Crystal Packing of **1**,

View along [0 0 1]; thermal ellipsoids are drawn on the 50% probability level

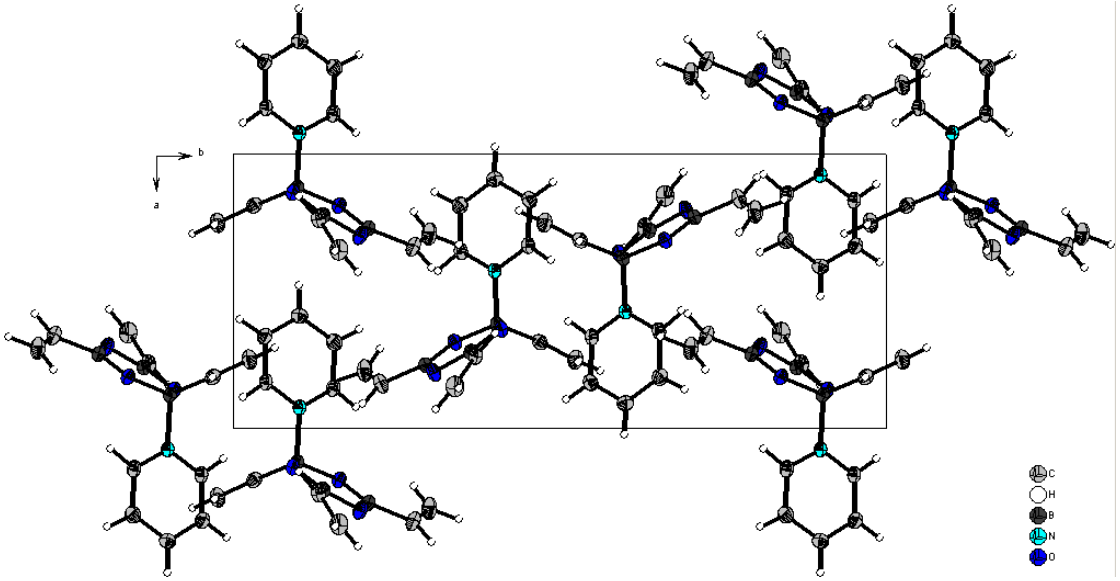

Table 1. Crystal data and structure refinement for **1**.

Identification code	**1**	
Empirical formula	$C_{11}H_{14}B_3NO_3$	
Formula weight	240.66	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$ (#14)	
Unit cell dimensions	a = 8.2029(8) Å	α= 90°.
	b = 19.488(2) Å	β= 90.423(2)°.
	c = 8.3016(8) Å	γ = 90°.
Volume	1327.0(2) $Å^3$	
Z	4	
Density (calculated)	1.205 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	504	
Crystal size	0.80 x 0.80 x 0.60 mm^3	
Theta range for data collection	2.09 to 28.29°.	
Index ranges	–10<=h<=10, –25<=k<=25, –11<=l<=11	
Reflections collected	10960	
Independent reflections	3088 [R(int) = 0.0223]	
Completeness to theta = 28.29°	93.8 %	
Absorption correction	Numerical	
Max. and min. transmission	0.9524 and 0.9373	
Refinement method	Full–matrix least–squares on F^2	
Data / restraints / parameters	3088 / 0 / 219	
Goodness–of–fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.1165	
R indices (all data)	R1 = 0.0483, wR2 = 0.1198	
Largest diff. peak and hole	0.463 and –0.164 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.

Atom	x	y	z	U(eq)
B(1)	1222(2)	972(1)	7706(2)	17(1)
N	–756(1)	1008(1)	7389(1)	17(1)
C(1)	–1679(1)	494(1)	7965(1)	20(1)
C(2)	–3341(2)	477(1)	7725(2)	24(1)
C(3)	–4080(2)	1009(1)	6879(2)	25(1)
C(4)	–3129(2)	1540(1)	6306(2)	26(1)
C(5)	–1465(2)	1524(1)	6569(1)	21(1)
C(6)	1867(1)	316(1)	6744(1)	21(1)
C(7)	2504(2)	–244(1)	7400(2)	29(1)
O(1)	1396(1)	908(1)	9455(1)	18(1)
B(2)	2216(2)	1375(1)	10346(2)	18(1)
C(8)	2353(2)	1298(1)	12214(1)	22(1)
C(9)	3476(2)	1613(1)	13101(2)	29(1)
O(2)	2961(1)	1938(1)	9630(1)	22(1)
B(3)	2701(2)	2065(1)	8006(2)	18(1)
C(10)	3371(2)	2747(1)	7281(2)	26(1)
C(11)	2903(2)	2993(1)	5868(2)	31(1)
O(3)	1868(1)	1615(1)	7078(1)	18(1)

