

Fast and accurate Predictions of Protein Stability Changes upon Mutations using statistical potentials and neural networks: PoPMuSiC-2.0

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1. Complete dataset of 2648 mutants

The following criteria were applied to define the dataset used in this study:

- (a) Only mutations in globular proteins were considered, since the force fields used by PoPMuSiC are only valid for that class of proteins.
- (b) Only mutant proteins whose experimental structure (either X-ray or NMR) is available were taken into account, as PoPMuSiC uses the structure.
- (c) Only single-site mutations were considered. Multiple simultaneous mutations, including single mutations introduced in pseudo wild-type constructs, were removed, because these mutations are likely to be correlated and/or to entail structural modifications not modelled by PoPMuSiC.
- (d) Mutations in heme-proteins are considered only if the stability measurements were performed on the apo form of the protein, and the structure of this apo form is available. Indeed, the interactions between residues and the heme are not taken into account by PoPMuSiC.
- (e) We consider only mutations whose stability changes are measured with respect to the same reference state, *i.e.* the unfolded conformation.
- (f) In the case of homo-multimeric proteins, the measured free energy changes may correspond either to the whole protein or to a monomer only. Mutations for which this information could not be retrieved from the original papers were eliminated. All remaining values were adapted to correspond to the free energy change per mole of monomer.
- (g) Mutations that destabilize the structure by more than 5 kcal/mol and mutations involving a proline were not considered, as they are likely to induce significant structural modifications, which are not modelled by PoPMuSiC.

With these criteria, 2648 different point mutations, in 131 proteins, were selected. For some of these mutants, several measures of the variation in folding free energy ($\Delta\Delta G$) have been performed, sometimes in different conditions. To avoid any redundancy in our database, we considered only one value per mutant, which is noted $\Delta\Delta G_M$ and is defined as an average of all available measured $\Delta\Delta G$ values. Measurements performed with a pH close to 7, a temperature close to 25°C, and without additives, are given a higher weight in the averaging procedure :

$$\Delta\Delta G_M = \left(\sum_{i=1}^n w_i^{pH} w_i^T w_i^{add} \Delta\Delta G_i \right) / \left(\sum_{i=1}^n w_i^{pH} w_i^T w_i^{add} \right) , \quad \text{with :} \quad (1)$$

$$w_i^{pH} = 1 - \frac{|pH_i - 7|}{7} , \quad w_i^T = \max(0 ; 1 - \frac{|T_i - 25|}{25}) , \quad \begin{cases} w_i^{add} = \prod_{j=1}^m (1 - \frac{C_{ij}}{C_j^{\max}}) & \text{if } m > 0 \\ w_i^{add} = 1 & \text{if } m = 0 \end{cases} \quad (2)$$

where n is the number of available experimental values of $\Delta\Delta G$ for a given mutation, m is the number of additives (excluding buffers) present in solution during a given experiment, C_{ij} is the concentration of additive j in experiment i , and C_j^{\max} is the maximal concentration of additive j in all experiments included in our dataset. Note that w_i^T is systematically set to 1 in the case of $\Delta\Delta G$ values obtained by thermal denaturation.

PDB Code ^a	Chain name and residue position	Wild-type and mutant amino acid	$\Delta\Delta G_M$ (kcal/mol)	T (°C) ^a	pH ^b	PDB Code ^a	Chain name + Residue position	Wild-type and mutant amino acid	$\Delta\Delta G_M$ (kcal/mol)	T (°C) ^b	pH ^b
1a43_p	A 156	G A	2.40	25.0	7.3	1a43_p	A 159	E D	4.55	25.0	7.3
1a43_p	A 167	R A	4.55	25.0	7.3	1a43_p	A 184	W A	0.70	25.0	7.3
1a43_p	A 218	C S	3.70	25.0	7.3	1a5e	A 15	W D	-0.19	20.0	8.5
1a5e	A 37	L S	-0.81	20.0	8.5	1a5e	A 121	L R	-0.55	20.0	8.5
1aep	A 14	L K	1.18	25.0	7.4	1aep	A 28	T A	-0.48	25.0	7.4
1aep	A 137	A K	1.40	25.0	7.4	1aep	A 141	T A	1.03	25.0	7.4
1ag2	A 129	M V	0.11	25.0	7.0	1ag2	A 175	F W	0.05	22.0	7.0
1ag2	A 180	V I	0.25	25.0	7.0	1ag2	A 183	T A	4.04	25.0	7.0
1ag2	A 190	T V	-0.19	25.0	7.0	1ag2	A 198	F S	2.15	25.0	7.0
1ag2	A 200	E K	0.23	25.0	7.0	1ag2	A 208	R H	1.05	25.0	7.0
1ag2	A 210	V I	0.07	25.0	7.0	1ag2	A 217	Q R	1.88	25.0	7.0
1aj3	A 10	H A	-0.50	25.0	7.0	1aj3	A 10	H G	0.50	25.0	7.0
1aj3	A 12	F A	3.70	25.0	7.0	1aj3	A 12	F L	1.30	25.0	7.0
1aj3	A 14	R A	0.30	25.0	7.0	1aj3	A 14	R G	1.90	25.0	7.0
1aj3	A 16	M A	2.20	25.0	7.0	1aj3	A 17	D A	0.20	25.0	7.0
1aj3	A 17	D G	1.20	25.0	7.0	1aj3	A 21	S A	-0.50	25.0	7.0
1aj3	A 21	S G	0.50	25.0	7.0	1aj3	A 22	W F	1.31	25.0	7.5
1aj3	A 23	I A	3.60	25.0	7.0	1aj3	A 23	I V	1.60	25.0	7.0
1aj3	A 25	E A	-0.10	25.0	7.0	1aj3	A 25	E G	1.10	25.0	7.0
1aj3	A 26	K A	0.00	25.0	7.0	1aj3	A 30	V A	0.20	25.0	7.0
1aj3	A 40	T A	-0.30	25.0	7.0	1aj3	A 40	T G	0.10	25.0	7.0
1aj3	A 42	V A	0.40	25.0	7.0	1aj3	A 44	N A	-0.20	25.0	7.0
1aj3	A 44	N G	0.40	25.0	7.0	1aj3	A 45	L A	0.20	25.0	7.0
1aj3	A 47	K A	-0.40	25.0	7.0	1aj3	A 47	K G	0.50	25.0	7.0
1aj3	A 49	H A	1.40	25.0	7.0	1aj3	A 51	R A	-0.30	25.0	7.0
1aj3	A 51	R G	0.60	25.0	7.0	1aj3	A 52	L A	2.80	25.0	7.0
1aj3	A 54	A G	1.10	25.0	7.0	1aj3	A 56	L A	3.80	25.0	7.0
1aj3	A 58	A G	1.10	25.0	7.0	1aj3	A 59	H A	2.30	25.0	7.0
1aj3	A 63	I A	2.80	25.0	7.0	1aj3	A 63	I V	0.60	25.0	7.0
1aj3	A 64	Q A	0.70	25.0	7.0	1aj3	A 64	Q G	1.80	25.0	7.0
1aj3	A 66	V A	2.30	25.0	7.0	1aj3	A 68	D A	0.10	25.0	7.0
1aj3	A 68	D G	1.30	25.0	7.0	1aj3	A 72	K A	0.10	25.0	7.0
1aj3	A 72	K G	1.40	25.0	7.0	1aj3	A 73	L A	2.40	25.0	7.0
1aj3	A 84	I A	2.00	25.0	7.0	1aj3	A 84	I V	0.60	25.0	7.0
1aj3	A 86	Q A	0.00	25.0	7.0	1aj3	A 86	Q G	1.30	25.0	7.0
1aj3	A 88	L A	2.80	25.0	7.0	1aj3	A 89	A G	1.10	25.0	7.0
1aj3	A 91	F A	2.80	25.0	7.0	1aj3	A 91	F L	-0.50	25.0	7.0
1aj3	A 93	D A	-0.70	25.0	7.0	1aj3	A 93	D G	0.30	25.0	7.0
1aj3	A 95	W F	2.10	25.0	7.0	1aj3	A 96	K A	0.40	25.0	7.0
1aj3	A 96	K G	1.30	25.0	7.0	1aj3	A 98	L A	3.80	25.0	7.0
1aj3	A 100	Q A	-0.40	25.0	7.0	1aj3	A 100	Q G	0.70	25.0	7.0
1aj3	A 102	A G	2.60	25.0	7.0	1aj3	A 104	A G	1.80	25.0	7.0
1aj3	A 105	R A	0.00	25.0	7.0	1aky	A 8	V I	1.20	25.0	7.5
1aky	A 48	Q E	0.96	25.0	7.7	1aky	A 77	T H	0.90	25.0	6.4
1aky	A 110	T H	2.13	25.0	6.3	1aky	A 169	N D	2.15	25.0	7.5
1aky	A 213	I F	1.91	25.0	7.5	1am7_a	A 31	H D	1.60	25.0	7.0
1am7_a	A 48	H N	5.00	25.0	7.0	1amq_p	A 82	C A	0.45	25.0	7.5
1amq_p	A 82	C S	2.44	25.0	7.5	1amq_p	A 191	C A	1.12	25.0	7.5
1amq_p	A 191	C F	0.90	25.0	7.5	1amq_p	A 191	C G	0.02	25.0	7.5
1amq_p	A 191	C R	1.69	25.0	7.5	1amq_p	A 191	C S	1.44	25.0	7.5
1amq_p	A 191	C W	2.25	25.0	7.5	1amq_p	A 191	C Y	1.05	25.0	7.5
1amq_p	A 192	C A	1.21	25.0	7.5	1amq_p	A 192	C S	0.99	25.0	7.5
1amq_p	A 270	C A	1.68	25.0	7.5	1amq_p	A 401	C A	-1.06	25.0	7.5
1amq_p	A 401	C S	1.79	25.0	7.5	1ank_a	A 84	D H	1.40	51.8	7.2
1ank_a	A 85	G V	2.40	51.8	7.2	1ank_a	A 86	F L	0.80	51.8	7.2
1ank_a	A 88	R G	0.10	51.8	7.4	1aon_u	U 3	I C	0.44	25.0	7.8

laon_u	U 3	I W	0.25	25.0	7.8	laon_u	U 48	I W	0.20	25.0	7.8
laon_u	U 95	V C	0.25	25.0	7.8	laps	A 11	Y F	-1.04	28.0	5.5
laps	A 11	Y I	2.24	28.0	5.5	laps	A 13	V A	2.63	28.0	5.5
laps	A 17	V A	1.84	28.0	5.5	laps	A 20	V A	0.28	28.0	5.5
laps	A 22	F L	1.29	28.0	5.5	laps	A 25	Y A	-0.10	28.0	5.5
laps	A 30	A G	1.65	28.0	5.5	laps	A 36	V A	2.54	28.0	5.5
laps	A 38	W F	0.02	28.0	5.5	laps	A 39	V A	1.63	28.0	5.5
laps	A 42	T A	1.84	28.0	5.5	laps	A 45	G A	1.73	28.0	5.5
laps	A 47	V A	1.87	28.0	5.5	laps	A 51	V A	1.88	28.0	5.5
laps	A 64	W A	1.50	28.0	5.5	laps	A 75	I V	1.41	28.0	5.5
laps	A 78	T S	1.41	28.0	5.5	laps	A 83	E D	1.51	28.0	5.5
laps	A 86	I V	1.57	28.0	5.5	laps	A 89	L A	1.67	28.0	5.5
larr	A 9	Q G	-0.22	25.0	7.5	larr	A 13	R G	-0.27	25.0	7.5
larr	A 16	R G	0.64	25.0	7.5	larr	A 17	E G	0.57	25.0	7.5
larr	A 19	L Q	0.90	25.0	7.5	larr	A 20	D G	1.35	25.0	7.5
larr	A 23	R G	1.04	25.0	7.5	larr	A 24	K G	1.23	25.0	7.5
larr	A 24	K T	0.60	25.0	7.5	larr	A 27	E G	0.43	25.0	7.5
larr	A 28	E G	0.84	25.0	7.5	larr	A 34	N G	-0.23	25.0	7.5
larr	A 35	S G	0.24	25.0	7.5	larr	A 39	Q G	0.65	25.0	7.5
larr	A 46	K G	0.73	25.0	7.5	larr	A 47	K G	0.57	25.0	7.5
larr	A 48	E G	1.14	25.0	7.5	lazp	A 30	V I	-0.70	50.0	7.0
lb26	A 190	R A	0.36	39.0	7.0	lb26	A 193	K A	-0.38	39.0	7.0
lb26	A 231	E A	0.49	39.0	7.0	lb8e_p	A 19	W Y	3.45	30.0	7.1
lble	A 179	D N	0.44	20.0	6.5	lbni_a	A 4	I A	1.11	25.0	6.3
lbni_a	A 4	I V	0.69	25.0	6.3	lbni_a	A 5	N A	1.83	25.0	6.3
lbni_a	A 6	T A	2.21	25.0	6.3	lbni_a	A 6	T D	-0.11	25.0	6.3
lbni_a	A 6	T E	0.27	25.0	6.3	lbni_a	A 6	T G	1.09	25.0	6.3
lbni_a	A 6	T H	2.06	25.0	6.8	lbni_a	A 6	T N	1.27	25.0	6.3
lbni_a	A 6	T Q	1.87	25.0	6.3	lbni_a	A 6	T S	0.22	25.0	6.3
lbni_a	A 7	F L	4.35	25.0	6.2	lbni_a	A 8	D A	0.80	25.0	5.9
lbni_a	A 8	D G	1.23	25.0	6.3	lbni_a	A 8	D S	0.84	25.0	6.3
lbni_a	A 10	V A	3.46	25.0	6.3	lbni_a	A 10	V T	2.37	25.0	6.3
lbni_a	A 12	D A	0.09	25.0	6.3	lbni_a	A 12	D G	0.76	25.0	5.3
lbni_a	A 12	D S	0.77	25.0	6.3	lbni_a	A 13	Y A	3.49	25.0	6.3
lbni_a	A 13	Y F	0.52	25.0	6.3	lbni_a	A 14	L A	4.51	29.6	6.3
lbni_a	A 15	Q I	-1.19	25.0	6.3	lbni_a	A 16	T A	0.38	25.0	6.3
lbni_a	A 16	T G	1.48	25.0	6.3	lbni_a	A 16	T R	-0.24	25.0	6.0
lbni_a	A 16	T S	1.66	25.0	6.3	lbni_a	A 17	Y A	2.12	25.0	6.3
lbni_a	A 17	Y F	0.44	25.0	6.3	lbni_a	A 17	Y G	4.02	25.0	6.3
lbni_a	A 17	Y S	2.28	25.0	6.3	lbni_a	A 18	H A	1.99	25.0	6.3
lbni_a	A 18	H D	2.38	25.0	6.3	lbni_a	A 18	H G	0.65	25.0	6.6
lbni_a	A 18	H K	1.05	25.0	6.3	lbni_a	A 18	H N	1.74	25.0	6.3
lbni_a	A 18	H Q	1.52	25.0	6.3	lbni_a	A 18	H R	1.09	25.0	6.3
lbni_a	A 18	H S	2.19	25.0	6.3	lbni_a	A 19	K R	-0.54	25.0	6.3
lbni_a	A 22	D M	0.27	25.0	4.4	lbni_a	A 23	N A	2.27	25.0	6.3
lbni_a	A 24	Y F	-0.05	25.0	6.3	lbni_a	A 25	I A	3.59	25.0	6.3
lbni_a	A 25	I V	1.05	25.0	6.3	lbni_a	A 26	T A	1.95	25.0	6.3
lbni_a	A 26	T D	0.04	25.0	6.3	lbni_a	A 26	T E	0.05	25.0	6.3
lbni_a	A 26	T G	1.48	25.0	5.9	lbni_a	A 26	T N	1.29	25.0	6.3
lbni_a	A 26	T Q	1.72	25.0	6.3	lbni_a	A 26	T S	0.56	25.0	6.3
lbni_a	A 26	T V	2.31	25.0	6.3	lbni_a	A 27	K A	-0.44	25.0	6.3
lbni_a	A 27	K G	0.30	25.0	6.3	lbni_a	A 28	S A	-0.50	25.0	6.3
lbni_a	A 28	S E	-0.50	25.0	6.3	lbni_a	A 28	S G	0.47	25.0	6.3
lbni_a	A 29	E A	1.28	25.0	6.3	lbni_a	A 29	E G	1.91	25.0	6.3
lbni_a	A 29	E Q	0.11	25.0	6.3	lbni_a	A 29	E S	1.22	25.0	6.3
lbni_a	A 31	Q A	0.03	25.0	6.3	lbni_a	A 31	Q G	1.04	25.0	6.3
lbni_a	A 31	Q S	0.00	25.0	6.3	lbni_a	A 32	A C	1.42	25.0	6.3
lbni_a	A 32	A D	0.56	25.0	6.3	lbni_a	A 32	A E	0.24	25.0	6.3
lbni_a	A 32	A F	0.56	25.0	6.3	lbni_a	A 32	A G	0.82	25.0	6.3
lbni_a	A 32	A H	0.75	25.0	6.3	lbni_a	A 32	A I	0.74	25.0	6.3
lbni_a	A 32	A K	0.15	25.0	6.3	lbni_a	A 32	A L	0.11	25.0	6.3
lbni_a	A 32	A M	0.19	25.0	6.3	lbni_a	A 32	A N	0.51	25.0	6.3
lbni_a	A 32	A Q	0.43	25.0	6.3	lbni_a	A 32	A R	0.15	25.0	6.3
lbni_a	A 32	A S	0.28	25.0	6.3	lbni_a	A 32	A T	0.64	25.0	6.3

lbni_a	A 32	A V	0.62	25.0	6.3	lbni_a	A 32	A W	1.07	25.0	6.3
lbni_a	A 32	A Y	0.75	25.0	6.3	lbni_a	A 33	L Q	1.34	25.0	6.3
lbni_a	A 34	G A	2.91	25.0	6.3	lbni_a	A 34	G D	3.30	25.0	6.3
lbni_a	A 34	G H	2.62	25.0	6.6	lbni_a	A 34	G K	2.91	25.0	6.3
lbni_a	A 34	G N	2.72	25.0	6.3	lbni_a	A 34	G R	2.61	25.0	6.3
lbni_a	A 34	G S	3.05	25.0	6.3	lbni_a	A 34	G T	3.28	25.0	6.3
lbni_a	A 36	V A	1.40	25.0	6.3	lbni_a	A 36	V T	1.11	25.0	6.3
lbni_a	A 41	N D	2.54	25.0	6.3	lbni_a	A 44	D E	0.11	25.0	6.3
lbni_a	A 45	V A	1.61	25.0	6.3	lbni_a	A 45	V T	2.34	25.0	6.3
lbni_a	A 51	I A	4.71	25.0	6.3	lbni_a	A 51	I V	1.66	25.0	5.9
lbni_a	A 53	G A	3.40	54.1	6.3	lbni_a	A 54	D A	3.04	25.0	6.3
lbni_a	A 54	D N	2.42	25.0	6.0	lbni_a	A 55	I A	1.29	25.0	6.3
lbni_a	A 55	I T	0.94	25.0	6.3	lbni_a	A 55	I V	0.37	25.0	6.3
lbni_a	A 57	S A	-0.15	25.0	6.3	lbni_a	A 58	N A	2.27	25.0	6.3
lbni_a	A 58	N D	-0.40	25.0	6.3	lbni_a	A 59	R A	-0.64	25.0	6.3
lbni_a	A 62	K R	0.35	25.0	6.3	lbni_a	A 65	G S	-0.74	25.0	6.3
lbni_a	A 66	K A	-0.59	25.0	6.3	lbni_a	A 69	R K	3.20	25.0	6.3
lbni_a	A 69	R M	2.04	25.0	5.5	lbni_a	A 69	R S	2.83	25.0	6.3
lbni_a	A 73	E A	2.40	25.0	6.3	lbni_a	A 73	E F	2.10	25.0	6.3
lbni_a	A 73	E Q	2.70	25.0	6.3	lbni_a	A 73	E W	2.20	25.0	6.3
lbni_a	A 76	I A	1.71	25.0	6.3	lbni_a	A 76	I T	2.64	25.0	6.3
lbni_a	A 76	I V	0.87	25.0	6.3	lbni_a	A 77	N A	1.63	25.0	6.3
lbni_a	A 78	Y F	1.35	25.0	6.3	lbni_a	A 79	T V	-0.24	25.0	6.3
lbni_a	A 83	R K	4.43	25.0	6.3	lbni_a	A 83	R Q	1.47	25.0	5.5
lbni_a	A 84	N A	1.94	25.0	6.3	lbni_a	A 85	S A	-0.08	25.0	6.3
lbni_a	A 88	I A	4.01	29.9	6.3	lbni_a	A 88	I L	0.16	25.0	6.3
lbni_a	A 88	I V	1.41	29.0	6.1	lbni_a	A 89	L T	2.82	25.0	6.3
lbni_a	A 89	L V	0.30	25.0	6.3	lbni_a	A 91	S A	1.84	25.0	5.7
lbni_a	A 92	S A	2.89	25.0	5.9	lbni_a	A 93	D N	4.03	25.0	6.3
lbni_a	A 94	W F	1.04	25.0	7.3	lbni_a	A 94	W L	1.12	25.0	7.8
lbni_a	A 94	W Y	1.24	25.0	7.3	lbni_a	A 96	I A	3.31	28.4	6.3
lbni_a	A 96	I V	0.97	28.1	5.9	lbni_a	A 99	T V	2.87	25.0	6.3
lbni_a	A 102	H A	0.24	25.0	6.3	lbni_a	A 103	Y F	0.06	25.0	6.3
lbni_a	A 104	Q A	0.13	25.0	6.3	lbni_a	A 105	T V	2.21	25.0	6.3
lbni_a	A 108	K R	-0.84	25.0	6.3	lbni_a	A 109	I A	1.74	25.0	6.3
lbni_a	A 109	I V	0.80	25.0	6.3	lbni_a	A 110	R A	0.10	25.0	6.3
lboy	A 200	R W	-0.60	23.0	7.5	lbtA	A 21	K A	1.04	25.0	8.0
lbtA	A 21	K Q	1.09	25.0	8.0	lbtA	A 22	K Q	0.79	25.0	8.0
lbtA	A 40	C A	-0.10	25.0	7.0	lbtA	A 57	E K	0.70	25.0	8.0
lbtA	A 60	K E	1.17	25.0	8.0	lbtA	A 60	K L	-0.55	25.0	8.0
lbtA	A 75	R L	-0.75	25.0	8.0	lbtA	A 75	R Q	0.37	25.0	8.0
lbtA	A 78	K A	0.05	25.0	8.0	lbtA	A 78	K Q	-0.38	25.0	8.0
lbtA	A 82	C A	0.10	25.0	7.2	lbvc	A 7	W F	0.90	4.0	7.8
lbvc	A 14	W F	1.10	4.0	7.8	lbvc	A 24	H V	0.52	0.0	7.0
lbvc	A 28	I A	0.86	36.8	6.6	lbvc	A 28	I L	0.60	76.5	11.0
lbvc	A 28	I M	0.60	76.5	11.0	lbvc	A 28	I V	0.00	76.5	11.0
lbvc	A 29	L A	0.63	36.8	6.6	lbvc	A 29	L I	1.10	76.5	11.0
lbvc	A 29	L M	-0.10	76.5	11.0	lbvc	A 29	L V	1.70	76.5	11.0
lbvc	A 30	I A	0.65	25.0	5.2	lbvc	A 32	L A	0.92	25.0	5.2
lbvc	A 36	H Q	0.83	3.7	7.8	lbvc	A 48	H Q	0.62	0.0	7.0
lbvc	A 49	L I	0.80	76.5	11.0	lbvc	A 64	H Q	0.45	0.0	7.0
lbvc	A 68	V T	0.60	4.0	7.8	lbvc	A 69	L A	1.20	76.5	11.0
lbvc	A 69	L I	0.00	76.5	11.0	lbvc	A 69	L M	0.00	76.5	11.0
lbvc	A 69	L V	0.10	76.5	11.0	lbvc	A 82	H Q	0.05	0.0	7.0
lbvc	A 93	H G	-0.04	0.0	7.0	lbvc	A 111	I A	1.80	76.5	11.0
lbvc	A 111	I L	0.60	76.5	11.0	lbvc	A 111	I M	1.10	76.5	11.0
lbvc	A 113	H Q	0.26	0.0	7.0	lbvc	A 119	H F	0.68	0.0	7.0
lbvc	A 123	F K	2.10	4.0	7.8	lbvc	A 123	F T	2.62	0.0	7.5
lbvc	A 130	A K	2.17	3.8	7.8	lbvc	A 130	A L	0.99	3.8	7.8
lbvc	A 131	M A	2.20	4.0	7.8	lbvc	A 135	L I	1.50	76.5	11.0
lbvc	A 135	L M	0.80	76.5	11.0	lbvc	A 135	L V	2.20	76.5	11.0
lbvc	A 142	I A	1.10	76.5	11.0	lbvc	A 142	I L	-0.60	76.5	11.0
lbvc	A 142	I M	-0.90	76.5	11.0	lbvc	A 142	I V	0.10	76.5	11.0
lc9o_a	A 2	Q L	-0.48	47.6	7.0	lc9o_a	A 3	R A	1.88	70.0	7.0

