FR3D/BGSU Representative Set Benchmark (Length ≤ 400, non-rRNA)

January 11, 2026

1 Benchmark definition

This report evaluates secondary-structure prediction quality on the FR3D/BGSU representative set under the following constraints:

- Truth is extracted from 3D structures using Barnaba canonical base-pair annotations (WC and GU).
- Targets are filtered to truth length ≤ 400 nucleotides and at least 5 canonical base pairs (to avoid degenerate empty-truth metrics).
- Ribosomal RNAs (rRNAs) are excluded (protein-partner confounders).
- Metrics are reported for the top-1 prediction and the best structure within the top-K list, with $K = 100$.

2 Algorithm overview

For each target sequence, the predictor:

1. Runs Infernal `cmscan` to select a covariance model (CM) and aligns the sequence with `cmalign`.
2. Runs R-scape CaCoFold to produce an initial consensus scaffold (when covariation signal is present).
3. Refines unpaired regions using RNAstructure-generated candidates and heuristic masking/search.
4. Samples additional structures with an MCMC sampler over base-pair moves, returning a diverse top-K list.
5. Uses a length-adaptive compute schedule (scaled budgets for long RNAs; up to 5 minutes refinement for ≥ 300 nt).

Table 1: Overall performance on the FR3D/BGSU representative benchmark (N=804, best-of-100).

Metric	Top-1	Best-of-100
Mean Precision	0.588	0.754
Mean Recall	0.727	0.844
Mean F1	0.636	0.784
Median F1	0.701	0.872
Mean MCC	0.644	0.790
Mean ΔF1	0.148	
Min #preds	1	
Median rank(best@100)	29.0	
Frac(rank(best@100)$\leq$ 10)	30.47%	
Frac(ΔF1$\geq$ 0.3)	13.81%	
Frac(best-of-100 F1$\geq$ 0.7)	73.13%	
Frac(best-of-100 F1$\geq$ 0.9)	43.03%	

Table 2: Performance by truth length bucket (means).

Bucket	N	P@1	R@1	F1@1	MCC@1	P@100	R@100	F1@100	MCC@100	ΔF1
30-80	587	0.611	0.755	0.660	0.669	0.791	0.879	0.820	0.826	0.160
81-150	149	0.585	0.696	0.625	0.630	0.727	0.810	0.756	0.761	0.131
151-300	53	0.399	0.531	0.441	0.451	0.496	0.614	0.533	0.543	0.092
301-400	15	0.403	0.638	0.468	0.491	0.489	0.665	0.538	0.556	0.071

3 Results

4 Appendix: by-family breakdown

Table 7: Performance by Rfam ID using the rank-1 prediction (means).

Rfam	N	P@1	R@1	F1@1	MCC@1
RF00005	306	0.596	0.797	0.666	0.679
no_rfam_hit	90	0.534	0.611	0.555	0.560
RF00167	12	0.760	0.848	0.796	0.798
RF01852	11	0.708	0.751	0.718	0.721
RF00458	9	0.203	0.506	0.274	0.308
RF00386	9	0.806	0.854	0.818	0.822
RF00023	8	0.312	0.731	0.427	0.469
RF00027	8	0.595	0.888	0.695	0.715
RF00003	8	0.617	0.714	0.657	0.658
RF01684	7	0.779	0.824	0.792	0.794
RF03072	6	0.330	0.379	0.348	0.348
RF00017	6	0.459	0.534	0.488	0.490
RF00028	6	0.586	0.658	0.619	0.620

