

Crystal structure of *cis*-1-phenyl-8-(pyridin-2-ylmethyl)dibenzo[1,2-*c*:2,1-*h*]-2,14-dioxo-8-aza-1-borabicyclo[4.4.0]deca-3,8-diene

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The title compound, C₂₆H₂₃BN₂O₂, was obtained as by product during synthetic attempts of a complexation reaction between the tripodal ligand H₂L [*N,N*-bis(2-hydroxybenzyl)(pyridin-2-yl)methylamine] and manganese(III) acetate in the presence of NaBPh₄. The isolated *B*-phenyl dioxazaborocine contains an N→B dative bond with a *cis* conformation. In the crystal, C—H...O hydrogen bonds define chains parallel to the *b*-axis direction. A comparative analysis with other structurally related derivatives is also included, together with a rationalization of the unexpected production of this zwitterionic heterocycle.

1. Chemical context

As part of our research program directed at obtaining manganese complexes as bio-inspired mimetics with different nuclearity and properties (Ledesma *et al.*, 2014, 2015), we were interested in coordination reactions of the tripodal tetradentate ligand H₂L, namely *N,N*-bis(2-hydroxybenzyl)(pyridin-2-yl)methylamine. We envisaged a systematic study comprising the use of several metal-to-ligand ratios, with the idea of varying the nuclearity of the resulting compounds. Unexpectedly, however, during consecutive attempts to obtain manganese complexes derived from H₂L, we isolated the *B*-phenyl dioxazaborocine derivative, **I**. Here we report its synthesis and crystal structure and, in order to unravel its presence, we rationalize its production under the employed reaction conditions. A comparative analysis of its structural data with that of other dioxazaborocines is also presented.

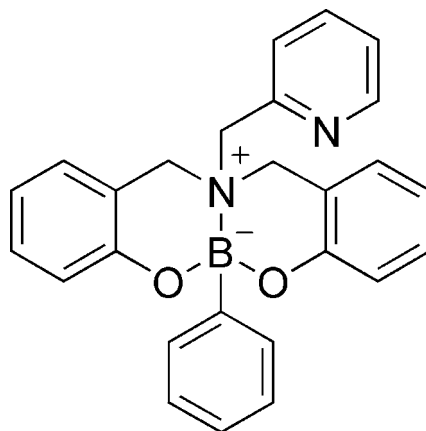
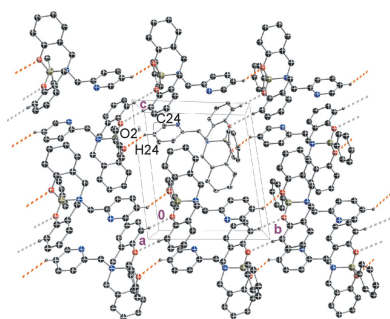


Table 1
 Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2\cdots O1^i$	0.95	2.57	3.503 (3)	168
$C24-H24\cdots O2^{ii}$	0.95	2.50	3.185 (3)	129

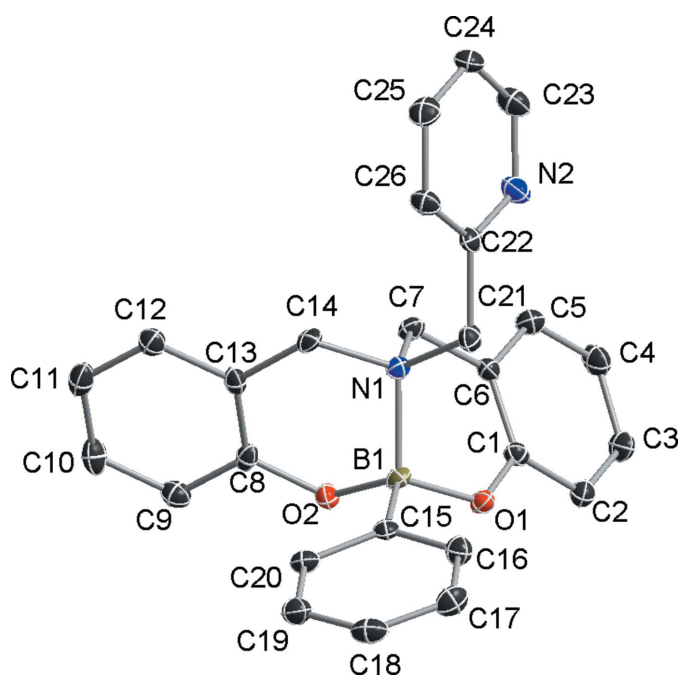
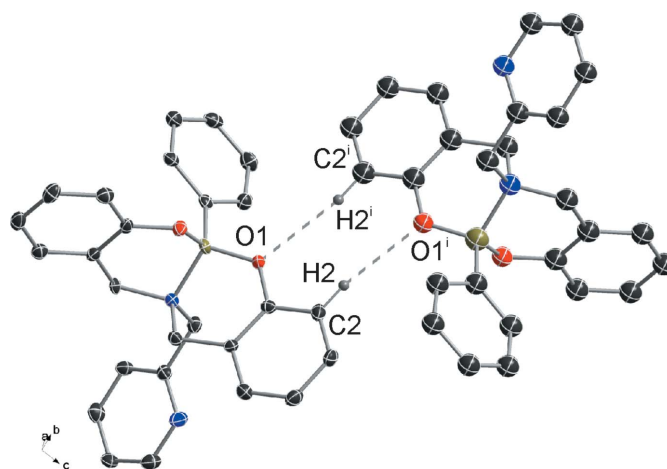
 Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $x, y-1, z$.

