

Modeling Backbone Flexibility Improves

Protein Stability Estimation

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Table S1. List of the Experimental and Calculated $\Delta\Delta G$ Values of All the Proteins and Their Mutants

PDB ID	Mutaton	Experimental $\Delta\Delta G$ (kcal/mol)	Calculated $\Delta\Delta G$ (kcal/mol) (w/ original reference energy)		Calculated $\Delta\Delta G$ (kcal/mol) (w/ improved reference energy)	
			Fixed BB	Flex BB	Fixed BB	Flex BB
1fkj	WILD TYPE	0	0.00	0.00	0.00	0.00
1fkj	V 2 A	2.43	4.88	5.65	6.44	7.21
1fkj	V 4 A	2.78	4.29	4.96	5.85	6.52
1fkj	V 23 A	2.97	4.17	4.83	5.73	6.39
1fkj	V 24 A	3.19	4.96	5.31	6.52	6.87
1fkj	F 36 A	3.54	5.62	5.78	6.03	6.19
1fkj	L 50 A	2.57	3.12	3.58	4.48	4.94
1fkj	V 55 A	2.13	0.82	0.65	2.38	2.21
1fkj	I 56 A	2.48	3.43	4.82	5.13	6.52
1fkj	I 56 D	3.16	3.41	4.51	6.17	7.27
1fkj	I 56 T	1.81	2.71	3.42	4.80	5.51
1fkj	V 63 A	2.97	4.30	4.55	5.86	6.11
1fkj	I 76 V	0.76	1.70	2.16	1.84	2.31
1fkj	I 76 A	3.81	6.60	6.55	8.31	8.25
1fkj	I 91 A	1.54	6.65	7.31	8.35	9.01
1fkj	I 91 V	0.38	1.47	1.64	1.62	1.79
1fkj	L 97 A	3.56	6.20	6.85	7.57	8.22
1fkj	V 98 A	2.16	2.45	2.86	4.01	4.42
1fkj	V 101 A	2.75	4.49	5.45	6.05	7.01
1fkj	L 106 A	2.32	5.36	5.63	6.72	7.00
1fkj	R 57 A	0.81	-0.07	0.24	0.64	0.95
1fkj	R 57 G	2.29	1.79	2.43	3.89	4.53
1fkj	E 60 A	2.13	1.31	1.58	0.19	0.45
1fkj	E 60 G	2.84	3.78	4.11	4.04	4.37
1fkj	E 61 A	0.84	1.17	0.91	0.05	-0.22
1fkj	E 61 G	2.49	3.47	2.66	3.73	2.93
1fkj	I 7 V	0.92	0.09	1.08	0.23	1.23
1fkj	T 21 V	-0.86	-1.61	-1.17	-3.56	-3.11
1fkj	T 21 A	1.6	1.14	1.11	0.76	0.73
1fkj	T 27 V	-0.23	-0.01	1.11	-1.95	-0.83
1fkj	T 27 A	1.97	1.33	2.70	0.94	2.32
1fkj	T 75 V	0.81	-2.75	-1.42	-4.69	-3.36
1fkj	T 75 A	2.65	0.79	0.95	0.40	0.57
1fkj	W 59 F	-2.72	6.21	1.89	3.11	-1.20

1fkj	W 59 L	-2.35	0.68	0.78	-3.36	-3.27
1bvc	WILD TYPE	0	0.00	0.00	0.00	0.00
1bvc	A 130 L	2.3	*	6.27	*	4.90
1bvc	A 130 K	3.7	*	9.29	*	11.46
1bvc	F 123 T	3.5	2.72	2.53	3.51	3.32
1bvc	N 132 G E 136 G	0.3	1.82	1.64	3.40	3.23
1bvc	L 115 A	1	3.86	4.43	5.23	5.80
1bvc	F 123 A	0.3	5.24	2.39	5.65	2.80
1bvc	L 135 A	0.8	6.00	4.84	7.37	6.21
1bvc	L 11 A	0.5	4.21	3.84	5.58	5.21
1bvc	F 106 A	0.2	2.56	1.93	2.97	2.35
1bvc	A 15 L	-0.2	2.01	0.76	0.65	-0.61
1bvc	A 125 L	-0.4	3.14	2.03	1.77	0.67
1bvc	A 144 L	-0.1	1.45	-0.14	0.08	-1.50
1bvc	I 28 A	2.06	4.65	4.62	6.35	6.32
1bvc	L 29 A	0.39	6.05	5.85	7.42	7.22
1bvc	I 30 A	1.9	3.07	3.10	4.77	4.80
1bvc	L 32 A	2.04	4.47	3.86	5.83	5.22
1bvc	G 129 A	-1.05	-0.60	-0.12	-1.99	-1.50
1bvc	V 66 A	-0.75	0.59	1.23	2.15	2.79
1bvc	V 13 A	0.67	1.57	2.66	3.13	4.22
1bvc	T 67 A	0.26	2.01	1.20	1.63	0.82
1bvc	L 11 A	0.44	4.22	3.49	5.59	4.86
1bvc	L 9 A	0.41	1.58	1.84	2.94	3.21
1bvc	L 137 A	1.78	2.85	2.34	4.21	3.70
1bvc	V 114 A	1.45	2.19	2.30	3.75	3.86
1bvc	I 142 A	1.92	3.52	3.03	5.23	4.73
1bvc	P 88 A	-0.59	-2.46	-2.86	-4.27	-4.68
1bvc	H 116 A	-0.16	-0.25	0.50	0.04	0.78
1bvc	S 117 A	0.26	0.33	1.80	-0.97	0.50
1bvc	G 23 A	1.12	1.93	2.18	0.54	0.79
1bvc	T 51 A	1.41	2.28	0.91	1.89	0.53
1bvc	L 149 A	1.6	3.04	2.75	4.41	4.12
1stn	WILD TYPE	0	0.00	0.00	0.00	0.00
1stn	K 1 A	-0.3	-0.95	0.33	-3.11	-1.84
1stn	K 1 G	-0.3	-0.05	1.20	-0.83	0.42
1stn	L 2 A	1.6	1.73	3.91	3.10	5.28
1stn	L 2 G	1.5	3.76	7.10	6.51	9.85
1stn	H 3 A	0.4	-1.95	-0.73	-1.67	-0.45
1stn	H 3 G	0.8	-1.56	-0.38	0.12	1.30
1stn	K 4 A	1.4	1.88	2.37	-0.29	0.20
1stn	K 4 G	1.9	3.07	2.70	2.29	1.92
1stn	E 5 A	1.3	1.84	1.95	0.71	0.82
1stn	E 5 G	1.8	3.94	3.66	4.20	3.93
1stn	P 6 A	0.4	-0.54	0.20	-2.36	-1.62
1stn	P 6 F	0.6	1.45	2.60	-0.78	0.37

