Supplementary Material

Statistical Potentials

i) Internal Loop Potentials (Bend and Torsion Angles)

An internal loop is defined by two double stranded regions connected by a bulge. In RAG-3D, these two double stranded regions are represented as two edges (V_1 and V_2) so that the vector V_1 points toward the bulge, and the vector V_2 points away from the bulge (see Figure S1). Then, the bending angle (θ) is defined as the angle between V_1 and V_2. This definition is consistent with the bend angle definition given by Lilley et al. in (1).

Let the third vector (V_3) connect V_1 and V_2. Then, the torsion angle (τ) is defined as the angle between the planes defined by V_1V_3 and V_3V_2 (n_1 and n_2, respectively). Specifically, the

$$\text{bend angle } \theta = \pi - \cos^{-1}\left(\left|V_1 \cdot V_2\right| \middle/ \left|V_1\right|\left|V_2\right|\right), \text{ and the}$$

$$\text{torsion angle } \tau = sign(n_1 \cdot V_3)\cos^{-1}\left(\left|n_1 \cdot n_2\right| \middle/ \left|n_1\right|\left|n_2\right|\right),$$

$$\text{where } sign(x) = \begin{cases} -1 & if \quad x < 0 \\ 0 & if \quad x = 0 \\ 1 & if \quad x > 0 \end{cases}.$$

ii) Radii of Gyration

The third potential of our scoring function is ΔG_{R_g} and is defined as the absolute difference of R_g from estimated radii of gyration $\overline{R_g}$:

$$\Delta G_{R_g} = \left|R - \overline{R}\right|.$$

R_g is defined as the mean distance from each vertex to the center of mass of all vertices in a RAG-3D graph representation, $R_g = \sum_i \left|V_i - \overline{V}\right| \big/ V$. The estimated $\overline{R_g}$ is calculated based on the sequence length (L) and the number of vertices (V) using the logarithmic relationship $\overline{R_g}(L,V) = a * \ln(L) + b * \ln(V) + c$, where $a = 8.58$, $b = 2.30$, and $c = -19.50$ (2). R_g was also used as a RNA 3D model selection criteria by Hofacker et al. (3).

iii) Pseudoknot Length

We add a term to the scoring function for structures with pseudoknot, using an additional edge to handle pseudoknot interactions:

$$\Delta G_{pk} = \left| D - \overline{D} \right| .$$

Here D is the length of the pseudoknot edge of the graph at each MC step, and $\overline{D}$ is the length of the pseudoknot edge of reference graph. At this point, we can only handle the pseudoknot structures if the reference is known.

Figure S1

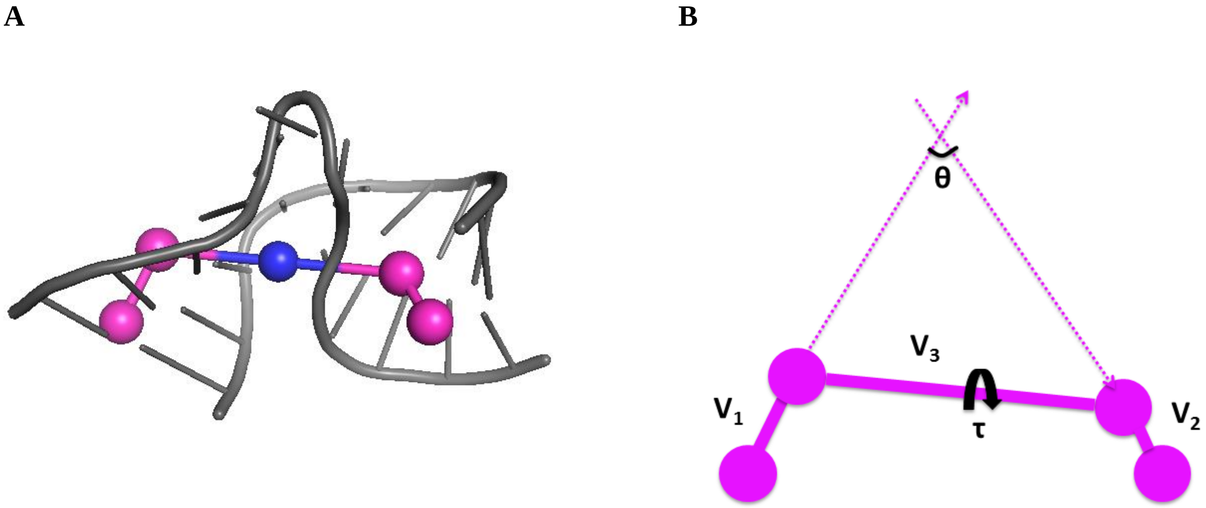
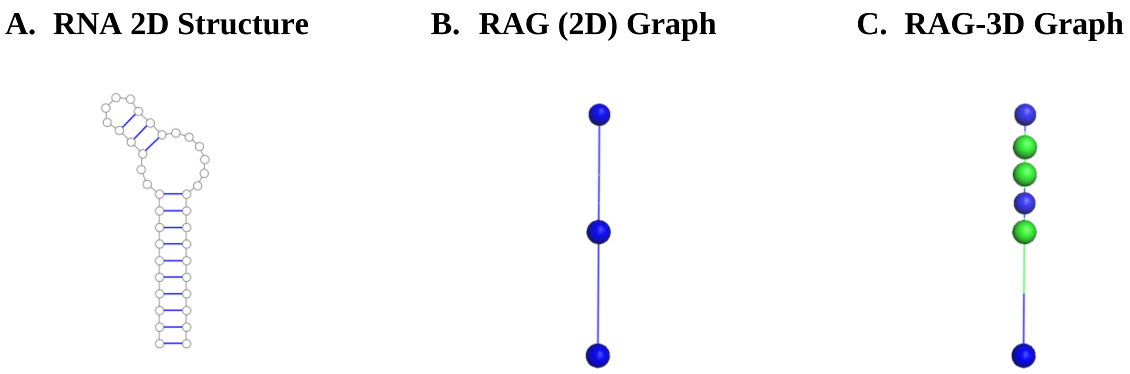


Figure S1. Knowledge-based internal loop potentials. (A) An internal loop defined by two helices and a connecting with a bulge represented as a RAG-3D graph. (B) Bend and torsion angles of the internal loop. The bend angle θ represents the angle between two helical axes V_1 and V_2. The torsion angle shows the angle between V_1V_3 and V_3V_2 planes.

Figure S2


A. RNA 2D Structure

B. RAG (2D) Graph

C. RAG-3D Graph

Figure S2. RNA graph representations. (A) RNA hairpin and internal loop elements. (B) RAG representation which defines hairpins and internal loops as vertices and stems as edges. (C) RAG-3D representation which defines each helix by one edge and two vertices.

Figure S3

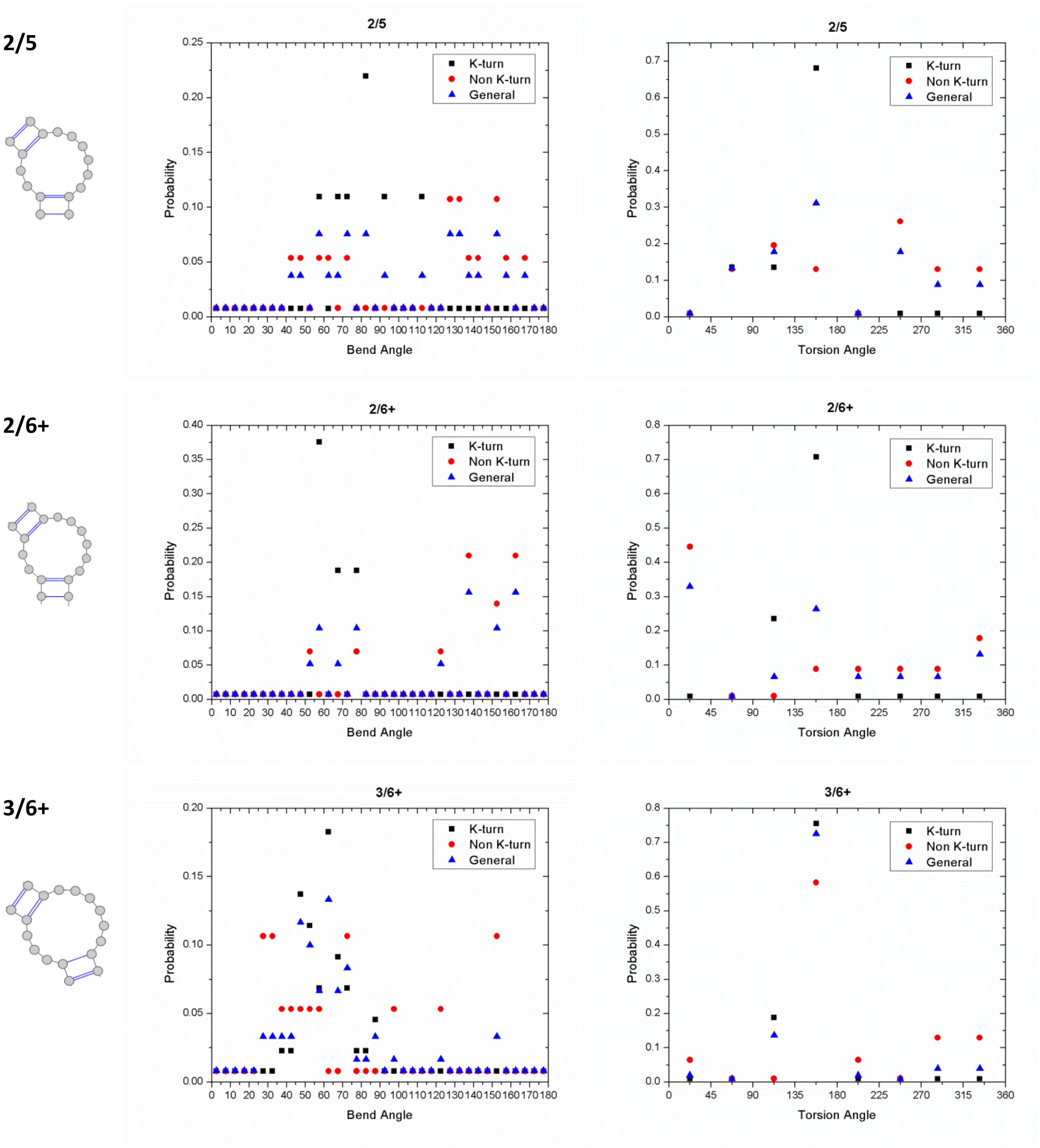


Figure S3. Statistical potential distributions of k-turn, and non k-turn motifs and all data

Figure S4

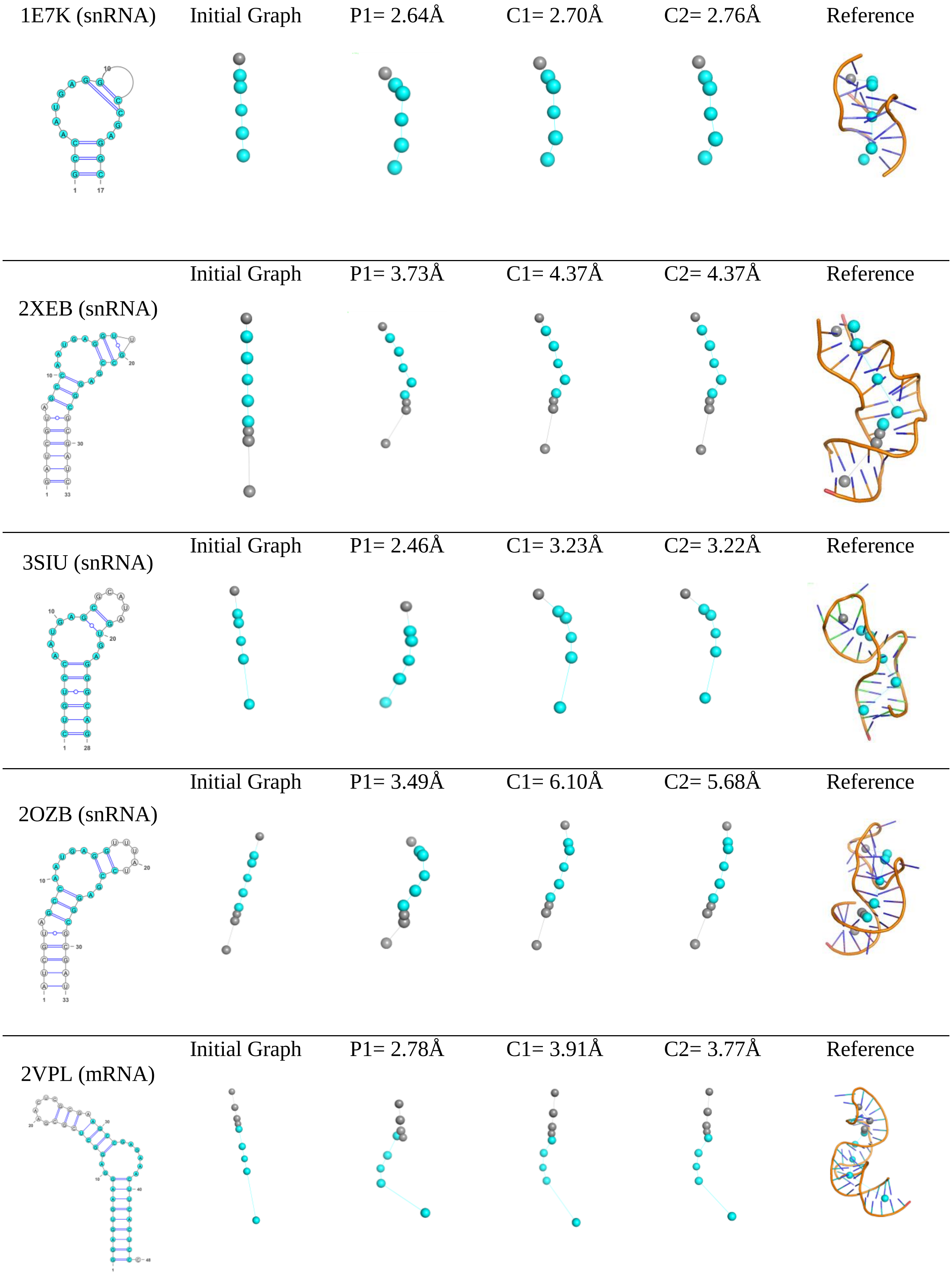

1E7K (snRNA)
Initial Graph
P1= 2.64Å
C1= 2.70Å
C2= 2.76Å
Reference
2XEB (snRNA)
Initial Graph
P1= 3.73Å
C1= 4.37Å
C2= 4.37Å
Reference
3SIU (snRNA)
Initial Graph
P1= 2.46Å
C1= 3.23Å
C2= 3.22Å
Reference
2OZB (snRNA)
Initial Graph
P1= 3.49Å
C1= 6.10Å
C2= 5.68Å
Reference
2VPL (mRNA)
Initial Graph
P1= 2.78Å
C1= 3.91Å
C2= 3.77Å
Reference

Figure S4

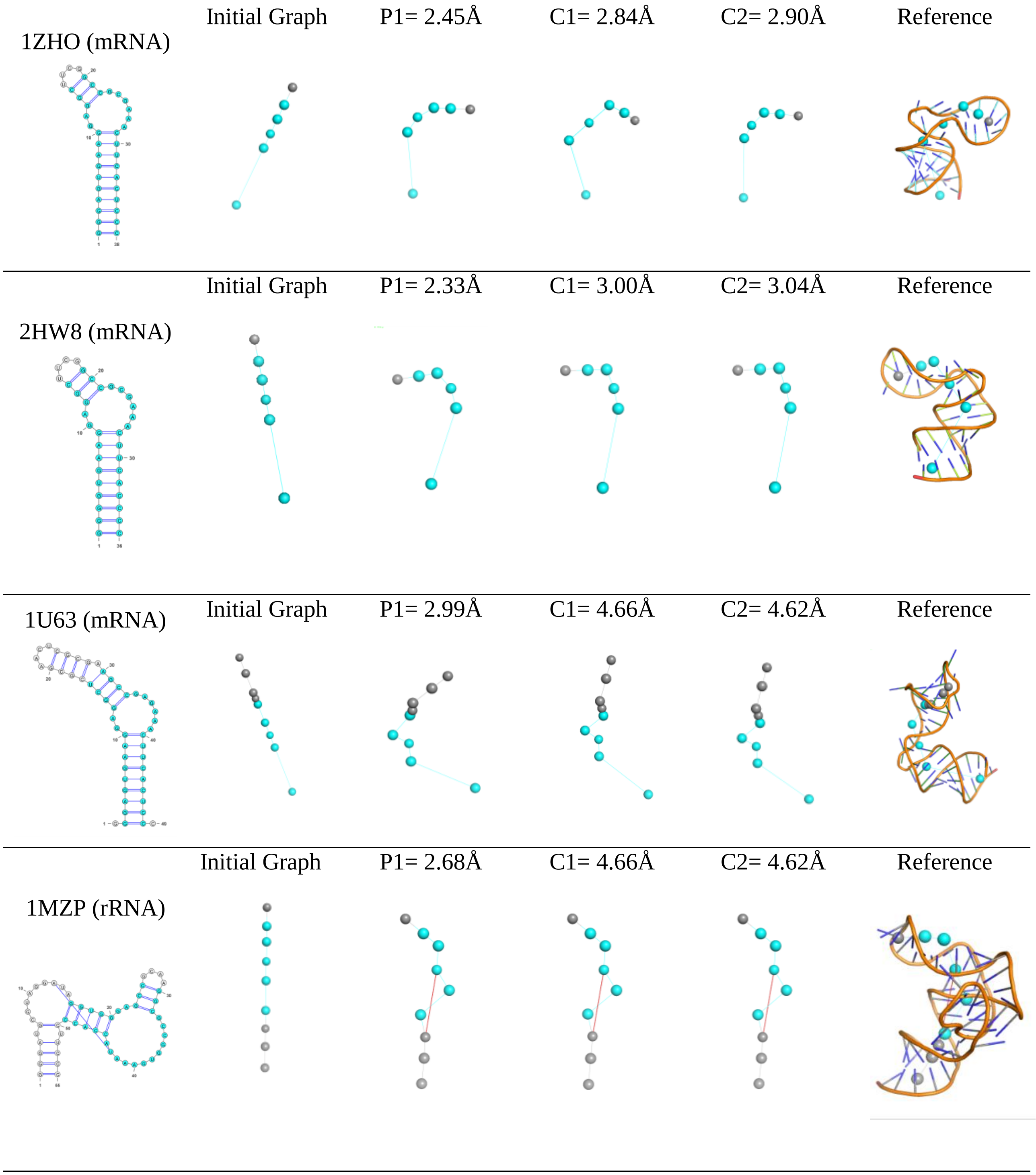

1ZHO (mRNA)
Initial Graph
P1= 2.45Å
C1= 2.84Å
C2= 2.90Å
Reference
2HW8 (mRNA)
Initial Graph
P1= 2.33Å
C1= 3.00Å
C2= 3.04Å
Reference
1U63 (mRNA)
Initial Graph
P1= 2.99Å
C1= 4.66Å
C2= 4.62Å
Reference
1MZP (rRNA)
Initial Graph
P1= 2.68Å
C1= 4.66Å
C2= 4.62Å
Reference

