Supporting Information

A Bulky Rhodium Complex Bound to an Adenosine-Adenosine DNA Mismatch: General Architecture of the Metalloinsertion Binding Mode †

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Figure S1. Crystal packing at the $Rh(bpy)_2(chrysi)^{3+}$ intercalation site in structure **2**.

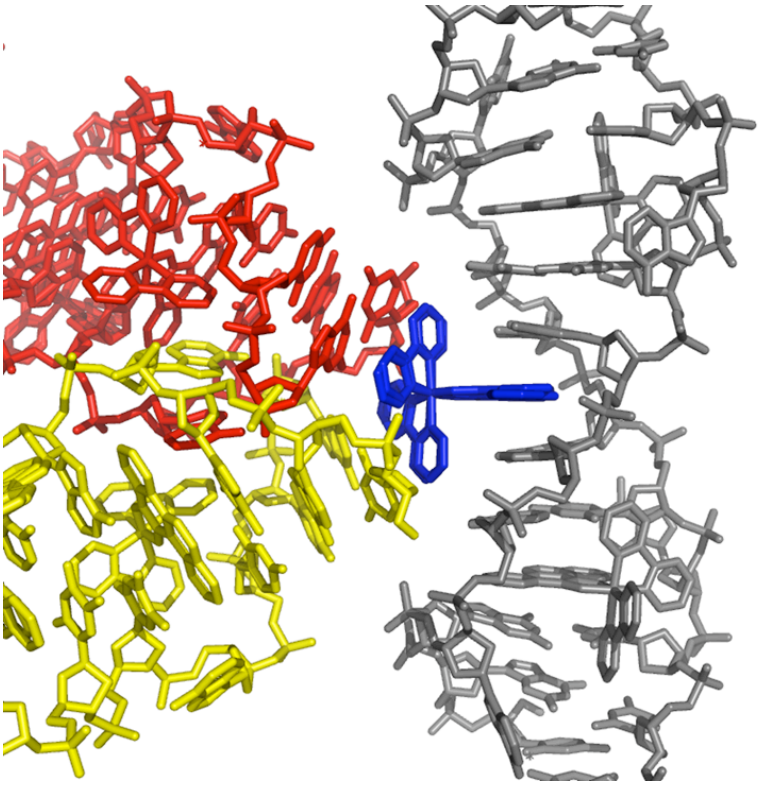


Figure S2. Superposition of entire duplex of structures **1** (green) and **2** (blue), illustrating the slight bending of the duplex in structure **1** relative to that in structure **2**.

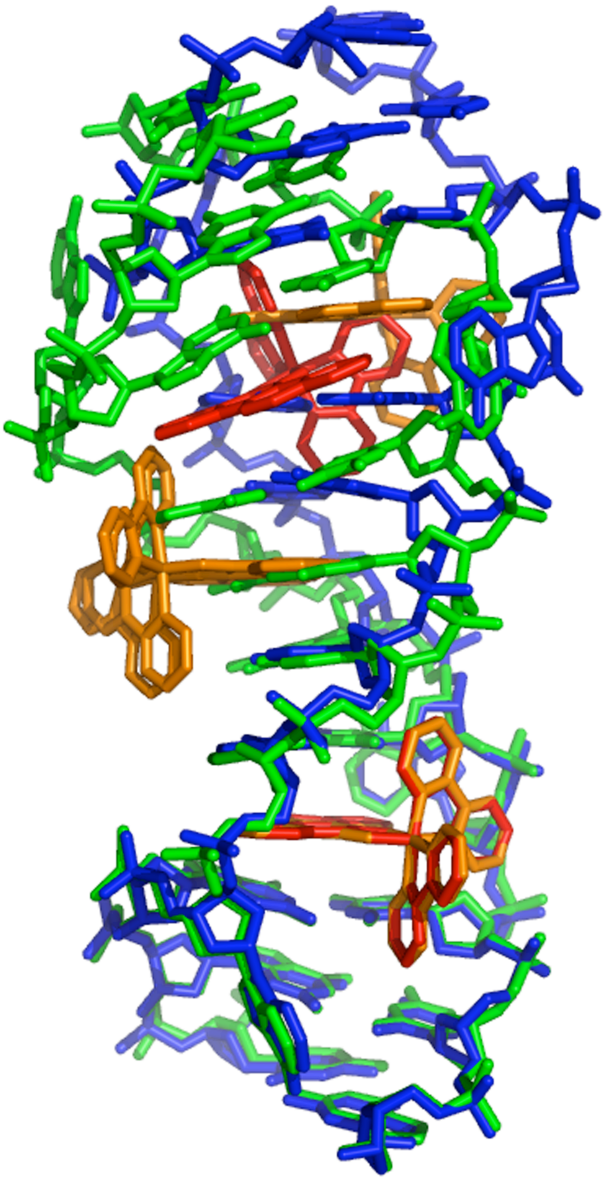


Figure S3. Interhelical stacking interactions for the ejected adenosines of a single duplex in structure **1.**