1stn	P 6 G	1	0.74	1.69	0.31	1.26
1stn	A 7 G	2.4	2.85	3.12	4.24	4.51
1stn	A 7 V	1.1	2.13	0.46	0.57	-1.10
1stn	T 8 A	0.7	-0.46	-0.78	-0.85	-1.17
1stn	T 8 G	1.1	0.54	0.88	1.54	1.88
1stn	T 8 S	0.3	1.03	1.59	1.95	2.50
1stn	T 8 V	0.4	-0.46	-0.04	-2.40	-1.98
1stn	L 9 A	2.3	1.73	2.86	3.09	4.23
1stn	L 9 G	3.7	4.43	4.56	7.18	7.31
1stn	I 10 A	2.65	2.31	0.84	4.02	2.55
1stn	I 10 G	3.3	3.35	3.74	6.44	6.83
1stn	I 10 V	0.8	1.68	3.03	1.82	3.18
1stn	K 11 A	0.2	-0.01	-0.78	-2.18	-2.95
1stn	K 11 F	0.5	4.15	4.59	1.57	2.01
1stn	K 11 G	0.7	1.27	2.65	0.49	1.87
1stn	A 12 G	0.3	2.58	4.26	3.97	5.65
1stn	A 12 V	1.9	-0.02	0.86	-1.58	-0.70
1stn	I 13 A	2.5	1.82	2.20	3.52	3.91
1stn	I 13 G	2.5	3.94	4.29	7.04	7.38
1stn	I 13 M	0.6	1.57	0.80	0.24	-0.53
1stn	I 13 V	1.1	0.41	0.45	0.55	0.60
1stn	D 14 A	0.1	4.09	4.37	3.04	3.32
1stn	D 14 G	0.4	5.03	4.59	5.36	4.92
1stn	G 15 A	0.3	1.60	1.15	0.21	-0.23
1stn	D 16 A	-0.7	1.18	-1.44	0.13	-2.50
1stn	D 16 G	-0.3	2.42	1.63	2.76	1.96
1stn	T 17 A	1.6	3.12	1.31	2.73	0.92
1stn	T 17 G	2.4	5.20	5.11	6.21	6.12
1stn	T 17 S	0.6	1.78	1.30	2.69	2.21
1stn	T 17 V	0.9	0.34	1.89	-1.60	-0.05
1stn	V 18 A	2.9	1.67	1.38	3.23	2.93
1stn	V 18 G	5.6	5.84	6.62	8.79	9.57
1stn	V 18 S	4.7	4.22	2.94	7.07	5.80
1stn	V 18 T	3.2	2.16	1.54	4.10	3.48
1stn	K 19 A	0.2	2.83	1.85	0.67	-0.32
1stn	K 19 G	1.2	4.15	3.80	3.37	3.02
1stn	L 20 A	2.7	5.99	6.79	7.36	8.16
1stn	L 20 G	4.5	9.10	9.17	11.85	11.92
1stn	M 21 A	1.5	0.01	0.45	3.04	3.48
1stn	M 21 G	2.2	2.74	4.25	7.16	8.67
1stn	M 21 I	0.9	2.59	1.63	3.91	2.96
1stn	M 21 L	0.5	-2.03	-0.66	-0.36	1.00
1stn	Y 22 A	3.5	4.25	3.81	6.50	6.05
1stn	Y 22 D	5.4	4.07	2.47	7.37	5.77
1stn	Y 22 E	5	2.87	2.76	6.25	6.13
1stn	Y 22 F	0.3	0.01	-0.85	1.85	0.99
1stn	Y 22 G	5.45	6.48	6.14	10.12	9.77
1stn	Y 22 H	1.6	1.77	1.81	3.73	3.77