Figure S4

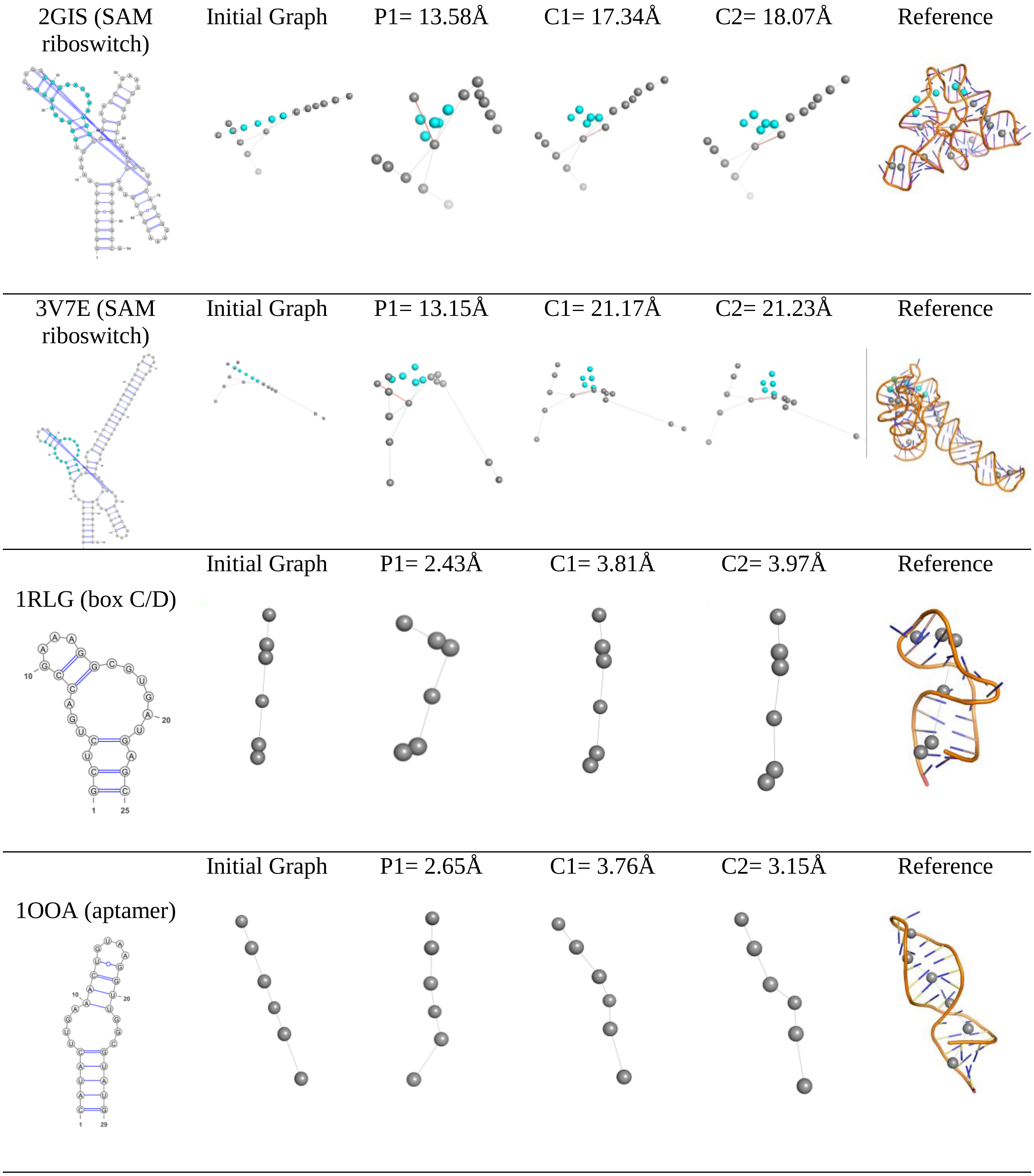

2GIS (SAM riboswitch)
Initial Graph
P1= 13.58Å
C1= 17.34Å
C2= 18.07Å
Reference
3V7E (SAM riboswitch)
Initial Graph
P1= 13.15Å
C1= 21.17Å
C2= 21.23Å
Reference
1RLG (box C/D)
Initial Graph
P1= 2.43Å
C1= 3.81Å
C2= 3.97Å
Reference
10
20
1
25
1OOA (aptamer)
Initial Graph
P1= 2.65Å
C1= 3.76Å
C2= 3.15Å
Reference
10
20
1
29

Figure S4

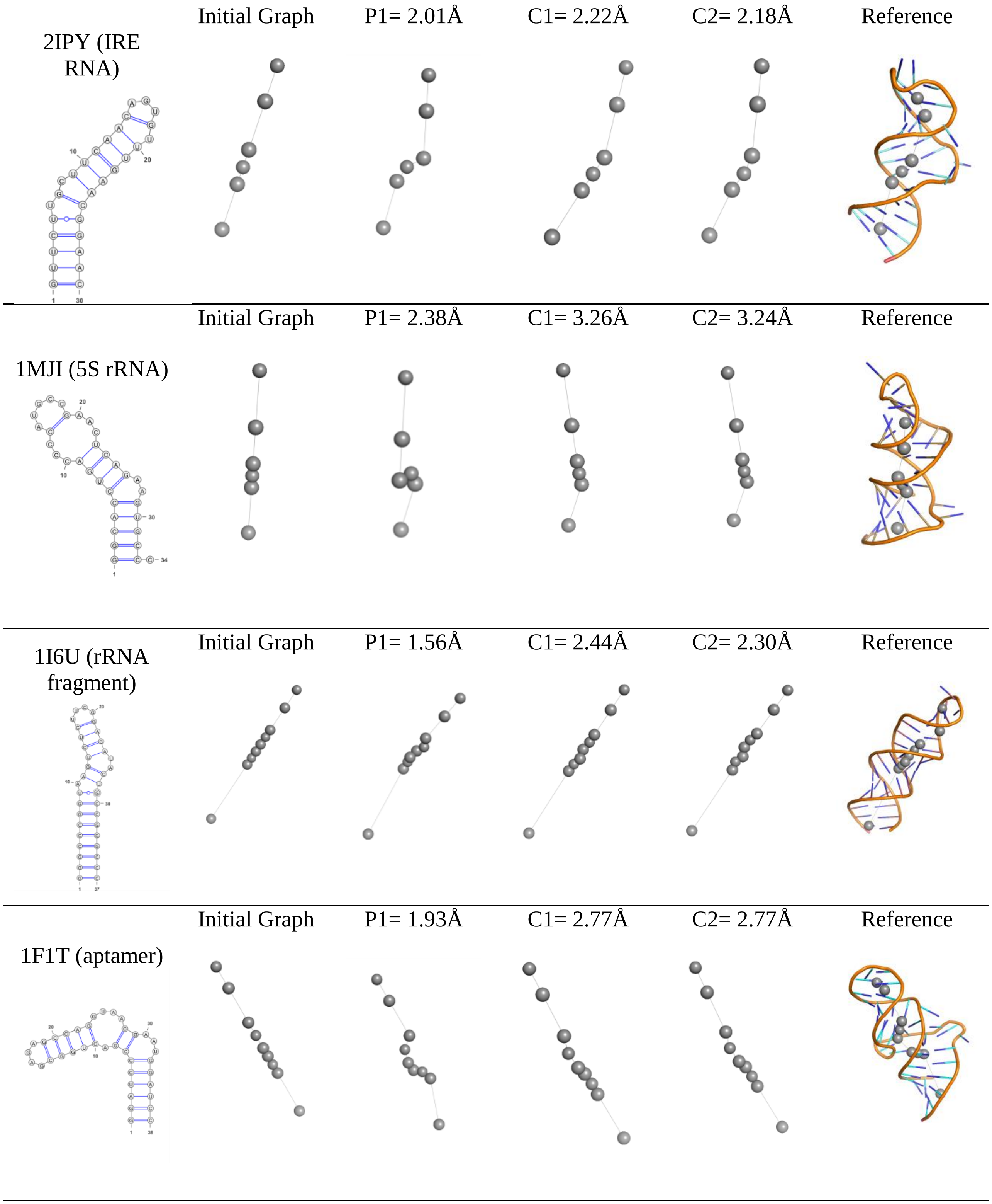

2IPY (IRE RNA)
Initial Graph
P1= 2.01Å
C1= 2.22Å
C2= 2.18Å
Reference
1MJI (5S rRNA)
Initial Graph
P1= 2.38Å
C1= 3.26Å
C2= 3.24Å
Reference
1I6U (rRNA fragment)
Initial Graph
P1= 1.56Å
C1= 2.44Å
C2= 2.30Å
Reference
1F1T (aptamer)
Initial Graph
P1= 1.93Å
C1= 2.77Å
C2= 2.77Å
Reference

Figure S4

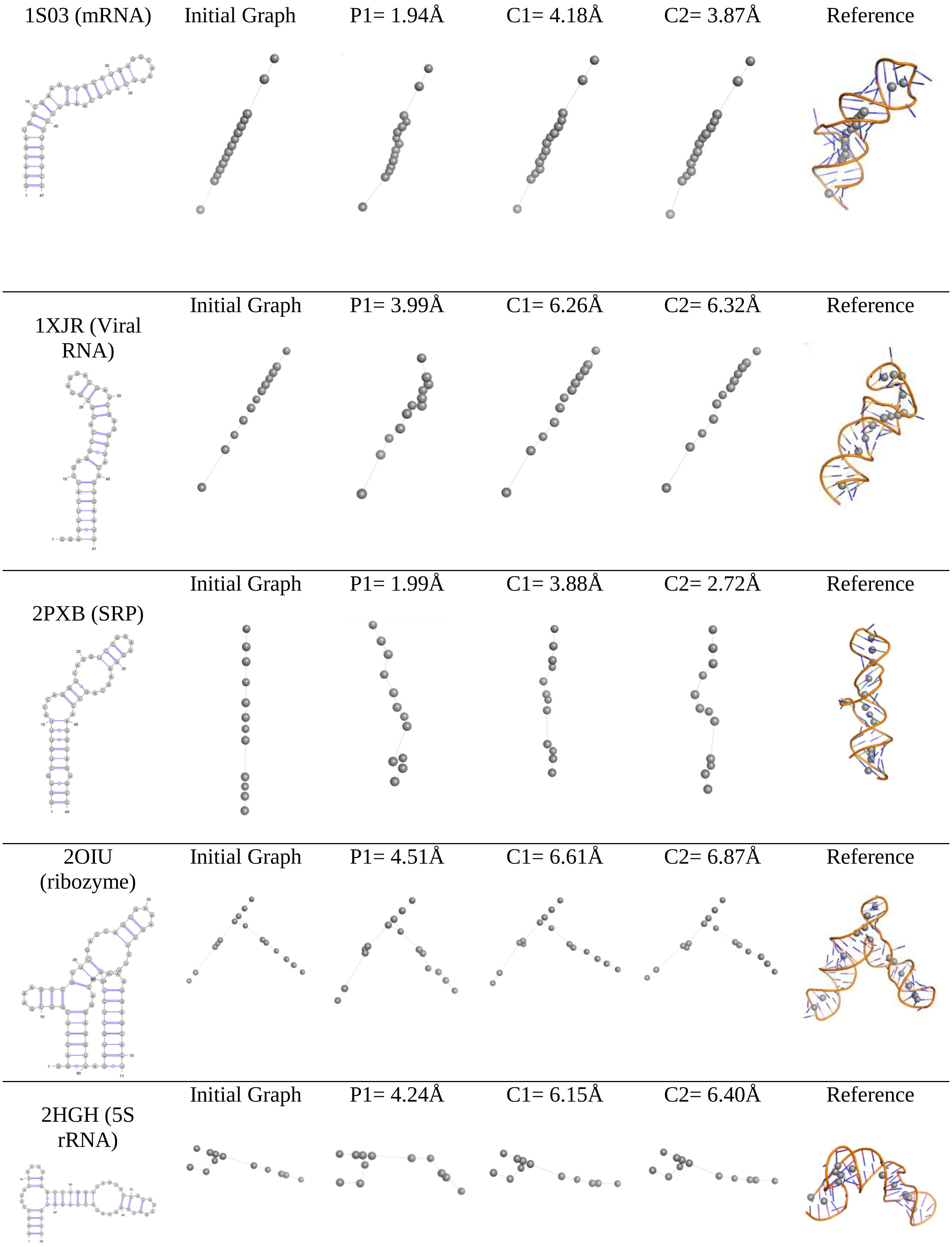

1S03 (mRNA)
Initial Graph
P1= 1.94Å
C1= 4.18Å
C2= 3.87Å
Reference
1XJR (Viral RNA)
Initial Graph
P1= 3.99Å
C1= 6.26Å
C2= 6.32Å
Reference
2PXB (SRP)
Initial Graph
P1= 1.99Å
C1= 3.88Å
C2= 2.72Å
Reference
2OIU (ribozyme)
Initial Graph
P1= 4.51Å
C1= 6.61Å
C2= 6.87Å
Reference
2HGH (5S rRNA)
Initial Graph
P1= 4.24Å
C1= 6.15Å
C2= 6.40Å
Reference

Figure S4

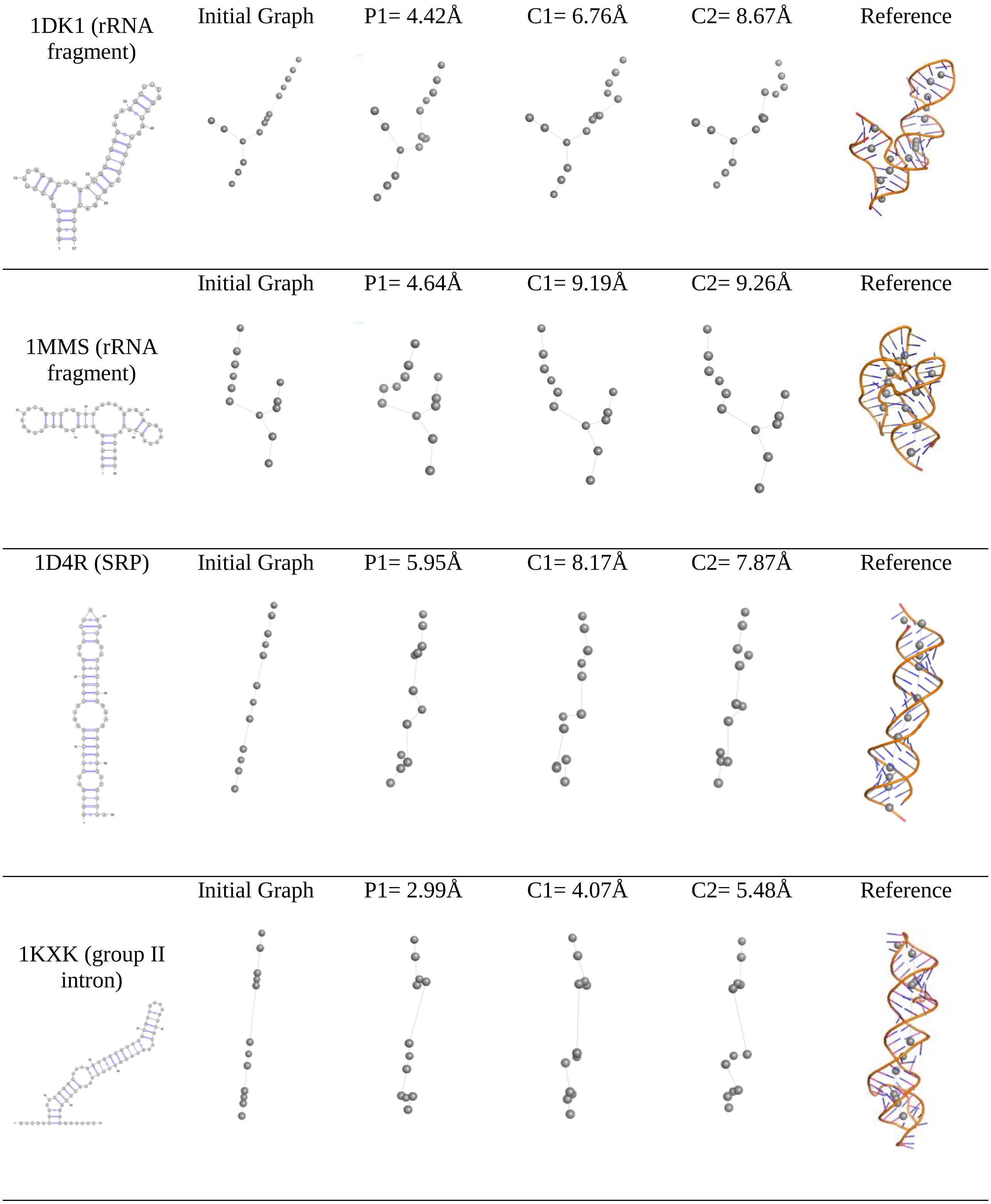

1DK1 (rRNA fragment)
Initial Graph
P1= 4.42Å
C1= 6.76Å
C2= 8.67Å
Reference
Initial Graph
P1= 4.64Å
C1= 9.19Å
C2= 9.26Å
Reference
1MMS (rRNA fragment)
1D4R (SRP)
Initial Graph
P1= 5.95Å
C1= 8.17Å
C2= 7.87Å
Reference
Initial Graph
P1= 2.99Å
C1= 4.07Å
C2= 5.48Å
Reference
1KXK (group II intron)

