Supplementary X-ray Crystallographic Information

Non-covalent interactions in paired DNA nucleobases investigated by terahertz spectroscopy and solid-state density functional theory

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Table 1. Crystal data and structure refinement for 1-methylthymine.

Identification code	p21c	
Empirical formula	C6 H8 N2 O2	
Formula weight	140.14	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 7.1579(8) Å	α= 90°.
	b = 12.0979(15) Å	β= 91.731(7)°.
	c = 7.5436(9) Å	γ = 90°.
Volume	652.94(13) $Å^3$	
Z	4	
Density (calculated)	1.426 Mg/m^3	
Absorption coefficient	0.109 mm^{-1}	
F(000)	296	
Crystal size	0.38 x 0.12 x 0.06 mm^3	
Theta range for data collection	2.85 to 27.99°.	
Index ranges	-9<=h<=9, -15<=k<=14, -9<=l<=9	
Reflections collected	8332	
Independent reflections	1528 [R(int) = 0.0822]	
Completeness to theta = 27.99°	97.1 %	
Absorption correction	None	
Max. and min. transmission	0.9935 and 0.9597	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1528 / 0 / 124	
Goodness-of-fit on F^2	0.852	
Final R indices [I>2sigma(I)]	R1 = 0.0530, wR2 = 0.1302	
R indices (all data)	R1 = 0.0903, wR2 = 0.1649	
Extinction coefficient	0.019(8)	
Largest diff. peak and hole	0.278 and -0.317 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1-methylthymine. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	10586(2)	3572(1)	-6(2)	27(1)
O(1)	5472(2)	5233(1)	2216(2)	36(1)
N(1)	5673(3)	3349(1)	2428(3)	28(1)
N(2)	7989(2)	4371(1)	1081(2)	24(1)
C(6)	3897(3)	3301(2)	3350(4)	31(1)
C(1)	6312(3)	4374(2)	1927(3)	26(1)
C(2)	9065(3)	3460(2)	719(3)	23(1)
C(3)	8314(3)	2414(2)	1231(3)	23(1)
C(5)	6672(3)	2406(2)	2063(3)	25(1)
C(4)	9380(3)	1380(2)	840(3)	30(1)

Table 3. Bond lengths [Å] and angles [°] for 1-methylthymine.

O(2)-C(2)	1.241(2)
O(1)-C(1)	1.224(2)
N(1)-C(1)	1.378(2)
N(1)-C(5)	1.379(2)
N(1)-C(6)	1.469(3)
N(2)-C(1)	1.377(3)
N(2)-C(2)	1.377(2)
N(2)-H(2)	0.93(3)
C(6)-H(6A)	0.94(3)
C(6)-H(6B)	0.94(3)
C(6)-H(6C)	0.97(3)
C(2)-C(3)	1.433(3)
C(3)-C(5)	1.349(3)
C(3)-C(4)	1.499(3)
C(5)-H(5)	0.90(3)
C(4)-H(4A)	1.01(3)
C(4)-H(4B)	1.00(3)
C(4)-H(4C)	0.98(3)
C(1)-N(1)-C(5)	120.77(17)
C(1)-N(1)-C(6)	117.72(17)
C(5)-N(1)-C(6)	121.51(17)
C(1)-N(2)-C(2)	126.52(17)
C(1)-N(2)-H(2)	116.8(17)
C(2)-N(2)-H(2)	116.7(17)
N(1)-C(6)-H(6A)	108.3(15)
N(1)-C(6)-H(6B)	110.9(16)
H(6A)-C(6)-H(6B)	114(2)
N(1)-C(6)-H(6C)	111.1(15)
H(6A)-C(6)-H(6C)	105(2)
H(6B)-C(6)-H(6C)	107(2)
O(1)-C(1)-N(2)	121.65(18)
O(1)-C(1)-N(1)	123.13(18)
N(2)-C(1)-N(1)	115.22(16)
O(2)-C(2)-N(2)	120.23(16)