1stn	Y 22 I	2.5	5.16	2.95	5.70	3.50
1stn	Y 22 K	3.9	2.84	4.09	7.26	8.50
1stn	Y 22 L	1.5	2.30	0.66	3.18	1.54
1stn	Y 22 M	2	4.50	4.25	3.72	3.46
1stn	Y 22 N	4	3.82	2.21	6.13	4.52
1stn	Y 22 Q	3.2	3.64	4.51	6.58	7.45
1stn	Y 22 R	2.9	5.22	4.38	6.76	5.91
1stn	Y 22 S	3	4.55	5.08	8.10	8.62
1stn	Y 22 T	3.3	2.67	3.68	5.30	6.31
1stn	Y 22 V	3	2.39	1.58	3.08	2.26
1stn	Y 22 W	0.6	4.03	2.04	8.96	6.97
1stn	K 23 A	0.7	-0.09	1.43	-2.26	-0.74
1stn	K 23 F	0.9	4.18	3.61	1.60	1.03
1stn	K 23 G	0.7	1.39	1.95	0.61	1.17
1stn	G 24 A	1.25	1.29	1.61	-0.10	0.22
1stn	G 24 F	1.25	4.52	5.80	2.72	4.00
1stn	Q 25 A	0.3	-1.79	-1.69	-2.48	-2.38
1stn	Q 25 G	0.9	0.03	0.19	0.72	0.89
1stn	P 26 A	0.55	-0.12	0.18	-1.94	-1.64
1stn	P 26 G	1.6	0.99	1.49	0.56	1.06
1stn	M 27 A	1.7	0.50	-0.13	3.53	2.90
1stn	M 27 G	2.4	2.84	3.89	7.26	8.31
1stn	M 27 I	0.6	0.80	2.64	2.13	3.97
1stn	M 27 L	0.8	0.44	1.33	2.11	3.00
1stn	T 28 A	1.4	0.18	0.33	-0.20	-0.05
1stn	T 28 G	2.5	3.01	2.78	4.02	3.78
1stn	T 28 S	1.15	1.13	0.13	2.04	1.04
1stn	T 28 V	-0.4	-1.12	-1.01	-3.06	-2.95
1stn	F 29 A	3.7	6.86	8.26	7.27	8.68
1stn	F 29 G	6.2	10.29	10.51	12.08	12.31
1stn	R 30 A	1.4	-1.74	0.57	-1.03	1.27
1stn	R 30 G	2.2	0.28	-0.28	2.38	1.81
1stn	L 31 A	3.5	2.51	2.38	3.88	3.75
1stn	L 31 G	5.3	5.31	6.33	8.06	9.08
1stn	L 32 A	1.7	1.59	3.48	2.95	4.85
1stn	L 32 G	3.8	5.30	5.92	8.05	8.68
1stn	L 33 A	1.65	4.19	5.51	5.55	6.88
1stn	L 33 G	0.55	5.18	4.78	7.93	7.53
1stn	V 34 A	2.2	4.75	4.19	6.31	5.75
1stn	V 34 G	4.7	7.42	8.02	10.37	10.97
1stn	V 34 S	2.4	4.97	5.13	7.82	7.98
1stn	V 34 T	1.3	1.96	2.12	3.90	4.06
1stn	D 35 A	-0.2	-0.83	0.04	-1.88	-1.01
1stn	D 35 G	0.5	0.58	1.96	0.92	2.29
1stn	T 36 A	0	2.29	2.04	1.90	1.66
1stn	T 36 G	2	3.26	4.71	4.26	5.71
1stn	T 36 S	1.1	2.39	2.60	3.31	3.52
1stn	T 36 V	-0.8	2.43	2.33	0.48	0.39

1stn	P 37 A	-0.1	0.94	2.19	-0.88	0.37
1stn	P 37 G	0.4	3.98	3.01	3.55	2.58
1stn	E 38 A	-0.3	2.73	3.47	1.60	2.35
1stn	E 38 D	-0.2	2.99	1.76	2.92	1.69
1stn	E 38 G	-0.5	3.73	4.05	3.99	4.32
1stn	T 39 A	0.4	2.21	2.07	1.83	1.69
1stn	T 39 G	0.6	3.33	4.20	4.34	5.20
1stn	T 39 S	0	1.18	2.12	2.10	3.03
1stn	T 39 V	-0.1	2.48	1.55	0.54	-0.39
1stn	K 40 A	-0.3	-0.49	-0.86	-2.66	-3.03
1stn	K 40 G	-0.2	0.09	-0.61	-0.69	-1.39
1stn	H 41 A	0.5	2.20	1.50	2.49	1.79
1stn	H 41 G	0.4	3.80	4.77	5.47	6.44
1stn	P 42 A	0.6	-1.60	-1.56	-3.42	-3.37
1stn	P 42 F	0.3	2.90	2.75	0.67	0.52
1stn	P 42 G	0.1	-0.59	2.30	-1.02	1.86
1stn	K 43 A	-0.1	0.45	0.38	-1.71	-1.79
1stn	K 43 F	0.5	1.67	2.21	-0.91	-0.37
1stn	K 43 G	-0.2	0.88	1.60	0.10	0.82
1stn	K 44 A	0.3	1.21	2.11	-0.96	-0.05
1stn	K 44 F	0	3.31	3.13	0.73	0.55
1stn	K 44 G	0.2	2.31	2.15	1.53	1.37
1stn	G 45 A	-0.25	1.22	0.13	-0.16	-1.26
1stn	G 45 F	0.6	2.94	4.43	1.14	2.63
1stn	G 45 V	1.1	0.68	0.85	-2.26	-2.09
1stn	V 46 A	0.25	1.47	1.27	3.03	2.83
1stn	V 46 G	0.35	2.65	3.20	5.60	6.15
1stn	V 46 S	0.1	1.46	2.33	4.32	5.18
1stn	V 46 T	-0.2	-0.01	1.65	1.93	3.59
1stn	E 47 A	0.1	3.02	3.17	1.90	2.04
1stn	E 47 G	0.4	4.80	5.79	5.06	6.05
1stn	K 48 A	0.2	0.35	1.78	-1.81	-0.39
1stn	K 48 G	0.3	2.75	1.61	1.97	0.83
1stn	P 51 A	0	-2.51	-1.62	-4.33	-3.44
1stn	P 51 G	1	-0.69	-1.35	-1.12	-1.78
1stn	E 52 A	0.2	1.37	1.79	0.24	0.66
1stn	E 52 F	0.8	3.21	2.00	1.67	0.46
1stn	E 52 G	1.6	2.92	3.28	3.19	3.54
1stn	A 53 G	2.6	4.07	4.04	5.46	5.43
1stn	A 53 V	2.8	4.53	3.26	2.97	1.70
1stn	S 54 A	-0.4	-0.41	-0.75	-1.70	-2.05
1stn	S 54 F	0	-1.77	-3.60	-3.47	-5.31
1stn	S 54 G	1.1	2.21	1.83	2.30	1.93
1stn	A 55 F	0.8	1.87	2.85	1.45	2.44
1stn	A 55 G	1.4	1.46	1.10	2.85	2.48
1stn	A 55 V	2.8	1.44	2.18	-0.12	0.62
1stn	F 56 A	2.3	0.13	0.46	0.55	0.87
1stn	F 56 G	4.8	2.86	3.62	4.66	5.42