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

B(1)–O(3)	1.4586(14)
B(1)–O(1)	1.4631(14)
B(1)–C(6)	1.5998(16)
B(1)–N	1.6433(15)
N–C(5)	1.3441(14)
N–C(1)	1.3466(15)
C(1)–C(2)	1.3763(17)
C(1)–H(1)	0.935(15)
C(2)–C(3)	1.3886(17)
C(2)–H(2)	0.947(16)
C(3)–C(4)	1.3826(18)
C(3)–H(3)	0.948(18)
C(4)–C(5)	1.3810(17)
C(4)–H(4)	0.970(16)
C(5)–H(5)	0.955(15)
C(6)–C(7)	1.3253(18)
C(6)–H(6)	0.983(19)
C(7)–H(7A)	0.967(18)
C(7)–H(7B)	0.987(18)
O(1)–B(2)	1.3489(14)
B(2)–O(2)	1.3906(15)
B(2)–C(8)	1.5617(16)
C(8)–C(9)	1.3257(18)
C(8)–H(8)	0.988(17)
C(9)–H(9A)	0.984(18)
C(9)–H(9B)	0.970(17)
O(2)–B(3)	1.3855(15)
B(3)–O(3)	1.3500(14)
B(3)–C(10)	1.5612(17)
C(10)–C(11)	1.3217(19)
C(10)–H(10)	0.98(2)
C(11)–H(11A)	0.992(18)
C(11)–H(11B)	0.966(19)

O(3)–B(1)–O(1)	113.20(9)
O(3)–B(1)–C(6)	112.70(9)
O(1)–B(1)–C(6)	113.43(9)
O(3)–B(1)–N	105.46(8)
O(1)–B(1)–N	104.59(8)
C(6)–B(1)–N	106.54(8)
C(5)–N–C(1)	119.64(10)
C(5)–N–B(1)	122.46(9)
C(1)–N–B(1)	117.89(9)
N–C(1)–C(2)	121.69(11)
N–C(1)–H(1)	115.7(9)
C(2)–C(1)–H(1)	122.6(9)
C(1)–C(2)–C(3)	118.92(11)
C(1)–C(2)–H(2)	120.0(9)
C(3)–C(2)–H(2)	121.1(9)
C(4)–C(3)–C(2)	119.17(11)
C(4)–C(3)–H(3)	121.4(10)
C(2)–C(3)–H(3)	119.4(10)
C(5)–C(4)–C(3)	119.25(11)
C(5)–C(4)–H(4)	118.1(10)
C(3)–C(4)–H(4)	122.6(10)
N–C(5)–C(4)	121.32(11)
N–C(5)–H(5)	115.7(8)
C(4)–C(5)–H(5)	122.9(8)
C(7)–C(6)–B(1)	125.70(11)
C(7)–C(6)–H(6)	115.1(11)
B(1)–C(6)–H(6)	119.2(11)
C(6)–C(7)–H(7A)	123.9(10)
C(6)–C(7)–H(7B)	120.7(11)
H(7A)–C(7)–H(7B)	115.4(15)
B(2)–O(1)–B(1)	122.12(9)
O(1)–B(2)–O(2)	121.10(10)
O(1)–B(2)–C(8)	120.79(10)
O(2)–B(2)–C(8)	118.11(10)
C(9)–C(8)–B(2)	123.49(12)
C(9)–C(8)–H(8)	117.9(9)

B(2)–C(8)–H(8)	118.6(9)
C(8)–C(9)–H(9A)	122.3(10)
C(8)–C(9)–H(9B)	121.6(10)
H(9A)–C(9)–H(9B)	116.1(14)
B(3)–O(2)–B(2)	119.47(9)
O(3)–B(3)–O(2)	120.81(10)
O(3)–B(3)–C(10)	120.76(10)
O(2)–B(3)–C(10)	118.42(10)
C(11)–C(10)–B(3)	123.41(12)
C(11)–C(10)–H(10)	117.1(11)
B(3)–C(10)–H(10)	119.4(11)
C(10)–C(11)–H(11A)	120.8(10)
C(10)–C(11)–H(11B)	121.6(11)
H(11A)–C(11)–H(11B)	117.6(15)
B(3)–O(3)–B(1)	122.58(9)

