Supporting Information

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Text S1. IS-score definition and calculation.

Pairwise interface structural alignments are performed by iAlign (Gao and Skolnick, 2010), which uses the IS-score to determine interface similarity. IS-score is defined as:

$$IS - score = \frac{S + s_0}{1 + s_0} \tag{S1}$$

where:

$$S = \frac{1}{L_Q} \sum_{i=1}^{N_a} \frac{f_i}{1 + \left(\frac{d_i}{d_0}\right)^2} \tag{S2}$$

is the raw similarity score, and $s_0 = 0.18 - \frac{0.35}{L_Q^{0.3}}$ is the scaling factor used to make the IS-score length independent. L_Q is the length of the query, N_a is the number of aligned interface residues, f_i is the fraction of conserved interface contacts at the ith aligned position, and d_i/d_0 is the normalized Cα distance at the ith aligned position. IS-score varies from (0, 1], where a larger value indicates a higher similarity.

Text S2. Physics-based $\Delta\Delta G_{EvoEF}$ calculation.

EvoEF is a physics-based energy function designed to describe the atomic interactions in proteins and was first implemented in our protein design protocol EvoDesign (Pearce, et al., 2019). In general, it consists of five energy terms as shown in Eq. S3:

$$E_{EvoEF} = E_{VDW} + E_{ELEC} + E_{HB} + E_{DESOLV} - E_{REF} \tag{S3}$$

$$E_{VDW} = \sum_{i,j} w_{vdw} E_{vdw}(i,j) \tag{S4}$$

$$E_{ELEC} = \sum_{i,j} w_{elec} E_{elec}(i,j) \tag{S5}$$

$$E_{HB} = \sum_{i,j} w_{hb} E_{hb}(i,j) \tag{S6}$$

$$E_{DESOLV} = \sum_{i,j} w_{desolv} E_{desolv}(i,j) \tag{S7}$$

$$E_{REF} = \sum_{l=1}^{L} E_{ref}(aa_l) \tag{S8}$$

In Eqs. S3-S8, E_{VDW}, E_{ELEC}, E_{HB}, E_{DESOLV}, and E_{REF} are the total van der Waals, electrostatic, hydrogen bonding, desolvation and reference energy of the protein system. $E_{vdw}(i,j)$, $E_{elec}(i,j)$, $E_{hb}(i,j)$, and $E_{desolv}(i,j)$ are the pairwise corresponding interaction between non-bonded atoms i and j. The w_{vdw}, w_{elec}, w_{hb} and w_{desolv} are the relative weights for the corresponding energy terms. $E_{ref}(aa_l)$ is the amino acid-specific reference energy used to model the energy of an amino acid in the unfolded state, and the reference energy of a protein (E_{REF}) is assumed to be the summation of each individual amino acid $E_{ref}(aa_l)$ at position l across the whole protein chain with length L. $E_{ref}(aa_l)$ is a parameter that was determined for each amino acid aa.

$E_{vdw}(i,j)$, is the van der Waals energy between atoms i and j, which was modified from the Lennard-Jones (LJ) 12-6 potential (Jones, 1924a; Jones, 1924b), and describes the atomic packing interactions as follows:

$$E_{vdw}(i,j) = \begin{cases} min\left\{5.0\varepsilon_{ij}, \varepsilon_{ij}\left[\left(\dfrac{\sigma_{ij}}{d_{ij}}\right)^{12} - 2\left(\dfrac{\sigma_{ij}}{d_{ij}}\right)^{6}\right]\right\}, & if\ d_{ij} < 0.8909\sigma_{ij} \\[3mm] \varepsilon_{ij}\left[\left(\dfrac{\sigma_{ij}}{d_{ij}}\right)^{12} - 2\left(\dfrac{\sigma_{ij}}{d_{ij}}\right)^{6}\right], & if\ 0.8909\sigma_{ij} \le d_{ij} < 5.0 \\[3mm] A * d_{ij}^3 + B * d_{ij}^2 + C * d_{ij} + D, & if\ 5.0 \le d_{ij} < 6.0 \\[1mm] 0, & if\ d_{ij} \ge 6.0 \end{cases} \tag{S9}$$

$$
\begin{cases}
A = -0.4\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{12} - 1.6\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{6} \\[2mm]
B = 7.8\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{12} + 25.2\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{6} \\[2mm]
C = -50.4\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{12} + 129.6\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{6} \\[2mm]
D = 108\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{12} + 216\varepsilon_{ij}\left(\dfrac{\sigma_{ij}}{5.0}\right)^{6}
\end{cases}
\qquad (S10)
$$

where d_{ij} is the distance between the two atoms i and j, $\sigma_{ij} = \sigma_i + \sigma_j$ is the sum of their van der Waals atomic radii and ε_{ij} is the combined well-depth for atoms i and j, which are taken from the CHARMM19 force field (Brooks, et al., 1983). The attractive and repulsive components of the van der Waals energy are split at $d_{ij} = 0.8909\sigma_{ij}$. A maximum distance cutoff of 6.0 Å is set to increase the computational efficiency of EvoEF, and a cubic function is used to continuously connect the LJ energy from its value at 5.0 Å to zero at the cutoff distance (6.0 Å). For the repulsive component of the LJ potential, the maximum energy cutoff is set to $5.0\varepsilon_{ij}$, which helps alleviate possible clashes, while not overly penalizing them due to the discrete rotameric conformations used in protein design. The weights for the attractive and repulsive energies were separately determined.

$E_{elec}(i,j)$ is used to determine the electrostatic interactions between partially charged non-bonded atoms i and j in a protein system:

$$
E_{elec}(i,j) = \begin{cases}
\dfrac{C_0 q_i q_j}{\varepsilon(0.8\sigma_{ij})}\dfrac{1}{0.8\sigma_{ij}}, & if\ d_{ij} < 0.8\sigma_{ij} \\[3mm]
\dfrac{C_0 q_i q_j}{\varepsilon(d_{ij})}\dfrac{1}{d_{ij}}, & if\ 0.8\sigma_{ij} < d_{ij} < 6.0 \\[3mm]
0, & if\ d_{ij} \geq 6.0
\end{cases}
\qquad (S11)
$$

where q_i and q_j are the PARSE atomic charges (Sitkoff, et al., 1994). Furthermore, $C_0 = 332$ Å kcal mol^{-1}e^{-2}, where e is the elementary charge, and $\varepsilon(d_{ij})$ is the distance-dependent dielectric constant, defined as $\varepsilon(d_{ij}) = 40d_{ij}$. The distance d_{ij} is set to $0.8\,\sigma_{ij}$ if d_{ij} is less than $0.8\,\sigma_{ij}$, when calculating the electrostatics term and dielectric constant. This avoids the electrostatics energy being an infinite value when d_{ij} is close to zero. Again, for the sake of computational efficiency, the electrostatics energy is set to zero if d_{ij} is beyond the maximum distance cutoff 6.0 Å.

$E_{hb}(i,j)$ is used to calculate the hydrogen-bonding interactions between potential hydrogen bond donor/acceptor pairs of atoms i and j, one of which should be a polar hydrogen. $E_{hb}(i,j)$ is a linear combination of three energy terms that depend on the hydrogen-acceptor distance (d_{ij}^{HA}), the angle between the donor atom, hydrogen and acceptor (θ_{ij}^{DHA}), and the angle between the hydrogen, acceptor and base atom (φ_{ij}^{HAB}):

$$
E_{hb}(i,j) = w_{d_{HA}}E\left(d_{ij}^{HA}\right) + w_{\theta_{DHA}}E\left(\theta_{ij}^{DHA}\right) + w_{\varphi_{HAB}}E\left(\varphi_{ij}^{HAB}\right) \qquad (S12)
$$

where:

$$
\begin{cases}
E(d_{ij}^{HA}) = \begin{cases} -cos\left[\dfrac{\pi}{2}(d_{ij}^{HA} - 1.9)/(1.9 - d_{min})\right], d_{min} \leq d_{HA} \leq 1.9 \\ -0.5\,cos[\pi\,(d_{ij}^{HA} - 1.9)/(d_{max} - 1.9)] - 0.5, \quad 1.9\,\text{Å} < d_{HA} \leq d_{max} \\ 0 \qquad\qquad\qquad\qquad\quad , \quad otherwise \end{cases} \\
E(\theta_{ij}^{DHA}) = -cos^4(\theta_{ij}^{DHA}) \\
E(\varphi_{ij}^{HAB}) = \begin{cases} -cos^4(\varphi_{ij}^{HAB} - 150), \quad for\ BBHB\ and\ for\ sp^2\ in\ SBHB\ or\ SSHB \\ -cos^4(\varphi_{ij}^{HAB} - 135), \quad for\ sp^3\ in\ SBHB\ or\ SSHB \end{cases}
\end{cases}
\tag{S13}
$$

The optimal distance between the hydrogen and its acceptor is set to 1.9 Å, which is taken from Kortemme $et\ al.$ (Kortemme, et al., 2003). Additionally, $d_{min} = 1.4$ Å and $d_{max} = 3.0$ Å are the lower and upper bounds on the distance between the hydrogen-acceptor pair. The optimal φ_{ij}^{HAB} value is set to either $150\,°$ or $135\,°$, depending on the acceptor hybridization (sp^2 or sp^3) and the locations of the donor and acceptor atoms (BBHB: Backbone-Backbone Hydrogen Bond; SBHB: Sidechain-Backbone Hydrogen Bond; SSHB: Sidechain-Sidechain Hydrogen Bond).

$E_{desolv}(i,j)$ is used to describe the desolvation energy using the pairwise Gaussian volume-excluded implicit solvation model developed by Lazaridis and Karplus (Lazaridis and Karplus, 1999). The pairwise $E_{desolv}(i,j)$ is counted as the sum of the energy of atom i being desolvated by atom j ($f_{desov}(i,j)$) and atom j being desolvated by atom i ($f_{desov}(j,i)$), as shown in Eq. S14:

$$
E_{desolv}(i,j) = f_{desov}(i,j) + f_{desov}(j,i)
\tag{S14}
$$

$$
f_{desolv}(i,j) = -V_j \frac{\Delta G_i^{free}}{2\pi^{\frac{3}{2}}\lambda_i d_{ij}^2} \exp\left[-\left(\frac{d_{ij} - \sigma_i}{\lambda_i}\right)^2\right]
\tag{S15}
$$

$$
f_{desolv}(j,i) = -V_i \frac{\Delta G_j^{free}}{2\pi^{\frac{3}{2}}\lambda_j d_{ij}^2} \exp\left[-\left(\frac{d_{ij} - \sigma_j}{\lambda_j}\right)^2\right]
\tag{S16}
$$

where $V_{i,j}$, $\Delta G_{i,j}^{free}$, and $\lambda_{i,j}$ are the volumes, reference solvation energies, and correlation lengths for atoms i and j, respectively. All types of carbon and sulphur atoms are considered to be nonpolar, while oxygen and nitrogen atoms are considered to be polar. The desolvation energy for hydrogen atoms is ignored in the Larzaridis-Karplus model, while the desolvation energy for other polar and nonpolar atoms are separately calculated and weighted. Specifically, $E_{DESOLV} = \sum w_{desolvPolar}f_{desolvPolar} + \sum w_{desolvNonP}f_{desolvNonP}$.

To estimate the $\Delta\Delta G_{bind}$ using EvoEF, we first need to minimize the energy of the user-provided structure, build a structural model for the mutant and calculate the binding energy of the wild-type (ΔG_{bind}^{WT}) and mutant (ΔG_{bind}^{mut}) complexes. Specifically, the following steps are performed:

Step 1: We extract the target dimeric protein chains, clean the structures and remove the water molecules and ligand that are not amino acids.

Step 2: We optimize the amino-acid side chains of the structure of the wild-type complex using EvoEF's "RepairStructure" command:

./EvoEF --command=RepairStructure --pdb=WT.pdb

Following this command, the minimized wild type complex will be output into a file named 'WT_Repair.pdb' and this minimized model is used as the initial structure to build the mutant model.

Step 3: Build the mutant model using EvoEF's "BuildMutant" command:

./EvoEF --command=BuildMutant --pdb=WT_Repair.pdb --mutant-file=mutation.txt

Here, the file "mutation.txt" contains the list of mutation(s). Following this command, a new file "WT_Repair_Mutant_1.pdb" that contains the modelled mutant structure will be generated if you have only one mutant in the file "mutation.txt". If you have more than one (i.e., N) mutations, N files named "WT_Repair_Mutant_1.pdb", "WT_Repair_Mutant_2.pdb", …, "WT_Repair_Mutant_N.pdb" will be generated for the corresponding mutations.

Step 4: We computed the binding energy of the wild-type and mutant complex using EvoEF's "ComputeBinding" command:

./EvoEF --command=ComputeBinding --pdb=WT_Repair.pdb

./EvoEF --command=ComputeBinding --pdb=WT_Repair_Mutant_1.pdb

Following the command, the ΔG_{bind}^{WT} and ΔG_{bind}^{mut} will be obtained, and then the $\Delta\Delta G_{bind}$ is calculated as $\Delta\Delta G_{bind}^{WT \rightarrow mut} = \Delta G_{bind}^{mut} - \Delta G_{bind}^{WT}$.

The source code and manual of EvoEF, as well as the estimated $\Delta\Delta G_{bind}$ values are freely available at: https://zhanglab.ccmb.med.umich.edu/SSIPe/download.

Table S1. The iPTM matrix for the interface structure alignments. A substitution probability is read as $M(i, j)$, where i and j are the amino acid in the column and row, respectively.

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	.30	.06	.03	.04	.04	.12	.04	.04	.04	.04	.06	.04	.07	.04	.04	.11	.07	.06	.03	.03
C	.01	.51	.00	.00	.00	.00	.00	.01	.00	.01	.01	.01	.02	.00	.00	.01	.01	.01	.00	.00
D	.02	.01	.42	.06	.01	.01	.03	.01	.03	.01	.02	.04	.02	.03	.03	.03	.02	.01	.01	.01
E	.05	.02	.13	.32	.02	.01	.05	.05	.13	.04	.05	.06	.03	.15	.09	.06	.07	.04	.02	.03
F	.02	.01	.01	.01	.39	.01	.03	.03	.01	.02	.04	.01	.01	.02	.01	.01	.01	.02	.11	.11
G	.08	.01	.01	.01	.01	.65	.02	.01	.01	.01	.01	.02	.02	.01	.01	.04	.02	.01	.02	.01
H	.01	.01	.01	.01	.02	.01	.41	.01	.01	.01	.01	.02	.01	.02	.02	.01	.01	.01	.01	.03
I	.04	.04	.02	.04	.05	.01	.03	.21	.05	.08	.09	.07	.02	.05	.04	.03	.05	.13	.03	.03
K	.04	.02	.05	.10	.02	.01	.03	.05	.21	.05	.04	.06	.02	.10	.12	.04	.05	.05	.02	.02
L	.12	.08	.06	.09	.13	.03	.07	.22	.14	.45	.24	.13	.03	.12	.09	.08	.12	.18	.08	.11
M	.02	.01	.01	.02	.03	.01	.01	.03	.02	.03	.16	.02	.01	.02	.02	.01	.02	.02	.01	.02
N	.03	.03	.05	.03	.02	.02	.05	.05	.04	.04	.03	.25	.01	.04	.04	.04	.04	.05	.01	.03
P	.02	.02	.01	.01	.01	.01	.01	.01	.01	.00	.00	.01	.60	.01	.01	.01	.01	.01	.01	.01
Q	.03	.01	.04	.09	.02	.01	.04	.03	.07	.03	.05	.04	.01	.22	.06	.03	.04	.03	.02	.02
R	.03	.01	.04	.06	.02	.01	.04	.03	.10	.03	.03	.04	.02	.06	.32	.03	.04	.03	.02	.02
S	.07	.04	.03	.03	.01	.03	.03	.02	.03	.02	.02	.04	.03	.03	.03	.30	.07	.03	.01	.03
T	.05	.05	.03	.04	.02	.01	.03	.04	.04	.03	.04	.05	.04	.04	.04	.07	.27	.04	.02	.02
V	.07	.05	.03	.04	.04	.02	.03	.15	.05	.08	.07	.09	.03	.04	.04	.05	.07	.26	.02	.03
W	.01	.00	.00	.00	.04	.00	.01	.01	.00	.01	.01	.00	.01	.00	.00	.00	.00	.00	.54	.02
Y	.01	.01	.01	.01	.10	.01	.04	.01	.01	.02	.02	.02	.01	.01	.01	.02	.01	.01	.05	.42
Sum	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Table S2. Number of interface structural and sequence analogs obtained by iAlign and PSI-BLAST for the 177 dimeric complexes. The IS-score cutoff was 0.5. The STRING link score cutoff as well as the maximum and minimum sequence identity cutoffs were 0.8, 0.6 and 0.3, respectively. '#struct' indicates the number of interface structural analogs, and '#seq' indicates the number of interface sequence analogs with the optimal cutoffs applied. As a comparison, '#rawseq' indicates the number of raw interface sequence analogs obtained without any cutoff.

PDB	#struct	#seq	#rawseq	PDB	#struct	#seq	#rawseq	PDB	#struct	#seq	#rawseq
1A22	4	2	93	1TM1	7	0	0	3EG5	1	0	179
1A4Y	1	1	52	1TM3	8	0	0	3EQS	5	0	0
1ACB	49	0	0	1TM4	7	0	0	3EQY	4	0	0
1AK4	7	0	0	1TM5	7	0	0	3F1S	1	1	157
1B2S	2	4	48	1TM7	9	0	0	3KBH	0	0	0
1B2U	3	4	47	1TMG	8	0	0	3KUD	1	1	110
1B3S	3	2	56	1TO1	8	0	0	3LB6	2	1	31
1B41	1	0	0	1UUZ	2	0	0	3M62	1	1	95
1BP3	2	3	93	1WQJ	1	2	79	3M63	1	1	221
1BRS	3	2	53	1X1X	3	3	48	3MZG	4	3	90
1C1Y	0	0	110	1XD3	4	0	203	3N06	4	3	89
1CSE	8	0	0	1Y1K	7	0	0	3NCB	4	2	89
1CSO	11	0	0	1Y33	7	0	0	3NCC	4	3	90
1CT0	8	0	0	1Y34	7	0	0	3NVN	1	2	245
1CT2	10	0	0	1Y3B	8	0	0	3NVQ	2	0	208
1CT4	12	0	0	1Y4A	7	0	0	3Q3J	2	1	141
1E50	1	1	78	1Z7X	2	0	52	3QHY	1	0	1
1E96	0	0	116	2A9K	0	0	0	3RF3	13	0	0
1EAW	40	1	153	2AJF	0	0	0	3S9D	1	4	34
1EFN	0	0	0	2AW2	0	1	22	3SF4	1	0	44
1EMV	1	2	25	2B0Z	0	1	123	3SGB	6	0	0
1F47	0	0	69	2B10	1	0	122	3TGK	6	0	147
1FC2	1	0	0	2B11	1	0	123	3U82	1	0	0
1FCC	0	0	0	2B42	1	0	0	3WWN	0	2	48
1FFW	1	0	73	2BTF	1	0	72	4BFI	0	3	88
1FSS	1	0	0	2C5D	0	0	119	4CPA	2	0	0
1FY8	5	0	146	2DVW	2	1	136	4CVW	0	0	0
1GC1	2	0	0	2FTL	57	0	137	4FZA	1	2	202
1GL0	26	0	0	2G2U	2	0	1	4G0N	1	0	110
1GL1	50	0	0	2G2W	3	0	1	4G2V	1	0	0
1GUA	1	0	112	2GOX	2	0	0	4GU0	1	0	93
1H9D	1	2	77	2HLE	1	2	153	4HRN	0	0	91
1HE8	0	0	179	2HRK	1	2	17	4KRL	0	0	15
1IAR	1	2	29	2I26	1	0	6	4KRO	0	0	16
1JCK	4	0	0	2J0T	6	1	144	4KRP	0	0	14
1JTD	1	0	1	2J1K	3	0	0	4L0P	3	2	154
1JTG	2	0	1	2KSO	0	1	84	4MYW	1	0	0
1K8R	1	0	2	2NOJ	3	0	0	4NZW	0	6	204
1KAC	3	0	0	2NU0	29	0	0	4O27	0	6	204
1KBH	0	1	59	2NU1	20	0	0	4OFY	0	3	163
1KTZ	1	0	53	2NU2	16	0	0	4RA0	1	0	120
1LFD	2	1	129	2NU4	10	0	0	4RS1	0	1	30
1M9E	6	0	0	2O3B	0	2	10	4WND	1	0	46
1MAH	1	0	0	2OOB	0	0	61	4Y61	0	0	147
1OHZ	3	1	19	2PCB	0	2	123	4YEB	0	1	82
1P69	3	0	0	2PCC	1	1	122	4YFD	0	0	55
1P6A	2	0	0	2REX	3	1	141	4YH7	0	0	132
1PPF	37	0	3	2SGP	8	0	0	5CXB	0	4	268
1R0R	8	0	0	2SGQ	10	0	0	5CYK	0	6	268

1S0W	2	0	1	2SIC	7	0	1	5E6P	1	0	96
1S1Q	2	0	192	2VLN	1	2	25	5F4E	0	1	33
1SBB	3	0	0	2VLQ	1	2	25	5K39	2	1	6
1SBN	7	0	0	2VN5	3	1	21	5M2O	0	0	2
1SGD	19	0	0	2WPT	1	2	24	5TAR	0	0	89
1SGE	11	0	0	3BK3	1	1	53	5UFE	0	0	0
1SGN	22	0	0	3BP8	1	1	194	5UFQ	0	0	0
1SGP	8	0	0	3BT1	0	1	36	5XCO	0	0	0
1SGQ	7	0	0	3BX1	1	0	0				
1SGY	28	0	0	3D5R	3	0	0				
1SMF	67	0	0	3D5S	3	0	0	**Average**	**5.0**	**0.7**	**52.5**

Table S3. Summary of the weights for the original EvoEF and the new weights optimized using the new training set.

Classification	Energy terms	EvoEF weight	
		Original	New (this work)
Inter-residue interactions in different chains	Van der Waals attractive	0.6384	0.6112
	Van der Waals repulsive	0.7904	0.8130
	Coulomb's electrostatics	0.0000	0.0000
	desolvP	0.4048	0.4137
	desolvH	0.3432	0.3756
	HBbb_dist	0.0000	0.5000
	HBbb_theta	0.7600	0.8800
	HBbb_phi	0.5000	0.7500
	HBsb_dist	0.0000	0.0000
	HBsb_theta	0.6552	0.6105
	HBsb_phi	0.5236	0.4096
	HBss_dist	0.7200	0.7516
	HBss_theta	0.6720	0.3576
	HBss_phi	0.5040	0.5014

Table S4. Summary of the parameters and pseudocounts in SSIPe.

Parameter name	Value
Pseudocounts	A (25), C (27), D (23), E (24), F (30), G (25), H (25), I (27), K (22), L (33), M (29), N (23), P (18), Q (22), R(24), S (23), T (28), V (28), W (32), Y (31)
$C_{IS-score}$	0.5
$C_{linkscore}$	0.8
C_{maxID}	0.6
C_{minID}	0.3
λ	5
w_1	1.55
w_2	0.734
w_3	0.341
w_4	0.205

Table S5. CD-HIT clustering results for the 177 protein-protein complexes.