1stn	T 57 A	2.4	1.99	1.72	1.61	1.33
1stn	T 57 G	3.5	5.63	4.99	6.64	6.00
1stn	T 57 S	2.1	2.41	1.41	3.33	2.33
1stn	T 57 V	0.2	3.11	2.07	1.17	0.13
1stn	K 58 A	0.5	1.45	1.40	-0.71	-0.76
1stn	K 58 F	2	1.95	1.80	-0.63	-0.78
1stn	K 58 G	1.5	2.67	2.99	1.89	2.21
1stn	K 59 A	-0.1	-0.29	0.23	-2.46	-1.94
1stn	K 59 F	0.3	0.36	1.48	-2.22	-1.10
1stn	K 59 G	0.4	1.50	1.43	0.72	0.65
1stn	M 60 A	2	-0.02	1.69	3.01	4.72
1stn	M 60 G	4.6	4.14	3.96	8.56	8.38
1stn	M 60 L	0.8	-0.73	-1.53	0.93	0.13
1stn	V 61 A	2.2	1.86	3.06	3.42	4.62
1stn	V 61 G	4.4	6.03	5.45	8.98	8.40
1stn	V 61 L	0.03	-1.50	-0.91	-1.31	-0.72
1stn	V 61 M	0.2	1.96	1.70	0.49	0.23
1stn	V 61 S	3.1	2.30	3.32	5.15	6.17
1stn	V 61 T	1.3	0.67	1.79	2.61	3.73
1stn	E 62 A	1	0.22	1.19	-0.91	0.07
1stn	E 62 F	1.4	4.52	4.44	2.99	2.91
1stn	E 62 G	0.9	1.49	2.27	1.75	2.54
1stn	N 63 A	0.5	1.20	0.39	1.14	0.32
1stn	N 63 G	0.5	1.57	2.42	2.89	3.74
1stn	A 64 G	2	2.54	2.31	3.93	3.69
1stn	A 64 T	3.077	6.31	6.32	6.70	6.70
1stn	K 65 A	0.1	-0.36	1.01	-2.53	-1.16
1stn	K 65 F	0.1	2.76	3.53	0.19	0.95
1stn	K 65 G	0.5	0.47	1.88	-0.31	1.10
1stn	K 65 W	0.495	5.42	7.07	5.94	7.58
1stn	K 66 A	0.4	0.98	0.46	-1.18	-1.71
1stn	K 66 F	0	3.07	6.08	0.49	3.50
1stn	K 66 G	1.1	1.82	3.41	1.04	2.63
1stn	I 67 A	5.1	4.84	7.23	6.54	8.93
1stn	I 67 G	6.5	7.49	7.43	10.58	10.52
1stn	I 67 V	1.8	0.95	1.15	1.10	1.29
1stn	E 68 A	1.2	1.32	1.05	0.20	-0.08
1stn	E 68 F	1.1	0.29	-1.24	-1.25	-2.78
1stn	E 68 G	2.7	3.66	4.61	3.93	4.87
1stn	V 69 A	3.1	2.27	2.10	3.83	3.66
1stn	V 69 G	6.6	5.58	5.69	8.52	8.64
1stn	V 69 S	5.4	3.17	3.97	6.02	6.82
1stn	V 69 T	3.8	1.29	2.20	3.23	4.15
1stn	E 70 A	2.2	4.73	3.94	3.61	2.81
1stn	E 70 G	3.5	6.57	6.27	6.83	6.53
1stn	E 70 V	2.31	4.90	4.67	2.22	1.99
1stn	F 71 A	4	3.61	4.66	4.03	5.07
1stn	F 71 G	4.7	4.94	5.79	6.74	7.59

1stn	D 72 A	3.1	3.83	3.22	2.77	2.16
1stn	D 72 G	2.2	2.90	2.41	3.24	2.74
1stn	K 73 A	0.6	-0.06	0.97	-2.23	-1.20
1stn	K 73 F	-0.1	1.41	0.35	-1.17	-2.23
1stn	K 73 G	1.1	1.45	1.81	0.67	1.03
1stn	Q 75 A	0.1	-1.34	-1.18	-2.04	-1.88
1stn	Q 75 F	0.7	2.17	2.98	1.07	1.87
1stn	Q 75 G	1.4	-0.17	-0.11	0.53	0.58
1stn	R 76 A	1.1	-0.68	-1.44	0.03	-0.73
1stn	R 76 G	2.2	1.65	1.92	3.74	4.02
1stn	T 77 A	0.9	0.29	0.54	-0.09	0.16
1stn	T 77 G	2	1.61	1.76	2.61	2.77
1stn	T 77 S	0.7	0.78	1.77	1.70	2.68
1stn	T 77 V	-0.2	-1.04	-0.62	-2.98	-2.56
1stn	D 78 A	3.8	6.85	5.49	5.79	4.44
1stn	D 78 F	5.2	6.51	7.23	5.05	5.76
1stn	D 78 G	2.7	6.26	4.98	6.60	5.31
1stn	K 79 A	-0.2	-0.30	-0.35	-2.46	-2.52
1stn	K 79 F	0.9	3.52	2.41	0.94	-0.17
1stn	K 79 G	0.3	0.49	0.62	-0.29	-0.16
1stn	Y 80 A	0.4	-1.15	-2.32	1.10	-0.08
1stn	Y 80 F	0.1	-0.19	0.21	1.65	2.05
1stn	Y 80 G	1	-0.94	-1.33	2.70	2.31
1stn	Y 80 L	0.1	-1.42	-1.03	-0.54	-0.15
1stn	G 81 A	0.55	1.90	2.00	0.51	0.61
1stn	R 82 A	0.9	0.09	0.46	0.80	1.17
1stn	R 82 G	2.6	2.35	3.14	4.45	5.24
1stn	G 83 A	0.1	1.63	0.83	0.24	-0.56
1stn	L 84 A	2.6	3.87	5.46	5.24	6.83
1stn	L 84 G	3.2	5.62	5.74	8.38	8.49
1stn	A 85 G	2	2.01	1.41	3.40	2.79
1stn	A 85 S	2	0.87	0.44	2.16	1.74
1stn	Y 86 A	5.3	10.52	10.63	12.77	12.88
1stn	Y 86 F	2.4	2.73	2.87	4.56	4.71
1stn	Y 86 G	6.7	12.72	14.60	16.36	18.23
1stn	Y 86 L	3.9	7.91	8.39	8.79	9.27
1stn	I 87 A	4	3.67	4.44	5.37	6.14
1stn	I 87 G	6.6	6.57	7.78	9.66	10.87
1stn	I 87 V	0.5	-0.34	0.54	-0.19	0.68
1stn	Y 88 A	6.5	6.80	6.66	9.05	8.91
1stn	Y 88 F	2	2.15	2.87	3.98	4.71
1stn	Y 88 G	7.5	9.09	10.91	12.72	14.55
1stn	Y 88 L	4.5	4.62	4.54	5.51	5.42
1stn	A 89 G	2.4	2.18	2.73	3.57	4.11
1stn	A 89 V	1.3	4.23	1.52	2.67	-0.04
1stn	D 90 A	3.3	4.08	3.86	3.02	2.81
1stn	D 90 F	5.3	7.97	6.64	6.50	5.17
1stn	D 90 G	2.7	3.53	3.62	3.87	3.95

