

Table S1. List of atom types and parameters of MedusaScore.

Name	Description	VDW parameters		EEF1 Parameters			
		E (kcal/mol)	$\sigma(\text{\AA})$	Vol (\AA^3)	ΔG^{free} (kcal/mol)	$\lambda(\text{\AA})$	r (\AA)
Hydrogen							
_H*	Hydrogen	0.00000	0.00000	0.00	0.00	0.00	0
Carbon							
_C*	Carbonyl carbon	0.12000	3.74177	14.70	0.00	3.50	2.100
_CR*	Carbon with no hydrogens	0.12000	3.74177	8.30	-1.40	3.50	2.100
_CH1E*	Extended aliphatic carbon with 1 H	0.04860	4.21395	14.70	0.00	3.50	2.490
_CH2E*	Extended aliphatic carbon with 2 H	0.11420	3.98232	22.40	0.52	3.50	2.235
_CH3E*	Extended aliphatic carbon with 3 H	0.18110	3.85759	30.00	1.50	3.50	2.165
_CR1E*	Extended aromatic carbon with 1 H	0.12000	3.74177	18.40	0.08	3.50	2.100
Oxygen bonded to one heavy atom							
_OC*	Carboxyl oxygen	0.21000	2.85088	10.80	-10.00	6.00	1.6
_O*	Carbonyl oxygen	0.15910	2.85088	10.80	-5.85	3.50	1.6
_OH1*	Hydroxyl oxygen	0.15910	2.85088	10.80	-6.70	3.50	1.6
_OPO	Oxygen in phosphate	0.21000	2.85088	10.80	-10.00	6.00	1.6
_ONO	Oxygen in O-N-O bond	0.15910	2.85088	10.80	-3	3.50	1.6
_ON	Oxygen bonded to a nitrogen atom, other cases	0.15910	2.85088	10.80	-3.000	3.50	1.6
_ONH	Oxygen bonded to a nitrogen atom with 1 H	0.15910	2.85088	10.80	-3.000	3.50	1.6
_OS	Oxygen in sulfone group	0.21000	2.85088	10.80	-10.00	6.00	1.6
Oxygen bonded to two heavy atoms							
_OCC	Ether oxygen	0.15910	2.85088	4.467	-4.0	3.5	1.6
_OCP	Phosphoric acid ester O	0.15910	2.85088	4.467	-4.0	3.5	1.6
_OCN	Oxygen in C-O-N group	0.15910	2.85088	4.467	-4.0	3.5	1.6
Nitrogen bonded to one heavy atom							
_NC	Nitrile nitrogen	0.23840	2.85088	11.20	-5	3.5	1.6
_NC2*	Guanidinium nitrogen	0.23840	2.85088	11.20	-10.00	6.00	1.6
_NH2*	Nitrogen bonded to 2 H	0.23840	2.85088	11.20	-7.80	3.50	1.6
_NH3*	Nitrogen bonded to 3 H	0.23840	2.85088	11.20	-20.00	6.00	1.6
_NNH2	Nitrogen bonded to a nitrogen and 2 H	0.23840	2.85088	11.20	-6.00	3.5	1.6
_NS	Nitrogen bonded to S	0.23840	2.85088	4.4	-4.00	3.50	1.6
Nitrogen bonded to two heavy atoms							
_NH1*	Amide nitrogen	0.23840	2.85088	4.4	-8.90	3.50	1.6
_NR*	Aromatic nitrogen with no H	0.23840	2.85088	4.4	-4.00	3.50	1.6
_NCCH2	Quaternary ammonium nitrogen with 2 H	0.23840	2.85088	4.4	-6.00	3.50	1.6
_NCN	Nitrogen bonded to a carbon and a nitrogen	0.23840	2.85088	4.4	-4	3.5	1.6
_NCNH	Nitrogen bonded to a carbon and a nitrogen with 1 H	0.23840	2.85088	4.4	-4	3.5	1.6
_NNN	Nitrogen bonded to a two nitrogens	0.23840	2.85088	4.4	0	3.5	1.6
_NXO	Nitrogen bonded to oxygen	0.23840	2.85088	4.4	-4	3.5	1.6
_NXSO	Nitrogen in sulfamide group	0.23840	2.85088	4.4	-10	6	1.6