#Cluster	Representative PDB	Member PDBs
1	3BX1	2SIC, 1TM1, 1TM7, 1TMG, 1Y1K, 1Y33, 1Y34, 1TM3, 1TM4, 1TM5, 1TO1, 1Y3B, 1SBN, 1Y4A, 1CSE, 1R0R
2	1CSO	1CT0, 1CT2, 1CT4, 1SGD, 1SGE, 1SGN, 1SGP, 1SGQ, 1SGY, 2NU0, 2NU1, 2NU2, 2NU4, 2SGP, 2SGQ, 3SGB
3	1HE8	5TAR, 1LFD, 1K8R, 4G0N, 3KUD, 5UFQ, 5UFE 5XCO
4	1ACB	1EAW, 2FTL, 1GL0, 1GL1, 3TGK, 1FY8, 1SMF
5	1JTD	3QHY, 2G2U, 2G2W, 1S0W, 1JTG
6	3MZG	3N06, 3NCB, 3NCC, 1BP3, 1A22
7	2B0Z	2B10, 2B11, 2PCC, 2PCB
8	1B2S	1B2U, 1B3S, 1X1X, 1BRS
9	2GOX	3D5R, 3D5S, 2NOJ
10	1KAC	1P69, 1P6A, 2J1K
11	2VLQ	1EMV, 2VLN, 2WPT
12	4YH7	4YFD, 4Y61
13	4KRO	4KRP, 4KRL
14	4O27	4FZA, 4NZW
15	1MAH	1FSS, 1B41
16	3SF4	4WND, 4G2V
17	2A9K	1C1Y, 1GUA
18	1XD3	1S1Q, 2OOB
19	3NVQ	3NVN
20	3M62	3M63
21	5CXB	5CYK
22	2AJF	3KBH
23	1Z7X	1A4Y
24	4RA0	2C5D
25	4MYW	3U82
26	3EG5	1E96
27	1JCK	1SBB
28	2HLE	4L0P
29	1AK4	1M9E
30	2REX	3Q3J
31	1FCC	1FC2
32	1UUZ	2I26
33	1H9D	1E50
34	2VN5	1OHZ
35	3EQY	3EQS
36	4CVW	
37	4GU0	
38	3F1S	
39	4OFY	
40	4YEB	
41	5E6P	
42	2B42	
43	2BTF	
44	1GC1	
45	3BP8	
46	5F4E	
47	3BT1	
48	4BFI	
49	2O3B	
50	4RS1	
51	3LB6	

52	4CPA	
53	5K39	
54	1IAR	
55	3WWN	
56	3S9D	
57	2DVW	
58	2HRK	
59	2J0T	
60	3RF3	
61	1PPF	
62	5M2O	
63	2AW2	
64	1FFW	
65	4HRN	
66	1KTZ	
67	3BK3	
68	1EFN	
69	1F47	
70	1WQJ	
71	2KSO	
72	1KBH	

Table S6. Experimental data for the training set (TrainSet).

PDB	Chains	Mutations	Experiment $\Delta\Delta G_{bind}$
1A22	AB	CA171A	1.019
1A22	AB	CB67A	0.000
1A22	AB	CB81A	0.000
1A22	AB	DA160A	0.974
1A22	AB	DB119A	1.530
1A22	AB	DB85A	0.984
1A22	AB	EA163A	-0.909
1A22	AB	EA56A	0.624
1A22	AB	EA56D,RA64M	2.002
1A22	AB	EA65A	-0.393
1A22	AB	EB12A	1.373
1A22	AB	EB34A	-0.099
1A22	AB	EB79A	-0.202
1A22	AB	EB79A,KB80A	-0.345
1A22	AB	EB86A	0.786
1A22	AB	FA165A	1.024
1A22	AB	FA165Y	1.269
1A22	AB	FA25A	-0.424
1A22	AB	FA25A,YA42A,QA46A	0.198
1A22	AB	HA18A	-0.346
1A22	AB	HA21A	0.155
1A22	AB	IA168A	0.698
1A22	AB	IB120A	2.154
1A22	AB	IB62A	1.272
1A22	AB	IB64A	1.350
1A22	AB	KA157A	-0.052
1A22	AB	KA157A,EA163A	-0.769
1A22	AB	KA161A	1.778
1A22	AB	KA161A,FA165A	3.779
1A22	AB	KB122A	-0.009
1A22	AB	KB80A	0.080
1A22	AB	LA45A	1.224
1A22	AB	NA63A	0.510
1A22	AB	NB173A	0.286
1A22	AB	PA48A	0.410
1A22	AB	PA61A	1.209
1A22	AB	PB65A	2.965
1A22	AB	QA22A	-0.220
1A22	AB	QA46A	0.108
1A22	AB	QA68A	0.787
1A22	AB	QB121A	0.009
1A22	AB	QB121A,KB122A,VB126A	-0.872
1A22	AB	QB33A	-0.194
1A22	AB	RA156A	0.060
1A22	AB	RA167A	2.424
1A22	AB	RA167K	0.953
1A22	AB	RA167N	1.269
1A22	AB	RA64A	1.721
1A22	AB	RA64A,DA160A	3.321
1A22	AB	RA64K	-0.314
1A22	AB	RB11A	1.523
1A22	AB	RB11L	0.521
1A22	AB	RB11M	1.000
1A22	AB	RB172A	0.261
1A22	AB	RB172A,NB173A	0.902
1A22	AB	RB30A	0.568
1A22	AB	SA51A	0.348

1A22	AB	SA62A	0.397
1A22	AB	SB174A	0.034
1A22	AB	SB57A	-0.169
1A22	AB	SB57A,SB61A	-0.569
1A22	AB	SB57A,SB61A,EB79A,KB80A	-0.895
1A22	AB	SB57A,SB61A,EB79A,KB80A,QB121A,KB122A,VB126A	-1.399
1A22	AB	SB61A	0.021
1A22	AB	SB83A	0.226
1A22	AB	TA164A	1.906
1A22	AB	TA164S	1.690
1A22	AB	TB60A	1.423
1A22	AB	VB126A	-0.670
1A22	AB	WB124A	4.729
1A22	AB	WB35A	0.545
1A22	AB	WB63A	4.681
1A22	AB	WB63F	2.783
1A22	AB	YA153A	0.348
1A22	AB	YA42A	0.199
1A22	AB	YA42A,QA46A	0.289
1AK4	AD	AD88G	2.654
1AK4	AD	AD88V	0.769
1AK4	AD	AD92G	0.581
1AK4	AD	AD92V	0.359
1AK4	AD	GD89A	2.076
1AK4	AD	GD89V	3.029
1AK4	AD	HD87A	1.009
1AK4	AD	HD87Q	0.972
1AK4	AD	HD87R	1.645
1AK4	AD	ID91A	0.240
1AK4	AD	ID91V	0.000
1AK4	AD	PD85A	1.085
1AK4	AD	PD90A	2.172
1AK4	AD	PD90V	3.029
1AK4	AD	PD93A	0.683
1AK4	AD	VD86A	0.991
1B41	AB	AB12S	0.707
1B41	AB	HB29K	-0.888
1B41	AB	HB29R	-0.409
1B41	AB	KB32R	0.391
1B41	AB	LB35W	1.304
1B41	AB	MB33F	0.778
1B41	AB	MB33L	1.811
1B41	AB	MB33Q	1.595
1B41	AB	MB33Y	0.707
1B41	AB	NB47F	-0.142
1B41	AB	NB47R	-0.030
1B41	AB	NB47W	0.037
1B41	AB	RB11K	0.625
1B41	AB	RB27F	2.107
1B41	AB	RB27M	1.483
1B41	AB	RB27Y	2.395
1B41	AB	TB8V	1.136
1B41	AB	TB8V,TB9I	0.394
1B41	AB	TB8V,TB9N	2.427
1B41	AB	TB9I	0.025
1B41	AB	TB9N	3.609
1B41	AB	VB34T	1.214
1BP3	AB	DA167A	0.068
1BP3	AB	EA170A	1.831

1BP3	AB	EA65A	0.546
1BP3	AB	FA172A	1.927
1BP3	AB	HA18A	1.549
1BP3	AB	HA21A	1.247
1BP3	AB	IA175A	0.354
1BP3	AB	IA175M	-0.164
1BP3	AB	KA164A	1.727
1BP3	AB	KA164A,EA170A	5.405
1BP3	AB	KA168A	2.605
1BP3	AB	KA168A,FA172A	5.352
1BP3	AB	NA63A	0.856
1BP3	AB	QA68A	0.114
1BP3	AB	RA163A	3.024
1BP3	AB	RA174A	1.150
1BP3	AB	RA179A	0.567
1BP3	AB	RA64A	0.354
1BP3	AB	RA64A,DA167A	0.378
1BP3	AB	SA184A	-0.297
1BP3	AB	SA62A	1.415
1BP3	AB	TA171S	0.494
1BP3	AB	YA160A	0.445
1C1Y	AB	DA38A	2.619
1C1Y	AB	KB11A	1.108
1C1Y	AB	KB11E	0.891
1C1Y	AB	KB11M	0.713
1C1Y	AB	KB30A	1.312
1C1Y	AB	KB30A,RB35G	2.619
1C1Y	AB	KB30E	2.232
1C1Y	AB	NB10A	0.502
1C1Y	AB	NB10D	1.476
1C1Y	AB	QB12A	1.580
1C1Y	AB	RB13A	1.455
1C1Y	AB	RB35L	2.619
1C1Y	AB	RB5A	1.906
1C1Y	AB	RB5A,NB10D	2.751
1C1Y	AB	TB14A	1.455
1C1Y	AB	VB15A	1.123
1CSE	EI	LI38D	4.350
1CSE	EI	LI38E	2.350
1CSE	EI	LI38G	2.249
1CSE	EI	LI38I	2.941
1CSE	EI	LI38P	6.671
1CSE	EI	LI38S	1.172
1CSO	EI	II13L	-4.419
1CT0	EI	SI13L	-4.100
1CT2	EI	TI13L	-3.160
1CT4	EI	VI13L	-2.992
1EFN	AB	IA12A	1.450
1EFN	AB	TA13H	1.243
1EMV	AB	CA21A	0.922
1EMV	AB	DA49A	5.915
1EMV	AB	EA28A	1.416
1EMV	AB	EA39A	2.083
1EMV	AB	FB86A	3.879
1EMV	AB	FB86A,LA31A	6.677
1EMV	AB	FB86A,VA32A	4.663
1EMV	AB	FB86A,VA35A	4.066
1EMV	AB	FB86A,YA52A	8.719
1EMV	AB	FB86A,YA53A	8.259

1EMV	AB	GA47A	1.485
1EMV	AB	IA51A	0.848
1EMV	AB	KB97A	1.960
1EMV	AB	LA31A	3.418
1EMV	AB	NA22A	0.139
1EMV	AB	NB72A	1.165
1EMV	AB	NB75A	2.334
1EMV	AB	PA45A	0.437
1EMV	AB	PA54A	1.242
1EMV	AB	QB92A	-0.278
1EMV	AB	RB54A	1.666
1EMV	AB	SA26A	0.173
1EMV	AB	SA27A	0.956
1EMV	AB	SA46A	0.007
1EMV	AB	SA48A	2.187
1EMV	AB	SB74A	-0.241
1EMV	AB	SB77A	-0.233
1EMV	AB	SB78A	-0.540
1EMV	AB	SB84A	-0.109
1EMV	AB	TA25A	0.728
1EMV	AB	TA36A	0.900
1EMV	AB	TB87A	0.158
1EMV	AB	VA32A	2.578
1EMV	AB	VA35A	1.664
1EMV	AB	VB98A	1.089
1EMV	AB	YA52A	4.834
1EMV	AB	YA53A	4.634
1F47	AB	DA4A	0.691
1F47	AB	DA7A	1.733
1F47	AB	DA7G	1.139
1F47	AB	DA7S	2.064
1F47	AB	FA11A	2.444
1F47	AB	IA8A	2.515
1F47	AB	LA12A	2.294
1F47	AB	LA6A	0.925
1F47	AB	QA15A	-0.046
1F47	AB	YA5A	0.869
1FFW	AB	AA102V	1.363
1FFW	AB	AA89V	0.091
1FFW	AB	CB55A	0.204
1FFW	AB	DB49A	0.096
1FFW	AB	EB13A	0.716
1FFW	AB	EB20A	0.639
1FFW	AB	FB56A	3.644
1FFW	AB	HB23A	0.034
1FFW	AB	IB58A	0.428
1FFW	AB	YA105W	0.713
1FSS	AB	AB12S	0.324
1FSS	AB	HB29K	-0.619
1FSS	AB	HB29R	-1.272
1FSS	AB	KB32R	1.135
1FSS	AB	LB35W	1.451
1FSS	AB	MB33F	0.937
1FSS	AB	MB33L	0.963
1FSS	AB	MB33Q	1.572
1FSS	AB	MB33Y	1.395
1FSS	AB	NB47F	0.493
1FSS	AB	NB47R	-0.535
1FSS	AB	NB47W	0.116

1FSS	AB	RB11K	0.317
1FSS	AB	RB27F	2.435
1FSS	AB	RB27M	2.663
1FSS	AB	RB27Y	2.628
1FSS	AB	TB8V	-0.085
1FSS	AB	TB8V,TB9I	0.442
1FSS	AB	TB8V,TB9N	0.357
1FSS	AB	TB8V,TB9N,RB11K,HB29R	-0.392
1FSS	AB	TB9I	-0.232
1FSS	AB	TB9N	1.250
1FSS	AB	VB34T	1.585
1GC1	GC	DC63A	-0.319
1GC1	GC	EC85A	1.323
1GC1	GC	HC27A	0.282
1GC1	GC	KC29A	0.536
1GC1	GC	KC35A	0.322
1GC1	GC	KC46A	1.430
1GC1	GC	LC44A	1.055
1GC1	GC	NC32A	0.183
1GC1	GC	NC52A	0.708
1GC1	GC	QC25A	0.032
1GC1	GC	QC33A	0.105
1GC1	GC	QC40A	-0.410
1GC1	GC	QC40A,DC63A	-0.499
1GC1	GC	QC64A	0.442
1GC1	GC	RC59A	1.175
1GC1	GC	SC42A	0.000
1GC1	GC	SC60A	-0.089
1GC1	GC	TC45A	-0.149
1GUA	AB	EA37A	1.300
1GUA	AB	KB10A	-0.400
1GUA	AB	KB29A	1.998
1GUA	AB	KB32A	0.799
1GUA	AB	NB9A	-0.400
1GUA	AB	QB11A	0.100
1GUA	AB	RB4A	1.000
1GUA	AB	RB4A,EA37A	1.300
1GUA	AB	SA39A	1.400
1GUA	AB	TB13A	0.701
1GUA	AB	VB14A	0.100
1GUA	AB	VB14A,EA37A	1.700
1GUA	AB	VB33A	0.200
1IAR	AB	EA9Q	3.111
1IAR	AB	FA82A	-0.086
1IAR	AB	FA82D	-0.580
1IAR	AB	IA5A	1.171
1IAR	AB	IA5R	0.796
1IAR	AB	KA12E	0.139
1IAR	AB	KA12S	-0.015
1IAR	AB	NA89A	1.558
1IAR	AB	QA78A	0.125
1IAR	AB	QA78E	0.245
1IAR	AB	RA53Q	0.835
1IAR	AB	RA81A	0.479
1IAR	AB	RA81E	1.461
1IAR	AB	RA85A	0.427
1IAR	AB	RA85E	1.224
1IAR	AB	RA88A	3.753
1IAR	AB	RA88Q	2.828

1IAR	AB	TA13A	0.978
1IAR	AB	TA13D	-0.219
1IAR	AB	TA6A	-0.104
1IAR	AB	TA6D	1.392
1IAR	AB	WA91A	0.729
1IAR	AB	WA91D	1.306
1JCK	AB	FB176A	1.960
1JCK	AB	GB102A	0.013
1JCK	AB	KB103A	0.403
1JCK	AB	NB23A	2.076
1JCK	AB	NB60A	1.329
1JCK	AB	QB210A	2.076
1JCK	AB	TB20A	1.488
1JCK	AB	VB91A	2.081
1JCK	AB	YB26A	1.760
1JCK	AB	YB90A	2.335
1JTD	AB	DB14A	1.507
1JTD	AB	DB168A	-1.061
1JTD	AB	DB93A	1.989
1JTD	AB	EA78A	0.835
1JTD	AB	EA84A	0.038
1JTD	AB	EB230A	1.849
1JTD	AB	FB171A	2.200
1JTD	AB	FB192A	3.960
1JTD	AB	FB36A	2.550
1JTD	AB	IB191A	2.889
1JTD	AB	KA85A	2.129
1JTD	AB	LA76A	1.721
1JTD	AB	LB53A	0.667
1JTD	AB	MA103A	2.504
1JTD	AB	MA244A	0.276
1JTD	AB	NA74A	0.795
1JTD	AB	NB12A	1.301
1JTD	AB	NB266A	2.669
1JTD	AB	NB74A	1.209
1JTD	AB	PA81A	1.721
1JTD	AB	QA73A	0.515
1JTD	AB	RB248A	0.888
1JTD	AB	SB131A	0.152
1JTD	AB	TB19A	0.295
1JTD	AB	VA190A	0.038
1JTD	AB	WB114A	3.255
1JTD	AB	WB15A	1.392
1JTD	AB	WB231A	5.809
1JTD	AB	YA79A	2.235
1JTD	AB	YB153A	3.298
1JTD	AB	YB170A	2.026
1JTD	AB	YB210A	0.824
1JTD	AB	YB35A	3.150
1JTD	AB	YB75A	0.480
1JTG	AB	DB163A	-1.340
1JTG	AB	DB163K	-1.982
1JTG	AB	DB49A	2.347
1JTG	AB	DB49A,KA208A	1.600
1JTG	AB	DB49A,RA217A	1.099
1JTG	AB	DB49A,SA105A	0.358
1JTG	AB	EA143A	-0.073
1JTG	AB	EA143A,DB49A	1.504
1JTG	AB	EA143A,FB142A	2.580

1JTG	AB	EA143A,KB74A	4.060
1JTG	AB	EA143A,RB160A	2.318
1JTG	AB	EA143A,WB112A	2.794
1JTG	AB	EA143A,WB150A	4.108
1JTG	AB	EA143A,WB162A	2.076
1JTG	AB	EA143G	-0.170
1JTG	AB	EA213K	-0.410
1JTG	AB	EA79A	1.978
1JTG	AB	EA79A,EB73M	1.842
1JTG	AB	EA79A,EB73M,FB142A	2.854
1JTG	AB	EA79A,EB73M,KB74A	2.102
1JTG	AB	EA79A,EB73M,KB74A,FB142A	2.589
1JTG	AB	EA79A,SB113A	1.864
1JTG	AB	EA79A,SB113A,SB71A	2.580
1JTG	AB	EA79A,YA80A	1.026
1JTG	AB	EA79D	3.654
1JTG	AB	EA79K	3.239
1JTG	AB	EA79K,DB49A	5.638
1JTG	AB	EA79K,FB142A	4.552
1JTG	AB	EA85A	1.377
1JTG	AB	EA85A,SB113A	4.563
1JTG	AB	EA85A,SB113A,SB71A	5.040
1JTG	AB	EA85A,SB71A	5.017
1JTG	AB	EA85A,YB50A	3.965
1JTG	AB	EA85G	-0.912
1JTG	AB	EA85G,EA143G	-0.610
1JTG	AB	EA85V	-0.672
1JTG	AB	EA85V,EA143G	-0.742
1JTG	AB	EB31A	0.821
1JTG	AB	EB73A	0.435
1JTG	AB	EB73A,YB50A	-1.496
1JTG	AB	EB73M	0.506
1JTG	AB	EB73M,FB142A	2.540
1JTG	AB	EB73M,KB74A	4.307
1JTG	AB	EB73M,KB74A,FB142A	4.569
1JTG	AB	FB142A	2.804
1JTG	AB	FB142A,EA79A	2.747
1JTG	AB	FB142A,EA79A,YA80A	1.504
1JTG	AB	FB142A,KA208A	3.393
1JTG	AB	FB142A,RA217A	3.393
1JTG	AB	FB142A,SA105A	2.842
1JTG	AB	FB142A,YA80A	0.694
1JTG	AB	FB142A,YB143A	2.842
1JTG	AB	FB142A,YB143A,EA79A	2.890
1JTG	AB	FB142A,YB143A,EA79A,YA80A	2.842
1JTG	AB	FB142A,YB143A,KA208A	4.680
1JTG	AB	FB142A,YB143A,RA217A	4.541
1JTG	AB	FB142A,YB143A,SA105A	4.156
1JTG	AB	FB142A,YB143A,YA80A	2.985
1JTG	AB	FB36A	3.225
1JTG	AB	GA212S	-0.268
1JTG	AB	GA212S,DB49A	2.634
1JTG	AB	GA212S,FB142A	3.680
1JTG	AB	GB141A	1.330
1JTG	AB	GB48A	1.113
1JTG	AB	HB148A	2.907
1JTG	AB	HB41A	3.316
1JTG	AB	KA208A	1.222
1JTG	AB	KA208A,DB49A	1.553

1JTG	AB	KA208A,SA105A	1.979
1JTG	AB	KA208A,SA105A,DB49A	1.318
1JTG	AB	KA208A,SA105A,RA217A	2.508
1JTG	AB	KA208A,SA105A,RA217A,DB49A	1.490
1JTG	AB	KA208A,SA209A,SA105A,RA217A	2.787
1JTG	AB	KA208A,SA209A,SA105A,RA217A,DB49A	1.726
1JTG	AB	KA86A	-0.852
1JTG	AB	KA86N	0.181
1JTG	AB	KB74A	3.616
1JTG	AB	KB74A,EA79A	1.576
1JTG	AB	KB74A,EA79A,YA80A	1.385
1JTG	AB	KB74A,FB142A	4.850
1JTG	AB	KB74A,FB142A,EA79A	3.129
1JTG	AB	KB74A,FB142A,EA79A,YA80A	3.129
1JTG	AB	KB74A,FB142A,KA208A	5.828
1JTG	AB	KB74A,FB142A,RA217A	5.494
1JTG	AB	KB74A,FB142A,SA105A	5.159
1JTG	AB	KB74A,FB142A,YA80A	4.777
1JTG	AB	KB74A,FB142A,YB143A	3.893
1JTG	AB	KB74A,FB142A,YB143A,EA79A	2.388
1JTG	AB	KB74A,FB142A,YB143A,EA79A,YA80A	2.412
1JTG	AB	KB74A,FB142A,YB143A,KA208A	5.470
1JTG	AB	KB74A,FB142A,YB143A,RA217A	5.255
1JTG	AB	KB74A,FB142A,YB143A,SA105A	5.064
1JTG	AB	KB74A,FB142A,YB143A,YA80A	4.227
1JTG	AB	KB74A,KA208A	6.545
1JTG	AB	KB74A,RA217A	6.617
1JTG	AB	KB74A,SA105A	3.177
1JTG	AB	KB74A,YA80A	3.321
1JTG	AB	KB74A,YB143A	3.057
1JTG	AB	KB74A,YB143A,EA79A	1.050
1JTG	AB	KB74A,YB143A,EA79A,YA80A	1.767
1JTG	AB	KB74A,YB143A,KA208A	4.874
1JTG	AB	KB74A,YB143A,RA217A	4.371
1JTG	AB	KB74A,YB143A,SA105A	3.727
1JTG	AB	KB74A,YB143A,YA80A	3.393
1JTG	AB	LA77A	0.864
1JTG	AB	MA104A	1.119
1JTG	AB	MA104A,FB36A	3.629
1JTG	AB	MA104A,SB113A,SB71A	1.672
1JTG	AB	MA104A,YB50A	0.358
1JTG	AB	MA104A,YB53A	3.607
1JTG	AB	MA244A	-0.051
1JTG	AB	NA75A	-0.962
1JTG	AB	NA75A,DB49A	1.576
1JTG	AB	NA75A,FB142A	2.292
1JTG	AB	NA75A,HB148A	2.102
1JTG	AB	NA75A,KB74A	3.510
1JTG	AB	NA75A,RB160A	1.576
1JTG	AB	NA75A,WB112A	2.794
1JTG	AB	NA75A,WB150A	4.347
1JTG	AB	NA75A,WB162A	2.102
1JTG	AB	PA82A	-0.074
1JTG	AB	PA82A,HB41A	2.652
1JTG	AB	PA82A,YB50A	-0.647
1JTG	AB	PA82A,YB53A	2.388
1JTG	AB	PA82Q	0.461
1JTG	AB	QA74A	0.507
1JTG	AB	QA74A,DB49A	2.197