Rfam	N	P@1	R@1	F1@1	MCC@1
RF00026	6	0.569	0.592	0.564	0.569
RF00036	6	0.803	0.936	0.858	0.863
RF00061	5	0.416	0.436	0.423	0.422
RF00442	5	0.540	0.610	0.569	0.569
RF00020	5	0.594	0.915	0.710	0.730
RF00059	5	0.453	0.508	0.475	0.474
RF01750	5	0.866	0.970	0.913	0.915
RF02925	4	0.362	0.463	0.403	0.406
RF00379	4	0.396	0.460	0.425	0.424
RF00024	4	0.485	0.645	0.533	0.543
RF00162	4	0.547	0.678	0.597	0.602
RF02340	4	0.570	0.782	0.652	0.662
RF03013	4	0.560	0.520	0.533	0.531
RF01689	3	0.289	0.393	0.333	0.333
RF00009	3	0.595	0.738	0.637	0.650
RF00010	3	0.619	0.714	0.657	0.661
RF00011	3	0.532	0.599	0.563	0.563
RF01857	3	0.545	0.689	0.602	0.608
RF01415	3	0.512	0.523	0.514	0.512
RF01051	3	0.660	0.618	0.637	0.635
RF00168	3	0.788	0.754	0.770	0.769
RF00174	3	0.675	0.763	0.713	0.715
RF01716	3	0.628	0.785	0.695	0.698
RF01834	3	0.875	0.905	0.875	0.881
RF01739	3	0.707	0.938	0.802	0.811
RF00507	3	0.838	0.955	0.888	0.891
RF03165	3	0.762	0.784	0.772	0.770
RF00173	3	0.767	0.926	0.838	0.840
RF00080	3	0.892	0.944	0.916	0.917
RF00100	3	0.795	0.898	0.842	0.842
RF00169	3	0.504	0.546	0.523	0.520
RF00094	2	0.000	0.000	0.000	-0.009
RF01988	2	0.000	0.000	0.000	-0.008
RF01792	2	0.400	0.500	0.444	0.443
RF00310	2	0.302	0.680	0.418	0.452
RF02477	2	0.340	0.590	0.431	0.446
RF01807	2	0.372	0.428	0.397	0.397
RF01854	2	0.320	0.473	0.371	0.380
RF03045	2	0.286	0.292	0.287	0.283
RF02348	2	0.272	0.326	0.296	0.294
RF02266	2	0.588	0.749	0.659	0.661
RF03016	2	0.676	0.593	0.631	0.631
RF02136	2	0.499	0.655	0.565	0.570
RF03160	2	0.452	0.375	0.410	0.405
RF01764	2	0.609	0.673	0.638	0.637
RF00233	2	0.463	0.519	0.489	0.487

Rfam	N	P@1	R@1	F1@1	MCC@1
RF00230	2	0.310	0.421	0.356	0.355
RF01831	2	0.657	0.750	0.697	0.698
RF01084	2	0.737	0.866	0.796	0.798
RF00254	2	0.837	0.819	0.828	0.827
RF00622	2	0.767	1.000	0.868	0.875
RF00015	2	0.683	0.938	0.790	0.798
RF01734	2	0.717	0.867	0.774	0.781
RF01054	2	0.720	0.976	0.829	0.837
RF01510	2	0.859	0.805	0.830	0.829
RF03093	2	0.667	0.750	0.706	0.702
RF00008	2	0.893	0.913	0.899	0.900
RF02553	2	0.787	0.774	0.780	0.778
RF00170	2	0.607	1.000	0.750	0.774
RF01767	2	0.721	0.800	0.755	0.755
RF02339	2	0.562	0.690	0.619	0.618
RF00065	2	0.845	0.933	0.885	0.885
RF02977	2	1.000	0.971	0.985	0.985
RF01850	2	0.958	1.000	0.978	0.978
RF02803	2	0.900	1.000	0.947	0.948
RF02805	1	0.000	0.000	0.000	-0.006
RF01666	1	0.074	0.400	0.125	0.171
RF01316	1	0.043	0.067	0.053	0.048
RF02975	1	0.000	0.000	0.000	-0.007
RF02359	1	0.099	0.500	0.165	0.221
RF00806	1	0.079	0.120	0.095	0.093
RF02295	1	0.150	0.429	0.222	0.250
RF02584	1	0.208	0.647	0.314	0.366
RF01838	1	0.000	0.000	0.000	-0.016
RF01826	1	0.000	0.000	0.000	-0.010
RF03166	1	0.205	0.600	0.305	0.349
RF00634	1	0.275	0.275	0.275	0.271
RF01554	1	0.211	0.500	0.296	0.319
RF01057	1	0.154	0.222	0.182	0.178
RF02561	1	0.130	0.214	0.162	0.162
RF00030	1	0.287	0.360	0.320	0.320
RF00172	1	0.417	0.556	0.476	0.478
RF03036	1	0.085	0.111	0.096	0.094
RF01713	1	0.303	0.909	0.455	0.523
RF01696	1	0.385	1.000	0.556	0.619
RF00050	1	0.517	0.600	0.556	0.555
RF00051	1	0.150	0.182	0.164	0.163
RF00950	1	0.409	0.900	0.563	0.605
RF01379	1	0.391	0.600	0.474	0.482
RF01762	1	0.375	1.000	0.545	0.607
RF00649	1	0.422	0.514	0.463	0.464
RF02056	1	0.533	0.727	0.615	0.622