_NXPO	Nitrogen in Phosphoramidite group	0.23840	2.85088	4.4	-10	6	1.6

Nitrogen bonded to three heavy atoms							
_N*	Proline nitrogen	0.23840	2.85088	0	-1.55	3.50	1.6
_NOOO	Nitrogen bonded to 3 O	0.23840	2.85088	0	0	3.5	1.6
_NCCCC	Quaternary ammonium nitrogen with 1 H	0.23840	2.85088	0	-5	3.5	1.6
_NXX-	Other amine nitrogen	0.23840	2.85088	0	0	3.5	1.6
_NXX-H	Other quaternary ammonium nitrogen with 1 H	0.23840	2.85088	0	0	3.5	1.6
_NXXSO	Nitrogen in sulfamide group	0.23840	2.85088	0	-10	6	1.6
_NXXPO	Nitrogen in Phosphoramidite group	0.23840	2.85088	0	-10	6	1.6
Nitrogen bonded to four heavy atoms							
_NXXXX	Other quaternary ammonium nitrogen	0.23840	2.85088	0	0	3.5	1.6
Sulphur							
_SC	Sulphur in S=C group	0.04300	3.36760	14.70	-3	3.50	1.89
_SH1E*	Extended sulfur with 1 H	0.04300	3.36760	21.40	-2.70	3.50	1.89
_S*	Sulfur in disulphide bond	0.04300	3.36760	14.70	-4.10	3.50	1.89
_SOXX	Sulphur in sulfinyl group	0.04300	3.36760	7.77	-8	3.5	1.89
_SXXXX	Other sulfur attached to 4 heavy atoms	0.04300	3.36760	7.77	0	3.5	1.89
Phosphorous							
_PXXXX	All phosphorous attached to 4 heavy atoms	0.314	3.6	0	0	3.5	2.02
Halogen atoms							
_FX	Fluorine	0.109	2.94	6.07	0	3.5	1.65
_ClX	Chlorine	0.314	3.5	18.1	0	3.5	1.96
_BrX	Bromine	0.434	3.7	26	0	3.5	2.07
_IX	Iodine	0.623	3.96	30.2	0	3.5	2.22
* Original EEF1 types. The parameters are from the original EEF1 model (Lazaridis and Karplus 1999).							

Table S2. MedusaScore calculation results using PDBBind core set.

PDBID	n	n _c	pK _d	Original Structure			Energy Minimized Structure		
				Total Score	VDWR term	VDWR excluded Score	Total Score	VDWR term	VDWR excluded Score
10gs	33	11	6.40	-22.9113	6.23369	-28.3645	-24.3789	4.73336	-28.5196
1a07	34	5	6.40	-13.2234	5.62081	-18.1405	-17.4475	3.48621	-20.4972
1a08	41	11	5.62	-25.8617	5.1007	-30.3238	-26.0411	5.66988	-31.0011
1a30	26	10	4.30	-14.211	6.29866	-19.7211	-14.1736	6.20064	-19.5979
1a69	19	8	5.30	-13.8989	6.27714	-19.3901	-13.9696	5.58126	-18.8521
1a94	60	19	7.85	-42.8708	14.5851	-55.6298	-43.072	14.2683	-55.5539
1abf	11	7	5.42	-15.9868	3.1755	-18.7647	-16.7407	2.90768	-19.2843
1ai5	13	4	3.72	-12.7813	6.73285	-18.6712	-12.7962	6.57268	-18.546
1ajp	12	5	2.23	-2.37437	12.6899	-13.4755	-2.9719	11.3353	-12.888
1ajq	9	3	4.31	-6.14428	6.44885	-11.7857	-5.48733	6.77782	-11.4166
1apw	35	9	8.00	-39.2021	4.75028	-43.3576	-39.6527	4.79643	-43.8486
1avn	8	2	3.90	-1.81941	0.698694	-2.43063	-1.88149	0.705845	-2.49896
1ax0	15	6	3.13	-13.2804	5.79579	-18.3506	-14.3394	4.40865	-18.1961

