

## Supplementary Materials for:

### Computational Protein Design with Explicit Consideration of Surface Hydrophobic Patches

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Experimental and predicted mutant free energy changes for all energy functions tested	

training set	size	fold	test set	size	fold
2igd	61	a/b	1a8o	70	all a
1orc	64	a/b	1hyp	75	a
1hoe	74	b	1bdo	80	all b
1aba	87	a/b	1opd	85	a/b
2acy	98	a/b	1opc	99	a/b
1bm8	99	a/b	1by2	110	a/b
1bxv	99	b	2mcm	112	b
1co6	107	a/b	1bea	116	a
1tmy	118	a/b	2a0b	118	all a
1mai	119	a/b	2mhr	118	a
3pyp	125	a/b	1b9o	123	a
1c52	131	a	1bqk	124	a/b
1vsr	134	a/b	1bfg	126	all b
1akr	147	a/b	1ifc	131	b
1bd8	156	all a	1bk9	134	a
1bgc	165	all a	1pne	139	a/b
1kao	167	a/b	2sns	141	a/b
1koe	172	a/b	1amx	150	b
1b2v	173	a/b	1bj7	150	a/b
2sga	181	a/b	1a6m	151	all a
1gbs	185	a/b	1ra9	159	a/b
1qf9	194	a/b	1qst	160	a/b
1nkr	195	all b	1cju	166	a/b
1cex	197	a/b	1mh1	181	a/b
1rgp	199	all a	3tss	190	a/b
1ppn	212	a/b	2pth	193	a/b
1a7s	225	a/b	2eng	210	a/b
1azo	226	a/b	1lbu	213	a/b
1uch	226	a/b	1g3p	217	a/b
1bio	228	b	3eug	225	a/b
1amf	231	a/b	1atg	231	a/b
3seb	238	a/b	1lst	240	a/b

Table SI

PDB codes of proteins used in design and weight optimization runs.

amino acid	average hydrophobic SASA ( $\text{\AA}^2$ )				
	nbs1-10	nbs11-13	nbs14-16	nbs17-20	nbs21-24
PHE	140.33	97.01	58.46	30.86	11.48
TRP	139.78	95.72	58.85	34.59	16.70
MET	129.12	97.25	61.79	33.03	11.05
LEU	119.66	85.25	53.91	26.87	7.93
TYR	114.72	83.56	55.49	30.61	13.05
ILE	114.64	80.00	52.77	25.21	7.48
LYS	101.83	81.16	63.23	42.99	23.74
VAL	97.18	70.04	47.46	23.49	6.79
PRO	93.59	72.40	52.45	31.07	12.69
HIS	90.26	68.55	48.19	30.81	15.02
CYS	80.59	53.46	32.72	16.52	5.64
ARG	71.21	56.79	42.58	26.33	11.48
THR	68.93	53.70	38.04	21.79	8.33
ALA	63.72	50.20	35.41	17.71	5.48
GLU	59.10	44.45	32.77	19.46	8.16
GLN	51.72	39.30	29.56	17.62	7.27
SER	47.41	37.45	27.29	14.82	5.37
ASP	42.50	31.62	22.33	12.67	5.78
GLY	38.24	31.12	23.67	13.42	5.24
ASN	36.32	27.02	19.65	10.92	4.51

Table SII

Average amount of hydrophobic accessible surface area exposed by each residue type at 5 levels of burial: 10 or fewer neighbors, 11 to 13 neighbors, 14 to 16 neighbors, 17-20 neighbors, and 21-24 neighbors. The aromatic residues expose the most hydrophobic surface area, while asparagine and glycine expose the least.

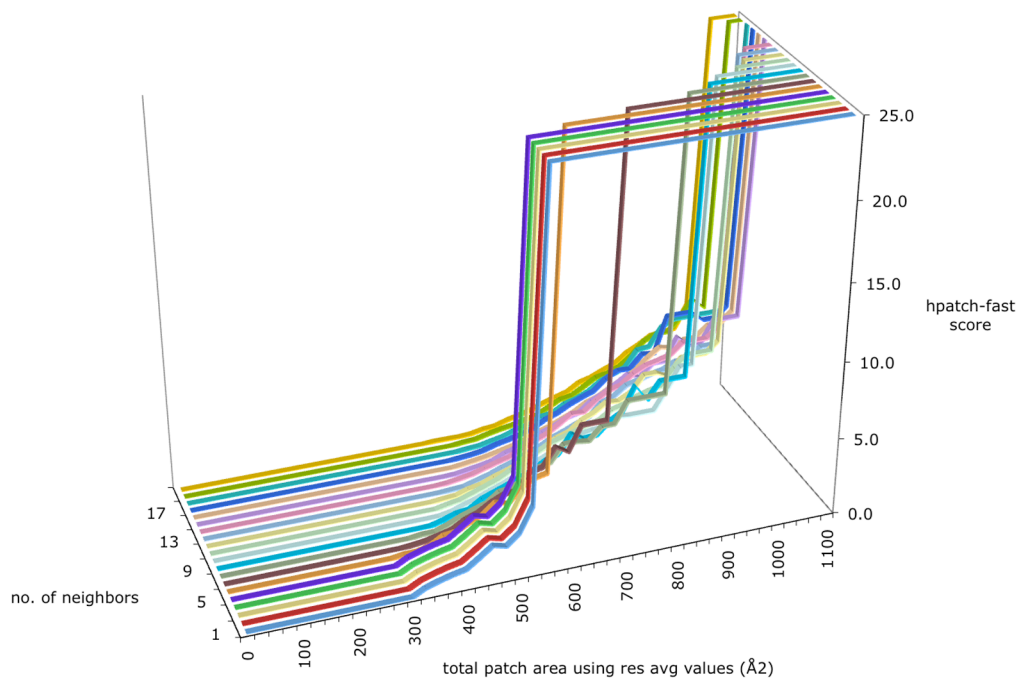


Figure S1

Plot of hpatch-fast score by hydrophobic patch area and number of neighbors. Each line represents the score for a given number of neighbors. Residues are only given hpatch-fast scores for having too much surrounding hydrophobic surface area. No score is given to residues with a patch area smaller than the most common patch area for that number of neighbors observed in native proteins. Patches of size 1100  $\text{\AA}^2$  and greater are given a score of 25.

patch area	nb1	nb2	nb3	nb4	nb5	nb6	nb7	nb8	nb9	nb10	nb11	nb12	nb13	nb14	nb15	nb16	nb17	nb18	nb19	nb20	
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
50	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
75	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
125	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
150	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
175	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
200	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
225	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
250	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
275	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
300	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
325	0.443	0.443	0.443	0.443	0.443	0.127	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
350	0.706	0.706	0.706	0.706	0.706	0.138	0.076	0	0	0	0	0	0	0	0	0	0	0	0	0	
375	0.929	0.929	0.929	0.929	0.929	0.348	0.182	0.113	0	0	0	0	0	0	0	0	0	0	0	0	
400	1.099	1.099	1.099	1.099	1.099	0.849	0.379	0.124	0.023	0	0	0	0	0	0	0	0	0	0	0	
425	1.686	1.686	1.686	1.686	1.686	0.937	0.579	0.418	0.243	0.017	0	0	0	0	0	0	0	0	0	0	
450	2.315	2.315	2.315	2.315	2.315	1.376	1.084	0.789	0.534	0.169	0.174	0.080	0.009	0	0	0	0	0	0	0	
475	2.092	2.092	2.092	2.092	2.092	1.713	1.372	1.079	0.628	0.472	0.320	0.145	0.066	0.063	0	0	0	0	0	0	
500	2.785	2.785	2.785	2.785	2.785	2.378	1.883	1.340	1.160	0.732	0.617	0.415	0.118	0.184	0.039	0	0	0.008	0	0.053	
525	4.394	4.394	4.394	4.394	4.394	2.133	2.261	1.960	1.470	1.055	0.910	0.571	0.362	0.330	0.165	0.100	0.071	0.018	0.005	0.049	
550	25	25	25	25	25	3.071	2.346	2.072	1.769	1.359	1.211	0.897	0.595	0.580	0.295	0.216	0.147	0.098	0.101	0.035	
575	25	25	25	25	25	3.476	3.387	2.531	2.103	1.741	1.660	1.154	0.911	0.815	0.466	0.354	0.279	0.152	0.149	0.087	
600	25	25	25	25	25	3.659	3.569	3.070	2.430	2.302	1.912	1.493	1.171	1.032	0.836	0.539	0.532	0.328	0.344	0.250	
625	25	25	25	25	25	4.773	3.267	2.920	2.552	2.503	2.038	1.572	1.443	1.039	0.725	0.694	0.490	0.515	0.322		
650	25	25	25	25	25	4.262	4.323	3.201	2.918	2.963	2.204	1.828	1.803	1.370	0.987	0.902	0.796	0.646	0.579		
675	25	25	25	25	25	5.872	4.323	4.414	3.059	3.196	2.747	2.297	2.126	1.789	1.340	1.161	0.961	0.831	0.766		
700	25	25	25	25	25	5.872	4.205	3.922	3.697	3.433	3.004	2.591	2.640	2.046	1.574	1.610	1.375	1.004	0.985		
725	25	25	25	25	25	5.872	5.016	3.979	3.851	3.743	3.633	2.947	3.209	2.482	1.927	1.903	1.469	1.407	1.284		
750	25	25	25	25	25	5.016	4.733	3.894	3.907	3.989	3.242	3.163	2.670	2.271	2.343	1.949	1.825	1.550			
775	25	25	25	25	25	6.402	5.203	4.464	4.467	4.549	4.057	3.812	3.309	2.766	2.687	2.175	1.953	1.780			
800	25	25	25	25	25	6.402	6.812	4.390	4.675	4.488	4.357	4.323	3.670	3.039	2.978	2.532	2.426	2.287			
825	25	25	25	25	25	6.402	5.714	4.390	5.042	4.924	4.955	4.534	4.156	3.504	3.686	3.092	2.914	2.498			
850	25	25	25	25	25	6.402	6.812	4.390	5.294	5.935	5.156	5.170	4.695	3.921	4.106	3.425	3.068	2.849			
875	25	25	25	25	25	6.812	5.643	5.448	5.935	5.407	5.576	4.338	4.343	4.063	3.720	3.401	3.171				
900	25	25	25	25	25	6.812	7.029	6.546	5.530	5.561	5.758	5.137	5.091	4.938	4.788	4.027	3.787				
925	25	25	25	25	25	25	25	7.029	7.239	6.628	5.967	5.981	5.137	5.678	4.843	4.883	4.860	4.193			
950	25	25	25	25	25	25	25	25	7.239	6.628	5.967	6.674	6.641	5.496	7.241	6.087	5.217	4.685			
975	25	25	25	25	25	25	25	25	7.239	6.628	6.660	6.674	5.948	5.902	7.241	6.493	5.217	4.781			
1000	25	25	25	25	25	25	25	25	25	7.322	6.660	6.674	5.948	5.902	7.241	6.493	6.064	4.886			
1025	25	25	25	25	25	25	25	25	25	25	25	25	7.368	7.334	6.595	6.548	6.493	7.163	6.390		
1050	25	25	25	25	25	25	25	25	25	25	25	25	25	7.334	6.595	6.548	6.493	6.470	25		
1075	25	25	25	25	25	25	25	25	25	25	25	25	25	7.334	7.288	7.241	6.493	25	25		
1100	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25	25

Table SIII

hpatch-fast score by hydrophobic patch area and number of neighbors.

The number of occurrences of each patch area and neighbor count for every residue with 20 or fewer neighbors in a set of monomeric proteins was determined using Rosetta. The inverse log of the probabilities was taken to obtain scores. The score for patch areas smaller than the most common patch area was set to the minimum score at that number of neighbors. The entire score was then shifted down so that the minimum hpatch-fast score at each number of neighbors is 0. Patches of size 1100 Å<sup>2</sup> and greater are given a score of 25.

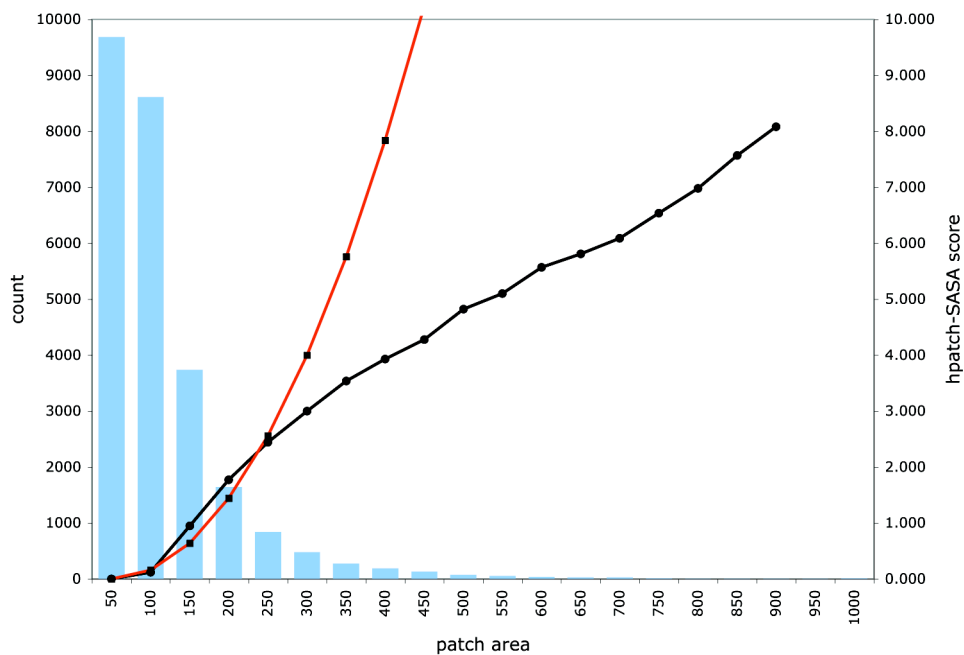


Figure S2

Plot of hpatch-SASA score by hydrophobic patch area. Blue bars represent the counts of the indicated patch size found in the set of monomeric structures. The red line is the hpatch-SASA score. The black line shows the score if the inverse log of the probabilities is used. Patches of size greater than 900 Å<sup>2</sup> are given a score of 100.

patch area	count	hpatch-SASA score
0	9692	0.00
50	8613	0.16
100	3740	0.64
150	1645	1.44
200	844	2.56
250	484	4.00
300	281	5.76
350	190	7.84
400	134	10.24
450	78	12.96
500	59	16.00
550	37	19.36
600	29	23.04
650	22	27.04
700	14	31.36
750	9	36.00
800	5	40.96
850	3	46.24
900		100.00
950		100.00

Table SIV

hpatch-SASA score by hydrophobic patch area.

The number of occurrences of each patch area in the set of monomeric proteins was determined using Rosetta. An exponential curve that more strongly penalizes large patches was used instead of the inverse log of the probabilities to obtain the score. The entire score was shifted down so that the minimum hpatch-SASA score is 0. Patches of size 900 Å<sup>2</sup> or greater are given a score of 100.

atom type	vdW radius
CNH2	1.76
COO	1.76
CH1	1.87
CH2	1.87
CH3	1.87
aroC	1.76
Ntrp	1.65
Nhis	1.65
NH2O	1.65
Nlys	1.5
Narg	1.65
Npro	1.65
OH	1.4
ONH2	1.4
OOC	1.4
Oaro	1.4
S	1.85
Nbb	1.65
CAbb	1.87
CObb	1.76
OCbb	1.4

Table SV

van der Waals radii used for SASA calculations



AA	fa_atr	fa_rep	fa_sol	fa_intra_rep	pro_close	fa_pair	hbond_sr_bb	hbond_lr_bb	hbond_bb_sc	hbond_sc	rama	omega	fa_dun	p_aa_pp
ALA	2.56	-0.57	-1.57	-0.23	-0.00	0	0.53	0.027	0.006	0	0.21	-0.15	0	0.16
ARG	3.18	-0.62	-2.22	-2.10	-0.01	0.09	0.49	0.017	0.021	0.013	0.26	-0.17	-2.33	0.10
ASN	2.87	-0.63	-2.41	-1.66	-0.01	0.08	0.39	0.017	0.031	0.006	-0.03	-0.18	-1.17	0.25
ASP	3.00	-0.68	-2.46	-1.50	-0.01	0.10	0.40	0.017	0.042	0.013	0.01	-0.16	-0.87	0.19
CYS	2.54	-0.62	-1.70	-0.40	-0.01	0	0.39	0.032	0.007	0	-0.02	-0.24	-0.55	-0.13
GLN	3.15	-0.67	-2.24	-1.55	-0.01	0.05	0.50	0.011	0.018	0.004	0.23	-0.17	-1.72	0.07
GLU	3.07	-0.63	-2.17	-1.56	-0.00	0.14	0.48	0.012	0.015	0.009	0.41	-0.14	-1.72	0.14
GLY	1.69	-0.49	-1.20	-0.02	-0.00	0	0.31	0.014	0.009	0	-0.66	-0.15	0	1.06
HIS	3.53	-0.70	-2.35	-0.99	-0.00	0.02	0.41	0.017	0.023	0.006	0.03	-0.21	-1.36	0.08
ILE	2.93	-0.61	-1.58	-4.74	-0.01	0	0.44	0.022	0.004	0	0.20	-0.17	-0.49	0.36
LEU	3.24	-0.65	-1.77	-2.05	-0.00	0	0.54	0.034	0.005	0	0.13	-0.17	-0.61	0.17
LYS	2.81	-0.66	-1.81	-1.08	-0.00	0.12	0.45	0.015	0.009	0.001	0.29	-0.16	-1.53	0.02
MET	3.27	-0.68	-1.87	-1.12	-0.01	0	0.53	0.027	0.005	0	0.10	-0.17	-1.92	0.07
PHE	3.68	-0.73	-1.73	-6.68	-0.01	0	0.43	0.022	0.006	0	0.12	-0.22	-1.03	0.10
PRO	2.23	-1.04	-1.14	-0.36	-0.39	0	0.18	0.002	0.002	0	0.15	-0.18	-0.63	1.13
SER	2.45	-0.62	-1.93	-0.37	-0.01	0.09	0.37	0.018	0.036	0.010	-0.02	-0.19	-0.62	0.08
THR	2.62	-0.61	-2.00	-1.82	-0.01	0.04	0.37	0.011	0.033	0.009	0.02	-0.18	-0.27	0.14
TRP	4.51	-0.87	-2.23	-6.39	-0.01	0	0.43	0.018	0.009	0.001	0.09	-0.21	-1.95	0.04
TYR	3.75	-0.74	-1.92	-6.55	-0.00	0	0.41	0.020	0.008	0.003	0.11	-0.23	-0.97	0.10
VAL	2.63	-0.58	-1.46	-3.26	-0.01	0	0.37	0.019	0.004	0	0.22	-0.18	-0.24	0.34