O(2)-C(2)-C(3)	123.89(17)
N(2)-C(2)-C(3)	115.89(18)
C(5)-C(3)-C(2)	118.14(18)
C(5)-C(3)-C(4)	122.77(18)
C(2)-C(3)-C(4)	119.09(18)
C(3)-C(5)-N(1)	123.42(18)
C(3)-C(5)-H(5)	121.2(15)
N(1)-C(5)-H(5)	115.4(15)
C(3)-C(4)-H(4A)	110.7(14)
C(3)-C(4)-H(4B)	111.3(16)
H(4A)-C(4)-H(4B)	113(2)
C(3)-C(4)-H(4C)	110.5(18)
H(4A)-C(4)-H(4C)	101(2)
H(4B)-C(4)-H(4C)	110(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1-methylthymine. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	25(1)	13(1)	43(1)	2(1)	8(1)	0(1)
O(1)	35(1)	16(1)	57(1)	-2(1)	13(1)	8(1)
N(1)	24(1)	16(1)	45(1)	2(1)	6(1)	-2(1)
N(2)	24(1)	9(1)	40(1)	1(1)	6(1)	0(1)
C(6)	23(1)	27(1)	42(1)	4(1)	6(1)	0(1)
C(1)	26(1)	14(1)	38(1)	0(1)	7(1)	2(1)
C(2)	24(1)	11(1)	33(1)	0(1)	4(1)	1(1)
C(3)	27(1)	12(1)	31(1)	-1(1)	3(1)	0(1)
C(5)	28(1)	11(1)	36(1)	0(1)	2(1)	-2(1)
C(4)	38(1)	11(1)	39(1)	3(1)	6(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for P21c.

	x	y	z	U(eq)
H(5)	6140(30)	1760(20)	2390(30)	28(6)
H(4A)	10590(40)	1360(20)	1550(30)	33(6)
H(2)	8460(40)	5050(30)	750(30)	39(7)
H(4B)	9560(40)	1290(20)	-470(40)	44(7)
H(4C)	8740(40)	730(30)	1300(40)	55(8)
H(6A)	2940(40)	3560(20)	2570(30)	33(6)
H(6B)	3990(40)	3680(20)	4440(40)	39(7)
H(6C)	3570(40)	2540(20)	3630(40)	46(8)

Table 6.Torsion angles [°] for 1-methylthymine.

C(2)-N(2)-C(1)-O(1)	178.7(2)
C(2)-N(2)-C(1)-N(1)	-0.7(3)
C(5)-N(1)-C(1)-O(1)	179.8(2)
C(6)-N(1)-C(1)-O(1)	0.0(3)
C(5)-N(1)-C(1)-N(2)	-0.8(3)
C(6)-N(1)-C(1)-N(2)	179.48(19)
C(1)-N(2)-C(2)-O(2)	-177.73(19)
C(1)-N(2)-C(2)-C(3)	2.2(3)
O(2)-C(2)-C(3)-C(5)	177.83(19)
N(2)-C(2)-C(3)-C(5)	-2.0(3)
O(2)-C(2)-C(3)-C(4)	-1.7(3)
N(2)-C(2)-C(3)-C(4)	178.46(19)
C(2)-C(3)-C(5)-N(1)	0.7(3)
C(4)-C(3)-C(5)-N(1)	-179.8(2)
C(1)-N(1)-C(5)-C(3)	0.8(3)
C(6)-N(1)-C(5)-C(3)	-179.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 7.Crystal data and structure refinement for 9-methyladenine.

Identification code	mo_9methyladenine_0m	
Empirical formula	C6 H7 N5	
Formula weight	149.17	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.4738(6) Å	α= 90°.
	b = 12.2720(9) Å	β= 112.110(6)°.
	c = 7.6927(6) Å	γ = 90°.
Volume	653.68(9) $Å^3$	
Z	4	
Density (calculated)	1.516 Mg/m^3	
Absorption coefficient	0.105 mm^{-1}	
F(000)	312	
Crystal size	0.42 x 0.25 x 0.06 mm^3	
Theta range for data collection	3.38 to 27.99°.	
Index ranges	-9<=h<=9, -16<=k<=15, -10<=l<=10	
Reflections collected	5917	
Independent reflections	1543 [R(int) = 0.0580]	
Completeness to theta = 27.99°	98.2 %	
Absorption correction	None	
Max. and min. transmission	0.9937 and 0.9573	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1543 / 0 / 128	
Goodness-of-fit on F^2	0.817	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1162	
R indices (all data)	R1 = 0.0646, wR2 = 0.1368	
Largest diff. peak and hole	0.306 and -0.265 e.$Å^{-3}$	

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for9-methyladenine. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	181(2)	8684(1)	2771(2)	18(1)
N(2)	1001(2)	10593(1)	3056(2)	18(1)
N(3)	3608(2)	10996(1)	6011(2)	17(1)
N(4)	4194(2)	9319(1)	7282(2)	18(1)
N(5)	1773(2)	7376(1)	4962(2)	19(1)
C(1)	1575(2)	8421(1)	4436(2)	16(1)
C(2)	-12(2)	9727(1)	2202(2)	18(1)
C(3)	2345(2)	10313(1)	4727(2)	16(1)
C(4)	3730(3)	12175(1)	5795(3)	22(1)
C(5)	4662(2)	10360(1)	7505(2)	19(1)
C(6)	2729(2)	9279(1)	5521(2)	15(1)

Table 9. Bond lengths [Å] and angles [°] for 9-methyladenine.