2. Structural commentary

The title compound **I**, Fig. 1, which represents one of the few examples of *B*-phenyl dioxazaborocine derivatives reported in the literature, crystallizes in the triclinic space group $P\bar{1}$ with two molecules in the unit cell. The boron atom shows a distorted tetrahedral coordination sphere described by one N atom (N1), two oxygen atoms (O1, O2) and one carbon atom from a phenyl ring (C15). The geometry about the intramolecular N1–B1 bond is *cis*, as inferred from the spatial arrangement of atoms C15–B1–N1–C21. The B–O bond lengths are 1.446 (3) and 1.471 (3) Å and the B–N bond length is 1.674 (4) Å. The BNC₃O six-membered rings adopt a half-chair conformation, with puckering parameters $Q_T = 0.502$ (2) Å, $\theta_2 = 135.4$ (2)°, $\varphi_2 = -138.4$ (4)° for B1/N1/C7/C6/C1/O1, and $Q_T = 0.525$ (2) Å, $\theta_2 = 132.2$ (3)°, $\varphi_2 = -144.8$ (4)° for B1/N1/C14/C13/C8/O2.

3. Supramolecular features

The crystal packing in **I** is defined by two sets of C–H⋯O hydrogen bonds. The first group implicates C2–H2⋯O1ⁱ atoms, giving rise to a dimeric system with a C–H⋯O angles


Figure 1
 The molecular structure of the title molecule, with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are omitted for clarity.

Figure 2
 Detail of the intermolecular interactions in the title compound forming a dimeric system through C–H⋯O hydrogen bonds (dashed lines). H atoms not involved in these hydrogen bonds are omitted [symmetry code: (i) = $1-x, 2-y, 2-z$].

of 167.5° (Fig. 2, Table 1). The remaining interaction, C24–H24⋯O2ⁱⁱ, shows a small C–H⋯O angle of 129.4°, indicating that this C–H⋯O hydrogen bond is quite weak. The two interactions link molecules into chains parallel to the *b* axis (Fig. 3), consolidating the three-dimensional molecular packing.

4. Database survey

A survey of the Cambridge Structural Database (CSD Version 5.38; Groom *et al.*, 2016) showed a few reported examples of dioxazaborocines (Geng & Wu, 2011; Gawdzik *et al.*, 2009; Zhu *et al.*, 2006; Thadani *et al.*, 2001; Woodgate *et al.*, 2000;

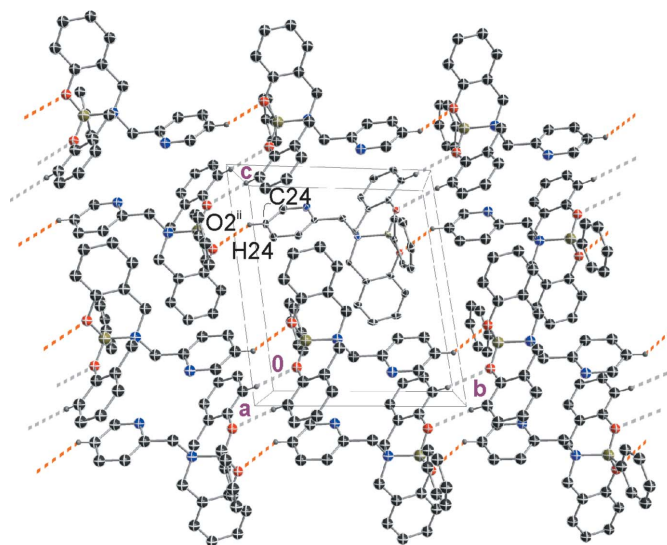

Figure 3
 Detail of C–H⋯O interactions in the title compound (grey and orange dashed lines denote C2–H2⋯O1 and C24–H24⋯O2ⁱⁱ interactions, respectively). H atoms not involved in these interactions are omitted for clarity [symmetry codes: (i) $1-x, 2-y, 2-z$; (ii) $x, -1+y, z$].

