

Supporting Information for

The landscape of RNA 3D structure modeling with transformer networks

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Supplementary Text:

Evaluation metrics and performance assessment

The predicted structural models were evaluated against the experimental coordinates provided by the CASP organizers for targets cleared for public access as of December 20, 2022 from https://predictioncenter.org/download_area/CASP15/targets/ for the of the 12 CASP targets or obtained from PDB for the remaining 60 targets. Below, we provide a brief description of the evaluation metrics and performance assessment.

TM-score. Template modeling score (TM-score) (1) is a superposition-based evaluation metric to calculate the topological or global fold similarity between two structures. The score is calculated using the following equation:

$$TM - score = \max \left[\frac{1}{L_N} \sum_{i=1}^{L_T} \frac{1}{1 + \left(\frac{d_i}{d_0}\right)^2} \right] \dots \dots \dots [1]$$

where L_N is the length of the reference RNA monomer, L_T is the length of the aligned region after superposition, d_i is the distance between the i^{th} pair of aligned nucleotides, and d_0 is a length dependent scale to make the TM-score length independent. We have used US-align tool (1) to compute TM-score for RNA structure comparison. TM-score values range between 0 and 1, where 1 defines a perfect global topological similarity and a score > 0.5 indicates similar fold between reference and prediction.

IDDT. The local distance difference test (IDDT) (2) provides a superposition-free method to determine structural similarity of the predicted model with respect to reference structure. IDDT compares the predicted coordinates to the reference coordinates by choosing a set of nearby atom distances in a default radius of 15Å and reports the accuracy of the model as a fraction of the preserved distances. We used the docker version of OpenStructure (3) from the OST registry: <https://git.scicore.unibas.ch/schwede/openstructure/-/tree/master/docker>. During evaluation, we used the option '--lddt-no-stereochecks' which does not remove nucleo-base or backbone atoms from nucleotides during calculation even if there is a presence of problematic stereochemistry (3) in the predicted model. IDDT also ranges between 0 and 1, with a higher score indicating better structural similarity.

INF. The interaction network fidelity (INF) (4), an environment-dependent local quality metric, was calculated using the official CASP15 assessment pipeline (5) available at <https://github.com/DasLab/casp-rna>. We used the "INF-all" variant of INF score that considers all types of base-pairing interaction patterns present in RNA molecules including stacking, canonical or Watson-Crick and non-Watson-Crick. INF score is computed from two interaction annotation sets S_R and S_P obtained from experimental and prediction models respectively as Matthews Correlation Coefficient using the following equation:

$$INF = \sqrt{\left(\frac{TP}{TP + FP}\right) \times \left(\frac{TP}{TP + FN}\right)} \dots \dots \dots [2]$$

where, TP = intersection of pairings from both sets, FP = Interactions that are only present in S_P and FN = Interactions that are only present in S_R . INF score ranges from (0,1) with a higher score indicating better base pairing orientation in the predictions.

Clash score. Clash score captures the steric violations of a structure and is defined as the number of “serious clashes” per thousand atoms including the hydrogen (H) atoms, where serious clash is identified as an overlap of non-H-bonds $\geq 0.4 \text{ \AA}$ (6). We computed clash-score from MolProbity (7) package for quantifying the steric clashes.

Supplementary Figures:

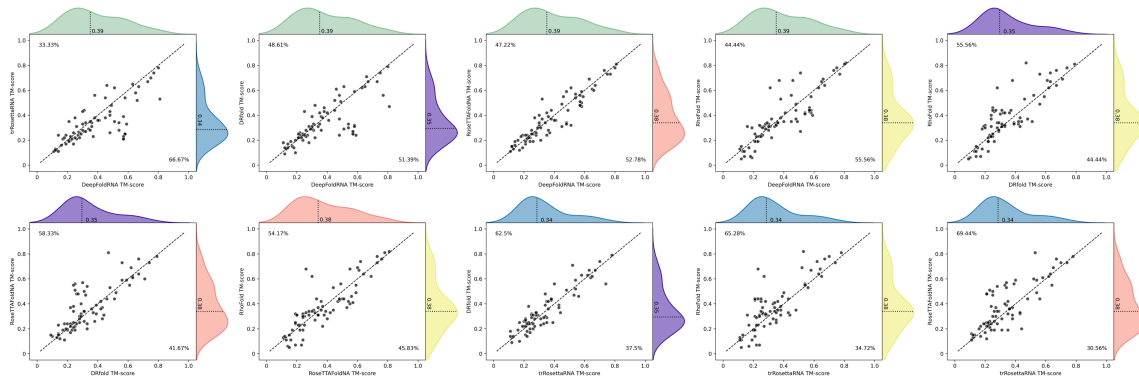


Figure S1: Head-to-head comparisons between all possible pairs of methods in terms of TM-score.

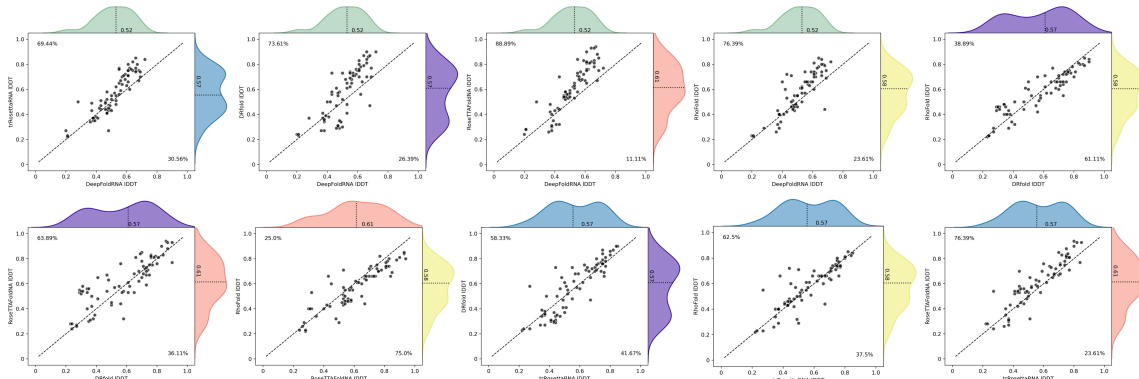


Figure S2: Head-to-head comparisons between all possible pairs of methods in terms of IDDT.

