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Supporting Material

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Supplementary Material #1
The dataset of domains with different folds

The table contains SCOP sid domain identifier, domain class, sequence length, root-mean-square-error (RMSE) of the structure regularization, and SPACI score as a measure of the structure quality.

SID	Class	Length	RMSE	SPACI
d1a1x__	β	106	0.039	0.43
d1a3aa_	α+β	145	0.029	0.51
d1a6m__	α	151	0.035	1.04
d1a6q_2	α+β	295	0.047	0.41
d1aa7a_	α	158	0.026	0.42
d1af7_1	α	81	0.031	0.41
d1ah7__	α	245	0.028	0.62
d1aie__	α	31	0.031	0.62
d1ail__	α	70	0.017	0.52
d1ako__	α+β	268	0.032	0.56
d1amj_2	α/β	527	0.043	0.45
d1axn__	α	323	0.041	0.51
d1ay7b_	α/β	89	0.033	0.57
d1b25a2	α+β	210	0.033	0.50
d1b2pa_	β	119	0.063	0.55
d1b2va_	α+β	173	0.036	0.47
d1b3aa_	α+β	67	0.048	0.60
d1b67a_	α	68	0.023	0.63
d1bd8__	α+β	156	0.022	0.51
d1bfd_2	α/β	180	0.025	0.62
d1bgf__	α	124	0.026	0.66
d1bkra_	α	108	0.025	0.91
d1bm8__	α+β	99	0.043	0.52
d1boua_	α	132	0.023	0.42
d1bx4a_	α/β	342	0.030	0.61
d1bxya_	α+β	60	0.064	0.45
d1byi__	α/β	224	0.042	1.06
d1c1da2	α/β	148	0.059	0.61
d1c1ka_	α	217	0.023	0.61
d1c75a_	α	71	0.039	1.06
d1c8za_	α+β	265	0.034	0.44
d1chd__	α/β	198	0.030	0.51
d1cipa1	α	121	0.023	0.59
d1cq3a_	β	224	0.047	0.45
d1csei_	α+β	63	0.062	0.79
d1ctf__	α+β	68	0.035	0.55
d1cy5a_	α	92	0.029	0.77
d1d3va_	α/β	308	0.030	0.57
d1d4oa_	α/β	177	0.028	0.66
d1dcia_	α/β	275	0.025	0.63
d1dd3a1	α	57	0.026	0.41
d1dfma_	α/β	223	0.046	0.61
d1dfup_	β	94	0.037	0.49
d1dj0a_	α+β	264	0.029	0.65
d1dj8a_	α	79	0.029	0.42
d1dkza2	β	118	0.036	0.45
d1dl5a2	α+β	104	0.037	0.52
d1ds1a_	β	323	0.032	0.90
d1duvg1	α/β	150	0.036	0.53
d1dvoa_	α	152	0.022	0.47
d1dw9a1	α	86	0.027	0.61
d1dw9a2	α+β	70	0.062	0.61
d1dzfa2	α+β	72	0.029	0.43
d1e19a_	α/β	313	0.030	0.64
d1e58a_	α/β	247	0.026	0.85
d1e7la1	α	54	0.024	0.79
d1e8ca1	α/β	101	0.032	0.44
d1eaqa_	β	124	0.062	0.80
d1eb6a_	α+β	177	0.038	1.06
d1ed1a_	α	114	0.024	0.41
d1eexg_	α	137	0.037	0.54
d1egwa_	α+β	71	0.052	0.54
d1el6a_	α+β	208	0.030	0.44
d1emua_	α	132	0.020	0.48
d1ew4a_	α+β	106	0.034	0.69
d1ewfa1	α+β	217	0.038	0.50
d1eyqa_	α+β	212	0.045	0.44
d1ez3a_	α	124	0.019	0.47
d1f3ua_	β	118	0.032	0.48
d1f5na1	α	300	0.020	0.53
d1f7ta_	α+β	119	0.039	0.49
d1f86a_	β	115	0.058	0.92
d1f8na1	α	690	0.021	0.65
d1f9ya_	α+β	158	0.041	1.17
d1fid__	α+β	258	0.037	0.44

