Table 1. Crystal data and structure refinement for 1.

Empirical formula	C20 H14 N4
Formula weight	310.35
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 7.3545(19) Å α= 90°. b = 9.7061(18) Å β= 90°. c = 21.074(4) Å γ = 90°.
Volume	1504.3(6) $Å^3$
Z	4
Density (calculated)	1.370 Mg/m^3
Absorption coefficient	0.084 mm^{-1}
F(000)	648
Crystal size	0.2 x 0.4 x 0.3 mm^3
Theta range for data collection	2.93 to 23.50°.
Index ranges	0<=h<=8, 0<=k<=10, -23<=l<=0
Reflections collected	1121
Independent reflections	1121 [R(int) = 0.0000]
Completeness to theta = 23.50°	85.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1121 / 0 / 217
Goodness-of-fit on F^2	0.998
Final R indices [I>2sigma(I)]	R1 = 0.0535, wR2 = 0.1244
R indices (all data)	R1 = 0.0865, wR2 = 0.1546
Absolute structure parameter	-7(8)
Largest diff. peak and hole	0.169 and -0.241 $e.Å^{-3}$

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

	x	y	z	U(eq)
N(2)	2558(7)	5895(6)	8465(2)	49(1)
N(1)	5014(6)	7215(6)	8018(2)	47(1)
N(4)	7297(7)	3322(6)	9444(3)	51(1)
N(3)	7664(7)	5481(6)	9993(2)	46(1)
C(7)	3319(7)	6628(7)	8004(3)	41(2)
C(12)	7444(10)	1338(8)	10137(4)	67(2)
C(14)	7547(7)	4054(7)	9973(3)	40(2)
C(17)	7372(9)	8435(7)	8560(3)	55(2)
C(3)	2528(9)	6968(7)	7413(3)	51(2)
C(16)	6264(7)	7297(7)	8536(3)	41(2)
C(13)	7259(9)	1958(7)	9547(4)	58(2)
C(20)	7600(8)	6434(7)	9488(3)	44(2)
C(15)	6351(7)	6283(7)	9001(3)	42(2)
C(10)	7790(8)	3544(8)	10597(3)	51(2)
C(11)	7720(9)	2136(9)	10669(4)	62(2)
C(8)	8016(8)	5823(9)	10618(3)	56(2)
C(2)	3796(10)	7774(9)	7075(4)	66(2)
C(5)	-17(10)	5698(9)	7767(4)	62(2)
C(9)	8086(9)	4716(10)	10985(3)	61(2)
C(6)	876(8)	5446(8)	8321(4)	61(2)
C(19)	8742(8)	7549(8)	9511(4)	58(2)
C(4)	792(10)	6473(9)	7297(4)	65(2)
C(18)	8617(9)	8555(8)	9037(4)	62(2)
C(1)	5281(10)	7901(9)	7446(4)	60(2)

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

N(2)-C(7)	1.328(8)
N(2)-C(6)	1.347(8)
N(1)-C(7)	1.371(7)
N(1)-C(1)	1.392(9)
N(1)-C(16)	1.429(8)
N(4)-C(14)	1.333(8)
N(4)-C(13)	1.342(9)
N(3)-C(8)	1.384(9)
N(3)-C(14)	1.388(9)
N(3)-C(20)	1.410(8)
C(7)-C(3)	1.413(8)
C(12)-C(11)	1.378(11)
C(12)-C(13)	1.388(10)
C(14)-C(10)	1.416(10)
C(17)-C(18)	1.364(10)
C(17)-C(16)	1.374(9)
C(3)-C(4)	1.385(10)
C(3)-C(2)	1.411(10)
C(16)-C(15)	1.392(9)
C(20)-C(19)	1.371(9)
C(20)-C(15)	1.385(8)
C(10)-C(11)	1.376(11)
C(10)-C(9)	1.418(11)