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: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	20(1)	16(1)	14(1)	0(1)	–2(1)	–2(1)
N	21(1)	15(1)	14(1)	–1(1)	–1(1)	–1(1)
C(1)	25(1)	16(1)	20(1)	2(1)	–1(1)	–1(1)
C(2)	24(1)	20(1)	26(1)	2(1)	1(1)	–3(1)
C(3)	21(1)	25(1)	28(1)	0(1)	–3(1)	1(1)
C(4)	27(1)	23(1)	28(1)	5(1)	–5(1)	2(1)
C(5)	27(1)	17(1)	19(1)	3(1)	–2(1)	–2(1)
C(6)	22(1)	21(1)	19(1)	–4(1)	1(1)	–3(1)
C(7)	35(1)	21(1)	30(1)	–3(1)	4(1)	3(1)
O(1)	25(1)	16(1)	14(1)	1(1)	–3(1)	–3(1)
B(2)	21(1)	16(1)	16(1)	–1(1)	–3(1)	2(1)
C(8)	30(1)	19(1)	16(1)	1(1)	–2(1)	2(1)
C(9)	40(1)	30(1)	19(1)	0(1)	–8(1)	–1(1)
O(2)	31(1)	19(1)	16(1)	–1(1)	–3(1)	–7(1)
B(3)	21(1)	17(1)	17(1)	0(1)	1(1)	–2(1)
C(10)	34(1)	19(1)	24(1)	–2(1)	5(1)	–8(1)
C(11)	47(1)	20(1)	27(1)	4(1)	8(1)	–2(1)
O(3)	23(1)	18(1)	14(1)	2(1)	–2(1)	–4(1)

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

Atom	x	y	z	U(eq)
H(1)	–1118(17)	150(8)	8526(17)	21(3)
H(2)	–3959(19)	105(8)	8126(18)	26(4)
H(3)	–5230(20)	1004(9)	6719(19)	34(4)
H(4)	–3583(19)	1926(8)	5720(20)	30(4)
H(5)	–746(17)	1872(8)	6186(17)	19(3)
H(6)	1820(20)	316(9)	5560(20)	40(4)
H(7A)	2910(20)	–629(9)	6790(20)	37(4)
H(7B)	2590(20)	–290(10)	8580(20)	41(5)
H(8)	1570(20)	997(8)	12770(20)	31(4)
H(9A)	3560(20)	1550(9)	14280(20)	37(4)
H(9B)	4300(20)	1901(9)	12620(20)	35(4)
H(10)	4130(20)	3027(10)	7920(20)	47(5)
H(11A)	3310(20)	3442(9)	5480(20)	40(5)
H(11B)	2120(20)	2756(10)	5200(20)	43(5)

Table 6. Torsion angles [°] for **1**.

O(3)–B(1)–N–C(5)	5.44(13)
O(1)–B(1)–N–C(5)	125.06(10)
C(6)–B(1)–N–C(5)	–114.54(11)
O(3)–B(1)–N–C(1)	–175.30(9)
O(1)–B(1)–N–C(1)	–55.68(12)
C(6)–B(1)–N–C(1)	64.71(12)
C(5)–N–C(1)–C(2)	0.59(17)
B(1)–N–C(1)–C(2)	–178.69(10)
N–C(1)–C(2)–C(3)	–0.57(18)
C(1)–C(2)–C(3)–C(4)	–0.18(19)
C(2)–C(3)–C(4)–C(5)	0.89(19)
C(1)–N–C(5)–C(4)	0.15(17)
B(1)–N–C(5)–C(4)	179.40(10)
C(3)–C(4)–C(5)–N	–0.89(19)
O(3)–B(1)–C(6)–C(7)	130.43(12)
O(1)–B(1)–C(6)–C(7)	0.15(17)
N–B(1)–C(6)–C(7)	–114.38(13)
O(3)–B(1)–O(1)–B(2)	–5.93(14)
C(6)–B(1)–O(1)–B(2)	124.10(11)
N–B(1)–O(1)–B(2)	–120.21(10)
B(1)–O(1)–B(2)–O(2)	–0.99(16)
B(1)–O(1)–B(2)–C(8)	178.93(10)
O(1)–B(2)–C(8)–C(9)	160.67(12)
O(2)–B(2)–C(8)–C(9)	–19.41(18)
O(1)–B(2)–O(2)–B(3)	7.52(16)
C(8)–B(2)–O(2)–B(3)	–172.40(10)
B(2)–O(2)–B(3)–O(3)	–6.51(17)
B(2)–O(2)–B(3)–C(10)	172.50(10)
O(3)–B(3)–C(10)–C(11)	14.36(19)
O(2)–B(3)–C(10)–C(11)	–164.65(12)
O(2)–B(3)–O(3)–B(1)	–1.01(17)
C(10)–B(3)–O(3)–B(1)	180.00(10)
O(1)–B(1)–O(3)–B(3)	6.95(15)
C(6)–B(1)–O(3)–B(3)	–123.45(11)
N–B(1)–O(3)–B(3)	120.71(10)