UK National Crystallography Service

Table 1. Crystal data and structure refinement.

Identification code	**2013ncs0027 / CLJ/MAB/1.47R**	
Empirical formula	$C_6H_{18}B_5NO_{10}$	
Formula weight	318.26	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P*–1	
Unit cell dimensions	a = 9.166(4) Å	α = 64.88(2)°
	b = 9.380(5) Å	β = 75.49(3)°
	c = 9.883(4) Å	γ = 84.73(4)°
Volume	744.7(6) Å^3	
Z	2	
Density (calculated)	1.419 Mg / m^3	
Absorption coefficient	0.123 mm^{-1}	
F(000)	332	
Crystal	Plate; Colourless	
Crystal size	0.230 × 0.100 × 0.030 mm^3	
θ range for data collection	3.081 – 27.478°	
Index ranges	$-11 \le h \le 10$, $-12 \le k \le 11$, $-12 \le l \le 12$	
Reflections collected	9366	
Independent reflections	3355 [R_{int} = 0.0428]	
Completeness to θ = 25.242°	98.8 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.822	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3355 / 0 / 205	
Goodness-of-fit on F^2	1.084	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0524, *wR2* = 0.1473	
R indices (all data)	*R1* = 0.0595, *wR2* = 0.1549	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.362 and –0.314 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100µm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b18* (Rigaku, 2012). **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 3.1 b18* (Rigaku, 2012). **Structure solution**: *SHELXS97* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Structure refinement**: *SHELXL-2012* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565

Special details:

All hydrogen atoms were fixed using a standard riding model.

Table 2. Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
B1	6938(2)	3895(2)	2483(2)	17(1)	1
B2	8875(2)	6083(2)	1298(2)	19(1)	1
B3	6794(2)	6104(2)	3308(2)	17(1)	1
B4	6694(2)	1029(2)	3283(2)	19(1)	1
B5	5308(2)	2760(2)	1489(2)	19(1)	1
O1	8372(1)	4691(1)	1446(1)	19(1)	1
O2	8075(1)	6831(1)	2197(1)	21(1)	1
O3	6279(1)	4694(1)	3512(1)	18(1)	1
O4	7230(1)	2264(1)	3408(1)	18(1)	1
O5	5708(1)	1246(1)	2356(1)	22(1)	1
O6	5880(1)	4031(1)	1529(1)	19(1)	1
O7	10177(1)	6802(1)	297(1)	26(1)	1
O8	6099(1)	6863(1)	4204(1)	21(1)	1
O9	7171(1)	–440(1)	4090(1)	24(1)	1
O10	4350(1)	2916(1)	582(1)	26(1)	1
C1	736(2)	7738(2)	4036(2)	30(1)	1
C2	1426(2)	6354(2)	3664(2)	34(1)	1
C3	2964(2)	6955(3)	2540(3)	41(1)	1
C4	3144(2)	8612(2)	2425(3)	40(1)	1
C5	915(2)	9566(2)	1320(2)	31(1)	1
C6	1417(2)	10572(2)	3065(2)	34(1)	1
N1	1543(2)	9167(2)	2701(2)	25(1)	1