Table 2
Structural data and calculated tetrahedral character THC_{DA} (\AA , $^\circ$) for compounds **I–III**.

	Compound I	II (MAWDET) ^a	III (EROJIF) ^b
<i>Bond lengths</i>			
B–N	1.674 (4) (B1–N1)	1.674 (5) (B1–N1)	1.641 (2) (B1–N2)
B–O	1.471 (3) (B1–O2)	1.443 (4) (B1–O2)	1.443 (2) (B1–O3)
B–O	1.446 (3) (B1–O1)	1.454 (4) (B1–O1)	1.463 (2) (B1–O5)
B–C	1.602 (4) (B1–C15)	1.608 (5) (B1–C15)	1.425 (2) (B1–O4)
<i>Angles</i>			
θ_1	113.0 (2) (C15–B1–O2)	110.3 (3) (C15–B–O2)	113.34 (15) (O4–B1–O3)
θ_2	109.5 (2) (C15–B1–O1)	115.5 (3) (C15–B–O1)	114.47 (16) (O4–B1–O5)
θ_3	109.0 (2) (O2–B1–O1)	109.5 (3) (O2–B–O1)	108.60 (15) (O3–B1–O5)
θ_4	113.5 (2) (N1–B1–C15)	110.0 (3) (N1–B–C15)	105.64 (14) (N2–B1–O4)
θ_5	104.5 (2) (N1–B1–O2)	106.7 (3) (N1–B–O2)	108.45 (14) (N2–B1–O3)
θ_6	107.1 (2) (N1–B1–O1)	104.4 (3) (N1–B–O1)	105.89 (13) (N2–B1–O5)
THC_{DA}^c	82.8	83.1	79.7

(a) Woodgate *et al.* (1999); (b) Geng *et al.* (2011); (c) Höpfl *et al.* (1999).

Woodgate *et al.*, 1999). Specifically, two members of this selected group are structurally related to the title compound: **II** (MAWDET; Woodgate *et al.*, 1999) and the recently described compound **III** (EROJIF; Geng & Wu, 2011) (Fig. 4).

Table 2 summarizes relevant bond lengths and angles for **I** compared with those observed in **II** and **III**. The intramolecular N–B bond lengths can vary, depending on the substituent groups to boron and nitrogen atoms. In particular, the covalent N1–B1 bond distance for **I** [1.674 (4) Å] is in the range observed for **III** and **II** [1.641 (2)–1.674 (5) Å]. The N–B bond distance for **III** is shorter than that in **II**, quite probably due to the extra oxygen atom bonded to the boron atom (from the –OCH₃ group).

The crystal structure of **I** shows that the phenyl group at the boron atom and the *N*-pyridin-2-ylmethyl substituent adopts a *cis* conformation around the N→B dative bond, in total agreement with that reported for **II** and **III**. The C21–N1–B1–C15 torsion angle assumes a value of 57.8 (3)°. Analysis of the structural data for **II** showed the corresponding torsion angle (C37–N1–B1–C15) is 56.71°. In compound **III**, the corresponding angle (C13–N2–B1–O4) is 62.34°. These two examples display a *cis* geometry around the intramolecular N–B bond, in concordance with compound **I** (Fig. 5).

We have performed an analysis of the experimental data of compounds **I–III** and calculated the tetrahedral character (THC_{DA}) at the boron atom (Höpfl *et al.*, 1999), making use of the values of the six angles around the boron atom (θ_1 – θ_6).

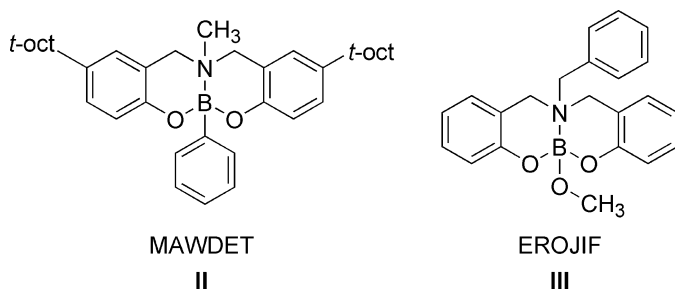


Figure 4
Oxazaborocine compounds structurally related to the title compound.

The quite high value of 82.8% for **I** is in the range observed for compounds **II** and **III**. Altogether, this parameter and the measured N–B bond lengths can be considered a clear indication of sp^3 -hybridization of the boron atom and of a resident negative charge (Sarina *et al.*, 2015). Therefore, we confirm that compound **I** adopts a zwitterionic form with a significant intramolecular N→B dative bond.

Based on previous observations (Barnes *et al.*, 1998), we hypothesize that employing an aqueous solution of NaBPh₄ led to the unexpected isolation of **I**. It is well known that NaBPh₄ in the presence of oxygen leads to the production of phenylboronic acid PhB(OH)₂ and phenol. Then, the *in situ* generated phenylboronic acid (derived in turn from an excess of NaBPh₄) is capable of reacting with the tripodal ligand H₂L, leading to the formation of compound **I** (Fig. 6).

Inspection of the reaction conditions already reported by Woodgate *et al.* (1999) indicates that compound **II** was obtained by reaction of phenylboronic acid and the corresponding tertiary amine. In turn, the authors reported that compound **III** was obtained unintentionally when using salicylaldehyde benzylamine and boron compounds (Geng *et al.*, 2011). We hypothesize that, in the case of **I**, the use of NaBPh₄ determined the course of the reaction, leading to the formation of the zwitterionic heterocycle in the described reaction conditions.

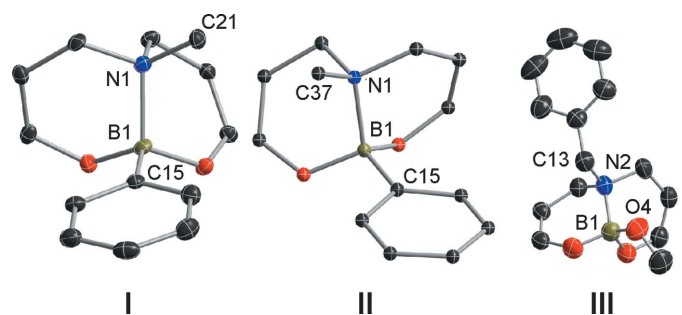


Figure 5
Comparison of the bonding environment at boron in **I** (title compound), **II** (MAWDET) and **III** (EROJIF). For clarity, only atoms closely involved in the N→B dative bonds are shown.

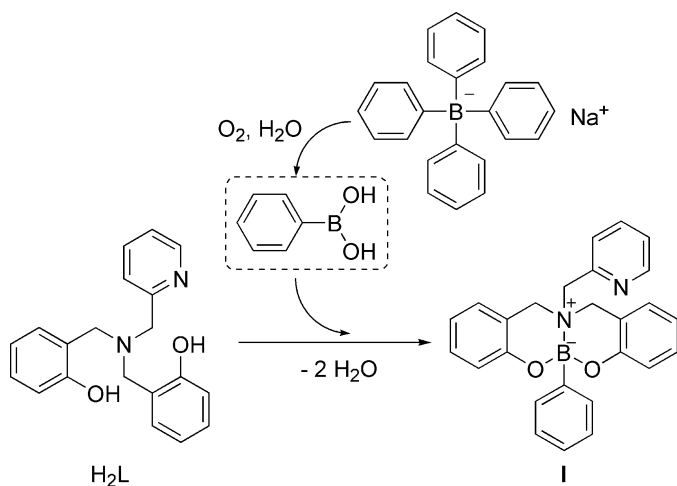


Figure 6
Synthesis of the title compound.

