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Predicting free energy changes using structural ensembles

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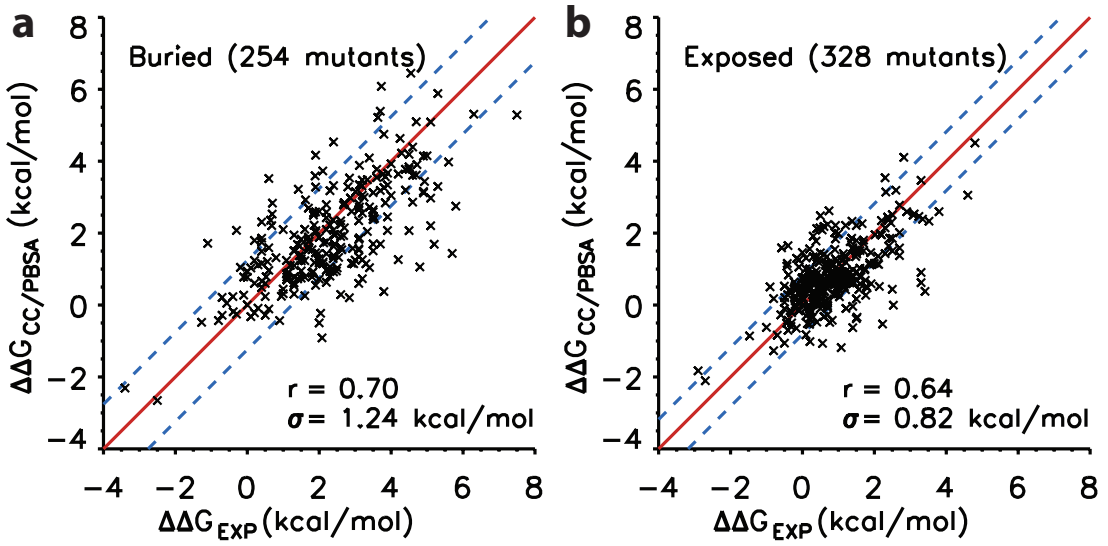
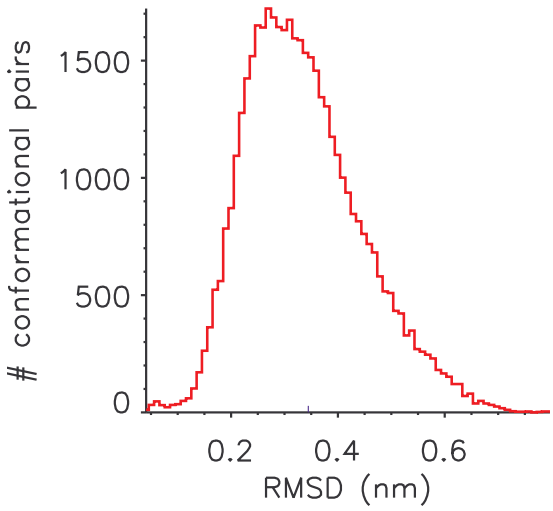
Supplementary Figure 1: Prediction of mutational changes of protein stability.



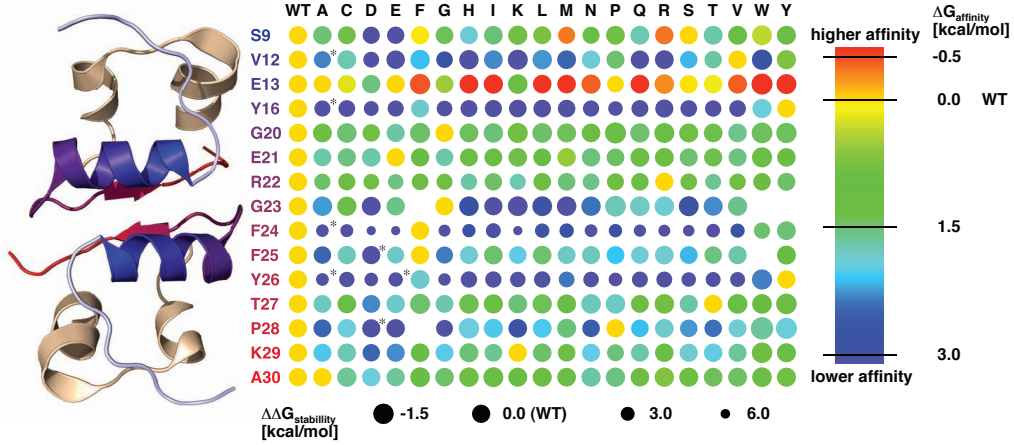
Computed values for the mutational change in folding free energies separately for buried (a) and for exposed (b) mutation sites. Mutation sites with a ratio of less than 0.2 between the solvent accessible surface areas of the residue placed in the protein and in a tripeptide GXG were considered to be buried. Correlations are $r = 0.70$ ($\sigma = 1.24\,\mathrm{kcal\,mol^{-1}}$) for mutations of buried positions and $r = 0.64$ ($\sigma = 0.82\,\mathrm{kcal\,mol^{-1}}$) for exposed sites.

Supplementary Figure 2: CONCOORD interconformer root mean square deviation distribution.



The interconformer root mean square deviation for 300 CONCOORD structures of the TEM1-BLIP complex ranged between 0.1 nm and 0.6 nm.

Supplementary Figure 3: Full mutational scan of insulin dimer interface.



Changes in binding affinity (color-coded red to blue) and changes in the stability of the monomers (radius of circles) are shown. Single-point mutants with known reduced self-association [1, 2] (marked by an asterisk) were all predicted to have a decreased binding affinity with respect to the wildtype.

[1] J. Brange and A. Vølund. Insulin analogs with improved pharmacokinetic profiles. *Adv. Drug Delivery Rev.*, 35:307–335, 1999.

[2] H. Chen, M. Shi, Z. Y. Guo, Y. H. Tang, Z. S. Qiao, Z. H. Liang, and Y. M. Feng. Four new monomeric insulins obtained by alanine scanning the dimer–forming surface of the insulin molecule. *Protein Eng.*, 13(11):779–782, 2000.

Supplementary Methods

Force field and minimization scheme

All minimizations were performed with the Gromacs simulation suite [1] using the GROMOS96 53a6 [2] force field. Tests with the OPLS-AA force field [3] yielded similar accuracy (not shown). For the minimization, a distance-dependent dielectric permittivity of $\epsilon(r) = 4r$ was used. The l-BFGS-algorithm was applied with an initial step size of 0.01 nm and a convergence criterium for the maximum force of $100\,\mathrm{kJmol^{-1}\,nm^{-1}}$. No cut-off was applied for both van der Waals and electrostatic interactions.

Processing of input structures

Crystal structures were taken as input structures. In some cases, the input structures were mutated to match the (pseudo) wild type sequence. Non-protein atoms were deleted, missing heavy side chain atoms were added using the *corall* routine of the program WhatIf [4], which was also used to fill small gaps. Structures of the mutants were generated using WhatIf [5]. Based on these input structures, structural ensembles were generated separately for the wild type and the mutant structures using the program CONCOORD [6]. Titratable groups were protonated according to their model pKa. All structures (including the mutated input conformations as well as the sampled ensembles) were shortly minimized as described above. No constraints were imposed.

Unfolded/unbound structures

For the prediction of the change of folding free energies upon mutation, the denatured state was approximated by structural ensembles generated for tripeptides `GXG` applying CONCOORD. For protein-protein binding prediction, the unbound state was taken from the complex structure, i.e. not sampled independently, similar to the MM/PBSA method [7, 8]. Thereby, it is assumed that the difference in conformational freedom between the protein-protein complex and the isolated proteins does not change significantly between the wildtype and the mutants.

Energy function and evaluation

The energy function for stability and affinity estimates reads

$$\Delta G_{\mathrm{CC/PBSA}} \quad = \quad \Delta G_{\mathrm{electrostatic}} + \Delta G_{\mathrm{vdW}} + \Delta G_{\mathrm{entropy}} \; . \tag{1}$$

All energies were averaged over all minimized CONCOORD structues (see above) (Boltzmann averaging did not improve the results), separately for the wild type and the mutant structures. Thereby, conformational flexibility is explicitly considered. Backbone flexibility was already shown before to improve the prediction accuracy for folding free energy differences upon mutation [9, 10].

The electrostatic contribution to the free energy, $\Delta G_{\mathrm{electrostatic}}$, can be sub-divided into the electrostatic interaction energy $\Delta G_{\mathrm{Coulomb}}$ and the polar contribution to the solvation free energy:

$$\Delta G_{\mathrm{electrostatic}} \quad = \quad \Delta G_{\mathrm{Coulomb}} + \Delta G^{\mathrm{polar}}_{\mathrm{solvation}} \; . \tag{2}$$

The polar solvation free energy was obtained from numerical solution of the Poisson-Boltzmann equation using the DelPhi package [11]. A dielectric constant of 78 was chosen for water, and the relative dielectric permittivity of the protein interior was set to 2. The box was chosen in a way that the proteins longest linear dimension fills 60% of the lattice linear dimension with two grid points per Å. Dipolar boundary conditions were applied. The ion concentration was set to 0 M. The van der Waals contribution to the free energy, ΔG_{vdW}, was approximated by a Lennard Jones potential for solute-solute interactions and a non-polar solvation contribution $\Delta G^{\mathrm{non\text{-}polar}}_{\mathrm{solvation}}$ for the solute-solvent interactions. The latter was assumed to be proportional to the solvent-accessible surface A_{SA} [12]:

$$\Delta G_{\mathrm{vdW}} \quad = \quad \Delta G_{\mathrm{LJ}} + \gamma \Delta A_{\mathrm{SA}} \; . \tag{3}$$

Entropic terms were explicitly considered only for the calculation of folding free energies. Here, we use a quasiharmonic approximation proposed by Schlitter [13] for the evaluation of the conformational entropy

$$S \quad = \quad \frac{1}{2} k_B \ln \det \left[1 + \frac{k_B T e^2}{\hbar^2} \mathbf{M}\sigma \right] \; , \tag{4}$$

where $\mathbf{M}\sigma$ denotes the mass weighted covariance-matrix and $e = \exp(1)$. This quasiharmonic expression was shown to yield an upper bound for the true entropy.

The change in folding free energy upon mutation can then be written as:

$$\Delta\Delta G^{\mathrm{stability}}_{\mathrm{CC/PBSA}} \quad = \quad \alpha \Delta\Delta G_{\mathrm{electrostatic}} + \beta \Delta\Delta G_{\mathrm{LJ}} + \gamma \Delta\Delta A_{\mathrm{SA}} - \tau T \Delta\Delta S \tag{5}$$

with the four fitted parameters $\alpha = 0.224$, $\beta = 0.217$, the surface tension $\gamma = 0.0166\,\mathrm{kcal\,mol^{-1}\,\AA^{-2}}$ and $\tau = 0.0287$. The correlation obtained using five-fold cross validation on the data set of 582 mutants (Supplementary Tables 1 and 2) is $R = 0.748 \pm 0.018$, the standard deviation $\sigma = 1.04 \pm 0.03\,\mathrm{kcal\,mol^{-1}}$. Without the entropic contribution to the change in free energy, the correlation decreases to 0.73.

Since minimized structures were used, values smaller than one are expected for α and β (see also the LIECE method [14]).

For the prediction of mutational changes on protein-protein binding affinities, an additional *cooperativity* contribution proportional to the (wildtype) protein-protein interaction surface (I_{wt}) was introduced ($G_{\mathrm{PPIS}} = \gamma I_{\mathrm{wt}} + c$):

$$\Delta\Delta G^{\mathrm{affinity}}_{\mathrm{CC/PBSA}} = \alpha\Delta\Delta G_{\mathrm{electrostatic}} + \beta\Delta\Delta G_{\mathrm{LJ}} + G_{\mathrm{PPIS}} + \Delta G_{\mathrm{pK}} \quad (6)$$

The four parameters were fitted using five-fold cross validation on the data set of 367 mutants of 9 protein-protein complexes (Supplementary Tables 3 and 4): $\alpha = 0.136$, $\beta = 0.259$, $\gamma = -0.841\,\mathrm{cal\,mol^{-1}\,\AA^{-2}}$, and $c = 2.573\,\mathrm{kcal\,mol^{-1}}$. G_{PPIS} varies between $0.316\,\mathrm{kcal\,mol^{-1}}$ and $1.50\,\mathrm{kcal\,mol^{-1}}$ for the nine investigated protein-protein complexes (interaction surface areas $I_{\mathrm{wt}} = 15.41 \ldots 29.74\,\mathrm{nm^2}$). The contribution is largest for small interfaces, i.e. here the binding is significantly disturbed for almost every substitution. Thus we conclude an increased degree of cooperativity for interface residues at small protein-protein interfaces. Entropy and the non-polar solvation contribution were neglected for the prediction of mutational changes on protein-protein binding affinity.

For the interleukin-4/receptor complex several computed affinity changes deviated significantly from the respective experimental values. Here, pKa calculations [15–17] revealed changes in the protonation states of some titratable goups upon mutation. For these, a correction term

$$\Delta G_{\mathrm{pK}} = k_B T \ln(10) \cdot (pK_a - pH_{\mathrm{exp}})$$

was computed [18, 19]. Both the unmodified and the pKa-corrected values are reported in Supplementary Table 4. Overall correlations were determined neglecting the influence of mutant-dependent protonation states.

Computation time

Typical cpu times for CC/PBSA range from 168 min (1YPC, 64 residues) to 249 min (1STN, 149 residues) for one processor (3.2 GHz Intel Xeon).

Supplementary Table 1: Proteins used for stability calculations.

Protein	PDB	Resolution	PDB-Reference	Mutation-References	#Mutations
colicin immunity protein Im7	1AYI	2.00Å	[20]	[21]	26
chymotrypsin inhibitor 2	1YPC	1.70Å	[22]	[23]	76
staphylococcal nuclease	1STN	1.70Å	[24]	[25–29]	265
B1 immunoglobulin-binding domain from streptococcal protein G	1PGA	2.07Å	[30]	[31]	30
B1 domain of protein L	1HZ6	1.70Å	[32]	[33]	68
bacteriophage T4 lysozyme	2LZM	1.70Å	[34]	[35–59]	82
salmonella typhimurium CheY	3CHY	1.66Å	[60]	[61]	35

Supplementary Table 2: Full list of protein mutations used for stability calculations. Experimental and calculated differences in folding free energies (in kcal/mol) relative to the wild type (both experimental and calculated). _pW denotes that the experimental and calculated free energies are taken relative to a pseudo wild type.

