

Table 1S. MT scoring result against a test set with 795 protein-ligand complexes.

PDB ID	exp.	MT	Original	Glide	Glide
	pK_d/pK_i	KECSA pK_d/pK_i	KECSA pK_d/pK_i	SP Score	XP Score
2aac	2.22	2.664	4.9983	-7.16	-9.79
1ajp	2.23	2.5618	4.3331	-6.75	-5.21
1uto	2.27	2.0579	3.9891	-7.05	-5.92
1qi0	2.35	2.4075	3.6334	-5.39	-12
6rnt	2.37	2.8461	3.8767	-4.97	-4.76
1oba	2.44	1.322	3.5455	-6.28	-5.45
2i2b	2.44	3.8577	3.9796	-7.36	-8.09
1tok	2.47	1.8589	4.2685	-7.14	-8.39
1utl	2.47	2.3736	4.4362	-7.09	-6.49
1gyx	2.48	3.1484	4.3568	-5.57	-4.95
1ai4	2.5	3.098	4.4551	-6.31	-6.1
2r5a	2.6	1.9313	3.0037	-3.87	-4.64
1ajn	2.63	3.3015	4.0577	-6.33	-4.47
3bra	2.7	1.1787	3.2605	-4.5	-3.84
2vyt	2.74	1.7871	3.0085	-3.75	-4.58
2bet	2.77	2.3554	4.2042	-8.21	-8.67
2bza	2.8	2.631	5.062	-7.29	-7.05
3c2u	2.9	4.0518	4.214	-6.3	-11.34
2fw6	2.92	3.8584	4.6623	-7.81	-9.03
2fwp	2.92	3.8049	4.7006	-7.5	-9.42
1tng	2.93	2.6603	4.9782	-6.8	-4.81
1f4e	2.96	2.6468	3.8846	-5.66	-3.9
1ws4	3	2.6475	3.9207	-7.19	-6.57
2v3u	3	2.4526	5.397	-6.66	-10.14
1utm	3.01	2.0138	3.81	-7.13	-6.36
1ogd	3.03	2.1464	4.3336	-6.32	-9.3
1ws5	3.03	2.553	3.9343	-6.67	-6.59
2ha3	3.03	1.92	4.5787	-6.59	-5.85
1uj6	3.05	2.7876	4.5937	-7.4	-8.9
1y1z	3.08	2.8456	6.0871	-8.29	-9.6
1ugw	3.09	2.2677	4.0581	-6.41	-6.47
3buf	3.1	1.327	3.3187	-5.77	-3.69
3c2r	3.11	3.1391	4.5721	-5.68	-6.26
1lbk	3.18	4.4072	4.6701	-6.47	-4.62
1br6	3.22	5.6011	4.4857	-7.36	-8.66
1e6s	3.22	3.4856	5.0717	-5.15	-7.89
1tog	3.22	2.9479	4.8069	-8.86	-10.16

2ri9	3.22	1.1861	3.6465	-5.57	-5.27
1v2j	3.25	2.9949	5.4962	-7.82	-7.36
5yas	3.26	1.6923	5.0446	-6.62	-8.18
1bcu	3.28	3.4763	4.0763	-7.18	-5.52
1phw	3.3	1.4194	3.7255	-6.09	-6.23
3c2o	3.35	2.9645	4.3105	-6.45	-7.61
1tnh	3.37	2.6968	5.254	-7.39	-6.8
1v2u	3.37	2.9762	5.0853	-7.99	-7.38
1toj	3.39	2.6151	4.6102	-8.83	-10.89
1uz4	3.4	3.2105	5.1311	-9.22	-11.13
2sim	3.42	3.5835	4.1985	-7.37	-9.91
1c5o	3.49	2.6805	4.6251	-8.62	-7.3
1utn	3.49	2.6387	5.2782	-7.16	-6.31
1jys	3.52	3.0372	3.5004	-5.77	-5.69
1v2r	3.55	4.4335	4.3488	-8.69	-9.32
2cle	3.55	4.5067	5.3899	-9.44	-8.37
2clf	3.55	4.4571	5.3387	-10.24	-10.05
1nli	3.59	3.5657	5.4153	-8.95	-8.89
1d7i	3.6	1.5447	4.4839	-5.46	-3.12
3jdw	3.6	1.6128	4.4861	-5.08	-6.84
1pb9	3.62	2.4378	6.0303	-6.65	-6.35
1gyy	3.64	3.4519	4.404	-5.48	-5.39
2azr	3.64	4.4901	5.0089	-8.8	-7.81
2v00	3.66	3.6029	4.7129	-5.71	-4.56
3buh	3.66	2.256	4.3891	-5.46	-5.18
1c3x	3.68	3.0748	6.0796	-6.73	-5.39
2a8g	3.69	4.3846	4.5471	-7.14	-8.75
3clp	3.69	4.7725	5.0314	-9.12	-8.44
1loq	3.7	3.2514	4.9435	-9.22	-9.96
1wht	3.7	4.4305	4.8214	-7.06	-6.92
2bvr	3.7	5.0684	4.9803	-7.49	-9.38
2fx6	3.7	3.8329	5.3124	-7.51	-5.37
2vfk	3.71	3.3798	3.8172	-6.75	-6.97
1ai5	3.72	3.4875	4.4963	-6.45	-4.52
1nje	3.8	3.3778	4.7316	-6.62	-5.61
2hb1	3.8	3.3349	4.531	-8.3	-7.08
1j16	3.84	2.7019	4.9749	-7.37	-8.8
1utj	3.84	2.4912	4.8234	-6.86	-6.01
1n1t	3.85	3.662	4.1336	-8.38	-10.97
1aj7	3.87	4.285	4.4864	-7.55	-7.89
1x9d	3.96	3.593	4.8447	-6.33	-10.03

2fpz	3.96	3.7076	5.323	-7.34	-4.71
2wec	3.96	5.7327	5.3741	-7.89	-8.88
2g8r	3.99	2.8193	3.6667	-5.43	-4.08
1lgw	4	2.2854	5.5125	-6.75	-6.17
1tni	4	3.3404	5.3365	-6.42	-6.32
2qrl	4	1.5169	3.5876	-5.75	-6.42
1c5z	4.01	2.767	4.8807	-8.34	-7.91
1v2w	4.01	4.1789	4.4761	-7.08	-9.77
3bxh	4.03	3.1856	4.9442	-7.93	-11.41
1toi	4.05	2.6407	4.5148	-8.55	-10.65
1tuf	4.05	3.0791	4.3788	-2.68	-3.34
2clh	4.06	5.0958	5.6612	-11.47	-9.92
1n2v	4.08	3.5139	4.1695	-8.46	-6.31
1c5t	4.1	3.2095	4.8202	-8.9	-7.98
1odj	4.1	4.8533	5.1038	-7.55	-8.02
2bvs	4.1	6.478	5.1266	-9.42	-9.18
1p19	4.11	3.2932	4.187	-8.84	-9.7
2exm	4.11	3.3649	3.9628	-7.75	-7.69
1v2q	4.13	4.1032	4.2877	-7.65	-9.63
1v2s	4.17	2.9064	5.1919	-8.18	-7.49
1c5y	4.2	3.4784	5.3927	-9.85	-8.08
1c87	4.2	4.4577	5.5213	-8.86	-9.53
1ghw	4.2	4.7093	5.1347	-10.39	-9.85
1odi	4.21	5.1161	5.2126	-8.09	-7.62
1pzi	4.22	2.8275	3.7161	-6.04	-6.88
1ua4	4.22	4.407	4.357	-11.74	-15.09
2bes	4.24	2.7484	4.5673	-6.89	-10.28
1li3	4.25	2.1262	4.9108	-6.58	-7.86
2qrk	4.26	4.0134	3.8684	-5.37	-4.82
1e2l	4.29	4.1337	5.2282	-10.2	-10.39
1v2l	4.29	2.825	4.9717	-7.8	-7.09
1det	4.3	3.1363	3.1401	-8.87	-11.79
1w3k	4.3	3.7197	4.8076	-6.93	-13.84
2cli	4.3	4.7232	5.6771	-10.82	-9.5
1ajq	4.31	2.9927	5.5685	-7.13	-5.77
2tpi	4.31	4.9528	5.1265	-7.41	-6.99
2ha6	4.32	4.2299	3.8678	-7.42	-10.41
4rsk	4.32	2.7314	3.6839	-5.1	-5.79
1e3v	4.34	2.7264	4.9337	-6.06	-5.83
1z6s	4.34	3.3092	3.9128	-5.57	-5.96
2ha5	4.34	1.9819	3.8873	-4.98	-6.98

1ghv	4.35	4.4051	4.6555	-10.12	-10.05
1sv3	4.35	2.3754	3.9835	-6.18	-4.45
1bhf	4.38	6.9337	4.2348	-7.99	-10.3
2hjb	4.39	3.6023	5.3495	-7.99	-7.31
1p57	4.4	4.3767	4.6952	-8.74	-7.91
2pwd	4.4	2.8279	5.5879	-8.03	-8.12
1no6	4.41	4.1804	4.7616	-6.84	-10.04
2pu2	4.43	4.028	4.1793	-7.25	-7.2
2r2w	4.47	5.233	5.2435	-9.48	-9.84
1qan	4.48	7.0459	5.4016	-10.45	-10.39
2ogy	4.48	4.8465	4.3359	-6.41	-6.57
1j14	4.49	2.8264	5.4131	-8.23	-8.83
1gi7	4.51	4.0084	4.4706	-10.42	-9.91
1gul	4.52	3.4531	5.3608	-7.3	-7.36
2a4m	4.52	2.9806	4.4376	-7.63	-5.37
1fj4	4.59	4.077	5.247	-6.86	-5.52
1l2s	4.59	3.6943	4.6801	-5.89	-5.17
2jiw	4.59	4.325	5.6277	-9.22	-10.01
1pa9	4.6	3.7412	5.1317	-8.87	-7.82
1upf	4.6	1.7618	3.5925	-6.06	-4.75
2ha2	4.66	4.0173	3.9433	-6.12	-8.61
2nsl	4.68	4.3015	4.7873	-9.96	-9.87
1c5n	4.7	2.8839	6.1171	-8.45	-6.28
1c86	4.7	4.7345	5.7959	-9.74	-10.72
2j9n	4.7	2.9922	5.5094	-8.42	-7.68
2qfo	4.7	2.1037	3.9792	-6.92	-4.61
3kiv	4.7	2.4156	4.6704	-5.19	-7.19
1v2t	4.71	3.9998	4.2367	-9.39	-10.65
1v2o	4.73	4.2498	4.3952	-8.61	-10.04
1ce5	4.74	3.0286	5.3831	-8.28	-7.16
1w4p	4.74	2.8825	3.8669	-5.92	-6.47
1q8t	4.76	3.9201	4.7309	-9.09	-8.09
2b4l	4.77	2.884	4.9468	-8.83	-7.22
1oss	4.79	2.5775	4.9359	-6.11	-3.77
2nsj	4.79	4.8625	4.8344	-10.05	-7.24
1bjv	4.8	4.5546	4.6839	-8.05	-8.53
2nta	4.8	5.2282	5.7505	-5.76	-4.99
1aid	4.82	3.2879	5.6256	-6.5	-6.16
1v1j	4.82	3.4875	5.2915	-7.13	-7.49
1xff	4.82	3.7152	5.2545	-10.92	-14.6
2gl0	4.82	4.5895	4.4237	-7.6	-9.32