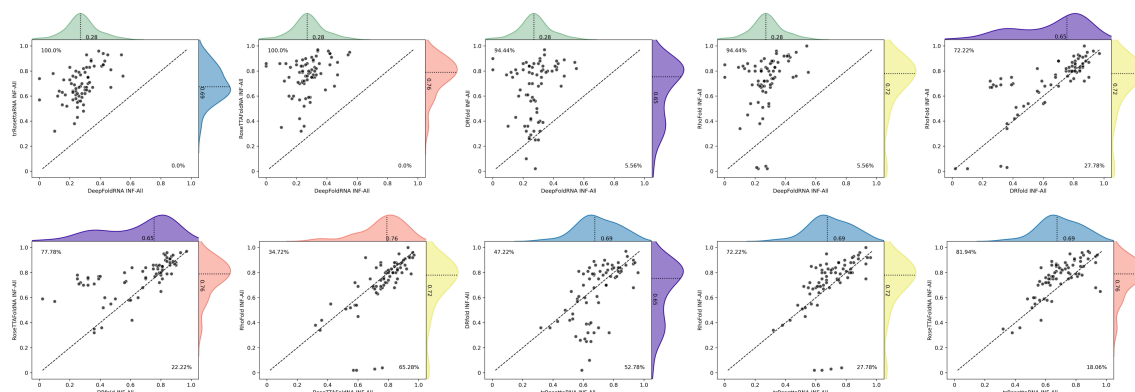


Figure S3: Head-to-head comparisons between all possible pairs of methods in terms of INF-All

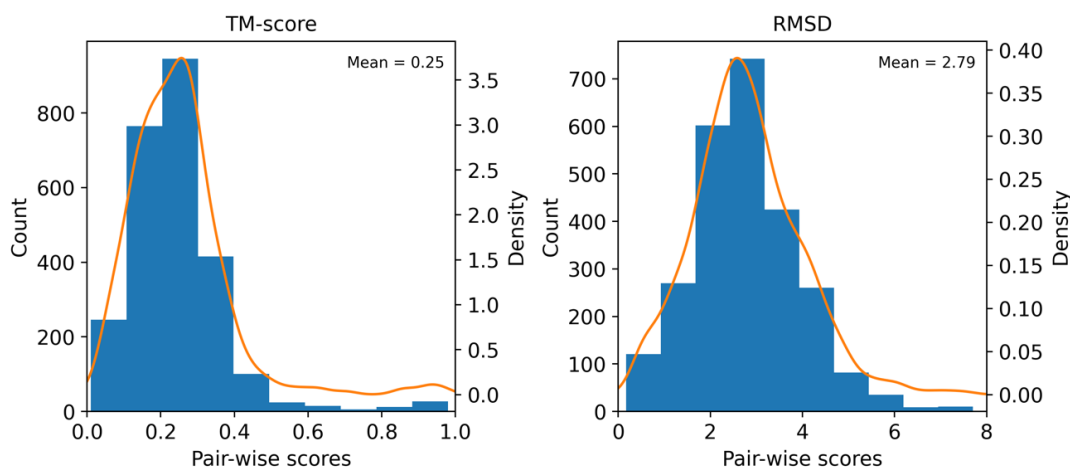


Figure S4: Unique pairwise similarity scores of the 72 structures in our benchmark set with mean values annotated on the top right showing the diversity of the evaluated experimental structures. A mean TM-score of 0.25 shows lack of fold similarity within the sequences in the set. The RMSD distribution on the other hand shows a varying range of values between 1 - 6 angstrom confirming structure dissimilarity among the experimental structures.

Supplementary Tables:

Table S1: Number of trainable parameters in each of the transformer-based models.

Method	Number of parameters(million/M)
DeepFoldRNA	7.44 M
trRosettaRNA	17.85 M
RoseTTAFoldNA	67.9 M
DRfold	13.12 M
RhoFold	27.39 M

Table S2: Average prediction accuracies for five deep learning-based and one deep learning-free prediction method RNAcomposer on the benchmark set on a common set of targets (70) excluding R1138 and 7QDU_Q (due to the limitation of <500 nucleotides for RNAcomposer). Bold denotes the best score.

Method/Score	TM-score	IDDT	INF-All	Clash-score
DeepFoldRNA	0.39	0.52	0.28	167.67
trRosettaRNA	0.35	0.57	0.7	27.25
DRfold	0.35	0.58	0.66	177.56
RoseTTAFoldNA	0.38	0.62	0.77	45.75
RhoFold	0.39	0.58	0.74	509.89
RNAcomposer	0.22	0.49	0.61	22.66

Table S3: Detailed scores for DeepFoldRNA predictions.