Rfam	N	P@1	R@1	F1@1	MCC@1
RF00502	1	0.455	0.714	0.556	0.564
RF02032	1	0.394	0.410	0.402	0.401
RF02922	1	0.562	0.600	0.581	0.578
RF03030	1	0.500	0.333	0.400	0.402
RF01725	1	0.000	0.000	0.000	-0.007
RF01753	1	0.120	0.300	0.171	0.184
RF01357	1	0.500	0.857	0.632	0.652
RF01786	1	0.522	0.500	0.511	0.506
RF00166	1	0.486	1.000	0.654	0.696
RF00295	1	0.000	0.000	0.000	-0.017
RF02505	1	0.385	1.000	0.556	0.615
RF02680	1	0.607	0.630	0.618	0.616
RF02802	1	0.543	0.826	0.655	0.668
RF00488	1	0.645	0.772	0.703	0.705
RF02926	1	0.385	0.333	0.357	0.350
RF03542	1	0.400	0.353	0.375	0.368
RF03509	1	0.625	0.909	0.741	0.752
RF00175	1	0.727	0.615	0.667	0.665
RF01317	1	0.357	1.000	0.526	0.596
RF02914	1	0.846	0.688	0.759	0.760
RF01406	1	0.500	0.636	0.560	0.561
RF00210	1	0.611	0.667	0.638	0.636
RF01356	1	0.700	0.875	0.778	0.781
RF03977	1	0.534	0.574	0.554	0.552
RF01232	1	0.417	0.357	0.385	0.381
RF02681	1	0.609	0.609	0.609	0.604
RF00198	1	0.375	0.429	0.400	0.391
RF01773	1	0.636	0.933	0.757	0.770
RF00521	1	0.769	0.909	0.833	0.835
RF03085	1	0.714	0.833	0.769	0.769
RF03570	1	0.000	0.000	0.000	-0.022
RF01519	1	0.643	0.818	0.720	0.723
RF03498	1	0.615	0.640	0.627	0.625
RF00176	1	0.694	0.962	0.806	0.816
RF00228	1	0.629	0.786	0.698	0.701
RF01763	1	0.385	0.417	0.400	0.391
RF02519	1	0.500	1.000	0.667	0.703
RF03404	1	0.789	0.909	0.845	0.846
RF00029	1	0.708	0.850	0.773	0.774
RF02001	1	0.937	0.832	0.881	0.883
RF01363	1	0.657	0.742	0.697	0.696
RF00163	1	0.767	0.958	0.852	0.857
RF03059	1	0.583	0.778	0.667	0.669
RF00785	1	1.000	0.600	0.750	0.774
RF01365	1	0.250	0.600	0.353	0.381
RF02869	1	0.421	1.000	0.593	0.647