2pwg	4.82	3.2875	5.3987	-8.7	-10.14
1c83	4.85	5.411	5.4174	-9.02	-10.26
1ecv	4.85	4.6006	6.3895	-8.75	-10.52
1xgi	4.85	4.2198	4.6665	-6.8	-5.17
3cj2	4.85	3.1582	4.0867	-5.49	-5.04
2brb	4.86	4.9193	4.6436	-7.15	-6.86
1p1q	4.89	3.8382	5.1087	-9.1	-10.55
2j77	4.89	3.1985	5.3591	-6.75	-9.94
3cf8	4.9	3.8902	4.4236	-7.65	-10.55
1bzc	4.92	6.6344	5.4375	-8.88	-10.99
1e1v	4.92	4.3913	4.8383	-9.04	-9.24
1h1p	4.92	3.9363	4.2877	-9.63	-9.21
1jqy	4.92	4.9842	4.4694	-6.54	-7.73
1e2k	4.94	4.3077	5.1935	-8.33	-7.31
2gss	4.94	2.6242	3.4028	-4.93	-5.48
1cea	4.96	2.3517	4.6516	-6.47	-9.31
1o5g	4.96	6.2261	5.6591	-11.35	-9.98
1tsy	4.96	3.8247	4.8436	-6.43	-6.45
3bxg	4.96	3.3732	5.1428	-8.28	-11.59
1c84	5	5.3155	5.4324	-8.94	-10.97
1nc3	5	6.012	5.1303	-10.2	-12.38
2oym	5	4.8272	4.6149	-8.75	-10.09
2glp	5.01	6.4223	4.8642	-7.61	-6.54
2d0k	5.02	5.4436	4.03	-7.18	-6.72
3bgc	5.02	9.039	6.6143	-10.6	-12.01
2qt5	5.03	4.8149	3.8697	-7.44	-8.55
2c3l	5.07	4.2388	5.0046	-8.66	-8.29
1enu	5.08	3.6426	4.4822	-9.55	-8.46
2qtg	5.08	5.0473	5.4328	-8.51	-7.5
1m48	5.09	5.7454	5.101	-7.14	-7.29
1nw7	5.09	5.3015	4.5902	-9.53	-10.97
1od8	5.1	4.2815	4.8132	-7.67	-10.2
1onz	5.1	4.2523	4.5169	-7.19	-7.06
1v0k	5.1	3.5742	4.6945	-6.91	-10.25
1w7g	5.1	5.52	5.7493	-8.3	-8.09
1k4h	5.11	4.5867	4.7998	-8.86	-8.83
2web	5.12	7.7628	5.8491	-8.08	-8.83
1gcz	5.13	5.3632	5.2819	-4.97	-6
2brl	5.14	5.3134	4.3464	-7.16	-7.17
1pb8	5.15	2.4005	5.5213	-7.49	-10.66
1s38	5.15	4.3545	5.6095	-8.67	-8.44

1thz	5.15	5.1262	4.7681	-6.46	-5.09
2f5t	5.17	5.1228	5.1776	-9.56	-19.08
3b7j	5.17	2.6927	4.1947	-6.25	-7.23
1ocq	5.19	3.9107	4.8855	-6.94	-12.4
1rnt	5.19	3.6469	4.1748	-10.96	-13.1
1j17	5.22	8.0626	6.3164	-8	-6.97
1o5c	5.22	5.4245	5.4365	-10.56	-10.86
1w4o	5.22	3.0231	4.0959	-6.8	-7.48
2hxm	5.22	5.4535	4.4156	-8.89	-8.76
1fh7	5.24	4.2526	5.058	-8.19	-12.61
2jfz	5.24	7.1965	5.2545	-8.51	-8.21
1w4q	5.26	3.7663	4.4614	-6.79	-6.45
1b46	5.28	7.3161	5.6057	-10.64	-13.2
1c88	5.29	4.9541	5.9343	-9.4	-9.38
1a69	5.3	4.7415	5.1567	-7.4	-7.63
1pr1	5.3	4.084	4.8786	-6.77	-8.36
1srg	5.3	6.6561	5.5636	-8.5	-4.48
1vyq	5.3	5.3695	5.2581	-8.56	-9.55
1xbb	5.3	5.2093	4.8339	-7.17	-10.04
2oyk	5.3	3.96	4.075	-7.06	-9.68
1lvu	5.32	5.3615	4.7289	-8.14	-8.77
1y20	5.32	2.6125	6.2781	-7.76	-6.52
2c80	5.33	6.1543	5.0641	-8.26	-9.87
1zgi	5.34	5.34	5.4515	-7.48	-8.87
2fxv	5.35	4.9427	4.7541	-9.64	
1adl	5.36	3.6317	4.0036	-4.93	-5.75
1sgu	5.37	8.4166	6.3141	-11.58	-9.15
1qbv	5.39	6.979	5.0251	-9.35	-8.08
2h6b	5.39	3.1212	4.9285	-9.41	-9.77
1bp0	5.4	3.2799	4.5452	-8.77	-10.85
1r9l	5.4	2.8799	5.2399	-9.78	-8.41
2c1p	5.4	5.3055	4.964	-8.33	-8.19
2f35	5.4	3.4295	4.0045	-6.11	-5.8
2i80	5.4	5.4206	5.9317	-7.67	-8.76
2qg2	5.4	5.5415	4.4649	-9.03	-8.95
3b4p	5.4	4.3024	5.1047	-7.49	-10.81
2j47	5.41	6.0606	5.3751	-7.63	-9.35
1gja	5.42	4.758	4.7325	-9.65	-10.66
1syi	5.44	5.2207	5.795	-10.32	-12.39
2iko	5.45	5.4642	5.1877	-7.38	-5.55
1lv8	5.46	5.2092	4.7339	-6.93	-5.57

1q65	5.46	4.6949	4.975	-8.68	-8.56
1gi1	5.47	4.3863	4.8842	-8.59	-9.48
1o2s	5.47	4.4604	4.6684	-9.49	-8.85
1g85	5.48	1.6341	2.9503	-4.46	-5.11
1pot	5.49	4.2313	5.6946	-8.47	-12.46
2h4k	5.49	4.1867	4.6617	-8.37	-9.03
2o0u	5.49	7.3414	6.0676	-10.49	-9.13
3bvb	5.49	7.7655	6.1028	-7.63	-9.68
1a8i	5.52	3.5389	4.4894	-7.77	-10.55
1oe8	5.52	3.6742	3.8493	-5.41	-7.13
1ydr	5.52	4.4115	5.1625	-9.26	-9.52
2cht	5.52	3.7169	4.855	-7.8	-7.16
1bjv	5.54	4.4735	4.5487	-5.93	-8.77
1y3n	5.55	4.3535	4.5061	-6.16	-11.8
2iuz	5.55	7.0726	4.9896	-9.29	-9.55
1jak	5.57	4.3057	5.642	-8.95	-10.31
1njd	5.57	3.8886	4.9167	-6.55	-7.75
3bex	5.57	3.4113	4.5001	-3.74	-5.79
1f4x	5.59	3.999	3.9112	-6.14	-8.5
1mfi	5.59	4.76	5.7851	-4.14	-2.92
1vfn	5.6	2.6303	5.0027	-6.14	-4.64
1a08	5.62	5.0818	5.0438	-8.4	-10.84
1ejn	5.62	5.9106	5.5761	-5.14	-4.83
2bmk	5.62	4.3	4.2946	-5.22	-3.06
2ojg	5.64	4.7883	5.0461	-10	-10.52
1nhu	5.66	3.6048	5.0186	-5.85	-6.16
2pqz	5.67	7.7347	6.7827	-9.18	-8.87
1ow4	5.68	5.0277	5.0792	-8.15	-9.03
2cbu	5.68	3.7911	5.739	-7.82	-9.49
1g98	5.7	2.7374	4.3913	-8.17	-6.48
1jsv	5.7	4.3373	4.9471	-8.2	-9.23
2f2h	5.7	6.4268	5.5272	-8.33	-11.58
1n7m	5.71	8.5755	5.8118	-7.49	-8.22
2qg0	5.72	4.983	4.8965	-6.31	-5.34
1o33	5.74	4.2467	4.6457	-9.2	-9.66
1o5e	5.74	6.2024	5.6436	-10.72	-10.8
1qy2	5.74	2.5931	3.5967	-6.44	-5.47
2b1v	5.74	3.2311	4.4951	-9.45	-9.09
2pgz	5.74	5.1342	5.0118	-10.99	-13.36
1p1o	5.76	3.8775	4.9342	-10.12	-11.64
1o5b	5.77	3.473	6.8263	-9.04	-8.06

1q66	5.77	6.3911	6.1982	-8.81	-8.42
1hmt	5.79	3.7702	3.9812	-1.4	-4.86
1kpm	5.8	6.5194	5.6171	-5.19	-6.75
2q88	5.8	4.1368	6.0205	-9.47	-10.76
1urg	5.82	4.0568	3.7509	-6.98	-10.46
3gss	5.82	7.6125	5.0154	-8.09	-8.83
1k4g	5.85	4.713	4.6239	-10.21	-10.24
1o2w	5.85	5.1379	4.142	-9.88	-9.73
1o2x	5.85	5.214	4.2974	-9.48	-9.64
1ogz	5.85	3.2376	4.476	-6.92	-7.46
1q63	5.85	5.1148	5.3377	-9.39	-9.4
1u1w	5.85	3.8606	5.469	-7.07	-5.69
2r3t	5.85	9.7872	7.1036	-12.44	-12.16
3e5u	5.85	3.3395	4.9651	-10.5	-10.58
1e1x	5.89	3.7685	4.1421	-5.55	-8.61
1ydk	5.89	5.1376	4.6723	-5.87	-8.56
2brm	5.89	4.5344	4.6435	-5.59	-5.81
1v2n	5.9	5.3435	5.6868	-9.79	-9.57
1ugx	5.91	3.0559	3.356	-6	-9.05
1a4w	5.92	6.9672	6.2565	-8.36	-11.7
1kyv	5.92	6.7477	5.1727	-10.52	-12.61
1pph	5.92	5.0626	5.3386	-8.98	-9.47
1yds	5.92	4.3972	5.0237	-9.73	-12.16
1fv0	5.93	5.0933	4.3642	-7.1	-3.16
1b9j	5.96	7.6125	5.3946	-10.51	-11.88
1nl9	5.96	6.2375	5.0672	-8.16	-8.67
1o36	5.96	6.7373	5.089	-9.64	-10.46
1c5s	6	3.3322	5.2842	-8.45	-7.64
1ceb	6	2.5461	4.7332	-6.68	-8.23
1hn2	6	3.8831	3.9206	-9.07	-9.47
1ssq	6	1.6734	4.7276	-5.92	-6.15
1xgj	6	3.6809	4.4833	-5.41	-6.15
2bvd	6	4.2255	5.0355	-6.2	-8.39
2izl	6	4.169	5.1382	-7.42	-9.57
2r43	6	8.1134	6.6149	-10.76	-10.71
1eb2	6.01	7.5101	6.0227	-8.96	-8.62
1tcw	6.02	5.9571	5.306	-6.73	-7.24
5er1	6.02	5.9137	4.9127	-8.25	-7.77
1n8v	6.03	2.585	3.5299	-3.02	-6.05
3bgb	6.05	6.8564	5.7051	-8.56	-7.38
1jmg	6.07	4.0192	5.216	-7.06	-5.25

2gst	6.07	7.255	5.8245	-10.05	-12.97
1dzk	6.1	2.0499	3.2115	-6.22	-5.62
1m2q	6.1	4.4387	4.825	-8.6	-8.73
2e7f	6.1	5.6366	4.9113	-5.88	-5.75
2flr	6.1	7.8232	5.8767	-7.79	-7.22
2p7a	6.1	2.4539	4.4441	-7.09	-6.35
2wed	6.1	6.5028	5.6187	-9.42	-7.67
1g32	6.11	7.7134	5.7176	-8.57	-8.96
1o2z	6.11	6.3572	4.8454	-9.02	-10.32
2qmq	6.11	8.0547	7.1362	-10.28	-8.9
1nc1	6.12	7.0555	5.8074	-11.83	-12.49
2fgv	6.12	9.6324	6.8101	-7.13	-8.37
1ppc	6.16	6.3419	5.7613	-8.89	-10.87
2i4j	6.16	7.4882	5.6922	-8.08	-9.74
1d6v	6.17	5.9801	5.0852	-9.53	-13.1
1ycl	6.17	4.8142	4.9157	-8.52	-8.77
1xhy	6.18	4.5297	5.3768	-9.26	-10.53
2qhm	6.18	4.1472	4.9191	-8.76	-8.54
1v2k	6.19	8.1203	6.2299	-9.17	-7.86
2bt9	6.19	2.7682	4.3992	-6.71	-8.08
2qbu	6.19	7.4919	5.7964	-11.39	-15.57
1owe	6.2	4.3292	4.8891	-9.19	-8.41
2aj8	6.2	5.7871	5.0164	-8.58	-10
1wcq	6.26	3.9979	4.2963	-7.4	-10.5
2ok1	6.26	5.954	5.4619	-8.68	-7.05
3bgz	6.26	4.8587	4.8054	-7.96	-8.07
1pbq	6.27	4.078	4.7463	-8.35	-8.99
3bfu	6.27	3.5509	5.2316	-8.97	-10.35
1lag	6.3	3.865	5.861	-9.28	-11.57
1wdn	6.3	3.5949	5.3743	-8.72	-8.46
1wm1	6.3	4.344	5.381	-7.79	-7.75
2q89	6.3	4.1263	5.5734	-9.67	-11.3
3ebl	6.3	4.4254	5.6038	-9.29	-9.59
2bal	6.31	5.0285	4.8527	-9.37	-9.74
1w3j	6.32	2.7937	5.2251	-6.54	-7.89
2qbr	6.33	5.4582	5.0918	-8.1	-7.27
3cj5	6.34	4.5055	4.8591	-5.95	-4.72
3ckp	6.35	8.0702	5.7918	-10.73	-11.32
1c5q	6.36	3.3495	6.3726	-8.22	-8.14
1ela	6.36	6.3088	5.4513	-4.59	-6.45
1o2o	6.36	5.6614	5.2847	-9.03	-8.78

1hbv	6.37	7.5044	5.7774	-6.68	-6.08
1hms	6.37	3.5581	3.6362	-2.21	-5
1i7z	6.4	5.0728	4.9574	-6.92	-5.39
1usk	6.4	3.7202	5.4496	-8.05	-5.21
2o2u	6.4	4.952	5.5164	-8.3	-8.11
1syh	6.41	5.2336	5.852	-10.38	-11.18
2cgf	6.41	3.8357	4.216	-6.75	-5.53
1o5a	6.42	5.8148	5.4493	-10.24	-10.22
1fh9	6.43	4.7664	5.1353	-7.36	-10.94
2b07	6.43	6.0967	6.2935	-8.89	-9.13
1gt3	6.46	2.3391	3.3745	-5.11	-6.09
1m2r	6.46	4.9688	5.0555	-8.21	-8.23
1r5y	6.46	4.4897	5.8472	-9.94	-8.61
1f4g	6.48	5.8068	4.6615	-8.12	-7.17
1gpn	6.48	5.2058	5.8471	-9.54	-9.01
1rpj	6.48	3.0888	5.4871	-6.67	-11.8
1dl7	6.49	4.0213	4.1896	-8.05	-7.44
3cj4	6.51	4.2676	4.4338	-6.38	-5.76
1ct8	6.52	6.8116	5.5033	-10.03	-10.99
1g74	6.52	4.2166	5.2252	-0.64	-2.98
1gt4	6.52	2.8188	3.5893	-0.28	-5.18
1qy1	6.52	3.1491	4.4036	-6.28	-5.45
1zhy	6.52	4.5891	5.7815	-10.11	-11.72
2nt7	6.52	7.525	6.4497	-8.09	-7.62
2oxy	6.52	2.5611	3.5675	-5.9	-5.39
3d0b	6.54	6.6552	5.2025	-10.96	-11.23
1dhj	6.55	5.5194	3.8509	-8.66	-9.68
1hmr	6.55	3.5621	3.9658	-1.33	-3.79
1n4h	6.55	4.2746	4.6754	-8.67	-11.01
1yc4	6.55	4.2911	4.8957	-7.86	-6.76
2bok	6.55	6.2133	5.487	-10.97	-12.09
2pwc	6.57	8.6919	6.7921	-10.13	-9.88
1k1i	6.58	5.4688	5.5559	-10.67	-11.9
1izi	6.59	9.6779	6.4208	-7.8	-5.84
2pvh	6.59	5.131	4.7414	-7.36	-8.25
2pwr	6.59	10.401	7.3191	-13.4	-12.58
1g7g	6.6	8.583	5.1613	-8.58	-10.9
2j4g	6.6	5.0311	5.9178	-6.51	-8.9
1ii5	6.62	2.8975	4.9083	-8.99	-9.66
2zb0	6.62	6.7669	5.5526	-5.47	-6.16
3f8f	6.63	6.4526	4.5849	-8.43	-11.1

2d3z	6.64	5.2624	5.3989	-7.71	-6.64
1o3p	6.66	5.268	5.1626	-11.31	-10.53
1pxp	6.66	6.264	5.277	-9.52	-10.62
1c5x	6.68	3.8298	6.9426	-9.67	-8.24
2fqw	6.68	4.6201	5.2953	-9.64	-8.9
2iwx	6.68	3.8636	4.3147	-7.05	-5.82
2qbs	6.68	5.3565	5.1377	-8.02	-7.61
1b0h	6.7	10.311	6.3311	-12.08	-15.46
1dfo	6.7	7.5527	5.0634	-8.77	-10.42
1eld	6.7	6.7	6.3768	-5.45	-4.85
2oxx	6.7	2.8828	4.4655	-6.12	-6.41
3eko	6.7	2.7217	4.4287	-6.61	-5.82
3gst	6.72	7.7753	5.7551	-11.82	-15.48
1usi	6.74	4.7704	5.7499	-9.16	-9.91
1o30	6.77	6.4856	5.2588	-10.06	-9.19
1o3j	6.77	4.9005	4.9001	-9.33	-9.23
1o3k	6.77	4.6365	4.5806	-9.12	-9.01
1ony	6.77	6.8495	5.3659	-7.91	-8.01
1qb1	6.77	6.9749	5.6204	-10.3	-11.26
2rcb	6.79	2.1363	5.7398	-9.05	-13.02
1fl3	6.8	6.478	5.1678	-10.15	-11.94
1nq7	6.8	4.8082	4.6944	-10.24	-11.88
1p1n	6.8	4.213	5.0131	-10.67	-12.24
3d94	6.8	8.0889	6.1271	-12.92	-12.07
1drk	6.82	2.681	5.6066	-7.67	-11.71
1fhd	6.82	5.1229	5.1034	-6.66	-9.51
1k1n	6.82	5.3705	5.3492	-9.07	-11.23
1uwf	6.82	2.5485	4.3102	-3.75	-5.36
2oxd	6.82	2.9152	4.2	-5.86	-5.59
1bhx	6.84	6.649	5.7074	-10.6	-10.72
1ele	6.85	6.6525	5.7495	-7.05	-6.41
1g30	6.85	7.3986	5.3654	-8.25	-9.7
1os5	6.85	4.9859	5.1812	-4.77	-6.48
1q72	6.85	4.6047	4.8041	-5.84	-5.06
1xk9	6.85	5.6821	5.0302	-8.2	-8.25
1xt8	6.85	2.304	5.7236	-9.48	-14.56
1xka	6.88	7.3442	5.345	-8.65	-11.29
1fh8	6.89	4.1008	4.9589	-8.48	-12.21
1sb1	6.89	7.6344	6.6908	-8.28	-7.23
2dri	6.89	2.6249	5.7372	-7.61	-11.44
2f34	6.89	3.6515	4.6812	-6.38	-9.23

2r3w	6.89	8.5329	6.8669	-11.47	-10.63
1swr	6.92	4.5607	5.8461	-10.5	-11.4
2d3u	6.92	4.9809	5.173	-7.72	-6.71
2g79	6.92	3.4841	4.7917	-5.76	-4.98
2uy0	6.92	10.582	6.5289	-12.75	-15.01
1tcx	6.95	7.2206	5.6192	-10.77	-12.42
1c5c	6.96	4.7501	5.3628	-9.36	-9.41
1ent	6.96	7.5441	5.7664	-7.66	-8.26
1gvw	6.96	7.9002	5.8947	-6.87	-6.81
1oyq	6.96	6.7109	5.0566	-10.41	-10.89
1x8j	6.96	2.3154	4.6055	-8.49	-9.13
1fki	7	4.8976	4.536	-7.14	-7.5
1fpc	7	6.4822	5.48	-7.34	-8.52
1gj6	7	6.2275	5.8558	-9.63	-9.35
2j7g	7	4.5805	4.93	-8.08	-10.92
3cdb	7.02	6.8822	6.6083	-9.17	-8.53
1b1h	7.03	8.9082	5.849	-11.77	-15
2bq7	7.05	7.3985	5.8359	-10.26	-9.7
1lpg	7.09	8.588	6.3105	-12.74	-11.73
2bz6	7.09	6.3241	5.2931	-10.07	-11.5
2il2	7.1	10.123	6.2642	-8.83	-10.59
#####	7.11	5.083	5.0481	-9.21	-9.12
1b05	7.12	7.208	5.6818	-10.77	-13.57
1nz7	7.12	7.7356	5.5446	-7.6	-9.57
1o3d	7.13	5.5022	5.531	-9.37	-8.45
1zog	7.15	3.4075	4.5135	-6.22	-6.63
2fqx	7.15	4.8711	5.3838	-10.36	-9.6
2qnn	7.15	10.126	8.2955	-14.04	-12.95
1f0u	7.16	7.3149	5.3722	-6.09	-10.89
1g36	7.17	6.4624	5.3767	-9.34	-10.57
2q63	7.18	7.9876	6.66	-9.72	-10.21
1fcx	7.19	7.7418	5.907	-14.2	-13.28
2j7h	7.19	2.5653	5.2064	-6.79	-8.66
3c79	7.2	5.1235	4.8524	-6.5	-7.86
1sw2	7.22	2.9803	5.3444	-9.39	-9.81
2epn	7.22	4.1489	5.4871	-6.92	-6.04
1g2l	7.24	9.2415	5.4971	-11.43	-12.6
1oyt	7.24	5.863	5.6245	-10.91	-12.1
2psv	7.24	7.3879	5.7297	-8.36	-10.55
1jet	7.25	7.1508	5.3119	-11.39	-11.8
1dhi	7.26	5.5957	3.8076	-9.03	-9.81

1mrx	7.26	8.5156	6.1386	-9.83	-11.73
1b40	7.28	8.8594	5.8463	-12.59	-14.97
1kel	7.28	4.9931	4.5523	-8.37	-3.66
2pql	7.28	4.0029	5.7451	-9.62	-9.69
2qhz	7.28	8.0748	7.474	-11.71	-10.69
3ccz	7.29	5.9571	5.4061	-6.93	-7.39
1o3i	7.3	4.5933	4.9723	-9.34	-9.81
2qi1	7.3	8.5764	6.5704	-10.51	-11.04
1ydt	7.32	6.5494	5.6083	-10.3	-11.35
2j7e	7.32	5.0617	5.1341	-8.27	-11.14
2j2u	7.33	7.8885	5.7066	-8.15	-7.67
2r2m	7.33	6.6687	5.5559	-6.71	-8.96
1uw6	7.34	4.2028	5.0051	-10.26	-9.77
2gv6	7.34	4.9646	5.6155	-10.06	-10.6
1swg	7.36	3.7419	5.1461	-7.87	-8.87
1bxq	7.38	8.2667	5.7159	-9.12	-8.77
2qi0	7.38	9.0885	7.0267	-11.41	-10.72
1k1m	7.4	6.2093	5.8475	-10.11	-10.51
1oar	7.4	5.9923	5.4548	-7.93	-9.5
1owh	7.4	4.66	4.9295	-9.4	-8.11
1r6n	7.4	5.6679	5.6575	-6.44	-4.63
2bpy	7.4	7.8581	6.2657	-10.3	-7
1q5k	7.42	4.5186	4.5579	-6.53	-8.15
1t32	7.42	8.2221	6.7969	-10.23	-10.18
2bak	7.43	9.3867	5.7818	-7.86	-11.07
1vzq	7.44	6.4506	5.8063	-12.6	-12.25
2qbk	7.44	5.533	5.4925	-8.38	-8.54
2r38	7.44	9.4655	7.0849	-8.4	-10.79
1sqo	7.46	5.1662	5.0563	-10.01	-9.43
2qhy	7.48	8.2714	6.9896	-10.03	-8.74
2hhn	7.49	8.7035	6.2939	-6.46	-6.71
1lah	7.52	3.2236	5.5473	-9.45	-11.34
1lf2	7.52	8.0601	5.9452	-10.01	-9.38
1lke	7.52	5.6216	5.718	-11.09	-12.49
3ekr	7.52	3.6719	4.867	-6.93	-6
2flg	7.54	6.2439	5.5449	-7.19	-6.9
1k1j	7.55	6.3883	5.8742	-7.9	-11.34
1lpk	7.55	7.7619	5.8529	-10.62	-11.49
1v0l	7.55	3.6986	4.9244	-7.68	-11.61
1vj9	7.55	7.7085	5.6896	-12.41	-13.12
3b50	7.55	3.7902	4.3178	-8.95	-14.16

3cct	7.56	6.9011	6.0928	-8.75	-9.19
1q95	7.57	4.0892	5.106	-9.69	-11.37
2avs	7.57	9.5432	6.6087	-11.78	-10
2pyn	7.57	7.7894	6.398	-10.42	-10.15
3cd0	7.57	6.4787	5.8952	-6.2	-6.51
3cda	7.58	7.4506	6.5062	-8.61	-9.86
1lpz	7.6	8.4485	5.9161	-12.04	-11.51
2psu	7.62	8.0051	5.7933	-8.49	-9.48
2pvl	7.62	6.1027	4.9991	-9.24	-7.63
3be9	7.62	5.9733	5.0621	-11.31	-11.33
1f0r	7.66	7.382	5.8006	-9.21	-8.76
1nny	7.66	8.9095	6.0687	-10.11	-8.03
1ppk	7.66	6.4718	5.3244	-8.27	-9.13
2bpv	7.67	7.4451	6.0971	-10.76	-10.76
1o2q	7.68	6.2684	5.7822	-6.2	-9.76
1t4v	7.68	5.634	4.9582	-8.72	-9.72
1w0z	7.68	6.4544	4.9102	-10.93	-12.39
3f8c	7.68	6.9206	5.5297	-7.53	-9.05
1izh	7.7	11.299	6.7563	-8.01	-7.29
1mes	7.7	8.1767	6.1974	-12.04	-14.47
1oau	7.7	4.5432	4.2886	-7.16	-6.86
1uou	7.7	4.2057	5.0943	-9.31	-9.17
1vja	7.7	7.5568	5.3854	-9.23	-13.24
1ajv	7.72	9.2868	6.6809	-10.36	-11.21
1j4r	7.72	7.4651	5.9758	-8.25	-8.97
1lee	7.74	8.3463	5.9912	-7.92	-12.44
1nfu	7.74	6.9148	6.2017	-10.69	-10.96
1qbo	7.74	6.12	5.3932	-9.02	-9.42
1qiw	7.74	5.8768	5.2688	-7.6	-8.34
1rd4	7.74	6.5757	5.6632	-8.72	-8.62
1sbg	7.74	8.1026	5.7441	-10.69	-11.37
2jh6	7.77	6.3475	5.8987	-7.39	-7.82
2qm9	7.77	5.9778	5.9238	-5.97	-6.12
3cyw	7.77	8.2908	6.0741	-6.16	-8.45
1v48	7.8	5.5701	5.4798	-9.07	-7.71
2ra0	7.8	9.6247	6.1517	-10.18	-8.65
1b6h	7.82	7.5559	5.3976	-9.98	-13.42
1nf8	7.82	4.5818	5.0218	-9.92	-12.41
1njs	7.82	7.8275	5.4613	-14.6	-18.84
1nvs	7.82	5.893	5.8481	-9.49	-9.67
2j34	7.82	6.9504	5.9429	-8.29	-7.73

3cd7	7.84	7.3393	6.3083	-8.7	-9.5
1laf	7.85	4.0616	5.5086	-9.45	-11.7
1lst	7.85	3.5688	5.6646	-9.43	-11.69
2gv7	7.85	6.7609	6.8304	-6.7	-10.72
3ccw	7.87	5.8546	5.5263	-6.84	-6.97
3cd5	7.9	7.0244	5.7584	-10.64	-10.85
1ajx	7.91	8.0018	6.114	-10.91	-13.05
3d7z	7.92	7.4981	5.7184	-11.48	-12.21
1epo	7.96	9.2981	6.6533	-5.59	-7.62
1g2k	7.96	9.2726	6.587	-12.91	-13.22
1hvh	7.96	6.9132	5.9207	-8.96	-13.38
2qe4	7.96	4.6377	4.9946	-9.7	-10.06
3bgq	7.96	4.3105	5.2627	-7.61	-5.8
#####	8	7.2362	4.2191	-10.13	-10.52
1a4k	8	5.41	5.4815	-8.79	-9.59
1apw	8	7.1043	5.0342	-10.11	-10.44
1fkg	8	4.9197	4.678	-8.32	-9.28
1gaf	8	4.6583	6.006	-8.8	-8.11
1r0p	8	7.4029	5.4674	-12.24	-12.98
1vyg	8	5.5565	5.3168	-5.32	-6.73
2vnt	8	6.0012	6.7139	-9.92	-11.44
3cyx	8	9.2302	5.7825	-9.94	-10.25
1b7h	8.02	7.7682	5.4098	-10.57	-13.13
1vyf	8.05	3.5027	4.3239	-1.88	-3.07
2bqv	8.05	8.1571	5.9662	-10.56	-14.02
1gni	8.07	4.8653	4.1056	-3.85	-10.06
2rkg	8.09	8.4171	6.203	-6.77	-6.25
1erb	8.1	5.2499	5.0361	-8.29	-9.83
1stc	8.1	7.5546	6.363	-12.99	-12.51
2pvj	8.1	6.5134	5.1206	-9.41	-9.9
1nvr	8.11	7.0232	6.0623	-11.29	-11.52
1g35	8.14	9.2306	6.4886	-13.3	-14.43
1yqj	8.14	8.0653	6.0161	-11	-10.87
1fkh	8.15	5.1133	5.3935	-7.48	-8.42
1w5v	8.15	11.991	7.4945	-12.55	-13.82
2fxu	8.15	7.7681	6.4011	-9.79	-11.48
3bu1	8.15	2.0095	4.5722	-7.47	-6.79
2f80	8.18	7.902	6.2148	-9.78	-10.71
2jds	8.2	6.589	5.3907	-11.82	-12.93
1efy	8.22	5.4246	4.6817	-8.5	-8
1h1s	8.22	6.4473	5.2445	-10.41	-12.74