Targets	TM-score	IDDT	INF	Clash-score
6YMC_A	0.48	0.67	0.34	158.65
7ECM_A	0.27	0.69	0.55	145.08
7EDL_A	0.36	0.68	0.34	192.36
7EDM_A	0.34	0.66	0.43	221.91
7EEM_A	0.45	0.61	0.42	144.23
7EFG_A	0.31	0.55	0.39	147.97
7EQJ_A	0.73	0.64	0.26	175.77
7EXY_A	0.24	0.48	0	138.61
7KUB_A	0.35	0.5	0.22	180.81
7KUC_A	0.49	0.62	0.31	159.92
7KUD_A	0.25	0.43	0	182.27
7KVT_B	0.37	0.4	0.26	181.44
7MLW_F	0.81	0.62	0.3	185.82
7Q48_A	0.13	0.21	0.25	148.25
7Q6L_A	0.14	0.2	0.1	133.9
7Q7X_B	0.26	0.69	0.54	172.28
7Q7X_C	0.24	0.42	0.32	123.06
7QA2_A	0.11	0.21	0.23	250
7QDU_Q	0.19	0.38	0.22	152.34
7QP2_A	0.46	0.66	0.42	144.93
7R6L_A	0.57	0.47	0.28	164.27
7R6L_B	0.17	0.43	0.17	164.61

7R6M_A	0.59	0.48	0.3	165.4
7RQ5_A	0.51	0.68	0.47	240.26
7RWR_A	0.38	0.47	0.29	139.44
7SHX_A	0.22	0.47	0.26	169.01
7UCR_A	0.51	0.64	0.41	140.53
7UGA_A	0.41	0.57	0.36	130.81
7UMC_A	0.32	0.56	0.27	132.82
7UMD_A	0.26	0.55	0.16	158.06
7UME_A	0.3	0.59	0.42	204.26
7UQ6_B	0.63	0.59	0.32	161.23
7UVT_A	0.58	0.49	0.31	197.29
7UZ0_A	0.77	0.63	0.24	155.95
7V06_A	0.45	0.6	0.2	158.87
7V9E_A	0.31	0.46	0.15	186.5
7VFT_A	0.21	0.66	0.45	114.56
7WIA_V	0.4	0.58	0.24	144.42
7XD3_N	0.57	0.47	0.25	180.91
7XJZ_B	0.75	0.61	0.09	189.89
7XK0_B	0.8	0.61	0.13	183.01
7XSN_N	0.58	0.49	0.33	184.93
7YC8_N	0.54	0.46	0.31	176.91
7YGC_N	0.54	0.48	0.3	184.46
8BGU_3	0.67	0.61	0.2	176.79
8D2A_A	0.3	0.55	0.33	193.4
8DMB_W	0.16	0.37	0.22	158.69
8DP3_R	0.3	0.52	0.33	185.15
8E0F_D	0.35	0.72	0.47	118.91
8EG0_C	0.65	0.61	0.3	146.87
8F4O_B	0.58	0.57	0.24	145.62
8FCS_A	0.66	0.66	0.31	163.48
8GXC_A	0.32	0.38	0.15	146.23
8HB8_A	0.22	0.41	0.25	175.3
8HBA_A	0.28	0.38	0.29	181.64
8HBA_B	0.19	0.38	0.29	183.98
8HD6_N	0.57	0.5	0.24	187.21
8I3Z_B	0.12	0.39	0.22	200.4
8I43_A	0.21	0.55	0.26	198.02
8I7N_N	0.57	0.47	0.24	186.68
R1107	0.48	0.53	0.23	162.62

R1108	0.48	0.56	0.35	152.25
R1116	0.38	0.53	0.24	184.94
R1117	0.21	0.43	0.18	196.54
R1126	0.18	0.37	0.21	154.74
R1128	0.36	0.61	0.32	162.87
R1136	0.14	0.28	0.27	131.86
R1138	0.12	0.36	0.28	140.9
R1149	0.28	0.53	0.12	164.71
R1156	0.29	0.53	0.28	165.26
R1189	0.23	0.46	0.27	148.38
R1190	0.25	0.5	0.25	148.38
Mean	0.39	0.52	0.28	167.08

Table S4: Detailed scores for trRosettaRNA predictions.

Targets	TM-score	IDDT	INF	Clash-score
6YMC_A	0.4	0.8	0.89	5.98
7ECM_A	0.24	0.7	0.76	2.57
7EDL_A	0.34	0.75	0.88	9.87
7EDM_A	0.29	0.75	0.88	2.82
7EEM_A	0.54	0.8	0.85	16.67
7EFG_A	0.44	0.77	0.96	17.57
7EQJ_A	0.67	0.75	0.79	28.23
7EXY_A	0.17	0.27	0.57	0
7KUB_A	0.35	0.55	0.76	14.53
7KUC_A	0.48	0.77	0.93	1.91
7KUD_A	0.38	0.44	0.74	0
7KVT_B	0.23	0.38	0.56	69.78
7MLW_F	0.53	0.6	0.67	35.17
7Q48_A	0.12	0.22	0.43	1.39
7Q6L_A	0.11	0.27	0.32	9.72
7Q7X_B	0.31	0.74	0.93	2.6
7Q7X_C	0.26	0.45	0.75	0
7QA2_A	0.11	0.23	0.38	0
7QDU_Q	0.17	0.37	0.64	42.67
7QP2_A	0.64	0.85	0.94	15.48
7R6L_A	0.39	0.44	0.62	43.53

