Accuracy of binding energy predictions achieved by Lead-Finder

PDB ID	R, Å	Properties						dG, kcal/mol	
		N_{frb}	cLogP	Mr	Charge	dHB	aHB	calc	exp
1a9u	2.5	3	4.10	377	0	1	3	-7.28	-10.11
1abe	1.7	0	-0.83	150	0	4	5	-8.12	-9.60
1acj	2.8	0	-	199	1	3	0	-7.57	-10.09
1ai6	2.55	2	0.77	150	-2	0	3	-5.95	-5.52
1apb	1.76	0	-0.34	164	0	4	5	-7.89	-8.05
1apv	1.8	14	4.82	522	0	6	6	-10.34	-12.43
1apw	1.8	14	3.79	506	0	5	5	-10.54	-11.05
1aq1	2	2	4.40	466	0	3	3	-12.34	-11.38
1atl	1.8	9	3.14	338	-1	2	4	-9.19	-8.63
1bap	1.75	0	-0.83	150	0	4	5	-6.64	-9.41
1bcu	2	0	-	210	1	5	0	-6.95	-6.79
1bnw	2.25	4	1.07	337	-1	2	6	-12.28	-12.46
1bqo	2.3	5	3.78	512	-1	1	9	-11.03	-10.69
1c5x	1.75	0	-	303	1	4	0	-9.52	-9.11
1c83	1.8	2	1.23	246	-2	2	10	-8.44	-6.71
1c84	2.35	2	2.54	257	-2	1	10	-8.63	-6.91
1cbx	2	5	1.60	206	-2	0	8	-10.53	-8.77
1cet	2.05	7	-	300	1	2	1	-5.82	-3.96
1d3p	2.1	11	7.52	543	0	1	9	-10.33	-10.14
1d4p	2.07	3	-	361	1	5	2	-10.36	-8.70
1d6v	2	6	3.05	380	-1	2	8	-9.82	-8.52
1d7j	1.85	2	-0.79	88	0	1	4	-3.46	-4.53
1dbb	2.7	1	4.04	314	0	0	4	-9.27	-12.29
1dbm	2.7	6	3.20	431	-1	1	12	-11.25	-12.89
1di9	2.6	4	3.39	327	0	1	6	-7.55	-7.40
1dm2	2.1	0	-2.28	322	0	3	7	-9.65	-9.88
1dwb	3.16	0	-	121	1	4	0	-5.67	-3.99
1dwd	3	7	-	522	1	6	9	-10.84	-11.15
1e1x	1.85	3	2.69	252	-1	5	6	-9.48	-8.08
1ejn	1.8	4	1.96	341	0	6	3	-10.02	-7.76
1ela	2	9	-	457	1	5	6	-9.92	-8.67
1ele	2	7	4.61	427	0	3	6	-9.05	-9.35
1enu	1.95	0	-1.23	177	-2	4	4	-6.88	-7.07
1etr	2.2	8	0.62	508	0	7	11	-10.55	-10.11
1f0s	2.1	4	-	428	1	3	8	-9.17	-10.70
1f4f	2	7	-0.83	425	-3	1	18	-6.74	-6.38
1fhd	1.9	2	-1.45	302	0	5	15	-10.00	-9.43
1fm9	2.1	2	7.12	301	-1	0	4	-11.67	-12.35
1g4j	1.84	3	1.75	379	-1	2	7	-12.22	-12.02
1h1s	2	4	-	403	1	5	9	-11.14	-11.29
1h4w	1.7	0	-	121	1	4	0	-6.47	-6.50
1h9u	2.7	3	6.46	362	-1	0	5	-12.28	-11.77
1hbv	2.3	14	-	587	2	7	11	-11.80	-8.80
1hef	2.2	19	-	668	1	8	14	-12.30	-12.43
1hsl	1.89	3	-	155	0	4	5	-7.93	-9.96
1hvi	1.8	19	4.14	794	0	6	14	-13.63	-13.83
1hvr	1.8	8	10.16	606	0	2	6	-12.95	-13.14
1i7z	2.3	5	-	304	1	1	8	-8.27	-8.84
1ijr	2.2	13	1.31	616	-3	4	20	-9.56	-7.60
