

Table S4. Running time (in minutes) and running time fold improvement for new ZDOCK versions 3.0.1, 3.0.2f, and 3.0.2 (versus ZDOCK 3.0) for all test cases in docking Benchmark 4.0.

L/R Switch indicates switching of ligand and receptor for that test case in ZDOCK 3.0.2.

Test Case	ZDOCK 3.0	ZDOCK 3.0.1		ZDOCK 3.0.2f		ZDOCK 3.0.2		L/R Switch
	Time	Time	Fold Improve	Time	Fold Improve	Time	Fold Improve	
1A2K	130.8	21.37	6.1	20.05	6.5	21.45	6.1	Y
1ACB	73.35	17.38	4.2	9.97	7.4	10	7.3	N
1AHW	302.63	50.28	6.0	45.5	6.7	35.22	8.6	Y
1AK4	96.75	21.25	4.6	21.15	4.6	12.48	7.8	Y
1AKJ	170.65	23.48	7.3	23.47	7.3	18.83	9.1	N
1ATN	165.6	20.62	8.0	20.68	8.0	19.33	8.6	N
1AVX	72.17	16.57	4.4	15.67	4.6	12.87	5.6	Y
1AY7	48.52	8.42	5.8	8.4	5.8	7.55	6.4	N
1AZS	178.35	35.17	5.1	34.5	5.2	25.58	7.0	Y
1B6C	122.18	27.28	4.5	25.95	4.7	15.23	8.0	Y
1BGX	391.65	66.13	5.9	60.32	6.5	46.72	8.4	Y
1BJ1	248.68	33.72	7.4	32.22	7.7	28.57	8.7	N
1BKD	296.85	24.5	12.1	22.75	13.0	23.73	12.5	N
1BUH	131.17	19.13	6.9	21.12	6.2	15.12	8.7	N
1BVK	103.12	19.97	5.2	19.5	5.3	12.83	8.0	N
1BVN	130.12	16	8.1	16.1	8.1	12.32	10.6	N
1CGI	76.7	9.7	7.9	9.53	8.0	9.57	8.0	N
1CLV	97.93	11.73	8.3	11.87	8.3	8.58	11.4	N
1D6R	72.8	13.97	5.2	10.88	6.7	9.97	7.3	N
1DF4	541.57	99.28	5.5	98.7	5.5	62.07	8.7	Y
1DFJ	166.35	27.83	6.0	26.32	6.3	21.15	7.9	Y
1DQJ	163.82	24.07	6.8	20.72	7.9	15.5	10.6	N
1E4K	211.43	37.28	5.7	31.72	6.7	24.98	8.5	N
1E6E	164.33	18.43	8.9	15.82	10.4	18.35	9.0	N
1E6J	128.77	16.72	7.7	14.75	8.7	14.43	8.9	N
1E96	130.3	22.88	5.7	23.9	5.5	20.82	6.3	Y
1EAW	57.82	10.23	5.7	9.52	6.1	9.53	6.1	N
1EER	249.03	53.42	4.7	53.75	4.6	29.82	8.4	Y
1EFN	42.25	7.03	6.0	5.8	7.3	5.8	7.3	N
1EWY	83.65	13.22	6.3	14.93	5.6	10.2	8.2	N
1EZU	133.22	25.75	5.2	25.73	5.2	17.53	7.6	Y
1F34	125.73	21.43	5.9	22.47	5.6	20	6.3	N
1F51	131.18	17.98	7.3	19.07	6.9	13.8	9.5	N
1F6M	131.28	16.23	8.1	17.97	7.3	11.78	11.1	N
1FAK	449.83	53.73	8.4	47.03	9.6	41.22	10.9	N
1FC2	163.65	28.25	5.8	28.03	5.8	18.33	8.9	Y
1FCC	128.48	16.82	7.6	15.25	8.4	14.38	8.9	N
