

Supplementary Information

for

DeepQA: Improving the estimation of single protein model quality
with deep belief networks

Renzhi Cao¹, Debswapna Bhattacharya², Jie Hou³, and Jianlin Cheng^{3,4*}

¹Department of Computer Science, Pacific Lutheran University, Tacoma, WA 98447, USA

²Department of Electrical Engineering and Computer Science, Wichita State University, Wichita, KS 67260, USA

³Department of Computer Science, University of Missouri, Columbia, MO 65211, USA

⁴Informatics Institute, University of Missouri, Columbia, MO 65211, USA

*To whom correspondence should be addressed. Phone: (573)-882-7306. Fax: (573)-882-8318. E-mail: chengji@missouri.edu.

Supplementary Item	Title
Supplementary Table 1	Z-score improvement of applying DeepQA for CASP11 top performance protein tertiary structure prediction methods
Supplementary Table 2	TM-score and RMSD score of DeepQA on <i>ab initio</i> datasets.
Supplementary Table 3	TM-score and RMSD score of ProQ2 on <i>ab initio</i> datasets.

Supplementary Table S1. Z-score improvement of applying DeepQA for CASP11 top performance protein tertiary structure prediction methods

Server name	Improvement on Z-score of GDT-TS score
Zhang-Server	6.38
QUARK	5.93
nns	-7.37
myprotein-me	-1.46
BAKER-ROSETTASERVER	16.34
MULTICOM-CONSTRUCT	-9.30
MULTICOM-CLUSTER	0.79
TASSER-VMT	11.46
RaptorX	6.66
MULTICOM-NOVEL	14.16

Supplementary Table S2. TM-score and RMSD score (and their Z-score) of DeepQA on ab initio datasets.

Target name (DeepQA)	TM-score for top 1	Z-score of TM-score for top 1	RMSD for top 1	Z-score of RMSD for top 1	TM-score for best of top 5	Z-score of TM-score for top 5	RMSD for best of top 5	Z-score of RMSD for top 5
T0761	0.19	-0.55	20.40	0.43	0.21	0.77	17.46	-1.35
T0763	0.18	-0.52	20.50	1.80	0.23	1.70	14.78	-2.05
T0767	0.21	0.08	23.07	1.43	0.23	0.91	19.33	-0.69
T0771	0.21	0.81	19.19	0.05	0.22	1.46	16.87	-1.41
T0777	0.29	2.17	16.03	-2.42	0.34	4.00	14.72	-3.17
T0781	0.22	1.73	21.59	-1.36	0.22	1.73	21.59	-1.36
T0785	0.22	0.58	13.38	-0.97	0.25	2.15	13.35	-1.00
T0789	0.25	0.87	19.98	0.48	0.27	1.65	18.12	-0.57
T0790	0.25	0.68	20.36	0.79	0.30	2.43	18.27	-0.41
T0791	0.27	2.63	16.53	-2.15	0.30	3.95	15.08	-3.00
T0794	0.27	1.93	20.23	-2.06	0.27	1.93	20.23	-2.06
T0806	0.25	0.48	16.89	-0.65	0.26	0.64	15.06	-1.78
T0808	0.17	-1.63	23.58	0.17	0.22	0.59	21.99	-0.81
T0810	0.25	1.01	24.85	1.01	0.25	1.14	22.14	-0.37
T0814	0.20	1.20	25.87	0.12	0.20	1.42	22.86	-1.79
T0820	0.23	1.06	14.01	-2.19	0.26	1.97	14.01	-2.19
T0824	0.24	0.95	12.12	-1.13	0.28	2.23	12.12	-1.13
T0827	0.23	-0.15	21.34	-0.19	0.29	1.41	17.64	-1.48
T0831	0.19	0.61	28.72	-0.03	0.22	1.90	26.29	-1.17
T0832	0.24	0.46	19.49	-0.14	0.25	1.08	17.56	-1.33
T0834	0.20	0.28	17.30	-2.41	0.23	1.50	17.30	-2.41
T0836	0.21	-0.75	19.38	0.68	0.29	1.89	17.01	-0.47
T0837	0.39	2.64	6.71	-2.65	0.39	2.64	6.71	-2.65
T0855	0.27	0.49	14.69	0.48	0.31	1.72	10.82	-1.82

Supplementary Table S3. TM-score and RMSD score of ProQ2 on ab initio datasets.

Target name (ProQ2)	TM-score for top one	RMSD for top one	TM-score for best of top 5	RMSD for best of top 5
T0834	0.18	23.64	0.23	21.32
T0790	0.20	22.10	0.26	16.19
T0824	0.21	14.29	0.25	11.99
T0806	0.21	20.26	0.27	16.37
T0767	0.21	23.07	0.24	17.92
T0836	0.21	17.46	0.27	16.73
T0791	0.24	20.18	0.25	17.19
T0785	0.22	12.88	0.23	12.88
T0855	0.29	11.04	0.30	10.82
T0814	0.20	25.87	0.20	25.73
T0781	0.18	24.17	0.21	23.26
T0831	0.22	26.79	0.22	26.29
T0789	0.23	18.04	0.25	18.04
T0820	0.21	16.36	0.26	16.36
T0808	0.21	23.80	0.22	21.99
T0810	0.23	22.44	0.23	20.86
T0771	0.17	21.18	0.20	18.15
T0827	0.25	17.90	0.28	17.90
T0761	0.21	20.22	0.21	18.96
T0777	0.20	22.52	0.34	14.72
T0832	0.24	18.39	0.25	17.81
T0763	0.19	18.03	0.21	16.71
T0794	0.27	20.23	0.27	20.23
T0837	0.23	12.61	0.33	11.79

Supplementary Table S4. Average per-target correlation and loss for DeepQA and ResQ on 54 targets of CASP11.

Target	ResQ		ResQ		DeepQA		DeepQA	
	Corr. on stage 1	Loss on stage 1	Corr. on stage 2	Loss on stage 2	Corr. on stage 1	Loss on stage 1	Corr. on stage 2	Loss on stage 2
T0760	0.93	0.01	0.72	0.02	0.61	0.34	0.40	0.02
T0762	1.00	0.00	0.76	0.04	0.81	0.00	0.44	0.04
T0763	0.06	0.06	0.16	0.06	0.26	0.03	0.14	0.02
T0764	0.99	0.00	0.93	0.01	0.88	0.00	0.44	0.00
T0765	0.39	0.00	-0.47	0.48	0.82	0.00	0.25	0.29
T0766	0.99	0.00	0.99	0.01	0.47	0.49	0.67	0.01
T0768	0.92	0.21	0.95	0.10	0.67	0.36	0.52	0.00
T0769	0.91	0.00	0.33	0.21	0.78	0.00	0.57	0.09
T0770	0.94	0.02	0.61	0.05	0.88	0.02	0.53	0.03
T0771	-0.57	0.08	-0.06	0.12	0.29	0.08	0.35	0.00
T0772	0.98	0.00	0.57	0.03	0.79	0.09	0.57	0.02
T0773	0.67	0.23	0.77	0.18	0.69	0.00	0.63	0.24
T0774	0.86	0.00	0.83	0.06	0.29	0.15	0.42	0.02

T0776	0.98	0.00	0.75	0.03	0.77	0.13	0.41	0.03
T0777	-0.41	0.07	0.39	0.06	0.70	0.03	0.62	0.04
T0782	0.84	0.00	0.86	0.20	0.32	0.22	0.30	0.20
T0784	0.98	0.00	0.90	0.07	0.53	0.43	0.14	0.02
T0785	-0.12	0.11	-0.05	0.08	0.67	0.05	0.48	0.09
T0786	0.95	0.00	0.84	0.07	0.44	0.33	0.71	0.03
T0792	0.96	0.00	0.43	0.12	0.50	0.29	0.57	0.02
T0796	0.84	0.00	0.89	0.07	0.75	0.26	0.54	0.03
T0800	0.68	0.00	0.74	0.11	0.70	0.25	0.38	0.01
T0801	0.99	0.00	0.64	0.03	0.90	0.00	0.67	0.02
T0803	0.95	0.00	0.88	0.08	0.31	0.13	0.07	0.08
T0805	0.99	0.00	0.79	0.02	0.64	0.23	0.44	0.09
T0806	-0.29	0.07	-0.11	0.14	0.79	0.00	0.45	0.01
T0807	0.99	0.08	0.68	0.06	0.95	0.11	0.70	0.03
T0811	0.99	0.00	0.77	0.01	0.77	0.00	0.58	0.01
T0812	0.65	0.00	0.96	0.03	0.32	0.23	0.45	0.00
T0813	0.96	0.00	0.40	0.05	0.58	0.27	0.23	0.02
T0815	0.99	0.00	0.81	0.03	0.84	0.01	0.44	0.08
T0816	-0.68	0.45	-0.42	0.35	0.79	0.00	0.49	0.21
T0818	0.70	0.00	0.69	0.03	0.42	0.00	0.09	0.02
T0819	0.99	0.00	0.85	0.05	0.87	0.16	0.64	0.04
T0821	0.36	0.22	0.88	0.07	0.64	0.00	0.67	0.03
T0822	-0.06	0.25	0.91	0.07	0.30	0.21	0.07	0.34
T0823	0.99	0.00	0.60	0.03	0.89	0.05	0.66	0.00
T0824	0.20	0.04	0.47	0.02	0.38	0.11	0.14	0.02
T0829	0.85	0.00	0.51	0.24	0.85	0.00	0.64	0.00
T0832	-0.28	0.02	-0.08	0.11	0.64	0.01	0.44	0.07
T0833	0.98	0.00	0.89	0.04	0.49	0.00	0.44	0.02
T0835	0.96	0.00	0.80	0.07	0.74	0.09	0.72	0.01
T0836	-0.35	0.09	0.16	0.09	0.45	0.03	0.46	0.07
T0837	0.49	0.00	-0.21	0.27	0.81	0.02	0.65	0.04
T0838	0.72	0.00	0.90	0.00	0.83	0.00	0.54	0.00
T0841	0.99	0.00	0.89	0.00	0.81	0.00	0.76	0.01
T0843	0.98	0.06	0.67	0.02	0.94	0.16	0.44	0.03
T0847	0.97	0.00	0.46	0.03	0.83	0.00	0.23	0.06
T0849	0.98	0.08	0.74	0.01	0.46	0.28	0.42	0.08
T0851	0.96	0.16	0.85	0.04	0.59	0.18	0.52	0.05
T0855	0.38	0.19	-0.40	0.26	0.74	0.00	0.64	0.13

T0856	1.00	0.00	0.69	0.07	0.87	0.06	0.34	0.06
T0857	0.88	0.00	0.94	0.07	0.42	0.25	0.04	0.30
T0858	0.99	0.00	0.74	0.04	0.88	0.00	0.62	0.03
Mean	0.67	0.05	0.58	0.09	0.65	0.11	0.46	0.06