1w11	8.22	7.2747	5.827	-11.62	-13.21
2cji	8.22	7.2689	5.5505	-8.66	-7.9
2zcs	8.22	4.6271	5.5811	-8.22	-6.5
3d1y	8.22	9.6403	6.7421	-13.34	-13.17
3e5a	8.23	6.619	5.5207	-6	-7.02
1nvq	8.25	7.679	6.2261	-11.75	-13.47
2e2r	8.26	4.7805	4.8246	-10.15	-10.46
1tom	8.3	5.9139	5.4995	-10.46	-10.56
2cen	8.3	10.202	6.6111	-12.01	-14.79
2v95	8.3	4.8671	5.3164	-8.09	-10.17
3d20	8.3	8.2904	6.2824	-7.69	-11.32
2hs2	8.31	7.6572	6.0941	-5.55	-12.39
1hwr	8.33	5.5722	5.3826	-8.49	-10.96
2qci	8.34	8.3958	6.2268	-10.42	-12.22
1h23	8.35	8.5015	6.2125	-9.84	-14.33
1mj7	8.35	7.2348	5.1713	-8.84	-9.75
1d4j	8.36	10.501	6.7429	-14.68	-16.47
3d83	8.36	7.4873	5.8894	-7.91	-11.95
2nmy	8.37	8.0759	6.444	-7.37	-12.61
2nmz	8.37	8.8074	6.7158	-8.71	-11.2
2nnk	8.37	9.0333	6.693	-8.66	-12.79
2nnp	8.37	9.1312	6.7055	-10.06	-10.5
1k21	8.38	6.2346	5.2216	-9.6	-10.96
1mu6	8.38	6.9052	5.2281	-9.42	-8.51
1fd0	8.4	8.2435	6.0347	-14.41	-17.06
1k22	8.4	7.0418	5.5673	-11.41	-11.5
1mtr	8.4	8.1323	5.5062	-11.76	-11.97
1w5x	8.4	12.608	7.9031	-11.1	-17.31
3b68	8.4	8.2214	6.055	-10.85	-10.75
1w96	8.41	6.5539	4.8207	-8.73	-9.4
2oag	8.47	7.1537	6.335	-8.63	-3.92
1w5y	8.48	10.981	7.7536	-12.7	-17.31
2hs1	8.48	7.9355	5.9407	-5.86	-6.26
2r5p	8.48	9.7456	6.5797	-13.76	-10.48
2uxz	8.48	10.049	6.1645	-12.42	-13.1
1ec0	8.49	11.87	7.3131	-10.73	-17.5
2ieo	8.49	7.5572	5.9707	-9.41	-12.34
2ihq	8.49	6.281	5.965	-10.09	-8.61
1fcy	8.52	8.012	6.001	-14.51	-13.45
1i5r	8.52	12.612	7.1517	-8.55	-15
1ta2	8.52	7.7881	5.887	-10.12	-9.54

1xkk	8.52	9.3159	6.3512	-6.96	-8
2boh	8.52	8.4247	6.7018	-8.7	-9.4
2bxt	8.52	8.8101	6.278		
2qu6	8.52	8.3573	5.5446	-13.42	-15.28
2vw5	8.52	5.2363	4.7805	-7.41	-7.64
1hos	8.55	8.1434	6.7648	-13.02	-11.61
1ppl	8.55	7.8562	5.7114	-5	-4.23
2byr	8.55	8.0888	6.2352	-8.99	-11.01
1bwa	8.6	11.205	8.1221	-16.76	-17.84
3b66	8.6	8.0442	5.7904	-11.5	-11.81
6std	8.64	4.3231	5.1926	-8.62	-9.27
3d1x	8.66	9.1823	6.7626	-13.02	-12.01
2qd6	8.68	7.9032	6.1042	-11.72	-10.44
2q55	8.69	9.304	6.5215	-7.8	-12.52
1jgl	8.7	5.346	5.7518	-12.97	-11.83
1lnm	8.7	5.755	5.6509	-9.38	-10.89
1ohr	8.7	7.6183	6.4961	-9.53	-11.03
1t7j	8.7	6.8621	5.3835	-9.54	-9.2
1w13	8.7	6.9904	5.3986	-12.02	-13.09
1xap	8.7	6.8717	5.5526	-12.92	-14.21
2f8g	8.7	7.8891	6.1767	-10.84	-12.95
2fr3	8.7	4.041	5.0332	-6.54	-6.74
2jh0	8.7	6.5278	6.1586	-8.23	-7.41
2ojj	8.7	5.8406	5.6648	-11.7	-12.53
2pcp	8.7	6.3489	6.1324	-9.42	-9.76
2uwo	8.7	7.6464	6.1971	-8.37	-7.37
3brn	8.7	3.4623	4.4311	-9.05	-7.06
3eqr	8.7	8.3973	5.6078	-9.3	-11.61
1b6k	8.74	8.7432	5.816	-12.77	-13.11
1mjj	8.74	7.0674	5.1151	-8.76	-10.37
1sdv	8.74	9.5499	6.5036	-13.33	-14.2
2vkm	8.74	13.284	7.1546	-9.55	-4.7
1d4l	8.77	8.1856	5.7948	-12.01	-14.81
1zp8	8.77	8.9601	6.3201	-7.59	-6.07
3b5r	8.77	7.3911	6.0245	-11.53	-12.12
1w5w	8.8	11.863	7.7385	-12.38	-17.24
3d1z	8.8	7.7036	6.147	-11.84	-12.19
#####	8.85	8.45	6.8287	-11.87	-11.11
1d4i	8.85	11.071	6.509	-14.23	-17.55
2avo	8.85	9.5101	6.4491	-11.61	-10.65
3b67	8.85	7.6976	6.4748	-10.45	-10.27

1nfy	8.89	7.0336	6.3846	-9.16	-7.48
1nt1	8.89	7.854	5.537	-11.51	-10.3
2idw	8.89	7.4357	5.8965	-7.05	-9.21
1ec1	8.92	10.638	7.1112	-7.44	-7.95
1kzn	8.92	6.719	5.7038	-6.38	-6.43
1nfw	8.96	7.6258	6.3678	-8.86	-7.95
1mq5	9	9.3752	6.685	-10.66	-12.73
1mu8	9	7.3929	5.4207	-9.54	-8.62
2ien	9	8.1125	6.1471	-9.41	-13.38
2j4i	9	8.4093	5.8723	-7.29	-6.43
2p4y	9	7.3566	6.134	-12.51	-11.74
2q54	9.01	8.8004	6.3437	-9.86	-11.11
1ebw	9.05	9.5807	6.1388	-9.84	-7.73
1ezq	9.05	10.172	6.0691	-8.44	-13.04
1kdk	9.05	4.3565	5.6141	-11.43	-10.87
2qd8	9.07	8.1525	6.1046	-11.91	-12.14
2rkf	9.08	8.703	6.2703	-6.89	-6.58
1msn	9.09	9.8292	6.5964	-10.56	-10.73
1h22	9.1	7.9734	6.0686	-10.98	-15.52
2qd7	9.1	8.1565	6.1727	-10.42	-12.66
1ta6	9.13	8.0567	5.6317	-10.53	-10.27
2qmg	9.15	10.868	7.1221	-13.65	-16.98
2fgu	9.18	9.5122	6.8505	-6.52	-6.15
1d4k	9.22	9.4814	6.4076	-8.97	-13.09
1fcz	9.22	7.8284	6.0045	-13.79	-12.73
1hps	9.22	8.9336	6.3573	-9.37	-9.35
1hpy	9.22	7.033	5.5889	-9.57	-9.99
1z1r	9.22	8.8352	5.8725	-12.7	-13.43
1db1	9.26	5.7885	5.9084	-12.5	-14.45
2avv	9.26	9.5564	6.6065	-11.03	-9.62
1sdt	9.27	9.802	6.5564	-13.63	-11.31
3b65	9.27	6.8101	6.6773	-10.88	-11.3
1xow	9.28	5.0132	5.9531	-11.51	-10.14
2ayr	9.29	8.7488	6.5818	-12.79	-14.1
1bv7	9.3	11.842	8.2025	-16.72	-19.84
2aqu	9.32	9.6081	5.9078	-7.21	-6.85
2r6w	9.36	7.1487	6.3733	-12.1	-10.65
2z4b	9.36	5.1731	5.7771	-10.45	-10.2
2p95	9.37	8.4914	6.213	-10.1	-8.39
1ebz	9.4	10.105	6.2826	-10.31	-15.11
1ksn	9.4	9.5438	5.7968	-10.64	-12.14

1met	9.4	8.6806	6.3808	-12.16	-15.05
2o4r	9.4	5.874	6.0693	-12.38	-13.51
1hsh	9.42	8.7644	6.2738	-11.98	-8.18
1qbs	9.47	8.3623	6.2397	-13.18	-16.45
2r6y	9.49	6.9147	6.07	-12.54	-11.83
1hvr	9.51	9.7345	6.9885	-13.45	-14.93
2bys	9.52	8.4206	6.0655	-14.39	-17.31
2g94	9.52	11.37	6.1675	-6.54	-8.33
1dmp	9.55	8.8469	6.4122	-12.84	-13.6
1df8	9.7	4.7893	5.1913	-9.73	-10.27
1eby	9.7	11.063	6.8259	-15.69	-17.37
1mrw	9.7	8.2186	6.1821	-12.11	-11.84
2vh6	9.7	9.0918	7.014	-9.63	-9.16
1z6e	9.72	10.27	6.4327	-11.04	-8.37
2std	9.85	3.9904	4.951	-8.43	-9.61
2drc	9.89	5.8698	3.9303	-8.17	-8.5
1hxb	9.92	9.1019	6.8337	-8.31	-9.21
1hvl	9.95	9.7635	6.4784	-6.09	-8.02
1bv9	9.96	11.535	8.2072	-16.51	-18.2
1bxo	10	8.5768	5.6179	-9.4	-7.04
1d4h	10	10.674	6.5464	-13.49	-14.79
1sdu	10.07	9.5182	6.4795	-12.55	-10.56
1sr7	10.1	7.1199	6.6614	-12.1	-13
2o4j	10.1	6.2573	6.1138	-11.22	-12.75
2p16	10.1	8.8746	5.781	-10.34	-8.68
1y6r	10.11	6.3656	5.7572	-12.49	-14.63
2qi3	10.2	6.7077	5.7047	-9.7	-11.8
2qi7	10.21	7.4998	5.7979	-9.3	-11.62
1qbu	10.24	7.963	6.7479	-12.44	-14.54
1hvs	10.3	9.5074	6.355	-7.55	-8.22
1kzk	10.39	9.2897	6.7259	-13.43	-14.01
2qi4	10.44	8.5335	6.5665	-11.04	-12.85
2o4k	10.46	10.287	6.2445	-8.08	-8.79
1msm	10.48	9.9681	6.7223	-12.5	-12.76
5std	10.49	7.05	5.4737	-11.22	-12
2o4s	10.51	10.055	6.4943	-8.16	-7.96
1n46	10.52	7.5437	5.7128	-11.08	-10.92
2f81	10.52	8.0104	6.1374	-7.22	-11.43
1qbr	10.57	11.178	8.179	-16.12	-17.33
2qi6	10.57	8.5358	6.5497	-11.36	-11.89
3djk	10.59	7.6862	5.7928	-11.09	-11.32

3cs7	10.68	8.425	6.4818	-9.57	-9.28
2pk5	10.7	12.885	7.8776	-10.52	-14.26
7std	10.72	4.1803	5.0554	-9.32	-10.4
1hxw	10.82	9.5279	6.9342	-7.03	-8.41
2qi5	10.85	8.5725	6.3559	-8.19	-13.33
2pk6	10.89	11.749	7.7518	-16.19	-16.52
1hvi	10.92	10.224	6.4833	-9.54	-8.52
1hvk	10.96	10.972	6.6657	-8.05	-8.49
1mq6	11.15	9.5741	6.13	-10.6	-10.34
2i4v	11.2	8.3801	6.1095	-6.51	-6.52
1hpx	11.26	7.8104	6.5794	-7.56	-7.61
2q5k	11.3	9.8163	6.4231	-7.69	-6.4
2hb3	11.35	7.9608	6.1581	-11.08	-11.46
1hvj	11.4	10.264	6.5103	-8.54	-8.89
2i0a	11.4	8.0905	6.0559	-6.46	-4.55
2i4u	11.57	8.0221	6.1305	-7.34	-10.74
2i4w	11.59	9.1315	6.3321	-11.17	-10.36
2i4d	11.68	8.2556	6.0726	-7.06	-5.74
1y6q	11.7	6.103	5.3171	-12.1	-12.5
2i4x	11.72	9.7985	6.3358	-11.4	-11.81

Table 2S. Heatmap docking RMSD result against a test set with 795 protein-ligand complexes.

PDB ID	RMSD			PDB ID	RMSD		
	for Heatmap	RMSD for Glide SP	RMSD for Glide XP		for Heatmap	RMSD for Glide SP	RMSD for Glide XP
2aac	0.77	0.28	0.66	lizi	1.46	9.08	9.08
1ajp	0.57	0.8	2.76	2pvh	2.53	5.01	4.86
luto	0.37	1.27	2.28	2pwr	1	0.43	0.55
1qi0	0.1	4.52	4.52	1g7g	3.43	6.2	0.00
6rnt	0.82	10.13	5.68	2j4g	2.72	0.25	0.28
1oba	1.94	3.31	2.85	1ii5	4.65	0.71	1.44
2i2b	2.46	0.55	0.38	2zb0	0.25	0.71	0.67
1tok	1.06	0.35	0.31	3f8f	0.31	6	1.72
1utl	0.17	0.71	2.68	2d3z	2.39	0.74	1.09
1gyx	1.16	1.99	1.90	1o3p	2.41	1.1	1.61
1ai4	1.04	0.74	1.12	1pxp	0.69	0.51	0.41
2r5a	1.16	1.23	1.72	1c5x	3.5	0.38	0.94
1ajn	1.16	1.36	0.48	2fqw	3.57	0.27	0.32

3bra	2.63	1.61	3.91	2iwx	2.49	0.17	0.19
2vyt	1.65	1.61	1.57	2qbs	2.29	0.87	0.90
2bet	0.72	1.38	1.40	1b0h	0.25	0.57	0.75
2bza	0.29	0.33	0.26	1dfo	1.48	0.75	0.98
3c2u	1.99	2.05	0.99	1eld	0.04	4.77	2.31
2fw6	1.63	1.14	2.07	2oxx	3.65	0.78	3.97
2fwp	1.53	2.13	1.81	3eko	3.68	0.57	0.57
1tng	0.47	0.28	0.29	3gst	1.83	0.69	0.51
1f4e	0.54	1.49	1.08	1usi	3.41	0.4	0.95
1ws4	0.61	0.24	0.30	1o30	0.49	3.89	4.46
2v3u	0.95	0.24	0.80	1o3j	3.24	1.73	1.97
1utm	1.73	0.24	1.60	1o3k	3.7	1.7	0.79
1ogd	1.53	0.24	1.98	1ony	0.14	3.55	3.71
1ws5	0.83	0.31	0.36	1qbl	0.35	2.67	4.53
2ha3	1.92	2.88	2.38	2rcb	3.66	0.18	0.34
1uj6	0.45	1.04	1.92	1fl3	0.56	1.01	0.97
1ylz	0.41	0.2	1.10	1nq7	3.45	0.65	0.94
1ugw	1.42	0.23	0.33	1p1n	4.48	0.94	1.52
3buf	3.07	2.77	4.70	3d94	2.23	1.19	1.34
3c2r	0.05	1.88	1.19	1drk	3.17	0.29	0.33
1lbk	2.13	0.36	0.88	1fhd	2.94	0.3	0.30
1br6	4.12	0.81	0.76	1k1n	2.51	5.17	2.01
1e6s	0.46	0.89	3.63	1uwf	2.14	5.12	3.25
1tog	0.47	0.89	0.72	2oxd	3.45	0.93	2.45
2ri9	3.52	0.89	2.30	1bhx	0.33	0.65	1.23
1v2j	0.44	0.5	1.18	1ele	0.34	0.47	0.88
5yas	2.72	1.08	2.28	1g30	0.95	3.68	2.52
1bcu	0.34	0.34	4.04	1os5	3.23	6.47	2.51
1phw	3.26	5.15	3.75	1q72	3.89	0.5	0.60
3c2o	0.67	1.62	2.95	1xk9	2.02	5.78	2.43
1tnh	1.17	0.22	0.78	1xt8	2.87	0.26	1.15
1v2u	0.68	0.33	0.31	1xka	0.8	0.82	1.68
1toj	1.34	0.42	0.60	1fh8	4.83	0.18	0.90
1uz4	0.33	0.39	0.49	1sb1	1.29	0.3	2.75
2sim	0.28	0.42	1.36	2dri	3.76	0.27	0.29
1c5o	1.4	1.17	1.11	2f34	2.61	1.73	1.73
1utn	1.47	0.29	0.83	2r3w	2.85	0.25	0.22
1jys	0.84	0.91	2.47	1swr	4.09	0.37	0.49
1v2r	1.53	2.48	3.39	2d3u	3.36	0.46	1.43
2cle	1.66	1	1.39	2g79	3.95	0.48	2.06
2clf	1.57	1.18	1.19	2uy0	3.11	2.69	0.94
1nli	0.04	0.32	0.21	1tcx	0.47	9.59	1.17
1d7i	3.56	1.02	3.39	1c5c	3.83	0.29	1.09
3jdw	3.44	1.35	4.08	1ent	1.01	8.19	8.19
1pb9	2.05	0.28	0.25	1gvw	1.63	10.73	9.19

1gyy	0.33	1.16	4.86	1oyq	0.43	1.8	3.94
2azr	1.47	1.03	1.26	1x8j	3.45	0.61	0.61
2v00	0.1	1.5	1.50	1fki	3.64	1.15	0.16
3buh	2.43	4.39	1.02	1fpc	0.9	5.52	1.32
1c3x	1.05	2.68	4.58	1gj6	1.34	0.41	0.26
2a8g	1.2	2.73	2.74	2j7g	3.7	0.77	1.19
3clp	1.87	0.25	0.31	3cdb	0.24	3.74	4.03
1loq	0.78	0.48	0.93	1b1h	2.25	0.77	0.71
1wht	1.27	0.91	0.61	2bq7	0.6	0.63	0.46
2bvr	2.37	7.61	7.61	1lpg	2.59	1.02	2.18
2fx6	0.23	0.54	0.39	2bz6	1.33	0.63	1.56
2vfk	0.57	7.61	7.87	2il2	5.24	6.91	0.84
1ai5	0.4	1.07	0.99	3.00E+64	3.51	0.93	2.77
1nje	0.73	1.09	1.09	1b05	0.15	0.9	1.14
2hb1	0.81	1.1	1.16	1nz7	1.07	8.58	8.49
1j16	1.97	1.08	0.56	1o3d	2.82	0.7	0.98
1utj	2.34	0.25	0.73	1zog	3.72	1.14	3.67
1n1t	0.33	1.09	1.24	2fqx	3.95	0.27	0.21
1aj7	0.72	1.14	1.99	2qnn	1.15	0.56	0.66
1x9d	0.64	0.26	0.39	1f0u	0.27	3.94	0.72
2fpz	0.44	0.47	2.29	1g36	1.23	1.79	1.85
2wec	3.07	2.43	2.43	2q63	1.4	1.51	1.51
2g8r	2.03	6.15	6.15	1fcx	0.96	0.33	0.26
1lgw	2.97	0.45	0.46	2j7h	2.42	0.33	3.69
1tni	1.14	1.83	2.74	3c79	3.6	0.86	3.16
2qrl	4.3	1.14	1.95	1sw2	3.76	0.21	0.50
1c5z	2.15	0.4	0.36	2epn	2.32	0.36	0.22
1v2w	0.29	1.88	4.29	1g2l	1.44	3.15	3.15
3bxh	1.46	0.43	0.90	1oyt	2.39	0.66	0.66
1toi	2.44	0.51	1.27	2psv	0.26	2.05	0.54
1tuf	1.68	8.46	7.60	1jet	0.17	0.65	1.24
2clh	1.79	0.94	1.35	1dhi	2.88	0.8	1.27
1n2v	0.98	0.49	3.22	1mrx	2.17	3.65	0.69
1c5t	1.54	0.37	0.99	1b40	2.74	0.46	0.77
1odj	1.3	0.73	0.73	1kel	3.96	1.13	1.92
2bvs	4.12	8.27	8.05	2pql	3.68	0.26	0.50
1p19	1.41	1.33	1.23	2qhz	1.38	0.32	0.47
2exm	1.29	0.47	0.77	3ccz	2.31	9.12	1.09
1v2q	0.05	2.59	4.81	1o3i	3.56	0.63	2.12
1v2s	2.19	1.13	1.13	2qil	1.21	0.57	0.27
1c5y	1.25	0.42	0.95	1ydt	1.33	0.7	0.87
1c87	0.45	0.82	0.29	2j7e	2.98	0.4	0.64
1ghw	0.88	0.72	1.06	2j2u	0.97	0.37	0.23
1odi	1.57	0.76	2.25	2r2m	1.15	2.4	2.58
1pzi	2.41	2.39	2.41	1uw6	3.36	0.3	0.39

1ua4	0.32	0.77	1.48	2gv6	4.11	3.38	3.61
2bes	2.58	1.12	1.28	1swg	3.27	2.53	2.46
1li3	3.68	0.28	0.65	1bxq	1.54	4.86	4.75
2qrk	0.43	3.11	0.64	2qi0	0.96	0.65	1.45
1e2l	0.27	0.57	0.51	1k1m	2.06	0.97	1.93
1v2l	2.54	0.34	0.23	1oar	2.44	0.97	1.35
1det	2.02	3.62	5.16	1owh	2.75	0.79	2.74
1w3k	1.01	0.25	0.26	1r6n	3	0.77	2.86
2cli	0.73	0.96	1.11	2bpy	0.79	11.82	1.71
1ajq	2.28	0.31	0.48	1q5k	3.03	1.66	1.66
2tpi	1.11	0.9	0.73	1t32	1.39	0.42	0.64
2ha6	0.16	3.46	2.17	2bak	3.39	9.13	3.28
4rsk	2.75	4.63	4.63	1vzq	1.71	0.61	0.27
1e3v	2.79	7.75	7.75	2qbk	3.3	0.57	1.05
1z6s	1.79	3.98	3.98	2r38	3.51	3.84	0.33
2ha5	4.08	4.3	2.63	1sqo	2.87	0.29	0.79
1ghv	0.1	0.58	1.92	2qhy	1.37	2.42	2.47
1sv3	3.42	2	2.58	2hhn	2.1	10.5	2.10
1bhf	4.42	11.9	5.14	1lah	3.25	0.24	0.21
2hjb	1.36	1.38	1.39	1lf2	0.94	1.09	1.09
1p57	0.04	1.01	1.09	1lke	2.29	0.42	0.43
2pwd	2.72	0.27	0.45	3ekr	3.46	3.11	3.27
1no6	0.4	1.02	0.81	2flg	2.24	1.52	2.10
2pu2	0.7	0.81	0.81	1klj	2.01	4.49	1.95
2r2w	1.32	0.67	0.94	1lpk	0.37	2.06	0.40
1qan	4.44	0.49	0.36	1v0l	1.28	0.3	0.34
2ogy	0.63	0.69	3.80	1vj9	0.27	1.66	2.81
1j14	2.88	1.09	1.18	3b50	3.11	0.82	0.67
1gi7	0.87	1.22	1.91	3cct	1.14	0.88	1.21
1gu1	1.85	0.28	0.91	1q95	2.15	1.23	1.18
2a4m	2.67	1.49	3.14	2avs	3.42	0.31	0.34
1fj4	0.89	0.77	0.97	2pyn	0.38	0.98	8.26
1l2s	1.55	1.56	1.56	3cd0	1.89	1.37	0.85
2jiw	0.46	0.22	0.39	3cda	0.22	0.79	0.37
1pa9	1.49	0.34	0.89	1lpz	1.47	0.72	0.62
1upf	4.92	1.51	3.06	2psu	0.67	1.97	0.60
2ha2	1.11	1.51	3.21	2pvl	2.63	0.56	0.40
2nsl	0.66	1.2	1.92	3be9	2.85	0.28	0.35
1c5n	3.15	0.93	0.27	1f0r	0.48	0.42	0.62
1c86	0.06	0.36	0.20	1nny	2.16	1.59	1.48
2j9n	2.96	0.19	1.08	1ppk	2.06	1.37	1.32
2qfo	4.5	0.49	0.57	2bpv	0.39	0.6	0.95
3kiv	3.96	0.68	1.76	1o2q	2.44	8.62	1.19
1v2t	1.23	2.92	3.85	1t4v	3.54	0.97	0.89
1v2o	0.83	7.08	3.11	1w0z	2.12	0.45	1.04

1ce5	2.96	1.02	0.24	3f8c	1.32	7.09	7.09
1w4p	3.22	4.14	4.14	lizh	0.23	8.49	8.49
1q8t	1.45	0.89	1.41	1mes	0.83	0.36	0.46
2b4l	3.27	0.4	0.57	1oau	5.47	1.25	1.32
1oss	3.83	1.02	1.83	1uou	2.05	0.49	0.44
2nsj	0.13	1.02	1.63	1vja	0.25	5.95	0.59
1bju	0.43	0.26	1.03	1ajv	2.71	0.45	0.52
2nta	0.74	0.37	0.61	1j4r	0.44	2.81	2.65
1aid	2.65	3.81	3.67	1lee	1.05	7.42	0.86
1v1j	2.31	0.3	0.68	1nfu	1.43	1.17	1.17
1xff	1.91	0.35	1.05	1qbo	2.81	3.09	3.56
2gl0	0.4	0.7	2.12	1qiw	3.23	3.18	3.90
2pwg	2.65	0.5	0.30	1rd4	2.02	2.93	1.19
1c83	0.97	0.31	0.77	1sbg	0.63	3.39	3.42
1ecv	0.43	0.19	0.86	2jh6	2.46	3.35	3.97
1xgi	1.09	1.09	2.74	2qm9	3.1	4.58	4.41
3cj2	2.93	0.33	0.35	3cyw	0.9	10.39	7.42
2brb	0.1	0.65	0.65	1v48	3.86	0.91	0.58
1plq	1.82	1.45	1.87	2ra0	3.16	0.72	0.75
2j77	2.93	0.58	2.32	1b6h	0.46	0.7	0.84
3cf8	1.75	6.3	2.94	1nf8	2.61	0.92	0.83
1bzc	2.97	1.12	0.97	1njs	0.01	0.92	1.27
1e1v	0.92	0.49	2.90	1nvs	3.34	0.51	0.25
1h1p	1.7	4.23	2.86	2j34	1.51	0.49	0.53
1jqy	0.11	2.65	3.07	3cd7	0.87	0.48	0.86
1e2k	1.1	0.58	2.31	1laf	2.56	0.9	0.90
2gss	4.01	3.05	2.91	1lst	1.42	0.23	1.23
1cea	4.52	1.13	1.46	2gv7	1.89	5.39	3.13
1o5g	2.19	0.83	1.50	3ccw	3.49	0.85	0.75
1tsy	1.97	2.13	2.13	3cd5	1.52	0.57	1.38
3bxg	2.75	0.93	0.94	1ajx	0.16	0.33	0.44
1c84	0.55	0.29	0.34	3d7z	0.73	0.45	0.40
1nc3	1.75	0.49	0.75	1epo	1.32	7.97	7.97
2oym	0.3	0.75	0.97	1g2k	0.27	0.6	0.57
2glp	1.18	8.23	8.23	1hvh	1.81	5.74	1.13
2d0k	0.73	1.03	0.99	2qe4	2.75	0.54	3.71
3bge	2.12	2.37	0.76	3bgq	3.32	0.31	2.45
2qt5	0.37	0.93	0.92	3.00E+92	1.32	0.5	0.38
2c3l	1.44	0.89	1.48	1a4k	3.49	1.66	2.04
1enu	2.49	0.25	0.18	1apw	1.55	0.48	1.01
2qtg	0.06	0.45	0.57	1fkg	2.34	1.24	1.52
1m48	1.14	0.84	1.20	1gaf	2.79	1.41	0.67
1nw7	0.37	0.68	0.64	1r0p	1.03	0.28	0.27
1od8	1.42	0.26	0.29	1vyg	2.23	1.27	3.10
1onz	1.47	0.83	0.81	2vnt	1.46	0.53	0.61

1v0k	2.64	0.32	0.38	3cyx	0.78	8.52	0.00
1w7g	0.73	6.61	5.90	1b7h	0.44	0.69	1.03
1k4h	0.91	0.66	0.84	1vyf	3.88	2.01	3.89
2web	1.46	5.65	5.65	2bqv	0.19	2.18	2.18
1gcz	0.4	4.99	4.99	1gni	4.03	2.08	2.75
2br1	0.3	0.98	1.32	2rkg	0.57	8.56	8.56
1pb8	2.27	0.4	1.38	1erb	4.94	2.19	1.39
1s38	1.38	0.25	0.30	1stc	0.94	0.31	0.31
1thz	0.04	1.02	1.02	2pvj	2.75	0.65	1.67
2f5t	0.08	0.16	0.15	1nvr	1.88	0.27	0.21
3b7j	3.81	7.02	7.02	1g35	1.89	0.53	0.52
1ocq	2.22	0.15	0.24	1yqj	0.13	0.26	0.33
1rnt	2.67	0.15	0.75	1fkh	1.26	1.48	1.24
1j17	0.53	0.48	1.38	1w5v	1.65	5.78	4.24
1o5c	0.35	1.58	2.01	2fxu	0.66	1.28	2.40
1w4o	3.81	7.67	7.67	3bul	2.36	0.57	1.15
2hxm	0.4	0.96	1.29	2f80	0.48	1.35	0.51
1fh7	1.71	0.27	0.40	2jds	2.79	0.46	1.46
2jtz	3.39	0.3	0.56	1efy	3.31	0.91	1.98
1w4q	2.59	1.55	1.55	1h1s	2.84	0.91	0.79
1b46	3.53	0.67	0.89	1w11	1.64	0.94	1.00
1c88	0.58	0.77	0.82	2cji	1.65	0.51	0.31
1a69	0.97	0.48	0.00	2zcs	2.22	1.94	2.88
1pr1	2.11	1.56	0.68	3d1y	2.46	0.51	0.53
1srg	2.35	6.62	6.62	3e5a	2.79	6.47	2.15
1vyq	0.12	0.83	0.57	1nvq	0.99	0.32	0.24
1xbb	0.16	6.02	3.82	2e2r	4.37	0.15	0.17
2oyk	2.32	0.5	0.57	1tom	2.13	0.46	0.88
1lvu	0.07	1.92	3.03	2cen	3.29	0.71	0.88
1y20	2.53	0.23	1.21	2v95	1.57	0.73	0.74
2c80	1.43	1.49	2.07	3d20	0.02	9.7	0.65
1zgi	0.33	7.75	0.39	2hs2	1.13	3.58	0.65
2fxv	0.71	0.66		1hwr	3.7	0.39	0.38
1adl	2.99	4.57	3.98	2qci	0.1	3.37	0.44
1sgu	0.87	0.52	0.94	1h23	0.26	6.42	2.09
1qbv	2.75	0.48	0.78	1mj7	1.93	5.53	1.80
2h6b	3.93	0.49	0.51	1d4j	1.71	1.33	1.52
1bp0	3.67	0.86	0.84	3d83	1.51	11.31	0.62
1r9l	2.41	0.44	1.15	2nmy	0.51	7.75	1.53
2c1p	0.16	0.3	0.34	2nmz	0.76	8.44	0.00
2f35	3.41	1.27	1.67	2nnk	1.15	7.59	0.84
2i80	0.04	0.74	0.47	2nnp	1.32	9.67	9.67
2qg2	0.25	0.5	4.93	1k21	3.72	1	0.52
3b4p	1.9	0.69	1.24	1mu6	2.55	0.39	0.33
2j47	1.13	0.67	0.56	1fd0	0.27	0.59	0.59

1gja	1.15	0.46	0.88	1k22	2.35	0.64	0.89
1syi	0.38	0.79	0.64	1mtr	0.46	0.75	0.49
2iko	0.02	1.03	1.03	1w5x	1.65	5.9	0.82
1lv8	0.43	0.94	2.97	3b68	0.31	0.76	0.57
1q65	1.33	1.63	1.78	1w96	3.21	0.45	0.52
1gi1	1.88	0.86	0.77	2oag	2.28	0.56	0.48
1o2s	1.75	0.92	0.65	1w5y	1.18	5.73	1.51
1g85	4.29	2.97	4.56	2hs1	0.94	13.97	0.43
1pot	2.18	1.01	1.63	2r5p	2.19	0.44	0.67
2h4k	2.26	0.77	2.09	2uxz	0.66	0.84	3.86
2o0u	3.21	0.85	2.69	1ec0	0.85	5.81	1.07
3bvb	3.94	6.07	6.07	2ieo	1.62	1.76	0.91
1a8i	3.43	0.67	0.71	2ihq	3.62	0.47	0.38
1oe8	3.2	8.6	7.42	1fcy	0.88	0.61	0.58
1ydr	1.92	0.69	1.12	1i5r	1.09	12.91	7.33
2cht	3.12	0.98	3.85	1ta2	1.27	0.35	0.24
1bjv	1.85	9.87	5.33	1xkk	1.38	8.74	8.74
1y3n	2.07	0.8	0.00	2boh	0.17	1.89	0.89
2iuz	2.64	0.54	1.49	2bxt	0.5		
1jak	2.19	0.17	0.23	2qu6	0.28	1.05	1.08
1njd	2.91	4.63	1.01	2vw5	1.69	0.36	0.35
3bex	3.74	0.41	1.53	1hos	0.7	2.07	2.39
1f4x	2.76	0.65	0.90	1ppl	1.2	6.87	6.55
1mfi	1.44	7.62	6.96	2byr	0.8	0.31	0.93
1vfn	2.13	1.54	4.32	1bwa	0.51	0.46	0.57
1a08	0.93	2.68	3.63	3b66	0.96	0.74	0.89
1ejn	0.5	2.68	2.04	6std	5.48	0.35	2.54
2bmk	2.29	1.24	2.25	3d1x	0.9	0.39	0.36
2ojg	1.48	0.38	0.37	2qd6	1.35	0.52	0.74
1nhu	3.56	4.1	5.75	2q55	1.06	2.67	0.49
2pqz	3.58	0.83	1.06	1jgl	0.95	0.19	0.35
1ow4	1.13	0.95	0.89	1lnm	4.45	1.1	1.10
2cbu	3.27	0.35	0.35	1ohr	1.87	0.63	1.34
1g98	3.14	2.85	2.85	1t7j	3.18	0.87	1.11
1jsv	2.36	1.47	1.48	1w13	2.96	0.26	0.96
2f2h	1.26	0.62	0.79	1xap	3.17	0.27	0.65
1n7m	1.92	1.34	2.11	2f8g	1.4	3.2	1.21
2qg0	1.28	1.34	1.83	2fr3	2.07	0.73	1.95
1o33	2.59	0.97	0.65	2jh0	3.27	1.21	4.10
1o5e	0.8	0.56	0.69	2ojj	3.94	0.49	1.28
1qy2	2.59	0.58	0.37	2pcp	3.07	0.52	0.57
2b1v	4.35	0.48	0.37	2uwo	1.82	1.79	2.22
2pgz	1.05	0.5	4.40	3brn	4.41	0.27	2.90
1p1o	3.26	0.35	0.60	3eqr	0.52	1.89	1.16
1o5b	3.98	0.37	0.18	1b6k	0.01	0.7	1.46