lc9o_a	A 3	R E	1.46	47.6	7.0	lc9o_a	A 3	R K	0.19	70.0	7.0
lc9o_a	A 3	R L	0.11	47.6	7.0	lc9o_a	A 11	N S	-0.11	47.6	7.0
lc9o_a	A 12	E K	0.32	75.0	7.0	lc9o_a	A 15	Y F	0.05	47.6	7.0
lc9o_a	A 21	E A	0.29	70.0	7.0	lc9o_a	A 21	E K	0.31	75.0	7.0
lc9o_a	A 23	G Q	0.13	47.6	7.0	lc9o_a	A 24	S D	-0.17	47.6	7.0
lc9o_a	A 29	H E	0.61	75.0	7.0	lc9o_a	A 31	T S	-0.10	47.6	7.0
lc9o_a	A 36	E K	0.45	75.0	7.0	lc9o_a	A 38	F W	-0.24	25.0	7.0
lc9o_a	A 46	E A	-0.01	47.6	7.0	lc9o_a	A 46	E K	0.57	75.0	7.0
lc9o_a	A 50	E K	0.58	75.0	7.0	lc9o_a	A 50	E W	-0.07	25.0	7.0
lc9o_a	A 53	Q E	0.03	47.6	7.0	lc9o_a	A 55	N K	0.03	75.0	7.0
lc9o_a	A 56	R E	-0.69	75.0	7.0	lc9o_a	A 64	V T	0.30	47.6	7.0
lc9o_a	A 66	L E	0.97	47.6	7.0	lcah	A 5	W F	1.80	23.0	7.5
lcah	A 206	C S	-2.35	23.0	7.5	lcey	A 12	D A	-2.50	25.0	7.0
lcey	A 13	D A	-2.70	25.0	7.0	lcey	A 14	F N	-2.64	25.0	7.5
lcey	A 48	A G	-0.06	25.0	8.0	lcey	A 57	D A	-3.30	25.0	7.0
lcey	A 74	A G	0.31	25.0	8.0	lcey	A 77	A G	0.31	25.0	8.0
lcey	A 80	A G	-0.43	25.0	8.0	lcey	A 88	A G	-0.04	25.0	8.0
lcey	A 90	A G	-0.35	25.0	8.0	lcey	A 99	A G	0.48	25.0	8.0
lcey	A 101	A G	0.95	25.0	8.0	lcey	A 113	A G	0.75	25.0	8.0
lcey	A 114	A G	0.50	25.0	8.0	lchk_a	A 28	W F	4.43	43.2	7.0
lchk_a	A 101	W F	4.27	43.2	7.0	lchk_a	A 227	W F	2.51	43.2	7.0
lcse_i	I 14	V A	1.04	25.0	7.0	lcse_i	I 18	V A	1.20	25.0	7.0
lcse_i	I 27	L A	0.16	25.0	7.0	lcse_i	I 54	V A	1.58	25.0	7.0
lcse_i	I 62	V A	1.01	25.0	7.0	lcs p	A 1	M R	-1.75	70.0	7.0
lcs p	A 3	E K	-2.75	70.0	7.0	lcs p	A 3	E L	-1.59	70.0	7.0
lcs p	A 3	E Q	-1.14	55.0	7.5	lcs p	A 3	E R	-1.77	52.8	7.3
lcs p	A 10	N D	-0.38	55.0	7.5	lcs p	A 15	F A	2.07	43.3	7.0
lcs p	A 17	F A	1.47	43.3	7.0	lcs p	A 25	D Q	0.79	55.0	7.5
lcs p	A 27	F A	0.84	43.3	7.0	lcs p	A 38	F A	-0.22	42.5	7.0
lcs p	A 43	E S	-0.29	70.0	7.0	lcs p	A 46	A E	0.59	70.0	7.0
lcs p	A 46	A K	-1.41	70.0	7.0	lcs p	A 48	S E	-0.04	55.0	7.5
lcs p	A 48	S R	-1.58	70.0	7.0	lcs p	A 50	E Q	1.16	55.0	7.5
lcs p	A 56	R Q	-0.28	55.0	7.5	lcs p	A 65	K I	-1.53	70.0	7.0
lcs p	A 66	E K	-2.18	70.0	7.0	lcs p	A 66	E L	-1.60	47.6	7.0
lcun_17	A 115	Q A	0.15	25.0	7.0	lcun_17	A 115	Q G	1.15	25.0	7.0
lcun_17	A 117	F L	2.55	25.0	7.0	lcun_17	A 119	A G	1.75	25.0	7.0
lcun_17	A 126	A G	1.65	25.0	7.0	lcun_17	A 128	I A	1.65	25.0	7.0
lcun_17	A 128	I V	2.85	25.0	7.0	lcun_17	A 152	K A	0.15	25.0	7.0
lcun_17	A 152	K G	1.45	25.0	7.0	lcun_17	A 156	A G	1.45	25.0	7.0
lcun_17	A 157	F L	1.85	25.0	7.0	lcun_17	A 163	V A	-0.15	25.0	7.0
lcun_17	A 163	V G	0.85	25.0	7.0	lcun_17	A 164	H A	2.35	25.0	7.0
lcun_17	A 171	V A	1.55	25.0	7.0	lcun_17	A 173	A G	1.95	25.0	7.0
lcun_17	A 191	A G	1.35	25.0	7.0	lcun_17	A 193	M A	2.65	25.0	7.0
lcun_17	A 196	L A	4.55	25.0	7.0	lcun_17	A 198	G A	-0.45	25.0	7.0
lcun_17	A 201	S A	-0.15	25.0	7.0	lcun_17	A 201	S G	0.95	25.0	7.0
lcun_17	A 203	L A	4.05	25.0	7.0	lcun_17	A 206	A G	2.25	25.0	7.0
lcun_17	A 212	A G	1.45	25.0	7.0	lcun_17	A 214	L A	3.65	25.0	7.0
ldkt_a	A 6	I V	0.57	10.0	7.5	ldkt_a	A 8	Y A	0.68	10.0	7.5
ldkt_a	A 9	S A	0.43	10.0	7.5	ldkt_a	A 11	K A	-0.62	10.0	7.5
ldkt_a	A 17	F L	2.58	10.0	7.5	ldkt_a	A 18	E A	0.81	10.0	7.5
ldkt_a	A 22	V A	1.36	10.0	7.5	ldkt_a	A 32	V A	1.07	10.0	7.5
ldkt_a	A 39	S A	0.60	10.0	7.5	ldkt_a	A 46	L A	2.04	10.0	7.5
ldkt_a	A 55	V A	0.73	10.0	7.5	ldkt_a	A 55	V G	2.04	10.0	7.5
ldkt_a	A 58	M L	0.23	10.0	7.5	ldkt_a	A 65	H A	0.51	10.0	7.5
ldkt_a	A 67	L A	1.98	10.0	7.5	ldkt_a	A 70	R A	2.80	10.0	7.5
ldkt_a	A 71	R A	0.59	10.0	7.5	le65_a	A 5	V A	0.00	25.0	7.0
le65_a	A 7	I A	3.11	25.0	7.0	le65_a	A 7	I S	3.44	26.5	7.3
le65_a	A 20	I A	1.56	25.0	7.0	le65_a	A 20	I T	2.39	25.0	7.0
le65_a	A 20	I V	0.38	25.0	7.0	le65_a	A 22	V A	1.44	25.0	7.0
le65_a	A 22	V T	0.96	25.0	7.0	le65_a	A 31	V T	1.08	25.0	7.0
le65_a	A 46	H G	2.50	20.0	7.0	le65_a	A 50	L T	2.34	25.0	7.0
le65_a	A 50	L V	0.36	25.0	7.0	le65_a	A 60	V G	3.11	25.0	7.0
le65_a	A 81	I A	2.39	25.0	7.0	le65_a	A 81	I T	2.51	25.0	7.0
le65_a	A 81	I V	0.07	25.0	7.0	le65_a	A 82	A G	3.11	25.0	7.0

1e65_a	A 95	V T	-0.96	25.0	7.0	1e65_a	A 110	F S	3.95	26.5	7.3
1e65_a	A 117	H G	2.18	20.0	7.0	1e65_a	A 125	L A	0.72	25.0	7.0
1ey0	A 6	K A	-0.19	20.0	7.0	1ey0	A 6	K G	-0.25	20.0	7.0
1ey0	A 7	L A	1.35	20.0	7.0	1ey0	A 7	L G	1.26	20.0	7.0
1ey0	A 7	L I	0.77	20.0	7.0	1ey0	A 7	L V	1.15	20.0	7.0
1ey0	A 8	H A	0.48	20.0	7.0	1ey0	A 8	H G	0.85	20.0	7.0
1ey0	A 9	K A	1.38	20.0	7.0	1ey0	A 9	K F	1.03	20.0	7.0
1ey0	A 9	K G	1.88	20.0	7.0	1ey0	A 10	E A	1.34	20.0	7.0
1ey0	A 10	E G	1.86	20.0	7.0	1ey0	A 10	E K	1.98	20.0	7.0
1ey0	A 10	E Q	0.97	20.0	7.0	1ey0	A 12	A G	2.37	20.0	7.0
1ey0	A 12	A V	0.89	20.0	7.0	1ey0	A 13	T A	0.73	20.0	7.0
1ey0	A 13	T C	1.20	20.0	7.0	1ey0	A 13	T G	1.16	20.0	7.0
1ey0	A 13	T I	0.05	20.0	7.0	1ey0	A 13	T S	0.35	20.0	7.0
1ey0	A 13	T V	0.26	20.0	7.0	1ey0	A 14	L A	2.38	20.0	7.0
1ey0	A 14	L G	3.84	20.0	7.0	1ey0	A 14	L I	1.60	20.0	7.0
1ey0	A 14	L V	1.63	20.0	7.0	1ey0	A 15	I A	2.73	20.0	7.0
1ey0	A 15	I G	3.43	20.0	7.0	1ey0	A 15	I L	0.62	20.0	7.0
1ey0	A 15	I M	0.15	20.0	7.0	1ey0	A 15	I V	0.88	20.0	7.0
1ey0	A 16	K A	0.06	20.0	7.0	1ey0	A 16	K F	0.38	20.0	7.0
1ey0	A 16	K G	0.76	20.0	7.0	1ey0	A 17	A G	-0.19	20.0	7.0
1ey0	A 17	A V	1.94	20.0	7.0	1ey0	A 18	I A	2.65	20.0	7.0
1ey0	A 18	I G	2.63	20.0	7.0	1ey0	A 18	I L	0.14	20.0	7.0
1ey0	A 18	I M	0.68	23.6	6.7	1ey0	A 18	I V	0.96	20.0	7.0
1ey0	A 19	D A	0.09	20.0	7.0	1ey0	A 19	D F	1.28	20.0	7.0
1ey0	A 19	D G	0.42	20.0	7.0	1ey0	A 19	D K	0.41	20.0	7.0
1ey0	A 19	D N	-0.07	20.0	7.0	1ey0	A 20	G A	0.12	20.0	7.0
1ey0	A 20	G V	2.18	20.0	7.0	1ey0	A 21	D A	-0.83	20.0	7.0
1ey0	A 21	D G	-0.46	20.0	7.0	1ey0	A 21	D K	-1.10	20.0	7.0
1ey0	A 21	D N	-1.43	20.0	7.0	1ey0	A 22	T A	1.69	20.0	7.0
1ey0	A 22	T C	0.95	20.0	7.0	1ey0	A 22	T G	2.54	20.0	7.0
1ey0	A 22	T I	0.61	20.0	7.0	1ey0	A 22	T S	0.74	20.0	7.0
1ey0	A 22	T V	0.85	20.0	7.0	1ey0	A 23	V A	2.70	22.5	6.2
1ey0	A 23	V F	1.93	29.2	6.2	1ey0	A 23	V I	-0.03	20.0	7.0
1ey0	A 23	V L	0.02	20.0	7.0	1ey0	A 23	V S	4.76	20.0	7.0
1ey0	A 23	V T	3.34	20.0	7.0	1ey0	A 24	K A	0.34	20.0	7.0
1ey0	A 24	K F	0.40	20.0	7.0	1ey0	A 24	K G	1.60	20.0	7.0
1ey0	A 25	L A	2.77	40.2	6.4	1ey0	A 25	L G	4.58	20.0	7.0
1ey0	A 25	L I	1.83	20.0	7.0	1ey0	A 25	L V	1.85	20.0	7.0
1ey0	A 26	M A	1.61	20.0	7.0	1ey0	A 26	M G	1.95	22.5	6.2
1ey0	A 26	M I	0.84	20.0	7.0	1ey0	A 26	M L	0.31	20.0	7.0
1ey0	A 27	Y A	3.63	20.0	7.0	1ey0	A 27	Y C	2.72	20.0	7.0
1ey0	A 27	Y F	0.40	20.0	7.0	1ey0	A 27	Y H	1.86	20.0	7.0
1ey0	A 27	Y I	2.28	20.0	7.0	1ey0	A 27	Y K	3.78	20.0	7.0
1ey0	A 27	Y L	1.55	20.0	7.0	1ey0	A 27	Y M	1.94	20.0	7.0
1ey0	A 27	Y N	3.83	20.0	7.0	1ey0	A 27	Y Q	3.31	20.0	7.0
1ey0	A 27	Y R	3.05	20.0	7.0	1ey0	A 27	Y S	3.21	20.0	7.0
1ey0	A 27	Y T	3.18	20.0	7.0	1ey0	A 27	Y V	2.65	20.0	7.0
1ey0	A 27	Y W	0.72	20.0	7.0	1ey0	A 28	K A	0.70	20.0	7.0
1ey0	A 28	K E	0.79	20.0	7.0	1ey0	A 28	K F	0.85	20.0	7.0
1ey0	A 28	K G	0.80	20.0	7.0	1ey0	A 28	K Q	0.28	20.0	7.0
1ey0	A 29	G A	1.41	20.0	7.0	1ey0	A 29	G C	1.26	20.0	7.0
1ey0	A 29	G F	1.46	20.0	7.0	1ey0	A 29	G V	3.11	20.0	7.0
1ey0	A 30	Q A	0.25	20.0	7.0	1ey0	A 30	Q G	0.93	20.0	7.0
1ey0	A 32	M A	1.81	20.0	7.0	1ey0	A 32	M G	2.54	20.0	7.0
1ey0	A 32	M I	0.56	20.0	7.0	1ey0	A 32	M L	0.76	20.0	7.0
1ey0	A 33	T A	1.52	20.0	7.0	1ey0	A 33	T C	1.04	20.0	7.0
1ey0	A 33	T G	2.62	20.0	7.0	1ey0	A 33	T I	-0.73	20.0	7.0
1ey0	A 33	T S	1.35	20.0	7.0	1ey0	A 33	T V	-0.47	20.0	7.0
1ey0	A 34	F A	3.80	20.0	7.0	1ey0	A 35	R A	1.38	20.0	7.0
1ey0	A 35	R G	2.26	20.0	7.0	1ey0	A 36	L A	3.66	20.0	7.0
1ey0	A 36	L I	3.09	20.0	7.0	1ey0	A 36	L V	3.58	20.0	7.0
1ey0	A 37	L A	1.51	20.0	7.0	1ey0	A 37	L G	3.79	20.0	7.0
1ey0	A 37	L I	1.82	20.0	7.0	1ey0	A 37	L V	2.78	20.0	7.0
1ey0	A 38	L A	1.51	20.0	7.0	1ey0	A 38	L G	0.28	20.0	7.0

ley0	A 38	L I	2.06	20.0	7.0	ley0	A 38	L V	0.14	20.0	7.0
ley0	A 39	V A	2.16	20.0	7.0	ley0	A 39	V G	4.61	20.0	7.0
ley0	A 39	V I	-0.11	20.0	7.0	ley0	A 39	V L	0.90	20.0	7.0
ley0	A 39	V S	2.44	20.0	7.0	ley0	A 39	V T	1.55	20.0	7.0
ley0	A 40	D A	-0.41	20.0	7.0	ley0	A 40	D G	0.38	20.0	7.0
ley0	A 41	T A	-0.07	20.0	7.0	ley0	A 41	T C	-0.74	20.0	7.0
ley0	A 41	T G	1.79	20.0	7.0	ley0	A 41	T I	-0.86	20.0	7.0
ley0	A 41	T S	0.88	20.0	7.0	ley0	A 41	T V	-0.90	20.0	7.0
ley0	A 43	E A	-0.32	20.0	7.0	ley0	A 43	E D	-0.20	20.0	7.0
ley0	A 43	E G	-0.59	20.0	7.0	ley0	A 44	T A	0.23	20.0	7.0
ley0	A 44	T C	0.04	20.0	7.0	ley0	A 44	T G	0.37	20.0	7.0
ley0	A 44	T I	0.56	20.0	7.0	ley0	A 44	T S	-0.04	20.0	7.0
ley0	A 44	T V	-0.09	20.0	7.0	ley0	A 45	K A	-0.19	20.0	7.0
ley0	A 45	K G	-0.20	20.0	7.0	ley0	A 46	H A	0.45	20.0	7.0
ley0	A 46	H G	0.17	20.0	7.0	ley0	A 46	H Y	0.00	40.0	5.4
ley0	A 48	K A	-0.09	20.0	7.0	ley0	A 48	K E	-0.10	20.0	7.0
ley0	A 48	K F	0.25	20.0	7.0	ley0	A 48	K G	-0.24	20.0	7.0
ley0	A 48	K Q	0.02	20.0	7.0	ley0	A 49	K A	0.25	20.0	7.0
ley0	A 49	K F	-0.20	20.0	7.0	ley0	A 49	K G	0.10	20.0	7.0
ley0	A 50	G A	-0.16	20.0	7.0	ley0	A 50	G C	0.75	20.0	7.0
ley0	A 50	G F	0.55	20.0	7.0	ley0	A 50	G V	1.00	20.0	7.0
ley0	A 51	V A	0.05	20.0	7.0	ley0	A 51	V G	0.17	20.0	7.0
ley0	A 51	V I	-0.09	20.0	7.0	ley0	A 51	V L	0.10	20.0	7.0
ley0	A 51	V S	-0.01	20.0	7.0	ley0	A 51	V T	-0.20	20.0	7.0
ley0	A 52	E A	0.05	20.0	7.0	ley0	A 52	E F	0.51	20.0	7.0
ley0	A 52	E G	0.27	20.0	7.0	ley0	A 53	K A	0.17	20.0	7.0
ley0	A 53	K G	0.08	20.0	7.0	ley0	A 54	Y A	1.97	20.0	7.0
ley0	A 54	Y F	0.38	20.0	7.0	ley0	A 54	Y G	1.72	20.0	7.0
ley0	A 54	Y L	3.31	20.0	7.0	ley0	A 55	G A	0.44	20.0	7.0
ley0	A 55	G V	1.48	20.0	7.0	ley0	A 57	E A	0.10	20.0	7.0
ley0	A 57	E C	0.64	20.0	7.0	ley0	A 57	E F	0.79	20.0	7.0
ley0	A 57	E G	1.41	20.0	7.0	ley0	A 57	E K	-0.01	20.0	7.0
ley0	A 57	E Q	0.14	20.0	7.0	ley0	A 58	A G	2.53	20.0	7.0
ley0	A 58	A V	2.63	20.0	7.0	ley0	A 59	S A	-0.62	20.0	7.0
ley0	A 59	S F	-0.56	20.0	7.0	ley0	A 59	S G	1.03	20.0	7.0
ley0	A 60	A C	1.12	20.0	7.0	ley0	A 60	A F	0.80	20.0	7.0
ley0	A 60	A G	1.45	20.0	7.0	ley0	A 60	A V	2.68	20.0	7.0
ley0	A 61	F A	2.34	20.0	7.0	ley0	A 61	F G	4.76	20.0	7.0
ley0	A 62	T A	2.23	20.0	7.0	ley0	A 62	T C	1.05	20.0	7.0
ley0	A 62	T G	3.52	20.0	7.0	ley0	A 62	T I	1.17	20.0	7.0
ley0	A 62	T S	2.15	20.0	7.0	ley0	A 62	T V	-0.10	20.0	7.0
ley0	A 63	K A	0.32	20.0	7.0	ley0	A 63	K E	1.47	20.0	7.0
ley0	A 63	K F	1.83	20.0	7.0	ley0	A 63	K G	1.57	20.0	7.0
ley0	A 63	K Q	0.89	20.0	7.0	ley0	A 64	K A	-0.16	20.0	7.0
ley0	A 64	K E	1.68	20.0	7.0	ley0	A 64	K F	0.09	20.0	7.0
ley0	A 64	K G	0.51	20.0	7.0	ley0	A 64	K Q	0.00	20.0	7.0
ley0	A 65	M A	2.06	20.0	7.0	ley0	A 65	M F	1.62	20.0	7.0
ley0	A 65	M G	4.66	20.0	7.0	ley0	A 65	M I	1.43	20.0	7.0
ley0	A 65	M L	0.73	20.0	7.0	ley0	A 66	V A	2.34	20.0	7.0
ley0	A 66	V G	4.49	20.0	7.0	ley0	A 66	V I	0.76	20.0	7.0
ley0	A 66	V K	4.83	20.0	9.2	ley0	A 66	V L	-0.37	28.9	6.8
ley0	A 66	V M	0.14	20.0	8.2	ley0	A 66	V S	3.09	20.0	7.0
ley0	A 66	V T	1.34	20.0	7.0	ley0	A 66	V W	2.69	20.0	7.0
ley0	A 67	E A	1.05	20.0	7.0	ley0	A 67	E F	1.33	20.0	7.0
ley0	A 67	E G	1.00	20.0	7.0	ley0	A 67	E Q	0.57	20.0	7.0
ley0	A 68	N A	0.38	20.0	7.0	ley0	A 68	N G	0.35	20.0	7.0
ley0	A 69	A G	2.10	20.0	7.0	ley0	A 69	A T	3.03	20.0	7.0
ley0	A 69	A V	2.80	20.0	7.0	ley0	A 70	K A	0.16	20.0	7.0
ley0	A 70	K C	0.48	20.0	7.0	ley0	A 70	K E	0.30	20.0	7.0
ley0	A 70	K F	0.03	20.0	7.0	ley0	A 70	K G	0.60	20.0	7.0
ley0	A 70	K Q	0.25	20.0	7.0	ley0	A 70	K W	0.40	20.0	7.0
ley0	A 71	K A	0.55	20.0	7.0	ley0	A 71	K F	-0.04	20.0	7.0
ley0	A 71	K G	1.31	20.0	7.0	ley0	A 72	I L	0.23	20.0	7.0
ley0	A 72	I M	1.88	20.0	7.0	ley0	A 72	I V	1.79	20.0	7.0

ley0	A 73	E A	1.46	20.0	7.0	ley0	A 73	E F	0.88	20.0	7.0
ley0	A 73	E G	2.76	20.0	7.0	ley0	A 73	E K	2.06	20.0	7.0
ley0	A 73	E Q	0.64	20.0	7.0	ley0	A 74	V A	3.23	20.0	7.0
ley0	A 74	V I	1.91	20.0	7.0	ley0	A 74	V L	1.12	20.0	7.0
ley0	A 74	V T	3.88	20.0	7.0	ley0	A 75	E A	1.69	22.5	6.2
ley0	A 75	E G	3.43	20.0	7.0	ley0	A 75	E K	2.22	20.0	7.0
ley0	A 75	E Q	0.61	20.0	7.0	ley0	A 75	E V	2.31	20.0	7.0
ley0	A 76	F A	4.10	20.0	7.0	ley0	A 76	F G	4.73	20.0	7.0
ley0	A 77	D A	2.39	21.6	6.5	ley0	A 77	D G	1.81	20.0	7.0
ley0	A 77	D K	3.28	20.0	7.0	ley0	A 77	D N	2.69	20.0	7.0
ley0	A 78	K A	0.50	20.0	7.0	ley0	A 78	K C	0.26	20.0	7.0
ley0	A 78	K E	0.69	20.0	7.0	ley0	A 78	K F	-0.05	20.0	7.0
ley0	A 78	K G	1.07	20.0	7.0	ley0	A 78	K Q	0.15	20.0	7.0
ley0	A 79	G A	2.17	20.0	7.0	ley0	A 79	G D	2.28	20.0	7.0
ley0	A 79	G S	2.14	31.5	6.5	ley0	A 79	G V	2.23	20.0	7.0
ley0	A 80	Q A	0.02	20.0	7.0	ley0	A 80	Q F	0.58	20.0	7.0
ley0	A 80	Q G	1.25	20.0	7.0	ley0	A 81	R A	1.10	20.0	7.0
ley0	A 81	R G	2.06	20.0	7.0	ley0	A 82	T A	0.89	20.0	7.0
ley0	A 82	T C	0.19	20.0	7.0	ley0	A 82	T G	2.03	20.0	7.0
ley0	A 82	T I	-0.51	20.0	7.0	ley0	A 82	T S	0.75	20.0	7.0
ley0	A 82	T V	-0.24	20.0	7.0	ley0	A 83	D A	3.76	20.0	7.0
ley0	A 83	D G	2.64	20.0	7.0	ley0	A 84	K A	-0.10	20.0	7.0
ley0	A 84	K E	0.00	20.0	7.0	ley0	A 84	K F	0.75	20.0	7.0
ley0	A 84	K G	0.39	20.0	7.0	ley0	A 84	K Q	0.15	20.0	7.0
ley0	A 85	Y A	0.41	20.0	7.0	ley0	A 85	Y F	0.07	20.0	7.0
ley0	A 85	Y G	1.05	20.0	7.0	ley0	A 85	Y L	0.15	20.0	7.0
ley0	A 86	G A	0.31	20.0	7.0	ley0	A 86	G F	1.99	20.0	7.0
ley0	A 86	G V	3.74	20.0	7.0	ley0	A 87	R A	0.79	20.0	7.0
ley0	A 87	R G	2.53	20.0	7.0	ley0	A 88	G A	-0.19	20.0	7.0
ley0	A 88	G V	0.24	28.9	6.8	ley0	A 88	G W	0.10	20.0	7.0
ley0	A 89	L A	2.60	20.0	7.0	ley0	A 89	L F	1.20	40.0	5.4
ley0	A 89	L G	3.18	20.0	7.0	ley0	A 89	L I	1.04	20.0	7.0
ley0	A 89	L V	1.42	20.0	7.0	ley0	A 90	A G	1.92	20.0	7.0
ley0	A 90	A S	2.24	30.3	6.7	ley0	A 90	A V	-0.04	20.0	7.0
ley0	A 91	Y F	2.27	20.0	7.0	ley0	A 91	Y L	3.83	20.0	7.0
ley0	A 92	I A	4.12	20.0	7.0	ley0	A 92	I L	0.60	20.0	7.0
ley0	A 92	I M	1.75	20.0	7.0	ley0	A 92	I V	0.46	20.0	7.0
ley0	A 93	Y F	1.81	20.0	7.0	ley0	A 93	Y L	4.53	20.0	7.0
ley0	A 94	A G	2.54	20.0	7.0	ley0	A 94	A V	1.13	20.0	7.0
ley0	A 95	D A	3.50	20.0	7.0	ley0	A 95	D G	2.93	20.0	7.0
ley0	A 96	G A	1.80	20.0	7.0	ley0	A 96	G F	2.55	20.0	7.0
ley0	A 96	G V	3.74	20.0	7.0	ley0	A 97	K A	0.22	20.0	7.0
ley0	A 97	K E	0.47	20.0	7.0	ley0	A 97	K F	0.58	20.0	7.0
ley0	A 97	K G	1.85	20.0	7.0	ley0	A 97	K Q	0.30	20.0	7.0
ley0	A 98	M A	4.43	20.0	7.0	ley0	A 98	M G	4.44	20.0	7.0
ley0	A 98	M I	4.39	20.0	7.0	ley0	A 98	M L	2.30	20.0	7.0
ley0	A 99	V A	3.35	20.0	7.0	ley0	A 99	V I	0.14	20.0	7.0
ley0	A 99	V L	0.15	20.0	7.0	ley0	A 99	V T	3.36	20.0	7.0
ley0	A 100	N G	4.98	20.0	7.0	ley0	A 101	E A	1.36	20.0	7.0
ley0	A 101	E F	2.74	20.0	7.0	ley0	A 101	E G	2.47	20.0	7.0
ley0	A 102	A F	1.71	20.0	7.0	ley0	A 102	A G	1.37	20.0	7.0
ley0	A 102	A V	1.84	20.0	7.0	ley0	A 103	L A	4.60	20.0	7.0
ley0	A 103	L I	1.11	20.0	7.0	ley0	A 103	L V	2.05	20.0	7.0
ley0	A 104	V A	2.82	20.0	7.0	ley0	A 104	V I	-0.27	20.0	7.0
ley0	A 104	V L	0.76	20.0	7.0	ley0	A 104	V S	4.86	20.0	7.0
ley0	A 104	V T	2.45	20.0	7.0	ley0	A 105	R A	1.32	20.0	7.0
ley0	A 105	R C	2.55	20.0	7.0	ley0	A 105	R F	2.84	20.0	7.0
ley0	A 105	R G	2.40	20.0	7.0	ley0	A 106	Q A	-0.25	20.0	7.0
ley0	A 106	Q G	1.50	20.0	7.0	ley0	A 107	G A	4.41	20.0	7.0
ley0	A 108	L I	3.34	20.0	7.0	ley0	A 108	L V	3.81	20.0	7.0
ley0	A 109	A G	0.98	20.0	7.0	ley0	A 109	A V	2.82	20.0	7.0
ley0	A 110	K A	1.13	20.0	7.0	ley0	A 110	K G	2.59	20.0	7.0
ley0	A 111	V A	4.26	20.0	7.0	ley0	A 111	V G	4.82	20.0	7.0
ley0	A 111	V I	0.74	20.0	7.0	ley0	A 111	V L	0.88	20.0	7.0

