

# Supplementary Data for Generating Atomic Coordinates from RNA Graphs by Fragment Assembly

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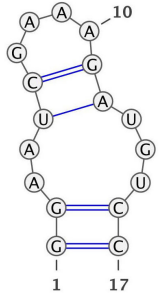

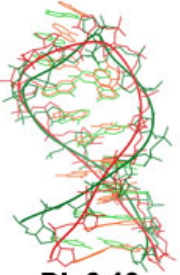
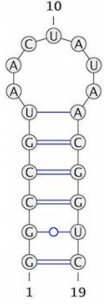

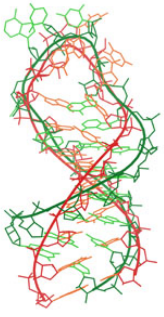
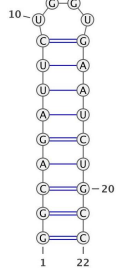

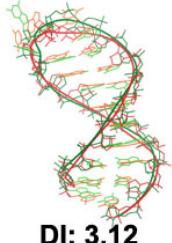
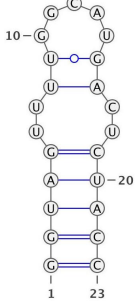
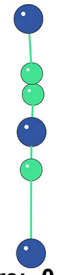
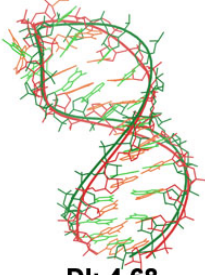
Table S1 : Lowest RMSD and lowest DI atomic models (of the top 20) generated for 50 structures by F-RAG using the fragments returned by RAG-3D search without the additional requirement for same types of loop present in the fragment as the target subgraph.

PDB	Lowest RMSD Model (Å)	Lowest DI Model (Å)
2M4W	4.489	5.80
2MEQ	5.857	8.49
2M5U	2.627	3.02
2N7X	3.588	6.07
1RLG	1.236	1.58
2MIS	2.210	2.79
2N0J	2.116	2.62
2NCI	9.916	13.25
3SIU	3.432	4.50
1OOA	5.793	7.90
2IPY	1.577	1.77
2OZB	3.389	3.85
2XEB	5.338	7.03
1MJI	3.246	4.27
2M57	5.063	8.38
4PCJ	1.116	1.23
2HW8	2.109	2.42
2N6S	2.714	3.07
5KQE	9.144	12.19
1I6U	0.828	0.93
1F1T	1.700	1.96
1ZHO	1.763	1.95
2MXL	5.235	6.73
2N6T	4.728	6.58
2N6X	10.285	13.40
5BTM	3.193	4.25
1S03	5.455	6.78
1XJR	7.767	11.16
2MTJ	13.255	21.27
2VPL	6.183	7.92
1U63	5.092	6.19
2PXB	0.687	0.77
2N4L	3.261	4.00
2HGH	3.375	3.99
1DK1	1.008	1.18
1MMS	0.647	0.73
1Y39	0.717	0.81
2N3Q	16.982	25.37
2MQT	6.352	7.94
2N6W	5.998	7.68
1KXK	0.872	1.03
2OIU	N/A	N/A
4LCK	5.162	6.90
1P5O	7.018	10.69
3D2G	1.285	1.52
2HOJ	2.747	3.45
2GDI	3.185	4.08
2GIS	0.737	0.84
1LNG	0.858	0.96
2LKR	20.682	32.91

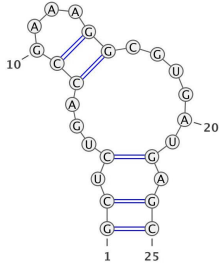
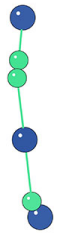

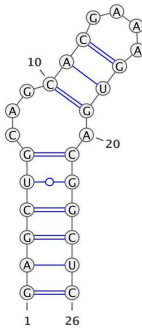
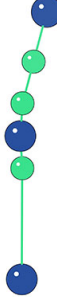
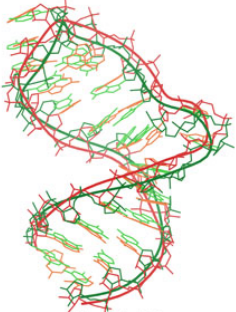
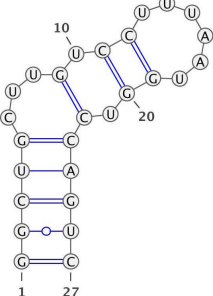
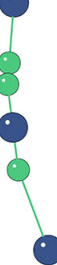
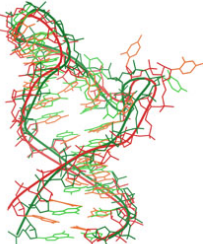
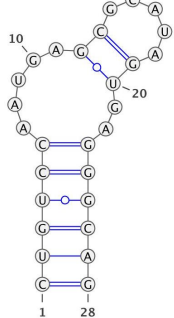

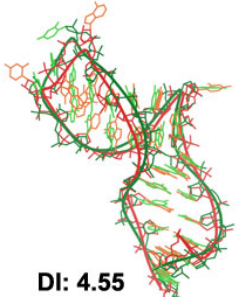
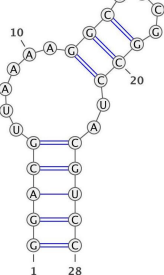
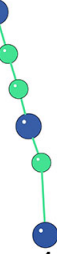

Table S2 : Comparison metrics for the top scoring atomic model (with the highest number of residues) generated by F-RAG.

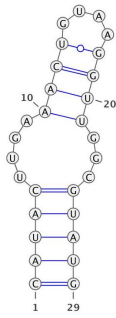
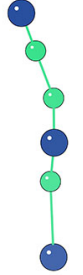
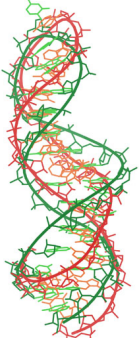
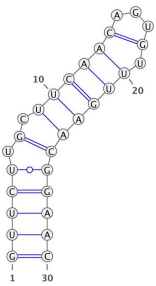
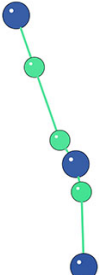
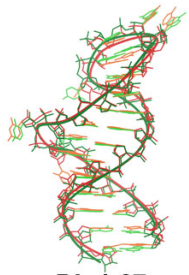
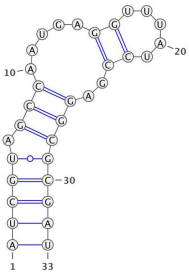
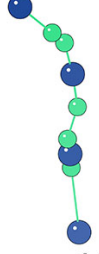
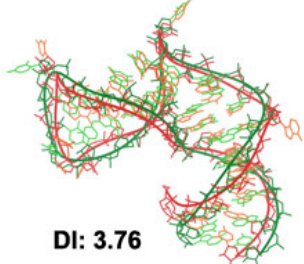
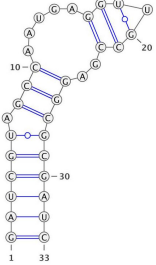
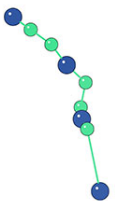
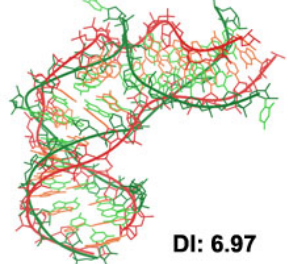
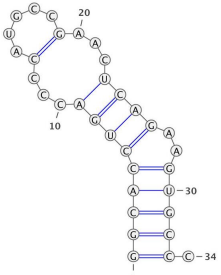
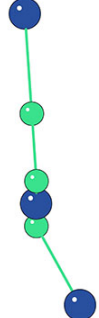

