG	108	410	-191.73261	-191.73262	8.54577e-14	900	210.84
49	1RIE	108	930	-117.91809	-117.91809	1.57208e-14	20200	17809.01
50	2SAK	111	214	-239.86975	-239.86975	1.08995e-12	500	37.26
51	1BGF	112	1180	-239.65571	-239.65571	1.52549e-13	56400	71503.54
52	2END	118	707	-8.22833	-8.22833	1.08596e-12	16100	8511.24
53	2SNS	119	634	620.86546	620.86546	1.79304e-14	6900	3082.12
54	1BD8	121	347	-219.12419	-219.12419	9.42666e-12	4970	760.81
55	1NPK	122	709	-205.56059	-205.56059	6.77231e-13	59075	31212.37
56	1A6M	124	613	-55.41007	-55.41008	4.93096e-14	22800	7608.82
57	2RN2	127	830	-198.37189	-198.37189	1.41057e-13	6073	4053.13
58	1RCF	130	733	-86.59895	-86.59775	1.38011e-05	100000	56927.20
59	1LCL	131	1246	-217.16433	-217.16433	2.53317e-14	3800	4821.11
60	2CPL	132	819	-284.97180	-284.97180	9.75693e-15	5900	3329.39
61	1VHH	133	844	-21.33604	-21.33604	3.59566e-14	3200	1843.96
62	1BJ7	135	917	-64.37915	-64.37915	5.69493e-14	11300	8946.94
63	119L	136	970	-234.21535	-234.21535	8.01617e-14	34200	30890.87
64	1RA9	136	1018	-185.07235	-185.07235	5.13076e-14	4400	4839.16
65	1L58	137	962	-285.60167	-285.60167	1.31131e-14	15600	13812.60
66	2ILK	142	708	-121.02712	-121.02712	1.82770e-13	4700	2750.13
67	1KOE	144	710	-13.87537	-13.87537	1.27269e-11	4124	2490.08
68	1HA1	146	538	-213.93793	-213.93793	1.44469e-13	3700	1229.31
69	1CEX	146	415	174.95279	174.95279	2.40438e-11	11447	2426.49
70	1CV8	146	730	-213.13554	-213.13554	3.28738e-13	5600	3442.13
71	153L	149	846	-170.13061	-170.13061	3.03488e-13	2100	1554.46
72	1BS9	150	935	103.16569	103.16569	1.31052e-13	2500	1736.57
73	2PTH	151	1198	-190.97344	-190.97344	1.39085e-13	1900	2233.17
74	1XNB	151	1233	-147.30040	-147.30040	2.69217e-15	13300	16562.76
75	1AQB	152	713	29.24537	29.24537	9.30418e-14	39300	17795.39
76	1LBU	152	1225	38.14603	38.14603	1.91397e-13	9900	11673.18
77	1KID	153	653	-351.91160	-351.91160	2.90337e-15	6600	2607.24
78	1CHD	154	489	-164.21510	-164.21510	3.27846e-14	19300	4097.50
79	1AMM	158	1480	-288.62671	-288.62671	2.75245e-15	3300	5793.13
80	2ENG	162	867	82.01797	82.01797	1.33295e-13	14200	8284.65
81	1G3P	165	921	-70.30769	-70.30769	6.66312e-14	7000	4469.99
82	1THV	167	902	5.12749	5.12749	4.63732e-12	4200	2637.88
83	1PPN	170	1259	-56.69346	-56.69346	1.23365e-13	11589	14139.22
84	1IAB	173	775	321.20652	321.20652	2.04964e-14	26500	13017.74
85	1DIN	175	1110	-264.73564	-264.73548	5.84356e-07	100000	93357.26
86	2AYH	176	1269	8428.18154	6089367.83709	1.99447e+00	100000	135879.29
87	1ZIN	177	853	-353.00431	-353.00431	3.18384e-14	23800	13742.52
88	1BYI	177	818	-242.78881	-242.78881	2.33646e-14	2400	1298.65
89	2BAA	178	1165	-43.77265	-43.77265	1.95480e-12	4600	4785.88
90	1A7S	179	524	-239.78218	-239.78218	1.00542e-14	1200	284.88
91	1WAB	183	1063	-317.46713	-317.46713	9.40337e-14	8500	7357.75
92	1MUN	185	1047	-378.01261	-378.01261	1.15635e-14	9500	7883.00
93	1LST	192	946	-244.76861	-244.76861	1.28627e-14	32300	21374.44
94	1GCI	194	1052	-205.63185	-205.63185	2.79899e-14	10300	8885.03
95	3CLA	198	857	-26.72768	-26.72768	9.89051e-14	3900	2287.99

