

Assessing the performance of MM/PBSA and MM/GBSA methods. 7. Entropy effects on the performance of end-point binding free energy calculation approaches

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Supporting Information

Table S1. Information of the used dataset.

PDB ID	ΔG_{exp}^a	Seq-length	PDBcode	ΔG_{exp}	Seq-length	PDBcode	ΔG_{exp}	Seq-length
2e27	-12.77	224	1sdv	-11.94	199	2v7d	-9	457
3e64	-9.71	292	1sgu	-7.34	199	2v8w	-9.32	361
3e85	-7.34	155	1sh9	-8.24	199	2v95	-11.34	343
3e92	-10.93	349	1siv	-11.03	199	2vb8	-6.29	809
3e93	-12.09	347	1sld	-8.97	485	2vba	-6.29	809
10gs	-8.74	417	1slg	-5.33	489	2vc9	-11.53	885
11gs	-7.96	417	1sqn	-12.84	249	2vfk	-5.07	206
1a1b	-8.74	210	1sqo	-10.18	246	2vh6	-13.25	287
1a1c	-8.74	210	1sqt	-8.47	246	2vix	-6.77	837
1a30	-5.88	199	1sr7	-13.79	499	2vk2	-9.41	297
1a4k	-10.93	870	1srg	-7.24	465	2vkm	-11.95	390
1a94	-10.73	199	1stc	-11.06	352	2vl4	-8.21	837
1a99	-7.78	683	1str	-6.52	489	2vmf	-8	836
1a9m	-9.46	199	1sts	-6.83	489	2vnt	-10.93	259
1aaq	-11.47	199	1sv3	-5.94	122	2vo4	-6.74	439
1adl	-7.32	263	1sw2	-9.87	271	2vo5	-6.67	834
1afk	-9.04	125	1swg	-10.05	464	2vot	-9.76	838
1ai4	-3.42	764	1swr	-9.45	472	2vqt	-8.2	837
1ai7	-5.58	764	1syh	-8.75	519	2vr4	-7.76	837
1aid	-6.59	199	1t4v	-10.49	276	2vt3	-5.68	394
1aj6	-8.09	195	1t5f	-5.77	943	2vvc	-11.64	286
1aj7	-5.29	432	1t7d	-8.23	209	2vvp	-4.64	315
1ajp	-3.05	764	1t7j	-11.88	199	2vvu	-11.06	288
1ajq	-5.89	764	1tew	-8.22	199	2vvv	-11.23	289
1ajv	-10.54	199	1tcx	-9.49	199	2vw5	-11.64	215
1ajx	-10.81	199	1td7	-5.96	120	2vwc	-9.04	215
1alw	-8.91	347	1tng	-4	224	2vwm	-9.61	285
1amw	-6.2	427	1tog	-4.4	791	2vwn	-10.93	281
1apv	-12.29	324	1toi	-5.53	791	2vx9	-10.17	757
1apw	-10.93	324	1toj	-4.63	791	2vxn	-6.83	499
1ax0	-4.27	479	1tok	-3.37	791	2vyt	-3.74	215
1axz	-4.37	240	1tom	-11.34	277	2vzr	-5.85	126
1b05	-9.73	518	1tpw	-4.51	491	2w26	-12.84	286
1b0h	-9.15	518	1trd	-7.37	527	2w47	-6.8	136

1b1h	-9.61	518	1tuf	-5.53	867	2w4x	-6.63	580
1b2h	-6.2	518	1tx7	-6.29	224	2w5g	-8.29	125
1b32	-9.7	518	1tys	-7.49	527	2w5i	-6.2	124
1b3f	-9.41	518	1u1b	-10.65	125	2w66	-5.53	648
1b3g	-9.15	518	1u1w	-8	558	2w67	-6.77	643
1b3h	-8.48	518	1u33	-6.29	496	2w7y	-8.31	381
1b3l	-8.04	518	1ua4	-5.77	455	2w87	-6.36	140
1b40	-9.94	518	1ucn	-7.13	907	2w8j	-4.04	799
1b46	-7.22	518	1ugp	-3.94	428	2w8w	-2.9	797
1b4h	-7.46	518	1ugw	-4.22	599	2w8y	-12.41	252
1b4z	-7.14	518	1ugx	-8.07	593	2wb5	-12.47	586
1b51	-10.06	518	1ui0	-9.64	193	2wca	-7.65	579
1b52	-9.72	516	1uj5	-4.17	226	2web	-6.99	647
1b58	-9	518	1uj6	-4.17	222	2wec	-5.41	647
1b5h	-8.21	518	1uou	-10.52	877	2wed	-8.33	647
1b5i	-9.62	518	1upf	-6.29	897	2weq	-8.05	427
1b5j	-10.15	518	1ur9	-7.88	996	2wer	-9.62	429
1b6h	-10.69	518	lurg	-7.96	374	2whp	-5.46	531
1b6j	-10.82	195	1usi	-9.21	693	2wk2	-9.32	540
1b6k	-11.95	195	lutc	-6.22	353	2wk6	-4.53	895
1b6l	-11.34	195	lutj	-5.25	223	2wky	-11.73	509
1b6m	-11.47	195	lutm	-4.11	223	2wl0	-10.65	199
1b7h	-10.96	518	luto	-3.11	224	2wly	-9.02	540
1b9j	-8.14	518	1uvt	-10.43	273	2wlz	-6.29	539
1bcu	-4.47	276	luz1	-9.41	440	2wm0	-6.18	539
1bdq	-8.66	199	luz4	-4.64	411	2wq5	-5.12	358
1bgq	-11.7	429	luz8	-6.77	431	2wqp	-7.52	679
1bhx	-9.34	283	1v0k	-6.96	303	2wtv	-11.95	263
1bjv	-7.56	224	1v0l	-10.32	303	2wtx	-3.94	895
1bq4	-7.13	939	1v2k	-8.45	224	2wuf	-5.86	565
1br6	-4.4	269	1v2n	-8.06	224	2wvt	-8.36	878
1bv7	-12.71	199	1v2q	-5.65	224	2wvz	-5.49	739
1bv9	-13.6	199	1v2r	-4.86	224	2wyg	-11.88	281
1bwa	-11.75	199	1v2s	-5.69	224	2wyj	-12.29	283
1bxo	-13.66	326	1v2t	-6.43	224	2wzm	-7.13	275
1bxq	-10.08	324	1v2u	-4.6	224	2wzs	-5.26	737
1byk	-6.83	511	1v2w	-5.48	224	2x09	-5.13	852
1bzc	-6.72	298	1vja	-10.52	248	2x4z	-11.7	292
1bjz	-6.36	298	1vjj	-7.88	676	2xab	-12.66	210
1c3x	-5.02	799	1vso	-6.45	487	2xb7	-12.55	287
1c4u	-14.16	283	1vwn	-7.96	485	2xba	-10.42	285
1c4v	-14.75	289	1vyf	-10.99	136	2xbw	-10.93	287
1c5n	-6.42	289	1vyq	-7.24	424	2xc4	-10.99	289
1c5q	-8.68	224	1w0z	-10.49	248	2xde	-7.47	138
1c5s	-8.2	224	1w11	-11.23	248	2xdk	-4.92	216
1c5t	-5.6	224	1w13	-11.88	248	2xdl	-4.24	417
1c5x	-9.12	249	1w2g	-6.24	403	2xht	-8.14	214
1c5y	-5.74	249	1w3j	-8.63	444	2xjg	-10.69	214
1c5z	-5.48	246	1w3k	-5.88	301	2xjj	-8.89	209
1c70	-14.07	199	1w3l	-8.58	301	2xjx	-12.5	222
1c83	-6.63	298	1w4q	-7.18	125	2xmy	-13.6	296
1c84	-6.84	298	1w5w	-12.02	199	2xnb	-9.33	297
1c86	-6.42	297	1w5x	-11.47	199	2ypi	-6.59	495
1c87	-5.74	298	1w6y	-7.32	253	2yxj	-12.71	138
1c88	-7.23	298	1w7x	-11.47	303	2z4b	-12.78	446
1ce5	-6.47	224	1w96	-11.49	550	2z4o	-13.07	199
1cea	-6.77	161	1w9u	-8.32	396	2za5	-11.52	973
1ceb	-8.2	81	1w9v	-8.66	396	2zaz	-8.74	346