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

B1–O4	1.452(2)	C1–C2	1.535(3)
B1–O6	1.476(2)	C1–H1A	0.9900
B1–O1	1.480(2)	C1–H1B	0.9900
B1–O3	1.4889(19)	C2–C3	1.539(3)
B2–O7	1.359(2)	C2–H2A	0.9900
B2–O1	1.361(2)	C2–H2B	0.9900
B2–O2	1.388(2)	C3–C4	1.531(3)
B3–O3	1.362(2)	C3–H3A	0.9900
B3–O8	1.3655(19)	C3–H3B	0.9900
B3–O2	1.384(2)	C4–N1	1.509(2)
B4–O4	1.362(2)	C4–H4A	0.9900
B4–O9	1.362(2)	C4–H4B	0.9900
B4–O5	1.386(2)	C5–N1	1.501(2)
B5–O10	1.362(2)	C5–H5A	0.9800
B5–O6	1.365(2)	C5–H5B	0.9800
B5–O5	1.384(2)	C5–H5C	0.9800
O7–H7	0.8400	C6–N1	1.495(2)
O8–H8	0.8400	C6–H6A	0.9800
O9–H9	0.8400	C6–H6B	0.9800
O10–H10	0.8400	C6–H6C	0.9800
C1–N1	1.509(2)		
O4–B1–O6	111.94(12)	C1–C2–H2A	110.5
O4–B1–O1	109.18(13)	C3–C2–H2A	110.5
O6–B1–O1	108.14(13)	C1–C2–H2B	110.5
O4–B1–O3	109.29(13)	C3–C2–H2B	110.5
O6–B1–O3	108.59(12)	H2A–C2–H2B	108.7
O1–B1–O3	109.68(12)	C4–C3–C2	104.68(17)
O7–B2–O1	122.66(14)	C4–C3–H3A	110.8
O7–B2–O2	116.50(13)	C2–C3–H3A	110.8
O1–B2–O2	120.83(14)	C4–C3–H3B	110.8
O3–B3–O8	122.11(14)	C2–C3–H3B	110.8
O3–B3–O2	121.53(14)	H3A–C3–H3B	108.9
O8–B3–O2	116.34(13)	N1–C4–C3	103.60(15)
O4–B4–O9	117.83(14)	N1–C4–H4A	111.0
O4–B4–O5	121.63(15)	C3–C4–H4A	111.0
O9–B4–O5	120.54(14)	N1–C4–H4B	111.0
O10–B5–O6	122.13(15)	C3–C4–H4B	111.0
O10–B5–O5	117.00(14)	H4A–C4–H4B	109.0
O6–B5–O5	120.86(14)	N1–C5–H5A	109.5
B2–O1–B1	124.40(12)	N1–C5–H5B	109.5
B3–O2–B2	119.14(12)	H5A–C5–H5B	109.5
B3–O3–B1	123.44(12)	N1–C5–H5C	109.5
B4–O4–B1	123.03(13)	H5A–C5–H5C	109.5
B5–O5–B4	119.09(13)	H5B–C5–H5C	109.5
B5–O6–B1	123.19(12)	N1–C6–H6A	109.5
B2–O7–H7	109.5	N1–C6–H6B	109.5
B3–O8–H8	109.5	H6A–C6–H6B	109.5
B4–O9–H9	109.5	N1–C6–H6C	109.5
B5–O10–H10	109.5	H6A–C6–H6C	109.5
N1–C1–C2	103.90(15)	H6B–C6–H6C	109.5
N1–C1–H1A	111.0	C6–N1–C5	108.81(14)
C2–C1–H1A	111.0	C6–N1–C4	112.50(14)
N1–C1–H1B	111.0	C5–N1–C4	110.51(15)
C2–C1–H1B	111.0	C6–N1–C1	112.22(14)
H1A–C1–H1B	109.0	C5–N1–C1	110.19(13)
C1–C2–C3	106.01(16)	C4–N1–C1	102.51(14)

Symmetry transformations used to generate equivalent atoms:

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

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B1	17(1)	16(1)	21(1)	–9(1)	–6(1)	–2(1)
B2	18(1)	20(1)	22(1)	–10(1)	–6(1)	–1(1)
B3	17(1)	16(1)	19(1)	–7(1)	–6(1)	–1(1)
B4	16(1)	20(1)	23(1)	–10(1)	–5(1)	–1(1)
B5	16(1)	20(1)	23(1)	–9(1)	–7(1)	–2(1)
O1	17(1)	19(1)	24(1)	–12(1)	–2(1)	–3(1)
O2	21(1)	19(1)	26(1)	–13(1)	–1(1)	–5(1)
O3	18(1)	17(1)	20(1)	–9(1)	–3(1)	–3(1)
O4	20(1)	16(1)	24(1)	–9(1)	–10(1)	–1(1)
O5	25(1)	17(1)	29(1)	–8(1)	–15(1)	–2(1)
O6	20(1)	17(1)	22(1)	–8(1)	–9(1)	0(1)
O7	23(1)	25(1)	31(1)	–18(1)	4(1)	–8(1)
O8	20(1)	19(1)	25(1)	–12(1)	0(1)	–5(1)
O9	28(1)	16(1)	33(1)	–11(1)	–17(1)	0(1)
O10	29(1)	21(1)	32(1)	–6(1)	–18(1)	–3(1)
C1	28(1)	31(1)	29(1)	–7(1)	–11(1)	–4(1)
C2	34(1)	33(1)	38(1)	–10(1)	–19(1)	2(1)
C3	31(1)	47(1)	47(1)	–20(1)	–13(1)	9(1)
C4	18(1)	45(1)	53(1)	–16(1)	–7(1)	–2(1)
C5	40(1)	30(1)	28(1)	–12(1)	–15(1)	–2(1)
C6	42(1)	33(1)	35(1)	–18(1)	–16(1)	–5(1)
N1	21(1)	28(1)	29(1)	–12(1)	–10(1)	–2(1)

Table 5. Hydrogen coordinates [× 10^4] and isotropic displacement parameters [Å^2 × 10^3].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H7	10564	6278	–210	38	1
H8	5371	6309	4877	32	1
H9	6754	–1105	3943	35	1
H10	4269	3875	22	40	1
H1A	–363	7789	4107	36	1
H1B	916	7643	5017	36	1
H2A	769	6029	3184	41	1
H2B	1555	5442	4611	41	1
H3A	3784	6268	2940	50	1
H3B	2976	6990	1522	50	1
H4A	3645	8582	3215	48	1
H4B	3737	9306	1395	48	1
H5A	920	8628	1119	47	1
H5B	1535	10400	425	47	1
H5C	–121	9930	1515	47	1
H6A	1967	11465	2175	50	1
H6B	1847	10332	3950	50	1
H6C	353	10839	3310	50	1

Table 6. Torsion angles [°].

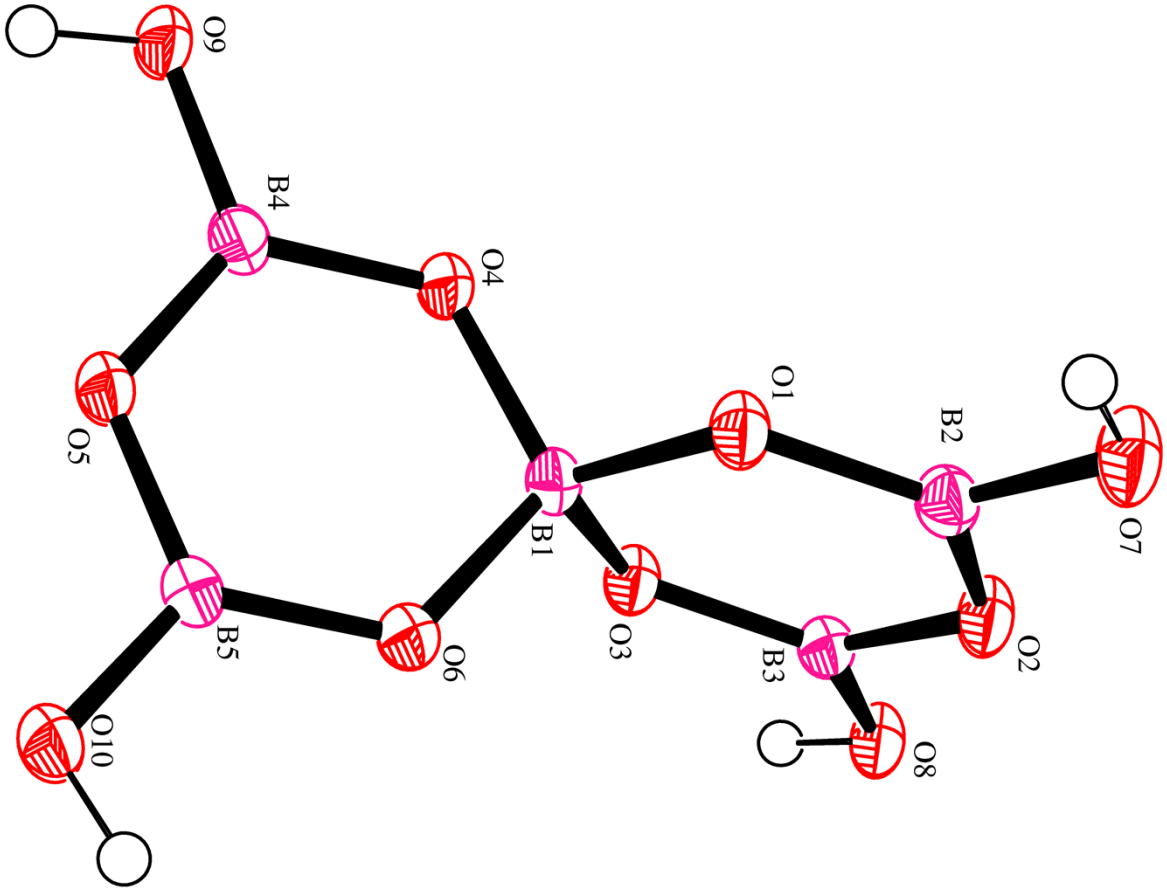
O7–B2–O1–B1	–177.89(14)
O2–B2–O1–B1	3.1(2)
O4–B1–O1–B2	–129.34(15)
O6–B1–O1–B2	108.65(15)
O3–B1–O1–B2	–9.6(2)
O3–B3–O2–B2	–1.8(2)
O8–B3–O2–B2	176.93(14)
O7–B2–O2–B3	–175.70(14)
O1–B2–O2–B3	3.4(2)
O8–B3–O3–B1	175.13(14)
O2–B3–O3–B1	–6.2(2)
O4–B1–O3–B3	130.75(14)
O6–B1–O3–B3	–106.88(15)
O1–B1–O3–B3	11.1(2)
O9–B4–O4–B1	173.14(12)
O5–B4–O4–B1	–6.1(2)
O6–B1–O4–B4	5.79(19)
O1–B1–O4–B4	–113.90(15)
O3–B1–O4–B4	126.14(14)
O10–B5–O5–B4	179.28(13)
O6–B5–O5–B4	0.6(2)
O4–B4–O5–B5	2.6(2)
O9–B4–O5–B5	–176.65(13)
O10–B5–O6–B1	–178.99(13)
O5–B5–O6–B1	–0.4(2)
O4–B1–O6–B5	–2.59(19)
O1–B1–O6–B5	117.72(15)
O3–B1–O6–B5	–123.34(14)
N1–C1–C2–C3	21.94(19)
C1–C2–C3–C4	4.6(2)
C2–C3–C4–N1	–29.5(2)
C3–C4–N1–C6	164.32(16)
C3–C4–N1–C5	–73.84(19)
C3–C4–N1–C1	43.57(19)
C2–C1–N1–C6	–161.33(14)
C2–C1–N1–C5	77.25(17)
C2–C1–N1–C4	–40.40(17)