Figure S4

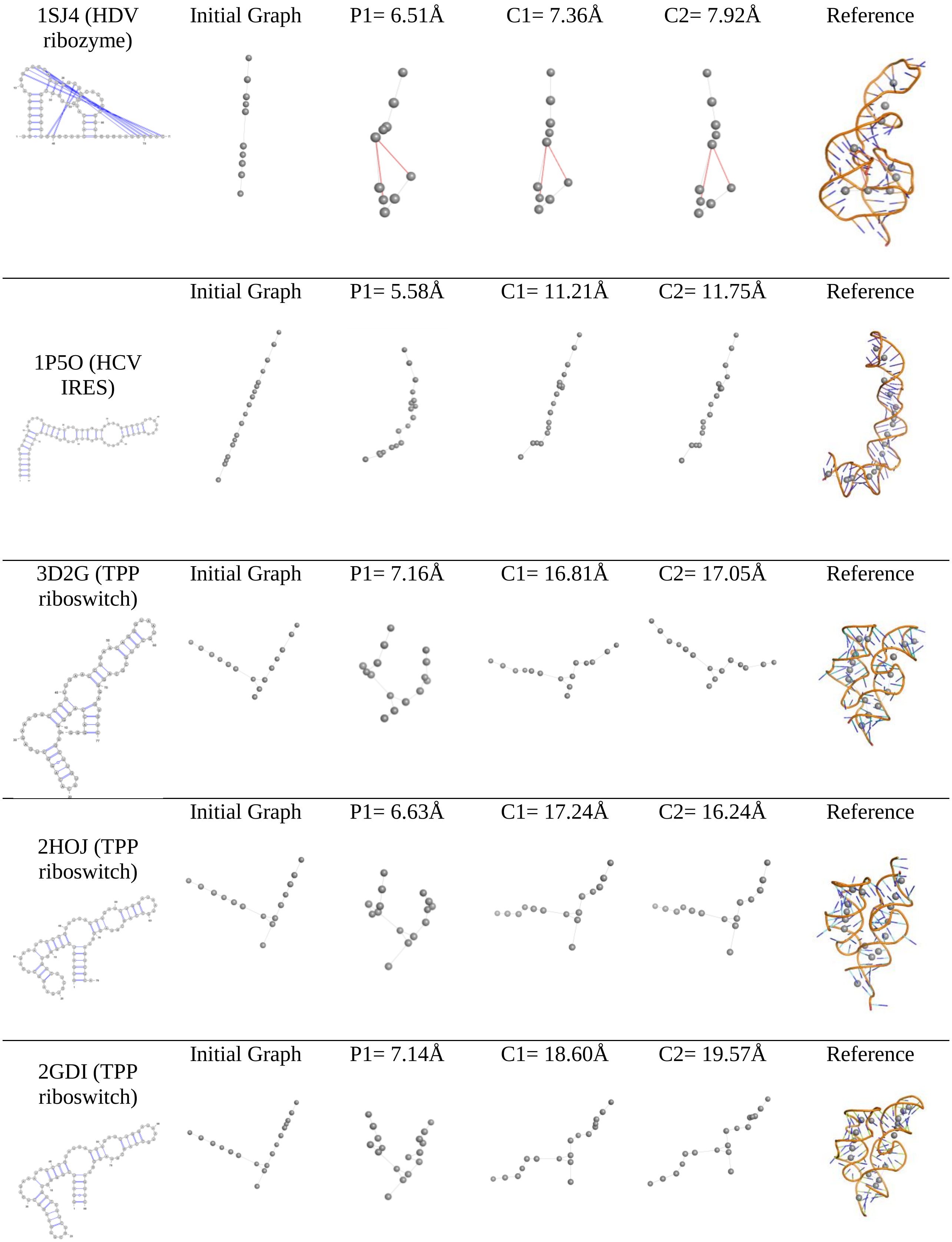

1SJ4 (HDV ribozyme)
Initial Graph
P1= 6.51Å
C1= 7.36Å
C2= 7.92Å
Reference
Initial Graph
P1= 5.58Å
C1= 11.21Å
C2= 11.75Å
Reference
1P5O (HCV IRES)
3D2G (TPP riboswitch)
Initial Graph
P1= 7.16Å
C1= 16.81Å
C2= 17.05Å
Reference
Initial Graph
P1= 6.63Å
C1= 17.24Å
C2= 16.24Å
Reference
2HOJ (TPP riboswitch)
2GDI (TPP riboswitch)
Initial Graph
P1= 7.14Å
C1= 18.60Å
C2= 19.57Å
Reference

Figure S4

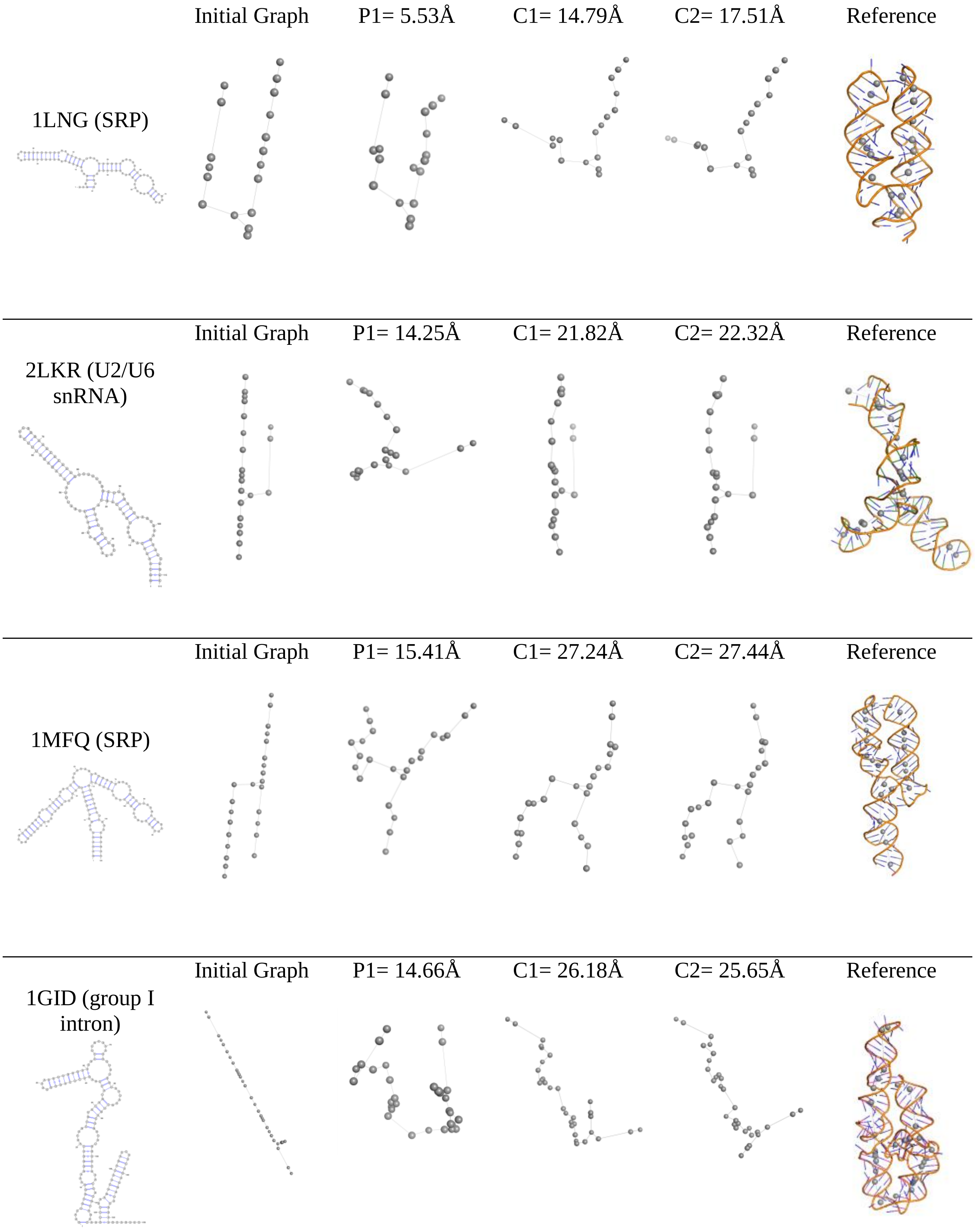


Figure S4. Graph results for 35 RNA structures based on k-turn and non k-turn potentials. The 2D structure is predicted using three 2D structure prediction algorithms (RNAView (4), MC-Annotate (5), and FR3D (6)). The initial graph is predicted based

Figure S4

on 2D structure. After MC/SA, P1 is the lowest RMSD graph with respect to the reference graph (when the reference is known), C1 is the lowest-scored graph, and C2 is the last accepted graph conformation. K-turn regions are indicated by cyan. Pseudoknot edges are shown in red.

Figure S5

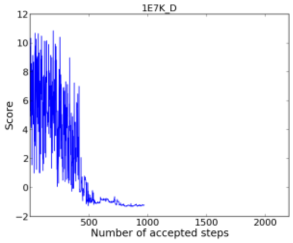
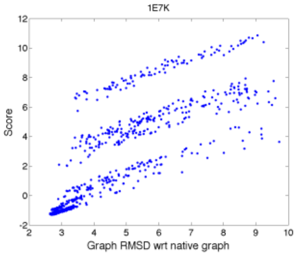
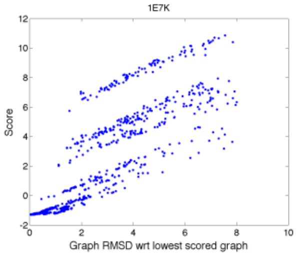
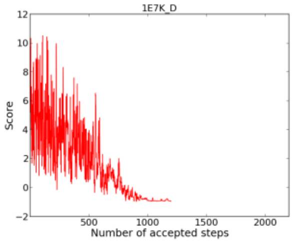
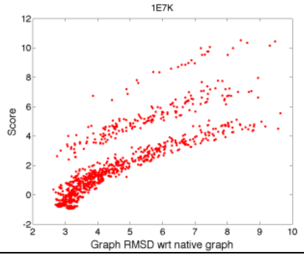
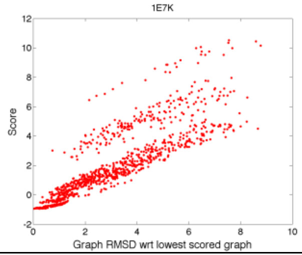
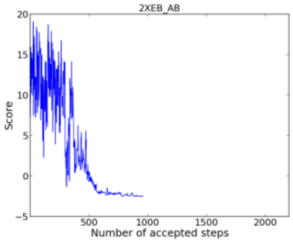
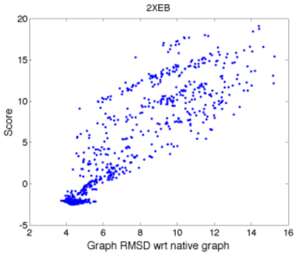
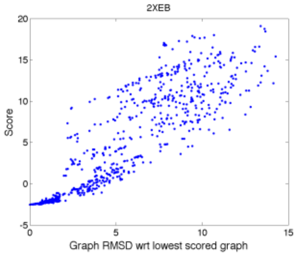
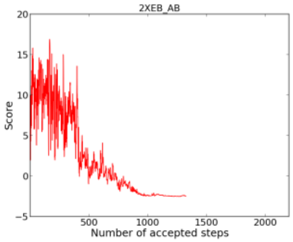
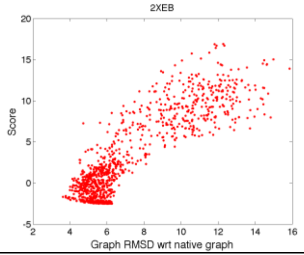
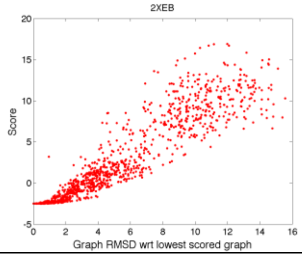
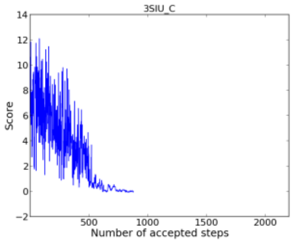
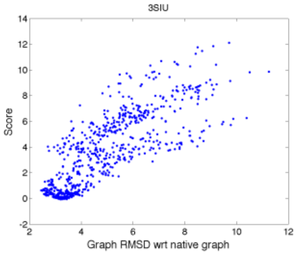
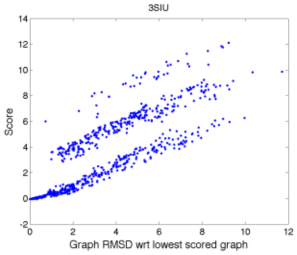
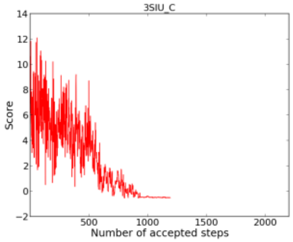
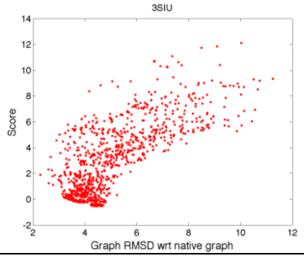
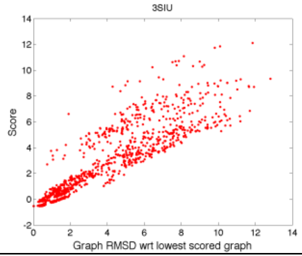
PDB		Convergence of MC scores	Score-RMSD wrt native graph	Score-RMSD wrt lowest scored graph
1E7K_D	K-turn pot.			
	General pot.			
2XEB_AB	K-turn pot.			
	General pot.			
3SIU_C	K-turn pot.			
	General pot.			

