Table 1. Crystal data and structure refinement for ham1.

Identification code	shelx	
Empirical formula	C12 H17 N O2	
Formula weight	207.26	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 18.380(4) Å	α= 90 °.
	b = 10.170(2) Å	β= 90 °.
	c = 6.0800(12) Å	γ = 90 °.
Volume	1136.5(4) $Å^3$	
Z	4	
Density (calculated)	1.211 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	448	
Crystal size	0.200 x 0.200 x 0.200 mm^3	
Theta range for data collection	2.216 to 23.248 °.	
Index ranges	-20<=h<=20, -11<=k<=10, -6<=l<=5	
Reflections collected	2430	
Independent reflections	1348 [R(int) = 0.0988]	
Completeness to theta = 23.248 °	95.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9915 and 0.991	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1348 / 91 / 138	
Goodness-of-fit on F^2	1.166	
Final R indices [I>2sigma(I)]	R1 = 0.0851, wR2 = 0.1541	
R indices (all data)	R1 = 0.1503, wR2 = 0.1861	
Absolute structure parameter	-1.7(10)	
Extinction coefficient	0.045(8)	
Largest diff. peak and hole	0.247 and -0.251 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ham1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4018(5)	5783(10)	3850(20)	41(2)
C(2)	4220(6)	6796(9)	5326(19)	43(2)
C(3)	4771(6)	7673(11)	4790(20)	47(2)
C(4)	4999(7)	8713(13)	6390(20)	65(3)
C(5)	5106(6)	7550(11)	2770(20)	49(2)
C(6)	4918(6)	6592(11)	1310(20)	49(2)
C(7)	4363(6)	5713(10)	1840(20)	46(2)
C(8)	3449(6)	4793(10)	4400(18)	39(2)
C(9)	2442(6)	4117(11)	6920(20)	48(2)
C(10)	2828(6)	2914(10)	7910(20)	52(3)
C(11)	2029(6)	4849(11)	8720(20)	58(3)
C(12)	1888(6)	3690(10)	5190(20)	49(2)
N(1)	2990(5)	5038(8)	6040(15)	39(2)
O(1)	3417(4)	3784(7)	3258(13)	55(2)
O(2)	2123(4)	2717(8)	3703(17)	65(3)

Table 3. Bond lengths [Å] and angles [°] for ham1.

C(1)-C(7)	1.376(16)
C(1)-C(2)	1.417(15)
C(1)-C(8)	1.489(13)
C(2)-C(3)	1.388(15)
C(2)-H(2)	0.9300
C(3)-C(5)	1.380(14)
C(3)-C(4)	1.495(16)
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-C(6)	1.364(17)
C(5)-H(5)	0.9300
C(6)-C(7)	1.394(14)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-O(1)	1.240(12)
C(8)-N(1)	1.330(13)
C(9)-N(1)	1.476(14)
C(9)-C(11)	1.523(16)
C(9)-C(12)	1.527(15)
C(9)-C(10)	1.536(15)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-O(2)	1.408(14)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
N(1)-H(1)	0.8600
O(2)-H(2A)	0.8200
C(7)-C(1)-C(2)	118.6(10)

C(7)-C(1)-C(8)	119.3(10)
C(2)-C(1)-C(8)	122.2(11)
C(3)-C(2)-C(1)	120.6(11)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
C(5)-C(3)-C(2)	118.4(11)
C(5)-C(3)-C(4)	121.1(11)
C(2)-C(3)-C(4)	120.4(11)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(3)	122.1(11)
C(6)-C(5)-H(5)	118.9
C(3)-C(5)-H(5)	118.9
C(5)-C(6)-C(7)	119.4(12)
C(5)-C(6)-H(6)	120.3
C(7)-C(6)-H(6)	120.3
C(1)-C(7)-C(6)	120.7(12)
C(1)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
O(1)-C(8)-N(1)	123.0(10)
O(1)-C(8)-C(1)	117.8(10)
N(1)-C(8)-C(1)	119.2(9)
N(1)-C(9)-C(11)	106.9(9)
N(1)-C(9)-C(12)	112.7(10)
C(11)-C(9)-C(12)	107.5(9)
N(1)-C(9)-C(10)	109.4(9)
C(11)-C(9)-C(10)	109.9(11)
C(12)-C(9)-C(10)	110.5(9)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5

H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(2)-C(12)-C(9)	116.0(9)
O(2)-C(12)-H(12A)	108.3
C(9)-C(12)-H(12A)	108.3
O(2)-C(12)-H(12B)	108.3
C(9)-C(12)-H(12B)	108.3
H(12A)-C(12)-H(12B)	107.4
C(8)-N(1)-C(9)	125.9(9)
C(8)-N(1)-H(1)	117.0
C(9)-N(1)-H(1)	117.0
C(12)-O(2)-H(2A)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ham1. 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(1)	43(3)	32(3)	47(3)	1(3)	4(3)	4(3)
C(2)	46(3)	35(3)	49(3)	1(3)	4(3)	1(3)
C(3)	48(3)	39(3)	55(3)	1(3)	5(3)	0(3)
C(4)	70(6)	56(6)	67(6)	-6(5)	0(6)	-18(5)
C(5)	48(4)	41(3)	57(4)	4(3)	8(3)	3(3)
C(6)	48(4)	43(3)	56(4)	2(3)	11(3)	6(3)
C(7)	47(3)	38(3)	52(4)	0(3)	9(3)	6(3)
C(8)	42(4)	30(4)	45(4)	1(4)	0(4)	4(3)
C(9)	49(5)	40(4)	54(5)	2(4)	1(4)	-4(4)
C(10)	64(6)	38(5)	54(6)	3(5)	-7(5)	-8(4)
C(11)	63(6)	53(5)	59(6)	-3(5)	12(5)	-8(5)
C(12)	49(5)	43(5)	56(5)	4(4)	0(4)	-1(4)
N(1)	47(5)	29(5)	42(6)	1(4)	13(5)	-1(4)
O(1)	68(5)	45(5)	52(6)	-23(5)	4(5)	-13(4)
O(2)	63(6)	59(5)	72(7)	-14(5)	-14(5)	-19(5)

Table 5. Hydrogen bonds for ham1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10B)...O(1)	0.96	2.58	3.154(15)	118.3
N(1)-H(1)...O(2)#1	0.86	2.33	3.176(12)	168.0
O(2)-H(2A)...O(1)	0.82	1.86	2.628(11)	156.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y+1/2,z+1/2