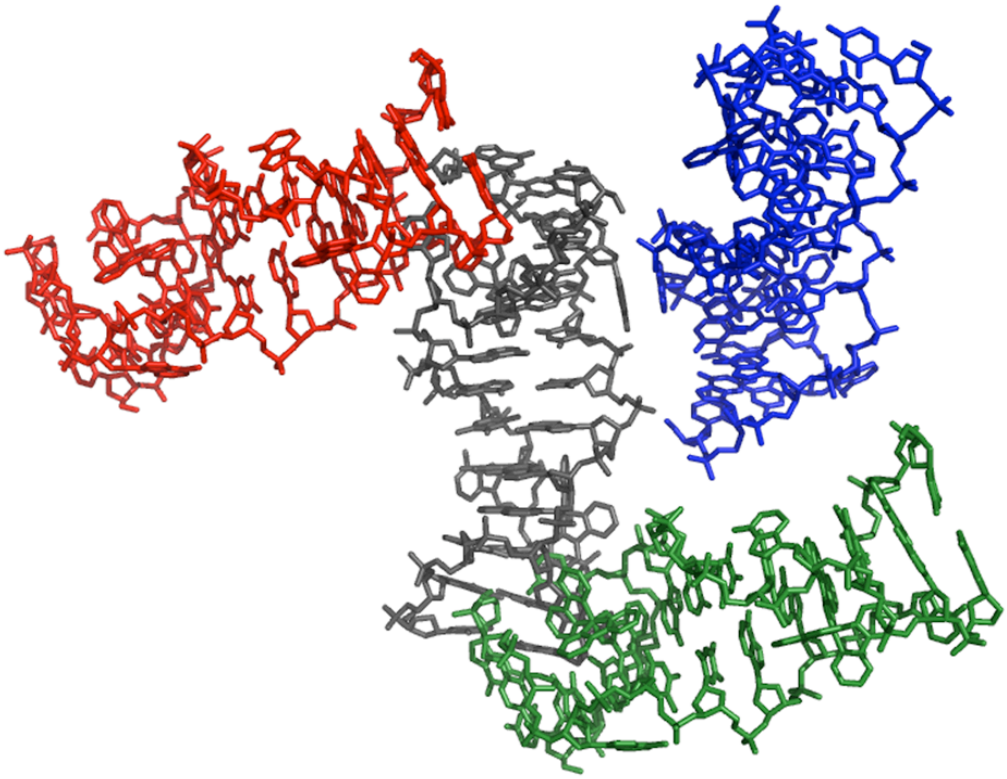
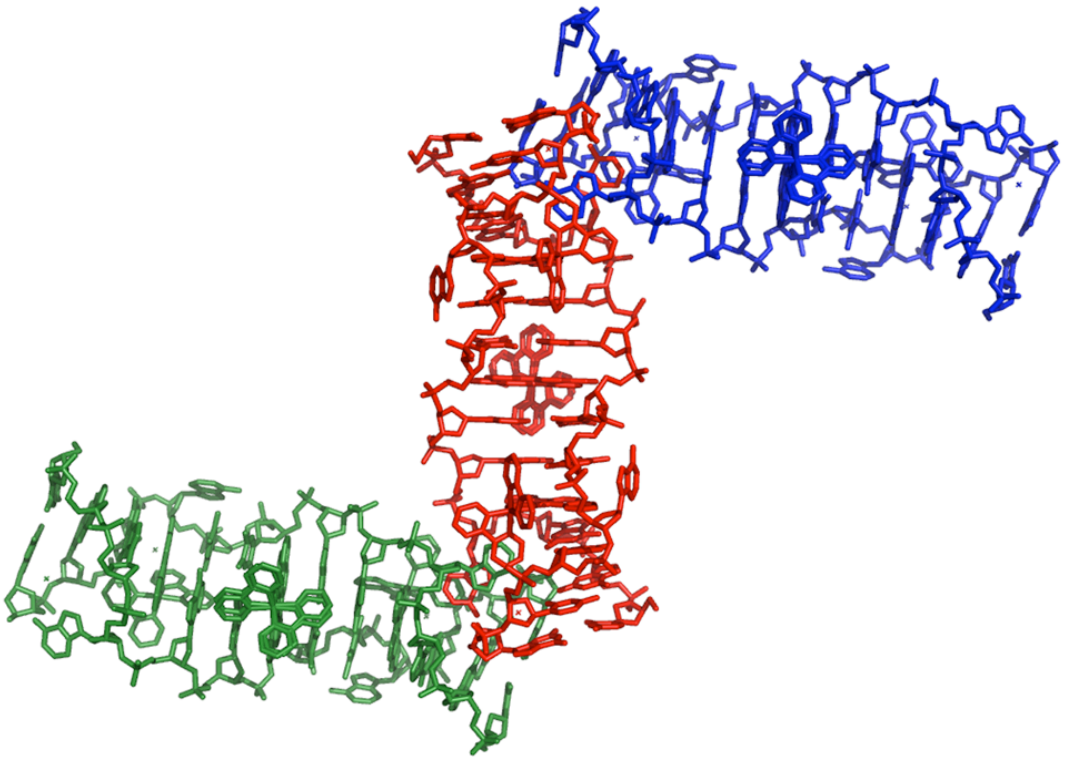