5. Synthesis and crystallization

H_2L (0.064 g; 0.2 mmol) was dissolved in methanol (4 mL), then solid manganese(III) acetate dihydrate (0.052 g; 0.2 mmol) was added. Immediately after, an excess of $NaBPh_4$ (0.2065 g, 0.60 mmol) in 2 mL of methanol/water was added to the reaction flask. The resulting dark-brown solution was sonicated at 313 K for 15 min and then stirred at reflux for additional 16 h (overnight). After cooling, the obtained precipitate was collected by filtration, washed with diethyl ether and dried *in vacuo*. Recrystallization from methanol gave colourless crystals of **I** suitable for X-ray diffraction. Yield: 21%. IR spectrum: $\nu(\text{cm}^{-1})$: 3043, 1630 (C=N), 1626, 1608 (C=C aromatic), 1462 (*br*, B—O), 1273, 1248, 1200, 1050 (C—O), 1002 (B—N), 702.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were placed at calculated positions, with $d(\text{C—H}) = 0.95\text{--}0.99 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Funding information

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Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{23}BN_2O_2$
M_r	406.27
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	8.8803 (7), 10.0871 (8), 11.7586 (10)
α, β, γ (°)	97.298 (2), 98.464 (2), 98.234 (2)
V (Å ³)	1019.21 (14)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.22 × 0.16 × 0.12
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Gaussian (<i>XPREP</i> and <i>SADABS</i> ; Bruker, 2008)
$T_{\text{min}}, T_{\text{max}}$	0.780, 0.875
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8344, 4004, 2161
R_{int}	0.088
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.059, 0.115, 0.92
No. of reflections	4004
No. of parameters	280
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.25, -0.31

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *DIAMOND* (Brandenburg, 2012).

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supporting information

Acta Cryst. (2017). E73, 1917-1920 [https://doi.org/10.1107/S2056989017016553]

Crystal structure of *cis*-1-phenyl-8-(pyridin-2-ylmethyl)dibenzo[1,2-*c*:2,1-*h*]-2,14-dioxa-8-aza-1-borabicyclo[4.4.0]deca-3,8-diene

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Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

cis-1-Phenyl-8-(pyridin-2-ylmethyl)dibenzo[1,2-*c*:2,1-*h*]-2,14-dioxa-8-aza-1-borabicyclo[4.4.0]deca-3,8-diene

Crystal data

C₂₆H₂₃BN₂O₂

M_r = 406.27

Triclinic, *P*1

Hall symbol: -*P* 1

a = 8.8803 (7) Å

b = 10.0871 (8) Å

c = 11.7586 (10) Å

α = 97.298 (2)°

β = 98.464 (2)°

γ = 98.234 (2)°

V = 1019.21 (14) Å³

Z = 2

F(000) = 428

D_x = 1.324 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 5951 reflections

θ = 2.4–28.2°

μ = 0.08 mm⁻¹

T = 100 K

Prism, colourless

0.22 × 0.16 × 0.12 mm

Data collection

Bruker APEXII CCD
diffractometer

Graphite monochromator

φ and ω scans

Absorption correction: gaussian
(XPREP and SADABS; Bruker, 2008)

T_{min} = 0.780, *T_{max}* = 0.875

8344 measured reflections

4004 independent reflections

2161 reflections with *I* > 2σ(*I*)

R_{int} = 0.088

θ_{max} = 26.0°, θ_{min} = 2.4°

h = -10→10

k = -12→10

l = -14→14

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.059

wR(*F*²) = 0.115

S = 0.92

4004 reflections

280 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O2	0.33571 (19)	0.80339 (16)	0.66654 (14)	0.0162 (4)
C7	0.2240 (3)	0.5768 (2)	0.7698 (2)	0.0154 (6)
H7A	0.186984	0.481569	0.777707	0.018*
H7B	0.15142	0.602455	0.707238	0.018*
O1	0.45343 (19)	0.81457 (16)	0.86313 (14)	0.0155 (4)
N1	0.3811 (2)	0.58730 (19)	0.73635 (17)	0.0142 (5)
N2	0.3294 (3)	0.3306 (2)	0.87553 (18)	0.0228 (6)
C1	0.3311 (3)	0.7832 (2)	0.9193 (2)	0.0141 (6)
C15	0.6210 (3)	0.7798 (2)	0.7133 (2)	0.0145 (6)
C6	0.2247 (3)	0.6666 (2)	0.8822 (2)	0.0143 (6)
C8	0.2760 (3)	0.7354 (2)	0.5582 (2)	0.0149 (6)
C22	0.4325 (3)	0.3686 (2)	0.8075 (2)	0.0164 (6)
C20	0.6479 (3)	0.8046 (2)	0.6034 (2)	0.0168 (6)
H20	0.562356	0.799166	0.543102	0.02*
C14	0.3653 (3)	0.5215 (2)	0.6124 (2)	0.0159 (6)
H14A	0.469245	0.515167	0.593371	0.019*
H14B	0.307445	0.428216	0.603349	0.019*
C13	0.2833 (3)	0.5988 (2)	0.5288 (2)	0.0154 (6)
C2	0.3191 (3)	0.8716 (3)	1.0178 (2)	0.0184 (6)
H2	0.391788	0.952737	1.042134	0.022*
C19	0.7968 (3)	0.8371 (3)	0.5794 (2)	0.0218 (7)
H19	0.811445	0.851654	0.503233	0.026*
C3	0.2016 (3)	0.8410 (3)	1.0797 (2)	0.0209 (7)
H3	0.192493	0.901899	1.145982	0.025*
C26	0.4860 (3)	0.2759 (2)	0.7329 (2)	0.0183 (6)
H26	0.56079	0.305733	0.687579	0.022*
C5	0.1087 (3)	0.6353 (3)	0.9472 (2)	0.0195 (6)
H5	0.036794	0.553633	0.923746	0.023*
C9	0.2030 (3)	0.8050 (3)	0.4773 (2)	0.0190 (7)
H9	0.198548	0.898346	0.497886	0.023*
C16	0.7521 (3)	0.7913 (2)	0.7980 (2)	0.0197 (7)
H16	0.738836	0.77471	0.873908	0.024*

