BindProfX: Assessing mutation-induced binding affinity change by protein interface profiles with pseudo counts

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Supplementary Material

Table S1. Probability transition matrix (iPTM) from interface structure alignments.

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	0.297	0.061	0.033	0.039	0.036	0.115	0.044	0.039	0.040	0.044	0.057	0.041	0.065	0.043	0.036	0.113	0.066	0.059	0.026	0.029
C	0.013	0.510	0.003	0.003	0.004	0.004	0.004	0.008	0.004	0.007	0.009	0.009	0.017	0.004	0.004	0.014	0.014	0.010	0.004	0.004
D	0.017	0.007	0.419	0.057	0.008	0.010	0.025	0.012	0.029	0.012	0.015	0.042	0.016	0.032	0.025	0.028	0.024	0.013	0.006	0.010
E	0.047	0.016	0.128	0.318	0.024	0.014	0.046	0.046	0.128	0.042	0.052	0.058	0.025	0.145	0.094	0.060	0.065	0.044	0.018	0.030
F	0.018	0.009	0.008	0.010	0.392	0.009	0.032	0.025	0.012	0.024	0.040	0.013	0.014	0.015	0.011	0.011	0.014	0.020	0.107	0.109
G	0.083	0.013	0.014	0.009	0.014	0.654	0.023	0.008	0.010	0.008	0.013	0.023	0.022	0.014	0.012	0.037	0.015	0.011	0.015	0.012
H	0.013	0.006	0.014	0.011	0.019	0.009	0.414	0.009	0.011	0.008	0.009	0.020	0.011	0.015	0.016	0.011	0.012	0.008	0.014	0.025
I	0.038	0.035	0.022	0.038	0.050	0.011	0.029	0.213	0.054	0.083	0.094	0.072	0.017	0.046	0.037	0.031	0.050	0.130	0.025	0.032
K	0.037	0.019	0.051	0.099	0.022	0.012	0.034	0.050	0.207	0.047	0.043	0.056	0.020	0.095	0.124	0.043	0.046	0.045	0.015	0.022
L	0.115	0.084	0.058	0.093	0.125	0.027	0.071	0.220	0.135	0.447	0.236	0.133	0.028	0.116	0.088	0.084	0.118	0.180	0.077	0.111
M	0.020	0.014	0.010	0.015	0.028	0.006	0.011	0.033	0.016	0.031	0.161	0.015	0.005	0.022	0.015	0.013	0.018	0.022	0.012	0.018
N	0.028	0.029	0.054	0.033	0.018	0.021	0.047	0.050	0.041	0.035	0.030	0.247	0.014	0.036	0.035	0.038	0.043	0.054	0.010	0.026
P	0.017	0.022	0.008	0.006	0.008	0.008	0.010	0.005	0.006	0.003	0.004	0.005	0.597	0.005	0.008	0.012	0.014	0.008	0.007	0.006
Q	0.030	0.014	0.042	0.086	0.021	0.014	0.036	0.033	0.073	0.031	0.046	0.037	0.014	0.221	0.061	0.032	0.038	0.028	0.015	0.019
R	0.026	0.012	0.035	0.058	0.017	0.012	0.041	0.028	0.100	0.025	0.033	0.038	0.023	0.064	0.318	0.031	0.037	0.025	0.016	0.022
S	0.072	0.041	0.034	0.032	0.014	0.033	0.025	0.021	0.030	0.021	0.024	0.036	0.029	0.029	0.027	0.303	0.065	0.026	0.011	0.026
T	0.046	0.047	0.032	0.039	0.019	0.014	0.029	0.036	0.035	0.032	0.037	0.045	0.037	0.037	0.035	0.071	0.274	0.044	0.015	0.021
V	0.065	0.052	0.026	0.041	0.044	0.016	0.032	0.146	0.054	0.076	0.070	0.088	0.032	0.044	0.037	0.045	0.069	0.257	0.016	0.034
W	0.005	0.003	0.002	0.003	0.040	0.004	0.009	0.005	0.003	0.005	0.007	0.003	0.005	0.004	0.004	0.003	0.004	0.003	0.535	0.023
Y	0.013	0.009	0.009	0.011	0.097	0.007	0.038	0.014	0.010	0.019	0.023	0.017	0.009	0.012	0.013	0.018	0.013	0.014	0.054	0.420

