

Table S3. Running time (in minutes) and running time fold improvement for new ZDOCK versions 2.3.1, 2.3.2f, and 2.3.2 (versus ZDOCK 2.3) for all test cases in docking Benchmark 4.0.

L/R Switch indicates switching of ligand and receptor for that test case in ZDOCK 2.3.2.

Test Case	ZDOCK 2.3	ZDOCK 2.3.1		ZDOCK 2.3.2f		ZDOCK 2.3.2		L/R Switch
	Time	Time	Fold Improve	Time	Fold Improve	Time	Fold Improve	
1A2K	42.97	11.87	3.6	9.97	4.3	10.8	4.0	Y
1ACB	23.1	8.97	2.6	4.85	4.8	4.9	4.7	N
1AHW	93.58	23.27	4.0	20.93	4.5	17.63	5.3	Y
1AK4	31.4	8.72	3.6	9.88	3.2	6.38	4.9	Y
1AKJ	54.32	13.55	4.0	11.83	4.6	9.95	5.5	N
1ATN	51.87	11.93	4.3	10.73	4.8	9.98	5.2	N
1AVX	23.92	9.22	2.6	7.77	3.1	6.85	3.5	Y
1AY7	15.92	4.63	3.4	4.13	3.9	3.83	4.2	N
1AZS	58.23	17.48	3.3	17.02	3.4	13.28	4.4	Y
1B6C	40.68	15.25	2.7	12.95	3.1	7.52	5.4	Y
1BGX	127.4	38.32	3.3	31.17	4.1	22.97	5.5	Y
1BJ1	78.03	16.33	4.8	15.17	5.1	13.7	5.7	N
1BKD	92.98	13.7	6.8	11.47	8.1	11.5	8.1	N
1BUH	40.92	9.48	4.3	9.65	4.2	7.15	5.7	N
1BVK	31.25	10.03	3.1	9.28	3.4	6.45	4.8	N
1BVN	41.27	8.1	5.1	7.58	5.4	6.03	6.8	N
1CGI	24.52	4.98	4.9	4.57	5.4	4.62	5.3	N
1CLV	30.32	5.53	5.5	5.45	5.6	4.18	7.3	N
1D6R	23.87	7.17	3.3	5.07	4.7	4.72	5.1	N
1DE4	181.1	55.6	3.3	50.32	3.6	30.77	5.9	Y
1DFJ	54.78	16.32	3.4	14.05	3.9	9.78	5.6	Y
1DQJ	51.05	11.5	4.4	9.62	5.3	7.78	6.6	N
1E4K	76.12	18.42	4.1	14.93	5.1	12.02	6.3	N
1E6E	51	9.05	5.6	7.88	6.5	8.77	5.8	N
1E6J	41.42	9.43	4.4	7.05	5.9	6.83	6.1	N
1E96	42.43	12.13	3.5	11.27	3.8	9.88	4.3	Y
1EAW	18.3	5.3	3.5	4.62	4.0	4.63	4.0	N
1EER	80.38	25.52	3.1	24.8	3.2	14.5	5.5	Y
1EFN	13.63	3.82	3.6	2.92	4.7	2.92	4.7	N
1EWY	26.42	7.78	3.4	7.17	3.7	5.23	5.1	N
1EZU	44	13	3.4	13.03	3.4	9.25	4.8	Y
1F34	38.87	10.2	3.8	10.63	3.7	9.83	4.0	N
1F51	41.63	8.75	4.8	9.22	4.5	6.8	6.1	N
1F6M	40.18	8.1	5.0	8.8	4.6	6.02	6.7	N
1FAK	137.9	25.77	5.4	21.17	6.5	19.05	7.2	N
1FC2	53.4	14.93	3.6	14.65	3.6	8.4	6.4	Y
1FCC	40.85	7.97	5.1	7.23	5.7	6.75	6.1	N