Rfam	N	P@1	R@1	F1@1	MCC@1
RF03918	1	0.889	0.571	0.696	0.706
RF03167	1	0.778	0.560	0.651	0.658
RF03054	1	0.714	0.769	0.741	0.738
RF00898	1	0.800	0.800	0.800	0.798
RF01836	1	0.235	0.267	0.250	0.240
RF00623	1	0.692	0.818	0.750	0.748
RF03081	1	0.778	0.875	0.824	0.824
RF03736	1	0.714	1.000	0.833	0.842
RF02683	1	0.645	0.690	0.667	0.665
RF01541	1	0.970	0.865	0.914	0.915
RF01622	1	1.000	0.846	0.917	0.919
RF01544	1	0.200	0.222	0.211	0.201
RF02521	1	0.906	0.879	0.892	0.891
RF00897	1	1.000	0.850	0.919	0.921
RF02678	1	0.783	0.947	0.857	0.860
RF00044	1	0.636	0.737	0.683	0.682
RF01344	1	0.733	0.815	0.772	0.772
RF02447	1	0.800	0.762	0.780	0.779
RF01472	1	0.607	0.773	0.680	0.682
RF01050	1	0.778	0.875	0.824	0.822
RF02538	1	0.875	1.000	0.933	0.935
RF02837	1	0.778	1.000	0.875	0.881
RF02984	1	0.800	0.857	0.828	0.825
RF01083	1	0.889	0.889	0.889	0.888
RF02888	1	0.727	0.889	0.800	0.802
RF01333	1	0.632	0.667	0.649	0.643
RF01082	1	0.385	0.556	0.455	0.457
RF03906	1	0.921	0.921	0.921	0.920
RF00419	1	0.857	0.857	0.857	0.856
RF01071	1	0.739	0.895	0.810	0.811
RF01107	1	0.909	1.000	0.952	0.953
RF04067	1	0.909	0.952	0.930	0.930
RF00102	1	0.913	0.977	0.944	0.944
RF00606	1	0.625	0.455	0.526	0.528
RF00504	1	0.920	0.920	0.920	0.919
RF02066	1	0.923	1.000	0.960	0.960
RF03863	1	0.852	0.885	0.868	0.867
RF00164	1	0.786	0.733	0.759	0.756
RF02871	1	0.743	0.897	0.812	0.815
RF00013	1	0.857	1.000	0.923	0.925
RF01241	1	0.882	1.000	0.938	0.939
RF02885	1	0.933	0.933	0.933	0.933
RF00380	1	0.902	0.920	0.911	0.911
RF00220	1	0.941	1.000	0.970	0.970
RF03900	1	1.000	0.889	0.941	0.941
RF03120	1	0.938	0.857	0.896	0.896

Rfam	N	P@1	R@1	F1@1	MCC@1
RF03790	1	1.000	0.947	0.973	0.973
RF00032	1	1.000	1.000	1.000	1.000
RF00234	1	0.857	1.000	0.923	0.925
RF00250	1	1.000	0.909	0.952	0.953
RF00381	1	0.000	0.000	0.000	-0.011
RF00455	1	0.944	1.000	0.971	0.971
RF00464	1	1.000	1.000	1.000	1.000
RF00480	1	0.846	0.917	0.880	0.879
RF02695	1	0.867	0.765	0.812	0.812
RF03031	1	1.000	0.933	0.966	0.965
RF03055	1	1.000	0.933	0.966	0.966
RF03339	1	0.895	1.000	0.944	0.945
RF03394	1	0.885	0.920	0.902	0.901
RF03493	1	1.000	1.000	1.000	1.000
RF04151	1	1.000	1.000	1.000	1.000
RF04217	1	1.000	0.923	0.960	0.960

Table 8: Performance by Rfam ID using best-of-100 (means).