1stn	G 91 A	1.75	2.61	2.38	1.23	0.99
1stn	K 92 A	0.1	0.50	-0.61	-1.67	-2.77
1stn	K 92 F	0.7	2.24	3.64	-0.34	1.06
1stn	K 92 G	1.7	2.31	1.90	1.53	1.12
1stn	M 93 A	4.6	2.08	2.64	5.11	5.67
1stn	M 93 G	4.5	4.47	6.41	8.88	10.83
1stn	M 93 I	4.4	2.10	2.63	3.43	3.96
1stn	V 94 A	3.2	3.18	3.99	4.74	5.55
1stn	V 94 G	5	6.39	4.14	9.34	7.09
1stn	V 94 S	5.1	4.05	3.98	6.90	6.84
1stn	V 94 T	3.3	1.59	1.72	3.53	3.66
1stn	N 95 A	5.2	0.92	1.38	0.85	1.31
1stn	N 95 G	5.1	4.57	4.28	5.90	5.61
1stn	E 96 A	1.9	-1.76	-2.22	-2.89	-3.35
1stn	E 96 G	3.1	0.32	1.16	0.58	1.42
1stn	A 97 F	1.9	5.21	5.00	4.80	4.58
1stn	A 97 G	1.3	1.75	1.43	3.14	2.82
1stn	L 98 A	4.6	4.32	5.19	5.69	6.56
1stn	L 98 G	6.6	7.77	8.17	10.53	10.92
1stn	V 99 A	2.9	2.62	2.29	4.18	3.85
1stn	V 99 G	6.5	5.41	4.81	8.36	7.76
1stn	V 99 S	4.9	2.29	2.43	5.14	5.28
1stn	V 99 T	2.5	2.16	2.08	4.10	4.02
1stn	R 100 A	1.4	-0.26	0.40	0.45	1.10
1stn	R 100 F	3.1	1.77	2.60	2.07	2.89
1stn	R 100 G	2.4	2.05	2.42	4.15	4.52
1stn	Q 101 A	-0.1	-0.67	-0.08	-1.36	-0.77
1stn	Q 101 G	1.5	1.35	1.54	2.04	2.23
1stn	L 103 A	5.8	5.49	6.75	6.85	8.11
1stn	L 103 G	7.2	7.34	8.01	10.09	10.77
1stn	A 104 G	1	3.27	2.10	4.65	3.49
1stn	K 105 A	1.3	1.12	2.50	-1.04	0.33
1stn	K 105 G	2.7	3.09	2.51	2.31	1.73
1stn	V 106 A	4.45	3.15	3.29	4.70	4.85
1stn	V 106 G	4.9	6.03	6.49	8.98	9.44
1stn	V 106 S	4.8	3.50	3.06	6.36	5.91
1stn	V 106 T	2.3	1.59	2.78	3.53	4.72
1stn	A 107 F	1.45	1.85	2.49	1.44	2.08
1stn	A 107 G	0	0.05	1.03	1.44	2.42
1stn	A 107 V	1.5	4.94	4.32	3.38	2.76
1stn	Y 108 A	-0.05	-3.23	-2.68	-0.98	-0.43
1stn	Y 108 F	0	0.14	1.13	1.97	2.96
1stn	Y 108 G	0.25	-1.03	-1.07	2.60	2.57
1stn	Y 108 L	-0.2	-1.45	-2.94	-0.57	-2.06
1stn	V 109 A	0	0.55	2.18	2.10	3.73
1stn	V 109 G	0.2	2.88	3.59	5.82	6.54
1stn	V 109 S	0	1.84	1.59	4.70	4.44
1stn	V 109 T	0.3	0.67	1.18	2.62	3.12