1b11	33	7	7.39	-25.4803	3.55969	-28.5943	-25.5714	3.39406	-28.5405
1b42	11	6	4.01	1.7187	11.5678	-8.40081	-2.41557	7.32621	-8.82454
1b7h	27	12	8.02	-28.1344	6.89242	-34.1639	-28.7627	6.99306	-34.8802
1b9j	27	10	5.96	-28.4242	4.5654	-32.418	-28.8635	4.24219	-32.5746
1bhf	45	11	4.38	-21.1725	6.79376	-27.1157	-20.0714	6.32552	-25.605
1bky	9	6	3.84	-3.11589	6.07293	-8.42849	-4.53491	4.92029	-8.83918
1bma	37	10	4.59	-29.6849	14.5912	-42.4493	-31.2638	12.4524	-42.1572
1bra	9	5	1.82	-7.32919	3.10638	-10.0467	-7.21598	3.08076	-9.91103
1bxo	44	13	10.00	-42.3088	8.36573	-49.6271	-42.9142	7.86705	-49.7963
1c5o	9	4	3.49	-10.7403	1.8478	-12.3568	-10.7524	1.77345	-12.3038
1c6y	45	15	9.51	-34.7688	21.0309	-53.1666	-34.4322	20.2192	-52.12
1d7j	6	2	3.30	-10.4357	2.564	-12.6787	-10.8866	2.15202	-12.7692
1det	24	6	4.30	-20.8348	2.06311	-22.6396	-20.3358	2.38985	-22.4264
1dhi	33	6	7.26	-26.8817	2.8613	-29.3848	-27.3311	2.49618	-29.5148
1dhj	33	7	6.55	-29.1356	2.08833	-30.9625	-29.5053	1.68751	-30.9815
1drj	10	8	7.40	-18.8381	6.34247	-24.3865	-19.7398	5.97102	-24.9632
1drk	10	9	6.82	-19.9835	6.9482	-26.0618	-21.4855	5.2896	-26.1128
1e1v	18	5	4.92	-12.8342	9.97303	-21.5586	-12.2417	10.1846	-21.1512
1e2k	18	6	4.94	-19.6487	11.5399	-29.7438	-20.4001	11.4662	-30.4307
1e2l	18	6	4.29	-20.7804	9.81847	-29.3696	-21.4932	8.64472	-29.0556
1e2p	15	8	4.57	-20.7917	4.55935	-24.7802	-20.6857	4.81473	-24.8976
1e3v	28	3	4.34	-21.1855	5.36672	-25.8803	-22.0201	4.2953	-25.7776
1e4h	12	3	8.41	-22.8977	3.10868	-25.6172	-23.8444	2.29366	-25.8509
1e5a	10	2	7.64	-18.115	4.05319	-21.6607	-17.8288	3.36173	-20.7696
1e66	21	7	9.89	-31.5818	10.9755	-41.1832	-33.4369	9.05167	-41.3553
1e6q	14	9	3.15	-14.9177	8.09191	-21.9965	-13.8602	8.72395	-21.4919
1e6s	13	10	3.22	-4.00972	13.0092	-15.3902	-4.40066	12.0833	-14.9711
1e70	11	6	3.05	-6.5666	12.6201	-17.6067	-6.54459	12.2818	-17.2887
1eed	45	12	4.79	-32.8573	10.8996	-42.3923	-32.6213	10.6186	-41.9105
1ela	32	6	6.36	-31.8415	5.52013	-36.6705	-30.2224	5.19274	-34.765
1elb	33	14	7.15	-13.0827	19.2842	-29.9525	-13.1394	18.5621	-29.3775
1epv	22	12	6.89	-0.660312	31.4696	-28.1899	-7.66156	26.5683	-30.9035
1ets	37	11	8.22	-32.7926	10.1392	-41.6624	-33.6358	8.6949	-41.2421
1ett	30	8	5.89	-19.9799	10.883	-29.5003	-20.0192	10.3696	-29.0905
1f3e	14	4	6.70	-18.8504	1.22294	-19.9202	-19.4213	0.753037	-20.0801
1f4e	18	6	2.96	-10.2333	4.60259	-14.2596	-11.5384	2.92885	-14.1006
1f4f	29	7	4.62	-7.36325	8.17637	-14.5159	-7.93091	7.36125	-14.3705
1f4g	34	8	6.48	-13.9983	8.99717	-21.869	-15.2508	7.5033	-21.8147
1f5k	9	3	3.74	-11.5466	1.98979	-13.2873	-11.5774	1.98244	-13.3116
1fcx	29	6	7.19	-46.0942	8.58078	-53.6007	-46.9729	7.75144	-53.7539
1fcz	27	6	9.22	-43.2333	8.81217	-50.9422	-44.7126	7.88582	-51.6111
1fd0	30	6	8.40	-46.1768	9.65782	-54.6255	-46.8002	8.65705	-54.3734
1fh7	18	9	5.24	-20.8123	8.50225	-28.2501	-20.0142	8.80695	-27.7185
1fh8	17	6	6.89	-22.8642	5.11895	-27.3423	-22.4124	4.77792	-26.5921
1fh9	20	13	6.43	-20.6357	9.62528	-29.0559	-19.6101	9.82132	-28.2018
1fkb	65	7	9.70	-43.2397	4.15745	-46.8766	-43.9743	3.69656	-47.2081
1fki	31	6	7.00	-30.944	3.33363	-33.8603	-31.7386	2.67892	-34.0821
1fo0	70	25	5.59	-60.0605	22.7777	-79.9864	-66.9518	20.0419	-84.4845

lftm	13	8	7.61	-18.8941	4.23066	-22.5951	-19.3138	3.69963	-22.5502
lfzk	68	13	8.40	-53.1741	10.8055	-62.6268	-55.0908	10.3529	-64.1475
lfzm	68	19	7.70	-60.2877	8.8434	-68.0239	-63.632	8.16893	-70.7782
lg85	9	2	5.48	-19.7552	2.99211	-22.3727	-19.1276	3.27621	-21.9936
lghz	19	5	4.80	-18.6604	0.869449	-19.421	-17.6991	0.607765	-18.2308
lgni	20	4	8.07	-33.3466	7.91667	-40.2721	-34.1276	8.00605	-41.1313
lgpk	18	5	5.37	-23.9615	4.21682	-27.6504	-23.419	5.21047	-27.9771
lgtl	15	4	6.00	-13.4866	15.6336	-27.1629	-12.3453	16.1322	-26.4577
lgz9	33	8	3.57	-17.2258	7.58717	-23.8631	-19.5574	6.29697	-25.066
lgzc	23	7	3.28	-6.83293	8.56511	-14.3257	-9.04124	7.95077	-15.9966
lh23	36	8	8.35	-46.5509	9.89606	-55.208	-48.8404	7.5735	-55.4657
lha2	23	3	5.54	-14.4526	13.873	-26.5887	-11.668	16.0914	-25.7448
lhi3	27	5	4.19	-9.61489	2.86326	-12.1197	-11.1412	2.38862	-13.2308
lhi4	27	12	4.49	-3.69047	13.0809	-15.1336	-6.11979	11.2158	-15.9314
lhi5	27	9	4.04	-10.8019	3.72532	-14.0608	-13.2119	2.98004	-15.8188
lhk4	24	8	5.31	-12.8951	18.3521	-28.9495	-15.72	14.7776	-28.6474
lhmr	20	3	6.55	-33.0268	2.70236	-35.3908	-33.4005	2.72513	-35.7844
lhms	20	3	6.37	-32.9952	1.92716	-34.6811	-33.316	1.90576	-34.9832
lhmt	20	3	5.79	-34.6804	1.63042	-36.1067	-35.844	1.23694	-36.9261
lhn2	15	3	6.00	-15.5722	13.3219	-27.2262	-14.4333	13.9815	-26.6643
lhsh	45	7	8.61	-48.153	10.5067	-57.3443	-49.3211	9.12475	-57.3034
li80	10	7	6.41	-15.1546	3.98773	-18.6431	-14.9855	3.86243	-18.3644
ligj	37	9	10.00	-27.3782	6.4241	-32.998	-26.9948	6.68328	-32.8413
lis0	47	11	7.00	-24.3881	9.04984	-32.3049	-23.0695	9.28604	-31.1929
livp	59	18	7.52	-30.3407	29.3773	-56.04	-32.2949	26.3639	-55.358
lizi	50	13	6.59	-45.9258	13.3516	-57.6058	-46.5284	12.9741	-57.8781
lj07	36	7	7.68	-23.8082	5.47476	-28.5975	-23.8752	5.41835	-28.6152
lj17	34	12	5.22	-24.4732	15.8557	-38.3438	-25.3442	13.9504	-37.548
lj8v	23	11	3.61	-16.4665	11.961	-26.93	-14.8111	12.3942	-25.6535