Table SVI

Unweighted unfolded state energies by energy term for all amino acids. The dot product of the unweighted energies for an amino acid with a set of weights gives the unfolded state energy of that amino acid.

	energy function						
	current Rosetta	standard, reweighted refEs	standard + hpatch-SASA, reweighted refEs	standard, all terms reweighted	standard + hpatch-SASA, all terms reweighted	unfoldedE, reweight all terms	unfolded + hpatch-SASA, reweight all terms
run_id	616	681/682	683/684b	653/654	663/664c	685/686	687/688
fa_atr	0.8	0.8	0.8	0.8	0.8	0.8	0.8
fa_rep	0.44	0.44	0.44	0.561	0.438	0.594	0.498
fa_sol	0.65	0.65	0.65	0.998	0.939	1.333	1.435
fa_intra_rep	0.004	0.004	0.004	0.182	0.220	0.056	0.558
pro_close	1	1	1	0.010	0.008	0.001	0.095
fa_pair	0.49	0.49	0.49	0.666	0.642	0.457	0.428
hbond_sr_bb	0.585	0.585	0.585	0.585	0.585	0.585	0.585
hbond_lr_bb	1.17	1.17	1.17	1.17	1.17	1.17	1.17
hbond_bb_sc	1.17	1.17	1.17	3.398	3.503	3.220	3.647
hbond_sc	1.1	1.1	1.1	1.348	1.236	1.303	1.834
dslf_ss_dst	1	1	1	1	1	1	1
dslf_cs_ang	1	1	1	1	1	1	1
dslf_ss_dih	1	1	1	1	1	1	1
dslf_ca_dih	1	1	1	1	1	1	1
rama	0.2	0.2	0.2	0.005	0.002	0.045	0.038
omega	0.5	0.5	0.5	0.5	0.5	0.5	0.5
fa_dun	0.56	0.56	0.56	0.508	0.333	0.283	0.280
p_aa_pp	0.32	0.32	0.32	0.981	1.047	0.950	1.026
ref/unfolded	1	1	1	1	1	1	1
hpatch			0.2		0.3		0.5
ALA	0.16	0.12	0.20	0.83	0.60	0.52	1.53
CYS	1.7	-0.04	0.07	0.44	0.36	-0.27	0.63
ASP	-0.67	-0.48	-0.42	-0.66	-0.45	-0.58	-0.26
GLU	-0.81	-0.61	-0.55	-0.65	-0.27	-0.42	-0.12
PHE	0.63	1.17	1.01	0.26	-0.18	0.29	-1.94
GLY	-0.17	-0.40	-0.27	0.42	0.18	1.07	2.29
HIS	0.56	0.98	0.97	1.02	1.11	-0.36	0.21
ILE	0.24	0.38	0.31	-0.03	-0.20	0.50	-0.73
LYS	-0.65	-0.42	-0.41	-0.28	-0.10	-0.27	0.29
LEU	-0.1	0.20	0.09	0.27	-0.03	0.48	0.57
MET	-0.34	-0.20	-0.25	0.02	0.13	-0.07	0.48
ASN	-0.89	-0.76	-0.72	-0.87	-0.59	-0.71	-0.47
PRO	0.02	-0.81	-0.89	0.57	0.88	1.02	2.10
GLN	-0.97	-0.82	-0.62	-0.80	-0.45	-0.59	-0.29
ARG	-0.98	-0.79	-0.74	-0.87	-0.47	-0.64	-0.62
SER	-0.37	-0.23	-0.26	0.27	0.14	-0.32	0.60
THR	-0.27	-0.18	-0.20	-0.19	-0.34	-0.22	-0.04
VAL	0.29	0.22	0.25	0.15	-0.03	0.53	0.05
TRP	0.91	1.73	1.50	0.29	0.12	-0.08	-2.20
TYR	0.51	0.95	0.91	-0.18	-0.42	0.11	-2.07
ddG	0.69	0.68	0.681	0.609	0.635		
core	49.2	51.7	52.5	51.6	52.3	47.7	48.4
overall	32.9	35.1	35.5	35.2	36.5	30.5	29.8
surface	24.9	27.9	27.3	27.3	28.9	21.0	19.9
%hp/surface	29.5	31.8	27.1	28.9	27.7	46.4	30.3
largest patch	813	694	446	735	433	1479	464

Table SVII

Final weights obtained from weight optimization runs for various energy functions including the hpatch score and/or the unfolded state energy term.

no. designed (surface positions)

Residue	natives	current Rosetta weights	current Rosetta, fit refEs only	current Rosetta + hpatch- SASA, fit refEs only	standard Rosetta, reweight all terms	standard + hpatch- SASA	standard, no refE + unfoldedE	standard, no refE + unfoldedE, hpatch- SASA
ALA	144	30	100	59	47	56	44	42
CYS	2	0	12	8	6	6	24	16
ASP	167	221	158	176	182	164	33	77
GLU	180	158	144	178	196	178	53	88
PHE	23	68	21	19	14	20	85	51
GLY	210	205	252	228	223	225	190	189
HIS	37	32	11	16	22	32	275	308
ILE	33	39	48	38	47	39	53	52
LYS	193	148	97	120	110	104	64	40
LEU	54	174	85	81	82	96	46	29
MET	20	5	15	7	12	5	83	32
ASN	110	120	144	182	163	131	77	85
PRO	144	40	143	140	178	141	127	69
GLN	94	110	142	44	134	124	69	174
ARG	85	76	81	97	90	79	71	153
SER	119	128	90	131	62	127	110	112
THR	145	110	146	181	137	178	52	67
VAL	60	37	104	75	75	64	33	30
TRP	12	56	3	9	12	22	314	168
TYR	23	98	59	66	63	64	52	73

Table VIII

Amino acid composition of surface residues for redesigns created with optimized energy functions.

The table shows the number of occurrences of each residue type in the set of native testing proteins and in redesigns created with the indicated energy functions. The counts shown are over surface positions only, here defined as positions with 15 or fewer neighbors.

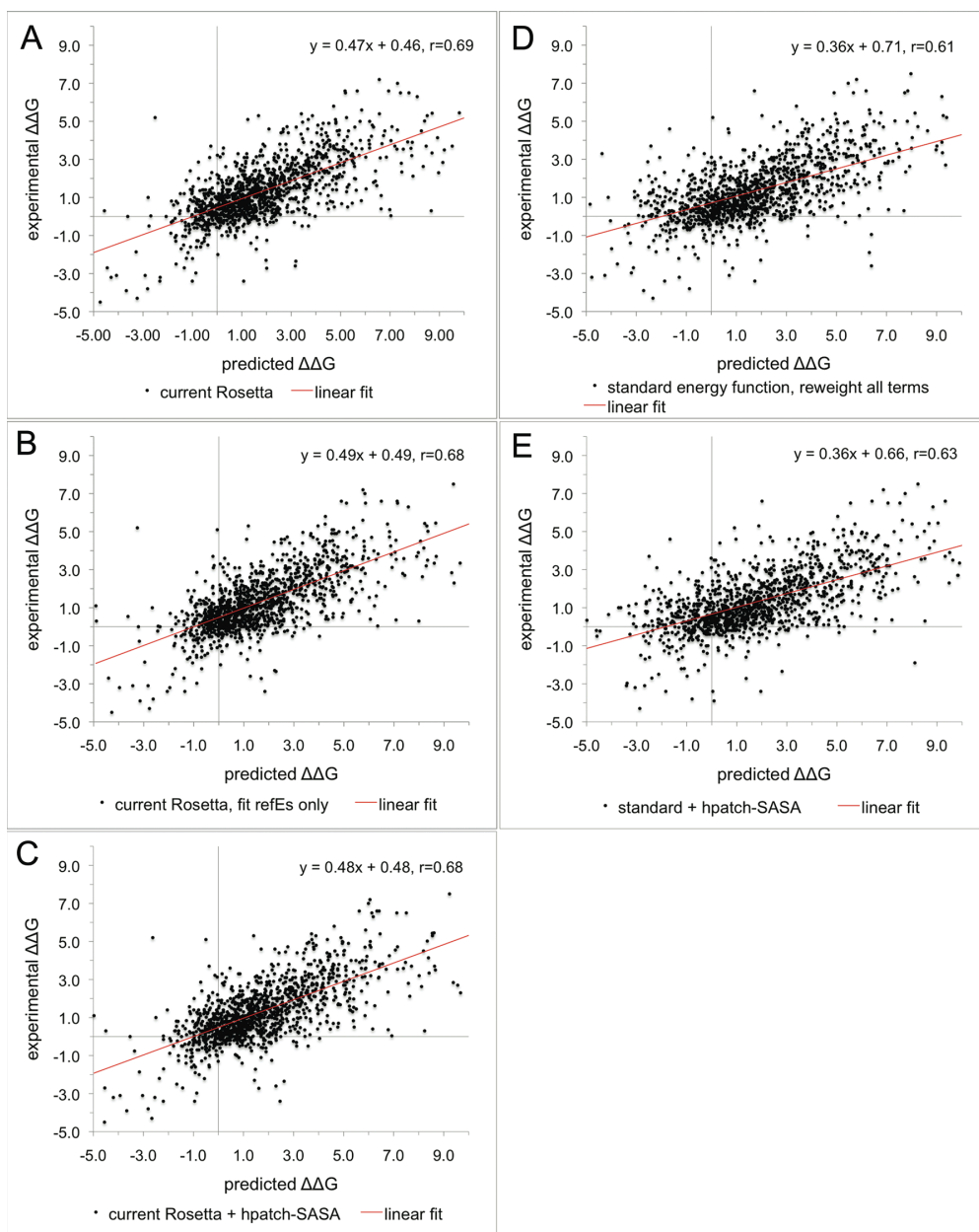


Figure S3

Performance of all energy functions tested in predicting mutant changes in free energy. Predicted values are plotted on the x-axis versus experimental values plotted on the y-axis (kcal/mol). The red-line indicates the best fit line. The equation of the best-fit line ( $y$ ) and the correlation coefficient ( $r$ ) are provided in the upper right hand corner. The energy functions tested are as follows: A) the current Rosetta energy function, B) current Rosetta with reweighted reference energies, C) current Rosetta with the hpatch-SASA score and reweighted reference energies, D) standard Rosetta with all terms reweighted, and E) standard Rosetta with the hpatch-SASA score with all terms reweighted.

Supplementary Table IX. Experimental and predicted changes in free energy for all mutants in the dataset for all energy functions tested.

Mutations are specified as PDB\_wild type amino acid\_position\_mutant amino acid

Example:

107L\_G\_44\_S is the point mutant glycine to serine at position 44 in the PDB file 107L.

Predicted  $\Delta\Delta G$ 's are reported for each of the following energy functions:

current Rosetta	the current Rosetta energy function previously optimized for native sequence recovery only
current Rosetta, fit refEs only	the current Rosetta energy function with the reference energies optimized for native sequence recovery and amino acid composition
current Rosetta + hpatch-SASA	the current Rosetta energy function using the hpatch-SASA score, with the reference energies optimized for native sequence recovery and amino acid composition
standard energy function, reweight all terms	A reweighted Rosetta energy function optimized for native sequence recovery and amino acid composition
standard + hpatch-SASA energy function	A reweighted Rosetta energy function using the hpatch-SASA score, optimized for native sequence recovery and amino acid composition

mutation	predicted ddG					
	experimental ddG	current Rosetta	current Rosetta, fit refEs only	current Rosetta + hpatch-SASA	standard energy function, reweight all terms	standard + hpatch-SASA
107L_G_44_S	-0.53	-0.61	-0.28	-0.34	1.15	1.13
160I_A_120_M	-0.20	-0.83	-0.60	-0.77	0.07	-4.61
161I_A_116_N	0.17	0.00	0.24	0.20	0.20	-0.27
162I_A_122_Q	-0.24	0.03	0.28	0.88	-1.58	6.51
163I_A_123_Q	-0.22	-1.43	-1.33	-1.90	-1.27	-0.22
164I_A_119_R	-0.18	0.64	0.76	0.45	2.82	2.95
165I_A_117_S	1.27	1.39	1.54	1.59	2.37	1.25
171I_A_45_E	0.01	1.57	1.08	-0.11	0.89	1.13
1a2p_A_30_C	0.90	2.31	0.83	0.57	1.79	1.62
1a2p_A_30_D	0.61	0.45	0.70	0.58	1.30	1.45
1a2p_A_30_F	0.59	-0.70	-0.18	-0.40	0.75	-0.07
1a2p_A_30_G	0.81	1.36	1.04	1.23	1.86	1.77
1a2p_A_30_H	0.70	0.32	0.69	0.54	1.05	1.42
1a2p_A_30_I	0.72	-0.28	0.07	-0.29	0.35	0.37
1a2p_A_30_K	0.10	-0.30	0.02	-0.12	0.87	0.71
1a2p_A_30_L	0.26	-0.76	-0.35	-0.43	-0.32	-0.48
1a2p_A_30_M	0.21	-0.13	-0.11	-0.08	0.04	0.21
1a2p_A_30_N	0.57	-0.26	-0.05	-0.10	1.02	1.10
1a2p_A_30_P	3.99	7.04	6.20	5.89	6.56	5.99
1a2p_A_30_Q	0.38	-0.50	-0.28	-0.07	0.22	0.72
1a2p_A_30_R	0.05	-0.15	0.19	0.16	0.31	0.52
1a2p_A_30_S	0.31	0.42	0.73	0.46	1.77	0.84
1a2p_A_30_T	0.69	0.69	0.69	0.76	0.95	1.51