7R6L_B	0.21	0.47	0.61	0
7R6M_A	0.33	0.43	0.65	31.77
7RQ5_A	0.35	0.67	0.81	8.1
7RWR_A	0.38	0.58	0.82	13.92
7SHX_A	0.2	0.52	0.6	27.28
7UCR_A	0.62	0.82	0.84	36.61
7UGA_A	0.36	0.7	0.84	22.43
7UMC_A	0.34	0.59	0.68	40.37
7UMD_A	0.21	0.56	0.73	28.64
7UME_A	0.43	0.68	0.85	14.38
7UQ6_B	0.65	0.72	0.7	40.56
7UVT_A	0.25	0.47	0.67	25.63
7UZ0_A	0.74	0.76	0.75	58.76
7V06_A	0.38	0.63	0.83	17.52
7V9E_A	0.27	0.5	0.63	48.26
7VFT_A	0.2	0.74	0.93	0
7WIA_V	0.36	0.71	0.8	20.89
7XD3_N	0.21	0.41	0.55	43.09
7XJZ_B	0.7	0.75	0.78	39.05
7XK0_B	0.78	0.75	0.64	41.91
7XSN_N	0.25	0.44	0.64	40.59
7YC8_N	0.28	0.44	0.65	31.75
7YGC_N	0.34	0.45	0.62	33.73
8BGU_3	0.63	0.71	0.73	51.52
8D2A_A	0.33	0.76	0.83	25.3
8DMB_W	0.16	0.43	0.63	17.56
8DP3_R	0.28	0.57	0.71	60.85
8E0F_D	0.28	0.84	0.67	23.37
8EG0_C	0.58	0.71	0.79	19.61
8F4O_B	0.54	0.64	0.64	81.24
8FCS_A	0.52	0.77	0.83	17.54
8GXC_A	0.27	0.35	0.53	19.18
8HB8_A	0.23	0.37	0.51	34.21
8HBA_A	0.22	0.37	0.53	38.49
8HBA_B	0.24	0.37	0.48	36.4
8HD6_N	0.23	0.43	0.61	31.91
8I3Z_B	0.13	0.35	0.57	5.96
8I43_A	0.19	0.65	0.67	18.12

8I7N_N	0.21	0.41	0.58	45.56
R1107	0.26	0.51	0.69	46.15
R1108	0.43	0.67	0.67	68.29
R1116	0.56	0.62	0.66	31.8
R1117	0.35	0.51	0.52	15.12
R1126	0.22	0.49	0.7	62.36
R1128	0.31	0.66	0.75	82.37
R1136	0.24	0.5	0.77	5.24
R1138	0.12	0.34	0.59	21.32
R1149	0.26	0.48	0.6	43.14
R1156	0.25	0.55	0.7	19.4
R1189	0.21	0.49	0.56	34.22
R1190	0.22	0.52	0.62	29.78
Mean	0.34	0.57	0.69	27.39

Table S5: Detailed scores for DRfold predictions.

Targets	TM-score	IDDT	INF	Clash-score
6YMC_A	0.56	0.86	0.93	19.12
7ECM_A	0.24	0.7	0.82	120.51
7EDL_A	0.39	0.87	0.97	11.25
7EDM_A	0.31	0.84	0.86	4.23
7EEM_A	0.52	0.83	0.83	93.94
7EFG_A	0.33	0.74	0.8	123.99
7EQJ_A	0.67	0.79	0.83	103.65
7EXY_A	0.25	0.58	0.81	63.24
7KUB_A	0.42	0.73	0.87	74.88
7KUC_A	0.51	0.78	0.9	47.71
7KUD_A	0.43	0.73	0.9	66.67
7KVT_B	0.38	0.5	0.59	251.26
7MLW_F	0.47	0.56	0.68	167.91
7Q48_A	0.13	0.23	0.41	115.76
7Q6L_A	0.14	0.24	0.36	41.61
7Q7X_B	0.23	0.77	0.87	48.3
7Q7X_C	0.2	0.5	0.7	65.81
7QA2_A	0.18	0.24	0.36	78.62
7QDU_Q	0.1	0.27	0.1	119.09

7QP2_A	0.61	0.9	0.88	83.14
7R6L_A	0.25	0.31	0.25	360.32
7R6L_B	0.15	0.56	0.6	181.19
7R6M_A	0.24	0.29	0.25	365.68
7RQ5_A	0.29	0.47	0.76	53.48
7RWR_A	0.43	0.57	0.77	213.58
7SHX_A	0.26	0.55	0.7	197.34
7UCR_A	0.63	0.87	0.84	96
7UGA_A	0.36	0.73	0.8	128.75
7UMC_A	0.48	0.68	0.86	89.98
7UMD_A	0.28	0.62	0.78	128.12
7UME_A	0.39	0.72	0.81	74.61
7UQ6_B	0.62	0.76	0.75	152.54
7UVT_A	0.32	0.34	0.32	389.35
7UZ0_A	0.56	0.66	0.7	122.15
7V06_A	0.44	0.75	0.81	81.62
7V9E_A	0.28	0.61	0.81	178.07
7VFT_A	0.22	0.7	0.68	79.73
7WIA_V	0.42	0.71	0.84	72.15
7XD3_N	0.26	0.3	0.29	347.05
7XJZ_B	0.74	0.76	0.77	67.07
7XK0_B	0.79	0.76	0.75	63.56
7XSN_N	0.31	0.34	0.39	400.67
7YC8_N	0.33	0.29	0.4	466.11
7YGC_N	0.3	0.35	0.39	433.38
8BGU_3	0.67	0.8	0.86	90.3
8D2A_A	0.29	0.69	0.84	102.25
8DMB_W	0.19	0.37	0.32	415.37
8DP3_R	0.31	0.68	0.81	172.06
8E0F_D	0.33	0.9	0.89	17.51
8EG0_C	0.63	0.75	0.86	91.61
8F4O_B	0.59	0.71	0.84	87.35
8FCS_A	0.71	0.81	0.88	76.82
8GXC_A	0.22	0.34	0.43	306.88
8HB8_A	0.24	0.38	0.42	292.22
8HBA_A	0.18	0.35	0.47	285.43
8HBA_B	0.2	0.36	0.5	280.43
8HD6_N	0.25	0.3	0.27	363.67
8I3Z_B	0.14	0.39	0.61	94.43