ljq9	47	15	8.45	23.1564	60.6111	-29.8662	23.9281	58.7145	-27.4353
ljqd	26	8	5.16	-12.2498	5.9302	-17.4375	-11.7208	6.79916	-17.6687
ljqe	28	11	6.44	-21.4092	27.6621	-45.608	-26.2048	22.1633	-45.5933
ljys	10	4	3.52	-5.75427	2.8097	-8.2122	-5.89351	2.57121	-8.1428
lk9s	20	6	6.52	-20.8448	2.77402	-23.2715	-20.7727	2.9305	-23.3363
lkpm	31	9	5.80	-26.4194	23.4761	-46.9563	-27.171	22.6268	-46.9649
lkv5	9	8	4.22	-5.84976	4.88779	-10.1256	-5.35225	5.25377	-9.94825
ll2s	19	5	4.59	-10.4645	4.03179	-13.9915	-10.2817	4.03915	-13.8151
ll83	6	1	3.40	-6.57812	6.66523	-12.4089	-6.58554	6.38569	-12.1717
llaf	12	7	7.85	-15.8596	3.67607	-19.0754	-16.4985	3.08901	-19.2008
llag	11	7	6.30	-8.1105	6.30465	-13.6258	-9.0564	5.5402	-13.903
llah	9	4	7.52	-12.6728	2.62236	-14.9668	-13.3635	2.05133	-15.158
lli3	8	3	4.25	-13.1258	4.63147	-17.1774	-12.9	4.84937	-17.1422
llkk	46	9	6.85	-29.909	4.90532	-34.2002	-34.7528	4.22099	-38.4453
llkl	42	12	5.81	-24.765	4.77524	-28.9424	-25.4584	4.35846	-29.2712
lloq	21	10	3.70	-25.5124	5.07239	-29.9497	-26.4679	4.95587	-30.8033
llos	21	9	7.19	-20.5412	4.82697	-24.7638	-22.4657	4.20846	-26.1473
llzq	50	18	8.39	-30.1619	28.1906	-54.823	-32.0394	24.9062	-53.8273
lm0n	25	15	2.22	-19.4047	15.7242	-33.1602	-19.1165	15.3026	-32.5032

1m0o	24	15	2.31	-23.645	12.5274	-34.604	-24.674	11.0342	-34.3267
1m0q	22	12	2.96	-22.2907	8.75	-29.9452	-25.1879	6.92345	-31.2445
1m2q	20	6	6.10	-13.4983	11.9092	-23.9165	-14.2252	10.3183	-23.2516
1m2r	20	10	6.46	-15.5909	8.59354	-23.1085	-15.2846	8.54944	-22.7637
1m7i	56	12	5.40	-33.5486	6.87656	-39.5642	-32.6093	7.95116	-39.565
1m9n	24	18	6.92	-19.6244	16.0441	-33.6598	-21.2015	15.3069	-34.592
1mh5	33	10	9.21	-27.3665	10.4652	-36.5215	-29.476	9.21285	-37.5354
1mj7	33	11	8.35	-28.57	12.723	-39.7001	-29.864	11.9491	-40.3171
1mjj	33	9	8.74	-34.669	9.137	-42.662	-34.7361	8.73804	-42.3801
1mq6	36	12	11.15	-36.3215	9.20848	-44.3771	-36.9655	8.65823	-44.5397
1n2v	15	2	4.08	-18.0303	2.20193	-19.9565	-18.3354	1.95427	-20.045
1n3i	19	8	8.89	-29.9523	4.43087	-33.8284	-32.1041	4.16673	-35.7492
1n5r	31	4	5.66	-22.8384	4.45069	-26.7319	-22.7731	4.27128	-26.5096
1nc1	20	9	6.12	-15.7237	14.9665	-28.8164	-17.1558	13.6725	-29.1165
1ndj	16	10	12.16	-24.7663	9.14932	-32.7701	-23.2876	10.4112	-32.3953
1ndw	19	6	5.23	-10.6629	15.5447	-24.2614	-12.1462	14.6185	-24.9345
1ndy	23	8	6.17	-18.1968	17.0066	-33.0742	-18.0953	16.4025	-32.4442
1nfy	30	11	8.89	-20.6833	9.40482	-28.9106	-19.2412	9.96097	-27.9551
1niu	22	11	7.10	-9.36241	18.6392	-25.668	-13.4984	15.9383	-27.4412