d1fjja_	β	159	0.047	0.57
d1fk5a_	α	93	0.040	0.77
d1fkma1	α	194	0.018	0.47
d1flma_	β	122	0.053	0.77
d1fmta1	β	108	0.058	0.41
d1fn9a_	α+β	365	0.030	0.52
d1fs1a1	α	41	0.036	0.48
d1fs1b1	α	55	0.030	0.48
d1fsga_	α/β	233	0.025	0.98
d1fw9a_	α+β	164	0.051	0.68
d1g2ra_	α+β	94	0.034	0.73
d1g2ya_	α	31	0.034	0.98
d1g3p_1	β	65	0.030	0.64
d1g61a_	α+β	225	0.036	0.74
d1g66a_	α/β	207	0.054	1.16
d1g6ga_	β	127	0.030	0.54
d1g7sa3	α/β	131	0.029	0.41
d1g8ea_	α	98	0.023	0.46
d1g8ma1	α/β	197	0.028	0.51
d1g8qa_	α	90	0.036	0.56
d1g8ta_	α+β	241	0.030	0.92
d1g9za_	α+β	152	0.031	0.48
d1gci__	α/β	269	0.041	1.33
d1gk8i_	α+β	125	0.036	0.71
d1gmua1	β	70	0.045	0.59
d1gmxa_	α/β	108	0.049	0.94
d1goia1	β	52	0.060	0.67
d1gp0a_	β	133	0.045	0.62
d1gpqa_	α+β	127	0.042	0.58
d1gwua_	α	306	0.043	0.73
d1gwya_	β	175	0.051	0.49
d1gxja_	α+β	161	0.029	0.41
d1gyxa_	α+β	76	0.028	0.75
d1h09a1	β	149	0.038	0.41
d1h16a_	α/β	759	0.030	0.51
d1h2ca_	β	124	0.041	0.60
d1h4ax1	β	85	0.045	0.85
d1h4xa_	α/β	111	0.042	0.87
d1h6wa1	β	82	0.063	0.44
d1h99a1	α	115	0.021	0.57
d1hdha_	α/β	525	0.038	0.71
d1hfel1	α/β	311	0.030	0.61
d1hfes_	α	88	0.033	0.61
d1hp1a1	α+β	188	0.047	0.56
d1hqsa_	α/β	423	0.031	0.58
d1hs6a2	β	208	0.099	0.44
d1hufa_	α+β	123	0.042	0.41
d1hw1a2	α	152	0.020	0.64
d1hxha_	α/β	253	0.045	0.82
d1hxn__	β	209	0.072	0.48
d1hyoa2	α+β	298	0.033	0.73
d1i27a_	α	73	0.034	1.00
d1i2ta_	α	61	0.019	0.98
d1i40a_	β	175	0.038	0.94
d1i4ja_	α+β	110	0.037	0.49
d1i4ma_	α+β	108	0.038	0.44
d1i6pa_	α/β	214	0.025	0.46
d1i7qa_	α+β	517	0.040	0.45
d1ig0a2	α/β	221	0.028	0.47
d1ihra_	α+β	73	0.057	0.64
d1ijya_	α	122	0.026	0.66
d1ikpa2	α+β	212	0.036	0.62
d1io0a_	α/β	166	0.022	0.63
d1ioma_	α	374	0.023	0.65
d1iq4a_	α+β	179	0.038	0.47
d1irqa_	α	48	0.034	0.60
d1itxa2	α+β	72	0.045	0.93
d1iw0a_	α	207	0.027	0.72
d1ix9a1	α	90	0.033	1.16
d1ix9a2	α+β	115	0.039	1.16
d1ixh__	α/β	321	0.051	1.05
d1izma_	α	170	0.045	0.45
d1j09a1	α	163	0.020	0.50
d1j0pa_	α	108	0.041	1.13
d1j2ra_	α/β	188	0.030	0.78
d1j31a_	α+β	262	0.039	0.60
d1j5ua_	α+β	127	0.044	0.42
d1j8ba_	α+β	92	0.043	0.52
d1j98a_	α+β	154	0.047	0.85
d1j9ja_	α/β	247	0.023	0.47
d1jata_	α+β	152	0.032	0.57
d1jb9a1	β	157	0.050	0.56
d1jf8a_	α/β	130	0.023	0.85
d1jfba_	α	399	0.037	1.01
d1jg1a_	α/β	215	0.037	0.82
d1jh6a_	α+β	181	0.051	0.50
d1jhda1	β	173	0.037	0.56
d1jhfa2	β	126	0.023	0.46
d1ji7a_	α	77	0.023	0.68
d1jida_	α+β	114	0.044	0.51
d1jixa_	α/β	351	0.028	0.55
d1jkea_	α/β	145	0.041	0.58
d1jkxa_	α/β	209	0.032	0.55
d1jm1a_	β	202	0.042	0.94
d1jnra1	α	141	0.030	0.59
d1jo0a_	α+β	97	0.049	0.73
d1jo8a_	β	58	0.054	0.78
d1josa_	α+β	100	0.048	0.51

