FR3D/BGSU under400: RNAnneal-ss + LinearFold-V + EternaFold Ensemble

Scope

This report evaluates an **ensemble** that injects **LinearFold-V** and **EternaFold suboptimal** structures into the RNAnneal-ss candidate set, targeting improved **F1@100** and reduced **Fail@100**.

Methods (high level)

- **RNAnneal-ss (pipeline)**: existing CaCoFold + refinement + MCMC pipeline outputting 100 candidates.

- **Ensemble (RNAnneal-ss + LF + EF)**: merges per-target candidates from RNAnneal-ss, LinearFold-V, and EternaFold, then selects 100 structures with **length-adaptive per-source quotas** and **diversity (Jaccard)**.

- **RNAstructure**: `Fold` MFE structure (padded to 100 for consistent @100 evaluation).

- **LinearFold-V**: `--zuker` suboptimal enumeration (first 100 used).

- **EternaFold**: MEA prediction plus additional structures from `contrafold sample` to reach 100 total candidates.

Results

Table 1: Overall performance on FR3D/BGSU under400 non-rRNA benchmark (N=804; metrics @1 and best-of-100).

Method	Mean F1@1	Med F1@1	Mean F1@100	Med F1@100	ΔF1	Fail@100
RNAnneal-ss	0.636	0.701	0.784	0.872	0.148	1.2%
Ensemble	0.636	0.701	0.828	0.886	0.192	0.1%
RNAstructure	0.627	0.688	0.627	0.688	0.000	5.7%
LinearFold-V	0.622	0.682	0.794	0.846	0.172	0.6%
EternaFold	0.656	0.733	0.820	0.872	0.163	0.1%

Table 2: Mean F1@1 / F1@100 by truth-length bucket (N=804).

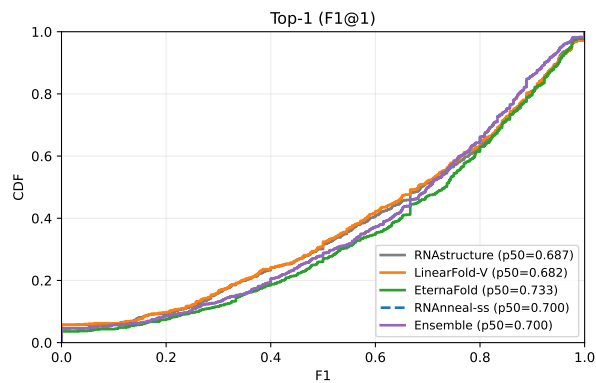| Bucket	Method	N	Mean F1@1	Mean F1@100
30-80	RNAnneal-ss	587	0.660	0.820
30-80	Ensemble	587	0.660	0.856
30-80	RNAstructure	587	0.647	0.647
30-80	LinearFold-V	587	0.637	0.815
30-80	EternaFold	587	0.670	0.845
81-150	RNAnneal-ss	149	0.625	0.756
81-150	Ensemble	149	0.625	0.820
81-150	RNAstructure	149	0.633	0.633
81-150	LinearFold-V	149	0.650	0.803
81-150	EternaFold	149	0.675	0.815
151-300	RNAnneal-ss	53	0.441	0.533
151-300	Ensemble	53	0.441	0.620
151-300	RNAstructure	53	0.439	0.439
151-300	LinearFold-V	53	0.429	0.603
151-300	EternaFold	53	0.496	0.628
301-400	RNAnneal-ss	15	0.468	0.538
301-400	Ensemble	15	0.468	0.574
301-400	RNAstructure	15	0.468	0.468
301-400	LinearFold-V	15	0.475	0.563
301-400	EternaFold	15	0.502	0.546

Empirical CDFs
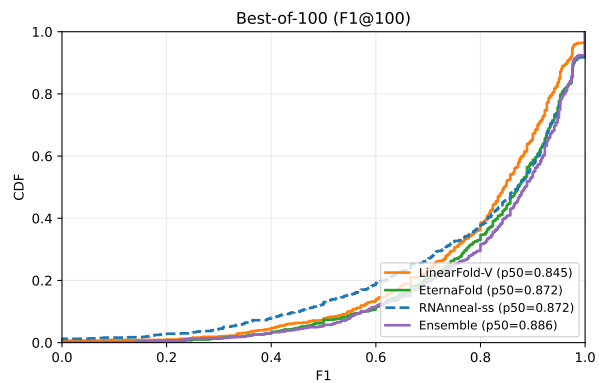

Figure 1: *
Top-1 (F1@1)

Figure 2: *
Best-of-100 (F1@100)

Figure 3: Empirical CDFs of per-target F1 (lines only; no markers). For F1@100, methods without a real top-100 search (e.g., MFE padded to 100) are omitted.