1k1j	2.2	7	-	523	1	5	11	-10.64	-10.37
1kv2	2.8	8	-	528	1	3	7	-12.61	-13.82

PDB ID	R, Å	Properties						dG, kcal/mol	
		N_{frb}	cLogP	Mr	Charge	dHB	aHB	calc	exp
1lah	2.06	4	-	132	1	5	5	-8.80	-10.39
1ldm	2.1	1	-1.58	88	-1	2	6	-5.88	-7.46
1lnm	1.9	1	4.88	373	-1	2	8	-11.73	-11.94
1mfe	2	6	-3.08	472	0	9	28	-8.82	-7.34
1mmq	1.9	6	2.70	456	0	4	8	-10.55	-10.39
1mq5	2.1	4	-	477	1	3	5	-12.69	-12.43
1n2v	2.1	3	0.43	206	0	1	7	-5.10	-5.69
1nhu	2	8	6.48	474.5	-1	0	6	-7.03	-7.77
1nhv	2.9	7	7.42	508	-1	0	8	-7.67	-7.82
1nli	1.93	0	-2.26	135	0	3	3	-5.27	-4.92
1nnb	2.8	5	-3.11	292	-1	5	16	-8.76	-6.91
1odw	2.1	16	-	544	1	6	12	-10.95	-9.67
1ohr	2.1	10	-	568	1	5	8	-10.94	-12.02
1oit	1.6	1	-	368	2	5	6	-10.67	-11.88
1om1	1.68	1	2.90	289	-1	0	7	-8.36	-9.29
1p1o	1.6	3	-1.86	189	0	4	10	-8.68	-7.91
1pbq	1.9	1	3.20	216	-1	1	6	-7.64	-8.60
1phf	1.6	1	1.46	143	-1	0	2	-5.71	-6.08
1pph	1.9	5	-	429	1	5	7	-9.23	-8.50
1ppl	1.7	18	4.82	610	-1	3	16	-11.73	-11.82
1ppm	1.7	17	4.22	604	-1	3	18	-10.87	-8.01
1pu7	1.93	0	-	164	1	2	2	-4.71	-4.25
1q65	2.1	5	-	294	1	6	3	-9.73	-7.62
1rne	2.4	21	-	729	-2	5	13	-15.15	-12.02
1rsi	2.2	1	1.21	187	0	3	3	-7.16	-6.17
1s38	1.81	0	1.06	175	0	3	3	-7.86	-7.19
1sj0	1.9	6	-	462	-1	1	8	-12.87	-12.57
1tng	1.8	1	-	114	1	3	0	-6.38	-4.05
1tni	1.9	4	-	150	1	3	0	-5.89	-5.49
1uwf	1.69	5	-1.10	236	0	4	12	-7.92	-9.37
1v2m	1.65	0	-	121	1	4	0	-5.80	-5.89
1w4q	1.68	4	-2.66	324	-2	2	16	-7.89	-7.22
1xp9	1.8	6	4.72	462	-1	3	8	-12.38	-12.40
1yds	2.2	4	0.37	266	1	3	6	-7.98	-8.18
1ydt	2.3	6	-	447	1	3	6	-10.55	-10.11
2dbl	2.9	6	5.40	417	-1	0	10	-11.44	-11.87
2dri	1.6	0	-0.83	150	0	4	10	-9.75	-9.45
2ifb	2	14	7.15	255	-1	0	4	-7.64	-7.38
2izl	1.48	5	-	243	2	4	4	-8.00	-8.24
2pax	2.4	0	-0.58	212	0	3	4	-7.78	-9.40
2phh	2.7	1	1.42	137	-1	1	6	-5.38	-6.39
2pk4	2.25	5	-	131	0	3	4	-5.15	-5.89
2r04	3	9	5.43	340	0	0	8	-8.88	-8.50
3tmn	1.7	6	-	303	0	5	6	-7.84	-8.15
4tmn	1.7	14	3.08	517	-2	3	15	-14.41	-14.08
5tln	2.3	8	-0.93	323	0	5	10	-8.55	-8.80
7est	1.8	8	5.14	441	0	3	6	-9.40	-10.50
7tim	1.9	3	-3.26	169	-2	2	12	-6.87	-7.37