d1jr2a_	α/β	260	0.052	0.48	d1m1na_	α/β	477	0.042	0.80
d1jsda_	β	317	0.037	0.48	d1m2da_	α/β	101	0.040	0.97
d1jtgb_	α+β	165	0.050	0.55	d1m44a_	α+β	177	0.040	0.59
d1jx4a1	α+β	101	0.047	0.51	d1m55a_	α+β	193	0.024	0.68
d1jyha_	α+β	155	0.035	0.50	d1m7ja1	β	55	0.042	0.65
d1jzta_	α/β	243	0.022	0.46	d1m9fc_	α	146	0.051	0.54
d1k0ra4	α+β	104	0.024	0.47	d1mc2a_	α	122	0.047	1.23
d1k20a_	α/β	310	0.031	0.64	d1me4a_	α+β	215	0.029	0.88
d1k3ia3	β	387	0.031	0.67	d1mixa1	α	114	0.022	0.52
d1k3xa1	α	89	0.024	0.79	d1mjna_	α/β	179	0.038	0.74
d1k3xa2	β	124	0.035	0.79	d1mk0a_	α+β	97	0.035	0.59
d1k3ya1	α	142	0.035	0.78	d1moga_	α+β	67	0.046	0.52
d1k4ia_	α+β	216	0.043	0.91	d1mqoa_	α+β	221	0.041	0.66
d1k5ca_	β	333	0.034	1.06	d1msk__	α+β	327	0.053	0.47
d1k5na2	α+β	181	0.049	0.95	d1mun__	α	225	0.035	0.88
d1k5nb_	β	100	0.055	0.95	d1mvfd_	β	44	0.036	0.53
d1k6ka_	α	142	0.022	0.50	d1mw5a_	α+β	162	0.039	0.41
d1k8ke_	α	173	0.030	0.40	d1mzga_	α+β	144	0.032	0.41
d1k92a2	α+β	256	0.029	0.61	d1n4wa2	α+β	132	0.043	0.98
d1kafa_	α+β	108	0.035	0.55	d1n5ua1	α	195	0.024	0.42
d1keka4	α/β	253	0.033	0.46	d1n62a1	α	82	0.074	0.92
d1khda1	α	69	0.017	0.46	d1n62b1	α+β	141	0.094	0.92
d1kid__	α/β	193	0.038	0.55	d1n62b2	α+β	663	0.103	0.92
d1kjqa1	β	74	0.054	0.88	d1n62c1	α+β	109	0.104	0.92
d1kjqa2	α/β	111	0.034	0.88	d1n62c2	α+β	177	0.086	0.92
d1kkoa2	α+β	160	0.049	0.74	d1n7za_	β	328	0.033	0.42
d1kmva_	α/β	185	0.052	0.82	d1n81a_	α	186	0.029	0.42
d1knma_	β	129	0.028	0.86	d1n8va_	α	101	0.021	0.71
d1kpf__	α+β	111	0.038	0.59	d1nbua_	α+β	118	0.049	0.56
d1kpta_	α+β	105	0.042	0.53	d1nc7a_	β	116	0.047	0.62
d1kq1a_	β	60	0.054	0.55	d1ng6a_	α	148	0.019	0.68
d1kq6a_	α+β	140	0.042	0.85	d1nh2b_	α	46	0.015	0.47
d1kqpa_	α/β	271	0.034	1.03	d1nkd__	α	59	0.039	0.90
d1kwfa_	α	363	0.033	1.12	d1nkia_	α+β	134	0.042	1.06
d1kyfa2	α+β	114	0.049	0.81	d1nkpb_	α	83	0.019	0.52
d1l5oa_	α/β	346	0.027	0.61	d1nlqa_	β	105	0.046	0.55
d1l9la_	α	74	0.035	1.10	d1nls__	β	237	0.039	1.06
d1lb6a_	β	155	0.037	0.49	d1nm8a1	α/β	377	0.033	0.56
d1lbu_1	α	83	0.027	0.50	d1nnha_	α+β	293	0.024	0.59
d1lc0a2	α+β	118	0.040	0.75	d1nox__	α+β	200	0.021	0.60
d1lc5a_	α/β	355	0.032	0.64	d1nppa1	β	81	0.053	0.40
d1lkka_	α+β	105	0.028	1.00	d1nqua_	α/β	154	0.038	0.58
d1lnia_	α+β	96	0.052	1.03	d1nrza_	α/β	163	0.032	0.50
d1lria_	α	98	0.034	0.67	d1ns5a_	α/β	153	0.041	0.60
d1luga_	β	258	0.059	1.07	d1ntya1	α	184	0.020	0.54
d1luqa_	β	119	0.101	1.04	d1nwwa_	α+β	145	0.045	0.84
d1lyva_	α/β	283	0.036	0.75	d1nwza_	α+β	125	0.067	1.24
d1m15a1	α	94	0.027	0.85	d1nxua_	α/β	332	0.030	0.49
d1m15a2	α+β	262	0.045	0.85	d1nz0a_	α+β	109	0.058	0.81