ld3d	-12.42	279	lwcq	-8.55	602	2zb0	-9.04	350
ld3p	-10.09	279	lwdn	-8.61	224	2zb1	-8.63	346
ld4h	-13.66	199	lwei	-12.29	221	2zc9	-9.21	280
ld4j	-11.42	199	lwht	-5.05	819	2zcs	-11.23	285
ld4k	-12.6	195	lwm1	-8.61	314	2zda	-11.47	281
ld4l	-11.98	195	lws1	-13.05	152	2zdk	-8.7	224
ld4p	-8.61	279	lws4	-4.1	599	2zdl	-8.74	224
ld4y	-15.16	199	lws5	-4.14	599	2zdm	-8.76	224
ld6v	-8.43	433	lwwj	-9.2	525	2zdn	-8.54	224
ld6w	-8.14	279	lx1z	-15.1	217	2zfp	-7.06	280
ld7j	-4.51	108	lx38	-11.98	603	2zfs	-8.94	224
ldb1	-12.65	251	lx39	-12.6	603	2zft	-8.91	224
ldet	-5.88	104	lx8d	-3.02	209	2zhd	-8.94	224
ldfo	-9.15	834	lx8j	-9.51	687	2zif	-5.96	483
ldhi	-9.92	319	lx8r	-8.37	428	2zjw	-10.52	333
ldhj	-8.95	319	lx8t	-10.65	428	2zm3	-8.49	301
ldif	-14.56	199	lx9d	-5.41	453	2zn7	-10.77	298
ldqx	-15.09	535	lxa5	-8.88	145	2zo3	-13.66	278
ldrj	-10.11	272	lxap	-11.88	233	2zpk	-10.6	419
ldrk	-9.32	272	lxbo	-8.25	300	2zq1	-9.05	224
ldud	-6.59	409	lxd0	-9.73	496	2zq2	-8.96	224
ldy4	-5.95	434	lxff	-6.59	478	2zy1	-10.11	280
ldzk	-8.33	149	lxgi	-6.63	359	2zym	-8.38	382
le1x	-8.04	291	lxgj	-8.2	352	2zz1	-6.2	431
le2k	-6.75	625	lxh4	-10.2	335	3a1t	-6.6	259
le2l	-5.86	615	lxh5	-7.47	336	3a2o	-12.4	199
le3v	-5.93	258	lxh6	-10	332	3a5y	-10.87	608
le4h	-11.49	465	lxhy	-8.44	519	3aaq	-4.51	350
le5j	-5.46	303	lxk5	-8.2	205	3acw	-6.5	285
lebw	-12.36	199	lxka	-9.4	326	3acx	-7.78	285
leby	-13.25	199	lxkk	-11.64	290	3ads	-6.85	514
lebz	-12.84	199	lxow	-12.68	244	3adv	-4.14	520
lec0	-11.6	199	lxr8	-9.15	376	3ag9	-10.99	318
lec1	-12.19	199	lxr9	-9.77	376	3agl	-10.65	339
lec2	-13.66	199	lxzx	-13.96	250	3aid	-9.38	199
lec3	-12.34	199	ly0l	-12.29	443	3b2q	-6.22	868
lecv	-6.63	298	ly1z	-4.21	283	3b3x	-4.92	511
lefy	-11.23	351	ly20	-7.27	288	3b50	-10.32	311
legh	-7.78	911	ly3n	-7.59	491	3b5j	-7.76	244
leix	-15.1	463	ly6q	-15.98	467	3b5r	-11.98	248
lejn	-7.68	248	ly6r	-13.82	467	3b65	-12.66	248
lela	-8.68	241	lyc1	-8.42	211	3b66	-11.75	248
lelb	-9.77	241	lydk	-8.04	427	3b67	-12.09	248
lelc	-9.09	241	lydr	-7.54	355	3b68	-11.47	248
leld	-9.15	241	lyds	-8.09	355	3b7j	-7.06	906
lele	-9.36	241	lydt	-10	355	3b9g	-6.45	634
lelr	-6.77	129	lyon	-5.76	293	3bbb	-9.56	901
lent	-9.51	331	lyqj	-11.11	357	3bc3	-9.3	215
lerb	-11.06	175	lyvm	-8.74	263	3bc4	-7.3	199
lez9	-6.96	371	lz1h	-11.47	195	3be9	-10.41	328
lezq	-12.36	286	lz1r	-12.6	195	3bex	-7.61	497
lf0r	-10.46	286	lz3t	-5.38	431	3bfu	-8.57	525
lf0t	-8.2	224	lz3v	-5.62	431	3bgb	-8.26	199
lf4e	-4.04	527	lz6e	-13.28	287	3bgc	-6.85	199
lf4f	-6.31	522	lz6s	-5.92	125	3bgq	-10.87	273
lf4g	-8.85	520	lz71	-12.54	277	3bgs	-12.87	859
lf4x	-7.63	427	lzc9	-4.4	432	3bgz	-8.55	268
lf5k	-5.12	248	lzea	-7.13	426	3bra	-3.69	371

1f5l	-7.21	246	1zgi	-7.29	277	3brn	-11.88	154
1fao	-10.06	101	1zhy	-8.91	437	3bu1	-11.13	145
1fch	-9.77	303	1zky	-8.54	479	3buh	-5	371
1fcy	-11.64	237	1zlv	-8.41	853	3bv9	-7.32	289
1fcz	-12.6	236	1zog	-9.77	651	3bva	-8.91	199
1fd0	-11.47	236	1zoh	-9.56	653	3bvb	-7.51	199
1fdq	-9.93	132	1zp8	-11.98	199	3bwj	-8.87	339
1fh8	-9.41	313	1zpa	-11.47	199	3bxo	-7.48	502
1fh9	-8.79	313	1zsf	-13.55	197	3bxf	-7.57	499
1fhd	-9.32	313	1zsr	-13.42	197	3bxg	-6.77	501
1fj4	-6.26	807	220l	-4.64	163	3bxh	-5.5	502
1fjs	-13.6	287	2a4m	-6.18	663	3bze	-8.2	374
1fkb	-13.25	108	2a5b	-5.37	497	3bzf	-6.18	374
1fkg	-10.93	108	2a5c	-6.31	493	3c1k	-12.9	277
1fki	-9.56	215	2a8g	-5.04	485	3c4h	-7.78	358
1fkn	-12.02	392	2aac	-3.04	327	3cf8	-6.69	902
1fl3	-9.28	423	2am4	-5.08	343	3cfn	-6.83	461
1flr	-13.66	436	2aoc	-6.67	199	3cft	-5.73	463
1fm9	-12.29	521	2aoe	-10.41	199	3cj2	-6.63	558
1fpc	-9.56	275	2aog	-8.57	199	3cj4	-8.89	559
1fq5	-11.47	330	2aou	-10.56	287	3cj5	-8.66	563
1fzk	-11.47	373	2aov	-9.62	289	3ckb	-4.07	505
1fzo	-10.77	373	2avm	-7.78	199	3ckp	-8.67	380
1fzq	-10.41	177	2avq	-5.99	199	3clp	-5.04	266
1g2k	-10.87	199	2avs	-10.34	199	3cow	-9.43	566
1g2o	-14.42	787	2avv	-12.65	199	3coy	-8.22	560
1g30	-9.36	280	2ayr	-12.69	247	3coz	-7.61	567
1g32	-8.34	280	2azr	-4.97	298	3ctt	-8.67	863
1g3d	-7.59	224	2b07	-8.79	298	3cwk	-9.02	138
1g74	-8.91	132	2b1v	-7.85	475	3cyw	-10.61	199
1g7g	-9.02	298	2b4l	-6.52	269	3cyx	-10.93	199
1g7q	-8.27	374	2b7d	-11.88	498	3d0b	-8.93	209
1g7v	-8.74	285	2baj	-11.47	338	3d0e	-11.47	645
1g85	-7.49	315	2bal	-8.62	338	3d1e	-7.88	733
1g9r	-7.78	272	2bet	-3.78	315	3d1x	-11.83	199
1gaf	-10.93	435	2bfq	-9.41	192	3d1y	-11.23	199
1gai	-10.93	473	2bmk	-7.68	438	3d1z	-12.02	199
1gar	-13.66	400	2boh	-11.64	290	3d20	-11.34	199
1gcz	-7.01	351	2boj	-7.88	457	3d6o	-5.62	125
1ghv	-5.94	287	2bok	-8.95	274	3d6p	-5.12	125
1ghw	-5.74	287	2bpy	-10.11	199	3d6q	-5.14	125
1gi1	-7.47	224	2bq7	-9.63	287	3d78	-10.43	239
1gi7	-6.16	246	2bqv	-10.99	199	3d7b	-5.04	125
1gj6	-9.56	224	2br1	-7.02	273	3d83	-11.42	348
1gj7	-10.77	247	2brb	-6.64	273	3d8z	-4.61	125
1gj8	-9.51	259	2bt9	-8.46	267	3da9	-7.52	279
1gja	-7.4	259	2bvd	-8.2	277	3dhv	-4.04	499
1gjb	-8.67	247	2bvr	-5.05	280	3djk	-14.46	199
1gjc	-8.67	247	2bz6	-9.69	308	3djo	-6	249
1gid	-7.13	259	2bza	-3.83	224	3djp	-5.74	249
1gni	-11.02	583	2c1p	-7.37	436	3djv	-6.22	249
1gnm	-8.54	199	2c3j	-8.44	258	3dix	-3.83	249
1gnn	-7.76	199	2c3l	-6.92	266	3dk1	-13.31	199
1gno	-10.52	199	2c80	-7.28	417	3dkf	-11.7	210
1gpk	-7.33	530	2c92	-7.75	735	3dkg	-6.83	282
1gpn	-8.85	530	2c94	-9.32	731	3dnd	-6.55	335
1gt1	-8.2	315	2c97	-8.39	734	3dne	-7.13	337
1gt3	-8.82	316	2ca8	-6.36	417	3dnj	-9.32	82