N(1)-C(2)	1.343(2)
N(1)-C(1)	1.352(2)
N(2)-C(2)	1.327(2)
N(2)-C(3)	1.345(2)
N(3)-C(3)	1.3669(19)
N(3)-C(5)	1.367(2)
N(3)-C(4)	1.4623(19)
N(4)-C(5)	1.319(2)
N(4)-C(6)	1.385(2)
N(5)-C(1)	1.335(2)
N(5)-H(5A)	0.86(3)
N(5)-H(5B)	0.95(3)
C(1)-C(6)	1.417(2)
C(2)-H(2)	0.95(2)
C(3)-C(6)	1.390(2)
C(4)-H(4A)	0.98(3)
C(4)-H(4B)	1.00(2)
C(4)-H(4C)	0.96(2)
C(5)-H(5)	0.97(2)
C(2)-N(1)-C(1)	119.11(13)
C(2)-N(2)-C(3)	110.46(13)
C(3)-N(3)-C(5)	106.25(13)
C(3)-N(3)-C(4)	125.48(14)
C(5)-N(3)-C(4)	128.26(14)
C(5)-N(4)-C(6)	103.58(13)
C(1)-N(5)-H(5A)	118.5(16)
C(1)-N(5)-H(5B)	115.9(15)
H(5A)-N(5)-H(5B)	122(2)
N(5)-C(1)-N(1)	118.31(14)
N(5)-C(1)-C(6)	124.20(14)
N(1)-C(1)-C(6)	117.50(14)
N(2)-C(2)-N(1)	129.15(15)
N(2)-C(2)-H(2)	116.0(12)
N(1)-C(2)-H(2)	114.8(12)

N(2)-C(3)-N(3)	126.71(14)
N(2)-C(3)-C(6)	127.60(14)
N(3)-C(3)-C(6)	105.68(13)
N(3)-C(4)-H(4A)	111.6(14)
N(3)-C(4)-H(4B)	108.6(13)
H(4A)-C(4)-H(4B)	108.2(19)
N(3)-C(4)-H(4C)	107.4(12)
H(4A)-C(4)-H(4C)	112.1(18)
H(4B)-C(4)-H(4C)	108.8(18)
N(4)-C(5)-N(3)	113.76(14)
N(4)-C(5)-H(5)	126.6(12)
N(3)-C(5)-H(5)	119.7(12)
N(4)-C(6)-C(3)	110.73(13)
N(4)-C(6)-C(1)	133.13(14)
C(3)-C(6)-C(1)	116.13(14)

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 9-methyladenine. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	21(1)	13(1)	16(1)	0(1)	3(1)	0(1)
N(2)	24(1)	12(1)	16(1)	2(1)	5(1)	2(1)
N(3)	22(1)	9(1)	17(1)	-1(1)	4(1)	-2(1)
N(4)	20(1)	13(1)	16(1)	-1(1)	2(1)	0(1)
N(5)	23(1)	10(1)	18(1)	1(1)	0(1)	0(1)
C(1)	20(1)	12(1)	14(1)	-1(1)	5(1)	0(1)
C(2)	21(1)	15(1)	15(1)	1(1)	3(1)	2(1)
C(3)	19(1)	11(1)	18(1)	-1(1)	6(1)	0(1)
C(4)	30(1)	9(1)	25(1)	1(1)	9(1)	-3(1)
C(5)	21(1)	12(1)	19(1)	-1(1)	3(1)	0(1)
C(6)	20(1)	12(1)	13(1)	0(1)	4(1)	0(1)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for9-methyladenine.

	x	y	z	U(eq)
H(2)	-1010(30)	9854(17)	1000(30)	21(5)
H(5)	5640(30)	10691(17)	8590(30)	24(5)
H(4A)	4800(30)	12490(20)	6850(30)	34(6)
H(5A)	2790(40)	7185(19)	5900(40)	38(6)
H(4B)	2510(30)	12513(19)	5760(30)	34(6)
H(5B)	1020(30)	6870(20)	4050(30)	43(6)
H(4C)	3850(30)	12300(17)	4620(30)	29(5)

Table 12.Torsion angles [°] for 9-methyladenine.