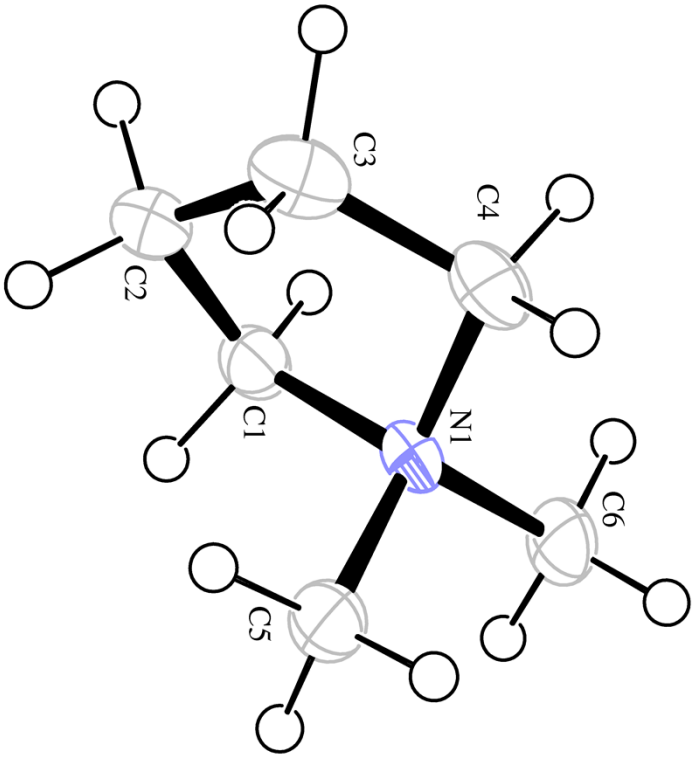
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds [Å and °].

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
O7–H7···O1^{i}	0.84	1.86	2.6933(18)	172.5
O8–H8···O3^{ii}	0.84	1.87	2.702(2)	171.4
O9–H9···O8^{iii}	0.84	1.94	2.746(2)	159.6
O10–H10···O6^{iv}	0.84	1.93	2.763(2)	170.7
C1–H1B···O4^{ii}	0.99	2.60	3.495(2)	149.6

Symmetry transformations used to generate equivalent atoms:
(i) –x+2,–y+1,–z (ii) –x+1,–y+1,–z+1 (iii) x,y–1,z
(iv) –x+1,–y+1,–z


O7
O2
B2
O1
O8
B3
O3
B1
O6
B5
O4
O10
O5
B4
O9


C6
C5
N1
C1
C4
C2
C3