lgt4	-8.91	316	2cbj	-11.29	586	3dp9	-13.23	460
lgt5	-8.33	316	2cbu	-7.76	441	3drf	-9.56	540
lgvw	-9.51	329	2cbv	-7.49	444	3drg	-9.56	563
lgvx	-9.87	329	2ce9	-8.24	675	3dri	-6.04	560
lgwv	-3.51	288	2cej	-11.77	199	3dsz	-10.61	173
lgyx	-3.39	153	2cen	-11.34	199	3dvp	-6.83	171
lgyy	-4.97	153	2ceq	-9.94	490	3dzt	-9.86	299
lgz9	-4.79	240	2ces	-9.91	441	3e3c	-7.68	237
lgzc	-4.77	240	2cet	-10.95	436	3e5a	-11.24	298
lh0a	-7.44	159	2cgf	-8.75	425	3e5u	-8	440
lh1p	-6.72	555	2cgr	-9.94	434	3e6y	-7.65	467
lh1s	-11.23	555	2cji	-11.23	287	3eb1	-6.54	284
lh22	-12.43	530	2csn	-6.02	587	3ebl	-8.61	324
lh23	-11.4	529	2d0k	-6.86	160	3ed0	-8.67	904
lh2t	-10.77	851	2d3u	-9.45	559	3eeb	-8.04	206
lh46	-4.87	431	2d3z	-9.07	561	3efs	-7.29	252
lh4w	-6.36	225	2drc	-13.5	319	3eko	-9.15	218
lh5v	-5.37	302	2dri	-9.41	272	3ekr	-10.28	218
lh6h	-7.24	144	2e2p	-6.48	596	3eks	-7.78	375
lh9z	-7.4	584	2e2r	-11.28	457	3eqr	-11.88	271
lha2	-7.56	584	2e7f	-8.34	525	3ew2	-9.11	236
lhbv	-8.7	199	2er6	-9.87	331	3eys	-7.54	434
lhi4	-6.14	136	2er9	-10.11	331	3f3t	-6.26	262
lhi5	-5.51	136	2erz	-7.73	355	3f3u	-6.48	262
lhii	-9.94	199	2euk	-9.02	205	3f68	-6.91	277
lhk4	-7.25	583	2eum	-9.15	206	3f78	-4.23	181
lhmr	-8.95	132	2evl	-9.15	206	3f80	-5.77	940
lhms	-8.7	132	2ewa	-10.85	331	3f82	-11.39	279
lhn2	-8.2	315	2exm	-5.61	299	3f8c	-10.49	207
lhnn	-8.52	262	2flg	-10.3	221	3f8f	-9.05	226
lhos	-11.68	199	2f34	-9.41	252	3fat	-10.44	518
lhp0	-9.15	642	2f35	-7.38	252	3ffg	-12.4	287
lhpo	-12.6	199	2f5t	-7.06	467	3fj7	-5.07	463
lhps	-12.6	199	2f80	-11.17	199	3fjg	-5.09	463
lhpv	-12.6	199	2f8g	-11.88	199	3fjz	-5.53	428
lhpx	-15.38	199	2fai	-8.53	476	3fk1	-3.57	428
lhqg	-4.1	940	2fdp	-10.36	374	3fl5	-9.95	325
lhsh	-12.87	199	2ffl	-11.21	631	3fqe	-11.34	270
lhvi	-14.92	199	2fgi	-10.03	547	3fql	-9.77	561
lhvj	-15.57	199	2fgu	-12.54	199	3fur	-10.93	257
lhvk	-14.97	199	2fgv	-8.36	199	3fv3	-13.01	340
lhvl	-13.59	199	2fle	-10.73	199	3fvh	-8.67	234
lhvr	-12.99	197	2flr	-8.33	502	3fwv	-7.7	129
lhvs	-14.07	199	2fpz	-5.41	973	3g08	-11.15	360
lhwr	-11.38	199	2fqo	-8.79	309	3g0i	-4.92	771
lhxb	-13.55	199	2fmt	-8.39	309	3g0w	-13.01	250
lhxw	-14.79	199	2fqw	-9.12	317	3g19	-9.11	85
li00	-8.66	557	2fqx	-9.77	317	3g2h	-5.22	807
li5r	-11.64	571	2fgy	-8.97	317	3g2i	-6.64	810
li7z	-8.74	440	2fr3	-11.88	138	3g2j	-6.48	810
li80	-8.75	792	2fvd	-11.64	285	3g2k	-6.55	810
li8i	-10.46	226	2fxs	-8.28	214	3g2l	-5.28	810
licj	-3.04	505	2fxu	-11.14	361	3g2n	-5.59	816
ligj	-13.66	867	2fxv	-7.3	381	3g30	-3.43	263
lii5	-9.04	443	2g5u	-11.6	455	3g31	-3.94	263
liih	-3.94	499	2g70	-10.61	262	3g34	-4.04	263
liiq	-10.22	199	2g71	-10.18	262	3g35	-6.39	260
lik4	-10.12	911	2g72	-8.88	265	3g3r	-8.85	287