1a2p_A_30_V	0.79	0.36	0.35	0.25	0.66	0.58
1a2p_A_30_W	0.88	-1.09	-0.22	-0.79	-0.30	-0.70
1a2p_A_30_Y	0.70	-0.84	-0.26	-0.32	0.47	0.15
1a2p_D_10_A	0.39	0.11	0.00	-0.20	-2.19	-2.15
1a2p_D_10_S	0.90	1.05	0.90	1.03	-0.48	0.05
1a2p_D_52_A	2.86	-0.76	-0.88	-0.71	0.13	0.16
1a2p_D_52_N	1.78	0.22	0.13	0.12	-0.36	-0.60
1a2p_D_6_A	0.85	0.10	0.05	0.13	-0.18	-0.58
1a2p_D_6_G	1.30	0.89	0.46	0.20	0.43	0.02
1a2p_D_6_S	0.70	0.82	0.44	0.39	0.36	0.13
1a2p_E_27_A	1.20	0.06	-0.20	-0.12	0.88	1.17
1a2p_E_27_G	2.13	2.45	1.92	1.91	3.56	3.94
1a2p_E_27_S	1.20	1.27	1.34	1.20	2.85	3.73
1a2p_G_32_A	2.70	15.93	16.12	15.86	19.57	16.42
1a2p_G_32_D	3.20	4.39	5.05	5.10	6.51	6.44
1a2p_G_32_H	2.30	4.50	5.04	5.24	6.78	6.61
1a2p_G_32_K	2.70	3.62	4.06	3.94	11.79	10.22
1a2p_G_32_N	2.70	3.00	3.59	3.35	10.50	9.84
1a2p_G_32_R	2.80	3.90	4.31	4.18	6.04	6.35
1a2p_G_32_S	2.90	4.56	5.10	4.71	7.07	6.68
1a2p_G_32_T	3.20	7.88	8.29	8.02	11.67	10.99
1a2p_H_16_A	1.90	3.78	3.02	3.18	3.17	3.16
1a2p_H_16_D	2.20	3.07	2.89	3.00	3.69	3.49
1a2p_H_16_G	0.70	2.20	1.60	1.68	-0.18	0.18
1a2p_H_16_K	0.90	1.80	1.51	1.55	1.22	1.45
1a2p_H_16_N	1.80	2.34	1.98	1.96	1.71	1.75
1a2p_H_16_R	1.00	2.04	1.88	1.83	1.87	2.28
1a2p_H_16_S	2.10	3.65	3.08	3.10	2.75	3.09
1a2p_I_107_A	2.07	1.33	0.86	0.81	0.43	1.99
1a2p_I_107_V	0.81	1.72	1.78	1.64	1.86	1.99
1a2p_I_23_A	3.68	4.58	4.35	4.55	4.59	4.14
1a2p_I_23_V	0.83	1.15	0.96	1.05	1.21	1.34
1a2p_I_2_A	0.75	3.29	2.94	3.15	3.40	2.98
1a2p_I_2_V	0.81	1.13	0.87	1.08	1.34	0.68
1a2p_I_49_A	4.72	2.83	2.74	2.77	2.49	2.33
1a2p_I_49_V	1.13	1.06	1.00	1.17	0.89	0.93
1a2p_I_53_A	1.48	0.84	0.81	0.78	0.73	0.79
1a2p_I_53_T	1.15	0.60	0.95	0.68	1.40	0.41
1a2p_I_53_V	0.63	0.09	-0.10	0.00	0.28	0.03
1a2p_I_74_A	1.66	2.37	2.61	2.52	2.07	3.57
1a2p_I_74_V	0.98	1.07	0.86	0.76	0.45	1.16
1a2p_I_86_A	4.02	4.52	4.22	4.38	4.28	5.07
1a2p_I_86_V	1.64	2.30	2.31	2.15	1.83	2.27
1a2p_I_94_A	3.15	3.98	3.53	3.96	3.86	4.28
1a2p_I_94_V	1.02	0.37	-0.13	0.08	-0.09	0.61
1a2p_K_25_G	0.38	1.42	1.47	1.23	-0.44	0.02
1a2p_K_60_R	0.32	0.63	0.59	0.63	3.21	5.02
1a2p_L_12_A	4.53	4.95	4.55	5.04	5.03	5.86
1a2p_L_31_Q	1.41	1.31	1.14	1.42	1.47	2.27
1a2p_L_87_T	3.28	4.05	3.85	3.73	4.78	5.45
1a2p_L_87_V	0.47	2.83	2.12	2.43	1.69	4.16
1a2p_N_21_A	2.20	0.00	0.05	-0.04	-0.76	-0.65
1a2p_N_39_D	2.62	0.35	0.71	0.54	0.78	0.97
1a2p_N_3_A	1.59	2.12	2.04	1.99	1.56	2.41
1a2p_N_56_A	2.00	3.14	2.82	3.11	5.08	7.44
1a2p_N_56_D	-0.31	3.13	3.02	3.12	5.36	5.09

1a2p_N_75_A	1.45	2.95	2.71	2.76	3.13	3.07
1a2p_N_82_A	1.59	3.59	3.38	3.25	4.24	5.00
1a2p_Q_29_A	0.19	1.48	1.25	1.00	-0.16	-0.15
1a2p_Q_29_G	1.10	2.72	2.49	2.32	1.94	1.45
1a2p_Q_29_S	-0.30	2.15	2.34	2.02	1.52	1.28
1a2p_R_108_A	-0.19	1.31	0.76	0.88	-0.41	-0.06
1a2p_S_26_A	-0.60	-0.38	-0.57	-0.48	-0.90	-0.88
1a2p_S_26_G	0.50	0.25	0.07	0.39	0.33	-0.08
1a2p_S_89_A	2.41	0.96	0.89	0.57	2.44	2.94
1a2p_S_90_A	3.22	0.01	-0.19	-0.14	-0.92	0.26
1a2p_T_103_V	2.14	1.72	1.52	1.45	0.53	2.09
1a2p_T_14_A	0.50	0.48	0.21	0.15	-0.94	-1.36
1a2p_T_14_G	1.30	1.97	1.60	1.86	1.32	1.07
1a2p_T_14_R	-0.74	-0.32	0.01	-0.10	-0.34	-0.38
1a2p_T_14_S	1.36	0.98	1.04	1.36	1.34	0.55
1a2p_T_24_A	1.67	1.30	1.20	1.22	2.98	2.95
1a2p_T_24_D	0.00	2.30	2.45	2.49	5.06	5.29
1a2p_T_24_G	1.01	1.61	1.13	1.29	1.33	2.07
1a2p_T_24_S	0.54	-0.16	-0.21	-0.19	-0.22	-0.03
1a2p_T_24_V	2.09	2.71	2.64	2.80	6.70	6.84
1a2p_T_4_A	2.02	1.31	1.17	1.41	3.32	3.57
1a2p_T_4_G	0.61	1.54	1.21	1.35	2.48	2.72
1a2p_T_4_P	3.30	4.41	3.40	3.61	5.10	5.28
1a2p_T_4_S	0.27	0.34	0.38	0.49	1.10	0.75
1a2p_T_97_V	2.92	3.59	3.63	3.43	4.01	4.89
1a2p_V_34_A	1.68	2.17	2.15	2.23	2.43	2.64
1a2p_V_34_T	1.05	1.05	1.17	1.17	2.04	0.44
1a2p_V_43_A	1.17	1.77	1.87	2.17	1.75	1.73
1a2p_V_43_T	2.22	1.71	1.87	1.69	1.97	2.32
1a2p_V_8_A	3.47	3.29	3.27	3.06	2.70	2.91
1a2p_V_8_T	1.99	1.47	1.81	1.71	2.85	2.76
1a2p_Y_101_F	0.18	-0.63	-0.45	-0.53	-1.25	0.51
1a2p_Y_11_A	3.00	5.01	4.40	4.43	2.75	2.83
1a2p_Y_15_A	1.67	3.76	3.32	3.17	3.32	3.91
1a2p_Y_15_G	4.00	5.80	5.10	5.49	5.52	6.22
1a2p_Y_15_S	2.00	4.84	4.29	4.33	4.43	4.77
1a2p_Y_22_F	-0.09	0.48	0.43	0.71	0.87	0.58
1a2p_Y_76_F	1.14	0.59	0.76	0.56	1.99	1.80
1bf4_A_44_G	1.27	2.52	1.99	-0.86	1.04	1.00
1bf4_A_50_G	2.10	4.72	4.17	4.22	1.16	1.30
1bf4_D_34_A	0.54	-1.14	-3.63	-1.68	-1.94	-1.52
1bf4_E_11_A	0.30	0.26	-0.31	-0.28	-0.04	-0.21
1bf4_F_31_A	2.70	10.21	7.43	9.56	9.36	9.83
1bf4_I_16_A	1.50	3.21	1.69	2.81	2.18	2.44
1bf4_I_29_A	2.57	4.58	4.09	4.12	4.94	5.21
1bf4_K_6_A	0.27	0.56	-1.02	-0.01	0.77	0.56
1bf4_L_54_A	3.92	7.72	7.04	6.26	4.89	5.61
1bf4_L_55_A	1.45	6.03	5.33	5.51	2.26	2.45
1bf4_L_58_A	0.67	5.04	0.20	1.34	2.04	2.42
1bf4_Q_56_G	0.70	0.70	-1.94	-0.05	-0.17	0.14
1bf4_R_24_A	0.38	0.09	-0.52	-0.46	-1.25	-0.78
1bf4_R_42_A	0.56	0.08	-0.52	-1.42	-2.83	-3.11
1bf4_S_17_A	0.13	1.26	-0.28	-0.15	0.52	0.54
1bf4_S_30_A	-0.72	-0.46	-1.33	-1.26	-1.50	-0.93
1bf4_S_46_A	-0.18	-0.59	-1.11	-1.02	-0.47	-0.15
1bf4_T_40_A	0.84	0.99	-0.38	-1.28	1.07	1.26

lbf4_V_14_A	2.29	3.18	1.89	2.87	3.31	3.84
lbf4_V_22_A	0.23	3.02	0.77	1.77	3.54	3.59
lbf4_V_3_A	2.12	7.93	6.65	7.65	5.27	5.46
lbf4_V_45_A	1.63	2.70	1.35	-0.49	3.25	3.15
lbp_i_D_3_A	-0.20	-0.54	-0.58	-0.59	-0.15	-0.80
lbp_i_D_50_A	0.40	-1.18	-1.25	-0.79	-2.23	-2.11
lbp_i_E_49_A	0.20	0.52	0.09	0.36	0.69	-0.02
lbp_i_E_7_A	1.50	-0.20	-0.50	-0.33	-0.39	-0.95
lbp_i_F_22_A	2.00	5.56	5.33	5.24	4.51	4.76
lbp_i_F_4_A	3.00	3.68	3.12	3.34	2.32	2.31
lbp_i_I_18_A	1.50	2.33	1.80	1.95	-0.49	-0.31
lbp_i_I_19_A	2.10	1.66	1.34	1.98	1.99	2.16
lbp_i_K_15_A	0.40	0.93	0.08	0.36	2.22	1.00
lbp_i_K_26_A	0.00	-0.04	-0.18	-0.12	-0.08	-0.31
lbp_i_K_41_A	0.40	0.31	0.08	0.62	0.45	-0.37
lbp_i_K_46_A	-0.10	0.15	0.18	0.34	0.00	-0.14
lbp_i_L_29_A	0.00	0.41	0.44	0.88	-0.51	-0.03
lbp_i_L_6_A	0.60	1.06	0.75	0.97	1.19	0.67
lbp_i_M_52_A	1.70	0.83	1.02	0.67	1.12	0.13
lbp_i_N_24_A	2.20	2.32	1.97	1.86	1.98	0.94
lbp_i_N_44_A	3.30	0.24	0.06	0.14	-4.37	-5.26
lbp_i_P_13_A	1.20	1.34	2.22	2.18	2.14	0.94
lbp_i_P_2_A	1.30	1.52	2.41	2.54	4.30	3.42
lbp_i_P_8_A	0.30	1.56	2.03	2.20	3.54	2.30
lbp_i_P_9_A	0.80	1.70	2.60	2.76	4.33	3.20
lbp_i_Q_31_A	1.00	1.90	1.51	1.39	1.63	0.89
lbp_i_R_17_A	0.30	1.01	0.52	0.58	0.98	0.72
lbp_i_R_1_A	0.50	-0.08	-0.36	-0.36	0.05	0.40
lbp_i_R_20_A	1.80	0.92	0.65	0.67	-2.37	-2.02
lbp_i_R_39_A	0.00	1.17	0.27	0.62	1.63	0.23
lbp_i_R_42_A	0.50	0.60	0.35	0.61	0.92	-0.21
lbp_i_R_53_A	0.10	0.67	0.39	0.44	-0.32	-0.29
lbp_i_S_47_A	1.60	0.23	0.21	0.02	1.05	0.98
lbp_i_T_11_A	0.00	1.11	1.25	1.37	3.04	2.01
lbp_i_T_32_A	0.10	0.92	0.42	0.91	1.06	1.29
lbp_i_T_54_A	0.10	-0.14	0.12	-0.20	0.49	0.30
lbp_i_V_34_A	1.20	2.43	2.52	2.71	2.97	3.66
lbp_i_Y_10_A	1.20	3.57	2.86	2.73	4.04	3.67
lbp_i_Y_35_A	1.10	4.50	4.23	4.35	1.53	1.41
lbvc_A_125_L	-0.40	-0.25	-0.10	0.45	0.41	-0.08
lbvc_A_130_K	3.70	9.52	8.69	8.63	11.52	10.63
lbvc_A_130_L	2.30	8.97	9.40	9.67	11.01	9.49
lbvc_A_144_L	-0.10	-0.71	-0.25	-0.57	0.17	0.23
lbvc_A_15_L	-0.20	-0.72	-0.01	-0.93	-0.38	0.19
lbvc_F_106_A	0.20	3.57	3.56	3.21	1.62	2.82
lbvc_F_123_A	0.30	8.67	8.00	8.24	7.70	8.52
lbvc_F_123_T	3.50	9.20	8.34	8.67	8.98	9.63
lbvc_G_129_A	-1.05	-1.28	-0.69	-1.04	-1.41	-1.58
lbvc_G_23_A	1.12	1.01	1.17	1.22	-0.97	-0.10
lbvc_H_116_A	-0.16	0.90	0.30	0.16	0.05	-0.38
lbvc_H_93_G	0.01	3.97	3.09	3.46	2.81	3.41
lbvc_I_142_A	1.92	3.16	3.24	3.71	3.28	3.19
lbvc_I_28_A	2.06	4.92	4.58	4.69	4.84	5.59
lbvc_I_30_A	1.90	2.13	1.24	1.63	0.97	2.49
lbvc_L_115_A	1.00	3.19	2.90	3.28	3.32	4.81
lbvc_L_11_A	0.47	3.50	3.31	3.27	3.19	3.33



lbvc_L_135_A	0.80	4.59	4.13	4.32	3.95	3.89
lbvc_L_137_A	1.78	1.85	1.01	1.32	1.16	0.78
lbvc_L_149_A	1.60	3.13	2.09	2.65	1.37	2.27
lbvc_L_29_A	0.39	4.51	4.37	4.47	4.51	4.24
lbvc_L_32_A	2.04	3.46	3.29	3.63	3.52	4.54
lbvc_L_9_A	0.41	2.00	1.60	1.77	1.83	2.25
lbvc_M_131_A	2.20	3.04	3.09	3.07	3.20	3.30
lbvc_N_132_G	0.30	-0.63	-0.50	-0.64	-1.58	-1.58
lbvc_P_88_A	-0.59	0.50	1.27	1.77	0.44	1.26
lbvc_S_117_A	0.26	-0.58	-0.65	-0.89	-1.52	-0.83
lbvc_T_51_A	1.41	0.21	0.02	0.67	0.62	0.52
lbvc_T_67_A	0.26	-0.73	-0.53	-0.65	-1.65	-1.53
lbvc_V_114_A	1.45	2.26	2.15	2.31	1.94	1.79
lbvc_V_13_A	0.67	1.75	2.47	1.82	0.52	0.86
lbvc_V_66_A	-0.75	0.80	0.93	1.32	2.07	0.61
lbvc_V_68_T	0.60	0.65	0.64	0.79	1.46	1.62
lcey_A_47_G	-0.20	1.65	1.22	0.99	-0.28	0.83
lcey_A_76_G	0.30	-4.56	-4.89	-4.50	-10.15	-8.61
lcey_A_79_G	-0.60	0.08	0.12	-0.20	1.11	-1.15
lcey_A_87_G	-0.10	1.20	1.12	0.84	0.84	2.15
lcey_A_89_G	-0.50	-1.14	-0.99	-1.44	-0.97	-2.72
lensp_F_15_A	2.27	3.91	3.31	3.56	2.43	3.14
lensp_F_17_A	1.53	3.34	2.74	2.99	2.76	3.24
lensp_F_27_A	0.76	4.69	4.09	4.34	4.57	4.10
lensp_F_38_A	-0.15	1.39	0.82	1.07	1.28	1.00
lcyo_F_35_L	1.87	2.53	2.28	2.34	1.13	0.72
ldyb_G_131_V	-0.68	-1.10	-0.92	-1.07	-0.07	-0.76
ldyj_D_27_N	-1.40	-0.62	-0.45	-1.29	-3.24	-1.70
ldyj_E_139_Q	0.42	0.34	-0.89	-1.32	-0.74	0.10
ldyj_P_66_A	-1.30	-1.67	0.13	-0.01	2.21	1.46
ldyj_T_113_V	1.20	-0.18	1.50	0.40	0.93	-0.52
ldyj_V_75_A	-0.10	2.20	3.40	4.04	2.94	3.07
ldyj_V_88_A	-0.20	1.63	2.75	1.87	2.12	3.05
lfkj_E_60_A	2.13	0.07	-0.24	-0.39	-2.50	-2.66
lfkj_E_60_G	2.84	2.06	1.75	1.71	-0.14	-0.38
lfkj_E_61_A	0.84	1.22	1.25	1.32	-0.80	-0.85
lfkj_E_61_G	2.49	2.28	2.84	1.86	0.14	0.83
lfkj_F_36_A	3.54	7.28	6.29	6.70	7.49	8.37
lfkj_I_56_A	2.48	3.48	3.45	3.37	2.66	2.60
lfkj_I_56_D	3.16	4.93	4.91	5.85	5.48	5.56
lfkj_I_56_T	1.81	3.75	3.83	3.34	3.68	3.77
lfkj_I_76_A	3.81	5.45	5.35	4.59	6.34	6.38
lfkj_I_76_V	0.76	1.92	0.88	1.45	1.03	1.12
lfkj_I_7_V	0.92	0.28	0.23	0.65	-0.35	0.68
lfkj_I_91_A	1.54	5.27	6.02	5.40	5.58	6.67
lfkj_I_91_V	0.38	1.26	1.04	0.84	0.96	1.37
lfkj_L_106_A	2.32	5.14	4.52	5.07	5.37	5.57
lfkj_L_50_A	2.57	3.40	3.50	4.21	3.39	4.59
lfkj_L_97_A	3.56	5.86	5.75	5.86	5.98	7.02
lfkj_R_57_A	0.81	1.43	0.45	0.99	0.27	-0.26
lfkj_R_57_G	2.29	3.08	2.62	2.38	1.17	0.66
lfkj_T_21_A	1.60	1.20	1.18	1.30	0.60	0.80
lfkj_T_21_S	1.44	1.99	1.67	2.01	2.18	2.37
lfkj_T_21_V	-0.86	-1.13	-0.82	-1.06	-1.67	-1.93
lfkj_T_27_A	1.97	1.49	1.41	1.48	-2.22	-2.11
lfkj_T_27_S	1.49	0.93	0.74	1.42	-1.85	-2.14

