Table 1. Crystal data and structure refinement for 2209.

Identification code	2209	
Empirical formula	C21 H23 Br2 N O2	
Formula weight	481.22	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.669(5) Å	α= 94.398(10)°.
	b = 10.054(5) Å	β= 97.815(10)°.
	c = 11.307(6) Å	γ = 110.743(9)°.
Volume	1009.0(9) $Å^3$	
Z	2	
Density (calculated)	1.584 Mg/m^3	
Absorption coefficient	4.032 mm^{-1}	
F(000)	484	
Crystal size	0.30 x 0.48 x 0.56 mm^3	
Theta range for data collection	1.83 to 27.50°.	
Index ranges	-12<=h<=12, -13<=k<=13, -14<=l<=14	
Reflections collected	13167	
Independent reflections	4628 [R(int) = 0.0193]	
Completeness to theta = 27.50°	99.9 %	
Absorption correction	Sadabs, (Sheldrick 2001)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4628 / 0 / 327	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0256, wR2 = 0.0631	
R indices (all data)	R1 = 0.0343, wR2 = 0.0661	
Largest diff. peak and hole	0.324 and -0.477 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2209. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	2556(1)	3453(1)	4028(1)	49(1)
Br(2)	1761(1)	-395(1)	6168(1)	46(1)
O(1)	7419(2)	1518(2)	8645(2)	60(1)
O(2)	9227(2)	1382(2)	7675(1)	45(1)
N(1)	6647(2)	3248(2)	7028(2)	33(1)
C(1)	10380(2)	4579(3)	6479(2)	52(1)
C(2)	11636(3)	5808(4)	6709(4)	81(1)
C(3)	11947(3)	6707(3)	7728(4)	87(1)
C(4)	10997(4)	6411(3)	8550(3)	86(1)
C(5)	9695(3)	5169(3)	8323(2)	61(1)
C(6)	9390(2)	4260(2)	7286(2)	35(1)
C(7)	7990(2)	2905(2)	7005(2)	30(1)
C(8)	8144(2)	1856(2)	7872(2)	34(1)
C(9)	9590(3)	500(3)	8526(3)	57(1)
C(10)	5249(2)	2178(2)	6338(2)	28(1)
C(11)	5285(2)	2238(2)	4995(2)	33(1)
C(12)	3823(2)	1280(2)	4206(2)	35(1)
C(13)	2486(2)	1592(2)	4532(2)	34(1)
C(14)	2439(2)	1644(2)	5861(2)	32(1)
C(15)	3930(2)	2557(2)	6675(2)	29(1)
C(16)	3796(2)	2605(2)	7996(2)	36(1)
C(17)	4096(3)	1653(3)	8719(2)	52(1)
C(18)	3929(3)	1749(4)	9924(2)	71(1)
C(19)	3471(3)	2772(4)	10406(3)	77(1)
C(20)	3170(4)	3710(4)	9709(3)	75(1)
C(21)	3336(3)	3639(3)	8510(2)	52(1)

Table 3. Bond lengths [Å] and angles [°] for 2209.

Br(1)-C(13)	1.978(2)
Br(2)-C(14)	1.9920(19)
O(1)-C(8)	1.188(2)
O(2)-C(8)	1.332(2)
O(2)-C(9)	1.447(3)
N(1)-C(7)	1.460(2)
N(1)-C(10)	1.465(2)
C(1)-C(2)	1.368(4)
C(1)-C(6)	1.384(3)
C(2)-C(3)	1.337(5)
C(3)-C(4)	1.370(5)
C(4)-C(5)	1.400(4)
C(5)-C(6)	1.359(3)
C(6)-C(7)	1.516(2)
C(7)-C(8)	1.525(2)
C(10)-C(11)	1.529(3)
C(10)-C(15)	1.540(2)
C(11)-C(12)	1.511(3)
C(12)-C(13)	1.519(3)
C(13)-C(14)	1.507(3)
C(14)-C(15)	1.530(2)
C(15)-C(16)	1.515(3)
C(16)-C(21)	1.386(3)
C(16)-C(17)	1.386(3)
C(17)-C(18)	1.393(3)
C(18)-C(19)	1.362(5)
C(19)-C(20)	1.357(5)
C(20)-C(21)	1.386(4)
C(8)-O(2)-C(9)	116.38(17)
C(7)-N(1)-C(10)	115.58(14)
C(2)-C(1)-C(6)	120.5(3)
C(3)-C(2)-C(1)	120.7(3)
C(2)-C(3)-C(4)	120.2(3)