ley0	A 111	V S	4.71	20.0	7.0	ley0	A 111	V T	2.36	20.0	7.0
ley0	A 112	A C	0.75	20.0	7.0	ley0	A 112	A F	1.35	20.0	7.0
ley0	A 112	A G	-0.20	20.0	7.0	ley0	A 112	A V	1.19	20.0	7.0
ley0	A 113	Y A	-0.06	20.0	7.0	ley0	A 113	Y F	-0.07	20.0	7.0
ley0	A 113	Y G	0.20	20.0	7.0	ley0	A 113	Y L	-0.20	20.0	7.0
ley0	A 114	V A	-0.14	20.0	7.0	ley0	A 114	V G	0.03	20.0	7.0
ley0	A 114	V I	0.15	20.0	7.0	ley0	A 114	V L	1.07	20.0	7.0
ley0	A 114	V S	0.04	20.0	7.0	ley0	A 114	V T	0.31	20.0	7.0
ley0	A 115	Y A	0.25	20.0	7.0	ley0	A 115	Y F	0.02	20.0	7.0
ley0	A 115	Y G	0.56	20.0	7.0	ley0	A 115	Y L	0.22	20.0	7.0
ley0	A 116	K A	-0.69	20.0	7.0	ley0	A 116	K F	-0.21	20.0	7.0
ley0	A 116	K G	-1.05	20.0	7.0	ley0	A 118	N A	1.88	20.0	7.0
ley0	A 118	N D	2.34	20.0	7.0	ley0	A 118	N G	1.61	20.0	7.0
ley0	A 119	N A	1.03	20.0	7.0	ley0	A 119	N G	0.97	20.0	7.0
ley0	A 120	T A	1.08	20.0	7.0	ley0	A 120	T C	1.59	20.0	7.0
ley0	A 120	T G	1.87	20.0	7.0	ley0	A 120	T I	1.54	20.0	7.0
ley0	A 120	T S	0.57	20.0	7.0	ley0	A 120	T V	1.63	20.0	7.0
ley0	A 121	H A	2.92	20.0	7.0	ley0	A 121	H G	4.09	20.0	7.0
ley0	A 122	E A	0.27	20.0	7.0	ley0	A 122	E F	0.44	20.0	7.0
ley0	A 122	E G	1.99	20.0	7.0	ley0	A 122	E K	2.53	20.0	7.0
ley0	A 122	E Q	1.52	20.0	7.0	ley0	A 123	Q A	0.10	20.0	7.0
ley0	A 123	Q F	0.51	20.0	7.0	ley0	A 123	Q G	0.44	20.0	7.0
ley0	A 124	H A	-0.57	20.0	7.0	ley0	A 124	H E	-0.46	20.0	7.0
ley0	A 124	H F	-0.51	20.0	7.0	ley0	A 124	H G	0.52	20.0	7.0
ley0	A 124	H L	-1.31	46.9	5.9	ley0	A 124	H Q	-0.69	20.0	7.0
ley0	A 125	L A	4.78	20.0	7.0	ley0	A 125	L I	0.96	20.0	7.0
ley0	A 125	L V	2.30	20.0	7.0	ley0	A 126	R A	1.64	20.0	7.0
ley0	A 126	R G	2.86	20.0	7.0	ley0	A 127	K A	-0.24	20.0	7.0
ley0	A 127	K E	-0.13	20.0	7.0	ley0	A 127	K F	0.22	20.0	7.0
ley0	A 127	K G	0.79	20.0	7.0	ley0	A 127	K Q	-0.06	20.0	7.0
ley0	A 128	S A	-0.83	20.0	7.0	ley0	A 128	S F	1.00	20.0	7.0
ley0	A 128	S G	1.52	20.0	7.0	ley0	A 129	E A	2.20	20.0	7.0
ley0	A 129	E F	3.88	20.0	7.0	ley0	A 129	E G	3.72	20.0	7.0
ley0	A 130	A G	1.00	20.0	7.0	ley0	A 130	A V	1.08	20.0	7.0
ley0	A 131	Q A	0.10	20.0	7.0	ley0	A 131	Q F	0.55	20.0	7.0
ley0	A 131	Q G	2.26	20.0	7.0	ley0	A 132	A G	3.60	20.0	7.0
ley0	A 132	A V	4.73	20.0	7.0	ley0	A 133	K A	1.32	20.0	7.0
ley0	A 133	K F	1.26	20.0	7.0	ley0	A 133	K G	3.22	20.0	7.0
ley0	A 133	K Q	0.44	20.0	7.0	ley0	A 134	K A	-0.12	20.0	7.0
ley0	A 134	K C	0.70	20.0	7.0	ley0	A 134	K F	0.26	20.0	7.0
ley0	A 134	K G	0.79	20.0	7.0	ley0	A 135	E A	0.73	20.0	7.0
ley0	A 135	E F	1.10	20.0	7.0	ley0	A 135	E G	1.64	20.0	7.0
ley0	A 135	E K	1.17	20.0	7.0	ley0	A 135	E Q	0.71	20.0	7.0
ley0	A 136	K A	0.75	20.0	7.0	ley0	A 136	K F	0.97	20.0	7.0
ley0	A 136	K G	0.02	20.0	7.0	ley0	A 137	L A	2.18	20.0	7.0
ley0	A 137	L G	4.43	20.0	7.0	ley0	A 137	L I	0.76	20.0	7.0
ley0	A 137	L V	1.42	20.0	7.0	ley0	A 138	N A	0.97	20.0	7.0
ley0	A 138	N G	-0.59	20.0	7.0	ley0	A 139	I A	3.29	20.0	7.0
ley0	A 139	I G	4.22	20.0	7.0	ley0	A 139	I L	0.09	20.0	7.0
ley0	A 139	I M	0.39	20.0	7.0	ley0	A 139	I V	1.37	20.0	7.0
ley0	A 141	S A	0.27	31.4	7.0	ley0	A 141	S G	0.82	20.0	7.0
lfkj	A 2	V A	2.18	25.0	7.5	lfkj	A 4	V A	2.26	25.0	7.5
lfkj	A 7	I V	0.90	25.0	7.5	lfkj	A 21	T A	1.24	25.0	7.5
lfkj	A 21	T S	1.06	25.0	7.5	lfkj	A 21	T V	-0.56	25.0	7.5
lfkj	A 23	V A	2.62	25.0	7.5	lfkj	A 24	V A	3.04	25.0	7.5
lfkj	A 27	T A	1.71	25.0	7.5	lfkj	A 27	T S	1.07	25.0	7.5
lfkj	A 27	T V	-0.58	25.0	7.5	lfkj	A 36	F A	3.07	25.0	7.5
lfkj	A 50	L A	2.22	25.0	7.5	lfkj	A 55	V A	1.78	25.0	7.5
lfkj	A 56	I A	2.04	25.0	7.5	lfkj	A 56	I D	2.88	25.0	7.5
lfkj	A 56	I T	1.95	25.0	7.5	lfkj	A 57	R A	0.55	25.0	7.5
lfkj	A 57	R G	1.89	25.0	7.5	lfkj	A 59	W F	-2.72	25.0	7.5
lfkj	A 59	W L	-2.35	25.0	7.5	lfkj	A 60	E A	1.71	25.0	7.5
lfkj	A 60	E G	2.62	25.0	7.5	lfkj	A 61	E A	0.73	25.0	7.5
lfkj	A 61	E G	2.20	25.0	7.5	lfkj	A 63	V A	2.56	25.0	7.5

1fkj	A 75	T A	2.27	25.0	7.5	1fkj	A 75	T V	0.70	25.0	7.5
1fkj	A 76	I A	3.36	25.0	7.5	1fkj	A 76	I V	0.33	25.0	7.5
1fkj	A 91	I A	1.33	25.0	7.5	1fkj	A 91	I V	0.10	25.0	7.5
1fkj	A 97	L A	3.01	25.0	7.5	1fkj	A 98	V A	1.99	25.0	7.5
1fkj	A 101	V A	2.39	25.0	7.5	1fkj	A 106	L A	2.08	25.0	7.5
1fna	A 8	L A	1.81	25.0	5.0	1fna	A 10	V A	1.17	25.0	5.0
1fna	A 13	A G	1.18	25.0	5.0	1fna	A 18	L A	0.99	25.0	5.0
1fna	A 20	I A	0.65	25.0	5.0	1fna	A 20	I V	0.18	25.0	5.0
1fna	A 22	W F	1.97	25.0	5.0	1fna	A 29	V A	1.37	25.0	5.0
1fna	A 32	Y A	4.23	25.0	5.0	1fna	A 32	Y F	0.54	25.0	5.0
1fna	A 32	Y L	2.74	25.0	5.0	1fna	A 34	I A	4.86	25.0	5.0
1fna	A 34	I V	0.11	25.0	5.0	1fna	A 36	Y A	1.49	25.0	5.0
1fna	A 48	F A	1.98	25.0	5.0	1fna	A 50	V A	2.85	25.0	5.0
1fna	A 57	A G	2.49	25.0	5.0	1fna	A 59	I A	3.33	25.0	5.0
1fna	A 59	I V	0.72	25.0	5.0	1fna	A 62	L A	2.88	25.0	5.0
1fna	A 66	V A	0.91	25.0	5.0	1fna	A 68	Y A	1.88	25.0	5.0
1fna	A 68	Y F	2.14	25.0	5.0	1fna	A 70	I A	4.11	25.0	5.0
1fna	A 70	I V	1.28	25.0	5.0	1fna	A 72	V A	3.17	25.0	5.0
1fna	A 74	A G	1.56	25.0	5.0	1fna	A 85	S A	-0.13	25.0	5.0
1fna	A 88	I A	0.67	25.0	5.0	1fna	A 88	I V	0.33	25.0	5.0
1fna	A 90	I A	0.69	25.0	5.0	1fna	A 90	I V	0.40	25.0	5.0
1fna	A 92	Y A	1.11	25.0	5.0	1fna	A 92	Y F	-0.13	25.0	5.0
1ftg	A 6	L A	3.11	34.6	7.0	1ftg	A 20	E K	-1.16	37.8	7.0
1ftg	A 22	I A	1.70	44.2	7.0	1ftg	A 22	I V	1.66	25.0	7.0
1ftg	A 31	V A	1.85	34.6	7.0	1ftg	A 40	E K	-1.61	37.8	7.0
1ftg	A 43	D A	-0.07	34.6	7.0	1ftg	A 51	I V	1.75	34.6	7.0
1ftg	A 52	I V	1.19	34.6	7.0	1ftg	A 61	E K	-0.51	34.6	7.0
1ftg	A 65	D K	0.10	34.6	7.0	1ftg	A 71	S A	0.44	34.6	7.0
1ftg	A 72	E K	-1.41	37.8	7.0	1ftg	A 75	D K	-1.03	37.8	7.0
1ftg	A 84	A G	1.90	34.6	7.0	1ftg	A 97	N A	0.58	34.6	7.0
1ftg	A 99	Q A	-1.59	34.6	7.0	1ftg	A 104	I V	0.57	34.6	7.0
1ftg	A 110	S A	0.73	34.6	7.0	1ftg	A 117	V A	2.02	34.6	7.0
1ftg	A 122	T S	-0.03	34.6	7.0	1ftg	A 126	D K	-0.81	37.8	7.0
1ftg	A 139	V A	1.09	34.6	7.0	1ftg	A 143	L A	0.17	34.6	7.0
1ftg	A 150	D K	0.21	37.8	7.0	1ftg	A 156	I V	3.16	34.6	7.0
1ftg	A 160	V A	2.07	34.6	7.0	1fvk_a	A 30	C S	1.79	25.0	7.5
1fvk_a	A 32	H L	-5.30	30.0	7.0	1fvk_a	A 32	H S	-5.20	30.0	7.0
1fvk_a	A 32	H Y	-6.80	30.0	7.0	1fvk_a	A 33	C S	1.15	25.0	7.5
1g4i	A 22	F A	-0.25	30.0	8.0	1g4i	A 22	F I	-1.43	30.0	8.0
1g4i	A 22	F Y	-0.83	30.0	8.0	1g4i	A 48	H A	1.93	30.0	8.0
1g4i	A 48	H N	2.44	30.0	8.0	1g4i	A 48	H Q	0.49	30.0	8.0
1g4i	A 106	F A	1.23	25.0	8.0	1g4i	A 106	F I	-0.95	30.0	8.0
1g4i	A 106	F Y	-0.07	30.0	8.0	1g6n_a	A 128	S A	0.26	20.0	7.9
1h7m	A 2	D A	0.53	25.0	7.4	1h7m	A 6	E A	0.77	25.0	7.4
1h7m	A 8	R A	0.77	25.0	7.4	1h7m	A 9	K A	0.29	25.0	7.4
1h7m	A 12	D A	-0.24	25.0	7.4	1h7m	A 15	K A	0.91	25.0	7.4
1h7m	A 21	R A	-0.07	25.0	7.4	1h7m	A 22	K A	-0.43	25.0	7.4
1h7m	A 28	K A	1.20	25.0	7.4	1h7m	A 33	K A	-0.12	25.0	7.4
1h7m	A 39	R A	0.07	25.0	7.4	1h7m	A 42	R A	-0.33	25.0	7.4
1h7m	A 44	D A	-0.05	25.0	7.4	1h7m	A 46	K A	1.10	25.0	7.4
1h7m	A 47	E A	0.05	25.0	7.4	1h7m	A 48	D A	-0.36	25.0	7.4
1h7m	A 50	E A	-0.57	25.0	7.4	1h7m	A 54	R A	0.26	25.0	7.4
1h7m	A 62	E A	1.29	25.0	7.4	1h7m	A 64	E A	0.26	25.0	7.4
1h7m	A 69	E A	0.74	25.0	7.4	1h7m	A 76	R A	-0.19	25.0	7.4
1h7m	A 78	H A	0.50	25.0	7.4	1h7m	A 87	D A	1.36	25.0	7.4
1h7m	A 90	E A	0.41	25.0	7.4	1h7m	A 92	R A	0.31	25.0	7.4
1hfz_a	A 32	H A	2.13	56.2	7.4	1hfz_a	A 32	H Y	-0.07	56.2	7.4
1hfz_a	A 42	V A	0.93	56.2	7.4	1hfz_a	A 42	V G	1.15	56.2	7.4
1hfz_a	A 42	V N	0.24	56.2	7.4	1hfz_a	A 54	Q A	0.41	56.2	7.4
1hfz_a	A 59	I W	0.93	56.2	7.4	1hfz_a	A 103	Y A	2.39	56.2	7.4
1hfz_a	A 104	W Y	2.44	56.2	7.4	1hfz_a	A 106	A S	1.05	56.2	7.4
1hfz_a	A 107	H A	0.79	56.2	7.4	1hfz_a	A 107	H W	1.72	56.2	7.4
1hfz_a	A 107	H Y	0.19	56.2	7.4	1hfz_a	A 110	L E	0.19	56.2	7.4
1hfz_a	A 110	L H	-1.39	56.2	7.4	1hfz_a	A 110	L R	-0.43	56.2	7.4

1hfz_a	A 114	K E	0.65	56.2	7.4	1hfz_a	A 114	K N	-2.66	56.2	7.4
1hfz_a	A 114	K Q	0.60	56.2	7.4	1hfz_a	A 117	Q A	0.96	56.2	7.4
1hfz_a	A 118	W H	0.60	56.2	7.4	1hfz_a	A 118	W Y	1.17	56.2	7.4
1hk0	X 43	M A	0.70	37.0	7.0	1hk0	X 54	Q A	-0.50	37.0	7.0
1hk0	X 56	F A	1.20	37.0	7.0	1hk0	X 79	R A	2.30	37.0	7.0
1hk0	X 81	I A	2.60	37.0	7.0	1hk0	X 132	V A	3.80	37.0	7.0
1hk0	X 143	Q A	0.40	37.0	7.0	1hk0	X 145	L A	2.60	37.0	7.0
1hk0	X 147	M A	1.10	37.0	7.0	1hk0	X 170	V A	-1.30	37.0	7.0
1hme	A 33	S H	1.85	20.0	7.0	1hme	A 34	I H	0.95	20.0	7.0
1hme	A 35	G H	0.33	20.0	7.0	1hmk	A 8	V A	0.83	25.0	7.0
1hmk	A 12	L A	2.73	25.0	7.0	1hmk	A 26	W F	2.11	25.0	7.5
1hmk	A 27	V A	1.24	25.0	7.0	1hmk	A 29	T I	-3.55	24.5	6.4
1hmk	A 29	T V	-2.26	25.0	7.0	1hmk	A 30	A I	-1.47	24.0	6.1
1hmk	A 30	A T	-0.48	24.0	6.1	1hmk	A 33	T I	0.64	24.0	6.1
1hmk	A 38	T A	1.30	58.8	7.0	1hmk	A 52	L A	3.22	25.0	7.0
1hmk	A 55	I V	2.72	25.0	7.0	1hmk	A 60	W A	2.01	25.0	7.0
1hmk	A 60	W F	0.68	25.0	7.5	1hmk	A 87	D N	1.14	25.0	7.0
1hmk	A 89	I V	0.86	25.0	7.0	1hmk	A 90	V A	-0.90	25.0	7.0
1hmk	A 93	K A	1.72	25.0	7.0	1hmk	A 95	I V	1.72	25.0	7.0
1hmk	A 96	L A	1.75	25.0	7.0	1hmk	A 103	Y F	2.13	25.0	7.0
1hmk	A 104	W F	1.96	25.0	7.5	1hmk	A 105	L A	0.28	25.0	7.0
1hmk	A 110	L A	0.35	25.0	7.0	1hmk	A 118	W F	0.31	25.0	7.0
1hms	A 4	F S	3.67	37.0	8.0	1hms	A 8	W E	3.82	37.0	8.0
1hms	A 16	F S	3.98	37.0	8.0	1hms	A 16	F Y	2.56	25.0	8.0
1hms	A 21	K I	0.00	37.0	8.0	1hms	A 40	T E	2.40	25.0	8.0
1hms	A 40	T Q	2.73	25.0	8.0	1hms	A 40	T V	0.76	25.0	8.0
1hms	A 57	F S	2.43	25.0	8.0	1hms	A 64	F S	3.82	37.0	8.0
1hms	A 66	L G	3.67	37.0	8.0	1hms	A 67	G S	1.22	37.0	8.0
1hms	A 72	E S	3.67	37.0	8.0	1hms	A 106	R T	2.84	25.0	8.0
1hms	A 126	R K	3.26	25.0	8.0	1hms	A 126	R Q	0.31	25.0	8.0
1hms	A 128	Y F	2.68	25.0	8.0	1hti	A 105	S D	0.65	25.0	8.0
1hti	A 179	Q A	-0.05	25.0	8.0	1hti	A 179	Q D	-0.75	25.0	8.0
1hti	A 193	K A	-0.50	25.0	8.0	1huu_p	A 27	A S	1.19	63.9	7.0
1huu_p	A 31	S T	-0.41	63.9	7.0	1huu_p	A 42	V I	0.82	63.9	7.0
1huu_p	A 56	A S	0.13	63.9	7.0	1huu_p	A 69	M I	0.00	63.9	7.0
1iet	A 60	D R	-0.14	25.0	7.2	1lfc	A 6	W Y	0.87	25.0	7.0
1lfc	A 23	I C	-0.51	20.0	8.1	1lfc	A 53	S C	-0.31	20.0	8.1
1lfc	A 60	V C	0.07	20.0	8.1	1lfc	A 60	V N	0.83	25.0	7.0
1lfc	A 64	L A	1.68	20.0	7.4	1lfc	A 64	L G	2.26	20.0	7.4
1lfc	A 65	G A	0.94	20.0	7.4	1lfc	A 68	F A	0.42	25.0	7.0
1lfc	A 72	L C	-0.02	20.0	8.1	1lfc	A 82	W Y	0.39	25.0	7.0
1lfc	A 89	L C	1.25	20.0	8.1	1lfc	A 93	F A	2.37	25.0	7.0
1lfc	A 104	A C	-1.32	20.0	8.1	1lqv	A 6	L V	1.72	25.0	7.0
1lqv	A 10	F A	4.12	25.0	7.0	1lqv	A 13	Y F	1.08	25.0	7.1
1lqv	A 17	E Q	-0.33	25.0	7.1	1lqv	A 19	D N	-0.83	25.0	7.0
1lqv	A 23	L A	3.24	25.0	7.0	1lqv	A 23	L G	3.95	25.0	7.0
1lqv	A 26	E Q	0.03	25.0	7.0	1lqv	A 28	L A	2.20	25.0	7.0
1lqv	A 61	V A	2.93	25.0	7.0	1lqv	A 61	V G	3.60	25.0	7.0
1lqv	A 66	F A	4.20	25.0	7.0	1lqv	A 66	F W	0.93	25.0	7.0
1lqv	A 70	V L	0.13	25.0	7.0	1lqv	A 73	I V	1.34	25.0	7.0
1lhb_a	A 37	F H	0.66	25.0	7.5	1lhb_a	A 55	R V	0.15	25.0	7.5
1lhb_a	A 71	F N	-0.46	25.0	7.5	1lhb_a	A 82	F Q	0.37	25.0	7.5
1lhb_a	A 92	F N	0.71	25.0	7.5	1lmq	A 19	V L	1.82	10.0	6.0
1lmq	A 25	A G	0.14	10.0	6.0	1lmq	A 31	E L	0.67	10.0	6.0
1lmq	A 34	V L	-0.33	10.0	6.0	1lmq	A 37	V L	0.26	10.0	6.0
1lmq	A 41	E V	-0.89	10.0	6.0	1lmq	A 68	V I	0.81	10.0	6.0
1lmq	A 71	V I	-0.07	10.0	6.0	1lio2	A 7	D N	-0.46	50.0	9.0
1lio2	A 8	E A	-1.77	50.0	9.0	1lio2	A 8	E Q	1.25	50.0	9.0
1lio2	A 105	D A	-1.72	50.0	9.0	1lio2	A 135	D A	-1.82	50.0	9.0
1lro	A 24	V I	-0.36	107.0	9.1	1lro	A 33	I L	-0.76	107.0	9.1
1ljiw_i	I 10	D A	0.70	25.0	7.1	1ljiw_i	I 15	W F	2.30	25.0	7.1
1k9q_a	A 20	A R	-0.89	56.7	7.0	1k9q_a	A 30	L Y	-0.27	56.7	7.0
1k9q_a	A 34	D T	-0.37	56.7	7.0	1kcq	A 187	D N	1.05	25.0	7.2
1kcq	A 187	D Y	2.03	15.0	7.2	1kdx_a	A 640	Y F	0.00	25.0	6.0

