

Docking performance of Lead-Finder

PDB ID	R, Å	N _{frb}	P		Time, s		dG, kcal/mol			RMSD converged		RMSD median	
			scr	doc	scr	doc	scr	doc	ref	scr	doc	scr	doc
121p	1.54	8	0.35	0.85	54.1	293.4	-16.2	-16.4	-18.2	1.7	1.4	2.59	1.50
186l	1.80	3	1.00	1.00	24.1	34.5	-5.3	-5.5	-5.5	0.8	0.8	0.78	0.78
1a28	1.80	1	1.00	1.00	5.1	10.4	-10.9	-10.9	-10.9	0.4	0.4	0.40	0.40
1a4q	1.90	8	1.00	1.00	32.4	118.4	-11.1	-11.2	-11.2	0.7	0.5	0.50	0.40
1a6w	1.80	4	1.00	1.00	9.7	14.7	-7.1	-7.1	-7.1	0.8	0.7	0.82	0.71
1a9u	2.50	3	0.95	0.95	25.3	36.1	-9.2	-9.4	-9.5	0.5	0.5	0.46	0.43
1aaq	2.50	17	0.45	0.50	577.4	998.4	-12.4	-12.2	-13.2	1.4	1.4	2.27	1.97
1abe	1.70	0	0.75	0.95	5.4	7.2	-7.0	-7.1	-7.2	0.7	0.5	0.82	0.65
1abf	1.90	0	0.95	1.00	5.7	7.4	-7.4	-7.2	-7.5	1.1	1.1	1.11	1.12
1acj	2.80	0	1.00	1.00	3.5	5.9	-7.8	-7.8	-7.8	0.6	0.7	0.64	0.65
1ack	2.80	2	0.85	0.75	5.7	15.2	-6.2	-6.2	-6.2	1.3	1.3	1.22	1.52
1acl	2.80	11	0.00	0.00	30.3	188.8	-	-	-7.0	-	-	4.76	4.81
1acm	2.80	6	1.00	1.00	11.7	17.7	-11.2	-11.2	-11.3	0.5	0.4	0.39	0.35
1aco	2.05	4	1.00	1.00	5.5	8.5	-9.7	-9.7	-9.7	0.5	0.3	0.37	0.30
1add	2.40	2	0.85	0.95	13.2	19.6	-7.6	-7.7	-7.8	0.5	0.5	0.48	0.55
1adf	2.90	10	0.05	0.00	514.8	858.8	-12.8	-	-12.3	1.9	-	7.73	6.06
1aec	1.86	13	1.00	1.00	101.6	105.3	-8.4	-8.6	-8.5	0.9	0.9	0.94	0.82
1aha	2.20	0	1.00	1.00	2.9	6.0	-6.1	-6.1	-6.1	0.3	0.3	0.29	0.28
1ake	1.90	16	0.15	0.10	628.6	1290	-22.5	-21.7	-25.5	1.7	1.9	2.39	2.62
1aoe	1.60	3	1.00	1.00	8.8	18.1	-7.7	-7.7	-7.7	0.5	0.5	0.53	0.51
1apb	1.76	0	0.95	1.00	5.7	7.7	-7.2	-7.2	-7.4	1.1	1.1	1.21	1.20
1apt	1.80	17	0.05	0.00	485.9	818.5	-11.9	-	-12.0	1.2	-	9.94	9.83
1apu	1.80	14	0.15	0.05	351.6	638.6	-9.9	-9.5	-9.7	0.9	1.0	3.94	8.94
1apv	1.80	14	0.45	0.50	392.3	674.5	-11.3	-11.6	-11.7	0.9	0.8	2.97	2.13
1apw	1.80	14	0.20	0.20	376.0	604.3	-10.8	-10.7	-11.1	0.7	0.9	5.22	3.64
1aqw	1.80	9	0.65	0.85	47.3	243.2	-8.1	-8.1	-8.2	1.3	1.3	1.40	1.21
1ase	2.50	5	1.00	1.00	9.2	14.0	-6.9	-6.8	-6.8	0.3	0.3	0.34	0.32
1atl	1.80	9	0.90	0.90	31.1	205.3	-9.2	-8.9	-9.2	1.3	1.3	1.36	1.37
1avd	2.70	5	1.00	1.00	22.2	88.5	-9.0	-9.1	-8.5	1.2	1.2	1.15	1.22
1azm	2.00	1	0.55	0.55	6.2	21.6	-7.7	-7.7	-7.9	1.3	1.4	1.84	1.95
1b40	2.20	15	1.00	1.00	496.5	710.0	-14.0	-14.0	-13.9	1.2	1.2	1.39	1.19
1b58	1.80	15	1.00	1.00	505.5	882.1	-15.7	-15.6	-15.7	1.1	1.1	1.05	1.10
1b59	1.80	6	1.00	1.00	32.9	38.1	-6.4	-6.4	-6.4	0.6	0.6	0.61	0.61
1b6j	1.85	13	0.80	0.65	569.2	872.5	-15.7	-16.3	-16.7	0.9	0.9	0.85	0.96
1b6k	1.85	12	0.95	1.00	562.1	844.1	-15.5	-15.3	-15.5	0.9	1.0	0.91	0.92
1b6l	1.75	7	0.85	0.90	51.4	210.5	-13.1	-13.0	-13.1	0.9	0.9	0.98	0.92
1b6m	1.85	11	0.75	0.70	94.4	451.7	-13.6	-13.8	-14.2	0.9	0.9	1.06	1.07
1baf	2.90	5	0.60	0.30	35.6	138.3	-6.3	-6.3	-6.3	1.4	1.4	1.45	7.09
1bap	1.75	0	0.85	0.95	5.4	7.3	-6.8	-6.9	-7.1	0.6	0.5	0.57	0.48
1bbp	2.00	8	1.00	1.00	35.6	155.3	-15.4	-15.5	-15.5	1.2	1.2	1.34	1.23
1bkm	2.00	16	0.00	0.00	447.3	778.2	-	-	-12.9	-	-	3.29	2.73
1blh	2.30	6	1.00	1.00	10.9	15.6	-5.5	-5.5	-5.3	1.2	1.2	1.34	1.35
1bma	1.80	12	0.95	1.00	88.0	342.4	-11.5	-11.5	-11.4	0.9	0.9	0.86	0.91
1bra	2.20	0	1.00	1.00	2.7	5.1	-6.2	-6.2	-6.1	1.2	1.1	1.27	1.12
1byb	1.90	10	0.35	0.65	936.9	1657	-15.3	-15.4	-16.9	1.4	1.4	3.02	1.65
1c1b	2.50	6	0.95	1.00	14.9	21.6	-9.7	-9.7	-9.7	0.5	0.5	0.54	0.48
1c1e	1.90	0	1.00	1.00	3.6	6.0	-10.7	-10.8	-10.8	0.3	0.3	0.31	0.31
1c3i	1.83	12	0.85	0.95	73.2	253.9	-12.9	-13.5	-12.7	1.3	1.1	1.26	1.12
1c5c	1.61	0	0.95	1.00	5.3	10.3	-10.1	-10.1	-10.1	0.3	0.3	0.23	0.24
1c5p	1.43	0	1.00	1.00	3.3	7.5	-5.9	-5.9	-5.9	0.3	0.3	0.29	0.32

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1c5x	1.75	0	1.00	1.00	3.8	7.2	-9.3	-9.3	-9.3	0.2	0.2	0.24	0.22