1nja	20	9	6.31	-13.5732	1.87074	-15.2097	-13.4689	2.58224	-15.7278
1nje	20	10	3.80	-14.3779	5.95415	-19.5866	-16.5004	4.29155	-20.2546
1nvq	36	11	8.25	-38.9031	9.29421	-47.0337	-39.3909	8.62271	-46.934
1nwl	31	8	2.39	-4.41217	14.2281	-16.8589	-4.99646	13.14	-16.4913
1o0h	27	13	5.92	-15.5219	6.08295	-20.8433	-17.2084	5.69835	-22.1933
1o0n	21	7	4.09	-16.6475	1.05054	-17.5665	-17.1212	1.1712	-18.1458
1ols	35	12	7.31	-27.2636	18.2072	-43.1913	-30.8899	16.4349	-45.2672
1o3p	25	9	6.66	-13.6877	7.09367	-19.8932	-15.1118	6.22115	-20.5541
1o5r	33	8	8.12	-26.4407	13.4333	-38.1922	-26.9284	13.005	-38.3052
1ocq	21	12	5.19	-22.3076	3.94804	-25.7613	-22.8752	3.82079	-26.2176
1ogg	43	10	5.19	-40.4216	8.94615	-48.2477	-40.5653	9.28865	-48.691
1ogx	20	4	6.09	-25.5561	4.08157	-29.1267	-26.7625	2.59076	-29.0289
1oif	10	6	7.72	-14.4279	7.10912	-20.647	-14.4186	6.68426	-20.266
1oim	11	6	5.32	-13.3478	8.06878	-20.4064	-13.7487	7.90684	-20.6656
1om1	22	7	6.77	-10.6086	17.5577	-25.9681	-10.328	18.3426	-26.3741
1oz0	57	19	7.70	-22.019	19.066	-38.6979	-23.7133	16.9079	-38.5043
1p1q	13	8	4.89	-9.11332	13.4208	-20.8538	-10.7685	10.73	-20.1551
1pb9	7	5	3.62	-4.80116	9.40914	-13.0323	-8.96267	7.04253	-15.1235
1pbq	16	6	6.27	-20.0773	8.12184	-27.1823	-19.3465	8.26984	-26.581
1ppm	42	15	5.80	-37.8207	6.50594	-43.5121	-38.1117	6.31049	-43.6321
1pr5	19	8	3.92	-8.91641	6.40576	-14.5202	-8.23188	6.37096	-13.8052
1pro	43	10	11.30	-46.4809	13.4943	-58.2857	-45.9574	13.3493	-57.6354
1pxh	48	14	8.74	-35.3169	11.9012	-45.7281	-37.7991	11.1035	-47.5124
1pxo	14	6	8.70	-9.80974	7.38571	-16.2708	-9.91626	6.93692	-15.9847
1pyn	43	14	5.49	-33.874	7.90639	-40.7905	-33.2901	7.72762	-40.0502
1q65	20	7	5.46	-23.9362	5.67133	-28.8975	-24.8785	4.93726	-29.1976
1q7a	24	7	7.19	-13.835	14.9331	-26.8985	-14.4363	13.764	-26.477
1q84	50	14	11.05	-62.3226	16.6002	-76.8445	-63.2863	15.8018	-77.1097
1q8t	18	7	4.76	-15.3579	7.27581	-21.7228	-15.2968	6.97055	-21.3946

lqbq	20	5	8.30	-22.7492	6.36998	-28.3217	-22.2164	6.63408	-28.0199
lqi0	23	11	2.35	-10.9977	6.45103	-16.6411	-12.184	6.24132	-17.6439
lre8	35	10	9.52	-34.2181	11.4155	-44.2044	-34.2433	11.5327	-44.3321
lrle	32	11	5.80	-11.8142	4.78869	-16.0033	-16.4715	4.55844	-20.4592
lrnt	24	7	5.19	-17.9386	6.94637	-24.0153	-17.5112	6.83216	-23.488
lsgx	24	7	5.80	-17.6506	2.18542	-19.5624	-18.1485	2.10978	-19.9941
lsl3	37	14	11.85	-43.0779	10.4015	-52.1771	-42.507	10.7168	-51.8821
lslg	59	9	3.90	-38.5997	5.5726	-43.4746	-38.4847	5.24534	-43.0733
lsqa	31	9	9.21	-21.4594	6.15714	-26.8457	-21.1741	6.22856	-26.6228