PDB	RMSD(Å)	PPV	STY	INF	DI(Å)	Clashscore
2M4W	4.038	0.75	0.71	0.73	5.55	10.83
2MEQ	6.849	0.73	0.73	0.73	9.34	3.27
2M5U	3.480	0.83	0.91	0.87	4.00	2.83
2N7X	3.625	0.69	0.46	0.56	6.46	1.36
1RLG	1.034	0.90	0.68	0.78	1.32	2.47
2MIS	5.150	0.69	0.80	0.74	6.93	2.36
2N0J	2.170	0.82	0.69	0.75	2.88	2.33
2NCI	11.412	0.73	0.95	0.83	13.70	0.00
3SIU	3.546	0.81	0.75	0.78	4.56	4.40
1OOA	5.005	0.70	0.66	0.68	7.38	10.73
2IPY	5.191	1.00	0.70	0.83	6.22	4.18
2OZB	3.579	0.83	0.94	0.88	4.07	4.70
2XEB	6.014	0.74	0.84	0.79	7.62	1.87
1MJI	3.246	0.87	0.67	0.76	4.27	13.72
2M57	5.416	0.62	0.68	0.65	8.37	14.20
4PCJ	1.116	0.93	0.89	0.91	1.23	0.89
2HW8	2.857	0.94	0.80	0.87	3.28	0.00
2N6S	14.538	0.73	0.54	0.63	23.18	38.36
5KQE	9.835	0.87	0.70	0.78	12.60	0.87
1I6U	3.258	0.90	0.78	0.84	3.90	11.74
1F1T	5.547	0.73	0.61	0.67	8.29	0.81
1ZHO	1.763	0.95	0.86	0.90	1.95	0.81
2MXL	8.419	0.78	0.60	0.68	12.37	20.50
2N6T	6.502	0.65	0.68	0.67	9.75	4.49
2N6X	12.616	0.62	0.88	0.74	16.99	3.64
5BTM	3.237	0.83	0.56	0.68	4.76	2.20
1S03	5.638	0.91	0.72	0.81	6.96	9.89
1XJR	8.622	0.80	0.59	0.69	12.55	3.27
2MTJ	13.255	0.71	0.54	0.62	21.27	3.52
2VPL	0.428	0.98	0.81	0.89	0.48	3.86
1U63	3.408	0.83	0.73	0.78	4.37	1.26
2PXB	5.367	0.90	0.62	0.75	7.15	4.40
2N4L	6.448	0.91	0.72	0.81	7.97	5.90
2HGH	4.563	0.91	0.61	0.74	6.15	1.71
1DK1	2.060	0.85	0.73	0.79	2.61	8.13
1MMS	2.337	0.95	0.71	0.82	2.86	6.43
1Y39	2.036	0.95	0.76	0.85	2.39	5.90
2N3Q	17.061	0.54	0.75	0.64	26.78	5.57
2MQT	12.310	0.80	0.68	0.74	16.65	5.50
2N6W	14.221	0.79	0.72	0.75	18.86	4.17
1KXX	1.800	0.90	0.73	0.81	2.23	3.99
2OIU	14.400	0.95	0.81	0.88	16.43	0.87
4LCK	1.336	0.93	0.76	0.84	1.59	3.72
1P5O	2.176	0.94	0.78	0.86	2.54	8.09
3D2G	2.131	0.90	0.69	0.79	2.70	6.43
2HOJ	2.747	0.92	0.69	0.80	3.45	4.71
2GDI	5.411	0.90	0.60	0.73	7.38	6.98
2GIS	0.929	0.92	0.82	0.87	1.07	5.25
1LNG	2.928	0.91	0.84	0.88	3.34	5.42
2LKR	20.741	0.65	0.61	0.63	32.92	7.75

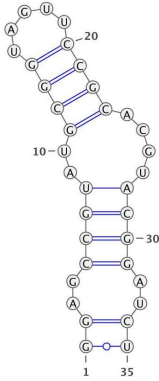
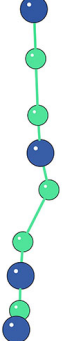
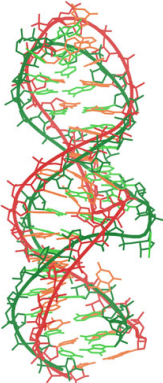
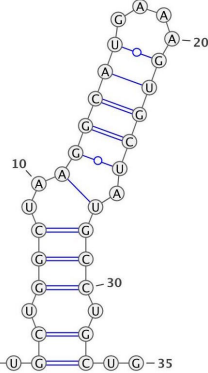
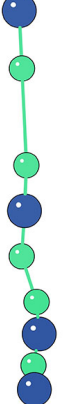

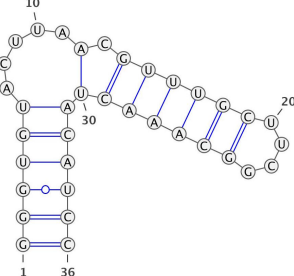

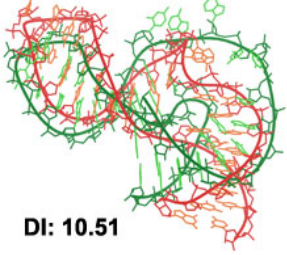
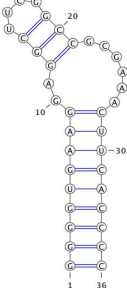
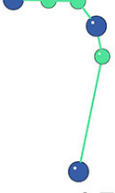
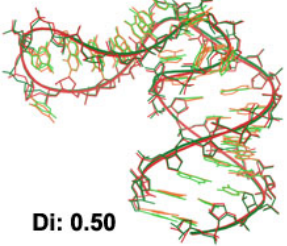
Table S3 : **Images of F-RAG atomic models:** the secondary structure, RAGTOP predicted candidate graph, and the lowest deformation index (DI) atomic model generated by F-RAG are shown for 50 RNA structures. The loop vertices are colored blue and helical vertices are colored sea green in the candidate 3D graphs. The reference model is colored red and the lowest DI atomic model generated by F-RAG is superimposed in green.