1FFW	15.72	4.82	3.3	4.75	3.3	3.93	4.0	Y
1FLE	15.45	4.83	3.2	4.13	3.7	3.78	4.1	N
1FQ1	43.02	12.95	3.3	10.98	3.9	7.97	5.4	Y
1FQJ	50.48	13.03	3.9	9.98	5.1	9.8	5.2	N
1FSK	51.12	13.05	3.9	11.2	4.6	11.15	4.6	N
1GCQ	26.07	6.13	4.3	5.68	4.6	4.75	5.5	N
1GHQ	42.08	10.58	4.0	10.1	4.2	8.85	4.8	Y
1GL1	23.33	6.52	3.6	4.3	5.4	4.1	5.7	N
1GLA	50.53	11.22	4.5	9.88	5.1	8.35	6.1	N
1GP2	79.87	23.52	3.4	17.25	4.6	14.78	5.4	Y
1GPW	33.57	9.92	3.4	10.13	3.3	9.67	3.5	Y
1GRN	41.77	9.98	4.2	11.02	3.8	8.38	5.0	N
1GXD	77.62	18.57	4.2	13.98	5.6	13.2	5.9	N
1H1V	126.08	30.38	4.2	27.83	4.5	19.68	6.4	Y
1H9D	34.25	11.22	3.1	7.28	4.7	5.98	5.7	Y
1HCF	52.98	16.43	3.2	10.8	4.9	9.07	5.8	Y
1HE1	41.6	9.05	4.6	8.45	4.9	8.07	5.2	Y
1HE8	77.67	15.63	5.0	14.35	5.4	11.32	6.9	N
1HIA	18.45	5.33	3.5	4.65	4.0	4.7	3.9	N
1I2M	41.52	13.67	3.0	13.45	3.1	11.32	3.7	Y
1I4D	193.4	32.05	6.0	20.57	9.4	14.4	13.4	N

1I9R	58.02	19.95	2.9	19.75	2.9	14.42	4.0	Y
1IB1	77.32	18.27	4.2	12.53	6.2	11.55	6.7	N
1IBR	58.97	20.33	2.9	19.97	3.0	10.48	5.6	Y
1IJK	76.95	13.78	5.6	11.57	6.7	9.27	8.3	N
1IQD	53.97	12.73	4.2	11.27	4.8	10.25	5.3	N
1IRA	41.3	10.48	3.9	9.65	4.3	8.9	4.6	N
1J2J	23.52	4.58	5.1	4.5	5.2	4.57	5.1	N
1JIW	53.1	10.1	5.3	7.93	6.7	7.27	7.3	N
1JK9	32.8	9.72	3.4	9.28	3.5	6.23	5.3	N
1JMO	52.83	12.68	4.2	11.12	4.8	11.45	4.6	N
1JPS	90.18	20.95	4.3	19.27	4.7	17.8	5.1	Y
1JTG	33.07	10.28	3.2	8.37	4.0	8.78	3.8	N
1JWH	91.8	18.03	5.1	17.78	5.2	16.68	5.5	N
1JZD	55.5	14.3	3.9	12.15	4.6	10.58	5.2	N
1K4C	67.37	19.5	3.5	18.65	3.6	15.37	4.4	N
1K5D	77.48	21.67	3.6	16.8	4.6	14.97	5.2	Y
1K74	44.2	14.72	3.0	12.82	3.4	9.25	4.8	Y
1KAC	26.53	9.4	2.8	6.75	3.9	5.72	4.6	N
1KKL	41.28	7.93	5.2	7.88	5.2	6.98	5.9	N
1KLU	78.53	16.95	4.6	15.25	5.1	12.57	6.2	N
1KTZ	41.65	7.7	5.4	7.57	5.5	6.02	6.9	N
1KXP	97.03	25.53	3.8	23.47	4.1	18.68	5.2	Y
1KXQ	50.55	9.62	5.3	8.82	5.7	8.77	5.8	N
1LFD	15.93	5.27	3.0	4.95	3.2	5	3.2	N
1M10	77.88	20.5	3.8	14.47	5.4	10.68	7.3	Y