966c	1.9	6	2.03	391	0	2	12	-11.07	-10.56
13gs	1.9	2	2.67	399	-1	4	6	-7.58	-6.38
1a42	2.25	7	0.69	382	-1	2	8	-11.59	-13.57

PDB ID	R, Å	Properties						dG, kcal/mol	
		N_{frb}	cLogP	Mr	Charge	dHB	aHB	calc	exp
1a4k	2.4	6	1.13	426	-1	2	7	-9.14	-11.05
1aaq	2.5	17	-1.03	579	0	8	7	-11.03	-11.53
1abf	1.9	0	-0.34	164	0	4	5	-8.02	-7.44
1acm	2.8	6	-2.85	251	-4	1	8	-10.68	-10.33
1apt	1.8	17	-	499	1	7	6	-10.36	-10.35
1apu	1.8	16	3.59	485	0	4	6	-9.21	-10.35
1azm	2	1	-0.26	221	-1	2	6	-9.25	-8.48
1b6k	1.85	12	-	678	1	6	8	-14.14	-12.08
1b6m	1.85	11	-	597	1	6	6	-14.01	-11.60
1bkm	2	16	1.70	595	-3	5	10	-8.57	-7.94
1bl7	2.5	3	-	339	1	4	3	-9.92	-10.67
1bma	1.8	12	-	521	1	3	3	-9.77	-6.33
1bra	2.2	0	-	121	1	4	0	-5.96	-5.91
1byb	1.9	10	-5.83	666	0	14	21	-16.14	-19.00
1c1b	2.5	6	4.10	330	0	1	6	-9.40	-10.22
1c3i	1.83	12	4.96	457	0	4	9	-10.63	-8.01
1c5c	1.61	0	-1.54	344	-2	2	14	-10.42	-9.50
1c5p	1.43	0	-	121	1	4	0	-6.43	-7.84
1c5z	1.85	5	-1.72	189	-3	1	14	-5.07	-5.51
1c88	1.8	2	-	269	-1	3	10	-9.12	-7.31
1c8k	1.76	2	-	400.5	-1	2	10	-7.34	-8.29
1cbs	1.8	1	6.83	299	-1	0	4	-9.55	-9.79
1cfv	2.1	3	1.38	445	-1	3	16	-12.69	-11.14
1cil	1.6	3	0.10	323	-1	2	10	-11.89	-11.12
1cim	2.1	1	-0.65	295	-1	3	10	-11.55	-12.10
1cnx	1.9	9	-	331	0	5	11	-10.26	-10.18
1cps	2.25	5	-	241	-1	4	6	-8.69	-9.20
1cqp	2.6	7	4.07	404	0	1	10	-7.76	-7.76
1ctr	2.45	5	3.53	403	0	0	0	-6.43	-5.85
1d3d	2.04	9	8.54	591	0	1	6	-10.50	-12.56
1d3h	1.8	2	2.51	269	-1	1	5	-8.99	-10.39
1d7x	2	5	-	346	1	4	13	-8.82	-7.40
1dbj	2.7	0	3.75	290	0	1	4	-9.38	-10.49
1dbk	3	0	3.17	288	0	0	4	-8.86	-11.06
1dhf	2.3	7	-2.46	439	-2	5	15	-10.22	-10.22
1dog	2.3	1	-	164	1	6	8	-7.81	-5.55
1dr1	2.2	2	-3.32	237	0	5	9	-7.23	-7.60
1dwc	3	8	-	508	0	7	11	-8.74	-10.11
1e1v	1.95	3	2.89	247	0	3	5	-7.86	-6.75
1eap	2.4	10	0.94	341	-2	1	12	-8.54	-8.47
1ecv	1.95	2	2.91	333	-2	1	10	-9.22	-6.71
1efy	2.2	1	1.93	267	0	3	5	-8.06	-11.48
1elb	2.1	13	-	473	1	6	6	-7.15	-9.88
1elc	1.75	13	-	507	1	6	6	-8.00	-11.05
1eld	2	8	5.58	475	0	3	6	-9.15	-9.25
1epb	2.2	1	6.83	299	-1	0	4	-9.93	-9.89
1ets	2.3	7	-	523	2	7	8	-11.63	-11.64