1c83	1.80	2	0.95	1.00	9.1	13.2	-8.2	-8.1	-8.2	0.4	0.3	0.35	0.33
1c84	2.35	2	0.90	1.00	8.6	12.3	-8.4	-8.4	-8.5	0.8	0.7	0.88	0.79
1c86	2.30	2	0.80	1.00	4.9	8.3	-9.8	-9.8	-9.8	0.7	0.7	0.73	0.71
1c87	2.10	2	0.95	1.00	8.6	13.5	-8.5	-8.8	-8.8	0.6	0.4	0.45	0.45
1c88	1.80	2	0.50	0.95	5.8	10.1	-8.9	-8.8	-8.7	0.6	0.5	1.90	0.54
1c8k	1.76	2	0.15	0.15	17.2	25.3	-7.9	-7.9	-7.8	1.0	1.0	5.78	5.78
1cbs	1.80	1	1.00	1.00	4.7	8.9	-9.7	-9.7	-9.8	0.7	0.7	0.72	0.72
1cbx	2.00	5	0.85	1.00	7.9	10.9	-9.6	-9.6	-9.5	0.7	0.7	0.75	0.74
1cde	2.50	5	1.00	1.00	39.2	203.3	-8.7	-8.7	-8.5	1.4	1.2	1.44	1.33
1cdg	2.00	4	0.30	0.90	257.4	524.4	-7.9	-6.4	-6.3	1.2	1.6	5.87	1.62
1cil	1.60	3	0.35	0.55	13.4	19.9	-8.6	-8.5	-8.3	0.8	0.8	3.91	1.06
1cnx	1.90	9	0.00	0.00	74.1	269.0	-	-	-9.5	-	-	6.57	6.56
1com	2.20	4	0.85	1.00	14.0	18.5	-8.4	-8.4	-8.5	0.8	0.6	0.87	0.67
1coy	1.80	0	1.00	1.00	4.8	7.9	-10.3	-10.3	-10.4	0.5	0.4	0.41	0.39
1cps	2.25	5	0.95	0.95	29.1	97.5	-9.0	-9.1	-9.0	0.9	1.0	0.87	1.01
1ctr	2.45	5	0.05	0.05	15.6	22.6	-7.0	-7.0	-7.2	1.8	1.3	7.61	7.64
1ctt	2.20	2	0.90	1.00	10.9	15.8	-9.4	-9.4	-9.4	0.7	0.7	0.78	0.70
1d0l	1.97	11	0.45	0.50	365.5	647.6	-10.5	-10.6	-10.8	1.6	1.6	2.65	1.90
1d3d	2.04	9	0.05	0.00	68.6	256.1	-11.4	-	-11.8	0.9	-	2.89	2.97
1d3h	1.80	4	1.00	1.00	12.0	16.9	-8.7	-8.7	-8.4	1.4	1.3	1.36	1.39
1d3p	2.10	11	0.00	0.20	338.5	454.8	-	-10.9	-10.9	-	1.6	3.02	2.81
1d7x	2.00	5	0.95	0.95	27.7	106.0	-9.4	-9.4	-9.3	0.8	0.8	0.81	0.82
1d8f	2.40	6	0.95	1.00	34.4	126.3	-10.2	-10.1	-10.1	1.2	1.2	1.16	1.16
1dbb	2.70	1	1.00	1.00	5.2	11.3	-9.0	-9.1	-9.2	0.6	0.6	0.61	0.63
1dbj	2.70	0	0.90	0.95	4.6	6.9	-9.2	-9.2	-9.2	0.9	0.9	0.94	0.95
1dbk	3.00	0	1.00	1.00	4.1	7.1	-8.6	-8.6	-8.6	1.3	1.3	1.32	1.33
1dbm	2.70	6	0.90	0.95	28.3	102.0	-11.1	-11.1	-10.9	1.9	1.9	1.94	1.90
1dd6	2.00	9	0.90	0.80	35.0	118.2	-12.6	-12.8	-12.7	1.7	1.7	1.71	1.71
1dds	2.20	7	0.70	0.50	41.9	159.1	-10.8	-10.9	-10.9	1.2	1.1	1.16	1.75
1dhf	2.30	5	1.00	1.00	17.0	24.1	-11.3	-11.4	-11.4	0.6	0.7	0.58	0.62
1did	2.50	2	0.45	0.55	20.2	79.2	-7.2	-7.4	-7.2	0.4	0.3	3.11	0.42
1die	2.50	1	1.00	1.00	9.2	13.7	-7.4	-7.8	-7.8	0.9	0.8	0.88	0.88
1dih	2.20	12	0.05	0.15	563.9	977.9	-12.8	-13.9	-14.0	1.6	1.7	3.19	3.13
1dm2	2.10	0	1.00	1.00	4.6	9.1	-9.5	-9.5	-9.5	0.2	0.2	0.23	0.23
1dog	2.40	1	0.65	0.80	9.5	13.2	-8.0	-7.9	-8.0	0.4	0.5	0.40	0.39
1dr1	2.20	2	0.70	0.85	11.5	16.6	-7.2	-7.3	-7.2	1.3	1.5	1.53	1.53
1dwb	3.16	0	1.00	1.00	3.0	5.5	-5.7	-5.7	-5.7	0.5	0.5	0.48	0.50
1dwc	3.00	8	0.35	0.90	59.4	285.9	-9.9	-10.0	-10.1	0.7	0.8	4.09	0.74
1dwd	3.00	7	0.75	1.00	53.8	157.4	-11.4	-11.7	-11.6	1.6	1.6	1.70	1.67
1e5i	2.10	4	0.40	0.05	6.1	11.2	-6.7	-6.7	-6.9	1.0	1.6	4.68	4.69
1eap	2.50	10	0.85	1.00	33.8	216.5	-10.1	-10.3	-10.2	0.9	0.9	0.93	0.88
1ebg	2.10	2	1.00	1.00	6.4	49.3	-8.6	-8.6	-8.3	1.6	1.6	1.64	1.64
1ecv	1.95	2	1.00	1.00	8.7	12.6	-8.5	-8.5	-8.5	0.5	0.5	0.48	0.44
1eed	2.00	19	0.25	0.20	585.1	1032	-10.9	-10.7	-11.5	1.3	1.5	5.15	8.94
1ejn	1.80	4	1.00	1.00	11.8	17.5	-10.4	-10.4	-10.3	0.7	0.6	0.56	0.55
1ela	1.80	9	0.95	0.70	59.7	288.0	-10.9	-10.9	-10.8	0.9	0.9	0.86	0.92
1elb	2.10	13	0.00	0.00	410.8	624.4	-	-	-8.1	-	-	5.27	5.21
1elc	1.75	13	0.00	0.00	433.2	654.9	-	-	-7.0	-	-	7.05	7.01
1eld	1.80	8	1.00	1.00	36.0	139.2	-11.0	-11.2	-11.0	1.2	1.0	1.12	0.97

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1ele	1.80	7	1.00	1.00	30.1	121.9	-9.9	-9.9	-9.9	0.9	0.8	0.85	0.84
1epb	2.20	1	1.00	1.00	4.7	9.3	-9.8	-9.8	-9.8	1.0	1.2	1.00	1.16
1eta	1.70	5	0.50	0.65	16.1	23.2	-10.9	-11.0	-10.9	1.5	1.5	2.00	1.89
1etr	2.20	8	0.50	1.00	57.2	283.9	-11.0	-11.0	-11.2	0.8	0.7	2.09	0.67
1ets	2.30	7	0.75	1.00	55.3	163.8	-12.5	-12.6	-12.8	0.6	0.5	0.48	0.37
1ett	2.50	5	0.55	0.60	23.7	35.8	-10.2	-10.2	-10.3	0.7	0.7	1.14	1.04