1stn	Y 110 A	0.3	-1.09	-1.89	1.16	0.35
1stn	Y 110 F	0.1	-0.25	0.11	1.59	1.95
1stn	Y 110 G	0.7	-1.15	0.03	2.49	3.66
1stn	Y 110 L	0.3	-1.13	-2.04	-0.25	-1.16
1stn	K 111 A	-0.7	-1.21	-0.36	-3.37	-2.52
1stn	K 111 F	0.1	3.67	3.92	1.09	1.34
1stn	K 111 G	-1	-0.70	-0.58	-1.48	-1.36
1stn	P 112 A	-0.8	-2.04	-1.77	-3.86	-3.58
1stn	P 112 F	-0.3	-0.12	-0.20	-2.35	-2.43
1stn	P 112 G	-1.25	-1.49	-0.70	-1.92	-1.13
1stn	P 112 L	-0.2	-2.05	-1.13	-5.23	-4.32
1stn	P 112 T	-1.1	-0.47	-0.98	-1.90	-2.42
1stn	N 113 A	2.05	2.81	2.79	2.75	2.72
1stn	N 113 D	2.4	3.04	3.53	4.03	4.52
1stn	N 113 G	1.85	5.66	6.91	6.99	8.23
1stn	N 114 A	1.25	-0.16	-0.04	-0.23	-0.11
1stn	N 114 G	1.25	0.63	0.02	1.96	1.34
1stn	T 115 A	1.2	-0.60	-0.92	-0.98	-1.31
1stn	T 115 G	2.1	0.97	-1.90	1.97	-0.89
1stn	T 115 S	0.6	0.31	1.16	1.22	2.07
1stn	T 115 V	1.8	3.46	2.39	1.52	0.45
1stn	H 116 A	3.1	2.02	2.98	2.30	3.26
1stn	H 116 G	4.2	3.07	3.36	4.74	5.03
1stn	E 117 A	0.4	0.69	1.56	-0.43	0.43
1stn	E 117 F	0.8	-0.71	0.24	-2.24	-1.30
1stn	E 117 G	2.2	2.65	3.04	2.92	3.30
1stn	Q 118 A	0.4	-0.90	-0.51	-1.60	-1.20
1stn	Q 118 F	0.7	1.46	1.87	0.36	0.76
1stn	Q 118 G	0.6	0.35	-0.73	1.04	-0.03
1stn	H 119 A	-0.4	-2.72	-1.33	-2.44	-1.04
1stn	H 119 F	-0.3	0.46	-0.45	0.34	-0.58
1stn	H 119 G	0.5	-0.21	0.35	1.47	2.02
1stn	L 120 A	4.9	5.04	5.03	6.40	6.40
1stn	L 120 G	7	8.40	8.60	11.15	11.35
1stn	R 121 A	1.7	0.90	1.71	1.61	2.41
1stn	R 121 G	2.9	2.82	3.83	4.92	5.93
1stn	K 122 A	-0.2	-0.34	-0.35	-2.51	-2.52
1stn	K 122 F	0.3	1.43	2.89	-1.15	0.31
1stn	K 122 G	0.7	1.98	2.65	1.20	1.87
1stn	S 123 A	-0.7	-1.36	-2.01	-2.65	-3.31
1stn	S 123 F	1	0.13	-1.36	-1.58	-3.07
1stn	S 123 G	1.6	0.30	0.49	0.39	0.58
1stn	E 124 A	2.4	0.16	0.84	-0.96	-0.29
1stn	E 124 G	3.8	3.97	3.97	4.23	4.24
1stn	A 125 G	1.1	1.94	1.47	3.32	2.86
1stn	A 125 V	1.2	0.59	0.99	-0.97	-0.57
1stn	Q 126 A	0.2	-0.19	-0.33	-0.88	-1.03
1stn	Q 126 F	0.7	2.75	1.84	1.65	0.73

1stn	Q 126 G	2.4	1.97	2.82	2.66	3.51
1stn	A 127 G	3.7	3.72	3.64	5.10	5.02
1stn	K 128 A	1.4	0.50	0.24	-1.67	-1.93
1stn	K 128 F	1.4	1.76	2.15	-0.82	-0.43
1stn	K 128 G	3.3	2.30	2.70	1.52	1.92
1stn	K 129 A	-0.1	-0.55	-0.44	-2.72	-2.61
1stn	K 129 F	0.4	2.84	1.37	0.26	-1.21
1stn	K 129 G	0.7	0.59	2.37	-0.19	1.59
1stn	E 130 A	0.7	2.27	2.40	1.15	1.27
1stn	E 130 F	1.2	3.12	4.26	1.58	2.72
1stn	E 130 G	1.7	4.11	4.25	4.38	4.51
1stn	K 131 A	0.8	1.05	1.41	-1.11	-0.76
1stn	K 131 F	1.2	2.30	2.71	-0.28	0.13
1stn	K 131 G	0.05	1.99	2.38	1.21	1.60
1stn	L 132 A	2.3	2.01	2.85	3.37	4.21
1stn	L 132 G	4.6	4.06	5.04	6.81	7.79
1stn	N 133 A	1.05	1.87	2.12	1.81	2.06
1stn	N 133 G	-0.15	1.50	1.55	2.82	2.87
1stn	I 134 A	3.5	1.13	1.94	2.83	3.64
1stn	I 134 G	4.4	3.75	2.51	6.84	5.60
1stn	I 134 V	1.5	0.44	0.39	0.58	0.53
1stn	S 136 A	0.4	0.76	0.84	-0.54	-0.45
1stn	S 136 G	0.9	2.04	1.50	2.13	1.59
2ci2	WILD TYPE	0	0.00	0.00	0.00	0.00
2ci2	L 27 A	1.91	4.39	4.34	5.76	5.70
2ci2	V 38 A	0	2.42	2.08	3.97	3.64
2ci2	I 39 V	0.91	3.02	2.34	3.16	2.48
2ci2	I 48 V	0.75	2.00	1.17	2.14	1.31
2ci2	I 48 A	3.4	5.31	4.70	7.01	6.40
2ci2	V 66 A	4.97	6.17	5.08	7.73	6.64
2ci2	L 68 A	3.56	5.17	4.65	6.54	6.02
2ci2	V 70 A	1.13	2.59	0.80	4.14	2.36
2ci2	I 76 V	0.08	0.12	-0.62	0.27	-0.47
2ci2	I 76 A	4.09	3.95	1.61	5.66	3.32
2ci2	I 48 A I 76 V	4.08	5.83	5.39	7.67	7.24
2ci2	T 58 D	0.04	-0.36	-0.19	0.31	0.49
2ci2	T 58 A	0.68	-0.90	0.11	-1.28	-0.27
2ci2	E 60 A	1.06	2.16	0.92	1.03	-0.21
2ci2	T 58 A E 60 A	0.67	2.66	1.61	1.15	0.10
2ci2	T 58 D E 60 A	0.24	2.00	0.45	1.55	-0.01
2ci2	I 39 V	1.17	2.97	2.34	3.11	2.48
2ci2	I 39 L	1.96	7.73	2.29	8.07	2.62
2ci2	R 67 A	1.21	2.08	1.60	2.79	2.30
2ci2	K 21 A	1.04	6.09	4.52	3.92	2.35
2ci2	K 21 A E 26 A	1.17	5.89	4.99	2.59	1.70
2ci2	K 21 M	0.73	5.11	4.83	-0.09	-0.37
2ci2	P 25 A	-3.4	-0.21	-0.69	-2.02	-2.51
2ci2	P 25 A A 35 G	1.3	3.00	0.35	2.57	-0.08

