Supporting information for Kortemme and Baker (2002) *Proc. Natl. Acad. Sci. USA*, 10.1073/pnas.202485799

Table 8. Glycine and proline residues were not considered as there might be significant changes in the backbone conformation upon mutation to alanine

PDB ID	Mutated partner	PDB residue no.	Amino acid	$\Delta\Delta G_{calc}$	$\Delta\Delta G_{obs}$	Interface residue 0, no; 1, yes
1A22	hGH	14	M	0.00	0.10	0
1A22	hGH	18	H	1.84	-0.50	1
1A22	hGH	21	H	0.78	0.20	1
1A22	hGH	22	Q	0.07	-0.20	1
1A22	hGH	25	F	1.30	-0.40	1
1A22	hGH	26	D	-0.05	-0.20	0
1A22	hGH	29	Q	0.01	-0.60	0
1A22	hGH	42	Y	2.00	0.20	1
1A22	hGH	45	L	1.15	1.20	1
1A22	hGH	46	Q	1.04	0.10	1
1A22	hGH	51	S	-0.02	0.30	0
1A22	hGH	56	E	0.97	0.40	1
1A22	hGH	62	S	-0.06	0.10	1
1A22	hGH	63	N	0.39	0.30	1

1A22	hGH	64	R	2.00	1.60	1
1A22	hGH	65	E	-0.11	-0.50	0
1A22	hGH	68	Q	1.81	0.60	1
1A22	hGH	164	Y	0.96	0.30	0
1A22	hGH	167	R	0.42	0.30	1
1A22	hGH	168	K	2.10	-0.20	1
1A22	hGH	171	D	8.73	0.80	1
1A22	hGH	172	K	0.74	2.00	1
1A22	hGH	174	E	0.85	-0.90	1
1A22	hGH	175	T	2.04	2.00	1
1A22	hGH	176	F	0.60	1.90	0
1A22	hGH	178	R	0.38	2.40	1
1A22	hGH	179	I	1.00	0.80	1
1A22	hGH	183	R	0.07	0.50	0
1A22	hGH	186	E	0.00	0.00	0
1A22	hGHbp	43	R	6.54	2.12	1
1A22	hGHbp	44	E	0.49	1.69	1
1A22	hGHbp	70	R	-0.06	0.69	0
1A22	hGHbp	71	R	1.31	0.54	1
1A22	hGHbp	73	T	0.00	0.11	0

1A22	hGHbp	74	Q	0.03	0.00	0
1A22	hGHbp	75	E	0.09	-0.10	1
1A22	hGHbp	76	W	2.86	0.51	1
1A22	hGHbp	80	W	0.04	-0.02	0
1A22	hGHbp	98	S	0.29	-0.05	0
1A22	hGHbp	102	S	-0.11	-0.20	1
1A22	hGHbp	103	I	0.31	1.61	1
1A22	hGHbp	104	W	5.38	>4.50	1
1A22	hGHbp	105	I	0.13	1.94	0
1A22	hGHbp	120	E	0.86	-0.19	1
1A22	hGHbp	121	K	0.05	0.08	0
1A22	hGHbp	124	S	-0.06	0.28	0
1A22	hGHbp	126	D	-0.31	0.99	1
1A22	hGHbp	127	E	1.11	0.97	1
1A22	hGHbp	164	D	1.37	1.49	1
1A22	hGHbp	165	I	0.09	2.13	0
1A22	hGHbp	166	Q	0.68	0.02	0
1A22	hGHbp	167	K	0.22	-0.02	1
1A22	hGHbp	169	W	3.63	>4.50	1