1JTG	AB	QA74A,FB142A	2.818
1JTG	AB	QA74A,HB148A	3.200
1JTG	AB	QA74A,KB74A	4.108
1JTG	AB	QA74A,RB160A	3.749
1JTG	AB	QA74A,WB112A	3.536
1JTG	AB	QA74A,WB150A	3.822
1JTG	AB	QA74A,WB162A	2.890
1JTG	AB	RA214Y	-0.143
1JTG	AB	RA217A	1.302
1JTG	AB	RA217A,DB49A	1.111
1JTG	AB	RA217A,KA208A	2.729
1JTG	AB	RA217A,KA208A,DB49A	1.903
1JTG	AB	RA217A,SA105A	1.849
1JTG	AB	RA217A,SA105A,DB49A	1.254
1JTG	AB	RA217A,SA209A	0.739
1JTG	AB	RA217A,SA209A,DB49A	0.408
1JTG	AB	RA217A,SA209A,KA208A	2.716
1JTG	AB	RA217A,SA209A,KA208A,DB49A	2.031
1JTG	AB	RA217A,SA209A,SA105A	1.687
1JTG	AB	RA217A,SA209A,SA105A,DB49A	0.894
1JTG	AB	RB144A	0.655
1JTG	AB	RB160A	2.736
1JTG	AB	SA105A	0.563
1JTG	AB	SA105A,DB49A	1.384
1JTG	AB	SA209A	1.238
1JTG	AB	SA209A,DB49A	1.640
1JTG	AB	SA209A,KA208A	2.093
1JTG	AB	SA209A,KA208A,DB49A	1.534
1JTG	AB	SA209A,SA105A	1.152
1JTG	AB	SA209A,SA105A,DB49A	1.094
1JTG	AB	SA209A,SA105A,KA208A	1.849
1JTG	AB	SA209A,SA105A,KA208A,DB49A	0.609
1JTG	AB	SB113A	-0.516
1JTG	AB	SB35A	0.000
1JTG	AB	SB39A	0.022
1JTG	AB	SB71A	0.139
1JTG	AB	SB71A,SB113A	0.456
1JTG	AB	TB140K	-0.014
1JTG	AB	VA190A	-0.493
1JTG	AB	VA190A,FB142A	2.197
1JTG	AB	VA190A,YB50A	-0.885
1JTG	AB	VA78A	1.910
1JTG	AB	VA78A,FB142A	4.514
1JTG	AB	VA78A,RB160A	4.347
1JTG	AB	VA78A,WB162A	4.227
1JTG	AB	WB112A	2.879
1JTG	AB	WB150A	4.314
1JTG	AB	WB162A	2.262
1JTG	AB	YA80A	-0.131
1JTG	AB	YB143A	0.710
1JTG	AB	YB143A,EA79A	1.864
1JTG	AB	YB143A,EA79A,YA80A	2.054
1JTG	AB	YB143A,KA208A	2.555
1JTG	AB	YB143A,RA217A	2.269
1JTG	AB	YB143A,SA105A	1.791
1JTG	AB	YB143A,YA80A	1.075
1JTG	AB	YB50A	-1.707
1JTG	AB	YB51A	0.799
1JTG	AB	YB53A	2.869

1KAC	AB	PA15S	-0.793
1KTZ	AB	DB8A	1.521
1KTZ	AB	DB8N	1.999
1KTZ	AB	EB31A	1.216
1KTZ	AB	EB95A	1.494
1KTZ	AB	EB95Q	1.626
1KTZ	AB	FB6A	2.979
1KTZ	AB	IB26A	1.896
1KTZ	AB	IB29A	1.370
1KTZ	AB	LB3A	1.824
1KTZ	AB	RA13A	1.481
1KTZ	AB	RA13K	1.151
1KTZ	AB	RA64A	2.883
1KTZ	AB	RA64K	2.200
1KTZ	AB	SB25A	0.326
1KTZ	AB	SB28A	0.216
1KTZ	AB	SB28L	4.036
1KTZ	AB	TB27A	1.513
1KTZ	AB	VA62I	0.243
1KTZ	AB	VB53A	0.415
1M9E	AD	AD76H	-1.009
1MAH	AF	WA276R	8.809
1MAH	AF	YA121Q	3.004
1MAH	AF	YA121Q,WA276R	9.706
1MAH	AF	YA69N	5.217
1MAH	AF	YA69N,WA276R	11.629
1MAH	AF	YA69N,YA121Q	6.644
1MAH	AF	YA69N,YA121Q,WA276R	11.837
1OHZ	AB	SB45A,TB46A	0.090
1P69	AB	SA15P	0.793
1P6A	AB	YA87S	1.252
1R0R	EI	AI10C	-0.477
1R0R	EI	AI10D	5.156
1R0R	EI	AI10D,LI13A	5.454
1R0R	EI	AI10D,LI13A,YI15D	8.820
1R0R	EI	AI10E	4.514
1R0R	EI	AI10F	-2.212
1R0R	EI	AI10G	1.096
1R0R	EI	AI10H	1.750
1R0R	EI	AI10I	-1.774
1R0R	EI	AI10K	3.030
1R0R	EI	AI10L	-1.731
1R0R	EI	AI10M	-1.715
1R0R	EI	AI10N	2.060
1R0R	EI	AI10P	3.299
1R0R	EI	AI10Q	1.786
1R0R	EI	AI10R	5.454
1R0R	EI	AI10R,LI13R	7.630
1R0R	EI	AI10R,TI12K,LI13R	9.171
1R0R	EI	AI10S	1.717
1R0R	EI	AI10T	1.250
1R0R	EI	AI10T,LI13M	0.255
1R0R	EI	AI10V	-0.956
1R0R	EI	AI10V,TI12S	0.093
1R0R	EI	AI10Y	-0.827
1R0R	EI	EI14A	2.060
1R0R	EI	EI14C	2.339
1R0R	EI	EI14D	0.255
1R0R	EI	EI14F	3.568

1R0R	EI	EI14G	2.674
1R0R	EI	EI14H	1.685
1R0R	EI	EI14I	0.727
1R0R	EI	EI14K	2.674
1R0R	EI	EI14L	0.562
1R0R	EI	EI14M	1.549
1R0R	EI	EI14N	2.089
1R0R	EI	EI14P	3.712
1R0R	EI	EI14Q	1.264
1R0R	EI	EI14R	2.060
1R0R	EI	EI14S	3.131
1R0R	EI	EI14T	4.193
1R0R	EI	EI14V	0.093
1R0R	EI	EI14W	1.824
1R0R	EI	EI14Y	1.864
1R0R	EI	KI8A	-0.602
1R0R	EI	KI8C	-0.607
1R0R	EI	KI8D	-0.585
1R0R	EI	KI8E	-0.109
1R0R	EI	KI8F	-0.783
1R0R	EI	KI8G	-0.827
1R0R	EI	KI8H	-0.585
1R0R	EI	KI8I	1.108
1R0R	EI	KI8L	-0.323
1R0R	EI	KI8M	-0.553
1R0R	EI	KI8N	-0.385
1R0R	EI	KI8P	1.329
1R0R	EI	KI8Q	-0.523
1R0R	EI	KI8R	0.134
1R0R	EI	KI8S	-0.303
1R0R	EI	KI8S,PI9D,AI10Y	-1.909
1R0R	EI	KI8S,PI9D,AI10Y,LI13G,EI14I,RI16K	0.790
1R0R	EI	KI8T	0.877
1R0R	EI	KI8T,PI9E,AI10Y	-0.864
1R0R	EI	KI8V	0.405
1R0R	EI	KI8W	-1.090
1R0R	EI	KI8Y	-0.686
1R0R	EI	LI13A	0.414
1R0R	EI	LI13C	-1.328
1R0R	EI	LI13D	4.476
1R0R	EI	LI13E	2.120
1R0R	EI	LI13F	0.608
1R0R	EI	LI13G	2.320
1R0R	EI	LI13H	0.562
1R0R	EI	LI13I	3.209
1R0R	EI	LI13K	3.051
1R0R	EI	LI13M	-0.509
1R0R	EI	LI13M,YI15Q	3.589
1R0R	EI	LI13N	1.480
1R0R	EI	LI13P	7.581
1R0R	EI	LI13Q	0.585
1R0R	EI	LI13R	2.895
1R0R	EI	LI13S	1.549
1R0R	EI	LI13T	0.158
1R0R	EI	LI13V	2.127
1R0R	EI	LI13W	1.503
1R0R	EI	LI13Y	0.441
1R0R	EI	PI9A	-0.630
1R0R	EI	PI9C	-0.973

1R0R	EI	PI9D	-2.486
1R0R	EI	PI9E	-2.212
1R0R	EI	PI9F	1.363
1R0R	EI	PI9G	-0.341
1R0R	EI	PI9H	-0.214
1R0R	EI	PI9I	1.717
1R0R	EI	PI9K	0.340
1R0R	EI	PI9L	1.168
1R0R	EI	PI9M	-0.033
1R0R	EI	PI9N	-0.905
1R0R	EI	PI9Q	-1.395
1R0R	EI	PI9R	1.087
1R0R	EI	PI9S	0.134
1R0R	EI	PI9S,AI10L,TI12K,LI13R	4.825
1R0R	EI	PI9T	1.181
1R0R	EI	PI9V	1.312
1R0R	EI	PI9W	0.479
1R0R	EI	PI9Y	0.846
1R0R	EI	RI16A	-0.095
1R0R	EI	RI16C	0.113
1R0R	EI	RI16D	-0.177
1R0R	EI	RI16E	0.340
1R0R	EI	RI16F	0.441
1R0R	EI	RI16G	2.060
1R0R	EI	RI16H	0.518
1R0R	EI	RI16I	0.204
1R0R	EI	RI16K	-0.095
1R0R	EI	RI16L	0.229
1R0R	EI	RI16M	0.441
1R0R	EI	RI16N	-0.050
1R0R	EI	RI16P	7.288
1R0R	EI	RI16Q	0.180
1R0R	EI	RI16S	-0.016
1R0R	EI	RI16T	0.340
1R0R	EI	RI16V	0.113
1R0R	EI	RI16W	0.932
1R0R	EI	RI16Y	0.812
1R0R	EI	TI12A	0.967
1R0R	EI	TI12C	0.802
1R0R	EI	TI12D	2.848
1R0R	EI	TI12E	2.976
1R0R	EI	TI12F	-0.065
1R0R	EI	TI12G	3.095
1R0R	EI	TI12H	0.518
1R0R	EI	TI12I	0.255
1R0R	EI	TI12K	1.907
1R0R	EI	TI12K,LI13R	5.186
1R0R	EI	TI12L	0.659
1R0R	EI	TI12M	1.312
1R0R	EI	TI12N	0.018
1R0R	EI	TI12P	4.881
1R0R	EI	TI12Q	2.191
1R0R	EI	TI12R	3.299
1R0R	EI	TI12R,LI13R	6.405
1R0R	EI	TI12S	0.847
1R0R	EI	TI12V	0.994
1R0R	EI	TI12W	2.895
1R0R	EI	TI12Y	-0.867
1R0R	EI	YI15A	5.398

1R0R	EI	YI15C	3.209
1R0R	EI	YI15D	5.544
1R0R	EI	YI15E	4.554
1R0R	EI	YI15F	0.608
1R0R	EI	YI15G	6.313
1R0R	EI	YI15H	3.212
1R0R	EI	YI15I	2.825
1R0R	EI	YI15K	5.436
1R0R	EI	YI15L	2.539
1R0R	EI	YI15M	3.095
1R0R	EI	YI15N	5.538
1R0R	EI	YI15P	6.562
1R0R	EI	YI15Q	4.440
1R0R	EI	YI15R	4.408
1R0R	EI	YI15S	5.091
1R0R	EI	YI15T	5.398
1R0R	EI	YI15V	3.461
1R0R	EI	YI15W	-0.359
1S0W	AC	AC142F	-2.102
1SBB	AB	LB20T	-0.100
1SBB	AB	LB20T,VB26Y,YB91V	0.132
1SBB	AB	VB26Y	-1.181
1SBB	AB	YB91V	0.085
1SBN	EI	RI38K	-0.310
1SGD	EI	DI13L	-5.590
1SGE	EI	EI13L	-5.899
1SGN	EI	NI13L	-3.352
1SGP	EI	AI13L	-2.948
1SGQ	EI	GI13L	-4.934
1SGY	EI	YI13L	-1.653
1TM1	EI	EI41A	2.988
1TM1	EI	EI41S	2.746
1TM1	EI	EI41S,MI40R	3.548
1TM1	EI	MI40A	1.027
1TM1	EI	MI40F	1.027
1TM1	EI	MI40G	2.232
1TM1	EI	MI40K	1.093
1TM1	EI	MI40Y	0.056
1TM1	EI	RI43A	1.256
1TM1	EI	TI39A	2.649
1TM1	EI	TI39A,EI41A	3.389
1TM1	EI	TI39D	2.098
1TM1	EI	TI39D,EI41A	0.754
1TM1	EI	TI39P	3.754
1TM1	EI	YI42A	2.579
1TM1	EI	YI42G	4.679
1TM3	EI	KI40M	-1.093
1TM4	EI	GI40M	-2.232
1TM5	EI	AI40M	-1.027
1TM7	EI	YI40M	-0.056
1TMG	EI	FI40M	-1.027
1TO1	EI	AI42Y	-2.980
1Y1K	EI	AI39T	-2.727
1Y33	EI	PI39T	-3.754
1Y34	EI	AI41E	-3.053
1Y3B	EI	SI41E	-2.746
1Y4A	EI	SI40E,RI39M	-3.548
2A9K	AB	EB65A	3.151
2A9K	AB	GB55D	2.410

2AJF	AE	DA20A	0.585
2AJF	AE	NE151K	2.012
2AJF	AE	TE159S	1.823
2AJF	AE	YA23A	1.452
2AJF	AE	YA23F	1.397
2B0Z	AB	IB87F	-2.528
2B10	AB	SB87F	-1.164
2B11	AB	WB87F	-0.754
2B42	AB	HA357A	1.621
2B42	AB	HA357Q	1.065
2BTF	AP	FP59A	1.595
2BTF	AP	GP120F	1.720
2BTF	AP	KP125A	0.460
2BTF	AP	VP60E	0.978
2DVW	AB	DA37A,DA69A	0.192
2DVW	AB	EA180A	0.438
2DVW	AB	EB21A,EB22A	0.038
2DVW	AB	KA114A	0.034
2DVW	AB	KB62E	0.205
2DVW	AB	RA39A	0.910
2DVW	AB	RA39A,KA114A	2.361
2DVW	AB	RB3A,RB4A,RB7A	2.789
2DVW	AB	RB3A,RB7A	2.152
2DVW	AB	RB7A	0.693
2G2U	AB	DA79A	-1.548
2G2U	AB	DA79A,EB73M	-2.153
2G2U	AB	DA79A,EB73M,FB142A	-0.694
2G2U	AB	DA79A,EB73M,KB74A	-1.561
2G2U	AB	DA79A,EB73M,KB74A,FB142A	-0.990
2G2U	AB	DA79E	-4.397
2G2U	AB	DA79K	-0.563
2G2U	AB	EB31A	0.651
2G2U	AB	EB73A	-1.978
2G2U	AB	EB73A,YB143A	-1.835
2G2U	AB	EB73A,YB50A	-2.451
2G2U	AB	EB73M	-3.004
2G2U	AB	EB73M,FB142A	0.323
2G2U	AB	EB73M,FB142W,YB143F	-1.108
2G2U	AB	EB73M,KB74A	0.474
2G2U	AB	EB73M,KB74A,FB142A	1.487
2G2U	AB	EB73M,YB143F	-1.592
2G2U	AB	FB142A	0.276
2G2U	AB	FB36A	2.763
2G2U	AB	GB141A	-0.414
2G2U	AB	GB48A	-0.426
2G2U	AB	HB148A	1.118
2G2U	AB	HB41A	1.716
2G2U	AB	KB74A	-0.217
2G2U	AB	RB144A	-0.342
2G2U	AB	RB160A	0.669
2G2U	AB	SB113A	-0.612
2G2U	AB	SB35A	-0.950
2G2U	AB	SB39A	-0.956
2G2U	AB	SB71A	-0.512
2G2U	AB	WB112A	0.958
2G2U	AB	WB112A,YB143A	-0.409
2G2U	AB	WB150A	1.784
2G2U	AB	WB150A,YB143A	0.989
2G2U	AB	WB162A	0.531

2G2U	AB	YB143A	-1.846
2G2U	AB	YB50A	-2.075
2G2U	AB	YB50A,YB143A	-2.075
2G2U	AB	YB51A	-0.628
2G2U	AB	YB53A	2.301
2G2W	AB	KA79D	0.453
2GOX	AB	NB38A	1.451
2GOX	AB	RB31A	1.883
2HLE	AB	KA141Q	-0.410
2HLE	AB	LA87R	2.286
2J0T	AD	CD70S	4.408
2J0T	AD	MD66A	1.680
2J0T	AD	SD68A	2.105
2J0T	AD	SD68E	2.184
2J0T	AD	SD68R	2.835
2J0T	AD	SD68Y	2.977
2J0T	AD	TD2A	4.388
2J0T	AD	TD2L	2.681
2J0T	AD	TD2L,VD4S	3.469
2J0T	AD	TD2R	5.043
2J0T	AD	TD2S	1.594
2J0T	AD	TD2S,VD4A	1.250
2J0T	AD	TD2S,VD4A,SD68Y	2.146
2J0T	AD	VD4A	0.000
2J0T	AD	VD4I	1.642
2J0T	AD	VD4K	1.824
2J0T	AD	VD4S	0.982
2J0T	AD	VD69I	0.809
2J0T	AD	VD69T	1.318
2J1K	CT	GC10D	0.184
2J1K	CT	RC24A	0.764
2NOJ	AB	RB24A,NB31A	0.748
2NU0	EI	WI13L	-1.839
2NU1	EI	HI13L	-1.690
2NU2	EI	RI13L	-3.320
2NU4	EI	KI13L	-3.138
2PCB	AB	DA34N	0.821
2PCB	AB	EA290N	0.871
2PCB	AB	EA32Q	0.605
2PCB	AB	EA35Q	0.676
2PCC	AB	AB86G	1.901
2PCC	AB	AB86G,DA34A	-0.098
2PCC	AB	AB86G,VA197A	2.102
2PCC	AB	DA34A	-0.897
2PCC	AB	EA290A	6.199
2PCC	AB	KB77A	0.304
2PCC	AB	KB77A,EA290A	1.102
2PCC	AB	KB77A,VA197A	2.800
2PCC	AB	KB92A	0.901
2PCC	AB	KB92A,DA34A	0.203
2PCC	AB	KB92A,VA197A	1.501
2PCC	AB	VA197A	2.102
2REX	AB	LA70Y	0.557
2REX	AB	YB97F	0.000
2SGP	EI	PI13L	-8.328
2SGQ	EI	QI13L	-2.567
2SIC	EI	MI67A	0.218
2SIC	EI	MI67D	0.751
2SIC	EI	MI67E	0.796

2SIC	EI	MI67G	0.145
2SIC	EI	MI67H	0.218
2SIC	EI	MI67I	1.604
2SIC	EI	MI67K	0.000
2SIC	EI	MI67L	-0.240
2SIC	EI	MI67R	0.000
2SIC	EI	MI67V	0.713
2VLN	AB	AB75N	-2.334
2VLQ	AB	AB86F	-3.879
2VN5	AB	AB14S,LB15T	1.318
2WPT	AB	DA30A	-0.776
2WPT	AB	DA30A,FB79A	-0.165
2WPT	AB	DA30L	-3.402
2WPT	AB	DA30L,NA31V,RA35T	-6.333
2WPT	AB	DA48A	5.214
2WPT	AB	EA27A	1.733
2WPT	AB	EA38A	4.501
2WPT	AB	FB79A	1.594
2WPT	AB	FB79A,DA30A	-0.132
2WPT	AB	FB79A,NA31A	1.352
2WPT	AB	FB79A,VA34A	3.111
2WPT	AB	KB90A	0.649
2WPT	AB	NA31A	-0.259
2WPT	AB	NA31V	-0.897
2WPT	AB	NA31V,RA35T	-2.587
2WPT	AB	NB65A	0.701
2WPT	AB	NB68A	1.251
2WPT	AB	PA53A	2.926
2WPT	AB	QB85A	0.384
2WPT	AB	RA35A	-1.110
2WPT	AB	RA35T	-1.038
2WPT	AB	RB47A	0.872
2WPT	AB	SA47A	2.424
2WPT	AB	SB67A	-0.134
2WPT	AB	SB70A	-0.457
2WPT	AB	SB71A	-0.095
2WPT	AB	SB77A	-0.074
2WPT	AB	SB77A,NA31A	-0.437
2WPT	AB	TB80A	0.377
2WPT	AB	VA34A	3.807
2WPT	AB	YA51A	5.214
2WPT	AB	YA52A	5.214
3BK3	AC	AC37R	1.382
3BK3	AC	IC19A	0.486
3BK3	AC	IC19R	0.424
3BK3	AC	IC22A	1.307
3BK3	AC	IC22R	2.120
3BK3	AC	IC28A	1.261
3BK3	AC	IC28R	1.175
3BK3	AC	IC3A	1.038
3BK3	AC	IC3R	0.651
3BK3	AC	LC2A	0.000
3BK3	AC	LC2R	0.026
3BK3	AC	TC4P	0.486
3BK3	AC	TC6P	1.742
3BP8	AC	AC51F	0.615
3BP8	AC	FA115A	0.709
3BP8	AC	FA115A,AC51F	-0.774
3BT1	AU	AU253S	0.201