1fkj_T_27_V	-0.23	-1.79	-2.44	-1.64	-4.03	-4.46
1fkj_T_75_A	2.65	0.78	0.74	0.87	1.00	0.76
1fkj_T_75_V	0.81	-1.85	-1.46	-1.68	-2.82	-2.65
1fkj_V_101_A	2.75	3.63	4.01	4.17	4.47	4.89
1fkj_V_23_A	2.97	2.73	2.03	2.86	2.50	2.49
1fkj_V_24_A	3.19	1.73	1.78	1.53	1.71	3.11
1fkj_V_2_A	2.43	2.33	1.56	2.68	2.09	2.51
1fkj_V_4_A	2.78	3.68	2.89	3.94	3.74	4.06
1fkj_V_55_A	2.13	3.56	3.26	3.60	5.05	5.25
1fkj_V_63_A	2.97	2.31	2.32	2.45	2.44	1.79
1fkj_V_98_A	2.16	3.00	3.04	3.63	3.65	4.72
1fkj_W_59_F	-2.72	2.01	1.70	1.61	0.85	1.38
1fkj_W_59_L	-2.35	3.19	2.29	2.62	0.55	2.81
1fxa_E_94_Q	-0.60	-0.93	-0.86	-0.65	-1.11	-0.59
1fxa_F_65_A	1.00	3.68	3.13	3.27	1.85	2.49
1fxa_R_42_A	2.40	1.10	0.93	0.86	-0.01	0.03
1fxa_T_48_A	-0.10	0.07	0.06	-0.04	-0.92	-1.86
1hfz_H_108_A	0.79	3.50	3.50	3.69	2.21	0.29
1hfz_H_33_A	2.13	2.36	1.69	1.78	1.65	0.33
1hfz_Q_118_A	0.96	0.85	0.53	0.32	0.47	0.45
1hfz_Q_55_A	0.41	-0.47	0.05	-0.35	0.22	-1.78
1hfz_V_43_A	0.93	-0.02	0.91	0.89	1.48	0.87
1hfz_V_43_G	1.15	0.93	1.06	1.61	2.04	1.94
1hfz_Y_104_A	2.39	6.41	5.67	5.72	5.48	6.80
1hz6_A_11_G	2.43	3.71	3.41	3.53	3.00	3.04
1hz6_A_32_G	2.54	2.83	2.90	2.97	3.06	3.35
1hz6_A_36_G	3.10	3.20	2.85	2.97	3.27	3.59
1hz6_A_38_G	1.32	1.57	0.90	1.31	1.66	1.88
1hz6_A_40_G	3.12	3.83	3.47	3.61	3.94	3.95
1hz6_A_55_G	0.49	0.71	-0.12	0.66	-1.17	-1.23
1hz6_D_41_A	1.21	-0.13	-0.89	-0.73	-2.43	-2.62
1hz6_D_41_G	2.14	1.81	0.99	0.81	-0.85	-0.52
1hz6_D_53_A	0.20	1.76	1.06	0.84	0.34	0.66
1hz6_E_24_A	0.59	1.20	0.75	0.85	0.16	0.29
1hz6_E_35_G	1.19	1.61	1.52	1.48	0.74	0.79
1hz6_E_49_A	0.23	-0.51	-0.29	-0.37	-0.34	-0.51
1hz6_F_15_A	3.12	6.02	5.44	5.74	5.40	5.96
1hz6_F_15_L	0.68	4.10	3.58	4.06	3.86	3.99
1hz6_F_25_A	4.25	6.74	6.87	6.83	6.04	7.04
1hz6_F_25_L	3.12	6.85	6.92	6.41	7.50	6.65
1hz6_F_29_G	3.08	6.60	5.77	6.40	5.82	6.54
1hz6_F_29_L	0.38	2.38	1.84	2.48	2.17	2.48
1hz6_F_65_L	3.34	8.70	8.61	8.42	6.73	6.50
1hz6_I_14_A	1.37	2.23	2.19	2.36	2.96	3.45
1hz6_I_14_V	0.47	0.07	0.07	-0.16	-0.48	0.10
1hz6_I_63_A	4.72	7.08	6.82	7.15	8.25	8.21
1hz6_I_63_V	1.69	2.79	2.35	2.49	2.36	2.34
1hz6_I_9_A	4.90	4.53	4.52	4.95	5.06	5.98
1hz6_I_9_V	0.56	1.36	0.98	0.80	1.20	1.40
1hz6_K_10_A	0.92	1.28	1.37	1.50	1.33	1.33
1hz6_K_26_A	1.13	0.75	1.03	0.72	0.46	0.49
1hz6_K_31_G	-0.16	1.72	1.44	1.30	1.57	1.60
1hz6_K_44_A	-0.58	0.87	0.66	1.27	-1.00	-0.61
1hz6_K_45_A	-0.35	0.25	0.01	0.15	-0.20	-0.30
1hz6_K_57_A	0.09	0.68	1.04	0.74	1.25	1.01
1hz6_K_64_A	0.45	1.39	1.62	1.27	1.58	1.46

1hz6_L_13_A	3.12	4.45	4.34	4.42	4.26	4.71
1hz6_L_43_A	2.44	3.20	2.41	2.89	2.92	3.08
1hz6_L_61_A	3.77	4.58	3.98	4.62	4.61	5.20
1hz6_N_12_A	1.87	0.54	0.46	0.36	-0.24	0.13
1hz6_N_17_A	1.78	1.33	0.92	1.04	1.01	1.03
1hz6_N_47_A	0.34	0.63	0.68	0.55	0.22	0.28
1hz6_N_62_A	1.73	0.39	0.43	0.25	-0.07	0.25
1hz6_S_19_A	0.30	0.47	0.09	0.42	0.24	0.13
1hz6_S_34_A	-0.41	-0.76	-0.68	-0.77	-1.86	-1.44
1hz6_S_34_G	0.82	1.10	0.09	0.33	-0.18	0.42
1hz6_T_20_A	1.17	1.03	0.98	0.79	0.90	1.18
1hz6_T_22_A	1.11	1.28	1.04	1.56	1.19	1.20
1hz6_T_28_A	1.25	-0.35	-0.28	-0.42	-0.26	-0.12
1hz6_T_33_A	1.09	0.19	0.07	-0.18	-2.18	-1.66
1hz6_T_42_G	0.17	0.15	-0.35	0.10	-0.34	0.14
1hz6_T_51_A	0.97	0.70	0.98	1.47	0.75	0.99
1hz6_T_60_A	1.83	1.51	1.12	1.17	1.58	1.83
1hz6_T_8_A	1.63	0.96	1.10	0.94	1.24	1.31
1hz6_V_52_A	0.92	3.08	2.67	2.34	2.39	2.58
1hz6_V_54_A	1.14	1.74	1.47	1.70	1.39	1.21
1hz6_V_7_A	1.22	2.82	2.99	3.43	3.45	3.68
1hz6_Y_37_G	2.82	4.91	4.72	4.39	4.35	4.94
1hz6_Y_39_A	2.46	3.08	2.34	2.82	2.46	2.62
1hz6_Y_59_A	1.66	4.40	3.87	3.96	4.40	4.28
1hz6_Y_59_L	-0.43	2.02	1.73	1.60	1.94	1.91
lffc_L_64_A	2.07	3.56	2.80	3.23	3.69	3.73
lffc_L_64_G	2.63	5.56	5.20	5.39	6.12	6.86
liob_K_97_G	1.20	0.73	0.33	1.41	0.65	-0.59
liob_T_9_A	0.80	0.27	0.61	1.16	0.35	2.11
liob_T_9_G	2.60	3.94	3.14	3.20	2.06	4.01
1100_A_105_Q	-0.60	-0.81	-0.78	-0.50	-0.81	0.84
1102_A_157_T	-0.50	-2.76	-1.72	-1.79	-3.45	-4.59
1108_G_157_T	-1.10	-1.70	-1.44	-1.11	0.51	0.84
1121_G_55_N	-0.60	0.79	1.67	1.90	1.72	2.20
1122_G_124_K	-0.10	-0.05	0.44	-0.07	1.75	2.73
1133_A_131_V	0.39	0.03	-0.03	0.28	1.24	1.00
1160_A_113_G	0.30	0.87	0.33	0.31	0.53	0.65
1165_A_47_D	-0.95	-0.32	0.33	0.68	6.40	2.68
1166_A_43_K	-1.03	-1.39	-0.98	-1.30	3.86	-1.78
1167_A_46_L	-1.86	-3.28	-2.96	-3.16	-2.21	-6.21
1168_A_44_S	0.34	0.60	0.79	0.73	-7.16	-4.99
1169_A_133_L	-4.30	-3.24	-2.77	-2.66	-2.33	-2.88
1185_A_153_F	-3.80	-2.81	-2.62	-2.81	-0.87	-0.79
1190_A_99_L	-4.50	-4.73	-4.28	-4.55	-5.46	-5.66
1199_G_105_Q	-1.50	-1.35	-0.89	-0.98	0.70	-2.84
llyh_G_59_T	-1.60	-1.08	-0.69	-0.92	-0.72	1.37
llyj_A_59_T	-1.50	-0.37	-0.55	-0.38	1.04	0.58
lmjc_F_17_L	1.00	2.20	1.98	2.02	3.58	3.60
lmjc_F_19_L	0.31	2.07	1.84	1.89	2.99	3.09
lmjc_F_30_L	0.66	2.34	2.12	2.16	1.98	2.06
lpga_A_20_G	2.39	1.49	1.31	1.34	0.52	0.23
lpga_A_26_G	2.96	3.66	3.46	3.51	4.86	4.34
lpga_A_34_G	2.48	2.94	2.75	2.82	3.26	3.33
lpga_D_22_A	1.75	0.03	-0.22	-0.24	-0.65	-0.51
lpga_D_46_A	1.74	1.04	0.76	0.77	0.34	0.33
lpga_D_47_A	-0.49	-1.27	-1.50	-1.47	-2.02	-2.01

lpga_E_15_A	0.47	1.53	1.23	1.28	0.34	-0.36
lpga_F_30_L	1.42	2.15	2.41	2.39	0.19	1.51
lpga_F_52_L	3.54	7.54	7.09	7.16	6.72	6.58
lpga_G_41_A	2.84	9.14	9.31	9.38	12.37	11.21
lpga_I_6_A	2.09	2.60	2.28	2.56	3.01	2.90
lpga_K_28_G	0.05	1.31	0.81	1.01	1.24	0.61
lpga_K_31_G	2.02	2.71	2.26	2.35	1.43	1.91
lpga_L_7_A	1.85	2.93	2.56	2.82	3.67	4.50
lpga_N_35_G	2.50	0.93	0.44	0.51	-0.24	-0.94
lpga_N_37_A	-0.17	0.14	-0.02	0.08	-0.63	-0.94
lpga_Q_32_G	1.00	1.29	0.88	0.87	1.34	1.00
lpga_T_11_A	0.60	0.52	0.38	0.48	0.78	0.96
lpga_T_16_A	0.38	2.26	2.13	2.23	3.36	3.52
lpga_T_18_A	0.46	0.19	0.07	0.16	0.10	0.16
lpga_T_25_A	-0.22	0.39	0.36	0.33	0.37	-0.35
lpga_T_49_A	0.72	0.94	0.85	0.96	0.56	0.84
lpga_T_51_A	1.87	1.33	1.43	1.35	2.54	2.42
lpga_T_53_A	1.91	0.18	0.07	0.13	-0.41	-0.15
lpga_V_29_A	0.70	0.99	0.95	1.02	1.25	0.34
lpga_V_39_A	1.72	3.23	3.22	3.29	3.72	3.65
lpga_V_54_A	2.93	1.48	1.48	1.52	2.48	3.18
lpga_Y_33_A	0.92	2.95	2.52	2.57	2.47	2.24
lpga_Y_3_L	1.62	6.46	6.29	6.25	5.07	5.09
lpga_Y_45_L	3.34	3.42	3.03	2.72	1.71	1.53
lqhe_A_83_G	1.80	2.93	2.40	2.55	3.02	3.01
lqhe_D_125_K	-1.01	0.44	0.06	-0.05	0.08	-0.22
lqhe_D_149_K	0.28	-0.23	-0.28	-0.44	0.00	-0.05
lqhe_D_42_A	-0.10	0.00	0.00	0.17	0.29	0.22
lqhe_D_64_K	0.26	-0.88	-0.41	-1.15	-1.51	-1.12
lqhe_D_74_K	-1.00	-1.66	-1.79	-1.60	-2.05	-1.13
lqhe_E_19_K	-1.60	-0.67	-0.88	-0.37	-1.04	-1.17
lqhe_E_39_K	-2.21	-1.00	-0.68	-0.56	-1.30	-1.22
lqhe_E_60_K	-0.88	-1.87	-1.76	-1.95	-3.33	-2.51
lqhe_E_71_K	-1.28	-0.76	-1.37	-0.67	-1.77	-1.41
lqhe_F_6_L	0.04	7.04	6.35	6.93	5.92	5.08
lqhe_H_33_A	0.83	5.84	5.60	5.39	4.33	4.48
lqhe_I_103_V	0.56	0.87	0.40	0.79	1.07	-0.67
lqhe_I_155_V	3.60	0.26	0.24	0.46	-0.70	-0.02
lqhe_I_21_V	1.39	2.59	2.35	2.49	2.82	2.82
lqhe_I_50_V	1.83	1.71	1.68	1.66	1.81	1.72
lqhe_I_51_V	1.40	1.41	1.15	0.89	1.54	1.78
lqhe_L_142_A	0.10	3.74	3.64	3.66	3.19	3.87
lqhe_L_5_A	2.94	5.47	5.15	5.41	5.87	6.55
lqhe_N_96_A	0.46	1.59	1.48	1.79	0.34	0.46
lqhe_Q_98_A	-1.72	1.59	1.15	1.48	-1.75	-1.33
lqhe_S_109_A	0.64	-0.19	-0.78	0.02	-0.63	-0.74
lqhe_V_116_A	1.74	0.54	0.87	0.89	2.42	3.07
lqhe_V_138_A	0.87	-0.74	-0.25	-0.37	-1.67	-1.27
lqhe_V_159_A	1.91	2.72	3.47	3.29	3.13	2.88
lqhe_V_30_A	1.72	4.03	3.77	3.47	3.69	3.49
lqhe_Y_46_F	0.59	0.96	0.91	0.99	0.95	0.96
lrex_I_106_A	0.93	3.55	3.31	3.67	3.10	2.93
lrex_I_106_V	0.72	2.23	2.12	2.56	2.58	2.68
lrex_I_23_A	2.54	4.67	4.29	4.60	4.49	5.15
lrex_I_23_V	0.36	1.20	0.72	1.28	0.83	1.24
lrex_I_56_A	3.71	4.72	4.17	3.96	3.92	4.22