Table A.2: Computational results on selected PDB instances up to 200 amino acids

Problem Data				Numerical Results			Timing	
#	name	p	n_0	lbd	ubd	rel-gap	iter	time(sec)
96	1AL3	201	1077	119.66598	119.66598	3.39407e-14	12500	10188.87
97	1ARB	202	1466	-61.52823	-61.52823	3.41363e-14	8900	14632.82
98	1XJO	202	776	-171.92443	-171.92443	8.24179e-15	3700	1455.50
99	1NLS	203	1060	-297.73578	-297.73578	5.33677e-15	2500	1976.08
100	1MRJ	208	1178	-295.13711	-295.13711	1.70740e-13	2300	2149.63
101	1OAA	208	854	-317.83422	-317.83422	1.44174e-12	3842	1823.52
102	2DRI	210	906	-398.45564	-398.45564	2.56465e-15	6200	3225.99
103	2CBA	223	1018	-86.52145	-86.52145	5.34000e-14	3400	2407.24
104	2POR	224	1304	-83.22221	-83.22221	5.55044e-14	6700	8044.39
105	3SEB	224	1412	77.15838	77.15852	1.84867e-06	100000	137194.81
106	1MLA	227	1322	-484.10542	-484.10542	1.68910e-14	62900	75257.79
107	1DCS	232	1170	-342.68600	-342.68600	1.39133e-14	8000	7459.07
108	1AKO	234	1387	-244.65691	-244.65691	1.18251e-14	7400	9809.00
109	1PDA	239	891	-423.50226	-423.50226	4.96037e-15	9100	4520.68
110	1EZM	239	1497	-217.36581	-217.36581	3.49620e-13	2300	3919.92
111	1C3D	243	1679	-400.69876	-400.69876	1.04846e-14	22100	134094.53
112	1RHS	244	1973	-341.20443	-341.20443	1.41400e-14	7300	62136.57
113	8ABP	245	1743	-273.90715	-273.90716	2.27865e-15	9000	59868.98
114	1CVL	246	910	-537.04249	-537.04249	2.11494e-16	14800	7522.51
115	1RYC	248	1831	-202.60568	-202.60568	4.81378e-14	15200	84674.22
116	1MRP	248	1648	-350.97062	-350.97062	1.39088e-14	11000	34303.23
117	1IXH	252	1134	-289.75241	-289.75241	4.11267e-14	1300	1087.30
118	1FNC	253	1940	-310.60999	-310.60999	6.54656e-13	34321	292924.91
119	1TCA	255	1062	-422.15387	-422.15387	4.24994e-14	8700	6424.87
120	1SBP	256	1704	-271.08838	-271.08838	3.59996e-14	40000	156330.60
121	2CTC	264	1536	-213.88596	-213.88596	2.17419e-14	15100	43642.85
122	1PGS	265	2190	-16.14049	-16.14049	2.28785e-12	21300	269611.15
123	1MSK	271	1798	-162.51007	-162.50978	1.77573e-06	100000	771330.61
124	1BG6	271	784	-452.62383	-452.62383	3.13620e-15	12700	4935.11
125	1ARU	271	939	-314.40612	-314.40589	7.15908e-07	100000	53858.54
126	1A8E	274	1096	-249.85499	-249.85499	3.58741e-14	96500	78746.74
127	1AXN	278	2343	-300.34291	-300.34291	7.55789e-15	12500	207625.02
128	1TAG	279	1330	-253.22167	-253.22167	1.68029e-14	4300	5038.43
129	1ADS	280	1560	733.91439	733.91440	1.39319e-13	18273	65301.22
130	3PTE	284	2006	161.17216	161.17216	5.09815e-15	13500	59169.60
131	1CEM	292	2400	-24.20196	-24.20196	3.85446e-14	7000	47701.70

Table A.3: Computational results on selected PDB instances up to 300 amino acids