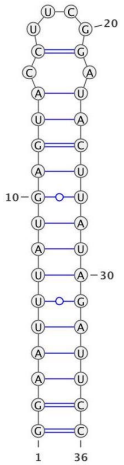

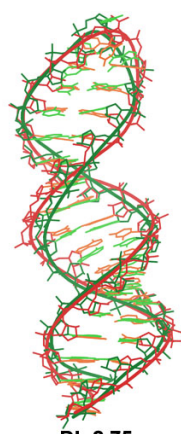
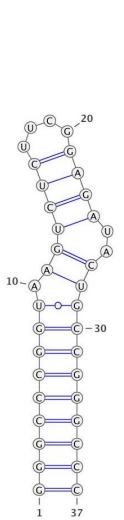
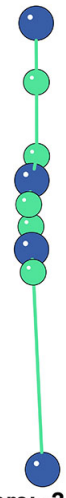
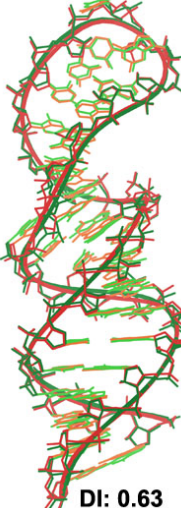
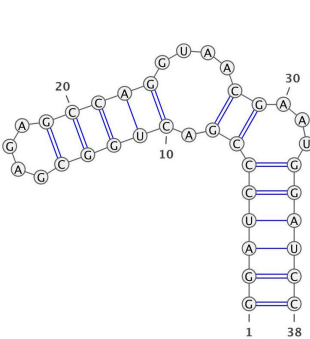


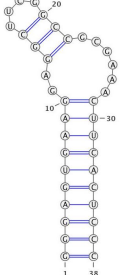
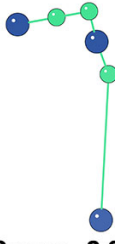
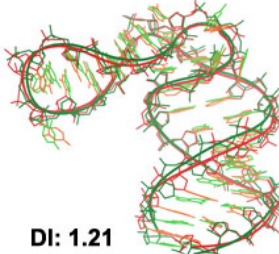
PDB	2D Structure	Candidate graph	Lowest DI atomic model
2M4W		 Score: -0.553	 DI: 3.19
2MEQ		 Score: 0.932	 DI: 8.49
2M5U		 Score: 3.20	 DI: 3.12
2N7X		 Score: -0.784	 DI: 4.68

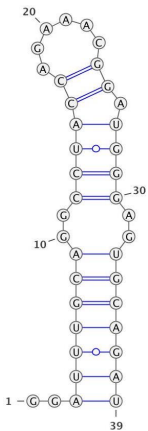
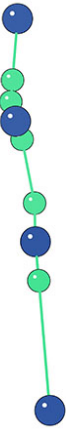
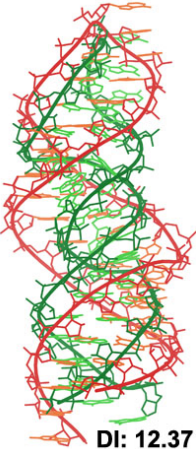
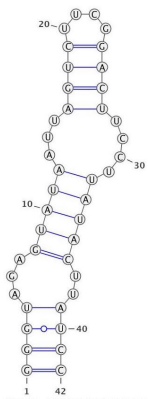
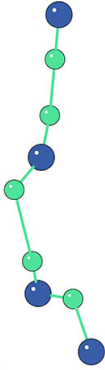
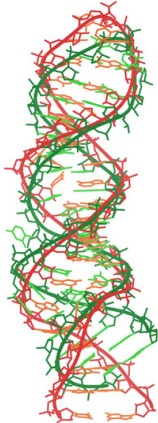
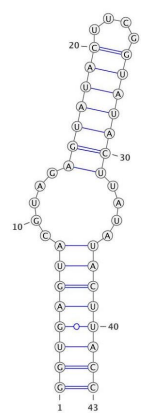

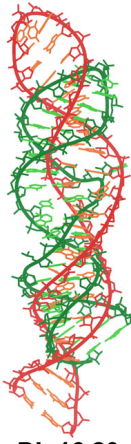


1RLG	 <p>Secondary structure diagram of RNA 1RLG. The sequence is numbered 1 to 25. The structure shows a stem-loop region at the top and a stem at the bottom.</p>	 <p>Score: <b>-0.988</b></p>	 <p>DI: <b>1.25</b></p>
2MIS	 <p>Secondary structure diagram of RNA 2MIS. The sequence is numbered 1 to 26. The structure shows a stem-loop region at the top and a stem at the bottom.</p>	 <p>Score: <b>-1.532</b></p>	 <p>DI: <b>2.46</b></p>
2N0J	 <p>Secondary structure diagram of RNA 2N0J. The sequence is numbered 1 to 27. The structure shows a stem-loop region at the top and a stem at the bottom.</p>	 <p>Score: <b>-0.011</b></p>	 <p>DI: <b>2.86</b></p>
3SIU	 <p>Secondary structure diagram of RNA 3SIU. The sequence is numbered 1 to 28. The structure shows a stem-loop region at the top and a stem at the bottom.</p>	 <p>Score: <b>-0.055</b></p>	 <p>DI: <b>4.55</b></p>
2NCI	 <p>Secondary structure diagram of RNA 2NCI. The sequence is numbered 1 to 28. The structure shows a stem-loop region at the top and a stem at the bottom.</p>	 <p>Score: <b>-1.373</b></p>	 <p>DI: <b>12.62</b></p>

100A		 <p><b>Score: -1.581</b></p>	 <p><b>DI: 7.22</b></p>
2IPY		 <p><b>Score: -1.586</b></p>	 <p><b>DI: 1.67</b></p>
2OZB		 <p><b>Score: -1.713</b></p>	 <p><b>DI: 3.76</b></p>
2XEB		 <p><b>Score: -2.521</b></p>	 <p><b>DI: 6.97</b></p>
1MJI		 <p><b>Score: 0.805</b></p>	 <p><b>DI: 4.27</b></p>

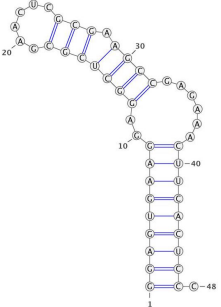
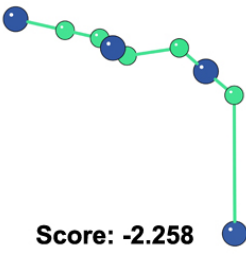
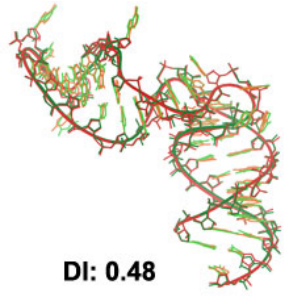
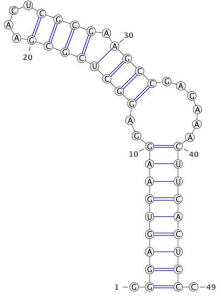
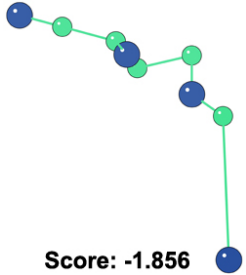