Figure S5

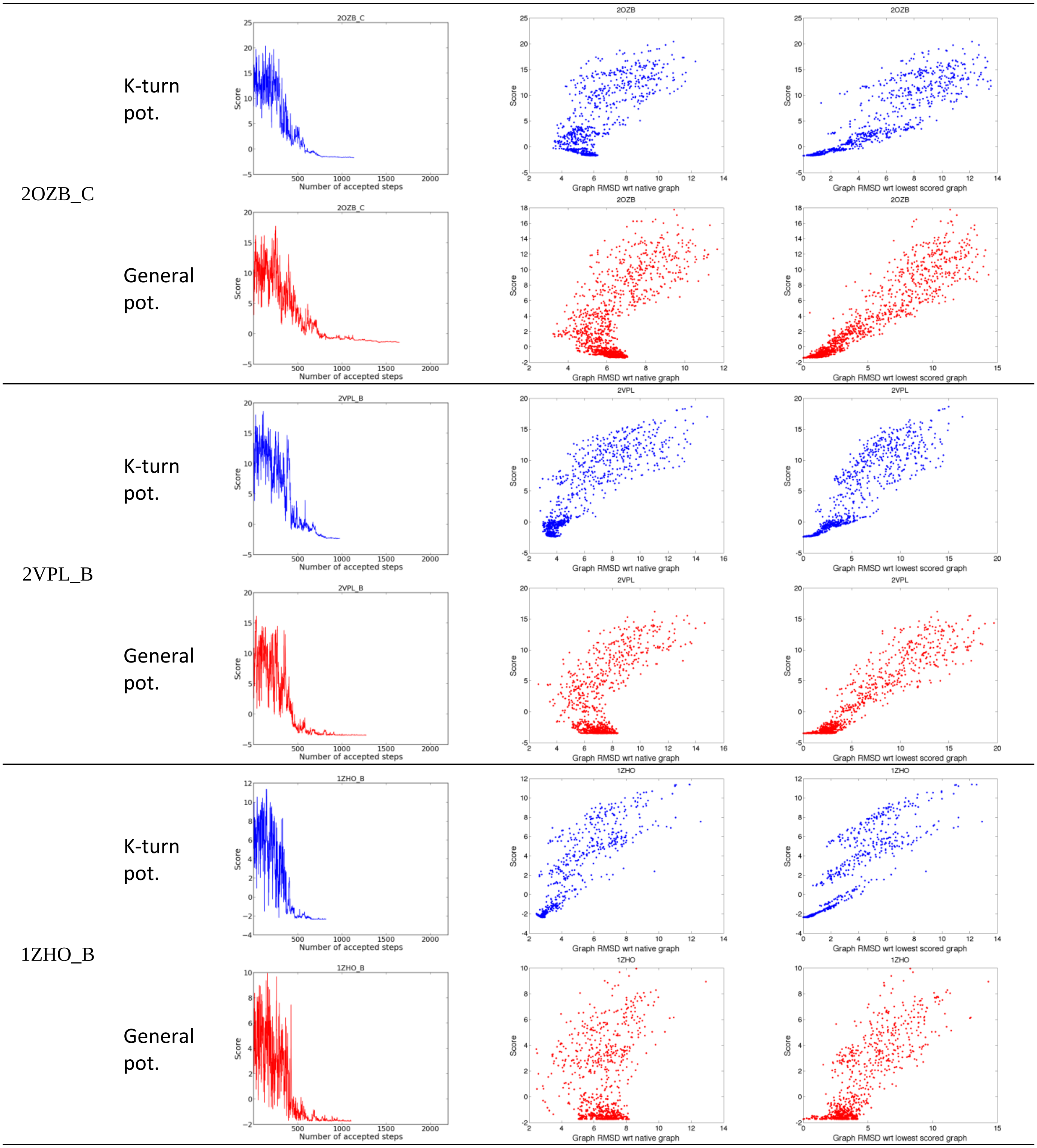

2OZB_C
K-turn pot.
General pot.
2VPL_B
1ZHO_B
2OZB_C
2OZB
2VPL_B
2VPL
1ZHO_B
1ZHO
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph
500
1000
1500
2000

Figure S5

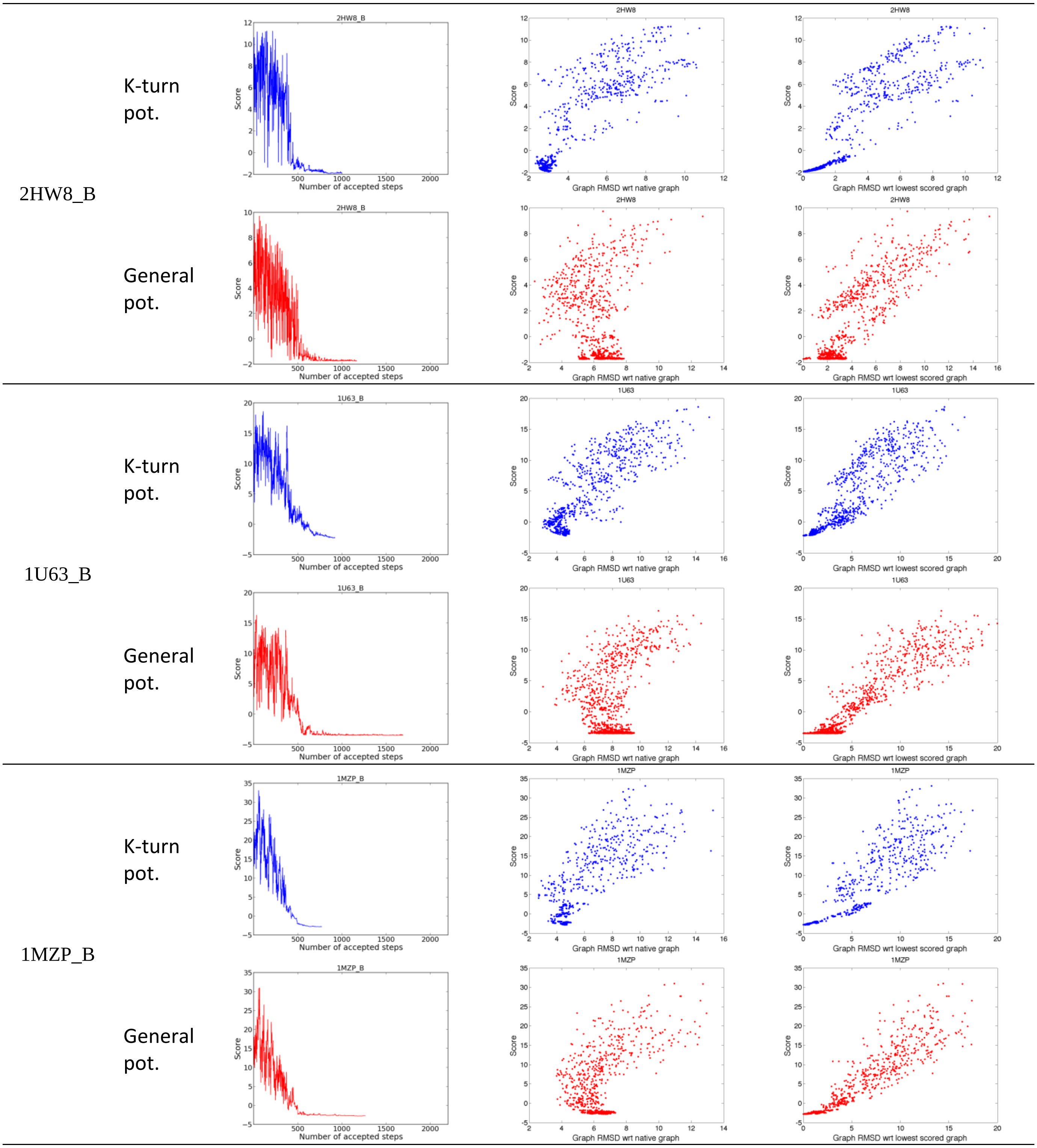
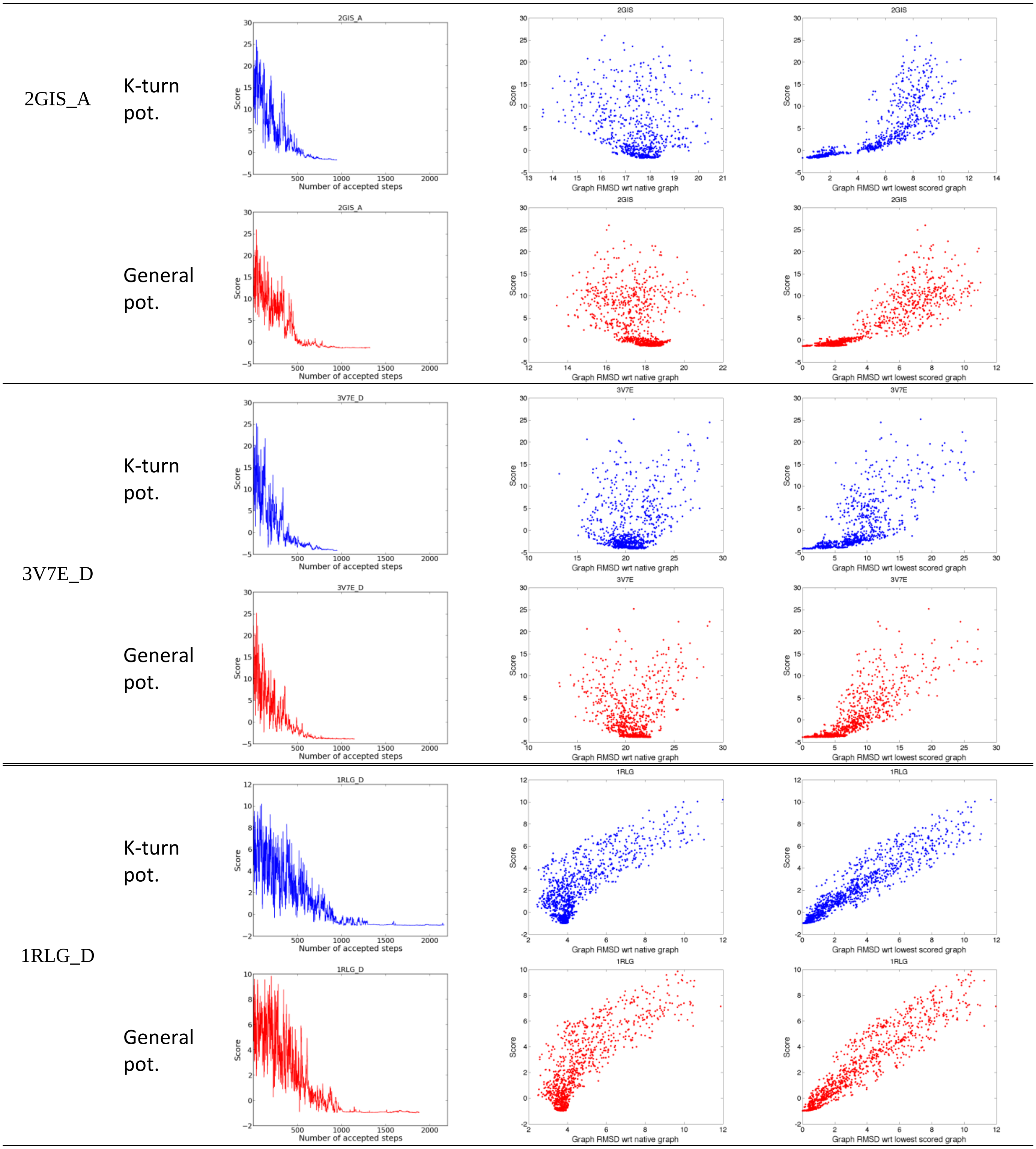

2HW8_B
K-turn pot.
General pot.
1U63_B
K-turn pot.
General pot.
1MZP_B
K-turn pot.
General pot.
2HW8_B
2HW8
1U63_B
1U63
1MZP_B
1MZP
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph
500
1000
1500
2000

Figure S5



2GIS_A
K-turn pot.
General pot.
3V7E_D
K-turn pot.
General pot.
1RLG_D
K-turn pot.
General pot.
2GIS_A
3V7E_D
1RLG_D
2GIS
3V7E
1RLG
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph
500
1000
1500
2000

Figure S5

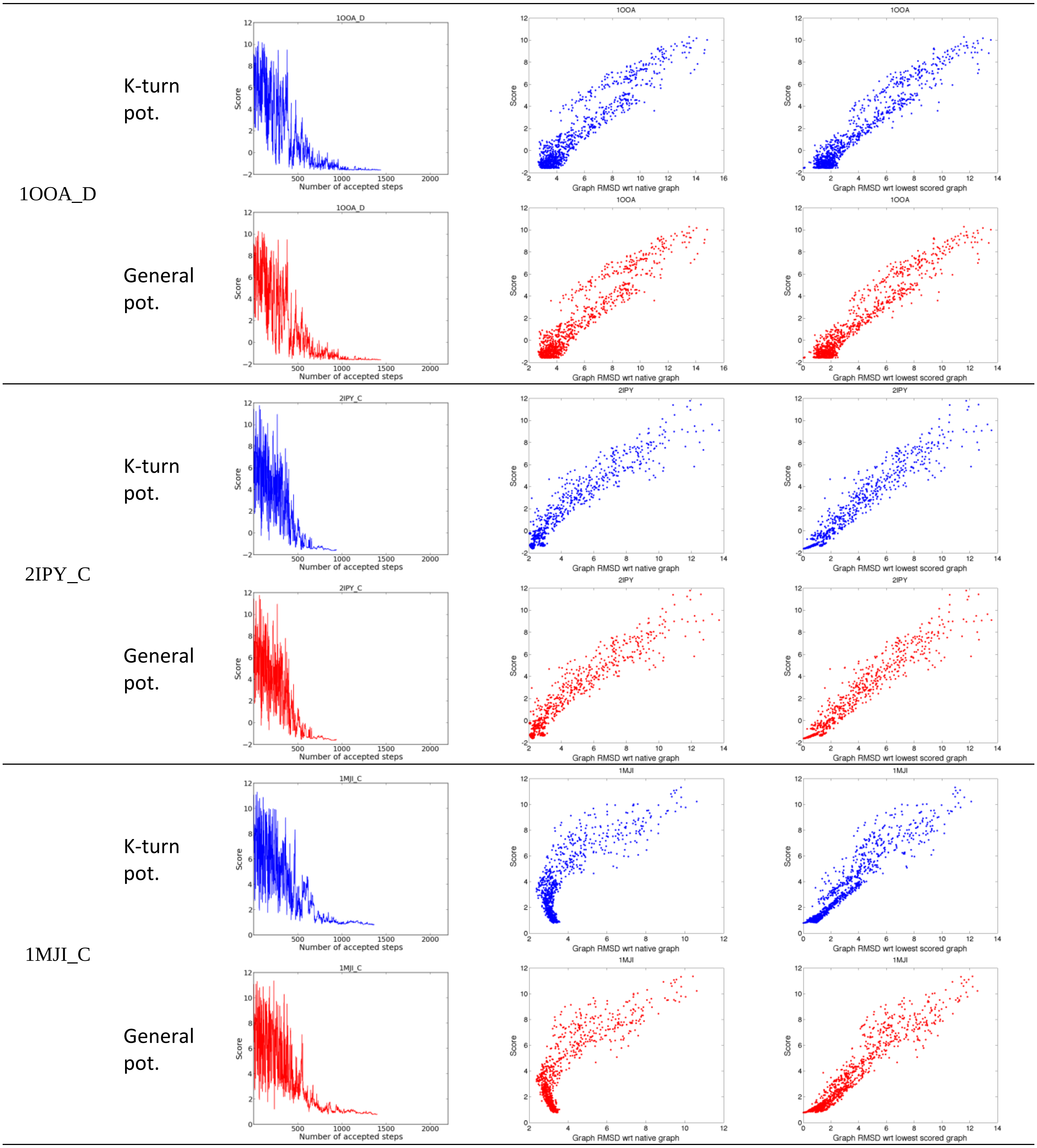
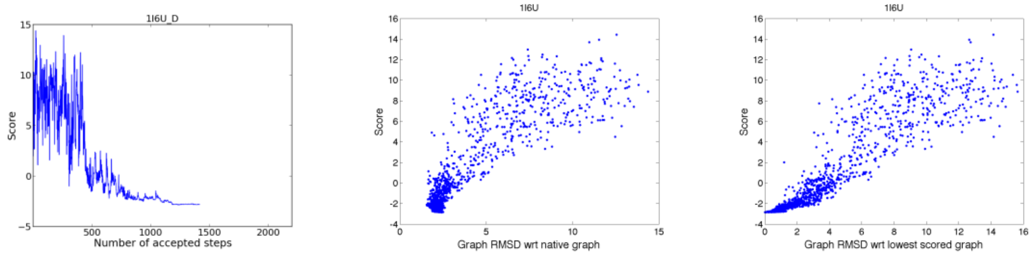

1OOA_D
K-turn pot.
General pot.
2IPY_C
1MJI_C
1OOA_D
2IPY_C
1MJI_C
1OOA
2IPY
1MJI
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph

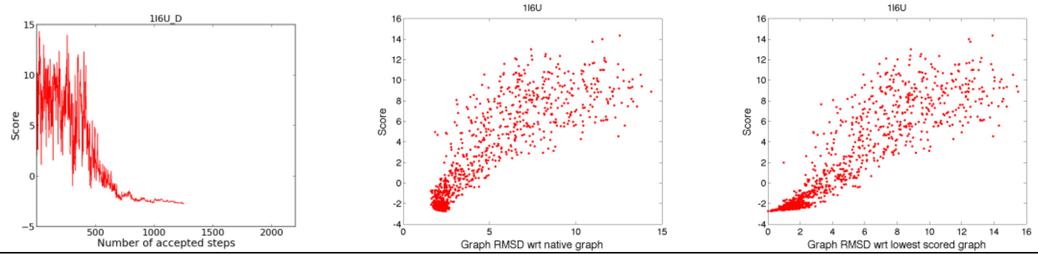
Figure S5

1I6U_D

K-turn pot.

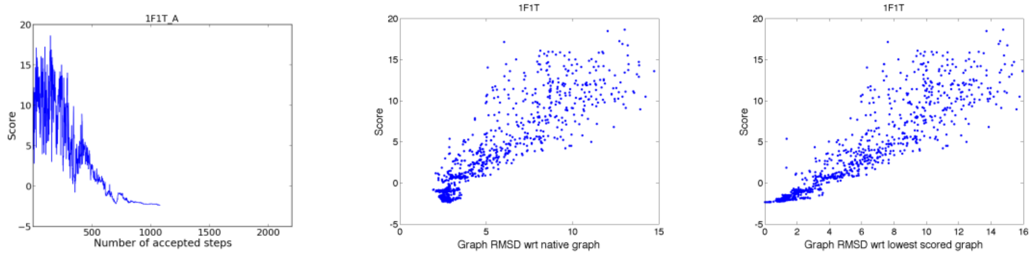


General pot.