lswr	16	10	6.92	-18.5875	9.14413	-26.5868	-24.2318	9.38488	-32.4417
lsyh	17	11	6.31	-26.0202	6.19589	-31.4404	-26.2952	5.30186	-30.9333
lt79	67	6	6.04	-23.4659	10.4965	-32.6482	-24.1592	10.1309	-33.0217
lt7f	66	6	5.74	-18.0124	12.439	-28.894	-20.9823	8.85356	-28.7274
lthz	33	10	5.15	-4.78119	13.1672	-16.2999	-4.83305	12.8712	-16.0928
ltnk	10	4	1.49	-6.59189	6.40876	-12.1983	-6.37927	6.34305	-11.9282
ltol	11	4	4.05	-14.4239	3.06663	-17.1066	-14.4124	2.55107	-16.6441
ltol	11	4	3.39	-13.4624	4.44681	-17.3525	-13.776	3.7724	-17.0761
ltok	8	4	2.47	-14.6233	1.21808	-15.6889	-14.5347	1.0967	-15.4941
ltrd	10	7	5.40	-10.7045	5.32003	-15.3585	-11.0573	4.93042	-15.3704
ltsy	20	11	4.96	-17.9473	4.84265	-22.1837	-18.9414	4.03348	-22.4699
ltyr	22	5	7.00	-6.50396	14.2584	-18.9772	-6.69381	13.3367	-18.3608
lu1b	51	13	7.80	-23.9981	9.07369	-31.9358	-22.78	8.67861	-30.372
lu2y	13	3	1.74	-7.09845	0.555182	-7.58412	-6.96608	0.439318	-7.3504
lu33	36	15	4.60	-21.2549	15.3606	-34.6924	-21.184	14.7176	-34.059
luxx	27	4	5.91	-16.8515	3.27657	-19.7178	-17.1109	2.76467	-19.5294
lur8	29	10	4.35	-31.6586	5.13049	-36.1468	-30.1639	6.21613	-35.6018
lur9	39	12	5.77	-42.0788	6.8317	-48.0552	-42.0889	7.72199	-48.8441
lutj	8	1	3.84	-8.92148	1.59364	-10.3156	-8.92238	1.59364	-10.3165
lutl	10	5	2.47	-4.15417	4.99405	-8.52296	-3.94758	5.01991	-8.339
lutm	9	2	3.01	-7.6763	0.237814	-7.88434	-7.64272	0.239747	-7.85245
lutt	27	7	7.64	-23.9945	9.70948	-32.4884	-24.3407	8.90207	-32.1282
lv0k	18	6	5.10	-9.40564	13.8868	-21.5538	-9.39864	12.2069	-20.0772
lv0l	17	8	7.55	-10.7607	11.347	-20.6871	-10.6587	10.9573	-20.2441
lv0n	17	7	7.55	-11.5278	10.6655	-20.858	-10.8186	10.7272	-20.2028
lv48	22	9	7.80	-24.3068	2.91122	-26.8535	-27.7256	2.50099	-29.9135
lvfn	10	5	5.60	-10.6627	2.35917	-12.7265	-11.5244	2.11357	-13.3734
lvjj	28	9	5.77	-13.097	4.14859	-16.7262	-14.0853	4.69298	-18.1907
lw2g	17	8	4.57	-21.185	5.82601	-26.2816	-21.6723	4.80063	-25.8719
lw3j	10	6	6.32	-9.85076	7.32687	-16.2603	-11.6392	6.52464	-17.347
lw3l	32	15	6.28	-9.32432	21.6842	-28.2937	-9.96259	19.3457	-26.8862
lw6y	20	5	5.36	-20.5423	5.00588	-24.9214	-21.5216	3.78996	-24.8371
lws4	13	5	3.00	-10.1612	7.495	-16.7178	-9.9821	7.33081	-16.3951
lws5	13	7	3.03	-8.85021	7.7315	-15.6137	-8.41086	8.03883	-15.4432
lx1z	22	11	11.06	-32.9518	5.95967	-38.1653	-32.9445	5.53276	-37.7846
lx38	20	13	8.77	-11.1182	15.9264	-25.0506	-11.7227	14.7083	-24.5895
lx39	22	13	9.22	-13.8797	14.1717	-26.2771	-14.3253	13.2638	-25.9285
lxd1	66	23	7.92	-32.536	14.2508	-45.0026	-33.9124	13.5958	-45.806
lxgi	21	6	4.85	-5.41481	8.21676	-12.6028	-5.64656	7.94405	-12.596