Figure S4. Interhelical stacking interactions for the ejected adenosines of a single duplex in structure **2**.



Supplementary Table 1. DNA helical parameters [a] relating consecutive base pairs of structure **2**.[b]

Base-pair	Shift (Å)	Slide (Å)	Rise (Å)	Tilt (°)	Roll (°)	Twist (°)
CG/CG	1.1	2.2	3.0	11.0	2.8	40.0
GG/CC	-0.4	2.7	3.3	-6.0	6.1	34.8
GA/TC	-	-	-	-	-	-
AA/TT	-0.8	0.8	3.3	0.4	4.3	32.2
AT/AT	0.0	-0.2	7.1	0.0	-10.4	27.3
TT/AA	0.8	0.8	3.3	0.4	4.3	32.2
TC/GA	-	-	-	-	-	-
CC/GG	0.4	2.7	3.3	6.0	6.1	34.8
CG/CG	-1.1	2.2	3.0	-11.0	2.8	40.0
B-DNA	-0.1	-0.8	3.3	-1.3	-3.6	36

[a] Geometrical relationships between consecutive base pairs: shift, translation into the groove; slide, translation toward the phosphodiester backbone; rise, translation along the helix axis; tilt, rotation about the pseudo-twofold axis relating the DNA strands; roll, rotation about a vector between the C1' atoms; and twist, rotation about the helix axis.
[b] Data were calculated by using the program 3DNA.[30]

Supplementary Table 2. DNA helical parameters [a] of base pairs of structure **2**.[b]

Base-pair	Shear (Å)	Stretch (Å)	Stagger (Å)	Buckle (°)	Propeller (°)	Opening (°)	Sugar pucker
C-G	0.0	-0.3	0.8	-16.2	-2.4	-4.9	C2'-endo
G-C	-0.2	-0.3	0.0	3.4	1.4	-2.1	C2'-endo
G-C	-0.3	-0.1	0.5	18.0	-6.0	0.2	C2'-endo
A-A	-	-	-	-	-	-	C2'-endo
A-T	-0.1	-0.1	0.1	-1.3	8.6	5.1	C2'-endo
A-T	0.1	-0.2	0.2	7.3	-6.9	1.2	C2'-endo
T-A	-0.1	-0.2	0.2	-7.3	-6.9	1.2	C2'-endo
T-A	0.1	-0.1	0.1	1.3	8.6	5.1	C2'-endo
A-A	-	-	-	-	-	-	C2'-endo
C-G	0.3	-0.1	0.5	-18.0	-6.0	0.2	C2'-endo
C-G	0.2	-0.3	0.0	-3.4	1.4	-2.1	C2'-endo
G-C	0.0	-0.3	0.8	16.2	-2.4	-4.9	C2'-endo
B-DNA	0	0.1	0.1	0.1	4.1	-4.1	C2'-endo

[a] Relationships between the bases that compose the pair, in directions that correspond with those of Table 2.
[b] Data were calculated by using the program 3DNA.[30]