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The influence of the axial group on the crystal structures of boron subphthalocyanines

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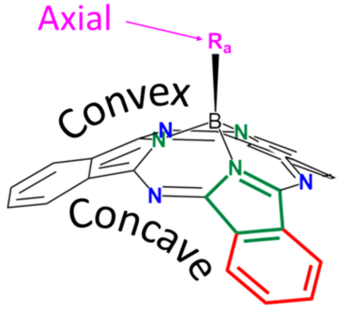
The crystal structures of 16 boron subphthalocyanines (BsubPcs) with structurally diverse axial groups were analyzed and compared to elucidate the impact of the axial group on the intermolecular π–π interactions, axial-group interactions, axial bond length and BsubPc bowl depth. π–π interactions between the isoindole units of adjacent BsubPc molecules most often involve concave–concave packing, whereas axial-group interactions with adjacent BsubPc molecules tend to favour the convex side of the BsubPc bowl. Furthermore, axial groups that contain O and/or F atoms tend to have significant hydrogen-bonding interactions, while axial groups containing arene site(s) can participate in π–π interactions with the BsubPc bowl, both of which can strongly influence the crystal packing. Bulky axial groups did tend to disrupt the π–π interactions and/or axial-group interactions, preventing some of the close packing that is seen in BsubPcs with less bulky axial groups. The atomic radius of the heteroatom bonded to boron directly influences the axial bond length, whereas the axial group has minimal impact on the BsubPc bowl depth. Finally, the crystal growth method did not generally appear to have a significant impact on the solid-state arrangement, with the exception of water occasionally being incorporated into crystal structures when hygroscopic solvents were used. These insights can help with the design and fine-tuning of the solid-state structures of BsubPcs as they continue to be developed as functional materials in organic electronics.

1. Introduction

Boron subphthalocyanines (BsubPcs) are a class of nonplanar aromatic organic compounds with a unique bowl-shaped structure. The BsubPcs are homologues of the phthalocyanine (Pc) family and are comprised of three diiminoisoindole units templated around a boron chelation centre (Fig. 1) (Claessens *et al.*, 2014). An additional substituent bonded to boron protrudes from the convex side of the bowl and is known as the axial group (Farac *et al.*, 2023; Zigelstein & Bender, 2024). BsubPcs were first synthesized accidentally by Meller and Ossko in 1972 when trying to incorporate boron as the central atom in a phthalocyanine (Pc) (Grant *et al.*, 2019; Meller & Ossko, 1972). Instead of the anticipated planar macrocycle with four repeating diiminoisoindole units that is a part of the Pc structure, they discovered Cl-BsubPc as a purple nonplanar compound with three diiminoisoindole units around the boron centre, with chlorine in the axial position [Fig. 1(*c*)] (Grant *et al.*, 2019). The characteristic nonplanar shape of BsubPcs is caused by the atomic radius of boron being slightly larger than the cavity it occupies (Morse & Bender, 2012*a*). Numerous BsubPc derivatives have been synthesized in the ~50 years since their discovery, with many physical properties, including



the solid-state arrangement, being influenced by substitution at the axial and/or peripheral positions of the BsubPc macrocycle (Morse *et al.*, 2014). The unique optical, electronic and physical properties of BsubPcs, as well as the ability to tune these properties through axial and/or peripheral derivatization, have led to the development of these materials for organic electronic applications, such as organic photovoltaics (OPVs) (Grant *et al.*, 2019; Mutolo *et al.*, 2006), organic light-emitting diodes (OLEDs) (Morse & Bender, 2012*a*: Morse *et al.*, 2010) and organic thin film transistors (OTFTs) (Yasuda & Tsutsui, 2006).

BsubPcs are typically employed in the solid state as photoactive materials in organic electronics, sparking the interest in using X-ray diffraction (XRD) to study the intermolecular interactions that impact their solid-state arrangements (Virdo *et al.*, 2016). The solid-state arrangement of BsubPcs can be described by the molecular fragment interactions between neighbouring BsubPcs and the relative alignment of the isoindoline fragments, with π–π interactions commonly being seen between adjacent BsubPcs in the crystal structure (Bukuroshi *et al.*, 2019). These interactions can provide information on the charge-transfer properties of BsubPcs, which is important for their application as organic semiconductors (Castrucci *et al.*, 2012).

In this study, single crystals were grown of an array of BsubPcs with structurally diverse axial groups (Fig. 2) to investigate how the axial group impacts the π–π interactions of BsubPcs in the solid state and explore the intermolecular interactions that involve the axial group. The influence of the axial group on the BsubPc bowl depth and axial bond length is also of interest. While crystal structures of some of the BsubPcs investigated in this study have been reported previously, past studies have largely focused on smaller subsets of axial substituents, such as halide (Fulford *et al.*, 2012), phenoxy (Paton *et al.*, 2011) or sulfonate (Paton *et al.*, 2012) derivatives, but different functional groups are rarely compared to each other. A review paper from Lavarda *et al.* (2022) provides a general summary of the crystal behaviour of axial halide, aryl and aryloxy derivatives, but the discussion does not extend to other boron–oxygen-bonded derivatives or include any boron–sulfur- or boron–nitrogen-bonded derivatives, and the crystals are from multiple laboratories. Therefore, herein, we provide the first report of a systematic comparison of BsubPc crystal structures with a comprehensive set of axial substituents, including halide (**1** and **2**), alkoxy (**3**–**8**), phenoxy (**9** and **10**), carboxylate (**11** and **12**), siloxy (**13**), thiophenoxy (**14** and **15**) and amino (**16**) derivatives. Furthermore, we report new polymorphs of some BsubPcs and use different crystal growth methods than have been reported previously.

2. Experimental

2.1. Materials and instrumentation

Toluene, heptane, acetone, dichloromethane (DCM), hexanes, tetrahydrofuran (THF) and pentane were purchased from Caledon Laboratories (Caledon, Ontario, Canada) and used as received. All X-ray crystal structure data were collected using a Bruker Kappa APEX DUO CMOS Photon II diffractometer. Experimental and refinement details are provided in Table 1. Structural analysis was conducted using *Mercury* software (Macrae *et al.*, 2020).

2.2. Synthesis and crystal growth

Briefly, with the exception of Br- and Cl-BsubPc, all other axially substituted BsubPcs were synthesized through an axial exchange reaction with Br-BsubPc and the appropriate nucleophile. In general, the axial exchange reactions were run in anhydrous chlorobenzene with 5–10 equivalents of the nucleophile at 75 °C until all of the Br-BsubPc was consumed, as monitored by high-performance liquid chromatography (HPLC). Full detailed synthetic procedures and characterization by ^{1}H NMR and ^{19}F NMR spectroscopy, direct analysis in real-time high-resolution mass spectrometry (DART-HRMS) and HPLC for the BsubPcs analysed within this study are provided in a recent publication (Zigelstein & Bender, 2024).

The train sublimation apparatus that was used to grow several of the crystals analysed in this study has been described previously (Morse *et al.*, 2010; Virdo *et al.*, 2016). For crystals grown by slow vapour diffusion of heptane into toluene, 5–10 mg of material was dissolved in toluene in a 20 ml scintillation vial. The vial was then suspended in a sealed jar containing ∼150 ml of heptane and left undisturbed for 2–4 weeks until crystals were seen. For crystals grown by slow evaporation of a common organic solvent (*i.e.* acetone or methanol), 5–10 mg of material was dissolved in solvent in a 20 ml scintillation vial. The vial was then covered with aluminium foil with 3–5 holes poked through and left undisturbed until crystals were seen. For crystals grown during a two-solvent recrystallization, the material was dissolved in THF, and pentane was added dropwise until crystals formed out of solution. These crystals were then collected by gravity filtration. Finally, some crystals formed after rotary evaporation to remove DCM/hexanes after purification by column chromatography on standard basic alumina. The crystal growth method used for each compound is provided in Table 1.

2.3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

3. Results and discussion

Single crystals of 16 axially substituted BsubPcs were grown by either train sublimation, slow vapour diffusion of heptane into toluene, slow evaporation of an organic solvent (*i.e.* acetone or methanol), two-solvent recrystallization or formed during rotary evaporation to remove solvent following purification by column chromatography. The influence of the axial group on

Table 1
Experimental details.

Experiments were carried out using a Bruker Kappa APEX DUO CMOS Photon II diffractometer at 150 K. H-atom parameters were constrained. Absorption was corrected for by multi-scan methods (*SADABS*; Krause *et al.*, 2015).

	Cl-BsubPc (**1**)	Br-BsubPc (**2**)	MeO-BsubPc (**3**)	EtO-BsubPc (**4-I**)
CCDC Deposition No.	2363922	2363923	2363924	2363925
Crystallization method	Sublimation (405 °C)	Sublimation (350 °C)	Sublimation (300 °C)	Sublimation (295 °C)
Crystal data				
Chemical formula	$C_{24}H_{12}BClN_6$	$C_{24}H_{12}BBrN_6$	$C_{25}H_{15}BN_6O$	$C_{26}H_{17}BN_6O$
M_r	430.66	475.12	426.24	440.26
Crystal system, space group	Orthorhombic, *Pnma*	Orthorhombic, *Pnma*	Orthorhombic, *Pnma*	Monoclinic, $P2_1/n$
a, b, c (Å)	12.0315 (10), 14.8174 (13), 10.3002 (8)	12.0010 (6), 15.0617 (8), 10.3879 (5)	12.3162 (11), 15.2325 (19), 10.4151 (10)	9.0313 (14), 14.220 (2), 16.474 (2)
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 102.667 (4), 90
V (Å^3)	1836.3 (3)	1877.67 (16)	1953.9 (4)	2064.3 (5)
Z	4	4	4	4
Radiation type	Cu $K\alpha$	Mo $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.07	2.22	0.75	0.09
Crystal size (mm)	0.15 × 0.06 × 0.02	0.27 × 0.16 × 0.14	0.10 × 0.04 × 0.02	0.21 × 0.12 × 0.03
Data collection				
T_{min}, T_{max}	0.646, 0.753	0.688, 0.746	0.659, 0.753	0.684, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19930, 1647, 1416	23127, 2243, 1955	27808, 1762, 1570	49575, 4744, 3311
R_{int}	0.061	0.027	0.057	0.101
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.593	0.650	0.592	0.650
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.097, 1.06	0.021, 0.057, 1.09	0.032, 0.078, 1.08	0.047, 0.098, 1.04
No. of reflections	1647	2243	1762	4744
No. of parameters	151	151	159	308
No. of restraints	0	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.35	0.38, −0.26	0.22, −0.19	0.21, −0.23

	EtO-BsubPc (**4-II**)	F_3EtO-BsubPc (**5**)	ButO-BsubPc (**6**)	tButO-BsubPc (**7**)
CCDC Deposition No.	2363926	2363927	2363928	2363929
Crystallization method	Slow evaporation – acetone	Sublimation (305 °C)	Sublimation (265 °C)	Rotovap – DCM/hexanes
Crystal data				
Chemical formula	$C_{26}H_{17}BN_6O$	$C_{26}H_{14}BF_3N_6O$	$C_{28}H_{21}BN_6O$	$C_{28}H_{21}BN_6O$
M_r	440.26	494.24	468.32	468.32
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$	Orthorhombic, *Pbca*	Monoclinic, $P2_1/c$
a, b, c (Å)	9.0304 (5), 14.2423 (8), 16.4452 (9)	10.4664 (6), 15.4986 (8), 14.3171 (8)	14.6398 (8), 15.2842 (9), 20.5313 (12)	14.3815 (7), 8.2702 (4), 19.8660 (9)
α, β, γ (°)	90, 102.476 (3), 90	90, 110.221 (3), 90	90, 90, 90	90, 102.074 (2), 90
V (Å^3)	2065.1 (2)	2179.3 (2)	4594.0 (5)	2310.55 (19)
Z	4	4	8	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.72	0.96	0.68	0.68
Crystal size (mm)	0.15 × 0.15 × 0.10	0.14 × 0.09 × 0.04	0.15 × 0.07 × 0.06	0.17 × 0.09 × 0.02
Data collection				
T_{min}, T_{max}	0.654, 0.753	0.624, 0.753	0.661, 0.753	0.673, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	46104, 3555, 3148	39716, 3759, 3043	45733, 3951, 3295	41764, 3994, 3363
R_{int}	0.059	0.083	0.065	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.593	0.594	0.594	0.594
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.102, 1.05	0.039, 0.107, 1.04	0.038, 0.095, 1.07	0.035, 0.089, 1.05
No. of reflections	3555	3759	3951	3994
No. of parameters	308	335	326	329
No. of restraints	0	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.50, −0.21	0.27, −0.28	0.33, −0.22	0.22, −0.17