3BT1	AU	DU11A	-0.026
3BT1	AU	DU138A	1.274
3BT1	AU	DU139A	1.030
3BT1	AU	DU252A	0.060
3BT1	AU	EU33A	0.371
3BT1	AU	EU36A	0.093
3BT1	AU	EU42A	-0.193
3BT1	AU	EU68A	0.049
3BT1	AU	GU10A	0.261
3BT1	AU	HU164A	1.011
3BT1	AU	KU137A	0.641
3BT1	AU	KU50A	0.631
3BT1	AU	KU62A	0.410
3BT1	AU	LU142A	0.711
3BT1	AU	LU148A	1.634
3BT1	AU	LU166A	0.733
3BT1	AU	LU31A	0.307
3BT1	AU	LU38A	0.513
3BT1	AU	LU40A	0.856
3BT1	AU	LU55A	1.092
3BT1	AU	LU66A	1.353
3BT1	AU	NU9A	0.300
3BT1	AU	PU136A	0.329
3BT1	AU	PU149A	0.587
3BT1	AU	RU25A	0.999
3BT1	AU	RU53A	0.873
3BT1	AU	SU99A	0.292
3BT1	AU	TU125A	0.986
3BT1	AU	TU27A	0.895
3BT1	AU	TU54A	0.384
3BT1	AU	TU64A	0.648
3BT1	AU	TU67A	0.183
3BT1	AU	TU8A	0.174
3BT1	AU	VU124A	0.733
3BT1	AU	VU29A	0.704
3BT1	AU	YU57A	1.180
3BX1	AC	AC86T	1.836
3BX1	AC	FC84V	0.410
3BX1	AC	RC85G	0.355
3BX1	AC	TC88V	2.837
3BX1	AC	TC89A	0.170
3BX1	AC	YC87A	1.298
3BX1	AC	YC87I	1.781
3D5R	AC	AC38N	-1.451
3D5S	AC	AC31R	-1.883
3F1S	AB	DA200A	0.554
3F1S	AB	DA255A	3.759
3F1S	AB	DA36A	2.184
3F1S	AB	KA201A	-2.079
3F1S	AB	KA201C	-1.694
3F1S	AB	MA33A	1.238
3F1S	AB	YA202A	2.995
3KBH	AE	SE54A	1.856
3KBH	AE	SE54T	2.489
3KBH	AE	YA23A	1.812
3KBH	AE	YA23F	1.615
3KBH	AE	YE17A	0.100
3LB6	AC	FA103A	5.115
3LB6	AC	IA10A	3.721

3LB6	AC	KA100A	5.812
3LB6	AC	KA101A	2.544
3M62	AB	DA46A	2.799
3M62	AB	EA32A	0.829
3M62	AB	EA55A	1.051
3M62	AB	FB7A	0.995
3M62	AB	GA102A	1.264
3M62	AB	IA110A	1.853
3M62	AB	IB43A	2.882
3M62	AB	LA50A	2.828
3M62	AB	MB69A	0.681
3M62	AB	QB50A	1.054
3M62	AB	QB65A	0.284
3M62	AB	RA98A	0.788
3M62	AB	SB45A	1.278
3M62	AB	TA54A	0.017
3M62	AB	VB48A	1.090
3M62	AB	VB67A	1.138
3M62	AB	YA103A	4.475
3M63	AB	DA46A	2.233
3M63	AB	EA55A	0.346
3M63	AB	FA113A	1.791
3M63	AB	GA102A	0.125
3M63	AB	IA110A	1.089
3M63	AB	LA50A	0.576
3M63	AB	RA98A	-0.185
3M63	AB	TA54A	0.311
3M63	AB	VA106A	1.838
3M63	AB	YA103A	3.649
3MZG	AB	HA14A	-0.019
3MZG	AB	HA167A	1.487
3MZG	AB	HA167A,HB188A	2.653
3MZG	AB	HA17A	0.062
3MZG	AB	HB188A	1.776
3N06	AB	AA14H	0.019
3NCB	AB	AA167H	-1.487
3NCC	AB	AB188H	-1.776
3NVN	BA	RA193E	2.527
3NVN	BA	RB186S	1.289
3NVQ	BA	RA157E	1.571
3NVQ	BA	RA159E	1.586
3Q3J	AB	YB100F	0.211
3QHY	AB	DB127A	0.380
3QHY	AB	DB12A	2.254
3QHY	AB	DB130A	0.961
3QHY	AB	DB166A	3.496
3QHY	AB	DB91A	1.888
3QHY	AB	EB228A	3.011
3QHY	AB	FB169A	2.061
3QHY	AB	FB190A	3.074
3QHY	AB	FB34A	3.982
3QHY	AB	IB189A	3.066
3QHY	AB	LB51A	0.816
3QHY	AB	NB10A	2.254
3QHY	AB	NB264A	2.695
3QHY	AB	NB72A	1.605
3QHY	AB	RB246A	0.535
3QHY	AB	WB112A	3.788
3QHY	AB	WB13A	2.862

3QHY	AB	WB229A	5.430
3QHY	AB	YB151A	3.422
3QHY	AB	YB168A	1.743
3QHY	AB	YB208A	0.240
3QHY	AB	YB33A	2.902
3QHY	AB	YB73A	0.801
3RF3	AC	AC8K	1.728
3S9D	AB	AA116G	2.118
3S9D	AB	AA116M	1.073
3S9D	AB	AA12W	-0.181
3S9D	AB	AB67M	-0.168
3S9D	AB	DA28A	0.301
3S9D	AB	EB39A	0.206
3S9D	AB	EB39R	0.651
3S9D	AB	EB66A	2.414
3S9D	AB	EB66A,AA116G	5.039
3S9D	AB	EB66A,LA124A	3.768
3S9D	AB	EB66A,LA23A	6.055
3S9D	AB	EB66A,LA8A	4.090
3S9D	AB	EB66A,MA119A	4.978
3S9D	AB	EB66A,RA120A	3.631
3S9D	AB	EB66A,SA123A	3.542
3S9D	AB	FA20A	0.710
3S9D	AB	HA27A	0.541
3S9D	AB	HB166A	0.000
3S9D	AB	HB65A	0.823
3S9D	AB	HB65A,LA124A	2.938
3S9D	AB	HB65A,LA19A	3.055
3S9D	AB	HB65A,LA8A	4.015
3S9D	AB	HB65A,RA120A	3.844
3S9D	AB	HB65A,RA5A	2.213
3S9D	AB	HB65A,SA123A	1.135
3S9D	AB	IB34A	1.852
3S9D	AB	IB34A,AA116G	4.472
3S9D	AB	IB34A,LA124A	3.560
3S9D	AB	IB34A,MA119A	4.233
3S9D	AB	IB34A,RA120A	4.999
3S9D	AB	IB34A,SA123A	3.005
3S9D	AB	IB90A	1.617
3S9D	AB	IB90A,FA20A	2.815
3S9D	AB	IB90A,LA124A	3.345
3S9D	AB	IB90A,LA19A	3.034
3S9D	AB	IB90A,LA23A	5.447
3S9D	AB	IB90A,LA8A	3.739
3S9D	AB	IB90A,MA119A	4.033
3S9D	AB	IB90A,RA120A	4.906
3S9D	AB	IB90A,SA123A	3.255
3S9D	AB	KB37A	0.504
3S9D	AB	LA124A	1.447
3S9D	AB	LA19A	1.105
3S9D	AB	LA23A	3.808
3S9D	AB	LA23V	2.436
3S9D	AB	LA8A	1.536
3S9D	AB	MA119A	2.253
3S9D	AB	MA9A	0.062
3S9D	AB	MB35A	2.998
3S9D	AB	MB35V	2.374
3S9D	AB	MB35V,AA116G	5.298
3S9D	AB	MB35V,LA124A	4.531

3S9D	AB	MB35V,LA19A	4.315
3S9D	AB	MB35V,LA23A	7.110
3S9D	AB	MB35V,LA8A	4.425
3S9D	AB	MB35V,MA119A	5.454
3S9D	AB	MB35V,RA120A	6.064
3S9D	AB	MB35V,SA123A	4.078
3S9D	AB	NA127A	-0.043
3S9D	AB	NB85A	-0.171
3S9D	AB	RA120A	3.021
3S9D	AB	RA120A,EB66A	3.601
3S9D	AB	RA15A	0.195
3S9D	AB	RA26A	5.123
3S9D	AB	RA26K	4.586
3S9D	AB	RA26Q	6.079
3S9D	AB	RA5A	0.622
3S9D	AB	SA123A	1.122
3S9D	AB	SA18A	-0.099
3S9D	AB	SB36A	0.505
3S9D	AB	TB33A	1.730
3S9D	AB	TB33A,AA116G	4.349
3S9D	AB	TB33A,FA20A	3.020
3S9D	AB	TB33A,LA124A	3.311
3S9D	AB	TB33A,LA19A	3.393
3S9D	AB	TB33A,LA23A	5.958
3S9D	AB	TB33A,LA8A	3.577
3S9D	AB	TB33A,MA119A	4.462
3S9D	AB	TB33A,RA120A	5.266
3S9D	AB	TB33A,SA123A	3.062
3S9D	AB	VB69A	2.317
3S9D	AB	WB87A	1.112
3S9D	AB	WB87A,LA124A	2.943
3S9D	AB	WB87A,LA8A	3.075
3S9D	AB	WB87A,MA119A	3.844
3S9D	AB	WB87A,RA5A	2.340
3S9D	AB	WB87A,SA123A	2.750
3SGB	EI	AI9C	0.041
3SGB	EI	AI9D	0.470
3SGB	EI	AI9D,GI26A	1.066
3SGB	EI	AI9D,GI26A,NI27S	2.153
3SGB	EI	AI9D,LI12A	2.583
3SGB	EI	AI9D,LI12A,YI14D	5.688
3SGB	EI	AI9E	0.662
3SGB	EI	AI9F	-1.164
3SGB	EI	AI9G	2.452
3SGB	EI	AI9H	-0.447
3SGB	EI	AI9I	-0.447
3SGB	EI	AI9K	2.457
3SGB	EI	AI9L	0.166
3SGB	EI	AI9M	0.088
3SGB	EI	AI9N	-0.088
3SGB	EI	AI9P	0.545
3SGB	EI	AI9Q	0.424
3SGB	EI	AI9R	2.007
3SGB	EI	AI9R,LI12R	5.077
3SGB	EI	AI9R,TI11K,LI12R	6.686
3SGB	EI	AI9R,TI11K,LI12R,EI13S	7.095
3SGB	EI	AI9R,TI11K,LI12R,RI15L	6.885
3SGB	EI	AI9R,TI11P,LI12R	8.449
3SGB	EI	AI9S	0.898

3SGB	EI	AI9T	0.326
3SGB	EI	AI9T,LI12M	0.470
3SGB	EI	AI9V	-0.712
3SGB	EI	AI9V,TI11S	1.585
3SGB	EI	AI9W	-1.532
3SGB	EI	AI9Y	-1.624
3SGB	EI	EI13A	1.005
3SGB	EI	EI13C	1.158
3SGB	EI	EI13D	0.545
3SGB	EI	EI13F	1.917
3SGB	EI	EI13G	2.076
3SGB	EI	EI13H	0.519
3SGB	EI	EI13I	-0.615
3SGB	EI	EI13K	0.166
3SGB	EI	EI13L	0.768
3SGB	EI	EI13M	-0.187
3SGB	EI	EI13N	1.087
3SGB	EI	EI13P	2.243
3SGB	EI	EI13Q	0.181
3SGB	EI	EI13R	1.257
3SGB	EI	EI13S	1.917
3SGB	EI	EI13T	2.114
3SGB	EI	EI13V	0.126
3SGB	EI	EI13W	1.526
3SGB	EI	EI13Y	0.768
3SGB	EI	GI26A	1.276
3SGB	EI	GI26C	2.575
3SGB	EI	GI26D	1.602
3SGB	EI	GI26E	1.945
3SGB	EI	GI26F	2.980
3SGB	EI	GI26H	2.700
3SGB	EI	GI26I	4.036
3SGB	EI	GI26K	2.490
3SGB	EI	GI26L	2.621
3SGB	EI	GI26M	2.755
3SGB	EI	GI26N	2.243
3SGB	EI	GI26P	1.082
3SGB	EI	GI26Q	2.915
3SGB	EI	GI26R	3.459
3SGB	EI	GI26S	1.585
3SGB	EI	GI26T	2.992
3SGB	EI	GI26V	2.788
3SGB	EI	GI26W	3.858
3SGB	EI	GI26Y	3.053
3SGB	EI	KI7A	-2.536
3SGB	EI	KI7C	-0.577
3SGB	EI	KI7D	-0.615
3SGB	EI	KI7E	0.032
3SGB	EI	KI7F	-0.715
3SGB	EI	KI7G	-0.715
3SGB	EI	KI7H	-0.396
3SGB	EI	KI7I	-1.326
3SGB	EI	KI7L	-1.792
3SGB	EI	KI7M	-1.150
3SGB	EI	KI7N	-0.650
3SGB	EI	KI7P	0.000
3SGB	EI	KI7Q	-0.615
3SGB	EI	KI7R	-0.683
3SGB	EI	KI7R,AI9R,TI11K,LI12R	5.515

3SGB	EI	KI7R,PI8F,AI9R,TI11K,LI12R	5.656
3SGB	EI	KI7S	-2.552
3SGB	EI	KI7S,PI8D,AI9Y	-4.094
3SGB	EI	KI7S,PI8D,AI9Y,LI12G,EI13I,RI15K	0.095
3SGB	EI	KI7T	-1.922
3SGB	EI	KI7T,PI8E,AI9Y	-3.817
3SGB	EI	KI7T,PI8E,AI9Y,LI12G,RI15M,GI26P,NI30V	1.828
3SGB	EI	KI7V	-0.942
3SGB	EI	KI7W	-0.013
3SGB	EI	KI7Y	-0.577
3SGB	EI	LI12A	2.931
3SGB	EI	LI12C	-0.013
3SGB	EI	LI12D	5.590
3SGB	EI	LI12E	6.089
3SGB	EI	LI12F	1.355
3SGB	EI	LI12G	4.934
3SGB	EI	LI12H	1.690
3SGB	EI	LI12I	4.419
3SGB	EI	LI12I,GI26D	5.764
3SGB	EI	LI12K	3.138
3SGB	EI	LI12M	0.447
3SGB	EI	LI12M,GI26D	2.243
3SGB	EI	LI12M,YI14Q	3.724
3SGB	EI	LI12N	3.352
3SGB	EI	LI12P	8.328
3SGB	EI	LI12Q	2.510
3SGB	EI	LI12R	3.320
3SGB	EI	LI12S	4.100
3SGB	EI	LI12T	3.160
3SGB	EI	LI12V	2.992
3SGB	EI	LI12W	1.839
3SGB	EI	LI12Y	1.653
3SGB	EI	NI30A	0.326
3SGB	EI	NI30C	0.345
3SGB	EI	NI30D	0.898
3SGB	EI	NI30E	0.949
3SGB	EI	NI30F	-0.139
3SGB	EI	NI30G	0.307
3SGB	EI	NI30H	-0.123
3SGB	EI	NI30I	0.195
3SGB	EI	NI30K	0.571
3SGB	EI	NI30L	0.730
3SGB	EI	NI30M	0.139
3SGB	EI	NI30P	0.571
3SGB	EI	NI30Q	0.240
3SGB	EI	NI30R	0.571
3SGB	EI	NI30S	0.403
3SGB	EI	NI30T	0.010
3SGB	EI	NI30V	-0.239
3SGB	EI	NI30W	0.519
3SGB	EI	NI30Y	-0.107
3SGB	EI	PI8A	-0.187
3SGB	EI	PI8C	-0.323
3SGB	EI	PI8D	-1.019
3SGB	EI	PI8E	-0.615
3SGB	EI	PI8F	-0.340
3SGB	EI	PI8G	0.053
3SGB	EI	PI8H	0.274
3SGB	EI	PI8I	-0.023

3SGB	EI	PI8K	0.112
3SGB	EI	PI8L	-0.139
3SGB	EI	PI8M	-0.494
3SGB	EI	PI8N	-0.123
3SGB	EI	PI8Q	-0.312
3SGB	EI	PI8R	0.307
3SGB	EI	PI8S	0.065
3SGB	EI	PI8S,AI9L,TI11K,LI12R	4.906
3SGB	EI	PI8S,AI9R,TI11P,LI12R	8.102
3SGB	EI	PI8T	-0.107
3SGB	EI	PI8V	-0.306
3SGB	EI	PI8W	-0.494
3SGB	EI	PI8Y	-0.396
3SGB	EI	RI15A	0.053
3SGB	EI	RI15C	0.545
3SGB	EI	RI15D	0.630
3SGB	EI	RI15E	0.662
3SGB	EI	RI15F	0.225
3SGB	EI	RI15G	1.092
3SGB	EI	RI15H	0.447
3SGB	EI	RI15I	0.240
3SGB	EI	RI15K	-0.274
3SGB	EI	RI15L	0.225
3SGB	EI	RI15M	0.126
3SGB	EI	RI15N	0.326
3SGB	EI	RI15P	7.578
3SGB	EI	RI15Q	0.041
3SGB	EI	RI15S	0.274
3SGB	EI	RI15T	0.447
3SGB	EI	RI15V	-0.023
3SGB	EI	RI15W	0.307
3SGB	EI	RI15Y	0.290
3SGB	EI	TI11A	3.363
3SGB	EI	TI11C	2.886
3SGB	EI	TI11D	4.887
3SGB	EI	TI11E	4.564
3SGB	EI	TI11F	3.589
3SGB	EI	TI11G	5.507
3SGB	EI	TI11H	3.459
3SGB	EI	TI11I	1.729
3SGB	EI	TI11K	2.007
3SGB	EI	TI11K,LI12R	5.233
3SGB	EI	TI11L	2.437
3SGB	EI	TI11M	2.007
3SGB	EI	TI11M,LI12S,GI26V	6.814
3SGB	EI	TI11N	3.209
3SGB	EI	TI11P	3.138
3SGB	EI	TI11P,LI12K	6.232
3SGB	EI	TI11P,LI12K,GI26D	6.452
3SGB	EI	TI11Q	2.899
3SGB	EI	TI11R	1.945
3SGB	EI	TI11R,LI12R	5.475
3SGB	EI	TI11S	2.468
3SGB	EI	TI11V	2.228
3SGB	EI	TI11W	2.992
3SGB	EI	TI11Y	3.320
3SGB	EI	YI14A	1.917
3SGB	EI	YI14C	1.672
3SGB	EI	YI14D	2.825

3SGB	EI	YI14E	2.007
3SGB	EI	YI14F	0.166
3SGB	EI	YI14G	2.803
3SGB	EI	YI14H	1.538
3SGB	EI	YI14I	3.542
3SGB	EI	YI14K	3.385
3SGB	EI	YI14L	1.554
3SGB	EI	YI14M	1.975
3SGB	EI	YI14N	3.115
3SGB	EI	YI14P	6.189
3SGB	EI	YI14Q	3.235
3SGB	EI	YI14R	2.722
3SGB	EI	YI14S	2.007
3SGB	EI	YI14T	4.804
3SGB	EI	YI14V	4.360
3SGB	EI	YI14W	0.383
3WWN	AB	KA225E	0.175
3WWN	AB	RA221E	-0.376
4BFI	AB	FB95A	2.076
4BFI	AB	FB95D	2.727
4BFI	AB	KB99E	2.317
4BFI	AB	LB29K	2.076
4BFI	AB	LB91A	1.307
4BFI	AB	NB43A	2.317
4BFI	AB	NB43D	2.727
4BFI	AB	NB93K	2.727
4CPA	AI	PI35G	2.595
4CPA	AI	VI37A	2.324
4CPA	AI	VI37F	0.000
4CPA	AI	VI37G	3.733
4CPA	AI	VI37I	0.199
4CPA	AI	VI37L	1.279
4CPA	AI	YI36F	0.000
4CPA	AI	YI36G	0.502
4CVW	AC	DA720R	3.046
4CVW	AC	DA720W	1.221
4CVW	AC	LC34G	2.727
4CVW	AC	LC34G,VC35D	7.742
4CVW	AC	LC34W	0.335
4CVW	AC	RC27A	1.828
4CVW	AC	RC31A	2.076
4CVW	AC	RC31W	1.490
4CVW	AC	VC35D	4.918
4FZA	AB	EB122A	0.425
4FZA	AB	FA168E	0.543
4FZA	AB	RA217A	1.027
4FZA	AB	YA213A	1.270
4GU0	AE	LE20A,TE22A,RE26A	0.894
4HRN	AD	FD47A	2.459
4HRN	AD	LD17A	2.597
4HRN	AD	SD43A	0.803
4HRN	AD	VD44A	2.811
4L0P	AB	EA27K	2.665
4L0P	AB	TA76Q	1.471
4NZW	AB	EB124A	0.357
4NZW	AB	EB49A	0.325
4NZW	AB	KA77A	0.076
4O27	AB	EB42A	0.371
4O27	AB	YA215A	1.195

4OFY	AD	DA38A	0.549
4OFY	AD	EA88A	0.282
4OFY	AD	FA40A	4.602
4OFY	AD	LD42A	2.567
4OFY	AD	MA36A	0.084
4OFY	AD	QA34A	1.176
4OFY	AD	QA34A,FA40A	4.139
4OFY	AD	QA34A,MA36A,FA40A,SA87A	4.459
4OFY	AD	QA85A	1.732
4OFY	AD	QD34A	2.869
4OFY	AD	QD86A	4.643
4OFY	AD	RD96A	3.419
4OFY	AD	SA87A	0.142
4Y61	AB	FB219A,HB222A	0.289
4Y61	AB	RB86A	-0.193
4Y61	AB	YA246A	-0.078
4YFD	AB	DB7A	-0.055
4YFD	AB	EA259A	1.216
4YFD	AB	KB71A	1.474
4YFD	AB	RA169A	0.159
4YFD	AB	WB4A	1.132
4YH7	AB	DB7A	1.642
4YH7	AB	RA169A	1.438
4YH7	AB	YA246A	1.034
5E6P	AB	AA494E	1.099
5E6P	AB	AA495E	1.577
5E6P	AB	IB22A	0.274
5E6P	AB	LB24A	0.913
5E6P	AB	RB42A	0.677
5E6P	AB	RB42E	1.744
5E6P	AB	YA468A	0.358
5K39	AB	FB142A	2.898
5K39	AB	IB148A	2.190
5K39	AB	MB108A	-0.510
5K39	AB	MB112A	-0.249
5M2O	AB	EA80A	0.723
5M2O	AB	EA80A,HA117A	2.614
5M2O	AB	EA80A,NA120A	1.251
5M2O	AB	HA117A	0.912
5M2O	AB	HA117A,NA120A	2.416
5M2O	AB	IB17A	2.093
5M2O	AB	KA73A	-0.782
5M2O	AB	KB32A	1.099
5M2O	AB	LA75A	1.681
5M2O	AB	LB65A	0.879
5M2O	AB	NA120A	0.465
5M2O	AB	NA64A	0.043
5M2O	AB	NA71A	0.160
5M2O	AB	NA71A,EA80A	1.063
5M2O	AB	NA71A,HA117A	2.362
5M2O	AB	NA71A,NA120A	2.541
5M2O	AB	QB25A	1.183
5M2O	AB	QB61A	-0.163
5M2O	AB	SB18A	0.049
5M2O	AB	VB21A	2.525
5M2O	AB	VB21A,QB25A	3.427

Table S7. Experimental data for TestSet1.