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1AYI	A13G	0.60	0.5601	0.1007	0.0442	0.1754	0.1488	0.0911
1AYI	A28G	0.19	0.7808	-2.1241	1.1374	0.6986	0.8327	0.2362
1AYI	A77G	1.27	0.7952	-0.3600	0.1481	0.3659	0.3988	0.2424
1AYI	A78G	1.31	0.6711	0.3473	-0.1665	0.1557	0.0169	0.3177
1AYI	F15A	3.63	5.2159	-1.1149	0.8079	2.6032	3.2166	-0.2970
1AYI	F41L	1.89	3.5927	-1.6453	1.2238	1.6611	2.2866	0.0665
1AYI	I22V	2.13	1.7274	-1.9938	1.6072	1.0373	1.1593	-0.0827
1AYI	I44V	0.53	0.7856	-0.8839	0.4800	0.6172	0.5622	0.0101
1AYI	I54V	2.63	1.5377	0.0560	-0.1799	0.7512	0.8876	0.0228
1AYI	I68V	0.60	1.5933	-0.6934	0.3681	0.9892	1.0288	-0.0994
1AYI	I72V	0.41	0.6623	-1.5447	1.2690	0.5399	0.4120	-0.0139
1AYI	I7V	1.46	1.6385	-1.5114	1.1684	1.1061	0.9641	-0.0888
1AYI	L18A	3.01	3.1499	-1.0577	0.3183	1.7862	2.3529	-0.2498
1AYI	L19A	3.39	4.0922	-2.1251	2.0346	2.1057	2.6135	-0.5366
1AYI	L34A	1.84	2.5004	-2.5351	1.8163	1.6684	1.9637	-0.4129
1AYI	L37A	2.84	3.5325	-1.4392	1.1593	1.8233	2.3595	-0.3704
1AYI	L38A	2.68	2.7843	-2.1132	1.6817	1.5828	1.9007	-0.2677
1AYI	L3A	0.74	2.6208	-2.1330	1.8226	1.5041	1.8662	-0.4391
1AYI	L53A	3.25	2.9949	-0.4211	-0.0970	1.5761	2.2153	-0.2784
1AYI	T51S	0.96	1.2195	1.2429	-0.8859	0.3420	0.4038	0.1167
1AYI	V16A	1.48	1.3472	-1.3197	1.0826	0.6848	0.8159	0.0835
1AYI	V27A	-0.50	0.5258	-1.1799	1.0039	0.3757	0.2327	0.0934
1AYI	V33A	0.24	0.4607	0.0536	-0.4417	0.4104	0.3701	0.0682
1AYI	V36A	0.10	1.0071	-1.3101	0.9411	0.6262	0.5666	0.1833
1AYI	V42A	0.69	1.1035	-2.1862	1.8430	0.6759	0.7272	0.0436

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1AYI	V69A	0.69	2.5279	0.5616	-0.3882	0.9603	1.3753	0.0190
1HZ6	A13P	-0.10	-0.1675	-0.0568	0.2051	-0.2003	-0.2934	0.1779
1HZ6	A13V	0.83	-0.4249	-0.1227	0.3005	-0.3010	-0.3088	0.0072
1HZ6	A20G	2.17	1.9766	-0.8456	0.8085	0.7725	1.2346	0.0066
1HZ6	A20V	-1.47	-0.8600	-0.3769	0.3439	-0.2107	-0.6048	-0.0115
1HZ6	A29G	2.54	1.3253	-0.0541	0.1571	0.4726	0.8127	-0.0630
1HZ6	A33G	3.10	1.8246	-0.0114	0.0559	0.7397	0.9144	0.1260
1HZ6	A35G	1.32	0.6115	-0.1323	0.1967	0.2171	0.2615	0.0686
1HZ6	A37G	3.12	1.8632	-0.1205	0.1746	0.7737	1.0839	-0.0484
1HZ6	A52G	0.49	0.6651	-0.0872	-0.0795	0.3456	0.4545	0.0317
1HZ6	A8G	2.43	1.6962	-0.0597	0.0055	0.6436	0.9595	0.1473
1HZ6	D38A	1.21	-0.0952	0.9933	-1.7402	0.6426	0.4048	-0.3957
1HZ6	D38G	2.14	0.5166	0.8314	-1.5389	0.7424	0.7382	-0.2566
1HZ6	D50A	0.20	-0.0297	3.0007	-3.3558	0.3681	0.3048	-0.3475
1HZ6	E21A	0.59	0.5404	-5.7066	5.3347	0.6591	0.6927	-0.4395
1HZ6	E32G	1.19	0.9244	-3.3186	2.3335	1.0327	1.1869	-0.3101
1HZ6	E32I	1.08	-1.1835	-3.4160	2.2837	0.1817	0.0572	-0.2901
1HZ6	E46A	0.23	-0.1624	-0.7381	0.2225	0.5007	0.3591	-0.5067
1HZ6	F12A	3.12	3.8833	-1.2154	1.0719	2.2375	2.1992	-0.4100
1HZ6	F12L	0.68	2.2094	-0.6396	0.7497	1.0005	1.1623	-0.0635
1HZ6	F22A	4.25	4.6338	-0.3584	0.3827	2.3547	2.7607	-0.5059
1HZ6	F22L	3.12	2.7270	0.0309	0.1092	1.1821	1.4738	-0.0690
1HZ6	F26G	3.08	2.5028	-1.3187	1.2992	1.2805	1.5663	-0.3245
1HZ6	F26L	0.38	1.7796	-0.5183	0.6398	0.6764	0.9112	0.0705
1HZ6	F62L	3.34	3.4836	-0.6449	0.7240	1.6761	1.8708	-0.1423
1HZ6	F62V	3.73	6.0822	-0.5184	0.7187	3.0106	3.1729	-0.3015
1HZ6	G15A	1.52	-0.3397	-0.1995	-0.1001	0.1571	-0.2355	0.0384
1HZ6	G15V	2.53	-0.0044	0.0543	-0.3389	0.2787	-0.1439	0.1453
1HZ6	G24A	2.08	-0.9119	0.0127	-0.0098	-0.2792	-0.6147	-0.0208
1HZ6	G45A	2.23	-0.5297	-0.0180	-0.0930	-0.0287	-0.3437	-0.0462

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1HZ6	G55A	2.04	-0.2295	-0.1894	0.1417	0.0178	-0.1561	-0.0435
1HZ6	I11A	1.37	1.8571	-0.5683	0.3520	1.1682	0.9612	-0.0560
1HZ6	I11V	0.47	0.3975	-0.3787	0.1804	0.4483	0.2176	-0.0700
1HZ6	I60A	4.72	3.9042	-0.1717	0.2549	1.9396	2.0936	-0.2121
1HZ6	I60V	1.69	1.6095	-0.2867	0.0481	1.0343	1.0375	-0.2238
1HZ6	I6A	4.90	4.1407	-0.8583	0.6503	2.1135	2.5337	-0.2985
1HZ6	I6V	0.56	1.2084	0.2734	-0.4428	0.7364	0.7446	-0.1032
1HZ6	K23A	0.88	0.2723	-15.4783	14.9158	0.7143	0.6067	-0.4862
1HZ6	K28G	-0.16	1.2971	-18.2561	17.8394	0.9205	1.0042	-0.2109
1HZ6	K41A	-0.58	1.5894	-23.8278	23.7891	1.0412	1.3644	-0.7774
1HZ6	K42A	-0.35	0.4221	-12.9648	13.2956	0.2351	0.1002	-0.2440
1HZ6	K54A	0.09	0.3662	-11.1482	11.3491	0.2398	0.3957	-0.4702
1HZ6	K61A	0.45	0.6771	-18.9566	17.8887	1.0550	1.1747	-0.4846
1HZ6	K7A	0.92	1.8398	-11.6481	11.8167	0.9740	1.2984	-0.6011
1HZ6	L10A	3.12	3.3422	-0.3246	0.5151	1.6332	1.8789	-0.3603
1HZ6	L40A	2.44	1.9611	-0.7887	0.4541	1.3480	1.3049	-0.3571
1HZ6	L58A	3.77	3.6404	-1.1118	1.0642	1.8470	2.2668	-0.4258
1HZ6	N14A	1.78	0.5149	-1.0652	1.2635	0.2105	0.2915	-0.1854
1HZ6	N44A	0.34	0.8270	-0.9788	0.6197	0.6807	0.7673	-0.2619
1HZ6	N59A	1.73	0.9768	-2.6702	2.5380	0.6210	0.8483	-0.3602
1HZ6	N9A	1.87	1.1695	-2.1320	1.7570	0.7912	1.0402	-0.2870
1HZ6	S16A	0.30	0.2733	-0.1138	-0.1612	0.3040	0.2854	-0.0411
1HZ6	S31A	-0.41	0.2857	0.0222	0.1023	0.1614	0.1466	-0.1468
1HZ6	S31G	0.82	0.7510	0.0266	0.1830	0.2708	0.3272	-0.0566
1HZ6	T17A	1.17	0.5087	-0.4447	0.2518	0.3316	0.3816	-0.0116
1HZ6	T19A	1.11	0.5899	0.0587	-0.4029	0.4845	0.5990	-0.1493
1HZ6	T25A	1.25	0.6667	-0.3058	-0.0014	0.4849	0.5151	-0.0262
1HZ6	T30A	1.09	0.8650	-0.6745	-0.1653	0.7987	0.8619	0.0443
1HZ6	T39G	0.17	0.5338	-0.1459	-0.1148	0.4909	0.3178	-0.0142
1HZ6	T48A	0.97	0.3118	-0.4021	-0.0006	0.5296	0.2187	-0.0338
1HZ6	T57A	1.83	0.9248	-0.4459	0.1342	0.6153	0.7636	-0.1425
1HZ6	T5A	1.63	0.7914	-0.7461	0.4503	0.6025	0.5536	-0.0689

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1HZ6	V49A	0.92	1.2834	-0.0017	-0.0047	0.6317	0.7509	-0.0927
1HZ6	V4A	1.22	1.3426	-0.2647	0.1658	0.5960	0.8128	0.0327
1HZ6	V51A	1.14	1.4277	-0.3181	0.4315	0.6088	0.7101	-0.0046
1HZ6	Y34A	2.82	4.1066	-0.8121	0.7679	2.1667	2.4927	-0.5086
1HZ6	Y36A	2.46	2.2851	-0.8959	0.8023	1.2214	1.3986	-0.2412
1HZ6	Y56A	1.66	2.2630	-0.9055	1.1427	1.1525	1.2870	-0.4137
1HZ6	Y56L	-0.43	1.0794	-0.7064	0.8066	0.4270	0.5515	0.0007
1PGA	A20G	2.39	1.2928	-0.2647	0.3917	0.3845	0.7199	0.0615
1PGA	A26G	2.96	1.1477	0.3069	0.0538	0.1832	0.5308	0.0731
1PGA	A34G	2.48	0.9462	-0.1419	0.2174	0.3288	0.4736	0.0685
1PGA	D22A	1.75	0.6876	-2.4317	2.5629	0.4086	0.5000	-0.3522
1PGA	D46A	1.74	1.0053	-1.0807	0.9005	0.8387	0.8581	-0.5114
1PGA	D47A	-0.49	0.2058	-3.3969	3.4021	0.2080	0.4282	-0.4356
1PGA	E15A	0.47	0.6919	-2.5704	2.3584	0.5198	0.7449	-0.3608
1PGA	F30L	1.42	3.2195	-0.6007	0.6431	1.3480	2.0304	-0.2013
1PGA	F52L	3.54	2.4051	-1.0619	1.1255	1.0702	1.2460	0.0254
1PGA	G41A	2.84	0.2048	-0.0500	-0.1669	0.3426	0.0689	0.0102
1PGA	I6A	2.09	1.1464	-0.2032	0.0413	0.8441	0.6042	-0.1401
1PGA	K28G	0.05	0.7607	-18.4931	18.4774	0.3974	0.7170	-0.3379
1PGA	K31G	2.02	1.9553	-21.7903	20.8941	1.6453	1.6566	-0.4505
1PGA	L7A	1.85	2.5673	-0.3608	0.4667	1.4664	1.4125	-0.4175
1PGA	N35G	2.50	0.4387	-0.8234	0.7603	0.3138	0.2130	-0.0250
1PGA	N37A	-0.17	0.4446	-1.5450	1.5063	0.2832	0.3965	-0.1964
1PGA	Q32G	1.00	0.8596	-1.4854	1.5801	0.4717	0.4317	-0.1384
1PGA	T11A	0.60	-0.3199	-0.5766	0.3568	0.0651	-0.0934	-0.0718
1PGA	T16A	0.38	0.9497	-0.8242	0.2519	0.7288	0.8229	-0.0296
1PGA	T18A	0.46	1.1855	-0.4932	0.1472	0.5332	1.0713	-0.0730
1PGA	T25A	-0.22	0.4244	-1.0224	0.8409	0.2614	0.4998	-0.1553
1PGA	T49A	0.72	1.1610	-2.0040	2.2167	0.4744	0.6735	-0.1996
1PGA	T51A	1.87	1.1826	-0.8600	0.6659	0.5970	0.8718	-0.0921

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1PGA	T53A	1.91	0.5922	-0.3023	-0.2811	0.5969	0.5964	-0.0176
1PGA	V29A	0.70	0.7745	-0.2865	0.2876	0.3509	0.4160	0.0065
1PGA	V39A	1.72	1.7804	-1.0123	0.8355	0.9524	1.0786	-0.0738
1PGA	V54A	2.93	1.5742	-0.4462	0.3730	0.6820	0.9450	0.0204
1PGA	Y33A	0.92	2.2149	-1.0146	0.9977	1.4269	1.2732	-0.4682
1PGA	Y3L	1.62	2.9239	-1.9023	1.8883	1.4221	1.5621	-0.0463
1PGA	Y45L	3.34	2.3901	-2.3604	2.3793	1.1403	1.2569	-0.0260
1STN	A102G	1.30	1.5013	-0.5213	0.7949	0.4365	0.8157	-0.0244
1STN	A109G	1.00	0.4421	-0.2000	0.1425	0.1241	0.3235	0.0519
1STN	A112G	0.00	0.7729	0.0250	0.0699	0.3007	0.3795	-0.0022
1STN	A12G	2.40	0.9205	0.2246	-0.0611	0.2789	0.3479	0.1303
1STN	A130G	1.10	0.5677	-0.2209	0.2202	0.1743	0.2632	0.1309
1STN	A132G	3.70	1.6953	-0.5367	0.5651	0.6948	0.8474	0.1248
1STN	A17G	0.30	1.1174	-0.3059	0.5200	0.2785	0.6650	-0.0403
1STN	A58G	2.60	1.6058	0.3349	-0.1076	0.5648	0.7551	0.0587
1STN	A60G	1.40	0.5957	-0.2958	0.2480	0.2504	0.3138	0.0792
1STN	A69G	2.00	0.7216	0.4736	-0.1305	0.0908	0.3724	-0.0848
1STN	A90G	2.00	1.1758	0.2089	-0.1092	0.4389	0.4641	0.1730
1STN	A94G	2.40	1.6317	0.2320	0.2101	0.3797	0.8289	-0.0190
1STN	D19A	0.10	-0.3230	-26.2932	24.3017	1.0900	1.1984	-0.6198
1STN	D19G	0.50	0.2376	-26.5624	24.2792	1.2381	1.6400	-0.3572
1STN	D21A	-0.70	-0.2863	-23.2144	22.5008	0.3976	0.6109	-0.5811
1STN	D21G	-0.30	-0.2530	-23.6294	22.1986	0.6312	0.9819	-0.4352
1STN	D40A	-0.20	0.0106	-21.9955	21.7449	0.3703	0.3175	-0.4267
1STN	D40G	0.50	0.7988	-21.4422	21.3188	0.5540	0.6389	-0.2707
1STN	D77A	3.10	0.6014	-30.3757	31.2967	0.0717	0.3117	-0.7030
1STN	D77G	2.20	0.6310	-29.3614	29.8875	0.0911	0.5044	-0.4906
1STN	D83A	3.80	2.5975	-30.4607	31.5486	1.0548	0.8850	-0.4301
1STN	D83G	2.70	2.7752	-31.7083	32.3364	1.3171	1.2457	-0.4157
1STN	D95A	3.30	0.9063	-28.0377	27.9875	0.8244	0.7541	-0.6219