C(2)-N(1)-C(1)-N(5)	-178.64(15)
C(2)-N(1)-C(1)-C(6)	1.8(2)
C(3)-N(2)-C(2)-N(1)	-1.5(2)
C(1)-N(1)-C(2)-N(2)	0.0(3)
C(2)-N(2)-C(3)-N(3)	-177.87(15)
C(2)-N(2)-C(3)-C(6)	1.2(2)
C(5)-N(3)-C(3)-N(2)	178.58(15)
C(4)-N(3)-C(3)-N(2)	-0.1(3)
C(5)-N(3)-C(3)-C(6)	-0.69(17)
C(4)-N(3)-C(3)-C(6)	-179.41(15)
C(6)-N(4)-C(5)-N(3)	-0.18(18)
C(3)-N(3)-C(5)-N(4)	0.56(18)
C(4)-N(3)-C(5)-N(4)	179.24(15)
C(5)-N(4)-C(6)-C(3)	-0.28(18)
C(5)-N(4)-C(6)-C(1)	-179.14(17)
N(2)-C(3)-C(6)-N(4)	-178.64(14)
N(3)-C(3)-C(6)-N(4)	0.62(18)
N(2)-C(3)-C(6)-C(1)	0.4(2)
N(3)-C(3)-C(6)-C(1)	179.69(13)
N(5)-C(1)-C(6)-N(4)	-2.7(3)
N(1)-C(1)-C(6)-N(4)	176.82(15)
N(5)-C(1)-C(6)-C(3)	178.50(15)
N(1)-C(1)-C(6)-C(3)	-2.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 13. Crystal data and structure refinement for cocrystal.

Identification code	p21m	
Empirical formula	C12 H15 N7 O2	
Formula weight	289.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/m	
Unit cell dimensions	a = 8.2751(3) Å	α= 90°.
	b = 6.3547(2) Å	β= 106.818(2)°.
	c = 12.8257(4) Å	γ = 90°.
Volume	645.60(4) $Å^3$	
Z	2	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	0.108 mm^{-1}	
F(000)	304	
Crystal size	0.50 x 0.16 x 0.12 mm^3	
Theta range for data collection	3.32 to 33.14°.	
Index ranges	-12<=h<=12, -9<=k<=9, -16<=l<=19	
Reflections collected	10864	
Independent reflections	2603 [R(int) = 0.0227]	
Completeness to theta = 33.14°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9871 and 0.9478	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2603 / 0 / 166	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.1234	
R indices (all data)	R1 = 0.0457, wR2 = 0.1293	
Largest diff. peak and hole	0.652 and -0.281 $e.Å^{-3}$	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) forcocrystal. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3199(1)	2500	10225(1)	15(1)
O(2)	8915(1)	2500	11088(1)	18(1)
N(1)	6056(1)	2500	10623(1)	11(1)
N(2)	7424(1)	2500	9272(1)	13(1)
N(3)	7752(1)	2500	4710(1)	13(1)
N(4)	5392(1)	2500	5484(1)	15(1)
N(5)	2694(1)	2500	4082(1)	15(1)
N(6)	6328(1)	2500	2931(1)	13(1)
N(7)	2449(1)	2500	2234(1)	17(1)
C(1)	4463(1)	2500	9895(1)	11(1)
C(2)	7556(1)	2500	10369(1)	12(1)
C(3)	5872(1)	2500	8506(1)	13(1)
C(4)	4396(1)	2500	8765(1)	12(1)
C(5)	8983(1)	2500	8942(1)	18(1)
C(6)	2690(1)	2500	7951(1)	17(1)
C(7)	6067(1)	2500	4648(1)	12(1)
C(8)	3711(1)	2500	5110(1)	16(1)
C(9)	3424(1)	2500	3263(1)	12(1)
C(10)	5202(1)	2500	3546(1)	11(1)
C(11)	7829(1)	2500	3656(1)	14(1)
C(12)	9155(1)	2500	5701(1)	19(1)

Table 15. Bond lengths [Å] and angles [°] for cocrystal.