1ezq	2.20	8	0.30	0.60	62.3	178.1	-13.0	-12.6	-13.4	1.8	1.7	8.87	1.87
1f0r	2.10	4	0.40	0.85	18.9	27.6	-11.6	-11.7	-11.7	1.5	1.8	2.28	1.84
1f0s	2.10	4	0.35	0.60	17.7	28.5	-9.9	-9.9	-9.5	1.5	1.5	4.72	1.74
1f0t	1.80	4	0.30	0.60	19.8	28.5	-9.1	-9.1	-9.2	1.5	1.4	5.14	1.93
1f0u	1.90	8	0.30	0.55	75.4	193.3	-9.2	-10.1	-10.1	1.3	1.7	3.18	1.92
1f3d	1.87	2	0.85	0.90	6.9	21.3	-6.4	-6.4	-6.4	0.7	0.8	0.80	0.78
1fen	1.90	1	1.00	1.00	5.7	20.3	-10.4	-10.4	-10.4	0.9	0.8	0.88	0.80
1fh8	1.95	2	0.95	1.00	24.5	96.3	-8.6	-8.7	-9.0	1.1	0.6	0.84	0.49
1fh9	1.72	2	0.15	0.85	26.2	237.9	-9.2	-9.4	-9.9	0.7	0.5	5.17	0.42
1fhd	1.90	2	0.60	0.60	26.3	120.6	-8.6	-9.5	-9.6	1.0	0.7	1.67	1.50
1fjs	1.92	8	0.35	0.25	73.8	212.4	-11.5	-11.8	-11.8	1.7	1.8	2.22	2.33
1fkg	2.00	10	0.50	0.95	47.4	261.5	-10.3	-10.5	-10.6	1.4	1.4	1.87	1.42
1fki	2.20	0	1.00	1.00	5.8	9.1	-12.1	-12.1	-12.1	0.2	0.2	0.23	0.23
1flr	1.85	2	1.00	1.00	9.1	20.5	-6.4	-6.4	-6.4	0.4	0.4	0.39	0.39
1fq5	2.40	10	0.90	1.00	86.6	438.7	-16.6	-16.5	-16.9	0.3	0.2	0.29	0.20
1frp	2.00	4	0.85	0.85	32.6	120.6	-9.6	-9.6	-9.6	1.1	1.0	0.96	0.97
1fvt	2.20	2	1.00	1.00	13.6	41.5	-9.4	-9.4	-9.4	0.7	0.6	0.66	0.65
1g45	1.83	3	0.15	0.15	13.3	20.5	-8.3	-8.8	-7.8	1.4	2.0	3.71	2.22
1g46	1.84	3	0.05	0.00	13.0	19.5	-8.2	-	-7.8	1.7	-	4.63	4.69
1g48	1.86	3	0.20	0.00	12.3	19.1	-8.6	-	-8.8	1.6	-	2.89	2.84
1g4j	1.84	3	0.75	0.80	13.4	20.5	-10.3	-10.4	-10.1	1.1	1.1	1.11	1.07
1g4o	1.96	3	0.25	0.45	13.1	19.7	-8.3	-8.3	-8.4	0.7	0.7	4.33	4.20
1g52	1.80	3	0.55	0.40	11.7	19.0	-9.1	-9.0	-9.3	1.0	1.1	1.57	4.20
1g53	1.94	3	0.30	0.15	13.3	20.6	-8.7	-8.7	-8.7	1.1	1.3	4.65	4.82
1g54	1.86	3	0.35	0.35	12.4	18.7	-9.8	-9.8	-10.0	1.1	1.1	2.55	5.15
1g9v	2.00	6	0.00	0.15	19.1	27.0	-	-7.7	-7.2	-	1.6	5.45	5.36
1ghb	1.90	4	0.55	0.50	8.6	13.2	-8.2	-8.3	-8.1	1.1	1.3	1.94	1.98
1gkc	1.80	8	1.00	1.00	37.2	109.4	-9.0	-9.0	-9.1	1.3	1.2	1.22	1.21
1glp	2.20	10	0.60	1.00	49.3	264.4	-8.3	-8.5	-8.7	1.4	1.3	1.56	1.33
1glq	2.30	13	0.15	0.15	323.5	517.4	-10.7	-10.9	-11.3	1.4	1.7	2.36	2.45
1gm8	2.20	4	0.00	0.00	12.1	17.2	-	-	-6.8	-	-	5.94	5.27
1gpk	2.50	0	0.05	0.00	5.1	8.9	-7.3	-	-7.5	0.5	-	3.60	3.59
1gsp	2.20	2	0.85	0.95	12.1	18.1	-9.4	-9.6	-9.6	0.6	0.5	0.51	0.50
1hbv	1.56	14	0.50	0.70	479.8	733.7	-12.9	-13.0	-13.1	1.1	1.2	1.91	1.27
1hdc	2.90	6	1.00	1.00	29.3	110.7	-11.8	-11.8	-11.8	1.4	1.5	1.48	1.60
1hdy	2.70	0	1.00	1.00	3.0	17.2	-5.1	-5.0	-4.8	1.5	1.5	1.48	1.47
1hef	2.70	19	0.00	0.05	729.9	1179	-	-13.2	-14.4	-	2.0	3.58	3.77
1hfc	2.70	9	0.90	1.00	45.2	124.6	-11.6	-11.7	-11.7	1.3	1.2	1.38	1.20
1hgg	2.20	3	1.00	1.00	8.0	14.7	-1.0	-1.0	-1.0	0.7	0.7	0.71	0.73
1hgh	2.30	3	1.00	1.00	8.1	14.9	-1.1	-1.1	-1.0	0.8	0.8	0.80	0.80
1hgi	1.90	3	1.00	1.00	8.0	14.2	-1.3	-1.3	-1.3	0.7	0.7	0.71	0.71
1hgj	2.00	3	1.00	1.00	8.0	14.1	-1.1	-1.1	-1.1	0.6	0.6	0.64	0.65
1hih	3.00	15	0.65	0.90	367.0	702.7	-13.0	-13.4	-13.9	1.3	1.1	1.75	1.10
1hnn	1.90	1	1.00	1.00	6.4	18.3	-6.8	-6.9	-6.8	0.7	0.6	0.70	0.71

PDB ID	R, Å	N _{frb}	P		Time, s		dG, kcal/mol			RMSD converged		RMSD median	
			scr	doc	scr	doc	scr	doc	ref	scr	doc	scr	doc
1hp0	2.00	2	0.65	0.60	13.5	19.3	-9.8	-9.8	-9.9	0.6	0.5	0.67	0.64
1hps	1.89	16	0.35	0.65	468.9	856.2	-12.7	-12.4	-13.2	1.5	1.6	3.77	1.83
1hpx	2.80	11	1.00	1.00	284.2	498.6	-11.7	-11.7	-11.8	0.9	0.9	0.95	0.86
1hpx	2.20	14	0.05	0.05	479.4	823.5	-13.9	-13.5	-14.4	1.9	2.0	2.62	2.62
1hq2	2.80	1	0.80	0.85	6.5	17.1	-9.1	-9.2	-9.2	0.5	0.5	0.60	0.48
1hri	1.80	9	0.55	0.65	31.0	115.9	-7.9	-7.9	-7.9	1.3	1.3	1.89	1.35
1hsb	1.70	7	0.65	0.85	36.3	129.7	-7.1	-7.4	-7.5	1.3	1.2	1.52	1.33
1hsg	1.74	12	0.60	0.90	400.1	776.0	-12.8	-13.1	-14.4	1.2	1.2	1.48	1.20
1hsl	1.70	3	0.95	0.65	7.3	11.7	-7.3	-7.3	-7.3	0.6	0.8	0.46	1.19