PDB	Chains	Mutations	Experimental $\Delta\Delta G_{bind}$
1A4Y	AB	DA435A	3.484
1A4Y	AB	EA344A	0.179
1A4Y	AB	EA401A	0.883
1A4Y	AB	EB108A	-0.323
1A4Y	AB	HB114A	0.656
1A4Y	AB	HB13A	-0.297
1A4Y	AB	HB84A	0.170
1A4Y	AB	HB8A	0.904
1A4Y	AB	IA459A	0.679
1A4Y	AB	KA320A	-0.310
1A4Y	AB	KB40G	3.235
1A4Y	AB	KB40G,DA435A	4.105
1A4Y	AB	KB40G,YA434A,DA435A	6.211
1A4Y	AB	KB40G,YA434A,YA437A	9.119
1A4Y	AB	KB40G,YA434F	6.662
1A4Y	AB	KB40G,YA437A	6.451
1A4Y	AB	KB40Q	4.250
1A4Y	AB	NB68A	0.118
1A4Y	AB	QA430A,VA432A	0.072
1A4Y	AB	QB12A	0.300
1A4Y	AB	RB31A	0.250
1A4Y	AB	RB32A	0.910
1A4Y	AB	RB5A	2.308
1A4Y	AB	RB5A,DA435A	6.770
1A4Y	AB	RB5A,YA434A	6.976
1A4Y	AB	RB5A,YA434A,DA435A	10.102
1A4Y	AB	RB5A,YA434A,YA437A	8.527
1A4Y	AB	SA289A	0.042
1A4Y	AB	WA261A	0.101
1A4Y	AB	WA263A	1.171
1A4Y	AB	WA318A	1.500
1A4Y	AB	WA375A	1.035
1A4Y	AB	WA438A,SA439A,EA440A	1.785
1A4Y	AB	WB89A	0.240
1A4Y	AB	YA434A	3.260
1A4Y	AB	YA434A,DA435A	6.817
1A4Y	AB	YA434A,YA437A	6.642
1A4Y	AB	YA434F	0.558
1A4Y	AB	YA437A	0.836
1A4Y	AB	YA437F	0.245
1ACB	EI	LI38D	6.771
1ACB	EI	LI38E	6.554
1ACB	EI	LI38G	6.033
1ACB	EI	LI38I	4.230
1ACB	EI	LI38P	6.852
1ACB	EI	LI38S	4.951
1B2S	AD	AA27K	-3.864
1B2S	AD	AA27K,AD43T	-5.721
1B2S	AD	AD43T	-0.343
1B2U	AD	AD36D	-4.166
1B3S	AD	AA102H	-5.679
1B3S	AD	AA102H,FD30Y	-5.547
1B3S	AD	FD30Y	0.596
1BRS	AD	DD35A	4.284
1BRS	AD	DD39A	6.790
1BRS	AD	EA58A	0.095
1BRS	AD	EA71A	2.352

1BRS	AD	EA71A,DD35A	6.437
1BRS	AD	EA71A,DD39A	7.182
1BRS	AD	EA71C	2.527
1BRS	AD	EA71F	2.234
1BRS	AD	EA71F,DD35A	6.407
1BRS	AD	EA71F,DD39A	7.468
1BRS	AD	EA71Q	1.451
1BRS	AD	EA71Q,DD39A	7.204
1BRS	AD	EA71Q,ED74A	3.525
1BRS	AD	EA71S	3.009
1BRS	AD	EA71W	1.656
1BRS	AD	EA71W,DD35A	5.710
1BRS	AD	EA71W,DD39A	6.662
1BRS	AD	EA71W,ED74A	3.548
1BRS	AD	EA71Y	2.413
1BRS	AD	ED74A	1.093
1BRS	AD	HA100A	6.344
1BRS	AD	HA100A,DD39A	8.987
1BRS	AD	HA100A,ED74A	7.559
1BRS	AD	HA100A,TD42A	8.132
1BRS	AD	HA100A,WD38F	7.638
1BRS	AD	HA100A,YD29A	6.304
1BRS	AD	HA100A,YD29F	5.547
1BRS	AD	HA100D	4.548
1BRS	AD	HA100G	6.817
1BRS	AD	HA100Q	4.548
1BRS	AD	HA100Q,RA57A	9.304
1BRS	AD	HA100Q,RA57K	6.909
1BRS	AD	KA25A	5.124
1BRS	AD	KA25A,DD35A	9.544
1BRS	AD	KA25A,DD39A	8.274
1BRS	AD	KA25A,ED74A	6.693
1BRS	AD	KA25A,TD42A	5.721
1BRS	AD	KA25A,WD38F	5.111
1BRS	AD	KA25A,YD29A	8.620
1BRS	AD	NA56A	3.090
1BRS	AD	RA57A	4.986
1BRS	AD	RA57A,DD35A	6.331
1BRS	AD	RA57A,DD39A	11.356
1BRS	AD	RA57A,ED74A	4.968
1BRS	AD	RA57A,TD42A	6.817
1BRS	AD	RA57A,WD38F	6.275
1BRS	AD	RA57A,YD29A	8.119
1BRS	AD	RA57K	2.487
1BRS	AD	RA81Q	5.417
1BRS	AD	RA81Q,DD35A	9.601
1BRS	AD	RA81Q,DD39A	6.436
1BRS	AD	RA81Q,ED74A	6.718
1BRS	AD	RA81Q,TD42A	6.104
1BRS	AD	RA81Q,WD38F	6.755
1BRS	AD	RA81Q,YD29A	8.289
1BRS	AD	RA85A	5.755
1BRS	AD	RA85A,DD39A	7.182
1BRS	AD	RA85A,ED74A	6.863
1BRS	AD	RA85A,TD42A	7.017
1BRS	AD	RA85A,WD38F	7.037
1BRS	AD	RA85A,YD29A	8.049
1BRS	AD	TD42A	1.857
1BRS	AD	WA33F	1.260

1BRS	AD	WD38F	1.642
1BRS	AD	WD44F	0.056
1BRS	AD	YD29A	3.469
1BRS	AD	YD29F	-0.132
1E50	AB	DA8A	-0.316
1E50	AB	MA48A	1.320
1E50	AB	NA11A	0.678
1E50	AB	NA51A	1.919
1E50	AB	NB62A	0.964
1E50	AB	NB99A	1.407
1E50	AB	RB32A	1.774
1E50	AB	SA56A	0.978
1E50	AB	SB64A	0.115
1E50	AB	TA103A	2.184
1E50	AB	TA91A	1.277
1E50	AB	VA101A	-0.044
1E50	AB	VB57A	0.000
1E50	AB	YA55A	0.914
1E96	AB	IA33N	2.008
1E96	AB	NA26H	1.085
1EAW	AB	DA47A	1.502
1EAW	AB	DA91A	0.654
1EAW	AB	FA92A	0.892
1EAW	AB	HA138A	-0.014
1EAW	AB	IA26A	-0.822
1EAW	AB	QA23A	-0.519
1EAW	AB	RA48A	0.587
1EAW	AB	YA141A	0.502
1EAW	AB	YA52A	-0.079
1FC2	CD	FC1M	0.912
1FC2	CD	IC27A	3.729
1FC2	CD	KC31A	1.379
1FC2	CD	LC13D	1.127
1FC2	CD	NC24A	0.593
1FC2	CD	NC24F	0.845
1FC2	CD	NC2F	-0.108
1FC2	CD	NC2Q	0.000
1FC2	CD	NC7F	0.091
1FC2	CD	QC28K	0.170
1FC2	CD	QC28L	0.458
1FC2	CD	YC10F	1.027
1FC2	CD	YC10W	0.410
1FCC	AC	DC40A	0.272
1FCC	AC	EC27A	4.936
1FCC	AC	EC42A	0.385
1FCC	AC	KC28A	1.256
1FCC	AC	KC31A	3.476
1FCC	AC	NC35A	2.364
1FCC	AC	TC25A	0.240
1FCC	AC	TC44A,YC45A	1.953
1FCC	AC	WC43A	3.771
1FY8	EI	DE168N	0.170
1GL0	EI	MI28K	-0.558
1GL0	EI	MI28K,LI27R	3.835
1GL1	AI	KI30M,AI31G	-0.132
1GL1	AI	LI29V	4.257
1H9D	AB	GB60A	1.902
1H9D	AB	LB93A	0.861
1H9D	AB	NB94A	2.110

1H9D	AB	QB66A	1.249
1H9D	AB	RB2A	1.064
1H9D	AB	VB3A	1.284
1HE8	AB	KA80V	0.467
1HE8	AB	KA80V,FA78S	2.125
1HE8	AB	KA80V,KA108A	2.125
1HE8	AB	KA80V,KA108E	2.125
1HE8	AB	KA80V,KA112A	2.125
1HE8	AB	KA80V,KA91A	1.497
1HE8	AB	KA80V,TA89D	2.125
1K8R	AB	DA33A	1.596
1K8R	AB	DA38A	1.780
1K8R	AB	DA38E	3.574
1K8R	AB	DA38N	1.972
1K8R	AB	EA37A	0.318
1K8R	AB	KB31A	2.837
1K8R	AB	QB11A	1.870
1K8R	AB	RA41A	1.227
1K8R	AB	RB13A	2.912
1K8R	AB	RB77A	1.494
1K8R	AB	SA39A	0.744
1K8R	AB	YA40C	3.574
1K8R	AB	YA40F	1.551
1KBH	AB	LA37W	0.679
1KBH	AB	QA3W	0.025
1KBH	AB	YB51W	0.314
1KBH	AB	YB51W,AA22G	0.695
1KBH	AB	YB51W,AB42G	0.695
1KBH	AB	YB51W,AB42G,AA22G	1.600
1KBH	AB	YB51W,AB42G,IA28V	2.037
1KBH	AB	YB51W,AB42G,IA34V	2.171
1KBH	AB	YB51W,AB42G,LA10A	2.535
1KBH	AB	YB51W,AB42G,LA16A	2.026
1KBH	AB	YB51W,AB42G,LA9A	2.665
1KBH	AB	YB51W,AB42G,VA38A	1.207
1KBH	AB	YB51W,IA28V	1.269
1KBH	AB	YB51W,IA34V	1.328
1KBH	AB	YB51W,IB44V	0.608
1KBH	AB	YB51W,IB44V,AA22G	1.353
1KBH	AB	YB51W,IB44V,IA28V	1.978
1KBH	AB	YB51W,IB44V,IA34V	2.357
1KBH	AB	YB51W,IB44V,LA10A	2.968
1KBH	AB	YB51W,IB44V,LA16A	1.826
1KBH	AB	YB51W,IB44V,LA9A	2.439
1KBH	AB	YB51W,IB44V,VA38A	1.022
1KBH	AB	YB51W,IB5V	0.812
1KBH	AB	YB51W,IB5V,IA28V	2.193
1KBH	AB	YB51W,IB5V,IA34V	2.120
1KBH	AB	YB51W,IB5V,LA10A	2.713
1KBH	AB	YB51W,IB5V,LA16A	2.048
1KBH	AB	YB51W,IB5V,LA9A	2.593
1KBH	AB	YB51W,IB5V,VA38A	1.326
1KBH	AB	YB51W,LA10A	1.990
1KBH	AB	YB51W,LA16A	1.078
1KBH	AB	YB51W,LA17A	2.838
1KBH	AB	YB51W,LA25A	2.158
1KBH	AB	YB51W,LA32A	2.793
1KBH	AB	YB51W,LA9A	1.690
1KBH	AB	YB51W,LB10A	0.096

1KBH	AB	YB51W,LB10A,AA22G	0.960
1KBH	AB	YB51W,LB10A,IA28V	1.686
1KBH	AB	YB51W,LB10A,IA34V	1.554
1KBH	AB	YB51W,LB10A,LA10A	1.687
1KBH	AB	YB51W,LB10A,LA16A	1.754
1KBH	AB	YB51W,LB10A,LA9A	1.346
1KBH	AB	YB51W,LB10A,VA38A	0.579
1KBH	AB	YB51W,LB13A	0.747
1KBH	AB	YB51W,LB13A,AA22G	2.382
1KBH	AB	YB51W,LB13A,IA28V	2.347
1KBH	AB	YB51W,LB13A,IA34V	2.363
1KBH	AB	YB51W,LB13A,LA10A	2.218
1KBH	AB	YB51W,LB13A,LA16A	2.645
1KBH	AB	YB51W,LB13A,LA9A	2.667
1KBH	AB	YB51W,LB17A	0.785
1KBH	AB	YB51W,LB17A,AA22G	2.250
1KBH	AB	YB51W,LB17A,IA28V	2.295
1KBH	AB	YB51W,LB17A,IA34V	2.392
1KBH	AB	YB51W,LB17A,LA10A	2.284
1KBH	AB	YB51W,LB17A,LA16A	2.323
1KBH	AB	YB51W,LB17A,LA9A	2.625
1KBH	AB	YB51W,LB30A	2.979
1KBH	AB	YB51W,LB30A,AA22G	3.264
1KBH	AB	YB51W,LB30A,IA28V	3.598
1KBH	AB	YB51W,LB30A,IA34V	3.557
1KBH	AB	YB51W,LB30A,LA16A	3.417
1KBH	AB	YB51W,LB30A,LA9A	3.659
1KBH	AB	YB51W,LB30A,VA38A	2.892
1KBH	AB	YB51W,LB39A	2.590
1KBH	AB	YB51W,LB39A,AA22G	4.006
1KBH	AB	YB51W,LB39A,LA16A	3.788
1KBH	AB	YB51W,LB39A,LA9A	4.271
1KBH	AB	YB51W,LB39A,VA38A	3.153
1KBH	AB	YB51W,VA38A	0.393
1KBH	AB	YB51W,VB29A	1.381
1KBH	AB	YB51W,VB29A,AA22G	2.347
1KBH	AB	YB51W,VB29A,IA28V	3.150
1KBH	AB	YB51W,VB29A,IA34V	2.838
1KBH	AB	YB51W,VB29A,LA10A	3.449
1KBH	AB	YB51W,VB29A,LA16A	2.779
1KBH	AB	YB51W,VB29A,LA9A	3.433
1KBH	AB	YB51W,VB29A,VA38A	1.844
1KBH	AB	YB51W,VB52A	0.410
1KBH	AB	YB51W,VB52A,IA28V	1.589
1KBH	AB	YB51W,VB52A,IA34V	1.788
1KBH	AB	YB51W,VB52A,LA10A	2.531
1KBH	AB	YB51W,VB52A,LA16A	1.559
1KBH	AB	YB51W,VB52A,LA17A	3.378
1KBH	AB	YB51W,VB52A,LA9A	2.080
1KBH	AB	YB51W,VB52A,VA38A	0.953
1LFD	AB	DA38A	-0.445
1LFD	AB	DA38A,DB33A	0.200
1LFD	AB	DA38K	-0.994
1LFD	AB	DB33A	1.100
1LFD	AB	DB38A	3.311
1LFD	AB	EB37A	1.196
1LFD	AB	IA5A	1.449
1LFD	AB	KA19A	1.955
1LFD	AB	KA19A,QB25A	2.500

1LFD	AB	KA39A	2.144
1LFD	AB	KA39A,DB38A	6.095
1LFD	AB	MA17K	-0.661
1LFD	AB	NA14A	0.949
1LFD	AB	NA14A,EB37A	1.996
1LFD	AB	NA14A,RB41A	1.548
1LFD	AB	NA14K	0.400
1LFD	AB	NA16A	0.499
1LFD	AB	NA16A,QB25A	0.302
1LFD	AB	NA16A,RB41A	1.099
1LFD	AB	NA16A,SB39A	0.000
1LFD	AB	NA16A,YB40F	2.300
1LFD	AB	NA41K	-0.634
1LFD	AB	QB25A	0.900
1LFD	AB	RA7A	1.832
1LFD	AB	RA7A,EB37A	2.097
1LFD	AB	RB41A	0.849
1LFD	AB	SA20A	0.949
1LFD	AB	SA20A,DB38A	3.296
1LFD	AB	SA20A,EB37A	2.296
1LFD	AB	SA20A,YB40F	1.798
1LFD	AB	SB39A	-0.751
1LFD	AB	YA18A	3.596
1LFD	AB	YA18A,DB38A	4.895
1LFD	AB	YA18A,EB37A	3.596
1LFD	AB	YA18A,SB39A	4.095
1LFD	AB	YA18F	1.348
1LFD	AB	YA18F,EB37A	1.297
1LFD	AB	YA18F,RB41A	1.798
1LFD	AB	YA18F,SB39A	0.800
1LFD	AB	YA18F,YB40F	2.600
1LFD	AB	YB40A	3.696
1LFD	AB	YB40F	2.148
1PPF	EI	AI15C	-0.664
1PPF	EI	AI15D	1.122
1PPF	EI	AI15D,GI32A	1.143
1PPF	EI	AI15D,LI18A,YI20D	8.616
1PPF	EI	AI15E	0.104
1PPF	EI	AI15F	-0.072
1PPF	EI	AI15G	1.122
1PPF	EI	AI15H	0.545
1PPF	EI	AI15I	0.325
1PPF	EI	AI15K	1.112
1PPF	EI	AI15L	0.018
1PPF	EI	AI15M	-0.396
1PPF	EI	AI15N	0.903
1PPF	EI	AI15P	1.968
1PPF	EI	AI15Q	0.246
1PPF	EI	AI15R	-0.261
1PPF	EI	AI15R,LI18R	7.226
1PPF	EI	AI15S	0.746
1PPF	EI	AI15T	0.949
1PPF	EI	AI15T,LI18M	-1.472
1PPF	EI	AI15V	0.198
1PPF	EI	AI15V,TI17S	1.741
1PPF	EI	AI15W	-0.632
1PPF	EI	AI15Y	-0.182
1PPF	EI	EI19A	1.187
1PPF	EI	EI19C	1.383

1PPF	EI	EI19D	0.570
1PPF	EI	EI19F	1.345
1PPF	EI	EI19G	2.091
1PPF	EI	EI19H	0.681
1PPF	EI	EI19I	0.713
1PPF	EI	EI19K	2.091
1PPF	EI	EI19L	1.056
1PPF	EI	EI19M	1.133
1PPF	EI	EI19N	1.196
1PPF	EI	EI19P	3.166
1PPF	EI	EI19Q	0.651
1PPF	EI	EI19R	1.461
1PPF	EI	EI19S	1.821
1PPF	EI	EI19T	1.484
1PPF	EI	EI19V	1.143
1PPF	EI	EI19W	1.509
1PPF	EI	EI19Y	1.232
1PPF	EI	GI32A	0.254
1PPF	EI	GI32C	1.163
1PPF	EI	GI32D	2.462
1PPF	EI	GI32E	1.437
1PPF	EI	GI32F	1.461
1PPF	EI	GI32H	1.484
1PPF	EI	GI32I	4.311
1PPF	EI	GI32K	3.260
1PPF	EI	GI32L	3.086
1PPF	EI	GI32M	2.165
1PPF	EI	GI32N	1.591
1PPF	EI	GI32P	0.260
1PPF	EI	GI32Q	2.761
1PPF	EI	GI32R	4.781
1PPF	EI	GI32S	0.903
1PPF	EI	GI32T	2.773
1PPF	EI	GI32V	2.513
1PPF	EI	GI32W	1.621
1PPF	EI	GI32Y	1.187
1PPF	EI	LI18A	1.002
1PPF	EI	LI18C	-0.088
1PPF	EI	LI18D	7.508
1PPF	EI	LI18E	6.965
1PPF	EI	LI18F	5.098
1PPF	EI	LI18G	3.287
1PPF	EI	LI18H	6.381
1PPF	EI	LI18I	-0.723
1PPF	EI	LI18I,GI32D	2.488
1PPF	EI	LI18K	5.614
1PPF	EI	LI18M	1.224
1PPF	EI	LI18M,GI32D	3.930
1PPF	EI	LI18M,TI30S,GI32D	4.118
1PPF	EI	LI18M,YI20Q	5.758
1PPF	EI	LI18N	5.153
1PPF	EI	LI18P	6.062
1PPF	EI	LI18Q	3.301
1PPF	EI	LI18R	7.085
1PPF	EI	LI18S	3.049
1PPF	EI	LI18T	0.903
1PPF	EI	LI18V	-0.486
1PPF	EI	LI18W	7.439
1PPF	EI	LI18Y	6.543

1PPF	EI	NI36A	-1.623
1PPF	EI	NI36C	0.596
1PPF	EI	NI36D	-3.035
1PPF	EI	NI36E	-1.004
1PPF	EI	NI36F	1.821
1PPF	EI	NI36G	-0.564
1PPF	EI	NI36H	-0.526
1PPF	EI	NI36I	0.859
1PPF	EI	NI36K	2.585
1PPF	EI	NI36L	2.610
1PPF	EI	NI36M	1.056
1PPF	EI	NI36P	-2.918
1PPF	EI	NI36Q	0.378
1PPF	EI	NI36R	1.844
1PPF	EI	NI36S	-1.328
1PPF	EI	NI36T	0.545
1PPF	EI	NI36V	0.341
1PPF	EI	NI36W	1.698
1PPF	EI	NI36Y	1.654
1PPF	EI	PI14A	-0.122
1PPF	EI	PI14C	-1.977
1PPF	EI	PI14D	-0.486
1PPF	EI	PI14E	-1.409
1PPF	EI	PI14F	-1.831
1PPF	EI	PI14G	0.092
1PPF	EI	PI14H	-1.741
1PPF	EI	PI14I	-1.628
1PPF	EI	PI14K	-0.442
1PPF	EI	PI14L	-2.883
1PPF	EI	PI14M	-1.553
1PPF	EI	PI14N	-0.632
1PPF	EI	PI14Q	-0.800
1PPF	EI	PI14R	-0.136
1PPF	EI	PI14S	-0.564
1PPF	EI	PI14T	-0.261
1PPF	EI	PI14V	-1.504
1PPF	EI	PI14W	-1.977
1PPF	EI	PI14Y	-0.949
1PPF	EI	RI21A	0.205
1PPF	EI	RI21C	-0.080
1PPF	EI	RI21D	0.205
1PPF	EI	RI21E	0.454
1PPF	EI	RI21F	-0.968
1PPF	EI	RI21G	0.570
1PPF	EI	RI21H	-0.486
1PPF	EI	RI21I	-0.800
1PPF	EI	RI21K	0.596
1PPF	EI	RI21L	-0.847
1PPF	EI	RI21M	-0.749
1PPF	EI	RI21N	0.325
1PPF	EI	RI21P	6.612
1PPF	EI	RI21Q	-0.018
1PPF	EI	RI21S	0.414
1PPF	EI	RI21T	-0.018
1PPF	EI	RI21V	-0.345
1PPF	EI	RI21W	-0.526
1PPF	EI	RI21Y	0.218
1PPF	EI	TI17A	3.145
1PPF	EI	TI17C	2.058