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	D95G	2.70	1.5888	-28.0151	28.2599	0.7701	1.1004	-0.5266
1STN	E101A	1.90	1.4550	-23.8361	24.3302	0.5709	0.8046	-0.4146
1STN	E101G	3.10	2.6518	-24.0677	24.6815	0.9664	1.4982	-0.4266
1STN	E10A	1.30	0.6155	-29.4380	28.3160	0.9343	1.3257	-0.5225
1STN	E10G	1.80	1.5407	-29.0969	28.0328	1.2690	1.8127	-0.4768
1STN	E122A	0.40	1.1536	-26.2732	26.2230	0.7085	1.0796	-0.5844
1STN	E122G	2.20	1.7557	-26.1469	25.9943	0.9599	1.3769	-0.4286
1STN	E129A	0.40	2.3108	-28.9364	29.1813	1.1204	1.2929	-0.3474
1STN	E129G	2.20	2.7916	-28.5309	28.7856	1.2306	1.7127	-0.4065
1STN	E135A	0.70	0.9366	-25.6083	25.3471	0.6456	1.0861	-0.5339
1STN	E135G	1.70	1.8052	-25.3368	25.2288	0.9347	1.3979	-0.4193
1STN	E43A	-0.30	-0.4952	-20.7365	18.7243	1.0737	0.7047	-0.2613
1STN	E43G	-0.50	0.0777	-20.9341	18.7028	1.3883	1.1763	-0.2556
1STN	E52A	0.10	1.0293	-24.3149	23.5314	1.2965	1.2495	-0.7333
1STN	E52G	0.40	1.8576	-22.9614	22.4045	1.4366	1.5329	-0.5550
1STN	E57A	0.20	0.8297	-19.9217	20.0254	0.5690	0.5641	-0.4069
1STN	E57G	1.60	1.5130	-19.7465	20.2497	0.5760	0.7146	-0.2808
1STN	E67A	1.00	0.7028	-27.7204	27.6817	0.4892	0.7151	-0.4628
1STN	E67G	0.90	1.5461	-27.7952	28.0610	0.7459	1.0746	-0.5403
1STN	E73A	1.20	1.1026	-25.5534	24.8580	1.2021	1.1393	-0.5433
1STN	E73G	2.70	2.1511	-25.6342	25.0727	1.4545	1.6152	-0.3573
1STN	E75A	2.20	0.9688	-30.3462	28.8360	1.4525	1.6023	-0.5757
1STN	E75G	3.50	2.4666	-30.3258	29.3301	1.7823	2.2629	-0.5829
1STN	F34A	3.70	5.3888	-0.8624	1.1624	2.7929	2.8480	-0.5521
1STN	F61A	2.30	3.5398	-0.8591	1.0692	1.8211	2.0856	-0.5770
1STN	F61G	4.80	4.5079	-0.1626	0.6683	2.0755	2.3077	-0.3810
1STN	F76A	4.00	3.9248	-2.1878	1.6568	2.3871	2.5972	-0.5285
1STN	F76G	4.70	5.0978	-2.5148	2.0486	2.7928	3.2433	-0.4721
1STN	H121A	3.10	2.3434	-2.1560	1.8755	1.4425	1.7208	-0.5394
1STN	H121G	4.20	3.6445	-2.6064	2.2922	1.9491	2.4946	-0.4850
1STN	H124A	-0.40	1.6527	-1.9150	1.9765	0.9080	1.1464	-0.4632
1STN	H124G	0.50	2.4835	-1.1050	1.6109	0.9301	1.3854	-0.3379

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	H46A	0.50	1.4512	-2.1923	2.6222	0.9086	0.6303	-0.5176
1STN	H46G	0.40	2.1265	-3.2347	3.2294	1.4062	1.3625	-0.6369
1STN	H8A	0.40	0.3093	-1.0297	0.5409	0.6223	0.6474	-0.4717
1STN	H8G	0.80	0.8769	-1.0606	0.6735	0.8169	0.8658	-0.4187
1STN	I139A	3.50	2.3786	1.8742	-1.3990	0.9331	1.2988	-0.3285
1STN	I139G	4.40	3.1952	1.5130	-1.1617	1.2573	1.7452	-0.1586
1STN	I139V	1.50	0.7465	0.6896	-0.7918	0.5219	0.5502	-0.2234
1STN	I15A	2.70	1.3739	-0.9962	0.5396	1.1060	0.8769	-0.1524
1STN	I15G	3.30	3.4662	-0.4888	0.7388	1.6096	1.6827	-0.0760
1STN	I15V	0.80	0.6489	-0.0104	-0.0543	0.5292	0.2681	-0.0837
1STN	I18A	2.50	1.8509	-0.7693	0.8631	0.9524	0.9668	-0.1620
1STN	I18G	2.50	2.5124	-0.8870	0.9647	1.1719	1.3777	-0.1149
1STN	I18V	1.10	0.8976	-0.1916	0.1579	0.5418	0.5490	-0.1596
1STN	I72A	5.10	2.9746	-0.2773	0.3084	1.4221	1.7289	-0.2073
1STN	I72V	1.80	0.8877	-0.1768	0.0261	0.5875	0.5197	-0.0687
1STN	I92A	4.00	3.0453	0.3607	0.0949	1.1367	1.6631	-0.2101
1STN	I92V	0.50	0.5995	-0.1527	0.2525	0.3208	0.3880	-0.2092
1STN	K110A	1.30	0.9215	9.6488	-9.3489	0.5508	0.6251	-0.5542
1STN	K110G	2.70	2.0141	9.1902	-8.9054	0.9970	1.1936	-0.4613
1STN	K116A	-0.70	-0.8388	11.4308	-12.0254	0.0960	0.1807	-0.5210
1STN	K116G	-1.00	-0.6213	11.2647	-11.7244	-0.0943	0.3116	-0.3789
1STN	K127A	-0.20	0.1590	11.7477	-11.9632	0.4145	0.3541	-0.3941
1STN	K127G	0.70	0.5503	11.8935	-11.9525	0.5199	0.3991	-0.3097
1STN	K133A	1.40	-0.0392	5.7398	-7.0522	0.7524	1.0562	-0.5354
1STN	K133G	3.30	0.6233	5.6631	-6.7778	0.8959	1.3092	-0.4671
1STN	K134A	-0.10	0.3531	6.2081	-6.4285	0.3521	0.6665	-0.4451
1STN	K134G	0.70	1.0108	7.3147	-7.0523	0.4139	0.6386	-0.3041
1STN	K136A	0.90	0.2869	5.1239	-5.1528	0.3908	0.2437	-0.3187
1STN	K136G	0.20	0.8347	5.1193	-4.7924	0.3254	0.5426	-0.3602
1STN	K16A	0.20	-0.5397	11.6700	-13.0584	0.5929	0.6768	-0.4210
1STN	K16G	0.70	0.0558	12.6190	-13.6365	0.6477	0.8000	-0.3745
1STN	K24A	0.20	1.0035	12.6060	-13.2086	1.1835	1.0263	-0.6037

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	K24G	1.20	2.2131	13.3991	-13.4035	1.3376	1.3766	-0.4967
1STN	K28A	0.70	-0.0767	5.7800	-6.5042	0.6009	0.6335	-0.5868
1STN	K28G	0.70	1.0379	5.8173	-6.1328	0.9065	0.9800	-0.5331
1STN	K45A	-0.30	-0.2155	7.3391	-8.3085	0.6994	0.7329	-0.6784
1STN	K45G	-0.20	0.4938	7.4318	-8.4091	0.9452	0.9642	-0.4382
1STN	K48A	-0.10	-0.1357	9.3867	-9.3989	0.1592	0.0027	-0.2854
1STN	K48G	-0.20	0.4301	9.6613	-9.5248	0.2844	0.1780	-0.1688
1STN	K49A	0.30	0.1018	5.5292	-5.8542	0.5158	0.5748	-0.6638
1STN	K49G	0.20	1.5598	5.6596	-5.4317	0.8447	1.0259	-0.5388
1STN	K53A	0.20	-0.1809	2.7480	-3.3022	0.2787	0.4557	-0.3612
1STN	K53G	0.30	0.3650	3.2742	-3.4852	0.4529	0.5340	-0.4108
1STN	K63A	0.50	0.0391	4.8028	-5.4630	0.6133	0.6601	-0.5741
1STN	K63G	1.50	0.9272	4.8553	-5.4446	0.9010	1.0449	-0.4293
1STN	K64A	-0.10	0.0394	7.2724	-7.3782	0.3453	0.2777	-0.4778
1STN	K64G	0.40	0.8612	7.2267	-7.0294	0.4951	0.5397	-0.3709
1STN	K70A	0.10	-0.2989	9.8046	-9.8046	0.1931	0.0409	-0.5329
1STN	K70G	0.50	0.4143	9.4285	-9.2030	0.3782	0.2468	-0.4362
1STN	K71A	0.40	0.2465	10.3521	-10.1245	0.3320	0.1723	-0.4854
1STN	K71G	1.10	1.2321	10.2666	-9.8169	0.6797	0.4725	-0.3698
1STN	K78A	0.60	0.6331	11.9663	-12.8597	1.0082	1.1589	-0.6407
1STN	K78G	1.10	0.9267	12.7764	-13.3500	0.9061	1.0490	-0.4547
1STN	K84A	-0.20	0.5424	9.8495	-10.3713	0.5431	0.9272	-0.4061
1STN	K84G	0.30	0.2938	9.9647	-10.4056	0.4670	0.6089	-0.3413
1STN	K97A	0.10	-0.0738	9.7106	-9.7721	0.4595	0.2106	-0.6825
1STN	K97G	1.70	1.5065	9.5331	-9.0734	0.8271	0.8043	-0.5844
1STN	K9A	1.40	0.6607	5.0377	-6.1310	1.1119	1.1374	-0.4953
1STN	K9G	1.90	1.4596	5.5774	-6.2323	1.1145	1.3751	-0.3750
1STN	L103A	4.60	4.3931	-0.4545	0.5924	2.2416	2.5737	-0.5601
1STN	L108A	5.80	2.7486	0.0922	0.0985	1.4616	1.5580	-0.4616
1STN	L125A	4.90	3.1211	-0.6992	0.5365	1.6724	2.0716	-0.4602
1STN	L137A	2.30	1.4284	-0.4526	0.1671	1.1217	0.9984	-0.4062
1STN	L137G	4.60	3.0542	-0.3677	0.5735	1.5874	1.5705	-0.3095

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	L14A	2.30	2.2228	-0.0147	0.0257	1.3245	1.3895	-0.5022
1STN	L14G	3.70	3.1842	-0.4292	0.4329	1.6019	1.9109	-0.3323
1STN	L25A	2.70	2.8423	-0.3262	0.6344	1.3823	1.6088	-0.4569
1STN	L25G	4.50	4.1893	-0.2839	0.7731	1.8238	2.2112	-0.3348
1STN	L36A	3.50	1.5066	0.2894	-0.5186	0.8215	1.3541	-0.4398
1STN	L36G	5.30	3.2976	0.3727	-0.2088	1.3272	2.1541	-0.3477
1STN	L37A	1.70	1.8877	-0.1365	-0.3202	1.3558	1.3231	-0.3344
1STN	L37G	3.80	3.2679	-0.8232	0.1857	2.1082	2.2073	-0.4102
1STN	L38A	1.70	2.6967	-0.0752	-0.0250	1.4921	1.7249	-0.4202
1STN	L38G	0.60	3.5184	-0.7579	0.6358	1.7830	2.2530	-0.3955
1STN	L7A	1.60	1.0227	-0.2662	-0.2944	0.9087	1.0652	-0.3906
1STN	L7G	1.50	1.7933	-0.4642	-0.2722	1.1825	1.6166	-0.2694
1STN	L89A	2.60	2.3422	-0.6101	0.3164	1.6439	1.5142	-0.5223
1STN	L89G	3.20	3.4725	-0.1929	0.0483	1.9104	1.9862	-0.2794
1STN	M26A	1.50	1.4533	-0.8873	0.8831	1.1896	0.8904	-0.6226
1STN	M26G	2.20	2.3474	-0.0559	0.4944	1.2939	1.1072	-0.4922
1STN	M32A	1.70	1.7683	-0.4270	0.3334	1.2081	1.1518	-0.4981
1STN	M32G	2.40	3.3217	-0.5955	0.7052	1.8378	1.9457	-0.5716
1STN	M65A	2.00	2.6022	0.0213	-0.0808	1.6714	1.8419	-0.8516
1STN	M65G	4.60	3.6078	0.2228	0.0577	1.9296	2.0932	-0.6955
1STN	M98A	4.60	2.8607	-0.7370	0.3928	1.8699	1.9025	-0.5675
1STN	M98G	4.50	3.8393	-0.0894	-0.1329	2.1441	2.3150	-0.3976
1STN	N100A	5.20	1.6906	-1.2930	1.6802	0.6031	1.0681	-0.3678
1STN	N100G	5.10	2.2059	-1.4714	1.5724	0.8428	1.5644	-0.3023
1STN	N118A	2.10	1.1494	-2.6708	2.0465	1.0168	1.1116	-0.3547
1STN	N118D	2.40	4.5357	20.1100	-16.5478	0.0926	0.7617	0.1193
1STN	N118G	1.90	2.0195	-2.5338	2.0129	1.2716	1.6184	-0.3496
1STN	N119A	1.30	0.5361	-0.6713	0.6852	0.2511	0.6583	-0.3873
1STN	N119G	1.30	0.7852	-0.5619	0.0515	0.4405	1.1155	-0.2603
1STN	N138A	1.10	1.0841	-0.8758	0.9472	0.5930	0.7833	-0.3636
1STN	N138G	-0.10	1.2543	-1.4432	1.3099	0.7527	0.9442	-0.3094
1STN	N68A	0.50	0.4247	-2.0261	2.2055	0.2718	0.3128	-0.3392

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	N68G	0.50	0.5282	-1.4423	1.6138	0.2797	0.2767	-0.1996
1STN	P117A	-0.80	0.1780	-0.5441	0.4732	0.1084	0.1558	-0.0153
1STN	P117G	-0.90	0.5060	-0.4360	0.5834	-0.0317	0.3707	0.0196
1STN	P11A	0.40	0.1457	-0.8895	0.8226	0.3027	0.0183	-0.1084
1STN	P11G	1.00	0.3442	-0.9281	1.0373	0.2401	-0.0352	0.0301
1STN	P31A	0.50	-0.0964	-0.9344	0.5756	0.3506	0.0494	-0.1376
1STN	P31G	1.60	0.5901	-0.2303	0.3608	0.2715	0.1593	0.0288
1STN	P42A	-0.10	0.7782	-0.8941	0.4941	0.6388	0.6679	-0.1284
1STN	P42G	0.40	1.4920	-1.1770	1.0732	0.8308	0.8432	-0.0782
1STN	P47A	0.60	0.1017	-0.3234	0.3290	0.2232	-0.0299	-0.0974
1STN	P47G	0.10	0.4926	-1.3305	0.9439	0.5641	0.2642	0.0510
1STN	P56A	0.00	0.6074	-0.7857	0.7148	0.3622	0.4410	-0.1249
1STN	P56G	1.00	0.7761	-1.0196	0.8039	0.4894	0.5565	-0.0541
1STN	Q106A	-0.10	1.0579	-0.4712	0.6932	0.5704	0.7402	-0.4748
1STN	Q106G	1.50	2.2114	-0.1596	0.6656	0.9998	1.0962	-0.3905
1STN	Q123A	0.40	0.0845	0.0989	-0.0649	0.3001	0.2140	-0.4636
1STN	Q123G	0.60	0.3652	-0.1096	0.2658	0.3599	0.3015	-0.4523
1STN	Q131A	0.20	-0.0975	-1.3330	1.0159	0.2495	0.4542	-0.4840
1STN	Q131G	2.40	1.6414	-1.7049	1.7006	0.7698	1.2532	-0.3773
1STN	Q30A	0.30	0.5882	-0.5161	0.5549	0.4552	0.5790	-0.4848
1STN	Q30G	0.90	0.7660	0.3815	-0.1588	0.5221	0.4212	-0.4000
1STN	Q80A	0.10	1.3076	-2.3253	2.3466	0.8506	1.0038	-0.5682
1STN	Q80G	1.40	1.5938	-2.2310	2.1762	1.0028	1.0377	-0.3917
1STN	R105A	1.40	1.5608	3.0525	-3.4123	1.1891	1.7097	-0.9782
1STN	R105G	2.40	2.3779	2.7361	-3.2029	1.5798	2.1384	-0.8735
1STN	R126A	1.70	1.7153	6.3429	-6.8060	1.3391	1.6163	-0.7769
1STN	R126G	2.90	2.5957	6.8774	-6.9289	1.4507	1.9196	-0.7232
1STN	R35A	1.40	1.6823	3.7206	-4.9258	1.6402	2.0226	-0.7752
1STN	R35G	2.20	2.0984	4.3914	-5.4154	1.7101	2.1511	-0.7389
1STN	R81A	1.10	0.7332	9.4355	-10.6498	1.3853	1.0747	-0.5124
1STN	R81G	2.20	1.9497	9.0455	-10.0041	1.6605	1.6176	-0.3698
1STN	R87A	0.90	2.0129	6.9026	-7.7137	1.5213	2.0346	-0.7318