8I43_A	0.22	0.73	0.78	49.34
8I7N_N	0.27	0.31	0.26	323.8
R1107	0.24	0.41	0.61	135.59
R1108	0.37	0.65	0.79	165.08
R1116	0.46	0.61	0.79	209.02
R1117	0.25	0.58	0.65	195.02
R1126	0.14	0.41	0.36	525.35
R1128	0.28	0.7	0.8	249.9
R1136	0.17	0.37	0.32	414.27
R1138	0.09	0.27	0.02	66.67
R1149	0.31	0.65	0.79	164.21
R1156	0.29	0.48	0.56	286.65
R1189	0.22	0.47	0.57	355.28
R1190	0.24	0.52	0.56	355.28
Mean	0.35	0.57	0.65	175.21

Table S6: Detailed scores for RoseTTAFoldNA predictions.

Targets	TM-score	IDDT	INF	Clash-score
6YMC_A	0.59	0.94	0.96	9.56
7ECM_A	0.38	0.85	0.95	0
7EDL_A	0.39	0.88	0.97	7.03
7EDM_A	0.34	0.83	0.91	9.86
7EEM_A	0.49	0.9	0.94	8.32
7EFG_A	0.2	0.71	0.65	191.39
7EQJ_A	0.76	0.82	0.9	22.06
7EXY_A	0.22	0.54	0.84	31.5
7KUB_A	0.42	0.59	0.79	27.45
7KUC_A	0.44	0.81	0.88	113.03
7KUD_A	0.28	0.7	0.86	94.79
7KVT_B	0.26	0.43	0.58	64.77
7MLW_F	0.81	0.76	0.81	50.98
7Q48_A	0.13	0.28	0.36	69.93
7Q6L_A	0.16	0.24	0.35	24.9
7Q7X_B	0.19	0.75	0.93	15.56
7Q7X_C	0.19	0.45	0.75	6.43
7QA2_A	0.11	0.28	0.32	93.92
7QDU_Q	0.14	0.27	0.57	49.55

7QP2_A	0.55	0.93	0.94	9.5
7R6L_A	0.56	0.58	0.78	44.93
7R6L_B	0.12	0.44	0.58	35.42
7R6M_A	0.55	0.53	0.75	58.37
7RQ5_A	0.32	0.67	0.77	66.13
7RWR_A	0.37	0.53	0.79	58.24
7SHX_A	0.24	0.58	0.76	66.34
7UCR_A	0.62	0.93	0.96	8
7UGA_A	0.36	0.67	0.78	70.71
7UMC_A	0.53	0.7	0.86	59.14
7UMD_A	0.25	0.58	0.83	32.56
7UME_A	0.32	0.72	0.85	111.36
7UQ6_B	0.69	0.83	0.83	44.26
7UVT_A	0.47	0.56	0.75	44.98
7UZ0_A	0.73	0.81	0.84	30.26
7V06_A	0.31	0.67	0.85	48.83
7V9E_A	0.3	0.53	0.75	71.76
7VFT_A	0.17	0.78	0.68	25.37
7WIA_V	0.36	0.68	0.79	52.5
7XD3_N	0.48	0.52	0.7	50.29
7XJZ_B	0.73	0.81	0.86	25.15
7XK0_B	0.78	0.82	0.86	28.07
7XSN_N	0.5	0.53	0.77	48.46
7YC8_N	0.54	0.55	0.77	47.49
7YGC_N	0.57	0.56	0.75	46.19
8BGU_3	0.64	0.76	0.88	36.79
8D2A_A	0.4	0.84	0.92	46.9
8DMB_W	0.2	0.42	0.7	47.94
8DP3_R	0.34	0.62	0.82	41.84
8E0F_D	0.24	0.77	0.87	9.72
8EG0_C	0.61	0.75	0.91	31.46
8F4O_B	0.59	0.74	0.89	29.86
8FCS_A	0.6	0.81	0.89	31.11
8GXC_A	0.37	0.4	0.6	29.53
8HB8_A	0.21	0.32	0.52	66
8HBA_A	0.24	0.3	0.55	34.57
8HBA_B	0.24	0.31	0.59	43.69
8HD6_N	0.51	0.54	0.72	68.33
8I3Z_B	0.15	0.35	0.42	49.7

8I43_A	0.24	0.73	0.85	54.55
8I7N_N	0.48	0.54	0.71	61.28
R1107	0.34	0.65	0.84	35.65
R1108	0.33	0.68	0.86	40.2
R1116	0.44	0.61	0.8	48.34
R1117	0.19	0.32	0.6	59.2
R1126	0.23	0.48	0.71	34.25
R1128	0.28	0.65	0.8	42.87
R1136	0.19	0.5	0.76	47.45
R1138	0.15	0.26	0.59	51.67
R1149	0.26	0.53	0.72	62.31
R1156	0.3	0.63	0.8	41.77
R1189	0.22	0.54	0.73	43.51
R1190	0.25	0.57	0.72	37.55
Mean	0.38	0.61	0.76	45.88

Table S7: Detailed scores for RhoFold predictions.