1hte	2.50	8	0.15	0.05	48.1	159.6	-9.0	-8.6	-8.6	1.1	0.9	5.67	6.99
1htf	2.20	12	0.05	0.20	411.9	642.6	-11.4	-11.4	-11.4	1.6	1.6	8.71	8.43
1hti	2.40	3	1.00	1.00	12.0	57.3	-4.7	-4.8	-4.7	1.2	1.2	1.13	1.15
1hvr	2.40	8	0.95	1.00	42.4	312.1	-14.2	-14.3	-14.3	0.5	0.5	0.45	0.49
1hvy	1.80	5	0.60	0.70	15.5	21.8	-10.7	-10.8	-10.3	1.9	1.9	1.94	1.93
1hwi	2.40	8	0.80	1.00	44.5	236.3	-11.3	-11.4	-11.7	1.1	1.0	1.24	1.01
1hww	2.40	0	0.85	0.90	5.6	6.9	-7.3	-7.6	-7.7	0.5	0.3	0.37	0.31
1hyt	1.82	5	0.85	1.00	7.9	11.5	-6.9	-6.9	-6.5	1.1	1.1	1.03	1.06
1ia1	1.90	2	0.95	1.00	9.2	31.0	-8.9	-8.9	-8.9	0.6	0.4	0.44	0.34
1icn	2.06	15	0.00	0.05	222.5	387.7	-	-7.9	-7.6	-	1.9	8.94	6.93
1ida	1.65	14	0.60	0.60	520.1	971.4	-15.0	-14.9	-15.9	1.3	1.4	1.54	1.62
1ig3	2.10	4	0.90	0.75	12.5	19.6	-8.6	-8.2	-8.9	1.5	1.6	1.84	1.88
1igj	1.60	3	0.60	0.50	32.1	241.0	-8.8	-8.8	-8.8	1.5	1.5	1.64	2.04
1imb	1.80	2	0.25	0.20	13.4	66.3	-8.4	-8.6	-7.4	1.9	2.0	2.31	2.07
1ivb	1.90	3	1.00	1.00	8.6	12.9	-6.3	-6.4	-6.4	0.8	0.7	0.85	0.63
1ivc	2.20	1	0.85	1.00	6.0	10.9	-4.9	-4.9	-5.0	1.3	1.2	1.26	1.16
1ivd	1.80	3	0.00	0.00	8.0	19.4	-	-	-4.7	-	-	4.69	4.75
1ive	2.00	2	0.55	0.60	6.2	17.5	-4.2	-4.2	-3.9	1.6	1.8	1.99	1.98
1ivf	2.70	5	0.65	1.00	25.8	190.8	-8.5	-8.5	-8.4	1.7	1.7	1.71	1.69
1j3j	2.10	2	1.00	1.00	7.5	17.8	-9.1	-9.1	-9.1	0.4	0.3	0.34	0.32
1jap	2.00	7	0.90	0.85	50.0	140.5	-7.2	-7.3	-7.6	1.2	1.0	1.29	1.12
1jd0	1.90	1	0.10	0.00	8.9	30.7	-7.1	-	-6.8	0.3	-	4.24	4.34
1jje	1.90	7	0.45	0.55	22.4	92.8	-11.7	-11.9	-12.2	1.1	1.1	3.55	1.77
1jla	2.10	7	1.00	1.00	32.2	113.0	-10.1	-10.1	-10.1	0.5	0.5	0.52	0.50
1k3u	1.80	6	0.65	0.70	14.3	22.3	-8.5	-8.6	-8.9	1.1	0.8	1.89	0.77
1ke5	1.60	1	1.00	1.00	6.3	17.2	-9.8	-9.8	-9.8	0.5	0.4	0.34	0.33
1kel	1.90	10	0.90	0.80	37.9	203.0	-7.9	-8.0	-8.2	1.6	1.6	1.63	1.78
1kzk	2.40	9	0.85	0.95	70.7	363.2	-11.9	-12.0	-12.9	1.2	1.0	1.60	0.82
1l2s	1.80	3	1.00	1.00	11.7	34.6	-8.1	-8.1	-8.0	0.7	0.8	0.74	0.73
1l7f	2.05	7	1.00	1.00	29.8	133.7	-10.9	-10.9	-10.9	0.5	0.5	0.45	0.49
1lah	2.80	4	1.00	1.00	14.6	18.8	-8.2	-8.2	-8.2	0.6	0.7	0.75	0.78
1lcp	1.70	3	0.55	0.80	10.4	16.4	-8.2	-8.5	-8.1	1.0	1.0	1.21	1.03
1ldm	1.80	1	1.00	1.00	3.3	21.4	-5.7	-5.7	-5.1	0.6	0.6	0.64	0.62
1lic	2.10	15	0.45	0.60	220.6	378.4	-7.7	-7.8	-7.7	1.5	1.6	5.88	1.69
1lmo	2.10	6	0.00	0.00	282.5	551.8	-	-	-7.2	-	-	8.54	8.57
1lna	2.30	8	0.90	0.90	32.7	219.1	-7.1	-7.3	-7.2	1.5	1.4	1.60	1.49
1lpm	2.50	9	1.00	1.00	21.8	26.6	-7.3	-7.3	-7.3	0.9	1.0	0.92	0.93
1lpz	1.63	4	0.45	0.70	18.7	26.6	-12.6	-12.5	-12.6	0.8	0.7	2.19	0.69
1lrh	1.60	2	1.00	1.00	4.6	15.9	-7.0	-7.0	-7.1	0.5	0.5	0.46	0.42
1lst	1.60	5	1.00	1.00	15.5	73.3	-8.4	-8.3	-8.2	0.9	0.9	0.94	0.93
1m2z	1.60	2	1.00	1.00	13.8	18.4	-11.7	-11.7	-11.8	0.3	0.3	0.33	0.31

PDB ID	R, Å	N _{frb}	P		Time, s		dG, kcal/mol			RMSD converged		RMSD median	
			scr	doc	scr	doc	scr	doc	ref	scr	doc	scr	doc
1mbi	2.00	0	1.00	1.00	2.7	15.8	-3.6	-3.7	-3.7	0.4	0.3	0.43	0.25
1mcr	1.80	5	0.40	0.50	14.6	21.0	-6.3	-6.4	-6.1	1.6	1.9	2.04	2.02
1mdr	1.90	2	1.00	1.00	5.8	17.3	-5.7	-5.6	-5.5	1.4	1.3	1.58	1.56
1meh	2.20	6	0.05	0.00	23.0	24.5	-8.1	-	-8.3	0.8	-	2.74	2.49
1mfe	1.80	6	0.00	0.00	446.5	824.9	-	-	-7.8	-	-	5.98	6.05
1mld	1.70	5	1.00	0.95	9.6	13.7	-8.2	-8.2	-7.9	1.3	1.3	1.37	1.38
1mmq	1.70	6	1.00	1.00	44.6	154.8	-10.2	-10.5	-10.5	0.7	0.4	0.61	0.40
1mmv	1.80	8	0.65	0.65	40.6	129.0	-8.7	-8.8	-9.1	1.4	1.3	1.42	1.35
1mnc	2.00	9	1.00	1.00	37.4	126.5	-10.4	-10.4	-10.2	1.1	1.0	1.08	1.01
1mrg	1.80	0	0.95	1.00	3.8	9.1	-5.1	-5.1	-5.1	0.5	0.5	0.51	0.49
1mrk	1.80	2	0.85	0.90	16.4	22.1	-8.2	-8.2	-8.3	1.2	1.2	1.27	1.20
1mts	2.00	6	0.85	1.00	37.6	123.6	-10.0	-10.4	-10.4	1.2	1.2	1.20	1.28