d1o08a_	α/β	221	0.028	0.84	d1pfva1	α	162	0.022	0.55
d1o0wa1	α	169	0.025	0.46	d1pjxa_	β	314	0.058	1.21
d1o1xa_	α/β	145	0.034	0.56	d1pm4a_	β	117	0.070	0.52
d1o22a_	α+β	149	0.042	0.46	d1pq7a_	β	224	0.057	1.29
d1o26a_	α+β	219	0.029	0.58	d1ptf__	α+β	87	0.024	0.61
d1o4wa_	α/β	125	0.035	0.48	d1pu5a_	β	164	0.050	0.45
d1o6aa_	β	87	0.055	0.53	d1puc__	α+β	101	0.043	0.44
d1o7ja_	α/β	325	0.030	0.95	d1pv5a_	α+β	261	0.034	0.51
d1o7na2	α+β	293	0.046	0.67	d1pz4a_	α+β	113	0.047	0.64
d1o7qa_	α/β	287	0.026	0.80	d1q5za_	α	145	0.020	0.52
d1o98a1	α/β	234	0.031	0.67	d1q9ia3	α+β	146	0.030	0.60
d1oa8a_	β	128	0.052	0.50	d1qdda_	α+β	144	0.027	0.75
d1oaia_	α	59	0.024	1.03	d1qgwa_	α+β	76	0.031	0.61
d1oc7a_	α/β	364	0.034	0.94	d1qhva_	β	195	0.040	0.69
d1ocya_	α+β	198	0.037	0.66	d1qksa2	β	432	0.042	0.74
d1od3a_	β	131	0.048	1.01	d1qlma_	α+β	316	0.024	0.44
d1ogca_	α/β	131	0.031	0.44	d1qopb_	α/β	390	0.030	0.73
d1ogox1	β	199	0.034	0.55	d1qqqa_	α+β	264	0.037	0.58
d1ojha_	α	52	0.025	0.54	d1qrea_	β	210	0.036	0.64
d1ojra_	α/β	274	0.038	0.77	d1qv9a_	α/β	282	0.032	0.61
d1ok0a_	β	74	0.066	1.11	d1qw2a_	α+β	102	0.045	0.61
d1ok7a1	α+β	122	0.049	0.54	d1qwna1	α	111	0.022	0.80
d1on2a2	α	74	0.019	0.57	d1qwza_	β	235	0.034	0.53
d1oo0a_	α+β	144	0.055	0.45	d1qxoa_	α+β	388	0.035	0.47
d1oqja_	α+β	90	0.028	0.59	d1qxya_	α+β	249	0.053	0.97
d1oqva_	α+β	171	0.050	0.79	d1r0da_	α	194	0.027	0.46
d1or7a2	α	113	0.033	0.45	d1r0va3	α+β	75	0.062	0.45
d1or7c_	α	66	0.033	0.45	d1r29a_	α+β	122	0.028	0.79
d1orua_	β	182	0.032	0.50	d1r2ma_	β	70	0.031	1.00
d1os1a1	α/β	313	0.039	0.49	d1r4va_	α	151	0.023	0.49
d1os1a2	α/β	224	0.030	0.49	d1r6ja_	β	82	0.035	1.45
d1ospo_	β	251	0.038	0.42	d1r6la2	α+β	88	0.037	0.44
d1ou8a_	β	106	0.034	0.57	d1r7la_	α+β	103	0.037	0.40
d1ovna1	α	107	0.057	0.43	d1r89a1	α	115	0.028	0.49
d1owla1	α	271	0.019	0.51	d1r89a2	α+β	142	0.028	0.49
d1owla2	α/β	202	0.029	0.51	d1rj1a_	α	148	0.020	0.51
d1ox0a1	α/β	256	0.030	0.78	d1rlha_	α+β	151	0.040	0.52
d1oxca_	β	114	0.053	0.81	d1rlka_	α/β	116	0.035	0.45
d1oyga_	β	440	0.035	0.64	d1ro7a_	α/β	258	0.027	0.48
d1p3da1	α/β	96	0.036	0.56	d1rqwa_	β	207	0.047	0.96
d1p3da2	α/β	152	0.025	0.56	d1rtqa_	α/β	291	0.033	1.08
d1p57a_	α+β	110	0.055	0.52	d1rv9a_	α+β	242	0.047	0.59
d1p5gx1	α/β	146	0.029	0.62	d1rwha2	β	113	0.061	0.83
d1p6oa_	α/β	156	0.052	0.91	d1rwha3	β	272	0.048	0.83
d1p9ya_	α+β	117	0.035	0.41	d1rxqa_	α	174	0.026	0.54
d1pbja1	α+β	59	0.028	0.67	d1ry9a_	α+β	133	0.030	0.49
d1pcfa_	α+β	66	0.033	0.54	d1ryaa_	α+β	160	0.036	0.74
d1pda_2	α+β	88	0.044	0.55	d1rzhh1	β	213	0.031	0.48
d1pdo__	α/β	129	0.036	0.55	d1s0pa_	α	176	0.037	0.70

