

SUPPLEMENTARY DATA

Table 1. Prototypical RNA molecules included in Figure 1d for simulation with iFoldRNA and comparison against the corresponding experimentally-derived native structures. O5* RMSD of NDB-generated RNA vs. iFoldRNA prediction is limited to the backbone O5* atoms. O5* RMSD of canonical double-stranded A-RNA of equal length is used as an effective control metric for iFoldRNA predicted structures.

NDB Identifier	RNA Length	Simulation Time (min)	Heavy-atom RMSD with iFoldRNA Prediction (Å)	O5* RMSD with iFoldRNA Prediction (Å)	O5* RMSD with A-RNA (Å)
2F87	12	12	2.3	1.9	2.1
2EVY	14	9	2.2	1.6	3.3
1XWU	16	9	2.1	1.8	3.2
1Z30	18	16	2.4	1.8	3.0
1BN0	20	17	2.4	1.7	3.2
1K6G	22	17	2.7	1.7	1.8
1SY4	24	14	2.7	2.3	2.5
1YSV	27	14	2.4	1.7	2.0
28SR	28	15	5.3	3.4	4.6
1XHP	32	24	4.1	2.4	3.5
2F88	34	20	4.9	2.8	3.6
1N8X	36	25	2.6	2.2	3.6
1M5L	38	20	6.2	5.6	7.2
1ZC5	41	22	4.9	5.4	6.7