Table S2. Probability transition matrix (PTM) converted from BLOSUM62

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	0.304	0.068	0.042	0.058	0.036	0.082	0.044	0.049	0.060	0.047	0.056	0.046	0.059	0.059	0.048	0.115	0.077	0.073	0.032	0.042
C	0.021	0.470	0.007	0.007	0.011	0.010	0.009	0.016	0.008	0.015	0.015	0.010	0.009	0.009	0.007	0.018	0.018	0.018	0.011	0.010
D	0.028	0.016	0.385	0.088	0.016	0.033	0.035	0.018	0.041	0.015	0.018	0.081	0.031	0.047	0.030	0.048	0.036	0.018	0.012	0.018
E	0.044	0.017	0.100	0.323	0.020	0.028	0.057	0.020	0.077	0.022	0.030	0.054	0.040	0.112	0.057	0.056	0.044	0.025	0.022	0.029
F	0.020	0.019	0.013	0.015	0.358	0.015	0.029	0.042	0.015	0.051	0.044	0.016	0.013	0.015	0.017	0.019	0.021	0.033	0.060	0.122
G	0.088	0.035	0.053	0.040	0.028	0.571	0.041	0.023	0.049	0.024	0.033	0.072	0.040	0.045	0.037	0.075	0.048	0.028	0.035	0.029
H	0.014	0.009	0.017	0.024	0.016	0.012	0.338	0.008	0.019	0.010	0.015	0.031	0.012	0.029	0.023	0.018	0.014	0.008	0.011	0.045
I	0.039	0.041	0.021	0.020	0.059	0.017	0.020	0.248	0.025	0.105	0.092	0.020	0.024	0.024	0.022	0.027	0.048	0.150	0.025	0.039
K	0.043	0.020	0.044	0.073	0.019	0.033	0.044	0.022	0.267	0.024	0.035	0.053	0.039	0.087	0.116	0.052	0.044	0.026	0.020	0.030
L	0.055	0.059	0.026	0.034	0.106	0.026	0.035	0.156	0.039	0.349	0.183	0.029	0.034	0.044	0.044	0.039	0.061	0.121	0.052	0.064
M	0.017	0.015	0.008	0.012	0.024	0.009	0.014	0.035	0.015	0.048	0.156	0.011	0.010	0.021	0.015	0.014	0.019	0.030	0.015	0.017
N	0.024	0.016	0.064	0.037	0.015	0.035	0.050	0.013	0.039	0.013	0.019	0.291	0.021	0.041	0.035	0.050	0.040	0.015	0.011	0.020
P	0.032	0.016	0.026	0.029	0.012	0.021	0.020	0.017	0.030	0.016	0.018	0.022	0.552	0.028	0.021	0.032	0.030	0.019	0.012	0.016
Q	0.026	0.012	0.031	0.065	0.011	0.018	0.040	0.013	0.053	0.016	0.029	0.034	0.022	0.212	0.048	0.033	0.027	0.016	0.017	0.021
R	0.031	0.016	0.029	0.049	0.019	0.023	0.047	0.018	0.106	0.024	0.032	0.044	0.025	0.072	0.340	0.039	0.035	0.021	0.020	0.028
S	0.087	0.044	0.054	0.056	0.026	0.053	0.043	0.026	0.055	0.025	0.035	0.073	0.045	0.057	0.045	0.227	0.095	0.033	0.023	0.033
T	0.054	0.041	0.038	0.041	0.026	0.032	0.031	0.043	0.044	0.036	0.044	0.054	0.038	0.044	0.037	0.089	0.266	0.054	0.024	0.032
V	0.067	0.054	0.024	0.031	0.054	0.024	0.024	0.174	0.033	0.095	0.091	0.027	0.032	0.034	0.030	0.041	0.071	0.266	0.027	0.047
W	0.006	0.006	0.003	0.005	0.019	0.006	0.006	0.006	0.005	0.008	0.009	0.004	0.004	0.007	0.006	0.005	0.006	0.005	0.534	0.030
Y	0.018	0.015	0.012	0.017	0.094	0.012	0.061	0.021	0.018	0.024	0.024	0.017	0.012	0.021	0.019	0.019	0.019	0.022	0.072	0.334

Table S3. The non-redundant protein group division for five-fold cross-validation, in which proteins in different groups have a sequence identity below 30%.

