Supplementary Materials for:

Hg(II) Binding to Thymine Bases in DNA

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TABLE OF CONTENTS

Table S1. Crystal data and structure refinement.

Empirical formula	C12 H14 Hg N4 O4
Formula weight	478.86
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 4.3903(2) Å; α = 90°
	b = 11.7232(4) Å; β = 91.5640(10)°
	c = 13.2976(5) Å; γ = 90°
Volume	684.15(5) $Å^3$
Z	2
Density (calculated)	2.325 Mg/m^3
Absorption coefficient	11.271 mm^{-1}
F(000)	452
Crystal size	0.190 x 0.070 x 0.040 mm^3
Theta range for data collection	3.065 to 27.438°
Index ranges	$-5 \leq h \leq 5$
	$-11 \leq k \leq 15$
	$-17 \leq l \leq 16$
Reflections collected	6670
Independent reflections	1560 [R(int) = 0.0172]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Multi-scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1560 / 0 / 99
Goodness-of-fit on F^2	1.193
Final R indices [I > 2sigma(I)]	R1 = 0.0124, wR2 = 0.0272
R indices (all data)	R1 = 0.0147, wR2 = 0.0280
Extinction coefficient	n/a
Largest diff. peak and hole	0.455 and –0.364 $e.Å^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for 1579c_0m. U (eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. Anisotropic displacement parameters ($Å^2 \times 10^3$) for 1579c_0m. The anisotropic displacement factor exponent takes the form: $-2p^2$ [h2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]. Numeric values in parentheses specify the estimated standard deviation on the last decimal place given.

	x	**y**	**z**	**U(eq)**	**U^{11}**	**U^{22}**	**U^{33}**	**U^{23}**	**U^{13}**	**U^{12}**
Hg(1)	5000	5000	5000	15(1)	17(1)	16(1)	13(1)	3(1)	1(1)	-2(1)
N(1)	9521(5)	7465(2)	3284(2)	21(1)	21(1)	18(1)	23(1)	5(1)	2(1)	0(1)
O(2)	10035(4)	6770(2)	4908(1)	24(1)	27(1)	28(1)	18(1)	0(1)	-4(1)	-4(1)
N(3)	6614(4)	5924(2)	3845(1)	15(1)	18(1)	15(1)	13(1)	4(1)	2(1)	-2(1)
O(4)	3274(4)	5001(2)	2810(1)	26(1)	28(1)	22(1)	27(1)	-2(1)	-3(1)	-7(1)
C(2)	8814(5)	6722(2)	4063(2)	17(1)	18(1)	16(1)	19(1)	1(1)	3(1)	3(1)
C(4)	5234(5)	5742(2)	2910(2)	17(1)	19(1)	14(1)	18(1)	0(1)	1(1)	5(1)
C(5)	6223(5)	6474(2)	2123(2)	16(1)	19(1)	16(1)	14(1)	4(1)	1(1)	3(1)
C(6)	8243(5)	7310(2)	2342(2)	20(1)	21(1)	20(1)	19(1)	8(1)	3(1)	4(1)
C(9)	11559(6)	8440(2)	3503(2)	26(1)	25(1)	22(1)	32(1)	7(1)	-1(1)	-4(1)
C(10)	4916(6)	6297(3)	1083(2)	28(1)	34(1)	33(2)	17(1)	5(1)	-3(1)	2(1)
H(6)	8806	7814	1819	24						
H(9A)	11856	8877	2885	39						
H(9B)	13531	8158	3761	39						
H(9C)	10644	8932	4008	39						
H(10A)	5560	6921	647	42						
H(10B)	2686	6285	1104	42						
H(10C)	5644	5570	817	42						

Table S3. Bond lengths for Hg-bis(1-methylthymine). Numeric values in parentheses specify the estimated standard deviation on the last decimal places given.

Atoms	Bond lengths (Å)
Hg(1)-N(3)	2.0235(18)
Hg(1)-N(3)#1	2.0235(18)
Hg(1)-C(1)	2.9233(18)
Hg(1)-C(2)	2.9161(18)
Hg(1)-O(4)	2.9897(18)
Hg(1)-O(2)	3.0368(18)
Hg(1)-O(2)axial	3.0094(19)
O(2)-C(2)	1.233(3)
O(4)-C(4)	1.228(3)
N(1)-C(6)	1.371(3)
N(1)-C(2)	1.395(3)
N(1)-C(9)	1.475(3)
N(3)-C(2)	1.370(3)
N(3)-C(4)	1.384(3)
C(4)-C(5)	1.431(3)
C(5)-C(6)	1.348(3)
C(5)-C(10)	1.497(3)
C(6)-H(6)	0.9500
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800

#1 –x+1, –y+1, –z+1 symmetry transformations

Table S4. Bond angles for Hg–bis(1–methylthymine). Numeric values in parentheses specify the estimated standard deviation on the last decimal place given.

Atoms	Angles (°)
N(3)-Hg(1)-N(3)#1	180.0
C(6)-N(1)-C(2)	120.1(2)
C(6)-N(1)-C(9)	121.0(2)
C(2)-N(1)-C(9)	118.9(2)
C(2)-N(3)-C(4)	125.74(19)
C(2)-N(3)-Hg(1)	117.67(15)
C(4)-N(3)-Hg(1)	116.45(15)
O(2)-C(2)-N(3)	120.7(2)
O(2)-C(2)-N(1)	123.2(2)
N(3)-C(2)-N(1)	116.1(2)
O(4)-C(4)-N(3)	119.7(2)
O(4)-C(4)-C(5)	124.8(2)
N(3)-C(4)-C(5)	115.5(2)
C(6)-C(5)-C(4)	119.3(2)
C(6)-C(5)-C(10)	122.3(2)
C(4)-C(5)-C(10)	118.5(2)
C(5)-C(6)-N(1)	123.0(2)
C(5)-C(6)-H(6)	118.5
N(1)-C(6)-H(6)	118.5
N(1)-C(9)-H(9A)	109.5
N(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
N(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

#1 –x+1, –y+1, –z+1 symmetry transformations