C12	0.2147 (3)	0.5337 (3)	0.4180 (2)	0.0183 (6)
H12	0.216587	0.439785	0.397566	0.022*
C4	0.0970 (3)	0.7221 (3)	1.0458 (2)	0.0226 (7)
H4	0.017669	0.699995	1.089651	0.027*
C25	0.4296 (3)	0.1387 (3)	0.7247 (2)	0.0222 (7)
H25	0.464256	0.073442	0.673508	0.027*
C17	0.9002 (3)	0.8257 (3)	0.7761 (2)	0.0217 (7)
H17	0.986288	0.834068	0.836496	0.026*
C10	0.1376 (3)	0.7395 (3)	0.3682 (2)	0.0223 (7)
H10	0.087663	0.787534	0.313513	0.027*
C21	0.4862 (3)	0.5193 (2)	0.8156 (2)	0.0168 (6)
H21A	0.591196	0.534146	0.795601	0.02*
H21B	0.492924	0.562668	0.896988	0.02*
C24	0.3225 (3)	0.0994 (3)	0.7923 (2)	0.0204 (7)
H24	0.2805	0.006461	0.788101	0.024*
C11	0.1438 (3)	0.6029 (3)	0.3371 (2)	0.0224 (7)
H11	0.099895	0.557761	0.260997	0.027*
C18	0.9221 (3)	0.8480 (2)	0.6656 (2)	0.0226 (7)
H18	1.023545	0.870859	0.649451	0.027*
C23	0.2776 (3)	0.1973 (3)	0.8658 (2)	0.0239 (7)
H23	0.204908	0.168795	0.913098	0.029*
B1	0.4511 (3)	0.7520 (3)	0.7450 (3)	0.0153 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0199 (11)	0.0149 (10)	0.0135 (10)	0.0035 (8)	0.0013 (8)	0.0025 (8)
C7	0.0131 (15)	0.0146 (15)	0.0167 (15)	-0.0010 (12)	0.0014 (12)	0.0005 (12)
O1	0.0169 (10)	0.0147 (10)	0.0132 (10)	-0.0016 (8)	0.0041 (8)	-0.0008 (8)
N1	0.0138 (12)	0.0135 (12)	0.0141 (12)	0.0002 (9)	0.0017 (10)	0.0012 (9)
N2	0.0325 (15)	0.0179 (14)	0.0204 (14)	0.0036 (11)	0.0096 (12)	0.0061 (11)
C1	0.0124 (15)	0.0148 (15)	0.0151 (15)	0.0013 (12)	0.0020 (12)	0.0038 (12)
C15	0.0188 (15)	0.0087 (14)	0.0155 (15)	0.0021 (11)	0.0023 (12)	0.0002 (11)
C6	0.0158 (15)	0.0140 (15)	0.0131 (14)	0.0009 (12)	0.0021 (12)	0.0043 (12)
C8	0.0127 (14)	0.0195 (15)	0.0113 (14)	-0.0002 (12)	0.0030 (12)	0.0000 (12)
C22	0.0192 (16)	0.0147 (15)	0.0143 (15)	0.0030 (12)	-0.0025 (13)	0.0046 (12)
C20	0.0165 (16)	0.0133 (15)	0.0195 (16)	-0.0007 (12)	0.0029 (13)	0.0018 (12)
C14	0.0213 (16)	0.0119 (14)	0.0131 (14)	0.0016 (12)	0.0041 (12)	-0.0036 (11)
C13	0.0164 (15)	0.0186 (15)	0.0120 (14)	0.0025 (12)	0.0037 (12)	0.0043 (12)
C2	0.0231 (17)	0.0171 (15)	0.0140 (15)	0.0029 (13)	0.0009 (13)	0.0013 (12)
C19	0.0253 (17)	0.0179 (15)	0.0210 (16)	-0.0003 (13)	0.0055 (14)	0.0015 (13)
C3	0.0284 (17)	0.0200 (16)	0.0146 (15)	0.0036 (13)	0.0080 (13)	-0.0008 (12)
C26	0.0182 (16)	0.0173 (16)	0.0209 (16)	0.0019 (12)	0.0071 (13)	0.0052 (12)
C5	0.0200 (16)	0.0170 (15)	0.0196 (16)	-0.0012 (12)	0.0022 (13)	0.0018 (12)
C9	0.0208 (16)	0.0172 (15)	0.0208 (16)	0.0049 (12)	0.0065 (13)	0.0043 (13)
C16	0.0224 (17)	0.0198 (16)	0.0170 (16)	0.0034 (13)	0.0049 (13)	0.0021 (12)
C12	0.0174 (15)	0.0202 (15)	0.0174 (16)	0.0014 (12)	0.0049 (13)	0.0029 (12)
C4	0.0281 (18)	0.0237 (17)	0.0183 (16)	0.0047 (14)	0.0095 (14)	0.0051 (13)