Rfam	N	P@100	R@100	F1@100	MCC@100
RF00005	306	0.777	0.895	0.818	0.825
no_rfam_hit	90	0.698	0.752	0.714	0.718
RF00167	12	0.891	0.887	0.887	0.887
RF01852	11	0.867	0.887	0.871	0.873
RF00458	9	0.303	0.651	0.392	0.428
RF00386	9	0.861	0.941	0.895	0.897
RF00023	8	0.410	0.786	0.528	0.560
RF00027	8	0.659	0.915	0.757	0.770
RF00003	8	0.895	0.931	0.906	0.909
RF01684	7	0.898	0.902	0.898	0.898
RF03072	6	0.472	0.512	0.484	0.486
RF00017	6	0.570	0.588	0.576	0.576
RF00028	6	0.660	0.680	0.668	0.668
RF00026	6	0.797	0.918	0.848	0.851
RF00036	6	0.867	0.950	0.905	0.906
RF00061	5	0.640	0.617	0.625	0.625
RF00442	5	0.735	0.777	0.751	0.752
RF00020	5	0.655	0.915	0.752	0.767
RF00059	5	0.790	0.802	0.793	0.793
RF01750	5	0.941	0.970	0.955	0.955
RF02925	4	0.457	0.549	0.496	0.498
RF00379	4	0.515	0.559	0.533	0.533
RF00024	4	0.711	0.851	0.753	0.765
RF00162	4	0.706	0.831	0.754	0.760

Rfam	N	P@100	R@100	F1@100	MCC@100
RF02340	4	0.699	0.924	0.789	0.799
RF03013	4	0.922	0.888	0.901	0.902
RF01689	3	0.577	0.681	0.620	0.622
RF00009	3	0.643	0.702	0.666	0.669
RF00010	3	0.680	0.668	0.671	0.672
RF00011	3	0.668	0.707	0.687	0.686
RF01857	3	0.672	0.812	0.729	0.734
RF01415	3	0.737	0.794	0.764	0.763
RF01051	3	0.768	0.774	0.766	0.767
RF00168	3	0.804	0.819	0.811	0.810
RF00174	3	0.806	0.897	0.843	0.847
RF01716	3	0.848	0.897	0.858	0.864
RF01834	3	0.875	0.905	0.875	0.881
RF01739	3	0.836	0.979	0.897	0.901
RF00507	3	0.865	0.968	0.908	0.912
RF03165	3	0.921	0.909	0.915	0.914
RF00173	3	0.921	0.926	0.922	0.922
RF00080	3	0.948	0.954	0.950	0.950
RF00100	3	0.933	0.972	0.952	0.952
RF00169	3	0.912	1.000	0.953	0.954
RF00094	2	0.130	0.150	0.139	0.133
RF01988	2	0.293	0.700	0.411	0.448
RF01792	2	0.444	0.500	0.471	0.469
RF00310	2	0.349	0.780	0.482	0.520
RF02477	2	0.407	0.618	0.486	0.498
RF01807	2	0.505	0.534	0.519	0.518
RF01854	2	0.498	0.580	0.521	0.528
RF03045	2	0.528	0.646	0.580	0.580
RF02348	2	0.590	0.708	0.635	0.640
RF02266	2	0.638	0.749	0.689	0.689
RF03016	2	0.745	0.660	0.698	0.699
RF02136	2	0.657	0.770	0.705	0.708
RF03160	2	0.750	0.686	0.714	0.713
RF01764	2	0.776	0.743	0.759	0.758
RF00233	2	0.815	0.722	0.764	0.765
RF00230	2	0.718	0.868	0.781	0.786
RF01831	2	0.839	0.819	0.828	0.827
RF01084	2	0.779	0.907	0.838	0.840
RF00254	2	0.902	0.863	0.882	0.881
RF00622	2	0.842	0.969	0.901	0.902
RF00015	2	0.838	1.000	0.911	0.914
RF01734	2	0.885	0.967	0.918	0.921
RF01054	2	0.865	1.000	0.927	0.929
RF01510	2	0.952	0.912	0.932	0.931
RF03093	2	0.889	1.000	0.941	0.942
RF00008	2	0.929	0.977	0.950	0.951