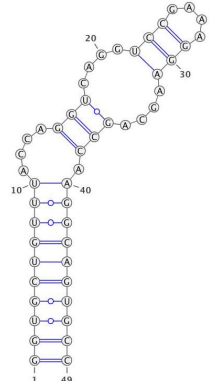
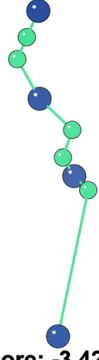
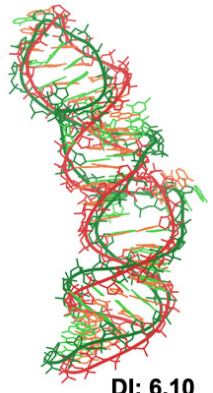
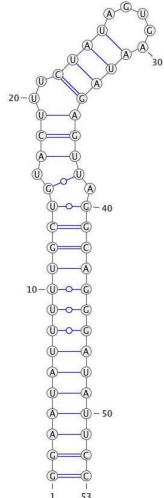
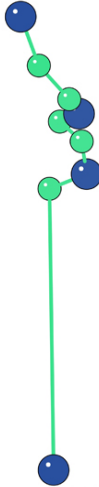
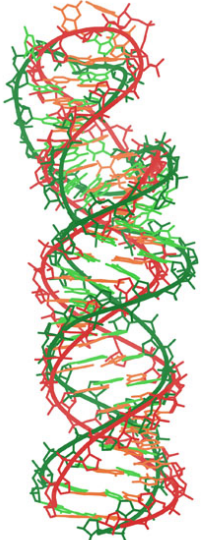
2M57		 <p><b>Score: -2.810</b></p>	 <p><b>DI: 7.75</b></p>
4PCJ		 <p><b>Score: -1.727</b></p>	 <p><b>DI: 1.23</b></p>
5KQE		 <p><b>Score: -1.121</b></p>	 <p><b>DI: 10.51</b></p>
2HW8		 <p><b>Score: -1.799</b></p>	 <p><b>DI: 0.50</b></p>

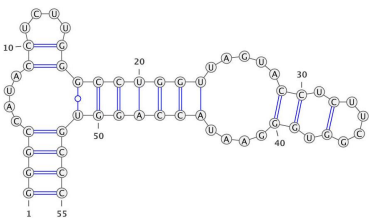
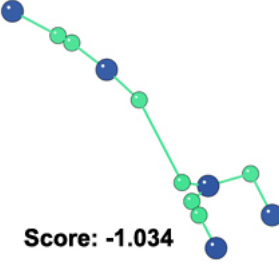
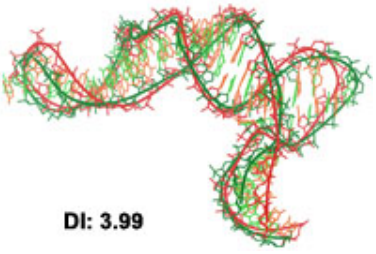
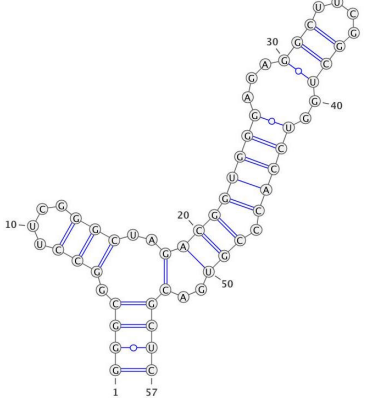
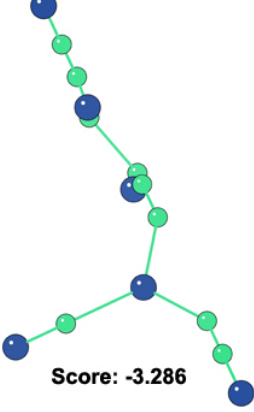

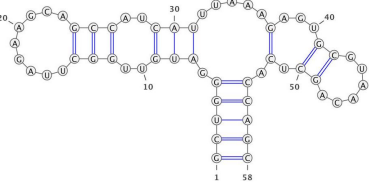
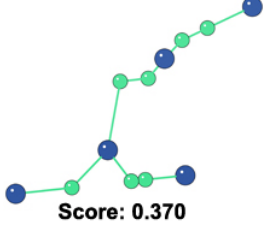
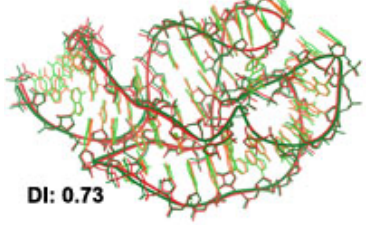
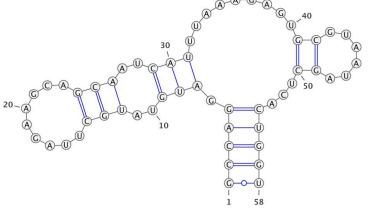
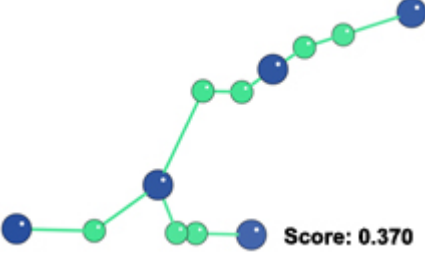
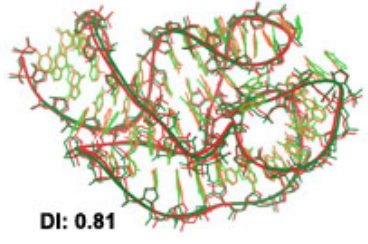
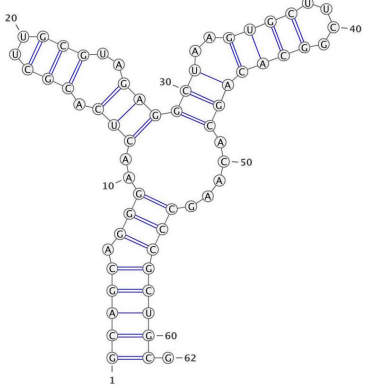
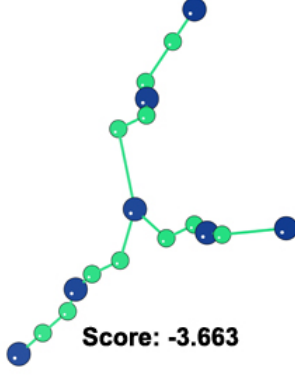
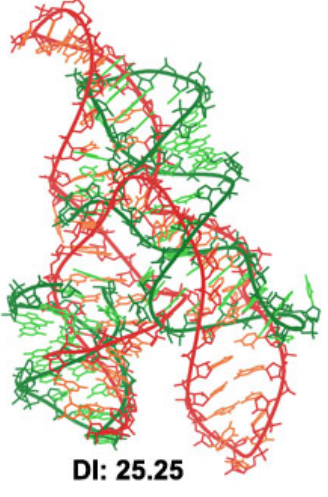
2N6S		 <p>Score: 6.852</p>	 <p>DI: 2.75</p>
1I6U		 <p>Score: -2.867</p>	 <p>DI: 0.63</p>
1F1T		 <p>Score: -2.265</p>	 <p>DI: 7.30</p>
1ZHO		 <p>Score: -2.343</p>	 <p>DI: 1.21</p>