C25	0.0270 (17)	0.0165 (16)	0.0229 (16)	0.0074 (13)	0.0031 (14)	-0.0005 (12)
C17	0.0152 (16)	0.0222 (16)	0.0258 (17)	0.0028 (13)	0.0003 (13)	-0.0001 (13)
C10	0.0196 (16)	0.0322 (17)	0.0162 (16)	0.0085 (13)	0.0012 (13)	0.0056 (13)
C21	0.0193 (15)	0.0170 (15)	0.0137 (15)	0.0050 (12)	-0.0010 (12)	0.0028 (12)
C24	0.0257 (17)	0.0131 (15)	0.0217 (16)	0.0003 (12)	0.0027 (13)	0.0049 (12)
C11	0.0181 (16)	0.0306 (17)	0.0155 (15)	-0.0012 (13)	0.0013 (13)	0.0001 (13)
C18	0.0218 (17)	0.0160 (16)	0.0307 (18)	0.0002 (13)	0.0111 (15)	0.0019 (13)
C23	0.0266 (18)	0.0220 (17)	0.0259 (17)	0.0037 (13)	0.0094 (14)	0.0089 (13)
B1	0.0192 (18)	0.0107 (16)	0.0141 (17)	0.0007 (13)	0.0022 (14)	-0.0022 (13)

Geometric parameters (Å, °)

O2—C8	1.360 (3)	C2—H2	0.95
O2—B1	1.471 (3)	C19—C18	1.372 (4)
C7—N1	1.497 (3)	C19—H19	0.95
C7—C6	1.504 (3)	C3—C4	1.382 (4)
C7—H7A	0.99	C3—H3	0.95
C7—H7B	0.99	C26—C25	1.389 (4)
O1—C1	1.372 (3)	C26—H26	0.95
O1—B1	1.446 (3)	C5—C4	1.387 (3)
N1—C14	1.501 (3)	C5—H5	0.95
N1—C21	1.517 (3)	C9—C10	1.370 (4)
N1—B1	1.674 (4)	C9—H9	0.95
N2—C23	1.343 (3)	C16—C17	1.381 (4)
N2—C22	1.348 (3)	C16—H16	0.95
C1—C6	1.378 (3)	C12—C11	1.381 (3)
C1—C2	1.396 (3)	C12—H12	0.95
C15—C20	1.396 (3)	C4—H4	0.95
C15—C16	1.396 (3)	C25—C24	1.374 (3)
C15—B1	1.602 (4)	C25—H25	0.95
C6—C5	1.395 (3)	C17—C18	1.383 (3)
C8—C13	1.391 (3)	C17—H17	0.95
C8—C9	1.391 (3)	C10—C11	1.391 (4)
C22—C26	1.383 (3)	C10—H10	0.95
C22—C21	1.513 (3)	C21—H21A	0.99
C20—C19	1.394 (4)	C21—H21B	0.99
C20—H20	0.95	C24—C23	1.371 (3)
C14—C13	1.501 (3)	C24—H24	0.95
C14—H14A	0.99	C11—H11	0.95
C14—H14B	0.99	C18—H18	0.95
C13—C12	1.391 (3)	C23—H23	0.95
C2—C3	1.380 (3)		
C8—O2—B1	121.39 (18)	C22—C26—C25	119.4 (2)
N1—C7—C6	111.9 (2)	C22—C26—H26	120.3
N1—C7—H7A	109.2	C25—C26—H26	120.3
C6—C7—H7A	109.2	C4—C5—C6	120.8 (3)
N1—C7—H7B	109.2	C4—C5—H5	119.6