1PPF	EI	TI17D	4.855
1PPF	EI	TI17E	3.015
1PPF	EI	TI17F	1.686
1PPF	EI	TI17G	3.550
1PPF	EI	TI17H	1.670
1PPF	EI	TI17I	1.461
1PPF	EI	TI17K	3.342
1PPF	EI	TI17L	2.248
1PPF	EI	TI17M	2.468
1PPF	EI	TI17N	2.661
1PPF	EI	TI17P	3.031
1PPF	EI	TI17Q	1.941
1PPF	EI	TI17R	3.404
1PPF	EI	TI17S	1.510
1PPF	EI	TI17V	1.492
1PPF	EI	TI17W	2.165
1PPF	EI	TI17Y	2.446
1PPF	EI	YI20A	3.166
1PPF	EI	YI20C	3.404
1PPF	EI	YI20D	6.330
1PPF	EI	YI20E	6.330
1PPF	EI	YI20F	0.475
1PPF	EI	YI20G	4.128
1PPF	EI	YI20H	2.383
1PPF	EI	YI20I	3.877
1PPF	EI	YI20K	4.432
1PPF	EI	YI20L	1.356
1PPF	EI	YI20M	2.773
1PPF	EI	YI20N	3.593
1PPF	EI	YI20P	5.292
1PPF	EI	YI20Q	4.632
1PPF	EI	YI20R	4.311
1PPF	EI	YI20S	3.593
1PPF	EI	YI20T	4.985
1PPF	EI	YI20V	4.128
1PPF	EI	YI20W	0.232
1S1Q	AB	DA44A	0.949
1S1Q	AB	FA42A	0.196
1S1Q	AB	FA86A	0.762
1S1Q	AB	NA43A	1.211
1S1Q	AB	VA41A	0.659
1SMF	EI	EI8A	1.019
1SMF	EI	II5A	3.533
1SMF	EI	KI3A	5.724
1SMF	EI	SI4A	1.912
1SMF	EI	TI2A	2.059
1UUZ	AD	CA64A	0.651
1UUZ	AD	HA62A	1.774
1UUZ	AD	HA62D	3.378
1UUZ	AD	HA62N	1.519
1UUZ	AD	HA62Q	1.519
1WQJ	IB	RI20A	0.679
1X1X	AD	AD76E	-0.823
1XD3	AB	DB39A	-0.420
1XD3	AB	HB68N	0.000
1XD3	AB	IB44A	0.272
1XD3	AB	KB11R	1.435
1XD3	AB	LB8A	2.738
1XD3	AB	RB42L	-0.882

1XD3	AB	RB72L	1.332
1XD3	AB	RB74L	2.432
1Z7X	WX	DW435A	3.661
1Z7X	WX	EW287A	1.321
1Z7X	WX	EW401A	1.306
1Z7X	WX	IW459A	0.337
1Z7X	WX	KW320A	1.321
1Z7X	WX	QW430A,VW432A	0.939
1Z7X	WX	RW457A	0.848
1Z7X	WX	SW289A	0.814
1Z7X	WX	WW261A	1.335
1Z7X	WX	WW263A	2.211
1Z7X	WX	WW318A	0.993
1Z7X	WX	WW375A	1.669
1Z7X	WX	WW438A,SW439A,EW440A	1.971
1Z7X	WX	YW434A	5.953
1Z7X	WX	YW434A,DW435A	7.168
1Z7X	WX	YW434A,YW437A	7.237
1Z7X	WX	YW434F	0.121
1Z7X	WX	YW437A	2.623
1Z7X	WX	YW437F	2.165
2AW2	AB	PB16A	2.574
2AW2	AB	VB35A	1.096
2AW2	AB	YB22A	1.884
2C5D	AC	EC33R,TC51R	6.110
2C5D	AC	VC66A	-0.599
2FTL	EI	GI12A	4.346
2FTL	EI	GI36A	4.891
2FTL	EI	GI37A	4.049
2FTL	EI	II18A	4.969
2FTL	EI	II19A	4.049
2FTL	EI	PI13A	4.049
2FTL	EI	RI17A	4.049
2FTL	EI	RI39A	4.049
2FTL	EI	TI11A	4.049
2FTL	EI	VI34A	4.049
2HRK	AB	KA140A	0.953
2HRK	AB	TA108V	0.721
2HRK	AB	TB55V	0.624
2I26	NL	AN29V	0.030
2KSO	AB	HB20E	-0.155
2KSO	AB	KA10D	0.331
2KSO	AB	KA10D,DB25K	0.387
2KSO	AB	KA49D	1.340
2KSO	AB	KA49D,DB36K	0.176
2KSO	AB	KA49E	1.340
2KSO	AB	RA43E	-0.662
2KSO	AB	RA43E,HB20E	0.454
2KSO	AB	RA43E,HB20R	-0.821
2O3B	AB	DB75E	5.435
2O3B	AB	DB75N	5.900
2O3B	AB	EB24A	5.472
2O3B	AB	EB24D	0.599
2O3B	AB	EB24Q	5.396
2O3B	AB	WB76A	4.072
2OOB	AB	AA9E	3.102
2OOB	AB	AA9E,GA13S	3.102
2OOB	AB	GA13S	0.235
3EG5	AB	HA104F	-2.049

3EG5	AB	TB73N,SB74N,HB75N	1.035
3EG5	AB	TB73N,SB74N,HB75N,HA104F	-1.304
3EQS	AB	FB3A	5.556
3EQS	AB	LB10A	3.333
3EQS	AB	LB9A	-0.170
3EQS	AB	NB8A	-1.111
3EQS	AB	SB11A	0.117
3EQS	AB	SB2A	1.263
3EQS	AB	TB1A	0.392
3EQS	AB	WB7A	6.407
3EQS	AB	YB6A	3.109
3EQY	AC	FC3A	5.658
3EQY	AC	LC10A	2.323
3EQY	AC	PC12A	0.295
3EQY	AC	SC11A	0.153
3EQY	AC	SC2A	0.871
3EQY	AC	TC1A	0.375
3EQY	AC	WC7A	6.043
3EQY	AC	YC6A	2.586
3KUD	AB	KB30A	1.953
3KUD	AB	KB30A,VB33I	2.758
3SF4	AD	ED19R	1.925
3SF4	AD	KD27D	0.410
3SF4	AD	NA264R	1.225
3SF4	AD	RA202E	2.364
3SF4	AD	WD8A	3.072
3TGK	EI	NE170D	-0.170
3U82	AB	IB45A	2.595
3U82	AB	TB28A,QB29A,EB90A,NB98A	-1.010
4G0N	AB	DA33A	0.895
4G0N	AB	DA38A	2.917
4G0N	AB	EA31A	0.945
4G0N	AB	EA37A	1.801
4G0N	AB	IA21A	0.900
4G0N	AB	IA36A	1.801
4G0N	AB	KB12A	1.831
4G0N	AB	KB12E	1.916
4G0N	AB	KB12M	1.322
4G0N	AB	KB31A	2.607
4G0N	AB	KB31A,DA33A	2.700
4G0N	AB	KB31A,EA31A	2.100
4G0N	AB	KB31A,EA37A	3.499
4G0N	AB	KB31A,RB36G	5.356
4G0N	AB	KB31E	5.063
4G0N	AB	NB11A	0.681
4G0N	AB	NB11A,RA41A	-0.600
4G0N	AB	NB11D	1.808
4G0N	AB	QB13A	2.242
4G0N	AB	QB13A,RA41A	1.300
4G0N	AB	QB13A,SA39A	2.100
4G0N	AB	RA41A	-0.354
4G0N	AB	RB14A	1.941
4G0N	AB	RB14A,SA39A	2.300
4G0N	AB	RB36L	5.356
4G0N	AB	RB6A	2.158
4G0N	AB	RB6A,DA33A	2.600
4G0N	AB	RB6A,DA38A	4.599
4G0N	AB	RB6A,EA31A	2.200
4G0N	AB	RB6A,EA37A	2.400

4G0N	AB	RB6A,IA36A	4.398
4G0N	AB	RB6A,NB11D	3.419
4G0N	AB	SA39A	0.300
4G0N	AB	TB15A	1.829
4G0N	AB	TB15A,DA38A	3.100
4G0N	AB	TB15A,EA31A	1.603
4G0N	AB	TB15A,EA37A	2.900
4G0N	AB	TB15A,IA21A	2.200
4G0N	AB	TB15A,IA36A	3.100
4G0N	AB	TB15A,SA39A	2.001
4G0N	AB	VB16A	1.166
4G0N	AB	VB16A,EA37A	2.800
4G0N	AB	VB16A,IA21A	1.603
4G0N	AB	VB16A,IA36A	2.700
4G0N	AB	VB35A	-0.004
4G0N	AB	VB35A,IA21A	0.300
4G0N	AB	VB35I	0.552
4G2V	AB	RA198E	2.236
4KRL	AB	DA49T,FA51A	1.852
4KRL	AB	DB112A	0.650
4KRL	AB	RB30A	1.720
4KRO	AB	DB92A	1.504
4KRO	AB	RB15A	1.583
4KRP	AB	EB105A	1.606
4MYW	AB	IB48A	2.572
4MYW	AB	TB31A,QB32A,EB93A,NB101A	-0.530
4RA0	AC	AC66V	0.931
4RS1	AB	DA28A	2.591
4RS1	AB	DA28K	3.618
4RS1	AB	DA28K,DA92K	4.121
4RS1	AB	DA92A	1.865
4RS1	AB	DA92K	3.476
4RS1	AB	DA92N	1.329
4RS1	AB	DA92R	2.908
4RS1	AB	EA25A	1.502
4RS1	AB	EA25K	2.139
4RS1	AB	EA25K,DA28K	4.121
4RS1	AB	EA25K,DA92K	4.121
4RS1	AB	FA99A	3.625
4RS1	AB	KB174A	0.871
4RS1	AB	KB203A	0.276
4RS1	AB	LA95A	2.364
4RS1	AB	LA95A,FA99A	4.121
4RS1	AB	LB204A	0.072
4RS1	AB	QA79A	0.470
4RS1	AB	QA79E	1.212
4RS1	AB	RA10D	0.178
4RS1	AB	SB205A	0.616
4WND	AB	NA263R	-0.021
4WND	AB	RA201E	2.794
4WND	AB	RA201E,NA263R	3.855
4YEB	AB	FB131A	2.416
5CXB	AB	EB49D	0.365
5CXB	AB	RB54A	0.564
5CXB	AB	RB54E	2.679
5CXB	AB	TB52Q	0.062
5CXB	AB	VB56W	0.564
5CYK	AB	EB52A	-2.115
5CYK	AB	EB52R	-2.679

5CYK	AB	EB52R,EB47D	-2.314
5CYK	AB	EB52R,TB50Q	-2.617
5CYK	AB	EB52R,VB54W	-2.115
5F4E	AB	EA50A	0.283
5F4E	AB	EA50K	0.408
5F4E	AB	EB26A	1.424
5F4E	AB	EB26K	2.247
5F4E	AB	HA136A	1.990
5F4E	AB	KB139A	0.289
5F4E	AB	KB139E	0.478
5F4E	AB	LB62A	2.934
5F4E	AB	RA139A	1.465
5F4E	AB	RA139E	2.107
5F4E	AB	WB43A	1.055
5TAR	AB	EB86A	1.126
5TAR	AB	QB114A	0.157
5TAR	AB	TA183A,KA184E	2.730
5TAR	AB	WB88A	0.384
5UFE	AB	QB25R	0.292
5UFQ	AC	QC25R,KC55G	0.246
5XCO	AB	DB12A	2.796
5XCO	AB	IB9A	2.796
5XCO	AB	LB7A	2.747
5XCO	AB	PB6A	1.078
5XCO	AB	SB10A	1.285
5XCO	AB	VB14A	0.000
5XCO	AB	YB11A	1.899
5XCO	AB	YB8A	1.363

Table S8. Experimental data for TestSet2. The multi-chain complexes were split into dimers and only the mutations at the interfaces of the split dimers are listed.

PDB	Chains	Mutations	Experimental $\Delta\Delta G_{bind}$
1AHW	AC	DC167A	-0.485
1AHW	AC	TC159A	1.106
1AHW	BC	RC189A,KC190A	4.016
1AHW	BC	TC186A	1.346
1AHW	BC	VC187A	-0.314
1AHW	BC	YC145A	3.805
1AO7	AC	EA63A	0.158
1AO7	AC	HA70A	3.154
1AO7	AC	KA146A	0.462
1AO7	AC	TA80A	0.076
1AO7	AC	VA67A	-0.558
1AO7	AC	VA76A	0.597
1AO7	AD	AA158G	0.312
1AO7	AD	DD26A	0.979
1AO7	AD	DD26A,EA58A	0.749
1AO7	AD	DD26M	0.211
1AO7	AD	DD26V	1.363
1AO7	AD	DD26W	-1.080
1AO7	AD	EA154A	0.361
1AO7	AD	EA166A	2.199
1AO7	AD	EA58A	-0.487
1AO7	AD	KA68A	0.193
1AO7	AD	KD66A	1.211
1AO7	AD	KD66A,EA166A	3.032
1AO7	AD	KD66H	0.953
1AO7	AD	ND52A	0.355
1AO7	AD	ND52A,EA166A	3.142
1AO7	AD	RA170A	-0.077
1AO7	AD	RA65A	3.042
1AO7	AD	RD27A	0.490
1AO7	AD	RD27A,RA170A	1.186
1AO7	AD	RD27F	-0.199
1AO7	AD	RD27P	0.308
1AO7	AD	SD51M	-0.378
1AO7	AE	AA149G	-0.154
1AO7	AE	HA151A	-0.302
1AO7	CE	EE28A	2.021
1AO7	DE	KD97P	-0.268
1BD2	AD	ED93A	1.315
1BJ1	HW	HH101Y	-1.584
1BJ1	HW	HH101Y,SH105T	-1.343
1BJ1	HW	HH101Y,YH103I,GH104A,SH105K	-0.431
1BJ1	HW	HH101Y,YH103R,GH104D,SH105N	-0.995
1BJ1	HW	HH101Y,YH103R,GH104N,SH105T	-0.763
1BJ1	HW	HH101Y,YH103R,SH105T	-1.173
1BJ1	HW	HH101Y,YH103W,SH105T	-1.041
1BJ1	HW	SH105T	-0.390
1BJ1	HW	TH59A	0.851
1C4Z	AD	AD56G	0.566
1C4Z	AD	AD95G	0.410
1C4Z	AD	DA145A	-0.387
1C4Z	AD	DA145K	0.208
1C4Z	AD	DA156A	0.518
1C4Z	AD	DA156R	1.375
1C4Z	AD	ED57A	0.088
1C4Z	AD	ED57R	0.067

1C4Z	AD	FA194A	1.596
1C4Z	AD	FD60A	3.013
1C4Z	AD	IA159A	0.410
1C4Z	AD	KD61A	0.293
1C4Z	AD	KD61E	0.725
1C4Z	AD	KD6A	0.610
1C4Z	AD	KD6E	1.554
1C4Z	AD	KD93A	1.135
1C4Z	AD	KD93E	1.169
1C4Z	AD	KD97A	1.301
1C4Z	AD	KD97E	1.420
1C4Z	AD	LA139A	1.216
1C4Z	AD	LA143A	0.999
1C4Z	AD	LD30A	-0.343
1C4Z	AD	MA157A	1.929
1C4Z	AD	MA158A	0.759
1C4Z	AD	MA174A	-0.573
1C4Z	AD	PD59A	1.409
1C4Z	AD	PD94A	0.850
1C4Z	AD	QA141A	-0.387
1C4Z	AD	RD2A	0.518
1C4Z	AD	RD2E	1.288
1C4Z	AD	RD3A	0.467
1C4Z	AD	RD3E	1.185
1C4Z	AD	SA142A	0.410
1C4Z	AD	SA164A	-0.410
1C4Z	AD	SD1A	0.566
1C4Z	AD	TA160A	0.566
1C4Z	AD	TA166A	-0.132
1C4Z	AD	VA138A	0.566
1C4Z	AD	WD92A	0.821
1C4Z	AD	YA198L	0.821
1CBW	GI	GI37A	0.803
1CBW	GI	II19A	0.120
1CBW	GI	RI39A	0.209
1CBW	HI	GI12A	0.637
1CHO	FI	RI18A	3.147
1CHO	FI	RI18C	3.471
1CHO	FI	RI18D	3.730
1CHO	FI	RI18E	3.471
1CHO	FI	RI18F	2.912
1CHO	FI	RI18G	3.438
1CHO	FI	RI18H	2.755
1CHO	FI	RI18I	2.080
1CHO	FI	RI18K	0.654
1CHO	FI	RI18L	2.791
1CHO	FI	RI18M	2.579
1CHO	FI	RI18N	3.471
1CHO	FI	RI18P	7.188
1CHO	FI	RI18Q	2.444
1CHO	FI	RI18S	3.142
1CHO	FI	RI18T	2.632
1CHO	FI	RI18V	2.037
1CHO	FI	RI18W	2.405
1CHO	FI	RI18Y	2.959
1CHO	GI	AI12C	-0.322
1CHO	GI	AI12D	0.000
1CHO	GI	AI12E	0.222
1CHO	GI	AI12F	-0.725

1CHO	GI	AI12G	0.065
1CHO	GI	AI12H	-0.322
1CHO	GI	AI12I	0.646
1CHO	GI	AI12K	2.464
1CHO	GI	AI12L	0.139
1CHO	GI	AI12M	0.139
1CHO	GI	AI12N	-0.285
1CHO	GI	AI12P	3.066
1CHO	GI	AI12Q	0.436
1CHO	GI	AI12R	0.462
1CHO	GI	AI12S	0.065
1CHO	GI	AI12T	0.956
1CHO	GI	AI12V	0.925
1CHO	GI	AI12W	-1.899
1CHO	GI	AI12Y	-0.863
1CHO	GI	KI10A	0.179
1CHO	GI	KI10C	0.496
1CHO	GI	KI10D	-0.504
1CHO	GI	KI10E	0.179
1CHO	GI	KI10F	1.078
1CHO	GI	KI10G	1.797
1CHO	GI	KI10H	0.139
1CHO	GI	KI10I	1.524
1CHO	GI	KI10L	0.375
1CHO	GI	KI10M	0.420
1CHO	GI	KI10N	-0.356
1CHO	GI	KI10P	2.047
1CHO	GI	KI10Q	-0.565
1CHO	GI	KI10R	-0.373
1CHO	GI	KI10S	-0.421
1CHO	GI	KI10S,PI11D,AI12Y	-1.022
1CHO	GI	KI10T	0.375
1CHO	GI	KI10T,PI11E,AI12Y	-0.932
1CHO	GI	KI10V	1.185
1CHO	GI	KI10W	1.005
1CHO	GI	KI10Y	1.060
1CHO	GI	PI11A	0.375
1CHO	GI	PI11C	-0.970
1CHO	GI	PI11D	-0.839
1CHO	GI	PI11E	-0.710
1CHO	GI	PI11F	-0.303
1CHO	GI	PI11G	0.628
1CHO	GI	PI11H	-0.111
1CHO	GI	PI11I	-0.504
1CHO	GI	PI11K	0.381
1CHO	GI	PI11L	-0.517
1CHO	GI	PI11M	-0.817
1CHO	GI	PI11N	-0.769
1CHO	GI	PI11Q	-0.718
1CHO	GI	PI11R	0.393
1CHO	GI	PI11S	-0.435
1CHO	GI	PI11T	-0.542
1CHO	GI	PI11V	-0.542
1CHO	GI	PI11W	-0.206
1CHO	GI	PI11Y	-0.390
1DAN	HT	DT39A	1.438
1DAN	HT	GT38A	0.067
1DAN	HT	QT32A	0.652
1DAN	HT	RH125A	0.744

1DAN	HT	ST37A	-0.069
1DAN	LT	DT53A	1.988
1DAN	LT	DT53E	1.380
1DAN	LT	ET19A	0.658
1DAN	LT	FT45A	0.438
1DAN	LT	IT17A	0.645
1DAN	LT	KT41A	0.563
1DAN	LT	KT41A,KT43A	1.135
1DAN	LT	KT43A	0.685
1DAN	LT	ST42A	-0.044
1DAN	LT	YT46A	-0.132
1DAN	LU	EU114A	-0.005
1DAN	LU	EU38A	0.086
1DAN	LU	FU50A	1.748
1DAN	LU	QU20A	1.305
1DAN	LU	SU69A	0.023
1DAN	LU	TU109A	0.135
1DAN	LU	VU113A	0.690
1DAN	LU	WU68F	0.123
1DAN	TU	EU9A	-0.176
1DAN	TU	FU57A	-0.060
1DAN	TU	IT58A	0.000
1DAN	TU	KT63A	-0.070
1DAN	TU	KT63A,QT64A	-0.206
1DAN	TU	LT67A	-0.060
1DAN	TU	NU17A	0.000
1DAN	TU	QT64A	0.000
1DAN	TU	ST11A	-0.130
1DAN	TU	TT16A	-0.159
1DAN	TU	TT55A	2.312
1DAN	TU	TU16A	-0.060
1DAN	TU	VT59A	0.000
1DAN	TU	VU56A	0.199
1DAN	TU	WT9F	0.691
1DAN	TU	YT73A	0.653
1DQJ	AC	NA31A	2.013
1DQJ	AC	NA32A	4.090
1DQJ	AC	NC93A	0.650
1DQJ	AC	SA91A	1.432
1DQJ	AC	TC89A	0.841
1DQJ	BC	DB32A	2.013
1DQJ	BC	DB32A,KC97A	1.122
1DQJ	BC	DC101A	1.377
1DQJ	BC	KC97A	3.520
1DQJ	BC	LC75A	1.452
1DQJ	BC	WC62A	0.758
1DQJ	BC	WC63A	1.346
1DQJ	BC	YB33A	5.524
1DQJ	BC	YB53A	1.180
1DQJ	BC	YB53A,DC101A	2.727
1DQJ	BC	YB53A,LC75A	1.217
1DQJ	BC	YB53A,WC62A	1.286
1DQJ	BC	YB53A,WC63A	2.199
1DVF	AC	HA30A	1.649
1DVF	AC	SA93A	1.162
1DVF	BD	DB100A	2.789
1DVF	BD	DB100A,DD52A	4.319
1DVF	BD	DB100A,HD33A	4.148
1DVF	BD	DD52A	1.682