1ett	2.5	5	-	429	1	5	7	-9.73	-8.55
1eve	2.5	6	-	378	1	1	6	-8.91	-11.72
1ezq	2.2	7	-	459	1	7	7	-12.39	-12.62
1f0q	2.63	0	5.03	270	0	3	10	-7.40	-8.36

PDB ID	R, Å	Properties						dG, kcal/mol	
		N_{frb}	cLogP	Mr	Charge	dHB	aHB	calc	exp
1f0r	2.1	4	-	455	2	5	7	-11.44	-10.58
1f0t	1.8	4	0.71	445	0	5	10	-8.80	-8.29
1f0u	1.9	8	-	459	1	7	7	-9.11	-9.89
1f3e	1.85	0	-	192	2	6	4	-8.53	-9.19
1f4e	1.9	2	-	270	1	2	8	-5.77	-4.09
1fbm	2.7	6	7.51	292	0	1	2	-9.49	-8.67
1fcx	1.47	3	7.40	387	-1	1	6	-13.46	-9.84
1fcz	1.38	3	6.40	365	-1	1	6	-14.18	-12.74
1fh8	1.95	2	-	250	1	6	12	-9.33	-9.51
1fh9	1.72	2	-	295	1	8	16	-10.26	-8.89
1fjs	1.92	8	-	520	-4	4	12	-11.24	-13.40
1fkb	1.7	6	3.86	915	0	4	26	-12.50	-13.17
1fkg	2	10	5.18	449	0	0	8	-7.21	-8.79
1fki	2.2	0	3.84	438	-1	1	12	-9.96	-9.67
1frb	1.7	5	3.43	419	-2	1	7	-11.67	-10.73
1fvt	2.2	2	2.84	396	-1	5	7	-9.63	-8.60
1g35	1.8	13	3.23	662	0	3	19	-12.97	-11.17
1g45	1.83	3	1.62	307	-1	2	7	-10.40	-11.93
1g46	1.84	3	1.58	325	-1	2	7	-10.70	-12.15
1g48	1.86	3	1.71	325	-1	2	7	-10.73	-10.24
1g4o	1.96	3	1.57	289	-1	2	7	-9.62	-11.33
1g52	1.8	3	1.58	325	-1	2	7	-11.62	-13.18
1g53	1.94	3	1.71	325	-1	2	7	-11.55	-11.11
1g54	1.86	3	1.75	379	-1	2	7	-12.78	-12.19
1gaf	1.95	8	0.82	301	-2	0	14	-8.47	-10.98
1gt1	1.71	2	0.71	166	0	1	3	-5.27	-8.24
1gwx	2.5	9	7.23	577.5	0	1	8	-13.00	-10.09
1hdq	2.3	4	0.80	222	-2	2	8	-8.08	-8.04
1hdt	2.6	16	-	555	1	9	13	-9.99	-10.81
1hfc	1.5	9	0.91	348	-1	3	8	-11.93	-11.26
1hih	2.2	15	3.52	573	0	5	11	-12.22	-11.12
1hps	2.3	16	6.86	638	0	4	11	-11.24	-12.74
1hpv	1.9	11	4.20	505	0	4	12	-9.83	-12.66
1hpx	2	14	4.52	667	0	4	13	-12.81	-15.56
1hri	3	9	4.04	308.5	0	0	5	-7.18	-5.92
1hsg	2	12	-	614	1	5	10	-13.37	-13.17
1hte	2.8	8	3.54	440	-1	3	9	-7.48	-7.79
1htf	2.2	12	-	575	1	6	8	-9.60	-9.44
1hti	2.8	3	-1.95	153	-3	0	12	-6.03	-7.00
1hwr	1.8	8	5.01	406	0	2	6	-9.31	-11.62
1hyt	1.7	5	1.60	206	-2	0	8	-9.12	-11.63
1i8z	1.93	5	-	473	0	2	14	-12.37	-12.29
1ida	1.7	14	-	725	1	5	10	-13.23	-11.82
1idb	2.2	13	-	651	1	4	13	-11.16	-11.10
1iig	2.6	3	-1.95	154	-2	1	12	-5.34	-6.31