C6—C7—H7B	109.2	C6—C5—H5	119.6
H7A—C7—H7B	107.9	C10—C9—C8	120.3 (2)
C1—O1—B1	120.8 (2)	C10—C9—H9	119.9
C7—N1—C14	108.67 (19)	C8—C9—H9	119.9
C7—N1—C21	110.68 (18)	C17—C16—C15	122.9 (2)
C14—N1—C21	110.23 (16)	C17—C16—H16	118.6
C7—N1—B1	107.64 (16)	C15—C16—H16	118.6
C14—N1—B1	108.46 (18)	C11—C12—C13	121.2 (2)
C21—N1—B1	111.07 (19)	C11—C12—H12	119.4
C23—N2—C22	116.7 (2)	C13—C12—H12	119.4
O1—C1—C6	121.5 (2)	C3—C4—C5	119.5 (3)
O1—C1—C2	118.0 (2)	C3—C4—H4	120.3
C6—C1—C2	120.5 (2)	C5—C4—H4	120.3
C20—C15—C16	115.9 (2)	C24—C25—C26	118.6 (2)
C20—C15—B1	122.7 (2)	C24—C25—H25	120.7
C16—C15—B1	121.2 (2)	C26—C25—H25	120.7
C1—C6—C5	119.0 (2)	C16—C17—C18	119.5 (3)
C1—C6—C7	121.8 (2)	C16—C17—H17	120.3
C5—C6—C7	119.1 (2)	C18—C17—H17	120.3
O2—C8—C13	121.4 (2)	C9—C10—C11	120.4 (2)
O2—C8—C9	118.4 (2)	C9—C10—H10	119.8
C13—C8—C9	120.3 (2)	C11—C10—H10	119.8
N2—C22—C26	122.3 (2)	C22—C21—N1	113.5 (2)
N2—C22—C21	116.5 (2)	C22—C21—H21A	108.9
C26—C22—C21	121.2 (2)	N1—C21—H21A	108.9
C19—C20—C15	121.9 (3)	C22—C21—H21B	108.9
C19—C20—H20	119	N1—C21—H21B	108.9
C15—C20—H20	119	H21A—C21—H21B	107.7
C13—C14—N1	112.13 (17)	C23—C24—C25	118.5 (3)
C13—C14—H14A	109.2	C23—C24—H24	120.8
N1—C14—H14A	109.2	C25—C24—H24	120.8
C13—C14—H14B	109.2	C12—C11—C10	119.2 (3)
N1—C14—H14B	109.2	C12—C11—H11	120.4
H14A—C14—H14B	107.9	C10—C11—H11	120.4
C8—C13—C12	118.6 (2)	C19—C18—C17	119.7 (3)
C8—C13—C14	121.8 (2)	C19—C18—H18	120.1
C12—C13—C14	119.6 (2)	C17—C18—H18	120.1
C3—C2—C1	119.9 (3)	N2—C23—C24	124.5 (3)
C3—C2—H2	120.1	N2—C23—H23	117.8
C1—C2—H2	120.1	C24—C23—H23	117.8
C18—C19—C20	120.1 (3)	O1—B1—O2	108.95 (17)
C18—C19—H19	120	O1—B1—C15	109.5 (2)
C20—C19—H19	120	O2—B1—C15	113.0 (2)
C2—C3—C4	120.3 (2)	O1—B1—N1	107.1 (2)
C2—C3—H3	119.8	O2—B1—N1	104.5 (2)
C4—C3—H3	119.8	C15—B1—N1	113.46 (17)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C2—H2 \cdots O1 ⁱ	0.95	2.57	3.503 (3)	168
C24—H24 \cdots O2 ⁱⁱ	0.95	2.50	3.185 (3)	129

Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $x, y-1, z$.