lis0	-9.56	103	2g78	-9.45	138	3g5d	-10.87	257
lizh	-10.52	199	2g79	-9.45	138	3g90	-8.68	346
lj01	-8.84	313	2g8r	-5.45	125	3g9l	-8.37	337
lj14	-6.14	224	2g94	-13.01	390	3ga5	-7.51	306
lj16	-5.25	224	2gek	-10.28	362	3gba	-12.39	258
lj17	-7.13	224	2gfd	-8.58	433	3gbb	-9.42	256
lj4r	-10.55	108	2gj5	-11.37	162	3gbe	-6.83	559
ljak	-7.61	500	2gl0	-6.59	977	3gcp	-10.69	338
ljet	-9.91	518	2glp	-6.85	906	3gcq	-8.83	338
ljeu	-9.32	518	2gss	-6.75	417	3gcs	-9.91	332
ljev	-9.41	518	2gst	-8.29	435	3gcu	-9.26	677
ljfh	-2.79	496	2gv7	-10.73	242	3gcv	-9.74	339
ljgl	-11.88	420	2gvj	-13.01	926	3ggt	-11.52	199
ljlr	-4.55	941	2gvv	-5.33	310	3ggv	-13.35	199
ljmf	-7.88	633	2gz2	-7.13	719	3gi4	-14.75	199
ljmg	-8.29	633	2h4g	-8.91	298	3gi5	-15.33	199
ljmi	-8.28	643	2h4k	-7.51	298	3gi6	-15.33	199
ljqd	-7.05	287	2hb1	-5.19	298	3gjw	-11.34	351
ljqe	-8.8	281	2hb3	-15.5	199	3gk1	-5.6	177
ljqy	-6.72	516	2hhn	-10.24	218	3gkz	-10.93	234
ljsv	-7.78	289	2hjb	-6	947	3gm0	-10.61	238
ljwt	-10.73	300	2hkf	-8.71	430	3gnw	-12.43	561
ljqy	-11.88	193	2hr6	-6.59	412	3gpo	-7.24	159
ljys	-4.81	453	2hrm	-4.86	412	3gqz	-2.97	359
lkl1	-8.99	224	2hs1	-11.59	199	3gr2	-3.45	359
lklj	-10.32	224	2hs2	-11.35	199	3gs6	-9	323
lkl1	-9.43	224	2hw2	-4.06	139	3gsg	-3.69	359
lklm	-10.11	224	2hxm	-7.13	224	3gsm	-8.85	325
lkl1n	-9.31	224	2hzi	-8.97	672	3gss	-7.96	417
lkl1y	-4.4	637	2hzy	-10.09	835	3gst	-9.18	435
lk21	-11.44	277	2i0a	-15.57	199	3gtc	-3.21	359
lk22	-11.47	281	2i0g	-13.28	444	3gus	-8.26	418
lk27	-12.29	811	2i4d	-15.95	199	3gv9	-2.9	359
lkav	-7.96	298	2i4j	-8.42	541	3gvb	-3.53	359
lkdk	-12.36	355	2i4u	-15.8	199	3gx0	-4.76	409
lkel	-9.95	436	2i4v	-15.3	199	3gy2	-7.85	224
lkpm	-7.92	122	2i4w	-15.83	199	3gy4	-6.96	224
lkv1	-8.11	332	2i4z	-7.79	541	3gy7	-6.18	224
lkv5	-5.77	499	2i80	-7.37	693	3h30	-6.19	334
lkyv	-8.09	743	2idw	-12.14	199	3h5b	-13.67	199
lkzk	-14.19	199	2ieo	-11.6	199	3h78	-5.8	666
lkzn	-12.19	187	2ihj	-6.27	379	3h89	-10.43	216
ll2s	-6.26	356	2ihq	-11.6	249	3h8b	-8.59	216
ll83	-4.64	163	2imd	-11.34	395	3h8c	-10.55	215
llaf	-10.73	239	2itk	-10.51	146	3hb4	-12.36	569
llag	-8.61	239	2iuz	-7.59	396	3hcm	-4.51	182
llah	-10.28	239	2ivu	-8.78	552	3hec	-6.1	330
llbf	-10.73	248	2iwx	-9.12	215	3heg	-9.21	334
llbk	-4.34	417	2iyf	-5.12	385	3hek	-11.29	444
llce	-10.58	332	2izl	-8.2	487	3hit	-11.19	258
llf2	-10.28	330	2j27	-4.81	499	3hjo	-8.91	419
lli2	-5.52	163	2j2u	-10.01	282	3hkw	-11.8	562
lli3	-5.81	163	2j34	-10.69	287	3hky	-9.69	565
lli6	-5.19	163	2j47	-7.39	573	3hl7	-10.43	337
llke	-10.27	158	2j4g	-9.02	587	3hll	-11.25	338
llkk	-9.36	106	2j62	-15.49	586	3hmo	-10.27	258
llkl	-7.94	105	2j75	-9.08	439	3hrf	-6.81	285
llol	-8.72	206	2j77	-6.68	437	3hub	-11.05	336

lloq	-5.05	417	2j78	-8.76	444	3huc	-8.18	338
llor	-15.1	419	2j79	-8.14	438	3hv7	-10.82	331
llpg	-9.68	235	2j7b	-9.04	438	3hv8	-9.54	243
llpz	-10.38	235	2j7d	-9.74	438	3hx3	-10.93	246
llyb	-15.6	677	2j7e	-10	437	3hxi	-8.64	197
llyx	-6.2	493	2j7f	-8.68	436	3i25	-11.62	374
lm0b	-12.04	199	2j7g	-9.56	438	3i4b	-11.14	707
lm13	-10.34	274	2j7h	-9.82	439	3i6o	-14.13	199
lm2p	-8.34	326	2j94	-8.57	287	3i73	-7.5	513
lm2q	-8.33	328	2j95	-11.47	287	3i7e	-14.83	199
lm2r	-8.82	328	2jdh	-8.89	457	3ie3	-9.12	418
lm4h	-13.01	392	2jdk	-8.93	457	3ies	-13.55	432
lm6p	-6.96	293	2jdm	-7.38	457	3ifl	-11.03	433
lm7d	-8.51	436	2jdn	-7.59	457	3ifo	-9.92	435
lm7i	-7.37	436	2jdp	-9.02	457	3ilq	-7.11	361
lm7y	-14.97	849	2jds	-11.2	355	3imc	-4.04	563
lmes	-10.52	199	2jdu	-9.18	457	3ime	-4.1	556
lmfa	-6.89	231	2jdv	-11.2	355	3iob	-4.67	563
lmh5	-12.59	370	2jdy	-5.97	457	3ioc	-5.02	548
lmhw	-10.04	215	2jf4	-11.14	487	3iod	-5.6	549
lmjj	-11.94	429	2jfh	-4.18	431	3ioe	-4.46	567
lmoq	-4.72	733	2jfb	-7.15	505	3ioi	-8.57	549
lmq5	-12.29	285	2jg0	-10.69	508	3iok	-10.87	286
lmq6	-15.24	285	2jh0	-11.88	280	3ip8	-3.12	233
lmrx	-9.92	199	2jh5	-8.79	279	3ipq	-10.34	471
lmsm	-14.32	199	2jh6	-10.61	280	3ipu	-10	504
lmsn	-12.42	199	2jiw	-6.26	591	3iqh	-6.27	310
lmtr	-11.47	195	2jj3	-13.05	452	3iqi	-6.03	310
lmu8	-12.29	277	2jkh	-10.99	289	3isj	-5.02	288
ln1t	-5.26	629	2jkp	-5.78	688	3iss	-8.26	419
ln3i	-12.14	787	2jxr	-9.62	330	3iub	-6.2	565
ln46	-14.37	488	2nmy	-11.43	199	3iue	-7.96	567
ln4h	-8.95	245	2nmz	-11.43	199	3ivc	-5.63	576
ln4k	-13.72	293	2nn8	-4.9	139	3ivg	-5.88	563
lncl	-8.37	467	2nnd	-8.28	149	3ivx	-7.85	564
lncl	-8.37	467	2nnd	-8.28	149	3ivx	-7.85	564
lncl	-8.37	467	2nnd	-8.28	149	3ivx	-7.85	564
ln3	-6.83	466	2nnp	-11.43	199	3iw5	-8.3	337
lnf8	-10.69	415	2nt7	-8.91	298	3iw6	-7.49	338
lnfu	-10.58	287	2nta	-6.55	298	3iw7	-7.7	336
lnfx	-11.64	288	2o0u	-7.51	332	3iw8	-6.66	335
lnfy	-12.14	288	2o1c	-6.45	148	3jdw	-4.91	721
lnh0	-13.31	199	2o2u	-8.74	320	3jrs	-5.85	175
lnhu	-7.73	559	2o4j	-13.79	241	3jrx	-12.29	497
lnja	-8.62	643	2o4k	-14.28	199	3juo	-6.92	314
lnjc	-7.59	643	2o4n	-10.69	199	3jup	-7.62	315
lnjd	-7.61	633	2o4p	-14.65	199	3jvk	-5.37	129
lnje	-5.19	633	2o4r	-12.84	241	3jvr	-7.82	259
lnjs	-10.69	201	2o4s	-14.35	199	3jvs	-8.93	257
lnl9	-8.14	284	2ogy	-6.12	525	3jy9	-12.29	283
lnli	-4.9	249	2ojg	-7.7	338	3jyj	-7.85	114
lnm6	-13.72	277	2ojj	-11.88	345	3jyr	-7.56	371
lnny	-10.46	284	2ok1	-8.55	334	3jzg	-5.42	360
lno6	-6.02	284	2olb	-7.56	518	3jzj	-4.93	389
lnq7	-9.28	245	2on6	-9.24	847	3k00	-7.88	389
lnu3	-5.46	285	2oxd	-9.32	326	3k02	-6.83	389
lnvr	-11.08	265	2oxn	-10.17	334	3k4q	-7.29	439
lnvs	-10.69	265	2oxx	-9.15	326	3k5v	-8.61	287
lnw5	-7.12	271	2oxy	-8.91	328	3k8o	-15.12	851
lnz7	-9.72	284	2oyk	-7.24	435	3k8q	-15.41	859

lo0f	-7.24	125	2oyl	-8.61	435	3k97	-10.93	211
lo0h	-8.09	125	2oym	-6.83	435	3k99	-9.87	219
lo0m	-7.03	125	2p15	-14.07	485	3kdb	-13.46	199
lo0n	-5.58	125	2p2a	-8.37	514	3kdc	-12.68	199
lo2h	-9.79	224	2p3a	-10.87	197	3kdm	-9.56	439
lo2j	-9.45	224	2p3b	-11.59	198	3kgp	-3.51	240
lo2n	-8.32	224	2p3i	-4.76	162	3kgt	-7.52	457
lo2o	-8.68	224	2p4j	-12.24	390	3kgu	-8.09	461
lo2q	-10.49	224	2p4y	-12.29	472	3kjd	-11.66	351
lo2s	-7.47	224	2p7a	-8.34	224	3kku	-7.78	216
lo2w	-8	224	2p7g	-8.92	223	3kmx	-6.59	785
lo2z	-8.34	224	2p7z	-8.99	208	3kmy	-6.14	785
lo33	-7.85	224	2p95	-12.79	287	3kqb	-12.71	287
lo3d	-9.74	224	2pbw	-11.28	502	3kqc	-11.83	287
lo3f	-10.87	224	2pfy	-8.91	296	3kqe	-11.05	287
lo3h	-9.97	224	2pk5	-14.61	199	3kv2	-8.59	940
lo3i	-9.97	224	2pk6	-14.87	199	3kyg	-10.2	455
lo3j	-9.25	224	2pmk	-8.09	244	3kyq	-5.77	194
lo3k	-9.25	224	2pog	-13.03	445	3kze	-5.4	274
lo3p	-9.09	247	2pq9	-11.08	428	3l1n	-7.69	153
lo5a	-8.77	247	2pqb	-9.84	446	3l4u	-10.28	865
lo5b	-7.88	246	2pqc	-7.85	446	3l4v	-9.18	864
lo5c	-7.13	247	2pqz	-7.74	199	3l4w	-8.2	864
lo5g	-6.77	284	2psj	-10.52	307	3l4x	-9.41	864
lo7o	-6.14	288	2psu	-10.41	199	3l4y	-9.56	864
lo8b	-3.66	370	2pu2	-6.05	359	3l4z	-9.18	864
lo9d	-7.65	465	2pv1	-9.75	104	3l59	-5.05	391
loar	-10.11	231	2pvh	-9	328	3l5b	-5.34	388
loba	-3.34	339	2pvj	-11.06	327	3l6h	-7.37	255
locq	-7.09	301	2pvl	-10.41	328	3l8s	-9.57	335
lod8	-6.96	303	2pvm	-8.8	328	3lbl	-10.17	95
lody	-11.06	199	2pwc	-8.97	199	3lbz	-5.27	245
loe8	-7.54	410	2pwd	-6.01	558	3lc3	-7.14	293
lofz	-6.31	625	2pwg	-6.59	557	3lcu	-4.81	258
logg	-7.09	995	2pym	-9.32	199	3lcv	-6.48	257
logx	-8.32	253	2pyn	-10.34	199	3le8	-8.29	565
logz	-8	251	2q54	-12.31	199	3lf0	-7.81	313
lohr	-11.88	199	2q55	-11.87	199	3lgs	-6.29	492
loif	-10.55	445	2q5k	-15.44	199	3liw	-10.38	286
loko	-6.2	485	2q6f	-7.44	590	3ljo	-9.05	224
lom1	-9.25	326	2q88	-7.92	258	3lk1	-5.82	177
lony	-9.25	284	2q89	-8.61	258	3lp7	-7.44	940
lonz	-6.96	284	2q8h	-4.1	731	3lpi	-11.64	780
los5	-9.36	564	2q8z	-7.76	652	3lpk	-12.43	780
low4	-7.76	240	2qbp	-11.47	298	3lxo	-6.59	125
lowe	-8.47	246	2qbp	-10.17	298	3lzu	-13.74	199
lowh	-10.11	246	2qbr	-8.64	299	3lzv	-14.46	199
loxr	-7.09	120	2qbs	-9.12	298	3lzz	-5.24	323
loyt	-9.9	278	2qbu	-8.46	457	3m36	-13.42	287
lp19	-5.62	372	2qbw	-9.91	190	3m37	-12.35	287
lp1n	-9.28	517	2qci	-11.39	199	3m89	-8.42	385
lp1o	-7.87	521	2qd6	-11.85	199	3m8u	-6.68	509
lpb8	-7.04	283	2qd7	-12.43	199	3mfv	-3.45	940
lpb9	-4.94	282	2qd8	-12.39	199	3mfw	-4.81	946
lpbq	-8.56	541	2qe4	-10.87	412	3mhw	-3.14	247
lpdz	-5.05	867	2qfo	-6.42	208	3mi2	-10.61	513
lpgp	-7.78	947	2qft	-7.18	428	3miy	-10.49	240
lpme	-12.84	334	2qfu	-5.71	428	3mj1	-10.69	229

lpot	-7.51	323	2qg0	-7.82	415	3moe	-5.88	619
lpph	-8.09	224	2qg2	-7.37	208	3mof	-4.19	625
lppi	-6.85	497	2qhd	-7.34	245	3moh	-3.87	605
lppk	-10.46	324	2qhm	-8.44	269	3ms9	-7.13	266
lppl	-11.68	324	2qhz	-9.94	199	3mss	-6.36	265
lppm	-7.92	324	2qi0	-10.08	199	3mxd	-12.07	199
lpro	-15.44	199	2qi1	-9.97	199	3mxe	-13.68	199
lpu7	-4.23	215	2qi3	-13.93	199	3mxf	-9.99	128
lpu8	-4.23	216	2qi5	-14.83	199	3n3g	-9.89	218
lpxn	-9.77	295	2qm7	-8.04	626	3n7o	-9.76	224
lpxo	-11.88	297	2qm9	-10.61	272	3nee	-7.29	463
lpxp	-9.09	295	2qmg	-12.51	391	3neo	-8.09	461
lpye	-8.76	267	2qmj	-5.75	864	3nes	-7.68	463
lpyn	-7.51	284	2qnn	-9.77	199	3nex	-8.2	465
lpzi	-5.77	516	2qnp	-8.75	199	3nhi	-11.52	296
lpzo	-4.53	264	2qnq	-8.35	199	3nht	-9.57	296
lpzp	-4.52	264	2qpu	-4.92	405	3nkx	-7	458
lq5k	-10.14	690	2qrk	-5.82	366	3npc	-11.39	358
lq72	-9.36	439	2qrl	-5.46	372	3nq3	-5.16	163
lq7a	-9.83	122	2qry	-11.8	305	3nq9	-5.51	163
lq8t	-6.5	359	2qt5	-6.87	195	3nu3	-13.42	199
lq8u	-8.14	362	2qtg	-6.94	492	3nu4	-12.05	199
lq8w	-7.16	355	2qtt	-5.9	494	3nu5	-11.4	199
lqan	-6.12	237	2qu6	-11.64	284	3nu6	-12.71	199
lqaw	-7	750	2qw1	-5.33	306	3nu9	-12.36	199
lqb1	-9.25	224	2r0h	-4.79	637	3nuj	-12.82	199
lqb6	-8.28	224	2r2w	-6.1	248	3o6m	-10.22	435
lqbn	-8	224	2r38	-10.17	199	3o84	-9.89	434
lqbo	-10.58	224	2r3t	-8	199	3obu	-5.88	143
lqbr	-14.44	199	2r3w	-9.42	199	3odu	-11.11	761
lqbs	-12.93	197	2r58	-2.73	213	3ok9	-15.34	199
lqbu	-13.98	199	2r5a	-3.55	213	3oka	-6.45	390
lqbv	-7.36	276	2r5p	-11.59	199	3okc	-6.06	379
lqca	-7.2	634	2r6w	-12.78	453	3okp	-6.45	379
lqft	-11.98	176	2r6y	-12.97	454	3oy8	-5	263
lqhc	-10.34	125	2r9w	-6.96	359	3oyw	-5.61	263
lqi0	-3.21	303	2ra0	-10.65	286	3p2e	-8.5	202
lqiw	-10.58	289	2rcb	-9.27	283	3p5o	-9.97	128
lqka	-8.09	518	2reg	-7.7	291	3p8p	-6.22	276
lqkb	-10.04	518	2rin	-5.46	289	3pb3	-8.5	200
lqkt	-12.34	249	2rk7	-5.53	611	3pd2	-7.47	291
lql7	-6.83	224	2rk8	-4.97	623	3pd3	-6.07	289
lql9	-7.31	224	2rka	-4.1	612	3pd4	-6.12	290
lqxk	-6.89	284	2rkd	-3.72	614	3pd9	-8.5	519
lqy1	-8.91	158	2rke	-5.58	613	3std	-15.18	487
lqy2	-7.85	158	2rkf	-12.4	199	4er1	-9.04	331
lqy5	-9.15	226	2rkm	-5.33	518	4er2	-12.71	331
lr4w	-5.53	443	2sim	-4.67	382	4rsk	-5.91	125
lr6n	-10.11	197	2std	-13.46	487	4std	-14.11	493
lr9l	-7.37	310	2tpi	-5.89	278	4tim	-2.95	499
lrbp	-9.18	176	2uwl	-11.47	287	4ts1	-6.74	629
lrd4	-10.57	185	2uwo	-11.88	285	5er1	-8.22	331
lrdt	-9.15	465	2uxi	-9.97	412	5er2	-8.97	331
lre8	-13.01	338	2uxu	-6.48	412	5std	-14.34	493
lrej	-11.34	334	2uy0	-9.45	199	5tmp	-10.2	211
lrek	-9.15	337	2uy3	-4.4	286	5yas	-4.45	257
lrnt	-7.09	105	2uy4	-6.39	285	6rnt	-3.23	105
lro7	-4.35	965	2uy5	-7.51	287	6std	-11.8	493

1rr6	-14	847	2v00	-5	331	7std	-14.65	493
1s5z	-4.38	901	2v2c	-4.66	499	8a3h	-5.54	301
1s89	-7.15	913	2v2h	-5.15	724			
1sdt	-12.66	199	2v3d	-5.38	497			
1sdu	-13.75	199	2v3u	-4.1	254			

^aExperimental binding free energy estimated from $\Delta G_{\text{bind}}=RT\ln 1/K_i$ or $\Delta G_{\text{bind}}=RT\ln 1/K_d$. T was set to 300 K.

Table S2. Overall accuracy of MM/GBSA results based on various calculation protocols.

ϵ_{in}	ff02	ff03	ff14SB	ff99	ff99SB	ff99SBildn
Enthalpies based on minimized structures (enthalpy_{min})						
1	0.343±0.002	0.379±0.002	0.339±0.002	0.336±0.002	0.339±0.002	0.335±0.003
1.5	0.477±0.002	0.502±0.002	0.477±0.003	0.474±0.002	0.477±0.002	0.474±0.002
2	0.534±0.002	0.551±0.003	0.536±0.002	0.533±0.002	0.536±0.002	0.533±0.002
2.5	0.561±0.002	0.573±0.002	0.563±0.002	0.560±0.004	0.562±0.002	0.561±0.002
3	0.574±0.002	0.583±0.002	0.576±0.002	0.574±0.002	0.576±0.002	0.574±0.002
3.5	0.582±0.003	0.589±0.002	0.584±0.002	0.581±0.003	0.583±0.002	0.582±0.002
4	0.586±0.002	0.593±0.002	0.588±0.002	0.586±0.002	0.588±0.002	0.587±0.002
Enthalpies based on MD trajectories (enthalpy_{md})						
1	0.327±0.002	0.362±0.002	0.325±0.002	0.318±0.003	0.342±0.002	0.318±0.002
1.5	0.449±0.003	0.478±0.002	0.455±0.002	0.447±0.002	0.465±0.003	0.447±0.002
2	0.504±0.002	0.526±0.004	0.513±0.002	0.505±0.004	0.519±0.002	0.505±0.002
2.5	0.531±0.002	0.549±0.002	0.541±0.002	0.533±0.002	0.545±0.002	0.533±0.002
3	0.545±0.002	0.560±0.002	0.555±0.003	0.548±0.002	0.558±0.002	0.548±0.002
3.5	0.553±0.002	0.567±0.002	0.564±0.003	0.556±0.002	0.565±0.003	0.557±0.002
4	0.558±0.002	0.571±0.002	0.569±0.002	0.561±0.002	0.570±0.002	0.562±0.003
Binding free energies based on 9Å-truncated NMEs of the minimized structures ($\Delta G_{\text{nmode_min_9Å}}$)						
1	0.323±0.002	0.375±0.002	0.327±0.002	0.323±0.002	0.324±0.003	0.321±0.002
1.5	0.468±0.002	0.507±0.002	0.478±0.002	0.472±0.002	0.470±0.002	0.469±0.002
2	0.528±0.002	0.555±0.003	0.538±0.002	0.532±0.002	0.527±0.002	0.527±0.004
2.5	0.552±0.002	0.573±0.002	0.562±0.004	0.556±0.002	0.551±0.002	0.551±0.002
3	0.563±0.002	0.582±0.002	0.573±0.003	0.567±0.002	0.561±0.002	0.562±0.002
3.5	0.568±0.002	0.585±0.002	0.578±0.002	0.573±0.002	0.567±0.002	0.567±0.002
4	0.571±0.002	0.587±0.002	0.581±0.002	0.575±0.004	0.569±0.002	0.569±0.002
Binding free energies based on IEs of the MD trajectories ($\Delta G_{\text{interaction_entropy}}$)						
1	0.404±0.002	0.407±0.003	0.394±0.002	0.400±0.002	0.401±0.002	0.389±0.002
1.5	0.497±0.003	0.503±0.002	0.491±0.002	0.496±0.002	0.499±0.002	0.487±0.003
2	0.539±0.002	0.547±0.002	0.538±0.002	0.540±0.003	0.544±0.002	0.533±0.002
2.5	0.558±0.002	0.567±0.002	0.560±0.002	0.560±0.002	0.564±0.002	0.556±0.002
3	0.567±0.002	0.578±0.002	0.572±0.002	0.569±0.002	0.574±0.003	0.568±0.002
3.5	0.572±0.002	0.583±0.002	0.578±0.003	0.574±0.002	0.579±0.002	0.574±0.002
4	0.574±0.002	0.586±0.002	0.581±0.002	0.576±0.002	0.582±0.002	0.577±0.002
Binding free energies based on 9Å-truncated NMEs of the MD trajectories ($\Delta G_{\text{nmode_md_9Å}}$)						
1	-	0.340±0.004	-	-	-	-
1.5	-	0.481±0.002	-	-	-	-
2	-	0.541±0.002	-	-	-	-
2.5	-	0.566±0.002	-	-	-	-

3	-	0.578±0.003	-	-	-	-
3.5	-	0.584±0.002	-	-	-	-
4	-	0.588±0.002	-	-	-	-

The standard deviations were estimated by randomly sampling 80% of the tested dataset for 100 times.

Table S3. Overall accuracy of MM/PBSA results based on various calculation protocols.

ϵ_{in}	enthalpy _{min}	$\Delta G_{nmode_min_9\text{\AA}}$	enthalpy _{md}	$\Delta G_{nmode_md_9\text{\AA}}$	$\Delta G_{interaction_entropy}$
1	-0.060±0.002	-0.089±0.003	0.184±0.003	0.050±0.002	0.285±0.002
2	0.130±0.003	0.084±0.002	0.423±0.002	0.414±0.003	0.479±0.002
4	0.402±0.003	0.349±0.004	0.538±0.002	0.557±0.002	0.561±0.003

The standard deviations were estimated by randomly sampling 80% of the tested dataset for 100 times.

Table S4. Prediction accuracy of MM/GBSA results of kinases based on various calculation protocols.

ϵ_{in}	enthalpy _{min}	enthalpy _{md}	$\Delta G_{interaction_entropy}$	$\Delta G_{nmode_min_9\text{\AA}}$	$\Delta G_{nmode_md_9\text{\AA}}$	$\Delta G_{nmode_md_full_length}$
ff03						
1	0.442±0.008	0.425±0.008	0.359±0.011	0.426±0.008	0.357±0.009	0.392±0.008
1.5	0.466±0.009	0.451±0.009	0.441±0.008	0.445±0.012	0.401±0.008	0.439±0.012
2	0.474±0.008	0.461±0.008	0.474±0.010	0.451±0.008	0.419±0.010	0.456±0.008
2.5	0.479±0.008	0.466±0.008	0.488±0.008	0.453±0.008	0.428±0.008	0.465±0.008
3	0.481±0.010	0.469±0.009	0.494±0.008	0.454±0.009	0.433±0.008	0.469±0.009
3.5	0.482±0.008	0.471±0.008	0.498±0.008	0.454±0.008	0.436±0.008	0.472±0.009
4	0.483±0.008	0.472±0.008	0.500±0.009	0.454±0.009	0.438±0.011	0.474±0.008
ff14SB						
1	0.463±0.009	0.447±0.008	0.375±0.008	0.432±0.010	0.433±0.009	-
1.5	0.478±0.008	0.465±0.008	0.447±0.009	0.447±0.008	0.476±0.012	-
2	0.482±0.008	0.470±0.009	0.473±0.008	0.450±0.008	0.490±0.010	-
2.5	0.483±0.008	0.472±0.008	0.482±0.008	0.451±0.008	0.497±0.008	-
3	0.483±0.010	0.473±0.009	0.486±0.008	0.451±0.008	0.500±0.009	-
3.5	0.484±0.008	0.474±0.008	0.488±0.008	0.451±0.011	0.502±0.008	-
4	0.484±0.008	0.474±0.008	0.489±0.011	0.450±0.009	0.503±0.008	-
ff02						
1	0.435±0.009	0.483±0.008	0.375±0.007	0.350±0.008	0.483±0.008	-
1.5	0.456±0.009	0.491±0.009	0.446±0.008	0.379±0.012	0.510±0.008	-
2	0.463±0.008	0.491±0.008	0.467±0.008	0.389±0.008	0.515±0.009	-
2.5	0.465±0.010	0.489±0.008	0.473±0.010	0.393±0.009	0.516±0.009	-
3	0.467±0.008	0.488±0.012	0.474±0.008	0.395±0.008	0.516±0.008	-
3.5	0.467±0.008	0.487±0.008	0.475±0.008	0.396±0.008	0.515±0.009	-

4	0.468±0.011	0.486±0.008	0.477±0.009	0.397±0.012	0.514±0.008	-
ff99						
1	0.449±0.008	0.445±0.008	0.362±0.008	0.283±0.009	0.397±0.008	-
1.5	0.472±0.007	0.461±0.008	0.442±0.008	0.311±0.008	0.437±0.008	-
2	0.479±0.008	0.465±0.009	0.467±0.008	0.321±0.009	0.452±0.008	-
2.5	0.483±0.008	0.466±0.008	0.475±0.009	0.326±0.010	0.459±0.009	-
3	0.484±0.008	0.467±0.008	0.477±0.011	0.329±0.008	0.463±0.012	-
3.5	0.485±0.008	0.467±0.008	0.476±0.008	0.331±0.008	0.465±0.008	-
4	0.486±0.010	0.466±0.011	0.474±0.008	0.333±0.008	0.466±0.008	-
ff99SB						
1	0.455±0.008	0.456±0.008	0.331±0.008	0.388±0.010	0.389±0.009	-
1.5	0.473±0.009	0.473±0.008	0.424±0.008	0.407±0.008	0.428±0.008	-
2	0.479±0.008	0.477±0.009	0.457±0.009	0.413±0.008	0.441±0.010	-
2.5	0.481±0.008	0.479±0.008	0.470±0.008	0.415±0.007	0.447±0.008	-
3	0.482±0.008	0.479±0.010	0.475±0.009	0.416±0.008	0.451±0.008	-
3.5	0.482±0.008	0.480±0.008	0.476±0.008	0.416±0.008	0.453±0.008	-
4	0.483±0.008	0.480±0.008	0.477±0.008	0.416±0.011	0.454±0.011	-
ff99SBildn						
1	0.453±0.010	0.444±0.008	0.406±0.008	0.415±0.008	0.398±0.009	-
1.5	0.471±0.008	0.459±0.009	0.468±0.009	0.441±0.009	0.431±0.008	-
2	0.477±0.008	0.464±0.008	0.485±0.008	0.449±0.008	0.442±0.010	-
2.5	0.479±0.008	0.466±0.010	0.490±0.011	0.453±0.008	0.447±0.008	-
3	0.480±0.011	0.467±0.008	0.491±0.008	0.454±0.009	0.449±0.008	-
3.5	0.480±0.010	0.467±0.009	0.492±0.008	0.455±0.008	0.450±0.008	-
4	0.481±0.008	0.467±0.008	0.493±0.010	0.455±0.008	0.451±0.011	-

The standard deviations were estimated by randomly sampling 80% of the tested dataset for 100 times.

Table S5. Prediction accuracy of MM/GBSA results of HIV proteases based on various calculation protocols.

ϵ_{in}	enthalpy _{min}	enthalpy _{md}	$\Delta G_{interaction_entropy}$	$\Delta G_{nmode_min_9\text{\AA}}$
ff03				
1	-0.060±0.012	-0.010±0.013	0.204±0.011	0.007±0.015
1.5	0.064±0.013	0.086±0.015	0.235±0.012	0.131±0.012
2	0.135±0.012	0.138±0.012	0.244±0.012	0.196±0.014
2.5	0.178±0.015	0.169±0.012	0.252±0.013	0.234±0.012
3	0.206±0.012	0.188±0.016	0.258±0.012	0.259±0.012
3.5	0.226±0.012	0.202±0.012	0.263±0.012	0.275±0.013
4	0.241±0.014	0.212±0.011	0.268±0.014	0.287±0.012
ff14SB				
1	-0.038±0.012	0.025±0.011	0.160±0.012	0.006±0.012
1.5	0.071±0.013	0.111±0.012	0.187±0.013	0.115±0.012
2	0.132±0.012	0.155±0.012	0.201±0.012	0.173±0.012
2.5	0.169±0.013	0.181±0.013	0.208±0.012	0.207±0.013
3	0.193±0.012	0.196±0.015	0.214±0.013	0.229±0.012
3.5	0.210±0.014	0.207±0.012	0.219±0.012	0.244±0.014
4	0.222±0.012	0.215±0.013	0.224±0.012	0.255±0.012
ff02				
1	-0.007±0.012	0.018±0.012	0.234±0.011	0.070±0.012
1.5	0.096±0.013	0.099±0.013	0.253±0.012	0.171±0.014
2	0.153±0.012	0.142±0.012	0.248±0.012	0.224±0.013
2.5	0.187±0.012	0.167±0.012	0.237±0.013	0.254±0.012
3	0.209±0.013	0.183±0.014	0.231±0.012	0.273±0.012
3.5	0.224±0.012	0.194±0.012	0.227±0.012	0.287±0.012

