

# Supporting Material

## Chapter 8

June 18, 2016

The information about validation set of 1322 complexes that belong to seven protein clusters is provided in Table 1, in which the PDB ID, cluster information and corresponding binding affinity data can be retrieved.

Table S1: The PDB ID and cluster ID of the validation set ( $N = 1322$ ). The energy data are all in the unit of kcal/mol.

PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy
1a94	1	-10.67	7upj	1	-11.54	2hnc	3	-9.81	2baj	5	-11.41
1a9m	1	-9.40	9hvp	1	-11.35	2hoc	3	-12.94	2bak	5	-10.10
1aaq	1	-11.41	1fkn	2	-11.96	2nng	3	-7.28	2bal	5	-8.57
1aid	1	-6.55	1m4h	2	-12.94	2nno	3	-8.70	2ewa	5	-10.79
1ajv	1	-10.49	1tqf	2	-7.95	2nns	3	-8.22	2gfs	5	-8.36
1ajx	1	-10.75	1w51	2	-8.56	2nnv	3	-10.22	2i0h	5	-10.94
1b6j	1	-10.76	1xs7	2	-10.33	2o4z	3	-8.49	2qd9	5	-10.72
1b6k	1	-11.88	1ym2	2	-10.87	2osf	3	-5.20	2rg5	5	-11.56
1b6l	1	-11.28	1ym4	2	-10.07	2osm	3	-8.42	2rg6	5	-11.77
1b6m	1	-11.41	2b8l	2	-10.63	2pou	3	-10.08	2y8o	5	-6.96
1bdl	1	-7.95	2b8v	2	-9.52	2pov	3	-9.67	2yis	5	-11.92
1bdq	1	-8.61	2f3e	2	-9.25	2pow	3	-9.78	2yiw	5	-12.36
1bdr	1	-9.08	2f3f	2	-9.13	2q1q	3	-11.07	2yix	5	-11.52
1bv7	1	-14.00	2fdp	2	-10.31	2q38	3	-7.11	2zaz	5	-8.70
1bv9	1	-13.53	2g94	2	-12.94	2qo8	3	-11.51	2zb0	5	-9.00
1bwa	1	-11.69	2hiz	2	-9.44	2qoa	3	-9.89	2zb1	5	-8.59
1bwb	1	-11.44	2hm1	2	-11.82	2qp6	3	-9.08	3bv2	5	-12.72
1c6y	1	-12.92	2iqg	2	-11.28	2wd3	3	-9.61	3bv3	5	-12.69
1c70	1	-14.00	2irz	2	-10.76	2weg	3	-8.83	3bx5	5	-11.50
1cpi	1	-10.07	2is0	2	-9.10	2weh	3	-8.08	3c5u	5	-11.13
1d4h	1	-13.59	2oah	2	-10.82	2wej	3	-8.26	3ctq	5	-10.05
1d4i	1	-12.03	2ohk	2	-3.67	2weo	3	-9.42	3d7z	5	-10.76
1d4j	1	-11.36	2ohl	2	-4.14	2x7s	3	-7.85	3d83	5	-11.36
1d4k	1	-12.53	2ohm	2	-4.77	2x7t	3	-9.01	3ds6	5	-12.36
1d4l	1	-11.92	2ohp	2	-5.48	2x7u	3	-7.16	3dt1	5	-11.71
1d4y	1	-15.08	2ohq	2	-6.25	3b4f	3	-11.06	3e92	5	-10.87
1dif	1	-14.48	2ohr	2	-5.44	3bet	3	-7.91	3e93	5	-12.03
1dmp	1	-12.98	2ohs	2	-5.98	3bl0	3	-9.40	3fc1	5	-10.87
1ebw	1	-12.30	2oht	2	-6.85	3bl1	3	-7.61	3gc7	5	-12.53
1eby	1	-13.18	2ohu	2	-7.31	3c7p	3	-13.59	3gcp	5	-10.63
1ebz	1	-12.77	2p4j	2	-12.17	3caj	3	-11.01	3gcq	5	-8.79
1ec0	1	-11.54	2p83	2	-10.82	3cyu	3	-9.81	3gcs	5	-9.85
1ec1	1	-12.12	2p8h	2	-9.72	3d8w	3	-11.07	3gcu	5	-9.21
1ec2	1	-13.59	2ph6	2	-10.29	3d9z	3	-11.82	3gcv	5	-9.69
1ec3	1	-12.28	2ph8	2	-7.80	3daz	3	-10.78	3gfe	5	-11.54
1g2k	1	-10.82	2q11	2	-8.22	3dbu	3	-10.95	3hec	5	-6.07
1g35	1	-11.06	2q15	2	-10.82	3dc3	3	-11.29	3heg	5	-9.16
1gnm	1	-8.49	2qk5	2	-11.01	3dcc	3	-12.17	3hl7	5	-10.38
1gnn	1	-7.72	2qmd	2	-11.28	3dcs	3	-10.79	3hll	5	-11.20
1gno	1	-10.46	2qmf	2	-11.58	3dcw	3	-12.23	3hp2	5	-8.38
1hbv	1	-8.66	2qmg	2	-12.43	3dd0	3	-12.23	3hp5	5	-9.72

**Table 1 – continued**

PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy
1hef	1	-12.23	2qp8	2	-11.01	3dd8	3	-10.67	3hrb	5	-10.44
1heg	1	-10.52	2qu2	2	-7.38	3f8e	3	-9.82	3hub	5	-10.99
1hih	1	-10.94	2qu3	2	-8.47	3ffp	3	-9.70	3huc	5	-8.14
1hiv	1	-12.23	2qzl	2	-11.01	3hkn	3	-7.27	3hv3	5	-8.60
1hos	1	-11.62	2va5	2	-5.53	3hkq	3	-7.26	3hv4	5	-8.85
1hpo	1	-12.53	2va6	2	-8.38	3hkt	3	-7.32	3hv5	5	-9.54
1hps	1	-12.53	2va7	2	-9.10	3hku	3	-11.28	3hv6	5	-7.66
1hpx	1	-12.53	2vie	2	-10.16	3hs4	3	-10.87	3hv7	5	-10.76
1hsg	1	-15.30	2viy	2	-7.80	3ibi	3	-11.67	3hvc	5	-8.45
1hte	1	-12.80	2viz	2	-8.45	3ibl	3	-10.65	3iph	5	-10.33
1hte	1	-7.66	2vj6	2	-10.72	3ibn	3	-10.34	3itz	5	-12.03
1htf	1	-9.28	2vj7	2	-10.05	3ibu	3	-12.43	3iw5	5	-8.26
1htg	1	-11.44	2vj9	2	-9.16	3ieo	3	-8.80	3iw6	5	-7.45
1hvh	1	-10.82	2vkm	2	-11.88	3igp	3	-9.54	3iw7	5	-7.66
1hvi	1	-14.84	2vnm	2	-11.58	3k2f	3	-9.78	3iw8	5	-6.62
1hvj	1	-15.49	2vnn	2	-11.82	3kig	3	-8.98	3k3i	5	-7.77
1hvk	1	-14.89	2wez	2	-10.38	3kwa	3	-5.54	3k3j	5	-6.66
1hvl	1	-13.52	2wf0	2	-9.08	3m1k	3	-7.32	3kf7	5	-10.05
1hvr	1	-12.92	2wf1	2	-11.82	3m3x	3	-9.27	3l8s	5	-9.51
1hvs	1	-14.00	2wf2	2	-10.31	3m40	3	-9.20	3l8x	5	-10.87
1hwr	1	-11.32	2wf3	2	-10.49	3m5e	3	-10.01	3lhj	5	-12.92
1hxb	1	-13.48	2wf4	2	-10.72	3m67	3	-9.16	3mpt	5	-8.97
1hxx	1	-14.70	2xfi	2	-10.63	3m96	3	-9.81	3mvl	5	-10.72
1iiq	1	-10.16	2xfj	2	-10.72	3mhc	3	-10.82	3mvm	5	-11.43
1izh	1	-10.46	2xfk	2	-11.58	3mhi	3	-9.10	3mw1	5	-12.35
1izi	1	-8.95	2zdz	2	-8.36	3mhl	3	-9.85	3new	5	-6.79
1k6c	1	-10.16	2ze1	2	-8.45	3mhm	3	-9.51	3nnu	5	-9.95
1k6p	1	-10.00	3bra	2	-3.67	3mho	3	-8.82	3nnv	5	-10.29
1k6t	1	-10.35	3buf	2	-4.21	3ml2	3	-10.94	3nnw	5	-10.94
1k6v	1	-9.40	3bug	2	-4.32	3mmf	3	-10.10	3nnx	5	-10.82
1kzk	1	-14.12	3buh	2	-4.97	3mna	3	-10.04	3nww	5	-11.07
1lqz	1	-11.40	3cib	2	-10.67	3myq	3	-10.22	3o8p	5	-8.78
1m0b	1	-11.98	3cic	2	-11.58	3mzc	3	-9.04	3ocg	5	-11.58
1mes	1	-10.46	3cid	2	-11.28	3n0n	3	-9.92	3p5k	5	-9.67
1met	1	-12.77	3ckp	2	-8.63	3n2p	3	-10.63	3p78	5	-9.46
1meu	1	-8.29	3ckr	2	-7.20	3n3j	3	-11.52	3p79	5	-7.66
1mrw	1	-13.18	3dm6	2	-10.10	3n4b	3	-9.54	3p7a	5	-8.53
1mrx	1	-9.86	3duy	2	-7.95	3nb5	3	-10.52	3p7b	5	-10.52
1msm	1	-14.24	3dv1	2	-8.47	3ni5	3	-10.26	3p7c	5	-10.41
1msn	1	-12.35	3dv5	2	-10.41	3oik	3	-8.38	3que	5	-11.98
1mtr	1	-11.41	3exo	2	-6.28	3oil	3	-7.72	3rin	5	-12.08
1mui	1	-16.16	3ftk	2	-7.54	3oim	3	-9.16	3roc	5	-11.13
1nh0	1	-13.23	3h0b	2	-7.46	3oku	3	-8.64	3s3i	5	-10.60
1ody	1	-11.01	3hvg	2	-3.67	3okv	3	-8.47	3s4q	5	-11.41
1ohr	1	-11.82	3hw1	2	-4.16	3oy0	3	-10.87	3u8w	5	-12.23
1pro	1	-15.35	3i25	2	-11.56	3oyq	3	-10.86	3uyp	5	-10.14
1qbr	1	-14.36	3igb	2	-6.01	3oys	3	-10.94	3uvq	5	-10.56
1qbs	1	-12.87	3in3	2	-9.81	3p4v	3	-6.93	3zya	5	-9.51
1qbt	1	-14.43	3in4	2	-10.22	3p58	3	-10.33	4aa0	5	-10.14
1qbu	1	-13.91	3ind	2	-7.91	3p5l	3	-10.04	4aa4	5	-10.94
1sbg	1	-10.52	3ine	2	-9.20	3po6	3	-9.59	4aa5	5	-10.60
1sdt	1	-12.60	3inf	2	-10.05	3r16	3	-9.92	4aac	5	-11.10
1sdu	1	-13.68	3inh	2	-10.46	3r17	3	-8.71	4dli	5	-7.64
1sdv	1	-11.88	3ivh	2	-9.96	3ryj	3	-10.60	4dlj	5	-8.04
1sgu	1	-7.30	3ivi	2	-10.76	3ryv	3	-9.61	4e6c	5	-6.55
1sh9	1	-8.19	3ixj	2	-12.89	3ryx	3	-11.06	4eh2	5	-4.29
1t7j	1	-11.82	3ixk	2	-11.11	3ryy	3	-10.08	4eh3	5	-4.80
1tcx	1	-9.44	3k5c	2	-10.56	3ryz	3	-11.71	4eh4	5	-3.82

**Table 1 – continued**

PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy
1vij	1	-12.94	3k5d	2	-9.89	3rz0	3	-10.26	4eh5	5	-4.20
1vik	1	-12.94	3k5f	2	-7.38	3rz1	3	-11.88	4eh6	5	-3.34
1w5v	1	-11.07	3k5g	2	-11.69	3rz5	3	-10.72	4eh7	5	-4.46
1w5w	1	-11.96	3kmx	2	-6.55	3rz7	3	-12.17	4eh8	5	-2.99
1w5x	1	-11.41	3kmy	2	-6.10	3rz8	3	-11.10	4eh9	5	-3.07
1w5y	1	-11.52	3kn0	2	-4.89	3s71	3	-11.74	4ehv	5	-3.11
1z1h	1	-11.41	3kyr	2	-9.13	3s73	3	-11.82	4f9w	5	-9.43
1z1r	1	-12.53	3l38	2	-9.51	3s74	3	-11.41	4f9y	5	-9.16
1zp8	1	-11.92	3l58	2	-11.01	3s76	3	-6.86	4kin	5	-11.30
1zpa	1	-11.41	3l59	2	-5.03	3s77	3	-9.80	4kip	5	-11.07
1zsf	1	-13.48	3l5b	2	-5.31	3s78	3	-8.79	4kiq	5	-10.38
1zsr	1	-13.34	3l5c	2	-7.00	3s8x	3	-9.92	4l8m	5	-12.23
2aoc	1	-6.64	3l5d	2	-5.58	3s9t	3	-9.27	4loo	5	-11.07
2aod	1	-7.69	3l5e	2	-10.29	3sap	3	-10.31	4lop	5	-11.07
2aoe	1	-10.35	3l5f	2	-8.45	3sax	3	-8.93	4loq	5	-11.07
2aog	1	-8.53	3lhg	2	-10.46	3sbh	3	-9.89	1uy6	6	-5.03
2aqu	1	-12.66	3lnk	2	-8.07	3sbi	3	-10.76	1uy7	6	-5.03
2avm	1	-7.74	3lpi	2	-11.58	3t5u	3	-10.31	1uy8	6	-5.60
2avo	1	-12.03	3lpj	2	-9.40	3t82	3	-9.51	1uy9	6	-6.55
2avq	1	-5.97	3lpk	2	-12.36	3t83	3	-9.48	1uyc	6	-5.97
2avs	1	-10.29	3msj	2	-4.23	3t84	3	-9.47	1uyd	6	-5.03
2avv	1	-12.58	3msk	2	-6.24	3t85	3	-10.80	1uye	6	-5.03
2bbb	1	-11.71	3msl	2	-7.00	3v5g	3	-9.69	1uyf	6	-6.14
2bpv	1	-10.42	3n4l	2	-9.82	3v7x	3	-11.64	1uyg	6	-5.80
2bpx	1	-12.77	3nsh	2	-8.60	3vbd	3	-10.97	1uyh	6	-6.58
2bpy	1	-10.05	3ohf	2	-9.55	4bcw	3	-5.44	1uyi	6	-7.32
2bqv	1	-10.94	3ohh	2	-10.52	4bf1	3	-11.71	1uyk	6	-6.48
2cej	1	-11.71	3ooz	2	-10.67	4bf6	3	-11.35	1yc1	6	-8.38
2cen	1	-11.28	3pi5	2	-8.18	4cq0	3	-6.92	1yc4	6	-8.90
2f3k	1	-10.72	3qbh	2	-9.27	4e3d	3	-3.13	1yet	6	-8.04
2f80	1	-11.11	3qi1	2	-10.41	4e3f	3	-3.42	2byh	6	-8.95
2f81	1	-14.29	3r2f	2	-12.03	4e3g	3	-6.75	2byi	6	-8.61
2f8g	1	-11.82	3rsv	2	-12.43	4e3h	3	-9.58	2bz5	6	-8.36
2fgu	1	-12.47	3rsx	2	-5.99	4e49	3	-6.94	2ccs	6	-7.74
2fgv	1	-8.32	3rth	2	-7.08	4e4a	3	-2.79	2cct	6	-6.82
2fle	1	-10.67	3rtm	2	-6.01	4g0c	3	-10.76	2ccu	6	-8.33
2hb3	1	-15.42	3rtn	2	-9.69	4ht0	3	-10.87	2fwy	6	-9.10
2hs1	1	-11.52	3ru1	2	-6.59	4itp	3	-9.88	2fwz	6	-9.92
2hs2	1	-11.29	3rvi	2	-10.82	4iwz	3	-9.91	2qf6	6	-8.82
2i0a	1	-15.49	3s2o	2	-6.86	4jsa	3	-6.74	2qfo	6	-6.39
2i0d	1	-16.44	3s7l	2	-9.65	4jss	3	-4.48	2qg0	6	-7.77
2i4d	1	-15.87	3s7m	2	-10.87	4jsz	3	-3.13	2qg2	6	-7.34
2i4u	1	-15.72	3skf	2	-11.28	4kni	3	-10.57	2uwd	6	-11.35
2i4v	1	-15.22	3skg	2	-11.01	4knj	3	-10.80	2vci	6	-10.44
2i4w	1	-15.75	3tpp	2	-10.63	4m2r	3	-11.54	2vcj	6	-10.44
2i4x	1	-15.92	3tpr	2	-10.46	4m2u	3	-10.92	2wi1	6	-3.26
2idw	1	-12.08	3u6a	2	-8.82	4m2v	3	-10.11	2wi2	6	-4.70
2ien	1	-12.23	3udh	2	-3.87	4m2w	3	-9.89	2wi3	6	-4.70
2ieo	1	-11.54	3udj	2	-4.92	4mo8	3	-10.87	2wi4	6	-7.89
2nmy	1	-11.37	3udk	2	-6.10	4q6d	3	-10.00	2wi5	6	-8.22
2nmz	1	-11.37	3udm	2	-6.09	4q6e	3	-8.40	2wi6	6	-9.02
2nnk	1	-11.37	3udp	2	-7.09	4qy3	3	-9.27	2wi7	6	-9.84
2nnp	1	-11.37	3udq	2	-8.15	4r59	3	-10.82	2xab	6	-12.60
2o4k	1	-14.21	3udr	2	-6.74	4r5a	3	-11.82	2xdk	6	-4.89
2o4l	1	-12.53	3ufl	2	-9.27	4r5b	3	-9.14	2xdl	6	-4.21
2o4n	1	-10.63	3uqp	2	-9.93	1b38	4	-8.97	2xdx	6	-8.78
2o4p	1	-14.57	3uqr	2	-9.84	1b39	4	-9.40	2xhr	6	-11.30
2o4s	1	-14.28	3veu	2	-9.86	1e1v	4	-6.69	2xht	6	-8.10

**Table 1 – continued**

PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy
2p3a	1	-10.82	3vf3	2	-7.96	1e1x	4	-8.00	2xhx	6	-8.97
2p3b	1	-11.52	3vg1	2	-9.86	1e9h	4	-10.14	2xjg	6	-10.63
2p3c	1	-10.35	3vv6	2	-5.16	1fvt	4	-9.81	2xjj	6	-8.85
2pk5	1	-14.54	3vv7	2	-7.26	1g5s	4	-9.95	2xjx	6	-12.43
2pk6	1	-14.80	3vv8	2	-6.48	1h00	4	-6.01	2yi0	6	-11.03
2pqz	1	-7.70	3wb4	2	-6.03	1h01	4	-6.33	2yi5	6	-10.07
2psu	1	-10.35	3wb5	2	-6.21	1h07	4	-7.50	2yi7	6	-11.30
2psv	1	-9.84	3zmg	2	-10.38	1h08	4	-6.18	2yjl	6	-6.96
2pwc	1	-8.93	3zov	2	-9.81	1h0w	4	-6.64	2yjk	6	-6.96
2pwr	1	-8.95	4acu	2	-10.04	1h1p	4	-6.69	2yk9	6	-6.92
2pym	1	-9.27	4acx	2	-9.66	1h1q	4	-8.15	2ykb	6	-8.10
2pyn	1	-10.29	4azy	2	-9.10	1h1r	4	-7.66	2ykc	6	-8.30
2q54	1	-12.24	4b00	2	-11.70	1h1s	4	-11.17	2yke	6	-8.10
2q55	1	-11.81	4b05	2	-10.30	1h26	4	-7.53	2yki	6	-12.85
2q5k	1	-15.35	4b1c	2	-9.65	1h27	4	-7.61	2yjk	6	-8.44
2q63	1	-9.76	4b1d	2	-10.18	1jsv	4	-7.74	3b24	6	-5.95
2q64	1	-11.58	4b70	2	-7.07	1jvp	4	-7.88	3b25	6	-8.25
2qci	1	-11.33	4b72	2	-8.42	1ke5	4	-8.49	3b26	6	-9.02
2qd6	1	-11.79	4b77	2	-6.93	1ke6	4	-11.20	3b27	6	-7.01
2qd7	1	-12.36	4b78	2	-6.79	1ke7	4	-10.94	3b28	6	-11.51
2qd8	1	-12.32	4bek	2	-5.97	1ke8	4	-8.15	3bm9	6	-9.13
2qhy	1	-10.16	4bfd	2	-9.54	1ke9	4	-8.40	3bmy	6	-10.22
2qhz	1	-9.89	4d83	2	-9.86	1ogu	4	-10.15	3d0b	6	-8.89
2qi0	1	-10.03	4d85	2	-9.31	1oi9	4	-9.73	3eko	6	-9.10
2qi1	1	-9.92	4d88	2	-9.93	1oiq	4	-7.53	3ekr	6	-10.22
2qi3	1	-13.86	4d89	2	-11.82	1oir	4	-10.18	3ft5	6	-6.55
2qi4	1	-14.19	4d8c	2	-11.82	1oit	4	-11.58	3ft8	6	-10.22
2qi5	1	-14.74	4dh6	2	-10.56	1oiu	4	-9.08	3hhu	6	-10.04
2qi6	1	-14.36	4di2	2	-11.22	1oiy	4	-9.77	3k97	6	-10.87
2qi7	1	-13.87	4dju	2	-7.39	1okv	4	-8.38	3k99	6	-9.81
2qnn	1	-9.72	4djv	2	-9.13	1okw	4	-7.13	3ow6	6	-9.05
2qnp	1	-8.71	4djw	2	-8.53	1ol1	4	-6.36	3owb	6	-10.49
2qnq	1	-8.30	4djx	2	-9.82	1ol2	4	-8.53	3owd	6	-10.22
2r38	1	-10.11	4djy	2	-11.24	1p2a	4	-10.76	3qdd	6	-11.92
2r3t	1	-7.95	4dpf	2	-8.70	1p5e	4	-6.54	3qtf	6	-9.46
2r3w	1	-9.36	4dpi	2	-9.66	1pf8	4	-10.20	3r4m	6	-8.04
2r43	1	-8.15	4dus	2	-11.28	1pxi	4	-6.48	3r4n	6	-9.36
2r5p	1	-11.52	4dv9	2	-9.13	1pxj	4	-6.64	3r4o	6	-11.07
2upj	1	-10.04	4dvf	2	-9.36	1pxk	4	-7.69	3r91	6	-9.57
2uxz	1	-11.52	4ewo	2	-10.00	1pxl	4	-8.22	3r92	6	-9.54
2uy0	1	-9.40	4exg	2	-10.97	1pxm	4	-9.81	3rkz	6	-9.62
2wkz	1	-11.92	4fgx	2	-9.70	1pxn	4	-9.72	3rlp	6	-9.62
2wl0	1	-10.60	4fm7	2	-9.84	1pxo	4	-11.82	3rlq	6	-10.05
2xye	1	-11.33	4fm8	2	-8.11	1pxp	4	-9.05	3rlr	6	-10.22
2xyf	1	-11.47	4fri	2	-7.54	1pye	4	-8.71	3vha	6	-10.05
2z4o	1	-13.00	4frj	2	-8.90	1r78	4	-11.58	3vhc	6	-12.08
2zga	1	-8.59	4frk	2	-11.01	1urc	4	-6.41	3vhd	6	-12.61
3a2o	1	-12.34	4frs	2	-11.92	1urw	4	-11.58	3wha	6	-12.66
3aid	1	-9.32	4fs4	2	-8.93	1v1k	4	-6.06	4awo	6	-10.35
3bc4	1	-7.27	4fse	2	-10.05	1vyw	4	-10.10	4awp	6	-9.63
3bgb	1	-8.22	4fsl	2	-10.46	1vyz	4	-8.89	4awq	6	-8.59
3bgc	1	-6.82	4gid	2	-14.63	1wcc	4	-4.70	4b7p	6	-12.85
3bva	1	-8.86	4h1e	2	-11.58	1y91	4	-9.82	4bqg	6	-8.45
3bvb	1	-7.46	4h3f	2	-12.23	1ykr	4	-8.49	4cwf	6	-6.10
3bxs	1	-6.93	4h3g	2	-11.17	2a0c	4	-9.92	4cwn	6	-7.60
3ckt	1	-8.59	4h3i	2	-11.58	2b52	4	-11.01	4cwo	6	-7.08
3cyw	1	-10.56	4h3j	2	-9.58	2b53	4	-8.45	4cwp	6	-9.20
3cyx	1	-10.87	4ha5	2	-9.84	2b54	4	-10.46	4cwq	6	-9.59

**Table 1 – continued**

PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy
3d1x	1	-11.77	4hzt	2	-8.32	2b55	4	-9.54	4cwr	6	-11.28
3d1y	1	-11.17	4i0d	2	-8.44	2bkz	4	-11.07	4cws	6	-10.76
3d1z	1	-11.96	4i0f	2	-8.63	2bpm	4	-11.82	4cwt	6	-9.17
3d20	1	-11.28	4i0z	2	-8.60	2btr	4	-9.54	4eeh	6	-5.91
3djk	1	-14.39	4i10	2	-9.20	2bts	4	-10.46	4eft	6	-5.53
3dk1	1	-13.23	4i11	2	-6.21	2c4g	4	-8.07	4efu	6	-8.97
3ekp	1	-12.08	4i12	2	-8.68	2c5n	4	-9.05	4egh	6	-4.43
3ekq	1	-9.17	4i1c	2	-11.01	2c5o	4	-7.05	4egi	6	-5.19
3ekt	1	-14.39	4ivs	2	-10.00	2c5x	4	-8.97	4egk	6	-10.49
3ekv	1	-12.79	4ivt	2	-8.15	2c5y	4	-8.97	4fcq	6	-9.51
3ekw	1	-10.82	4j0p	2	-9.91	2c68	4	-7.80	4fcr	6	-12.77
3ekx	1	-12.79	4j0t	2	-9.16	2c69	4	-6.24	4jql	6	-8.15
3eky	1	-13.10	4j0v	2	-10.26	2c6i	4	-6.74	4nh7	6	-11.41
3el0	1	-10.15	4j0y	2	-8.64	2c6k	4	-8.34	4nh8	6	-11.58
3el1	1	-13.10	4j0z	2	-9.66	2c6l	4	-8.93	4o04	6	-8.37
3el4	1	-9.74	4j17	2	-9.88	2c6m	4	-8.78	4o05	6	-10.10
3el5	1	-10.49	4j1c	2	-9.93	2c6o	4	-11.17	4o07	6	-10.03
3el9	1	-11.41	4j1e	2	-10.49	2clx	4	-6.63	4o09	6	-10.46
3ggg	1	-13.28	4j1f	2	-10.76	2ds1	4	-11.51	4o0b	6	-11.28
3ggv	1	-14.74	4j1h	2	-8.30	2duv	4	-9.59	4u93	6	-10.72
3gi4	1	-14.67	4j1i	2	-10.05	2exm	4	-5.58	4w7t	6	-8.22
3gi5	1	-15.25	4j1k	2	-10.72	2fvd	4	-11.58	1a8i	7	-7.50
3gi6	1	-15.25	4joo	2	-6.02	2g9x	4	-9.99	1axr	7	-4.44
3h5b	1	-13.59	4jp9	2	-10.35	2i40	4	-7.88	1c50	7	-8.80
3hau	1	-8.67	4jpc	2	-9.55	2iw6	4	-9.31	1c8k	7	-8.15
3i6o	1	-14.06	4jpe	2	-9.95	2iw8	4	-9.50	1c8l	7	-11.09
3i7e	1	-14.74	4k8s	2	-10.11	2iw9	4	-10.94	1e1y	7	-7.61
3kdb	1	-13.38	4k9h	2	-9.67	2r3f	4	-8.56	1em6	7	-11.17
3kdc	1	-12.61	4ke0	2	-10.56	2r3g	4	-8.29	1exv	7	-9.99
3kdd	1	-11.50	4ke1	2	-11.69	2r3h	4	-6.39	1gfz	7	-5.44
3kfn	1	-6.44	4l7g	2	-5.44	2r3i	4	-8.15	1ggg	7	-7.49
3lzs	1	-14.89	4l7h	2	-5.03	2r3j	4	-10.87	1h5u	7	-9.17
3lzu	1	-13.67	4l7j	2	-5.03	2r3k	4	-9.51	1hlf	7	-7.66
3lzv	1	-14.39	4lxa	2	-11.82	2r3l	4	-9.51	1k06	7	-7.26
3m9f	1	-15.15	4lxx	2	-11.41	2r3n	4	-9.72	1k08	7	-7.26
3mxd	1	-12.00	4lxm	2	-9.59	2r3o	4	-8.45	1kti	7	-4.66
3mxe	1	-13.60	4n00	2	-10.90	2r3p	4	-8.22	1noi	7	-4.28
3nu3	1	-13.34	4pzw	2	-9.46	2r64	4	-10.22	1noj	7	-4.28
3nu4	1	-11.98	4pzx	2	-8.15	2uue	4	-8.33	1nok	7	-4.28
3nu5	1	-11.35	4r5n	2	-9.67	2uzb	4	-9.40	1p2g	7	-2.89
3nu6	1	-12.64	4r8y	2	-8.41	2uzd	4	-9.16	1z6p	7	-8.22
3nu9	1	-12.30	4r91	2	-8.66	2uze	4	-5.88	1z6q	7	-9.10
3nuj	1	-12.76	4r92	2	-10.07	2uzl	4	-8.44	2amv	7	-11.96
3nuo	1	-13.32	4r93	2	-10.60	2uzn	4	-10.22	2g9q	7	-8.70
3o99	1	-14.70	4r95	2	-10.67	2uzo	4	-6.21	2g9u	7	-8.26
3o9a	1	-14.54	4rce	2	-11.82	2v22	4	-7.32	2g9v	7	-8.04
3o9d	1	-14.57	4rcf	2	-11.41	2vta	4	-5.07	2gj4	7	-8.83
3o9e	1	-15.35	4rrn	2	-9.95	2vth	4	-5.33	2gm9	7	-10.04
3o9f	1	-17.26	4rro	2	-10.31	2vti	4	-8.40	2off	7	-8.86
3o9g	1	-16.71	4rrs	2	-9.08	2vtj	4	-7.77	2prj	7	-6.10
3o9h	1	-16.44	4x7i	2	-10.45	2vtl	4	-5.45	2pyi	7	-5.10
3o9i	1	-16.06	1a42	3	-13.44	2vtm	4	-4.08	2qlm	7	-7.66
3ok9	1	-15.26	1avn	3	-5.30	2vtn	4	-8.25	2qln	7	-7.38
3oxc	1	-11.43	1bcd	3	-11.82	2vto	4	-9.31	2qn1	7	-6.48
3pwm	1	-12.36	1bn1	3	-12.69	2vtp	4	-11.58	2qn2	7	-6.18
3qaa	1	-15.68	1bn3	3	-13.44	2vtq	4	-9.31	2qn3	7	-7.28
3r0y	1	-6.58	1bn4	3	-12.65	2vtr	4	-7.91	2qnb	7	-7.26
3s43	1	-11.69	1bnm	3	-13.59	2vts	4	-10.22	2qrg	7	-7.04

**Table 1 – continued**

PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy
3s53	1	-13.10	1bnn	3	-13.59	2vtt	4	-10.00	2qrh	7	-6.40
3s54	1	-13.10	1bnq	3	-12.89	2vu3	4	-9.96	2qrm	7	-5.48
3s56	1	-13.07	1bnt	3	-13.32	2vv9	4	-10.56	2qrp	7	-8.42
3so9	1	-11.63	1bnu	3	-13.18	2w05	4	-12.23	2qrr	7	-6.93
3spk	1	-11.58	1bnv	3	-11.92	2w06	4	-9.62	3amv	7	-10.83
3st5	1	-15.35	1bnw	3	-12.34	2w17	4	-11.82	3bcs	7	-7.08
3t3c	1	-13.90	1cil	3	-12.81	2w1h	4	-9.89	3ebo	7	-6.41
3th9	1	-10.46	1cim	3	-11.98	2wev	4	-10.87	3ebp	7	-8.03
3tkw	1	-7.16	1cin	3	-11.86	2wih	4	-9.99	3g2h	7	-5.19
3tlh	1	-11.98	1cnw	3	-10.49	2wpa	4	-11.01	3g2i	7	-6.60
3ttp	1	-12.39	1cnx	3	-10.01	2wxv	4	-11.82	3g2j	7	-6.45
3u7s	1	-11.45	1cny	3	-10.67	2xmy	4	-13.53	3g2k	7	-6.51
3vf5	1	-12.69	1eou	3	-10.11	2xnb	4	-9.28	3g2l	7	-5.26
3vf7	1	-12.36	1g1d	3	-12.83	3ddp	4	-9.70	3g2n	7	-5.56
3vfa	1	-12.49	1g45	3	-11.74	3ddq	4	-9.08	3l79	7	-3.34
3vfb	1	-12.28	1g46	3	-11.96	3dog	4	-10.05	3l7a	7	-5.88
3zps	1	-11.28	1g48	3	-11.43	3eid	4	-8.63	3l7b	7	-3.26
3zpt	1	-11.56	1g4j	3	-11.82	3ej1	4	-9.40	3l7c	7	-3.32
3zpu	1	-11.39	1g4o	3	-11.21	3eoc	4	-9.02	3l7d	7	-2.96
4a4q	1	-12.77	1g52	3	-12.96	3ezr	4	-6.79	3mqf	7	-7.12
4a6b	1	-11.39	1g53	3	-12.28	3ezv	4	-8.13	3mrt	7	-5.03
4a6c	1	-10.76	1g54	3	-11.98	3fz1	4	-10.76	3mrv	7	-5.08
4cp7	1	-11.02	1h4n	3	-6.69	3ig7	4	-9.78	3mrx	7	-4.61
4cpq	1	-10.52	1i8z	3	-12.09	3igg	4	-9.76	3ms2	7	-5.05
4cpr	1	-10.14	1i90	3	-12.08	3le6	4	-10.14	3ms4	7	-4.46
4cps	1	-11.24	1i91	3	-12.15	3lfn	4	-7.47	3ms7	7	-4.66
4cpt	1	-10.46	1i9l	3	-11.52	3lfs	4	-7.61	3msc	7	-4.50
4cpu	1	-10.23	1i9m	3	-11.52	3my5	4	-5.69	3mt7	7	-5.48
4cpw	1	-10.19	1i9n	3	-11.77	3ns9	4	-11.58	3mt8	7	-6.18
4cpx	1	-10.56	1i9o	3	-11.44	3pj8	4	-10.05	3mt9	7	-6.24
4dfg	1	-15.95	1i9p	3	-11.43	3pxf	4	-6.02	3mta	7	-5.84
4djo	1	-15.65	1i9q	3	-11.43	3pxq	4	-6.02	3mtb	7	-6.29
4djp	1	-14.34	1if7	3	-14.29	3pxy	4	-7.11	3mtd	7	-4.71
4djg	1	-14.02	1if8	3	-13.10	3pxz	4	-7.11	3nc4	7	-6.22
4djr	1	-15.65	1kwq	3	-12.51	3py0	4	-9.36	3np7	7	-5.46
4ej8	1	-7.32	1kwr	3	-8.97	3py1	4	-9.36	3np9	7	-5.98
4ejl	1	-6.98	1okl	3	-8.19	4i3z	4	-5.83	3npa	7	-5.26
4eyr	1	-9.01	1oq5	3	-10.44	1m7q	5	-11.67	3s0j	7	-5.12
4fe6	1	-13.59	1ttm	3	-9.99	1ouk	5	-13.44	3sym	7	-6.21
4hdb	1	-10.94	1xpz	3	-9.62	1ouy	5	-11.37	3syr	7	-6.93
4hdf	1	-11.54	1xq0	3	-8.61	1ove	5	-12.41	3t3d	7	-6.67
4hdp	1	-10.20	1yda	3	-8.90	1w7h	5	-4.08	3t3e	7	-8.14
4he9	1	-11.50	1ydb	3	-11.20	1w82	5	-9.12	3t3g	7	-7.46
4heg	1	-12.12	1ydd	3	-9.61	1w83	5	-9.77	3t3h	7	-7.76
4hla	1	-14.67	1z9y	3	-9.77	1w84	5	-6.06	3t3i	7	-6.48
4i8w	1	-14.81	1ze8	3	-10.44	1wbn	5	-8.78	4ej2	7	-3.38
4i8z	1	-15.01	1zfk	3	-10.76	1wbo	5	-4.08	4eke	7	-6.09
4kb9	1	-14.95	1zfq	3	-10.22	1wbs	5	-8.42	4eky	7	-4.78
4ll3	1	-15.72	1zge	3	-9.92	1wbt	5	-8.79	4el0	7	-6.10
4mc1	1	-10.67	1zsb	3	-0.82	1wbv	5	-5.15	4el5	7	-7.30
4mc2	1	-11.13	2aw1	3	-10.01	1wbw	5	-5.92	4mho	7	-6.90
4mc6	1	-13.03	2ez7	3	-5.92	1yqj	5	-11.06	4mhs	7	-7.19
4mc9	1	-12.83	2f14	3	-12.49	1yw2	5	-9.31	4mi3	7	-5.60
4phv	1	-12.46	2gd8	3	-10.07	1ywr	5	-10.72	4mi6	7	-5.86
4qgi	1	-5.30	2h15	3	-7.70	1zyj	5	-7.91	4mi9	7	-4.65
4u8w	1	-15.27	2h4n	3	-11.82	1zz2	5	-7.09	4mic	7	-7.20
5hvp	1	-10.46	2hd6	3	-10.60	1zzl	5	-11.28	4mra	7	-6.07
7hvp	1	-13.07	2hl4	3	-10.38						

**Table 1 – continued**

PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy	PDB ID	Class	Energy
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The data involved in this work from the training set of 3589 complexes is provided in Table 2.

Table S2: The PDB ID and binding affinity of the data from the training set. Totally 3589 complexes are used. The energy data are all in the unit of kcal/mol.

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1a08	-7.64	1p1n	-9.24	2o4j	-13.72	3ebh	-8.59	3suv	-6.18	4j22	-10.52
1a1b	-8.70	1p1o	-7.83	2o4k	-14.21	3ebi	-9.65	3suw	-6.39	4j28	-7.74
1a46	-7.74	1p57	-5.98	2o4l	-12.53	3ebl	-8.56	3sv2	-5.69	4j3l	-10.60
1a5g	-13.79	1pa9	-6.25	2o4n	-10.63	3ebo	-6.41	3sw8	-6.11	4j44	-7.79
1a69	-7.20	1pb8	-7.00	2o4p	-14.57	3ed0	-8.63	3sww	-11.41	4j45	-7.84
1abe	-8.86	1pb9	-4.92	2o4r	-12.77	3eeb	-8.00	3sxf	-11.69	4j46	-7.17
1abf	-7.36	1pbq	-8.52	2o4s	-14.28	3efs	-7.26	3sym	-6.21	4j47	-6.69
1adb	-11.41	1pdz	-5.03	2o4z	-8.49	3egt	-12.09	3syr	-6.93	4j48	-7.64
1add	-9.16	1pgp	-7.74	2o8h	-10.33	3ehx	-10.33	3t01	-6.09	4j74	-6.24
1af2	-4.21	1phw	-4.48	2oag	-11.51	3ejp	-11.62	3t1a	-11.37	4j7d	-6.39
1ai5	-5.05	1pkx	-9.40	2oax	-11.75	3ejq	-11.64	3t1l	-4.43	4j7e	-6.59
1ajp	-3.03	1pme	-12.77	2oc2	-11.58	3eko	-9.10	3t1m	-4.13	4j93	-6.39
1ajq	-5.86	1pot	-7.46	2oi0	-10.26	3ekp	-12.08	3t2q	-4.97	4jal	-6.25
1apb	-7.91	1ppc	-8.37	2oi2	-8.56	3ekr	-10.22	3t2w	-10.14	4jc1	-5.84
1apt	-12.77	1pph	-8.04	2oiq	-6.79	3ekt	-14.39	3t3c	-13.90	4je7	-8.70
1apw	-10.87	1ppi	-6.81	2ojg	-7.66	3ekv	-12.79	3t5u	-10.31	4je8	-7.08
1avn	-5.30	1ppk	-10.41	2ojj	-11.82	3ekw	-10.82	3t60	-9.10	4jfk	-8.75
1ax0	-4.25	1ppl	-11.62	2olb	-7.53	3ekx	-12.79	3t64	-9.10	4jfm	-7.45
1axz	-4.35	1ppm	-7.88	2on6	-9.19	3el1	-13.10	3t6b	-8.64	4jfs	-7.16
1b0h	-9.10	1pr5	-5.33	2ot1	-5.44	3el4	-9.74	3t82	-9.51	4jh0	-12.27
1b11	-10.04	1pro	-15.35	2ov4	-6.44	3el5	-10.49	3t83	-9.48	4jia	-12.53
1b1h	-9.55	1pvn	-13.34	2ovv	-10.76	3el9	-11.41	3t84	-9.47	4jkw	-5.65
1b2h	-6.17	1pxn	-9.72	2ovy	-11.41	3elc	-3.66	3t85	-10.80	4jn2	-15.87
1b32	-9.65	1pxo	-11.82	2oxd	-9.27	3eqr	-11.82	3t8v	-8.95	4jne	-7.96
1b38	-8.97	1pxp	-9.05	2oxn	-10.11	3evd	-9.39	3ta0	-4.71	4jpx	-7.00
1b3f	-9.36	1pyn	-7.46	2oxx	-9.10	3ewc	-10.46	3ta1	-4.42	4jpy	-6.02
1b3g	-9.10	1pz5	-7.34	2oxy	-8.86	3ewj	-9.29	3tao	-6.98	4jsa	-6.74
1b3h	-8.44	1pzi	-5.73	2oym	-6.79	3exe	-9.46	3tay	-4.59	4jss	-4.48
1b3l	-8.00	1pzo	-4.51	2p09	-8.63	3exh	-6.63	3tb6	-6.90	4jsz	-3.13
1b40	-9.89	1pzp	-4.50	2p15	-14.00	3f15	-11.01	3tcg	-7.98	4jv6	-9.05
1b46	-7.17	1q1g	-11.64	2p16	-13.72	3f16	-11.18	3td4	-7.69	4jv8	-7.95
1b4h	-7.42	1q54	-7.95	2p2a	-8.32	3f18	-10.05	3tf6	-8.70	4jwk	-11.31
1b4z	-7.11	1q5k	-10.08	2p3a	-10.82	3f19	-9.77	3tfn	-8.93	4jx9	-11.71
1b51	-10.01	1q65	-7.42	2p3b	-11.52	3f1a	-9.80	3tfp	-8.79	4jxs	-6.44
1b52	-9.67	1q72	-9.31	2p3c	-10.35	3f37	-3.56	3tfu	-4.46	4jyb	-9.46
1b55	-10.05	1q7a	-9.77	2p3i	-4.73	3f3d	-9.73	3th9	-10.46	4jyc	-9.10
1b57	-10.87	1q84	-15.01	2p4j	-12.17	3f3u	-6.44	3tif	-7.31	4jym	-6.85
1b58	-8.95	1q8w	-7.12	2p4s	-12.92	3f48	-8.55	3tk2	-6.28	4jyt	-10.05
1b5g	-10.87	1q91	-5.64	2p53	-10.14	3f5j	-5.82	3tkw	-7.16	4jz1	-9.10
1b5h	-8.17	1qan	-6.09	2p7a	-8.29	3f5k	-6.28	3tmk	-9.33	4jzi	-10.05
1b5i	-9.58	1qaw	-6.96	2p7g	-8.87	3f5l	-5.05	3tmn	-8.02	4k0o	-4.08
1b5j	-10.10	1qb1	-9.20	2p7z	-8.94	3f68	-6.88	3ts4	-11.85	4k0y	-10.63
1b6h	-10.63	1qb6	-8.23	2p95	-12.73	3f6e	-3.23	3tsk	-9.74	4k3h	-9.31
1b6j	-10.76	1qb9	-10.11	2pbw	-11.21	3f6g	-6.41	3tt4	-11.25	4k4j	-8.32
1b6k	-11.88	1qbn	-7.95	2pfy	-8.86	3f70	-6.59	3ttm	-11.58	4k55	-7.49
1b6l	-11.28	1qbo	-10.52	2pgz	-7.80	3f78	-4.21	3ttn	-10.65	4k5p	-4.70
1b7h	-10.90	1qbq	-11.28	2pk4	-5.87	3f7g	-10.01	3ttp	-12.39	4k6i	-8.42
1b8n	-14.29	1qbr	-14.36	2pk5	-14.54	3f7h	-9.63	3tu7	-10.99	4k77	-9.01
1b8o	-14.46	1qbs	-12.87	2pk6	-14.80	3f7i	-9.97	3tvc	-10.52	4k7i	-3.83
1b8y	-10.67	1qbt	-14.43	2pmk	-8.04	3f8c	-10.44	3twp	-5.33	4k7n	-4.73

**Table 2 – continued**

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1b9j	-8.10	1qbu	-13.91	2pnc	-4.52	3f8e	-9.82	3tz0	-6.85	4k7o	-5.84
1ba8	-12.23	1qbv	-7.32	2pou	-10.08	3f8f	-9.01	3tza	-7.47	4k9y	-9.44
1bai	-10.46	1qf0	-10.03	2pov	-9.67	3fas	-9.20	3tzm	-10.56	4kao	-8.30
1bap	-9.31	1qf1	-9.95	2pow	-9.78	3fat	-10.38	3u10	-7.39	4kax	-6.48
1bb0	-11.36	1qf2	-8.04	2pqb	-9.78	3fed	-10.14	3u15	-9.66	4kb9	-14.95
1bcd	-11.82	1qft	-11.92	2ppc	-7.80	3fee	-9.02	3u3u	-9.35	4kcx	-6.02
1bdq	-8.61	1qhc	-10.29	2pql	-9.89	3ff3	-4.85	3u5j	-7.62	4keq	-5.19
1bgq	-11.64	1qin	-10.87	2pqz	-7.70	3ffg	-12.34	3u5l	-8.41	4kif	-6.58
1bhf	-5.95	1qji	-6.59	2psu	-10.35	3fh7	-10.33	3u6h	-12.23	4kiu	-5.23
1bhx	-9.29	1qk3	-7.00	2psv	-9.84	3fhb	-7.74	3u6i	-12.23	4km0	-8.21
1bju	-6.52	1qk4	-5.72	2ptz	-10.63	3fj7	-5.04	3u7k	-9.61	4km2	-7.94
1bjv	-7.53	1qka	-8.04	2pu1	-7.95	3fjg	-5.07	3u7l	-9.89	4kmz	-11.64
1bm7	-10.22	1qkb	-9.99	2pu2	-6.02	3fjz	-5.50	3u7m	-10.12	4kni	-10.57
1bma	-6.24	1qkt	-12.28	2pv1	-9.70	3fl5	-9.89	3u7n	-10.80	4knj	-10.80
1bn1	-12.69	1ql7	-6.79	2pvh	-8.95	3fqe	-11.28	3u7s	-11.45	4knm	-10.87
1bn3	-13.44	1ql9	-7.27	2pvj	-11.01	3fql	-9.72	3u81	-6.03	4knn	-10.57
1bn4	-12.65	1qxk	-6.86	2pvk	-11.28	3fuc	-13.21	3u8j	-11.56	4kow	-5.86
1bnn	-13.59	1qxl	-10.82	2pvl	-10.35	3fur	-10.87	3u8k	-11.77	4kp5	-8.26
1bnq	-12.89	1qy1	-8.86	2pvm	-8.75	3fuz	-8.89	3u8l	-10.94	4kp8	-7.45
1bnt	-13.32	1qy2	-7.80	2pwc	-8.93	3fv2	-11.02	3u8n	-13.82	4kqp	-8.22
1bnu	-13.18	1qyg	-9.31	2pwd	-5.98	3fv3	-12.94	3u90	-6.28	4ks1	-11.98
1bnv	-11.92	1r0p	-10.87	2pwg	-6.55	3fvh	-8.63	3u92	-10.16	4ks4	-9.70
1bnw	-12.34	1r1h	-12.12	2pwr	-8.95	3fvk	-11.98	3u93	-8.57	4ksy	-11.44
1bp0	-7.34	1r1j	-11.74	2py4	-9.10	3fvl	-8.25	3ubd	-7.53	4kwf	-6.55
1bq4	-7.09	1r4w	-5.50	2pym	-9.27	3fvn	-9.20	3ucj	-8.15	4kwo	-8.76
1br6	-4.38	1r6n	-10.05	2pyn	-10.29	3fwv	-7.66	3udd	-9.65	4kx8	-9.69
1bra	-2.47	1r9l	-7.34	2pyy	-6.25	3fx2	-12.64	3uev	-8.00	4kxb	-5.60
1bty	-6.44	1rbp	-9.13	2q1q	-11.07	3fx6	-9.24	3uew	-8.57	4kxn	-8.29
1bv7	-14.00	1rd4	-10.52	2q2a	-10.07	3fzn	-5.45	3ug2	-11.21	4kyh	-8.04
1bv9	-13.53	1rdi	-2.80	2q38	-7.11	3fzy	-9.16	3ui7	-12.23	4kyk	-6.44
1bwa	-11.69	1rdj	-2.26	2q54	-12.24	3g08	-11.09	3uil	-8.15	4kz3	-3.76
1bwb	-11.44	1rdl	-3.04	2q55	-11.81	3g0e	-10.46	3uj9	-6.29	4kz4	-5.64
1bxo	-13.59	1re8	-12.94	2q5k	-15.35	3g0i	-4.89	3ujb	-6.93	4kz7	-3.38
1bxq	-10.03	1rgk	-5.86	2q63	-9.76	3g19	-9.06	3ujc	-6.24	4kzb	-3.93
1bxr	-4.62	1rgl	-6.02	2q64	-11.58	3g1d	-4.73	3ujd	-6.37	4kzq	-8.29
1byk	-6.79	1rjk	-13.59	2q6f	-7.39	3g1v	-4.33	3umo	-5.29	4kzu	-8.83
1bzc	-6.69	1rmz	-10.87	2q7q	-7.20	3g2h	-5.19	3umq	-6.28	4l19	-8.29
1bzj	-6.33	1rnm	-4.17	2q7y	-5.84	3g2i	-6.60	3uod	-9.93	4l2l	-7.74
1bzy	-11.33	1rnt	-7.05	2q88	-7.88	3g2j	-6.45	3up2	-10.05	4l4v	-7.85
1c1r	-10.37	1ro6	-8.78	2q89	-8.56	3g2k	-6.51	3upk	-5.84	4l4z	-7.72
1c1u	-11.21	1rp7	-11.58	2q8h	-4.08	3g2l	-5.26	3upv	-7.20	4l50	-8.23
1c1v	-10.38	1rpf	-5.42	2q8z	-7.72	3g30	-3.41	3usx	-6.82	4l51	-4.08
1c3e	-8.95	1rpj	-8.80	2qbq	-10.11	3g31	-3.93	3uu1	-7.07	4l6t	-10.18
1c3x	-5.00	1rql	-3.74	2qbs	-9.08	3g32	-5.04	3uug	-6.13	4l9i	-6.64
1c4u	-14.09	1rr6	-13.93	2qbu	-8.41	3g34	-4.02	3uuo	-10.82	4lar	-6.36
1c5c	-9.46	1rtf	-4.13	2qbw	-9.85	3g35	-6.36	3uw4	-10.56	4lbu	-8.91
1c5n	-6.39	1s19	-12.92	2qci	-11.33	3g3r	-8.80	3uw5	-10.67	4lch	-14.43
1c5o	-4.74	1s38	-7.00	2qd6	-11.79	3g5k	-12.94	3uxd	-5.99	4leq	-8.89
1c5p	-6.36	1s39	-10.46	2qd7	-12.36	3ga5	-7.46	3uxk	-6.70	4lhm	-4.61
1c5q	-8.64	1s5z	-4.36	2qd8	-12.32	3gba	-12.32	3uxl	-7.57	4lhv	-13.59
1c5s	-8.15	1s63	-12.30	2qdt	-7.05	3gbe	-6.79	3uyr	-9.38	4lj5	-8.55
1c5t	-5.57	1s89	-7.12	2qe4	-10.82	3gc4	-10.33	3uz5	-9.81	4lj8	-7.91
1c5x	-9.08	1sb1	-9.36	2qfo	-6.39	3gc5	-9.86	3uzj	-7.54	4ljh	-6.40
1c5y	-5.71	1sbg	-10.52	2qfu	-5.68	3gcp	-10.63	3v2n	-8.29	4lk7	-6.85
1c5z	-5.45	1sbr	-6.79	2qg0	-7.77	3gcu	-9.21	3v2p	-8.64	4lkk	-8.04
1c70	-14.00	1sdt	-12.60	2qg2	-7.34	3gdt	-9.77	3v2q	-8.55	4lko	-11.17
1c83	-6.59	1sdu	-13.68	2qhd	-7.31	3ggg	-13.28	3v3q	-8.97	4lkq	-4.55
1c84	-6.79	1sdv	-11.88	2qhy	-10.16	3gi4	-14.67	3v4t	-5.58	4ll3	-15.72



Table 2 – continued

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1c86	-6.39	1sgu	-7.30	2qhz	-9.89	3gi5	-15.25	3v51	-11.62	4llj	-4.65
1c87	-5.71	1sh9	-8.19	2qi0	-10.03	3gi6	-15.25	3v5t	-11.17	4llk	-4.08
1c88	-7.19	1siv	-10.98	2qi1	-9.92	3giw	-11.28	3v78	-7.53	4llp	-6.52
1cbx	-8.63	1sl3	-16.10	2qi3	-13.86	3gk1	-5.57	3v7t	-9.80	4llx	-3.93
1ceb	-8.15	1sld	-8.93	2qi4	-14.19	3gkz	-10.87	3v7x	-11.64	4lm0	-4.42
1cet	-3.93	1slg	-5.30	2qi5	-14.74	3gm0	-10.56	3vbd	-10.97	4lm2	-4.12
1cgl	-9.33	1sqo	-10.14	2qi6	-14.36	3gpo	-7.20	3veh	-6.74	4lm3	-3.97
1ch8	-9.51	1sqt	-8.42	2qi7	-13.87	3gqz	-2.95	3vf5	-12.69	4lm4	-4.13
1ciz	-10.11	1sr7	-13.72	2qm9	-10.56	3gr2	-3.42	3vf7	-12.36	4loh	-9.46
1cla	-7.17	1sre	-5.44	2qmg	-12.43	3gs6	-8.95	3vfa	-12.49	4loi	-9.20
1cnw	-10.49	1srg	-7.20	2qnn	-9.72	3gsm	-8.80	3vfb	-12.28	4loo	-11.07
1cnx	-10.01	1ssq	-8.15	2qnp	-8.71	3gss	-7.91	3vha	-10.05	4lov	-10.56
1cny	-10.67	1stc	-11.01	2qnq	-8.30	3gst	-9.13	3vhc	-12.08	4loy	-10.99
1cps	-9.05	1str	-6.48	2qpq	-8.66	3gt9	-5.38	3vhd	-12.61	4lps	-7.80
1ct8	-8.86	1sv3	-5.91	2qpu	-4.89	3gta	-5.82	3vhk	-6.25	4lrr	-7.09
1ctt	-6.14	1sw1	-9.92	2qrh	-6.40	3gtc	-3.19	3vjc	-10.49	4luz	-6.39
1ctu	-16.20	1sw2	-9.81	2qrk	-5.79	3guz	-5.95	3vje	-10.88	4lvt	-14.08
1d09	-10.29	1swg	-10.00	2qrl	-5.44	3gv9	-2.88	3vtr	-7.57	4lw1	-4.28
1d3d	-12.35	1swr	-9.40	2qrm	-5.48	3gvb	-3.52	3vvy	-6.58	4lxd	-9.82
1d3p	-10.04	1syh	-8.71	2qrp	-8.42	3gvu	-10.87	3vw1	-6.35	4lxz	-9.16
1d4h	-13.59	1syi	-7.39	2qrq	-6.93	3gx0	-4.73	3vw2	-6.45	4ly1	-9.86
1d4i	-12.03	1szd	-6.17	2qry	-11.74	3gxy	-7.60	3vx3	-10.63	4ly9	-11.07
1d4j	-11.36	1t31	-11.74	2qta	-7.83	3gy2	-7.80	3w07	-4.59	4lyw	-4.93
1d4k	-12.53	1t32	-10.08	2qtg	-6.90	3gy3	-7.65	3w37	-7.04	4lzt	-6.39
1d4l	-11.92	1t4v	-10.44	2qtn	-4.65	3gy7	-6.14	3w5n	-5.26	4lzs	-6.52
1d4p	-8.56	1t5f	-5.73	2qtt	-5.87	3h1x	-8.00	3w9k	-8.59	4m0e	-8.45
1d4y	-15.08	1t7d	-8.19	2qu6	-11.58	3h30	-6.16	3w9r	-8.40	4m0f	-11.92
1d6v	-8.38	1t7j	-11.82	2qv7	-4.97	3h5b	-13.59	3wgg	-5.98	4m0r	-7.08
1d6w	-8.10	1ta6	-12.41	2qw1	-5.30	3h89	-10.38	3wha	-12.66	4m0y	-8.78
1d7i	-4.89	1tcw	-8.18	2qwb	-3.72	3hb4	-12.30	3wjw	-5.26	4m0z	-7.05
1d7j	-4.48	1tcx	-9.44	2qwc	-4.82	3hcm	-4.48	3wmc	-8.85	4m12	-8.22
1d9i	-12.38	1td7	-5.94	2qwd	-6.59	3hek	-11.24	3wqm	-8.49	4m13	-9.10
1det	-5.84	1tet	-8.42	2qwe	-10.16	3hf8	-8.85	3zbx	-11.17	4m14	-9.10
1df8	-13.18	1thz	-7.00	2qwf	-7.70	3hfb	-10.22	3zc5	-9.69	4m2r	-11.54
1dgm	-6.86	1tjp	-6.01	2qwg	-11.41	3hig	-10.72	3zcl	-10.87	4m2u	-10.92
1dhf	-10.05	1tkb	-10.87	2qx0	-8.30	3hit	-11.13	3zdg	-9.65	4m2v	-10.11
1dhi	-9.86	1tmn	-9.92	2qzr	-9.86	3hk1	-8.38	3zdh	-9.99	4m2w	-9.89
1dhj	-8.90	1tng	-3.98	2r0h	-4.77	3hkn	-7.27	3zdv	-7.45	4m3p	-7.34
1dif	-14.48	1tnh	-4.58	2r0z	-7.43	3hkq	-7.26	3zhx	-9.08	4m6u	-3.72
1dl7	-8.82	1tni	-5.44	2r1y	-6.13	3hkt	-7.32	3zi0	-10.05	4m7j	-8.30
1dmp	-12.98	1tnj	-2.66	2r2b	-5.71	3hku	-11.28	3zi8	-7.69	4m8e	-10.72
1dqn	-10.87	1tnk	-2.02	2r2m	-9.96	3hkw	-11.74	3zj6	-9.05	4m8h	-10.33
1dr1	-7.57	1tnl	-2.55	2r2w	-6.07	3hky	-9.65	3zk6	-8.61	4m8x	-13.86
1drf	-10.11	1tog	-4.38	2r38	-10.11	3hl5	-6.07	3zll	-8.70	4m8y	-13.53
1drj	-10.05	1toi	-5.50	2r3t	-7.95	3hl7	-10.38	3zln	-11.51	4mc1	-10.67
1drk	-9.27	1toj	-4.61	2r3w	-9.36	3hl8	-6.10	3zlr	-12.58	4mc2	-11.13
1drv	-8.89	1tok	-3.36	2r43	-8.15	3hll	-11.20	3zm9	-10.08	4mc6	-13.03
1dud	-6.55	1tom	-11.28	2r58	-2.72	3hmo	-10.22	3znr	-10.11	4mc9	-12.83
1duv	-16.03	1tpw	-4.48	2r59	-11.13	3hmp	-7.46	3zns	-10.07	4mdn	-8.45
1dzk	-8.29	1tq4	-8.41	2r5a	-3.53	3hp9	-6.24	3zps	-11.28	4mgd	-6.37
1e1v	-6.69	1tsy	-6.74	2r5p	-11.52	3hs4	-10.87	3zpu	-11.39	4mhy	-8.79
1e1x	-8.00	1ttm	-9.99	2r9w	-6.93	3hu3	-9.36	3zq9	-8.18	4mhz	-9.33
1e2k	-6.71	1tuf	-5.50	2r9x	-6.59	3hub	-10.99	3zqe	-5.75	4mjo	-8.45
1e2l	-5.83	1tx7	-6.25	2ra0	-10.60	3hv8	-9.48	3zsq	-6.74	4mjp	-5.27
1e3g	-12.23	1txr	-10.52	2ra6	-6.14	3hvh	-11.58	3zsy	-4.39	4mme	-8.83
1e3v	-5.90	1tys	-7.46	2rcb	-9.23	3hvj	-11.82	3zt2	-3.86	4mmm	-5.19
1e4h	-11.43	1u0g	-8.36	2rcn	-8.15	3hvk	-11.58	3zt3	-3.89	4mmp	-10.48
1e5a	-10.38	1u1w	-7.95	2reg	-7.66	3hww	-9.67	3zv7	-8.04	4mn3	-7.81

**Table 2 – continued**

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1e5j	-5.44	1u2y	-2.36	2rfh	-9.27	3hx3	-10.87	3zxx	-11.41	4mnp	-9.97
1e6q	-4.28	1u71	-10.16	2rin	-5.44	3hzk	-9.10	3zyf	-6.59	4mo4	-5.73
1e6s	-4.38	1ua4	-5.73	2rio	-6.37	3hzm	-7.50	3zyu	-9.51	4mo8	-10.87
1e96	-7.09	1ucn	-7.09	2rk8	-4.95	3hzv	-8.86	3zze	-12.08	4mpn	-9.00
1eb2	-8.17	1ugp	-3.93	2rka	-4.08	3i25	-11.56	456c	-13.28	4mr3	-8.07
1ebw	-12.30	1ugx	-8.03	2rkd	-3.70	3i4b	-11.07	4a4q	-12.77	4mr6	-8.97
1eby	-13.18	1uho	-12.53	2rke	-5.54	3i4y	-9.58	4a4v	-8.89	4mre	-2.98
1ebz	-12.77	1ui0	-9.59	2rkf	-12.34	3i51	-10.46	4a4w	-10.49	4mrg	-4.02
1ec0	-11.54	1uj5	-4.14	2rkg	-10.99	3i5z	-11.82	4a6b	-11.39	4mrw	-4.48
1ec1	-12.12	1uj6	-4.14	2rkm	-5.30	3i60	-11.82	4a6c	-10.76	4mrz	-4.78
1ec2	-13.59	1uml	-10.22	2sim	-4.65	3i6o	-14.06	4a6l	-10.87	4msa	-4.48
1ec3	-12.28	1uou	-10.46	2sns	-9.10	3i73	-7.46	4a6s	-7.07	4msc	-8.10
1ec9	-4.21	1upf	-6.25	2std	-13.38	3i7e	-14.74	4a7i	-11.82	4mss	-8.70
1ecq	-4.08	1ur9	-7.84	2tmn	-8.00	3i9g	-12.17	4a95	-7.83	4muv	-7.83
1ecv	-6.59	1usi	-9.16	2tpi	-5.86	3iae	-5.29	4ab9	-4.52	4myd	-6.18
1efy	-11.17	1usk	-8.70	2usn	-8.85	3ibi	-11.67	4aba	-5.19	4n07	-8.78
1egh	-7.74	1usn	-10.52	2uwd	-11.35	3ibl	-10.65	4abb	-6.13	4n3l	-9.51
1ejn	-7.64	1utj	-5.22	2uwl	-11.41	3ibn	-10.34	4abd	-5.98	4n5d	-4.38
1ela	-8.64	1utl	-3.36	2uwo	-11.82	3ibu	-12.43	4abe	-4.62	4n6g	-7.43
1elb	-9.72	1utm	-4.09	2uwp	-9.25	3ies	-13.48	4abf	-6.28	4n6h	-12.61
1elc	-9.05	1utn	-4.74	2uxi	-9.92	3ifl	-10.98	4abg	-4.85	4n6z	-10.60
1eld	-9.10	1utp	-1.96	2uxz	-11.52	3igp	-9.54	4abh	-5.64	4n7m	-7.43
1ele	-9.31	1uv6	-6.96	2uy0	-9.40	3ijh	-5.44	4acc	-10.46	4n7u	-8.55
1elr	-6.74	1uvt	-10.38	2uy3	-4.38	3ikd	-9.17	4aci	-3.02	4n8q	-4.65
1eoc	-8.22	1uw6	-9.97	2uy4	-6.36	3ikg	-9.84	4ad2	-8.42	4n9a	-5.69
1epo	-10.82	1uwf	-9.27	2uy5	-7.46	3ime	-4.08	4ad3	-6.28	4n9c	-5.30
1erb	-11.01	1uwt	-8.11	2uyn	-3.67	3iob	-4.65	4ad6	-6.49	4na9	-10.04
1etr	-10.07	1uwu	-8.13	2uyq	-7.72	3ioc	-5.00	4afg	-11.28	4nbk	-5.26
1ets	-11.17	1uz1	-9.36	2uz9	-7.76	3iod	-5.57	4ag8	-12.17	4nbl	-8.60
1ew8	-3.07	1uz4	-4.62	2v25	-7.77	3ioe	-4.44	4agc	-14.54	4nbn	-5.92
1ew9	-4.38	1uz8	-6.74	2v2c	-4.63	3iof	-7.09	4agl	-4.96	4ncn	-7.70
1ex8	-8.60	1v0k	-6.93	2v2h	-5.12	3iog	-7.50	4agm	-5.41	4ndu	-3.72
1exw	-5.30	1v0l	-10.26	2v2q	-5.64	3ip5	-8.45	4agn	-5.39	4ngm	-14.06
1ez9	-6.93	1v11	-5.41	2v2v	-5.53	3ip6	-8.97	4ago	-6.54	4ngn	-10.26
1ezq	-12.30	1v16	-5.26	2v3d	-5.35	3ip8	-3.10	4agp	-6.37	4ngp	-10.82
1f0r	-10.41	1v1j	-6.55	2v3u	-4.08	3ip9	-7.64	4agq	-6.81	4nh7	-11.41
1f0s	-10.52	1v1m	-5.35	2v54	-6.25	3iph	-10.33	4ahr	-2.98	4nh8	-11.58
1f0t	-8.15	1v2j	-4.42	2v57	-9.65	3ipq	-10.29	4ahs	-2.98	4nkt	-8.11
1f0u	-9.73	1v2k	-8.41	2v58	-12.35	3ipu	-9.95	4ahu	-3.08	4nku	-6.35
1f3e	-9.10	1v2l	-5.83	2v59	-10.52	3iqu	-6.48	4ai5	-3.97	4nl1	-5.29
1f4e	-4.02	1v2n	-8.02	2v77	-6.88	3isj	-5.00	4aia	-4.97	4nnr	-9.86
1f4f	-6.28	1v2o	-6.43	2v8w	-9.27	3iss	-8.22	4aj4	-5.29	4non	-7.12
1f4g	-8.80	1v2r	-4.82	2v95	-11.28	3iub	-6.17	4aje	-5.00	4np2	-3.07
1f4x	-7.60	1v2s	-5.67	2vb8	-6.25	3iue	-7.91	4aji	-4.82	4np3	-4.48
1f57	-7.66	1v2t	-6.40	2vba	-6.25	3ivc	-5.60	4ajl	-5.16	4np9	-6.83
1f5k	-5.08	1v2u	-4.58	2vc7	-4.57	3ivx	-7.80	4alx	-9.89	4nra	-5.69
1f5l	-7.17	1v2w	-5.45	2vc9	-11.47	3iw5	-8.26	4aoi	-11.41	4nuc	-8.21
1f73	-3.25	1v48	-10.60	2ves	-10.46	3iw6	-7.45	4ap7	-10.82	4nue	-9.27
1f74	-4.14	1v7a	-10.88	2vfk	-5.04	3iww	-10.82	4app	-9.77	4nvp	-10.29
1f8e	-6.55	1vfn	-7.61	2vh0	-11.56	3jdw	-4.89	4aq4	-8.38	4nwc	-7.83
1fao	-10.01	1vyf	-10.94	2vh6	-13.18	3jrs	-5.82	4aqh	-8.89	4nxu	-7.53
1fch	-9.72	1vyg	-10.87	2vhj	-5.30	3jrx	-12.23	4ara	-8.22	4nxv	-7.36
1fcx	-9.77	1vzq	-10.11	2vj8	-11.82	3juk	-6.64	4arb	-8.00	4nyf	-9.93
1fcy	-11.58	1w0z	-10.44	2vjx	-6.74	3juo	-6.89	4arw	-9.69	4nze	-9.24
1fcz	-12.53	1w11	-11.17	2vk6	-7.20	3jup	-7.58	4asd	-12.61	4o04	-8.37
1fd0	-11.41	1w13	-11.82	2vkm	-11.88	3juq	-6.67	4ase	-14.95	4o05	-10.10
1fh7	-7.12	1w3j	-8.59	2vmc	-3.99	3jvr	-7.77	4asj	-10.26	4o07	-10.03
1fh8	-9.36	1w4p	-6.44	2vmd	-4.10	3jy0	-11.28	4att	-9.48	4o09	-10.46

**Table 2 – continued**

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1fh9	-8.74	1w4q	-7.15	2vmf	-7.95	3jya	-9.36	4auj	-10.52	4o0a	-9.13
1fhd	-9.27	1w5v	-11.07	2vnp	-13.48	3jyr	-7.53	4av4	-9.55	4o0b	-11.28
1fiv	-8.95	1w5w	-11.96	2vnt	-10.87	3jzg	-5.98	4avh	-9.82	4o0x	-9.74
1fjs	-13.53	1w5x	-11.41	2vo4	-6.71	3jzh	-4.62	4avi	-10.37	4o0y	-9.81
1flb	-13.18	1w5y	-11.52	2vpe	-6.71	3jzj	-4.91	4avj	-10.11	4o2b	-7.80
1flf	-12.77	1w7g	-6.93	2vpn	-9.13	3k00	-7.84	4avs	-4.74	4o3c	-3.52
1flg	-10.87	1w96	-11.43	2vpo	-7.36	3k02	-6.79	4ax9	-13.00	4o3f	-7.55
1flh	-11.07	1w9u	-8.27	2vqt	-8.15	3k2f	-9.78	4axd	-6.02	4o61	-5.84
1flk	-9.51	1w9v	-8.61	2vrj	-8.56	3k37	-12.12	4ayp	-8.32	4o6w	-11.58
1fln	-11.96	1wc1	-5.44	2vsl	-11.41	3k4d	-6.94	4ayq	-9.96	4o97	-11.58
1flw	-6.86	1wcq	-8.51	2vt3	-5.64	3k5i	-6.39	4ayu	-6.43	4o9v	-10.87
1fl3	-9.24	1wht	-5.03	2vuk	-5.30	3k5x	-8.71	4az5	-8.14	4o9w	-9.73
1flr	-13.59	1wm1	-8.56	2vvc	-11.58	3k8c	-3.97	4az6	-12.36	4oak	-5.73
1fm9	-12.23	1wn6	-6.36	2vvp	-4.62	3k8o	-15.04	4azb	-9.84	4oc1	-8.97
1fmo	-11.74	1ws1	-12.98	2vvs	-9.97	3k8q	-15.33	4azc	-7.96	4oc2	-11.25
1fpc	-9.51	1ws4	-4.08	2vvu	-11.01	3k97	-10.87	4azg	-9.65	4oc3	-11.25
1fq5	-11.41	1wur	-9.05	2vvv	-11.17	3kdb	-13.38	4azi	-10.12	4oc5	-9.61
1ftm	-10.34	1wvj	-9.14	2vw1	-4.78	3kdc	-12.61	4b0b	-4.52	4ocq	-6.26
1fv0	-8.06	1x1z	-15.03	2vw2	-4.48	3kdd	-11.50	4b1j	-9.92	4oct	-6.86
1fzj	-11.01	1x38	-11.92	2vwc	-9.00	3kek	-11.36	4b2i	-4.08	4oeu	-10.41
1fzo	-10.72	1x39	-12.53	2vwl	-9.54	3kgq	-3.13	4b2l	-4.40	4og3	-8.90
1g1d	-12.83	1x8d	-3.00	2vwm	-9.55	3kgt	-7.49	4b32	-4.54	4og4	-8.18
1g2k	-10.82	1x8j	-9.46	2vwo	-10.20	3kgu	-8.04	4b33	-4.58	4ogj	-9.23
1g2l	-9.84	1x8r	-8.32	2vxn	-6.79	3kiv	-6.39	4b34	-4.27	4oks	-6.09
1g2o	-14.34	1x8t	-10.60	2vyt	-3.72	3kjd	-11.60	4b35	-3.93	4oma	-5.67
1g30	-9.31	1xap	-11.82	2vzr	-5.82	3kku	-7.74	4b3b	-4.89	4omc	-14.65
1g32	-8.30	1xbo	-8.21	2w08	-4.65	3kmc	-8.70	4b3c	-3.64	4ouj	-3.89
1g35	-11.06	1xd1	-10.76	2w26	-12.77	3kmx	-6.55	4b3d	-3.64	4owm	-4.02
1g36	-9.74	1xff	-6.55	2w47	-6.77	3kmy	-6.10	4b5d	-10.72	4owv	-5.91
1g3d	-7.54	1xge	-6.36	2w4x	-6.59	3kqr	-6.02	4b5s	-4.74	4ozj	-7.34
1g3e	-7.31	1xgi	-6.59	2w5g	-8.25	3kr8	-11.01	4b5t	-4.52	4p3h	-8.15
1g45	-11.74	1xgj	-8.15	2w67	-6.74	3kyq	-5.73	4b5w	-4.52	4p58	-6.25
1g46	-11.96	1xh4	-10.15	2w7y	-8.26	3l1n	-7.65	4b6o	-9.51	4p5d	-7.91
1g48	-11.43	1xh5	-7.43	2w8j	-4.02	3l3l	-10.16	4b6p	-9.69	4p5z	-10.07
1g4j	-11.82	1xh9	-10.56	2w8w	-2.88	3l3m	-11.17	4b6r	-7.95	4p6x	-9.57
1g4o	-11.21	1xhy	-8.40	2w8y	-12.35	3l4v	-9.13	4b6s	-8.17	4pb2	-6.52
1g52	-12.96	1xjd	-12.88	2w9h	-8.66	3l4x	-9.36	4b73	-9.80	4pcs	-10.67
1g53	-12.28	1xk5	-8.15	2wb5	-12.41	3l4y	-9.51	4b76	-6.17	4pee	-11.31
1g54	-11.98	1xk9	-9.31	2wc4	-7.19	3l4z	-9.13	4b7j	-10.80	4pf5	-7.45
1g74	-8.86	1xka	-9.35	2we3	-6.02	3l59	-5.03	4b7p	-12.85	4pft	-11.74
1g7f	-7.43	1xkk	-11.58	2web	-6.96	3l6h	-7.34	4b7r	-13.10	4pfu	-8.38
1g7g	-8.97	1xow	-12.61	2wec	-5.38	3l79	-3.34	4b8y	-10.94	4phu	-10.76
1g7q	-8.23	1xpz	-9.62	2wed	-8.29	3l7a	-5.88	4b9k	-8.38	4pin	-7.34
1g7v	-8.70	1xr9	-9.72	2weh	-8.08	3l7c	-3.32	4b9z	-5.56	4pmm	-10.29
1g85	-7.45	1xt8	-9.31	2wej	-8.26	3l7d	-2.96	4bah	-11.82	4poh	-10.87
1g98	-7.74	1xug	-9.58	2weo	-9.42	3lbj	-6.74	4bak	-12.11	4poj	-11.01
1gaf	-10.87	1xws	-10.87	2weq	-8.02	3lbz	-5.24	4bam	-12.15	4pow	-8.56
1gai	-10.87	1y0l	-12.23	2wer	-9.58	3lc3	-7.11	4ban	-11.70	4pox	-7.38
1gar	-13.59	1y1m	-2.47	2wgj	-11.82	3lcu	-4.78	4bao	-11.37	4pp0	-5.98
1gcz	-6.97	1y1z	-4.19	2whp	-5.44	3lcv	-6.44	4baq	-12.24	4pp3	-10.63
1gfy	-6.90	1y20	-7.23	2wjg	-9.65	3ldp	-7.64	4bb9	-8.15	4pp5	-10.52
1ghv	-5.91	1y3n	-7.54	2wk6	-4.51	3ldq	-7.28	4bc5	-6.25	4psb	-6.30
1ghw	-5.71	1y3p	-6.55	2wky	-11.67	3le9	-11.17	4bck	-11.41	4pum	-9.14
1ghy	-11.01	1y3v	-7.66	2wkz	-11.92	3lea	-12.36	4bcm	-9.39	4pzv	-7.74
1ghz	-6.52	1y3x	-6.98	2wl0	-10.60	3lgs	-6.26	4bcn	-10.76	4q0k	-6.62
1gi1	-7.43	1y6q	-15.90	2wly	-8.97	3liw	-10.33	4bco	-9.35	4q19	-10.94
1gi4	-9.77	1y6r	-13.74	2wlz	-6.25	3ljg	-10.50	4bcp	-8.49	4q3t	-8.80
1gi7	-6.13	1yc4	-8.90	2wm0	-6.14	3ljo	-9.00	4bcs	-9.50	4q3u	-8.75

**Table 2 – continued**

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1gj6	-9.51	1yda	-8.90	2wn9	-11.58	3ljz	-11.06	4bf1	-11.71	4q4o	-10.14
1gj7	-10.72	1ydb	-11.20	2wnc	-8.59	3lk8	-10.48	4bi6	-5.37	4q4p	-8.68
1gj8	-9.46	1ydd	-9.61	2wnj	-8.80	3lmk	-8.07	4bi7	-6.22	4q4q	-7.87
1gja	-7.36	1ydk	-8.00	2wor	-5.30	3lp4	-6.63	4bj8	-11.26	4q4r	-8.74
1gjc	-8.63	1ydr	-7.50	2wos	-5.30	3lp7	-7.39	4bks	-5.19	4q4s	-9.44
1gjd	-7.09	1yds	-8.04	2wq5	-5.08	3lpi	-11.58	4bkt	-4.92	4q6d	-10.00
1gni	-10.97	1ydt	-9.95	2wqp	-7.49	3lpk	-12.36	4bny	-9.65	4q6e	-8.40
1gnm	-8.49	1yei	-10.14	2wr8	-7.39	3lpl	-7.64	4bqg	-8.45	4q93	-6.32
1gnn	-7.72	1yej	-10.14	2wuf	-5.83	3lpp	-8.45	4bqh	-7.60	4q9o	-7.84
1gno	-10.46	1yet	-8.04	2wva	-14.54	3lq2	-7.09	4bqs	-5.72	4qac	-12.77
1gpn	-8.80	1yfb	-5.91	2wvt	-8.32	3lvw	-3.63	4br3	-7.77	4qem	-10.60
1grp	-5.05	1yp9	-6.94	2wvz	-5.46	3lxe	-8.97	4bs0	-7.74	4qer	-10.25
1gu1	-6.14	1ype	-11.01	2wyf	-6.02	3lxx	-13.32	4bt3	-4.24	4qf7	-11.69
1gvw	-9.46	1ypg	-10.87	2wyg	-11.82	3lzs	-14.89	4bt4	-4.54	4qf8	-10.20
1gvx	-9.81	1ypj	-9.54	2wyj	-12.23	3lzu	-13.67	4bt5	-3.75	4qgd	-10.10
1gwv	-3.49	1yq7	-9.63	2wzf	-9.51	3lzz	-5.22	4btk	-9.00	4qge	-12.64
1gx8	-8.66	1yqj	-11.06	2wzm	-7.09	3m1k	-7.32	4bup	-6.73	4qgi	-5.30
1gyx	-3.37	1yqy	-10.35	2wzs	-5.23	3m35	-9.81	4buq	-11.06	4qij	-7.53
1gyy	-4.95	1yvm	-8.70	2x09	-5.11	3m36	-13.34	4bxk	-10.80	4qnb	-8.95
1gz9	-4.77	1yyy	-6.92	2x2r	-9.67	3m37	-12.28	4bzs	-9.67	4qsu	-2.72
1h0a	-7.39	1z1h	-11.41	2x4z	-11.64	3m3c	-5.52	4c1t	-9.72	4qsv	-2.72
1h1d	-11.17	1z4o	-6.14	2x7t	-9.01	3m3e	-6.02	4c1u	-9.63	4qxo	-7.49
1h1s	-11.17	1z6e	-13.21	2x7u	-7.16	3m3o	-4.89	4c2v	-12.23	4qxq	-7.74
1h22	-12.36	1z6s	-5.90	2x91	-9.16	3m3x	-9.27	4c6u	-6.24	4qxr	-8.15
1h2k	-3.97	1z71	-12.47	2x95	-6.73	3m3z	-7.79	4c9x	-9.95	4qy3	-9.27
1h2t	-10.72	1z9g	-7.66	2x96	-5.48	3m40	-9.20	4ca5	-12.76	4qyy	-9.92
1h4w	-6.33	1z9y	-9.77	2xab	-12.60	3m5e	-10.01	4ca6	-9.16	4r3w	-4.08
1h5v	-5.34	1zc9	-4.38	2xb7	-12.49	3m67	-9.16	4ca7	-10.00	4r4c	-7.53
1h6h	-7.20	1zfk	-10.76	2xbp	-6.82	3m6r	-10.18	4ca8	-9.08	4r4o	-7.91
1ha2	-7.53	1zfq	-10.22	2xbw	-10.87	3m8t	-5.44	4cc5	-6.01	4r4t	-8.51
1hbv	-8.66	1zge	-9.92	2xbx	-10.63	3m8u	-6.64	4cd0	-13.18	4r59	-10.82
1hdq	-7.91	1zgi	-7.26	2xc0	-9.13	3m96	-9.81	4cd1	-6.64	4r5a	-11.82
1hee	-7.26	1zhy	-8.86	2xc4	-10.94	3mam	-5.60	4cd4	-8.94	4r5b	-9.14
1hi3	-5.69	1zoe	-10.05	2xd9	-8.78	3mdz	-12.36	4cd5	-9.12	4r5t	-8.29
1hi4	-6.10	1zog	-9.72	2xda	-8.45	3mf5	-7.28	4cfl	-7.99	4r76	-10.67
1hi5	-5.49	1zoh	-9.51	2xde	-7.43	3mfw	-4.78	4cg8	-9.46	4rak	-10.67
1hih	-10.94	1zp8	-11.92	2xdk	-4.89	3mhc	-10.82	4cg9	-8.44	4rdn	-8.04
1hii	-9.89	1zpa	-11.41	2xdx	-8.78	3mhi	-9.10	4cga	-8.70	4rj8	-10.56
1hk4	-7.22	1zs0	-8.36	2xeg	-14.54	3mhl	-9.85	4cgi	-4.24	4rpn	-9.46
1hlk	-6.79	1zsf	-13.48	2xei	-14.43	3mhm	-9.51	4cig	-4.99	4rpo	-10.38
1hmr	-8.90	1zvx	-12.53	2xej	-12.05	3mho	-8.82	4ciw	-6.55	4rqk	-7.91
1hms	-8.66	1zzz	-6.97	2xg9	-5.64	3mhw	-3.13	4cj4	-4.57	4rqv	-6.86
1hmt	-7.87	2a14	-7.74	2xht	-8.10	3mi2	-10.56	4cjp	-4.51	4rsk	-5.87
1hn4	-5.19	2a4m	-6.14	2xib	-9.86	3mi3	-7.41	4cjq	-4.88	4sga	-9.92
1hos	-11.62	2a5b	-5.34	2xii	-9.78	3miy	-10.44	4cjr	-4.21	4std	-14.04
1hp5	-8.90	2a5c	-6.28	2xim	-3.10	3mjl	-3.32	4ck3	-4.85	4tim	-2.93
1hps	-12.53	2a5s	-9.10	2xis	-7.91	3ml5	-11.58	4cla	-7.43	4tln	-5.05
1hpu	-12.53	2a8g	-5.01	2xj1	-10.26	3mmf	-10.10	4clj	-12.43	4tmk	-10.46
1hpx	-15.30	2aac	-3.02	2xj2	-9.76	3mna	-10.04	4cmo	-12.32	4tpw	-6.37
1hsh	-12.80	2afw	-6.48	2xj7	-9.05	3moe	-5.84	4cp7	-11.02	4ts1	-6.71
1hsl	-9.77	2afx	-7.00	2xjg	-10.63	3mof	-4.17	4cpr	-10.14	4tt2	-6.33
1hvh	-10.82	2aj8	-8.42	2xjj	-8.85	3moh	-3.86	4cps	-11.24	4tte	-5.01
1hvi	-14.84	2ak3	-5.24	2xjx	-12.43	3ms9	-7.09	4cpt	-10.46	4tu4	-5.11
1hvj	-15.49	2al5	-11.41	2xm1	-6.89	3mtw	-9.57	4cpw	-10.19	4tun	-7.35
1hvk	-14.89	2am4	-5.05	2xm2	-6.28	3mxd	-12.00	4cpy	-8.57	4ty6	-10.22
1hvl	-13.52	2amt	-6.03	2xmy	-13.53	3mxe	-13.60	4cs9	-2.85	4ty7	-12.94
1hvr	-12.92	2ans	-8.04	2xn3	-8.04	3myq	-10.22	4csd	-8.03	4tz2	-4.70
1hvs	-14.00	2aoc	-6.64	2xn5	-9.09	3mz6	-9.78	4cu7	-10.31	4u0f	-8.04

Table 2 – continued

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1hwr	-11.32	2aod	-7.69	2xog	-4.66	3mzc	-9.04	4cu8	-6.07	4u43	-5.87
1hxb	-13.48	2aog	-8.53	2xp7	-7.84	3n0n	-9.92	4cwf	-6.10	4u4s	-3.97
1hwx	-14.70	2aou	-10.50	2xpc	-5.30	3n1c	-7.09	4cwn	-7.60	4u4x	-6.81
1hyo	-5.53	2aqu	-12.66	2xpk	-15.35	3n2p	-10.63	4cwo	-7.08	4u8w	-15.27
1i00	-8.61	2arm	-10.44	2xxr	-8.90	3n2u	-10.65	4cwp	-9.20	4ua8	-8.51
1i1e	-6.83	2ate	-9.61	2xxt	-10.94	3n2v	-10.20	4cwq	-9.59	4uac	-8.89
1i2s	-4.50	2avm	-7.74	2xyd	-9.27	3n35	-4.58	4cwr	-11.28	4ual	-11.41
1i37	-13.00	2avo	-12.03	2xye	-11.33	3n3g	-9.84	4cws	-10.76	4uma	-7.35
1i5r	-11.58	2avq	-5.97	2xyf	-11.47	3n3j	-11.52	4cwt	-9.17	4umb	-5.44
1i7z	-8.70	2avs	-10.29	2xyt	-8.55	3n4b	-9.54	4d1j	-8.57	4umc	-4.67
1i80	-8.71	2ax9	-12.94	2y5f	-11.82	3n76	-9.31	4d3h	-8.74	4uof	-6.58
1i9l	-11.52	2ayr	-12.62	2y5g	-9.29	3n7h	-6.11	4d8z	-8.55	4uoh	-6.48
1i9m	-11.52	2azr	-4.95	2y7i	-7.53	3n7o	-9.70	4da5	-8.75	4up5	-3.53
1i9n	-11.77	2b07	-8.74	2y7x	-12.08	3n8k	-5.50	4daf	-9.67	4us3	-7.23
1i9o	-11.44	2b1g	-9.02	2y7z	-11.82	3n9r	-9.72	4db7	-8.91	4uye	-10.90
1i9p	-11.43	2b1i	-9.27	2y81	-11.82	3n9s	-7.15	4dbm	-10.35	4uyf	-10.33
1i9q	-11.43	2b1v	-7.80	2y82	-11.41	3nb5	-10.52	4ddh	-4.48	4v01	-11.02
1ie9	-13.85	2b4l	-6.48	2y8c	-8.70	3nee	-7.26	4ddk	-3.11	4v24	-11.37
1if7	-14.29	2b7d	-11.82	2y9g	-5.12	3neo	-8.04	4ddm	-3.34	4v27	-9.05
1if8	-13.10	2b9a	-10.94	2ya6	-7.74	3nes	-7.64	4dds	-6.81	4w97	-9.65
1igb	-8.70	2baj	-11.41	2ya7	-4.27	3nex	-8.15	4ddy	-7.64	4w9c	-6.32
1ii5	-9.00	2bak	-10.10	2ya8	-7.81	3nhi	-11.45	4de3	-7.50	4w9d	-6.78
1iih	-3.93	2bal	-8.57	2yay	-8.29	3nht	-9.52	4de5	-4.28	4w9f	-7.46
1iiq	-10.16	2bet	-3.76	2yaz	-6.98	3ni5	-10.26	4del	-10.44	4w9h	-9.14
1ik4	-10.07	2bfq	-9.36	2yb0	-5.23	3nim	-6.45	4der	-8.57	4w9i	-8.10
1ikt	-4.62	2bfr	-7.13	2ybu	-8.67	3njq	-6.64	4det	-7.72	4w9j	-8.47
1inc	-10.87	2bmK	-7.64	2ydt	-7.50	3nkk	-6.39	4deu	-7.66	4w9k	-8.89
1is0	-9.51	2bo4	-6.26	2ydw	-9.97	3npc	-11.33	4dff	-10.14	4w9l	-6.82
1ivp	-10.22	2boh	-11.58	2yek	-9.80	3nq9	-5.48	4dfg	-15.95	4w9o	-10.56
1iy7	-8.41	2boj	-7.84	2yel	-9.89	3nsn	-9.77	4dhl	-6.09	4w9p	-10.60
1izh	-10.46	2bok	-8.90	2yfa	-6.89	3nu3	-13.34	4djo	-15.65	4whs	-5.60
1izi	-8.95	2bpv	-10.42	2yfx	-10.99	3nu4	-11.98	4djp	-14.34	4wiv	-8.51
1j01	-8.79	2bpy	-10.05	2ygf	-6.92	3nu5	-11.35	4djQ	-14.02	4wk1	-8.00
1j14	-6.10	2bq7	-9.58	2yi0	-11.03	3nu6	-12.64	4dju	-7.39	4wt2	-14.16
1j16	-5.22	2bqv	-10.94	2yi7	-11.31	3nu9	-12.30	4djw	-8.53	4xia	-2.09
1j17	-7.09	2br1	-6.98	2yix	-11.52	3nuj	-12.76	4djx	-9.82	5abp	-9.02
1j36	-10.52	2brm	-8.00	2yk1	-11.05	3nuo	-13.32	4djy	-11.24	5cna	-2.72
1j4r	-10.49	2bt9	-8.41	2ylc	-10.72	3nw3	-8.82	4dko	-8.86	5er1	-8.18
1jak	-7.57	2buv	-5.44	2yln	-10.44	3nx7	-11.01	4dkp	-7.77	5er2	-8.93
1jao	-8.04	2bvd	-8.15	2yme	-10.41	3nxq	-11.07	4dkq	-8.97	5p21	-7.23
1jaq	-6.09	2bvr	-5.03	2ypi	-6.55	3ny3	-6.40	4dkr	-8.86	5sga	-3.87
1jcx	-7.00	2bvs	-5.57	2ypo	-6.36	3nyd	-4.73	4dld	-7.91	5std	-14.25
1jet	-9.85	2byr	-11.62	2ypp	-5.99	3nyx	-10.18	4dli	-7.64	5tln	-8.66
1jeu	-9.27	2bys	-12.94	2yxj	-12.64	3nzk	-12.60	4dmw	-6.71	5tmp	-10.15
1jev	-9.36	2bz6	-9.63	2yz3	-9.05	3o4k	-10.35	4do4	-9.91	5upj	-9.67
1jgl	-11.82	2bza	-3.80	2z1w	-5.54	3o56	-12.36	4do5	-7.92	5yas	-4.43
1jlr	-4.52	2bzz	-8.74	2z4o	-13.00	3o5n	-6.47	4dq2	-10.22	6abp	-7.66
1jmf	-7.84	2c02	-5.49	2z94	-7.95	3o5x	-7.17	4dst	-4.02	6cpa	-15.65
1jmg	-8.25	2c1p	-7.34	2za0	-9.02	3o75	-9.08	4dsu	-3.83	6fiv	-10.98
1jn4	-6.73	2c3i	-10.33	2za5	-11.45	3o84	-9.84	4dsy	-6.02	6rnt	-3.22
1jq8	-8.15	2c3l	-6.89	2zb1	-8.59	3o8p	-8.78	4duh	-7.04	6std	-11.74
1jq9	-11.48	2c80	-7.24	2zc9	-9.16	3o99	-14.70	4dv8	-12.56	6tim	-4.36
1jqd	-7.01	2c92	-7.72	2zcs	-11.17	3o9a	-14.54	4dy6	-5.98	6upj	-8.59
1jqe	-8.75	2c94	-9.27	2zda	-11.41	3o9d	-14.57	4dzy	-7.64	7cpa	-18.97
1jqy	-6.69	2c97	-8.34	2zdk	-8.66	3o9e	-15.35	4e0x	-9.67	7std	-14.57
1jsv	-7.74	2ca8	-6.33	2zdl	-8.70	3o9i	-16.06	4e1k	-8.56	7tln	-3.36
1jvu	-7.00	2cbu	-7.72	2zdm	-8.71	3o9p	-8.86	4e3g	-6.75	7upj	-11.54
1jys	-4.78	2cbv	-7.45	2zdn	-8.49	3oaf	-11.96	4e4l	-11.92	8a3h	-5.52

Table 2 – continued

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1jzs	-8.97	2cc7	-10.88	2zfp	-7.02	3obq	-4.81	4e4n	-12.30	8abp	-10.87
1k1i	-8.94	2ccb	-10.12	2zfs	-8.89	3ocp	-10.29	4e5w	-10.41	8cpa	-12.43
1k1j	-10.26	2ccc	-10.54	2zft	-8.86	3ocz	-10.14	4E+67	-8.80	8xia	-4.01
1k1l	-9.38	2ce9	-8.19	2zgx	-9.16	3odu	-11.06	4e6d	-12.12	966c	-10.38
1k1m	-10.05	2cej	-11.71	2zkj	-7.45	3oe4	-10.15	4e6q	-11.36	9aat	-11.17
1k1n	-9.27	2cen	-11.28	2zmm	-10.33	3ohi	-6.59	4e7r	-10.46	9abp	-10.87
1k1o	-8.38	2ceq	-9.89	2zn7	-10.72	3oil	-7.72	4e9u	-7.91	1a30	-5.84
1k1y	-4.38	2cer	-12.53	2zq0	-9.27	3oim	-9.16	4ea2	-8.75	1bcu	-4.46
1k21	-11.39	2ces	-9.85	2zq2	-8.91	3ok9	-15.26	4eb8	-13.34	1e66	-13.44
1k22	-11.41	2cex	-6.39	2zx7	-14.25	3oku	-8.64	4ef6	-3.97	1f8b	-7.34
1k27	-12.23	2cf8	-11.01	2zx8	-13.10	3okv	-8.47	4efk	-3.38	1f8d	-4.62
1k4g	-7.95	2cf9	-10.63	2zxc	-11.98	3old	-8.02	4efs	-11.69	1gpk	-7.30
1k4h	-6.94	2cgf	-8.71	2zy1	-10.05	3ouj	-8.22	4egk	-10.49	1h23	-11.35
1k6c	-10.16	2cgr	-9.89	2zym	-8.34	3ove	-8.93	4ehz	-10.87	1hfs	-11.82
1k6p	-10.00	2cht	-7.50	2zz1	-6.17	3ovn	-3.46	4ei4	-11.88	1hnn	-8.48
1k6t	-10.35	2cle	-4.82	2zz2	-6.17	3own	-10.15	4ej8	-7.32	1igj	-13.59
1k6v	-9.40	2clh	-5.52	3a1c	-5.44	3oy0	-10.87	4ejl	-6.98	1jyq	-11.82
1kav	-7.91	2cli	-5.84	3a1d	-5.60	3oy8	-4.97	4ek9	-6.01	1kel	-9.89
1kc7	-7.50	2csc	-4.57	3a1e	-3.61	3oyq	-10.86	4el0	-6.10	1lbk	-4.32
1kdk	-12.30	2csn	-5.99	3a1s	-6.56	3oyw	-5.58	4el5	-7.30	1lol	-8.68
1kjr	-8.23	2ctc	-5.29	3a2o	-12.34	3ozg	-12.49	4elf	-10.91	1loq	-5.03
1km3	-6.67	2d0k	-6.82	3a5y	-10.82	3ozj	-6.94	4elg	-11.09	1mq6	-15.15
1kmy	-6.93	2d1n	-11.07	3a6t	-9.89	3ozp	-9.00	4elh	-10.99	1n1m	-7.74
1koj	-9.10	2d3z	-9.02	3a9i	-5.64	3ozr	-7.00	4emf	-9.62	1n2v	-5.54
1kpm	-7.88	2doo	-9.74	3aas	-6.13	3ozs	-7.24	4emr	-10.18	1nvq	-11.21
1ksn	-12.77	2dri	-9.36	3aau	-6.86	3p17	-6.09	4en4	-7.50	1o3f	-10.82
1kug	-5.16	2dw7	-6.39	3acx	-7.74	3p2e	-8.45	4eo6	-11.82	1o5b	-7.84
1kui	-5.12	2e1w	-10.82	3adv	-4.12	3p3g	-13.23	4eo8	-11.07	1oyt	-9.84
1kuk	-5.31	2e27	-12.70	3afk	-4.89	3p3r	-9.85	4eoh	-5.84	1p1q	-6.64
1kv1	-8.07	2e2p	-6.44	3ahn	-9.58	3p3s	-10.31	4eor	-8.56	1ps3	-3.10
1kv5	-5.73	2e2r	-11.22	3aho	-9.58	3p3t	-9.84	4epy	-4.71	1q8u	-8.10
1kyv	-8.04	2e5y	-7.95	3ai8	-5.18	3p4v	-6.93	4er1	-9.00	1qi0	-3.19
1kzk	-14.12	2e91	-8.95	3aid	-9.32	3p58	-10.33	4er2	-12.64	1r5y	-8.78
1kzn	-12.12	2e92	-9.36	3alt	-3.97	3p5l	-10.04	4erf	-12.77	1sln	-9.02
1l2s	-6.24	2e94	-10.87	3ama	-8.87	3p5o	-9.92	4etz	-8.56	1sqa	-12.51
1l6m	-11.01	2e9u	-11.01	3ao1	-3.07	3p7i	-10.46	4eu0	-8.70	1u1b	-10.60
1l83	-4.62	2eg7	-8.00	3ao2	-5.12	3p8n	-12.61	4euo	-6.86	1uto	-3.08
1l8g	-8.45	2eg8	-6.11	3ao5	-3.03	3p8o	-11.85	4ew2	-9.08	1vso	-6.41
1laf	-10.67	2epn	-9.81	3ap4	-5.33	3p8p	-6.18	4ew3	-9.16	1w3k	-5.84
1lag	-8.56	2er9	-10.05	3aqt	-9.13	3p8z	-8.27	4ewn	-9.10	1w3l	-8.53
1lah	-10.22	2erz	-7.69	3arp	-9.72	3p9l	-7.20	4exs	-5.99	1w4o	-7.09
1lbf	-10.67	2eum	-9.10	3arq	-8.70	3p9t	-8.42	4ezr	-7.07	1yc1	-8.38
1lee	-10.52	2evl	-9.10	3arr	-7.34	3pb7	-7.80	4ezx	-7.88	1zea	-7.09
1lf2	-10.22	2ewa	-10.79	3aru	-4.38	3pb8	-7.12	4f09	-9.10	2brb	-6.60
1lgt	-8.29	2ews	-9.00	3arv	-7.66	3pb9	-8.94	4f2w	-15.35	2cbj	-11.24
1lgw	-5.44	2exm	-5.58	3arw	-8.36	3pbb	-9.54	4f39	-7.74	2cet	-10.90
1lhu	-12.00	2ez7	-5.92	3arx	-7.24	3pce	-2.72	4f3c	-16.06	2d1o	-10.46
1li2	-5.49	2f01	-17.66	3ary	-8.15	3pcf	-8.22	4f3k	-13.81	2d3u	-9.40
1li3	-5.77	2f1g	-10.25	3axz	-4.66	3pcg	-3.13	4f5y	-7.38	2fvd	-11.58
1li6	-5.16	2f34	-9.36	3b1m	-11.52	3pch	-7.34	4f7v	-7.31	2g70	-10.56
1like	-10.22	2f35	-7.34	3b24	-5.95	3pcn	-4.97	4f9u	-8.19	2gss	-6.71
1lkl	-7.89	2f6t	-6.28	3b25	-8.25	3pd8	-8.78	4f9w	-9.43	2hb1	-5.16
1lnm	-11.82	2f7i	-9.65	3b26	-9.02	3pd9	-8.45	4f9y	-9.16	2iwx	-9.08
1lpg	-9.63	2f7o	-10.11	3b27	-7.01	3pe1	-13.11	4fai	-9.50	2j62	-15.41
1lpk	-10.26	2f7p	-8.97	3b2q	-6.18	3pfp	-8.75	4fcf	-11.71	2j78	-8.72
1lpz	-10.33	2f80	-11.11	3b3x	-4.89	3pgl	-7.20	4fev	-7.36	2jdm	-7.34
1lrh	-9.27	2f81	-14.29	3b4f	-11.06	3pgu	-9.10	4few	-7.08	2jdu	-9.13
1lst	-10.67	2f8g	-11.82	3b4p	-7.34	3pju	-6.63	4ffs	-14.19	2jdy	-5.94

**Table 2 – continued**

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1lvu	-7.23	2f94	-9.12	3b50	-10.26	3pn1	-9.46	4fht	-8.38	2obf	-12.03
1lyb	-15.52	2f9k	-9.61	3b5j	-7.72	3pn4	-9.31	4fiv	-8.86	2ole	-9.85
1lyx	-6.17	2fai	-8.48	3b5r	-11.92	3po1	-5.46	4fk6	-13.18	2p4y	-12.23
1lzq	-11.40	2fdp	-10.31	3b65	-12.60	3po6	-9.59	4fl1	-4.46	2pq9	-11.02
1m0b	-11.98	2fgu	-12.47	3b66	-11.69	3ppm	-12.96	4fl2	-4.97	2qbp	-11.41
1m0n	-3.02	2fgv	-8.32	3b67	-12.03	3ppp	-7.09	4flp	-9.13	2qbr	-8.60
1m0q	-5.29	2flb	-7.80	3b7j	-7.02	3ppq	-6.18	4fm7	-9.84	2qft	-7.15
1m1b	-6.33	2fle	-10.67	3b7r	-10.46	3ppr	-3.83	4fm8	-8.11	2qmj	-5.72
1m2p	-8.30	2flr	-8.29	3b7u	-10.52	3prs	-10.63	4fnn	-10.29	2r23	-5.05
1m2q	-8.29	2fmb	-11.82	3b92	-10.87	3ptb	-6.11	4fp1	-6.21	2v00	-4.97
1m2r	-8.78	2fpz	-5.38	3bbb	-9.51	3pwd	-9.05	4fs4	-8.93	2v7a	-11.28
1m2x	-5.64	2fqo	-8.74	3bbf	-7.17	3pwk	-4.55	4fsl	-10.46	2vl4	-8.17
1m48	-6.92	2fmt	-8.34	3be9	-10.35	3pwm	-12.36	4fut	-8.85	2vo5	-6.64
1m4h	-12.94	2fqw	-9.08	3bex	-7.57	3pyy	-9.32	4fxp	-5.56	2vot	-9.70
1m5w	-5.80	2fqx	-9.72	3bf1	-3.42	3q1x	-7.24	4fxq	-7.84	2vvn	-9.92
1m7d	-8.47	2fqy	-8.93	3bft	-8.82	3q2j	-5.68	4fys	-6.55	2vw5	-11.58
1m7i	-7.34	2fu8	-6.39	3bgb	-8.22	3q44	-8.57	4fz3	-5.07	2w66	-5.50
1m7y	-14.89	2fw6	-3.97	3bgc	-6.82	3q6w	-10.29	4fzj	-4.28	2wbg	-6.05
1m83	-4.62	2fx6	-5.03	3bgq	-10.82	3q6z	-5.05	4g0p	-4.09	2wca	-7.61
1mai	-9.08	2fxs	-8.23	3bgs	-12.80	3q7q	-7.68	4g0q	-3.42	2weg	-8.83
1mes	-10.46	2fxu	-11.07	3bgz	-8.51	3qaa	-15.68	4g0y	-3.13	2wtv	-11.88
1met	-12.77	2fxv	-7.27	3bkl	-8.38	3qbc	-6.75	4g0z	-3.00	2x00	-15.39
1mfa	-6.85	2g5u	-11.54	3bl0	-9.40	3qdd	-11.92	4g4p	-9.36	2x0y	-6.25
1mfd	-7.22	2g71	-10.14	3bl1	-7.61	3qfd	-5.67	4g5f	-4.14	2x8z	-10.82
1mfi	-7.60	2g72	-8.83	3bqc	-7.79	3qfy	-8.32	4g8n	-9.78	2x97	-7.69
1mh5	-12.51	2g8r	-5.42	3bra	-3.67	3qgw	-8.00	4g8v	-7.88	2xb8	-10.31
1mmq	-10.22	2g94	-12.94	3brn	-11.82	3qgy	-10.60	4g8y	-6.24	2xbv	-11.45
1mmr	-7.34	2g9q	-8.70	3bu1	-11.07	3qin	-9.33	4g90	-6.13	2xdl	-4.21
1mnc	-12.23	2gbp	-10.05	3buf	-4.21	3qkd	-11.39	4g95	-10.34	2xhm	-9.24
1moq	-4.70	2gh9	-8.15	3bug	-4.32	3qlm	-8.66	4gbd	-15.38	2xnb	-9.28
1mq5	-12.23	2gj5	-11.31	3buh	-4.97	3qnd	-6.59	4ge1	-8.74	2xy9	-12.49
1mrn	-6.14	2gkl	-7.27	3bv9	-7.28	3qox	-8.93	4gfm	-9.81	2xys	-10.08
1mrs	-5.38	2gl0	-6.55	3bva	-8.86	3qps	-7.61	4gfo	-9.00	2y5h	-7.87
1mrw	-13.18	2glp	-6.81	3vvb	-7.46	3qqa	-7.91	4gg7	-11.14	2yfe	-9.01
1mrx	-9.86	2gst	-8.25	3bwj	-8.83	3qqs	-7.91	4ggz	-13.83	2yge	-6.88
1msm	-14.24	2gsu	-4.88	3bxg	-7.45	3qto	-5.61	4ghi	-9.63	2yki	-12.85
1msn	-12.35	2gv6	-9.97	3bxf	-7.53	3qtv	-6.32	4gih	-11.31	2ymd	-4.29
1mtr	-11.41	2gv7	-10.67	3bxg	-6.74	3qw5	-8.76	4gj3	-12.03	2zcq	-11.98
1mu6	-11.39	2gvj	-12.94	3bxh	-5.48	3qwc	-5.79	4gkh	-6.35	2zcr	-9.33
1mu8	-12.23	2gvv	-5.30	3bzf	-6.14	3qx5	-5.71	4gki	-6.06	2zjw	-10.46
1mue	-11.74	2gz2	-7.09	3c2f	-2.72	3qx8	-3.89	4gkm	-7.02	2zxd	-7.09
1my4	-9.48	2gzl	-6.55	3c2o	-4.55	3qx9	-5.50	4gny	-5.73	3acw	-6.47
1n0s	-10.12	2h15	-7.70	3c2r	-4.23	3qxt	-7.09	4gq4	-10.41	3ag9	-10.94
1n3i	-12.08	2h21	-8.89	3c2u	-3.94	3qxv	-11.41	4gql	-13.03	3ao4	-2.81
1n3z	-5.71	2h3e	-7.74	3c39	-5.38	3qyy	-6.90	4gqp	-13.04	3b3s	-3.46
1n46	-14.29	2h4g	-8.86	3c4h	-7.74	3r0y	-6.58	4gr0	-12.98	3b3w	-5.69
1n4h	-8.90	2h4k	-7.46	3c56	-10.72	3r16	-9.92	4gr3	-10.61	3b68	-11.41
1n4k	-13.66	2h4n	-11.82	3c79	-9.78	3r17	-8.71	4gr8	-10.64	3bfu	-8.52
1n51	-6.59	2h5a	-6.93	3c84	-10.67	3r1v	-9.40	4gu6	-10.00	3bkk	-8.26
1n8v	-8.19	2h6t	-9.81	3c88	-9.24	3r24	-7.13	4gu9	-5.94	3bpc	-6.52
1nc1	-8.32	2ha2	-6.33	3c89	-8.25	3r4m	-8.04	4gue	-7.12	3cft	-5.69
1nc3	-6.79	2ha3	-4.12	3c8a	-8.40	3r4n	-9.36	4gzp	-10.65	3cj2	-6.59
1ndv	-8.04	2ha5	-5.90	3c8b	-8.29	3r4p	-10.82	4gzt	-10.56	3coy	-8.18
1ndw	-7.11	2ha6	-5.87	3c8e	-5.64	3r5t	-11.66	4gzw	-6.14	3cyx	-10.87
1ndy	-8.38	2hah	-10.87	3cct	-10.27	3r6c	-6.41	4gzx	-4.33	3d4z	-6.64
1ndz	-11.02	2haw	-6.69	3ccw	-10.69	3r6u	-6.14	4h3f	-12.23	3dd0	-12.23
1nf8	-10.63	2hb3	-15.42	3ccz	-9.91	3r7o	-11.36	4h3g	-11.17	3dxg	-3.26
1nfu	-10.52	2hdq	-1.90	3cd0	-10.29	3r88	-6.55	4h3j	-9.58	3e93	-12.03

**Table 2 – continued**

PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy	PDB ID	Energy
1nfw	-12.17	2hf8	-7.43	3cd5	-10.73	3rbu	-12.81	4h42	-4.71	3ebp	-8.03
1nfx	-11.58	2hhn	-10.18	3cd7	-10.65	3rdo	-13.38	4h75	-8.97	3ehy	-7.95
1nfy	-12.08	2hjb	-5.97	3cdb	-9.54	3rdq	-12.65	4h7q	-6.88	3ejr	-11.64
1nh0	-13.23	2hl4	-10.38	3cf8	-6.66	3rdv	-6.67	4h81	-6.96	3f17	-11.73
1nhu	-7.69	2hmu	-10.46	3cfn	-6.79	3re4	-10.05	4h85	-7.00	3f3a	-5.69
1nhz	-8.26	2hmv	-10.46	3cj4	-8.85	3rf4	-8.49	4hbm	-10.76	3f3c	-8.18
1nja	-8.57	2hnc	-9.81	3cj5	-8.61	3rf5	-7.65	4hdb	-10.94	3f3e	-10.46
1njc	-7.54	2hnx	-9.62	3ckb	-4.05	3rlb	-13.48	4hdf	-11.54	3f80	-5.73
1njd	-7.57	2hoc	-12.94	3ckz	-11.85	3rlp	-9.62	4hdp	-10.20	3fcq	-3.76
1nje	-5.16	2hs1	-11.52	3cl0	-9.61	3rlq	-10.05	4heg	-12.12	3fk1	-3.56
1njs	-10.63	2hu6	-5.18	3cla	-6.71	3rlr	-10.22	4hf4	-11.71	3fv1	-12.64
1nki	-9.10	2hw2	-4.04	3cm2	-8.79	3rm4	-7.84	4hfp	-10.03	3g0w	-12.94
1nl9	-8.10	2hxm	-7.09	3cow	-9.38	3rm9	-6.48	4hge	-10.76	3g2n	-5.56
1nli	-4.88	2hzi	-8.93	3coz	-7.57	3roc	-11.13	4hj2	-3.44	3g2z	-3.21
1nm6	-13.66	2hzy	-10.04	3cpa	-5.44	3rr4	-6.18	4hla	-14.67	3gbb	-9.38
1nny	-10.41	2i0a	-15.49	3cr5	-5.69	3rsr	-5.92	4hp0	-8.32	3gcs	-9.85
1no6	-5.99	2i0d	-16.44	3cs7	-14.51	3rsx	-5.99	4hpi	-6.59	3ge7	-11.82
1np0	-4.85	2i19	-10.60	3ctt	-8.63	3rt4	-11.96	4ht0	-10.87	3gnw	-12.36
1nq7	-9.24	2i2b	-3.32	3cyw	-10.56	3rt8	-8.63	4ht2	-8.89	3gy4	-6.93
1nt1	-12.08	2i2c	-6.39	3cyz	-9.81	3rtf	-9.99	4hu1	-10.25	3huc	-8.14
1nu3	-5.44	2i3h	-10.05	3cz1	-9.86	3ru1	-6.59	4hw3	-8.82	3imc	-4.02
1nvr	-11.02	2i3i	-9.92	3czv	-10.60	3rux	-12.61	4hws	-12.36	3ivg	-5.84
1nvs	-10.63	2i3v	-8.90	3d0b	-8.89	3rv4	-3.13	4hy1	-11.82	3jvs	-8.89
1nw4	-12.32	2i4d	-15.87	3d0e	-11.41	3rv8	-6.69	4hym	-11.17	3k5v	-8.56
1nw5	-7.08	2i4j	-8.37	3d1x	-11.77	3rwp	-12.53	4hzm	-6.29	3kgp	-3.49
1nw7	-6.92	2i4u	-15.72	3d1y	-11.17	3ryj	-10.60	4i3z	-5.83	3kv2	-9.95
1nwl	-3.25	2i4v	-15.22	3d1z	-11.96	3ryv	-9.61	4i54	-9.46	3kwa	-5.54
1nz7	-9.67	2i4w	-15.75	3d2e	-8.72	3ryy	-10.08	4i5c	-11.98	3l3n	-11.11
1o0f	-7.20	2i4x	-15.92	3d4y	-7.74	3ryz	-11.71	4i71	-10.52	3l4u	-10.22
1o0h	-8.04	2i4z	-7.74	3d50	-6.48	3rz0	-10.26	4i72	-12.30	3l4w	-8.15
1o0m	-7.00	2i6b	-9.74	3d51	-5.64	3rz1	-11.88	4i74	-9.13	3l7b	-3.26
1o0n	-5.56	2i80	-7.34	3d52	-4.46	3rz5	-10.72	4i7j	-4.51	3lka	-3.83
1o1s	-9.93	2idw	-12.08	3d6o	-5.58	3rz7	-12.17	4i7k	-4.13	3mfv	-3.42
1o2h	-9.74	2igv	-3.03	3d6p	-5.10	3rz8	-11.10	4i7l	-5.42	3mss	-6.33
1o2j	-9.40	2ihj	-6.24	3d6q	-5.11	3s0b	-8.82	4i7m	-5.63	3myg	-14.54
1o2n	-8.27	2ihq	-11.54	3d78	-10.38	3s0d	-9.58	4i7p	-4.76	3n7a	-5.03
1o2o	-8.64	2iko	-7.41	3d7b	-5.01	3s0e	-8.90	4i8n	-6.06	3n86	-7.66
1o2q	-10.44	2il2	-9.65	3d7k	-6.25	3s2v	-9.24	4i8w	-14.81	3nox	-11.77
1o2r	-7.08	2iuz	-7.54	3d7z	-10.76	3s3v	-8.47	4i8x	-3.59	3nq3	-5.14
1o33	-7.80	2izl	-8.15	3d83	-11.36	3s43	-11.69	4i8z	-15.01	3nw9	-12.23
1o35	-6.79	2j27	-4.78	3d8w	-11.07	3s45	-11.54	4i9u	-5.24	3oe5	-9.35
1o36	-8.10	2j2u	-9.96	3d8y	-4.62	3s54	-13.10	4ibb	-4.85	3ov1	-7.07
1o38	-9.27	2j34	-10.63	3d8z	-4.58	3s56	-13.07	4ibc	-4.05	3owj	-8.25
1o3d	-9.69	2j47	-7.35	3d91	-12.43	3s6t	-9.99	4ibd	-4.99	3ozt	-5.61
1o3i	-9.92	2j4g	-8.97	3d9z	-11.82	3s71	-11.74	4ibe	-5.64	3pe2	-13.26
1o3j	-9.20	2j4i	-12.23	3da9	-7.49	3s73	-11.82	4ibf	-6.02	3pww	-9.95
1o3l	-8.89	2j75	-9.04	3dbu	-10.95	3s76	-6.86	4ibg	-5.39	3pxf	-6.02
1o3p	-9.05	2j77	-6.64	3dc3	-11.29	3s77	-9.80	4ibi	-5.63	3s8o	-9.31
1o5a	-8.72	2j79	-8.10	3dcc	-12.17	3s78	-8.79	4ibj	-5.88	3su2	-9.99
1o5c	-7.09	2j7b	-9.00	3dd8	-10.67	3s8l	-7.66	4ibk	-5.84	3su3	-12.41
1o5e	-7.80	2j7d	-9.69	3ddf	-6.33	3s8n	-8.44	4idn	-7.12	3su5	-7.58
1o5g	-6.74	2j7e	-9.95	3ddg	-8.15	3s8x	-9.92	4ido	-6.70	3u9q	-5.95
1o5r	-11.03	2j7f	-8.63	3dgo	-9.16	3s9e	-6.97	4ieh	-10.67	3udh	-3.87
1o7o	-6.10	2j7g	-9.51	3dhv	-4.02	3s9t	-9.27	4igt	-10.72	3ueu	-7.12
1o86	-13.00	2j7h	-9.77	3djk	-14.39	3sap	-10.31	4ih3	-6.55	3uex	-9.40
1oar	-10.05	2j94	-8.52	3djo	-5.97	3sax	-8.93	4ih5	-5.58	3uo4	-8.86
1oau	-10.46	2j95	-11.41	3djp	-5.71	3sbh	-9.89	4ih6	-6.44	3utu	-14.84
1oba	-3.32	2jdh	-8.85	3djg	-4.05	3sbi	-10.76	4ih7	-7.12	3vh9	-8.48





**Table 3 – continued**

PDB ID	Energy	Special Treatment
9aat	-11.17	
1bzm	-8.19	wrong resonance structure of ligand
1cbx	-8.63	
2ctc	-5.29	
3cpa	-5.44	
1cla	-7.17	
3cla	-6.71	
4cla	-7.43	
2csc	-4.57	
5cna	-2.72	
1af2	-4.21	
1dr1	-7.57	
1dhf	-10.05	
1drf	-10.11	
1ela	-8.63	
7est	-10.33	Delete lonely pair atom
3fx2	-12.64	
2gbp	-10.05	
1hsl	-9.92	
2qwd	-6.59	
2qwe	-10.16	
2qwf	-7.70	
2qwg	-11.41	
2qwc	-4.82	
2qwb	-3.72	
1mnc	-12.23	
1exw	-5.30	
1apw	-10.87	
1apt	-12.77	
1bxo	-13.59	
1fmo	-11.74	
2pk4	-5.87	
1inc	-10.87	
4sga	-4.44	
5sga	-3.87	
5p21	-7.23	
1rbp	-9.13	
1rgk	-5.86	
6rnt	-3.22	
1rgl	-6.02	
1rnt	-7.04	
1zzz	-6.97	
1yyy	-6.92	
1b5g	-10.87	
1ba8	-12.23	
1bb0	-11.36	
2sns	-9.10	
1sre	-5.44	
7tln	-3.36	
4tln	-5.05	
1tmn	-10.15	
2tmn	-8.00	
3tmn	-8.02	
5tln	-8.66	
1tlp	-10.27	No atom type for OXT atom in ligand after schrodinger processing.
1etr	-10.07	
1ets	-11.17	
1d3d	-12.35	

Table 3 – continued		
PDB ID	Energy	Special Treatment
1d3p	-10.04	overlap atoms at OE1/OE2 at GLU62 B chain, delete OE2 atom.
1a46	-7.74	
1a5g	-13.79	
1bcu	-6.79	
1tha	-7.27	
4tim	-2.93	
6tim	-4.36	
7tim	-7.34	
1bra	-2.47	
1tnj	-2.66	
1pph	-8.45	Delete lonely pair atom
1tnk	-2.02	
1tnh	-4.58	
1tni	-2.31	
1ppc	-8.37	
1tng	-3.98	
3ptb	-6.11	
1tnl	-2.55	
1bhf	-5.95	
2xis	-7.91	

Table S4: The information about the PDBBind v2007 core set ( $N = 195$ ). Special treatments are emphasized. The energy data are all in the unit of kcal/mol.

PDB ID	Energy	Special Treatment
1HK4	-7.22	
1HA2	-7.53	
1GNI	-10.97	
1NHU	-7.69	
2D3Z	-9.02	
2D3U	-9.40	
1AJP	-3.03	
1AI5	-5.05	
1AJQ	-5.86	
1GPK	-7.30	
1H23	-11.35	
1E66	-13.44	
2RKM	-5.30	
1B9J	-8.10	
1B7H	-10.90	
1U2Y	-2.36	
1U33	-6.25	
1XD1	-10.76	
1UWT	-8.11	
2CEQ	-9.89	
2CER	-12.53	
2QWB	-3.72	
2QWD	-6.59	
2QWE	-10.16	
2J77	-6.64	
2J78	-8.72	
2CET	-10.90	
1M0N	-3.02	
1ZC9	-4.38	
1M0Q	-5.29	
2FDP	-10.31	

**Table 4 – continued**

PDB ID	Energy	Special Treatment
1FKN	-11.96	
2G94	-12.94	
1V16	-5.26	
1OLU	-5.99	
1OLS	-7.91	
1TOK	-3.36	
1TOJ	-4.61	
1TOI	-5.50	
1N2V	-5.54	
1K4G	-7.95	
1S39	-10.46	
1KV1	-8.07	
2BAK	-10.10	
2BAJ	-11.41	
1NDW	-7.11	
1NDY	-8.38	
1NDZ	-11.02	
2HDQ	-1.90	
1L2S	-6.24	
1XGJ	-8.15	
1Q8T	-6.47	
1YDT	-9.95	
1RE8	-12.94	
1G7Q	-8.23	
1FZJ	-11.01	
1FZK	-11.41	
1M2Q	-8.29	
1OM1	-9.20	
1ZOE	-10.05	
2AZR	-4.95	
1G7F	-7.43	
1NNY	-10.41	
5ER1	-8.18	
2ER9	-10.05	
4ER2	-12.64	
1PPM	-7.88	
1APW	-10.87	
1BXO	-13.59	
1NJE	-5.16	
1TSY	-6.74	
1NJA	-8.57	
4TLN	-5.05	
1TMN	-9.92	
4TMN	-13.82	
1FH7	-7.12	
1FH9	-8.74	
1FH8	-9.36	
2FZC	-3.67	
2H3E	-7.74	
1D09	-10.29	
2CTC	-5.29	
8CPA	-12.43	
7CPA	-18.97	
1E1V	-6.69	
1B39	-9.40	wrong separation of Schrodinger, not convergence when bcc charge calculation (QM). Re-optimize ligand structure.
1PXO	-11.82	
1BCU	-4.46	
1VZQ	-10.11	

**Table 4 – continued**

PDB ID	Energy	Special Treatment
1SL3	-16.10	
2BRB	-6.60	
2BRM	-8.00	
1NVQ	-11.21	
1JQD	-7.01	
2AOV	-9.57	
2AOU	-10.50	
1Y1M	-2.47	
1PB9	-4.92	
1PBQ	-8.52	
1VFN	-7.61	
1V48	-10.60	
1B8O	-14.46	
1P1Q	-6.64	
1SYH	-8.57	
1FTM	-10.34	
1FCX	-9.77	
1FD0	-11.41	
1FCZ	-12.53	
1F4E	-4.02	
1F4F	-6.28	
1F4G	-8.80	
1F5K	-5.08	
1O3P	-9.05	
1SQA	-12.51	
2B1V	-7.80	
2FAI	-8.48	
2AYR	-12.62	
1AVN	-5.30	
1TTM	-9.99	
1IF7	-14.29	
2BOK	-8.90	
1NFY	-12.08	
1MQ6	-15.15	
2USN	-8.85	
2D1O	-10.46	
1HFS	-11.82	
2FLB	-7.80	
2BZ6	-9.63	
2B7D	-11.82	
1LOQ	-5.03	
1LOL	-8.68	
1X1Z	-15.03	
4TIM	-2.93	
1KV5	-5.73	
1TRD	-7.34	
1BRA	-2.47	
1J16	-5.22	
1J17	-7.09	
1UTP	-1.96	
1V2O	-6.43	
1O3F	-10.82	
1JYS	-4.78	
1NC1	-8.32	
1Y6Q	-15.90	
1BMA	-6.24	
1ELA	-8.64	
1ELB	-9.72	

Table 4 – continued		
PDB ID	Energy	Special Treatment
1PR5	-5.33	
1A69	-7.20	
1K9S	-8.86	
3PCE	-2.72	
3PCH	-7.34	
3PCJ	-9.81	
1PZ5	-7.34	
2CGR	-9.89	
1FLR	-13.59	
2GSS	-6.71	
3GSS	-7.91	
10GS	-8.70	
6STD	-11.74	
2STD	-13.38	
3STD	-15.10	
1JAQ	-6.09	
1ZS0	-8.36	
1ZVX	-12.53	
2D0K	-6.82	
1DHI	-9.86	
2DRC	-13.44	
1SLG	-5.30	
1DF8	-13.18	
2F01	-17.66	
2G8R	-5.42	
1O0H	-8.04	
1U1B	-10.60	
2C02	-5.49	
1HI4	-6.10	
2BZZ	-8.74	
1TYR	-9.51	conflict of water to ligand in origin structure. ambiguous ligand Z/E structure.
1E5A	-10.38	
2G5U	-11.54	
1SV3	-6.44	
1Q7A	-9.77	
1JQ9	-11.48	
1A08	-7.64	
1A1B	-8.70	
1IS0	-9.51	
1A30	-5.84	
2F80	-11.11	
2I0D	-16.44	
1D7J	-4.48	
1FKI	-9.51	
1FKB	-13.18	
6RNT	-3.22	
1DET	-5.84	
1RNT	-7.05	

Table S5: The information about the PDBBind v2015 core set ( $N = 195$ ). Special treatments are emphasized. The energy data are all in the unit of kcal/mol.

PDB ID	Energy	Special Treatment
10gs	-8.69613	
1a30	-5.84271	
1bcu	-4.45677	

**Table 5 – continued**

PDB ID	Energy	Special Treatment
1e66	-13.4382	
1f8b	-7.33736	
1f8c	-10.0549	
1f8d	-4.61982	
1gpk	-7.29659	
1h23	-11.3457	
1hfs	-11.8213	
1hnn	-8.47872	
1igj	-13.5877	
1jyq	-11.8213	
1kel	-9.89185	
1lbk	-4.32089	
1lol	-8.68254	
1loq	-5.02745	
1lor	-15.028	
1mq6	-15.1503	
1n1m	-7.74499	
1n2v	-5.54378	
1nvq	-11.2099	
1o3f	-10.8158	
1o5b	-7.8401	
1os0	-8.19338	Error extract structure from Schrodinger result. Error atom type (None to O.co2 for OXT) in output ligand.
1oyt	-9.83749	
1p1q	-6.64439	
1ps3	-3.098	
1q8t	-6.46775	
1q8u	-8.09827	
1qi0	-3.19311	
1r5y	-8.77765	
1sln	-9.02223	
1sqa	-12.5143	
1u1b	-10.5984	
1u33	-6.25034	
1uto	-3.08441	
1vso	-6.41339	
1w3k	-5.84271	
1w3l	-8.53308	
1w4o	-7.09278	
1xd0	-9.67444	Error repeat H in tleap. Delete atom name H in NTYR2 (A chain) in pqr file.
1yc1	-8.38361	
1z95	-9.67444	
1zea	-7.09278	
2brb	-6.60362	
2cbj	-11.237	
2cet	-10.8973	
2d1o	-10.4625	
2d3u	-9.40269	
2fvd	-11.5767	
2g70	-10.5576	
2gss	-6.71232	
2hb1	-5.16333	
2iwx	-9.07658	
2j62	-15.4085	
2j78	-8.7233	
2jdm	-7.33736	
2jdu	-9.13093	
2jdy	-5.93782	
2obf	-12.0251	

**Table 5 – continued**

PDB ID	Energy	Special Treatment
2ole	-9.85108	carbon atom named CL be identified as CI in sqm, rename it. Optional residue exist in A/B chain.
2p4y	-12.2289	
2pcp	-11.8213	
2pq9	-11.0196	
2qbp	-11.4137	
2qbr	-8.60101	
2qft	-7.14713	
2qmj	-5.72042	
2r23	-5.05462	
2v00	-4.9731	
2v7a	-11.2778	
2vl4	-8.16621	
2vo5	-6.64439	
2vot	-9.70162	
2vvn	-9.91902	
2vw5	-11.5767	
2w66	-5.50302	
2wbg	-6.04653	
2wca	-7.60911	
2weg	-8.83201	
2wtv	-11.8756	
2x00	-15.3949	
2x0y	-6.25034	
2x8z	-10.8158	
2x97	-7.69064	
2xb8	-10.3131	
2xbv	-11.4544	
2xdl	-4.21219	
2xhm	-9.23964	
2xnb	-9.2804	
2xy9	-12.4871	
2xys	-10.0821	
2y5h	-7.86728	
2yfe	-9.00865	
2yge	-6.87538	
2yki	-12.854	
2ymd	-4.29371	
2zcq	-11.9844	
2zcr	-9.33475	
2zjw	-10.4625	
2zwz	-10.5848	
2zx6	-14.403	
2zxd	-7.09278	
3acw	-6.46775	
3ag9	-10.9381	
3ao4	-2.81265	
3b3s	-3.46486	
3b3w	-5.69325	
3b68	-11.4137	
3bfu	-8.51949	
3bkk	-8.26132	
3bpc	-6.5221	
3cft	-5.69325	
3cj2	-6.59003	
3coy	-8.1798	
3cyx	-10.8702	
3d4z	-6.64439	
3dd0	-12.2289	



**Table 5 – continued**

PDB ID	Energy	Special Treatment
3dxg	-3.26105	
3e93	-12.0251	
3ebp	-8.03033	
3ehy	-7.9488	
3ejr	-11.6447	
3f17	-11.7262	
3f3a	-5.69325	
3f3c	-8.1798	
3f3e	-10.4625	
3f80	-5.73401	
3fcq	-3.76379	
3fk1	-3.55998	
3fv1	-12.6366	
3g0w	-12.9355	
3g2n	-5.55737	
3g2z	-3.2067	
3gbb	-9.37551	
3gcs	-9.85108	
3ge7	-11.8213	
3gnw	-12.3648	
3gy4	-6.92973	
3huc	-8.13903	
3i3b	-3.03006	
3imc	-4.02196	
3ivg	-5.84271	
3jvs	-8.88636	
3k5v	-8.56025	
3kgp	-3.49204	
3kv2	-9.9462	
3kwa	-5.54378	
3l3n	-11.1147	
3l4u	-10.218	
3l4w	-8.15262	
3l7b	-3.26105	
3lka	-3.83173	
3mfv	-3.4241	
3mss	-6.33187	
3muz	-4.70134	
3myg	-14.5388	
3n7a	-5.02745	
3n86	-7.66346	
3nox	-11.7669	
3nq3	-5.13615	
3nw9	-12.2289	
3oe5	-9.34834	
3ov1	-7.0656	
3owj	-8.24773	
3ozt	-5.61172	
3pe2	-13.2616	
3pww	-9.9462	
3pxf	-6.01935	
3s8o	-9.30757	
3su2	-9.98696	
3su3	-12.4056	
3su5	-7.58194	
3u9q	-5.95141	
3udh	-3.87249	
3ueu	-7.11995	

Table 5 – continued		
PDB ID	Energy	Special Treatment
3uex	-9.40269	4 polymer of protein, too large to calculate (more than 4000 residues).
3uo4	-8.85918	
3uri	-12.2289	
3utu	-14.8378	
3vd4	-6.54927	
3vh9	-8.47872	
3zso	-6.9569	
3zsx	-4.45677	
4de1	-8.09827	
4de2	-5.59813	
4des	-7.9488	Error repeat H in tleap. Delete atom name H in NTYR2 (A chain) in pqr file.
4dew	-9.51139	
4djr	-15.653	
4djv	-9.13093	
4g8m	-10.7207	
4gid	-14.634	
4gqq	-3.92685	
4tmn	-13.8187	
		Error atom type (None to O.co2 for OXT) in output ligand.

Tables 6-10 list the most important 50 features that contribute to the binding affinity prediction in the different tests referred in this work.

Table S6: The most important 50 features in the learning to rank algorithm for the five-fold cross validation on the validation set ( $N = 1322$ ).

Feature
Volume change
Sum of atomic Coulombic energy of S atom in Ligand
van der Waals interaction between C and P atoms
The sum of area change of C atom in protein ligand complex
The average change of area of C atoms in protein
van der Waals interaction between C and S atoms
Electrostatics binding free energy
van der Waals interaction between C and O atoms
van der Waals interaction between S and O atoms
van der Waals interaction between C and N atoms
The max of area change of C atom in protein ligand complex
van der Waals interaction between N and O atoms
van der Waals interaction between C and C atoms
van der Waals interaction between N and P atoms
The average change of area of all atoms in protein
The max area change of O atoms in protein ligand complex
The max area change of C atoms in protein
The max area change of N atoms in protein
The sum of atomic reaction field energy of O atoms in protein
The max of atomic Coulombic energy of O atoms in protein
The average of atomic Coulombic energy of S atoms in protein
The sum of atomic area change of O atoms in ligand
van der Waals interaction between C and N atoms
The sum of atomic area change of N atoms in protein ligand complex
The max of atomic area change of N atoms in protein
The max of atomic area change of C atoms in protein ligand complex
The max of the reaction field energy of C atoms in ligand.
The max of atomic reaction field energy of all atoms in ligand
The sum of atomic area change of N atoms in ligand
The average of atomic area change of C atoms in ligand
van der Waals interaction between N and S atoms

**Table 6 – continued**

Feature
The max of atomic area change of N atoms in protein ligand complex
The max of atomic area change of all atoms in protein ligand complex
The min atomic reaction field energy of C atoms in ligand
The min atomic area change of O atoms in protein ligand complex
van der Waals interaction between N and N atoms
The average atomic area change of O atoms in protein
The max of atomic reaction field energy of C atoms in protein ligand complex
The min of atomic Coulombic energy of C atoms in prtein
The average of the atomic area change of N atoms in ligand
The average of the atomic area change of C atoms in ligand
The max of atomic area change of O atoms in ligand
The min of atomic reaction field energy of C in ligand
The sum of atomic reaction field energy of all atoms in protein ligand complex
The max of atomic reaction field energy of all atoms in protein
The max of the change of atomic reaction field energy of C atoms in protein ligand complex
The max of the change of atomic reaction field energy of all atoms in protein
The min of atomic Coulombic energy of C atoms in protein
The average of the atomic area change of O atoms in protein ligand complex
The sum of atomic reaction field energy of all atoms in protein

Table S7: The most important 50 features in the learning to rank algorithm for the five-fold cross validation on the training set ( $N = 3589$ ).

Feature
Volume change
Electrostatics binding free energy
van der Waals interaction between C and O atoms
van der Waals interaction between C and S atoms
van der Waals interaction between C and N atoms
van der Waals interaction between C and C atoms
The max of atomic area change of C atoms in ligand
van der Waals interaction between C and P atoms
The sum of atomic area change of all atoms in ligand
The sum of Coulombic energy of S atoms in ligand
The max of atomic area change of C atoms in protein
van der Waals interaction between S and O atoms
The average of atomic area change of all atoms in ligand
The max of atomic area change of all atoms in protein ligand complex
The max of atomic area change of N atoms in protein ligand complex
van der Waals interaction between N and O atoms
The max of atomic area change of N atoms in protein
The min of reaction field energy change of N atoms in protein
The sum of atomic area change of N atoms in ligand
van der Waals interaction between N and N atoms
van der Waals interaction between O and S atoms
The min of atomic reaction field energy of C atoms in protein
The average change of atomic area of C atoms in ligand
The sum of atomic area change of C atoms in protein
The max of atomic reaction field energy of all atoms in protein
The max of atomic area change of O atoms in protein ligand complex
van der Waals interaction between N and P atoms
The sum of atomic area change of N atoms in protein
The average of atomic reaction field energy of all atoms in protein ligand complex
van der Waals interaction between C and N atoms
The max of atomic area change of C atoms in protein ligand complex
The average of atomic area change of N atoms in protein
The min of atomic area change of C atoms in ligand

Table 7 – continued
Feature
The min of atomic reaction field energy of C atoms in ligand
van der Waals interaction between C and S atoms
The average of atomic reaction field energy of all atoms in ligand
The average of atomic area change of N atoms in protein ligand complex
The max of atomic area change of C atoms in protein
The average of atomic area change of C atoms in ligand
The sum of atomic area change of C atoms in ligand
The min of atomic area change of N atoms in protein
van der Waals interaction between N and S atoms
The sum of atomic area change of C atoms in protein ligand complex
The sum of atomic reaction field energy of S atoms in protein ligand complex
The min of the change of atomic reaction field energy of C atoms in protein
The sum of atomic area change of O atoms in protein
The min of atomic area change of O atoms in ligand
The min of the change of the reaction field energy of N atoms in protein ligand complex
The max of atomic Coulombic energy of all atoms in ligand
The sum of atomic reaction field energy of all atoms in ligand

Table S8: The most important 50 features in the learning to rank algorithm for the blind prediction of the benchmark set ( $N = 100$ ). The method was trained on the training set ( $N = 3589$ ) excluding the benchmark set ( $N = 100$ ).

Feature
Volume change
Electrostatics binding free energy
van der Waals interaction between C and S atoms
van der Waals interaction between C and C atoms
The max of atomic area change of all atoms in protein ligand complex
The max of atomic area change of O atoms in protein ligand complex
The max of atomic area change of C atoms in ligand
The min of atomic reaction field energy of C atoms in ligand
van der Waals interaction between C and O atoms
van der Waals interaction between S and O atoms
The max of atomic area change of N atoms in protein
The min of atomic Coulombic energy of all atoms in ligand
van der Waals interaction between N and O atoms
The min of atomic reaction field energy of C atoms in protein
van der Waals interaction between N and S atoms
The average of atomic reaction field energy change of all atoms in protein
The sum of atomic area change of N atoms in ligand
van der Waals interaction between N and N atoms
The max of atomic area change of C atoms in protein
The max of atomic area change of all atoms in protein
van der Waals interaction between C and P atoms
The min of atomic area change of all atoms in protein ligand complex
The average of atomic reaction field energy of all atoms in ligand
van der Waals interaction between O and S atoms
The sum of atomic Coulombic energy of S atomic in ligand
van der Waals interaction between N and P atoms
The sum of atomic area change of C atoms in protein
The sum of atomic area change of N atoms in protein ligand complex
The sum of atomic area change of all atoms in ligand
The max of the atomic reaction field energy change of C atoms in protein ligand complex
The max of atomic area change of C atoms in protein
The max of atomic reaction field energy change of O atoms in protein ligand complex
The max of atomic reaction field energy change of N atoms in ligand
The average of atomic area change of all atoms in ligand

**Table 8 – continued**

Feature
The sum of atomic reaction field energy change of C atoms in ligand
van der Waals interaction of C and N atoms
The sum of atomic area change of C atoms in ligand
The sum of atomic area change of C atoms in protein
The max of atomic Coulombic energy of C atoms in ligand
van der Waals interaction of C and S atoms
The min of atomic Coulombic energy of N atoms in protein
The min of atomic Coulombic energy of all atoms in protein
The max of atomic Coulombic energy of C atoms in protein
The max of atomic reaction field energy of O atoms in ligand
The sum of atomic area change of O atoms in protein ligand complex
The average of atomic area change of O atoms in ligand
The min of atomic area change of C atoms in protein
The sum of atomic area change of N atoms in protein
The sum of atomic area change of O atoms in protein
The max of atomic Coulombic energy of N atoms in ligand

Table S9: The most important 50 features in the learning to rank algorithm for the blind prediction of the PDBBind v2007 core set ( $N = 195$ ). The method was trained on the training set ( $N = 3589$ ) excluding the PDBBind v2007 core set ( $N = 195$ ).

Feature
Electrostatics binding free energy
Volume change
van der Waals interaction between C and O atoms
The max of atomic area change of all atoms in protein ligand complex
van der Waals interaction between C and C atoms
van der Waals interaction between N and N atoms
The max of atomic area change of C atoms in protein ligand complex
The max of atomic area change of N atoms in protein
The sum of atomic area change of C atoms in protein
The sum of atomic area change of O atoms in protein
van der Waals interaction between C and N atoms
The max of atomic area change of O atoms in protein ligand complex
The average of atomic area change of all atoms in protein ligand complex
The max of atomic reaction field energy of all atoms in protein ligand complex
The sum of atomic area change of N atoms in protein
The min of atomic reaction field energy change of O atoms in protein
The sum of atomic Coulombic energy of S atoms in ligand
van der Waals interaction between S and O atoms
The sum of atomic area change of C atoms in ligand
van der Waals interaction between N and S atoms
van der Waals interaction between C and P atoms
The average of reaction field energy of all atoms in protein ligand complex
The sum of atomic area change of N atoms in protein
The average of atomic reaction field energy of all atoms in ligand
The average of atomic area change of C atoms in protein
The min of atomic Coulombic energy of all atoms in protein
The max of atomic reaction field energy change of C atoms in protein ligand complex
The sum of the atomic area change of O atoms in protein ligand complex
The average of the atomic reaction field energy change of C atoms in ligand
The max of the atomic reaction field energy of O atoms in protein
The sum of atomic area change of N atoms in protein ligand complex
The average of atomic area change of C atoms in ligand
van der Waals interaction between C and S atoms
The min of the atomic reaction field energy of C atoms in protein ligand complex
The max of atomic area change of C atoms in protein

**Table 9 – continued**

Feature
van der Waals interaction between N and O atoms
The min of atomic reaction field energy of C atoms in protein
The max of atomic reaction field energy of all atoms in protein
van der Waals interaction between O and P atoms
The sum of atomic area change of N atoms in ligand
The max of atomic reaction field energy of O atoms in ligand
The average of atomic area change of all atoms in ligand
The sum of atomic Coulombic energy of O atoms in ligand
van der Waals interaction between C and S atoms
The max of atomic area change of O atoms in protein ligand complex
The max of atomic reaction field energy of C atoms in ligand
The min of atomic reaction field energy change of N atoms in protein ligand complex
The max of atomic area change of all atoms in protein
The average of atomic area change of O atoms in ligand
The max of atomic reaction field energy of C atoms in ligand

Table S10: The most important 50 features in the learning to rank algorithm for the blind prediction of the PDBBind v2015 core set ( $N = 195$ ). The method was trained on the training set ( $N = 3589$ ) excluding the PDBBind v2015 core set ( $N = 195$ ).

Feature
Volume change
Electrostatics binding free energy
van der Waals interaction between N and S atoms
The max atomic area change of all atoms in protein ligand complex
The max atomic area change of N atoms in protein
van der Waals interaction between C and O atoms
van der Waals interaction between C and C atoms
The sum of atomic Coulombic energy of S atoms in ligand
van der Waals interaction between C and N atoms
van der Waals interaction between C and S atoms
The max of atomic area change of O atoms in protein ligand complex
The max of atomic area change of C atoms in protein
The max of atomic area change of C atoms in ligand
The sum of atomic area change of C atoms in ligand
The max of atomic area change of C atoms in protein ligand complex
The sum of atomic area change of C atoms in protein
The average of atomic area change of all atoms in ligand
The max of atomic reaction field energy change of all atoms in protein ligand complex.
The min of reaction field energy of C atoms in protein
The average of atomic reaction field energy of all atoms in protein
The max of atomic area change of O atoms in protein
The sum of atomic area change of O atoms in protein ligand complex
The min of atomic reaction field energy of C atoms in protein ligand complex
The max of atomic reaction field energy of O atoms in ligand
The sum of atomic area change of O atoms in protein
The average of atomic area change of C atoms in protein
The min of atomic reaction field energy of N atoms in protein ligand complex
The average of atomic area change of N atoms in protein ligand complex
The average of the reaction field energy change of N atoms in ligand
The max of atomic area change of O atoms in protein ligand complex
The average of atomic area change of C atoms in protein
van der Waals interaction between N and P atoms
van der Waals interaction between N and N atoms
The sum of atomic area change of all atoms in ligand
The sum of atomic reaction field energy of C atoms in ligand
The min of atomic area change of C atoms in protein

**Table 10 – continued**

Feature

The average of atomic area change of O atoms in ligand  
 The average of atomic area change of all atoms in protein ligand complex  
 The sum of atomic reaction field energy of S atoms in protein ligand complex  
 The sum of atomic area change of N atoms in ligand  
 The min of atomic reaction field energy change of N atoms in protein  
 The max of atomic Coulombic energy of all atoms in protein  
 The average of atomic area change of all S atoms in protein  
 van der Waals interaction between C and P atoms  
 The sum of atomic area change of N atoms in ligand  
 The min of atomic area change of all atoms in protein  
 The min of atomic reaction field energy change of O atoms in protein  
 The max of atomic reaction field energy of C atoms in ligand  
 The min of atomic reaction field energy of C atoms in protein  
 van der Waals interaction between O and S atoms