2MXL		 <p><b>Score: -2.827</b></p>	 <p><b>DI: 12.37</b></p>
2N6T		 <p><b>Score: -3.132</b></p>	 <p><b>DI: 7.72</b></p>
2N6X		 <p><b>Score: -1.081</b></p>	 <p><b>DI: 16.20</b></p>

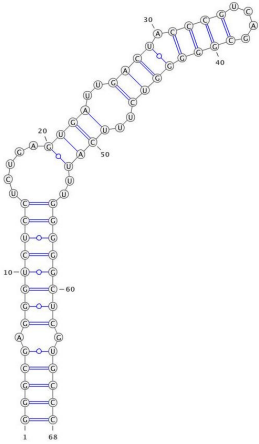
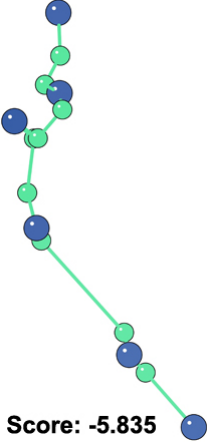
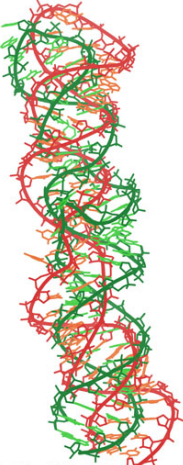
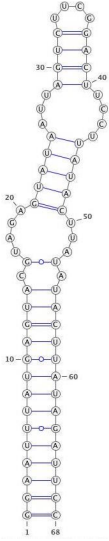
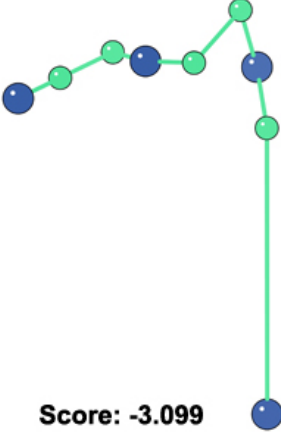
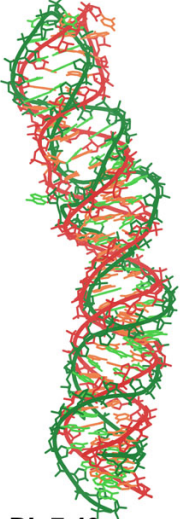
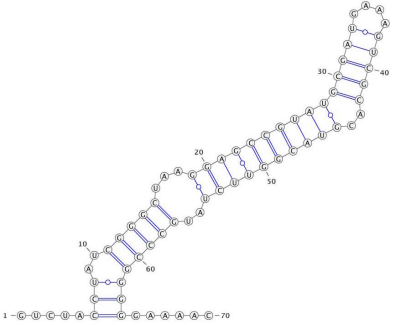
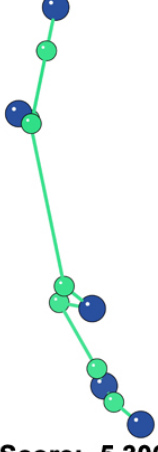
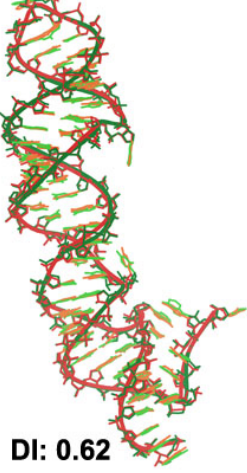


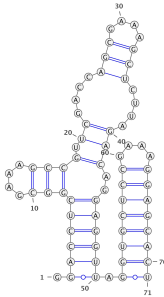
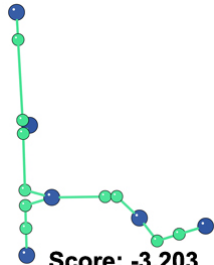
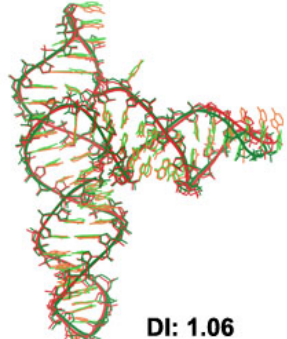
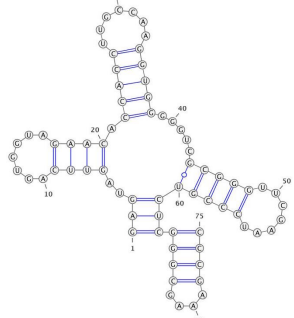
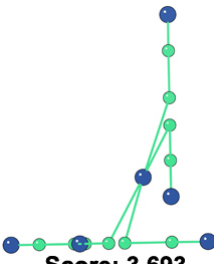
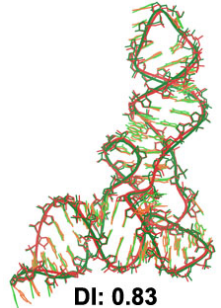
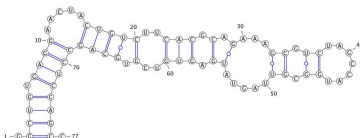
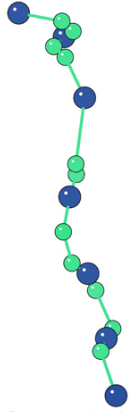

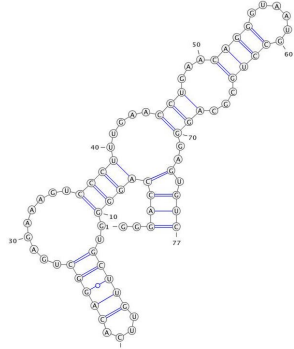
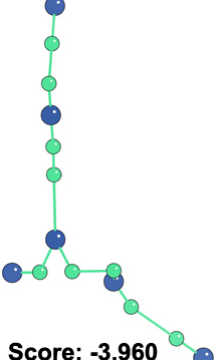
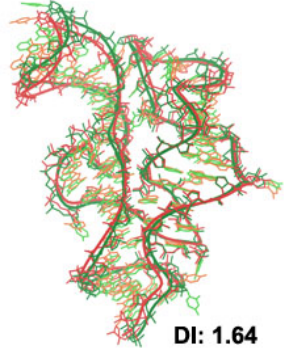