4	0.235±0.012	0.202±0.012	0.224±0.012	0.296±0.015
ff99				
1	-0.027±0.012	-0.033±0.012	0.197±0.011	0.012±0.012
1.5	0.079±0.012	0.051±0.012	0.214±0.012	0.115±0.011
2	0.139±0.013	0.098±0.012	0.214±0.012	0.170±0.012
2.5	0.176±0.012	0.126±0.012	0.209±0.013	0.202±0.013
3	0.200±0.015	0.144±0.013	0.204±0.012	0.223±0.012
3.5	0.217±0.014	0.157±0.012	0.200±0.012	0.237±0.013
4	0.229±0.012	0.166±0.013	0.197±0.014	0.248±0.012
ff99SB				
1	-0.035±0.015	0.078±0.012	0.253±0.011	-0.010±0.012
1.5	0.075±0.012	0.152±0.012	0.285±0.012	0.102±0.013
2	0.138±0.012	0.191±0.012	0.289±0.012	0.164±0.012
2.5	0.176±0.013	0.213±0.012	0.283±0.014	0.201±0.013
3	0.201±0.012	0.226±0.012	0.276±0.012	0.225±0.012
3.5	0.219±0.012	0.235±0.013	0.271±0.012	0.242±0.012
4	0.232±0.012	0.242±0.012	0.267±0.012	0.254±0.013
ff99SBildn				
1	-0.051±0.013	-0.021±0.013	0.132±0.011	-0.027±0.013
1.5	0.064±0.013	0.082±0.012	0.182±0.012	0.088±0.012
2	0.130±0.012	0.138±0.011	0.206±0.012	0.152±0.012
2.5	0.170±0.012	0.171±0.012	0.219±0.013	0.190±0.013
3	0.196±0.012	0.191±0.012	0.229±0.012	0.214±0.012
3.5	0.214±0.013	0.206±0.014	0.237±0.012	0.231±0.012
4	0.228±0.012	0.216±0.012	0.243±0.013	0.244±0.014

The standard deviations were estimated by randomly sampling 80% of the tested dataset for 100 times.

Table S6. Prediction accuracy of MM/GBSA results of thrombin-like proteins based on various calculation protocols.

ϵ_{in}	enthalpy _{min}	enthalpy _{md}	$\Delta G_{interaction_entropy}$	$\Delta G_{nmode_min_9\text{\AA}}$
ff03				
1	0.678±0.005	0.641±0.006	0.403±0.004	0.340±0.005
1.5	0.782±0.005	0.742±0.005	0.597±0.005	0.493±0.006
2	0.797±0.007	0.766±0.005	0.679±0.005	0.546±0.005
2.5	0.798±0.005	0.773±0.006	0.718±0.005	0.569±0.005
3	0.796±0.006	0.776±0.005	0.738±0.006	0.582±0.007
3.5	0.794±0.006	0.778±0.005	0.750±0.005	0.589±0.005
4	0.792±0.005	0.778±0.005	0.757±0.005	0.594±0.005
ff14SB				
1	0.630±0.005	0.541±0.005	0.348±0.005	0.448±0.006
1.5	0.766±0.006	0.698±0.005	0.562±0.006	0.581±0.005
2	0.792±0.005	0.737±0.008	0.657±0.005	0.618±0.007
2.5	0.797±0.005	0.749±0.005	0.702±0.005	0.631±0.005
3	0.797±0.005	0.754±0.005	0.725±0.005	0.638±0.005
3.5	0.796±0.006	0.755±0.006	0.738±0.005	0.641±0.006
4	0.794±0.005	0.756±0.005	0.747±0.006	0.643±0.005
ff02				
1	0.681±0.006	0.651±0.005	0.403±0.005	0.525±0.006
1.5	0.773±0.005	0.734±0.005	0.595±0.006	0.638±0.007
2	0.789±0.005	0.749±0.005	0.664±0.005	0.672±0.005
2.5	0.792±0.005	0.753±0.006	0.692±0.005	0.686±0.005
3	0.792±0.006	0.753±0.005	0.705±0.006	0.692±0.006

3.5	0.791±0.005	0.753±0.005	0.714±0.005	0.695±0.005
4	0.790±0.007	0.752±0.006	0.719±0.005	0.697±0.005
ff99				
1	0.628±0.007	0.582±0.005	0.301±0.006	0.500±0.005
1.5	0.762±0.005	0.716±0.006	0.539±0.006	0.619±0.006
2	0.788±0.005	0.747±0.005	0.637±0.005	0.649±0.005
2.5	0.794±0.005	0.756±0.006	0.680±0.005	0.659±0.005
3	0.794±0.006	0.759±0.005	0.701±0.005	0.663±0.007
3.5	0.793±0.006	0.760±0.005	0.714±0.005	0.665±0.005
4	0.792±0.005	0.761±0.007	0.721±0.006	0.666±0.005
ff99SB				
1	0.634±0.005	0.585±0.005	0.364±0.004	0.491±0.006
1.5	0.764±0.005	0.706±0.005	0.564±0.005	0.609±0.005
2	0.789±0.005	0.735±0.007	0.649±0.007	0.639±0.005
2.5	0.793±0.006	0.745±0.005	0.689±0.005	0.649±0.006
3	0.792±0.005	0.749±0.005	0.710±0.005	0.653±0.005
3.5	0.791±0.006	0.750±0.007	0.721±0.005	0.655±0.006
4	0.789±0.005	0.751±0.005	0.730±0.006	0.656±0.005
ff99SBildn				
1	0.627±0.006	0.613±0.005	0.413±0.005	0.359±0.005
1.5	0.760±0.005	0.726±0.005	0.609±0.005	0.494±0.004
2	0.785±0.005	0.752±0.005	0.678±0.005	0.539±0.006
2.5	0.790±0.005	0.760±0.006	0.707±0.006	0.559±0.005
3	0.790±0.006	0.763±0.005	0.720±0.007	0.569±0.006
3.5	0.789±0.006	0.764±0.007	0.726±0.006	0.575±0.005
4	0.788±0.006	0.765±0.005	0.730±0.005	0.580±0.005

The standard deviations were estimated by randomly sampling 80% of the tested dataset for 100 times.

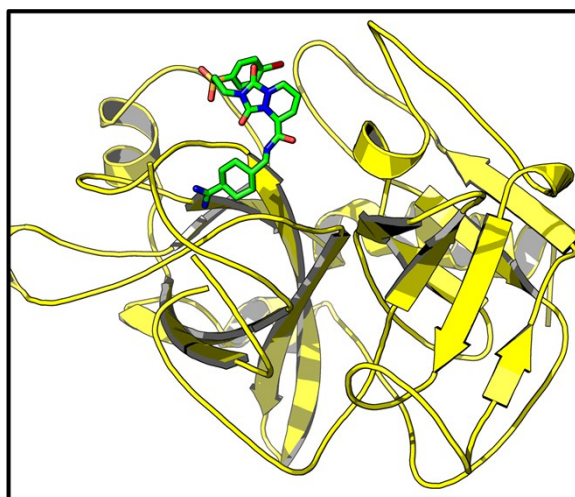


Figure S1. Structure of thrombin-like protein. The protein and co-crystallized ligand are shown in yellow cartoon model and green stick model, respectively. PDB code of 1C4U is used for the illustration.