1mup	1.80	2	0.50	0.65	6.1	25.4	-5.1	-5.1	-5.0	1.8	1.9	1.97	1.99
1mzc	1.95	7	0.35	0.50	48.9	165.3	-9.9	-10.3	-10.2	0.7	0.7	4.40	3.29
1n1m	1.90	2	0.95	1.00	7.4	11.1	-7.4	-7.4	-7.4	0.6	0.7	0.52	0.53
1n2j	2.40	3	0.10	0.05	7.6	10.9	-4.8	-4.8	-4.7	0.7	0.9	2.82	3.33
1n2v	1.90	3	0.50	0.40	9.2	32.8	-6.9	-7.3	-7.3	1.0	1.2	1.71	2.35
1n46	1.60	4	1.00	1.00	13.6	20.2	-12.1	-12.2	-12.2	0.4	0.4	0.37	0.34
1nav	2.30	5	0.85	0.95	14.0	21.9	-10.9	-10.9	-10.9	0.5	0.5	0.50	0.48
1nco	1.70	8	0.35	0.55	80.7	412.6	-13.7	-14.0	-14.2	1.1	0.6	7.25	1.23
1nis	1.90	5	0.90	0.95	8.9	13.6	-7.9	-8.2	-8.1	1.1	0.9	1.19	0.71
1nnb	1.65	5	0.65	0.95	28.4	173.6	-8.1	-8.1	-8.2	1.2	1.4	1.62	1.51
1nsc	1.78	5	0.85	1.00	28.6	191.0	-9.4	-9.4	-9.5	1.2	1.4	1.39	1.56
1nsd	1.80	5	0.60	0.90	26.6	174.7	-8.1	-8.1	-8.5	1.3	1.2	1.38	1.19
1odw	2.60	16	0.60	0.60	410.8	757.5	-11.4	-11.3	-12.1	1.1	1.2	1.80	1.71
1of1	2.65	2	1.00	1.00	9.0	13.3	-9.0	-9.1	-9.0	0.5	0.5	0.39	0.40
1of6	2.90	3	1.00	1.00	9.6	13.4	-8.2	-8.3	-8.3	0.5	0.5	0.48	0.47
1okl	2.70	2	0.90	0.90	12.0	37.2	-7.7	-7.7	-7.8	0.5	0.6	0.43	0.42
1opk	2.30	2	1.00	1.00	11.1	30.6	-13.1	-13.1	-13.2	0.6	0.6	0.58	0.56
1oq5	1.90	4	0.55	1.00	15.2	22.6	-11.3	-11.2	-11.3	0.7	0.7	0.95	0.74
1owe	1.80	2	0.70	0.55	11.2	36.1	-8.3	-8.3	-8.6	0.9	0.8	1.50	1.64
1oyt	1.80	3	0.80	1.00	12.4	17.4	-12.2	-12.2	-12.2	0.7	0.7	0.77	0.77
1p2y	1.90	1	0.90	1.00	4.5	16.5	-6.6	-6.6	-6.7	1.3	1.5	1.80	1.83
1p62	1.80	2	0.70	0.75	10.4	15.9	-7.9	-7.9	-7.6	0.8	0.7	0.82	0.69
1pbd	1.80	1	1.00	1.00	2.9	5.1	-4.4	-4.3	-4.3	0.5	0.5	0.46	0.44
1pgp	1.90	7	0.50	0.65	195.8	361.4	-10.0	-10.2	-9.5	1.8	1.8	1.96	1.92
1pha	1.80	8	0.45	0.55	32.8	112.3	-9.5	-9.6	-9.2	1.1	1.1	2.14	1.23
1phd	1.40	1	1.00	1.00	3.6	10.7	-5.7	-5.7	-5.8	1.0	0.9	0.96	0.95
1phf	2.00	1	1.00	1.00	4.1	15.6	-5.8	-5.8	-5.3	1.1	1.1	1.21	1.20
1phg	1.90	3	0.90	0.90	8.7	28.0	-7.2	-7.7	-8.1	1.2	0.8	1.31	0.81
1pmn	1.90	6	1.00	0.95	39.1	129.9	-12.2	-12.2	-12.3	0.8	0.8	0.71	0.85
1poc	2.75	23	0.05	0.00	596.2	976.5	-13.4	-	-13.4	1.9	-	2.55	2.70
1ppc	1.90	7	0.70	1.00	65.5	181.1	-11.2	-11.1	-11.0	1.0	1.3	1.25	1.27
1pph	1.80	5	0.45	0.60	25.7	38.6	-9.9	-9.9	-9.9	0.5	0.5	2.90	0.74
1ppi	1.70	11	0.00	0.15	1582	2432	-	-16.1	-18.1	-	1.3	5.13	4.99
1ppk	1.70	14	0.35	0.55	358.5	570.0	-9.9	-9.8	-10.0	0.9	0.9	4.61	1.18
1ppl	2.40	18	0.45	0.65	486.9	826.6	-12.6	-12.8	-13.1	1.4	1.3	2.16	1.51
1ppm	2.40	17	0.05	0.10	449.3	817.9	-11.0	-11.4	-11.7	0.9	1.6	5.51	4.51
1pro	1.85	10	0.80	0.95	287.1	527.6	-14.4	-14.4	-14.4	0.5	0.5	0.48	0.47
1pso	2.20	22	0.05	0.00	890.8	1403	-12.4	-	-13.0	1.6	-	12.49	13.14

PDB ID	R, Å	N _{frb}	P		Time, s		dG, kcal/mol			RMSD converged		RMSD median	
			scr	doc	scr	doc	scr	doc	ref	scr	doc	scr	doc
1q1g	2.20	3	1.00	1.00	14.4	21.4	-10.7	-10.8	-11.0	0.8	0.5	0.74	0.47
1q41	1.87	0	1.00	1.00	5.3	8.4	-8.6	-8.6	-8.5	0.3	0.3	0.31	0.32
1q4g	1.63	3	1.00	1.00	7.3	21.2	-8.0	-8.1	-7.7	0.9	0.9	0.86	0.92
1qbr	1.40	6	0.95	1.00	42.0	209.2	-17.0	-17.1	-17.2	0.3	0.3	0.30	0.27
1qbu	2.90	8	0.85	1.00	48.8	341.9	-14.4	-14.6	-14.5	0.8	0.8	0.76	0.75
1r1h	2.00	9	0.75	0.90	45.4	261.2	-11.4	-11.2	-11.6	1.2	1.3	1.32	1.25
1r55	1.80	8	0.85	0.90	43.8	131.5	-9.6	-9.6	-9.4	1.3	1.3	1.37	1.39
1r58	1.90	7	0.60	0.50	52.5	147.3	-9.8	-9.9	-9.0	1.2	1.2	1.34	2.13
1r9o	1.90	3	1.00	1.00	8.7	28.3	-7.4	-7.5	-6.6	1.0	1.0	0.93	0.92
1rbp	2.00	2	1.00	1.00	7.1	9.5	-10.9	-10.9	-10.8	0.6	0.6	0.61	0.61
1rds	2.80	8	0.90	0.80	478.1	583.1	-11.6	-11.8	-12.1	1.0	1.0	0.77	1.03
1rhl	3.10	4	0.75	0.95	38.9	152.9	-8.4	-8.4	-8.5	1.1	1.3	1.40	1.50
1rls	1.90	4	0.95	1.00	31.8	104.3	-9.5	-9.5	-9.5	0.6	0.7	0.67	0.67
1rne	2.70	21	0.25	0.55	713.4	1149	-15.8	-15.2	-15.6	1.3	1.4	6.64	1.77
1rnt	2.25	4	0.75	0.90	40.5	151.9	-8.6	-8.6	-7.7	1.6	1.5	1.71	1.65