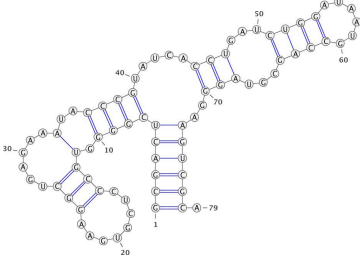
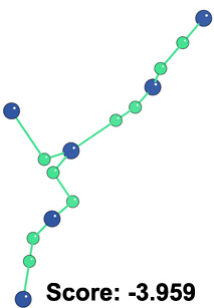
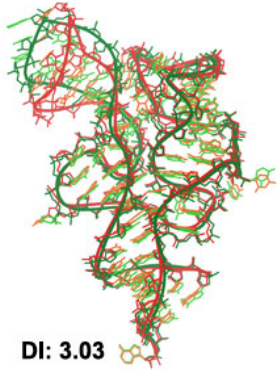
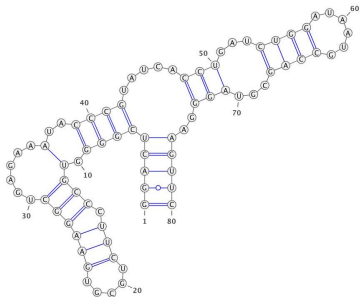
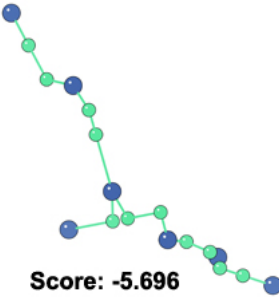
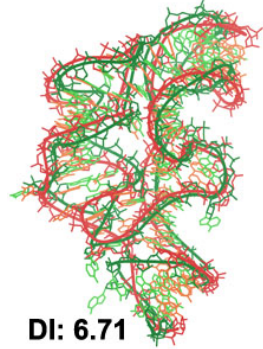
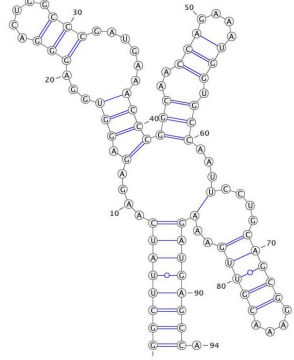
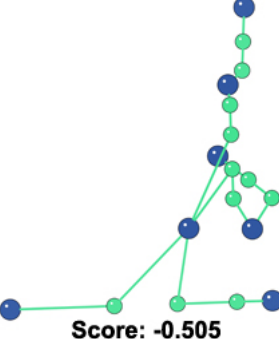
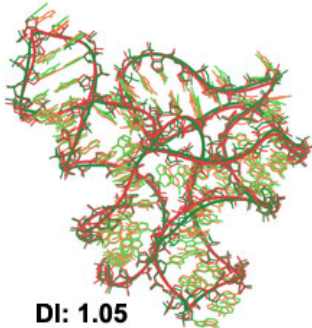
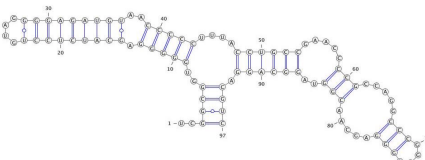
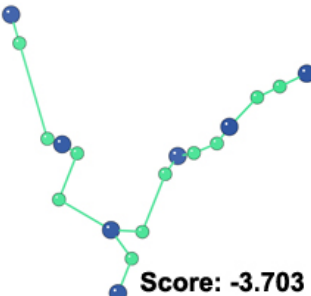
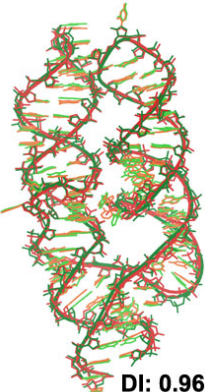
2VPL	 <p>Secondary structure diagram of RNA 2VPL, showing a stem-loop structure with residues numbered 1 to 48.</p>	 <p>Score: <b>-2.258</b></p>	 <p>DI: <b>0.48</b></p>
1U63	 <p>Secondary structure diagram of RNA 1U63, showing a stem-loop structure with residues numbered 1 to 49.</p>	 <p>Score: <b>-1.856</b></p>	 <p>DI: <b>4.37</b></p>
2PXB	 <p>Secondary structure diagram of RNA 2PXB, showing a stem-loop structure with residues numbered 1 to 49.</p>	 <p>Score: <b>-3.427</b></p>	 <p>DI: <b>6.10</b></p>
2N4L	 <p>Secondary structure diagram of RNA 2N4L, showing a stem-loop structure with residues numbered 1 to 53.</p>	 <p>Score: <b>-3.197</b></p>	 <p>DI: <b>7.15</b></p>

2HGH	 <p>Secondary structure diagram of RNA 2HGH, showing base pairing between nucleotides 1 and 55. The structure features several stem-loops and internal loops.</p>	 <p>Simplified secondary structure diagram of RNA 2HGH, represented by green and blue nodes connected by lines. <b>Score: -1.034</b></p>	 <p>3D ribbon model of RNA 2HGH, colored in red and green. <b>DI: 3.99</b></p>
1DK1	 <p>Secondary structure diagram of RNA 1DK1, showing base pairing between nucleotides 1 and 57. The structure is highly branched with multiple stem-loops.</p>	 <p>Simplified secondary structure diagram of RNA 1DK1, represented by green and blue nodes connected by lines. <b>Score: -3.286</b></p>	 <p>3D ribbon model of RNA 1DK1, colored in red and green. <b>DI: 1.18</b></p>
1MMS	 <p>Secondary structure diagram of RNA 1MMS, showing base pairing between nucleotides 1 and 58. The structure is relatively compact with several stem-loops.</p>	 <p>Simplified secondary structure diagram of RNA 1MMS, represented by green and blue nodes connected by lines. <b>Score: 0.370</b></p>	 <p>3D ribbon model of RNA 1MMS, colored in red and green. <b>DI: 0.73</b></p>
1Y39	 <p>Secondary structure diagram of RNA 1Y39, showing base pairing between nucleotides 1 and 58. The structure is highly branched and complex.</p>	 <p>Simplified secondary structure diagram of RNA 1Y39, represented by green and blue nodes connected by lines. <b>Score: 0.370</b></p>	 <p>3D ribbon model of RNA 1Y39, colored in red and green. <b>DI: 0.81</b></p>
2N3Q	 <p>Secondary structure diagram of RNA 2N3Q, showing base pairing between nucleotides 1 and 62. The structure is highly branched and complex.</p>	 <p>Simplified secondary structure diagram of RNA 2N3Q, represented by green and blue nodes connected by lines. <b>Score: -3.663</b></p>	 <p>3D ribbon model of RNA 2N3Q, colored in red and green. <b>DI: 25.25</b></p>

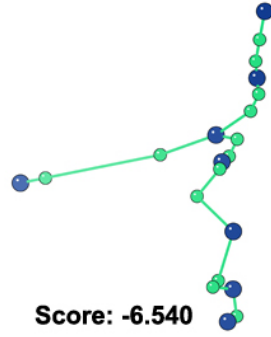
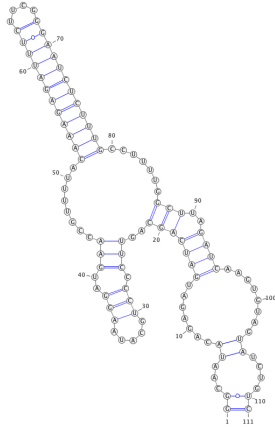