1ke4_a	A 150	Y F	2.05	38.9	6.8	1kfw	A 197	N K	-0.81	16.0	7.5
1kfw	A 405	G Q	-0.62	16.0	7.5	1lbi	A 84	K L	0.20	25.0	7.4
1lni_a	A 2	V T	0.90	48.4	7.0	1lni_a	A 5	T V	0.00	48.4	7.0
1lni_a	A 16	T V	-0.30	48.4	7.0	1lni_a	A 17	D K	1.10	25.0	7.0
1lni_a	A 18	T V	1.40	48.4	7.0	1lni_a	A 25	D K	-0.90	36.1	7.0
1lni_a	A 30	Y F	-0.40	25.0	7.0	1lni_a	A 36	V T	1.30	48.4	7.0
1lni_a	A 38	Q A	-0.74	51.9	6.3	1lni_a	A 39	N A	2.20	48.4	7.0
1lni_a	A 39	N D	1.50	48.4	7.0	1lni_a	A 39	N S	2.30	48.4	7.0
1lni_a	A 41	E K	1.11	42.2	6.6	1lni_a	A 43	V T	0.50	48.4	7.0
1lni_a	A 49	Y F	0.20	25.0	7.0	1lni_a	A 51	Y F	2.30	25.0	7.0
1lni_a	A 52	Y F	3.60	25.0	7.0	1lni_a	A 54	E Q	1.96	51.9	6.3
1lni_a	A 55	Y F	0.60	25.0	7.0	1lni_a	A 56	T V	1.90	48.4	7.0
1lni_a	A 57	V T	4.40	48.4	7.0	1lni_a	A 59	T V	1.70	48.4	7.0
1lni_a	A 65	R A	1.13	51.9	6.3	1lni_a	A 67	T V	0.00	48.4	7.0
1lni_a	A 72	T V	0.20	48.4	7.0	1lni_a	A 74	E K	-0.84	43.5	6.7
1lni_a	A 79	D A	-2.48	49.1	6.8	1lni_a	A 79	D E	0.40	52.6	7.0
1lni_a	A 79	D F	-2.73	49.1	6.8	1lni_a	A 79	D H	-1.70	52.6	7.0
1lni_a	A 79	D I	-2.85	52.6	7.0	1lni_a	A 79	D K	-2.35	52.6	7.0
1lni_a	A 79	D L	-2.65	52.6	7.0	1lni_a	A 79	D N	-1.46	49.1	6.8
1lni_a	A 79	D R	-2.70	52.6	7.0	1lni_a	A 79	D W	-2.25	52.6	7.0
1lni_a	A 79	D Y	-2.90	52.6	7.0	1lni_a	A 80	Y F	1.50	25.0	7.0
1lni_a	A 81	Y F	1.20	25.0	7.0	1lni_a	A 82	T V	1.70	48.4	7.0
1lni_a	A 85	H Q	0.00	51.9	6.3	1lni_a	A 86	Y F	0.30	25.0	7.0
1lni_a	A 94	Q K	-0.56	47.5	6.8	1luc	A 81	A H	2.70	25.0	7.0
1luc	B 81	H A	2.10	25.0	7.0	1luc	B 82	H A	2.70	25.0	7.0
1lve_p	A 4	M L	-1.04	25.0	7.5	1lve_p	A 27C	L N	0.57	25.0	7.5
1lve_p	A 27C	L Q	-0.63	25.0	7.5	1lve_p	A 27B	V L	-1.67	25.0	7.5
1lve_p	A 27D	Y D	-2.19	25.0	7.5	1lve_p	A 28	N F	2.41	25.0	7.5
1lve_p	A 29	S N	-0.39	25.0	7.5	1lve_p	A 30	K R	0.55	25.0	7.5
1lve_p	A 30	K T	1.33	25.0	7.5	1lve_p	A 38	Q N	1.60	25.0	7.5
1lve_p	A 39	K T	2.29	25.0	7.5	1lve_p	A 89	Q H	0.90	25.0	7.5
1lve_p	A 89	Q N	1.26	25.0	7.5	1lve_p	A 94	T H	-0.73	25.0	7.5
1lve_p	A 96	Y Q	2.09	25.0	7.5	1lve_p	A 97	S T	-0.13	25.0	7.5
1lve_p	A 106	I L	0.51	25.0	7.5	1lzl	A 1	K A	0.60	64.9	2.7
1lzl	A 1	K M	0.12	64.9	2.7	1lzl	A 2	V A	1.51	64.9	2.7
1lzl	A 2	V D	1.44	64.9	2.7	1lzl	A 2	V F	0.86	64.9	2.7
1lzl	A 2	V G	2.30	64.9	2.7	1lzl	A 2	V I	-1.10	64.9	2.7
1lzl	A 2	V L	0.05	64.9	2.7	1lzl	A 2	V M	0.31	64.9	2.7
1lzl	A 2	V N	1.34	64.9	2.7	1lzl	A 2	V R	0.38	64.9	2.7
1lzl	A 2	V S	1.41	64.9	2.7	1lzl	A 2	V Y	0.36	64.9	2.7
1lzl	A 7	E Q	0.94	65.0	3.5	1lzl	A 8	L T	3.73	64.9	2.7
1lzl	A 9	A S	0.02	64.9	2.7	1lzl	A 16	G A	1.39	64.9	2.7
1lzl	A 18	D N	1.28	65.0	3.4	1lzl	A 19	G A	1.77	64.9	2.7
1lzl	A 20	Y F	0.50	64.9	2.7	1lzl	A 21	R A	-1.32	64.9	2.7
1lzl	A 21	R G	-1.15	64.9	2.7	1lzl	A 22	G A	1.79	64.9	2.7
1lzl	A 23	I A	2.54	64.9	2.7	1lzl	A 23	I V	0.36	64.9	2.7
1lzl	A 32	A L	0.10	64.9	2.7	1lzl	A 32	A S	0.33	64.9	2.7
1lzl	A 35	E L	0.53	64.9	2.7	1lzl	A 37	G A	0.29	64.9	2.7
1lzl	A 37	G Q	0.40	52.3	3.0	1lzl	A 38	Y A	2.49	64.9	2.7
1lzl	A 38	Y F	0.19	64.9	2.7	1lzl	A 38	Y G	2.32	64.9	2.7
1lzl	A 45	Y F	-0.07	64.9	2.7	1lzl	A 48	G A	-0.45	64.9	2.7
1lzl	A 49	D N	0.65	65.0	3.4	1lzl	A 50	R A	-0.43	64.9	2.7
1lzl	A 50	R G	-0.32	52.3	3.0	1lzl	A 54	Y F	0.96	64.9	2.7
1lzl	A 56	I A	3.71	64.9	2.7	1lzl	A 56	I F	4.09	64.9	2.7
1lzl	A 56	I L	0.10	64.9	2.7	1lzl	A 56	I M	1.77	64.9	2.7
1lzl	A 56	I T	4.31	52.3	3.0	1lzl	A 56	I V	1.20	64.9	2.7
1lzl	A 58	Q A	-0.91	64.9	2.7	1lzl	A 58	Q G	-1.91	52.3	3.0
1lzl	A 59	I A	1.72	64.9	2.7	1lzl	A 59	I F	0.81	64.9	2.7
1lzl	A 59	I G	3.83	64.9	2.7	1lzl	A 59	I L	0.00	64.9	2.7
1lzl	A 59	I M	1.29	64.9	2.7	1lzl	A 59	I S	3.59	64.9	2.7
1lzl	A 59	I T	2.22	64.9	2.7	1lzl	A 59	I V	1.10	64.9	2.7
1lzl	A 59	I Y	3.78	64.9	2.7	1lzl	A 63	Y F	0.24	64.9	2.7
1lzl	A 67	D H	3.73	10.0	4.0	1lzl	A 67	D N	1.39	65.0	3.5
1lzl	A 68	G A	0.12	64.9	2.7	1lzl	A 72	G A	0.36	64.9	2.7

1lz1	A 74	V A	0.36	64.9	2.7	1lz1	A 74	V D	0.43	64.9	2.7
1lz1	A 74	V F	0.29	64.9	2.7	1lz1	A 74	V G	0.22	64.9	2.7
1lz1	A 74	V I	-0.45	64.9	2.7	1lz1	A 74	V L	-0.19	64.9	2.7
1lz1	A 74	V M	-0.65	64.9	2.7	1lz1	A 74	V N	0.33	64.9	2.7
1lz1	A 74	V R	0.07	64.9	2.7	1lz1	A 74	V S	0.38	64.9	2.7
1lz1	A 74	V Y	0.24	64.9	2.7	1lz1	A 77	C A	4.60	57.0	3.0
1lz1	A 78	H A	0.14	64.9	2.7	1lz1	A 78	H G	0.21	52.3	3.0
1lz1	A 89	I A	2.70	64.9	2.7	1lz1	A 89	I V	0.48	64.9	2.7
1lz1	A 92	A S	-0.81	64.9	2.7	1lz1	A 93	V A	0.74	64.9	2.7
1lz1	A 93	V T	0.67	64.9	2.7	1lz1	A 96	A M	-0.02	64.9	2.7
1lz1	A 96	A S	1.00	64.9	2.7	1lz1	A 99	V A	0.98	64.9	2.7
1lz1	A 99	V T	0.50	64.9	2.7	1lz1	A 100	V A	0.26	64.9	2.7
1lz1	A 100	V F	1.65	64.9	2.7	1lz1	A 100	V T	0.29	64.9	2.7
1lz1	A 102	D N	0.15	65.0	3.5	1lz1	A 105	G A	0.62	64.9	2.7
1lz1	A 106	I A	0.93	64.9	2.7	1lz1	A 106	I V	0.72	64.9	2.7
1lz1	A 110	V A	-0.53	64.9	2.7	1lz1	A 110	V D	-0.17	64.9	2.7
1lz1	A 110	V F	0.05	64.9	2.7	1lz1	A 110	V G	-0.48	64.9	2.7
1lz1	A 110	V I	-0.86	64.9	2.7	1lz1	A 110	V L	-0.07	64.9	2.7
1lz1	A 110	V M	-0.53	64.9	2.7	1lz1	A 110	V N	-0.07	64.9	2.7
1lz1	A 110	V R	-0.89	64.9	2.7	1lz1	A 110	V Y	0.14	64.9	2.7
1lz1	A 118	N A	-0.19	64.9	2.7	1lz1	A 118	N G	-0.05	64.9	2.7
1lz1	A 120	D N	0.17	65.0	3.5	1lz1	A 121	V A	1.44	64.9	2.7
1lz1	A 124	Y F	0.36	64.9	2.7	1lz1	A 125	V A	1.32	64.9	2.7
1lz1	A 127	G A	0.55	64.9	2.7	1lz1	A 129	G A	-0.14	64.9	2.7
1lz1	A 130	V A	0.84	64.9	2.7	1mbg	A 103	V A	2.32	25.0	7.5
1mbg	A 103	V I	-0.69	25.0	7.5	1mbg	A 103	V L	-2.08	21.4	7.4
1mgr	A 11	Y F	0.60	25.0	7.0	1mgr	A 33	Y F	-0.50	25.0	7.0
1mgr	A 54	Y F	2.60	25.0	7.0	1mgr	A 55	Y F	2.10	25.0	7.0
1mgr	A 58	Y F	0.70	25.0	7.0	1mgr	A 83	Y F	1.50	25.0	7.0
1mgr	A 84	Y F	1.00	25.0	7.0	1mgr	A 89	Y F	0.00	25.0	7.0
1mjc	A 18	F L	1.00	25.0	7.0	1mjc	A 18	F S	1.54	25.0	7.0
1mjc	A 20	F L	0.31	25.0	7.0	1mjc	A 20	F S	1.16	25.0	7.0
1mjc	A 31	F L	0.66	25.0	7.0	1mjc	A 31	F S	1.03	25.0	7.0
1mjc	A 42	Y W	-0.15	25.0	7.0	1mjc	A 52	S W	0.20	25.0	7.0
1mjc	A 68	T W	-0.70	25.0	7.0	1msi	A 23	R A	0.89	25.0	7.0
1msi	A 25	E A	0.09	25.0	7.0	1msi	A 36	D A	-0.30	25.0	7.0
1msi	A 39	R A	0.80	25.0	7.0	1msi	A 47	R A	0.74	25.0	7.0
1msi	A 58	D N	0.20	25.0	7.0	1n0j_p	A 34	Y F	-4.75	88.9	7.8
1n0j_p	A 58	I T	2.95	88.9	7.8	1n0j_p	A 143	Q N	-1.04	88.9	7.8
1oh0_q	A 16	Y F	1.79	25.0	7.0	1oh0_q	A 32	Y F	-0.20	25.0	7.0
1oh0_q	A 57	Y F	1.22	25.0	7.0	1oh0_q	A 57	Y S	4.53	25.0	7.0
1oh0_q	A 101	V L	1.72	25.0	7.0	1oia_a	A 13	Y F	0.70	22.0	7.0
1oia_a	A 13	Y T	1.30	22.0	7.0	1oia_a	A 31	Y F	0.00	22.0	7.0
1oia_a	A 31	Y S	2.30	22.0	7.0	1oia_a	A 78	Y F	0.00	22.0	7.0
1oia_a	A 86	Y F	2.60	22.0	7.0	1oia_a	A 86	Y T	2.90	22.0	7.0
1onc	A 23	M L	2.76	0.4	7.0	1onc	A 28	F A	5.00	20.0	5.5
1onc	A 36	F Y	4.67	20.0	5.5	1otr_b	B 11	K A	0.14	25.0	5.0
1otr_b	B 30	I F	3.32	50.0	3.0	1otr_b	B 30	I L	1.96	50.0	3.0
1otr_b	B 30	I V	1.58	50.0	3.0	1otr_b	B 34	E D	1.00	25.0	5.0
1otr_b	B 34	E L	-0.96	25.0	5.0	1otr_b	B 34	E S	0.60	25.0	5.0
1otr_b	B 36	I F	0.86	50.0	3.0	1otr_b	B 36	I L	1.32	50.0	3.0
1otr_b	B 36	I V	0.79	50.0	3.0	1p2p	A 48	H K	2.12	20.0	7.0
1p2p	A 48	H N	1.69	20.0	7.0	1p2p	A 48	H Q	0.64	20.0	7.0
1pdo_p	A 12	W F	-1.79	22.0	7.4	1pdo_p	A 33	W F	1.08	22.0	7.4
1pdo_p	A 69	W F	2.15	22.0	7.4	1pga	A 6	I L	1.39	25.0	5.4
1pga	A 6	I N	1.73	44.0	5.2	1pga	A 6	I T	1.79	44.0	5.2
1pga	A 22	D G	1.52	25.0	5.5	1pga	A 53	T A	0.51	20.0	5.2
1pga	A 53	T D	1.15	20.0	5.2	1pga	A 53	T E	0.40	20.0	5.2
1pga	A 53	T F	-0.55	37.1	5.2	1pga	A 53	T I	0.10	37.1	5.2
1pga	A 53	T R	0.28	20.0	5.2	1pga	A 53	T V	0.58	44.0	5.2
1pga	A 53	T Y	-0.52	44.0	5.2	1poh	A 31	S A	0.40	30.0	7.0
1poh	A 46	S A	1.01	30.0	7.0	1poh	A 46	S D	-1.44	30.0	7.0
1poh	A 46	S N	-0.39	30.0	7.0	1poh	A 49	K A	-1.39	25.0	7.0
1poh	A 49	K D	-1.41	25.0	7.0	1poh	A 49	K E	-1.85	36.2	7.0

lpoh	A 49	K G	-1.05	25.0	7.0	lpoh	A 49	K M	-0.94	25.0	7.0
lpoh	A 49	K N	-0.35	25.0	7.0	lpoh	A 49	K Q	-1.39	25.0	7.0
lpoh	A 49	K R	0.15	25.0	7.0	lpoh	A 49	K S	-0.95	25.0	7.0
lqgv	A 126	G D	0.93	20.0	7.8	lqlp	A 31	A I	-0.90	25.0	6.5
lqlp	A 31	A L	-0.90	25.0	6.5	lqlp	A 31	A V	-0.60	25.0	6.5
lqlp	A 51	F C	-3.01	23.0	6.5	lqlp	A 51	F L	-2.10	25.0	6.5
lqlp	A 55	V I	0.20	25.0	6.5	lqlp	A 55	V L	0.30	25.0	6.5
lqlp	A 59	T A	-1.00	25.0	6.5	lqlp	A 68	T A	-1.00	25.0	6.5
lqlp	A 70	A G	-1.60	25.0	6.5	lqlp	A 145	V I	-0.20	25.0	6.5
lqlp	A 145	V L	0.70	25.0	6.5	lqlp	A 160	Y A	0.21	25.0	7.8
lqlp	A 160	Y W	-1.18	25.0	7.8	lqlp	A 173	V I	-0.50	25.0	6.5
lqlp	A 173	V L	0.60	25.0	6.5	lqlp	A 183	A F	-1.50	25.0	6.5
lqlp	A 183	A I	-1.80	25.0	6.5	lqlp	A 183	A L	-1.40	25.0	6.5
lqlp	A 183	A V	-3.80	25.0	6.5	lqlp	A 194	W F	0.47	25.0	7.8
lqlp	A 238	W F	-0.98	25.0	7.8	lqlp	A 248	A F	-1.80	25.0	6.5
lqlp	A 248	A I	-2.20	25.0	6.5	lqlp	A 248	A L	-0.35	25.0	6.5
lqlp	A 248	A V	-2.30	25.0	6.5	lqlp	A 250	A I	0.40	25.0	6.5
lqlp	A 250	A L	1.00	25.0	6.5	lqlp	A 250	A V	0.40	25.0	6.5
lqlp	A 284	A I	0.00	25.0	6.5	lqlp	A 284	A V	-0.80	25.0	6.5
lqlp	A 321	V I	-0.60	25.0	6.5	lqlp	A 321	V L	1.20	25.0	6.5
lqlp	A 330	S R	2.44	25.0	7.8	lqlp	A 331	K F	-1.75	25.0	7.8
lqlp	A 331	K I	-0.84	25.0	7.8	lqlp	A 331	K T	0.54	25.0	7.8
lqlp	A 331	K V	-0.89	25.0	7.8	lqlp	A 364	V I	-0.40	25.0	6.5
lqlp	A 364	V L	0.30	25.0	6.5	lqlp	A 374	M I	-2.30	25.0	6.5
lqlp	A 381	S A	-1.00	25.0	6.5	lqlp	A 387	K R	-1.00	25.0	6.5
lqm4	A 265	R H	3.11	25.0	8.0	lqnd	A 71	C S	1.38	20.0	6.8
lrg8_a	A 16	C S	2.81	25.0	6.6	lrg8_a	A 21	H Y	-0.79	34.5	7.3
lrg8_a	A 44	L F	-0.59	34.5	7.3	lrg8_a	A 62	G A	1.48	24.9	6.6
lrg8_a	A 62	G N	0.97	24.9	6.6	lrg8_a	A 73	L V	1.46	40.0	6.6
lrg8_a	A 83	C S	1.78	29.6	6.6	lrg8_a	A 93	H A	0.60	24.9	6.6
lrg8_a	A 93	H G	-1.34	28.6	6.6	lrg8_a	A 93	H N	-0.19	24.9	6.6
lrg8_a	A 102	H Y	-0.39	34.5	7.3	lrg8_a	A 103	A G	0.46	24.9	6.6
lrg8_a	A 106	N G	-0.16	24.9	6.6	lrg8_a	A 108	F Y	-0.49	34.5	7.3
lrg8_a	A 109	V I	0.05	34.5	7.3	lrg8_a	A 109	V L	0.57	40.0	6.6
lrg8_a	A 117	C S	0.64	29.6	6.6	lrhg_a	A 26	G A	-1.93	25.0	7.0
lrhg_a	A 28	G A	-2.35	25.0	7.0	lrhg_a	A 33	E A	-0.31	25.0	5.9
lrhg_a	A 46	E A	0.32	25.0	5.9	lrhg_a	A 50	L E	0.19	25.0	5.9
lrhg_a	A 73	G A	-0.89	25.0	7.0	lrhg_a	A 81	G A	0.76	25.0	7.0
lrhg_a	A 87	G A	0.97	25.0	7.0	lrhg_a	A 149	G A	-1.38	25.0	7.0
lrhg_a	A 150	G A	-1.94	25.0	7.0	lris	A 6	V A	2.93	25.0	8.0
lris	A 8	I A	3.56	25.0	8.0	lris	A 21	L A	0.16	25.0	8.0
lris	A 22	E Q	1.12	25.0	8.0	lris	A 26	I A	2.84	25.0	8.0
lris	A 33	Y A	-0.41	25.0	8.0	lris	A 35	A G	0.77	25.0	8.0
lris	A 37	V A	2.55	25.0	8.0	lris	A 48	L A	0.21	25.0	8.0
lris	A 52	I A	0.36	25.0	8.0	lris	A 60	F A	0.81	25.0	8.0
lris	A 65	V A	2.89	25.0	8.0	lris	A 75	L A	1.35	25.0	8.0
lris	A 79	L A	3.91	25.0	8.0	lris	A 85	V A	3.02	25.0	8.0
lris	A 88	V A	1.68	25.0	8.0	lrl_c	C 16	V A	2.34	25.0	7.0
lrl_c	C 16	V C	4.99	25.0	7.0	lrl_c	C 16	V S	4.68	25.0	7.0
lrl_c	C 16	V T	3.65	25.0	7.0	lrl_c	C 21	A G	1.10	25.0	7.4
lrl_c	C 23	G A	1.20	25.0	7.4	lrl_c	C 24	Y W	-1.24	25.0	6.0
lrl_c	C 25	Q K	-0.88	36.8	7.0	lrl_c	C 40	H T	0.26	25.0	6.0
lrl_c	C 42	Y W	0.14	25.0	6.0	lrl_c	C 44	N A	1.88	37.9	7.0
lrl_c	C 44	N D	1.58	35.8	6.3	lrl_c	C 44	N S	1.77	37.9	7.0
lrl_c	C 45	Y W	-0.74	25.0	6.0	lrl_c	C 49	D A	-0.50	37.3	6.3
lrl_c	C 49	D F	-0.10	52.7	7.0	lrl_c	C 49	D H	-1.10	40.7	6.5
lrl_c	C 49	D Y	0.00	52.4	7.0	lrl_c	C 58	E A	0.42	31.5	7.0
lrl_c	C 59	W Y	0.93	25.0	6.0	lrl_c	C 76	D A	3.76	15.0	7.0
lrl_c	C 76	D N	3.39	17.2	7.0	lrl_c	C 76	D S	3.17	15.0	7.0
lrl_c	C 78	V A	4.08	25.0	7.0	lrl_c	C 78	V C	3.67	25.0	7.0
lrl_c	C 78	V S	4.73	25.0	7.0	lrl_c	C 78	V T	3.59	25.0	7.0
lrl_c	C 89	V C	3.54	25.0	7.0	lrl_c	C 89	V S	4.87	25.0	7.0
lrl_c	C 89	V T	3.07	25.0	7.0	lrl_c	C 92	H A	0.62	25.0	6.0
lrop_p	A 30	D A	-0.30	69.0	7.0	lrop_p	A 30	D C	-0.80	69.0	7.0

lrop_p	A 30	D E	-1.00	69.0	7.0	lrop_p	A 30	D F	0.10	69.0	7.0
lrop_p	A 30	D G	-2.00	69.0	7.0	lrop_p	A 30	D H	-0.90	69.0	7.0
lrop_p	A 30	D I	0.80	69.0	7.0	lrop_p	A 30	D K	-0.90	69.0	7.0
lrop_p	A 30	D L	0.10	69.0	7.0	lrop_p	A 30	D M	-0.60	69.0	7.0
lrop_p	A 30	D N	-0.80	69.0	7.0	lrop_p	A 30	D Q	-1.80	69.0	7.0
lrop_p	A 30	D R	-0.80	69.0	7.0	lrop_p	A 30	D S	-1.00	69.0	7.0
lrop_p	A 30	D T	0.40	69.0	7.0	lrop_p	A 30	D V	0.40	69.0	7.0
lrop_p	A 30	D W	0.40	69.0	7.0	lrop_p	A 30	D Y	-0.20	69.0	7.0
lrop_p	A 41	L A	3.06	25.0	6.0	lrop_p	A 41	L V	1.26	25.0	6.0
lrtb	A 4	A S	0.45	62.0	7.1	lrtb	A 5	A S	0.27	62.0	7.1
lrtb	A 46	F L	3.21	24.9	6.0	lrtb	A 46	F V	4.55	24.9	6.0
lrtb	A 47	V A	3.80	40.0	5.0	lrtb	A 54	V A	2.58	40.0	5.0
lrtb	A 54	V G	4.87	40.0	5.0	lrtb	A 54	V I	1.95	40.0	5.0
lrtb	A 54	V L	1.09	40.0	5.0	lrtb	A 57	V A	2.85	40.0	5.0
lrtb	A 57	V I	1.30	40.0	5.0	lrtb	A 57	V L	2.37	40.0	5.0
lrtb	A 63	V A	2.03	40.0	5.0	lrtb	A 63	V G	3.50	40.0	5.0
lrtb	A 64	A G	0.44	40.0	5.0	lrtb	A 81	I A	2.99	40.0	5.0
lrtb	A 81	I G	4.81	40.0	5.0	lrtb	A 81	I V	0.43	40.0	5.0
lrtb	A 97	Y F	3.54	63.3	5.0	lrtb	A 106	I A	4.38	40.0	5.0
lrtb	A 106	I L	1.79	40.0	5.0	lrtb	A 106	I V	0.80	40.0	5.0
lrtb	A 107	I A	2.85	40.0	5.0	lrtb	A 107	I L	2.20	40.0	5.0
lrtb	A 107	I V	0.08	40.0	5.0	lrtb	A 108	V A	4.20	40.0	5.0
lrtb	A 108	V I	0.44	40.0	5.0	lrtb	A 108	V L	0.70	40.0	5.0
lrtb	A 109	A G	0.43	40.0	5.0	lrtb	A 116	V A	0.67	40.0	5.0
lrtb	A 116	V G	1.18	40.0	5.0	lrtb	A 118	V A	1.92	40.0	5.0
lrtb	A 118	V G	2.78	40.0	5.0	lrtb	A 119	H A	-0.35	25.0	5.2
lrtb	A 121	D A	1.95	25.0	5.2	lrtb	A 121	D N	1.71	25.0	5.2
lrtb	A 123	S A	-0.69	62.0	7.1	lrtb_a	A 80	K S	0.29	45.8	7.4
lsak	A 326	E A	0.40	25.0	7.0	lsak	A 328	F A	2.36	25.0	7.0
lsak	A 328	F L	1.43	25.0	7.0	lsak	A 329	T A	1.02	25.0	7.0
lsak	A 330	L F	1.80	25.0	7.0	lsak	A 331	Q A	0.46	25.0	7.0
lsak	A 332	I V	0.99	25.0	7.0	lsak	A 333	R A	1.05	25.0	7.0
lsak	A 335	R A	0.75	25.0	7.0	lsak	A 336	E A	-0.40	25.0	7.0
lsak	A 337	R A	2.41	25.0	7.0	lsak	A 338	F A	2.03	25.0	7.0
lsak	A 339	E A	0.66	25.0	7.0	lsak	A 340	M A	1.90	25.0	7.0
lsak	A 340	M I	0.38	25.0	7.0	lsak	A 341	F I	2.01	25.0	7.0
lsak	A 341	F L	0.91	25.0	7.0	lsak	A 342	R A	0.38	25.0	7.0
lsak	A 343	E A	0.25	25.0	7.0	lsak	A 344	L F	1.62	25.0	7.0
lsak	A 344	L I	0.41	25.0	7.0	lsak	A 345	N A	0.98	25.0	7.0
lsak	A 346	E A	0.27	25.0	7.0	lsak	A 347	A G	0.97	25.0	7.0
lsak	A 349	E A	1.18	25.0	7.0	lsak	A 350	L A	0.50	25.0	7.0
lsak	A 351	K A	-0.57	25.0	7.0	lsak	A 352	D A	0.62	25.0	7.0
lshf_a	A 107	E A	1.27	25.0	8.0	lshf_a	A 107	E D	-0.68	25.0	8.0
lshf_a	A 107	E F	1.63	25.0	8.0	lshf_a	A 107	E G	2.29	25.0	8.0
lshf_a	A 107	E H	0.99	25.0	8.0	lshf_a	A 107	E I	2.71	25.0	8.0
lshf_a	A 107	E K	0.97	25.0	8.0	lshf_a	A 107	E L	3.02	25.0	8.0
lshf_a	A 107	E Q	0.74	25.0	8.0	lshf_a	A 107	E R	3.38	25.0	8.0
lshf_a	A 107	E S	1.64	25.0	8.0	lshf_a	A 107	E T	0.60	25.0	8.0
lshf_a	A 107	E V	2.00	25.0	8.0	lshf_a	A 107	E Y	2.40	25.0	8.0
lshf_a	A 111	I A	2.84	25.0	7.0	lshf_a	A 111	I L	0.71	25.0	7.0
lshf_a	A 111	I V	0.63	25.0	7.0	lshf_a	A 124	S A	0.71	25.0	8.0
lshf_a	A 124	S D	2.02	25.0	8.0	lshf_a	A 124	S F	1.90	25.0	8.0
lshf_a	A 124	S G	1.68	25.0	8.0	lshf_a	A 124	S H	1.25	25.0	8.0
lshf_a	A 124	S I	1.41	25.0	8.0	lshf_a	A 124	S K	-0.11	25.0	8.0
lshf_a	A 124	S L	0.37	25.0	8.0	lshf_a	A 124	S N	0.73	25.0	8.0
lshf_a	A 124	S R	0.18	25.0	8.0	lshf_a	A 124	S T	1.65	25.0	8.0
lshf_a	A 124	S V	1.10	25.0	8.0	lshf_a	A 124	S Y	2.27	25.0	8.0
lshf_a	A 127	T A	2.59	25.0	8.0	lshf_a	A 128	G A	1.78	25.0	8.0
lshf_a	A 138	V A	2.34	25.0	7.0	lshf_a	A 138	V G	3.65	25.0	7.0
lshf_a	A 138	V M	0.52	25.0	7.0	lshf_a	A 138	V T	2.40	25.0	7.0
lshg	A 48	D G	-0.82	24.9	2.9	lshg	A 52	F Y	-0.44	24.9	7.0
lshg	A 59	K F	0.92	24.9	7.0	lshg	A 59	K Y	0.84	24.9	7.0
lssso	A 29	I V	0.40	50.0	7.0	lsup	A 50	M F	-0.48	58.8	8.0
lsup	A 76	N D	-0.45	58.8	8.0	lsup	A 169	G A	-0.30	58.8	8.0