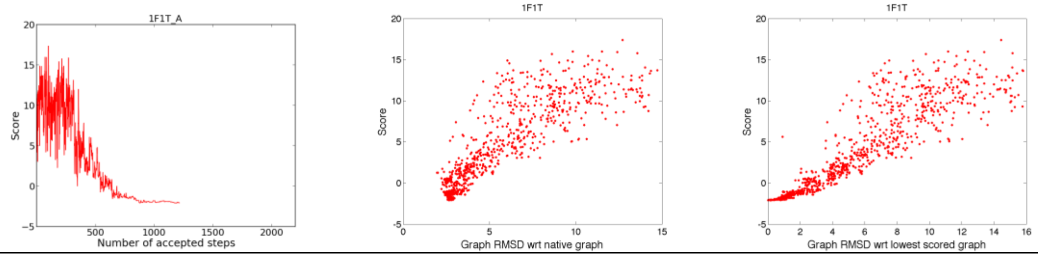


1F1T_A

K-turn pot.

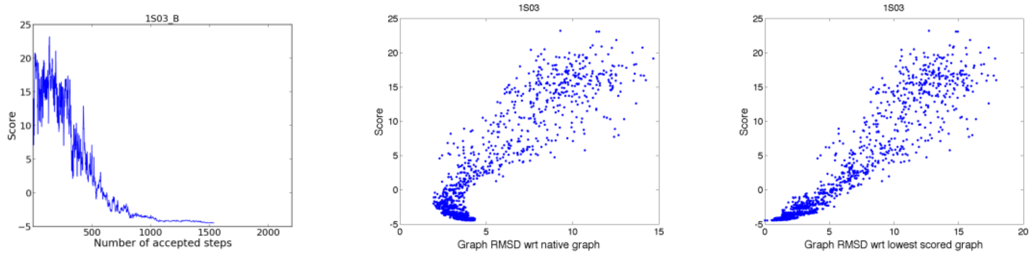


General pot.



1S03_B

K-turn pot.



General pot.

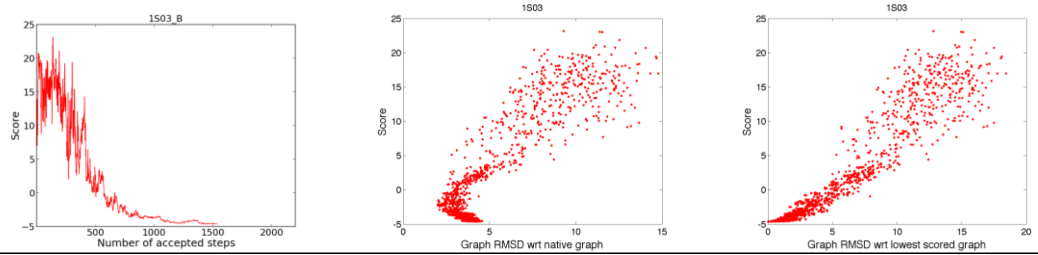


Figure S5

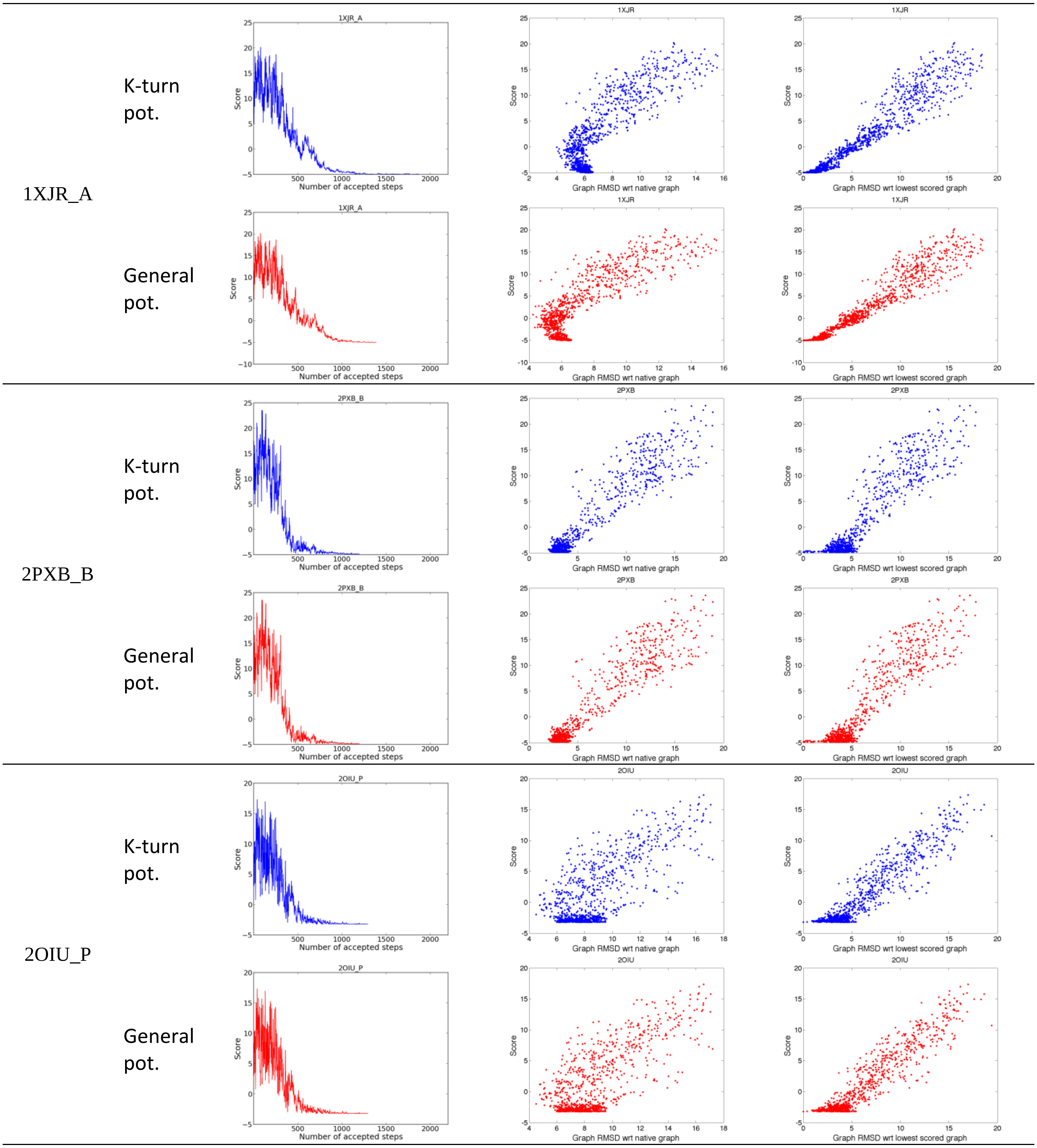

1XJR_A
K-turn pot.
General pot.
2PXB_B
K-turn pot.
General pot.
2OIU_P
K-turn pot.
General pot.
1XJR_A
2PXB_B
2OIU_P
1XJR
2PXB
2OIU
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph
500
1000
1500
2000

Figure S5

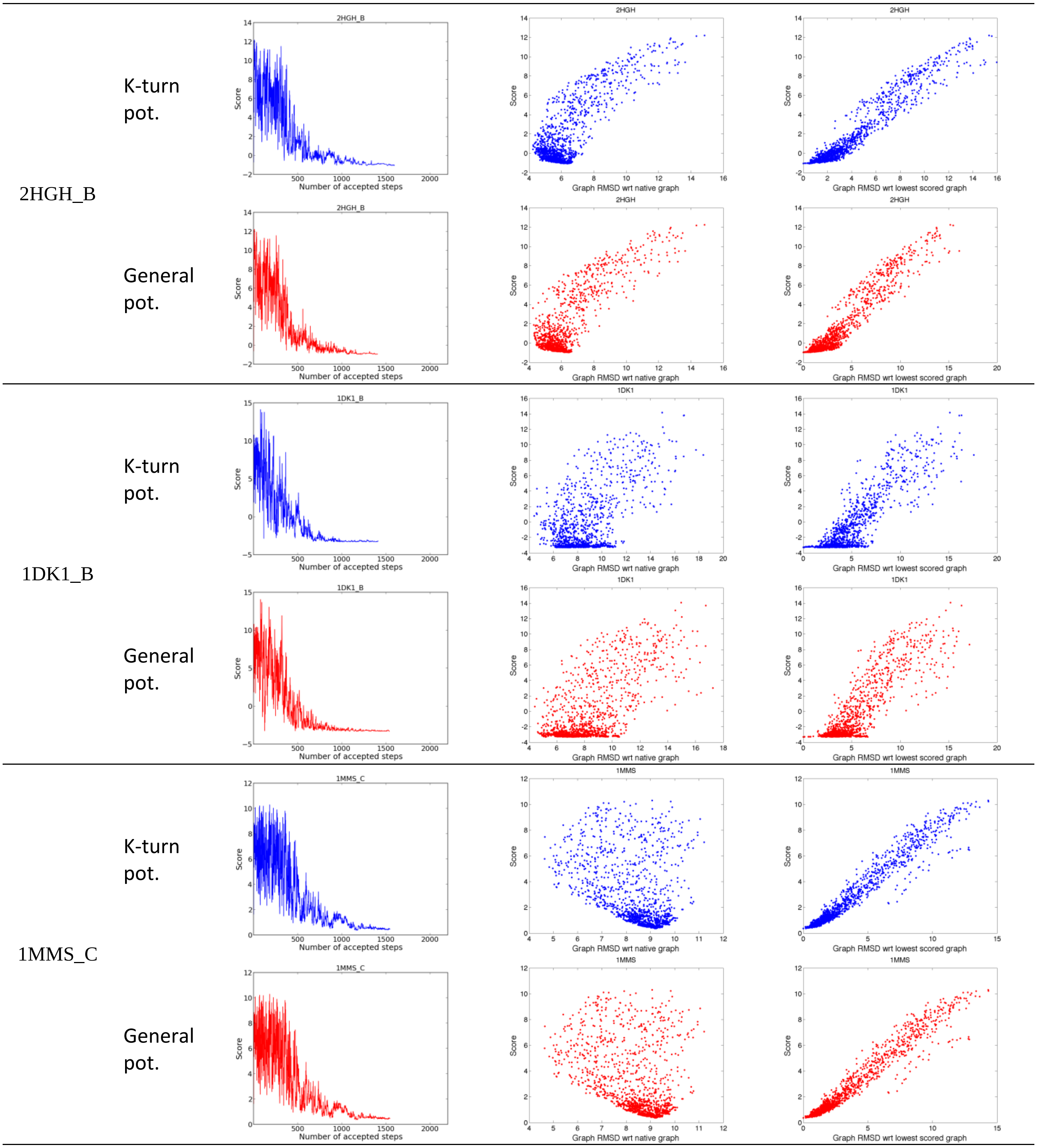

2HGH_B
K-turn pot.
General pot.
1DK1_B
K-turn pot.
General pot.
1MMS_C
K-turn pot.
General pot.
2HGH_B
2HGH
1DK1_B
1DK1
1MMS_C
1MMS
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph
500
1000
1500
2000

Figure S5

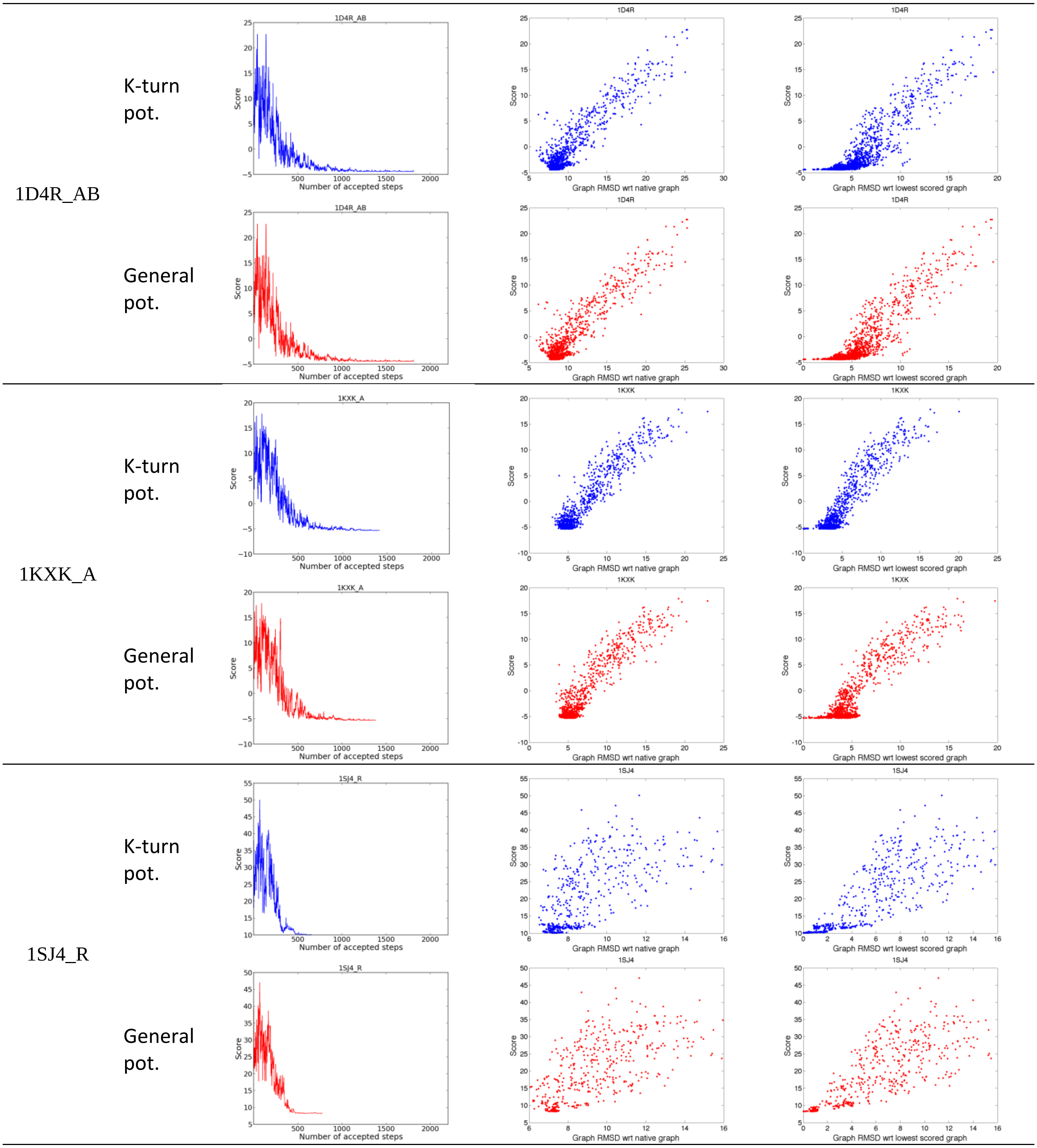

1D4R_AB
K-turn pot.
General pot.
1KXK_A
K-turn pot.
General pot.
1SJ4_R
K-turn pot.
General pot.
1D4R_AB
1D4R
1KXK_A
1KXK
1SJ4_R
1SJ4
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph
500
1000
1500
2000

Figure S5

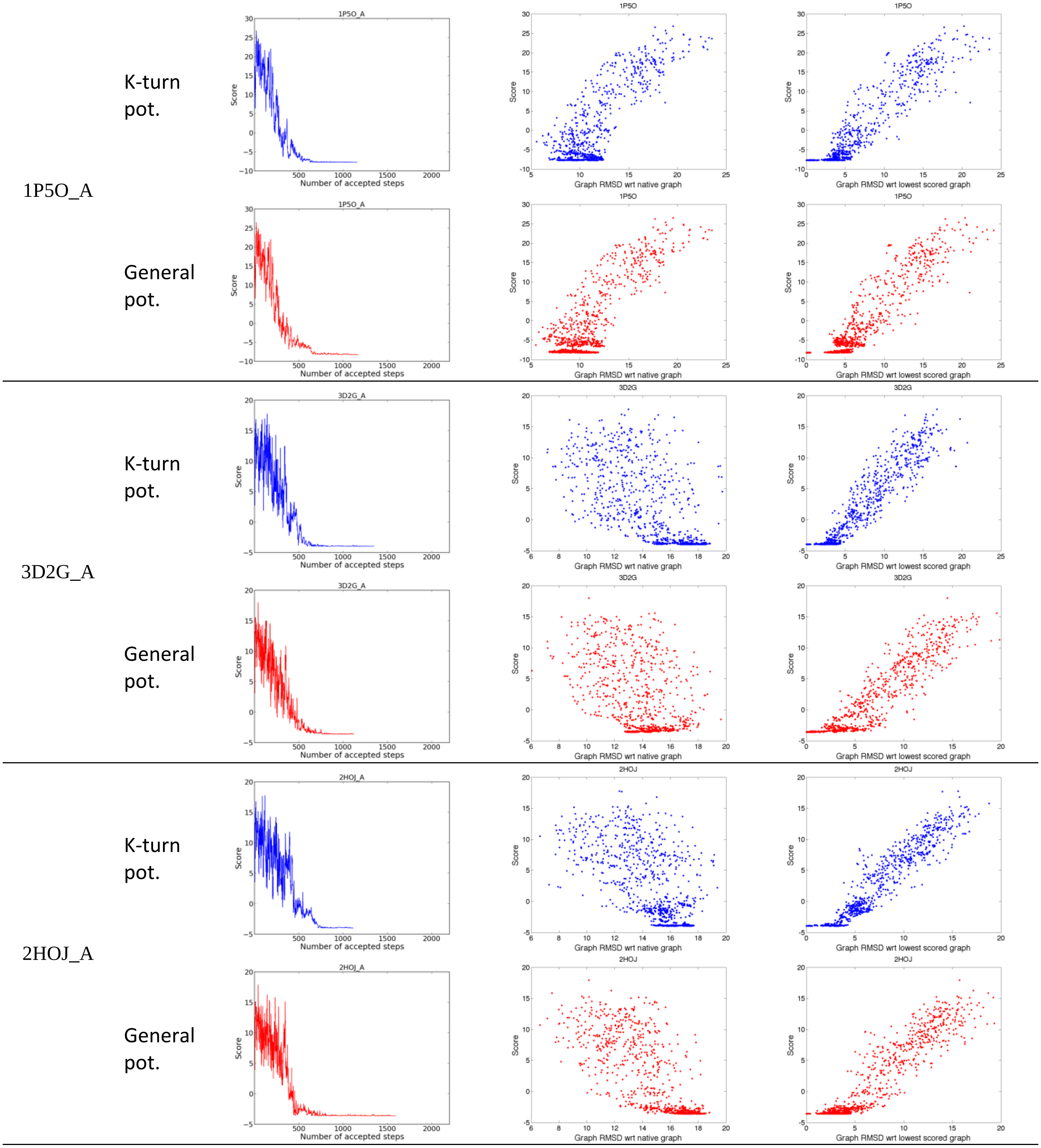
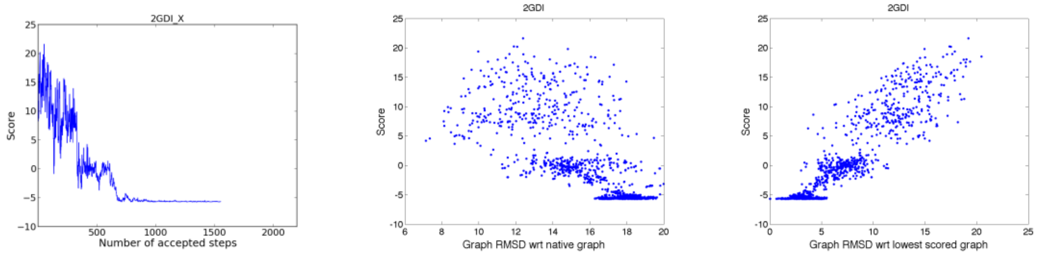

1P5O_A
K-turn pot.
General pot.
3D2G_A
K-turn pot.
General pot.
2HOJ_A
K-turn pot.
General pot.
1P5O_A
1P5O
3D2G_A
3D2G
2HOJ_A
2HOJ
Score
Number of accepted steps
Graph RMSD wrt native graph
Graph RMSD wrt lowest scored graph
500
1000
1500
2000
30
25
20
15
10
5
0
−5
−10

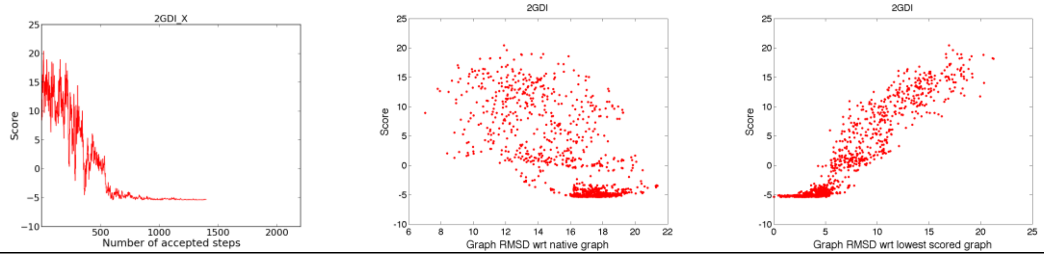
Figure S5

2GDI_X

K-turn pot.

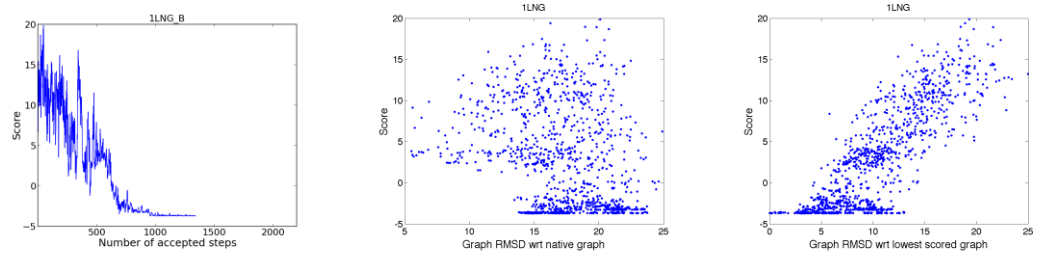


General pot.

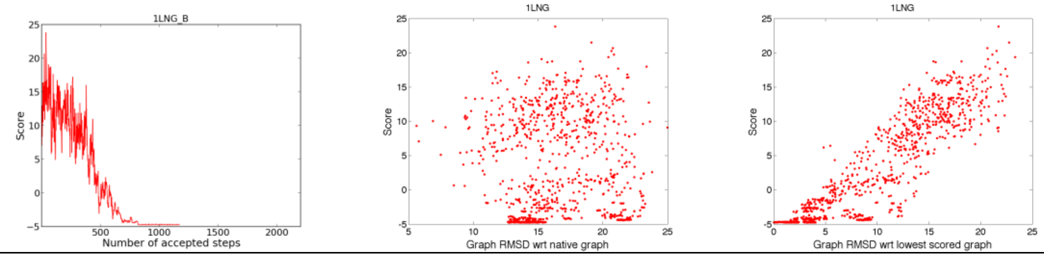


1LNG_B

K-turn pot.

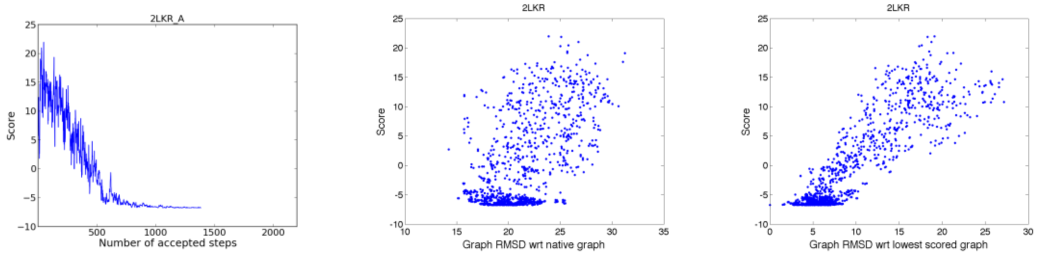


General pot.



2LKR_A

K-turn pot.



General pot.

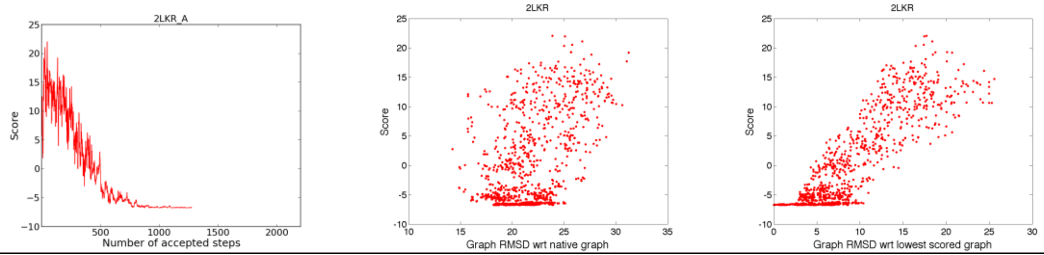


Figure S5

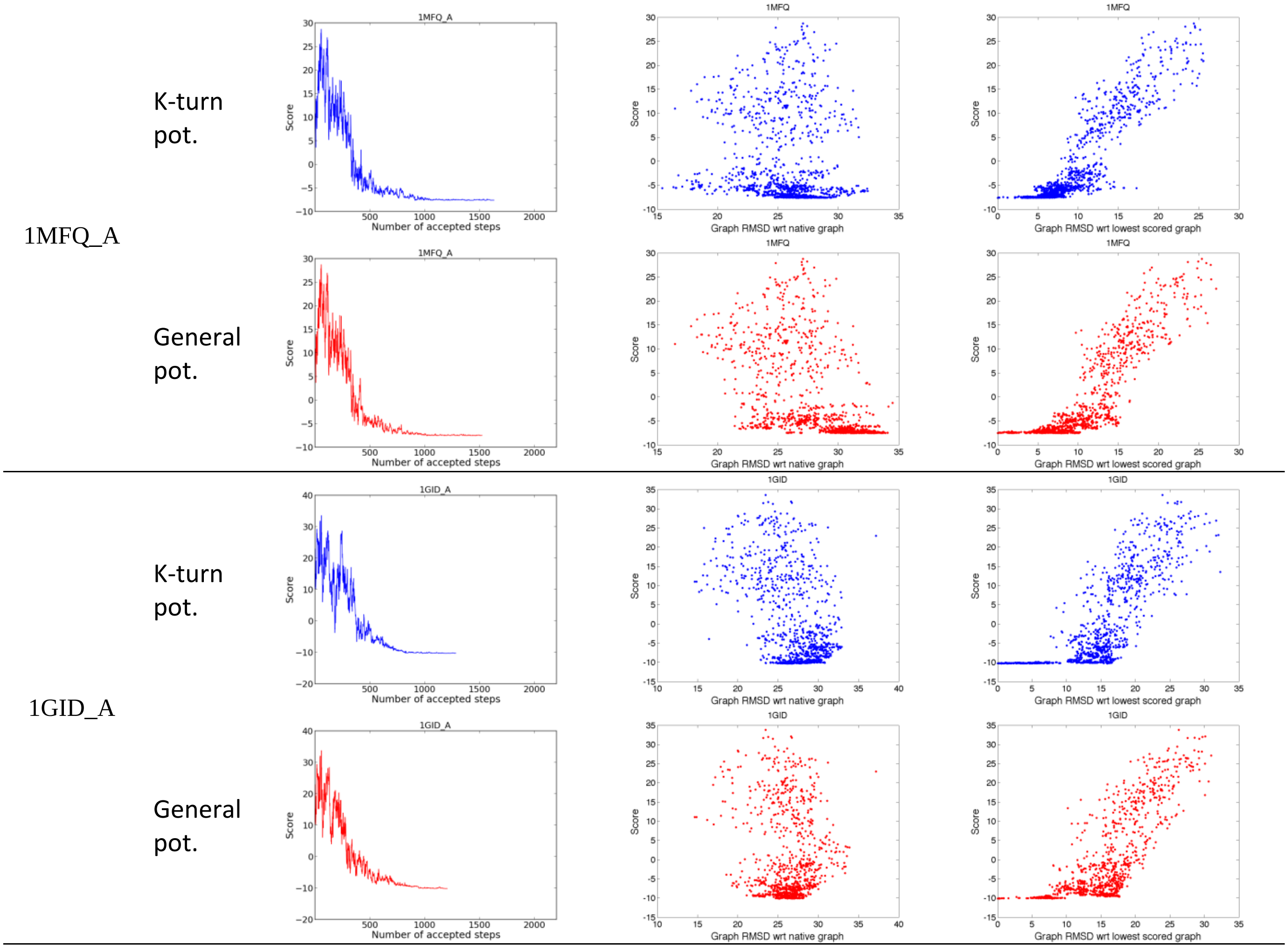


Figure S5. MC/SA behavior. For each of the 35 RNAs simulated, we show the convergence of the MC/SA procedure along the accepted moves (left), score-RMSD landscapes with respect to native graph (middle), and score-RMSD landscapes with respect to the lowest scored structure (right) based on k-turn and general potentials (in blue and in red, respectively).

Figure S6

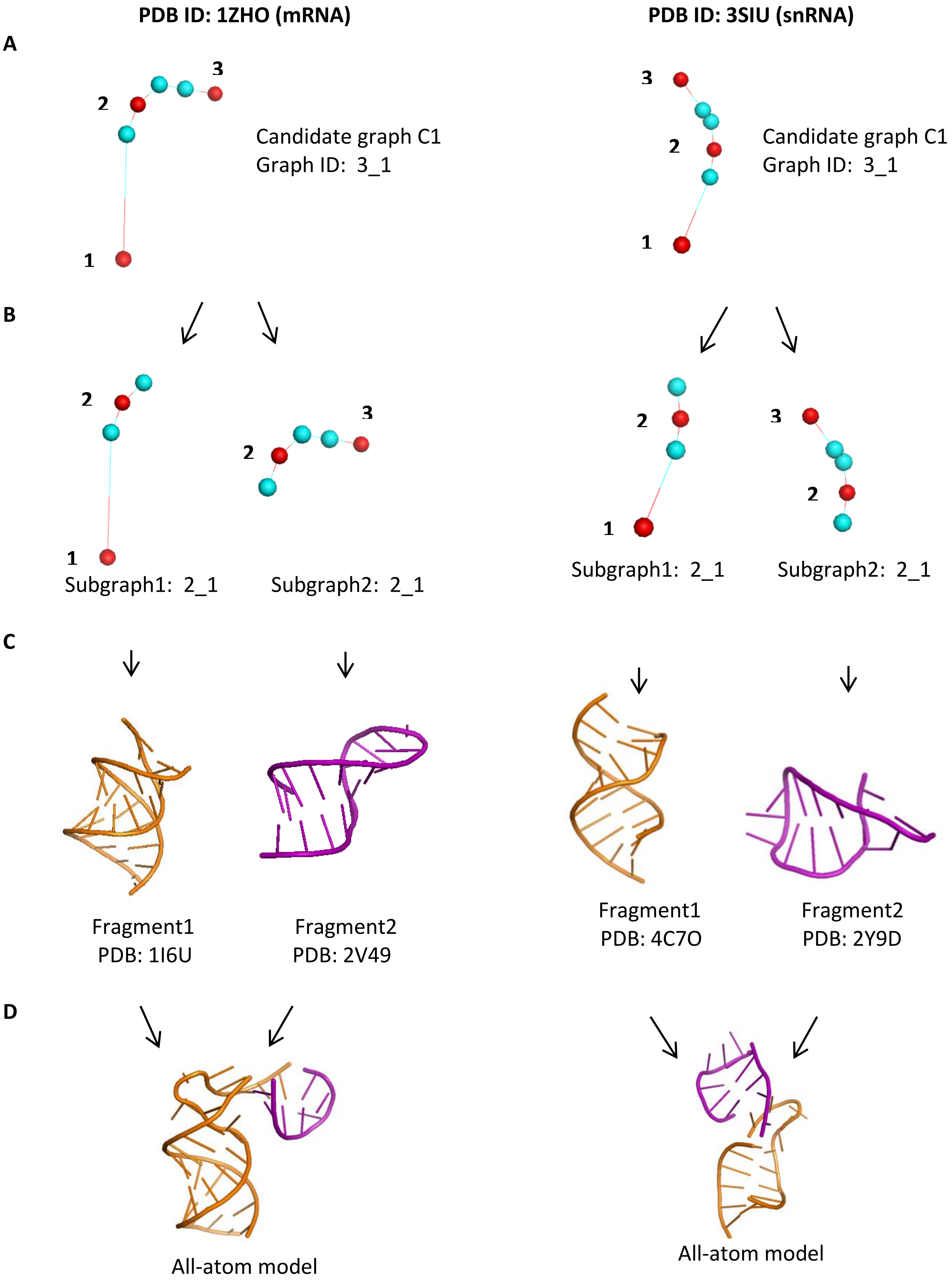

PDB ID: 1ZHO (mRNA)
PDB ID: 3SIU (snRNA)
A
3
2
1
Candidate graph C1
Graph ID: 3_1
3
2
1
Candidate graph C1
Graph ID: 3_1
B
2
1
3
2
Subgraph1: 2_1
Subgraph2: 2_1
2
1
3
2
Subgraph1: 2_1
Subgraph2: 2_1
C
Fragment1
PDB: 1I6U
Fragment2
PDB: 2V49
Fragment1
PDB: 4C7O
Fragment2
PDB: 2Y9D
D
All-atom model
All-atom model

Figure S6

RMSD= 1.89 Å

RMSD= 3.62 Å

Figure S6. All-atom model generation for 1ZHO and 3SIU. A) C1 candidate graph returned by MC/SA simulations. The additional vertices included for RAG-3D are shown in cyan, the main vertices are shown in red. B) Partitioning the graph using RAG-3D search tool. C) Finding best matching fragments in RAG-3D database. Only one example is shown here, but the program considers 15. D) Assembling of the fragments by adjustment of bases, helix and loop lengths, and geometry optimization. E) Alignment of the predicted all atom model to the reference structure. All atom RMSD = 1.89 Å for 1ZHO, 3.62 Å for 3SIU. The reference structure is shown in red, and the predicted model is shown in blue.