1A22	hGHbp	171	V	0.26	-0.64	1
1A22	hGHbp	195	D	0.00	-0.09	0
1A22	hGHbp	216	Q	-0.03	0.89	0
1A22	hGHbp	217	R	0.23	0.28	1
1A22	hGHbp	218	N	0.79	0.30	1
1A22	hGHbp	219	S	0.98	0.03	1
1A22	hGHbp	42	E	0.00	0.18	0
1A22	hGHbp	72	N	0.00	0.28	0
1A22	hGHbp	77	T	0.00	0.20	0
1A22	hGHbp	101	T	0.02	1.76	0
1A22	hGHbp	194	T	0.00	0.20	0
1A22	hGHbp	215	K	-0.02	0.79	0
1A4Y	Rnase Inh	261	W	1.05	0.10	1
1A4Y	Rnase Inh	263	W	2.27	1.20	1
1A4Y	Rnase Inh	287	E	-0.02	0.10	0
1A4Y	Rnase Inh	289	S	0.55	0.00	1
1A4Y	Rnase Inh	318	W	2.19	1.50	1
1A4Y	Rnase Inh	320	K	-0.21	-0.30	1
1A4Y	Rnase Inh	344	E	1.37	0.20	1
1A4Y	Rnase Inh	375	W	2.83	1.00	1

1A4Y	Rnase Inh	401	E	0.02	0.90	1
1A4Y	Rnase Inh	434	Y	3.03	3.30	1
1A4Y	Rnase Inh	435	D	0.58	3.50	1
1A4Y	Rnase Inh	437	Y	3.13	0.80	1
1A4Y	Rnase Inh	457	R	-0.04	-0.20	0
1A4Y	Rnase Inh	459	I	0.63	0.70	1
1A4Y	Angiogenin	5	R	2.54	2.30	1
1A4Y	Angiogenin	8	H	0.84	0.90	1
1A4Y	Angiogenin	12	Q	1.07	0.30	1
1A4Y	Angiogenin	13	H	0.02	-0.30	0
1A4Y	Angiogenin	31	R	2.77	0.20	1
1A4Y	Angiogenin	32	R	0.18	0.90	1
1A4Y	Angiogenin	33	R	-0.00	0.30	0
1A4Y	Angiogenin	66	R	0.00	0.20	0
1A4Y	Angiogenin	68	N	0.52	0.20	1
1A4Y	Angiogenin	70	R	1.02	-0.20	0
1A4Y	Angiogenin	84	H	1.01	0.20	1
1A4Y	Angiogenin	89	W	2.71	0.20	1
1A4Y	Angiogenin	108	E	1.73	-0.30	1

1A4Y	Angiogenin	114	H	1.69	0.65	1
1AHW	TF	156	Y	4.60	>4.00	1
1AHW	TF	167	T	-0.19	0.00	1
1AHW	TF	170	T	-0.06	1.00	0
1AHW	TF	176	L	0.01	1.00	0
1AHW	TF	178	D	-0.08	-0.50	0
1AHW	TF	197	T	-0.02	1.30	0
1AHW	TF	198	V	-0.01	-0.30	0
1AHW	TF	199	N	-0.01	1.10	0
1BRS	Barnase	27	K	1.91	5.40	1
1BRS	Barnase	54	D	-0.04	-0.80	0
1BRS	Barnase	58	N	-0.03	3.10	0
1BRS	Barnase	59	R	3.01	5.20	1
1BRS	Barnase	60	E	1.65	-0.20	1
1BRS	Barnase	73	E	-0.20	2.80	0
1BRS	Barnase	87	R	4.44	5.50	1
1BRS	Barnase	102	H	5.08	6.00	1
1BRS	Barstar	29	Y	3.13	3.40	1
1BRS	Barstar	35	D	1.42	4.50	1
1BRS	Barstar	39	D	9.40	7.70	1