lrex_I_56_L	0.10	0.19	-0.25	0.31	-0.35	-0.12
lrex_I_56_M	1.77	1.54	1.56	1.59	1.86	1.95
lrex_I_56_T	3.64	4.31	3.47	4.20	5.05	5.10
lrex_I_56_V	1.20	2.49	2.12	2.21	3.34	3.20
lrex_I_59_A	1.72	4.82	4.08	4.79	5.39	5.23
lrex_I_59_G	3.83	6.67	6.37	6.56	7.41	7.48
lrex_I_59_L	0.00	0.51	0.48	0.74	0.81	0.16
lrex_I_59_M	1.29	2.89	2.87	3.21	3.75	3.01
lrex_I_59_S	3.59	5.62	5.10	5.71	6.90	6.67
lrex_I_59_T	2.22	4.97	4.79	5.05	5.85	5.57
lrex_I_59_V	1.10	2.58	2.16	2.04	2.75	2.41
lrex_I_89_A	2.70	3.75	3.52	4.15	3.63	3.40
lrex_I_89_V	0.48	1.86	1.81	2.10	2.35	1.99
lrex_S_24_A	0.53	1.10	0.26	0.18	0.63	0.57
lrex_S_36_A	1.12	1.35	1.44	1.74	4.20	4.62
lrex_S_51_A	0.24	2.85	3.01	3.17	2.72	2.70
lrex_S_61_A	1.36	2.41	2.37	2.68	5.10	4.81
lrex_S_80_A	-0.48	0.13	-0.02	-0.15	0.73	0.82
lrex_T_11_A	-0.38	-0.32	0.03	0.14	-0.83	-0.81
lrex_T_11_V	-0.31	-1.29	-1.16	-1.16	-1.34	-1.58
lrex_T_40_A	1.51	0.26	0.12	0.01	-0.49	-0.05
lrex_T_40_V	1.34	1.90	2.07	1.61	3.86	3.46
lrex_T_43_A	0.36	0.40	0.41	0.38	0.06	0.04
lrex_T_43_V	-0.96	-0.44	-0.33	-0.09	-0.27	-0.43
lrex_T_52_A	0.91	0.77	0.95	0.56	0.53	1.04
lrex_T_70_V	0.69	4.45	4.57	4.59	10.20	10.27
lrex_V_100_A	0.26	0.51	0.93	0.63	-0.23	-0.18
lrex_V_110_A	-0.53	-0.40	-0.38	-0.52	-0.72	-0.82
lrex_V_121_A	1.44	1.22	1.30	2.05	1.36	1.38
lrex_V_125_A	1.32	2.70	2.47	3.14	3.12	3.30
lrex_V_2_A	1.51	1.95	1.99	1.86	2.74	2.70
lrex_V_74_A	0.36	1.18	1.30	1.21	1.73	1.45
lrex_V_93_A	0.74	-0.27	0.36	0.22	-0.44	0.14
lrex_V_99_A	0.98	2.17	2.43	2.54	1.49	1.48
lrex_Y_124_F	0.36	-0.24	-0.26	-0.37	-0.27	-0.41
lrex_Y_20_F	0.50	-0.71	-0.42	-0.19	0.60	0.56
lrex_Y_38_F	0.19	-0.07	0.62	0.15	-0.42	-1.19
lrex_Y_45_F	-0.07	-0.01	-0.30	-0.61	-0.50	-0.70
lrex_Y_54_F	0.96	-0.46	0.09	-0.04	-0.04	-0.19
lrex_Y_63_F	0.24	-0.07	0.10	0.02	0.14	-0.26
lrm1_D_48_A	0.50	0.89	0.61	0.59	1.31	1.22
lrm1_D_75_A	3.70	-0.26	-0.23	-0.37	-2.42	-2.51
lrm1_D_75_N	2.87	0.73	0.22	0.25	-2.54	-1.27
lrm1_E_57_A	0.64	-0.80	-1.05	-0.93	-4.85	-4.12
lrm1_N_35_A	-0.03	0.63	0.52	0.52	1.15	0.85
lrm1_N_43_A	2.00	1.67	1.39	1.51	2.44	2.30
lrm1_N_43_D	2.00	1.19	1.34	1.37	1.40	1.03
lrm1_N_80_A	2.87	2.72	2.67	2.68	3.34	3.96
lrm1_N_8_A	0.90	0.02	0.09	-0.01	-0.55	-0.20
lrm1_P_38_A	4.33	3.40	4.24	4.45	4.97	4.51
lrm1_S_11_A	1.23	1.32	1.31	1.29	1.58	1.67
lrm1_S_16_A	-0.67	-0.59	-0.87	-0.52	-1.42	-1.27
lrm1_S_63_A	1.44	0.74	0.47	0.61	0.74	0.81
lrm1_Y_10_F	2.11	0.85	1.05	0.91	0.76	0.31
lrm1_Y_41_F	-1.14	-0.52	-0.29	-0.53	-0.31	-1.23
lrm1_Y_55_F	0.78	-0.81	-0.56	-0.82	-1.87	-1.25

1rn1_Y_56_F	0.50	0.84	0.99	0.80	1.54	1.31
1rn1_Y_67_F	1.36	-0.70	-0.61	-0.56	-1.78	-1.69
1shf_E_24_A	1.27	-0.32	-0.53	-0.50	-2.33	-0.02
1shf_E_24_Q	0.74	0.99	0.97	1.11	3.28	4.19
1shf_S_41_A	0.71	0.86	0.70	0.81	3.02	3.86
1shf_S_41_G	1.68	3.51	3.14	3.28	5.84	6.94
1shg_A_50_G	2.00	2.57	2.23	2.27	2.74	2.87
1shg_A_6_G	1.40	3.61	3.36	3.39	3.02	3.24
1shg_D_24_A	1.20	-0.53	-0.86	-0.83	-0.92	-0.42
1shg_D_43_G	-1.40	1.37	0.88	0.95	0.06	-0.18
1shg_F_47_A	2.70	4.10	3.48	3.73	0.57	1.53
1shg_K_38_A	1.00	2.36	2.07	2.14	1.42	1.54
1shg_M_20_A	2.50	4.00	3.75	3.89	2.76	2.91
1shg_N_42_A	0.30	2.47	2.18	2.23	2.24	2.43
1shg_N_42_G	-0.40	-1.00	-1.42	-1.34	-0.37	-0.16
1shg_T_19_A	1.10	0.45	0.25	0.35	1.50	1.69
1shg_V_18_A	2.00	2.34	2.30	2.36	2.05	2.49
1shg_V_39_A	3.40	4.06	4.01	4.07	3.95	3.53
1shg_V_41_A	0.90	3.18	2.94	3.00	3.13	3.33
1shg_V_48_A	2.20	3.66	3.59	3.65	3.31	3.63
1shg_V_53_A	2.40	2.75	2.96	3.02	2.61	3.28
1stn_A_104_G	1.00	2.02	1.88	2.13	-4.12	-3.63
1stn_A_107_F	1.45	0.94	1.01	1.30	3.39	2.97
1stn_A_107_G	0.00	0.60	0.91	0.76	-1.47	-1.05
1stn_A_107_V	1.50	4.31	4.10	3.53	4.41	4.82
1stn_A_125_G	1.10	1.08	1.02	0.56	1.77	0.56
1stn_A_125_V	1.20	-0.19	0.83	-0.44	0.26	-1.12
1stn_A_127_G	3.70	1.93	3.02	2.19	1.95	1.75
1stn_A_12_G	0.30	2.21	2.51	1.56	3.24	1.67
1stn_A_12_V	1.90	-0.46	-0.98	0.02	-0.79	0.03
1stn_A_53_G	2.60	2.98	3.07	2.84	3.48	3.29
1stn_A_53_V	2.80	5.54	5.85	5.95	4.32	2.38
1stn_A_55_F	0.80	-0.95	-0.41	0.44	0.22	0.48
1stn_A_55_G	1.40	0.47	1.14	1.28	1.35	1.25
1stn_A_55_V	2.80	0.81	1.75	0.16	0.00	0.67
1stn_A_64_G	2.00	3.65	2.32	2.16	0.68	2.66
1stn_A_64_T	3.08	3.70	2.65	3.78	4.43	2.38
1stn_A_7_G	2.40	2.89	2.98	2.95	1.41	2.23
1stn_A_7_V	1.10	-0.51	-0.95	-0.18	0.02	-0.72
1stn_A_85_G	2.00	0.63	0.71	0.48	-0.69	-0.56
1stn_A_85_S	2.00	0.07	0.27	1.27	2.02	1.30
1stn_A_89_G	2.40	4.36	3.87	3.56	2.21	3.20
1stn_A_89_V	1.30	-0.27	0.14	-0.05	-1.66	-1.40
1stn_A_97_F	1.90	0.57	0.27	1.11	2.33	0.63
1stn_A_97_G	1.30	2.20	2.28	2.23	3.07	2.85
1stn_D_14_A	0.10	2.33	1.72	2.00	3.29	4.48
1stn_D_14_G	0.40	1.58	1.26	2.37	1.89	4.07
1stn_D_16_A	-0.70	0.53	-0.85	-0.37	-0.95	-0.77
1stn_D_16_G	-0.30	1.31	0.47	0.96	-0.31	-1.34
1stn_D_35_A	-0.20	0.88	-0.41	-0.52	-0.38	-1.04
1stn_D_35_G	0.50	2.16	1.46	1.05	0.82	2.21
1stn_D_72_A	3.10	1.10	0.83	1.69	2.61	4.03
1stn_D_72_G	2.20	2.31	1.84	1.49	0.55	1.33
1stn_D_78_A	3.80	4.35	3.92	3.59	6.18	6.40
1stn_D_78_F	5.20	5.24	5.39	4.90	9.40	11.13
1stn_D_78_G	2.70	3.51	3.65	3.16	4.15	6.10

1stn_D_90_A	3.30	1.20	0.38	0.80	2.84	1.86
1stn_D_90_F	5.30	1.68	1.18	1.41	2.03	1.88
1stn_D_90_G	2.70	1.01	0.34	0.21	0.49	0.26
1stn_E_117_A	0.40	1.30	0.26	0.15	-0.60	-0.69
1stn_E_117_F	0.80	-0.59	-0.13	-1.02	-2.27	-2.57
1stn_E_117_G	2.20	2.24	1.37	1.52	3.51	3.79
1stn_E_124_A	2.40	-1.09	-0.54	-0.66	-0.35	-0.53
1stn_E_124_G	3.80	2.54	2.15	2.12	3.15	4.00
1stn_E_130_A	0.70	0.78	0.00	-0.19	-2.60	-1.60
1stn_E_130_F	1.20	-1.49	-0.57	-0.75	-2.49	-1.71
1stn_E_130_G	1.70	2.05	1.51	1.38	-0.07	-0.07
1stn_E_38_A	-0.30	0.18	-0.19	-0.31	-2.63	-2.57
1stn_E_38_D	-0.20	1.24	0.69	1.81	0.46	0.97
1stn_E_38_G	-0.50	1.05	0.50	1.10	-2.76	-2.44
1stn_E_47_A	0.10	2.37	1.39	1.71	2.48	3.21
1stn_E_47_G	0.40	3.26	2.60	3.06	1.16	1.02
1stn_E_52_A	0.20	-0.33	-0.77	-1.01	-2.15	-1.50
1stn_E_52_F	0.80	-1.66	-0.89	-1.61	-2.52	-2.00
1stn_E_52_G	1.60	1.54	0.85	0.81	1.12	2.09
1stn_E_5_A	1.30	0.44	0.95	0.68	0.16	-0.18
1stn_E_5_G	1.80	2.74	1.58	2.01	2.15	1.52
1stn_E_62_A	1.00	-0.92	0.29	0.73	-0.75	-0.23
1stn_E_62_F	1.40	-0.59	0.22	-0.79	1.08	-1.29
1stn_E_62_G	0.90	1.96	0.39	1.64	0.36	0.96
1stn_E_68_A	1.20	-1.33	-0.52	0.00	-1.50	-2.04
1stn_E_68_F	1.10	-5.35	-4.91	-4.97	-6.31	-7.46
1stn_E_68_G	2.70	3.16	2.04	1.93	0.15	2.37
1stn_E_70_A	2.20	1.42	1.78	1.58	-0.22	0.03
1stn_E_70_G	3.50	4.90	4.04	4.15	2.23	2.26
1stn_E_70_V	2.31	-0.22	0.61	-0.23	-1.87	-1.63
1stn_E_96_A	1.90	-1.25	-1.23	-0.41	-2.84	-2.34
1stn_E_96_G	3.10	1.21	0.64	1.62	0.38	1.68
1stn_F_29_A	3.70	8.46	7.91	7.71	9.01	9.33
1stn_F_29_G	6.20	11.65	10.99	10.36	11.35	12.63
1stn_F_56_A	2.30	4.36	3.59	4.29	4.40	4.07
1stn_F_56_G	4.80	6.28	5.49	6.05	6.20	6.65
1stn_F_71_A	4.00	5.14	4.55	5.30	5.02	4.94
1stn_F_71_G	4.70	6.33	6.11	6.09	6.88	6.13
1stn_G_15_A	0.30	-1.17	-1.61	-1.75	-1.69	-0.93
1stn_G_24_A	1.25	2.00	2.56	2.21	5.88	5.87
1stn_G_24_F	1.25	0.83	2.12	2.35	2.99	3.33
1stn_G_45_A	-0.25	1.95	2.63	2.99	1.83	2.31
1stn_G_45_F	0.60	1.01	1.10	1.20	1.44	2.28
1stn_G_45_V	1.10	6.64	6.22	5.86	4.88	5.01
1stn_G_81_A	0.55	2.17	4.30	2.98	4.82	5.95
1stn_G_83_A	0.10	-1.01	-1.39	-1.28	-2.35	-1.84
1stn_G_91_A	1.75	1.92	2.98	3.02	5.72	4.48
1stn_H_116_A	3.10	4.24	3.22	3.33	2.50	1.81
1stn_H_116_G	4.20	5.27	4.76	4.39	3.45	3.36
1stn_H_119_A	-0.40	1.10	0.32	0.30	-0.50	-0.21
1stn_H_119_F	-0.30	0.71	0.68	0.92	0.39	-0.17
1stn_H_119_G	0.50	2.46	1.98	1.04	1.96	1.69
1stn_H_3_A	0.40	0.38	0.00	0.93	-0.47	-0.41
1stn_H_3_G	0.80	1.90	1.26	0.42	1.29	0.41
1stn_H_41_A	0.50	4.75	4.57	4.77	4.34	4.93
1stn_H_41_G	0.40	6.64	6.06	6.16	6.27	6.56

1stn_I_10_A	2.65	3.85	3.25	3.42	4.54	4.86
1stn_I_10_G	3.30	5.48	5.11	4.60	5.29	4.15
1stn_I_10_V	0.80	1.30	0.99	1.15	1.37	1.79
1stn_I_134_A	3.50	2.59	2.53	2.14	1.27	0.16
1stn_I_134_G	4.40	4.41	3.35	3.41	3.67	3.85
1stn_I_134_V	1.50	1.81	0.73	1.26	1.48	1.95
1stn_I_13_A	2.50	2.54	2.27	2.80	2.39	1.66
1stn_I_13_G	2.50	4.21	4.43	5.11	4.76	3.73
1stn_I_13_M	0.60	0.96	1.52	1.68	1.07	0.93
1stn_I_13_V	1.10	1.07	1.79	0.73	1.12	0.93
1stn_I_67_A	5.10	4.79	4.53	4.35	5.01	4.86
1stn_I_67_G	6.50	7.77	5.86	7.51	7.73	7.04
1stn_I_67_V	1.80	0.88	1.70	0.55	0.38	1.57
1stn_I_87_A	4.00	4.55	4.21	3.84	5.36	5.38
1stn_I_87_G	6.60	6.95	7.13	6.42	7.85	9.33
1stn_I_87_V	0.50	1.16	1.31	1.07	0.27	1.61
1stn_K_105_A	1.30	1.88	0.63	1.00	1.56	0.54
1stn_K_105_G	2.70	1.93	0.83	2.08	1.20	0.95
1stn_K_111_A	-0.70	-0.49	-0.92	-0.85	-0.86	-0.54
1stn_K_111_F	0.10	-0.39	0.55	0.50	1.36	0.55
1stn_K_111_G	-1.00	0.73	0.04	0.73	0.08	-0.15
1stn_K_11_A	0.20	0.20	0.17	0.29	-0.61	-0.84
1stn_K_11_F	0.50	-0.68	-1.72	-0.95	-0.12	0.28
1stn_K_11_G	0.70	1.21	0.55	0.96	-1.15	-0.66
1stn_K_122_A	-0.20	0.74	-0.89	0.47	-1.09	0.42
1stn_K_122_F	0.30	-0.30	-0.44	-0.71	-0.72	-0.28
1stn_K_122_G	0.70	2.18	1.61	2.39	1.41	1.01
1stn_K_128_A	1.40	-1.01	-0.78	-0.98	-1.39	-1.63
1stn_K_128_F	1.40	-0.30	-0.76	-0.08	-0.75	-0.35
1stn_K_128_G	3.30	0.85	1.30	0.86	-0.28	0.47
1stn_K_129_A	-0.10	-0.21	-0.37	-0.50	-1.62	-0.44
1stn_K_129_F	0.40	-0.86	-0.95	-0.06	0.42	-1.77
1stn_K_129_G	0.70	1.71	0.86	1.38	0.57	0.58
1stn_K_131_A	0.80	0.90	0.74	0.46	1.62	0.73
1stn_K_131_F	1.20	-1.02	-0.71	-1.11	0.84	-0.49
1stn_K_131_G	0.05	0.36	0.03	-0.96	-2.91	-2.53
1stn_K_19_A	0.20	1.37	1.23	0.27	0.67	0.99
1stn_K_19_G	1.20	4.18	4.18	3.98	4.51	3.44
1stn_K_1_A	-0.30	0.54	-0.29	-0.12	0.22	0.47
1stn_K_1_G	-0.30	0.26	-0.46	-0.53	-0.09	0.23
1stn_K_23_A	0.70	0.24	0.80	0.35	0.73	0.12
1stn_K_23_F	0.90	-0.22	0.02	-0.06	0.28	1.55
1stn_K_23_G	0.70	0.07	-0.04	-0.29	-2.15	-1.44
1stn_K_40_A	-0.30	-0.48	-0.55	-0.52	0.38	-0.85
1stn_K_40_G	-0.20	0.38	0.42	0.48	-0.80	0.69
1stn_K_43_A	-0.10	1.51	1.50	0.69	0.66	1.92
1stn_K_43_F	0.50	-0.44	-0.15	-0.37	-0.93	-1.42
1stn_K_43_G	-0.20	2.40	1.64	2.31	0.63	0.58
1stn_K_44_A	0.30	1.51	0.32	0.10	0.28	0.03
1stn_K_44_F	0.00	0.29	0.99	0.20	-0.06	-0.70
1stn_K_44_G	0.20	2.48	2.22	2.68	1.87	1.65
1stn_K_48_A	0.20	1.37	1.39	0.48	-0.56	-0.19
1stn_K_48_G	0.30	1.94	1.14	0.79	1.04	0.22
1stn_K_4_A	1.40	1.08	0.80	0.19	-0.67	0.36
1stn_K_4_G	1.90	2.31	2.08	1.91	0.74	1.57
1stn_K_58_A	0.50	1.17	0.06	1.18	0.68	0.88