C(8)-C(9)	1.325(11)
C(2)-C(1)	1.348(10)
C(5)-C(6)	1.361(10)
C(5)-C(4)	1.378(11)
C(19)-C(18)	1.400(10)
C(7)-N(2)-C(6)	113.3(5)
C(7)-N(1)-C(1)	108.0(5)
C(7)-N(1)-C(16)	128.7(5)
C(1)-N(1)-C(16)	123.0(6)
C(14)-N(4)-C(13)	113.2(6)
C(8)-N(3)-C(14)	106.3(6)
C(8)-N(3)-C(20)	124.5(6)
C(14)-N(3)-C(20)	129.0(5)
N(2)-C(7)-N(1)	126.1(6)
N(2)-C(7)-C(3)	126.6(6)
N(1)-C(7)-C(3)	107.3(6)
C(11)-C(12)-C(13)	120.0(7)
N(4)-C(14)-N(3)	124.5(6)
N(4)-C(14)-C(10)	127.3(6)
N(3)-C(14)-C(10)	108.2(5)
C(18)-C(17)-C(16)	119.6(7)
C(4)-C(3)-C(2)	135.5(7)
C(4)-C(3)-C(7)	117.0(6)
C(2)-C(3)-C(7)	107.6(6)
C(17)-C(16)-C(15)	121.0(6)
C(17)-C(16)-N(1)	117.1(6)
C(15)-C(16)-N(1)	121.9(6)
N(4)-C(13)-C(12)	124.8(7)
C(19)-C(20)-C(15)	121.0(6)
C(19)-C(20)-N(3)	118.1(6)
C(15)-C(20)-N(3)	120.8(5)
C(20)-C(15)-C(16)	118.6(6)
C(11)-C(10)-C(14)	116.5(7)
C(11)-C(10)-C(9)	137.5(8)
C(14)-C(10)-C(9)	106.0(7)
C(10)-C(11)-C(12)	118.2(7)
C(9)-C(8)-N(3)	111.6(7)
C(1)-C(2)-C(3)	107.1(7)
C(6)-C(5)-C(4)	120.4(7)
C(8)-C(9)-C(10)	107.9(6)
N(2)-C(6)-C(5)	125.3(7)
C(20)-C(19)-C(18)	119.0(6)
C(5)-C(4)-C(3)	117.4(7)
C(17)-C(18)-C(19)	120.7(7)
C(2)-C(1)-N(1)	110.1(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. 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(2)	47(3)	51(3)	48(3)	1(3)	4(3)	0(3)
N(1)	51(3)	46(4)	44(3)	5(3)	1(2)	-3(3)

N(4)	54(3)	43(3)	55(3)	-5(3)	-9(3)	1(3)
N(3)	52(3)	45(3)	42(3)	-4(3)	-12(3)	-1(3)
C(7)	47(3)	38(4)	39(4)	-5(3)	3(3)	3(3)
C(12)	68(5)	49(5)	83(6)	20(4)	-14(4)	6(4)
C(14)	41(3)	49(4)	31(3)	-2(3)	-11(3)	8(3)
C(17)	59(4)	40(4)	65(4)	5(4)	2(3)	-6(4)
C(3)	68(4)	46(4)	39(4)	0(3)	-1(3)	13(4)
C(16)	37(3)	44(4)	42(4)	4(4)	6(2)	4(3)
C(13)	64(4)	45(5)	64(5)	-2(4)	-12(4)	2(3)
C(20)	42(3)	45(4)	43(4)	-2(3)	-2(3)	1(3)
C(15)	39(3)	35(4)	52(4)	-5(3)	6(3)	-2(3)
C(10)	38(3)	66(5)	49(4)	2(4)	-3(3)	0(3)
C(11)	61(4)	68(5)	56(5)	7(4)	-7(4)	1(4)
C(8)	60(4)	56(5)	52(4)	-11(4)	-14(3)	1(3)
C(2)	90(6)	65(6)	42(4)	13(4)	1(4)	7(4)
C(5)	51(4)	66(6)	69(5)	-8(5)	-11(4)	4(4)
C(9)	57(4)	84(6)	42(4)	-5(5)	-13(3)	3(4)
C(6)	43(4)	57(5)	81(5)	-2(5)	3(3)	-3(3)
C(19)	50(4)	53(5)	69(5)	-7(4)	-9(3)	-14(3)
C(4)	64(5)	68(6)	61(5)	-11(5)	-19(4)	21(4)
C(18)	56(4)	46(5)	83(6)	5(4)	-7(4)	-11(4)
C(1)	77(5)	68(6)	37(4)	10(4)	10(3)	-8(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H(12)	7382	385	10174	80
H(17)	7275	9120	8254	65
H(13)	7097	1386	9198	69
H(15)	5587	5520	8986	50
H(11)	7856	1734	11067	74
H(8)	8183	6719	10763	67
H(2)	3638	8147	6673	79
H(5)	-1178	5344	7705	74
H(9)	8292	4708	11421	73
H(6)	274	4920	8625	73
H(19)	9588	7636	9836	69
H(4)	195	6658	6918	77
H(18)	9389	9313	9047	74
H(1)	6330	8378	7335	72

Table 1. Crystal data and structure refinement for 4.