lsup	A 206	Q C	-1.25	58.8	8.0	lsup	A 217	Y K	-0.72	58.8	8.0
lsup	A 218	N S	-1.07	58.8	8.0	lten	A 809	I A	2.74	25.0	5.0
lten	A 809	I V	-0.02	25.0	5.0	lten	A 811	V A	1.40	25.0	5.0
lten	A 819	A G	2.67	25.0	5.0	lten	A 821	I A	3.58	25.0	5.0
lten	A 821	I V	0.28	25.0	5.0	lten	A 830	I A	1.63	25.0	5.0
lten	A 830	I V	0.37	25.0	5.0	lten	A 833	I A	3.30	25.0	5.0
lten	A 833	I V	0.80	25.0	5.0	lten	A 835	L A	4.13	25.0	5.0
lten	A 837	Y A	3.96	25.0	5.0	lten	A 849	I A	2.40	25.0	5.0
lten	A 851	L A	2.88	25.0	5.0	lten	A 858	Y A	1.21	25.0	5.0
lten	A 858	Y G	4.06	25.0	5.0	lten	A 860	I A	1.91	25.0	5.0
lten	A 860	I V	0.88	25.0	5.0	lten	A 863	L A	3.96	25.0	5.0
lten	A 867	T S	1.26	25.0	5.0	lten	A 869	Y F	3.09	25.0	5.0
lten	A 871	V A	2.69	25.0	5.0	lten	A 873	L A	2.81	25.0	5.0
lten	A 875	S A	0.27	25.0	5.0	lten	A 882	S A	2.58	25.0	5.0
lten	A 885	A G	0.92	25.0	5.0	lten	A 887	E A	-1.55	25.0	5.0
lten	A 887	E G	0.14	25.0	5.0	ltit	A 13	V A	2.15	25.0	7.4
ltit	A 23	I A	2.70	25.0	7.4	ltit	A 41	L A	2.70	25.0	7.4
ltit	A 58	L A	3.23	25.0	7.4	ltit	A 60	L A	4.88	25.0	7.4
ltit	A 63	C S	2.08	25.0	7.3	ltit	A 73	F L	3.83	25.0	7.4
ltit	A 86	V A	4.45	25.0	7.4	ltpk_a	A 65	V A	2.00	64.3	4.5
ltpk_a	A 65	V I	-0.30	64.3	4.5	ltpk_a	A 65	V L	1.90	64.3	4.5
ltpk_a	A 65	V M	2.20	64.3	4.5	ltpk_a	A 65	V S	2.40	64.3	4.5
ltpk_a	A 65	V T	1.00	64.3	4.5	lttq_a	A 18	A G	2.70	25.0	7.8
lttq_a	A 18	A V	2.30	25.0	7.8	lttq_a	A 22	F I	4.58	25.0	7.8
lttq_a	A 22	F L	1.05	25.0	7.8	lttq_a	A 22	F V	3.44	25.0	7.8
lttq_a	A 175	Y Q	1.65	25.0	7.8	lttq_a	A 209	L V	3.20	25.0	7.8
lttq_a	A 232	I V	3.30	25.0	7.8	ltyv_p	A 177	G R	0.70	88.4	7.4
ltyv_p	A 235	T I	0.53	88.4	7.4	ltyv_p	A 244	G R	1.33	88.4	7.4
ltyv_p	A 285	R K	3.43	88.4	7.4	ltyv_p	A 309	E V	0.77	88.4	7.4
ltyv_p	A 323	G D	0.13	88.4	7.4	lubq	A 6	K E	-0.53	25.0	5.0
lubq	A 6	K Q	-0.26	25.0	5.0	lubq	A 18	E D	0.08	25.0	3.0
lubq	A 27	K Q	1.91	25.0	5.0	lubq	A 29	K N	1.48	25.0	5.0
lubq	A 29	K Q	1.67	25.0	5.0	lubq	A 42	R E	-1.63	25.0	5.0
lubq	A 45	F W	-0.46	25.0	5.0	lubq	A 68	H E	-0.77	25.0	5.0
lubq	A 68	H Q	-0.55	25.0	5.0	lubq	A 72	R Q	0.33	25.0	5.0
luze	A 11	W F	0.31	9.9	5.7	luze	A 13	T A	0.99	9.9	5.7
luze	A 13	T S	-0.10	9.9	5.7	luze	A 15	E A	0.40	9.9	5.7
luze	A 15	E G	1.02	9.9	5.7	luze	A 17	A G	0.70	9.9	5.7
luze	A 19	Q A	0.08	9.9	5.7	luze	A 19	Q G	1.23	9.9	5.7
luze	A 20	A G	2.30	9.9	5.7	luze	A 24	L A	1.04	9.9	5.7
luze	A 26	K A	-0.11	9.9	5.7	luze	A 26	K G	0.74	9.9	5.7
luze	A 27	E A	0.62	9.9	5.7	luze	A 27	E G	1.57	9.9	5.7
luze	A 30	V A	3.28	9.9	5.7	luze	A 32	S A	0.00	9.9	5.7
luze	A 33	N G	0.42	9.9	5.7	luze	A 35	S A	1.04	9.9	5.7
luze	A 36	W F	-0.30	9.9	5.7	luze	A 38	Q A	0.37	9.9	5.7
luze	A 38	Q G	1.57	9.9	5.7	luze	A 39	A G	1.93	9.9	5.7
luze	A 42	M A	1.37	9.9	5.7	luze	A 43	I V	1.21	9.9	5.7
luze	A 44	I A	0.09	9.9	5.7	luze	A 44	I G	0.40	9.9	5.7
luze	A 44	I V	0.30	9.9	5.7	luze	A 46	D N	2.51	9.9	5.7
luze	A 49	Y A	2.46	9.9	5.7	luze	A 49	Y F	0.31	9.9	5.7
luze	A 50	S A	0.02	9.9	5.7	luze	A 50	S G	0.02	9.9	5.7
luze	A 51	A G	1.12	9.9	5.7	luze	A 52	L A	2.71	9.9	5.7
luze	A 53	A G	0.30	9.9	5.7	luze	A 56	S A	0.40	9.9	5.7
luze	A 56	S G	0.54	9.9	5.7	luze	A 58	K A	2.10	9.9	5.7
luze	A 60	Q A	-0.31	9.9	5.7	luze	A 60	Q G	0.80	9.9	5.7
luze	A 61	A G	2.07	9.9	5.7	luze	A 64	A G	0.94	9.9	5.7
luze	A 65	Y F	0.72	9.9	5.7	luze	A 67	V A	-0.51	9.9	5.7
luze	A 67	V G	0.00	9.9	5.7	lvqb_p	A 6	I V	0.35	25.0	7.0
lvqb_p	A 13	F T	0.35	25.0	7.0	lvqb_p	A 19	V C	0.15	25.0	7.0
lvqb_p	A 19	V T	0.30	25.0	7.0	lvqb_p	A 24	K V	-0.40	25.0	7.0
lvqb_p	A 26	Y R	0.20	25.0	7.0	lvqb_p	A 28	L V	-0.55	25.0	7.0
lvqb_p	A 30	E F	-1.02	25.0	7.0	lvqb_p	A 30	E M	-0.32	25.0	7.0
lvqb_p	A 30	E N	0.55	25.0	7.0	lvqb_p	A 32	L H	0.45	25.0	7.0
lvqb_p	A 32	L R	0.80	25.0	7.0	lvqb_p	A 32	L W	-1.40	25.0	7.0

lvqb_p	A 32	L Y	-0.50	25.0	7.0	lvqb_p	A 33	C A	0.25	25.0	7.0
lvqb_p	A 33	C I	0.45	25.0	7.0	lvqb_p	A 33	C L	1.30	25.0	7.0
lvqb_p	A 33	C M	1.75	25.0	7.0	lvqb_p	A 33	C S	2.12	25.0	7.0
lvqb_p	A 33	C T	2.30	25.0	7.0	lvqb_p	A 33	C V	0.10	25.0	7.0
lvqb_p	A 35	V A	1.02	25.0	7.0	lvqb_p	A 35	V C	0.55	25.0	7.0
lvqb_p	A 35	V F	1.50	25.0	7.0	lvqb_p	A 35	V I	0.32	25.0	7.0
lvqb_p	A 35	V L	1.07	25.0	7.0	lvqb_p	A 35	V M	0.53	25.0	7.0
lvqb_p	A 35	V T	2.65	25.0	7.0	lvqb_p	A 36	D C	1.02	25.0	7.0
lvqb_p	A 36	D N	0.50	25.0	7.0	lvqb_p	A 37	L A	3.85	25.0	7.0
lvqb_p	A 37	L C	2.30	25.0	7.0	lvqb_p	A 37	L I	0.70	25.0	7.0
lvqb_p	A 37	L T	2.60	25.0	7.0	lvqb_p	A 37	L V	1.75	25.0	7.0
lvqb_p	A 40	E C	0.80	25.0	7.0	lvqb_p	A 40	E T	0.20	25.0	7.0
lvqb_p	A 41	Y A	0.20	25.0	7.0	lvqb_p	A 41	Y F	0.30	25.0	7.0
lvqb_p	A 43	V C	1.05	25.0	7.0	lvqb_p	A 43	V T	0.80	25.0	7.0
lvqb_p	A 45	V A	1.05	25.0	7.0	lvqb_p	A 45	V C	0.05	25.0	7.0
lvqb_p	A 45	V L	1.50	25.0	7.0	lvqb_p	A 45	V T	1.75	25.0	7.0
lvqb_p	A 47	I A	3.32	25.0	7.0	lvqb_p	A 47	I C	2.33	25.0	7.0
lvqb_p	A 47	I F	0.85	25.0	7.0	lvqb_p	A 47	I L	0.28	25.0	7.0
lvqb_p	A 47	I M	1.00	25.0	7.0	lvqb_p	A 47	I T	3.70	25.0	7.0
lvqb_p	A 47	I V	1.18	25.0	7.0	lvqb_p	A 48	T C	0.40	25.0	7.0
lvqb_p	A 48	T V	0.00	25.0	7.0	lvqb_p	A 49	L A	3.05	25.0	7.0
lvqb_p	A 49	L C	2.05	25.0	7.0	lvqb_p	A 49	L I	0.95	25.0	7.0
lvqb_p	A 49	L T	2.85	25.0	7.0	lvqb_p	A 49	L V	1.45	25.0	7.0
lvqb_p	A 50	D H	0.77	25.0	7.0	lvqb_p	A 62	T C	0.35	25.0	7.0
lvqb_p	A 62	T V	-0.65	25.0	7.0	lvqb_p	A 63	V C	2.05	25.0	7.0
lvqb_p	A 63	V T	2.50	25.0	7.0	lvqb_p	A 64	H C	-0.25	25.0	7.0
lvqb_p	A 67	S C	1.85	25.0	7.0	lvqb_p	A 67	S T	0.80	25.0	7.0
lvqb_p	A 68	F L	2.12	25.0	7.0	lvqb_p	A 68	F V	2.50	25.0	7.0
lvqb_p	A 69	K H	0.62	25.0	7.0	lvqb_p	A 69	K M	-0.08	25.0	7.0
lvqb_p	A 70	V C	1.60	25.0	7.0	lvqb_p	A 70	V T	1.75	25.0	7.0
lvqb_p	A 73	F W	-0.40	25.0	7.0	lvqb_p	A 77	M A	1.05	25.0	7.0
lvqb_p	A 77	M C	0.00	25.0	7.0	lvqb_p	A 77	M F	0.10	25.0	7.0
lvqb_p	A 77	M I	-0.80	25.0	7.0	lvqb_p	A 77	M L	0.60	25.0	7.0
lvqb_p	A 77	M T	0.40	25.0	7.0	lvqb_p	A 77	M V	-0.60	25.0	7.0
lvqb_p	A 78	I C	2.20	25.0	7.0	lvqb_p	A 78	I T	3.30	25.0	7.0
lvqb_p	A 78	I V	0.65	25.0	7.0	lvqb_p	A 81	L C	1.85	25.0	7.0
lvqb_p	A 81	L T	2.55	25.0	7.0	lvqb_p	A 81	L V	0.10	25.0	7.0
lvqb_p	A 82	R C	0.75	25.0	7.0	lvqb_p	A 86	A T	0.35	25.0	7.0
lvqb_p	A 86	A V	-0.25	25.0	7.0	lwit	A 73	Y F	2.15	20.0	7.0
lwq5_a	A 22	F L	-1.40	25.0	7.8	lwq5_a	A 37	I A	4.42	25.0	7.8
lwq5_a	A 49	E A	-0.41	25.0	7.8	lwq5_a	A 49	E C	-1.33	25.0	7.8
lwq5_a	A 49	E D	-0.07	25.0	7.8	lwq5_a	A 49	E F	-1.15	25.0	7.8
lwq5_a	A 49	E G	0.03	25.0	7.8	lwq5_a	A 49	E H	-1.51	25.0	7.8
lwq5_a	A 49	E I	-3.79	25.0	7.8	lwq5_a	A 49	E K	-0.42	25.0	7.8
lwq5_a	A 49	E L	-3.67	25.0	7.8	lwq5_a	A 49	E M	-3.13	25.1	7.4
lwq5_a	A 49	E N	0.05	25.0	7.8	lwq5_a	A 49	E Q	0.58	25.1	7.3
lwq5_a	A 49	E S	0.01	25.0	7.4	lwq5_a	A 49	E T	-0.16	25.0	7.8
lwq5_a	A 49	E V	-2.43	25.0	7.4	lwq5_a	A 49	E W	0.02	25.0	7.8
lwq5_a	A 49	E Y	-0.41	25.0	7.4	lwq5_a	A 50	L A	2.99	25.0	7.8
lwq5_a	A 81	C A	0.69	50.0	9.0	lwq5_a	A 81	C G	1.58	50.0	9.0
lwq5_a	A 81	C S	1.41	50.0	9.0	lwq5_a	A 81	C V	1.32	50.0	9.0
lwq5_a	A 99	L A	4.07	25.0	7.8	lwq5_a	A 118	C A	1.36	50.0	9.0
lwq5_a	A 118	C S	2.27	50.0	9.0	lwq5_a	A 118	C V	1.34	50.0	9.0
lwq5_a	A 127	L A	1.28	25.0	7.8	lwq5_a	A 139	F W	0.64	23.0	7.8
lwq5_a	A 154	C A	1.03	50.0	9.0	lwq5_a	A 154	C S	1.72	50.0	9.0
lwq5_a	A 154	C V	1.12	50.0	9.0	lwq5_a	A 175	Y C	0.60	25.0	7.8
lwq5_a	A 176	L A	4.01	25.0	7.8	lwq5_a	A 211	G D	0.80	25.0	7.8
lwq5_a	A 211	G E	-1.10	33.2	7.8	lwq5_a	A 211	G R	0.12	50.4	7.8
lwq5_a	A 211	G S	0.15	25.0	7.8	lwq5_a	A 211	G V	-1.05	25.0	7.8
lwq5_a	A 211	G W	1.95	25.0	7.8	lwq5_a	A 234	G D	-3.40	25.0	7.8
lwq5_a	A 234	G K	-0.20	25.0	7.8	lwq5_a	A 258	F W	1.17	23.0	7.8
lyu5	X 41	H Y	-1.11	25.0	5.6	lyyj	A 3	L A	1.60	25.0	5.0
lyyj	A 7	W M	0.85	25.0	5.0	lyyj	A 10	L A	1.86	25.0	5.0
lyyj	A 14	L A	1.92	25.0	5.0	lyyj	A 15	K A	0.20	25.0	5.0

lyyj	A 17	I A	1.30	25.0	5.0	lyyj	A 18	E A	-1.30	25.0	5.0
lyyj	A 20	A G	1.97	25.0	5.0	lyyj	A 23	A G	2.38	25.0	5.0
lyyj	A 27	K A	0.17	25.0	5.0	lyyj	A 27	K G	1.00	25.0	5.0
lyyj	A 30	L A	2.83	25.0	5.0	lyyj	A 33	M A	2.97	25.0	5.0
lyyj	A 34	R A	2.25	25.0	5.0	lyyj	A 34	R G	3.26	25.0	5.0
lyyj	A 36	A G	2.61	25.0	5.0	lyyj	A 37	A G	4.15	25.0	5.0
lyyj	A 38	L G	1.44	25.0	5.0	lyyj	A 40	A G	1.41	25.0	5.0
lyyj	A 48	L A	3.73	25.0	5.0	lyyj	A 51	K G	1.32	25.0	5.0
lyyj	A 58	M A	2.91	25.0	5.0	lyyj	A 61	F A	4.52	25.0	5.0
lyyj	A 65	F A	1.92	25.0	5.0	lyyj	A 68	L A	3.88	25.0	5.0
lyyj	A 69	V G	3.61	25.0	5.0	lyyj	A 72	I A	4.79	25.0	5.0
lyyj	A 73	D A	1.57	25.0	5.0	lyyj	A 76	L A	3.48	25.0	5.0
lyyj	A 84	V A	3.42	25.0	5.0	lyyj	A 87	A G	3.20	25.0	5.0
lyyj	A 90	A G	2.34	25.0	5.0	lyyj	A 91	A G	1.60	25.0	5.0
lyyj	A 94	L A	1.50	25.0	5.0	lyyj	A 98	I A	3.48	25.0	5.0
lyyj	A 101	Y A	-0.52	25.0	5.0	lyyj	A 105	Y A	2.36	25.0	5.0
lzg4	A 77	C S	3.36	25.0	7.0	lzg4	A 290	W F	0.83	25.0	7.0
lznj_b	B 9	S D	-0.06	25.0	8.0	lznj_b	B 10	H D	-0.76	24.0	7.2
lznj_b	B 10	H E	-1.11	25.0	8.0	lznj_b	B 10	H T	-0.03	25.0	8.0
lznj_b	B 25	F D	-0.48	25.0	8.0	lznj_b	B 25	F H	-0.75	25.0	8.0
lznj_b	B 26	Y T	0.22	25.0	8.0	lznj_b	B 29	K G	0.05	23.0	7.5
2a01_a	A 141	L R	0.65	25.0	7.4	2a36	A 22	T A	-0.40	25.0	6.0
2a36	A 22	T D	-1.50	25.0	6.0	2a36	A 22	T F	-1.30	25.0	6.0
2a36	A 22	T G	-3.59	20.1	6.0	2a36	A 22	T K	0.00	25.0	6.0
2a36	A 22	T L	-0.50	25.0	6.0	2a36	A 22	T N	-1.30	25.0	6.0
2a36	A 22	T S	-0.60	25.0	6.0	2abd	A 5	F A	2.61	5.0	5.3
2abd	A 9	A G	1.88	5.0	5.3	2abd	A 12	V A	1.54	5.0	5.3
2abd	A 15	L A	3.28	5.0	5.3	2abd	A 21	D A	-0.03	5.0	5.3
2abd	A 21	D H	0.56	5.0	5.3	2abd	A 25	L A	1.60	5.0	5.3
2abd	A 26	F A	1.79	5.0	5.3	2abd	A 28	Y A	2.74	5.0	5.3
2abd	A 28	Y F	1.23	5.0	5.3	2abd	A 28	Y N	2.48	5.0	5.3
2abd	A 31	Y N	1.86	5.0	5.3	2abd	A 32	K A	1.34	5.0	5.3
2abd	A 32	K E	1.48	5.0	5.3	2abd	A 32	K R	1.83	5.0	5.3
2abd	A 33	Q A	3.64	5.0	5.3	2abd	A 34	A G	1.33	5.0	5.3
2abd	A 35	T A	1.47	5.0	5.3	2abd	A 39	I A	1.05	5.0	5.3
2abd	A 52	K M	-0.24	5.0	5.3	2abd	A 54	K A	0.97	5.0	5.3
2abd	A 54	K M	-0.10	5.0	5.3	2abd	A 67	E A	0.60	5.0	5.3
2abd	A 69	A G	2.28	5.0	5.3	2abd	A 73	Y A	4.77	5.0	5.3
2abd	A 73	Y F	-0.29	5.0	5.3	2abd	A 74	I A	1.70	5.0	5.3
2abd	A 77	V A	1.57	5.0	5.3	2abd	A 80	L A	4.15	5.0	5.3
2ci2	I 21	K A	0.79	25.0	6.2	2ci2	I 21	K M	0.70	25.0	6.2
2ci2	I 22	T A	0.93	35.7	6.3	2ci2	I 22	T G	1.07	25.0	6.3
2ci2	I 22	T V	0.76	25.0	6.3	2ci2	I 26	E A	0.75	25.0	6.2
2ci2	I 26	E Q	0.60	25.0	6.2	2ci2	I 27	L A	2.44	33.7	5.7
2ci2	I 30	K A	0.39	25.0	6.2	2ci2	I 31	S A	0.96	31.2	5.8
2ci2	I 31	S G	0.49	25.0	5.7	2ci2	I 33	E D	0.65	25.0	6.2
2ci2	I 33	E N	0.55	32.2	6.3	2ci2	I 33	E Q	0.39	25.0	6.2
2ci2	I 34	E D	0.19	25.0	6.2	2ci2	I 34	E N	0.58	25.0	6.2
2ci2	I 34	E Q	0.58	25.0	6.2	2ci2	I 35	A G	1.25	25.0	6.2
2ci2	I 36	K A	0.70	35.8	6.3	2ci2	I 36	K G	2.16	25.0	6.2
2ci2	I 37	K A	0.18	35.8	6.3	2ci2	I 37	K G	1.18	35.8	6.3
2ci2	I 38	V A	0.31	31.2	5.8	2ci2	I 39	I L	1.96	30.0	7.0
2ci2	I 39	I V	1.16	30.3	5.8	2ci2	I 40	L A	1.27	25.0	6.2
2ci2	I 40	L G	1.73	25.0	6.2	2ci2	I 41	Q A	0.28	25.0	6.2
2ci2	I 41	Q G	0.76	25.0	6.2	2ci2	I 42	D A	1.00	25.0	6.2
2ci2	I 43	K A	0.82	39.8	5.9	2ci2	I 43	K G	3.34	25.0	6.2
2ci2	I 45	E A	0.64	37.2	5.8	2ci2	I 48	I A	3.68	25.0	5.3
2ci2	I 48	I V	0.97	33.4	5.7	2ci2	I 49	I A	1.05	35.7	6.3
2ci2	I 49	I G	3.23	25.0	6.3	2ci2	I 49	I T	1.21	25.0	6.3
2ci2	I 49	I V	0.10	35.7	6.3	2ci2	I 51	L A	2.16	35.8	6.3
2ci2	I 51	L I	0.63	25.0	6.2	2ci2	I 51	L V	0.67	35.8	6.3
2ci2	I 53	V A	0.88	35.7	6.3	2ci2	I 53	V G	2.26	25.0	6.3
2ci2	I 53	V T	1.31	35.7	6.3	2ci2	I 55	T A	0.59	25.0	6.2
2ci2	I 55	T S	0.50	25.0	6.2	2ci2	I 55	T V	1.16	25.0	6.2