2ci2	E 26 A	1.03	2.75	2.92	1.62	1.80
2ci2	E 26 Q	0.57	3.26	3.79	2.83	3.36
2ci2	K 30 A	1.2	1.74	1.78	-0.43	-0.39
2ci2	S 31 G	0.06	3.81	2.97	3.90	3.06
2ci2	S 31 A	1.02	1.66	0.86	0.36	-0.44
2ci2	E 33 Q	0.4	1.34	1.09	0.91	0.66
2ci2	E 33 D	0.77	-0.09	1.30	-0.16	1.23
2ci2	E 33 N	0.28	2.13	1.09	1.07	0.03
2ci2	E 34 Q	0.68	0.72	-0.81	0.28	-1.24
2ci2	E 34 D	-0.36	2.20	0.98	2.13	0.91
2ci2	E 34 N	0.08	3.41	2.60	2.35	1.54
2ci2	E 33 A E 34 A	-0.02	2.74	2.54	0.49	0.29
2ci2	S 31 G E 33 A E 34 A	0.81	4.98	4.47	2.82	2.31
2ci2	A	0.75	3.46	3.42	-0.09	-0.13
2ci2	S 31 A E 33 A E 34 A	1.41	3.77	1.30	5.16	2.68
2ci2	A 35 G	1.13	0.89	2.14	-1.28	-0.03
2ci2	K 36 A	2.01	2.92	3.38	2.14	2.60
2ci2	K 36 G	0.99	0.37	-0.34	-1.80	-2.51
2ci2	K 37 A	1.58	1.67	1.86	0.89	1.08
2ci2	K 37 G	0.06	2.36	2.08	3.92	3.64
2ci2	V 38 A	0.97	3.02	2.34	3.16	2.49
2ci2	I 39 V	1.21	2.16	-0.07	3.53	1.30
2ci2	L 40 A	2.09	4.75	4.10	7.50	6.86
2ci2	L 40 G	0.54	-0.33	0.63	-1.03	-0.07
2ci2	Q 41 A	0.92	-0.68	-1.36	0.02	-0.67
2ci2	Q 41 G	1.05	3.93	4.23	2.87	3.17
2ci2	D 42 A	1.85	3.75	6.17	1.58	4.00
2ci2	K 43 A	3.49	5.51	6.82	4.73	6.04
2ci2	K 43 G	1.22	0.71	0.72	-1.11	-1.10
2ci2	P 44 A	0.78	2.09	1.76	0.97	0.63
2ci2	E 45 A	0.18	2.02	0.38	-0.04	-1.68
2ci2	Q 47 M M 59 L	1.74	3.03	3.36	4.40	4.73
2ci2	L 51 A	1.01	7.01	4.61	6.67	4.28
2ci2	L 51 I	1.02	2.70	-0.25	2.51	-0.44
2ci2	L 51 V	1.08	4.12	3.37	2.97	2.22
2ci2	L 51 V F 69 L	3.26	6.53	6.19	6.75	6.41
2ci2	L 51 V F 69 A	3.25	6.24	4.37	6.65	4.78
2ci2	L 51 A F 69 L	5.16	8.07	7.58	9.85	9.36
2ci2	L 51 A F 69 A	2.95	4.83	3.87	7.76	6.79
2ci2	L 51 A V 57 A	1.93	3.83	2.79	5.20	4.16
2ci2	L 51 V V 57 A	3.34	6.33	4.60	8.31	6.57
2ci2	L 51 A V 57 A F 69 L	2.84	5.10	4.68	5.51	5.09
2ci2	L	0.58	0.14	0.49	-1.68	-1.32
2ci2	P 52 A	0.98	1.93	2.15	2.84	3.07
2ci2	T 55 S					

2ci2	T 55 V	1.57	2.98	1.32	1.04	-0.62
2ci2	T 55 A	1.42	1.69	1.45	1.31	1.06
2ci2	I 56 A	1.28	0.38	-0.22	2.08	1.48
2ci2	V 57 A	0.67	2.19	1.56	3.75	3.12
2ci2	V 57 A F 69 L	2.2	4.28	2.26	4.88	2.87
2ci2	V 57 A V 79 A	3.78	3.29	3.12	6.41	6.24
2ci2	E 60 A	1.12	2.16	0.92	1.03	-0.21
2ci2	R 62 A	1.02	2.73	3.29	3.44	4.00
2ci2	R 62 A D 64 A	2.46	3.45	3.75	3.10	3.40
2ci2	D 64 A	1.02	0.52	1.19	-0.54	0.13
2ci2	F 69 L	1.92	2.84	1.47	1.89	0.51
2ci2	F 69 V	1.41	8.67	4.06	7.52	2.92
2ci2	F 69 A	3.21	6.25	4.53	6.67	4.94
2ci2	D 71 A	3.14	5.85	4.43	4.79	3.37
2ci2	K 72 N	1.21	0.50	0.74	-1.61	-1.36
2ci2	N 75 D	1.51	1.08	0.84	2.07	1.83
2ci2	N 75 A	1.22	2.03	1.00	1.97	0.94
2ci2	P 80 A	3.5	2.38	2.66	0.56	0.84
2ci2	R 67 A	1.4	2.08	1.60	2.79	2.30
2ci2	K 43 A	-0.64	3.66	4.88	1.49	2.71
2ci2	E 45 A	-0.57	2.10	2.13	0.97	1.00
2ci2	K 43 A E 45 A	-0.95	4.74	4.27	1.44	0.98
2ci2	P 44 A	-1.93	0.70	0.72	-1.11	-1.10
1u5p	WILD TYPE	0	0.00	0.00	0.00	0.00
1u5p	P 60 A	-0.4	-1.87	-1.63	-3.68	-3.45
1u5p	W 94 F	2.1	6.76	5.33	3.67	2.24
1u5p	F 11 L	1.3	4.51	-0.49	3.55	-1.44
1u5p	F 11 A	3.7	6.27	4.34	6.69	4.76
1u5p	L 11 A	3.7	6.27	4.34	7.64	5.71
1u5p	M 15 A	2.2	3.52	4.01	6.55	7.04
1u5p	I 22 V	1.6	2.61	2.61	2.76	2.76
1u5p	I 22 A	3.6	7.40	6.86	9.10	8.56
1u5p	V 22 A	3.7	7.40	6.86	8.95	8.41
1u5p	K 25 A	0	3.61	3.63	1.44	1.47
1u5p	V 29 A	0.2	0.10	1.57	1.66	3.13
1u5p	V 41 A	0.4	-1.93	-1.71	-0.37	-0.15
1u5p	L 44 A	0.2	0.90	3.25	2.27	4.61
1u5p	H 48 A	1.4	2.20	1.24	2.48	1.53
1u5p	L 51 A	2.8	2.17	3.23	3.54	4.59
1u5p	L 55 A	3.8	3.07	3.28	4.44	4.65
1u5p	H 58 A	2.3	0.40	3.35	0.68	3.64
1u5p	I 62 V	0.6	0.54	0.05	0.69	0.19
1u5p	I 62 A	2.8	3.65	2.80	5.35	4.51
1u5p	V 62 A	2.8	3.65	2.80	5.20	4.36
1u5p	V 65 A	2.3	2.86	3.07	4.41	4.63
1u5p	L 72 A	2.4	1.77	2.75	3.13	4.12
1u5p	I 83 V	0.6	2.60	-0.20	2.74	-0.05
1u5p	I 83 A	2	2.30	5.33	4.01	7.03

