

Supporting Information for

DynaRNA: Accurate Dynamic RNA Conformation

Ensemble Generation with Diffusion Model

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Notes

The authors declare that there is no conflict of interest.

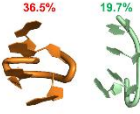
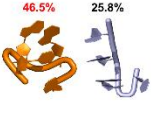
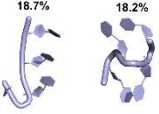
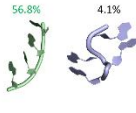
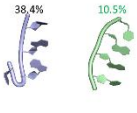
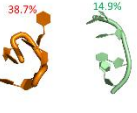
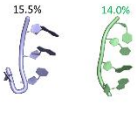
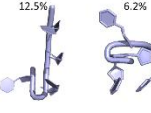
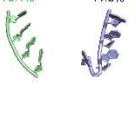
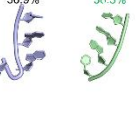
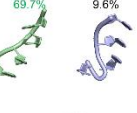
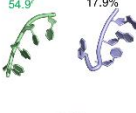
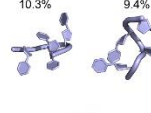
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BSFF1					
BSFF2					
DynaRNA					

Figure S1. Clustering results of tetranucleotides conformation ensembles generated with molecular dynamics simulations with OL3, BSFF1, BSFF2, and DynaRNA initialized from A-form structures. The orange color represents the intercalated conformation, the green color represents the A-form conformation, the blue color represents the other conformations.

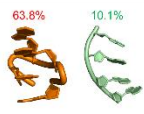
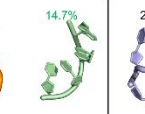
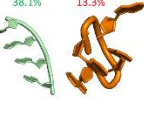
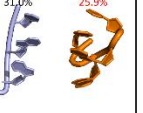
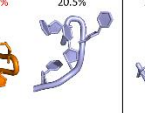
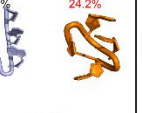
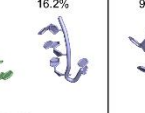
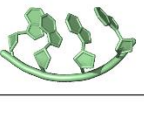
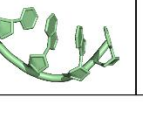
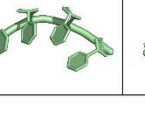
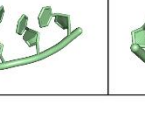
	AAAA	CAAU	CCCC	GACC	UUUU
<i>ff99bsc0xOL3</i>					
BSFF1					
BSFF2					
DynaRNA					

Figure S2. Clustering results of tetranucleotides conformation ensembles generated with molecular dynamics simulations with OL3, BSFF1, BSFF2, and DynaRNA initialized from intercalated structures. The orange color represents the intercalated conformation, the green color represents the A-form conformation, the blue color represents the other conformations.

