

Table S4: Values of ϵ_{ij}^0 (kcal/mol) of the Gay-Berne potential (J.G.Gay, B.J. Berne, J. Chem. Phys., 1981, 74, 3316-3319) determined in this work by hierarchical optimization using the 1ENH and 1E0L proteins.

	Cys	Met	Phe	Ile	Leu	Val	Trp	Tyr	Ala	Gly	Thr	Ser	Gln	Asn	Glu	Asp	His	Arg	Lys	Pro
Cys	1.40	1.56	1.55	1.61	1.55	1.49	1.36	1.22	1.32	1.37	1.07	1.09	1.07	0.92	0.89	0.93	1.18	0.85	0.95	1.13
Met		1.66	1.67	1.70	1.71	1.59	1.54	1.38	1.37	1.23	1.07	1.01	1.05	0.88	0.86	0.70	1.20	0.97	0.90	1.16
Phe			1.41	1.77	1.48	1.63	1.52	1.13	1.07	1.05	0.78	0.74	0.73	0.74	0.52	0.75	1.20	0.72	0.83	0.95
Ile				1.67	1.57	1.76	1.58	1.20	1.24	1.36	0.93	0.87	1.06	0.97	0.76	0.91	1.15	0.87	1.03	1.47
Leu					1.61	1.86	1.57	1.65	1.26	1.47	0.80	1.31	0.84	1.14	0.63	0.65	1.13	0.76	0.75	1.15
Val						1.63	1.61	1.37	1.43	1.26	0.80	1.26	0.95	1.10	0.62	0.69	1.01	0.91	1.01	1.10
Trp							1.07	1.46	1.35	1.33	0.64	1.14	1.23	1.19	0.74	0.85	1.16	0.81	1.18	1.13
Tyr								1.23	1.10	0.75	0.94	0.99	1.01	0.45	0.92	0.47	0.97	0.61	0.66	1.27
Ala									0.91	0.80	0.51	0.60	0.37	0.79	0.24	0.37	0.78	0.26	0.52	1.16
Gly										0.62	0.47	0.66	0.34	0.37	-0.31	0.11	0.72	0.19	-0.08	0.98
Thr											0.50	0.31	0.14	0.35	0.13	0.50	0.71	0.28	-0.12	0.99
Ser												0.18	0.33	0.44	-0.13	0.09	0.61	0.12	0.09	0.61
Gln													-0.42	-0.00	-0.38	-0.10	0.42	0.18	-0.24	0.81
Asn														0.06	-0.00	0.04	0.53	0.10	-0.18	0.56
Glu															-1.10	-0.44	0.46	0.45	0.74	0.20
Asp																-0.34	0.64	0.70	0.18	0.47
His																	0.93	0.57	-0.01	0.78
Arg																		-0.27	-0.61	0.55
Lys																			-0.86	0.84
Pro																				1.05