1rob	2.88	4	1.00	1.00	30.2	106.3	-8.3	-8.4	-8.0	1.1	1.1	1.09	1.09
1s19	1.80	4	1.00	1.00	16.8	177.4	-14.3	-14.3	-14.4	0.8	0.7	0.69	0.65
1s3v	3.00	5	0.15	0.55	19.3	26.4	-9.6	-9.6	-9.6	0.8	0.6	7.83	0.73
1sbg	3.00	14	1.00	1.00	321.6	641.9	-12.2	-12.1	-12.4	0.8	0.7	0.82	0.61
1sbp	1.60	0	1.00	1.00	3.6	55.1	-5.1	-5.1	-5.0	0.4	0.4	0.37	0.38
1sg0	1.60	0	1.00	1.00	7.5	14.3	-8.5	-8.5	-8.6	0.8	0.7	0.93	0.79
1sj0	2.10	6	1.00	1.00	51.8	147.3	-13.4	-13.4	-13.5	0.7	0.8	0.75	0.74
1slt	3.00	5	0.70	0.90	256.8	508.6	-6.3	-6.3	-5.7	1.7	1.7	1.89	1.83
1snc	1.71	6	0.55	0.65	30.3	97.7	-12.0	-11.6	-12.3	1.3	1.1	1.75	1.24
1sq5	2.10	6	0.00	0.00	25.1	93.0	-	-	-5.5	-	-	4.34	4.31
1sqn	2.50	1	1.00	1.00	5.7	8.8	-10.6	-10.7	-10.6	0.4	0.3	0.27	0.21
1sre	2.40	1	1.00	1.00	4.8	8.2	-7.1	-7.1	-7.1	0.5	0.5	0.43	0.44
1srj	1.75	1	0.85	1.00	6.2	11.7	-6.8	-7.2	-7.2	0.8	0.8	0.84	0.85
1stp	2.00	5	1.00	1.00	11.1	16.8	-8.8	-8.9	-8.9	0.6	0.6	0.63	0.61
1t40	1.70	5	1.00	1.00	14.0	22.0	-14.0	-14.1	-14.1	0.5	0.5	0.45	0.37
1t46	1.90	3	1.00	1.00	12.3	18.1	-14.5	-14.5	-14.4	0.7	0.6	0.74	0.59
1t9b	1.90	2	1.00	1.00	9.1	32.2	-8.1	-8.3	-8.3	0.8	0.7	0.83	0.77
1tdb	2.90	4	0.95	0.95	16.8	24.5	-6.7	-7.3	-7.1	1.1	1.2	1.06	1.13
1thy	1.90	4	0.50	0.50	14.9	21.8	-6.1	-6.2	-6.0	0.7	0.8	1.94	1.84
1tka	1.70	8	0.90	0.95	55.1	138.8	-13.9	-14.1	-13.8	1.3	1.3	1.42	1.27
1tlp	1.90	11	0.25	0.20	522.7	752.2	-11.7	-11.7	-11.4	1.7	1.8	2.35	7.66
1tmn	2.40	13	0.70	0.70	368.7	515.2	-11.6	-11.5	-12.0	1.7	1.6	1.78	1.66
1tng	2.90	1	1.00	1.00	5.0	14.0	-6.4	-6.4	-6.4	1.0	0.9	0.99	0.99
1tnh	1.70	1	1.00	0.95	5.2	14.2	-6.2	-6.2	-6.1	0.6	0.6	0.61	0.57
1tni	1.78	4	0.65	0.35	10.2	14.6	-6.5	-6.5	-6.5	1.0	1.2	1.22	2.31
1tnj	2.70	2	1.00	0.95	7.7	23.0	-5.9	-5.9	-5.8	1.4	1.5	1.40	1.57
1tnk	2.50	3	1.00	1.00	7.6	11.5	-6.2	-6.2	-6.2	0.9	0.9	0.91	0.95
1tnl	1.80	1	1.00	1.00	4.9	12.7	-6.4	-6.3	-6.5	0.5	0.5	0.53	0.52
1tow	3.00	4	1.00	1.00	9.1	13.0	-7.0	-7.0	-7.0	0.9	0.9	0.82	0.80
1tph	2.10	3	1.00	1.00	7.3	12.1	-6.3	-6.3	-6.0	0.8	0.9	0.65	0.97
1tpp	2.40	4	1.00	1.00	12.0	16.9	-9.2	-9.2	-9.2	0.2	0.2	0.23	0.23
1trk	2.30	8	1.00	1.00	55.3	140.7	-14.4	-14.4	-14.6	1.4	1.5	1.64	1.66
1tt1	1.70	4	1.00	1.00	8.0	11.7	-8.8	-8.8	-8.8	0.5	0.5	0.52	0.53
1tyl	2.20	1	1.00	1.00	5.2	18.4	-4.2	-4.2	-4.2	1.0	0.9	0.97	0.91
1tz8	2.50	4	1.00	1.00	12.8	17.5	-8.2	-8.2	-8.2	0.6	0.6	0.60	0.60

PDB ID	R, Å	N _{frb}	P		Time, s		dG, kcal/mol			RMSD converged		RMSD median	
			scr	doc	scr	doc	scr	doc	ref	scr	doc	scr	doc
1u1c	1.80	6	1.00	1.00	24.6	99.3	-9.6	-9.8	-9.7	1.3	1.6	1.47	1.66
1u4d	2.08	0	1.00	1.00	5.2	10.2	-7.5	-7.5	-7.5	0.3	0.4	0.34	0.35
1ukz	1.90	4	0.55	0.55	29.6	110.4	-11.8	-11.8	-11.9	0.6	0.6	0.84	0.81
1ulb	2.40	0	0.50	0.80	3.5	8.2	-6.0	-6.0	-5.9	0.7	0.6	2.01	0.58
1uml	1.83	8	0.45	0.65	59.6	168.0	-10.4	-10.7	-10.0	1.2	1.3	6.44	1.62
1unl	2.30	6	1.00	1.00	31.3	121.6	-9.3	-9.3	-9.3	0.5	0.5	0.55	0.46
1uou	1.60	2	1.00	1.00	8.0	26.3	-8.2	-8.2	-8.2	1.4	1.4	1.50	1.50
1v0p	1.67	6	1.00	1.00	37.2	132.0	-10.4	-10.4	-10.4	0.7	0.8	0.60	0.62
1v48	2.00	6	0.85	0.85	21.0	31.2	-9.2	-9.4	-9.7	1.1	0.8	1.16	0.79
1v4s	1.80	2	0.90	1.00	10.1	33.1	-10.5	-10.8	-10.7	1.0	1.0	0.72	0.81
1vcj	2.00	7	1.00	1.00	31.5	222.2	-10.4	-10.4	-10.3	0.9	0.9	0.96	0.95
1vgc	2.20	5	1.00	1.00	25.5	29.6	-7.4	-7.5	-7.4	0.6	0.5	0.55	0.54
1w1p	1.60	0	1.00	1.00	3.3	8.4	-5.0	-5.0	-4.9	0.3	0.3	0.34	0.34
1w2g	1.67	2	1.00	1.00	9.5	14.1	-8.5	-8.5	-8.5	0.9	0.8	0.90	0.82
1wap	2.00	3	0.95	1.00	9.9	13.1	-7.9	-7.9	-7.9	0.5	0.5	0.38	0.42
1x8x	2.00	3	0.95	1.00	11.1	16.0	-7.6	-7.6	-7.7	0.7	0.6	0.59	0.57
1xid	1.90	2	1.00	1.00	6.9	10.8	-7.9	-7.7	-7.7	0.9	0.9	1.06	0.98
1xie	1.49	1	1.00	1.00	6.5	10.2	-7.8	-8.0	-8.1	0.5	0.5	0.52	0.48