1xgj	22	7	6.00	-0.464472	9.5418	-8.81164	-0.03731	9.65183	-8.48073
1xqk	22	10	2.68	-16.4014	13.2146	-27.9615	-19.072	10.7142	-28.4448
1ylm	9	5	1.82	-11.7877	3.54369	-14.8877	-13.2967	2.67929	-15.6405
1y6q	20	7	11.70	-31.1921	4.36299	-35.0088	-31.1466	4.51766	-35.0986
1ydt	27	6	7.32	-24.9762	12.3461	-35.7766	-25.1803	11.593	-35.3219
1z95	29	9	4.30	-30.0284	10.9855	-39.6385	-29.2862	11.3287	-39.1965
220l	6	3	3.00	-5.57722	7.50092	-12.139	-5.3638	7.36366	-11.8055
2aou	25	9	7.73	-27.0183	16.6317	-41.5677	-29.0024	14.2386	-41.4583
2baj	27	5	8.40	-41.8663	8.7929	-49.5583	-42.2476	7.73945	-49.0181
2bak	43	10	7.43	-46.9608	13.6114	-58.8681	-45.8325	14.2515	-58.2997
2bal	28	4	6.31	-33.7598	2.62458	-36.0558	-33.6685	2.62458	-35.9645
2bok	29	8	6.55	-30.0738	7.53499	-36.6654	-28.8292	8.52369	-36.2857
2brb	25	4	4.86	-19.3508	8.18848	-26.5141	-19.411	7.88999	-26.3132
2brm	25	6	5.89	-17.0304	9.33609	-25.1976	-17.148	8.90413	-24.9373
2cgr	29	10	7.28	-27.598	6.88645	-33.6223	-28.9186	8.03996	-35.952
2drc	33	8	9.89	-28.9697	2.43539	-31.1002	-29.2703	2.20409	-31.1984
2dri	10	10	6.89	-21.156	6.87502	-27.1703	-22.5358	5.56797	-27.4067
2gss	19	3	4.94	-18.3587	1.65903	-19.81	-18.8977	1.0968	-19.8572
2qwb	21	9	2.74	-10.4914	2.75683	-12.9031	-11.8135	1.28636	-12.9388
2qwd	20	8	4.85	-11.9083	4.90668	-16.2007	-13.1757	3.54323	-16.2753
2qwe	23	11	7.48	-18.1504	5.34845	-22.8292	-16.0214	5.75595	-21.0567
2rkm	19	7	3.90	-14.6704	1.71692	-16.1724	-15.2119	1.41426	-16.4491
2std	20	4	9.85	-36.573	6.68392	-42.4201	-36.2349	6.52642	-41.9442
3er3	57	16	7.09	-43.5035	9.67093	-51.9636	-43.0353	9.74909	-51.5638
3gss	39	13	5.82	-29.4209	7.70201	-36.1586	-31.704	6.40692	-37.3088
3mag	11	6	4.07	-1.72653	7.03735	-7.8828	-4.89603	4.16982	-8.54379
3std	28	4	11.11	-35.4292	10.6141	-44.7144	-35.4451	10.5272	-44.6543
4apr	47	14	6.70	-36.1573	10.1754	-45.0587	-37.7698	9.07533	-45.7089
4er2	48	10	9.30	-42.1761	4.34821	-45.9799	-41.4755	4.97019	-45.8234
4fiv	58	19	6.52	-53.9064	19.0465	-70.5683	-56.9801	16.3896	-71.3177
4tim	11	7	2.16	-1.79786	7.32705	-8.20756	-1.20511	7.72945	-7.96683
5abp	12	8	6.64	-14.7004	4.1803	-18.3573	-15.6185	3.45383	-18.6399
6apr	48	15	7.77	-39.2912	11.4985	-49.3501	-39.1035	11.9446	-49.5526
6fiv	33	10	8.08	-23.03	5.74706	-28.0575	-23.053	5.60992	-27.9606
6rnt	23	8	2.37	-9.84233	3.90351	-13.2571	-11.3317	3.58447	-14.4674
6std	21	4	8.64	-32.4014	6.7383	-38.2961	-32.5686	6.43172	-38.1951
6upj	22	5	6.32	-26.6046	3.50085	-29.6671	-26.9543	3.40518	-29.9332
8abp	12	7	8.00	-19.0497	3.32242	-21.9562	-19.0594	3.80549	-22.3884