d1s7za_	α	106	0.041	0.54	d1uptb_	α	58	0.023	0.49
d1s95a_	α+β	324	0.050	0.59	d1uq5a_	α+β	263	0.057	0.68
d1sbxa_	α	106	0.036	0.60	d1us0a_	α/β	313	0.047	1.42
d1sdia_	α	213	0.041	0.62	d1utg__	α	70	0.028	0.65
d1seda_	α	112	0.023	0.47	d1uuja_	α	76	0.034	0.56
d1seia_	α+β	130	0.053	0.42	d1uuya_	α/β	161	0.038	0.68
d1sfda_	β	105	0.045	1.02	d1uyla_	α+β	207	0.041	0.64
d1shea_	α+β	94	0.021	0.47	d1uz5a2	β	176	0.035	0.41
d1smba_	α+β	149	0.029	0.62	d1uzba_	α/β	516	0.033	0.68
d1soxa3	α+β	250	0.031	0.47	d1v16b2	α/β	138	0.031	0.53
d1sxra_	α+β	173	0.034	0.60	d1v1ha1	β	74	0.049	0.49
d1sy1a_	β	184	0.059	1.01	d1v33a_	α+β	346	0.035	0.48
d1szha_	α	147	0.024	0.62	d1v54h_	α	79	0.027	0.50
d1t07a_	α+β	81	0.031	0.51	d1v6sa_	α/β	390	0.030	0.61
d1t15a1	α/β	109	0.034	0.45	d1v74a_	α+β	107	0.030	0.46
d1t1ja_	α/β	119	0.031	0.53	d1v7ra_	α/β	186	0.047	0.66
d1t2da2	α+β	165	0.030	0.77	d1v7za_	α/β	257	0.026	0.59
d1t3ta3	α+β	152	0.025	0.47	d1vcc__	α+β	77	0.040	0.55
d1t56a2	α	120	0.013	0.54	d1vcla3	α+β	149	0.039	0.55
d1t6t1_	α/β	108	0.025	0.53	d1vf6a_	α	58	0.019	0.41
d1t7ra_	α	250	0.020	0.69	d1vh5a_	α+β	138	0.041	0.71
d1t8ka_	α	77	0.024	0.93	d1vhua_	α/β	192	0.033	0.76
d1t95a2	α+β	76	0.043	0.45	d1vhva_	α/β	251	0.034	0.49
d1tbfa_	α	326	0.031	0.78	d1vioa2	α+β	58	0.029	0.58
d1teaa1	α	133	0.021	0.63	d1vk1a_	α+β	232	0.044	0.82
d1tfe__	α+β	142	0.031	0.52	d1vk5a_	α	121	0.031	0.64
d1tjya_	α/β	316	0.032	0.77	d1vkia_	α+β	165	0.042	0.62
d1tlua_	α+β	117	0.044	0.62	d1vkka_	α+β	137	0.069	0.73
d1tqga_	α	105	0.035	1.02	d1vkma_	α/β	291	0.040	0.51
d1tuaa1	α+β	84	0.027	0.62	d1vlya1	β	82	0.058	0.77
d1tvfa1	β	68	0.056	0.47	d1vlya2	α+β	241	0.049	0.77
d1tx4a_	α	196	0.025	0.56	d1vns__	α	574	0.024	0.56
d1tzba_	α/β	301	0.025	0.86	d1w53a_	α	84	0.028	0.59
d1tzva_	α	141	0.025	0.70	d1whi__	β	122	0.036	0.62
d1u0ka1	α+β	129	0.044	0.64	d1xbfa_	α+β	131	0.037	0.44
d1u55a_	α+β	188	0.031	0.49	d2cbla2	α	131	0.024	0.40
d1u94a2	α+β	60	0.024	0.49	d2cpl__	β	164	0.042	0.57
d1uc2a_	α+β	480	0.034	0.43	d2end__	α	137	0.034	0.70
d1ucda_	α+β	190	0.049	0.71	d2erl__	α	40	0.055	1.01
d1ucsa_	β	64	0.039	1.62	d2igd__	α+β	61	0.047	0.97
d1udxa1	β	156	0.041	0.40	d2ilk__	α	155	0.040	0.58
d1udxa3	α+β	76	0.025	0.40	d2lisa_	α	131	0.024	0.78
d1udza_	β	179	0.042	0.47	d2pvba_	α	107	0.032	1.15
d1ufya_	α+β	121	0.048	0.93	d3euga_	α/β	225	0.038	0.68
d1ugpa_	α+β	203	0.023	0.58	d3ezma_	β	101	0.044	0.61
d1ukka_	α+β	141	0.053	0.59	d3lzt__	α+β	129	0.064	1.14
d1umwa1	α+β	128	0.031	0.42	d3sici_	α+β	107	0.053	0.48
d1unqa_	β	117	0.046	1.03	d4ubpa_	α+β	100	0.039	0.64
d1uowa_	β	156	0.056	0.93					

Reconstruction and stability of secondary structure elements in the context of protein structure prediction

Alexei A. Podtelezhnikov and David L. Wild

Supplementary Material #2
Supplementary Figures

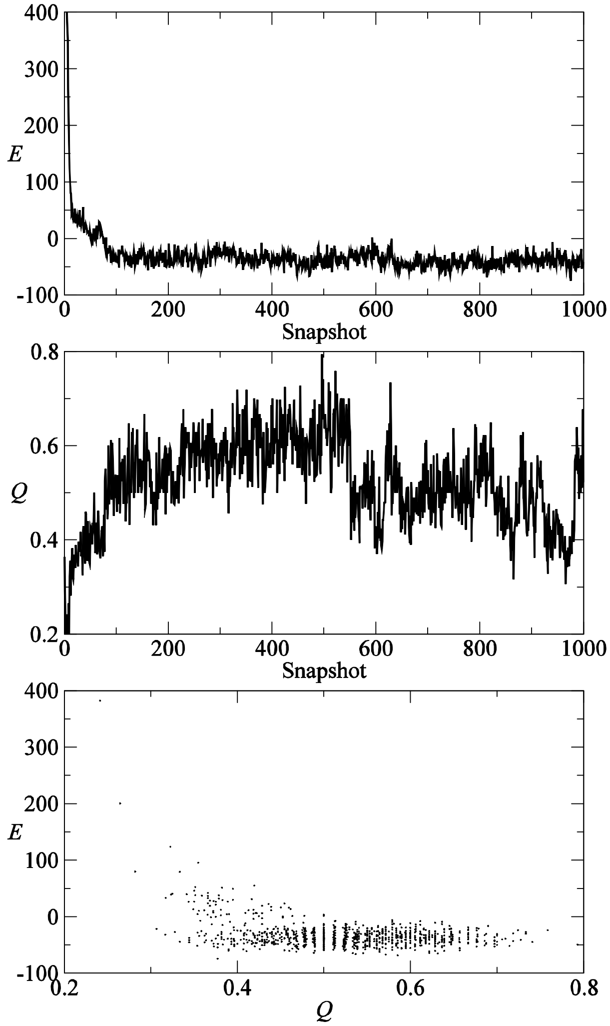

Figure 5S. Reconstruction of the protein G fold by specifying predicted interactions (Case 1). The graphs demonstrate the evolution of the microscopic energy, *E*, and fraction of the native contacts, *Q*, during the simulation run in the top and middle panel respectively. The bottom panel demonstrated the relationship between *Q* and *E*.

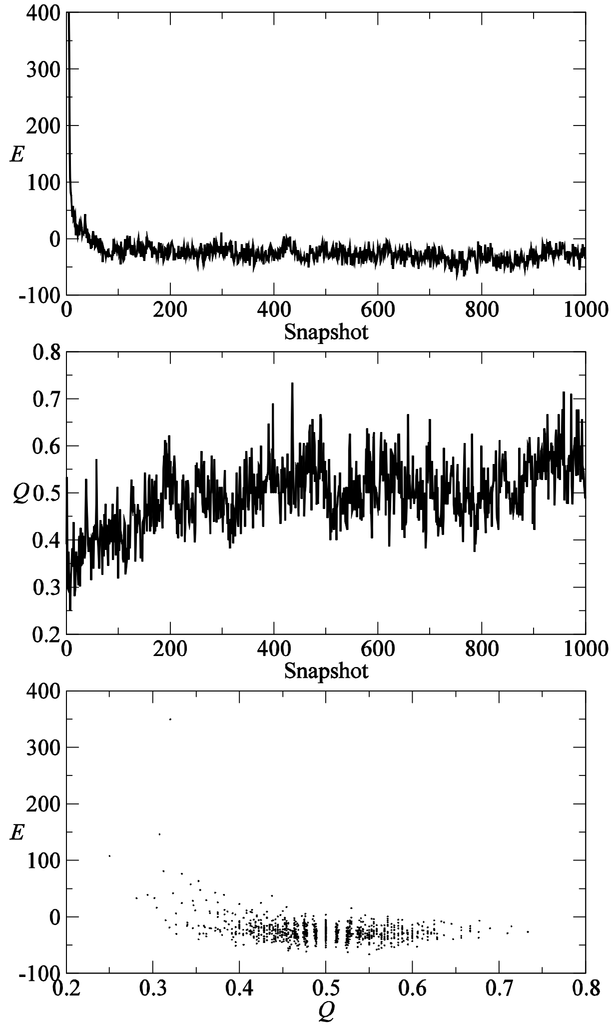

Figure 6S. Reconstruction of the protein G fold by specifying predicted interactions (Case 2). The graphs demonstrate the evolution of the microscopic energy, *E*, and fraction of the native contacts, *Q*, during the simulation run in the top and middle panel respectively. The bottom panel demonstrated the relationship between *Q* and *E*.

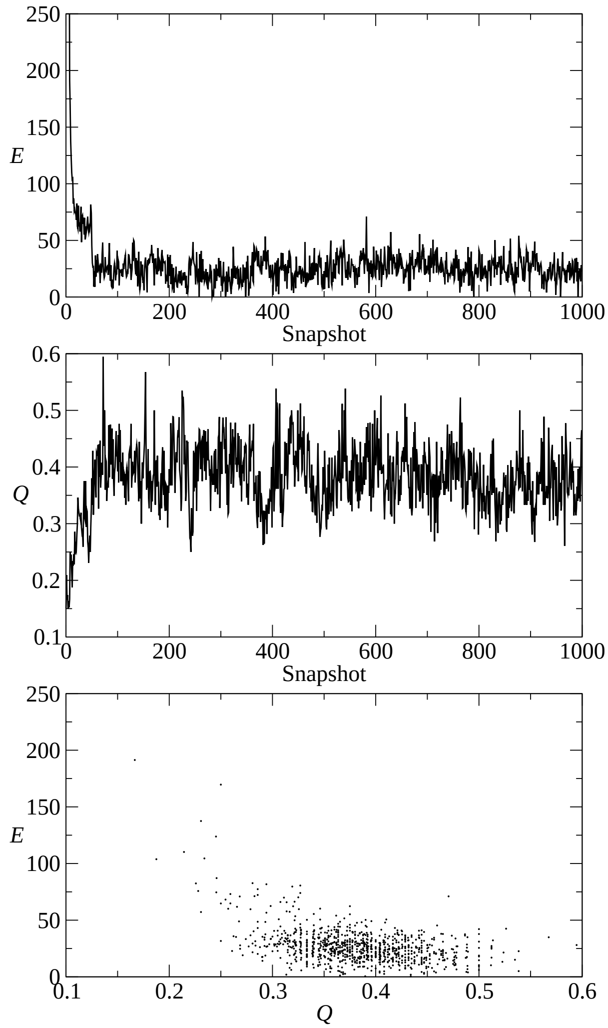

Figure 7S. Reconstruction of chymotrypsin inhibitor 2 CI2 fold by specifying predicted interactions. The graphs demonstrate the evolution of the microscopic energy, *E*, and fraction of the native contacts, *Q*, during the simulation run in the top and middle panel respectively. The bottom panel demonstrated the relationship between *Q* and *E*.

