

## Supplementary Materials

**Supplementary Table 1.** PDB IDs and running time of benchmark proteins, ranked in ascending order of number of residues.

PDB ID	Number of residues	GPU Time/s	CPU Time/s
1edmB	39	750	10244
1j2jB	41	1932	6282
1n13A	46	105	1377
1irqA	48	985	9167
2a26A	48	2936	24662
1i2tA	61	338	3551
1jniA	62	1099	6787
1ahoA	64	4469	10410
1gutA	67	2682	47057
1egwa	71	1368	14638
1i27A	73	4569	114661
1dp7p	76	6847	69845
1hq1A	76	2023	11736
1zzkA	80	3024	23587
1iqzA	81	2742	11462
1ugiA	83	77	1719
1cy5A	92	1530	14382
1bteA	92	672	5779
1gmxA	107	1120	72800
1j0pA	108	1380	22968
1bkrA	108	899	8810
1h4xA	110	4354	125733
1hxiA	112	1740	6974
1ifra	113	2395	13077
1t6uA	117	110	2000
2a0bA	118	1328	12748
1e58A	124	6458	32562
1eaqA	124	1471	28716
1bgfA	124	378	2196
1e71A	124	2645	33129
1jbeA	126	1669	12860
1jb3A	127	1877	8629
1j3aA	129	1563	14486
1jf8A	130	4237	25107
1gp0A	133	2581	10971
1j3wA	134	1623	13355
1e29A	135	560	10192
1ccwC	137	1740	43152

1f46A	139	26260	129151
1cxqA	143	530	5180
1i5gA	144	2938	35843
1id0A	146	1390	16026
1h97B	147	2220	16370
1idpA	147	1592	20922
1dg6A	149	150	2774
1jl1A	152	2550	14877
1j98A	153	3570	31903
1jhjA	161	1567	41864
1eb6A	177	3079	43043
1e5kA	188	2549	37236
1jg1A	215	1012	12144
1gppA	217	2456	14865
1c1kA	217	1398	36348
1gv9A	223	15720	137032
1dfmA	223	1242	14986
1byiA	224	2952	17712
1atgA	231	3826	138855
1fsgC	233	3680	37897
1ah7A	245	3873	23535
1djoA	264	985	8174
1hz4A	266	8183	111780
3hp7A	275	1307	31486
1i1wA	302	2757	127140
1dd9A	310	1924	12121
1f9vA	313	4537	70658
1ds1A	323	1242	14986
1gxmA	324	16576	111840
2a3nA	336	2215	27799
1iuqA	357	5122	141840
1c0pA	363	1311	19605
1jfBA	399	24107	91440

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**Supplementary Table 2:** Benchmark results of accuracy of GPU-I-TASSER models on a set of 80 proteins on a Tesla P100 GPU.

Range of Residue	Average GPU TM-score to Native	Average CPU TM-score to Native	Average TM-score GPU to CPU	Average GPU time (seconds)	Average CPU time (seconds)	Average speedup
10-50	0.84	0.99	0.83	1342	10346	7.71
51-100	0.90	0.84	0.95	2418	25816	10.67
101-200	0.92	0.90	0.93	2766	27989	10.11
201-300	0.96	0.96	0.96	3886	48734	12.54
301-400	0.97	0.98	0.98	6643	68603	10.32
Average	0.90	0.91	0.93	0.93	36298	10.27