1DVF	BD	HD33A	1.860
1DVF	BD	ID101A	2.681
1DVF	BD	KD30A	1.003
1DVF	BD	RB99A	1.875
1DVF	BD	TB30A	0.907
1DVF	BD	YB32A	1.831
1GCQ	AC	GC21V	-0.025
1GCQ	AC	PC18A	0.121
1GCQ	AC	PC19A	0.085
1GCQ	BC	AC42G	1.353
1GCQ	BC	PC5A	0.767
1GCQ	BC	PC67A	1.316
1GCQ	BC	WC47Y	2.146
1JRH	HI	DH56A	1.886
1JRH	HI	DH58A	1.855
1JRH	HI	GI40A	4.450
1JRH	HI	KI42A	3.386
1JRH	HI	KI42M	4.911
1JRH	HI	NI69A	-0.200
1JRH	HI	RH100A	0.543
1JRH	HI	VI41A	1.679
1JRH	HI	WH55A	2.421
1JRH	HI	YH104A	1.061
1JRH	HI	YH32A	1.433
1JRH	IL	DL28A	0.435
1JRH	IL	EL27A	0.543
1JRH	IL	KI37A	3.713
1JRH	IL	KI37M	3.292
1JRH	IL	KI88A	0.312
1JRH	IL	RI74A	0.392
1JRH	IL	SL93A	-0.651
1JRH	IL	WI46F	-0.253
1JRH	IL	WI46Y	0.298
1JRH	IL	WI72A	4.429
1JRH	IL	WI72F	1.103
1JRH	IL	WI72Y	1.188
1JRH	IL	WL92A	2.818
1JRH	IL	YL30A	1.108
1KIP	BC	AB32Y	-0.801
1KIR	AC	SA50Y	-1.387
1MHP	AH	GH53A	0.513
1MHP	AH	GH53N	1.255
1MHP	AH	GH53S	0.676
1MHP	AH	RH31Q	1.307
1MHP	AH	SH52M	2.076
1MHP	AH	TH33E,GH53Q	1.667
1MHP	AH	TH33N	2.727
1MHP	AH	TH33V	0.434
1MHP	AH	YH58E	2.076
1MHP	AH	YH58Q	2.076
1MHP	AH	YH58W	0.821
1MHP	AL	GL91Q	1.573
1MHP	AL	GL91S	0.513
1MHP	AL	HL30K	1.164
1MHP	AL	HL30R	1.124
1MHP	AL	HL30W	1.255
1MHP	AL	NL29V	1.049
1MHP	AL	NL29W	1.573
1MHP	AL	NL29Y	1.907

1MHP	AL	NL29Y,SL90I	0.434
1MHP	AL	SL90Q	1.774
1MHP	AL	SL90R	2.727
1MHP	AL	SL90R,NL29E	2.727
1MHP	AL	SL90T	2.317
1MHP	HL	FH99W	0.000
1MHP	HL	FH99Y	0.755
1MHP	HL	LH60D	-0.061
1MHP	HL	SH35A	1.573
1MHP	HL	SH35Q	2.727
1MI5	AD	AD91G	0.608
1MI5	AD	GD92A	0.764
1MI5	AD	LD49A	1.231
1MI5	AD	SD26A	-0.039
1MI5	AD	SD51A	0.482
1MI5	AD	TD94A	0.943
1MI5	AE	EE50A	0.819
1MI5	AE	GE95A	1.231
1MI5	AE	LE94A	0.116
1MI5	AE	NE49A	-0.433
1MI5	AE	QE48A	-0.070
1MI5	AE	SE29A	1.063
1MI5	AE	VE28A	0.293
1MI5	DE	EE99A	0.120
1MI5	DE	GD97A	1.231
1MI5	DE	KD98A	1.231
1MI5	DE	QE100A	1.231
1MLC	AE	NA32G	-0.877
1MLC	AE	NA32G,NA92A	-0.687
1MLC	AE	NA32Y	0.000
1MLC	AE	NA92A	-1.253
1MLC	BE	SB57A	-0.379
1MLC	BE	SB57V	-0.494
1MLC	BE	TB31A	0.447
1MLC	BE	TB31V	0.526
1MLC	BE	TB31W	0.132
1N8Z	AB	YB109V	0.232
1N8Z	AC	NA30S	0.067
1NCA	HN	DH101K	0.714
1NCA	HN	EH100D	0.410
1NCA	HN	NH102Q	0.543
1NCA	HN	NH31Q	0.000
1NMB	HN	DH57E	2.953
1NMB	HN	DH57N	2.953
1NMB	HN	YH103A	2.141
1NMB	LN	TL93F	-0.024
1NMB	LN	TL93W	0.184
1OGA	AC	EA63A	-0.018
1OGA	AC	HA70A	0.517
1OGA	AC	TA80A	0.195
1OGA	AC	VA67A	-0.139
1OGA	AD	EA154A	0.612
1OGA	AD	SD29A	0.627
1OGA	AE	AA149G	0.123
1OGA	AE	AA150G	0.448
1OGA	AE	DE52A	0.117
1OGA	AE	KA68A	0.248
1OGA	AE	NE51A	1.115
1OGA	AE	NE51D	0.495

1OGA	AE	QA72A	-0.459
1OGA	AE	RA65A	-0.365
1OGA	AE	RA75A	0.711
1OGA	DE	QD32A	0.988
1OGA	DE	SD30A	1.019
1REW	AC	QC55A	2.657
1U7F	AB	RB65A	1.807
1U7F	BC	DB140A	2.780
1VFB	AB	DB58A	-0.207
1VFB	AB	DB58E	0.078
1VFB	AB	DB58N	-0.128
1VFB	AB	EB98A	1.156
1VFB	AB	LA46D	5.628
1VFB	AB	LA46E	5.628
1VFB	AC	DC18A	0.340
1VFB	AC	HA30A	0.845
1VFB	AC	IC124A	1.231
1VFB	AC	LC129A	0.172
1VFB	AC	NC19A	0.396
1VFB	AC	RC125A	1.837
1VFB	AC	SA93A	0.343
1VFB	AC	TA53R	1.646
1VFB	AC	WA92A	3.037
1VFB	AC	WA92A,IC124A	3.850
1VFB	AC	WA92A,LC129A	3.307
1VFB	AC	WA92A,RC125A	3.393
1VFB	AC	YA50A	0.456
1VFB	AC	YA50A,DC18A	1.266
1VFB	AC	YA50K	1.716
1VFB	AC	YA50R	0.844
1VFB	BC	DB100A	3.005
1VFB	BC	DB54A	0.816
1VFB	BC	DB54A,TC118A	1.255
1VFB	BC	DC119A	0.953
1VFB	BC	GB31A	0.306
1VFB	BC	GB31E	-0.510
1VFB	BC	GB31W	0.004
1VFB	BC	KC116A	0.713
1VFB	BC	RB99A	-0.100
1VFB	BC	RB99W	0.705
1VFB	BC	RB99Y	1.235
1VFB	BC	TB30A	-0.056
1VFB	BC	TC118A	0.765
1VFB	BC	VC120A	0.917
1VFB	BC	YB32A	0.791
1VFB	BC	YB32A,KC116A	1.586
1VFB	BC	YB32E	1.902
1VFB	BC	YC23A	0.410
1XGQ	BC	VB33A	1.153
1XGQ	BC	VB33F	-2.908
1XGQ	BC	VB33I	-1.108
1XGQ	BC	VB33L	-1.046
1XGR	BC	IB33A	2.260
1XGR	BC	IB33F	-1.800
1XGR	BC	IB33L	0.061
1XGR	BC	IB33V	1.108
1XGT	BC	LB33A	2.199
1XGT	BC	LB33F	-1.862
1XGT	BC	LB33I	-0.061

1XGT	BC	LB33V	1.046
1XGU	BC	FB33A	4.060
1XGU	BC	FB33I	1.800
1XGU	BC	FB33L	1.862
1XGU	BC	FB33V	2.908
1YY9	AC	NC93A	-0.742
1YY9	AD	GD54P	0.268
1YY9	AD	ND56A	-0.057
1YY9	AD	SD53P	0.817
1YY9	AD	WD52P	1.478
1YY9	AD	YD101P	1.651
1YY9	CD	TD61E	-0.057
2AK4	AD	AA158G	0.873
2AK4	AD	EA161A	0.465
2AK4	AD	ND51A	1.403
2AK4	AD	RA157A	1.403
2AK4	AD	TD30A	-0.127
2AK4	AE	RA151A	1.367
2AK4	CD	SD94A	1.403
2AK4	CE	NE26A	0.209
2AK4	CE	QC9A	0.066
2B0U	AC	FC52A	0.000
2B0U	AC	FC52E	0.000
2B0U	BC	VC15E	0.000
2B2X	AL	QL28S,YL52N	0.863
2B2X	AL	YL52E	-0.224
2BDN	AH	DH31E	1.085
2BDN	AL	YL30K	0.675
2BNQ	AC	VC9C	0.502
2BNR	AC	CC9V	-0.502
2BNR	AC	EA63A	0.335
2BNR	AC	HA70A	1.695
2BNR	AC	TA80A	0.535
2BNR	AC	VA152A	0.903
2BNR	AC	VA67A	0.393
2BNR	AD	EA154A	0.018
2BNR	AD	HA151A	0.533
2BNR	AE	KA68A	0.006
2BNR	AE	QA72A	-0.096
2BNR	AE	RA75A	0.531
2JCC	AC	AA167W	-0.299
2JEL	HP	EP68A	0.410
2JEL	HP	EP70A	2.727
2JEL	HP	EP70K	4.090
2JEL	HP	EP75R	2.727
2JEL	HP	FP2W	2.619
2JEL	HP	FP2Y	0.000
2JEL	HP	HP76A	-0.410
2JEL	HP	HP76D	-0.651
2JEL	HP	KP72E	0.410
2JEL	HP	KP72R	0.000
2JEL	HP	QP4K	1.363
2JEL	HP	QP71E	2.727
2JEL	LP	SP41C	1.496
2JEL	LP	SP64T	4.090
2JEL	LP	TP34N	6.817
2JEL	LP	TP34Q	0.000
2JEL	LP	TP36Q	0.410
2NYY	AC	DC30Y	0.641

2NYY	AC	FA925A	4.058
2NYY	AC	HC34R	0.101
2NYY	AC	IA928A	-0.009
2NYY	AC	NA926A	0.099
2NYY	AC	RA1266A	0.300
2NYY	AC	SA927A	0.000
2NYY	AC	SC31N	-0.353
2NYY	AD	DA1030A	0.009
2NYY	AD	EA892A	2.839
2NYY	AD	FA889A	0.419
2NYY	AD	KA1028A	-0.029
2NYY	AD	LA891A	2.589
2NYY	AD	NA890A	0.890
2NYY	AD	RA1033A	0.820
2NYY	AD	SA874A	-0.230
2NYY	AD	YD30D	0.065
2NYY	AD	YD30Q	0.129
2NYY	AD	YD56Q	0.520
2NYY	CD	VD36I	-0.213
2NZ9	AC	FA925A	3.340
2NZ9	AC	IA928A	0.069
2NZ9	AC	NA926A	-0.152
2NZ9	AC	RA1266A	0.390
2NZ9	AC	SA927A	-0.079
2NZ9	AD	DA1030A	-0.031
2NZ9	AD	EA892A	2.770
2NZ9	AD	FA889A	-0.050
2NZ9	AD	KA1028A	-0.009
2NZ9	AD	KA875A	0.541
2NZ9	AD	LA891A	2.280
2NZ9	AD	NA890A	2.160
2NZ9	AD	RA1033A	0.291
2NZ9	AD	SA874A	-0.119
2UWE	AE	AA163T	0.404
2VIR	BC	SC115L	3.680
2VIR	BC	TC89I	4.911
2VIS	BC	IC89T	-4.911
3AAA	AC	DC43A	5.037
3AAA	AC	EC77A	1.932
3AAA	AC	EC77R	4.022
3AAA	AC	RA258A	2.207
3AAA	AC	RA258E	3.502
3B4V	AC	LC53A	3.391
3B4V	AC	LC53E	4.090
3B4V	BC	LC16E	0.821
3BN9	BD	DB214A	0.566
3BN9	BD	DB47A	0.311
3BN9	BD	DB91A	6.695
3BN9	BD	IB45A	0.835
3BN9	BD	NB90A	0.773
3BN9	BD	PD104H	2.427
3BN9	BD	QB218A	0.706
3BN9	BD	QD105V	1.224
3BN9	BD	RB48A	-0.045
3BN9	BD	SD30G	1.186
3BN9	BD	SD30N	1.145
3BN9	BD	TB93A	1.132
3BN9	BD	TD28R	0.333
3BN9	BD	YB141A	1.085

3BN9	BD	YD103S	0.459
3C60	AD	ED79A	0.047
3C60	AD	HD91A	1.085
3C60	AD	TD87A	1.166
3C60	BC	KC40A	1.594
3C60	BC	LC61A	0.943
3C60	BD	RD80A	2.025
3D3V	CE	EE30A	2.671
3HFM	HY	DH32A	1.898
3HFM	HY	DH32A,KY97A	4.592
3HFM	HY	DH32A,KY97M	1.123
3HFM	HY	DH32N	0.170
3HFM	HY	DH32N,KY97A	4.891
3HFM	HY	DH32N,KY97M	0.302
3HFM	HY	DY101A	1.232
3HFM	HY	DY101E	2.132
3HFM	HY	DY101F	2.328
3HFM	HY	DY101G	0.359
3HFM	HY	DY101K	2.124
3HFM	HY	DY101N	1.491
3HFM	HY	DY101Q	2.085
3HFM	HY	DY101R	2.279
3HFM	HY	DY101S	1.869
3HFM	HY	GY102V	0.395
3HFM	HY	IY98A	0.000
3HFM	HY	KY97A	5.861
3HFM	HY	KY97D	6.768
3HFM	HY	KY97E	3.604
3HFM	HY	KY97G	6.430
3HFM	HY	KY97M	0.947
3HFM	HY	KY97R	3.053
3HFM	HY	LY75A	0.704
3HFM	HY	RY73A	-0.331
3HFM	HY	SH31A	0.170
3HFM	HY	WY63A	0.319
3HFM	HY	YH33A	6.035
3HFM	HY	YH33A,KY97A	7.228
3HFM	HY	YH33F	1.071
3HFM	HY	YH33L	2.007
3HFM	HY	YH33W	1.749
3HFM	HY	YH53A	3.250
3HFM	HY	YH53F	0.620
3HFM	HY	YH53L	0.807
3HFM	HY	YH53W	0.706
3HFM	LY	HY15A	-0.445
3HFM	LY	KY96A	6.737
3HFM	LY	KY96M	6.777
3HFM	LY	KY96R	5.353
3HFM	LY	NL31A	5.214
3HFM	LY	NL31A,KY96A	7.468
3HFM	LY	NL31D	1.343
3HFM	LY	NL31E	5.707
3HFM	LY	NL32A	5.107
3HFM	LY	NY19D	0.410
3HFM	LY	NY19K	0.240
3HFM	LY	NY19Q	-0.042
3HFM	LY	NY93A	0.211
3HFM	LY	QL53A	0.953
3HFM	LY	TY89A	0.000

3HH2	AC	FC52A	1.272
3HH2	AC	FC52E	0.816
3HH2	BC	VC15E	0.684
3L5X	HL	YL94A	-0.829
3N85	AH	SH32A	-0.134
3N85	AH	SH32Y	0.057
3N85	AH	SH52Y	-0.785
3N85	AH	WH30K	-0.785
3N85	AH	WH30R	-0.554
3N85	HL	SH50G	0.488
3NGB	GH	AH57G	-0.056
3NGB	GH	AH57G,VH58T,PH63K,VH74T	1.673
3NGB	GH	DH103A	0.060
3NGB	GH	GH55A	-1.277
3NGB	GH	GH55S	0.743
3NGB	GH	GH56A	1.266
3NGB	GH	IH30A	-0.003
3NGB	GH	IH30T	0.073
3NGB	GH	KH52A	0.623
3NGB	GH	KH52N	0.175
3NGB	GH	NH105A	1.119
3NGB	GH	NH59A	1.767
3NGB	GH	PH63A	-0.043
3NGB	GH	PH63K	0.233
3NGB	GH	QH65A	-0.340
3NGB	GH	RH54A	-0.259
3NGB	GH	RH54N	0.046
3NGB	GH	RH62A	0.996
3NGB	GH	RH62Q	0.097
3NGB	GH	RH72A	1.643
3NGB	GH	VH58A	1.358
3NGB	GH	VH58T	0.138
3NGB	GH	VH74A	1.088
3NGB	GH	VH74T	0.165
3NGB	GH	WH50A	1.292
3NGB	GH	YH60A	0.548
3NGB	GH	YH75A	-0.199
3NGB	GH	YH75S	0.333
3NGB	GL	FL89A	0.859
3NGB	GL	QL25A	-0.231
3NGB	GL	VL1A	-0.773
3NGB	GL	YL26A	0.985
3NGB	GL	YL26S	0.651
3NPS	AB	DA214A	1.467
3NPS	AB	DA91A	1.507
3NPS	AB	FA92A	0.464
3NPS	AB	IA26A	0.642
3NPS	AB	QA168A	-0.059
3NPS	AB	QA169A	0.741
3NPS	AB	TA93A	0.724
3NPS	AC	HA138A	1.875
3NPS	AC	QA140A	0.296
3QDG	AD	DD26W	-1.561
3QDG	AD	DD26Y	-1.793
3QDG	AD	RD27P	0.138
3QDG	AD	RD27W	0.596
3QDJ	AD	DD26W	-2.171
3QDJ	AD	DD26Y	-1.337
3QDJ	AD	GD28I	-0.105

3QDJ	AD	GD28L	0.655
3QDJ	AD	GD28N	0.410
3QDJ	AD	GD28P	1.224
3QDJ	AD	GD28Y	0.556
3QDJ	AD	RD27P	0.040
3QDJ	AD	RD27W	0.217
3QIB	AD	AA61G	0.892
3QIB	AD	AA64G	0.610
3QIB	AD	AA68G	0.845
3QIB	AD	KA67A	0.566
3QIB	BC	AB71G	2.203
3QIB	BC	DB74A	0.862
3QIB	BC	EB67A	1.821
3QIB	BD	QB62A	1.763
3R9A	AB	AA323W	0.339
3R9A	AB	YA325A	1.014
3R9A	AB	YA325W	0.482
3SE3	BA	DA117A	0.543
3SE3	BA	FA223A	1.497
3SE3	BA	FA81A	0.410
3SE3	BA	LA116A	0.000
3SE3	BA	NA140T	0.133
3SE3	BA	NA230A	0.211
3SE3	BA	NA53A	-0.348
3SE3	BA	RA226A	0.410
3SE3	BA	SA120A	0.543
3SE3	BA	SA167A	-0.239
3SE3	BA	TA166A	-0.156
3SE3	BA	YA55A	1.497
3SE3	BA	YB43A,NB44A,SB47A	0.590
3SE3	BA	YB43A,NB44E,SB47Q	1.917
3SE3	BA	YB43H,NB44A,SB47Q	1.445
3SE3	BA	YB43H,NB44E,SB47A	1.823
3SE3	BA	YB43H,NB44E,SB47Q	2.456
3SE3	BA	YB43H,NB44E,SB47Q,EB82A	2.761
3SE3	BA	YB43H,NB44E,SB47Q,FB50A	2.850
3SE3	BA	YB43H,NB44E,SB47Q,IB88A	2.326
3SE3	BA	YB43H,NB44E,SB47Q,KB56A	2.695
3SE3	BA	YB43H,NB44E,SB47Q,KB93A	2.609
3SE3	BA	YB43H,NB44E,SB47Q,NB51A	3.093
3SE3	BA	YB43H,NB44E,SB47Q,NB79A	2.827
3SE3	BA	YB43H,NB44E,SB47Q,QB48A	2.490
3SE3	BA	YB43H,NB44E,SB47Q,QB76A	2.348
3SE3	BA	YB43H,NB44E,SB47Q,RB92A	2.835
3SE3	BA	YB43H,NB44E,SB47Q,RB92K	2.609
3SE3	BA	YB43H,NB44E,SB47Q,TB72A	2.741
3SE3	BA	YB43H,NB44E,SB47Q,YB71A	2.985
3SE3	BA	YB43H,NB44E,SB47Q,YB75A	3.125
3SE3	BA	YB43M,NB44D,SB47L	0.713
3SE4	BA	DA117A	0.132
3SE4	BA	FA223A	1.363
3SE4	BA	LA116A	0.132
3SE4	BA	NA140T	0.410
3SE4	BA	NA227A	0.000
3SE4	BA	RA226A	0.303
3SE4	BA	SA120A	0.000
3SE4	BA	TA166A	-0.543
3SE4	BA	YA55A	1.363
3SE4	BC	HC172A	-0.410

3SE4	BC	HC68A	-0.610
3SE4	BC	IC95A	1.209
3SE4	BC	KB134A	1.788
3SE4	BC	KB134R	-0.936
3SE4	BC	LB31A	2.727
3SE4	BC	MB130A	0.573
3SE4	BC	MC38A	1.665
3SE4	BC	MC38V	1.165
3SE4	BC	PB27A	-0.170
3SE4	BC	PB27L	0.924
3SE4	BC	SC39A	0.212
3SE4	BC	TC36A	1.363
3SE4	BC	VC72A	1.165
3SE8	GH	DH110A	-0.389
3SE8	GH	DH114A	-0.244
3SE8	GH	GH56A	0.357
3SE8	GH	KH52A	1.111
3SE8	GH	LH54A	0.055
3SE8	GH	PH78A	0.019
3SE8	GH	PH81A	-0.071
3SE8	GH	QH63A	1.114
3SE8	GH	QH65A	0.550
3SE8	GH	QH76A	0.097
3SE8	GH	RH30A	-0.039
3SE8	GH	RH62A	1.206
3SE8	GH	RH72A	2.644
3SE8	GH	SH59A	1.151
3SE8	GH	VH58A	1.250
3SE8	GH	WH50A	1.333
3SE8	GH	WH55A	0.761
3SE8	GH	YH60A	0.856
3SE8	GL	EL1A	-0.556
3SE8	GL	FL92A	0.832
3SE8	GL	NL30A	0.194
3SE8	HL	DL49A	0.856
3SE9	GH	DH77A	-0.766
3SE9	GH	GH106A	-0.308
3SE9	GH	GH57A	0.452
3SE9	GH	GH62A	0.046
3SE9	GH	LH34A	0.566
3SE9	GH	NH60A	1.522
3SE9	GH	PH64A	-0.442
3SE9	GH	RH67A	1.469
3SE9	GH	RH74A	2.679
3SE9	GH	RH76A	-0.232
3SE9	GH	TH105A	-0.442
3SE9	GH	TH56A	-0.859
3SE9	GH	VH55A	-0.859
3SE9	GH	VH59A	0.983
3SE9	GH	WH51A	1.276
3SE9	GH	YH104A	0.464
3SE9	GL	FL91A	0.024
3SE9	GL	VL3A	-0.494
3SEK	AC	LC48A	3.407
3SEK	AC	LC48E	4.213
3SEK	BC	LC11E	2.886
3SZK	AC	FC44A	2.089
3SZK	AC	NC66A	0.194
3SZK	AC	SC69A	1.437