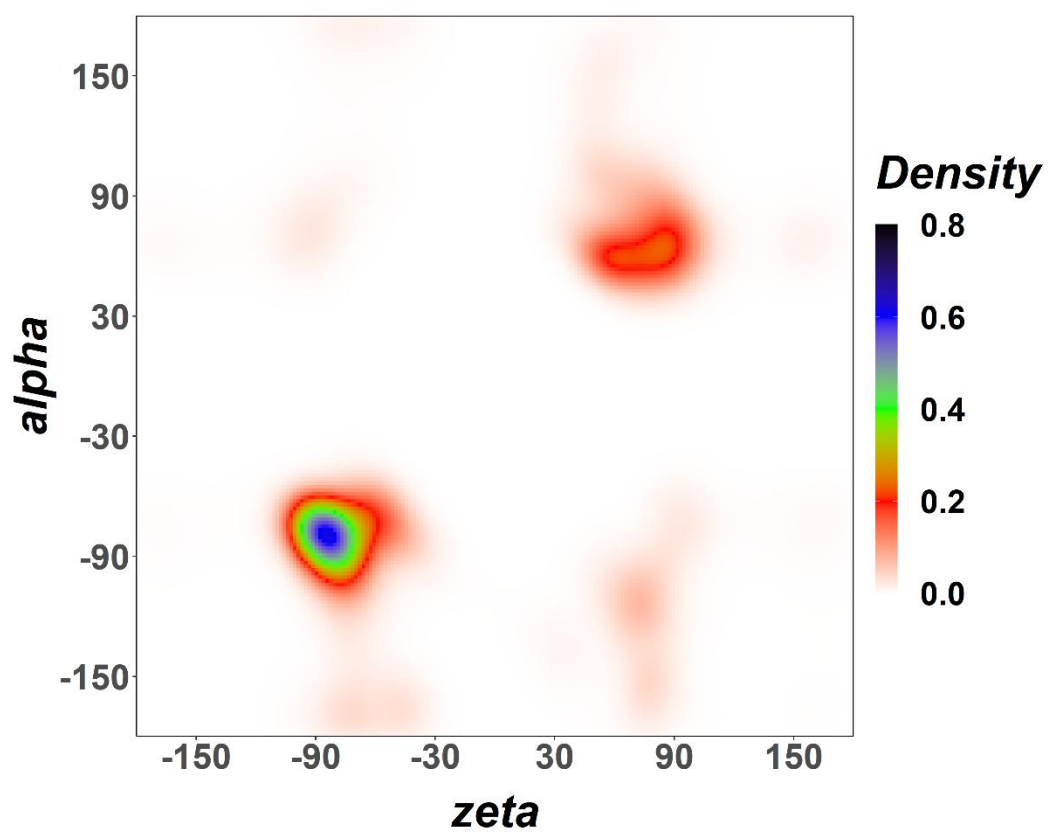


Figure S3. Dihedral statistical distribution of conformation ensemble generated with molecular dynamics simulations with BSFF1 initialized from A-form structures.

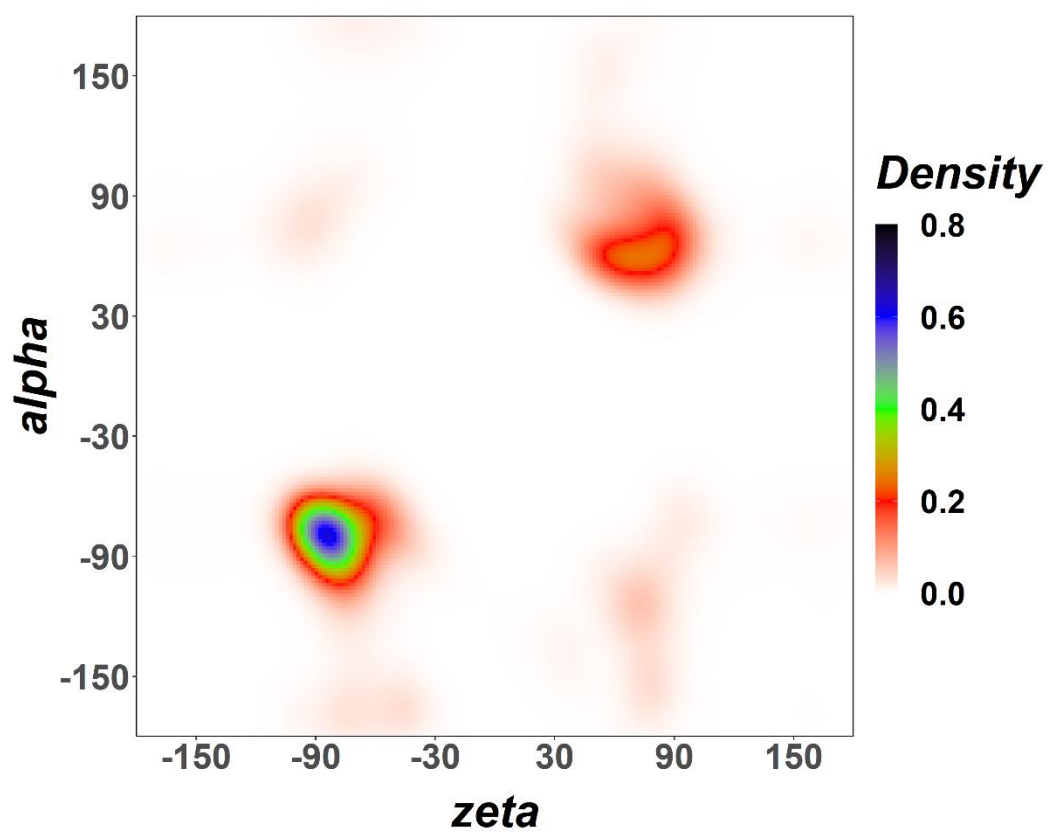


Figure S4. Dihedral statistical distribution of conformation ensemble generated with molecular dynamics simulations with BSFF1 initialized from intercalated structures.