O(1)-C(1)	1.2363(11)
O(2)-C(2)	1.2313(12)
N(1)-C(2)	1.3716(12)
N(1)-C(1)	1.3779(12)
N(1)-H(1)	1.02(2)
N(2)-C(3)	1.3728(13)
N(2)-C(2)	1.3789(13)
N(2)-C(5)	1.4690(13)
N(3)-C(11)	1.3711(12)
N(3)-C(7)	1.3738(12)
N(3)-C(12)	1.4524(13)
N(4)-C(8)	1.3334(14)
N(4)-C(7)	1.3440(12)
N(5)-C(8)	1.3433(13)
N(5)-C(9)	1.3541(12)
N(6)-C(11)	1.3190(12)
N(6)-C(10)	1.3839(12)
N(7)-C(9)	1.3326(12)
N(7)-H(7A)	0.819(19)
N(7)-H(7B)	0.89(2)
C(1)-C(4)	1.4340(13)
C(3)-C(4)	1.3549(13)
C(3)-H(3)	0.954(19)
C(4)-C(6)	1.4934(14)
C(5)-H(5A)	0.976(16)
C(5)-H(5B)	0.99(2)
C(6)-H(6A)	0.991(13)
C(6)-H(6B)	1.04(2)
C(7)-C(10)	1.3882(12)
C(8)-H(8)	1.009(19)
C(9)-C(10)	1.4105(13)
C(11)-H(11)	0.996(15)
C(12)-H(12A)	0.953(14)
C(12)-H(12B)	0.97(2)

C(2)-N(1)-C(1)	126.35(8)
C(2)-N(1)-H(1)	113.7(12)
C(1)-N(1)-H(1)	119.9(12)
C(3)-N(2)-C(2)	120.71(8)
C(3)-N(2)-C(5)	120.81(9)
C(2)-N(2)-C(5)	118.48(9)
C(11)-N(3)-C(7)	106.24(8)
C(11)-N(3)-C(12)	127.53(9)
C(7)-N(3)-C(12)	126.24(9)
C(8)-N(4)-C(7)	110.15(9)
C(8)-N(5)-C(9)	117.90(9)
C(11)-N(6)-C(10)	104.47(8)
C(9)-N(7)-H(7A)	119.1(15)
C(9)-N(7)-H(7B)	116.3(12)
H(7A)-N(7)-H(7B)	124.5(18)
O(1)-C(1)-N(1)	120.38(9)
O(1)-C(1)-C(4)	123.85(9)
N(1)-C(1)-C(4)	115.76(8)
O(2)-C(2)-N(1)	121.00(9)
O(2)-C(2)-N(2)	123.33(9)
N(1)-C(2)-N(2)	115.67(9)
C(4)-C(3)-N(2)	123.25(9)
C(4)-C(3)-H(3)	122.5(12)
N(2)-C(3)-H(3)	114.3(12)
C(3)-C(4)-C(1)	118.25(9)
C(3)-C(4)-C(6)	124.47(9)
C(1)-C(4)-C(6)	117.28(8)
N(2)-C(5)-H(5A)	110.7(9)
N(2)-C(5)-H(5B)	110.6(15)
H(5A)-C(5)-H(5B)	108.0(12)
C(4)-C(6)-H(6A)	109.9(8)
C(4)-C(6)-H(6B)	110.3(14)
H(6A)-C(6)-H(6B)	109.4(11)
N(4)-C(7)-N(3)	127.15(9)
N(4)-C(7)-C(10)	126.97(9)
N(3)-C(7)-C(10)	105.88(8)
N(4)-C(8)-N(5)	130.15(9)

N(4)-C(8)-H(8)	116.0(12)
N(5)-C(8)-H(8)	113.9(12)
N(7)-C(9)-N(5)	119.35(9)
N(7)-C(9)-C(10)	122.81(9)
N(5)-C(9)-C(10)	117.84(9)
N(6)-C(10)-C(7)	110.32(8)
N(6)-C(10)-C(9)	132.70(9)
C(7)-C(10)-C(9)	116.98(9)
N(6)-C(11)-N(3)	113.10(8)
N(6)-C(11)-H(11)	124.6(9)
N(3)-C(11)-H(11)	122.3(9)
N(3)-C(12)-H(12A)	108.7(9)
N(3)-C(12)-H(12B)	109.9(13)
H(12A)-C(12)-H(12B)	112.7(11)