Empirical formula	C26 H18 N4	
Formula weight	386.44	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.6984(19) Å	α= 90°.
	b = 8.1737(17) Å	β= 101.537(5)°.
	c = 12.176(3) Å	γ = 90°.
Volume	945.7(3) $Å^3$	
Z	2	
Density (calculated)	1.357 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	404	
Crystal size	0.10x 0.20 x 0.20 mm^3	
Theta range for data collection	2.14 to 23.27°.	
Index ranges	-10<=h<=7, -8<=k<=9, -13<=l<=11	
Reflections collected	4595	
Independent reflections	1353 [R(int) = 0.0313]	
Completeness to theta = 23.27°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1353 / 0 / 136	
Goodness-of-fit on F^2	0.877	
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.1208	
R indices (all data)	R1 = 0.0651, wR2 = 0.1317	
Largest diff. peak and hole	0.179 and -0.161 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(11)	3363(2)	5576(3)	-1041(2)	60(1)
N(1)	2968(2)	4945(2)	-4090(1)	54(1)
C(7)	1890(2)	5889(3)	-4685(2)	53(1)
C(12)	2789(2)	5562(3)	-2165(2)	62(1)
C(10)	4694(2)	4980(2)	-607(2)	46(1)
N(2)	1187(2)	7041(2)	-4254(1)	59(1)
C(13)	3536(2)	4963(2)	-2922(2)	48(1)
C(9)	5416(2)	4354(3)	-1386(2)	70(1)
C(8)	4860(2)	4336(3)	-2516(2)	68(1)
C(1)	3401(2)	3915(3)	-4850(2)	68(1)
C(6)	1680(2)	5427(3)	-5821(2)	63(1)
C(5)	181(2)	7763(3)	-5003(2)	70(1)
C(2)	2659(3)	4161(3)	-5889(2)	75(1)
C(3)	641(3)	6243(4)	-6555(2)	77(1)
C(4)	-121(3)	7408(3)	-6136(2)	78(1)

Table 3. Bond lengths [Å] and angles [°] for 4.

C(11)-C(12)	1.370(3)
C(11)-C(10)	1.382(3)
N(1)-C(1)	1.378(3)
N(1)-C(7)	1.381(2)
N(1)-C(13)	1.419(2)
C(7)-N(2)	1.331(3)
C(7)-C(6)	1.409(3)
C(12)-C(13)	1.372(3)
C(10)-C(9)	1.385(3)
C(10)-C(10)#1	1.480(4)
N(2)-C(5)	1.333(3)
C(13)-C(8)	1.378(3)
C(9)-C(8)	1.373(3)
C(1)-C(2)	1.339(3)
C(6)-C(2)	1.418(3)
C(6)-C(3)	1.378(3)
C(5)-C(4)	1.383(4)
C(3)-C(4)	1.366(4)
C(12)-C(11)-C(10)	122.7(2)
C(1)-N(1)-C(7)	106.79(18)
C(1)-N(1)-C(13)	124.74(18)
C(7)-N(1)-C(13)	128.46(18)
N(2)-C(7)-N(1)	125.56(18)
N(2)-C(7)-C(6)	126.3(2)
N(1)-C(7)-C(6)	108.1(2)
C(11)-C(12)-C(13)	120.68(19)
C(9)-C(10)-C(11)	115.49(19)
C(9)-C(10)-C(10)#1	122.4(2)
C(11)-C(10)-C(10)#1	122.1(2)
C(7)-N(2)-C(5)	114.0(2)
C(8)-C(13)-N(1)	120.22(19)

C(8)-C(13)-C(12)	118.09(19)
N(1)-C(13)-C(12)	121.68(18)
C(10)-C(9)-C(8)	122.6(2)
C(13)-C(8)-C(9)	120.4(2)
C(2)-C(1)-N(1)	111.4(2)
C(7)-C(6)-C(2)	106.6(2)
C(7)-C(6)-C(3)	116.8(3)
C(2)-C(6)-C(3)	136.6(2)
N(2)-C(5)-C(4)	124.8(3)
C(1)-C(2)-C(6)	107.1(2)
C(4)-C(3)-C(6)	118.4(2)
C(3)-C(4)-C(5)	119.8(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 4. 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}
C(11)	57(1)	76(2)	47(1)	-5(1)	7(1)	19(1)
N(1)	56(1)	62(1)	41(1)	-1(1)	6(1)	1(1)
C(7)	58(1)	51(1)	48(1)	6(1)	4(1)	-12(1)
C(12)	53(1)	81(2)	49(1)	-5(1)	2(1)	17(1)
C(10)	47(1)	47(1)	45(1)	4(1)	8(1)	4(1)
N(2)	60(1)	51(1)	60(1)	11(1)	0(1)	-4(1)
C(13)	50(1)	52(1)	42(1)	2(1)	8(1)	1(1)
C(9)	57(1)	101(2)	50(2)	4(1)	9(1)	29(1)
C(8)	63(1)	98(2)	45(1)	1(1)	14(1)	23(1)
C(1)	73(1)	80(2)	52(2)	-11(1)	13(1)	3(1)
C(6)	71(2)	69(2)	44(1)	7(1)	0(1)	-23(1)
C(5)	66(1)	56(2)	79(2)	20(1)	-5(1)	-8(1)
C(2)	86(2)	91(2)	46(2)	-12(1)	11(1)	-12(2)
C(3)	89(2)	81(2)	51(2)	12(1)	-7(1)	-28(2)
C(4)	77(2)	72(2)	72(2)	31(2)	-19(1)	-20(2)

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

	x	y	z	U(eq)
H(11)	2835	6004	-550	72
H(12)	1884	5964	-2417	75
H(9)	6313	3928	-1135	83
H(8)	5379	3899	-3010	82
H(1)	4118	3148	-4666	82
H(5)	-356	8564	-4745	83
H(2)	2765	3605	-6533	90
H(3)	462	6005	-7318	92
H(4)	-841	7962	-6611	94