Supplementary Materials: Template-free detection of macromolecular complexes in cryo electron tomograms

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1 Classification performance on additional benchmark sets

Besides benchmark sets 1 and 2, we tested our method on additional 50 benchmark sets for which tomograms were reconstructed at SNR level 0.5 using the same parameters as in benchmark sets 1 and 2. Each tomogram contains 4 types of randomly chosen complexes with 10 instances for each type randomly oriented and located, generated in the same way as in benchmark sets 1 and 2. The GHMRF classification performance for all sets is listed in Table 1.

Table 1: Classification performance

		Voxel based		Object based	
Tomogram id	Protein complexes	Precision	Recall	Precision	Recall
1	3K7A 2REC 2BO9 2H12	0.48	0.52	0.62	0.62
2	2REC 1W6T 1QO1 1DPB	0.33	0.39	0.53	0.53
3	2GLS 1VRG 2AW7_2AWB 1F1B	0.55	0.59	0.70	0.70
4	2GHO 1EQR 1VRG 1AON	0.43	0.49	0.62	0.62
5	2REC 1QO1 3K7A 2IDB	0.67	0.72	0.90	0.88
6	3K7A 1W6T 1F1B 2GHO	0.48	0.52	0.50	0.50
7	1VPX 1GYT 2AW7_2AWB 3GPT	0.72	0.77	0.85	0.85
8	1QO1 1VRG 2GHO 1W6T	0.25	0.34	0.62	0.62
9	2AW7_2AWB 2GLS 2REC 1DPB	0.46	0.56	0.72	0.72
10	2REC 3GPT 2GLS 1QO1	0.44	0.48	0.47	0.47
11	2H12 1DPB 2BYU 1EQR	0.45	0.51	0.65	0.65
12	1F1B 1DPB 1W6T 1A1S	0.56	0.62	0.76	0.78
13	1VPX 3K7A 1EQR 2AW7_2AWB	0.45	0.50	0.53	0.53
14	1YG6 2AW7_2AWB 1A1S 2GLS	0.44	0.49	0.60	0.60
15	1A1S 1QO1 2IDB 1W6T	0.41	0.44	0.35	0.35
16	1A1S 3K7A 2REC 2IDB	0.45	0.50	0.55	0.55
17	3K7A 1QO1 2AW7_2AWB 1F1B	0.27	0.30	0.39	0.40
18	2AW7_2AWB 1A1S 1DPB 2H12	0.67	0.71	0.80	0.80
19	1BXR 1F1B 2GLS 1VRG	0.59	0.67	0.68	0.68
20	2AW7_2AWB 2GHO 2IDB 2BO9	0.40	0.44	0.57	0.57
21	3K7A 1VPX 2REC 1DPB	0.27	0.31	0.39	0.40
22	1BXR 2REC 1GYT 2GHO	0.45	0.51	0.72	0.72
23	1AON 1YG6 2GHO 2GLS	0.30	0.32	0.49	0.50
24	1DPB 3GPT 1BXR 1VPX	0.46	0.50	0.55	0.55
25	1VRG 1KP8 2AW7_2AWB 1GYT	0.48	0.50	0.57	0.57
26	3K7A 1DPB 1A1S 2GHO	0.17	0.29	0.57	0.57

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27	1KP8 3GPT 1YG6 1VPX	0.63	0.68	0.78	0.78
28	1A1S 2BYU 3GPT 2REC	0.38	0.40	0.40	0.40
29	1AON 1A1S 2GHO 2GLS	0.52	0.57	0.62	0.62
30	3K7A 2GHO 1VPX 2AW7_2AWB	0.36	0.39	0.50	0.50
31	2GLS 1DPB 2BYU 1A1S	0.40	0.44	0.50	0.50
32	1VRG 1DPB 1KP8 2GHO	0.40	0.48	0.65	0.65
33	1F1B 1VPX 2H12 1EQR	0.69	0.74	0.88	0.88
34	1GYT 1QO1 1KP8 2IDB	0.28	0.37	0.55	0.55
35	1VPX 1EQR 1GYT 2AW7_2AWB	0.47	0.54	0.68	0.68
36	1BXR 1QO1 2H12 2BYU	0.37	0.41	0.50	0.50
37	1A1S 1QO1 2IDB 1DPB	0.39	0.47	0.70	0.70
38	1VRG 1AON 2GHO 2BO9	0.44	0.51	0.50	0.50
39	2GHO 1VPX 1QO1 2IDB	0.50	0.56	0.70	0.70
40	2IDB 1AON 1EQR 2GLS	0.41	0.46	0.65	0.65
41	1YG6 2BO9 1DPB 1VRG	0.63	0.73	0.97	0.97
42	2IDB 3GPT 1GYT 1A1S	0.50	0.53	0.53	0.53
43	2H12 1DPB 1W6T 1A1S	0.55	0.65	0.85	0.82
44	3K7A 1F1B 1AON 1VRG	0.34	0.36	0.50	0.50
45	2AW7_2AWB 1VRG 1W6T 1VPX	0.35	0.42	0.46	0.45
46	2GLS 2H12 1QO1 1W6T	0.55	0.57	0.75	0.75
47	1BXR 3K7A 1VPX 1A1S	0.50	0.54	0.60	0.60
48	3GPT 2REC 1YG6 1A1S	0.52	0.60	0.78	0.80
49	2REC 2AW7_2AWB 3K7A 1GYT	0.42	0.45	0.45	0.45
50	1EQR 1QO1 2H12 1A1S	0.49	0.52	0.62	0.62