1stn_K_58_F	2.00	-0.29	0.08	-0.97	1.06	1.09
1stn_K_58_G	1.50	3.69	2.50	2.24	2.30	1.29
1stn_K_59_A	-0.10	-0.21	0.57	-0.42	-0.16	-0.70
1stn_K_59_F	0.30	-1.16	-0.27	-0.26	0.68	-0.47
1stn_K_59_G	0.40	1.75	0.92	0.75	0.91	1.77
1stn_K_65_A	0.10	0.84	0.59	-0.21	-0.13	1.14
1stn_K_65_F	0.10	0.47	1.29	-0.11	1.47	-0.64
1stn_K_65_G	0.50	0.73	0.68	0.43	-0.96	-1.31
1stn_K_65_W	0.50	1.25	0.96	1.39	1.86	0.57
1stn_K_66_A	0.40	0.38	0.61	0.63	0.06	0.66
1stn_K_66_F	0.00	-1.02	-0.79	-0.27	-0.70	-0.75
1stn_K_66_G	1.10	2.46	2.02	2.29	1.15	1.48
1stn_K_73_A	0.60	0.35	-0.74	0.31	-0.66	0.07
1stn_K_73_F	-0.10	-1.70	-1.28	-1.94	-1.35	-1.11
1stn_K_73_G	1.10	1.63	0.12	0.45	0.19	-0.10
1stn_K_79_A	-0.20	0.01	0.34	0.21	0.61	0.91
1stn_K_79_F	0.90	0.88	1.10	0.67	1.85	1.19
1stn_K_79_G	0.30	0.51	0.24	0.33	0.28	0.07
1stn_K_92_A	0.10	0.74	0.33	0.35	0.46	0.92
1stn_K_92_F	0.70	-0.56	-0.58	-0.84	-1.24	-0.62
1stn_K_92_G	1.70	2.18	1.93	1.81	1.98	3.31
1stn_L_103_A	5.80	4.72	4.26	4.62	3.40	5.03
1stn_L_103_G	7.20	6.57	5.76	6.05	5.80	6.86
1stn_L_120_A	4.90	4.52	3.68	3.54	3.82	3.95
1stn_L_120_G	7.00	7.30	5.84	5.99	5.47	7.73
1stn_L_132_A	2.30	2.59	1.75	2.66	2.24	2.71
1stn_L_132_G	4.60	3.67	3.94	3.48	3.90	3.44
1stn_L_20_A	2.70	5.12	4.30	5.00	4.25	4.72
1stn_L_20_G	4.50	8.27	8.06	8.19	8.64	8.89
1stn_L_2_A	1.60	2.14	1.84	1.92	1.31	1.85
1stn_L_2_G	1.50	2.96	1.83	1.89	0.28	1.59
1stn_L_31_A	3.50	3.31	2.35	3.00	3.13	0.09
1stn_L_31_G	5.30	3.86	3.97	3.89	11.31	13.12
1stn_L_32_A	1.70	2.09	2.22	1.29	1.34	1.14
1stn_L_32_G	3.80	4.85	4.73	4.81	3.48	5.51
1stn_L_33_A	1.65	3.31	3.47	3.08	3.35	3.94
1stn_L_33_G	0.55	2.06	1.82	1.65	-0.94	2.36
1stn_L_84_A	2.60	3.35	3.13	2.87	2.18	3.60
1stn_L_84_G	3.20	5.42	5.26	4.83	5.58	7.11
1stn_L_98_A	4.60	2.68	2.50	2.26	-1.67	-1.67
1stn_L_98_G	6.60	5.18	4.90	5.62	1.72	2.01
1stn_L_9_A	2.30	4.13	3.44	3.31	2.68	3.51
1stn_L_9_G	3.70	4.12	5.03	5.10	4.55	6.32
1stn_M_21_A	1.50	1.72	1.42	1.41	1.90	1.59
1stn_M_21_G	2.20	3.26	3.86	2.77	3.82	4.98
1stn_M_21_I	0.90	0.17	-0.01	-0.17	0.66	0.53
1stn_M_21_L	0.50	-0.63	-0.54	0.24	0.68	-1.13
1stn_M_27_A	1.70	2.26	1.83	1.54	1.82	0.76
1stn_M_27_G	2.40	4.29	4.22	4.65	2.88	3.21
1stn_M_27_I	0.60	-0.63	-0.86	-0.67	-0.23	-1.35
1stn_M_27_L	0.80	0.22	0.25	0.27	0.30	1.55
1stn_M_60_A	2.00	2.15	1.94	1.72	0.72	0.99
1stn_M_60_G	4.60	4.23	2.63	3.81	3.75	3.10
1stn_M_60_L	0.80	-1.00	-0.06	-0.63	0.18	-0.78
1stn_M_93_A	4.60	2.10	1.11	1.71	0.67	0.97
1stn_M_93_G	4.50	4.86	4.27	4.65	3.03	2.44

1stn_M_93_I	4.40	2.88	2.83	3.14	0.70	0.32
1stn_N_113_A	2.05	0.47	-0.25	-0.37	2.02	3.43
1stn_N_113_D	2.40	1.01	1.42	2.46	3.46	3.80
1stn_N_113_G	1.85	1.76	2.67	1.83	3.83	4.46
1stn_N_114_A	1.25	0.42	0.78	1.37	0.47	-0.15
1stn_N_114_G	1.25	2.19	2.49	1.90	-2.45	-1.80
1stn_N_133_A	1.05	-0.05	0.88	0.91	2.21	2.15
1stn_N_133_G	-0.15	-0.83	-1.88	-2.20	2.75	2.68
1stn_N_63_A	0.50	0.56	0.12	0.96	0.35	-0.15
1stn_N_63_G	0.50	1.14	0.44	0.96	0.58	1.78
1stn_N_95_A	5.20	-2.51	-3.25	-2.63	0.06	0.91
1stn_N_95_G	5.10	1.24	-0.06	-0.50	3.64	5.25
1stn_P_112_A	-0.80	1.09	1.57	1.90	0.38	1.89
1stn_P_112_F	-0.30	-0.35	0.56	1.31	0.58	0.19
1stn_P_112_G	-1.25	2.01	1.65	2.13	1.02	0.27
1stn_P_112_L	-0.20	-0.56	1.82	0.62	1.04	1.10
1stn_P_112_T	-1.10	1.61	1.24	1.70	1.81	0.25
1stn_P_26_A	0.55	-0.18	0.41	0.60	2.87	2.06
1stn_P_26_G	1.60	1.00	1.14	2.85	3.67	4.50
1stn_P_37_A	-0.10	1.19	1.40	1.81	-1.63	-1.83
1stn_P_37_G	0.40	3.59	4.28	3.96	-0.37	0.62
1stn_P_42_A	0.60	0.33	1.26	0.82	2.47	1.66
1stn_P_42_F	0.30	1.01	2.45	1.63	2.61	2.96
1stn_P_42_G	0.10	1.13	1.97	1.99	2.54	1.63
1stn_P_51_A	0.00	1.42	1.52	2.03	2.75	2.88
1stn_P_51_G	1.00	3.20	3.10	3.49	3.24	3.15
1stn_P_6_A	0.40	-0.02	1.48	0.21	1.76	2.36
1stn_P_6_F	0.60	-1.76	-1.22	-0.91	0.86	0.35
1stn_P_6_G	1.00	0.85	2.44	1.13	2.39	2.79
1stn_Q_101_A	-0.10	1.42	1.37	0.80	0.63	1.54
1stn_Q_101_G	1.50	3.07	2.59	2.75	2.41	2.87
1stn_Q_118_A	0.40	0.15	-0.08	0.25	1.41	0.25
1stn_Q_118_F	0.70	0.46	0.54	-0.89	0.52	-1.08
1stn_Q_118_G	0.60	1.49	1.69	1.69	2.13	1.19
1stn_Q_126_A	0.20	1.25	0.38	0.94	-0.49	-1.64
1stn_Q_126_F	0.70	-1.59	-1.29	-0.45	-2.65	-3.30
1stn_Q_126_G	2.40	2.04	0.70	1.90	1.30	0.30
1stn_Q_25_A	0.30	-0.33	-0.24	-0.55	0.13	-0.87
1stn_Q_25_G	0.90	2.57	1.02	0.58	0.95	0.83
1stn_Q_75_A	0.10	0.27	-0.68	-0.73	0.52	-0.15
1stn_Q_75_F	0.70	0.55	0.94	-0.31	0.50	0.10
1stn_Q_75_G	1.40	0.53	0.38	0.68	1.15	1.13
1stn_R_100_A	1.40	-0.46	0.79	-0.37	-2.32	-2.48
1stn_R_100_F	3.10	-0.30	-0.22	0.31	-2.06	-2.19
1stn_R_100_G	2.40	1.55	2.15	0.96	-1.11	-0.62
1stn_R_121_A	1.70	0.47	0.66	1.30	-0.88	-1.31
1stn_R_121_G	2.90	1.16	1.47	1.53	1.28	2.18
1stn_R_30_A	1.40	-0.54	-0.74	-2.04	-0.82	-0.28
1stn_R_30_G	2.20	1.11	0.63	0.81	0.08	1.51
1stn_R_76_A	1.10	0.16	0.45	-0.72	-0.39	-1.07
1stn_R_76_G	2.20	1.08	0.69	0.98	1.81	1.46
1stn_R_82_A	0.90	1.21	1.52	0.55	0.50	2.37
1stn_R_82_G	2.60	3.71	3.09	2.92	2.90	3.96
1stn_S_123_A	-0.70	-1.28	-0.65	-0.78	-1.64	-2.07
1stn_S_123_F	1.00	-2.79	-2.66	-2.50	-3.07	-3.72
1stn_S_123_G	1.60	1.67	2.03	1.16	-0.93	-0.58

1stn_S_136_A	0.40	-0.02	0.32	-0.41	-0.96	-0.16
1stn_S_136_G	0.90	0.19	0.06	0.71	0.09	-0.55
1stn_S_54_A	-0.40	-1.15	-1.08	-0.02	-3.31	-3.27
1stn_S_54_F	0.00	-3.62	-3.21	-3.53	-2.40	-3.03
1stn_S_54_G	1.10	0.95	1.33	0.79	-0.16	-0.50
1stn_T_115_A	1.20	-0.45	0.39	-0.59	-1.44	-3.03
1stn_T_115_G	2.10	1.87	1.09	1.43	-0.04	-0.38
1stn_T_115_S	0.60	-0.04	0.96	0.32	-1.97	-0.19
1stn_T_115_V	1.80	1.22	0.72	0.99	1.78	0.77
1stn_T_17_A	1.60	2.20	1.17	1.46	-0.05	0.62
1stn_T_17_G	2.40	4.44	3.63	3.77	2.41	2.52
1stn_T_17_S	0.60	1.06	1.96	1.15	0.39	0.59
1stn_T_17_V	0.90	-0.82	-0.54	-0.30	0.00	-2.13
1stn_T_28_A	1.40	0.45	0.11	0.84	0.00	-0.52
1stn_T_28_G	2.50	2.09	2.34	2.34	2.70	3.57
1stn_T_28_S	1.15	0.60	1.55	1.25	0.57	1.45
1stn_T_28_V	-0.40	-0.42	-1.35	-1.20	-1.01	-0.23
1stn_T_36_A	0.00	0.52	-0.33	-0.37	-0.22	-0.25
1stn_T_36_G	2.00	1.84	2.23	2.32	-0.66	0.51
1stn_T_36_S	1.10	-0.35	-0.31	0.50	-2.94	-3.32
1stn_T_36_V	-0.80	0.54	0.74	-0.47	1.18	1.43
1stn_T_39_A	0.40	2.53	2.33	1.79	1.95	0.01
1stn_T_39_G	0.60	2.86	2.52	3.12	3.80	2.16
1stn_T_39_S	0.00	0.79	1.23	0.46	1.33	0.00
1stn_T_39_V	-0.10	1.91	2.27	2.29	3.18	1.33
1stn_T_57_A	2.40	1.73	1.57	1.52	3.69	2.96
1stn_T_57_G	3.50	4.51	3.84	4.26	7.52	7.00
1stn_T_57_S	2.10	1.09	1.09	0.71	0.36	2.23
1stn_T_57_V	0.20	1.76	1.01	1.81	3.93	3.65
1stn_T_77_A	0.90	0.69	0.58	1.36	-0.88	-0.08
1stn_T_77_G	2.00	2.43	2.39	2.44	2.76	2.22
1stn_T_77_S	0.70	0.88	0.82	0.86	0.91	0.66
1stn_T_77_V	-0.20	-0.88	-0.16	0.27	-0.33	0.37
1stn_T_8_A	0.70	0.59	-0.37	1.27	-0.09	0.74
1stn_T_8_G	1.10	1.92	1.72	1.31	2.18	1.24
1stn_T_8_S	0.30	0.31	1.25	0.25	0.64	1.26
1stn_T_8_V	0.40	-0.46	-0.59	-0.53	-2.18	-0.77
1stn_V_106_A	4.45	2.67	2.21	2.68	3.87	4.24
1stn_V_106_G	4.90	4.81	4.70	5.20	6.71	6.19
1stn_V_106_S	4.80	4.08	3.67	3.90	4.05	5.26
1stn_V_106_T	2.30	3.44	2.49	3.07	3.85	3.08
1stn_V_109_A	0.00	0.94	0.36	0.05	-0.83	0.28
1stn_V_109_G	0.20	2.36	2.23	2.07	2.24	2.42
1stn_V_109_S	0.00	0.48	1.11	1.19	2.96	1.32
1stn_V_109_T	0.30	1.60	1.56	1.08	1.66	1.04
1stn_V_18_A	2.90	2.72	1.68	2.21	3.76	3.02
1stn_V_18_G	5.60	5.85	5.76	5.88	6.31	7.62
1stn_V_18_S	4.70	3.20	3.77	3.80	4.76	5.04
1stn_V_18_T	3.20	1.85	1.67	1.97	2.73	3.16
1stn_V_34_A	2.20	3.55	3.27	3.30	3.59	3.16
1stn_V_34_G	4.70	5.58	5.37	5.86	6.07	6.57
1stn_V_34_S	2.40	3.56	4.77	3.85	4.79	4.44
1stn_V_34_T	1.30	1.69	1.91	2.39	2.46	3.41
1stn_V_46_A	0.25	1.57	2.21	1.75	2.97	2.17
1stn_V_46_G	0.35	3.31	2.97	3.45	4.53	4.68
1stn_V_46_S	0.10	2.56	2.53	2.31	2.78	4.18

1stn_V_46_T	-0.20	0.27	0.82	0.74	-1.53	-2.37
1stn_V_61_A	2.20	1.03	2.01	2.09	2.92	1.37
1stn_V_61_G	4.40	4.04	4.01	4.34	4.75	5.33
1stn_V_61_L	0.03	-2.68	-2.42	-2.20	-2.50	-2.72
1stn_V_61_M	0.20	-0.16	0.28	-0.63	0.75	1.54
1stn_V_61_S	3.10	2.48	3.71	2.66	3.49	3.99
1stn_V_61_T	1.30	1.46	1.21	0.70	1.93	1.44
1stn_V_69_A	3.10	2.31	3.17	2.97	3.39	3.99
1stn_V_69_G	6.60	5.67	6.50	6.33	6.18	6.40
1stn_V_69_S	5.40	3.41	4.25	3.72	4.95	5.72
1stn_V_69_T	3.80	1.86	2.72	2.82	3.33	3.82
1stn_V_94_A	3.20	2.83	3.56	3.46	3.71	4.39
1stn_V_94_G	5.00	5.79	4.80	4.95	6.51	5.59
1stn_V_94_S	5.10	3.69	4.59	3.73	4.45	5.27
1stn_V_94_T	3.30	2.34	3.15	2.24	3.97	4.32
1stn_V_99_A	2.90	2.38	3.18	2.04	2.06	3.12
1stn_V_99_G	6.50	5.20	5.10	6.13	4.91	5.54
1stn_V_99_S	4.90	4.30	4.63	3.78	5.32	5.60
1stn_V_99_T	2.50	2.88	2.28	2.81	4.36	3.74
1stn_Y_108_A	-0.05	1.12	1.17	0.07	1.63	1.35
1stn_Y_108_F	0.00	-0.21	0.15	-0.11	0.80	0.91
1stn_Y_108_G	0.25	3.08	1.97	2.31	3.98	4.20
1stn_Y_108_L	-0.20	0.88	1.64	0.42	0.83	0.78
1stn_Y_110_A	0.30	2.40	2.60	2.87	2.16	2.77
1stn_Y_110_F	0.10	0.03	1.06	0.52	0.01	0.14
1stn_Y_110_G	0.70	5.47	4.97	4.80	5.27	5.60
1stn_Y_110_L	0.30	1.45	1.22	1.59	0.73	0.69
1stn_Y_22_A	3.50	5.00	4.90	4.77	3.25	5.12
1stn_Y_22_D	5.40	6.57	6.74	6.46	6.34	8.00
1stn_Y_22_E	5.00	6.18	6.82	6.07	7.83	7.29
1stn_Y_22_F	0.30	-0.78	0.09	-0.36	-0.83	0.55
1stn_Y_22_G	5.45	9.81	8.67	8.61	6.78	9.04
1stn_Y_22_H	1.60	2.16	1.32	1.84	2.03	1.02
1stn_Y_22_I	2.50	1.99	1.93	2.69	0.15	0.99
1stn_Y_22_K	3.90	3.82	4.31	4.10	4.87	6.07
1stn_Y_22_L	1.50	1.66	2.10	2.35	2.13	1.94
1stn_Y_22_M	2.00	2.94	3.31	4.19	1.06	2.96
1stn_Y_22_N	4.00	6.15	5.82	5.75	5.65	5.58
1stn_Y_22_Q	3.20	4.30	4.35	4.75	5.67	7.01
1stn_Y_22_R	2.90	5.49	4.89	5.02	7.26	6.07
1stn_Y_22_S	3.00	5.25	5.70	5.23	4.99	6.27
1stn_Y_22_T	3.30	5.15	4.02	4.44	4.70	4.77
1stn_Y_22_V	3.00	3.15	2.16	2.47	1.67	2.14
1stn_Y_22_W	0.60	0.19	0.49	0.60	0.86	1.44
1stn_Y_80_A	0.40	0.65	0.00	-0.10	0.85	3.66
1stn_Y_80_F	0.10	1.05	0.88	0.76	0.77	1.26
1stn_Y_80_G	1.00	2.49	1.31	0.61	1.76	1.85
1stn_Y_80_L	0.10	1.94	1.85	2.13	4.10	4.67
1stn_Y_86_A	5.30	8.51	8.31	8.55	9.27	11.67
1stn_Y_86_F	2.40	1.06	1.34	2.11	3.20	4.84
1stn_Y_86_G	6.70	11.53	11.11	11.58	12.33	12.95
1stn_Y_86_L	3.90	7.90	7.97	7.47	9.21	9.51
1stn_Y_88_A	6.50	7.42	7.15	7.13	5.68	7.52
1stn_Y_88_F	2.00	-0.75	0.69	0.61	0.86	0.27
1stn_Y_88_G	7.50	10.42	9.38	9.23	7.98	8.24
1stn_Y_88_L	4.50	6.79	5.80	5.01	4.64	4.08