1BRS	Barstar	42	T	1.69	1.80	1
1BRS	Barstar	76	E	1.54	1.30	1
1BRS	Barstar	80	E	-0.12	0.50	0
1BXI	Im9	24	N	0.00	0.14	0
1BXI	Im9	26	D	0.00	0.34	0
1BXI	Im9	27	T	0.59	0.73	1
1BXI	Im9	28	S	0.00	0.17	0
1BXI	Im9	29	S	0.35	0.96	0
1BXI	Im9	30	E	2.97	1.41	1
1BXI	Im9	31	E	0.13	0.31	0
1BXI	Im9	32	E	-0.01	0.22	0
1BXI	Im9	33	L	1.02	3.42	1
1BXI	Im9	34	V	0.98	2.58	1
1BXI	Im9	35	K	0.00	0.19	0
1BXI	Im9	36	L	0.00	0.91	0
1BXI	Im9	37	V	0.50	1.66	1
1BXI	Im9	38	T	1.34	0.90	1
1BXI	Im9	41	E	-0.08	2.08	1
1BXI	Im9	42	E	-0.03	0.66	0

1BXI	Im9	44	T	0.00	0.30	0
1BXI	Im9	45	E	0.00	0.21	0
1BXI	Im9	46	H	0.00	0.83	0
1BXI	Im9	48	S	-0.01	0.01	0
1BXI	Im9	50	S	5.40	2.19	1
1BXI	Im9	51	D	0.82	5.92	1
1BXI	Im9	52	L	0.00	0.60	0
1BXI	Im9	53	I	0.17	0.85	1
1BXI	Im9	54	Y	2.86	4.83	1
1BXI	Im9	55	Y	3.31	4.63	1
1BXI	Im9	60	D	0.00	0.51	0
1BXI	Im9	63	S	0.00	0.87	0
1BXI	Im9	68	V	0.00	1.86	0
1BXI	Im9	69	N	0.00	0.28	0
1CBW	BPTI	11	T	0.18	0.20	1
1CBW	BPTI	15	K	1.58	2.00	1
1CBW	BPTI	17	R	1.53	0.50	1
1CBW	BPTI	19	I	0.68	0.10	0
1CBW	BPTI	20	R	-0.02	0.30	0
1CBW	BPTI	34	V	0.30	0.00	0

1CBW	BPTI	39	R	1.58	0.20	1
1CBW	BPTI	46	K	0.00	0.10	0
1DAN	TF	15	K	-0.02	-0.40	0
1DAN	TF	17	T	0.13	0.10	1
1DAN	TF	18	N	0.04	0.20	0
1DAN	TF	20	K	1.50	2.60	1
1DAN	TF	21	T	0.00	-0.20	0
1DAN	TF	22	I	0.65	0.70	1
1DAN	TF	24	E	0.64	0.70	1
1DAN	TF	26	E	0.00	0.10	0
1DAN	TF	28	K	0.00	0.10	0
1DAN	TF	37	Q	1.41	0.55	1
1DAN	TF	41	K	-0.04	0.35	0
1DAN	TF	42	S	-0.05	-0.10	0
1DAN	TF	44	D	0.89	0.70	1
1DAN	TF	46	K	0.10	0.25	0
1DAN	TF	47	S	0.56	0.05	1
1DAN	TF	48	K	0.43	0.40	1
1DAN	TF	50	F	2.61	0.40	1

1DAN	TF	52	T	0.00	0.40	0
1DAN	TF	58	D	1.24	2.18	1
1DAN	TF	68	K	0.00	-0.10	0
1DAN	TF	94	Y	2.70	1.00	1
1DAN	TF	99	E	0.00	-0.20	0
1DAN	TF	122	K	0.00	-0.10	0
1DAN	TF	128	E	-0.11	0.10	1
1DAN	TF	129	D	0.00	0.00	0
1DAN	TF	133	L	1.62	0.00	1
1DAN	TF	135	R	0.94	0.55	1
1DAN	TF	139	T	0.00	0.00	0
1DAN	TF	140	F	1.54	1.50	1
1DAN	TF	144	R	0.00	0.00	0
1DAN	TF	145	D	0.00	0.00	0
1DAN	TF	152	I	0.00	0.20	0
1DAN	TF	163	S	0.42	0.00	1
1DAN	TF	167	T	0.00	0.20	0
1DAN	TF	169	K	0.00	0.10	0
1DAN	TF	172	T	0.00	0.00	0
1DAN	TF	176	L	0.00	0.10	0

