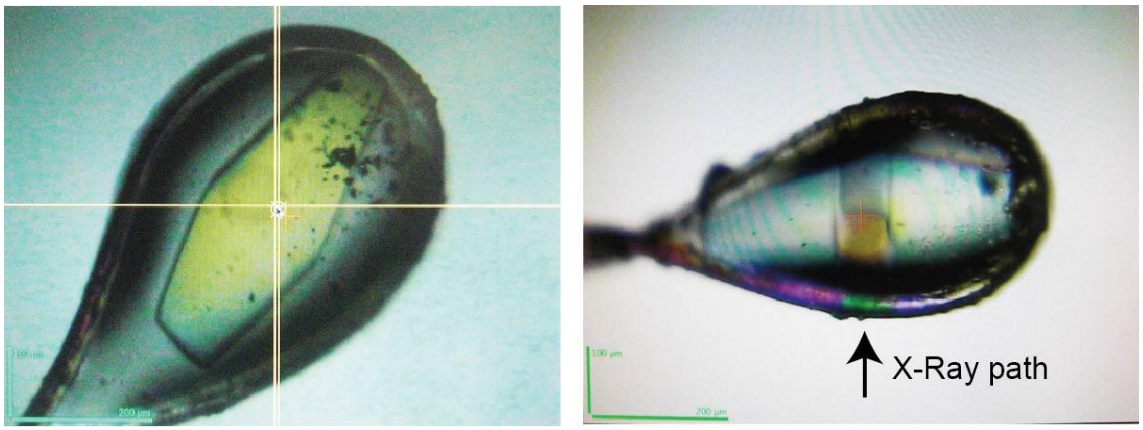
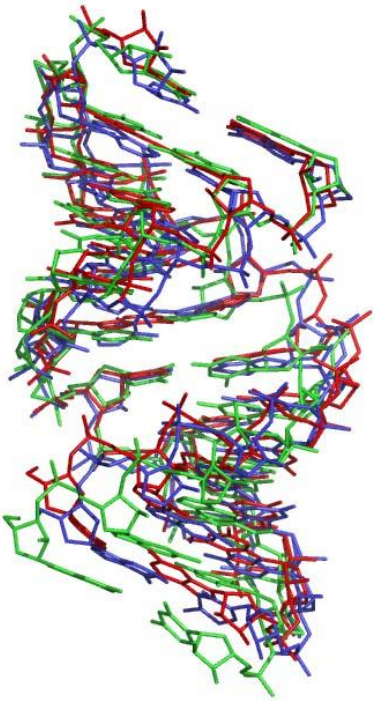
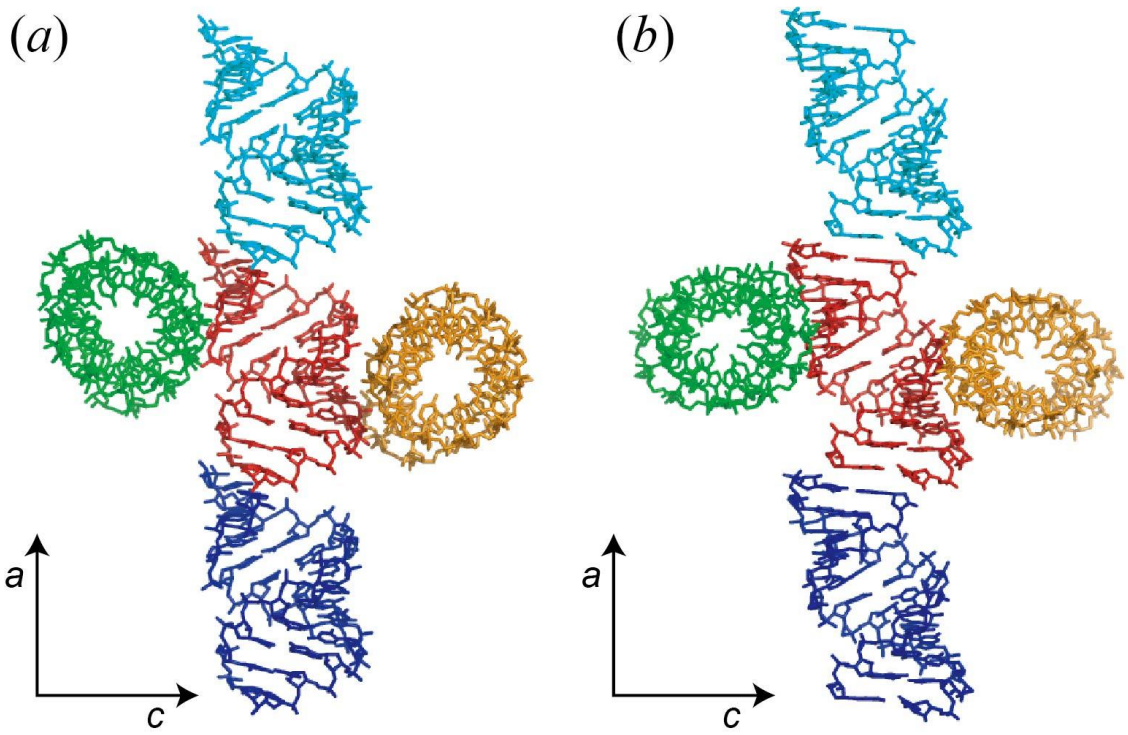
Supplementary Material



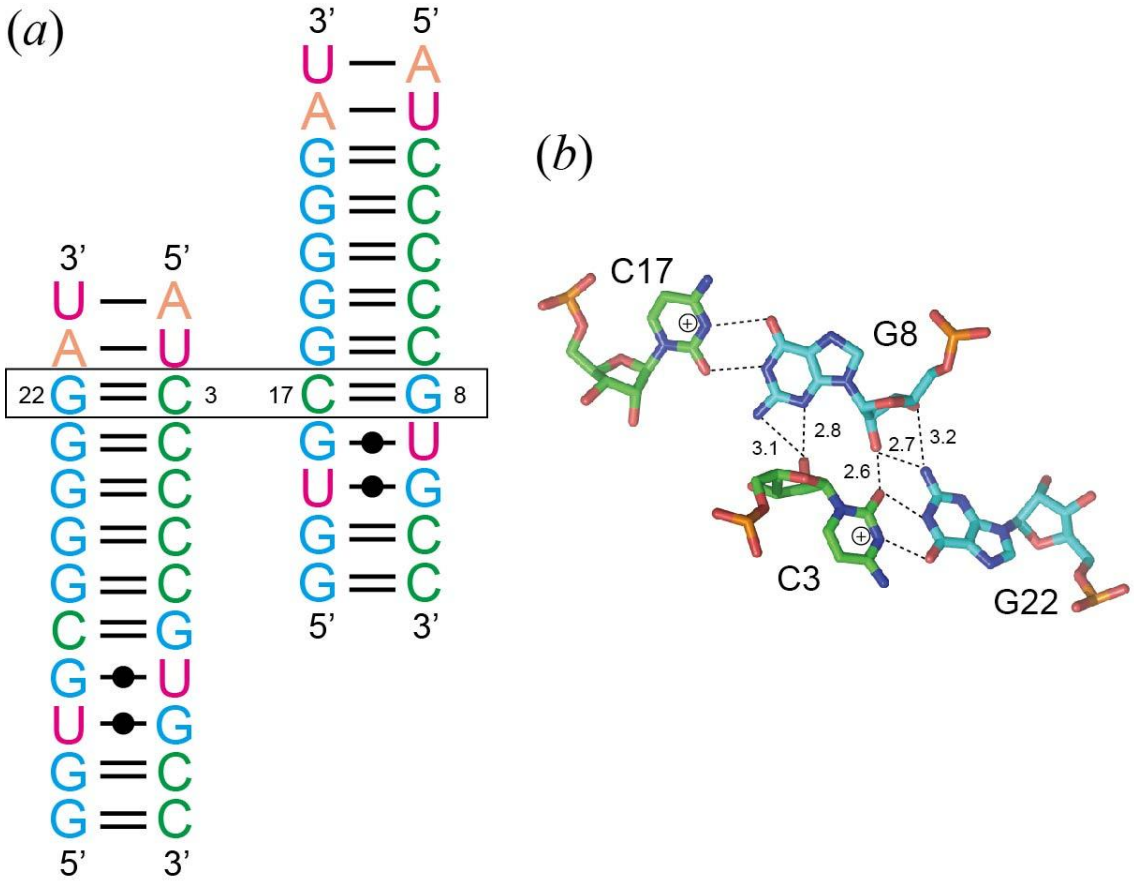
Supplementary Figure S1. The plate-shaped crystal of the 132-nt 6S RNA variant before and after X-ray exposure. In the right panel, radiation damage on the crystal is clearly seen along the X-ray path.



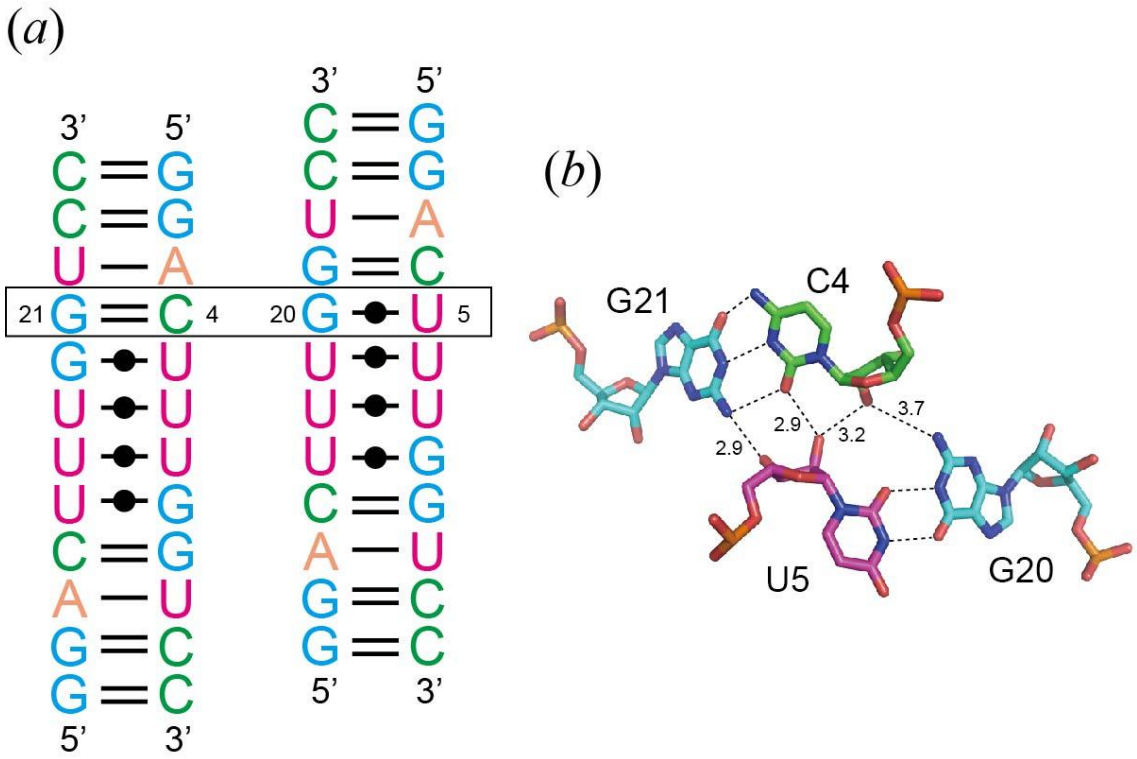
Supplementary Figure S2. Superimpositions among the RNA duplex obtained in this study (red), the 5S rRNA domain A (blue: PDB-ID 353D) and an RNA duplex containing tandem UoU base pairs (green: PDB-ID 205D).



Supplementary Figure S3. Crystal packing interactions observed in the crystals of the 5S rRNA domain A (a) and of an RNA duplex containing tandem UoU base pairs (*b*). The view is down the crystallographic *b* axis.



Supplementary Figure S4. A ribose zipper motif, boxed in (*a*) and detailed views in (*b*), observed at the packing interface of the 5S rRNA domain A crystal (PDB-ID 353D). Hydrogen bonds involved in the motifs are represented by dashed lines with distances in Å in panel (*b*).. In the original article (Betzel *et al*., 1994), there is no mention of protonation of cytosine residues. However, from distances and angles of hydrogen bonds observed in G=C base pairs, it is possible that cytosine residues are protonated to form wobble-type G-C^+ pairs in the crystal as illustrated in panel (*b*). The crystals were obtained at pH 6.5.



Supplementary Figure S5. A ribose zipper motif, boxed in (*a*) and detailed views in (*b*), observed at the packing interface of the crystal of an RNA duplex containing tandem UoU base pairs (PDB-ID 205D). Hydrogen bonds involved in the motifs are represented by dashed lines with distances in Å in panel (*b*).

Supplementary Table S1. Local base pair parameters of the RNA duplex obtained in this study.

Base pair	Inclination (°)	Tip (°)	Twist (°)	Rise (Å)	Propeller (°)	Buckle (°)	Opening (°)	C1'...C1' (Å)
G_1=C_{24}					-7	-6	-5	11.2
	0	-2	33	3.1				
G_2=C_{23}					-1	2	8	10.7
	33	2	36	1.8				
G_3=C_{22}					-7	-9	5	10.5
	12	1	40	2.7				
U_4oG_{21}					-1	0	3	10.5
	40	7	23	1.2				
G_5oU_{20}					-16	-11	6	10.2
	12	-6	38	2.9				
G_6=C_{19}					-9	-12	6	10.4
	12	-3	33	2.6				
U_7-A_{18}					-5	0	2	10.7
	25	3	34	2.4				
G_8=C_{17}					-12	4	6	10.6
	21	4	34	2.7				
C_9=G_{16}					-11	7	-3	10.6
	33	-3	31	1.7				
G_{10}oU_{15}					-16	-3	2	10.2
	9	-1	36	3.1				
G_{11}=C_{14}					-14	-11	5	10.7
	15	7	35	3.1				
G_{12}=C_{13}					-13	-14	7	10.5
Average	15	1	34	2.5	-9	-5	4	10.6
A-form	20	0	33	2.3	12	0	-2	10.7