Rfam	N	P@100	R@100	F1@100	MCC@100
RF02553	2	0.958	0.958	0.958	0.958
RF00170	2	0.929	1.000	0.962	0.963
RF01767	2	0.929	1.000	0.962	0.962
RF02339	2	0.929	1.000	0.962	0.963
RF00065	2	0.967	1.000	0.983	0.983
RF02977	2	1.000	0.971	0.985	0.985
RF01850	2	1.000	1.000	1.000	1.000
RF02803	2	1.000	1.000	1.000	1.000
RF02805	1	0.000	0.000	0.000	-0.006
RF01666	1	0.105	0.400	0.167	0.204
RF01316	1	0.158	0.200	0.176	0.173
RF02975	1	0.188	0.188	0.188	0.183
RF02359	1	0.130	0.438	0.200	0.237
RF00806	1	0.235	0.320	0.271	0.271
RF02295	1	0.231	0.429	0.300	0.312
RF02584	1	0.226	0.618	0.331	0.373
RF01838	1	1.000	0.222	0.364	0.468
RF01826	1	0.308	0.444	0.364	0.363
RF03166	1	0.268	0.733	0.393	0.443
RF00634	1	0.390	0.400	0.395	0.392
RF01554	1	0.333	0.500	0.400	0.405
RF01057	1	0.333	0.556	0.417	0.425
RF02561	1	0.400	0.571	0.471	0.475
RF00030	1	0.448	0.520	0.481	0.482
RF00172	1	0.455	0.556	0.500	0.500
RF03036	1	0.447	0.583	0.506	0.509
RF01713	1	0.357	0.909	0.513	0.569
RF01696	1	0.385	1.000	0.556	0.619
RF00050	1	0.577	0.600	0.588	0.586
RF00051	1	0.553	0.636	0.592	0.592
RF00950	1	0.450	0.900	0.600	0.634
RF01379	1	0.600	0.600	0.600	0.599
RF01762	1	0.429	1.000	0.600	0.650
RF00649	1	0.656	0.568	0.609	0.609
RF02056	1	0.533	0.727	0.615	0.622
RF00502	1	0.556	0.714	0.625	0.625
RF02032	1	0.670	0.590	0.628	0.628
RF02922	1	0.655	0.633	0.644	0.642
RF03030	1	0.688	0.611	0.647	0.644
RF01725	1	0.655	0.679	0.667	0.665
RF01753	1	0.526	1.000	0.690	0.724
RF01357	1	0.600	0.857	0.706	0.715
RF01786	1	0.667	0.750	0.706	0.704
RF00166	1	0.548	1.000	0.708	0.740
RF00295	1	0.625	0.833	0.714	0.717
RF02505	1	0.556	1.000	0.714	0.742

Rfam	N	P@100	R@100	F1@100	MCC@100
RF02680	1	0.731	0.704	0.717	0.715
RF02802	1	0.600	0.913	0.724	0.739
RF00488	1	0.692	0.783	0.735	0.736
RF02926	1	0.833	0.667	0.741	0.742
RF03542	1	0.722	0.765	0.743	0.740
RF03509	1	0.667	0.909	0.769	0.777
RF00175	1	0.769	0.769	0.769	0.767
RF01317	1	0.625	1.000	0.769	0.790
RF02914	1	0.917	0.688	0.786	0.791
RF01406	1	0.647	1.000	0.786	0.803
RF00210	1	0.794	0.818	0.806	0.805
RF01356	1	0.697	0.958	0.807	0.816
RF03977	1	0.780	0.852	0.814	0.814
RF01232	1	0.846	0.786	0.815	0.814
RF02681	1	1.000	0.696	0.821	0.832
RF00198	1	0.700	1.000	0.824	0.834
RF01773	1	0.737	0.933	0.824	0.829
RF00521	1	0.769	0.909	0.833	0.835
RF03085	1	0.833	0.833	0.833	0.832
RF03570	1	0.889	0.800	0.842	0.840
RF01519	1	0.826	0.864	0.844	0.844
RF03498	1	0.909	0.800	0.851	0.852
RF00176	1	0.743	1.000	0.852	0.861
RF00228	1	0.857	0.857	0.857	0.856
RF01763	1	1.000	0.750	0.857	0.864
RF02519	1	0.750	1.000	0.857	0.864
RF03404	1	0.816	0.939	0.873	0.874
RF00029	1	0.857	0.900	0.878	0.877
RF02001	1	0.937	0.832	0.881	0.883
RF01363	1	0.929	0.839	0.881	0.882
RF00163	1	0.821	0.958	0.885	0.887
RF03059	1	0.889	0.889	0.889	0.887
RF00785	1	1.000	0.800	0.889	0.894
RF01365	1	1.000	0.800	0.889	0.894
RF02869	1	0.800	1.000	0.889	0.894
RF03918	1	0.923	0.857	0.889	0.886
RF03167	1	0.955	0.840	0.894	0.895
RF03054	1	0.812	1.000	0.897	0.900
RF00898	1	0.900	0.900	0.900	0.899
RF01836	1	0.875	0.933	0.903	0.902
RF00623	1	0.909	0.909	0.909	0.907
RF03081	1	0.882	0.938	0.909	0.909
RF03736	1	0.833	1.000	0.909	0.911
RF02683	1	0.929	0.897	0.912	0.912
RF01541	1	0.970	0.865	0.914	0.915
RF01622	1	1.000	0.846	0.917	0.919

Rfam	N	P@100	R@100	F1@100	MCC@100
RF01544	1	0.895	0.944	0.919	0.918
RF02521	1	0.967	0.879	0.921	0.921
RF00897	1	0.947	0.900	0.923	0.923
RF02678	1	0.900	0.947	0.923	0.923
RF00044	1	0.864	1.000	0.927	0.929
RF01344	1	0.897	0.963	0.929	0.929
RF02447	1	0.909	0.952	0.930	0.930
RF01472	1	0.913	0.955	0.933	0.933
RF01050	1	1.000	0.875	0.933	0.934
RF02538	1	0.875	1.000	0.933	0.935
RF02837	1	0.875	1.000	0.933	0.935
RF02984	1	0.875	1.000	0.933	0.934
RF01083	1	1.000	0.889	0.941	0.942
RF02888	1	1.000	0.889	0.941	0.942
RF01333	1	0.944	0.944	0.944	0.944
RF01082	1	0.900	1.000	0.947	0.948
RF03906	1	0.925	0.974	0.949	0.949
RF00419	1	1.000	0.905	0.950	0.951
RF01071	1	0.905	1.000	0.950	0.951
RF01107	1	0.909	1.000	0.952	0.953
RF04067	1	0.952	0.952	0.952	0.952
RF00102	1	0.915	1.000	0.956	0.956
RF00606	1	0.917	1.000	0.957	0.957
RF00504	1	0.960	0.960	0.960	0.960
RF02066	1	0.923	1.000	0.960	0.960
RF03863	1	1.000	0.923	0.960	0.960
RF00164	1	1.000	0.933	0.966	0.966
RF02871	1	0.935	1.000	0.967	0.967
RF00013	1	0.938	1.000	0.968	0.968
RF01241	1	0.938	1.000	0.968	0.968
RF02885	1	0.938	1.000	0.968	0.968
RF00380	1	1.000	0.940	0.969	0.969
RF00220	1	0.941	1.000	0.970	0.970
RF03900	1	1.000	0.944	0.971	0.971
RF03120	1	0.946	1.000	0.972	0.972
RF03790	1	1.000	0.947	0.973	0.973
RF00032	1	1.000	1.000	1.000	1.000
RF00234	1	1.000	1.000	1.000	1.000
RF00250	1	1.000	1.000	1.000	1.000
RF00381	1	1.000	1.000	1.000	1.000
RF00455	1	1.000	1.000	1.000	1.000
RF00464	1	1.000	1.000	1.000	1.000
RF00480	1	1.000	1.000	1.000	1.000
RF02695	1	1.000	1.000	1.000	1.000
RF03031	1	1.000	1.000	1.000	1.000
RF03055	1	1.000	1.000	1.000	1.000

Rfam	N	P@100	R@100	F1@100	MCC@100
RF03339	1	1.000	1.000	1.000	1.000
RF03394	1	1.000	1.000	1.000	1.000
RF03493	1	1.000	1.000	1.000	1.000
RF04151	1	1.000	1.000	1.000	1.000
RF04217	1	1.000	1.000	1.000	1.000

Table 3: Performance split by whether Infernal found an Rfam CM hit (means).

Group	N	P@1	R@1	F1@1	MCC@1	P@100	R@100	F1@100	MCC@100	ΔF1
rfam_hit	714	0.595	0.742	0.646	0.654	0.761	0.856	0.793	0.799	0.147
no_rfam_hit	90	0.534	0.611	0.555	0.560	0.698	0.752	0.714	0.718	0.159

Table 4: Top Rfam IDs by frequency in this benchmark (means).

Rfam	N	F1@1	F1@100	ΔF1
RF00005	306	0.666	0.818	0.151
no_rfam_hit	90	0.555	0.714	0.159
RF00167	12	0.796	0.887	0.091
RF01852	11	0.718	0.871	0.153
RF00458	9	0.274	0.392	0.118
RF00386	9	0.818	0.895	0.077
RF00023	8	0.427	0.528	0.101
RF00027	8	0.695	0.757	0.062
RF00003	8	0.657	0.906	0.249
RF01684	7	0.792	0.898	0.107
RF03072	6	0.348	0.484	0.136
RF00017	6	0.488	0.576	0.088
RF00028	6	0.619	0.668	0.049
RF00026	6	0.564	0.848	0.283
RF00036	6	0.858	0.905	0.046

Table 5: Worst targets by best-of-100 F1 (lower is worse).

Target	Rfam	L	$\lvert P_{ref} \rvert$	F1@1	F1@100	Rank(best)
8FVY|1|g	RF00005	74	9	0.000	0.000	37
8FKW|1|L2	no_rfam_hit	69	19	0.000	0.000	30
8EUY|1|6	RF01792	56	5	0.000	0.000	93
9FXO|1|L6	no_rfam_hit	71	9	0.000	0.000	75
6ZJ3|1|LL	RF02805	91	24	0.000	0.000	44
4XNR|1|X	no_rfam_hit	73	22	0.000	0.000	1
7OGM|1|P	no_rfam_hit	38	6	0.000	0.000	37
6AZ3|1|6	no_rfam_hit	67	6	0.000	0.000	99
2B63|1|R	no_rfam_hit	31	9	0.000	0.000	3
1Y26|1|X	no_rfam_hit	73	25	0.000	0.000	1
4PRF|1|B	RF00094	74	16	0.000	0.051	73
9BUQ|1|S7	RF00005	74	8	0.000	0.067	67

Table 6: Targets with the largest improvement from rank-1 to best-of-100 (ranking/sampling sensitivity).

Target	Rfam	L	F1@1	F1@100	ΔF1	Rank(best)
7M5O|1|B	RF00381	37	0.000	1.000	1.000	27
8FN6|1|g	no_rfam_hit	46	0.000	0.909	0.909	4
9ERF|1|T	RF00005	48	0.000	0.857	0.857	19
2XXA|1|F	RF00169	102	0.088	0.941	0.853	81
9RVP|1|B	RF03570	30	0.000	0.842	0.842	6
7D7V|1|A	RF03013	57	0.000	0.812	0.812	81
4O26|1|E	RF00024	47	0.194	0.933	0.740	37
8QEQ|1|R	RF00295	30	0.000	0.714	0.714	50
1KUQ|1|B	RF01544	57	0.211	0.919	0.708	81
9P8B|1|Pt	RF00005	74	0.227	0.927	0.700	97
5FJ4|1|H	RF00003	35	0.316	1.000	0.684	8
6PMO|1|A	RF00230	59	0.244	0.923	0.679	83