Targets	TM-score	IDDT	INF	Clash-score
6YMC_A	0.49	0.8	0.96	442
7ECM_A	0.31	0.69	0.79	466.84
7EDL_A	0.34	0.79	0.94	505.08
7EDM_A	0.31	0.8	0.91	431.46
7EEM_A	0.56	0.81	0.93	507.92
7EFG_A	0.31	0.74	0.92	479.81
7EQJ_A	0.76	0.78	0.9	435.57
7EXY_A	0.23	0.55	0.85	478.87
7KUB_A	0.33	0.55	0.72	565.03
7KUC_A	0.35	0.73	0.87	524.27
7KUD_A	0.31	0.72	0.75	447.37
7KVT_B	0.68	0.66	0.72	495.11
7MLW_F	0.82	0.7	0.77	454.69
7Q48_A	0.11	0.22	0.42	465.44
7Q6L_A	0.11	0.23	0.34	461.1
7Q7X_B	0.24	0.75	1	514.02
7Q7X_C	0.32	0.6	0.88	565.5
7QA2_A	0.13	0.23	0.38	506.28
7QDU_Q	0.06	0.29	0.02	65.59

7QP2_A	0.68	0.84	0.92	519.46
7R6L_A	0.46	0.46	0.72	777.45
7R6L_B	0.14	0.42	0.54	562.41
7R6M_A	0.4	0.43	0.67	730.32
7RQ5_A	0.27	0.44	0.76	503.28
7RWR_A	0.38	0.51	0.8	467.84
7SHX_A	0.19	0.47	0.68	477.43
7UCR_A	0.74	0.85	0.92	507.6
7UGA_A	0.42	0.64	0.8	571.85
7UMC_A	0.37	0.66	0.83	419.65
7UMD_A	0.3	0.57	0.8	473.06
7UME_A	0.33	0.66	0.88	425.17
7UQ6_B	0.62	0.74	0.8	479.02
7UVT_A	0.42	0.48	0.74	624.84
7UZ0_A	0.73	0.77	0.88	486.44
7V06_A	0.35	0.66	0.8	454.48
7V9E_A	0.62	0.71	0.86	449.9
7VFT_A	0.19	0.71	0.75	504.8
7WIA_V	0.35	0.63	0.81	455.19
7XD3_N	0.43	0.45	0.68	669.36
7XJZ_B	0.78	0.73	0.83	446.84
7XK0_B	0.81	0.74	0.82	440.24
7XSN_N	0.44	0.48	0.75	631.33
7YC8_N	0.42	0.46	0.7	738.82
7YGC_N	0.41	0.46	0.69	762.75
8BGU_3	0.64	0.7	0.84	504.55
8D2A_A	0.28	0.66	0.83	433.82
8DMB_W	0.31	0.43	0.69	608.81
8DP3_R	0.31	0.61	0.83	389.85
8E0F_D	0.32	0.82	0.95	440.32
8EG0_C	0.67	0.72	0.86	434.78
8F4O_B	0.55	0.66	0.8	465.75
8FCS_A	0.69	0.74	0.88	401.72
8GXC_A	0.22	0.4	0.45	716.79
8HB8_A	0.23	0.4	0.51	595.38
8HBA_A	0.29	0.4	0.52	592.47
8HBA_B	0.3	0.4	0.54	593.77
8HD6_N	0.44	0.46	0.69	627.91
8I3Z_B	0.15	0.34	0.55	703.11

8I43_A	0.11	0.66	0.72	461.93
8I7N_N	0.44	0.44	0.67	637.06
R1107	0.37	0.5	0.68	566.14
R1108	0.44	0.66	0.87	476.1
R1116	0.53	0.62	0.8	444.77
R1117	0.25	0.53	0.69	509.39
R1126	0.07	0.32	0.03	41.83
R1128	0.34	0.6	0.74	531.13
R1136	0.07	0.29	0.04	139.17
R1138	0.05	0.26	0.02	123.8
R1149	0.33	0.57	0.84	532.1
R1156	0.34	0.61	0.82	499.04
R1189	0.19	0.5	0.63	509.37
R1190	0.23	0.55	0.64	509.37
Mean	0.38	0.58	0.72	498.36

Table S8: Detailed scores for RNAComposer predictions (Predictions of 7QDU_Q and R1138 are absent since there is a limitation of <500 nucleotides for this tool)

Targets	TM-score	IDDT	INF	Clash-score
6YMC_A	0.38	0.82	0.92	23.95
7ECM_A	0.17	0.56	0.53	12.89
7EDL_A	0.18	0.58	0.44	13.55
7EDM_A	0.11	0.66	0.71	20.35
7EEM_A	0.28	0.55	0.7	20.62
7EFG_A	0.17	0.46	0.47	17.6
7EQJ_A	0.23	0.29	0.47	21.29
7EXY_A	0.15	0.51	0.76	7.91
7KUB_A	0.39	0.62	0.83	16.1
7KUC_A	0.33	0.69	0.83	15.3
7KUD_A	0.2	0.66	0.89	7.18
7KVT_B	0.22	0.33	0.43	20.6
7MLW_F	0.37	0.54	0.39	12.59
7Q48_A	0.12	0.21	0.49	16.76
7Q6L_A	0.03	0.22	0.4	19.47
7Q7X_B	0.09	0.67	0.79	18.21
7Q7X_C	0.21	0.52	0.62	11.6
7QA2_A	0.07	0.2	0.44	16.57
7QP2_A	0.25	0.57	0.61	20.62