<p>2MQT</p>	 <p>Secondary structure diagram of RNA 2MQT, showing a stem-loop structure with residues numbered 1 to 68.</p>	 <p>Simplified RNA secondary structure diagram for 2MQT, showing a path of blue and green nodes connected by a green line.</p> <p><b>Score: -5.835</b></p>	 <p>3D ribbon model of RNA 2MQT, colored in red and green.</p> <p><b>DI: 11.24</b></p>
<p>2N6W</p>	 <p>Secondary structure diagram of RNA 2N6W, showing a stem-loop structure with residues numbered 1 to 68.</p>	 <p>Simplified RNA secondary structure diagram for 2N6W, showing a path of blue and green nodes connected by a green line.</p> <p><b>Score: -3.099</b></p>	 <p>3D ribbon model of RNA 2N6W, colored in red and green.</p> <p><b>DI: 7.40</b></p>
<p>1KXK</p>	 <p>Secondary structure diagram of RNA 1KXK, showing a stem-loop structure with residues numbered 1 to 70.</p>	 <p>Simplified RNA secondary structure diagram for 1KXK, showing a path of blue and green nodes connected by a green line.</p> <p><b>Score: -5.306</b></p>	 <p>3D ribbon model of RNA 1KXK, colored in red and green.</p> <p><b>DI: 0.62</b></p>

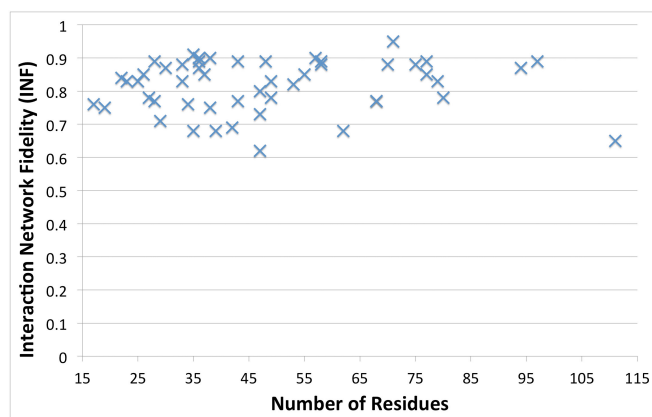
2OIU	 <p>2D schematic of RNA structure 2OIU, showing nucleotides 1 through 71. The structure features a stem-loop region at the top and a larger stem-loop at the bottom.</p>	 <p>Simplified representation of RNA structure 2OIU, with nucleotides represented by green and blue spheres. <b>Score: -3.203</b></p>	 <p>3D ribbon model of RNA structure 2OIU, colored in red and green. <b>DI: 1.06</b></p>
4LCK	 <p>2D schematic of RNA structure 4LCK, showing nucleotides 1 through 70. The structure is highly branched with multiple stem-loops.</p>	 <p>Simplified representation of RNA structure 4LCK, with nucleotides represented by green and blue spheres. <b>Score: 3.693</b></p>	 <p>3D ribbon model of RNA structure 4LCK, colored in red and green. <b>DI: 0.83</b></p>
1P5O	 <p>2D schematic of RNA structure 1P5O, showing nucleotides 1 through 77. The structure is a long, relatively linear stem-loop.</p>	 <p>Simplified representation of RNA structure 1P5O, with nucleotides represented by green and blue spheres. <b>Score: -8.516</b></p>	 <p>3D ribbon model of RNA structure 1P5O, colored in red and green. <b>DI: 2.53</b></p>
3D2G	 <p>2D schematic of RNA structure 3D2G, showing nucleotides 1 through 77. The structure is highly branched and complex.</p>	 <p>Simplified representation of RNA structure 3D2G, with nucleotides represented by green and blue spheres. <b>Score: -3.960</b></p>	 <p>3D ribbon model of RNA structure 3D2G, colored in red and green. <b>DI: 1.64</b></p>

2HOJ		 <p><b>Score: -3.959</b></p>	 <p><b>DI: 3.03</b></p>
2GDI		 <p><b>Score: -5.696</b></p>	 <p><b>DI: 6.71</b></p>
2GIS		 <p><b>Score: -0.505</b></p>	 <p><b>DI: 1.05</b></p>
1LNG		 <p><b>Score: -3.703</b></p>	 <p><b>DI: 0.96</b></p>

2LKR



**(a) INF**



**(b) Clashscore**

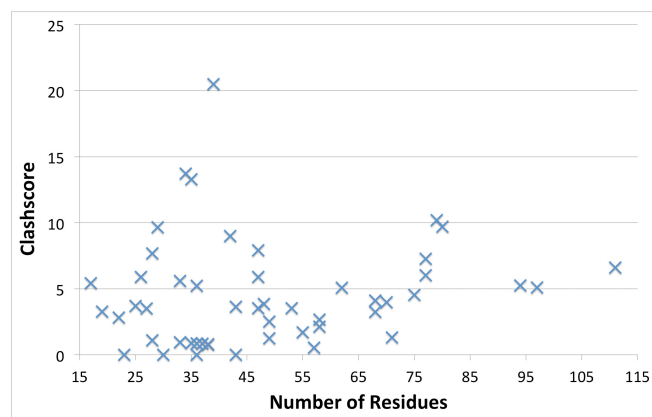


Figure S1 : **Statistics for the lowest DI atomic model generated by F-RAG for 50 RNA structures.** (a) Number of Residues vs Interaction Network Fidelity (INF) (b) Number of residues vs Clashscore. See the main text for definitions of these measures.