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	R87G	2.60	3.1915	7.6570	-8.0079	1.7236	2.4967	-0.6780
1STN	S128A	-0.70	0.2127	-0.5739	1.1922	-0.2584	0.0379	-0.1852
1STN	S128G	1.60	1.2335	-0.4693	1.0666	0.1954	0.4988	-0.0580
1STN	S141A	0.40	0.0506	0.4031	-0.0915	-0.0939	-0.0799	-0.0871
1STN	S141G	0.90	1.0126	-0.7829	0.7959	0.4091	0.6856	-0.0951
1STN	S59A	-0.40	0.2343	-0.8333	0.4591	0.3817	0.3826	-0.1558
1STN	S59G	1.10	0.7055	-1.0764	0.8460	0.4831	0.4587	-0.0057
1STN	T120A	1.20	0.7220	-1.7079	2.2783	-0.0079	0.5212	-0.3617
1STN	T120G	2.10	1.3556	-1.0999	1.4080	0.2229	0.9131	-0.0886
1STN	T120V	1.80	0.4789	-1.3242	1.9636	-0.2243	0.0726	-0.0088
1STN	T13A	0.70	-0.0193	-0.3414	0.0519	0.2762	0.1281	-0.1340
1STN	T13G	1.10	0.6306	-0.4097	0.4186	0.3879	0.3033	-0.0695
1STN	T13V	0.40	-0.4753	0.4051	-0.6676	0.0172	-0.1651	-0.0648
1STN	T22A	1.60	0.7769	-1.5995	1.3371	0.5201	0.8057	-0.2866
1STN	T22G	2.40	1.9623	-2.0068	1.6027	1.0039	1.5153	-0.1527
1STN	T22V	0.90	-0.4324	-0.7659	1.0221	-0.2802	-0.2277	-0.1807
1STN	T33A	1.40	0.7675	-1.0931	0.8396	0.4831	0.6468	-0.1090
1STN	T33G	2.50	1.5041	-0.8219	0.7991	0.6030	0.8859	0.0380
1STN	T33V	-0.40	-0.4242	-0.5079	0.5018	-0.0945	-0.1170	-0.2066
1STN	T41A	0.00	0.0042	-0.1129	-0.4487	0.1020	0.5622	-0.0985
1STN	T41G	2.00	1.2875	-0.3168	-0.5304	0.8198	1.3464	-0.0315
1STN	T41V	-0.80	-0.4324	0.0431	-0.8062	0.2369	0.2210	-0.1273
1STN	T44A	0.40	0.4870	-1.0430	0.5822	0.6124	0.5727	-0.2373
1STN	T44G	0.60	0.9638	-1.7226	1.0613	0.8528	1.0000	-0.2277
1STN	T44V	-0.10	0.2750	-0.7304	1.1512	-0.0469	-0.0297	-0.0692
1STN	T62A	2.40	2.0847	-0.5277	0.6334	0.9482	1.1755	-0.1447
1STN	T62G	3.50	3.1250	-0.0614	0.2112	1.4482	1.8121	-0.2851
1STN	T62V	0.20	-0.2184	-0.5408	0.1562	0.1190	0.1535	-0.1063
1STN	T82A	0.90	0.5994	-0.0079	0.2023	0.3275	0.2519	-0.1745
1STN	T82G	2.00	1.1567	0.3046	0.3297	0.3246	0.3215	-0.1238
1STN	T82V	-0.20	-0.0653	-0.5064	0.3060	0.0849	0.0910	-0.0409
1STN	V104A	2.90	1.1620	2.8348	-1.6831	-0.2568	0.1091	0.1581

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	V104T	2.50	1.0310	0.6801	0.3303	-0.0441	0.1562	-0.0915
1STN	V111A	4.20	1.2623	0.1295	-0.2885	0.8479	0.6710	-0.0975
1STN	V111G	4.90	3.1587	-0.1399	0.1131	1.4898	1.7837	-0.0880
1STN	V111T	2.30	0.8025	0.5967	-0.6186	0.4348	0.3749	0.0147
1STN	V114A	0.00	0.9366	0.4369	-0.3679	0.4638	0.5261	-0.1222
1STN	V114G	0.20	1.7955	1.1858	-0.9023	0.5295	1.0957	-0.1131
1STN	V114T	0.30	-0.0885	1.0764	-1.0950	0.1201	-0.0587	-0.1313
1STN	V23A	2.90	2.6043	-0.2558	0.2570	1.1513	1.5194	-0.0676
1STN	V23G	5.60	3.9772	-1.0338	1.0276	1.8498	2.2213	-0.0876
1STN	V23T	3.20	0.7316	1.0175	-0.7237	0.2628	0.1195	0.0555
1STN	V39A	2.20	1.4265	0.2196	-0.1129	0.6831	0.8308	-0.1941
1STN	V39G	4.70	3.6131	0.6215	-0.0163	1.2058	1.9180	-0.1159
1STN	V39T	1.30	0.7638	1.1493	-0.2978	-0.1190	0.0429	-0.0116
1STN	V51A	0.30	0.8479	-0.3336	0.3558	0.4950	0.3389	-0.0082
1STN	V51G	0.40	1.2378	-0.2073	0.5432	0.4415	0.4761	-0.0157
1STN	V51T	-0.20	0.2434	-0.4014	0.4969	0.0950	0.0433	0.0096
1STN	V66A	2.20	2.4276	-0.2868	0.4504	1.1309	1.4027	-0.2696
1STN	V66G	4.40	3.7745	-0.4106	0.6801	1.5049	2.0545	-0.0543
1STN	V66T	1.40	0.7255	0.7047	-0.0745	0.0198	0.1200	-0.0445
1STN	V74A	3.10	1.5303	1.2013	-0.6315	0.3032	0.7195	-0.0621
1STN	V74T	3.80	0.3745	0.6778	0.4095	-0.4247	-0.3038	0.0158
1STN	V99A	3.20	3.0577	-0.7166	0.8963	1.3821	1.7902	-0.2943
1STN	V99G	5.00	4.1522	-0.0660	0.3771	1.7616	2.3291	-0.2495
1STN	V99T	3.30	1.1498	0.0626	0.5585	0.2900	0.3520	-0.1133
1STN	Y113A	0.00	1.4595	-0.6002	1.2327	0.6656	0.6494	-0.4880
1STN	Y113F	0.00	0.4047	0.0743	-0.1009	0.3863	0.3351	-0.2901
1STN	Y113G	0.30	1.9153	-0.3495	1.1760	0.6836	0.7742	-0.3689
1STN	Y113L	-0.20	0.5078	0.4658	0.2162	0.0569	-0.0795	-0.1517
1STN	Y115A	0.30	1.3440	-0.0595	0.6423	0.7562	0.4657	-0.4607
1STN	Y115F	0.10	0.5968	-0.5913	0.5812	0.4671	0.2778	-0.1380
1STN	Y115G	0.70	2.2419	-0.2223	0.6956	1.1457	0.9909	-0.3681
1STN	Y115L	0.30	0.6395	0.1439	0.3586	0.1070	0.1493	-0.1193

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1STN	Y27A	2.80	3.2876	-1.7758	1.5343	1.9953	2.2307	-0.6970
1STN	Y27F	0.60	-0.1096	-1.2456	0.4417	0.3749	0.4825	-0.1630
1STN	Y27G	5.10	5.0879	-1.9411	1.9953	2.5184	3.1789	-0.6636
1STN	Y27L	1.50	0.9493	-1.0637	0.4801	0.8472	0.7952	-0.1095
1STN	Y54A	2.20	2.5804	-2.0564	1.6834	1.7646	1.8960	-0.7073
1STN	Y54F	0.50	-0.2829	-0.7245	0.4812	-0.0245	0.0186	-0.0338
1STN	Y54G	1.90	3.2809	-1.1359	0.5751	1.8423	2.5577	-0.5582
1STN	Y54L	3.40	1.0415	-2.0854	1.7220	0.8535	0.7831	-0.2316
1STN	Y85A	0.40	1.3363	-1.9932	1.7530	0.8058	1.1640	-0.3933
1STN	Y85F	0.00	0.1794	-2.7739	1.9688	0.4054	0.7786	-0.1995
1STN	Y85G	1.00	1.9862	-1.8889	1.7673	1.0503	1.3716	-0.3140
1STN	Y85L	0.10	0.5694	-1.3162	1.5246	0.1146	0.2842	-0.0378
1STN	Y91A	5.30	5.8830	-2.2727	2.4729	2.9380	3.3826	-0.6379
1STN	Y91F	2.40	1.3753	-0.3629	1.2265	0.3848	0.3115	-0.1845
1STN	Y91L	3.90	3.6663	-2.5424	2.9937	1.6424	1.8027	-0.2301
1STN	Y93F	2.00	-0.4976	-0.0346	-0.5540	0.1737	0.0020	-0.0848
1STN	Y93G	7.50	5.2864	-1.7187	0.7603	3.2402	3.3975	-0.3929
1STN	Y93L	4.50	2.0697	-1.4929	1.0409	1.3813	1.3289	-0.1885
1YPC	A16G	1.09	1.2403	0.4285	-0.1703	0.3401	0.6109	0.0311
1YPC	A58G	1.88	1.1118	-0.0263	0.1706	0.3199	0.5145	0.1330
1YPC	D23A	0.96	0.5965	-8.4956	8.0910	0.6877	0.6922	-0.3789
1YPC	D45A	0.80	0.8935	-13.7760	13.6185	0.6428	0.8960	-0.4878
1YPC	D52A	3.41	0.3808	-6.2983	5.9802	0.6156	0.4618	-0.3786
1YPC	E14D	0.52	0.1497	-2.9044	2.7208	0.1746	0.2593	-0.1007
1YPC	E14N	0.70	-0.2674	-5.7170	5.3266	0.0396	0.1669	-0.0836
1YPC	E14Q	0.29	-0.3253	-6.5794	6.4307	-0.1593	-0.1303	0.1129
1YPC	E15D	0.74	0.5800	-2.0380	1.9967	0.3157	0.3465	-0.0408
1YPC	E15N	1.07	0.8665	-7.4612	6.9863	0.7368	0.6341	-0.0296
1YPC	E15Q	0.47	0.3592	-7.8167	7.7602	0.1109	0.3345	-0.0298
1YPC	E26A	0.32	0.6901	-2.0388	3.2741	-0.3737	-0.3606	0.1891

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1YPC	E41A	0.70	0.1743	-14.8275	14.0037	0.5808	0.8596	-0.4423
1YPC	E7A	0.47	0.6013	-10.7589	9.4409	1.2150	1.1155	-0.4113
1YPC	E7Q	0.62	0.3861	-9.2458	8.0435	0.8874	0.9216	-0.2205
1YPC	F50A	3.84	3.5671	-0.5165	0.6075	1.8865	2.0846	-0.4950
1YPC	F50L	2.11	1.1937	0.4516	-0.2017	0.2613	0.5586	0.1240
1YPC	F50V	2.39	2.3602	-0.5586	0.7860	1.0670	1.4496	-0.3837
1YPC	I20V	1.30	1.5113	0.4794	-0.3292	0.7306	0.7910	-0.1606
1YPC	I29A	3.90	2.4516	0.5641	-0.2568	0.9039	1.3512	-0.1108
1YPC	I29V	1.11	0.7030	0.3455	-0.3459	0.4463	0.3399	-0.0828
1YPC	I30A	2.12	1.1280	0.3445	-0.3446	0.4946	0.7653	-0.1318
1YPC	I30G	3.52	2.3319	0.3770	-0.1084	0.7924	1.3204	-0.0495
1YPC	I30T	1.34	0.7181	0.1000	0.4595	0.0732	0.1697	-0.0843
1YPC	I30V	-0.08	0.0380	0.0511	-0.1106	0.0896	0.1567	-0.1487
1YPC	I37A	0.03	0.1403	0.3827	-0.2235	0.1221	-0.2365	0.0955
1YPC	I57A	4.29	4.2241	-0.1962	0.5183	1.7200	2.3444	-0.1624
1YPC	I57V	-0.19	1.0475	-0.1721	0.1328	0.5009	0.5554	0.0304
1YPC	K11A	-0.42	1.1565	-11.8812	12.0504	0.7534	0.7190	-0.4851
1YPC	K17A	0.49	2.1406	-12.6573	12.6137	1.2494	1.5653	-0.6304
1YPC	K17G	2.32	3.1426	-12.6028	12.7046	1.5615	2.0722	-0.5929
1YPC	K18A	-0.21	0.2072	-5.6350	5.9773	0.1686	-0.0369	-0.2668
1YPC	K18G	0.99	0.7773	-5.4867	6.0104	0.3268	0.0795	-0.1527
1YPC	K24A	0.65	2.3588	-9.8790	9.1568	1.5920	2.1131	-0.6242
1YPC	K24G	3.19	3.3130	-9.5684	9.0081	1.9114	2.4876	-0.5258
1YPC	K2A	0.55	2.0867	-15.3362	14.9584	1.3445	1.6399	-0.5200
1YPC	K2M	0.67	0.9960	-14.9989	15.5176	-0.0534	0.5195	0.0113
1YPC	L21A	1.33	1.7644	-0.1406	0.2497	1.1047	1.0333	-0.4827
1YPC	L21G	1.38	2.3293	0.2172	0.1816	1.1622	1.2102	-0.4419
1YPC	L32A	2.37	2.4447	-0.4825	0.6756	1.1480	1.5456	-0.4421
1YPC	L32I	0.26	-0.1857	0.8183	-0.3815	-0.1932	-0.3274	-0.1019
1YPC	L32V	0.50	0.3627	0.2133	0.0635	0.2486	0.1383	-0.3010
1YPC	L49A	3.84	2.8431	0.2499	-0.0615	1.1252	1.8472	-0.3176
1YPC	L8A	2.68	1.9316	0.5701	-0.3564	0.8745	1.0538	-0.2104