2ci2	I 56	I A	0.65	25.0	6.2	2ci2	I 57	V A	1.07	25.0	6.2
2ci2	I 58	T A	0.69	25.0	6.3	2ci2	I 58	T D	0.00	25.0	6.3
2ci2	I 60	E A	0.89	25.0	6.3	2ci2	I 62	R A	0.80	25.0	6.2
2ci2	I 64	D A	0.91	25.0	6.2	2ci2	I 66	V A	4.92	25.0	5.3
2ci2	I 67	R A	1.21	30.1	7.0	2ci2	I 68	L A	3.70	25.0	5.3
2ci2	I 69	F A	3.53	25.0	6.2	2ci2	I 69	F L	2.05	35.8	6.3
2ci2	I 69	F V	1.90	25.0	6.2	2ci2	I 70	V A	1.74	33.7	5.7
2ci2	I 71	D A	3.28	25.0	6.2	2ci2	I 72	K N	0.61	25.0	6.2
2ci2	I 75	N A	1.02	25.0	6.2	2ci2	I 75	N D	1.36	25.0	6.2
2ci2	I 76	I A	4.21	25.0	4.8	2ci2	I 76	I V	-0.10	33.7	5.7
2ci2	I 77	A G	1.42	25.0	6.3	2ci2	I 79	V A	1.46	25.0	6.3
2ci2	I 79	V G	2.38	25.0	6.3	2ci2	I 79	V T	0.89	25.0	6.3
2ci2	I 82	V A	1.36	25.0	6.3	2ci2	I 82	V G	3.24	25.0	6.3
2ci2	I 82	V T	1.33	25.0	6.3	2dri	A 27	A T	3.30	25.0	7.7
2dri	A 50	V E	3.50	25.0	7.7	2h61_ab	A 3	L A	0.64	25.0	7.2
2h61_ab	A 3	L S	1.25	25.0	7.2	2h61_ab	A 7	M A	2.00	25.0	7.2
2h61_ab	A 11	I A	1.65	25.0	7.2	2h61_ab	A 14	F A	2.85	25.0	7.2
2hpr	A 46	S D	-0.72	54.2	7.0	2imm	A 15	A L	-1.36	20.0	7.4
2imm	A 21	M I	-0.24	20.0	7.4	2imm	A 21	M L	0.31	20.0	7.4
2imm	A 24	K R	0.17	20.0	7.4	2imm	A 32	F Y	-0.38	20.0	7.4
2imm	A 63	T S	-0.29	20.0	7.4	2imm	A 79	Q E	0.41	20.0	7.4
2imm	A 90	N Q	-1.05	20.0	7.4	2imm	A 100	A G	-0.02	20.0	7.4
2imm	A 106	L I	-0.36	20.0	7.4	2lzm	A 3	I A	0.79	59.3	5.4
2lzm	A 3	I C	-0.07	59.3	5.4	2lzm	A 3	I D	2.87	59.3	5.4
2lzm	A 3	I E	1.72	53.0	4.0	2lzm	A 3	I F	1.02	53.0	4.0
2lzm	A 3	I G	2.03	59.3	5.4	2lzm	A 3	I L	-0.77	56.2	4.2
2lzm	A 3	I M	0.76	59.3	5.4	2lzm	A 3	I S	1.75	59.3	5.4
2lzm	A 3	I T	2.15	53.0	4.0	2lzm	A 3	I V	0.45	59.3	5.4
2lzm	A 3	I W	2.80	64.7	6.5	2lzm	A 3	I Y	2.39	59.3	5.4
2lzm	A 6	M I	3.10	43.5	6.5	2lzm	A 11	E A	-1.10	66.5	5.4
2lzm	A 11	E F	-1.70	66.5	5.4	2lzm	A 11	E M	-1.60	66.5	5.4
2lzm	A 16	K E	-0.15	61.2	4.4	2lzm	A 25	Y G	4.55	22.0	7.0
2lzm	A 30	G A	-0.10	66.5	5.4	2lzm	A 30	G F	1.50	66.5	5.4
2lzm	A 38	S A	0.77	53.4	3.0	2lzm	A 38	S D	0.01	50.1	5.7
2lzm	A 41	A V	-0.37	57.0	3.9	2lzm	A 44	S A	-0.44	47.8	2.5
2lzm	A 51	G D	2.63	22.0	7.0	2lzm	A 54	C T	-0.87	67.6	6.2
2lzm	A 54	C V	0.70	70.0	6.5	2lzm	A 55	N G	0.58	59.3	5.4
2lzm	A 58	I Y	3.11	22.0	7.0	2lzm	A 60	K H	0.26	54.9	5.4
2lzm	A 68	N A	-0.05	47.8	2.5	2lzm	A 77	G A	0.20	48.4	5.9
2lzm	A 83	K H	0.42	54.9	5.4	2lzm	A 90	S H	1.09	59.0	5.5
2lzm	A 96	R H	2.91	63.6	5.6	2lzm	A 98	A T	3.83	22.0	7.0
2lzm	A 98	A V	4.98	27.8	5.7	2lzm	A 102	M V	3.00	47.0	3.0
2lzm	A 103	V A	1.91	22.0	7.0	2lzm	A 105	Q A	0.68	59.8	4.8
2lzm	A 105	Q E	0.94	59.8	4.8	2lzm	A 105	Q G	2.30	41.7	5.9
2lzm	A 113	G A	-0.39	53.3	4.0	2lzm	A 115	T E	-0.03	60.8	5.0
2lzm	A 116	N D	-0.47	60.9	4.6	2lzm	A 117	S F	-1.10	66.5	5.4
2lzm	A 117	S I	-1.70	66.5	5.4	2lzm	A 117	S V	-2.00	66.5	5.4
2lzm	A 119	R E	0.06	46.9	4.8	2lzm	A 119	R M	-0.00	59.8	4.8
2lzm	A 123	Q E	-0.27	61.9	5.5	2lzm	A 124	K G	0.08	59.3	5.4
2lzm	A 128	E A	-0.16	40.8	2.0	2lzm	A 128	E K	1.16	47.0	3.0
2lzm	A 129	A V	0.74	47.7	2.5	2lzm	A 131	V A	-0.30	53.2	3.4
2lzm	A 131	V D	-0.08	53.1	3.0	2lzm	A 131	V E	-0.20	53.1	3.0
2lzm	A 131	V G	0.68	53.1	3.0	2lzm	A 131	V I	-0.16	53.1	3.0
2lzm	A 131	V L	-0.09	53.1	3.0	2lzm	A 131	V M	-0.12	53.1	3.0
2lzm	A 131	V S	0.05	53.1	3.0	2lzm	A 131	V T	0.09	49.7	2.7
2lzm	A 132	N F	-1.30	66.5	5.4	2lzm	A 132	N I	-1.20	66.5	5.4
2lzm	A 132	N M	-1.50	66.5	5.4	2lzm	A 133	L A	4.19	40.8	2.0
2lzm	A 133	L F	0.26	47.7	2.5	2lzm	A 135	K E	0.83	46.9	4.8
2lzm	A 138	W Y	2.62	26.4	6.0	2lzm	A 144	N D	-0.39	61.2	5.2
2lzm	A 144	N E	-0.46	61.9	5.5	2lzm	A 146	A I	4.31	22.0	7.0
2lzm	A 146	A T	2.25	44.5	6.1	2lzm	A 146	A V	4.31	22.0	7.0
2lzm	A 147	K E	0.53	46.9	4.8	2lzm	A 149	V A	2.87	22.0	7.0
2lzm	A 149	V C	2.20	40.0	3.0	2lzm	A 152	T S	2.60	40.0	3.0
2lzm	A 153	F C	3.11	22.0	7.0	2lzm	A 154	R E	0.65	61.2	4.4

2lzm	A 156	G D	3.03	41.6	6.2	2lzm	A 157	T A	0.90	46.3	2.5
2lzm	A 157	T C	1.30	42.0	2.0	2lzm	A 157	T D	2.12	26.1	6.0
2lzm	A 157	T E	1.22	46.3	2.5	2lzm	A 157	T F	3.73	26.1	6.0
2lzm	A 157	T G	1.10	42.0	2.0	2lzm	A 157	T H	2.10	42.0	2.0
2lzm	A 157	T I	1.79	54.6	3.8	2lzm	A 157	T L	1.63	46.3	2.5
2lzm	A 157	T N	0.99	46.3	2.5	2lzm	A 157	T R	0.54	46.3	2.5
2lzm	A 157	T S	0.66	42.0	2.0	2lzm	A 157	T V	1.49	46.3	2.5
2lzm	A 160	A T	3.12	43.5	6.5	2nvh	A 4	R Q	0.57	25.0	6.5
2nvh	A 6	L A	2.13	25.0	6.5	2nvh	A 7	N D	-0.09	25.0	6.5
2nvh	A 7	N G	1.91	25.0	6.5	2nvh	A 8	C A	2.02	25.0	6.5
2nvh	A 8	C S	3.74	25.0	6.5	2nvh	A 9	T A	1.45	25.0	6.5
2nvh	A 9	T G	2.91	25.0	6.5	2nvh	A 9	T L	1.90	25.0	6.5
2nvh	A 9	T Q	2.53	25.0	6.5	2nvh	A 10	L A	3.90	25.0	6.5
2nvh	A 97	K G	1.65	25.0	6.5	2nvh	A 97	K R	1.80	25.0	6.5
2nvh	A 97	K V	-1.15	25.0	6.5	2ocj_a	A 175	R H	3.47	10.0	7.2
2ocj_a	A 242	C S	3.30	10.0	7.2	2ocj_a	A 248	R Q	2.03	10.0	7.2
2ocj_a	A 249	R S	1.81	10.0	7.2	2ocj_a	A 273	R H	0.13	10.0	7.2
2rn2	A 10	D A	-3.40	48.1	6.8	2rn2	A 10	D E	-1.04	48.1	6.8
2rn2	A 10	D H	-1.65	48.1	6.8	2rn2	A 10	D N	-0.99	48.1	6.8
2rn2	A 10	D S	-1.95	48.1	6.8	2rn2	A 23	G A	-0.57	51.9	4.6
2rn2	A 24	A V	-0.83	51.8	4.6	2rn2	A 41	R C	-0.33	51.8	4.6
2rn2	A 48	E A	0.23	48.1	6.8	2rn2	A 48	E D	0.05	48.1	6.8
2rn2	A 48	E Q	-0.15	48.1	6.8	2rn2	A 52	A C	-0.80	53.0	3.2
2rn2	A 52	A D	1.90	53.0	3.2	2rn2	A 52	A E	1.50	53.0	3.2
2rn2	A 52	A F	0.50	53.0	3.2	2rn2	A 52	A G	2.70	53.0	3.2
2rn2	A 52	A H	3.60	53.0	3.2	2rn2	A 52	A I	-1.90	53.0	3.2
2rn2	A 52	A L	-1.30	53.0	3.2	2rn2	A 52	A M	-0.50	53.0	3.2
2rn2	A 52	A N	1.80	53.0	3.2	2rn2	A 52	A Q	1.20	53.0	3.2
2rn2	A 52	A S	1.80	53.0	3.2	2rn2	A 52	A T	0.80	53.0	3.2
2rn2	A 52	A V	-1.70	51.6	3.1	2rn2	A 52	A Y	2.30	53.0	3.2
2rn2	A 53	I D	3.10	25.0	5.5	2rn2	A 53	I F	3.90	25.0	5.5
2rn2	A 53	I L	1.40	25.0	5.5	2rn2	A 53	I V	0.20	25.0	5.5
2rn2	A 62	H A	-0.44	25.0	6.4	2rn2	A 62	H D	-0.13	51.8	4.6
2rn2	A 62	H R	-0.22	51.8	4.6	2rn2	A 68	S A	0.20	34.0	4.6
2rn2	A 68	S G	2.17	34.0	4.6	2rn2	A 68	S L	0.82	34.0	4.6
2rn2	A 68	S T	0.01	34.0	4.6	2rn2	A 68	S V	-0.70	34.0	4.6
2rn2	A 70	D A	-0.65	48.1	6.8	2rn2	A 70	D E	-0.25	48.1	6.8
2rn2	A 70	D N	-0.89	48.1	6.8	2rn2	A 74	V A	2.98	51.2	4.6
2rn2	A 74	V I	-0.64	51.2	4.6	2rn2	A 74	V L	-0.97	51.6	4.6
2rn2	A 76	Q L	-0.24	50.1	3.0	2rn2	A 77	G A	0.90	49.8	3.0
2rn2	A 80	Q L	-0.30	50.1	3.0	2rn2	A 83	H A	-0.07	25.0	6.4
2rn2	A 91	K R	-0.07	49.8	4.6	2rn2	A 94	D E	0.40	49.8	4.6
2rn2	A 95	K A	-0.10	49.8	4.6	2rn2	A 95	K G	-1.83	49.8	4.6
2rn2	A 95	K N	-0.89	50.8	4.6	2rn2	A 114	H A	1.87	25.0	5.5
2rn2	A 117	K R	0.00	51.8	4.6	2rn2	A 119	E V	-0.51	51.8	4.6
2rn2	A 124	H A	-0.17	25.0	6.4	2rn2	A 125	A T	-0.04	51.2	4.6
2rn2	A 127	H A	0.32	25.0	6.4	2rn2	A 134	D A	-1.42	50.1	5.7
2rn2	A 134	D E	-0.81	52.0	4.6	2rn2	A 134	D H	-1.42	52.0	4.6
2rn2	A 134	D I	-1.07	52.0	4.6	2rn2	A 134	D L	-1.38	52.0	4.6
2rn2	A 134	D N	-0.81	50.1	5.7	2rn2	A 134	D Q	-1.02	52.0	4.6
2rn2	A 134	D S	-0.79	52.0	4.6	2rn2	A 134	D T	-0.74	52.0	4.6
2rn2	A 134	D V	-0.83	52.0	4.6	2rn2	A 135	E K	0.53	51.8	4.6
2trt_p	A 128	R E	-0.31	22.0	7.5	2trx_a	A 26	D A	-4.20	25.0	7.7
2trx_a	A 26	D I	-3.37	25.0	7.0	2trx_a	A 32	C A	3.50	25.0	7.0
2trx_a	A 35	C A	3.03	25.0	7.0	2trx_a	A 66	T L	1.03	25.0	7.0
2trx_a	A 77	T V	0.72	25.0	7.0	2trx_a	A 78	L K	1.95	85.3	7.0
2trx_a	A 78	L R	2.00	85.3	7.0	2tsl_p	A 52	I L	-0.10	25.0	7.8
2tsl_p	A 105	L V	3.15	25.0	7.8	3eca_q	A 12	T A	0.00	25.0	7.4
3eca_q	A 12	T S	0.24	25.0	7.4	3eca_q	A 119	T A	0.00	25.0	7.4
3eca_q	A 122	S A	-0.96	25.0	7.4	3gly	A 137	G A	0.31	30.0	4.5
3gly	A 139	G A	1.40	30.0	4.5	3gly	A 251	G A	0.14	30.0	4.5
3gly	A 383	G A	-0.11	30.0	4.5	3hhr_a	A 71	S A	1.12	20.0	8.0
3hhr_a	A 71	S Q	1.37	20.0	8.0	3hhr_a	A 71	S T	0.20	20.0	8.0
3hhr_a	A 71	S V	1.26	20.0	8.0	3hhr_a	A 74	E A	0.95	20.0	8.0

3hrh_a	A 74	E D	1.26	20.0	8.0	3hrh_a	A 74	E L	1.01	20.0	8.0
3hrh_a	A 74	E Q	0.71	20.0	8.0	3hrh_a	A 74	E S	1.01	20.0	8.0
3hrh_a	A 74	E T	1.13	20.0	8.0	3mbp	A 8	V G	-0.38	25.0	7.6
3mbp	A 10	W A	4.31	25.0	7.6	3mbp	A 19	G C	2.15	25.0	7.6
3mbp	A 55	D N	-0.69	25.0	7.6	3mbp	A 276	A G	1.10	25.0	7.6
3mbp	A 283	Y D	2.30	25.0	7.6	3mbp	A 345	T I	-0.17	25.0	7.6
3pgk	A 48	Y W	1.62	25.0	7.5	3pgk	A 122	Y W	2.19	25.0	7.5
3pgk	A 194	F W	1.12	25.0	7.5	3pgk	A 308	W F	2.46	25.0	7.5
3pgk	A 308	W Y	1.06	23.6	7.5	3pgk	A 333	W F	1.88	24.1	7.5
3pgk	A 333	W Y	1.13	25.0	7.5	3pgk	A 388	H Q	0.84	25.0	6.5
3pgk	A 399	L W	2.56	25.0	7.5	3sil	A 53	A L	-0.90	25.0	7.0
3sil	A 69	A V	-0.45	25.0	7.0	3ssi_p	A 13	V A	3.42	82.2	8.0
3ssi_p	A 13	V F	2.78	82.2	8.0	3ssi_p	A 13	V G	4.96	82.2	8.0
3ssi_p	A 13	V I	0.44	82.2	8.0	3ssi_p	A 13	V L	1.17	82.2	8.0
3ssi_p	A 13	V M	2.86	82.2	8.0	3ssi_p	A 73	M A	-0.21	53.4	6.9
3ssi_p	A 73	M D	-0.69	53.4	6.9	3ssi_p	A 73	M E	-0.37	53.4	6.9
3ssi_p	A 73	M G	0.11	53.4	6.9	3ssi_p	A 73	M I	0.50	53.4	6.9
3ssi_p	A 73	M K	-0.23	53.4	6.9	3ssi_p	A 73	M L	0.16	53.4	6.9
3ssi_p	A 73	M V	0.35	53.4	6.9	3ssi_p	A 103	M A	1.13	75.5	6.9
3ssi_p	A 103	M G	3.46	81.6	8.0	3ssi_p	A 103	M I	1.01	75.5	6.9
3ssi_p	A 103	M L	-0.08	75.5	6.9	3ssi_p	A 103	M V	0.93	75.5	6.9
4lyz	A 3	F Y	0.45	74.0	6.4	4lyz	A 12	M F	-0.28	66.0	2.7
4lyz	A 12	M L	0.57	66.0	2.7	4lyz	A 15	H L	-0.76	74.0	6.4
4lyz	A 19	N K	1.06	74.0	6.4	4lyz	A 21	R Q	0.15	74.0	6.4
4lyz	A 31	A I	-1.40	74.0	6.4	4lyz	A 31	A L	-1.80	74.0	6.4
4lyz	A 31	A V	-1.20	74.0	6.4	4lyz	A 34	F Y	-0.19	74.0	6.4
4lyz	A 35	E A	-1.24	35.0	4.6	4lyz	A 35	E H	2.45	35.0	4.6
4lyz	A 35	E Q	0.64	35.0	4.6	4lyz	A 40	T I	2.20	74.0	6.4
4lyz	A 40	T S	0.27	74.0	6.4	4lyz	A 46	N D	0.44	35.0	4.6
4lyz	A 49	G A	1.91	48.8	4.2	4lyz	A 49	G N	0.96	20.0	9.5
4lyz	A 55	I A	4.40	74.0	6.4	4lyz	A 55	I F	2.46	74.0	6.4
4lyz	A 55	I L	0.45	74.0	6.4	4lyz	A 55	I M	2.27	74.0	6.4
4lyz	A 55	I T	4.12	52.5	5.8	4lyz	A 55	I V	0.91	74.0	6.4
4lyz	A 58	I M	1.18	35.0	5.5	4lyz	A 67	G A	1.19	48.8	4.2
4lyz	A 68	R K	0.04	74.0	6.4	4lyz	A 71	G A	0.38	65.6	2.7
4lyz	A 73	R K	-0.23	74.0	6.4	4lyz	A 77	N H	0.38	74.0	6.4
4lyz	A 78	I M	0.90	35.0	5.5	4lyz	A 91	S A	0.15	74.0	6.4
4lyz	A 91	S D	2.31	74.0	6.4	4lyz	A 91	S T	-0.99	74.0	6.4
4lyz	A 91	S V	0.08	74.0	6.4	4lyz	A 91	S Y	3.07	74.0	6.4
4lyz	A 94	C A	4.78	20.0	9.5	4lyz	A 98	I M	0.90	35.0	5.5
4lyz	A 101	D A	-0.76	74.0	6.4	4lyz	A 101	D E	0.00	74.0	6.4
4lyz	A 101	D F	-0.72	74.0	6.4	4lyz	A 101	D G	-0.45	74.0	6.4
4lyz	A 101	D K	-0.19	74.0	6.4	4lyz	A 101	D N	-0.04	74.0	6.4
4lyz	A 101	D Q	0.08	74.0	6.4	4lyz	A 101	D R	-0.27	74.0	6.4
4lyz	A 101	D S	-0.87	74.0	6.4	4lyz	A 102	G A	-0.02	65.6	2.7
4lyz	A 102	G R	-0.38	74.0	6.4	4lyz	A 102	G V	0.04	74.0	6.4
4lyz	A 103	N D	-0.24	20.0	9.5	4lyz	A 105	M T	0.24	20.0	9.5
4lyz	A 108	W Q	3.95	35.0	4.6	4lyz	A 108	W Y	1.92	35.0	4.6
4lyz	A 114	R H	-0.68	74.0	6.4	4lyz	A 117	G A	1.46	65.6	2.7
4lyz	A 121	Q H	0.45	74.0	6.4	5cro_q	A 16	Q L	-1.40	45.0	3.0
5cro_q	A 26	Y C	-1.10	45.0	5.8	5cro_q	A 26	Y D	-1.35	45.0	7.0
5cro_q	A 26	Y F	-0.20	45.0	7.0	5cro_q	A 26	Y H	-0.95	45.0	7.0
5cro_q	A 26	Y L	-0.55	45.0	7.0	5cro_q	A 26	Y Q	-0.70	45.0	7.0
5cro_q	A 26	Y V	-0.45	45.0	7.0	5cro_q	A 26	Y W	0.05	45.0	7.0
5cro_q	A 36	A S	-0.20	45.0	3.0	5dfr	A 2	I V	0.55	15.0	7.8
5dfr	A 15	G A	-0.44	15.0	7.8	5dfr	A 22	W L	0.31	15.0	7.8
5dfr	A 24	L V	1.29	15.0	7.8	5dfr	A 27	D N	-1.21	15.0	7.8
5dfr	A 28	L R	-1.08	15.0	7.8	5dfr	A 30	W A	2.03	15.0	7.8
5dfr	A 30	W E	2.42	15.0	7.8	5dfr	A 30	W H	2.44	15.0	7.8
5dfr	A 30	W M	1.94	15.0	7.8	5dfr	A 30	W N	2.07	15.0	7.8
5dfr	A 30	W R	2.09	15.0	7.8	5dfr	A 30	W S	2.29	15.0	7.8
5dfr	A 30	W Y	1.79	15.0	7.8	5dfr	A 31	F A	1.72	15.0	7.8
5dfr	A 31	F V	1.46	15.0	7.8	5dfr	A 35	T A	1.10	15.0	7.8
5dfr	A 40	V A	1.59	15.0	7.8	5dfr	A 40	V F	1.99	15.0	7.8

5dfr	A 40	V H	2.76	15.0	7.8	5dfr	A 40	V I	0.50	15.0	7.8
5dfr	A 40	V L	0.78	15.0	7.8	5dfr	A 40	V M	1.27	15.0	7.8
5dfr	A 40	V N	1.82	15.0	7.8	5dfr	A 40	V R	1.38	15.0	7.8
5dfr	A 40	V S	2.04	15.0	7.8	5dfr	A 43	G A	0.48	15.0	7.8
5dfr	A 44	R A	0.94	15.0	7.8	5dfr	A 44	R L	-0.78	15.0	7.8
5dfr	A 54	L V	0.32	15.0	7.8	5dfr	A 59	N C	-0.24	15.0	7.8
5dfr	A 59	N E	1.36	15.0	7.8	5dfr	A 59	N G	2.01	15.0	7.8
5dfr	A 59	N H	0.81	15.0	7.8	5dfr	A 59	N I	-0.13	15.0	7.8
5dfr	A 59	N K	1.55	15.0	7.8	5dfr	A 59	N L	-0.01	15.0	7.8
5dfr	A 59	N M	0.14	15.0	7.8	5dfr	A 59	N Q	0.35	15.0	7.8
5dfr	A 59	N S	1.26	15.0	7.8	5dfr	A 59	N T	0.05	15.0	7.8
5dfr	A 59	N V	-0.36	15.0	7.8	5dfr	A 59	N W	0.79	15.0	7.8
5dfr	A 61	I L	0.36	15.0	7.8	5dfr	A 61	I V	0.83	15.0	7.8
5dfr	A 67	G A	0.05	15.0	7.0	5dfr	A 67	G C	0.51	15.0	7.0
5dfr	A 67	G D	0.58	15.0	7.0	5dfr	A 67	G L	0.51	15.0	7.0
5dfr	A 67	G S	0.27	15.0	7.0	5dfr	A 67	G T	0.62	15.0	7.0
5dfr	A 67	G V	0.70	15.0	7.0	5dfr	A 74	W F	1.20	15.0	7.8
5dfr	A 75	V A	0.05	15.0	7.8	5dfr	A 75	V C	0.05	15.0	7.8
5dfr	A 75	V H	1.72	15.0	7.1	5dfr	A 75	V I	1.65	15.0	7.8
5dfr	A 75	V R	2.00	15.0	7.8	5dfr	A 75	V S	0.80	15.0	7.8
5dfr	A 75	V Y	1.80	15.0	7.8	5dfr	A 85	C S	0.97	15.0	7.8
5dfr	A 88	V A	-0.29	20.0	7.2	5dfr	A 88	V I	0.49	20.0	7.2
5dfr	A 91	I L	1.50	15.0	7.8	5dfr	A 91	I V	1.34	15.0	7.8
5dfr	A 94	I L	0.63	15.0	7.8	5dfr	A 94	I V	0.67	15.0	7.8
5dfr	A 95	G A	0.90	15.0	7.8	5dfr	A 112	L I	0.25	15.0	7.8
5dfr	A 112	L V	1.39	15.0	7.8	5dfr	A 113	T V	0.91	15.0	7.8
5dfr	A 121	G A	0.01	15.0	7.0	5dfr	A 121	G C	0.22	15.0	7.0
5dfr	A 121	G D	0.34	15.0	7.0	5dfr	A 121	G H	0.56	15.0	7.0
5dfr	A 121	G L	0.58	15.0	7.0	5dfr	A 121	G S	0.08	15.0	7.0
5dfr	A 121	G V	0.99	15.0	7.0	5dfr	A 121	G Y	0.51	15.0	7.0
5dfr	A 122	D A	1.00	15.0	7.8	5dfr	A 139	E K	1.59	15.0	7.8
5dfr	A 139	E Q	0.89	15.0	7.8	5dfr	A 148	S A	0.42	15.0	7.8
5dfr	A 148	S E	0.61	15.0	7.8	5dfr	A 148	S K	0.38	15.0	7.8
5dfr	A 148	S N	0.88	15.0	7.8	5dfr	A 148	S R	0.66	15.0	7.8
5dfr	A 148	S T	0.41	15.0	7.8	5dfr	A 148	S V	0.35	15.0	7.8
5dfr	A 152	C E	0.97	15.0	7.8	5dfr	A 155	I A	2.99	15.0	7.8
5dfr	A 155	I D	3.19	15.0	7.8	5dfr	A 155	I E	2.62	15.0	7.8
5dfr	A 155	I K	2.69	15.0	7.8	5dfr	A 155	I L	1.63	15.0	7.8
5dfr	A 155	I Q	3.01	15.0	7.8	5dfr	A 155	I R	2.65	15.0	7.8
5dfr	A 155	I S	3.09	15.0	7.8	5dfr	A 155	I T	2.53	15.0	7.8
5dfr	A 155	I V	0.03	15.0	7.8	5dfr	A 155	I W	3.21	15.0	7.8
5dfr	A 155	I Y	2.85	15.0	7.8	5pti	A 4	F L	2.20	25.0	8.7
5pti	A 10	Y L	2.90	25.0	8.7	5pti	A 12	G D	4.30	25.0	8.7
5pti	A 12	G V	4.10	25.0	8.7	5pti	A 16	A T	1.70	25.0	8.7
5pti	A 16	A V	1.30	25.0	8.7	5pti	A 21	Y A	3.90	20.0	2.0
5pti	A 21	Y L	3.40	25.0	8.7	5pti	A 22	F A	1.11	22.7	2.0
5pti	A 33	F I	2.40	25.0	8.7	5pti	A 33	F L	2.70	25.0	8.7
5pti	A 35	Y A	4.70	25.0	8.7	5pti	A 35	Y D	3.80	25.0	8.7
5pti	A 35	Y F	0.60	25.0	8.7	5pti	A 35	Y G	5.00	25.0	5.4
5pti	A 35	Y N	3.70	25.0	8.7	5pti	A 36	G D	2.80	25.0	8.7
5pti	A 36	G S	0.70	72.6	4.6	5pti	A 37	G A	3.01	23.9	5.5
5pti	A 37	G D	1.70	25.0	8.7	5pti	A 44	N G	4.70	25.0	2.0

^a We checked that the multimeric state of each protein structure corresponds to its naturally occurring biological conformation. PDB records followed by '_a', '_b', '_c', '_i' or '_u' indicate that only the chain (A,B,C,I or U, respectively) was taken into account. For PDB records followed by '_p' or '_q', the multimeric forms were those retrieved from the PQS server (<http://www.ebi.ac.uk/msd-srv/pqs>), or referred to as “biological unit” on the PDB (www.rcsb.org), respectively. PDB record 1cun is followed by '_17' to indicate that only domain 17 (chain A, residues 107-219) is taken into account, since the experiments were performed on this domain only.