1u5p	V 83 A	2	2.30	5.33	3.86	6.89
1u5p	L 87 A	2.8	4.95	3.88	6.31	5.25
1u5p	F 90 L	-0.5	3.36	2.47	2.40	1.51
1u5p	F 90 A	2.8	8.08	6.76	8.49	7.17
1u5p	L 97 A	3.8	5.11	4.54	6.48	5.91
1u5p	A 101 G	2.6	3.94	2.49	5.33	3.87
1u5p	R 104 A	0	2.92	2.16	3.63	2.87
1u5p	L 108 A	1.4	0.00	-0.50	1.37	0.87
1u5p	H 9 A	-0.5	-3.50	-2.47	-3.21	-2.18
1u5p	H 9 G	0.5	-2.14	-1.29	-0.46	0.38
1u5p	R 13 A	0.3	0.78	0.33	1.48	1.04
1u5p	R 13 G	1.9	0.00	-0.50	0.00	-0.50
1u5p	D 16 A	0.2	0.74	2.08	-0.32	1.02
1u5p	D 16 G	1.2	1.89	6.97	2.22	7.30
1u5p	E 24 A	-0.1	0.61	0.89	-0.51	-0.24
1u5p	E 24 G	1.1	2.99	1.21	3.25	1.47
1u5p	T 39 A	-0.3	0.33	-1.46	-0.06	-1.84
1u5p	T 39 G	0.1	0.25	-0.24	1.26	0.76
1u5p	N 43 A	-0.2	1.05	0.81	0.99	0.74
1u5p	N 43 G	0.4	2.22	2.27	3.54	3.59
1u5p	K 46 A	-0.4	0.83	-0.52	-1.34	-2.68
1u5p	K 46 G	0.5	2.42	1.57	1.64	0.79
1u5p	R 50 A	-0.3	-1.03	-1.70	-0.32	-0.99
1u5p	R 50 G	0.6	0.16	1.37	2.26	3.46
1u5p	A 53 G	1.1	1.72	1.10	3.11	2.49
1u5p	A 57 G	1.1	0.93	0.74	2.32	2.13
1u5p	Q 63 A	0.7	1.19	-0.16	0.50	-0.85
1u5p	Q 63 G	1.8	2.70	4.26	3.40	4.95
1u5p	D 67 A	0.1	1.16	2.46	0.10	1.41
1u5p	D 67 G	1.3	3.48	3.44	3.81	3.78
1u5p	K 71 A	0.1	-0.05	0.77	-2.22	-1.40
1u5p	K 71 G	1.4	2.20	2.23	1.42	1.45
1u5p	Q 85 A	0	0.86	2.24	0.17	1.55
1u5p	Q 85 G	1.3	3.55	2.02	4.25	2.71
1u5p	A 88 G	1.1	1.06	1.52	2.45	2.91
1u5p	D 92 A	-0.7	-0.17	0.83	-1.22	-0.23
1u5p	D 92 G	0.3	1.71	2.86	2.05	3.20
1u5p	K 95 A	0.4	0.46	-0.50	-1.71	-2.67
1u5p	K 95 G	1.3	2.39	3.48	1.61	2.70
1u5p	Q 99 A	-0.4	-1.05	-1.26	-1.75	-1.96
1u5p	Q 99 G	0.7	0.70	0.34	1.39	1.04
1u5p	A 103 G	1.8	1.68	1.65	3.07	3.04
1u5p	D 106 A	-0.5	-1.66	-1.61	-2.72	-2.66
1u5p	D 106 G	1.3	0.74	1.32	1.07	1.65

Table S2. The Correlation Coefficients between the Calculated and Experimental $\Delta\Delta G$ for Mutations of Buried and Solvent-Exposed Residues

Mutation type	N_{mut}	Fixed backbone		Flexible backbone	
		r	p	r	p
Buried	364	0.69	9.2×10^{-53}	0.70	7.0×10^{-55}
Solvent-exposed	207	0.52	9.78×10^{-16}	0.51	4.2×10^{-15}

Table S3. The Correlation Coefficients between the Calculated and Experimental $\Delta\Delta G$ for Mutations at Different Types of Secondary Structures

Mutation type	N_{mut}	Fixed backbone		Flexible backbone	
		r	p	r	P
H	209	0.69	7.0×10^{-31}	0.70	4.3×10^{-32}
E	161	0.81	1.1×10^{-38}	0.82	2.3×10^{-40}
C	78	0.57	5.1×10^{-8}	0.53	6.0×10^{-7}
T	65	0.67	1.0×10^{-9}	0.65	4.6×10^{-9}
S	25	0.68	1.8×10^{-4}	0.65	4.4×10^{-4}
B	24	0.54	6.5×10^{-3}	0.42	4.1×10^{-2}

DSSP program is used for the assignment of secondary structures. In DSSP, H denotes α -helix; B denotes isolated β -bridge; E denotes extended strand; T denotes hydrogen bonded turn; S denotes bend; and C denotes loop or irregular structure.