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
1YPC	N56A	0.83	0.9080	-0.8584	0.6149	0.6948	0.6923	-0.2356
1YPC	N56D	1.21	1.1854	-7.2129	8.4501	-0.2180	0.0010	0.1652
1YPC	P25A	1.76	0.2720	-0.5476	0.5815	0.2359	-0.0198	0.0220
1YPC	P33A	0.17	0.7477	-0.6362	0.7952	0.3940	0.1995	-0.0048
1YPC	P61A	3.34	2.0440	0.0723	0.2993	0.8860	0.7380	0.0484
1YPC	P6A	1.57	0.4341	0.6977	-0.4116	0.1798	-0.0318	-0.0000
1YPC	Q22A	0.02	0.0171	0.0638	0.1173	0.0737	0.0815	-0.3192
1YPC	Q22G	0.60	0.6081	0.0624	0.2004	0.3366	0.2791	-0.2704
1YPC	R43A	0.58	-0.0192	-8.2401	7.6462	0.5273	0.6464	-0.5989
1YPC	S12A	0.89	0.7659	-1.6847	1.7977	0.3527	0.4208	-0.1206
1YPC	S12G	0.80	1.1538	-1.9382	1.9975	0.5072	0.6465	-0.0591
1YPC	T36A	-0.23	0.6401	-0.3233	0.2284	0.1882	0.3603	0.1866
1YPC	T36S	0.02	0.3450	0.0703	0.2032	-0.1481	-0.1263	0.3460
1YPC	T36V	0.76	-0.4830	-0.0448	-0.3456	-0.0805	-0.0250	0.0131
1YPC	T39A	0.72	0.7860	-0.9800	1.1623	0.2246	0.3885	-0.0094
1YPC	T39D	-0.02	0.2278	1.6136	-1.8685	0.1504	0.1430	0.1893
1YPC	T3A	0.85	0.9336	-0.1627	0.4289	0.3458	0.3676	-0.0460
1YPC	T3G	1.16	1.3482	-0.1011	0.5805	0.3329	0.4382	0.0977
1YPC	T3V	0.32	0.1331	-0.1343	0.4544	-0.1380	-0.1574	0.1083
1YPC	V19A	0.49	0.6258	-0.4082	-0.0386	0.6639	0.6313	-0.2228
1YPC	V34A	0.64	1.1104	0.2060	-0.0258	0.4172	0.6010	-0.0880
1YPC	V34G	2.43	1.8569	0.7133	-0.3379	0.5466	0.8930	0.0419
1YPC	V34T	1.03	0.2301	1.0971	-0.2066	-0.5772	-0.3410	0.2578
1YPC	V38A	1.47	1.5283	-0.6213	0.7162	0.5695	0.8870	-0.0230
1YPC	V47A	4.93	3.4354	-0.3759	0.7360	1.4114	1.7651	-0.1013
1YPC	V51A	1.98	1.4299	0.2914	-0.0967	0.5699	0.7676	-0.1022
1YPC	V60A	1.51	1.4186	0.1746	-0.1213	0.6402	0.7277	-0.0026
1YPC	V60G	3.24	2.4654	-0.2603	0.3708	0.9501	1.3596	0.0451
1YPC	V60T	0.38	0.2593	0.1901	0.0795	-0.0932	-0.1435	0.2265
1YPC	V63A	1.45	1.3707	0.2495	-0.1267	0.6052	0.6549	-0.0122
1YPC	V63G	3.50	2.6512	-0.4164	0.1437	1.1537	1.6921	0.0780
1YPC	V63T	1.15	0.8996	0.4821	-0.0127	0.1408	0.1986	0.0908

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
2LZM	E11A	-1.10	1.7152	-18.0360	17.7297	0.8522	1.4931	-0.3240
2LZM	E128A	0.16	0.7588	-22.4257	22.5744	0.5121	0.5065	-0.4086
2LZM	I3A	0.70	2.8336	-0.1031	0.3016	1.2255	1.5548	-0.1453
2LZM	I3G	2.10	3.7282	0.3379	0.2060	1.3812	1.8447	-0.0415
2LZM	I3T	2.30	1.0609	0.8662	-0.2569	0.2863	0.1999	-0.0347
2LZM	I3V	0.40	1.7426	-0.3124	0.6587	0.7314	0.7130	-0.0481
2LZM	K124G	0.10	-0.8264	4.0245	-6.2053	0.8276	0.9636	-0.4368
2LZM	L133A	3.60	3.5470	0.0838	0.0432	1.8469	2.0013	-0.4282
2LZM	N116D	-0.60	-0.2713	21.4054	-21.7141	0.0261	-0.2210	0.2322
2LZM	N144D	-0.50	-1.0599	18.3443	-18.7242	-0.3021	-0.4406	0.0628
2LZM	N55G	0.60	0.7410	-1.7963	2.2431	0.0651	0.3880	-0.1589
2LZM	P37A	0.00	0.3662	-0.5165	0.7338	0.1004	0.1134	-0.0649
2LZM_pW	D20A	0.30	0.0143	-18.3642	18.5994	-0.0150	0.0669	-0.2729
2LZM_pW	D47A	0.95	0.2427	-21.1740	20.1132	0.7186	0.8644	-0.2793
2LZM_pW	D92N	1.40	-0.6302	-26.1845	26.0719	-0.1333	-0.2149	-0.1694
2LZM_pW	E45A	-0.01	0.7393	-18.7687	19.0294	0.3347	0.4995	-0.3555
2LZM_pW	F153A	3.80	4.7497	-0.4937	0.6420	2.4228	2.5375	-0.3589
2LZM_pW	F153L	-0.30	2.0754	-0.2152	0.3984	1.0017	0.8944	-0.0038
2LZM_pW	F67A	1.90	4.1671	-0.5669	0.7109	2.0105	2.3950	-0.3825
2LZM_pW	I100A	3.40	2.7283	-0.1956	0.3929	1.0574	1.5052	-0.0316
2LZM_pW	I17A	2.70	2.8361	0.5077	-0.2110	1.2202	1.3648	-0.0456
2LZM_pW	I27A	3.10	1.5650	0.8058	-0.9398	0.7858	1.0365	-0.1232
2LZM_pW	I29A	2.60	1.9056	-0.0554	-0.1791	1.0096	1.3035	-0.1730
2LZM_pW	I50A	2.00	1.8815	-0.2804	0.4837	0.7113	1.0482	-0.0813
2LZM_pW	I58A	3.20	2.5577	0.3032	-0.2265	1.2653	1.3401	-0.1244
2LZM_pW	I78A	1.60	2.1050	0.5966	-0.3818	1.0841	0.9553	-0.1492
2LZM_pW	K43A	1.03	0.8240	4.9887	-5.9595	0.9357	1.4177	-0.5586
2LZM_pW	K48A	0.56	-1.0669	-3.1758	2.5862	-0.0682	0.0277	-0.4369
2LZM_pW	L118A	3.50	2.5925	-0.2382	0.6490	1.1195	1.3018	-0.2397
2LZM_pW	L121A	2.30	3.1791	-0.2176	0.2766	1.7228	1.6908	-0.2935

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
2LZM_pW	L33A	3.60	3.7743	0.1607	0.0642	1.8963	1.9727	-0.3196
2LZM_pW	L39A	0.90	0.6282	0.0951	0.1327	0.4421	0.2351	-0.2768
2LZM_pW	L46A	1.86	2.2193	-0.1106	0.1248	1.1284	1.5875	-0.5107
2LZM_pW	L66A	3.90	2.0730	0.0201	-0.0270	1.1684	1.3024	-0.3910
2LZM_pW	L7A	2.60	2.2460	0.1949	-0.6337	1.4595	1.6089	-0.3836
2LZM_pW	L84A	3.90	3.3378	-0.3001	0.5352	1.5394	1.8805	-0.3173
2LZM_pW	L91A	3.10	2.8153	-0.2833	0.3113	1.3672	1.6616	-0.2415
2LZM_pW	L99A	4.50	3.7784	-0.0125	0.2190	1.7623	2.1142	-0.3046
2LZM_pW	L99G	6.30	5.3065	-0.0914	0.3768	2.3473	2.9269	-0.2531
2LZM_pW	M106A	2.30	2.1443	-0.4873	0.4350	1.2023	1.3531	-0.3588
2LZM_pW	M120A	0.20	1.2386	-0.1547	-0.5951	1.4820	1.0753	-0.5688
2LZM_pW	M6A	1.90	2.5891	-1.2993	0.4073	2.0546	1.9564	-0.5299
2LZM_pW	N116A	-0.17	-0.6469	-1.0628	1.3542	-0.2914	-0.4281	-0.2187
2LZM_pW	N163D	0.21	-1.0151	11.2314	-11.7342	-0.3249	-0.3586	0.1711
2LZM_pW	N40A	-0.32	-0.5934	-0.8664	1.2323	-0.3858	-0.3979	-0.1755
2LZM_pW	N40D	-0.44	-0.5018	16.5729	-16.6910	-0.2385	-0.3540	0.2087
2LZM_pW	N68A	-0.05	0.4464	-0.5166	0.2869	0.4475	0.4300	-0.2014
2LZM_pW	Q122A	0.24	0.8014	-0.0972	-0.3749	0.7602	0.8079	-0.2945
2LZM_pW	Q123A	0.22	-0.3968	-0.4491	-0.3304	0.2565	0.5231	-0.3970
2LZM_pW	R119A	0.18	-0.0615	11.5935	-12.3886	0.6251	0.6813	-0.5728
2LZM_pW	S117A	-1.27	-0.4807	-0.9039	0.2057	0.1947	0.0550	-0.0323
2LZM_pW	S44A	-0.34	-0.1581	0.4219	-0.1990	-0.1245	-0.1658	-0.0906
2LZM_pW	S44G	0.53	0.1874	0.4750	-0.2384	0.0612	-0.0789	-0.0315
2LZM_pW	T115A	0.14	-0.5169	0.2747	-0.3520	-0.0893	-0.3871	0.0368
2LZM_pW	T151S	-0.39	-0.1861	-0.0303	-0.3146	-0.0512	0.1323	0.0776
2LZM_pW	T152S	2.60	0.2912	0.2094	-0.4149	0.1998	0.2426	0.0542
2LZM_pW	T26S	-0.57	0.0512	0.1894	-0.7130	0.3203	0.2077	0.0467
2LZM_pW	T59A	1.50	0.1698	-0.4709	0.3013	0.2453	0.1770	-0.0829
2LZM_pW	T59G	1.60	0.7761	-0.7091	0.3616	0.5319	0.4808	0.1108
2LZM_pW	T59S	0.20	-0.3686	0.1901	-0.5007	-0.0752	-0.0445	0.0617
2LZM_pW	T59V	1.50	-0.3798	-0.3257	0.3572	-0.1460	-0.2101	-0.0551
2LZM_pW	V111A	1.10	0.7774	0.1273	-0.3041	0.5018	0.5634	-0.1110

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
2LZM_pW	V149T	3.00	1.2467	0.8021	0.4159	0.0400	-0.0596	0.0482
2LZM_pW	V71A	1.50	1.8297	0.2675	-0.0877	0.7717	0.9641	-0.0860
2LZM_pW	V75T	1.30	0.3072	0.5199	0.1310	-0.1879	-0.1678	0.0121
2LZM_pW	V87A	1.70	1.5537	0.4393	-0.2999	0.6740	0.6789	0.0613
2LZM_pW	V87T	1.60	0.2560	0.6656	-0.2236	-0.0592	-0.1333	0.0064
2LZM_pW	V94A	1.80	0.7833	0.0581	-0.1377	0.4197	0.3698	0.0735
2LZM	Q105A	0.60	2.1824	-2.3017	2.0274	1.1825	1.5670	-0.2928
2LZM	Q105E	1.10	0.6802	21.0233	-19.3742	-0.8489	-0.4436	0.3237
2LZM	Q105G	3.11	2.5340	-2.9951	2.1051	1.5786	2.0454	-0.2000
2LZM	Q123E	-0.40	-0.7031	20.7350	-21.1032	-0.3720	-0.0424	0.0795
2LZM	T157A	0.50	0.7614	-1.0694	1.5674	0.0794	0.2635	-0.0795
2LZM	T157G	1.10	1.2508	-1.0551	1.3893	0.2936	0.6761	-0.0530
2LZM	T157S	0.66	0.4842	0.2009	-0.1649	0.1019	0.3221	0.0242
2LZM	T157V	1.20	0.4266	-1.2121	1.8563	-0.2488	-0.0149	0.0462
2LZM	V103A	1.91	2.0695	0.0659	0.2962	0.7185	0.9742	0.0147
2LZM	V131A	-0.39	0.8371	-0.0861	0.2540	0.2871	0.4229	-0.0408
2LZM	V131G	0.68	1.3444	-0.1656	0.3664	0.5514	0.5246	0.0676
2LZM	V131T	0.12	0.6522	-0.3257	0.5288	0.1030	0.1973	0.1488
2LZM	V149A	2.87	2.9766	-0.3222	0.5285	1.3631	1.3667	0.0406
2LZM	Y25G	4.55	6.4469	-1.7923	2.1667	2.9194	3.6985	-0.5453
3CHY	A101G	1.00	0.9925	0.4378	-0.2242	0.1691	0.3703	0.2395
3CHY	A113G	1.30	1.0997	1.5854	-1.2318	0.0561	0.4022	0.2878
3CHY	A114G	0.80	0.6208	1.2532	-0.9232	-0.0141	0.0417	0.2633
3CHY	A74G	0.30	0.3430	0.7524	-0.2867	-0.1284	-0.1873	0.1930
3CHY	A99G	0.50	0.6634	2.6903	-2.2020	-0.0336	-0.1444	0.3531
3CHY	D12A	-2.50	-2.6546	0.1073	-4.4995	1.1990	1.0226	-0.4841
3CHY	D13A	-2.70	-2.1046	3.7135	-6.8440	0.7855	0.6535	-0.4131
3CHY	D57A	-3.40	-2.3101	-1.2608	-2.8374	1.0669	1.1166	-0.3954
3CHY	F14A	-0.80	-1.2703	0.6169	-1.5190	0.1721	-0.3906	-0.1497
3CHY	F14N	-2.90	-1.8279	-0.6377	-0.9711	0.1121	-0.3111	-0.0202

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	SAS	-TS
3CHY	P61G	0.60	1.4092	-0.6386	0.7873	0.4974	0.5954	0.1677
3CHY_pW	A103G	1.70	1.5571	-0.8915	0.8438	0.6183	1.1206	-0.1341
3CHY_pW	A36G	3.10	1.3395	-0.5105	0.4658	0.7001	0.8031	-0.1190
3CHY_pW	A42G	2.30	0.9322	-0.0696	0.1725	0.3712	0.5168	-0.0587
3CHY_pW	A97G	1.40	0.9794	-0.3129	0.3044	0.4343	0.6198	-0.0662
3CHY_pW	A98G	1.30	1.9445	-1.2940	1.1883	0.9109	1.3317	-0.1924
3CHY_pW	D38A	1.90	0.5499	4.9449	-5.3753	0.6839	1.0041	-0.7076
3CHY_pW	D38G	1.00	2.0989	4.5779	-5.2099	1.2416	2.0911	-0.6018
3CHY_pW	D64A	1.00	0.6460	4.5537	-4.7136	0.7155	0.6625	-0.5722
3CHY_pW	G39A	1.00	0.3150	-0.4938	0.1599	0.5814	0.3093	-0.2418
3CHY_pW	G76A	-0.50	-0.1014	-0.5814	0.2516	0.1928	0.2956	-0.2601
3CHY_pW	I123V	0.80	1.3167	0.1489	-0.0263	0.6339	0.7360	-0.1757
3CHY_pW	I55V	1.50	1.2284	-0.6284	0.4589	0.8134	0.8941	-0.3097
3CHY_pW	I72V	1.50	1.3813	-1.1092	0.9833	0.7856	0.9928	-0.2712
3CHY_pW	N23G	0.00	0.7547	0.0728	-0.1918	0.5884	0.6015	-0.3162
3CHY_pW	T112A	1.50	0.6972	-0.9192	0.8823	0.4440	0.5664	-0.2764
3CHY_pW	T112G	1.00	0.4311	-0.0477	0.0745	0.2233	0.1772	0.0038
3CHY_pW	V108T	1.00	0.5349	-1.3685	0.8094	0.5757	0.6063	-0.0881
3CHY_pW	V10T	5.70	1.4345	-0.2716	0.6643	0.5221	0.6388	-0.1192
3CHY_pW	V11T	3.20	1.2605	-0.2689	0.7141	0.6241	0.4388	-0.2476
3CHY_pW	V21T	0.20	0.6043	-0.2153	0.3600	0.2697	0.3044	-0.1144
3CHY_pW	V33T	1.50	1.2890	-0.1063	0.4512	0.4952	0.5751	-0.1262
3CHY_pW	V40T	0.70	0.4737	-0.7862	0.7578	0.2468	0.3784	-0.1231
3CHY_pW	V54T	4.80	1.0595	0.1663	0.4776	0.1593	0.3825	-0.1262
3CHY_pW	V83T	3.50	1.6970	0.0722	0.8459	0.2970	0.5514	-0.0696

Supplementary Table 3: Protein complexes used for affinity calculations.

Protein	PDB	Resolution	PDB-Reference	Mutation-References	#Mutations
colicin E9 DNAse domain/immunity protein Im9	1BXI	2.05Å	[62]	[63]	31
bovine chymotrypsin/BPTI	1CBW	2.60Å	[64]	[65–67]	24
ribonuclease inhibitor/angiogenin	1A4Y	2.00Å	[68]	[69–73]	39
TEM-1 beta-lactamase/ beta-lactamase inhibitor protein	1JTG	1.73Å	[74]	[75–77]	105
IGG1-KAPPA D1.3 FV/hen egg white lysozyme	1VFB	1.80Å	[78]	[79–82]	46
alpha-chymotrypsin A/turkey ovomucoid third domain	1CHO	1.80Å	[83]	[84]	16
anti-hen-egg-white lysozyme antibody (D1.3)/anti-idiotopic antibody (E5.2)	1DVF	1.90Å	[85]	[79, 86]	32
hyhel-10 FV/hen egg lysozyme	2DQJ	1.80Å	[87]	[88–92]	26
interleukin-4/receptor alpha chain	1IAR	2.30Å	[93]	[94, 95]	48

Supplementary Table 4: Full list of protein mutations used for binding affinity calculations. Experimental and calculated differences in binding free energies (in kcal/mol) relative to the wild type (both experimental and calculated).

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1BXI	A_C21A	0.92	1.3476	-0.6699	0.1701	0.4131	1.4343	0.0000
1BXI	A_N22A	0.14	1.2573	-0.2645	-0.0424	0.1299	1.4343	0.0000
1BXI	A_D24A	0.34	1.2445	-7.2749	6.7741	0.3110	1.4343	0.0000
1BXI	A_T25A	0.73	1.2124	-0.0766	-0.0846	-0.0608	1.4343	0.0000
1BXI	A_S26A	0.17	1.2682	-0.7448	0.3100	0.2688	1.4343	0.0000
1BXI	A_S27A	0.96	1.0165	0.3441	-0.5741	-0.1878	1.4343	0.0000
1BXI	A_E28A	1.41	1.6237	-8.3385	7.1583	1.3697	1.4343	0.0000
1BXI	A_E29A	0.31	1.4982	-5.8151	5.4195	0.4595	1.4343	0.0000
1BXI	A_E30A	0.22	1.1369	-5.0862	4.8303	-0.0415	1.4343	0.0000
1BXI	A_L31A	3.42	1.6981	0.1196	-0.4168	0.5610	1.4343	0.0000
1BXI	A_V32A	2.58	1.6268	1.3267	-1.7393	0.6051	1.4343	0.0000
1BXI	A_K33A	0.19	0.9224	5.6179	-5.8851	-0.2447	1.4343	0.0000
1BXI	A_L34A	0.91	0.9728	-0.1285	-0.2361	-0.0968	1.4343	0.0000
1BXI	A_V35A	1.66	1.3909	0.5272	-0.7146	0.1440	1.4343	0.0000
1BXI	A_T36A	0.90	1.4288	-0.1372	-0.1358	0.2676	1.4343	0.0000
1BXI	A_E39A	2.08	1.3952	-11.3435	10.6348	0.6697	1.4343	0.0000
1BXI	A_E40A	0.66	1.3857	-5.2638	5.0338	0.1814	1.4343	0.0000
1BXI	A_T42A	0.30	1.2292	-0.6667	0.1401	0.3214	1.4343	0.0000
1BXI	A_E43A	0.21	1.2703	-4.7769	4.5970	0.0159	1.4343	0.0000
1BXI	A_H44A	0.83	0.9517	-1.0335	0.5807	-0.0298	1.4343	0.0000
1BXI	A_S46A	0.01	1.0903	1.0431	-1.3240	-0.0631	1.4343	0.0000
1BXI	A_S48A	2.19	1.3440	-0.8261	0.2338	0.5020	1.4343	0.0000
1BXI	A_D49A	5.92	1.2814	-8.5634	7.7934	0.6171	1.4343	0.0000
1BXI	A_L50A	0.60	1.2650	-0.0684	-0.2856	0.1847	1.4343	0.0000
1BXI	A_I51A	0.85	1.6083	0.0666	-0.4907	0.5981	1.4343	0.0000
1BXI	A_Y52A	4.83	2.7668	0.3162	-0.8114	1.8277	1.4343	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1BXI	A_Y53A	4.63	2.9420	-0.1570	-0.3013	1.9661	1.4343	0.0000
1BXI	A_D58A	0.51	1.1851	-5.7722	5.5521	-0.0291	1.4343	0.0000
1BXI	A_S61A	0.87	1.0221	0.2869	-0.3853	-0.3137	1.4343	0.0000
1BXI	A_V66A	1.86	1.1066	1.6811	-1.7324	-0.2763	1.4343	0.0000
1BXI	A_N67A	0.28	1.3359	-0.3005	-0.1705	0.3726	1.4343	0.0000
1CBW	D_T11A	0.22	1.8837	-0.1656	0.6305	-0.1026	1.5215	0.0000
1CBW	D_K15A	2.00	1.2947	-1.5445	-0.2369	1.5546	1.5215	0.0000
1CBW	D_R17A	0.29	3.0740	-4.3534	3.8722	2.0338	1.5215	0.0000
1CBW	D_I18A	1.41	1.8345	-0.0025	-0.1771	0.4927	1.5215	0.0000
1CBW	D_I19A	0.14	1.6742	-0.1525	-0.0708	0.3760	1.5215	0.0000
1CBW	D_R20A	0.35	1.3562	1.3174	-1.4232	-0.0596	1.5215	0.0000
1CBW	D_F33A	0.14	1.2949	-0.2156	0.0965	-0.1074	1.5215	0.0000
1CBW	D_V34A	0.05	1.6185	-0.4653	0.4239	0.1384	1.5215	0.0000
1CBW	D_Y35A	0.88	1.7256	-0.1383	0.1047	0.2377	1.5215	0.0000
1CBW	D_R39A	0.22	2.1752	4.3495	-4.9445	1.2487	1.5215	0.0000
1CBW	D_K46A	0.14	1.6572	2.1599	-2.3932	0.3690	1.5215	0.0000
1CBW	D_K15D	5.25	4.5723	4.6528	-1.8943	0.2923	1.5215	0.0000
1CBW	D_K15E	3.89	3.8162	4.7551	-2.1518	-0.3086	1.5215	0.0000
1CBW	D_K15H	0.10	1.2596	1.1093	-1.4816	0.1104	1.5215	0.0000
1CBW	D_K15I	2.95	0.6550	-0.6688	-0.5847	0.3870	1.5215	0.0000
1CBW	D_K15L	-1.59	-0.4871	-0.9823	-0.5083	-0.5179	1.5215	0.0000
1CBW	D_K15M	-1.42	-0.1305	-0.6054	-0.5659	-0.4806	1.5215	0.0000
1CBW	D_K15N	1.33	0.8637	-0.0666	-0.6729	0.0817	1.5215	0.0000
1CBW	D_K15Q	0.31	0.3217	0.0518	-0.8036	-0.4480	1.5215	0.0000
1CBW	D_K15S	3.41	1.7383	-0.6929	-0.4060	1.3157	1.5215	0.0000
1CBW	D_K15T	2.10	1.2869	-1.1372	0.3422	0.5604	1.5215	0.0000
1CBW	D_K15V	2.15	0.7117	-0.9158	-0.5992	0.7053	1.5215	0.0000
1CBW	D_K15W	-2.45	-0.9332	0.4398	-0.7176	-2.1768	1.5215	0.0000
1CBW	D_K15Y	-2.63	-1.4412	-0.0241	-0.8465	-2.0921	1.5215	0.0000
1A4Y	B_E108A	-0.30	-1.0725	25.5571	-26.8504	-0.0956	0.3164	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1A4Y	B_H114A	0.65	0.6551	0.7557	0.0643	-0.4812	0.3164	0.0000
1A4Y	B_Q12A	0.30	-0.2047	1.6929	-1.7654	-0.4486	0.3164	0.0000
1A4Y	B_H13A	-0.30	0.0214	0.6755	0.2326	-1.2030	0.3164	0.0000
1A4Y	A_W261A	0.10	0.6771	2.6132	-1.7487	-0.5037	0.3164	0.0000
1A4Y	A_W261A A_W263A A_W318A	5.20	2.8225	-2.1194	1.0076	3.6179	0.3164	0.0000
1A4Y	A_W263A	1.20	1.1721	1.0560	-1.0955	0.8952	0.3164	0.0000
1A4Y	A_E287A	0.10	0.5874	-7.2457	7.2400	0.2767	0.3164	0.0000
1A4Y	A_S289A	0.00	0.2505	0.9882	-0.7648	-0.2893	0.3164	0.0000
1A4Y	A_W318A	1.50	1.0920	-0.3362	-0.2149	1.3267	0.3164	0.0000
1A4Y	B_R31A	0.20	1.3146	-26.1951	26.6757	0.5177	0.3164	0.0000
1A4Y	A_K320A	-0.30	-0.2978	10.7372	-11.1009	-0.2505	0.3164	0.0000
1A4Y	B_R32A	0.90	1.0712	-25.9905	26.6934	0.0520	0.3164	0.0000
1A4Y	B_R33A	0.30	1.0677	-22.4089	23.0742	0.0861	0.3164	0.0000
1A4Y	A_E344A	0.20	-0.0406	-6.9071	7.5325	-0.9825	0.3164	0.0000
1A4Y	A_W375A	1.00	0.6484	1.0630	-0.9593	0.2284	0.3164	0.0000
1A4Y	A_E401A	0.90	-1.3446	-10.2848	8.3970	0.2268	0.3164	0.0000
1A4Y	A_Q430A A_V432A	0.10	-0.2470	-0.7044	0.0665	0.0746	0.3164	0.0000
1A4Y	A_Y434A	3.30	2.1175	0.0258	-0.3371	2.1125	0.3164	0.0000
1A4Y	A_Y434A A_D435A	6.80	2.2753	-18.9742	18.5172	2.4160	0.3164	0.0000
1A4Y	A_Y434A A_Y437A	6.60	2.6861	-0.5212	-0.2503	3.1413	0.3164	0.0000
1A4Y	A_D435A	3.50	0.6041	-18.6180	18.9068	-0.0010	0.3164	0.0000
1A4Y	A_Y437A	0.80	1.0330	0.8998	-0.8302	0.6471	0.3164	0.0000
1A4Y	A_W438A A_S439A A_E440A	1.80	1.5294	-14.2052	13.8320	1.5862	0.3164	0.0000
1A4Y	A_R457A	-0.20	0.8412	10.2259	-9.5129	-0.1883	0.3164	0.0000
1A4Y	A_I459A	0.70	0.0746	0.2236	-0.8044	0.3391	0.3164	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1A4Y	B_R5A	2.30	3.6835	-28.5985	30.4765	1.4892	0.3164	0.0000
1A4Y	B_R5A A_Y434A	7.00	5.0221	-29.3520	30.6711	3.3867	0.3164	0.0000
1A4Y	B_R5A A_Y434A A_D435A	10.10	4.9350	-44.0506	46.3006	2.3687	0.3164	0.0000
1A4Y	B_R5A A_Y434A A_R457A	8.50	5.6140	-31.0757	31.2080	5.1653	0.3164	0.0000
1A4Y	B_R5A A_D435A	6.70	3.5313	-45.6252	47.2642	1.5760	0.3164	0.0000
1A4Y	B_R66A	0.20	1.1578	-19.2988	20.1346	0.0057	0.3164	0.0000
1A4Y	B_N68A	0.20	0.3052	-0.8367	1.0387	-0.2132	0.3164	0.0000
1A4Y	B_R70A	-0.20	0.5893	-13.7767	15.0630	-1.0134	0.3164	0.0000
1A4Y	B_H84A	0.20	0.6922	-0.2335	0.4046	0.2047	0.3164	0.0000
1A4Y	B_W89A	0.20	0.1402	-1.7141	-0.0300	1.5680	0.3164	0.0000
1A4Y	B_H8A	0.90	0.5930	-0.7020	0.8178	0.1609	0.3164	0.0000
1A4Y	A_Y434F	0.60	0.5104	0.1864	-0.1768	0.1844	0.3164	0.0000
1A4Y	A_Y437F	0.20	0.8271	-0.4226	0.2380	0.6953	0.3164	0.0000
1JTG	A_S105A	0.80	0.7443	-0.0551	0.6091	-0.2364	0.4267	0.0000
1JTG	A_S105A B_D49A	1.40	1.4412	-0.6408	0.8650	0.7903	0.4267	0.0000
1JTG	B_D163A	-1.35	-0.4538	7.8099	-8.9297	0.2394	0.4267	0.0000
1JTG	A_K209A	1.40	2.3751	-3.8622	5.8101	0.0005	0.4267	0.0000
1JTG	A_K209A A_S105A	2.00	2.5685	-4.6876	6.8651	-0.0357	0.4267	0.0000
1JTG	A_K209A A_S105A A_R218A	2.50	3.4830	-6.9296	10.4894	-0.5034	0.4267	0.0000
1JTG	A_K209A A_S105A	1.50	1.4952	-2.1085	1.8345	1.3426	0.4267	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	A_R218A B_D49A							
1JTG	A_K209A A_S105A B_D49A	1.30	1.3263	-1.5087	1.5427	0.8656	0.4267	0.0000
1JTG	A_K209A A_S210A A_S105A A_R218A	2.80	3.6961	-7.6241	10.8138	0.0797	0.4267	0.0000
1JTG	A_K209A A_S210A A_S105A A_R218A B_D49A	1.70	1.5557	-2.3819	1.9787	1.5322	0.4267	0.0000
1JTG	A_K209A B_D49A	1.60	0.9966	-1.0741	0.9531	0.6909	0.4267	0.0000
1JTG	A_S210A	1.30	0.7783	-0.5796	1.0596	-0.1283	0.4267	0.0000
1JTG	A_S210A A_S105A	1.20	1.4027	0.0824	1.5015	-0.6078	0.4267	0.0000
1JTG	A_S210A A_S105A A_K209A	1.90	2.8759	-4.4725	7.2215	-0.2998	0.4267	0.0000
1JTG	A_S210A A_S105A A_K209A B_D49A	0.60	1.3640	-2.1159	1.9449	1.1084	0.4267	0.0000
1JTG	A_S210A A_S105A B_D49A	1.10	1.6593	-0.5867	0.9848	0.8346	0.4267	0.0000
1JTG	A_S210A A_K209A	2.10	2.9159	-4.4572	6.3122	0.6341	0.4267	0.0000
1JTG	A_S210A	1.50	0.8763	-1.3659	1.2933	0.5223	0.4267	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	A_K209A B_D49A							
1JTG	A_R218A	1.40	1.2032	-3.0212	4.0887	-0.2910	0.4267	0.0000
1JTG	A_R218A A_S105A	1.80	1.8255	-2.5364	3.6497	0.2856	0.4267	0.0000
1JTG	A_R218A A_S105A B_D49A	1.30	1.7049	-2.0547	1.2887	2.0442	0.4267	0.0000
1JTG	A_R218A A_K209A	2.70	2.9751	-7.2705	9.8637	-0.0448	0.4267	0.0000
1JTG	A_R218A A_K209A B_D49A	1.90	1.3783	-2.1903	1.7640	1.3779	0.4267	0.0000
1JTG	A_R218A A_S210A	0.70	1.6343	-2.9497	4.7023	-0.5449	0.4267	0.0000
1JTG	A_R218A A_S210A A_S105A	1.70	2.2799	-3.0173	5.0426	-0.1720	0.4267	0.0000
1JTG	A_R218A A_S210A A_S105A B_D49A	0.90	1.4237	-1.5421	1.4752	1.0640	0.4267	0.0000
1JTG	A_R218A A_S210A A_K209A	2.80	3.1874	-7.2653	10.2425	-0.2165	0.4267	0.0000
1JTG	A_R218A A_S210A A_K209A B_D49A	2.00	1.1469	-2.1206	1.8554	0.9855	0.4267	0.0000
1JTG	A_R218A A_S210A B_D49A	0.40	0.8579	-0.8034	0.8503	0.3843	0.4267	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1JTG	A_R218A B_D49A	1.10	1.1317	-1.4555	1.1860	0.9745	0.4267	0.0000
1JTG	B_D49A	1.80	1.5237	-0.9674	0.8559	1.2086	0.4267	0.0000
1JTG	B_T140K	-0.01	0.1398	6.5688	-6.6547	-0.2010	0.4267	0.0000
1JTG	B_T140K B_Q157K	-0.40	-0.0449	12.1425	-11.7076	-0.9066	0.4267	0.0000
1JTG	B_D163K	-1.99	-0.7458	23.0416	-22.1882	-2.0258	0.4267	0.0000
1JTG	B_V165K B_D163K B_D135K B_N89K	-3.38	-1.2166	46.3128	-46.4779	-1.4781	0.4267	0.0000
1JTG	B_V165K B_D163A B_N89K	-2.41	-0.9029	33.4925	-33.1423	-1.6798	0.4267	0.0000
1JTG	B_T32K	0.20	0.1700	2.4313	-2.2550	-0.4330	0.4267	0.0000
1JTG	B_N89K	-0.46	-0.0443	5.0465	-5.0971	-0.4204	0.4267	0.0000
1JTG	B_V93K	-0.48	0.0538	5.1587	-4.7551	-0.7765	0.4267	0.0000
1VFB	B_D100A	3.10	2.4177	-10.9751	11.7294	0.1636	1.4999	0.0000
1VFB	B_D100A C_S24A	3.40	2.2798	-11.9228	12.2400	0.4628	1.4999	0.0000
1VFB	C_K116A	0.70	1.2878	1.9655	-2.6760	0.4984	1.4999	0.0000
1VFB	C_T118A	0.80	1.2178	-0.6767	0.4770	-0.0824	1.4999	0.0000
1VFB	C_D119A	1.00	0.9943	0.0460	-0.8256	0.2740	1.4999	0.0000
1VFB	C_V120A	0.90	1.1151	-0.7715	0.3435	0.0432	1.4999	0.0000
1VFB	C_Q121A	2.90	2.6328	-0.9372	1.0199	1.0503	1.4999	0.0000
1VFB	C_I124A	1.20	1.6442	0.0323	0.1425	-0.0305	1.4999	0.0000
1VFB	C_R125A	1.80	1.4992	-0.7659	0.1712	0.5941	1.4999	0.0000
1VFB	C_L129A	0.20	1.1274	-0.9500	0.6539	-0.0763	1.4999	0.0000
1VFB	C_D18A	0.30	0.8271	-1.6643	0.8806	0.1110	1.4999	0.0000
1VFB	C_N19A	0.30	1.7292	-1.7741	1.0274	0.9761	1.4999	0.0000
1VFB	C_Y23A	0.40	1.2024	-0.9009	0.5338	0.0695	1.4999	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1VFB	C_S24A	0.80	1.0192	-1.2507	1.1624	-0.3924	1.4999	0.0000
1VFB	A_H30A	0.80	0.6700	-1.5070	0.7366	-0.0595	1.4999	0.0000
1VFB	B_T30A	0.10	1.2281	-0.5833	0.6303	-0.3188	1.4999	0.0000
1VFB	A_Y32A	1.30	1.2895	-1.9321	0.9352	0.7865	1.4999	0.0000
1VFB	A_Y32A C_Q121A	2.60	2.7116	-2.2999	1.5078	2.0037	1.4999	0.0000
1VFB	B_Y32A	0.50	1.4590	-1.3201	0.9261	0.3531	1.4999	0.0000
1VFB	A_Y49A	0.80	1.2181	-1.0446	0.4746	0.2883	1.4999	0.0000
1VFB	A_Y50A	0.40	1.8983	-1.9510	1.1694	1.1800	1.4999	0.0000
1VFB	A_Y50A C_D18A	1.30	2.0551	-2.2311	1.5778	1.2085	1.4999	0.0000
1VFB	B_W52A	0.40	1.8058	-1.3398	0.8047	0.8411	1.4999	0.0000
1VFB	B_W52A C_D119A	2.20	1.1113	-0.9509	-0.3333	0.8957	1.4999	0.0000
1VFB	A_T53A	-0.23	0.6678	-1.4492	0.7661	-0.1490	1.4999	0.0000
1VFB	B_D54A	0.60	0.9395	-9.2651	8.7146	-0.0099	1.4999	0.0000
1VFB	B_D54A C_T118A	1.20	1.3974	-8.5928	8.3817	0.1087	1.4999	0.0000
1VFB	B_N56A	0.20	1.1551	-0.7167	0.4746	-0.1026	1.4999	0.0000
1VFB	B_D58A	-0.20	1.3102	-7.3295	7.2998	-0.1599	1.4999	0.0000
1VFB	A_W92A	2.70	2.1364	-1.4682	0.8876	1.2172	1.4999	0.0000
1VFB	A_W92A C_Q121A	3.50	3.0926	-2.1091	1.3205	2.3813	1.4999	0.0000
1VFB	A_W92A C_I124A	3.80	2.6595	-0.9354	0.7752	1.3199	1.4999	0.0000
1VFB	A_W92A C_R125A	3.40	2.6016	-0.6333	-0.0016	1.7366	1.4999	0.0000
1VFB	A_W92A C_L129A	3.30	2.5839	-1.3471	1.0129	1.4183	1.4999	0.0000
1VFB	A_W92A	0.30	1.1981	-0.7815	0.7138	-0.2341	1.4999	0.0000
1VFB	B_E98A	1.10	1.5779	-7.7037	8.0474	-0.2657	1.4999	0.0000
1VFB	B_R99A	0.10	0.1380	5.2790	-6.8356	0.1947	1.4999	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1VFB	B_Y101F	1.00	1.4310	-0.5568	0.0582	0.4298	1.4999	0.0000
1VFB	B_Y101F C_D119A	2.70	1.8384	-0.1315	-0.6244	1.0944	1.4999	0.0000
1VFB	B_Y101F C_V120A	2.50	1.6706	-0.0610	0.1661	0.0656	1.4999	0.0000
1VFB	A_Y32F	2.15	0.9622	-1.0498	0.4046	0.1075	1.4999	0.0000
1VFB	B_Y32F	0.21	1.6924	-0.2024	0.6080	-0.2131	1.4999	0.0000
1VFB	A_Y50F	0.48	1.0107	-1.0457	1.0207	-0.4642	1.4999	0.0000
1VFB	B_R102K	1.58	1.7003	-0.1645	0.2865	0.0785	1.4999	0.0000
1VFB	B_R102M	3.23	0.7737	6.2869	-7.0594	0.0463	1.4999	0.0000
1VFB	B_D100N	3.72	1.9187	-10.4789	11.4023	-0.5046	1.4999	0.0000
1cho	I_L15A	4.73	3.8263	2.2593	-2.2499	2.3578	1.4591	0.0000
1cho	I_L15D	7.14	5.3253	6.3283	-2.8938	0.4316	1.4591	0.0000
1cho	I_L15E	6.60	5.6202	5.4060	-1.1292	-0.1156	1.4591	0.0000
1cho	I_L15F	-1.49	1.0299	2.5726	-1.9146	-1.0872	1.4591	0.0000
1cho	I_L15H	2.98	2.0733	2.7430	-1.8085	-0.3203	1.4591	0.0000
1cho	I_L15I	4.44	2.0731	1.4896	-1.1198	0.2443	1.4591	0.0000
1cho	I_L15K	4.43	3.7759	5.9987	-3.9054	0.2234	1.4591	0.0000
1cho	I_L15M	0.38	1.7293	2.1258	-1.3666	-0.4890	1.4591	0.0000
1cho	I_L15N	3.33	3.2964	2.5610	-1.7533	1.0296	1.4591	0.0000
1cho	I_L15Q	2.93	2.5695	1.8852	-1.0480	0.2732	1.4591	0.0000
1cho	I_L15R	3.97	3.5983	5.2164	-1.8195	-1.2577	1.4591	0.0000
1cho	I_L15S	4.94	3.2505	1.9713	-1.7431	1.5632	1.4591	0.0000
1cho	I_L15T	4.45	2.9806	1.2953	-1.1174	1.3438	1.4591	0.0000
1cho	I_L15V	4.24	2.3678	1.1095	-1.2764	1.0755	1.4591	0.0000
1cho	I_L15W	-1.68	0.1753	3.8182	-2.7450	-2.3569	1.4591	0.0000
1cho	I_L15Y	-2.20	0.8289	2.7404	-1.7930	-1.5776	1.4591	0.0000
1DVF	B_D100A	2.80	1.6268	-5.6829	6.2807	-0.2160	1.2449	0.0000
1DVF	B_D100A D_H33A	4.10	1.7724	-5.3476	5.7098	0.1653	1.2449	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1DVF	B_D100A D_D52A	4.30	2.1519	-11.0801	12.2821	-0.2951	1.2449	0.0000
1DVF	B_D100A D_N55A	4.20	1.6683	-5.1610	5.5549	0.0295	1.2449	0.0000
1DVF	A_H30A	1.70	1.4966	-0.0517	0.4062	-0.1029	1.2449	0.0000
1DVF	B_T30A	0.90	1.1305	0.1346	0.3923	-0.6414	1.2449	0.0000
1DVF	D_K30A	1.00	0.5697	3.8149	-3.3046	-1.1856	1.2449	0.0000
1DVF	A_Y32A	2.00	1.2730	-0.7953	0.8259	-0.0025	1.2449	0.0000
1DVF	B_Y32A	1.80	1.3134	0.5431	-0.0263	-0.4484	1.2449	0.0000
1DVF	D_H33A	1.90	1.2869	-0.1319	-0.0869	0.2608	1.2449	0.0000
1DVF	A_Y49A	1.70	1.1245	1.4841	-0.8640	-0.7405	1.2449	0.0000
1DVF	A_Y49A D_H33A	2.60	1.1530	-0.1153	0.1082	-0.0849	1.2449	0.0000
1DVF	A_Y49A D_N55A	2.00	1.0600	0.4935	-0.1774	-0.5009	1.2449	0.0000
1DVF	C_Y49A	1.90	1.1523	0.5692	-0.7374	0.0756	1.2449	0.0000
1DVF	A_Y50A	0.70	1.7554	0.5088	-0.2278	0.2294	1.2449	0.0000
1DVF	B_W52A	4.20	2.8871	0.6102	-0.3280	1.3600	1.2449	0.0000
1DVF	B_W52A D_N55A	4.20	3.5673	-1.4282	0.7760	2.9745	1.2449	0.0000
1DVF	D_D52A	1.70	1.6874	-2.1572	2.8550	-0.2553	1.2449	0.0000
1DVF	B_D54A	4.30	1.3836	-3.1595	3.3968	-0.0986	1.2449	0.0000
1DVF	B_D54A D_Q104A	4.50	1.4486	-3.6980	3.2033	0.6983	1.2449	0.0000
1DVF	B_N56A	1.20	1.2161	-0.2523	0.8624	-0.6389	1.2449	0.0000
1DVF	B_N56A D_Q104A	1.50	1.8711	-1.1691	1.3253	0.4700	1.2449	0.0000
1DVF	B_N56A D_H33A	2.50	1.5215	-0.5323	0.4116	0.3973	1.2449	0.0000
1DVF	B_N56A D_N55A	2.30	1.0984	0.1799	0.4776	-0.8040	1.2449	0.0000
1DVF	B_D58A	1.60	1.6608	-3.7644	4.5136	-0.3334	1.2449	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1DVF	B_D58A D_Q104A	1.50	1.9631	-4.3845	4.4617	0.6410	1.2449	0.0000
1DVF	A_W92A	0.30	1.7954	-0.2083	0.8157	-0.0570	1.2449	0.0000
1DVF	A_S93A	1.20	1.2473	0.3111	0.2214	-0.5301	1.2449	0.0000
1DVF	D_I101A	2.70	1.5153	0.1848	0.4497	-0.3641	1.2449	0.0000
1DVF	B_E98A	4.20	2.8823	-1.1701	3.8732	-1.0657	1.2449	0.0000
1DVF	D_Y102A	4.70	2.8817	-1.7586	1.0794	2.3160	1.2449	0.0000
1DVF	B_Y101F	2.00	1.0379	0.2627	-0.1747	-0.2950	1.2449	0.0000
1JTG	A_E79A	1.60	0.2545	-3.2871	2.3356	0.7793	0.4267	0.0000
1JTG	A_Y80A	-0.20	2.6494	-1.2951	0.6292	2.8886	0.4267	0.0000
1JTG	A_E79A A_Y80A	1.00	2.0063	-2.8691	2.2024	2.2463	0.4267	0.0000
1JTG	B_K74A	3.60	3.4456	-6.2862	10.6383	-1.3332	0.4267	0.0000
1JTG	B_K74A A_E79A	1.60	-0.1750	-6.8212	7.1150	-0.8955	0.4267	0.0000
1JTG	B_K74A A_Y80A	3.30	5.1951	-9.4696	11.5829	2.6551	0.4267	0.0000
1JTG	B_K74A A_E79A A_Y80A	1.40	3.0125	-9.0000	7.4946	4.0913	0.4267	0.0000
1JTG	B_K74A A_R218A	6.60	4.1667	-12.1602	16.4495	-0.5493	0.4267	0.0000
1JTG	B_K74A A_K209A	6.50	5.7045	-12.8909	18.3925	-0.2238	0.4267	0.0000
1JTG	B_K74A A_S105A	3.20	3.6749	-6.2275	10.9515	-1.4759	0.4267	0.0000
1JTG	B_K74A A_S105A A_S210A A_R218A	5.00	5.6782	-11.3868	17.5921	-0.9538	0.4267	0.0000
1JTG	B_K74A	5.50	7.4968	-18.8028	25.0247	0.8482	0.4267	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	A_S105A A_S210A A_R218A A_K209A							
1JTG	B_F142A	2.10	1.9358	-0.8632	-0.2270	2.5993	0.4267	0.0000
1JTG	B_F142A A_E79A	2.70	1.7711	-4.8323	2.6167	3.5600	0.4267	0.0000
1JTG	B_F142A A_Y80A	0.70	3.9020	-3.5855	0.9521	6.1087	0.4267	0.0000
1JTG	B_F142A A_E79A A_Y80A	1.50	3.2359	-5.2503	2.7488	5.3106	0.4267	0.0000
1JTG	B_F142A A_R218A	3.40	2.6837	-4.9166	4.0611	3.1126	0.4267	0.0000
1JTG	B_F142A A_K209A	3.40	3.9478	-5.2705	5.7637	3.0279	0.4267	0.0000
1JTG	B_F142A A_S105A	2.80	2.1252	-0.5401	-0.2653	2.5040	0.4267	0.0000
1JTG	B_F142A A_S105A A_S210A A_R218A	3.50	4.0930	-5.7958	5.7712	3.6909	0.4267	0.0000
1JTG	B_F142A A_S105A A_S210A A_R218A A_K209A	4.30	5.6109	-10.8135	11.1030	4.8947	0.4267	0.0000
1JTG	B_Y143A	0.40	0.6019	0.1243	-0.4014	0.4522	0.4267	0.0000
1JTG	B_Y143A A_E79A	1.90	0.8014	-3.3981	2.0275	1.7453	0.4267	0.0000
1JTG	B_Y143A A_Y80A	1.10	2.9314	-0.5701	0.1519	2.9229	0.4267	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1JTG	B_Y143A A_E79A A_Y80A	2.10	2.0788	-3.6067	2.3980	2.8609	0.4267	0.0000
1JTG	B_Y143A A_R218A	2.30	1.4015	-2.5591	3.7121	-0.1782	0.4267	0.0000
1JTG	B_Y143A A_K209A	2.60	2.8083	-2.9957	5.3918	-0.0144	0.4267	0.0000
1JTG	B_Y143A A_S105A	1.80	0.8092	0.5992	0.2157	-0.4324	0.4267	0.0000
1JTG	B_Y143A A_S105A A_S210A A_R218A	2.70	2.8207	-2.9006	5.1093	0.1852	0.4267	0.0000
1JTG	B_Y143A A_S105A A_S210A A_R218A A_K209A	3.70	4.1985	-7.8031	10.8404	0.7345	0.4267	0.0000
1JTG	B_K74A B_F142A	4.80	4.2012	-8.6434	11.0416	1.3763	0.4267	0.0000
1JTG	B_K74A B_F142A A_E79A	3.10	1.1325	-8.7381	7.4479	1.9961	0.4267	0.0000
1JTG	B_K74A B_F142A A_Y80A	4.80	6.3416	-11.0386	11.9107	5.0429	0.4267	0.0000
1JTG	B_K74A B_F142A A_E79A A_Y80A	3.10	3.7878	-9.8509	7.6816	5.5305	0.4267	0.0000
1JTG	B_K74A B_F142A	5.50	5.1991	-14.9447	17.1915	2.5257	0.4267	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	A_R218A							
1JTG	B_K74A	5.80	6.3699	-14.9217	18.7529	2.1120	0.4267	0.0000
	B_F142A							
	A_K209A							
1JTG	B_K74A	5.20	4.8225	-9.8837	12.0280	2.2515	0.4267	0.0000
	B_F142A							
	A_S105A							
1JTG	B_K74A	5.80	6.6267	-14.3863	18.3965	2.1899	0.4267	0.0000
	B_F142A							
	A_S105A							
	A_S210A							
	A_R218A							
1JTG	B_K74A	5.70	7.8240	-20.2795	25.2632	2.4136	0.4267	0.0000
	B_F142A							
	A_S105A							
	A_S210A							
	A_R218A							
	A_K209A							
1JTG	B_K74A	3.00	2.4053	-9.1525	10.4778	0.6534	0.4267	0.0000
	B_Y143A							
1JTG	B_K74A	1.00	0.4465	-7.4803	7.1209	0.3791	0.4267	0.0000
	B_Y143A							
	A_E79A							
1JTG	B_K74A	3.40	4.6074	-10.0176	11.0591	3.1393	0.4267	0.0000
	B_Y143A							
	A_Y80A							
1JTG	B_K74A	1.80	3.0476	-8.9649	7.5559	4.0299	0.4267	0.0000
	B_Y143A							
	A_E79A							
	A_Y80A							
1JTG	B_K74A	4.40	3.1848	-12.9526	16.0722	-0.3614	0.4267	0.0000
	B_Y143A							

