

Ultra-Fast FFT Protein Docking On Graphics Processors

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SUPPLEMENTARY MATERIAL

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Supplementary Table 1. Comparison of *Hex* docking results for the 63 “rigid body” complexes of the Docking Benchmark (version 2) using the 3D and 1D FFT calculation schemes on the CPU and GPU.*

PDB Code	<u>3D CPU</u>		<u>3D GPU</u>		<u>1D CPU</u>		<u>1D GPU</u>	
	Rank (RMS)	Hits	Rank (RMS)	Hits	Rank (RMS)	Hits	Rank (RMS)	Hits
1AVX	–	–	–	–	–	–	–	–
1AY7	–	–	–	–	–	–	–	–
1BVN	298 (4.1)	4	291 (4.1)	4	393 (4.1)	4	380 (4.1)	3
1CGI	344 (6.4)	4	434 (9.1)	4	427 (6.9)	6	416 (6.9)	5
1D6R	261 (9.1)	5	205 (9.7)	5	230 (9.7)	4	231 (9.7)	2
1DFJ	1 (6.8)	13	1 (6.8)	8	1 (6.8)	6	1 (6.8)	3
1E6E	12 (4.2)	8	12 (4.2)	5	13 (4.2)	5	13 (4.2)	4
1EAW	2 (4.5)	34	2 (4.5)	35	2 (4.5)	30	2 (4.5)	27
1EWY	27 (4.2)	18	26 (4.2)	17	28 (4.2)	14	28 (4.2)	15
1EZU	–	–	–	–	–	–	–	–
1F34	–	–	–	–	–	–	–	–
1HIA	14 (9.9)	21	14 (9.9)	22	4 (9.4)	21	4 (9.4)	18
1MAH	1 (0.9)	25	1 (0.9)	27	2 (0.9)	30	2 (0.9)	23
1PPE	3 (3.4)	45	3 (3.4)	47	3 (3.4)	36	3 (3.4)	41
1TMQ	16 (1.4)	14	16 (1.4)	15	19 (1.4)	12	19 (1.4)	12
1UDI	246 (4.0)	13	227 (4.0)	14	348 (2.6)	13	262 (4.1)	12
2MTA	10 (8.5)	3	10 (8.5)	3	9 (8.5)	3	9 (8.5)	3
2PCC	301 (2.2)	26	135 (1.3)	26	18 (5.3)	29	18 (5.3)	29
2SIC	–	–	–	–	–	–	–	–
2SNI	870 (4.3)	12	847 (4.3)	12	44 (7.5)	10	44 (7.5)	10
7CEI	39 (4.4)	18	28 (4.4)	17	120 (4.5)	13	119 (4.5)	14
1AHW	363 (3.6)	2	359 (6.6)	2	–	–	–	–
1BVK	–	–	–	–	–	–	–	–
1DQJ	101 (9.7)	5	101 (9.7)	5	128 (9.7)	4	128 (9.7)	4
1E6J	–	–	–	–	574 (9.1)	2	571 (9.1)	2
1JPS	252 (8.6)	2	251 (8.6)	2	280 (8.6)	1	279 (8.6)	1
1MLC	–	–	–	–	–	–	–	–
1VFB	–	–	–	–	–	–	–	–
1WEJ	16 (1.5)	9	16 (1.5)	9	336 (2.2)	6	334 (2.2)	7
2VIS	–	–	–	–	–	–	–	–
1A2K	–	–	–	–	–	–	–	–
1AK4	–	–	–	–	–	–	–	–
1AKJ	41 (3.4)	21	41 (3.4)	18	5 (6.1)	27	5 (6.1)	29
1B6C	–	–	–	–	–	–	–	–
1BUH	175 (4.9)	7	175 (4.9)	7	179 (4.9)	7	178 (4.9)	7
1E96	390 (8.6)	4	386 (8.6)	4	499 (8.6)	2	492 (8.6)	2
1F51	–	–	–	–	–	–	–	–
1FC2	–	–	–	–	–	–	–	–
1FQJ	7 (8.7)	11	7 (8.7)	11	15 (9.5)	9	15 (9.5)	9
1GCQ	–	–	–	–	–	–	–	–
1GHQ	–	–	–	–	–	–	–	–
1HE1	93 (6.6)	16	91 (6.6)	13	103 (6.7)	11	103 (6.7)	13
1I4D	–	–	–	–	–	–	–	–
1KAC	250 (8.0)	4	249 (8.0)	4	316 (8.0)	5	317 (8.0)	5
1KLU	–	–	–	–	–	–	–	–
1KTZ	–	–	–	–	–	–	–	–
1KXP	57 (4.9)	2	57 (4.9)	2	1 (6.7)	1	1 (6.7)	1
1ML0	–	–	–	–	–	–	–	–
1QA9	–	–	–	–	–	–	–	–
1RLB	–	–	–	–	–	–	–	–
1SBB	–	–	–	–	–	–	–	–
2BTF	–	–	–	–	–	–	–	–
1BJ1	–	–	–	–	–	–	–	–
1FSK	10 (2.3)	12	10 (2.3)	13	8 (2.3)	11	8 (2.3)	11

(continued)

Supplementary Table 1. (continued).

PDB Code	3D CPU		3D GPU		1D CPU		1D GPU	
	Rank (RMS)	Hits	Rank (RMS)	Hits	Rank (RMS)	Hits	Rank (RMS)	Hits
1I9R	14 (1.8)	9	14 (1.8)	8	13 (1.8)	9	13 (1.8)	8
1IQD	74 (8.6)	10	72 (8.6)	6	176 (9.3)	7	168 (9.3)	4
1K4C	–	–	–	–	–	–	–	–
1KXQ	741 (4.6)	6	724 (4.6)	6	942 (4.6)	5	923 (4.6)	5
1NCA	11 (0.6)	10	11 (0.6)	10	14 (0.6)	11	14 (0.6)	11
1NSN	347 (2.6)	3	340 (2.6)	3	538 (4.2)	3	529 (4.2)	3
1QFW	–	–	–	–	–	–	–	–
2QFW	–	–	–	–	–	–	–	–
2JEL	204 (6.4)	8	202 (6.4)	8	226 (6.4)	9	223 (6.4)	8
Mean	147 (7.8)	6.4	147 (7.9)	6.2	166 (7.9)	5.8	165 (7.9)	5.6

*Each blind docking run used default search parameters with an initial steric scan using $N=18$ followed by shape plus electrostatic re-scoring using $N=25$. For each FFT docking scheme, the results are tabulated as triples consisting of the mean rank, the average ligand C_{α} root-mean-squared (RMS) deviation with respect to the crystal structure of the complex, and the average number of hits found within the top 1,000 docking predictions. Means of ranks were calculated using the mean log rank (MLR) formula of Ritchie *et al.* (2008). A hyphen denotes no acceptable solution within the top 1,000, in which case a value of 10 Å is used when calculating the mean RMS deviation. For the antibody/antigen complexes (1AHW, 1BVK, 1DQJ, 1E6J, 1DQJ, 1JPS, 1MLC, 1VFB, 1WEJ, 2VIS, 1BJ1, 1FSK, 1I9R, 1IQD, 1K4C, 1KXQ, 1NCA, 1NSN, 1QFW, 2QFW, 2JEL), the C_{α} coordinates of heavy chain residue 37 were used as the the antibody coordinate origin. For all other structures, the centre of mass was used as the coordinate origin. The Docking Benchmark includes several antibody complexes (1BJ1, 1FSK, 1I9R, 1IQD, 1K4C, 1KXQ, 1NCA, 1NSN, 1QFW, 2QFW, 2JEL) for which only the *bound* antibody Fab coordinates are available.