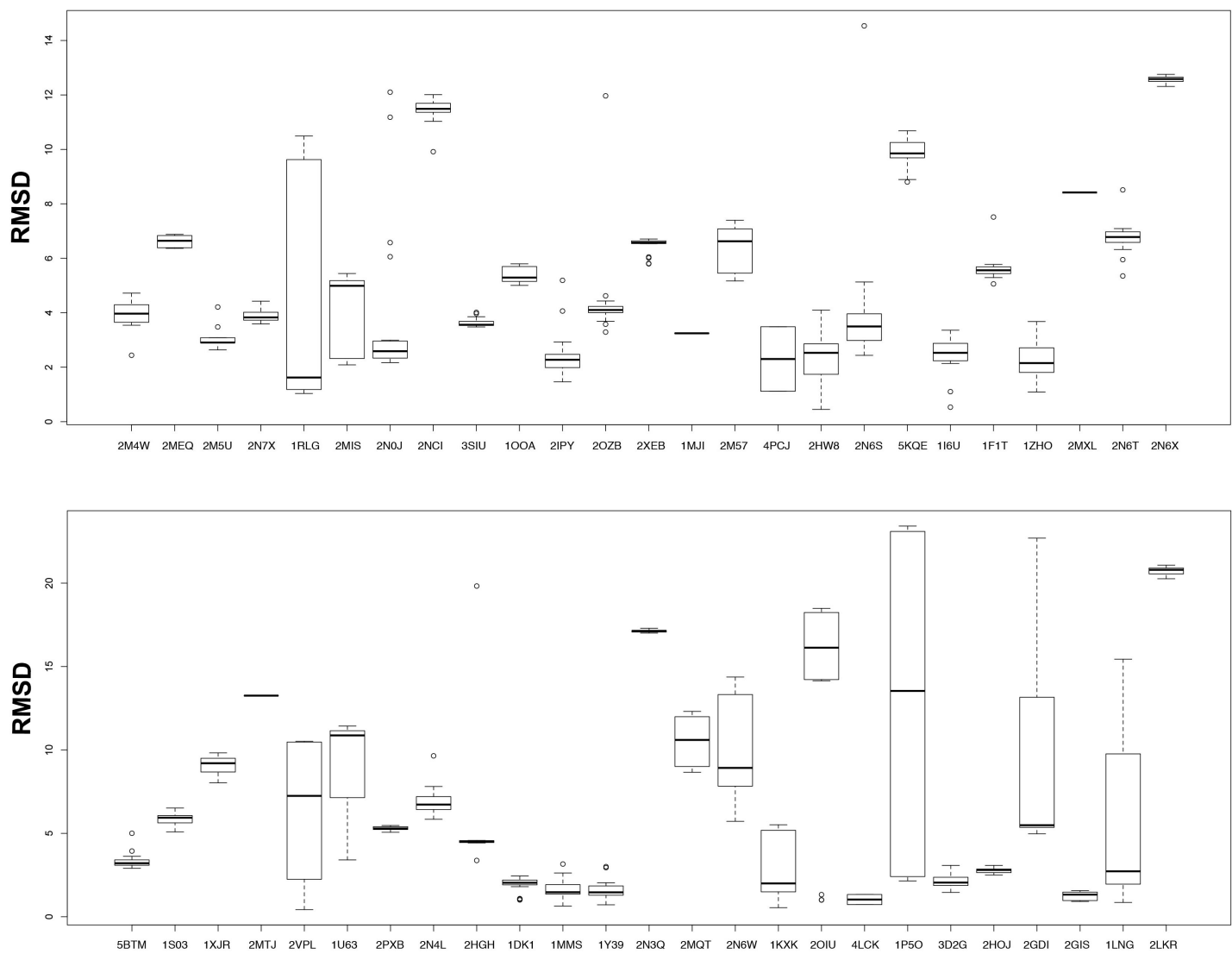


Figure S2 : RMSD of top atomic models generated by F-RAG for 50 RNA structures after geometry optimization with PHENIX.

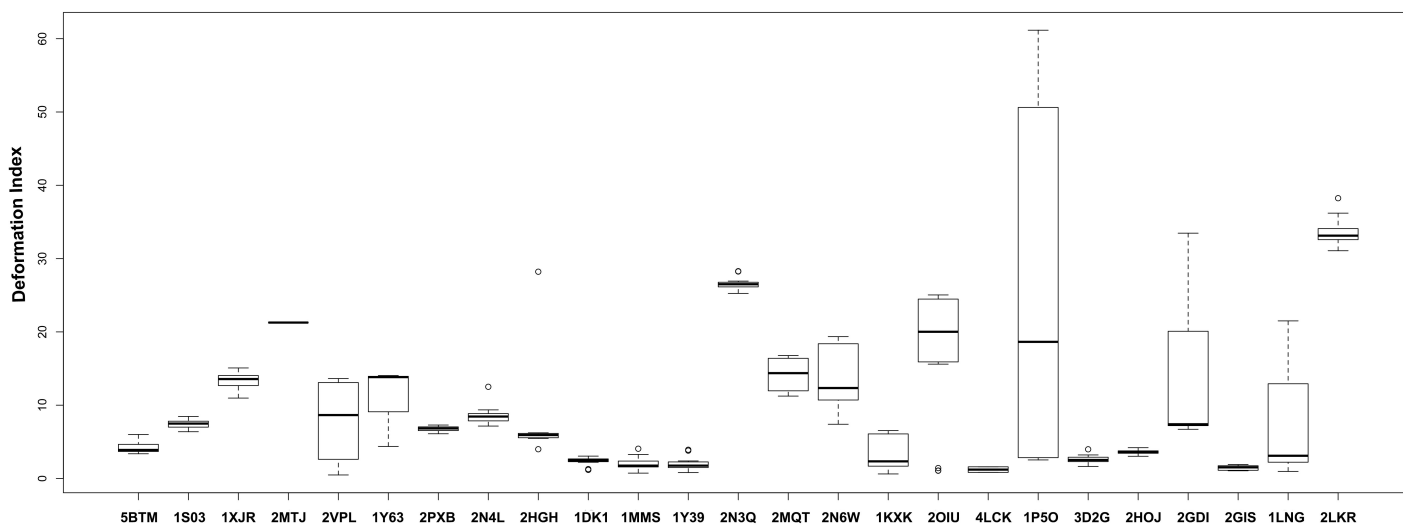
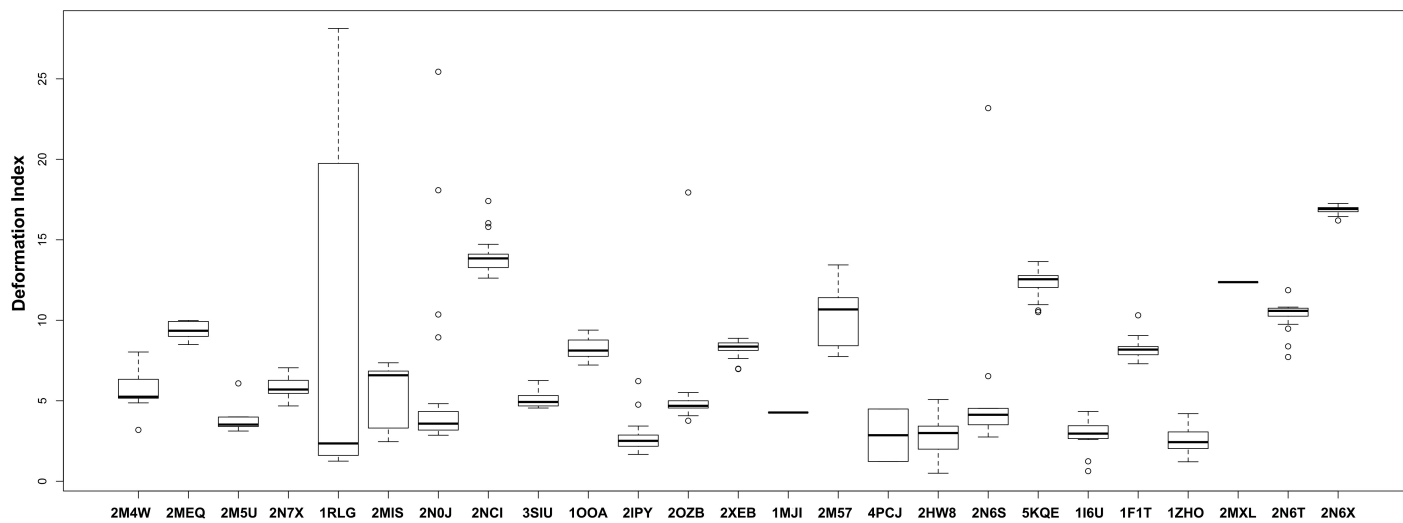


Figure S3 : Deformation Index (DI) values of top atomic models generated by F-RAG for 50 RNA structures after geometry optimization with PHENIX.