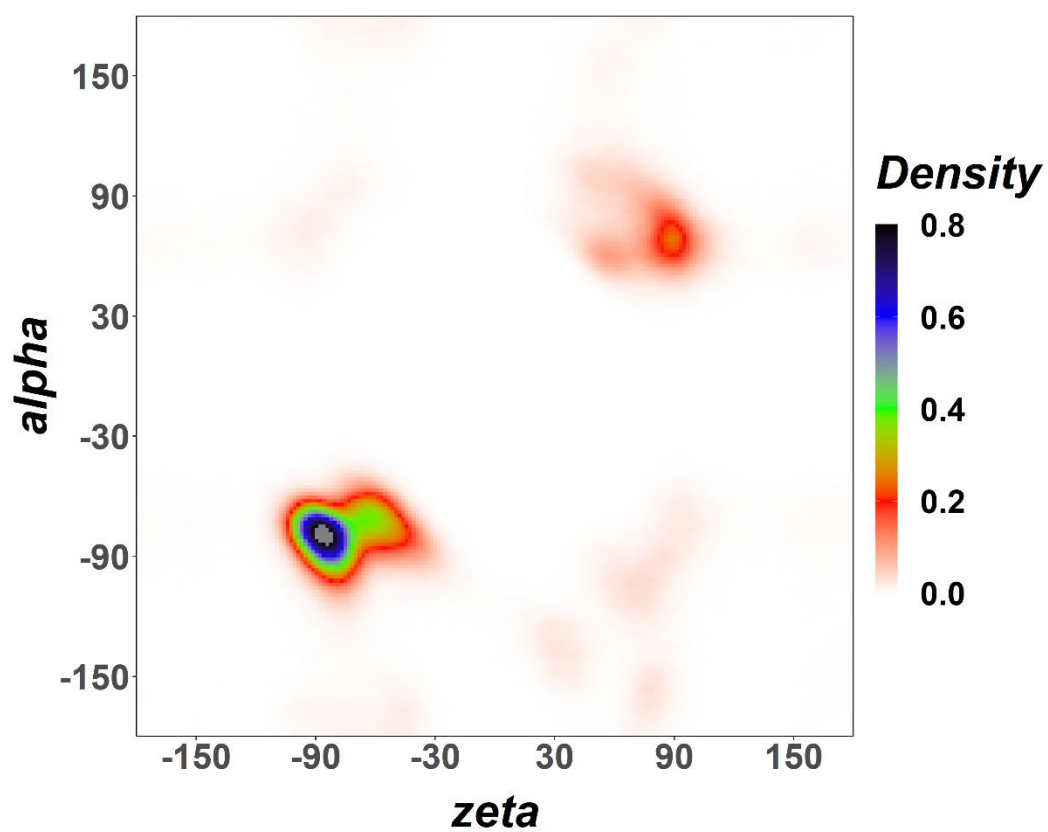


Figure S5. Dihedral statistical distribution of conformation ensemble generated with molecular dynamics simulations with BSFF2 initialized from A-form structures.