C(3)-C(4)-C(5)	120.0(3)
C(6)-C(5)-C(4)	119.4(3)
C(5)-C(6)-C(1)	119.2(2)
C(5)-C(6)-C(7)	121.05(19)
C(1)-C(6)-C(7)	119.76(19)
N(1)-C(7)-C(6)	110.58(15)
N(1)-C(7)-C(8)	113.46(14)
C(6)-C(7)-C(8)	109.03(14)
O(1)-C(8)-O(2)	123.73(18)
O(1)-C(8)-C(7)	124.95(17)
O(2)-C(8)-C(7)	111.31(15)
N(1)-C(10)-C(11)	108.70(14)
N(1)-C(10)-C(15)	108.12(14)
C(11)-C(10)-C(15)	109.85(14)
C(12)-C(11)-C(10)	112.77(15)
C(11)-C(12)-C(13)	112.42(15)
C(14)-C(13)-C(12)	112.80(15)
C(14)-C(13)-Br(1)	108.86(12)
C(12)-C(13)-Br(1)	109.38(13)
C(13)-C(14)-C(15)	114.43(15)
C(13)-C(14)-Br(2)	105.33(12)
C(15)-C(14)-Br(2)	111.44(11)
C(16)-C(15)-C(14)	111.85(14)
C(16)-C(15)-C(10)	115.72(14)
C(14)-C(15)-C(10)	112.15(14)
C(21)-C(16)-C(17)	118.0(2)
C(21)-C(16)-C(15)	118.78(18)
C(17)-C(16)-C(15)	123.24(18)
C(16)-C(17)-C(18)	120.1(3)
C(19)-C(18)-C(17)	120.8(3)
C(20)-C(19)-C(18)	119.8(3)
C(19)-C(20)-C(21)	120.4(3)
C(20)-C(21)-C(16)	121.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 2209. 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}
Br(1)	61(1)	51(1)	44(1)	14(1)	4(1)	33(1)
Br(2)	34(1)	36(1)	66(1)	15(1)	15(1)	6(1)
O(1)	57(1)	83(1)	61(1)	39(1)	29(1)	39(1)
O(2)	43(1)	56(1)	49(1)	20(1)	12(1)	28(1)
N(1)	24(1)	37(1)	37(1)	1(1)	3(1)	10(1)
C(1)	38(1)	62(1)	62(2)	29(1)	19(1)	16(1)
C(2)	42(1)	76(2)	120(3)	52(2)	23(2)	6(1)
C(3)	42(1)	54(2)	141(3)	47(2)	-12(2)	-8(1)
C(4)	87(2)	54(2)	83(2)	-7(2)	-29(2)	5(2)
C(5)	58(2)	52(1)	53(1)	-2(1)	3(1)	2(1)
C(6)	25(1)	38(1)	38(1)	12(1)	2(1)	9(1)
C(7)	23(1)	36(1)	30(1)	3(1)	4(1)	10(1)
C(8)	26(1)	36(1)	36(1)	4(1)	3(1)	8(1)
C(9)	55(2)	66(2)	63(2)	27(1)	10(1)	36(1)
C(10)	22(1)	27(1)	35(1)	6(1)	5(1)	8(1)
C(11)	26(1)	37(1)	36(1)	6(1)	10(1)	12(1)
C(12)	34(1)	38(1)	34(1)	2(1)	5(1)	14(1)
C(13)	27(1)	33(1)	39(1)	3(1)	0(1)	10(1)
C(14)	24(1)	31(1)	43(1)	7(1)	7(1)	12(1)
C(15)	26(1)	29(1)	34(1)	8(1)	8(1)	12(1)
C(16)	26(1)	46(1)	35(1)	8(1)	8(1)	12(1)
C(17)	47(1)	71(2)	48(1)	25(1)	17(1)	27(1)
C(18)	55(2)	112(2)	50(1)	36(2)	17(1)	27(2)
C(19)	65(2)	115(3)	38(1)	6(2)	19(1)	15(2)
C(20)	77(2)	93(2)	55(2)	-14(2)	22(1)	32(2)
C(21)	53(1)	59(1)	46(1)	-1(1)	12(1)	24(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for 2209.

	x	y	z	U(eq)
H(1A)	6570(30)	3270(30)	7730(20)	52(7)
H(1)	10120(30)	4020(30)	5710(30)	73(9)
H(2)	12340(40)	6060(40)	6160(30)	95(10)
H(3)	12960(40)	7590(40)	7960(30)	110(11)
H(4)	10990(40)	6940(30)	9150(30)	86(10)
H(5)	9030(30)	5000(30)	8800(20)	54(7)
H(7)	7960(19)	2438(18)	6207(16)	22(4)
H(9A)	10520(40)	470(30)	8410(30)	94(10)
H(9B)	9850(40)	1020(40)	9330(40)	111(13)
H(9C)	8830(40)	-250(40)	8590(30)	94(11)
H(11A)	5510(20)	3170(20)	4870(18)	36(5)
H(11B)	6050(20)	1940(20)	4779(19)	42(5)
H(12A)	3850(20)	1360(20)	3400(20)	46(6)
H(12B)	3640(20)	310(20)	4329(18)	39(5)
H(13)	1630(20)	950(20)	4066(18)	34(5)
H(14)	1660(20)	1920(20)	6065(18)	38(5)
H(15)	4100(20)	3500(20)	6487(17)	36(5)
H(10)	5110(20)	1207(19)	6505(15)	25(4)
H(17)	4420(30)	980(30)	8380(20)	57(7)
H(18)	4200(30)	1190(30)	10390(30)	80(9)
H(19)	3390(40)	2800(30)	11220(30)	95(10)
H(20)	2970(40)	4410(40)	9990(30)	93(11)
H(21)	3150(30)	4300(30)	8040(20)	55(7)

Table 6. Hydrogen bonds for 2209 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(1)	0.81(2)	2.43(2)	2.822(2)	110.7(19)

Symmetry transformations used to generate equivalent atoms: