

Supplementary Information

Table S1. Comparison three different types of energy model with the QUARK.

No.	SCOP	PDB-ID	Length	GA_{FCC}^{HP}	$NSGA_{KA+FCC'}^{HP}$	$NSGAI_{KA+FCC'}^{HP}$	QUARK
01	All α	2erl-	40	4.64	4.32	3.46	5.47
02		2utga	70	7.35	6.42	5.29	4.81
03		1cei	85	6.62	6.72	5.27	4.05
04		1cc5	83	6.35	6.53	5.52	3.52
05		1rpo	61	10.58	7.16	6.29	1.02
06		2or1l	63	5.36	5.69	4.84	1.67
07		1lmb3	87	7.01	6.69	5.61	3.66
08		3icb	75	5.97	6.23	5.2	2.22
09		1hcra	52	7.22	5.47	4.95	4.41
10		4fisb	73	10.81	6.61	5.77	4.79
11		1hyp	75	6.43	6.06	5.69	2.89
12		1fc2c	43	5.01	4.64	4.45	2.21
13	All β	4rhv4	40	19.83	12.9	11.2	18.03
14		2mev4	58	28.1	10.72	14.4	25.99
15		2ltnb	47	12.67	9.29	9	10.34
16		1pht	83	7.44	8.06	6.42	6.24
17		1mjc	69	6.01	7.71	5.39	2.89
18		1bovb	69	6.49	6.98	5.65	4.47
19		2gn5	87	9.24	7.61	8.08	8.68
20		3ait	74	7.47	7.32	6.53	5.88
21		1htrp	43	15.36	7.59	7.34	12.44
22		1wapv	67	7.37	7.47	6.14	5.08
23		1bdo-	80	7.3	7.59	6.63	5.86
24	α and β (a/b)	1aazb	87	7.45	6.7	5.92	3.13
25		1brse	86	7.02	6	5.95	3.73
26	α and β (a + b)	1vcc	77	6.54	6.96	5.69	3.15
27		1pga	56	6.28	6.42	5.48	9.63
28		1ubq	76	7.14	6.64	6.49	2.34
29		1tif	76	6.07	6.51	5.76	4.68
30		1tiic	36	15.13	6.23	5.2	0.79
31		1csei	63	6.39	6.93	5.69	2.44
32		1ctf	68	6.06	6.82	5.53	3.64
33		1spbp	71	8.11	7.43	6.21	5.36
34		2bopa	85	8.77	9.11	7.61	6.45
35		1tig	88	7.65	6.77	6.99	2.37
36	1il8a	71	8.82	7.81	6.86	6.48	
37	2hpr	87	6.68	6.65	5.91	2.53	
38	1cksc	78	16.31	10.74	11.42	15.14	

Table S1. *Cont.*

No.	SCOP	PDB-ID	Length	GA_{FCC}^{HP}	$NSGA_{KA+FCC'}^{HP}$	$NSGAI_{KA+FCC'}^{HP}$	QUARK	
39	Multi-domain	9apib	36	10.59	7.71	6.38	7.92	
40		1bpha	21	4.78	3.37	3.09	5.01	
41		9insb	30	5.2	3.57	3.84	4.14	
42		1crn	46	5.4	5.45	4.46	3.54	
43		1mcti	28	4.16	4.22	3.6	4.34	
44		1cbh-	36	5.28	5.11	4.91	4.30	
45		1tabi	36	6.75	6.55	5.72	6.35	
46		4cpai	37	4.7	4.87	4.26	4.52	
47		1edmc	39	7.2	6.13	5.17	3.52	
48		6hir	49	5.51	5.7	4.94	5.02	
49		1hcgb	51	9.41	5.8	4.18	6.73	
50		1ptx	64	6.39	7.16	5.54	4.81	
51		1lpba	85	6.94	7.82	5.85	7.06	
52		1isub	62	5.49	6.71	5.01	5.70	
53		Small proteins	2hipb	71	5.71	6.32	5.29	4.98
54			1hip	85	5.92	7.06	5.56	6.10
55			1latb	74	6.57	7.28	5.72	5.29
56			4rxn	54	5.32	5.29	4.92	3.97
57			2mhu-	30	3.9	3.77	3.56	4.50
58			1mrt-	31	3.88	4.13	2.87	2.94
59			1ptr	50	6.33	4.98	5.18	1.83
60			1ovoa	56	6.98	5.95	5.54	3.28
61			4sgbi	51	6.41	6.37	5.21	4.53
62			1cdta	60	7.25	7.14	6.35	6.34
63			2tgpi	58	6.81	6.74	5.82	5.88
64			1dfnb	30	5.19	4.43	4.19	2.34
65			1bds	43	4.73	5.33	4.57	4.90
66			1shl	48	5.56	6.12	4.89	5.46
67		Coiled coil	1gcmc	33	12.97	5.27	3	0.58
68			1mof	53	14.28	7.68	5.75	4.21
69		Peptides	1atpi	20	8.92	3.83	2.62	8.01
70			2mltb	26	7.9	2.6	2.74	6.17
71	1wfb		37	5.61	7.73	3.07	0.32	
72	1edn-		21	4.42	2.84	2.71	4.10	
73	1ppt-		36	7.32	5.12	4.09	2.83	
74	Designed		1coi-	29	10.95	4.12	3.16	0.67
75		1cdlg	20	6.11	1.84	2.77	1.19	
Average of RMSD				7.76	6.34	5.5	5.09	

Words in bold indicate the lowest RMSD.