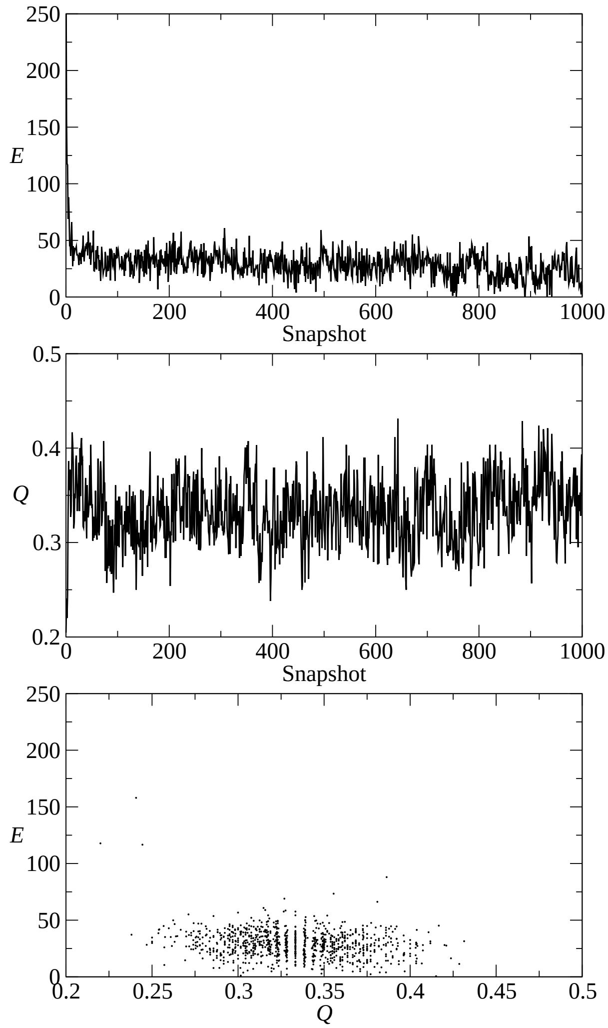

Figure 8S. Reconstruction of the SH3 domain fold by specifying predicted interactions. The graphs demonstrate the evolution of the microscopic energy, *E*, and fraction of the native contacts, *Q*, during the simulation run in the top and middle panel respectively. The bottom panel demonstrated the relationship between *Q* and *E*.

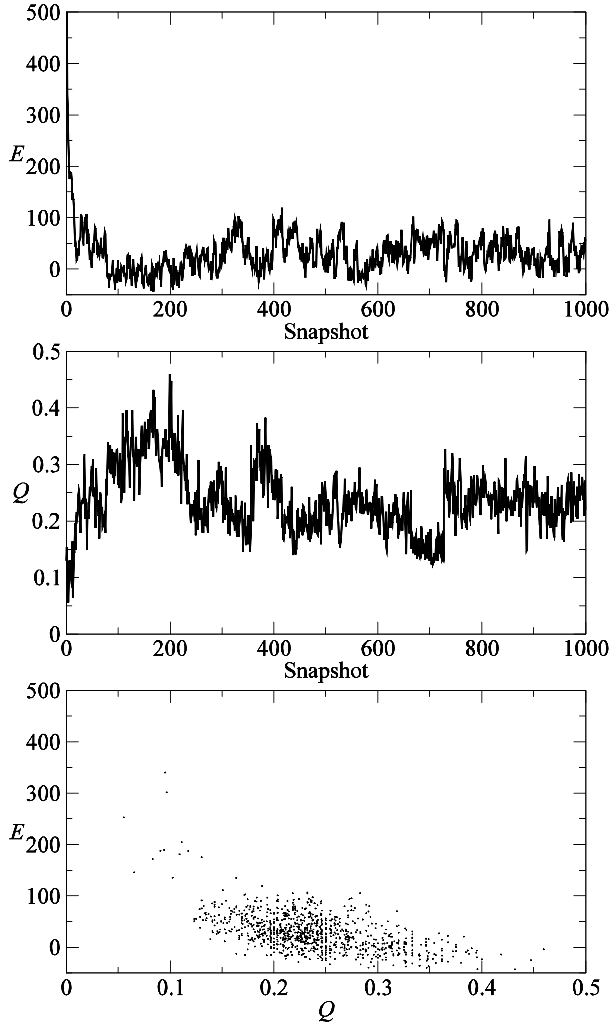

Figure 9S. Reconstruction of the cold-shock protein CspA fold by specifying predicted interactions. The graphs demonstrate the evolution of the microscopic energy, *E*, and fraction of the native contacts, *Q*, during the simulation run in the top and middle panel respectively. The bottom panel demonstrated the relationship between *Q* and *E*.