1xm6	2.50	5	0.00	0.00	10.4	15.4	-	-	-7.9	-	-	2.51	2.53
1xoq	1.60	6	0.90	0.85	19.3	31.2	-10.1	-10.1	-10.0	0.7	0.7	0.68	0.67
1xoz	1.97	1	1.00	1.00	7.9	22.0	-8.2	-8.1	-8.2	0.7	0.6	0.43	0.40
1y6b	2.80	6	0.70	1.00	26.5	36.1	-11.8	-11.9	-12.1	0.6	0.5	0.61	0.53
1ygc	2.00	8	1.00	1.00	112.8	277.1	-12.9	-13.0	-12.9	1.5	1.6	1.65	1.64
1yqy	2.30	4	0.55	0.90	11.5	18.6	-10.6	-10.6	-10.9	0.9	0.7	1.75	0.73
1yv3	2.00	0	1.00	1.00	5.2	8.5	-10.3	-10.2	-10.4	0.4	0.4	0.37	0.38
1yvf	2.50	4	1.00	0.95	12.2	17.8	-9.8	-9.8	-9.9	0.7	0.8	0.54	0.57
1ywr	1.95	5	0.90	0.95	22.9	34.8	-12.0	-12.1	-12.3	0.5	0.6	0.55	0.56
1z95	1.80	6	1.00	1.00	23.6	124.6	-12.1	-12.2	-12.2	0.5	0.5	0.48	0.48
2ack	2.40	2	1.00	1.00	5.8	15.7	-5.6	-5.6	-5.6	0.9	1.0	0.90	0.99
2ada	2.40	2	0.90	1.00	24.3	95.1	-9.2	-9.3	-9.4	0.4	0.3	0.35	0.31
2ak3	1.85	4	0.45	0.75	30.8	109.4	-9.2	-9.2	-9.2	0.7	0.6	2.84	0.75
2bm2	2.20	6	0.95	0.95	39.9	129.5	-10.8	-10.7	-10.9	0.6	0.7	0.49	0.59
2br1	2.00	5	1.00	1.00	19.1	26.6	-8.4	-8.4	-8.4	1.4	1.4	1.38	1.35
2bsm	2.05	4	1.00	1.00	17.1	23.8	-10.0	-10.0	-10.0	0.8	0.8	0.79	0.79
2cgr	2.20	7	1.00	1.00	25.8	120.3	-6.9	-7.0	-6.9	0.7	0.7	0.75	0.74
2cht	2.20	2	1.00	1.00	5.9	10.5	-8.7	-8.7	-8.7	0.4	0.4	0.44	0.38
2cmd	1.87	5	1.00	1.00	10.1	15.6	-8.3	-8.4	-8.4	1.4	1.3	1.41	1.40
2cpp	1.63	0	1.00	1.00	2.6	5.0	-5.9	-5.9	-5.9	0.5	0.5	0.51	0.51
2ctc	1.40	3	1.00	1.00	5.9	8.6	-6.8	-6.9	-6.9	0.7	0.7	0.65	0.67
2dbl	2.90	6	1.00	1.00	24.9	88.5	-11.5	-11.5	-11.5	0.8	0.9	0.87	0.88
2er6	2.00	29	0.05	0.00	2213	3038	-13.4	-	-13.6	1.3	-	9.89	10.71
2fox	1.80	7	0.90	1.00	50.8	277.1	-11.0	-11.1	-11.3	0.7	0.6	0.71	0.55
2gbp	1.90	1	1.00	1.00	16.0	72.5	-9.3	-9.3	-9.3	0.3	0.3	0.32	0.31
2h4n	1.90	1	0.95	0.85	6.9	27.2	-7.6	-7.7	-7.6	1.0	1.2	1.34	1.57
2ifb	2.00	14	0.65	0.80	203.7	342.8	-7.9	-7.9	-7.9	1.5	1.6	1.67	1.76
2lgs	2.80	4	0.70	0.80	9.4	13.8	-6.8	-6.8	-6.7	0.7	0.6	0.70	0.67
2mcp	3.10	4	1.00	1.00	6.1	9.6	-4.6	-4.7	-4.5	1.6	1.6	1.57	1.66
2mth	1.90	2	0.80	0.90	5.6	18.0	-5.1	-5.1	-5.2	1.1	1.1	1.06	1.06
2phh	2.70	1	1.00	1.00	3.6	6.4	-5.3	-5.4	-5.4	0.6	0.6	0.60	0.59
2pk4	2.25	5	1.00	1.00	11.6	18.0	-5.7	-5.7	-5.4	1.0	1.0	0.96	0.94

PDB ID	R, Å	N _{frb}	P		Time, s		dG, kcal/mol			RMSD converged		RMSD median	
			scr	doc	scr	doc	scr	doc	ref	scr	doc	scr	doc
2plv	2.88	15	0.00	0.00	313.4	591.9	-	-	-8.0	-	-	9.12	8.46
2qwk	1.80	6	1.00	1.00	14.9	72.3	-9.4	-9.4	-9.5	0.7	0.6	0.52	0.52
2r04	3.00	9	0.55	0.75	41.9	120.8	-9.0	-9.1	-9.0	1.7	1.6	1.79	1.65
2r07	3.00	7	0.65	0.70	29.2	106.3	-9.1	-9.1	-9.0	1.6	1.7	1.81	1.81
2sim	1.60	5	0.55	0.95	31.5	177.6	-8.9	-9.1	-8.9	1.3	1.4	1.53	1.46
2tmn	1.60	5	0.60	0.80	10.9	17.7	-8.4	-8.7	-8.3	1.2	1.2	1.61	1.32
2tpi	2.10	6	1.00	1.00	23.3	95.6	-8.8	-8.8	-8.9	0.6	0.5	0.47	0.45
2tsc	1.97	7	0.2	0.25	73.2	124.4	-12.5	-12.7	-12.8	1.8	2.1	2.18	2.18
2upj	3.00	13	0.30	0.60	376.7	554.6	-10.9	-10.9	-10.7	1.8	1.9	2.06	1.97
2xis	1.71	4	1.00	0.95	24.2	93.2	-6.9	-6.9	-7.0	0.6	0.7	0.37	0.38
2yhx	2.10	3	0.95	1.00	19.9	95.3	-10.8	-10.9	-10.8	1.2	1.2	1.26	1.28
2ypi	2.50	3	1.00	1.00	14.0	65.1	-5.5	-5.6	-5.2	1.0	1.1	0.97	1.07
3aah	2.40	3	0.90	0.90	7.6	12.3	-12.4	-12.5	-12.6	0.6	0.6	0.64	0.63
3cla	1.75	6	0.00	0.00	28.7	110.6	-	-	-6.4	-	-	6.29	7.55
3cpa	2.00	5	0.45	0.80	26.4	98.6	-9.2	-9.0	-9.0	0.8	0.8	2.14	0.85
3dfr	1.70	7	0.80	0.85	44.6	150.5	-12.2	-12.3	-12.4	0.6	0.8	0.69	0.80
3ert	1.90	8	1.00	1.00	36.6	113.1	-11.1	-11.1	-11.2	1.6	1.5	1.57	1.53
3gch	1.90	2	1.00	1.00	5.9	9.9	-5.6	-5.6	-5.6	0.4	0.4	0.42	0.42
3hvt	2.90	1	1.00	1.00	5.2	12.0	-8.0	-8.0	-8.0	0.4	0.4	0.33	0.34
3mth	1.90	2	0.70	0.45	5.7	18.3	-5.1	-5.1	-5.1	1.0	1.0	1.12	4.20
3ptb	1.70	0	1.00	1.00	2.9	5.6	-6.2	-6.2	-6.2	0.1	0.1	0.14	0.14
3tpi	1.90	6	1.00	1.00	20.3	89.0	-9.0	-9.0	-9.2	0.5	0.4	0.43	0.41
4aah	2.40	3	0.85	0.95	10.1	13.5	-12.2	-12.2	-12.1	0.7	0.7	0.73	0.67
4cts	2.90	3	1.00	1.00	8.0	40.7	-7.1	-7.1	-7.0	0.6	0.5	0.39	0.38
4dfr	1.70	7	0.75	0.80	55.0	145.7	-11.5	-11.6	-11.5	1.3	1.2	1.36	1.32
4est	1.78	13	0.00	0.00	115.3	122.3	-	-	-10.4	-	-	3.70	3.71
4fab	2.70	2	0.75	0.70	7.9	20.2	-6.7	-6.7	-6.7	0.9	0.9	0.93	0.94
4fbp	2.50	4	0.35	0.50	30.4	106.4	-8.6	-8.6	-9.1	1.4	1.4	2.74	1.99
4fxn	1.80	7	0.95	1.00	45.9	269.4	-11.8	-11.8	-11.7	0.8	0.6	0.87	0.61
4hmg	3.00	3	1.00	1.00	8.0	14.4	-1.3	-1.3	-1.3	0.4	0.5	0.40	0.40
4phv	2.10	12	0.25	0.25	442.5	789.4	-12.8	-15.0	-15.3	1.6	0.9	3.96	4.02
4tim	2.40	4	1.00	1.00	7.5	12.1	-7.4	-7.5	-7.1	1.2	1.3	1.26	1.28
4tln	2.30	3	0.65	0.65	10.2	16.2	-5.9	-6.2	-5.7	1.8	1.9	1.91	1.97
4tmn	1.70	14	0.30	0.40	380.3	600.3	-12.6	-12.1	-13.0	1.3	1.4	6.65	6.51
4tpi	2.20	5	1.00	1.00	13.8	20.3	-8.6	-8.6	-8.6	0.6	0.6	0.60	0.59
4ts1	2.50	3	0.95	1.00	9.7	14.1	-7.1	-7.2	-6.1	0.7	0.7	0.60	0.73
5abp	1.80	1	1.00	1.00	16.0	70.3	-8.2	-8.3	-8.3	0.7	0.6	0.56	0.46
5cpp	2.08	0	1.00	1.00	2.7	4.8	-6.0	-5.9	-5.9	1.1	1.3	0.94	1.41
5cts	1.90	3	1.00	1.00	9.0	45.4	-8.0	-8.0	-8.0	0.3	0.2	0.25	0.24
5p2p	2.40	20	0.80	0.70	478.0	771.5	-12.8	-12.8	-13.1	1.4	1.6	1.45	1.75
5tim	1.83	0	0.00	0.00	4.8	25.6	-	-	-5.7	-	-	2.99	3.00
5tln	2.30	8	0.90	1.00	45.1	244.8	-9.0	-9.0	-9.0	1.3	1.4	1.34	1.32
5tmn	1.60	14	0.15	0.05	336.7	501.0	-12.6	-12.6	-12.8	1.7	0.8	2.24	2.23
6abp	1.67	0	0.95	0.95	5.4	7.2	-6.8	-6.9	-7.0	0.7	0.8	0.54	0.83
6cpa	2.00	12	0.50	0.50	71.4	290.3	-13.3	-13.4	-13.8	1.1	1.0	2.50	2.47
6rnt	1.80	4	0.90	0.90	33.4	148.7	-7.4	-7.5	-7.5	0.9	1.0	0.85	0.90
6rsa	2.00	2	1.00	1.00	9.4	14.4	-7.1	-7.1	-7.2	0.8	0.8	0.75	0.80
6tim	2.20	4	1.00	1.00	10.3	16.9	-7.4	-7.4	-7.1	1.1	1.1	1.14	1.18
6tmn	1.60	14	0.05	0.00	324.2	500.5	-11.1	-	-11.3	2.0	-	2.77	2.72
7abp	1.67	0	0.85	1.00	5.7	7.4	-7.2	-7.2	-7.4	1.1	0.9	1.09	0.98

PDB ID	R, Å	N _{frb}	P		Time, s		dG, kcal/mol			RMSD converged		RMSD median	
			scr	doc	scr	doc	scr	doc	ref	scr	doc	scr	doc
7cpa	2.00	15	0.25	0.70	358.6	667.8	-14.4	-14.1	-14.6	1.8	1.6	2.66	1.86
7cpp	2.00	0	1.00	1.00	3.3	16.9	-4.5	-4.5	-4.5	1.3	1.3	1.30	1.30
7tim	1.90	3	1.00	1.00	7.6	12.1	-6.0	-6.1	-6.5	1.1	1.0	1.13	1.08
7upj	2.00	5	0.45	0.55	21.0	30.0	-12.9	-9.7	-10.0	1.2	1.3	2.15	1.35
8abp	1.49	1	1.00	1.00	15.4	69.9	-8.2	-8.2	-8.4	0.6	0.5	0.61	0.52
8atc	2.50	6	1.00	1.00	12.3	18.5	-12.8	-12.5	-13.0	0.7	0.8	0.75	0.76
8gch	1.60	8	1.00	1.00	46.8	52.7	-9.5	-9.5	-9.5	0.3	0.3	0.28	0.28
9abp	1.97	1	1.00	1.00	15.8	70.1	-8.2	-8.3	-8.3	0.7	0.4	0.49	0.39
9hvp	2.80	20	0.70	0.35	707.5	1148	-15.4	-15.1	-15.3	1.7	1.7	1.83	2.20

Docking performance of Lead-Finder was benchmarked on the set of 407 protein-ligand complexes in the default docking (doc) and screening (scr) regimes. Column 'PDBid' contains PDB codes of protein-ligand complexes used for current benchmarking studies, and column 'R' – structure resolution in Å; column 'N_{FRB}' contains the number of freely rotatable ligand bonds; column 'P' – probability of successful ligand docking (with RMSD of 2 Å and less) determined by 20 independent docking runs; column 'Time' contains time needed for ligand docking (Linux x86_64, Intel Core2Duo 2.4GHz); column 'dG' lists binding energies (dG-score) for the top-ranked poses (ref – reference ligand pose from PDB structure); column 'RMSD converged' contains RMSD of top-scored ligand poses from the corresponding reference poses averaged over successful docking runs (those of 20 independent runs, for which RMSD of 2 Å and less was obtained), while c 'RMSD median' contains data averaged over all 20 independent docking runs.