lsup_N_76_D	-0.45	0.67	0.86	0.96	1.51	0.40
lten_A_17_G	2.80	3.27	3.05	3.04	3.05	2.88
lten_A_83_G	1.09	2.23	2.03	2.06	1.84	1.93
lten_E_85_A	-1.61	-0.84	-1.15	-1.07	-2.50	-2.49
lten_E_85_G	0.34	0.72	0.27	0.34	-0.71	-0.65
lten_F_87_A	5.43	8.71	8.23	8.54	8.14	8.68
lten_I_19_A	3.67	5.11	4.96	5.08	6.33	6.70
lten_I_19_V	0.23	0.74	0.62	0.69	0.92	1.33
lten_I_28_A	1.38	4.02	3.93	4.00	3.79	3.90
lten_I_28_V	0.32	1.21	0.85	0.99	0.65	0.83
lten_I_31_A	3.28	4.20	4.01	4.14	5.38	5.75
lten_I_31_V	0.50	-0.10	-0.30	-0.24	-0.14	0.30
lten_I_47_A	2.19	1.14	0.92	0.94	1.40	2.01
lten_I_58_A	2.06	4.26	4.14	4.19	4.22	4.52
lten_I_58_V	0.83	2.64	2.42	2.47	2.10	2.38
lten_I_7_A	2.86	5.15	5.03	5.13	6.12	6.17
lten_I_7_V	0.18	1.75	1.46	1.59	1.74	1.77
lten_L_1_A	2.11	4.86	4.54	4.67	3.76	4.15
lten_L_33_A	4.29	4.93	4.61	4.75	6.13	6.93
lten_L_49_A	2.99	3.07	2.73	2.93	2.93	3.36
lten_L_61_A	4.22	4.47	4.17	4.45	3.64	4.05
lten_L_71_A	3.06	4.28	3.93	4.20	4.74	5.41
lten_P_24_A	1.73	3.23	4.04	4.20	4.83	4.60
lten_P_41_A	0.46	0.44	1.22	1.38	1.15	0.79
lten_P_4_A	2.74	2.86	3.63	3.79	4.41	3.99
lten_P_63_A	0.93	1.74	2.53	2.72	3.27	3.03
lten_P_82_A	0.11	0.79	1.56	1.70	2.03	1.67
lten_S_73_A	-0.04	-0.87	-1.09	-0.97	0.10	0.62
lten_S_80_A	2.82	1.63	1.63	1.60	5.65	6.00
lten_T_65_A	1.96	1.12	1.00	1.15	1.75	2.34
lten_T_65_S	1.22	1.47	1.52	1.59	1.40	1.81
lten_T_89_A	3.43	1.76	1.69	1.78	4.41	5.19
lten_T_89_S	1.92	2.98	3.08	2.93	6.72	7.23
lten_V_69_A	2.81	3.05	3.08	3.10	4.27	4.63
lten_V_9_A	1.36	3.52	3.57	3.64	5.29	5.63
lten_Y_35_A	4.22	6.25	5.81	5.93	4.98	5.44
lten_Y_35_F	0.44	-0.20	-0.05	-0.15	-0.48	-0.31
lten_Y_56_A	1.38	5.63	5.28	5.27	4.77	5.27
lten_Y_56_G	4.14	8.92	8.19	8.39	8.03	8.70
lten_Y_67_F	3.13	0.13	0.16	-0.05	1.51	1.65
lu5p_A_155_G	1.10	1.18	1.39	0.70	1.32	1.49
lu5p_A_159_G	1.10	0.74	0.95	0.97	0.93	1.92
lu5p_A_190_G	1.10	1.50	1.28	1.07	1.47	1.30
lu5p_A_203_G	2.60	2.55	2.04	2.38	2.54	3.08
lu5p_A_205_G	1.80	1.48	1.16	1.65	1.79	1.92
lu5p_D_118_A	0.20	-0.60	-0.62	-1.13	-1.84	-2.14
lu5p_D_118_G	1.20	0.65	0.36	0.41	-0.95	-0.70
lu5p_D_169_A	0.10	-0.68	-0.34	-0.52	-1.20	-1.85
lu5p_D_169_G	1.30	0.48	0.33	0.35	-0.16	0.23
lu5p_D_194_A	-0.70	-1.11	-1.02	-1.11	-1.95	-1.72
lu5p_D_194_G	0.30	0.43	-0.01	0.35	-0.50	-0.02
lu5p_E_126_A	-0.10	0.02	-0.47	-0.12	-0.48	-0.91
lu5p_E_126_G	1.10	1.74	1.17	1.21	1.58	1.22
lu5p_F_113_A	3.70	7.20	5.77	6.42	6.21	6.05
lu5p_F_113_L	1.30	5.24	5.28	5.36	4.63	5.19
lu5p_F_192_A	2.80	7.46	7.35	7.59	6.94	7.35

1u5p_F_192_L	-0.50	3.70	4.02	3.58	3.85	3.83
1u5p_H_111_A	-0.50	3.44	2.94	3.12	-0.11	0.57
1u5p_H_111_G	0.50	5.29	4.93	5.42	3.31	4.30
1u5p_H_150_A	1.40	2.41	1.52	1.56	-0.52	0.63
1u5p_H_160_A	2.30	2.30	1.55	1.47	1.15	1.97
1u5p_I_124_A	3.60	4.73	4.72	4.58	3.98	3.94
1u5p_I_124_V	1.60	2.25	2.15	2.59	2.15	2.56
1u5p_I_164_A	2.80	1.16	1.32	2.01	2.09	2.30
1u5p_I_164_V	0.60	0.03	-0.27	0.04	0.50	0.32
1u5p_I_185_A	2.00	2.36	2.17	2.56	2.76	3.73
1u5p_I_185_V	0.60	2.33	1.76	2.19	2.71	3.06
1u5p_K_127_A	0.00	2.25	1.65	1.70	-0.32	0.85
1u5p_K_148_A	-0.40	-0.08	0.09	-0.48	-0.67	-0.18
1u5p_K_148_G	0.50	0.98	1.20	0.84	1.39	1.26
1u5p_K_173_A	0.10	0.15	-0.22	-0.23	-1.08	-0.54
1u5p_K_173_G	1.40	1.55	1.23	1.23	0.80	1.56
1u5p_K_197_A	0.40	0.17	0.30	0.19	-1.07	-0.01
1u5p_K_197_G	1.30	1.64	1.14	1.26	1.24	1.71
1u5p_L_146_A	0.20	1.83	1.52	1.69	0.69	0.84
1u5p_L_153_A	2.80	3.02	2.19	2.59	2.70	2.34
1u5p_L_157_A	3.80	2.78	2.57	2.39	2.97	3.54
1u5p_L_174_A	2.40	2.87	2.90	3.10	3.49	3.56
1u5p_L_189_A	2.80	3.60	3.40	3.74	3.18	3.94
1u5p_L_199_A	3.80	4.06	3.25	3.69	3.79	3.81
1u5p_L_210_A	1.40	4.84	4.81	5.25	4.28	4.72
1u5p_M_117_A	2.20	2.64	2.66	2.74	1.75	2.37
1u5p_N_145_A	-0.20	-0.18	-0.16	-0.49	-0.60	-0.67
1u5p_N_145_G	0.40	1.10	1.20	1.15	0.23	0.57
1u5p_P_162_A	-0.40	0.43	1.56	1.80	1.43	1.68
1u5p_Q_165_A	0.70	0.42	0.49	0.15	-0.06	0.03
1u5p_Q_165_G	1.80	2.18	1.83	1.64	1.65	1.98
1u5p_Q_187_A	0.00	0.55	0.65	0.45	0.49	0.20
1u5p_Q_187_G	1.30	1.94	1.65	1.60	1.10	1.54
1u5p_Q_201_A	-0.40	0.64	0.19	0.07	0.22	0.07
1u5p_Q_201_G	0.70	1.89	1.76	1.34	1.68	2.09
1u5p_R_115_A	0.30	-0.69	-0.92	-1.59	-2.07	-2.39
1u5p_R_115_G	1.90	0.38	0.12	-0.03	-1.31	-0.49
1u5p_R_152_A	-0.30	0.10	-0.63	-0.87	-1.11	-0.71
1u5p_R_152_G	0.60	0.53	0.01	0.04	0.00	0.85
1u5p_R_206_A	0.00	0.43	-0.01	0.04	-2.21	-1.11
1u5p_T_141_A	-0.30	0.08	0.01	-0.21	-0.92	-0.92
1u5p_T_141_G	0.10	-0.03	-0.52	0.44	-1.06	-0.12
1u5p_V_131_A	0.20	0.75	0.81	0.97	1.22	1.92
1u5p_V_143_A	0.40	-0.62	-0.35	-0.16	-0.45	-0.03
1u5p_V_167_A	2.30	2.18	2.07	2.09	2.18	2.09
1u5p_W_196_F	2.10	2.71	2.89	2.56	2.49	3.79
lycc_K_78_A	0.45	0.17	-0.12	-0.10	0.53	-0.25
lycc_K_78_G	0.74	1.26	0.79	0.85	1.57	1.42
lycc_L_90_A	2.80	4.13	3.72	3.92	7.05	6.97
lycc_N_57_A	-2.97	-0.86	-0.88	-0.87	-3.20	-3.38
200l_A_121_L	-2.30	1.98	2.23	1.44	1.97	-0.53
227l_A_104_F	-3.10	-4.07	-3.44	-3.93	-4.25	-2.68
235l_A_111_V	-1.30	-0.52	-1.03	-1.08	-0.20	-0.33
236l_A_87_V	-1.70	-1.45	-1.25	-2.19	-3.98	-2.66
237l_A_149_V	-3.20	-2.31	-1.96	-2.54	-1.28	-3.06
238l_A_103_V	-2.20	-1.24	-1.74	-2.36	-0.52	-1.10

239I_A_17_I	-2.70	-4.45	-4.40	-4.54	-5.25	-5.62
240I_A_27_I	-3.10	-2.91	-2.83	-3.03	0.72	-3.41
241I_A_29_I	-2.60	3.16	1.26	2.30	6.40	-0.98
242I_A_50_I	-2.00	0.03	0.07	-0.77	-0.65	-0.29
243I_A_58_I	-3.20	-4.29	-3.97	-4.20	-4.78	-6.03
244I_A_100_I	-3.40	-2.32	-2.06	-2.20	-6.00	0.04
246I_A_67_F	-1.90	-1.18	-1.05	-0.93	6.31	8.12
247I_A_84_L	-3.90	-3.68	-3.15	-3.66	-2.71	0.09
253I_A_20_D	-0.30	-1.85	-0.67	-0.75	-1.73	-1.58
2bqa_I_106_V	0.98	2.39	2.05	3.15	2.22	2.26
2chf_A_100_G	1.00	2.10	1.95	1.97	3.23	2.11
2chf_A_102_G	1.70	2.54	2.43	2.56	1.72	2.36
2chf_A_112_G	1.30	1.69	1.53	1.78	1.68	1.75
2chf_A_113_G	0.80	1.00	0.66	0.77	0.90	0.97
2chf_A_35_G	3.10	3.05	2.80	2.72	2.41	2.96
2chf_A_41_G	2.30	3.29	2.92	3.32	3.23	3.72
2chf_A_73_G	0.30	0.94	0.92	0.88	1.17	1.18
2chf_A_96_G	1.40	1.64	1.54	1.77	2.24	2.14
2chf_A_97_G	1.30	2.02	1.91	2.10	2.16	2.67
2chf_A_98_G	0.50	1.75	1.13	1.27	1.74	2.02
2chf_D_11_A	-2.50	-1.66	-1.84	-1.67	-3.75	-2.12
2chf_D_12_A	-2.70	-1.33	-1.39	-1.43	-3.11	-2.40
2chf_D_37_A	1.90	1.38	1.19	0.95	2.50	3.66
2chf_D_37_G	1.00	1.79	1.67	1.73	1.27	1.99
2chf_D_56_A	-3.40	-1.00	-1.36	-0.95	-1.86	-1.84
2chf_D_63_A	1.00	0.19	-0.15	0.09	1.16	1.62
2chf_F_13_A	-0.80	0.38	-0.18	0.14	0.19	0.57
2chf_I_122_V	0.80	2.09	1.93	1.95	2.20	2.27
2chf_I_54_V	1.50	2.49	1.98	2.09	1.87	2.29
2chf_I_71_V	1.50	1.56	1.36	1.45	1.31	1.53
2chf_N_22_G	0.00	1.41	0.90	1.06	0.04	-0.53
2chf_P_60_G	0.60	1.94	2.31	2.49	2.69	3.51
2chf_T_111_A	1.50	1.44	1.42	1.59	2.85	1.80
2chf_T_111_G	1.00	0.99	0.81	1.04	0.27	0.57
2chf_V_107_T	1.00	1.00	1.17	1.44	1.82	1.72
2chf_V_10_T	3.20	2.47	2.66	2.54	3.66	3.59
2chf_V_20_T	0.20	2.23	2.39	2.20	2.91	2.82
2chf_V_32_T	1.50	3.74	4.03	3.93	6.74	6.75
2chf_V_39_T	0.80	-0.71	-0.34	-0.32	-1.44	-1.34
2chf_V_82_T	3.50	2.81	2.82	2.80	3.01	2.46
2chf_V_9_T	4.00	4.28	4.28	4.06	6.48	5.88
2ci2_A_17_G	1.41	1.77	1.71	1.78	1.76	2.51
2ci2_A_59_G	1.88	0.62	0.74	0.59	1.36	1.39
2ci2_D_24_A	1.05	0.23	0.16	0.28	-1.16	-1.13
2ci2_D_46_A	1.02	0.08	-0.39	-0.12	-0.67	-0.96
2ci2_D_53_A	3.14	1.59	1.34	1.48	2.96	3.29
2ci2_D_56_N	0.00	-2.06	-2.35	-1.47	-2.18	-2.16
2ci2_E_15_D	0.77	0.50	-0.25	0.49	0.45	0.33
2ci2_E_15_N	0.28	-0.21	-0.41	-0.26	0.20	0.24
2ci2_E_15_Q	0.40	-0.51	-0.14	-0.45	-0.60	-0.41
2ci2_E_16_D	-0.36	0.72	0.83	0.75	1.98	2.59
2ci2_E_16_N	0.08	0.11	0.32	0.02	1.62	2.13
2ci2_E_16_Q	0.68	-0.51	-0.51	-0.69	0.91	1.27
2ci2_E_27_A	0.11	0.93	0.65	0.52	-1.72	-1.95
2ci2_E_42_A	1.09	0.47	0.43	0.30	-0.42	-0.57
2ci2_E_8_A	1.03	0.03	-0.93	-0.18	-1.84	-1.32