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cocrystal. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	10(1)	24(1)	13(1)	0	5(1)	0
O(2)	9(1)	24(1)	18(1)	0	0(1)	0
N(1)	8(1)	16(1)	10(1)	0	2(1)	0
N(2)	10(1)	16(1)	15(1)	0	5(1)	0
N(3)	10(1)	18(1)	11(1)	0	1(1)	0
N(4)	13(1)	23(1)	10(1)	0	3(1)	0
N(5)	12(1)	20(1)	12(1)	0	4(1)	0
N(6)	10(1)	18(1)	12(1)	0	4(1)	0
N(7)	9(1)	31(1)	10(1)	0	2(1)	0
C(1)	9(1)	13(1)	10(1)	0	2(1)	0
C(2)	9(1)	13(1)	14(1)	0	2(1)	0
C(3)	12(1)	16(1)	11(1)	0	4(1)	0
C(4)	10(1)	15(1)	9(1)	0	2(1)	0
C(5)	12(1)	22(1)	23(1)	0	9(1)	0
C(6)	12(1)	26(1)	10(1)	0	1(1)	0
C(7)	10(1)	15(1)	10(1)	0	2(1)	0
C(8)	14(1)	25(1)	12(1)	0	5(1)	0
C(9)	10(1)	14(1)	12(1)	0	3(1)	0
C(10)	9(1)	14(1)	10(1)	0	2(1)	0
C(11)	10(1)	18(1)	13(1)	0	4(1)	0
C(12)	12(1)	27(1)	15(1)	0	-3(1)	0

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) forcocrystal.

	x	y	z	U(eq)
H(1)	6200(30)	2500	11443(19)	35(5)
H(3)	5920(30)	2500	7772(16)	26(4)
H(8)	3090(30)	2500	5680(17)	32(5)
H(11)	8921(19)	2500	3474(13)	12(3)
H(5A)	9660(20)	3750(20)	9219(13)	48(4)
H(6A)	2050(17)	3760(20)	8056(11)	30(3)
H(7A)	2890(30)	2500	1740(16)	27(5)
H(12A)	9043(18)	3680(20)	6132(11)	38(4)
H(5B)	8720(30)	2500	8139(19)	48(7)
H(6B)	2800(30)	2500	7160(20)	52(7)
H(7B)	1340(30)	2500	2136(16)	27(5)
H(12B)	10220(30)	2500	5521(17)	36(5)

Table 18. Torsion angles [°] for cocrystal.

C(2)-N(1)-C(1)-O(1)	180.0
C(2)-N(1)-C(1)-C(4)	0.0
C(1)-N(1)-C(2)-O(2)	180.0
C(1)-N(1)-C(2)-N(2)	0.0
C(3)-N(2)-C(2)-O(2)	180.0
C(5)-N(2)-C(2)-O(2)	0.0
C(3)-N(2)-C(2)-N(1)	0.0
C(5)-N(2)-C(2)-N(1)	180.0
C(2)-N(2)-C(3)-C(4)	0.0
C(5)-N(2)-C(3)-C(4)	180.0
N(2)-C(3)-C(4)-C(1)	0.0
N(2)-C(3)-C(4)-C(6)	180.0
O(1)-C(1)-C(4)-C(3)	180.0
N(1)-C(1)-C(4)-C(3)	0.0
O(1)-C(1)-C(4)-C(6)	0.0
N(1)-C(1)-C(4)-C(6)	180.0
C(8)-N(4)-C(7)-N(3)	180.0
C(8)-N(4)-C(7)-C(10)	0.0
C(11)-N(3)-C(7)-N(4)	180.0
C(12)-N(3)-C(7)-N(4)	0.0
C(11)-N(3)-C(7)-C(10)	0.0
C(12)-N(3)-C(7)-C(10)	180.0
C(7)-N(4)-C(8)-N(5)	0.0
C(9)-N(5)-C(8)-N(4)	0.0
C(8)-N(5)-C(9)-N(7)	180.0
C(8)-N(5)-C(9)-C(10)	0.0
C(11)-N(6)-C(10)-C(7)	0.0
C(11)-N(6)-C(10)-C(9)	180.0
N(4)-C(7)-C(10)-N(6)	180.0
N(3)-C(7)-C(10)-N(6)	0.0
N(4)-C(7)-C(10)-C(9)	0.0
N(3)-C(7)-C(10)-C(9)	180.0
N(7)-C(9)-C(10)-N(6)	0.0
N(5)-C(9)-C(10)-N(6)	180.0
N(7)-C(9)-C(10)-C(7)	180.0

N(5)-C(9)-C(10)-C(7)	0.0
C(10)-N(6)-C(11)-N(3)	0.0
C(7)-N(3)-C(11)-N(6)	0.0
C(12)-N(3)-C(11)-N(6)	180.0

Symmetry transformations used to generate equivalent atoms: