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SUPPLEMENTARY INFORMATION

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Crystal structure of Δ-$[Ru(bpy)_2dppz]^{2+}$ bound to mismatched DNA reveals side-by-side metalloinsertion and intercalation

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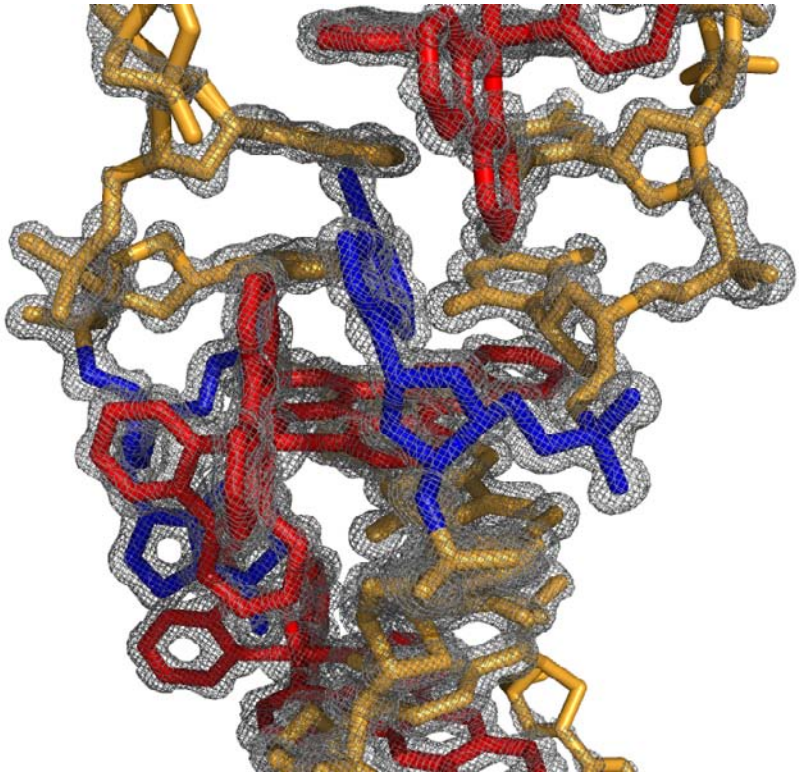
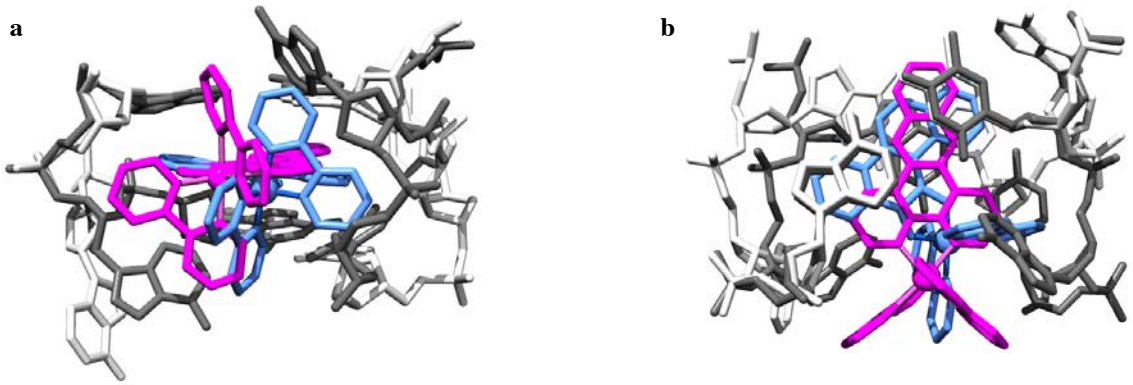
Supplementary Figure S1. Representative electron density map of a metalloinsertion site. The extruded adenosines (blue) stack with two ancillary bpy ligands, one from the inserted ruthenium complex (red, middle) and the other from a neighboring intercalated complex (red, top and bottom).

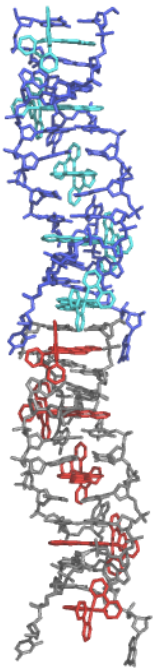


Supplementary Figure S2. Comparison of metalloinsertion by Δ-$[Ru(bpy)_2dppz]^{2+}$ (magenta, DNA in dark gray) and Δ-$[Rh(bpy)_2chrysi]^{3+}$ (blue, DNA in light gray). **a**, View from the minor groove. **b**, View down the helical axis. The mismatch binding sites are superimposed using the top flanking AT base pair (PDB accession code of the rhodium structure: 3GSK).

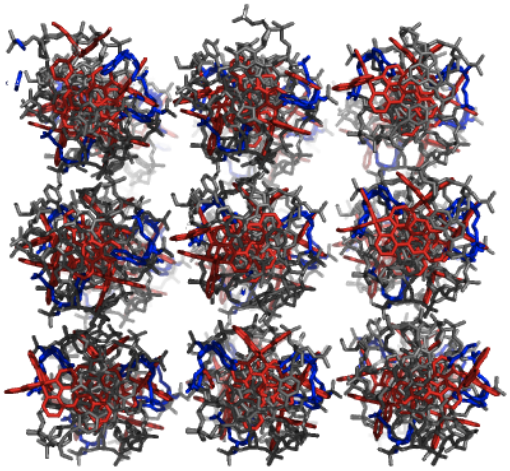


Supplementary Figure S3. Crystal packing. **a**, Two crystallographically-related duplexes stack head-to-tail, forming a long rod along the helical axis. **b**, View down the helical axis shows that parallel rods do not have appreciable contact with each other in the crystal lattice.

a



b



Supplementary Table S1. Data collection and refinement statistics.

Data collection	
space group	*P*1
cell dimensions	
a, b, c (Å)	24.039, 24.797, 37.521
α, β, γ (°)	74.669, 84.416, 76.208
wavelength	0.7749
Resolution*	36—0.92 (0.97—0.92)
R_{merge}*	0.030 (0.537)
R_{pim}*	0.018 (0.317)
$I/\sigma I$*	20.0 (2.4)
completeness (%)*	82.7 (64.5)
redundancy	3.9
Refinement	
no. of reflections (anomalous)	46920 (92014)
R_{work}/R_{free}	0.140/0.149
rmsd for bond lengths (Å)	0.011
rmsd for bond angles (°)	1.62

*Highest-resolution shell is shown in parentheses.

Supplementary Table S2. Helical parameters of DNA conformation relating bases that comprise each base pair.[a]

Base pair	Shear (Å)	Stretch (Å)	Stagger (Å)	Buckle (°)	Propeller (°)	Opening (°)	Sugar pucker
C_1-G_{12}	0.2	-0.2	-0.4	0.6	20.2	-1.1	C2'-endo, C1'-exo
G_2-C_{11}	-0.2	-0.2	-0.4	-8.1	3.2	-0.6	C3'-exo, C2'-endo
G_3-C_{10}	-0.2	-0.2	-0.2	14.9	19.6	-2.4	C2'-endo, C2'-endo
A_5-T_8	0.2	0.0	-0.7	-7.1	28.0	7.7	C2'-endo, C1'-exo
A_6-T_7	0.1	0.0	0.0	21.5	10.4	-2.2	C2'-endo, O4'-endo
T_7-A_6	-0.2	-0.2	0.0	-18.0	9.2	-0.7	O4'-endo, C1'-exo
T_8-A_5	-0.1	-0.1	-0.2	15.8	13.6	9.8	C1'-exo, C2'-endo
C_{10}-G_3	0.3	-0.2	0.1	-16.6	23.7	-1.5	C2'-endo, C1'-exo
C_{11}-G_2	0.2	-0.1	-0.2	6.4	10.0	-0.3	C1'-exo, C3'-exo
B-DNA	0	0.1	0.1	0.1	4.1	-4.1	C2'-endo

[a]Data were calculated using 3DNA.