1ivd	1.9	3	2.12	239	-1	2	12	-5.11	-4.27
1jgl	2.15	0	4.13	272	0	2	4	-9.79	-12.14
1jik	2.8	11	-	472	1	10	19	-11.09	-13.52
1jmi	2.5	4	-2.19	306	-2	2	16	-5.87	-8.45
1jsv	1.96	1	-0.55	265	0	5	7	-6.61	-7.87
1jwt	2.5	6	-0.90	491	-1	3	12	-10.93	-10.95

PDB ID	R, Å	Properties						dG, kcal/mol	
		N_{frb}	cLogP	Mr	Charge	dHB	aHB	calc	exp
1k22	1.93	8	-	431	2	8	8	-12.22	-11.53
1k4h	1.8	3	-0.49	262	0	4	4	-7.41	-7.14
1kel	1.9	10	-	344	-2	1	14	-7.94	-9.94
1kv1	2.5	3	4.16	306.5	0	2	3	-8.17	-8.21
1l2s	1.94	3	3.26	316.5	-1	1	8	-7.27	-6.34
1lbf	2.05	8	-0.83	348	-3	4	18	-12.20	-10.95
1lcp	1.65	3	-1.00	166	-1	3	7	-10.06	-9.17
1lgw	1.85	0	1.27	111	0	2	0	-4.55	-5.49
1lqd	2.7	5	-	425	1	5	2	-9.22	-11.21
1lyx	1.9	3	-1.95	153	-3	0	12	-6.83	-6.33
1m48	1.95	9	-	447	1	5	6	-9.55	-7.03
1m5c	1.65	3	0.51	251	0	4	8	-9.28	-8.79
1mbi	2	0	-0.16	68	0	1	1	-4.41	-2.60
1mdr	2.1	2	1.27	165	-1	1	6	-6.02	-5.32
1met	1.9	10	5.33	566	0	4	10	-12.72	-13.10
1mnc	2.1	9	0.91	348	-1	3	8	-10.44	-12.43
1mq6	2.1	3	-	524.5	1	2	11	-12.24	-15.31
1mtw	1.9	6	-	444	0	6	6	-11.09	-10.04
1n4k	2.2	6	-2.69	414	-6	3	30	-13.14	-14.00
1nja	2.5	4	-2.17	306	-1	4	15	-8.54	-8.66
1njb	2.74	4	-2.19	307	-1	3	16	-7.87	-8.95
1njc	2.5	4	-2.17	305	-2	3	15	-6.29	-7.74
1nox	1.59	7	-2.87	457	-1	7	18	-10.36	-9.83
1nvs	1.8	0	4.86	393	-2	1	6	-8.97	-10.74
1o32	1.78	0	-	254	1	6	3	-7.12	-8.02
1o39	1.59	1	-	328	1	5	3	-10.62	-9.95
1o86	2	10	-	400	-1	4	11	-11.80	-13.22
1ofz	1.5	0	-0.34	164	0	4	10	-5.59	-6.34
1oiq	2.31	0	0.60	267	0	1	5	-7.53	-7.71
1okl	2.1	2	2.01	250	0	2	6	-9.22	-8.33
1ow4	1.6	1	2.45	298	-1	1	6	-8.92	-7.79
1pb8	1.45	2	-	105	0	4	6	-7.86	-7.07
1pgp	2.5	7	3.20	275	-3	6	20	-7.13	-7.87
1phd	1.6	1	1.46	143	-1	0	2	-5.72	-6.08
1phh	2.3	1	1.16	153	-1	2	8	-5.59	-3.97
1pmv	2.5	0	-	221	1	2	3	-7.39	-9.52
1ppc	1.8	7	-	522	1	6	9	-9.86	-8.82
1ppk	1.8	13	3.24	435	0	5	13	-8.05	-10.58
1pro	1.8	10	3.32	583	0	3	13	-13.44	-15.76
1pso	2	22	2.16	684	-1	7	18	-12.46	-14.10
1pzo	1.9	4	2.97	295	0	3	1	-6.03	-4.56
1pzp	1.45	4	0.40	305	0	5	2	-6.61	-4.54
1qbr	1.8	6	-	756	2	4	12	-16.26	-14.51
1qbt	2.1	6	-	822	2	6	13	-17.92	-14.58