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	A_R218A							
1JTG	B_K74A	4.90	4.9541	-13.2848	17.6897	0.1225	0.4267	0.0000
	B_Y143A							
	A_K209A							
1JTG	B_K74A	3.70	2.8777	-8.0112	10.8774	-0.4152	0.4267	0.0000
	B_Y143A							
	A_S105A							
1JTG	B_K74A	4.40	4.6936	-12.8264	17.4048	-0.3115	0.4267	0.0000
	B_Y143A							
	A_S105A							
	A_S210A							
	A_R218A							
1JTG	B_K74A	6.60	6.1602	-19.2526	24.5389	0.4473	0.4267	0.0000
	B_Y143A							
	A_S205A							
	A_S210A							
	A_R218A							
	A_K209A							
1JTG	B_F142A	2.80	2.5190	-2.2882	0.0426	4.3379	0.4267	0.0000
	B_Y143A							
1JTG	B_F142A	2.90	1.4649	-4.5997	2.1384	3.4995	0.4267	0.0000
	B_Y143A							
	A_E79A							
1JTG	B_F142A	3.00	4.1138	-3.1377	0.2803	6.5446	0.4267	0.0000
	B_Y143A							
	A_Y80A							
1JTG	B_F142A	2.80	3.3705	-5.8410	2.5548	6.2299	0.4267	0.0000
	B_Y143A							
	A_E79A							
	A_Y80A							
1JTG	B_F142A	4.50	3.1365	-5.3911	4.0713	4.0297	0.4267	0.0000
	B_Y143A							

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	A_R218A							
1JTG	B_F142A	4.70	4.1450	-5.7847	5.8723	3.6308	0.4267	0.0000
	B_Y143A							
	A_K209A							
1JTG	B_F142A	4.20	2.6323	-1.8168	0.4298	3.5926	0.4267	0.0000
	B_Y143A							
	A_S105A							
1JTG	B_F142A	4.80	4.4294	-5.1485	5.2015	3.9497	0.4267	0.0000
	B_Y143A							
	A_S105A							
	A_S210A							
	A_R218A							
1JTG	B_F142A	4.90	5.3643	-9.7376	10.9620	3.7132	0.4267	0.0000
	B_Y143A							
	A_S105A							
	A_S210A							
	A_R218A							
	A_K209A							
1JTG	B_K74A	3.90	3.5779	-9.9073	10.7070	2.3515	0.4267	0.0000
	B_F142A							
	B_Y143A							
1JTG	B_K74A	2.40	1.7636	-9.2067	7.3460	3.1976	0.4267	0.0000
	B_F142A							
	B_Y143A							
	A_E79A							
1JTG	B_K74A	4.20	5.5065	-12.7215	11.7874	6.0140	0.4267	0.0000
	B_F142A							
	B_Y143A							
	A_Y80A							
1JTG	B_K74A	2.40	3.9119	-10.4518	7.8713	6.0657	0.4267	0.0000
	B_F142A							
	B_Y143A							

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	A_E79A							
	A_Y80A							
1JTG	B_K74A	5.30	4.6877	-13.9156	16.1662	2.0104	0.4267	0.0000
	B_F142A							
	B_Y143A							
	A_R218A							
1JTG	B_K74A	5.50	6.2419	-15.6440	18.3299	3.1293	0.4267	0.0000
	B_F142A							
	B_Y143A							
	A_K209A							
1JTG	B_K74A	5.10	4.1571	-10.2640	11.2812	2.7132	0.4267	0.0000
	B_F142A							
	B_Y143A							
	A_S105A							
1JTG	B_K74A	5.60	6.1025	-15.2544	17.8389	3.0913	0.4267	0.0000
	B_F142A							
	B_Y143A							
	A_S105A							
	A_S210A							
	A_R218A							
1JTG	B_K74A	5.50	7.4001	-20.3362	24.6667	2.6430	0.4267	0.0000
	B_F142A							
	B_Y143A							
	A_S105A							
	A_S210A							
	A_R218A							
	A_K209A							
2DQJ	L_Y50A	1.70	1.9369	-1.2960	0.9180	1.7625	0.5522	0.0000
2DQJ	L_Y50F	0.80	1.5880	-1.5595	1.3433	1.2519	0.5522	0.0000
2DQJ	L_Y96F	0.80	1.2697	-0.8451	1.3843	0.1782	0.5522	0.0000
2DQJ	H_Y33A	3.30	4.0917	-1.5938	0.9057	4.2275	0.5522	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
	H_Y53A							
2DQJ	H_Y33F	1.10	1.5733	-1.4316	1.5579	0.8947	0.5522	0.0000
2DQJ	H_Y50F	1.70	1.1113	-0.4393	1.0749	-0.0765	0.5522	0.0000
2DQJ	H_Y53A	0.20	2.1681	-1.6966	1.1571	2.1553	0.5522	0.0000
2DQJ	H_Y53F	0.70	2.1882	-1.9485	1.5987	1.9858	0.5522	0.0000
2DQJ	H_Y58A	1.70	1.7620	-1.9585	1.6571	1.5112	0.5522	0.0000
2DQJ	H_Y58F	0.40	1.1088	-1.1285	1.0888	0.5964	0.5522	0.0000
2DQJ	Y_D101G	-0.10	1.8868	0.8093	-0.5458	1.0711	0.5522	0.0000
2DQJ	Y_W62G	1.00	1.6379	-0.9329	1.0349	0.9838	0.5522	0.0000
2DQJ	H_Y53W	0.80	1.9149	-1.7158	1.3149	1.7635	0.5522	0.0000
2DQJ	H_Y53L	0.90	1.4322	-1.1660	0.9333	1.1127	0.5522	0.0000
2DQJ	H_Y33W	1.80	1.2976	1.1643	0.2616	-0.6806	0.5522	0.0000
2DQJ	H_Y33L	2.10	2.0653	-1.0164	1.2496	1.2799	0.5522	0.0000
2DQJ	H_Y50L	2.90	0.8636	-0.7873	1.4336	-0.3349	0.5522	0.0000
2DQJ	H_Y58L	1.60	1.8310	-2.2002	2.2855	1.1936	0.5522	0.0000
2DQJ	H_D32A	0.90	1.4029	-11.7844	12.0709	0.5642	0.5522	0.0000
2DQJ	H_D32N	0.40	1.3238	-10.1189	10.5276	0.3629	0.5522	0.0000
2DQJ	H_D32E	0.60	1.5651	-2.2763	3.0715	0.2177	0.5522	0.0000
2DQJ	H_Y53S H_S54F H_Y58F	1.20	1.9074	-1.4557	2.4088	0.4020	0.5522	0.0000
2DQJ	H_Y53A H_S54E H_S56A H_Y58F	1.90	3.1405	8.2086	-6.7844	1.1641	0.5522	0.0000
2DQJ	H_Y53E H_S54T H_S56K H_Y58F	2.10	2.7653	4.8838	-2.9095	0.2389	0.5522	0.0000
2DQJ	L_S91A	0.50	1.1039	-0.5784	0.7339	0.3962	0.5522	0.0000
2DQJ	L_S93A	0.10	1.1120	-0.6700	0.9381	0.2916	0.5522	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1IAR	B_D125A	0.80	0.4939	-22.4920	21.1531	0.4042	1.4286	0.0000
1IAR	B_N126A	0.68	0.4732	-3.9252	3.0860	-0.1160	1.4286	0.0000
1IAR	B_Y127A	2.17	2.9109	-0.8866	0.0033	2.3656	1.4286	0.0000
1IAR	B_Y127A	2.17	4.4728	-16.8611	13.7397	2.3656	1.4286	3.8000
1IAR	B_L128A	1.11	0.8887	-3.3215	2.7496	0.0321	1.4286	0.0000
1IAR	B_Y129A	0.28	1.2970	-0.3086	0.1023	0.0747	1.4286	0.0000
1IAR	B_Y13A	5.22	1.6589	-0.2175	0.2132	0.2347	1.4286	0.0000
1IAR	B_Y13A	5.22	3.7726	-13.4356	11.7450	0.2347	1.4286	3.7700
1IAR	B_M14A	0.17	0.7225	-3.8026	3.0996	-0.0030	1.4286	0.0000
1IAR	B_S15A	0.04	1.4835	-1.1377	0.9893	0.2034	1.4286	0.0000
1IAR	B_Y183A	3.68	2.1590	0.7935	-0.5175	0.4545	1.4286	0.0000
1IAR	B_Y183A	3.68	4.1868	-15.0098	13.2735	0.4545	1.4286	4.0400
1IAR	B_L39A	2.77	1.3562	-1.2382	1.0561	0.1098	1.4286	0.0000
1IAR	B_F41A	2.26	2.2598	-10.9180	9.5616	2.1876	1.4286	0.0000
1IAR	B_L42A	0.00	1.5531	-2.7409	2.1652	0.7003	1.4286	0.0000
1IAR	B_L43A	0.33	0.3319	-10.6422	8.7923	0.7533	1.4286	0.0000
1IAR	B_D66A	0.73	1.7048	-14.7284	14.8200	0.1847	1.4286	0.0000
1IAR	B_D67A	2.36	2.0750	-14.9390	15.2613	0.3242	1.4286	0.0000
1IAR	B_D67A	2.36	4.2946	-27.6107	26.1725	0.3242	1.4286	3.9800
1IAR	B_V68A	0.84	0.5388	-9.3231	7.5947	0.8387	1.4286	0.0000
1IAR	B_V69A	2.10	0.7826	-5.8669	5.3317	-0.1108	1.4286	0.0000
1IAR	B_S70A	-0.24	0.6158	-8.0329	6.7308	0.4893	1.4286	0.0000
1IAR	B_D72A	4.35	1.7584	-7.4910	7.9975	-0.1767	1.4286	0.0000
1IAR	B_D72A	4.35	3.6833	-20.0323	18.7437	-0.1767	1.4286	3.7200
1IAR	B_N73A	0.28	0.6137	-7.6394	6.4387	0.3859	1.4286	0.0000
1IAR	B_Y74A	2.73	1.8513	2.9172	-2.2246	-0.2699	1.4286	0.0000
1IAR	B_Y74A	2.73	3.0203	-15.7824	13.9040	-0.2699	1.4286	3.7400
1IAR	B_K91A	0.53	0.5936	4.1746	-5.1653	0.1558	1.4286	0.0000
1IAR	B_P92A	1.44	0.2566	-6.1148	5.0507	-0.1078	1.4286	0.0000
1IAR	B_S93A	-0.18	0.3741	-7.5079	6.1421	0.3113	1.4286	0.0000
1IAR	B_G94A	0.00	0.4589	-13.8037	12.7740	0.0601	1.4286	0.0000
1IAR	B_Y127F	-0.18	0.7807	-6.2295	5.2350	0.3467	1.4286	0.0000

PROT	MUTATION	EXP	CALC	SOLV	COUL	LJ	PPIS	PKA
1IAR	B_Y13F	1.91	1.5609	0.7464	-0.2589	-0.3552	1.4286	0.0000
1IAR	B_Y183F	3.16	1.7344	-2.1141	2.6177	-0.1977	1.4286	0.0000
1IAR	B_Y183F	3.16	3.6627	-15.0641	13.5859	-0.1977	1.4286	3.9100
1IAR	A_I5A	1.19	0.2394	-7.6545	6.3318	0.1335	1.4286	0.0000
1IAR	A_T6A	-0.08	0.8655	-3.5512	3.1266	-0.1385	1.4286	0.0000
1IAR	A_Q8A	0.00	0.4264	-6.9134	5.7945	0.1167	1.4286	0.0000
1IAR	A_I11A	0.07	0.9123	-4.9199	4.0209	0.3828	1.4286	0.0000
1IAR	A_K12S	-0.04	0.3611	-14.7536	12.6376	1.0486	1.4286	0.0000
1IAR	A_T13A	0.98	0.5779	-4.5476	3.6082	0.0888	1.4286	0.0000
1IAR	A_N15A	-0.04	1.8747	-0.5206	0.6295	0.3373	1.4286	0.0000
1IAR	A_S16A	-0.17	0.3398	-7.5369	6.3353	0.1129	1.4286	0.0000
1IAR	A_E19A	-0.32	0.2397	-3.9993	2.6961	0.1144	1.4286	0.0000
1IAR	A_R53Q	0.84	1.9467	-9.4901	9.9552	0.0530	1.4286	0.0000
1IAR	A_K77A	0.16	1.3129	-10.7589	10.2468	0.3965	1.4286	0.0000
1IAR	A_Q78A	0.13	0.2844	-6.9567	5.5415	0.2710	1.4286	0.0000
1IAR	A_R81A	0.48	1.0567	-20.2935	18.8593	1.0624	1.4286	0.0000
1IAR	A_F82A	-0.08	0.9892	-5.0910	4.2293	0.4224	1.4286	0.0000
1IAR	A_K84A	0.35	0.6522	-17.8271	16.5818	0.4690	1.4286	0.0000
1IAR	A_R85A	0.43	1.0411	-22.3990	20.6236	1.3880	1.4286	0.0000
1IAR	A_R88Q	2.83	1.7146	-17.6146	17.3713	0.5293	1.4286	0.0000
1IAR	A_N89A	1.58	1.4540	-3.7891	3.3001	0.5145	1.4286	0.0000
1IAR	A_W91A	0.73	1.5026	-2.0719	1.7817	0.3642	1.4286	0.0000
1IAR	A_E9Q	3.12	1.4306	6.3868	-6.0284	-0.3564	1.4286	0.0000
1IAR	A_E9Q	3.12	1.9904	-14.9473	11.8655	-0.3564	1.4286	4.0000

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