Table S1

Table S1. K-turn structure data used for potential calculation derived by DSSR

PDB	Length of Bulge1	Length of Bulge2	Initial BP of Helix1		Initial BP of Helix2		Seq1 (1b, 2b, 3b, 4b)	Seq2 (3n,4n)	Length of Helix1	Length of Helix2	K-turn type
1E7K_D	5	2	3	15	9	12	GAGG	CC	3	2	normal
1FJG_A	4	6	233	275	238	268	CAGC	GC	3	3	normal
1FJG_A	4	7	662	686	667	678	UAGC	GC	7	2	normal
1PNU_0	3	6	80	103	84	96	GAGC	GC	6	2	normal
1PNU_0	3	6	1370	1549	1374	1542	GAGU	AC	7	2	normal
1PNU_0	6	3	2065	2093	2072	2089	AACC	GG	3	7	normal
1PNX_A	4	6	237	279	242	272	CAGC	GC	3	3	normal
1PNX_A	4	7	676	700	681	692	UAGC	GC	7	2	normal
1S1H_A	4	6	223	265	228	258	CAGC	GC	3	3	normal
1S1H_A	4	7	637	661	642	653	UAGC	GC	7	2	normal
1S1I_3	3	6	68	91	72	84	GAGC	GC	6	3	normal
1S1I_3	4	5	1545	1566	1550	1560	AAGC	GC	5	3	normal
1S1I_3	4	8	923	993	928	984	AGGU	GC	6	2	normal
1S72_0	3	6	68	91	72	84	GAGC	GC	6	3	normal
1S72_0	7	3	1107	1176	1115	1172	CAGC	GC	10	5	normal
1S72_0	4	8	924	994	929	985	AGGU	GC	6	2	normal
1T0K_CD	3	6	4	24	8	17	GAGU	GC	4	5	normal
1U63_B	2	6	10	40	13	33	GAGG	CC	9	4	normal
1YSH_B	4	7	32	56	37	48	UAGC	GC	7	2	normal
1YSH_F	4	5	8	29	13	23	AAGC	GC	5	3	normal
1ZHO_B	2	6	10	29	13	22	GAGG	CC	10	3	normal

Table S1

2AW7_A	3	6	680	702	684	695	UAGC	GC	8	2	normal
2AW7_A	4	6	238	280	243	273	UAGC	GC	3	3	normal
2AW7_A	5	7	511	532	517	524	CAGC	GC	5	2	normal
2GIS_A	3	6	17	38	21	31	GAGG	CC	3	3	normal
2HW8_B	2	6	9	28	12	21	GAGG	CC	9	3	normal
2J37_Z	4	5	227	248	232	242	AAGC	GC	5	3	normal
2OZB_C	5	2	9	26	15	23	GAGG	CC	3	2	normal
2QBG_B	6	3	1189	1219	1196	1215	AAGG	CU	3	8	normal
2VPL_B	2	6	9	39	12	32	GAGG	CC	9	4	normal
2WWA_D	4	10	27	52	32	41	GAAU	AU	2	3	normal
2XEB_AB	5	2	10	25	16	22	GAGG	CC	3	3	normal
2ZJR_X	3	6	80	103	84	96	GAGC	GC	6	2	normal
2ZJR_X	6	3	1124	1154	1131	1150	AAGC	GU	2	5	normal
2ZJR_X	3	6	1329	1508	1333	1501	GAGU	AC	9	2	normal
3BBN_A	3	6	627	649	631	642	GAGC	GC	7	2	normal
3BBN_A	4	6	208	250	213	243	UAGC	GC	3	3	normal
3GX5_A	3	6	17	38	21	31	GAGG	CC	3	3	normal
3IZ7_A	5	7	294	338	300	330	CAAC	GU	2	3	normal
3IZ9_AB	7	3	1212	1281	1220	1277	CAGC	GC	2	5	normal
3IZF_A	7	3	1197	1266	1205	1262	CAGC	GC	9	5	normal
3JYV_A	5	7	544	565	550	557	CAGC	GC	4	2	normal
3Q3Z_A	6	3	10	52	17	48	AUGA	UU	2	9	normal
3SIU_C	5	2	6	23	12	20	GAGC	GU	6	2	normal
3SIV_CF	5	2	8	57	14	54	GAGC	GU	8	2	normal

Table S1

3SIV_CF	2	5	22	46	25	40	GAGG	CC	2	8	normal
3U5F_6	5	8	888	914	894	905	CAGA	UC	6	2	normal
3U5F_6	8	6	1219	1254	1228	1247	UUGA	UC	5	2	normal
3U5H_58	7	3	1169	1238	1177	1234	CAGC	GC	10	5	normal
3V2F_A	3	6	75	98	79	91	GAGC	GC	6	3	normal
3V2F_A	6	3	1152	1183	1159	1179	AAGG	CU	3	5	normal
3V2F_A	6	3	2048	2078	2055	2074	AACC	GG	3	5	normal
3V7E_D	3	6	17	38	21	31	GAGG	CC	3	3	normal
4A1B_1	7	3	1245	1266	1253	1262	CAGC	GC	10	5	normal
4AEB_A	3	6	17	38	21	31	AAGA	UU	3	3	normal
3UMY_B	6	3	2129	2159	2136	2155	AACC	GG	3	8	normal
4B5R_A	3	6	17	38	21	31	GAGC	GC	3	3	normal
4BW0_A	3	6	3	23	7	16	GAGC	GC	3	3	normal
4C4W_D	3	6	3	33	7	26	AAGA	UU	3	5	normal
4GXY_A	3	6	82	146	86	139	GAGU	GC	3	7	normal
4IOA_X	3	6	80	103	84	96	GAGC	GC	6	2	normal
4IOA_X	6	3	1221	1251	1228	1247	AAGC	GU	2	5	normal
4IOA_X	3	6	1426	1605	1430	1598	GAGU	AC	9	2	normal
4KQY_A	3	6	17	38	21	31	GAGG	CC	5	3	normal
4KZY_i	3	6	948	970	952	963	UAGA	UC	8	2	normal
4TZZ_BC	5	2	108	199	114	196	GAGA	UC	6	4	normal

Table S2

Table S2. List of k-turn structures with k-turn sequence signature, L, R, family types of internal loops and corresponding geometrical potentials (size, bend and torsion angles). The aptamer 1OOA has a reverse kink-turn.

PDB ID	k-turn seq signature	Class	L	R	Family	(1b,2b,3b,4b)	(3n,4n)	Size	Bend	Torsion
1E7K_D	Y	snRNA	2	5	2/5	GAGG	CC	8.92	65.75	-23.13
2XEB_AB	Y	snRNA	2	5	2/5	GAGG	CC	10.91	111.44	-109.99
3SIU_C	Y	snRNA	2	5	2/5	GAGC	GU	8.76	74.79	-14.85
2OZB_C	Y	snRNA	2	5	2/5	GAGG	CC	8.96	91.29	-18.39
2VPL_B	Y	mRNA	2	6	2/6+	GAGG	CC	9.12	69.80	-48.82
1ZHO_B	Y	mRNA	2	6	2/6+	GAGG	CC	9.09	58.75	-38.26
2HW8_B	Y	mRNA	2	6	2/6+	GAGG	CC	8.93	58.62	-35.29
1U63_B	Y	mRNA	2	6	2/6+	GAGG	CC	8.76	76.05	-44.07
1MZP_B	Y	rRNA	2	12	2/6+	GAGC	GC	8.72	71.61	-47.68
2GIS_A	Y	SAM Riboswitch	3	6	3/6+	GAGG	CC	9.31	64.89	-39.75
3V7E_D	Y	SAM Riboswitch	3	6	3/6+	GAGG	CC	8.76	67.53	-32.77
1OOA_D	N	Aptamer	3	4	3/4	GAAA	UU	9.59	100.19	24.07

Table S3

Table S3. RMSDs of kink-turn regions (5 vertices of the internal loop) with respect to native graph structure.

PDB	Kink-turn potentials	General potentials
1E7K_D	2.86	3.14
2XEB_AB	4.61	6.05
3SIU_C	3.92	4.33
2OZB_C	5.75	5.97
2VPL_B	3.94	7.68
1ZHO_B	2.88	6.94
2HW8_B	3.01	6.73
1U63_B	4.70	9.78
1MZP_B	3.57	4.85
2GIS_A	14.62	15.95
3V7E_D	17.74	20.23

Table S4

Table S4. 10-fold cross validation results compared to k-turn test results.

	10-fold cross validation			**K-turn test**		
PDB	P1	C1	C2	P1	C1	C2
1E7K_D	2.66	2.67	2.68	2.64	2.70	2.76
2XEB_AB	3.97	4.69	4.68	3.73	4.37	4.37
3SIU_C	2.40	3.23	3.15	2.46	3.23	3.22
2OZB_C	3.56	6.14	5.93	3.49	6.10	5.68
2VPL_B	2.67	3.77	3.87	2.78	3.91	3.77
1ZHO_B	2.33	2.90	3.11	2.45	2.84	2.90
2HW8_B	2.34	2.76	2.74	2.33	3.00	3.04
1U63_B	3.17	4.22	4.26	2.99	4.66	4.62
1MZP_B	2.54	4.43	4.23	2.68	4.66	4.62
2GIS_A	13.59	18.06	18.06	13.58	17.87	18.07
3V7E_D	13.15	20.08	21.09	13.15	21.17	21.23

Table S5

Table S5. Graph results for 35 RNA structures starting with a known 2D structure, and starting with a predicted 2D structure.

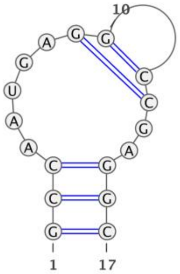
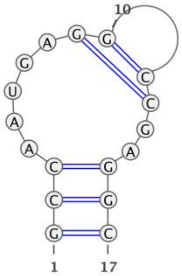
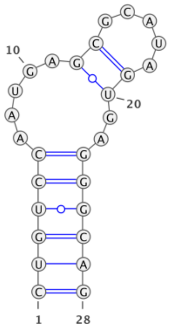
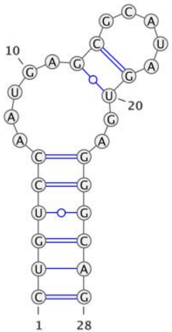
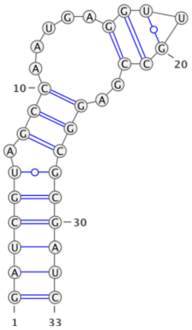
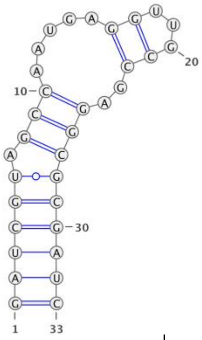
	Known structure		RNAFold prediction (Min. Free En.)	
1E7K				
	K-turn pot. P1= 2.64 P2= 2.70 P3= 2.76	General pot. P1= 2.63 P2= 3.16 P3= 3.15	K-turn pot. P1= 2.64 P2= 2.69 P3= 2.76	General pot. P1= 2.63 P2= 3.17 P3= 3.15
3SIU				
	K-turn pot. P1= 2.46 P2= 3.23 P3= 3.22	General pot. P1= 2.28 P2= 4.46 P3= 4.45	K-turn pot. P1= 2.46 P2= 3.23 P3= 3.22	General pot. P1= 2.28 P2= 4.46 P3= 4.45
2XEB				
	K-turn pot. P1= 3.73 P2= 4.37 P3= 4.37	General pot. P1= 3.61 P2= 6.27 P3= 6.05	K-turn pot. P1= 4.03 P2= 5.07 P3= 4.88	General pot. P1= 4.16 P2= 6.25 P3= 5.64

Table S5

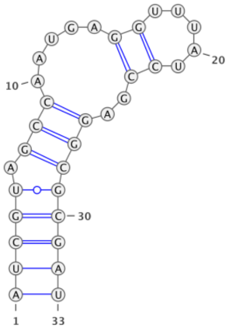
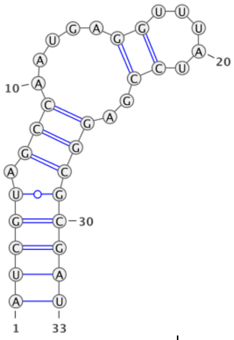
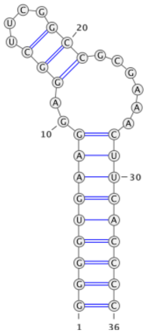
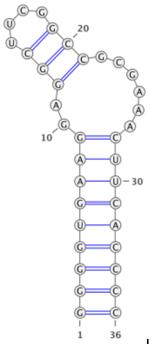
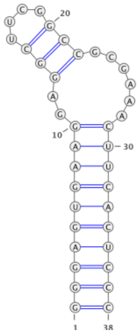
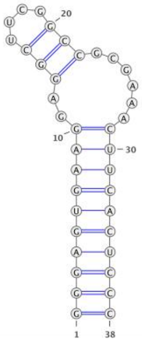
2OZB				
	K-turn pot. P1= 3.49 P2= 6.10 P3= 5.68	General pot. P1= 3.25 P2= 6.90 P3= 6.90	K-turn pot. P1= 3.49 P2= 6.10 P3= 5.68	General pot. P1= 3.25 P2= 6.90 P3= 6.90
2HW8				
	K-turn pot. P1= 2.33 P2= 3.00 P3= 3.04	General pot. P1= 2.34 P2= 7.16 P3= 6.44	K-turn pot. P1= 2.33 P2= 3.00 P3= 3.04	General pot. P1= 2.34 P2= 7.16 P3= 6.44
1ZHO				
	K-turn pot. P1= 2.45 P2= 2.84 P3= 2.90	General pot. P1= 2.45 P2= 7.11 P3= 6.55	K-turn pot. P1= 2.46 P2= 2.85 P3= 2.90	General pot. P1= 2.45 P2= 7.11 P3= 6.55

Table S5

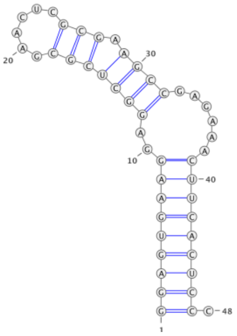
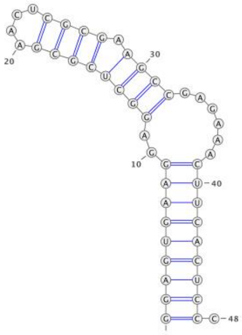
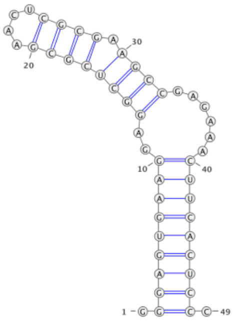
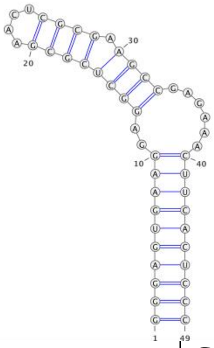
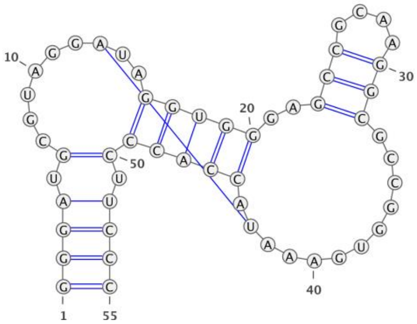
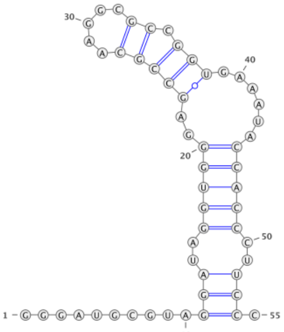
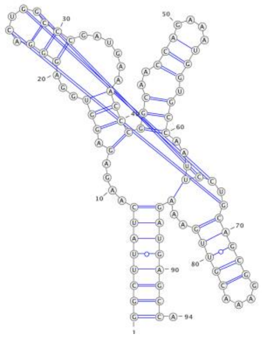
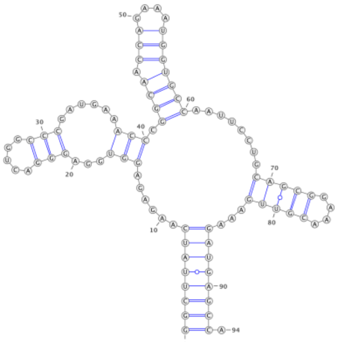
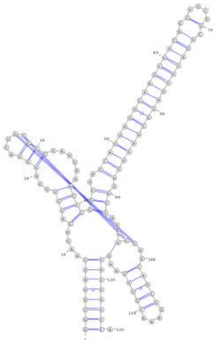
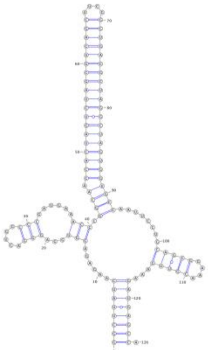
2VPL				
	K-turn pot. P1= 2.78 P2= 3.91 P3= 3.77	General pot. P1= 2.67 P2= 7.59 P3= 7.05	K-turn pot. P1= 2.91 P2= 4.15 P3= 4.16	General pot. P1= 3.60 P2= 7.87 P3= 7.42
1U63				
	K-turn pot. P1= 2.99 P2= 4.66 P3= 4.62	General pot. P1= 2.99 P2= 9.34 P3= 6.86	K-turn pot. P1= 2.56 P2= 4.63 P3= 4.55	General pot. P1= 3.71 P2= 7.68 P3= 8.09
1MZP				
	K-turn pot. P1= 2.68 P2= 4.66 P3= 4.62	General pot. P1= 3.70 P2= 6.72 P3= 6.60	K-turn pot. P1= 3.85 P2= 5.64 P3= 5.53	General pot. P1= 3.53 P2= 7.14 P3= 7.29