1qbu	1.8	8	6.74	596	0	3	9	-13.95	-13.98
1qhi	1.9	4	0.96	299	0	3	6	-11.44	-10.09
1qpe	2	2	-	302.5	1	3	2	-8.57	-10.64
1r09	2.9	2	2.16	286	0	2	4	-8.50	-6.77
1rbp	2	2	6.84	286	0	1	2	-10.82	-9.28
1rs4	2.7	3	3.19	430	0	4	7	-10.84	-10.00
1rzy	1.8	5	-1.97	374	0	5	16	-10.43	-8.24

PDB ID	R, Å	Properties						dG, kcal/mol	
		N_{frb}	cLogP	Mr	Charge	dHB	aHB	calc	exp
1s39	1.95	0	0.60	161	0	3	3	-6.90	-9.00
1sbg	2.3	14	4.87	534	0	4	9	-10.59	-10.70
1snc	1.65	6	-3.34	398	-4	1	22	-12.86	-9.26
1sqn	1.45	1	3.66	300	0	1	4	-10.76	-12.90
1sre	1.78	1	3.72	241	-1	1	8	-7.49	-5.42
1srj	1.8	1	4.22	293	-1	3	6	-7.00	-4.69
1swi	2.6	0	2.22	78	0	0	0	-2.79	-4.31
1thl	1.7	11	4.52	474	-2	2	10	-10.24	-8.87
1tlp	2.3	11	0.86	541	-2	6	21	-12.13	-10.43
1tmn	1.9	13	4.42	477	-2	3	11	-11.72	-10.09
1tnh	1.8	1	-	126	1	3	0	-6.49	-4.60
1tnj	1.8	2	1.46	121	0	2	1	-5.31	-2.71
1tnk	1.8	3	1.83	135	0	2	1	-5.37	-2.06
1tnl	1.9	1	1.26	133	0	2	1	-5.75	-2.59
1tv6	2.8	2	-	373	1	1	3	-10.83	-8.84
1u0g	1.7	5	-3.17	200	-2	3	14	-9.34	-8.45
1u1w	1.35	1	1.06	151	-2	2	6	-5.07	-8.03
1u59	2.3	2	4.40	466	0	3	6	-11.91	-10.12
1urg	1.8	4	-3.41	342	0	8	22	-9.15	-8.12
1utj	1.83	1	-	108	1	3	0	-5.83	-5.36
1utm	1.5	2	-	122	1	3	0	-5.97	-4.19
1uvt	2.5	6	-	384	1	3	6	-9.61	-10.56
1vjy	2	2	-1.04	287	-2	1	4	-9.11	-10.64
1vpo	2.15	0	4.01	290	0	2	4	-10.43	-13.29
1vyz	2.21	1	2.44	227	0	2	3	-6.91	-9.12
1wm1	2.1	2	-	224	1	2	6	-8.24	-8.79
1xap	2.1	1	8.62	347	-1	0	4	-12.95	-12.14
1xp1	1.8	6	-	478	1	3	8	-13.41	-12.98
1xp6	1.7	6	-	478	1	3	8	-13.65	-13.10
1yc1	1.7	3	-	367	1	3	13	-9.31	-8.47
1ydr	2.2	1	-	292	1	2	6	-7.82	-7.63
1zzz	1.9	7	-	420	2	9	10	-8.38	-7.10
2bt9	0.94	1	0.05	178	0	3	10	-7.41	-7.50
2cbr	2.8	1	6.48	350	-1	1	6	-9.64	-9.55
2cbs	2.1	1	7.61	337	-1	0	4	-10.70	-11.48
2cgr	2.2	7	2.00	384	0	3	5	-6.61	-9.89
2cht	2.2	2	-0.65	226	-2	1	12	-9.36	-7.63
2cpp	1.63	0	2.13	152	0	0	2	-5.94	-8.39
2csn	2.5	3	-	266	1	4	6	-6.52	-6.09
2ctc	1.4	3	1.05	165	-1	1	6	-7.03	-5.31
2gbp	1.9	1	-1.88	180	0	5	12	-10.08	-10.37
2h4n	1.9	1	-0.26	221	-1	2	9	-9.31	-10.94
2qwi	2	6	-	341	0	6	10	-9.63	-11.61