7R6L_A	0.14	0.35	0.4	18.05
7R6L_B	0.1	0.5	0.53	27.14
7R6M_A	0.21	0.35	0.47	68.71
7RQ5_A	0.22	0.63	0.76	17.86
7RWR_A	0.3	0.51	0.74	19.67
7SHX_A	0.2	0.5	0.66	18.74
7UCR_A	0.26	0.56	0.72	20.62
7UGA_A	0.32	0.53	0.71	15.21
7UMC_A	0.22	0.61	0.85	15.53
7UMD_A	0.23	0.61	0.81	18.59
7UME_A	0.29	0.65	0.88	17.72
7UQ6_B	0.2	0.5	0.3	20.58
7UVT_A	0.2	0.42	0.38	57.23
7UZ0_A	0.2	0.44	0.32	22.44
7V06_A	0.29	0.6	0.78	18.99
7V9E_A	0.25	0.54	0.72	18.29
7VFT_A	0.17	0.67	0.62	14.71
7WIA_V	0.43	0.72	0.51	17.36
7XD3_N	0.23	0.42	0.63	58.66
7XJZ_B	0.23	0.47	0.32	24.46
7XK0_B	0.24	0.47	0.31	24.46
7XSN_N	0.18	0.42	0.7	20.13
7YC8_N	0.14	0.4	0.38	18.05
7YGC_N	0.14	0.41	0.69	18.05
8BGU_3	0.52	0.6	0.79	12.63
8D2A_A	0.27	0.62	0.74	15.01
8DMB_W	0.13	0.33	0.42	20.34
8DP3_R	0.28	0.59	0.87	21.91
8E0F_D	0.14	0.57	0.5	12.67
8EG0_C	0.21	0.48	0.47	23.84
8F4O_B	0.17	0.32	0.39	14.98
8FCS_A	0.51	0.73	0.85	17.11
8GXC_A	0.12	0.22	0.47	20.9
8HB8_A	0.18	0.26	0.48	15.15
8HBA_A	0.15	0.27	0.33	16
8HBA_B	0.16	0.26	0.39	16
8HD6_N	0.21	0.43	0.65	34.44
8I3Z_B	0.13	0.33	0.4	14.93
8I43_A	0.16	0.6	0.68	21.45

8I7N_N	0.22	0.41	0.68	47.2
R1107	0.22	0.36	0.6	19.47
R1108	0.3	0.47	0.73	9.5
R1116	0.43	0.65	0.34	15.3
R1117	0.12	0.2	0.55	24.86
R1126	0.18	0.5	0.79	157.12
R1128	0.23	0.69	0.87	12.63
R1136	0.2	0.49	0.77	52.37
R1149	0.31	0.61	0.83	16.15
R1156	0.18	0.44	0.67	27.26
R1189	0.2	0.49	0.68	11.24
R1190	0.24	0.54	0.69	11.24
Mean	0.22	0.49	0.61	22.66

Table S9: Names and corresponding families of each of the 60 targets curated from rcsb PDB.

PDB ID	Chain	Name	Rfam Family
6YMC	A	26-mer stem-loop RNA	-
7ECM	A	RNA duplex containing C-A base pair	-
7EDL	A	Crystal structure of the bacterial ribosomal decoding site in complex with G418 and Hg(II)	-
7EDM	A	Crystal structure of the eukaryotic ribosomal decoding site in complex with G418 and Hg(II)	-
7EEM	A	RNA bulged-G motif	-
7EFG	A	RNA kink-turn motif	-
7EQJ	A	crystal structure of E. coli Valine tRNA	tRNA (RF00005)
7EXY	A	T-hairpin structure found in the RNA element involved in the piRNA biogenesis	-
7KUB	A	Au1 Domain of VEGF Readthrough Element	-
7KUC	A	Ax1 Domain of VEGF Readthrough Element	-
7KUD	A	Ax2 Domain of VEGF Readthrough Element	-
7KVT	B	Crystal structure of Squash RNA aptamer in complex with DFHBI-1T with iridium (III) ions	-
7MLW	F	Burkholderia sp. TJI49 Guanidine-I riboswitch	ykkC-yxkD (RF00442)
7Q48	A	Solution structure of an intramolecular RNA G-quadruplex formed by the 6A8U17U mutant from a 22mer guanine-rich sequence within the 5'UTR of BCL-2 proto onco-gene	-
7Q6L	A	Solution structure of an intramolecular RNA G-quadruplex formed by the 6A8A17U mutant from a 22mer guanine-rich sequence within the 5'UTR of BCL-2 proto-oncogene	-
7Q7X	B	Crystal structure of the methyltransferase-ribozyme 1 (with 1-methyl-adenosine)	-