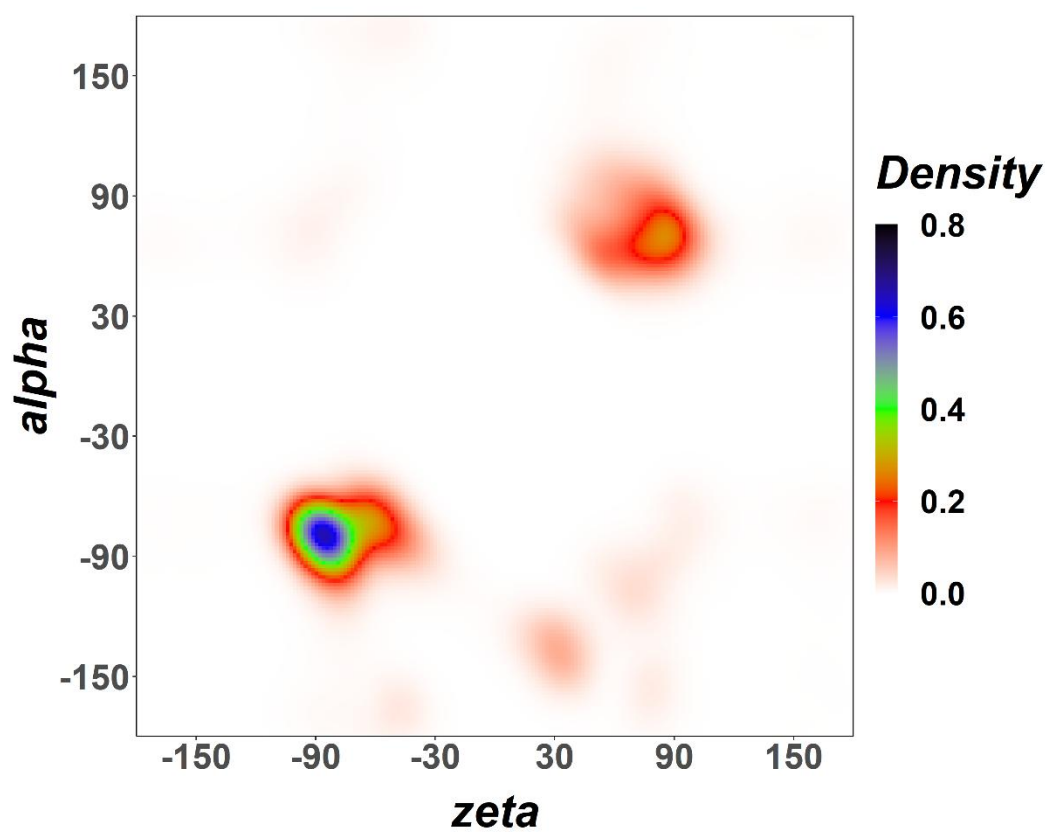


Figure S6. Dihedral statistical distribution of conformation ensemble generated with molecular dynamics simulations with BSFF2 initialized from intercalated structures.

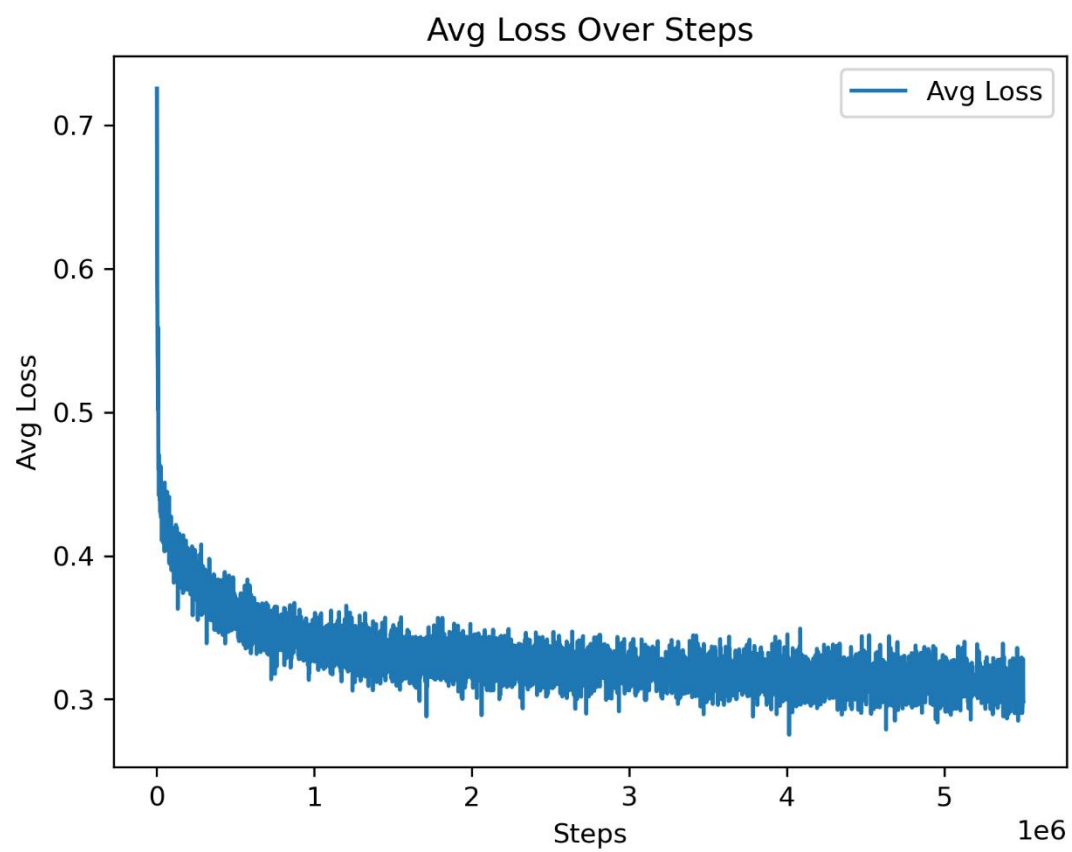


Figure S7. Loss curves of model over training steps.

Table S1. Radius of gyration of tetranucleotide conformation ensembles generated with molecular dynamics simulations and DynaRNA.

Rg (Å)	AAAA	CAAU	CCCC	GACC	UUUU
DynaRNA	5.9	5.8	5.8	5.8	5.8
OL3	5.7	5.6	5.2	5.5	5.8
Reference	5.8 ~ 8.0				