3SZK	AC	TC70A	1.395
3SZK	AC	YC40A	2.757
3SZK	AC	YC41A	2.831
3VR6	CG	LG139N	0.709
3VR6	DG	LG28N	0.310
4B0M	AM	LM40A	1.908
4B0M	AM	PM98A	0.406
4B0M	AM	PM98S	0.758
4B0M	AM	PM98S,PM99A	2.072
4B0M	AM	PM99A	1.915
4B0M	AM	PM99S	1.993
4B0M	AM	YM37A	1.652
4B0M	BM	YM9G	0.629
4FTV	AD	KD66A	-1.579
4FTV	AD	RA65A	3.506
4GXU	AM	DA189E	2.165
4GXU	AM	DA189E,DA224G	3.010
4GXU	AM	DA224G	1.961
4HFK	AB	EB46A	1.188
4HFK	AB	EB56A	0.942
4HFK	AB	LB45A	2.524
4HFK	AB	LB50A	0.030
4HFK	AB	NB49A	-0.020
4HFK	AB	RB22A	1.391
4HFK	AB	SB48A	0.201
4HFK	AD	TD72A	1.849
4HSA	AC	HA59S	-0.123
4HSA	AC	YA58I	0.118
4I77	HZ	DH54A	2.620
4I77	HZ	YH100A	0.000
4I77	HZ	YH100F	0.000
4I77	LZ	YL32A	0.815
4I77	LZ	YL32F	0.000
4J2L	AC	LA118E	-0.631
4J2L	AC	LC20S	1.688
4J2L	AC	SA34D	-0.970
4J2L	AC	SA34D,LA118E	0.697
4J2L	AC	WC17A	2.229
4JPK	AH	DA141R	3.857
4JPK	AH	FA144I	1.387
4JPK	AH	TA35S	-0.032
4JPK	AL	RA81T	0.759
4K71	AB	HA462A	1.051
4K71	AB	HA462F	1.009
4K71	AB	HB157A	0.644
4K71	AB	HB157F	0.185
4L3E	AD	EA166A	1.217
4N8V	AG	KG38A	0.588
4N8V	AG	YG124A	0.120
4N8V	AG	YG39F	0.515
4NKQ	AC	EC8R	2.639
4NKQ	AC	NC4E	-0.390
4NKQ	AC	RC11D	-0.205
4NKQ	BC	DC99K	-0.331
4NKQ	BC	DC99K,KB90D	-0.502
4NKQ	BC	DC99K,RB80D	0.176
4NKQ	BC	DC99K,RB80D,KB90D	0.535
4NKQ	BC	KB89A	0.386
4NKQ	BC	KB89D	1.061

4NKQ	BC	KB90A	-0.199
4NKQ	BC	KB90D	-0.199
4NKQ	BC	LB77A,TB78A,SB79A	0.110
4NKQ	BC	RB178A	0.360
4NKQ	BC	RB178D	-0.291
4NKQ	BC	RB178M	2.134
4NKQ	BC	RB80A	0.120
4NKQ	BC	RB80D	-0.077
4NKQ	BC	RB80D,KB90D	1.313
4NKQ	BC	RC10D	0.111
4NM8	BH	QB34R	2.975
4NM8	BH	QB34T	2.331
4NM8	BH	TB32E	-0.552
4NM8	BH	TB32I	-0.050
4NM8	BH	TB32R	1.221
4NM8	BL	LB38Y	-0.615
4OZG	AH	QH48A	0.791
4OZG	AH	YH46F	-0.636
4OZG	BG	LG50A	1.166
4OZG	BG	YG31A	1.714
4P23	BC	KC40A	1.193
4P23	BC	KC68A	0.683
4P23	BC	LC61A	0.953
4P23	BD	ED75A	0.170
4P23	BD	RD79A	2.070
4P5T	AD	DD84A	0.000
4P5T	AD	ED77A	1.009
4P5T	AD	HD89A	0.796
4P5T	AD	TD85A	0.821
4P5T	BC	KC40A	1.138
4P5T	BC	LC61A	1.009
4PWX	AC	EA201K	1.728
4PWX	AC	QA205A	1.013
4PWX	AC	QC20A	-0.178
4PWX	AC	RC28A	1.728
4PWX	AC	RC31A	0.335
4PWX	AC	YA198A	1.728
4PWX	BC	DC60K	0.371
4PWX	BC	KB65A	0.202
4PWX	BC	KB65D	0.119
4PWX	BC	KB68A	0.448
4PWX	BC	KB68D	0.262
4PWX	BC	RB71A	0.359
4U6H	AE	NE21A	-0.348
4X4M	BE	KE153A	0.639
4X4M	BE	KE153E	0.953
4ZS6	AH	EA156A	3.038
4ZS6	AH	YA160A	-0.110
5C6T	AH	EA194A	1.091
5C6T	AH	FA192A	1.997
5C6T	AH	FA199A	2.758
5C6T	AH	FA200A	0.410
5C6T	AH	IA201A	0.886
5C6T	AH	NA186A	0.363
5C6T	AH	NA188A	-0.367
5C6T	AH	NA195A,DA197A	0.586
5C6T	AH	NH97A	1.526
5C6T	AH	RH31S	0.312
5C6T	AH	SH32A	-0.868

5C6T	AH	YA182A	3.208
5C6T	AH	YA182A,NA195A,DA197A	2.942
5C6T	AH	YH104A	0.363
5C6T	AH	YH98A	1.717
5E9D	AD	SD50G	-0.036
5E9D	DE	KD96Q	0.187

Table S9. Experimental data for CAPRI target T55.

Chains	Mutation	Experiment enrichment value
AC	DC50A	-1.556
AC	DC50C	-5.283
AC	DC50E	-1.564
AC	DC50F	-6.055
AC	DC50G	-1.036
AC	DC50H	-4.238
AC	DC50I	-3.824
AC	DC50K	-7.443
AC	DC50L	-3.578
AC	DC50M	-6.598
AC	DC50N	-1.431
AC	DC50P	-1.670
AC	DC50Q	-7.275
AC	DC50R	-6.909
AC	DC50S	-1.708
AC	DC50T	-2.587
AC	DC50V	-2.452
AC	DC50W	-7.955
AC	DC50Y	-2.297
AC	AC62C	-5.335
AC	AC62D	-3.231
AC	AC62E	-4.152
AC	AC62F	-3.359
AC	AC62G	-0.448
AC	AC62H	-4.760
AC	AC62I	-5.027
AC	AC62K	0.275
AC	AC62L	-5.590
AC	AC62M	-5.826
AC	AC62N	-4.217
AC	AC62P	-4.158
AC	AC62Q	-3.053
AC	AC62R	-0.826
AC	AC62S	-0.070
AC	AC62T	-2.972
AC	AC62V	-3.500
AC	AC62W	-6.381
AC	AC62Y	-7.710
BC	SC47A	-1.429
BC	SC47C	-5.930
BC	SC47D	-4.528
BC	SC47E	-2.975
BC	SC47F	-1.381
BC	SC47G	-3.035
BC	SC47H	2.084
BC	SC47I	-2.392
BC	SC47K	-1.269
BC	SC47L	-3.048
BC	SC47M	-1.915
BC	SC47N	0.502
BC	SC47P	-3.533
BC	SC47Q	-0.948
BC	SC47R	-3.703
BC	SC47T	0.846
BC	SC47V	-2.157
BC	SC47W	-3.375
BC	SC47Y	-0.578

BC	MC56A	-3.985
BC	MC56C	-2.978
BC	MC56D	-5.257
BC	MC56E	-6.943
BC	MC56F	-6.040
BC	MC56G	-1.555
BC	MC56H	4.910
BC	MC56I	0.491
BC	MC56K	-1.642
BC	MC56L	-0.356
BC	MC56N	3.588
BC	MC56P	-5.720
BC	MC56Q	-2.720
BC	MC56R	-1.667
BC	MC56S	-1.679
BC	MC56T	-0.762
BC	MC56V	0.368
BC	MC56W	-7.408
BC	MC56Y	1.699
BC	VC60A	-2.202
BC	VC60C	-7.150
BC	VC60D	-2.704
BC	VC60E	-6.573
BC	VC60F	2.526
BC	VC60G	-4.036
BC	VC60H	-5.943
BC	VC60I	-0.198
BC	VC60K	-4.504
BC	VC60L	2.545
BC	VC60M	-4.616
BC	VC60N	4.115
BC	VC60P	-4.328
BC	VC60Q	0.504
BC	VC60R	-4.619
BC	VC60S	-2.384
BC	VC60T	1.327
BC	VC60W	-6.976
BC	VC60Y	0.203
BC	KC64A	-3.040
BC	KC64C	-6.233
BC	KC64D	-3.936
BC	KC64E	-2.508
BC	KC64F	-3.852
BC	KC64G	-4.679
BC	KC64H	-1.126
BC	KC64I	-6.600
BC	KC64L	-3.844
BC	KC64M	-2.880
BC	KC64N	-2.667
BC	KC64P	-4.613
BC	KC64Q	-3.167
BC	KC64R	0.240
BC	KC64S	-3.326
BC	KC64T	-3.841
BC	KC64V	-5.478
BC	KC64W	-4.803
BC	KC64Y	-5.966
BC	RC65A	-4.781
BC	RC65C	-4.834

BC	RC65D	-3.893
BC	RC65E	-4.021
BC	RC65F	-5.953
BC	RC65G	-3.289
BC	RC65H	-2.967
BC	RC65I	-3.076
BC	RC65K	1.002
BC	RC65L	-3.212
BC	RC65M	-3.030
BC	RC65N	-4.494
BC	RC65P	-4.456
BC	RC65Q	-2.488
BC	RC65S	-2.768
BC	RC65T	-3.343
BC	RC65V	-4.436
BC	RC65W	-4.182
BC	RC65Y	-4.940
BC	PC66A	0.592
BC	PC66C	-6.206
BC	PC66D	-3.820
BC	PC66E	-4.894
BC	PC66F	-3.433
BC	PC66G	-2.116
BC	PC66H	-0.473
BC	PC66I	-2.091
BC	PC66K	3.172
BC	PC66L	-2.859
BC	PC66M	-2.010
BC	PC66N	-0.198
BC	PC66Q	-1.135
BC	PC66R	1.404
BC	PC66S	0.501
BC	PC66T	0.660
BC	PC66V	-1.398
BC	PC66W	-5.041
BC	PC66Y	-2.872
BC	FC69A	-5.429
BC	FC69C	-3.395
BC	FC69D	-3.332
BC	FC69E	-8.112
BC	FC69G	-4.310
BC	FC69H	-2.691
BC	FC69I	-3.777
BC	FC69K	-4.439
BC	FC69L	-2.377
BC	FC69M	-2.662
BC	FC69N	-4.069
BC	FC69P	-4.824
BC	FC69Q	-4.325
BC	FC69R	-4.375
BC	FC69S	-4.016
BC	FC69T	-4.473
BC	FC69V	-4.724
BC	FC69W	-5.642
BC	FC69Y	0.385
BC	PC70A	4.293
BC	PC70C	-1.363
BC	PC70D	0.377
BC	PC70E	2.686

BC	PC70F	3.511
BC	PC70G	1.796
BC	PC70H	3.091
BC	PC70I	4.138
BC	PC70K	2.995
BC	PC70L	3.345
BC	PC70M	4.019
BC	PC70N	2.246
BC	PC70Q	3.124
BC	PC70R	3.545
BC	PC70S	3.410
BC	PC70T	3.066
BC	PC70V	4.580
BC	PC70W	1.564
BC	PC70Y	3.412

Table S10. Experimental data for CAPRI target T56.

Chains	Mutation	Experiment enrichment value
AG	EG20A	-0.903
AG	EG20C	-3.291
AG	EG20D	-0.980
AG	EG20F	-6.039
AG	EG20G	-1.731
AG	EG20H	-1.763
AG	EG20I	-3.268
AG	EG20K	-2.081
AG	EG20L	-1.115
AG	EG20M	-0.815
AG	EG20N	-1.425
AG	EG20P	-5.305
AG	EG20Q	0.735
AG	EG20R	-1.289
AG	EG20S	1.376
AG	EG20T	-1.519
AG	EG20V	-2.187
AG	EG20W	-2.096
AG	EG20Y	-4.147
BG	SG14A	3.332
BG	SG14C	-2.934
BG	SG14D	-6.673
BG	SG14E	-4.407
BG	SG14F	-1.278
BG	SG14G	3.089
BG	SG14H	-3.244
BG	SG14I	3.385
BG	SG14K	4.105
BG	SG14L	-1.572
BG	SG14M	-0.454
BG	SG14N	-1.109
BG	SG14P	-0.481
BG	SG14Q	-1.552
BG	SG14R	4.669
BG	SG14T	2.365
BG	SG14V	3.781
BG	SG14W	-3.209
BG	SG14Y	-2.842
BG	AG18C	-7.432
BG	AG18D	-1.177
BG	AG18E	-4.987
BG	AG18F	-4.965
BG	AG18G	-3.106
BG	AG18H	-8.537
BG	AG18I	-6.721
BG	AG18K	4.535
BG	AG18L	-4.917
BG	AG18M	-2.114
BG	AG18N	-1.500
BG	AG18P	-3.009
BG	AG18Q	-2.201
BG	AG18R	1.657
BG	AG18S	-4.842
BG	AG18T	-2.677
BG	AG18V	-2.178
BG	AG18W	-4.534
BG	AG18Y	-7.443

BG	NG27A	-3.148
BG	NG27C	-8.175
BG	NG27D	-1.901
BG	NG27E	-3.986
BG	NG27F	-3.023
BG	NG27G	-3.199
BG	NG27H	-0.177
BG	NG27I	-1.629
BG	NG27K	0.013
BG	NG27L	-1.942
BG	NG27M	-4.060
BG	NG27P	-1.661
BG	NG27Q	-1.502
BG	NG27R	1.835
BG	NG27S	-1.003
BG	NG27T	-0.334
BG	NG27V	-2.780
BG	NG27W	-2.315
BG	NG27Y	-1.643
BG	KG36A	-2.233
BG	KG36C	-9.063
BG	KG36D	-1.943
BG	KG36E	-1.863
BG	KG36F	-6.788
BG	KG36G	-7.833
BG	KG36H	-8.631
BG	KG36I	-3.194
BG	KG36L	-1.935
BG	KG36M	-3.274
BG	KG36N	-2.281
BG	KG36P	-9.369
BG	KG36Q	-4.332
BG	KG36R	0.220
BG	KG36S	-3.384
BG	KG36T	-5.875
BG	KG36V	-0.362
BG	KG36W	-8.867
BG	KG36Y	-9.007
BG	QG39A	0.033
BG	QG39C	-6.071
BG	QG39D	-3.770
BG	QG39E	-2.215
BG	QG39F	3.645
BG	QG39G	-0.745
BG	QG39H	-1.769
BG	QG39I	-1.519
BG	QG39K	-0.047
BG	QG39L	-0.571
BG	QG39M	1.132
BG	QG39N	-1.327
BG	QG39P	-4.214
BG	QG39R	3.943
BG	QG39S	-0.204
BG	QG39T	-2.545
BG	QG39V	-1.847
BG	QG39W	-1.505
BG	QG39Y	4.157
BG	YG40A	-4.425
BG	YG40C	-2.771

BG	YG40D	-0.321
BG	YG40E	-6.051
BG	YG40F	-2.459
BG	YG40G	-5.420
BG	YG40H	-2.547
BG	YG40I	-4.101
BG	YG40K	-5.856
BG	YG40L	-3.016
BG	YG40M	-2.094
BG	YG40N	-2.205
BG	YG40P	-4.310
BG	YG40Q	-7.172
BG	YG40R	-4.787
BG	YG40S	-2.026
BG	YG40T	-4.383
BG	YG40V	-4.329
BG	YG40W	-5.810
BG	SG42A	0.381
BG	SG42C	-1.989
BG	SG42D	-7.182
BG	SG42E	-6.816
BG	SG42F	-2.218
BG	SG42G	-0.003
BG	SG42H	0.354
BG	SG42I	-2.389
BG	SG42K	4.360
BG	SG42L	-2.261
BG	SG42M	0.093
BG	SG42N	-0.049
BG	SG42P	-1.071
BG	SG42Q	-1.624
BG	SG42R	4.766
BG	SG42T	-0.248
BG	SG42V	-2.978
BG	SG42W	-1.567
BG	SG42Y	-0.700

Table S11. Pairwise comparison of $\Delta\Delta G_{bind}$ estimation results for the common mutations in TestSet1.

Method	Number of common mutations [a]	R [b] / σ [c] / P-value [d]	
		Control method	SSIPe
BeAtMuSiC	508	0.47 / 1.80 / 8.6e-3	0.57 / 1.66 / -
BindProfX	314	0.33 / 2.12 / 3.2e-3	0.49 / 1.38 / -
ELASPIC	500	0.53 / 1.74 / 5.4e-3	0.56 / 1.65 / -
EvoEF	734	0.53 / 2.36 / 4.1e-5	0.61 / 1.93 / -
FlexddG	547	0.59 / 2.04 / 3.6e-2	0.60 / 1.98 / -
FoldX	734	0.48 / 2.51 / 1.0e-4	0.61 / 1.93 / -
mCSM	178	0.28 / 1.82 / 3.6e-3	0.60 / 1.48 / -
MutaBind	167	0.55 / 1.78 / 6.4e-3	0.56 / 1.47 / -
SAAMBE	236	0.33 / 1.82 / 1.7e-3	0.49 / 1.56 / -

[a]: The mutation data points that were used to train the control method were excluded for fair comparison. There were a total of 734 mutations in TestSet1, including 508 single and 226 multiple mutations. For BeAtMuSiC, EvoEF and FoldX, all of the mutations in TestSet1 have not been used for their training. For ELASPIC, it is not clear whether some of the data points in TestSet1 have been used for its training because its training dataset is not known.

[b]: R, PCC between predicted and experimental $\Delta\Delta G_{bind}$ values.

[c]: σ, RMSE of $\Delta\Delta G_{bind}$ estimation in kcal/mol.

[d]: P-value in Wilcoxon rank sum test for paired samples between the RMSE of SSIPe and that of the control method on the common mutations.

Table S12. Summary of reported prediction performance of methods tested in this work.

Method	Dataset	PCC	Error [a] (kcal/mol)	Comments
BeAtMuSiC	2007 mutations	0.40	1.80	Single mutation only
BindProfX [b]	1402 mutations (114 proteins)	0.66	>1.70	RMSE is for single mutation
ELASPIC	873 mutations from 54 proteins	0.75	1.26	Single mutation only
EvoEF	2204 mutations (177 proteins)	0.51	2.07	Both single and multiple mutation
FlexddG	1240 mutations	0.63	0.96	Both single and multiple mutation
mCSM	2317 mutations (150 proteins)	0.80	1.25	Single mutation only
MutaBind	1925 mutations (80 proteins)	0.68	1.41	Single mutation only
SAAMBE [c]	1326 mutations (43 proteins)	0.62	n. r.	Single mutation only

[a]: For FlexddG the reported standard error is MAE, while for the other methods the error is RMSE.

[b]: The RMSE for 1131 single mutations was 1.70 kcal/mol, but it's not shown for the overall dataset. As mentioned in the paper, the RMSE on multiple mutations was higher than single mutations.

[c]: The RMSE is not reported in the paper.

Table S13. Experimental and estimated $\Delta\Delta G_{bind}$ and absolute estimation errors for selected mutations in 1LFD and 4WND. Experimental $\Delta\Delta G_{bind}$ are used as ground truth, and the estimated $\Delta\Delta G_{bind}$ are shown outside the parenthesis. The absolute estimation errors in the parenthesis are calculated as $|\Delta\Delta G_{exp,bind} - \Delta\Delta G_{pre,bind}|$, and the least estimated errors for each mutation is highlight in bold.

Method	$\Delta\Delta G_{bind}$ and absolute estimation error (kcal/mol)	
	DB33A	NA263R
Experimental	1.100 (0.000)	-0.021 (0.000)
BeAtMuSiC	0.730 (0.370)	0.810 (0.831)
BindProfX	2.176 (1.076)	1.713 (1.734)
ELASPIC	2.665 (1.565)	1.335 (1.356)
EvoEF	0.790 (0.310)	-1.180 (1.159)
FlexddG	1.292 (0.192)	-1.283 (1.262)
FoldX	0.420 (0.680)	1.540 (1.561)
mCSM	0.338 (0.762)	0.594 (0.615)
MutaBind	1.280 (0.180)	2.050 (2.071)
SAAMBE	-0.236 (1.336)	1.698 (1.719)
SSIPe	1.068 (**0.032**)	0.201 (**0.222**)

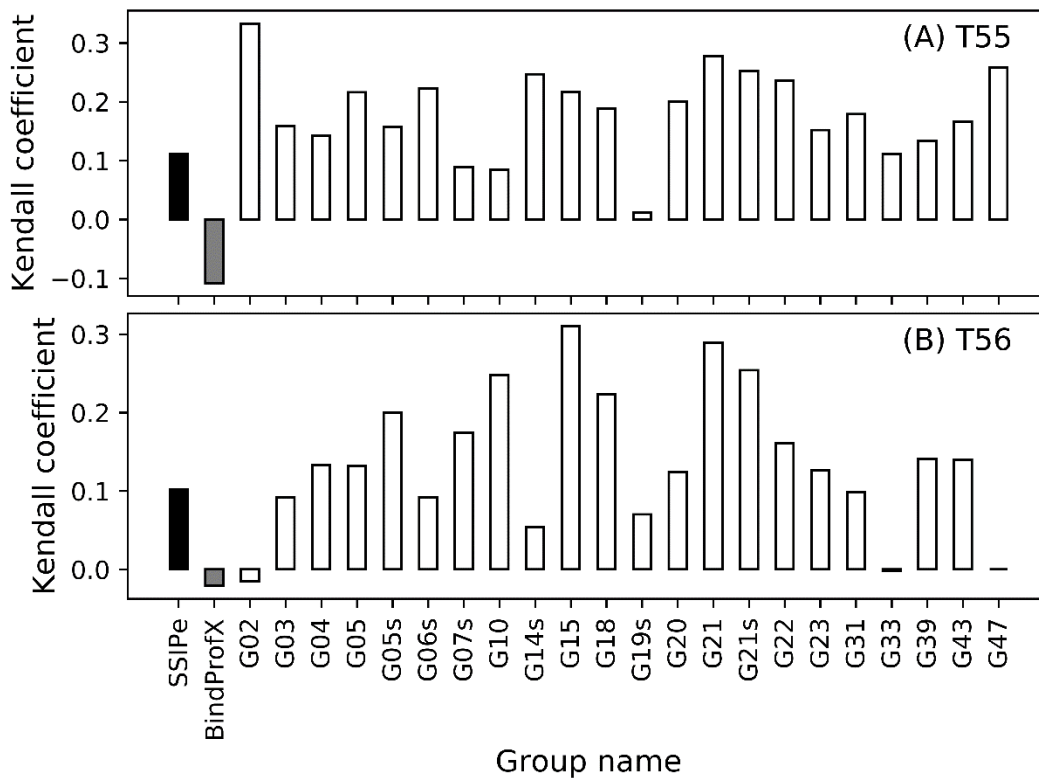**Fig. S1.** Kendall's tau rank correlation coefficient between predictions and experiments during the 26th round of the CAPRI experiment (http://www.ebi.ac.uk/msd-srv/capri/round26). Only the results for interface mutations are illustrated. The results for SSIPe and BindProfX are depicted in black and gray, respectively. The results of other groups are taken from (Moretti, et al., 2013). (A) Target T55. (B) Target 56.

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