1MAH	30.75	9.38	3.3	8.17	3.8	7.73	4.0	N
1ML0	63.43	12.72	5.0	11.03	5.8	11.02	5.8	N
1MLC	51.07	12.33	4.1	9.85	5.2	7.52	6.8	N
1MQ8	53.55	9.15	5.9	8.9	6.0	7.33	7.3	N
1N2C	173.25	41.48	4.2	41.32	4.2	36.57	4.7	N
1N80	31.45	11.62	2.7	8.82	3.6	7.42	4.2	Y
1NCA	79.38	18.63	4.3	18.4	4.3	15.13	5.2	N
1NSN	50.58	11.25	4.5	10.1	5.0	8.48	6.0	N
1NW9	33.97	8.97	3.8	7.88	4.3	5.82	5.8	N
1OC0	25.67	6.72	3.8	4.85	5.3	3.87	6.6	N
1OFU	39.95	11.58	3.4	11.52	3.5	10.3	3.9	Y
1OPH	54.27	12.55	4.3	11.2	4.8	11.08	4.9	N
1OYV	41	11.1	3.7	8.95	4.6	7.65	5.4	Y
1PPE	13.5	3.75	3.6	3.35	4.0	2.67	5.1	N
1PVH	64.53	14.65	4.4	11.58	5.6	8.62	7.5	N
1PXV	26.45	11.03	2.4	8.87	3.0	7.53	3.5	N
1QA9	118.75	20.85	5.7	16	7.4	15.33	7.7	N
1QFW	77.67	19.8	3.9	16.13	4.8	10.47	7.4	Y
1R0R	15.47	4.47	3.5	3.97	3.9	3.63	4.3	N
1R6Q	50.35	11.48	4.4	8.13	6.2	6.92	7.3	Y
1R8S	77.43	21.1	3.7	12.58	6.2	7.35	10.5	Y
1RLB	51.7	11.57	4.5	11.53	4.5	11.08	4.7	N
1RV6	32.35	6.83	4.7	6.33	5.1	5.98	5.4	N
1S1Q	19.27	4.7	4.1	4.02	4.8	3.48	5.5	N
1SBB	76.9	15.63	4.9	14.07	5.5	11.37	6.8	N
1SYX	18.45	5.05	3.7	3.95	4.7	3.35	5.5	N
1T6B	89.88	15.35	5.9	11.98	7.5	13.02	6.9	N
1TMQ	50.15	9.52	5.3	8.72	5.8	8.68	5.8	N
1UDI	24.12	8.63	2.8	6.67	3.6	4.88	4.9	N
1US7	42.07	10.82	3.9	10.1	4.2	7.28	5.8	Y
1VFB	40.58	10.5	3.9	10.28	3.9	6.6	6.1	N
1WDW	56.22	16.05	3.5	15.15	3.7	12.27	4.6	N
1WEJ	40.68	7.95	5.1	7.43	5.5	7	5.8	N
1WQ1	77.08	14.55	5.3	11.38	6.8	12.17	6.3	N
1XD3	15.62	4.65	3.4	4.38	3.6	4.52	3.5	N
1XQS	77.83	15.02	5.2	12.37	6.3	11.52	6.8	N
1XU1	30.15	8.25	3.7	8.22	3.7	6.45	4.7	N
1Y64	165.7	27.12	6.1	22.47	7.4	20.92	7.9	N

1YVB	38.25	10.15	3.8	7.68	5.0	7.73	4.9	N
1Z0K	23.63	6	3.9	4.47	5.3	4.28	5.5	N
1Z5Y	26.47	9.28	2.9	8.52	3.1	5.4	4.9	Y
1ZHH	53.85	13.82	3.9	13.6	4.0	11.37	4.7	N
1ZHI	53.02	10.82	4.9	9.7	5.5	7.78	6.8	N
1ZLI	41.52	9.78	4.2	7.48	5.6	6.03	6.9	N
1ZM4	166.97	22.43	7.4	21.08	7.9	17.35	9.6	N
2A5T	52.18	16.05	3.3	12.65	4.1	10.72	4.9	Y
2A9K	35.08	11.38	3.1	9.63	3.6	7.93	4.4	Y
2ABZ	23.05	6.18	3.7	4.93	4.7	4.63	5.0	N
2AJF	77.67	19.33	4.0	16.9	4.6	15.05	5.2	N
2AYO	41.25	7.67	5.4	6.5	6.3	7.18	5.7	N
2B42	42.1	10.65	4.0	7.83	5.4	8.07	5.2	N
2B4J	26.87	7.72	3.5	6.3	4.3	5.33	5.0	N
2BTF	40.97	10.33	4.0	8.25	5.0	7.12	5.8	N
2C0L	40.6	11.03	3.7	8.93	4.5	8.97	4.5	N
2CFH	32.82	9.48	3.5	8.78	3.7	6.45	5.1	Y
2FD6	57.38	16.02	3.6	15.9	3.6	14.23	4.0	N
2FJU	76.73	15.38	5.0	14.7	5.2	13.27	5.8	N
2G77	41.87	11.2	3.7	8.88	4.7	9.28	4.5	N
2H7V	93.5	15.4	6.1	13.57	6.9	11.9	7.9	N
2HLE	41.38	8.73	4.7	7.52	5.5	6.88	6.0	N
2HMI	140.35	34.6	4.1	30.4	4.6	26.15	5.4	N
2HQS	40.85	9.75	4.2	7.65	5.3	6.77	6.0	N
2HRK	50.22	11.57	4.3	7.1	7.1	6.35	7.9	N
2I25	23.35	8.55	2.7	6.08	3.8	5.42	4.3	N
2I9B	50.53	11.38	4.4	10.22	4.9	9.22	5.5	N
2IDO	25.92	8.13	3.2	6.57	3.9	5.9	4.4	Y
2J0T	24.18	9.42	2.6	7.42	3.3	5.63	4.3	Y
2J7P	78.63	17.98	4.4	14.4	5.5	14.47	5.4	N
2JEL	41	8.63	4.8	7.57	5.4	6.5	6.3	N
2MTA	38.3	9.78	3.9	9.75	3.9	7.7	5.0	N
2NZ8	54.13	14.45	3.7	13.03	4.2	10.97	4.9	N
2O3B	31.4	10.12	3.1	9.15	3.4	7.57	4.1	N
2O8V	24.55	7.9	3.1	5.77	4.3	5.12	4.8	N
2O0B	9.22	3.1	3.0	2.77	3.3	2.67	3.5	N
2OOR	77.12	14.18	5.4	13.85	5.6	12.68	6.1	N
2OT3	50.88	10.33	4.9	9.02	5.6	6.8	7.5	N
2OUL	41.1	9.95	4.1	9.83	4.2	7.32	5.6	N
2OZA	57.13	18.15	3.1	14.42	4.0	12.85	4.4	N
2PCC	23.55	9.05	2.6	7.92	3.0	6.03	3.9	N
2QFW	76.92	20.8	3.7	17.9	4.3	11.3	6.8	Y
2SIC	32.25	9.23	3.5	8.05	4.0	6.42	5.0	N
2SNI	23.9	6.55	3.6	5.1	4.7	4.83	4.9	N
2UUY	24.05	6.4	3.8	6.32	3.8	4.78	5.0	N
2VDB	54.7	13.28	4.1	8.9	6.1	8.23	6.6	N
2VIS	288.52	86.98	3.3	52.57	5.5	30.42	9.5	Y
2Z0E	32.9	10.2	3.2	9.12	3.6	7.45	4.4	N
3BP8	49.98	11.08	4.5	11.17	4.5	9.18	5.4	N
3CPH	50.98	12.77	4.0	11.07	4.6	9.87	5.2	N
3D5S	24.1	6.4	3.8	4.9	4.9	4.73	5.1	N
3SGQ	13.43	4.47	3.0	3.63	3.7	3.17	4.2	N
4CPA	25.38	6.18	4.1	4.67	5.4	4.4	5.8	N
7CEI	19.53	6.15	3.2	4.72	4.1	4.83	4.0	N
BOYV	41.43	11.23	3.7	9.37	4.4	7.68	5.4	Y
Average	53.20	13.13	4.0	11.23	4.7	9.32	5.5	