1FFW	48.32	9.88	4.9	9.85	4.9	7.17	6.7	Y
1FLE	47.88	10.2	4.7	8.53	5.6	7.68	6.2	N
1FQ1	127.77	22.32	5.7	21.13	6.0	15.8	8.1	Y
1FQJ	163.5	27.43	6.0	21.32	7.7	19.78	8.3	N
1FSK	172.45	23.9	7.2	22.78	7.6	22.28	7.7	N
1GCQ	83.77	12.52	6.7	11.78	7.1	9.7	8.6	N
1GHQ	132.57	21.93	6.0	21.93	6.0	16.3	8.1	Y
1GL1	77.22	13.57	5.7	9.23	8.4	8.53	9.1	N
1GLA	163.43	23.45	7.0	20.5	8.0	16.45	9.9	N
1GP2	249.3	49.55	5.0	34.5	7.2	29.67	8.4	Y
1GPW	102.55	20.22	5.1	20.08	5.1	18.88	5.4	Y
1GRN	131.43	22.62	5.8	23.1	5.7	16.72	7.9	N
1GXD	245.43	39.5	6.2	29.47	8.3	26.88	9.1	N
1H1V	394.47	58.87	6.7	54.2	7.3	40.33	9.8	Y
1H9D	96.85	24.42	4.0	14.78	6.6	12.08	8.0	Y
1HCF	167.78	43.17	3.9	23.65	7.1	18.2	9.2	Y
1HE1	133.25	16.73	8.0	16.67	8.0	16.8	7.9	Y
1HE8	246.88	32.1	7.7	30.05	8.2	22.37	11.0	N
1HIA	58.45	11.48	5.1	10.05	5.8	10.05	5.8	N
1I2M	124.03	25.58	4.8	25.1	4.9	22.82	5.4	Y
1I4D	655.48	67.83	9.7	44.1	14.9	30.15	21.7	N

1I9R	177.07	40.15	4.4	39.83	4.4	26.4	6.7	Y
1IB1	249.17	38.68	6.4	25.88	9.6	24.27	10.3	N
1IBR	179.38	47.52	3.8	47.12	3.8	20.6	8.7	Y
1IJK	255.88	24.77	10.3	23.33	11.0	18.35	13.9	N
1IQD	168.5	27.08	6.2	23.3	7.2	21.65	7.8	N
1IRA	131.8	21.07	6.3	19.55	6.7	17.6	7.5	N
1J2J	71.75	9.77	7.3	9.6	7.5	9.88	7.3	N
1JIW	167.97	20.42	8.2	16.25	10.3	14.82	11.3	N
1JK9	98.33	18.43	5.3	19.32	5.1	12.35	8.0	N
1JMO	170.5	21.35	8.0	20.97	8.1	22.37	7.6	N
1JPS	300.15	45.13	6.7	42.87	7.0	35.23	8.5	Y
1JTG	96.92	19.9	4.9	17.13	5.7	18.02	5.4	N
1JWH	300.35	36.07	8.3	36.07	8.3	33.25	9.0	N
1JZD	177.93	30.28	5.9	25.73	6.9	22.2	8.0	N
1K4C	209.68	43.18	4.9	37.55	5.6	30.12	7.0	N
1K5D	211.75	35.38	6.0	34.25	6.2	29.13	7.3	Y
1K74	127.73	28.75	4.4	25.35	5.0	17.82	7.2	Y
1KAC	83.27	19.88	4.2	13.83	6.0	11.45	7.3	N
1KKL	127.43	16.78	7.6	16.73	7.6	14.48	8.8	N
1KLU	211.43	31.53	6.7	31.03	6.8	24.78	8.5	N
1KTZ	131.93	16	8.2	15.83	8.3	12.57	10.5	N
1KXP	299.08	52.32	5.7	47.73	6.3	37.67	7.9	Y
1KXQ	165	17.2	9.6	17.53	9.4	18.45	8.9	N
1LFD	47.87	9.98	4.8	9.92	4.8	9.95	4.8	N
1M10	214.15	39.95	5.4	30.72	7.0	22.25	9.6	Y
1MAH	96.25	19.58	4.9	17.2	5.6	16.32	5.9	N
1ML0	211.57	27.32	7.7	23.2	9.1	22.85	9.3	N
1MLC	162.38	22.67	7.2	20.57	7.9	14.9	10.9	N
1MQ8	171.08	18.38	9.3	17.87	9.6	14.48	11.8	N
1N2C	447.17	85.8	5.2	85.8	5.2	70.08	6.4	N
1N80	96.95	24.55	3.9	17.82	5.4	13.95	6.9	Y
1NCA	247.35	36.7	6.7	36.52	6.8	28.43	8.7	N
1NSN	164.3	22.7	7.2	20.95	7.8	16.65	9.9	N
1NW9	102.45	18.35	5.6	16.4	6.2	11.72	8.7	N
1OC0	83.05	14.2	5.8	10.2	8.1	7.87	10.6	N
1OFU	123.67	22.48	5.5	22.42	5.5	19.73	6.3	Y
1OPH	170.48	22.08	7.7	21.77	7.8	22.73	7.5	N
1OYV	132.18	19.45	6.8	19.13	6.9	14.58	9.1	Y
1PPE	42.35	7.95	5.3	7.13	5.9	5.53	7.7	N
1PVH	210.5	26.82	7.8	23.57	8.9	17.53	12.0	N
1PXV	83.25	19.17	4.3	19.12	4.4	15.65	5.3	N
1QA9	366.82	39.78	9.2	34.42	10.7	33.55	10.9	N
1QFW	248.37	43.68	5.7	35.22	7.1	21.15	11.7	Y
1R0R	48.75	9.13	5.3	8.12	6.0	7.4	6.6	N
1R6Q	162.98	25.33	6.4	17.97	9.1	14.27	11.4	Y
1R8S	256.1	47.28	5.4	27.38	9.4	14.37	17.8	Y
1RLB	164	23.63	6.9	23.27	7.0	22.33	7.3	N
1RV6	102.83	13.78	7.5	12.93	8.0	12.08	8.5	N
1S1Q	60.78	8.77	6.9	8.17	7.4	6.83	8.9	N
1SBB	209.97	29.2	7.2	28.9	7.3	22.55	9.3	N
1SYX	58.42	9.6	6.1	7.92	7.4	6.53	8.9	N
1T6B	294.28	31.05	9.5	23.43	12.6	25.72	11.4	N
1TMQ	163.02	18.18	9.0	18	9.1	18.47	8.8	N
1UDI	76.18	13.77	5.5	13.75	5.5	9.93	7.7	N
1US7	132.78	23	5.8	22.18	6.0	13.78	9.6	Y
1VFB	131.48	22.9	5.7	22.07	6.0	13.42	9.8	N
1WDW	176.87	31.88	5.5	30.28	5.8	23.9	7.4	N
1WEJ	131.13	14.9	8.8	14.68	8.9	14.08	9.3	N
1WQ1	247.18	30.22	8.2	23.1	10.7	25.85	9.6	N
1XD3	47.78	8.63	5.5	8.6	5.6	9.3	5.1	N
1XQS	248.93	29.82	8.3	25.83	9.6	24.17	10.3	N
1XU1	96.62	17.87	5.4	18.03	5.4	13.75	7.0	N
1Y64	538.68	56.03	9.6	45.82	11.8	43.4	12.4	N

1YVB	122.52	18.7	6.6	16.3	7.5	16.15	7.6	N
1Z0K	75.87	10.43	7.3	9.52	8.0	8.92	8.5	N
1Z5Y	84.17	16.98	5.0	18.43	4.6	10.35	8.1	Y
1ZHH	169.28	28.25	6.0	28.2	6.0	22.98	7.4	N
1ZHI	171.62	21.17	8.1	21.25	8.1	16.18	10.6	N
1ZLI	132.5	21.22	6.2	16.2	8.2	12.28	10.8	N
1ZM4	528.27	51.9	10.2	45.38	11.6	36.57	14.4	N
2A5T	166.07	28.73	5.8	24.88	6.7	20.65	8.0	Y
2A9K	102.87	22.73	4.5	19.22	5.4	15.58	6.6	Y
2ABZ	72.27	11.92	6.1	10.13	7.1	9.38	7.7	N
2AJF	250.25	41.23	6.1	35.83	7.0	31.68	7.9	N
2AYO	132.77	16.17	8.2	13.22	10.0	15.32	8.7	N
2B42	126.72	20.98	6.0	15.28	8.3	15.48	8.2	N
2B4J	82.97	12.98	6.4	13.1	6.3	10.95	7.6	N
2BTF	128.9	18.38	7.0	16.93	7.6	14	9.2	N
2C0L	131.3	23.4	5.6	19.3	6.8	18.43	7.1	N
2CFH	98.43	19.3	5.1	18.7	5.3	12.68	7.8	Y
2FD6	179.37	32.77	5.5	32.32	5.5	28.57	6.3	N
2FJU	211.45	30.58	6.9	30.68	6.9	27.32	7.7	N
2G77	131.15	22.78	5.8	17.82	7.4	18.97	6.9	N
2H7V	302.15	31.9	9.5	28.27	10.7	25.9	11.7	N
2HLE	131.25	15.35	8.6	15.5	8.5	13.83	9.5	N
2HMI	436.12	70.43	6.2	63.13	6.9	52.8	8.3	N
2HQS	128.33	17.4	7.4	15.92	8.1	13.53	9.5	N
2HRK	164.03	21.82	7.5	15.17	10.8	13.22	12.4	N
2I25	72.12	15.35	4.7	12.37	5.8	10.58	6.8	N
2I9B	165.67	24.33	6.8	21.22	7.8	19.15	8.7	N
2IDO	82.68	16.38	5.0	14.3	5.8	11.1	7.4	Y
2J0T	76.57	19.42	3.9	15.02	5.1	10.65	7.2	Y
2J7P	248.77	37.7	6.6	29.62	8.4	30	8.3	N
2JEL	134.63	17.53	7.7	15.15	8.9	13.02	10.3	N
2MTA	121.42	20.62	5.9	20.77	5.8	15.95	7.6	N
2NZ8	171.95	35.43	4.9	27.87	6.2	22.8	7.5	N
2O3B	97.75	21.75	4.5	19.48	5.0	15.87	6.2	N
2O8V	72.08	13.82	5.2	11.65	6.2	10.08	7.2	N
2O0B	27.75	5.5	5.0	5.47	5.1	5.13	5.4	N
2OOR	247.9	30.63	8.1	29.63	8.4	26.8	9.3	N
2OT3	162.97	20.2	8.1	17.67	9.2	12.8	12.7	N
2OUL	131.03	21.37	6.1	21.1	6.2	15.17	8.6	N
2OZA	180.57	43.1	4.2	29.03	6.2	25.3	7.1	N
2PCC	72.6	18.77	3.9	16.27	4.5	11.93	6.1	N
2QFW	211.6	43.72	4.8	39.08	5.4	25.67	8.2	Y
2SIC	97.98	18.58	5.3	17.12	5.7	13.2	7.4	N
2SNI	75.78	12.68	6.0	10.48	7.2	10.05	7.5	N
2UUY	77.05	13.85	5.6	13.77	5.6	10.32	7.5	N
2VDB	173.82	28.68	6.1	18.83	9.2	17.48	9.9	N
2VIS	923.4	199.17	4.6	111.28	8.3	62.8	14.7	Y
2Z0E	98.17	21.38	4.6	19.03	5.2	15.17	6.5	N
3BP8	169.27	23.27	7.3	22.9	7.4	19.37	8.7	N
3CPH	164.98	26.02	6.3	22.5	7.3	19.1	8.6	N
3D5S	72.48	13.25	5.5	10.1	7.2	9.63	7.5	N
3SGQ	43.07	9.2	4.7	7.48	5.8	6.53	6.6	N
4CPA	84.55	12.72	6.6	9.98	8.5	9.28	9.1	N
7CEI	60.27	11.38	5.3	8.98	6.7	9.27	6.5	N
BOYV	130.48	24.68	5.3	20.55	6.3	14.5	9.0	Y
Average	166.64	26.48	6.3	23.24	7.1	18.86	8.6	