^b The temperature and pH are those of the experiment that led to the determination of $\Delta\Delta G_M$. When $\Delta\Delta G_M$ is an average value over several experiments, the given temperature and pH are also average values.

2. Dataset of 350 mutants for validation and comparison

PDB Code ¹	Chain name and residue position	Wild-type and mutant amino acid	$\Delta\Delta G_M$ (kcal/mol)	$\Delta\Delta G_P^2$ PoPMuSiC (v2)	$\Delta\Delta G_P^2$ PoPMuSiC (v1)	$\Delta\Delta G_P^2$ Automute	$\Delta\Delta G_P^2$ CUPSAT	$\Delta\Delta G_P^2$ Dmutant	$\Delta\Delta G_P^2$ Eris	$\Delta\Delta G_P^2$ I-mutant	Remarks
1aj3	A 10	H A	-0.50	-0.08	0.11	1.00	0.88	0.03	-1.14	0.54	[a1,c1]
1aj3	A 23	I A	3.60	2.18	2.28	2.63	0.84	1.20	-0.78	1.11	[a1,c1]
1aj3	A 25	E A	-0.10	0.30	0.18	0.64	1.26	0.20	1.41	0.84	[a1,c1]
1aj3	A 26	K A	0.00	2.34	0.63	0.57	-0.93	0.10	-7.05	0.66	[a1,c1]
1aj3	A 30	V A	0.20	1.48	1.02	2.96	-1.27	0.44	1.14	1.05	[a1,c1]
1aj3	A 40	T A	-0.30	-0.01	-0.34	0.35	0.90	0.15	-1.25	0.31	[a1,c1]
1aj3	A 42	V A	0.40	0.22	-0.14	2.81	-0.36	-0.12	0.56	1.47	[a1,c1]
1aj3	A 44	N G	0.40	0.99	1.63	1.82	0.67	0.90	2.76	2.93	[a1,c1]
1aj3	A 45	L A	0.20	0.57	0.15	2.55	1.03	0.84	2.14	2.15	[a1,c1]
1aj3	A 47	K A	-0.40	0.93	-0.01	1.06	1.16	0.06	-1.86	0.20	[a1,c1]
1aj3	A 47	K G	0.50	1.55	1.66	1.12	2.28	0.67	1.06	1.23	[a1,c1]
1aj3	A 84	I A	2.00	2.24	1.69	2.76	-0.04	1.21	4.42	2.23	[a1,c1]
1aj3	A 86	Q A	0.00	-0.20	0.05	0.43	-0.59	0.47	0.01	-0.37	[a1,c1]
1aj3	A 86	Q G	1.30	1.06	1.03	0.56	1.56	1.40	2.11	0.59	[a1,c1]
1aj3	A 88	L A	2.80	2.56	1.99	2.67	5.24	2.14	3.06	1.68	[a1,c1]
1aj3	A 93	D A	-0.70	-0.13	-0.03	0.59	1.54	0.03	-0.37	0.56	[a1,c1]
1aj3	A 93	D G	0.30	1.00	1.70	0.58	1.63	1.00	2.53	0.54	[a1,c1]
1aj3	A 96	K A	0.40	0.62	0.01	0.69	2.28	0.75	-0.11	0.10	[a1,c1]
1aj3	A 96	K G	1.30	1.50	1.00	0.51	2.40	1.72	1.38	0.96	[a1,c1]
1aj3	A 98	L A	3.80	2.35	1.79	2.39	1.56	1.94	6.04	2.02	[a1,c1]
1aky	A 48	Q E	0.96	-0.25	0.09	0.06	0.03	0.07	1.39	-0.66	[a2,c2]
1aon_u	U 48	I W	0.20	0.48	0.48	1.32	-1.28	-1.52	8.41	0.74	[a1,c1]
1aps	A 75	I V	1.41	1.24	1.56	2.20	-0.17	-4.20	0.39	0.53	[a3,c1]
1bni_a	A 27	K A	-0.44	0.20	-0.05	0.18	2.19	0.41	-2.54	0.68	[a1,c1]
1bni_a	A 59	R A	-0.64	-0.30	0.31	0.98	0.83	0.37	1.71	0.39	[a1,c1]
1bni_a	A 76	I T	2.64	2.15	1.32	1.89	1.69	1.14	5.29	2.25	[a3,c1]
1bta	A 22	K Q	0.79	-0.01	0.21	-0.34	1.38	-0.03	0.35	-0.72	[a3,c1]
1bta	A 60	K E	1.17	0.94	1.11	1.19	0.61	1.25	0.30	0.32	[a3,c1]
1bta	A 75	R L	-0.75	-0.11	0.21	1.66	1.56	-1.65	-0.25	-0.35	[a3,c1]
1bvce	A 24	H V	0.52	-0.00	-0.51	0.24	0.09	-1.45	1.25	-0.79	[a1,c1]

lbvc	A 48	H Q	0.62	0.04	0.20	0.29	0.42	-0.20	3.39	-0.10	[a1,c1]
lbvc	A 119	H F	0.68	0.42	0.71	0.36	0.00	-1.19	0.96	0.39	[a1,c1]
lc9o_a	A 12	E K	0.32	0.04	0.42	99.99	0.23	0.20	1.96	-0.19	[c2]
lc9o_a	A 21	E A	0.29	0.31	0.27	0.55	-0.64	0.22	-0.82	-0.44	[a2,c2]
lc9o_a	A 38	F W	-0.24	0.05	0.21	1.48	1.32	-0.59	4.82	-1.27	[a1,c1]
lc9o_a	A 50	E K	0.58	0.20	0.05	1.09	-0.56	-0.42	2.87	0.20	[a2,c2]
lc9o_a	A 56	R E	-0.69	-0.01	0.27	99.99	0.52	0.26	2.08	0.13	[c2]
lcey	A 12	D A	-2.50	0.69	1.36	0.25	0.61	-0.77	-2.09	1.45	[a1,c1]
lcey	A 14	F N	-2.64	0.54	-0.42	2.38	1.58	1.51	-5.21	1.04	[a3,c1]
lcey	A 57	D A	-3.30	0.37	0.08	1.81	0.02	-0.77	-1.00	2.48	[a1,c1]
lcey	A 77	A G	0.31	-0.48	-0.80	0.98	-0.60	0.09	-0.13	1.06	[a3,c1]
lcey	A 80	A G	-0.43	0.14	0.01	2.26	0.72	0.75	2.65	-1.06	[a3,c1]
lcey	A 88	A G	-0.04	0.30	-0.61	1.60	-0.10	0.45	2.79	1.06	[a3,c1]
lcey	A 99	A G	0.48	1.25	1.09	2.83	0.31	1.00	4.07	-1.06	[a3,c1]
lcse_i	I 54	V A	1.58	2.85	4.44	2.99	6.44	2.30	6.86	3.18	[a1,c1]
lcs p	A 3	E Q	-1.14	-0.08	-0.12	0.20	99.99	-0.65	0.12	-0.38	[a2]
lcs p	A 43	E S	-0.29	-0.16	0.23	0.43	99.99	0.24	0.11	-1.12	[a2]
lcs p	A 48	S R	-1.58	0.53	0.09	0.55	99.99	-0.98	-3.22	-0.33	[a2]
lcs p	A 56	R Q	-0.28	-0.34	0.10	1.14	99.99	0.04	3.19	0.26	[a2]
lcun_17	A 115	Q G	1.15	1.29	1.03	0.79	1.42	1.25	2.34	0.96	[a1,c1]
lcun_17	A 126	A G	1.65	1.11	2.18	1.67	1.52	0.95	3.67	0.73	[a1,c1]
lcun_17	A 128	I A	1.65	2.96	2.06	2.21	2.34	1.65	5.54	1.68	[a1,c1]
lcun_17	A 128	I V	2.85	1.40	1.75	0.72	3.78	0.69	2.06	-0.75	[a1,c1]
lcun_17	A 152	K A	0.15	0.47	0.01	-0.53	1.71	0.33	-2.72	0.16	[a1,c1]
lcun_17	A 152	K G	1.45	1.58	1.00	-0.51	0.69	1.17	0.38	0.31	[a1,c1]
lcun_17	A 156	A G	1.45	1.33	1.23	0.42	1.35	0.76	3.15	0.29	[a1,c1]
lcun_17	A 157	F L	1.85	0.88	0.38	1.81	1.07	1.44	1.01	1.14	[a1,c1]
lcun_17	A 173	A G	1.95	0.95	1.73	1.84	-0.27	0.78	2.91	1.88	[a1,c1]
lcun_17	A 191	A G	1.35	1.30	1.23	2.09	0.20	0.83	2.57	-1.88	[a1,c1]
lcun_17	A 193	M A	2.65	2.58	1.97	1.96	-0.39	0.96	5.31	2.03	[a1,c1]
lcun_17	A 196	L A	4.55	3.47	2.50	1.80	0.30	2.19	5.26	2.24	[a1,c1]
lcun_17	A 201	S A	-0.15	-0.16	-0.32	0.69	2.30	-0.40	-1.79	0.31	[a1,c1]
lcun_17	A 201	S G	0.95	0.87	0.66	0.77	0.78	0.60	2.00	0.19	[a1,c1]
lcun_17	A 203	L A	4.05	2.31	1.89	1.71	1.70	2.16	7.28	2.56	[a1,c1]
lcun_17	A 212	A G	1.45	1.14	2.09	0.95	0.31	0.89	2.77	0.78	[a1,c1]
lcun_17	A 214	L A	3.65	2.33	2.04	2.15	3.04	1.55	7.19	3.73	[a1,c1]
ldkt_a	A 9	S A	0.43	0.86	1.14	0.63	0.53	0.02	3.79	0.99	[a3,c1]
ldkt_a	A 11	K A	-0.62	0.49	0.31	-0.26	0.80	0.59	-0.28	0.59	[a3,c1]

ldkt a	A 39	S A	0.60	0.62	0.67	0.44	0.75	0.00	3.69	0.38	[a3,c1]
ldkt a	A 55	V A	0.73	1.05	1.01	1.19	1.74	0.85	3.10	1.53	[a3,c1]
ldkt a	A 58	M L	0.23	0.07	0.23	1.10	0.50	-0.60	2.67	0.47	[a3,c1]
ldkt a	A 71	R A	0.59	1.25	0.88	1.43	1.59	1.46	5.60	0.86	[a3,c1]
le65 a	A 7	I S	3.44	3.32	3.45	2.62	2.80	2.46	7.07	1.43	[a3,c1]
le65 a	A 20	I T	2.39	2.67	2.43	2.48	3.54	2.90	7.16	2.17	[a1,c1]
le65 a	A 31	V T	1.08	2.59	3.47	2.84	0.64	1.84	4.81	1.86	[a1,c1]
le65 a	A 50	L V	0.36	1.24	1.05	1.98	2.74	1.52	8.69	1.08	[a1,c1]
le65 a	A 60	V G	3.11	2.42	1.83	2.41	10.42	2.13	7.05	3.34	[a1,c1]
le65 a	A 82	A G	3.11	1.28	1.24	1.27	1.91	1.05	4.36	3.63	[a1,c1]
le65 a	A 95	V T	-0.96	1.75	1.91	1.15	0.94	1.18	3.42	1.90	[a1,c1]
le65 a	A 117	H G	2.18	2.66	1.91	1.16	1.49	1.42	-0.11	0.73	[a3,c1]
ley0	A 7	L V	1.15	0.48	0.37	1.49	0.22	0.41	0.74	0.33	[a3,c1]
ley0	A 9	K F	1.03	-0.33	-0.26	0.34	1.13	-0.67	6.08	-0.57	[a3,c1]
ley0	A 13	T C	1.20	0.08	0.23	1.16	1.23	-0.70	-1.22	0.59	[a3,c1]
ley0	A 14	L V	1.63	0.96	0.53	1.42	2.00	0.59	1.91	1.49	[a3,c1]
ley0	A 15	I M	0.15	0.41	0.48	1.09	1.05	0.27	0.69	0.03	[a3,c1]
ley0	A 19	D F	1.28	0.43	1.21	0.19	0.49	0.29	10.00	0.06	[a3,c1]
ley0	A 21	D K	-1.10	1.51	0.74	0.92	0.28	-0.45	3.89	1.94	[a3,c1]
ley0	A 22	T I	0.61	1.11	1.42	0.64	0.39	-1.01	-1.52	0.08	[a3,c1]
ley0	A 23	V I	-0.03	0.74	0.67	0.90	0.33	-1.02	-0.61	0.98	[a3,c1]
ley0	A 23	V L	0.02	1.08	1.45	1.07	0.19	-1.37	0.46	0.34	[a3,c1]
ley0	A 24	K F	0.40	-0.41	-1.45	0.31	0.05	-1.94	9.59	-0.98	[a3,c1]
ley0	A 27	Y C	2.72	2.51	1.30	2.13	-0.24	1.86	5.23	0.75	[a3,c1]
ley0	A 29	G V	3.11	1.38	2.33	1.29	3.05	-0.32	-2.95	0.97	[a3,c1]
ley0	A 33	T C	1.04	0.88	-0.09	0.83	1.88	-0.70	-2.31	1.57	[a3,c1]
ley0	A 36	L V	3.58	1.45	1.21	1.33	3.11	1.38	10.00	1.15	[a3,c1]
ley0	A 37	L I	1.82	0.80	0.85	1.33	2.22	0.63	5.99	-0.11	[a3,c1]
ley0	A 39	V I	-0.11	0.71	1.22	0.69	0.26	-0.68	0.47	0.50	[a3,c1]
ley0	A 39	V L	0.90	1.05	2.08	1.06	-0.61	-0.87	2.13	0.64	[a3,c1]
ley0	A 41	T I	-0.86	0.08	0.22	0.19	-0.30	-1.28	10.00	-0.19	[a3,c1]
ley0	A 44	T C	0.04	0.58	-0.19	0.31	-2.08	-0.21	-0.78	0.08	[a3,c1]
ley0	A 51	V L	0.10	0.42	0.57	1.24	0.85	-0.07	3.21	0.01	[a3,c1]
ley0	A 54	Y F	0.38	0.72	1.57	-0.39	0.53	0.32	1.83	0.41	[a3,c1]
ley0	A 55	G V	1.48	0.57	1.40	1.00	-3.49	0.88	10.00	2.31	[a3,c1]
ley0	A 63	K Q	0.89	0.12	0.55	0.68	0.65	0.27	0.15	0.28	[a3,c1]
ley0	A 65	M F	1.62	0.82	0.93	1.26	1.54	-1.50	6.32	0.50	[a3,c1]
ley0	A 65	M I	1.43	0.80	0.71	1.25	1.76	-0.39	2.15	1.01	[a3,c1]

ley0	A 66	V I	0.76	0.50	0.44	0.16	2.56	-1.15	2.06	0.62	[a3,c1]
ley0	A 70	K E	0.30	-0.08	0.32	0.37	0.29	0.16	-1.38	0.44	[a3,c1]
ley0	A 72	I L	0.23	1.37	1.92	0.62	1.28	-0.42	2.13	0.93	[a3,c1]
ley0	A 74	V L	1.12	1.01	1.26	0.99	1.73	-0.79	4.86	-0.37	[a3,c1]
ley0	A 77	D K	3.28	1.71	2.02	1.73	2.78	-0.35	10.00	0.87	[a3,c1]
ley0	A 78	K Q	0.15	0.14	0.36	-0.22	0.15	0.01	-1.74	0.28	[a3,c1]
ley0	A 82	T C	0.19	0.16	0.16	0.51	0.07	-0.69	-1.42	0.75	[a3,c1]
ley0	A 82	T I	-0.51	0.28	0.34	0.53	1.32	-0.64	-2.37	0.01	[a3,c1]
ley0	A 84	K Q	0.15	-0.08	0.38	99.99	0.29	0.09	0.09	-0.13	[c1]
ley0	A 86	G F	1.99	1.59	2.44	1.00	3.06	-1.34	-1.80	0.18	[a3,c1]
ley0	A 89	L I	1.04	0.66	0.70	1.68	1.44	0.03	1.77	0.17	[a3,c1]
ley0	A 92	I M	1.75	1.66	2.83	1.67	2.83	0.99	-0.25	1.40	[a3,c1]
ley0	A 96	G F	2.55	1.21	1.58	1.49	5.00	-0.67	3.90	2.07	[a3,c1]
ley0	A 96	G V	3.74	1.90	2.33	1.56	3.80	-0.26	-2.95	2.67	[a3,c1]
ley0	A 104	V I	-0.27	0.58	1.14	0.47	-1.41	-0.55	1.95	-0.03	[a3,c1]
ley0	A 105	R C	2.55	1.67	0.84	1.72	4.60	0.48	2.51	0.76	[a3,c1]
ley0	A 108	L V	3.81	1.31	1.09	1.12	2.08	0.75	10.00	0.85	[a3,c1]
ley0	A 111	V I	0.74	0.57	1.07	0.95	1.86	-0.30	3.10	-0.02	[a3,c1]
ley0	A 111	V L	0.88	0.71	1.51	1.14	1.66	-0.52	1.34	0.65	[a3,c1]
ley0	A 114	V I	0.15	0.43	1.01	0.64	0.27	-0.33	2.05	0.08	[a3,c1]
ley0	A 124	H E	-0.46	-0.04	-0.18	0.22	-0.81	-0.04	-2.78	0.31	[a3,c1]
ley0	A 125	L I	0.96	1.03	1.18	1.63	-0.10	0.48	3.12	0.37	[a3,c1]
ley0	A 137	L V	1.42	0.93	0.04	1.10	1.21	0.52	5.02	1.33	[a3,c1]
ley0	A 139	I L	0.09	0.60	0.60	0.85	0.30	-0.32	1.03	-0.34	[a3,c1]
lfna	A 34	I V	0.11	1.13	1.42	0.72	2.19	0.90	0.31	0.55	[a3,c1]
lfna	A 50	V A	2.85	1.99	2.59	1.99	2.73	1.42	4.55	2.35	[a3,c1]
lftg	A 6	L A	3.11	3.10	3.10	2.42	3.35	3.63	7.79	3.35	[a3,c3]
lftg	A 65	D K	0.10	0.73	0.71	0.78	0.43	-0.64	3.02	-0.23	[a3,c3]
lftg	A 72	E K	-1.41	0.09	0.45	0.88	0.81	-0.86	1.39	1.03	[a3,c3]
lftg	A 75	D K	-1.03	-0.10	0.36	0.51	-0.62	-0.87	-1.77	0.10	[a3,c3]
lftg	A 84	A G	1.90	2.00	0.95	1.85	1.68	1.75	4.93	1.68	[a3,c3]
lftg	A 97	N A	0.58	1.57	1.01	1.61	2.41	0.14	2.15	1.91	[a3,c3]
lftg	A 99	Q A	-1.59	1.28	0.26	0.78	0.67	-0.10	3.26	2.48	[a3,c3]
lftg	A 110	S A	0.73	-0.11	-0.66	0.50	-0.18	-0.34	-0.07	0.86	[a3,c3]
lftg	A 126	D K	-0.81	-0.08	0.06	1.38	0.75	-0.47	1.66	0.69	[a3,c3]
lftg	A 156	I V	3.16	1.35	1.55	0.95	0.97	0.86	2.59	0.70	[a3,c3]
lftg	A 160	V A	2.07	1.96	1.14	2.12	0.98	1.55	5.65	2.33	[a3,c3]
lg4i	A 22	F I	-1.43	2.22	2.11	0.69	0.36	2.15	3.08	1.86	[a3,a4,c1]

lg4i	A 22	F Y	-0.83	0.93	1.44	0.73	1.83	0.31	0.44	1.46	[a3,a4,c1]
lg4i	A 48	H A	1.93	1.81	1.06	2.38	1.42	1.75	0.93	1.73	[a3,a4,c1]
lg4i	A 48	H Q	0.49	1.29	2.27	1.44	1.53	1.35	0.07	1.77	[a3,a4,c1]
lg4i	A 106	F A	1.23	3.08	3.77	0.74	1.20	5.17	6.12	3.54	[a3,a4,c1]
1h7m	A 2	D A	0.53	0.50	0.61	99.99	0.90	-0.31	99.99	0.28	[c1]
1h7m	A 9	K A	0.29	0.79	-0.35	99.99	0.19	0.69	99.99	0.24	[c1]
1h7m	A 33	K A	-0.12	0.29	0.43	99.99	1.93	-0.37	99.99	-0.24	[c1]
1h7m	A 46	K A	1.10	1.25	1.01	99.99	1.64	0.42	99.99	0.24	[c1]
1h7m	A 47	E A	0.05	-0.03	0.18	99.99	0.32	0.16	99.99	1.12	[c1]
1h7m	A 54	R A	0.26	0.24	0.10	99.99	0.67	0.27	99.99	1.10	[c1]
1h7m	A 64	E A	0.26	-0.08	0.14	99.99	-0.06	-0.40	99.99	-0.17	[c1]
1h7m	A 87	D A	1.36	0.48	0.52	99.99	0.89	-0.04	99.99	0.95	[c1]
1hfz a	A 32	H Y	-0.07	0.29	0.25	99.99	-0.36	-1.74	-2.85	-2.27	[c2]
1hfz a	A 59	I W	0.93	0.35	0.33	99.99	0.73	-1.92	7.07	2.13	[c2]
1hfz a	A 107	H W	1.72	0.61	1.08	99.99	1.84	-2.20	2.17	-1.10	[c2]
1hfz a	A 107	H Y	0.19	0.75	1.13	99.99	0.90	-1.59	-6.35	-1.02	[c2]
1hfz a	A 110	L E	0.19	0.46	-0.08	99.99	-0.31	1.08	1.22	-0.08	[c2]
1hfz a	A 114	K E	0.65	0.06	0.48	99.99	0.18	0.65	-2.36	0.08	[c2]
1hme	A 35	G H	0.33	0.29	0.62	1.30	-2.14	-0.29	-1.64	2.07	[a2,c2]
1hmk	A 8	V A	0.83	2.06	2.18	1.66	0.19	1.54	3.80	1.38	[a3,c1]
1hmk	A 12	L A	2.73	2.71	2.21	2.84	2.55	3.55	7.13	1.83	[a3,c1]
1hmk	A 27	V A	1.24	1.93	1.53	1.87	3.15	1.82	5.66	1.70	[a3,c1]
1hmk	A 29	T V	-2.26	0.51	-0.86	-0.65	-1.10	-1.95	-2.69	-0.98	[a3,c1]
1hmk	A 55	I V	2.72	1.33	1.46	0.72	0.78	0.91	-1.02	2.38	[a3,c1]
1hmk	A 60	W A	2.01	3.84	1.56	1.87	1.64	3.90	0.29	3.76	[a3,c1]
1hmk	A 89	I V	0.86	1.17	1.52	0.79	1.66	0.59	2.15	0.98	[a3,c1]
1hmk	A 95	I V	1.72	1.40	2.27	0.85	1.97	0.91	0.66	-0.98	[a3,c1]
1hmk	A 96	L A	1.75	2.38	1.81	2.18	0.55	2.20	3.67	2.56	[a3,c1]
1hmk	A 103	Y F	2.13	0.60	0.44	0.73	-0.41	-0.56	5.07	0.39	[a3,c1]
1hmk	A 110	L A	0.35	0.69	0.08	1.42	-0.84	1.17	3.31	0.90	[a3,c1]
1hms	A 4	F S	3.67	2.73	3.39	2.21	-0.42	3.82	8.28	2.35	[a2,c1]
1hms	A 16	F S	3.98	2.51	2.06	1.85	1.23	3.92	5.61	-2.35	[a2,c1]
1hms	A 40	T E	2.40	2.06	3.12	1.25	-1.13	0.13	-1.07	0.53	[a3,c1]
1hms	A 57	F S	2.43	0.73	0.67	2.32	0.74	1.65	1.96	1.10	[a3,c1]
1hms	A 66	L G	3.67	1.94	1.44	3.00	0.22	3.25	9.89	2.78	[a2,c1]
1hms	A 106	R T	2.84	0.55	0.38	1.74	-0.84	-0.21	3.96	0.61	[a3,c1]
liet	A 60	D R	-0.14	-0.23	0.20	0.38	-1.69	-1.95	-3.68	-1.56	[a2,c2]
lifc	A 6	W Y	0.87	1.18	1.10	1.84	0.01	13.06	-2.88	1.64	[a3,a5,c1]