Table S5

2GIS				
	K-turn pot. P1= 13.58 P2= 17.87 P3= 18.07	General pot. P1= 13.45 P2= 18.31 P3= 18.52	K-turn pot. P1= 14.47 P2= 18.89 P3= 19.06	General pot. P1= 14.20 P2= 18.76 P3= 18.94
3V7E				
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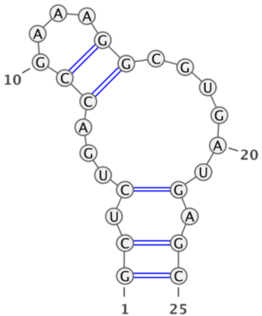
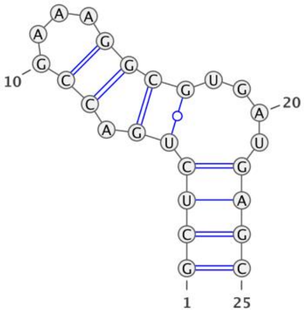
1RLG				
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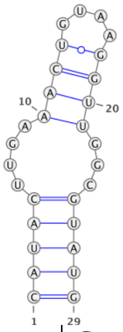
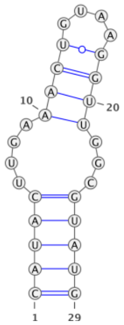
<tr><td rowspan="2">1OOA</td><td colspan="2">
</td><td colspan="2">
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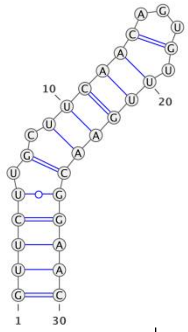
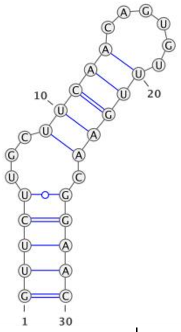
<tr><td rowspan="2">2IPY</td><td colspan="2">
</td><td colspan="2">
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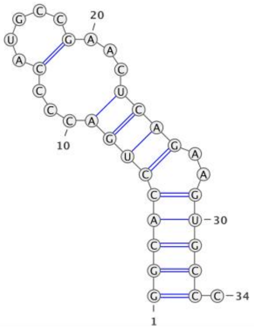
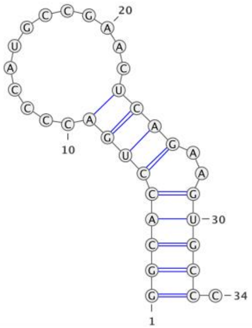
<tr><td rowspan="2">1MJI</td><td colspan="2">
</td><td colspan="2">
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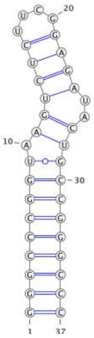
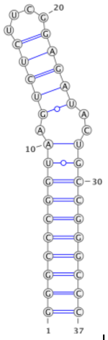
1I6U				
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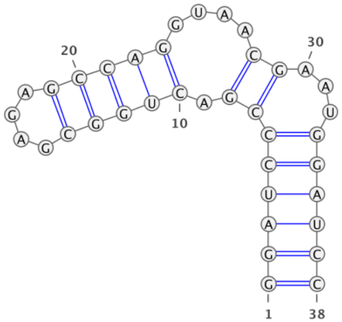
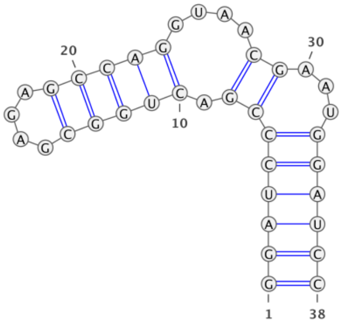
1F1T				
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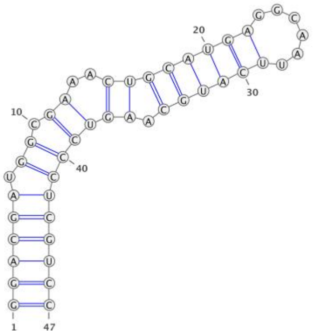
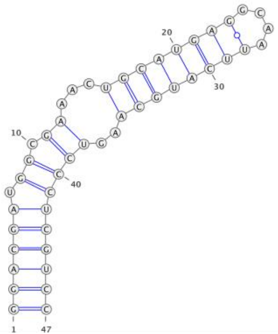
1S03				
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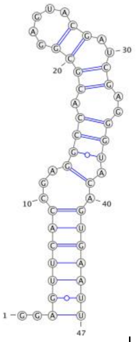
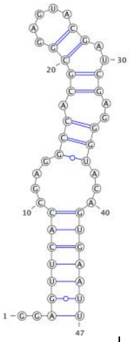
<tr><td rowspan="2">1XJR</td><td colspan="2">
</td><td colspan="2">
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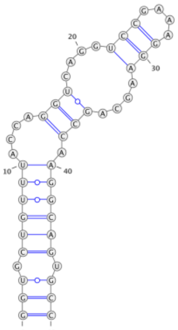
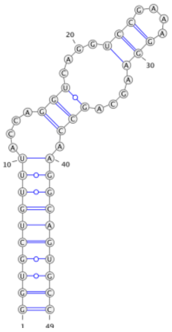
<tr><td rowspan="2">2PXB</td><td colspan="2">
</td><td colspan="2">
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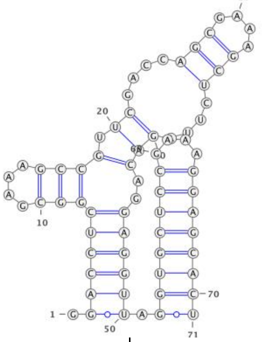
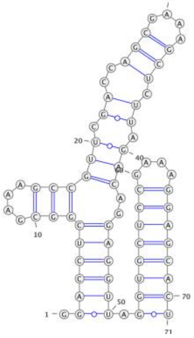
<tr><td rowspan="2">2OIU</td><td colspan="2">
</td><td colspan="2">
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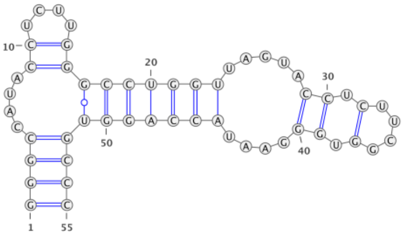
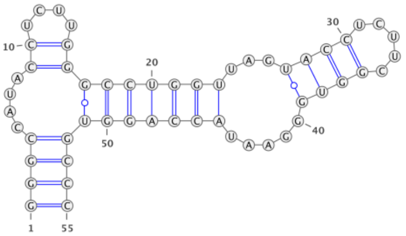
<tr><td>2HGH</td><td colspan="2">
</td><td colspan="2">
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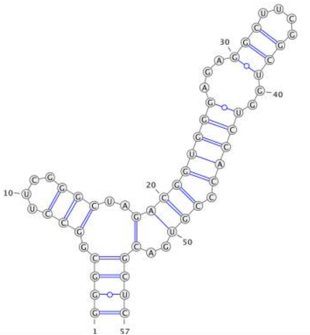
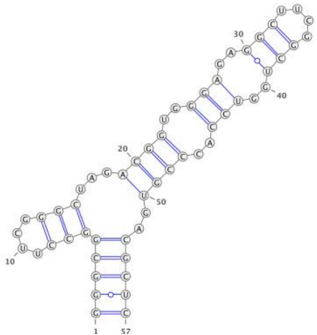
<tr><td>1DK1</td><td colspan="2">
</td><td colspan="2">
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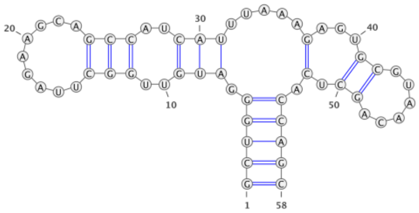
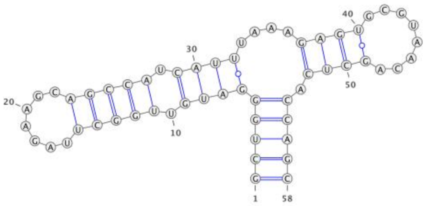
<tr><td>1MMS</td><td colspan="2">
</td><td colspan="2">
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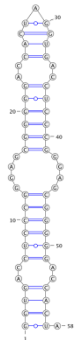
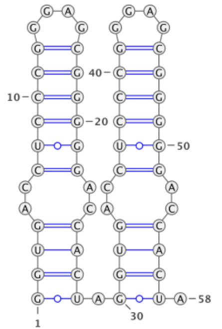
<tr><td rowspan="2">1D4R</td><td colspan="2"></td><td colspan="2">
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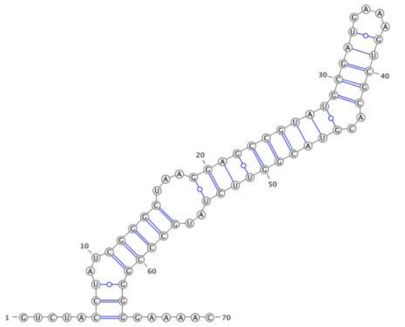
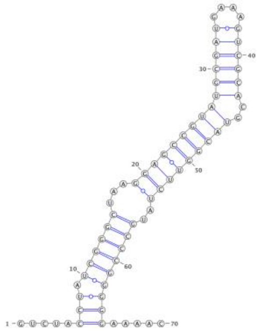
<tr><td rowspan="2">1KXK</td><td colspan="2">
</td><td colspan="2"></td></tr>
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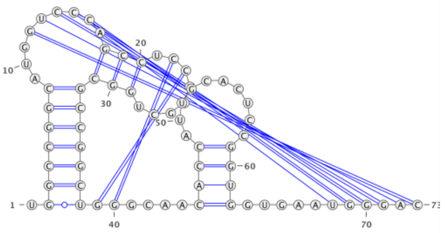
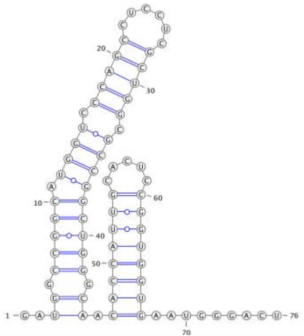
<tr><td rowspan="2">1SJ4</td><td colspan="2">
</td><td colspan="2"></td></tr>
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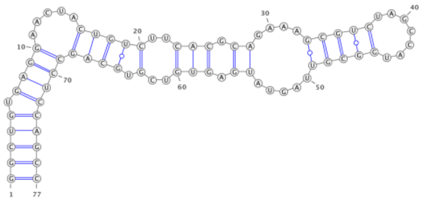
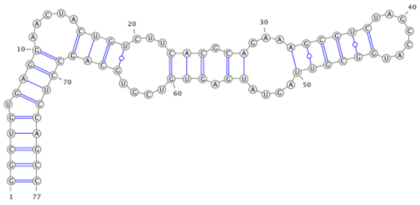
1P5O				
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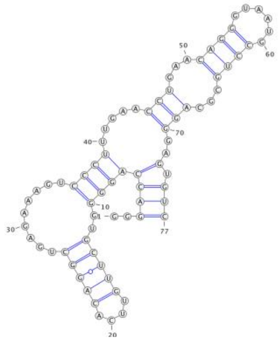
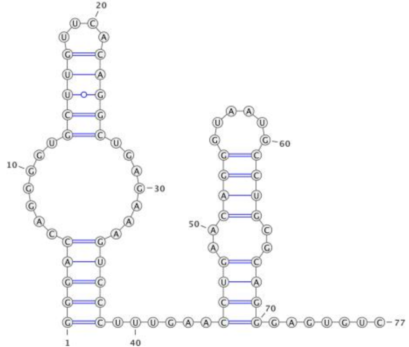
3D2G				
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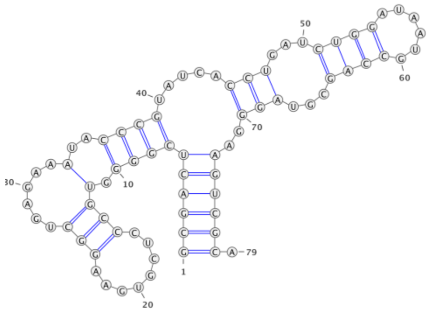
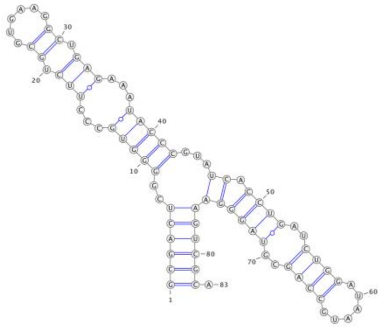
2HOJ				
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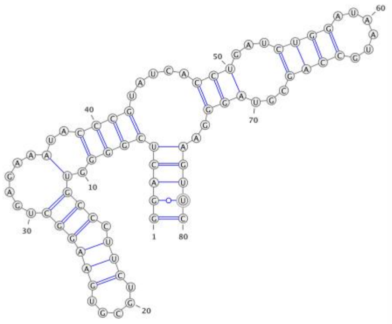
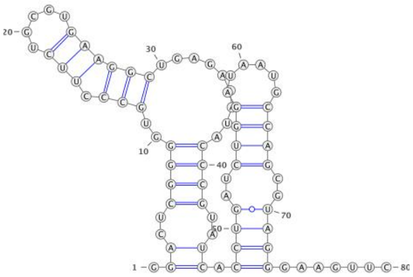
2GDI				
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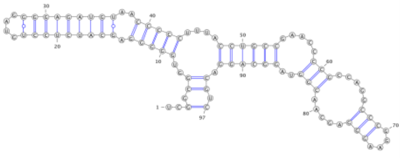
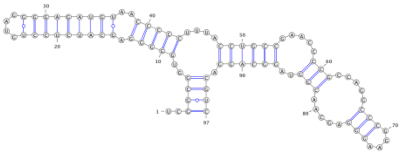
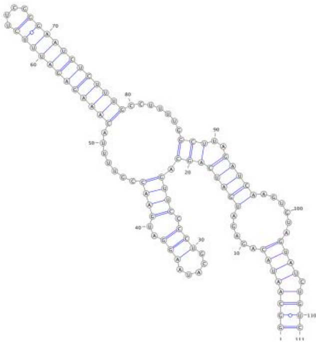
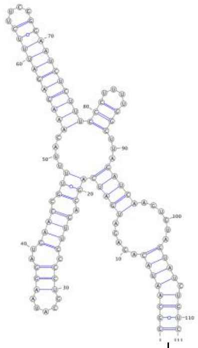
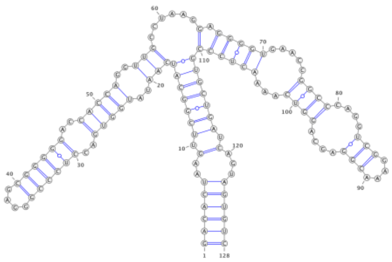
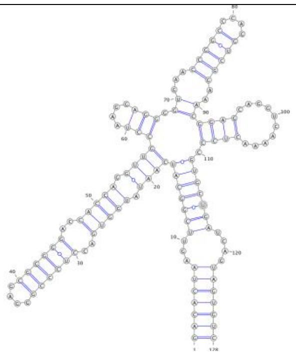
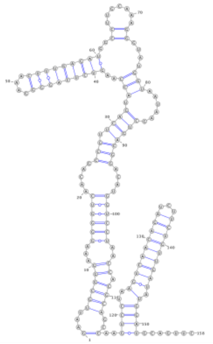
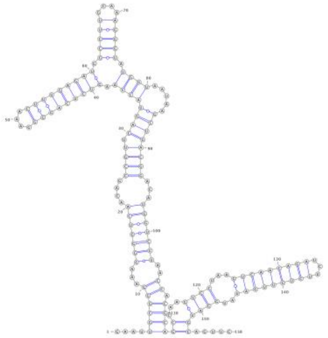
1LNG				
	K-turn pot. P1= 5.53 P2= 14.79 P3= 17.51	General pot. P1= 5.61 P2= 15.01 P3= 13.85	K-turn pot. P1= 6.06 P2= 14.86 P3= 17.62	General pot. P1= 6.06 P2= 19.22 P3= 22.07
2LKR				
	K-turn pot. P1= 14.25 P2= 21.82 P3= 22.32	General pot. P1= 14.25 P2= 18.20 P3= 20.66	K-turn pot. P1= 25.45 P2= 40.32 P3= 39.97	General pot. P1= 25.45 P2= 40.89 P3= 40.10

Table S5

<table>
<tr><td rowspan="2">1MFQ</td><td colspan="2"></td><td colspan="2"></td></tr>
<tr><td>K-turn pot.
P1= 15.41
P2= 27.24
P3= 27.44</td><td>General pot.
P1= 16.48
P2= 30.22
P3= 26.97</td><td>K-turn pot.
P1= 30.54
P2= 30.55
P3= 30.56</td><td>General pot.
P1= 30.54
P2= 30.55
P3= 30.56</td></tr>
<tr><td rowspan="2">1GID</td><td colspan="2"></td><td colspan="2"></td></tr>
<tr><td>K-turn pot.
P1= 14.66
P2= 26.18
P3= 25.65</td><td>General pot.
P1= 14.66
P2= 25.13
P3= 26.19</td><td>K-turn pot.
P1= 16.59
P2= 29.48
P3= 30.52</td><td>General pot.
P1= 18.61
P2= 29.67
P3= 30.74</td></tr>
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