1DAN	TF	181	K	0.00	0.00	0
1DAN	TF	185	Y	0.00	-0.35	0
1DAN	TF	195	S	0.00	0.00	0
1DAN	TF	203	T	0.21	0.10	1
1DAN	TF	207	V	1.12	-0.20	1
1DAN	TF	208	E	0.28	0.00	1
1DFJ	Rnase Inh	326	E	1.22	1.00	1
1DFJ	Rnase Inh	381	W	1.57	1.30	1
1DFJ	Rnase Inh	383	W	3.10	2.20	1
1DFJ	Rnase Inh	407	E	-0.10	1.30	1
1DFJ	Rnase Inh	409	S	-0.01	0.80	0
1DFJ	Rnase Inh	438	W	1.27	1.00	1
1DFJ	Rnase Inh	440	K	0.38	1.30	1
1DFJ	Rnase Inh	464	E	-0.12	1.60	0
1DFJ	Rnase Inh	521	E	0.42	1.30	1
1DFJ	Rnase Inh	577	R	0.21	0.80	1
1DFJ	Rnase Inh	579	I	0.50	0.30	1
1DFJ	Rnase Inh	434	Y	3.22	5.90	1
1DFJ	Rnase Inh	435	D	0.16	3.60	1

1DFJ	Rnase Inh	437	Y	3.73	2.60	1
1DN2	IgG	434	N	1.95	>1.50	1
1DN2	IgG	435	H	1.07	>1.50	1
1DN2	IgG	436	Y	4.32	>1.50	1
1DN2	Peptide	10	V	1.85	>2.00	1
1DN2	Peptide	11	W	3.99	>2.00	1
1F47	FTSZ fragm.	370	D	-0.15	0.70	1
1F47	FTSZ fragm.	371	Y	1.65	0.90	1
1F47	FTSZ fragm.	372	L	1.94	0.90	1
1F47	FTSZ fragm.	373	D	-0.08	1.80	0
1F47	FTSZ fragm.	374	I	2.07	2.50	1
1F47	FTSZ fragm.	377	F	2.43	2.50	1
1F47	FTSZ fragm.	378	L	1.13	2.30	1
1F47	FTSZ fragm.	380	K	-0.12	0.00	0
1F47	FTSZ fragm.	381	Q	0.03	0.00	1
1FC2	Protein A	28	N	0.61	0.60	1
1FC2	Protein A	31	I	0.78	2.20	1
1FC2	Protein A	35	K	0.16	1.20	1
1FCC	Protein G	25	T	0.10	0.24	0
1FCC	Protein G	27	E	3.21	>4.90	1

1FCC	Protein G	28	K	0.99	1.30	1
1FCC	Protein G	31	K	1.91	3.50	1
1FCC	Protein G	35	N	1.18	2.40	1
1FCC	Protein G	40	D	-0.15	0.30	1
1FCC	Protein G	42	E	0.03	0.40	1
1FCC	Protein G	43	W	2.71	3.80	1
1GC1	CD4	1	K	0.00	0.06	0
1GC1	CD4	2	K	0.00	-0.02	0
1GC1	CD4	8	K	0.00	0.10	0
1GC1	CD4	10	D	0.00	0.00	0
1GC1	CD4	11	T	0.00	0.00	0
1GC1	CD4	15	T	0.00	0.32	0
1GC1	CD4	19	S	0.00	0.00	0
1GC1	CD4	20	Q	0.00	-0.02	0
1GC1	CD4	21	K	0.00	-0.13	0
1GC1	CD4	22	K	0.00	0.24	0
1GC1	CD4	23	S	0.27	0.29	0
1GC1	CD4	25	Q	0.42	0.03	1
1GC1	CD4	27	H	0.80	0.28	1