#Groups	Protein IDs in SKEMPI
1	1CSOEI 1CT0EI 1CT2EI 1CT4EI 1SGDEI 1SGEEI 1SGNEI 1SGPEI 1SGQEI 1SGYEI 2NU0EI 2NU1EI 2NU2EI 2NU4EI 2SGPEI 2SGQEI 3SGBEI 1IARAB 1XD3AB 1F47AB 1ACBEI 1H9DAB 2HRKAB 3BP8AC 2OOBAB
2	1JTGAB 1S0WAC 2G2UAB 2G2WAB 1A4YAB 1Z7XWX 2GOXAB 2NOJAB 3D5RAC 3D5SAC 1KACAB 1P69AB 1P6AAB 3BK3AC 1JCKAB 1SBBAB 4CPAAI 1S1QAB 2B42AB 1E96AB 2I26NL
3	1PPFEI 1CSEEI 1SBNEI 1TM1EI 1TM3EI 1TM4EI 1TM5EI 1TM7EI 1TMGEI 1TO1EI 1Y1KEI 1Y33EI 1Y34EI 1Y3BEI 1Y4AEI 1GC1GC 2SICEI 2O3BAB 1FC2CD 2BTFAP 1EFNAB 2A9KAB
4	1R0REI 1EAWAB 2FTLEI 3BTDEI 3BTEEI 3BTFEI 3BTGEI 3BTHEI 3BTMEI 3BTQEI 3BTTEI 3BTWEI 1AK4AD 1M9EAD 2J0TAD 1FFWAB 1MAHAF 1UUZAD 1SMFEI 2AJFAE 2J1KCT
5	1B2SAD 1B2UAD 1B3SAD 1BRSAD 1X1XAD 1EMVAB 2VLNAB 2VLOAB 2VLQAB 2WPTAB 1A22AB 2B0ZAB 2B10AB 2B11AB 2B12AB 2PCBAB 2PCCAB 1KTZAB 1LFDAB 1FCCAC 1GL0EI 1GL1AI 1HE8AB 2HLEAB 2I9BAE

Table S4. $\Delta\Delta G$ calculations based on low-resolution complex structure models built from unbound monomer structures. The ZEMu results are collected from the Supplementary Information of the ZEMu paper (Dourado DF, Flores SC. Modeling and fitting protein-protein complexes to predict change of binding energy. Sci Rep. 2016;6:25406).

PDBID	Mutations	#mutation	$\Delta\Delta G$ (kcal/mol)		
			Exp.	ZEMu	BindProfX
1tgj_1m9z_1ktz	VA92I	1	0.24	0.5	0.942
1tgj_1m9z_1ktz	RA25K	1	1.15	0.87	1.205
1tgj_1m9z_1ktz	RA94K	1	2.2	-1.76	1.205
1tgj_1m9z_1ktz	RA25A	1	1.48	0.46	1.6
1tgj_1m9z_1ktz	RA94A	1	2.88	0.62	1.6
1tgj_1m9z_1ktz	LB27A	1	2.27	1.42	2.044
1tgj_1m9z_1ktz	FB30A	1	3.43	0.33	1.879
1tgj_1m9z_1ktz	DB32A	1	1.97	0.3	0
1tgj_1m9z_1ktz	DB32N	1	2.45	0.42	0
1tgj_1m9z_1ktz	SB49A	1	0.77	0.01	1.196
1tgj_1m9z_1ktz	IB50A	1	2.34	0.89	1.173
1tgj_1m9z_1ktz	TB51A	1	1.96	0.13	1.296
1tgj_1m9z_1ktz	SB52A	1	0.66	-2.27	1.196
1tgj_1m9z_1ktz	SB52L	1	4.48	NA	1.325
1tgj_1m9z_1ktz	IB53A	1	1.82	0.89	1.173
1tgj_1m9z_1ktz	EB55A	1	1.66	0.12	1.583
1tgj_1m9z_1ktz	VB77A	1	0.86	0.01	1.254
1tgj_1m9z_1ktz	DB118A	1	1.26	0.24	0.808
1tgj_1m9z_1ktz	EB119A	1	1.94	0.47	1.583
1tgj_1m9z_1ktz	EB119Q	1	2.07	0.07	1.374
1tgj_1m9z_1ktz	NB47A	1	0.73	0	0
1tgj_1m9z_1ktz	VB62A	1	1.09	0	0
1tgj_1m9z_1ktz	EB75A	1	1.53	0.21	0
1tgj_1m9z_1ktz	HB79A	1	0.74	-0.04	0
1tgj_1m9z_1ktz	FB110A	1	1.38	0	0
1tgj_1m9z_1ktz	MB112A	1	1.32	0	0
1tgj_1m9z_1ktz	IB125A	1	0.99	0	0
1zg4_3gmu_1jtg	KB74A,YA105A	2	3.32	0.2	1.687
1zg4_3gmu_1jtg	NA100A	1	-0.46	1.24	1.15
1zg4_3gmu_1jtg	NA100A,WB112A	2	2.79	-0.16	3.94
1zg4_3gmu_1jtg	NA100A,FB142A	2	2.29	1	3.395
1zg4_3gmu_1jtg	NA100A,HB148A	2	2.1	-1.1	3.435
1zg4_3gmu_1jtg	NA100A,WB150A	2	4.35	0.4	3.94
1zg4_3gmu_1jtg	NA100A,RB160A	2	1.58	0.35	3.127
1zg4_3gmu_1jtg	NA100A,WB162A	2	2.1	-1.15	3.94
1zg4_3gmu_1jtg	NA100A,KB74A	2	3.51	-1.02	1.15

1zg4_3gmu_1jtg	VA103A	1	1.91	0.02	1.641
1zg4_3gmu_1jtg	VA103A,FB142A	2	4.51	2.73	3.886
1zg4_3gmu_1jtg	VA103A,RB160A	2	4.35	0.63	3.618
1zg4_3gmu_1jtg	VA103A,WB162A	2	4.23	-1.16	4.431
1zg4_3gmu_1jtg	EA104A	1	1.55	-2.25	0.774
1zg4_3gmu_1jtg	EA104A,SB113A	2	1.86	-1.62	0.774
1zg4_3gmu_1jtg	EA110A,SB113A,SB71A	3	5.04	1.28	3.535
1zg4_3gmu_1jtg	EA104K	1	4.23	NA	0.726
1zg4_3gmu_1jtg	PA107A	1	-0.38	-1.36	2.82
1zg4_3gmu_1jtg	PA107A,HB41A	2	2.65	-2.23	5.106
1zg4_3gmu_1jtg	PA107A,YB53A	2	2.39	-1.51	5.197
1zg4_3gmu_1jtg	EA110A	1	4.06	-1.58	1.96
1zg4_3gmu_1jtg	EA110A,SB113A	2	4.56	1.41	1.96
1zg4_3gmu_1jtg	EA110A,SB113A,SB71A	3	5.04	-0.08	3.535
1zg4_3gmu_1jtg	EA110A,SB71A	2	5.02	1.08	3.535
1zg4_3gmu_1jtg	MA129A	1	0.74	1.09	0.864
1zg4_3gmu_1jtg	MA129A,SB113A,SB71A	3	1.67	2.89	2.439
1zg4_3gmu_1jtg	MA129A,FB36A	2	3.63	1.89	3.109
1zg4_3gmu_1jtg	MA129A,YB53A	2	3.61	2.17	3.241
1zg4_3gmu_1jtg	EA168A	1	-0.07	-0.14	1.96
1zg4_3gmu_1jtg	EA168A,WB112A	2	2.79	1.09	4.75
1zg4_3gmu_1jtg	EA168A,FB142A	2	2.58	2.41	4.205
1zg4_3gmu_1jtg	EA168A,WB150A	2	4.11	0.62	4.75
1zg4_3gmu_1jtg	EA168A,RB160A	2	2.32	1.18	3.937
1zg4_3gmu_1jtg	EA168A,WB162A	2	2.08	0.51	4.75
1zg4_3gmu_1jtg	EA168A,KB74A	2	4.06	-1.01	1.96
1zg4_3gmu_1jtg	VA216A	1	-0.41	0.68	1.129
1zg4_3gmu_1jtg	SA235A,SA130A,KA234A	3	1.85	0.51	1.576
1zg4_3gmu_1jtg	QA99A	1	0.43	0.36	1.128
1zg4_3gmu_1jtg	QA99A,WB112A	2	3.54	1.41	3.918
1zg4_3gmu_1jtg	QA99A,FB142A	2	2.82	2.95	3.373
1zg4_3gmu_1jtg	QA99A,HB148A	2	3.2	0.83	3.414
1zg4_3gmu_1jtg	QA99A,WB150A	2	3.82	1.54	3.918
1zg4_3gmu_1jtg	QA99A,RB160A	2	3.75	2.65	3.105
1zg4_3gmu_1jtg	QA99A,WB162A	2	2.89	1.68	3.918
1zg4_3gmu_1jtg	QA99A,KB74A	2	4.11	-1.76	1.128
1zg4_3gmu_1jtg	WB112A	1	3.01	0.87	2.79
1zg4_3gmu_1jtg	SB113A	1	-0.17	-0.21	0
1zg4_3gmu_1jtg	FB142A,EA104A	2	2.75	0.77	3.02
1zg4_3gmu_1jtg	FB142A,YB143A,EA104A,YA105A	4	2.84	0.91	7.084
1zg4_3gmu_1jtg	HB148A	1	2.75	0.11	2.286
1zg4_3gmu_1jtg	WB150A	1	4.25	0.78	2.79
1zg4_3gmu_1jtg	RB160A	1	2.22	0.55	1.977

1zg4_3gmu_1jtg	WB162A	1	2.34	1.43	2.79
1zg4_3gmu_1jtg	FB36A	1	3.2	2.11	2.245
1zg4_3gmu_1jtg	HB41A	1	3.25	0.47	2.286
1zg4_3gmu_1jtg	YB53A	1	2.08	0.56	2.377
1zg4_3gmu_1jtg	SB71A	1	0.36	1.57	1.576
2jwd_4dz8_1fc2	IC135W	1	0.58	-1.17	0
2jwd_4dz8_1fc2	FC149W	1	-0.04	-0.01	0
2jwd_4dz8_1fc2	LC163W	1	2.18	0	0
2jwd_4dz8_1fc2	LC136D	1	1.23	0.41	1.82
2jwd_4dz8_1fc2	NC147A	1	0.41	0.14	0.896
2jwd_4dz8_1fc2	FC149A	1	3.14	0.33	0
2jwd_4dz8_1fc2	IC150A	1	0	0.11	0
2jwd_4dz8_1fc2	KC154A	1	0	1.47	0
3r99_1nmi_2pcc	DA34A	1	-0.9	2.53	1.993
3r99_1nmi_2pcc	VA197A	1	2.1	0.44	1.254
3r99_1nmi_2pcc	EA290A	1	6.2	1.02	1.583
3r99_1nmi_2pcc	KB87A	1	0.9	2.12	1.141
3r99_1nmi_2pcc	KB87A,DA34A	2	0.2	0.89	3.134
3r99_1nmi_2pcc	KB87A,VA197A	2	1.5	2.19	2.396
3r99_1nmi_2pcc	KB72A	1	0.3	-0.61	1.141
3r99_1nmi_2pcc	KB72A,VA197A	2	2.8	-0.1	2.396
3r99_1nmi_2pcc	KB72A,EA290A	2	1.1	-0.01	2.724
3r99_1nmi_2pcc	AB81G	1	1.9	-0.29	0.71
3r99_1nmi_2pcc	AB81G,DA34A	2	-0.1	0.41	2.703
3r99_1nmi_2pcc	AB81G,VA197A	2	2.1	0.36	1.964
Correlation coefficient				0.118	0.454