lifc	A 60	V C	0.07	1.40	1.50	1.10	0.36	4.41	1.56	2.28	[a3,a5,c1]
lifc	A 60	V N	0.83	2.50	1.52	1.66	3.49	6.26	4.27	3.11	[a3,a5,c1]
lifc	A 64	L G	2.26	2.90	1.64	3.34	0.96	7.82	7.99	1.59	[a3,a5,c1]
lifc	A 65	G A	0.94	1.27	2.15	1.37	2.24	1.46	0.27	-1.31	[a3,a5,c1]
lifc	A 68	F A	0.42	2.86	1.74	2.08	2.69	7.17	3.85	2.54	[a3,a5,c1]
lifc	A 93	F A	2.37	3.87	2.11	1.84	2.25	11.26	9.18	-2.54	[a3,a5,c1]
ligv	A 13	Y F	1.08	0.74	1.12	0.75	1.18	-0.06	4.53	0.66	[a3,c1]
ligv	A 66	F W	0.93	0.78	1.79	2.35	0.12	-0.65	7.33	0.87	[a3,c1]
ligv	A 70	V L	0.13	0.50	0.18	1.12	0.96	-1.79	2.50	1.64	[a3,c1]
lih_b_a	A 37	F H	0.66	-0.28	-0.30	1.21	0.71	0.79	-1.39	0.04	[a3,c1]
lih_b_a	A 82	F Q	0.37	1.19	0.83	1.68	2.31	2.14	0.61	1.69	[a3,c1]
limq	A 19	V L	1.82	0.62	0.82	1.16	0.30	-1.06	5.61	0.53	[a1,c1]
limq	A 31	E L	0.67	0.08	0.43	0.72	0.90	-0.55	-6.86	-0.77	[a1,c1]
limq	A 41	E V	-0.89	0.86	0.83	0.58	1.20	-1.52	6.36	-0.65	[a1,c1]
liro	A 24	V I	-0.36	0.67	1.05	99.99	1.19	-0.09	-0.28	0.25	[c2]
liro	A 33	I L	-0.76	0.42	0.91	99.99	2.45	-0.18	4.35	0.26	[c2]
ljiw_i	I 10	D A	0.70	0.21	0.05	1.76	-0.07	-0.17	1.59	1.03	[a1,c1]
ljiw_i	I 15	W F	2.30	1.19	0.59	3.13	0.02	1.58	1.83	1.33	[a1,c1]
lk9q_a	A 30	L Y	-0.27	0.56	0.71	2.04	1.58	-0.81	-5.83	-0.43	[a3,c3]
lkfw	A 197	N K	-0.81	0.17	0.71	99.99	-2.75	-0.21	-2.45	0.40	[c2]
lkfw	A 405	G Q	-0.62	1.58	2.61	99.99	0.84	-0.65	-0.69	1.07	[c2]
lni_a	A 16	T V	-0.30	-0.07	-0.06	0.64	1.42	-0.89	-2.01	1.24	[a2,a6,c2]
lni_a	A 30	Y F	-0.40	0.49	0.75	1.21	0.46	0.16	2.30	-0.25	[a2,a6,c2]
lni_a	A 43	V T	0.50	1.17	2.33	2.09	0.96	0.56	3.84	1.69	[a2,a6,c2]
lni_a	A 55	Y F	0.60	0.53	0.92	0.85	-2.52	0.18	2.00	0.03	[a2,a6,c2]
lni_a	A 56	T V	1.90	0.40	0.92	0.17	4.32	-0.61	0.60	0.67	[a2,a6,c2]
lni_a	A 79	D F	-2.73	-1.31	-0.86	0.57	0.03	-3.94	-2.71	0.21	[a2,a6,c2]
lni_a	A 79	D I	-2.85	-1.24	-0.54	0.53	-0.20	-3.26	-1.41	-0.44	[a2,a6,c2]
lni_a	A 79	D K	-2.35	0.39	1.46	0.56	-2.18	-1.01	0.92	2.08	[a2,a6,c2]
lni_a	A 79	D L	-2.65	-0.95	-0.21	0.60	-0.70	-3.42	1.32	-0.36	[a2,a6,c2]
lni_a	A 79	D N	-1.46	0.31	1.01	0.63	1.30	-0.40	-3.10	1.51	[a2,a6,c2]
lni_a	A 79	D Y	-2.90	-0.96	-0.76	0.56	-1.07	-3.73	-4.85	0.57	[a2,a6,c2]
lni_a	A 80	Y F	1.50	0.83	1.37	0.03	0.08	0.04	5.54	0.46	[a2,a6,c2]
lni_a	A 85	H Q	0.00	0.24	0.48	0.97	0.99	0.24	1.16	0.35	[a2,a6,c2]
lni_a	A 94	Q K	-0.56	0.29	0.12	0.63	-0.16	-0.12	2.21	0.43	[a2,a6,c2]
llzl	A 48	G A	-0.45	-1.66	-0.59	99.99	0.59	-0.17	-2.70	0.95	[c2]
llzl	A 105	G A	0.62	2.00	1.74	0.05	0.43	-0.78	-1.47	-0.95	[a2,c2]
lmgr	A 54	Y F	2.60	1.01	1.38	0.85	1.31	0.90	4.16	0.26	[a3,c2]

lmgr	A 84	Y F	1.00	0.87	1.44	1.30	0.52	-0.01	2.61	-0.26	[a3,c2]
lmjc	A 20	F L	0.31	0.76	0.85	0.90	2.13	0.83	-0.69	0.80	[a1,c1]
lmjc	A 20	F S	1.16	1.97	1.42	1.46	3.24	2.56	5.04	0.87	[a1,c1]
lmjc	A 31	F S	1.03	1.69	1.53	1.40	1.17	3.26	4.11	-0.87	[a1,c1]
lmjc	A 52	S W	0.20	0.97	1.13	0.38	3.58	-1.03	10.00	-0.10	[a1,c1]
lmsi	A 25	E A	0.09	0.48	0.22	0.56	0.33	-0.31	-0.57	0.33	[a3,c1]
lmsi	A 47	R A	0.74	0.67	0.08	1.01	1.40	0.15	2.75	0.03	[a3,c1]
lmsi	A 58	D N	0.20	0.14	0.30	0.62	0.60	0.02	-0.21	0.63	[a3,c1]
loia_a	A 78	Y F	0.00	0.88	1.38	1.18	-0.61	1.36	2.79	0.47	[a1,c1]
loia_a	A 86	Y T	2.90	1.98	2.20	1.86	1.23	2.23	9.90	1.20	[a1,c1]
lp2p	A 48	H K	2.12	1.75	3.13	1.76	1.12	1.33	-1.66	1.77	[a3,c1]
lqlp	A 31	A L	-0.90	0.95	0.90	0.75	1.04	-2.71	-1.54	0.84	[a1,c1]
lqlp	A 55	V I	0.20	0.85	1.17	0.72	0.63	-1.00	0.71	0.87	[a1,c1]
lqlp	A 70	A G	-1.60	-1.18	-1.12	-0.29	3.72	0.34	0.25	0.82	[a1,c1]
lqlp	A 160	Y W	-1.18	0.65	1.23	2.29	0.31	-0.96	6.78	0.76	[a1,c1]
lqlp	A 183	A I	-1.80	-0.35	-0.79	1.39	-2.00	-3.08	1.12	0.48	[a1,c1]
lqlp	A 183	A V	-3.80	-0.25	-0.57	1.47	-0.89	-2.38	0.38	-0.35	[a1,c1]
lqlp	A 238	W F	-0.98	1.14	0.49	1.89	0.42	0.65	-0.71	1.16	[a1,c1]
lqlp	A 248	A F	-1.80	-0.25	-1.48	1.03	-1.14	-1.30	10.00	0.40	[a1,c1]
lqlp	A 248	A I	-2.20	0.03	-0.86	1.03	-0.26	-2.26	-2.96	0.36	[a1,c1]
lqlp	A 248	A L	-0.35	0.17	-0.54	1.05	0.21	-2.77	1.91	0.60	[a1,c1]
lqlp	A 248	A V	-2.30	0.04	-1.02	1.08	0.38	-1.37	-0.89	0.41	[a1,c1]
lqlp	A 284	A I	0.00	0.16	-0.99	0.53	-2.28	-1.68	3.30	0.46	[a1,c1]
lqlp	A 284	A V	-0.80	-0.01	-1.16	0.55	-2.08	-1.05	-0.57	0.71	[a1,c1]
lqlp	A 321	V I	-0.60	0.79	0.92	0.74	1.35	-1.11	-0.70	0.64	[a1,c1]
lqlp	A 330	S R	2.44	1.30	1.29	-0.42	0.75	-0.90	0.48	1.16	[a1,c1]
lqlp	A 331	K F	-1.75	-1.24	-0.54	0.53	-1.73	-4.40	-4.25	-0.88	[a1,c1]
lqlp	A 364	V L	0.30	1.06	0.77	1.54	0.53	-0.71	8.08	0.59	[a1,c1]
lqlp	A 374	M I	-2.30	-0.08	0.02	0.40	-2.40	-1.30	-3.51	1.41	[a1,c1]
lqlp	A 381	S A	-1.00	0.50	0.95	0.28	0.63	-1.77	-2.57	0.91	[a1,c1]
lrg8_a	A 16	C S	2.81	1.45	3.27	1.96	4.18	2.10	4.88	0.11	[a3,a7,c1]
lrg8_a	A 44	L F	-0.59	0.60	1.21	2.60	1.83	-0.99	0.97	-0.27	[a3,a7,c3]
lrg8_a	A 106	N G	-0.16	0.25	-0.85	0.98	-0.03	0.58	2.67	0.26	[a3,a7,c1]
lrg8_a	A 109	V I	0.05	0.60	0.44	1.09	1.50	-1.18	1.21	0.48	[a3,a7,c3]
lris	A 8	I A	3.56	3.16	3.54	2.41	2.40	3.38	8.03	4.42	[a3,c1]
lris	A 21	L A	0.16	0.52	0.15	1.65	1.51	0.81	1.20	3.99	[a3,c1]
lris	A 33	Y A	-0.41	2.50	3.71	0.03	-0.26	2.00	4.18	2.03	[a3,c1]
lris	A 48	L A	0.21	2.17	1.76	2.81	1.71	1.31	6.22	3.18	[a3,c1]

lris	A 60	F A	0.81	2.67	2.24	2.70	1.84	2.84	0.25	4.04	[a3,c1]
lris	A 75	L A	1.35	2.51	2.28	2.06	1.75	2.61	7.43	2.97	[a3,c1]
lris	A 79	L A	3.91	2.84	2.93	2.90	1.38	2.97	6.34	-2.97	[a3,c1]
lrm1_c	C 16	V T	3.65	2.30	2.76	1.95	2.78	1.35	4.17	1.94	[a3,c3]
lrm1_c	C 23	G A	1.20	0.06	0.20	1.63	8.96	-0.49	5.80	0.77	[a2,c1]
lrm1_c	C 49	D A	-0.50	-0.34	0.12	0.66	0.30	-0.10	-1.30	-0.65	[a3,c3]
lrm1_c	C 78	V S	4.73	3.58	3.78	3.17	3.70	2.67	6.59	2.00	[a1,c1]
lrm1_c	C 78	V T	3.59	2.46	2.99	2.74	2.22	1.72	3.05	1.64	[a3,c3]
lrtb	A 5	A S	0.27	1.28	1.49	1.40	1.23	0.32	1.65	-0.01	[a2,c2]
lrtb	A 46	F V	4.55	1.60	1.70	1.46	2.39	2.38	0.84	3.66	[a2,c2]
lrtb	A 57	V A	2.85	2.18	2.13	2.89	0.34	1.49	3.64	1.68	[a2,c2]
lrtb	A 57	V L	2.37	0.60	0.86	0.15	0.42	-0.65	6.75	0.65	[a2,c2]
lrtb	A 63	V A	2.03	2.05	1.96	0.81	1.49	0.89	5.14	1.13	[a2,c2]
lrtp_a	A 80	K S	0.29	0.65	0.59	99.99	-0.45	0.56	3.86	99.99	[c2]
lshf_a	A 107	E F	1.63	-0.17	-0.21	-1.29	2.32	-2.42	-1.79	-1.35	[a2,c1]
lshf_a	A 107	E H	0.99	0.40	0.13	1.46	1.55	-0.51	0.43	1.42	[a2,c1]
lshf_a	A 107	E K	0.97	0.92	1.22	1.95	2.20	0.13	3.19	2.02	[a2,c1]
lshf_a	A 107	E L	3.02	-0.01	-0.19	-0.46	3.44	-2.04	-1.50	-1.52	[a2,c1]
lshf_a	A 107	E Y	2.40	0.01	-0.18	-0.24	1.87	-2.31	-2.48	-0.82	[a2,c1]
lshf_a	A 111	I A	2.84	1.89	2.24	2.06	2.71	2.06	4.30	2.43	[a1,c1]
lshf_a	A 111	I L	0.71	0.61	1.48	0.92	0.60	-0.24	5.63	-0.63	[a1,c1]
lshf_a	A 124	S D	2.02	1.23	1.85	0.15	0.10	0.49	4.70	0.66	[a2,c1]
lshf_a	A 124	S F	1.90	1.32	0.43	-0.27	1.87	-0.53	10.00	-0.53	[a2,c1]
lshf_a	A 124	S G	1.68	1.97	1.54	-0.00	2.97	0.47	3.68	1.36	[a2,c1]
lshf_a	A 124	S H	1.25	1.66	1.17	0.20	-0.19	0.69	10.00	0.39	[a2,c1]
lshf_a	A 124	S L	0.37	1.39	0.65	-0.08	3.49	-1.39	3.44	-0.98	[a2,c1]
lshf_a	A 124	S N	0.73	1.15	1.68	-0.08	2.95	0.28	1.92	0.13	[a2,c1]
lshf_a	A 128	G A	1.78	2.41	2.74	0.68	1.26	-0.15	0.96	0.89	[a2,c1]
lshf_a	A 138	V M	0.52	1.00	1.96	0.97	3.30	-0.18	4.90	0.14	[a1,c1]
ltit	A 60	L A	4.88	2.54	2.64	2.41	5.11	2.93	7.92	2.55	[a1,c1]
ltit	A 63	C S	2.08	1.63	3.48	-0.49	-0.56	1.77	3.74	0.31	[a1,c1]
ltit	A 86	V A	4.45	2.97	4.12	1.55	2.78	0.24	-9.35	0.82	[a1,c1]
lttq_a	A 22	F L	1.05	1.53	1.41	99.99	-0.59	1.31	99.99	99.99	[c1]
lttq_a	A 22	F V	3.44	1.71	0.52	99.99	-0.12	2.13	99.99	99.99	[c1]
luzc	A 27	E A	0.62	0.15	0.28	0.80	0.08	0.79	-0.33	1.02	[a3,c1]
luzc	A 38	Q G	1.57	0.88	1.03	0.46	0.66	1.30	5.02	0.99	[a3,c1]
luzc	A 44	I V	0.30	0.36	0.85	1.87	0.52	0.10	-1.41	0.58	[a1,c1]
luzc	A 61	A G	2.07	2.03	2.39	3.22	3.08	1.40	0.65	0.87	[a3,c1]

lyyj	A 3	L A	1.60	0.69	-0.07	2.14	0.42	0.74	2.51	1.75	[a1,a8,c1,e1,i1]
lyyj	A 20	A G	1.97	1.12	1.73	1.14	1.25	0.60	0.78	1.03	[a1,a8,c1,e1,i1]
lyyj	A 61	F A	4.52	3.25	1.21	2.45	1.06	2.20	0.22	2.36	[a1,a8,c1,e1,i1]
lyyj	A 65	F A	1.92	2.89	1.84	2.10	1.06	2.86	1.55	-2.36	[a1,a8,c1,e1,i1]
lyyj	A 105	Y A	2.36	2.08	0.24	1.58	1.08	2.36	99.99	2.55	[a1,a8,c1,e1,i1]
lzg4	A 290	W F	0.83	0.51	0.46	99.99	1.91	1.30	0.97	0.90	[c1]
lznj_b	B 10	H E	-1.11	-0.22	-0.18	0.24	-0.41	0.35	0.57	-0.06	[a3,c1]
lznj_b	B 10	H T	-0.03	-0.12	0.34	-0.06	0.05	0.12	0.91	0.94	[a3,c1]
lznj_b	B 25	F D	-0.48	0.16	0.95	0.82	0.01	1.14	-3.30	0.95	[a3,c1]
2a01_a	A 141	L R	0.65	0.23	0.44	0.64	0.58	-0.96	-1.50	0.73	[a1,c1]
2a36	A 22	T A	-0.40	0.01	0.30	0.73	-2.49	1.68	-2.44	1.84	[a2,c2]
2a36	A 22	T F	-1.30	-0.16	0.27	0.67	12.80	-1.53	-0.79	1.16	[a2,c2]
2a36	A 22	T L	-0.50	-0.17	0.18	0.72	3.97	-1.09	-1.75	2.11	[a2,c2]
2a36	A 22	T N	-1.30	-0.75	-0.88	0.71	1.08	2.05	-2.09	1.41	[a2,c2]
2dri	A 50	V E	3.50	2.29	3.92	2.90	1.51	3.06	10.00	2.36	[a1,c1]
2imm	A 15	A L	-1.36	0.57	0.33	99.99	0.63	-0.94	99.99	0.84	[c1]
2imm	A 21	M L	0.31	0.35	0.97	99.99	1.13	-0.96	99.99	0.47	[c1]
2imm	A 24	K R	0.17	0.07	0.16	99.99	0.03	-0.74	99.99	0.73	[c1]
2imm	A 79	Q E	0.41	0.76	0.43	99.99	0.39	0.04	99.99	-0.09	[c1]
2imm	A 106	L I	-0.36	0.16	-0.31	99.99	1.34	0.18	99.99	0.55	[c1]
2lzm	A 51	G D	2.63	0.83	1.36	1.66	2.91	-0.22	-0.99	2.18	[a1,c1]
2lzm	A 58	I Y	3.11	0.89	2.13	2.67	1.78	1.22	10.00	2.20	[a1,c1]
2lzm	A 146	A I	4.31	0.44	1.98	3.24	2.43	0.09	10.00	1.52	[a1,c1]
2lzm	A 153	F C	3.11	2.49	2.80	2.95	4.38	3.59	-1.81	2.01	[a1,c1]
2nvh	A 4	R Q	0.57	-0.42	0.28	0.79	1.17	0.04	1.56	0.85	[a3,c1]
2nvh	A 7	N D	-0.09	0.47	0.97	0.50	0.70	0.05	1.81	0.28	[a3,c1]
2nvh	A 8	C S	3.74	2.54	5.15	2.24	4.06	1.98	5.31	0.63	[a3,c1]
2rn2	A 62	H A	-0.44	0.11	0.34	-0.36	0.22	0.32	-1.81	0.13	[a3,c1]
2rn2	A 83	H A	-0.07	-0.09	-0.25	-0.14	-0.38	0.15	-0.65	-0.13	[a3,c1]
2trx_a	A 26	D I	-3.37	-2.11	-2.58	99.99	-7.53	-5.10	-3.11	0.07	[c1]
2trx_a	A 66	T L	1.03	0.23	-0.15	99.99	0.09	-1.93	7.09	0.47	[c1]
3gly	A 139	G A	1.40	-0.49	-0.76	99.99	-2.23	-1.24	1.38	0.51	[c1]
3gly	A 383	G A	-0.11	-0.51	-1.19	99.99	-0.26	-1.27	2.23	-0.51	[c1]
3mbp	A 10	W A	4.31	3.34	2.54	3.07	1.63	4.81	-2.12	3.33	[a1,c1]
3pgk	A 48	Y W	1.62	0.11	-0.03	1.23	-0.21	-1.33	5.24	0.06	[a3,c1]
3pgk	A 122	Y W	2.19	0.05	0.62	1.37	0.65	-0.49	2.77	-0.06	[a3,c1]
3pgk	A 194	F W	1.12	0.82	1.73	1.55	2.75	0.29	-5.43	99.99	[a3,c1]
3pgk	A 388	H Q	0.84	1.48	2.77	0.42	2.39	0.30	-38.87	1.06	[a1,c1]

3sil	A 53	A L	-0.90	0.02	0.15	1.83	-0.09	0.55	6.11	0.71	[a3,a9,c1]
4lyz	A 35	E A	-1.24	0.46	-0.07	0.12	-0.36	-0.39	-4.16	0.72	[a3,c1]
5dfr	A 2	I V	0.55	1.21	2.23	1.16	2.44	0.62	-0.22	1.28	[a3,a10,c1,i2]
5dfr	A 30	W M	1.94	2.28	1.40	2.38	2.99	3.20	-2.05	0.78	[a3,a10,c1,i2]
5dfr	A 40	V H	2.76	1.72	2.86	2.34	1.00	3.78	10.00	2.69	[a3,a10,c1,i2]
5dfr	A 59	N T	0.05	-0.09	0.27	0.31	2.52	-0.61	3.93	0.98	[a3,a10,c1,i2]
5dfr	A 59	N W	0.79	-0.41	0.51	0.52	0.42	-0.86	10.00	0.91	[a3,a10,c1,i2]
5dfr	A 67	G S	0.27	0.34	-0.08	0.94	6.09	1.12	10.00	0.90	[a3,a10,c1,i2]
5dfr	A 67	G T	0.62	0.35	-0.06	0.95	5.98	2.62	10.00	0.91	[a3,a10,c1,i2]
5dfr	A 95	G A	0.90	1.85	2.06	0.53	3.31	-0.63	0.40	0.39	[a3,a10,c1,i2]
5dfr	A 121	G C	0.22	0.06	-0.47	1.22	3.58	-1.06	-2.19	0.88	[a3,a10,c1,i2]
5dfr	A 121	G H	0.56	0.53	-0.32	1.26	2.02	-0.75	0.03	0.98	[a3,a10,c1,i2]
5dfr	A 155	I T	2.53	1.66	2.49	2.28	0.47	1.41	3.24	1.75	[a3,a10,c1,i2]
5pti	A 16	A T	1.70	0.40	0.13	1.30	0.39	-0.05	3.45	0.34	[a1,c1,d1]
5pti	A 16	A V	1.30	0.66	0.33	1.27	0.30	-0.26	6.76	0.88	[a1,c1,d1]
5pti	A 35	Y D	3.80	2.69	2.27	3.24	3.64	1.87	1.87	1.37	[a1,c1,d1]

¹ PDB records followed by '_a','_b','_c','_i' or '_u' indicate that only the chain (A,B,C,I or U, respectively) was taken into account. PDB record 1cun is followed by '_17' to indicate that only domain 17 (chain A, residues 107-219) is taken into account.

² A $\Delta\Delta G_p$ value of 99.99 indicates that the server failed to provide any prediction for the corresponding mutation. In the procedure to evaluate the performances, these mutations are either removed from the dataset, or their values are set to 0.0 kcal/mol.

REMARKS

PoPMuSiC-2.0: new version of PoPMuSiC, not yet online.

PoPMuSiC-1.0: old version of PoPMuSiC. <http://babylone.ulb.ac.be/popmusic>

Automute: <http://proteins.gmu.edu/automute>

- The "Tree Regression (REPTree)" option was chosen
- All signs are inverted, since the server uses a different sign convention.
- The server failed to provide predictions for 35 of the 350 mutations, mostly because the structure could not be tessellated, or because of residues having "too few" neighbours. In such cases, a value of 99.99 is reported.
- The servers requires the input of the temperature and pH. The values used were those reported in Table 1 of Supplementary Material.
- The nature of the $\Delta\Delta G$ measure ($\Delta\Delta G$ or $\Delta\Delta G_{H_2O}$) has an impact on the prediction. We systematically used the option corresponding to the nature of the available experimental data ($\Delta\Delta G_M$). When the $\Delta\Delta G_M$ value in our database is an average of both types of values, the outputs of

the server were also averaged.

- a1: $\Delta\Delta G_{H_2O}$ value
- a2: $\Delta\Delta G$ value
- a3: average of $\Delta\Delta G_{H_2O}$ and $\Delta\Delta G$ values
- a4: the server could not handle PDB 1g4i, so 1bp2 was used instead
- a5: the server could not handle PDB 1ifc, so 1ifb was used instead
- a6: the server could not handle PDB 1lni, so 1rgg was used instead
- a7: the server could not handle PDB 1rg8, so 2afg was used instead
- a8: the server could not handle PDB 1yyj, so 1yyx was used instead
- a9: the server could not handle PDB 3sil, so 1dil was used instead
- a10: the server could not handle PDB 5dfr, so 1rx4 was used instead

CUPSAT: <http://cupsat.tu-bs.de>

- The nature of the $\Delta\Delta G$ measure (thermal or chemical denaturation) has an impact on the prediction. We systematically used the option corresponding to the nature of the available experimental data ($\Delta\Delta G_M$). When the $\Delta\Delta G_M$ value in our database is an average of both types of values, the outputs of the server were also averaged.
- With the "Thermal" option, all signs are inverted, since the server uses a different sign convention.
- With the "Denaturants" option, the signs are not inverted (this results apparently from a bug that counter-effects the sign convention).
- The server failed to provide predictions for 4 of the 350 mutations, for unknown reasons. In such cases, a value of 99.99 is reported.
- c1: computed with the "Denaturants" option
- c2: computed with the "Thermal" option
- c3: average of values computed with the "Denaturant" and "Thermal" options

Dmutant : <http://sparks.informatics.iupui.edu/hzhou/dmutation.html>

- d1: the server could not handle PDB 5pti, so 1bpi was used instead

Eris: <http://eris.dokhlab.org>

- Predictions reported here are with fixed backbone, and without pre-relaxation. Although the authors reported that predictions with flexible backbone are more efficient in some cases, they are also much more computationally intensive (the server needed several hours for one mutation) and thus not comparable with the other methods tested here.
- The server failed to provide predictions for 16 of the 350 mutations, for unknown reasons. In such cases, a value of 99.99 is reported.
- e1: the server could not handle PDB 1yyj, so 1yyx was used instead

I-mutant: <http://gpcr2.biocomp.unibo.it/cgi/predictors/I-Mutant2.0/I-Mutant2.0.cgi>

- We downloaded and used the stand-alone program, version 2.0.4
- All signs are inverted, since the program uses a different sign convention.
- The servers requires the input of the temperature and pH. The values used were those reported in Table 1 of Supplementary Material.
- The program failed to provide predictions for 4 of the 350 mutations, for unknown reasons. In such cases, a value of 99.99 is reported.
- i1: the program could not handle PDB 1yyj, so 1yyx was used instead
- i2: the program could not handle PDB 5dfr, so 1rx4 was used instead