1GC1	CD4	29	K	2.46	0.59	1
1GC1	CD4	30	N	0.00	0.17	0
1GC1	CD4	31	S	0.00	0.10	0
1GC1	CD4	32	N	0.00	0.18	0
1GC1	CD4	33	Q	0.03	0.10	0
1GC1	CD4	35	K	0.56	0.32	1
1GC1	CD4	39	N	0.00	0.46	0
1GC1	CD4	40	Q	0.75	-0.41	1
1GC1	CD4	42	S	0.20	0.00	1
1GC1	CD4	44	L	0.07	1.04	1
1GC1	CD4	45	T	0.32	-0.15	1
1GC1	CD4	49	S	0.00	0.60	0
1GC1	CD4	50	K	0.00	0.05	0
1GC1	CD4	52	N	1.01	0.70	1
1GC1	CD4	53	D	0.00	0.30	0
1GC1	CD4	56	D	-0.03	-0.07	0
1GC1	CD4	58	R	0.02	0.13	0
1GC1	CD4	59	R	1.02	1.16	1
1GC1	CD4	60	S	0.13	-0.09	1
1GC1	CD4	63	D	-0.05	-0.32	1

1GC1	CD4	64	Q	1.16	0.44	1
1GC1	CD4	66	N	0.00	-0.03	0
1GC1	CD4	72	K	0.00	-0.02	0
1GC1	CD4	73	N	0.00	-0.11	0
1GC1	CD4	75	K	0.00	0.16	0
1GC1	CD4	77	E	0.00	0.56	0
1GC1	CD4	81	T	0.00	>1.50	0
1GC1	CD4	85	E	2.10	1.31	0
1GC1	CD4	86	V	0.00	-0.07	0
1GC1	CD4	87	E	-0.06	0.22	0
1GC1	CD4	88	D	0.00	-0.07	0
1GC1	CD4	89	Q	0.00	0.17	0
1GC1	CD4	90	K	-0.04	0.05	0
1GC1	CD4	91	E	0.00	-0.13	0
1GC1	CD4	92	E	0.00	0.02	0
1GC1	CD4	94	Q	0.00	-0.11	0
1JCK	SEC3	20	T	1.26	1.40	1
1JCK	SEC3	23	N	1.98	>2.50	1
1JCK	SEC3	26	Y	0.92	1.70	1

1JCK	SEC3	60	N	0.82	1.30	1
1JCK	SEC3	90	Y	1.00	>2.50	1
1JCK	SEC3	91	V	1.02	2.10	1
1JCK	SEC3	103	K	-0.26	0.40	0
1JCK	SEC3	176	F	0.63	1.90	1
1JCK	SEC3	210	Q	1.12	>2.50	1
1JRH	A6	L27	E	0.67	0.54	1
1JRH	A6	L28	D	0.67	0.44	1
1JRH	A6	L30	Y	1.08	1.10	1
1JRH	A6	L91	Y	0.28	0.58	1
1JRH	A6	L92	W	3.01	2.80	1
1JRH	A6	L93	S	0.54	-0.65	1
1JRH	A6	L94	T	0.36	0.38	1
1JRH	A6	L96	W	0.59	1.70	1
1JRH	A6	H32	Y	1.63	1.40	1
1JRH	A6	H52	W	1.55	2.70	1
1JRH	A6	H53	W	0.73	2.40	1
1JRH	A6	H54	D	1.64	1.90	1
1JRH	A6	H55	D	0.00	1.70	0
1JRH	A6	H56	D	0.49	1.80	1

1JRH	A6	H58	Y	2.19	1.20	1
1JRH	A6	H95	R	1.49	0.54	1
1JRH	A6	H98	F	0.00	0.00	0
1JRH	A6	H99	Y	1.98	1.10	1
1JRH	A6	H100b	H	3.38	1.70	1
1JRH	Interferon	47	K	1.40	3.60	1
1JRH	Interferon	48	N	-0.01	-0.30	0
1JRH	Interferon	49	Y	3.87	3.40	1
1JRH	Interferon	51	V	1.00	1.90	1
1JRH	Interferon	52	K	2.36	3.00	1
1JRH	Interferon	53	N	2.74	3.90	1
1JRH	Interferon	54	S	-0.03	0.30	0
1JRH	Interferon	55	E	-0.10	-0.40	1
1JRH	Interferon	79	N	0.03	-0.40	0
1JRH	Interferon	82	W	1.35	4.50	1
1JRH	Interferon	84	R	0.37	-0.30	1
1JRH	Interferon	98	K	0.04	0.00	1
1NMB	NC10	H99	Y	1.27	1.50	1
1VFB	D1.3	L30	H	0.26	0.80	0

1VFB	D1.3	L32	Y	1.30	1.30	1
1VFB	D1.3	L49	Y	0.42	0.80	1
1VFB	D1.3	L50	Y	1.54	0.40	1
1VFB	D1.3	L53	T	0.58	-0.23	1
1VFB	D1.3	L92	W	2.06	1.71	1
1VFB	D1.3	L93	S	0.00	0.11	1
1VFB	D1.3	H30	T	1.22	0.09	0
1VFB	D1.3	H32	Y	0.64	0.50	1
1VFB	D1.3	H52	W	1.75	1.23	1
1VFB	D1.3	H56	N	0.01	0.20	0
1VFB	D1.3	H58	D	-0.05	-0.20	0
1VFB	D1.3	H98	E	-0.03	1.10	0
1VFB	D1.3	H99	R	0.73	0.47	1
1VFB	D1.3	H100	D	3.03	3.10	1
1VFB	D1.3	H101	Y	3.29	>4.00	1
1VFB	HEL	18	D	0.55	0.30	1
1VFB	HEL	19	N	0.96	0.30	1
1VFB	HEL	23	Y	0.00	0.40	0
1VFB	HEL	24	S	0.97	0.80	1
1VFB	HEL	116	K	0.83	0.70	1

1VFB	HEL	118	T	0.10	0.80	1
1VFB	HEL	119	D	1.75	1.00	1
1VFB	HEL	120	V	0.23	0.90	1
1VFB	HEL	121	Q	4.20	2.90	1
1VFB	HEL	124	I	0.46	1.20	0
1VFB	HEL	125	R	2.22	1.80	1
1VFB	HEL	129	L	0.06	0.20	0
2PTC	BPTI	15	K	4.16	10.00	1
3HFM	HYHEL-10	L31	N	1.86	5.25	1
3HFM	HYHEL-10	L32	N	1.27	5.20	1
3HFM	HYHEL-10	L50	Y	1.42	4.60	1
3HFM	HYHEL-10	L53	Q	0.83	1.00	1
3HFM	HYHEL-10	L96	Y	0.55	2.80	1
3HFM	HYHEL-10	H31	S	0.45	0.20	1
3HFM	HYHEL-10	H32	D	1.10	2.00	1
3HFM	HYHEL-10	H33	Y	2.90	6.00	1
3HFM	HYHEL-10	H50	Y	2.92	7.50	1
3HFM	HYHEL-10	W95	W	1.00	5.50	1
3HFM	HYHEL-10	H101	D	-0.04	3.75	0

3HFM	HYHEL-10	H53	Y	2.04	3.29	1
3HFM	HYHEL-10	H58	Y	1.77	1.70	1
3HFM	HEL	15	H	0.09	-0.50	0
3HFM	HEL	20	Y	2.72	5.00	1
3HFM	HEL	21	R	3.47	1.00	1
3HFM	HEL	63	W	0.83	0.30	1
3HFM	HEL	73	R	0.62	-0.20	1
3HFM	HEL	75	L	1.30	1.25	1
3HFM	HEL	89	T	0.17	0.00	1
3HFM	HEL	93	N	1.53	0.60	1
3HFM	HEL	96	K	2.13	7.00	1
3HFM	HEL	97	K	1.42	6.00	1
3HFM	HEL	98	I	0.10	-0.10	0
3HFM	HEL	100	S	0.95	0.25	1
3HFM	HEL	101	D	1.02	1.50	1