2ci2_E_8_Q	0.57	-0.35	-0.69	-0.34	-2.41	-1.58
2ci2_F_51_A	3.21	5.76	4.96	5.52	3.25	2.48
2ci2_F_51_L	1.92	1.58	1.27	1.65	0.52	0.78
2ci2_F_51_V	1.41	4.68	4.20	4.14	2.89	1.78
2ci2_I_21_L	1.96	1.59	2.09	1.93	1.79	0.15
2ci2_I_21_V	1.02	1.51	1.38	1.63	2.02	2.00
2ci2_I_30_A	3.40	5.31	4.73	5.39	6.38	6.36
2ci2_I_30_V	0.75	1.87	1.74	1.83	2.39	2.29
2ci2_I_31_A	2.12	3.76	3.55	3.81	3.69	2.94
2ci2_I_31_G	3.52	5.12	4.51	4.56	4.64	4.24
2ci2_I_31_V	-0.08	1.59	1.12	1.28	0.25	0.36
2ci2_I_38_A	1.28	0.22	0.06	0.35	1.16	1.20
2ci2_I_58_A	4.09	3.46	3.03	3.40	3.81	4.07
2ci2_I_58_V	0.08	0.44	0.40	0.42	0.12	0.37
2ci2_K_12_A	1.20	0.77	0.84	0.77	1.15	0.76
2ci2_K_18_A	1.13	0.32	0.31	0.12	0.15	0.23
2ci2_K_18_G	2.01	2.66	1.76	1.71	2.09	2.49
2ci2_K_19_A	0.99	0.42	0.32	0.30	-0.09	-0.19
2ci2_K_19_G	1.58	1.06	1.17	1.57	1.60	1.49
2ci2_K_25_A	0.61	2.25	1.71	1.88	-0.62	-0.61
2ci2_K_25_G	3.49	5.21	4.76	5.10	1.34	1.28
2ci2_K_3_A	1.04	1.86	0.62	1.26	-2.05	-1.77
2ci2_K_3_M	0.73	0.76	0.35	0.10	-1.95	-2.60
2ci2_K_54_N	1.21	-0.23	-0.47	-0.21	-0.11	0.08
2ci2_L_22_A	1.21	2.40	2.32	2.16	2.12	2.74
2ci2_L_22_G	2.09	3.51	3.25	3.38	4.08	4.77
2ci2_L_33_A	1.74	2.74	2.30	2.17	2.52	2.89
2ci2_L_33_I	1.01	0.49	0.42	0.32	0.45	0.50
2ci2_L_33_V	1.02	1.24	0.60	1.28	0.80	0.93
2ci2_L_50_A	3.56	4.78	3.83	4.77	5.47	5.93
2ci2_L_9_A	1.91	4.67	4.47	4.61	4.67	5.18
2ci2_N_57_A	1.22	0.20	0.05	0.11	-0.86	-0.91
2ci2_N_57_D	1.51	1.06	0.88	1.16	1.81	1.87
2ci2_P_26_A	-0.36	1.26	2.17	2.11	1.73	1.87
2ci2_P_34_A	0.58	0.15	1.26	1.55	2.04	1.80
2ci2_P_62_A	3.50	1.78	2.88	2.80	3.27	3.17
2ci2_P_7_A	-3.40	1.08	1.84	2.46	1.74	1.96
2ci2_Q_23_A	0.54	-0.43	-0.20	-0.53	-0.51	-0.66
2ci2_Q_23_G	0.92	0.64	0.65	0.14	0.90	0.59
2ci2_R_44_A	1.02	0.64	0.81	0.71	0.23	0.65
2ci2_R_49_A	1.31	-1.01	-1.10	-1.14	-3.07	-2.61
2ci2_S_13_A	1.02	-0.08	-0.31	-0.49	0.69	1.09
2ci2_S_13_G	0.06	0.63	0.50	0.52	0.13	0.68
2ci2_T_37_A	1.42	-1.08	-1.13	-0.57	-0.82	-1.15
2ci2_T_37_S	0.98	-0.01	-0.31	-0.21	0.75	0.52
2ci2_T_37_V	1.57	-0.97	-1.08	-1.16	-2.08	-1.87
2ci2_T_40_A	0.68	0.53	0.21	0.49	0.09	0.25
2ci2_T_40_D	0.04	0.88	1.95	1.96	1.58	0.99
2ci2_T_4_A	0.85	1.34	0.77	1.22	1.79	1.37
2ci2_T_4_G	1.16	2.43	1.82	1.87	3.19	2.09
2ci2_T_4_V	0.32	0.30	-0.19	-0.09	0.31	-0.03
2ci2_V_20_A	0.03	1.47	1.34	1.39	1.86	1.37
2ci2_V_35_A	0.64	-0.20	-0.36	-0.30	-0.13	0.15
2ci2_V_35_G	2.43	1.56	1.45	1.43	1.96	1.88
2ci2_V_35_T	1.03	-0.01	-0.05	0.25	0.91	1.12
2ci2_V_39_A	0.67	1.10	0.90	1.12	2.12	1.74



2ci2_V_48_A	4.97	4.81	5.13	4.97	5.44	6.01
2ci2_V_52_A	1.13	2.49	2.49	2.50	2.25	2.64
2ci2_V_61_A	1.51	1.67	1.61	1.76	1.38	1.47
2ci2_V_61_G	3.24	3.64	3.45	3.59	3.89	3.75
2ci2_V_61_T	0.38	1.29	1.41	1.52	1.35	1.18
2ci2_V_64_A	1.45	2.80	2.62	2.52	2.36	1.92
2ci2_V_64_G	3.50	4.88	4.58	4.51	4.67	4.26
2ci2_V_64_T	1.15	2.54	2.86	2.37	3.21	3.51
2lzm_D_20_A	0.30	-1.50	-1.38	-1.72	-1.10	-2.00
2lzm_D_47_A	0.95	-0.47	0.20	-0.78	-1.61	-1.01
2lzm_D_92_N	1.40	0.39	-0.38	0.20	0.93	1.95
2lzm_E_11_A	-1.10	0.75	-0.07	0.82	-1.63	-1.69
2lzm_E_128_A	0.16	0.47	0.02	0.31	0.22	-0.24
2lzm_E_45_A	-0.01	-0.90	0.07	-0.62	-2.72	-1.47
2lzm_F_104_A	3.10	5.55	5.53	4.41	4.53	5.17
2lzm_F_153_A	3.80	6.17	6.89	6.45	5.74	6.83
2lzm_F_153_L	-0.30	2.28	2.30	2.09	1.58	0.52
2lzm_F_67_A	1.90	4.15	3.83	4.09	5.73	6.48
2lzm_I_100_A	3.40	4.08	4.17	3.46	4.93	3.51
2lzm_I_17_A	2.70	4.98	4.75	5.06	3.64	3.53
2lzm_I_27_A	3.10	4.31	4.42	4.57	4.20	4.42
2lzm_I_29_A	2.60	3.96	2.86	3.20	4.38	4.50
2lzm_I_3_A	0.70	2.01	2.21	2.29	2.55	2.04
2lzm_I_3_G	2.10	5.07	4.06	3.87	4.33	6.00
2lzm_I_3_T	2.30	2.06	1.83	1.86	3.05	2.54
2lzm_I_3_V	0.40	1.31	0.35	-0.06	2.16	2.49
2lzm_I_50_A	2.00	2.90	2.89	2.89	3.11	3.65
2lzm_I_58_A	3.20	5.49	5.33	6.08	5.83	6.99
2lzm_I_78_A	1.60	3.71	4.57	5.23	5.19	4.39
2lzm_K_124_G	0.10	-0.37	-0.15	0.28	-2.39	-2.67
2lzm_K_43_A	1.03	1.59	0.83	1.02	0.09	0.08
2lzm_K_48_A	0.56	0.96	-0.47	1.03	1.02	-0.89
2lzm_L_118_A	3.50	3.89	3.56	4.21	4.30	4.25
2lzm_L_121_A	2.30	3.94	4.02	3.49	3.89	4.24
2lzm_L_133_A	4.30	4.22	4.25	5.01	4.47	4.25
2lzm_L_33_A	3.60	6.17	5.98	5.89	5.97	6.20
2lzm_L_39_A	0.90	1.22	0.72	0.95	1.34	1.24
2lzm_L_46_A	1.86	6.41	4.60	5.16	3.52	4.21
2lzm_L_66_A	3.90	3.51	3.28	4.08	3.01	3.64
2lzm_L_7_A	2.60	4.86	4.89	3.59	4.54	5.03
2lzm_L_84_A	3.90	4.44	4.60	5.64	5.57	5.77
2lzm_L_91_A	3.10	4.04	5.16	4.52	4.83	5.31
2lzm_L_99_A	4.50	5.32	4.44	4.66	5.58	6.44
2lzm_L_99_G	6.30	8.10	7.58	6.18	9.21	8.84
2lzm_M_106_A	2.30	4.53	3.78	4.08	2.28	2.42
2lzm_M_120_A	0.20	-0.47	0.65	0.78	0.32	0.62
2lzm_M_6_A	1.90	2.58	1.48	1.83	0.44	0.59
2lzm_N_116_A	-0.17	-0.34	-0.33	-0.14	0.33	-0.78
2lzm_N_116_D	-0.60	0.50	0.83	0.06	1.54	1.50
2lzm_N_144_D	-0.50	-0.66	0.16	0.85	0.82	-0.53
2lzm_N_163_D	0.21	1.10	0.26	0.59	0.78	1.35
2lzm_N_40_A	-0.32	-0.42	0.13	0.28	-1.41	-1.76
2lzm_N_40_D	-0.44	-0.32	-0.37	-0.18	-0.03	0.32
2lzm_N_55_G	0.60	0.40	-0.50	-0.87	-0.10	-0.17
2lzm_N_68_A	0.05	-0.02	-0.43	-0.52	-1.64	-2.35
2lzm_P_37_A	0.00	-0.62	-0.10	0.70	0.06	-0.54

2lzm_P_86_G	1.91	1.22	0.86	1.07	1.82	2.70
2lzm_Q_105_A	0.60	1.72	1.94	2.26	-1.03	-0.53
2lzm_Q_105_E	1.10	1.70	1.74	1.69	3.18	2.94
2lzm_Q_105_G	3.11	2.50	2.68	3.08	0.01	-0.02
2lzm_Q_122_A	0.24	0.59	0.02	-0.43	-0.83	-1.05
2lzm_Q_123_A	0.22	0.53	0.16	0.28	-0.17	-0.14
2lzm_Q_123_E	-0.40	1.70	1.21	1.19	1.57	2.02
2lzm_R_119_A	0.18	-0.56	-0.58	-0.02	-0.39	-0.93
2lzm_S_117_A	-1.27	-0.82	-0.67	-1.59	-2.31	-1.90
2lzm_S_44_A	-0.34	-0.93	-0.48	-0.99	-1.37	-1.87
2lzm_S_44_G	0.53	0.29	0.07	0.97	0.25	-0.54
2lzm_T_115_A	0.14	-0.20	-1.00	0.23	-1.09	-2.07
2lzm_T_151_S	-0.39	-0.82	-0.86	1.42	0.27	-0.10
2lzm_T_152_S	2.60	1.14	1.25	1.17	2.50	1.58
2lzm_T_157_A	0.50	1.31	3.11	2.85	4.76	4.96
2lzm_T_157_G	1.10	1.06	1.61	1.38	1.80	-0.06
2lzm_T_157_S	0.66	0.62	1.36	1.52	0.54	1.90
2lzm_T_157_V	1.20	1.88	2.20	1.87	3.05	4.45
2lzm_T_26_S	-0.57	-0.02	0.91	1.71	0.86	-0.61
2lzm_T_59_A	1.50	1.67	0.15	0.52	2.48	1.86
2lzm_T_59_G	1.60	0.81	1.14	1.23	0.49	2.28
2lzm_T_59_S	0.20	0.53	-1.01	0.15	-0.39	0.02
2lzm_T_59_V	1.50	2.21	2.14	2.37	3.37	4.83
2lzm_V_103_A	1.91	2.33	2.81	1.62	1.93	1.58
2lzm_V_111_A	1.30	2.49	2.72	2.83	1.74	2.30
2lzm_V_131_A	-0.39	-0.13	0.67	-0.07	-0.22	0.28
2lzm_V_131_G	0.68	1.30	0.65	0.68	-0.19	1.66
2lzm_V_131_T	0.12	-0.27	0.58	0.36	1.09	0.73
2lzm_V_149_A	2.87	2.41	2.08	1.93	0.78	0.67
2lzm_V_149_T	2.80	1.45	1.51	1.21	1.31	1.13
2lzm_V_71_A	1.50	2.88	2.40	1.61	3.28	3.81
2lzm_V_75_T	1.30	0.86	2.12	1.67	3.09	1.99
2lzm_V_87_A	1.70	1.63	2.54	2.70	3.87	3.17
2lzm_V_87_T	1.60	0.76	1.13	0.44	2.53	2.56
2lzm_V_94_A	1.80	1.33	0.89	1.87	2.23	2.19
2lzm_Y_25_G	4.55	7.30	7.08	7.07	6.12	7.57
4lyz_D_101_A	-0.76	-5.16	-3.17	-3.35	-1.81	-2.64
4lyz_D_101_G	-0.45	-0.53	-1.12	-1.01	-1.73	-1.08
4lyz_D_101_N	-0.04	-0.57	-0.60	-0.77	-5.22	-1.31
4lyz_I_55_A	4.40	2.59	2.50	2.42	3.61	1.98
4lyz_I_55_T	4.96	3.46	3.36	3.62	2.75	4.04
4lyz_I_55_V	0.91	0.82	0.89	0.89	2.77	0.29
4lyz_S_91_A	0.15	-1.52	-1.72	-1.60	-0.99	-3.13
5azu_A_82_G	1.67	2.31	1.84	2.27	1.67	1.69
5azu_F_110_A	5.02	8.40	8.36	8.34	7.34	8.50
5azu_F_97_A	2.63	8.35	8.14	8.12	7.92	8.10
5azu_I_20_A	1.98	5.61	5.74	5.40	6.09	5.96
5azu_I_20_T	2.39	4.34	3.83	4.12	5.35	5.57
5azu_I_20_V	0.38	2.45	2.03	1.70	2.05	2.06
5azu_I_7_A	3.35	4.15	4.11	4.57	2.99	3.94
5azu_I_81_A	1.91	3.85	3.04	3.20	3.25	3.68
5azu_I_81_T	2.51	2.87	2.58	2.93	3.01	3.36
5azu_I_81_V	0.16	0.99	0.86	1.10	0.21	0.80
5azu_L_33_A	1.67	5.34	4.55	4.78	4.81	5.18
5azu_L_50_A	1.79	6.33	5.49	5.91	6.31	6.72
5azu_L_50_T	2.34	7.48	6.37	6.78	7.77	8.24

5azu_L_50_V	0.36	6.99	7.09	6.78	7.08	7.20
5azu_M_121_A	2.87	3.73	3.18	3.36	2.00	3.03
5azu_V_22_A	1.67	4.54	4.68	4.87	6.17	5.85
5azu_V_31_A	1.67	4.00	4.23	4.25	5.02	5.07
5azu_V_5_A	0.96	2.17	2.09	2.24	1.95	1.88
5azu_V_60_G	3.11	4.01	3.93	3.82	3.45	3.45
5azu_V_95_A	0.96	3.01	2.78	3.19	2.64	2.94
5azu_W_48_A	3.35	10.52	9.64	10.17	9.23	9.90
5azu_Y_108_A	3.59	7.85	7.40	7.39	8.00	8.51
8tim_K_192_A	-1.00	0.19	0.32	-0.35	-2.22	0.72
8tim_Q_178_A	-0.10	0.61	0.32	0.40	0.08	0.89

## Command lines used in this work:

### Design runs

```
mini/bin/fixbb.macosgccrelease
-database minirosetta_database
-s 1FKB.pdb
-ex1 -ex2 -extrachi_cutoff 0 -linmem_ig 10
-ignore_unrecognized_res -no_optH false -skip_set_reasonable_fold_tree -no_his_his_pairE
-mute core.io core.scoring core.conformation
[-score:weights ./hpatch_weights.txt]
```

### Weight optimization runs

```
mpirun mini/bin/surface_optE_parallel.linuxgccrelease
-database minirosetta_database
-s nataa_recovery_pdbids.test.list
-optE:optimize_nat_aa true
-optE:fit_reference_energies_to_aa_profile_recovery true
-optE:n_design_cycles 10
-optE:mpi_weight_minimization true
-optE:optimize_starting_free_weights true
[ -optE:rescore:weights weights.txt -optE:rescore:outlog rescore.log ]
[ -optE:rescore:measure_sequence_recovery true ]
-optE:number_of_swarm_particles 75 -optE:number_of_swarm_cycles 30
-optE:repeat_swarm_optimization_until_fitness_improves true
-optE:free free_wts.txt -optE:fixed fixed_wts.txt
-ignore_unrecognized_res -no_optH false -skip_set_reasonable_fold_tree -no_his_his_pairE
-mute core.io core.pack core.scoring core.conformation
-ex1 -ex2 -extrachi_cutoff 0 -linmem_ig 10 -options:user
```

free.txt	fixed.txt
fa_rep	fa_atr 0.8
fa_sol	omega 0.5
fa_intra_rep	hbond_lr_bb 1.17
pro_close	hbond_sr_bb 0.585
fa_pair	dslf_ss_dst 1.0
hbond_bb_sc	dslf_cs_ang 1.0
hbond_sc	dslf_ss_dih 1.0
rama	dslf_ca_dih 1.0
fa_dun	hpatch 0.3
p_aa_pp	

### QUILT runs

```
quilt -n 252 -ep 1.4 -R 1FKB.pdb
```

### Sequence recovery runs

```
~/minibin/sequencerecovery.macosgccrelease -database ~/minidb/
-native_pdb_list seqrecovery.list -redesign_pdb_list redesigned.list
-ignore_unrecognized_res -mute core
```

### Scoring runs

```
~/minibin/score.macosgccrelease -database ~/minidb/
-l redesigns.list
-ignore_unrecognized_res -mute core
[-score:weights design_hpatch.wts]
```