2sim	1.6	5	-3.27	290	-1	5	16	-9.61	-8.74
2upj	3	12	6.11	558	0	3	12	-9.72	-10.21
2xis	1.71	4	-3.77	151	-1	4	10	-6.98	-8.14
2ypi	2.5	3	-1.95	153	-3	0	12	-5.88	-6.59
3cbs	2	1	-	298	7	2	6	-8.90	-10.10
3cla	1.75	6	1.02	323	0	3	10	-5.54	-6.82
3dfr	1.7	7	-1.63	452	-2	5	14	-11.81	-14.23
3erk	2.1	3	-	339	1	4	3	-9.11	-7.07

PDB ID	R, Å	Properties						dG, kcal/mol	
		N_{frb}	cLogP	Mr	Charge	dHB	aHB	calc	exp
3ert	1.9	8	-	388	1	2	4	-10.75	-13.26
3kiv	1.8	4	-0.13	129	0	3	4	-5.20	-6.55
3pax	2.4	1	0.85	151	0	2	4	-6.89	-6.98
3ptb	1.7	1	-	121	1	4	0	-6.03	-6.45
4pax	2.8	0	-0.03	176	0	2	5	-7.53	-8.93
4phv	2.1	12	5.49	618	0	5	10	-12.70	-12.67
4sga	1.8	8	0.66	471	-1	2	12	-9.08	-10.02
4tln	2.3	3	-	146	0	4	4	-5.59	-5.14
4ts1	2.5	3	-	181	0	4	6	-5.80	-7.64
5abp	1.8	1	-1.88	180	0	5	12	-9.40	-9.08
5cpp	2.08	0	1.60	150	0	0	2	-5.87	-8.12
5tim	1.83	0	0.52	152	0	2	4	-3.13	-3.14
6abp	1.67	0	-0.83	150	0	4	10	-8.21	-8.69
6cpa	2	12	2.24	476	-2	2	16	-14.60	-15.92
6rnt	1.8	4	-2.08	348	-1	6	16	-5.93	-3.27
6tim	2.2	4	-2.84	170	-2	2	12	-6.93	-4.43
7abp	1.67	0	-0.34	164	0	4	10	-8.14	-8.92
7cpa	2	15	4.97	580	-2	2	16	-15.50	-19.34
7cpp	2	0	0.62	110	0	0	2	-4.58	-5.25
830c	1.6	6	2.55	425.5	0	2	12	-10.07	-12.74
8abp	1.49	1	-1.88	180	0	5	12	-9.47	-9.12
8atc	2.5	6	-1.88	251	-4	1	16	-11.65	-10.46
9abp	1.97	1	-1.88	180	0	5	12	-9.27	-11.05
9hvp	2.8	20	7.52	736	0	5	14	-11.96	-11.54

Accuracy of binding energy (dG) predictions achieved by Lead-Finder on the set of 330 protein-ligand complexes with diverse physiochemical properties. Column 'PDBid' contains PDB codes of protein-ligand complexes; 'R' – structure resolution in Å; 'N_{FRB}' – the number of freely rotatable ligand bonds; 'cLogP' – calculated logP; 'Mr' – relative molecular weight; 'Charge' – net charge of the ligand molecule; 'dHB' and 'aHB' – numbers of hydrogen bond donors and acceptors in the ligand molecule; 'calc' and 'exp'- calculated and experimental binding energies correspondingly. PDB codes of protein-ligand complexes comprising the training set are typed with bold font.