7Q7X	C	Crystal structure of the methyltransferase-ribozyme 1 (with 1-methyl-adenosine)	-
7QA2	A	Solution structure of an intramolecular RNA G-quadruplex formed by the 6A mutant from a 22mer guanine-rich sequence within the 5'UTR of BCL-2 proto-oncogene	-
7QDU	Q	Twist-corrected RNA origami 5-helix Tile A	-
7QP2	A	1-deazaguanosine modified-RNA Sarcin Ricin Loop	-
7R6L	A	5 prime exon-free pre-2S intermediate of the Tetrahymena group I intron, symmetry-expanded monomer from a synthetic dimeric construct, chain A	-
7R6L	B	5 prime exon-free pre-2S intermediate of the Tetrahymena group I intron, symmetry-expanded monomer from a synthetic dimeric construct, chain B	-
7R6M	A	Post-2S intermediate of the Tetrahymena group I intron, symmetry-expanded monomer from a synthetic dimeric construct	-
7RQ5	A	Hairpin near 3'-Splice Site of Influenza A Segment 7 Bound to 5-nt Oligonucleotide	-
7RWR	A	An RNA aptamer that decreases flavin redox potential	-
7SHX	A	A functional SNP regulates E-cadherin expression by dynamically remodeling the 3D structure of a promoter-associated non-coding RNA transcript, NMR, minimized average structure	-
7UCR	A	Joint X-ray/neutron structure of the Sarcin-Ricin loop RNA	-
7UGA	A	Solution structure of NPSL2	-
7UMC	A	DENV1 SLA RNA (DenvSLATL)	DENV_SLA (RF02340)
7UMD	A	DENV1 SLA three-way junction RNA (DenvSLAsh)	-
7UME	A	DENV1 SLA top stemloop RNA (DenvTSL)	-
7UQ6	B	tRNA T-box antiterminator fusion, construct #4	tRNA (RF00005)
7UVT	A	Kinetically trapped misfolded state of the Tetrahymena ribozyme	Intron_gpl (RF00028)
7UZ0	A	AntiT-tRNA flip UCCA	tRNA (RF00005)
7V06	A	Encoded Conformational Dynamics of the HIV Splice Site A3 Regulatory Locus: Implications for differential binding of hnRNP Splicing Auxiliary Factors	-
7V9E	A	Crystal structure of a methyl transferase ribozyme	-
7VFT	A	Crystal structure of rGGGC(CAG)5GUCC oligo	-
7WIA	V	The apo-form of THF-II C22G riboswitch	Intron_gpl (RF00028)
7XD3	N	The relaxed pre-Tet-S1 state of wild-type Tetrahymena group I intron with 6nt 3'/5'-exon	-
7XJZ	B	Cryo-EM structure of Oryza sativa plastid glycyl-tRNA synthetase in complex with tRNA (tRNA binding state)	tRNA (RF00005)
7XK0	B	Cryo-EM structure of Oryza sativa plastid glycyl-tRNA synthetase in complex with tRNA (tRNA locked state)	tRNA (RF00005)
7XSN	N	Native Tetrahymena ribozyme conformation	Intron_gpl (RF00028)
7YC8	N	Cryo-EM structure of Tetrahymena ribozyme conformation 1 undergoing the first-step self-splicing	Intron_gpl (RF00028)
7YGC	N	Cryo-EM structure of Tetrahymena ribozyme conformation 4 undergoing the second-step self-splicing	-

8BGU	3	human MDM2-5S RNP	5S_rRNA (RF00001)
8D2A	A	Crystal structure of theophylline aptamer in complex with TAL3	-
8DMB	W	Structure of <i>Desulfovibrio thermocuniculi</i> IsrB (DtIsrB) in complex with omega RNA and target DNA	HEARO (RF02033)
8DP3	R	Crystal structure of coxsackievirus B3 cloverleaf RNA replication element	Enterovirus_5_CRE (RF00386)
8E0F	D	Human Adenosine Deaminase Acting on dsRNA (ADAR2-RD) bound to dsRNA containing a G-G pair adjacent to the target site	-
8EG0	C	CryoEM structure of human METTL1-WDR4 in complex with Lys-tRNA and SAH	tRNA (RF00005)
8F4O	B	Apo structure of the TPP riboswitch aptamer domain	TPP (RF00059)
8FCS	A	Structure of pre-miR-31 reveals an active role in Dicer processing	mir-31 (RF00661)
8GXC	A	Crystal structure of NAD ⁺ -II riboswitch in complex with NMN	-
8HB8	A	Crystal structure of NAD-II riboswitch (single strand) with NMN	-
8HBA	A	Crystal structure of NAD-II riboswitch (single strand) with NAD	-
8HBA	B	Crystal structure of NAD-II riboswitch (single strand) with NAD	-
8HD6	N	The relaxed pre-Tet-S1 state of G264A mutated <i>Tetrahymena</i> group I intron with 6nt 3'/5'-exon and 2-aminopurine nucleoside	Intron_gpl (RF00028)
8I3Z	B	Crystal structure of NAD-II riboswitch (two strands) with NMN at 1.67 angstrom	-
8I43	A	Interaction between a fluoroquinolone derivative KG022 and RNAs: effect of base pairs 3' adjacent to the bulge out residues	-
8I7N	N	The Tet-S1 state of G264A mutated <i>Tetrahymena</i> group I intron with 6nt 3'/5'-exon and 2-aminopurine nucleoside	Intron_gpl (RF00028)

Table S10: Names and corresponding families of each of the 12 CASP15 targets.

CASP ID	PDB ID	Name	Rfam Family
R1107	7QR4	human CPEB3 HDV-like ribozyme	CPEB3_ribozyme (RF00622)
R1108	7QR3	Chimpanzee CPEB3 HDV-like ribozyme	CPEB3_ribozyme (RF00622)
R1116	8S95	Crystal Structure of Poliovirus (type 1 Mahoney) cloverleaf RNA with tRNA scaffold	Enterovirus_5_CRE (RF00386)
R1117	8FZA	Class I type III preQ1 riboswitch from <i>E. coli</i>	-
R1126	-	Traptamer	-
R1128	8BTZA	Single-stranded Paranemic Crossover RNA Triangle (PXT)	-
R1136	7ZJ4	Ligand bound state of a broccoli-pepper aptamer FRET tile	-
R1138	7PTL	Mature conformer of a 6-helix bundle of RNA with clasp	-
R1149	8UYS	SARS-CoV-2 5' proximal stem-loop 5	-
R1156	8UYG	BtCoV-HKU5 5' proximal stem-loop 5, conformation 2	-
R1189	7YR7	Cryo-EM structure of <i>Pseudomonas aeruginosa</i> RsmZ RNA in complex with three RsmA protein dimers	PrrB_RsmZ (RF00166)

R1190	7YR6	Cryo-EM structure of <i>Pseudomonas aeruginosa</i> RsmZ RNA in complex with two RsmA protein dimers	PrrB_RsmZ (RF00166)
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