1q66	1.08	1.12	1.06	1mjj	0.9	4.67	4.16
lhmt	3.5	1.45	3.67	1sdv	1.4	0.49	0.20
1kpm	1.25	13.89	4.39	2vkm	1.87	7.65	7.65
2q88	2.88	0.24	0.21	1d4l	1.01	0.79	0.51
1urg	3.05	0.52	0.54	1zp8	0.33	9.35	9.35
3gss	3.1	4.37	4.37	3b5r	2.39	0.48	0.50
1k4g	1.97	0.9	1.40	1w5w	1.78	1.75	0.73
1o2w	1.23	2.58	3.80	3d1z	1.9	0.49	0.88
1o2x	1.1	1.34	3.74	3.00E+93	0.69	0.45	0.41
1ogz	4.52	0.62	0.55	1d4i	3.85	5.9	5.90
1q63	1.27	0.96	0.79	2avo	1.14	0.46	1.06
1u1w	3.45	0.24	0.29	3b67	2	0.35	0.69
2r3t	3.8	0.9	1.34	1nfy	3.22	0.72	0.50
3e5u	4.35	0.33	0.41	1nt1	1.79	0.42	0.29
1e1x	3.67	2.01	0.76	2idw	2.52	5.87	1.16
1ydk	1.3	1.05	1.13	1ec1	2.98	12.13	1.64
2brm	2.35	4.83	4.83	1kzn	1.91	11.76	1.76
1v2n	0.96	0.44	0.39	1nfw	2.31	0.47	2.27
lugx	4.94	1.13	1.70	1mq5	0.65	1.49	2.63
1a4w	1.81	1.19	1.74	1mu8	2.78	0.27	0.44
1kyv	1.43	0.64	1.39	2ien	1.54	2.22	0.89
1pph	1.49	0.75	4.59	2j4i	1.02	6.98	6.98
1yds	2.64	0.53	0.89	2p4y	2.85	0.62	0.56
1fv0	1.45	0.69	0.61	2q54	0.36	6.27	6.27
1b9j	2.86	0.79	1.06	1ebw	0.92	5.22	5.16
1n19	0.48	0.46	1.09	1ezq	1.94	6.01	0.58
1o36	1.35	0.95	4.45	1kdk	4.13	0.22	0.30
1c5s	4.62	0.5	0.74	2qd8	1.59	0.6	0.60
1ceb	3.33	0.95	0.84	2rkf	0.65	9.76	9.76
1hn2	3.67	0.52	2.67	1msn	1.28	7.78	7.78
1ssq	4.1	1.85	2.53	1h22	1.95	3.41	2.85
1xgj	4.02	3.64	3.64	2qd7	1.63	3.27	0.50
2bvd	3.07	0.19	0.28	1ta6	1.86	0.43	0.45
2izl	3.17	0.23	1.02	2qmg	2.98	0.31	0.75
2r43	3.66	0.23	0.55	2fgu	0.58	9.3	9.30
1eb2	2.6	0.38	0.58	1d4k	0.45	3.35	3.35
1tcw	0.11	3.87	3.63	1fcz	2.41	0.3	0.31
5er1	0.18	5.99	5.99	1hps	0.5	8.5	6.50
1n8v	3.69	1.37	1.50	1hps	3.79	9.01	9.01
3bgb	1.4	1.48	1.80	1z1r	0.67	0.45	0.44
1jmg	3.55	1.75	1.75	1db1	2.01	0.24	0.38
2gst	2.05	1.24	1.01	2avv	0.51	1.02	1.02
1dzk	2.08	2.69	2.55	1sdt	0.92	0.51	0.43
1m2q	2.88	0.67	4.93	3b65	3.66	0.38	0.40
2e7f	0.8	1.37	4.09	1xow	3.21	0.21	0.11

2flr	2.98	0.6	1.20	2ayr	0.94	0.41	0.85
2p7a	4.45	0.26	0.20	1bv7	4.4	0.33	0.42
2wed	0.7	1.99	0.76	2aqu	0.5	9.74	8.91
1g32	2.78	1.99	0.64	2r6w	3.83	0.35	1.19
1o2z	0.43	1.88	4.13	2z4b	5.88	0.36	0.34
2qnq	3.37	0.53	1.47	2p95	1.52	0.4	0.32
1nc1	1.62	0.44	0.80	1ebz	1.22	9.52	0.00
2fgv	1.55	10.05	0.05	1ksn	0.25	0.62	0.58
1ppc	0.32	1.53	1.53	1met	1.25	0.39	0.30
2i4j	2.3	2.3	2.30	2o4r	3.11	0.56	0.64
1d6v	0.33	2.46	4.15	1hsh	1.14	0.63	0.65
1yc1	2.35	0.65	1.12	1qbs	1.92	0.32	0.40
1xhy	2.86	0.33	0.30	2r6y	4.46	0.25	1.00
2qhm	3.52	0.34	0.36	1hvr	0.39	0.35	0.35
1v2k	3.34	0.5	0.45	2bys	1.9	0.36	0.61
2bt9	4.27	0.24	0.30	2g94	3.2	8.77	8.77
2qbu	2.25	0.7	0.63	1dmp	1.22	0.4	0.55
1owe	3.24	0.33	0.81	1df8	2.05	0.37	0.70
2aj8	0.72	0.46	0.63	1eby	2.36	0.48	0.62
1wcq	3.92	0.95	0.94	1mrw	2.57	0.29	1.38
2ok1	0.53	3.2	2.06	2vh6	1.05	0.68	1.33
3bgz	2.43	0.66	0.40	1z6e	0.95	0.89	1.28
1pbq	3.8	0.18	0.33	2std	4.32	0.57	1.17
3bfu	4.71	0.55	1.03	2drc	3.78	1.06	4.04
1lag	4.22	0.41	0.26	1hxb	1.42	9.63	9.63
1wdn	4.69	0.61	0.84	1hvl	0.32	8.63	8.63
1wm1	3.39	0.9	1.71	1bv9	2.73	0.34	0.34
2q89	3.76	0.93	0.98	1bxo	2.47	0.38	0.80
3ebl	3.25	0.37	0.54	1d4h	1.17	0.95	0.89
2bal	2.22	0.37	0.60	1sdu	0.96	0.3	0.42
1w3j	4.31	2.32	2.19	1sr7	2.6	0.32	0.39
2qbr	1.51	5.4	1.31	2o4j	3.66	1.83	1.85
3cj5	3.18	0.66	3.09	2p16	2.12	0.28	0.38
3ckp	2.98	0.52	0.54	1y6r	2.55	0.3	0.29
1c5q	3.9	0.3	0.42	2qi3	2.41	1.13	1.00
1ela	0.09	2.36	2.23	2qi7	1.69	1.95	1.33
1o2o	1.21	0.72	0.67	1qbu	3.94	0.65	0.68
1hbv	1.96	8.31	8.31	1hvs	1.37	8.07	8.07
1hms	3.37	1.31	3.73	1kzk	1.91	0.48	1.33
1i7z	2.3	0.46	2.27	2qi4	3.3	1.01	1.32
1usk	4.64	0.25	1.23	2o4k	0.3	11.14	0.05
2o2u	2.51	2.34	0.54	1msm	0.89	1.22	0.38
1syh	2.04	0.81	0.87	5std	3.96	0.49	0.53
2cgf	4.46	0.36	0.24	2o4s	0.79	10.91	0.79
1o5a	1.05	1.37	1.96	1n46	3.16	0.4	0.35

1fh9	2.88	0.41	0.45	2f81	1.57	6.64	1.59
2b07	0.58	2.75	2.59	1qbr	1.05	0.32	0.89
1gt3	4.14	5.37	4.89	2qi6	3.52	0.25	0.49
1m2r	2.58	4.85	0.27	3djk	3.03	0.44	0.27
1r5y	3.41	0.22	0.08	3cs7	3.91	0.46	2.18
1f4g	1.17	1.21	1.12	2pk5	3.78	12.21	2.21
1gpn	2.21	0.47	0.43	7std	4.46	0.37	0.62
1rpj	3.37	0.23	0.31	1hwx	2.24	10.89	9.01
1dl7	4.28	1.35	1.35	2qi5	3.94	3.96	3.96
3cj4	3.88	2.09	1.93	2pk6	1.49	2.26	2.16
1ct8	0.51	5.9	5.90	1hvi	1.21	4.87	4.87
1g74	3.99	5.49	4.73	1hvk	0.02	7.07	7.07
1gt4	2.41	5.21	3.11	1mq6	2.73	0.47	1.44
1qyl	3.57	0.7	0.56	2i4v	1.14	8.38	8.38
1zhy	3.34	0.66	0.78	1hpx	1.47	7.98	7.98
2nt7	1.74	9.76	7.40	2q5k	2.57	9.29	9.29
2oxy	3.86	2.52	3.87	2hb3	1.27	0.35	0.43
3d0b	0.2	0.42	0.94	1hvj	1.97	6.17	6.17
1dhj	1.79	1.21	1.00	2i0a	0.99	11.13	1.02
1hmr	3.58	4.21	4.04	2i4u	0.87	4.73	4.73
1n4h	3.94	0.65	0.57	2i4w	2.36	3.14	3.47
1yc4	3.91	0.87	0.58	2i4d	0.86	10.95	0.36
2bok	0.58	0.7	0.42	1y6q	2.82	0.35	0.31
2pwc	0.68	0.93	0.92	2i4x	1.49	1.09	1.02
1kli	1.92	3.5	2.11				