	OctO-BsubPc (**8**)	PhO-BsubPc (**9**)	Naphthoxy-BsubPc (**10**)	Acetate-BsubPc (**11**)
CCDC Deposition No.	2363930	2363931	2363932	2363933
Crystallization method	Slow Evaporation – methanol	SVD – toluene/heptane	Sublimation (315 °C)	Sublimation (290 °C)
Crystal data				
Chemical formula	$6C_{32}H_{29}BN_6O{\cdot}0.5H_2O$	$C_{30}H_{17}BN_6O$	$C_{34}H_{19}BN_6O$	$C_{26}H_{15}BN_6O_2$

Table 1 (continued)

	OctO-BsubPc (**8**)	PhO-BsubPc (**9**)	Naphthoxy-BsubPc (**10**)	Acetate-BsubPc (**11**)
M_r	3166.55	488.30	538.36	454.25
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Orthorhombic, *Pnma*	Triclinic, $P\overline{1}$
a, *b*, *c* (Å)	15.3028 (7), 16.2278 (7), 17.3604 (7)	10.0268 (10), 10.7263 (12), 11.8090 (13)	17.133 (3), 13.929 (2), 10.3669 (16)	9.3432 (9), 9.3548 (7), 12.3322 (12)
α, β, γ (°)	103.045 (3), 105.716 (3), 94.022 (3)	85.879 (4), 77.440 (3), 66.151 (3)	90, 90, 90	104.203 (2), 100.751 (3), 90.701 (2)
V (Å^3)	4003.0 (3)	1133.6 (2)	2474.0 (7)	1024.69 (16)
Z	1	2	4	2
Radiation type	Cu $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.65	0.09	0.09	0.10
Crystal size (mm)	0.24 × 0.16 × 0.06	0.28 × 0.15 × 0.09	0.26 × 0.15 × 0.08	0.24 × 0.22 × 0.13
Data collection				
T_{min}, T_{max}	0.622, 0.753	0.687, 0.746	0.609, 0.746	0.710, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	110436, 13816, 10618	26461, 5137, 3795	17347, 2963, 1878	21123, 4670, 3665
R_{int}	0.070	0.052	0.092	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.594	0.649	0.650	0.650
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.149, 1.05	0.039, 0.095, 1.03	0.052, 0.119, 1.05	0.038, 0.096, 1.03
No. of reflections	13816	5137	2963	4670
No. of parameters	1201	343	217	317
No. of restraints	499	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.61, −0.39	0.22, −0.23	0.26, −0.28	0.32, −0.28

	Benzoate-BsubPc (**12**)	TMSO-BsubPc (**13**)	F_5PhS-BsubPc (**14**)	MePhS-BsubPC (**15**)
CCDC Deposition No.	2363934	2363935	2363936	2363937
Crystallization method	Sublimation (355 °C)	Rotovap – DCM/hexanes	SVD – toluene/heptane	SVD – toluene/heptane
Crystal data				
Chemical formula	$C_{31}H_{17}BN_6O_2$	$C_{27}H_{21}BN_6OSi$	$C_{30}H_{12}BF_5N_6S$	$C_{31}H_{19}BN_6S$
M_r	516.31	484.40	594.33	518.39
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$	Monoclinic, $C2/c$
a, *b*, *c* (Å)	15.671 (2), 11.1920 (13), 15.2363 (19)	16.343 (3), 11.9655 (16), 12.5059 (19)	10.7010 (5), 11.8651 (6), 22.4968 (13)	49.653 (4), 12.1268 (10), 27.559 (2)
α, β, γ (°)	90, 115.386 (4), 90	90, 99.996 (11), 90	95.863 (2), 92.861 (2), 115.433 (2)	90, 114.838 (4), 90
V (Å^3)	2414.3 (5)	2408.4 (6)	2552.1 (2)	15059 (2)
Z	4	4	4	24
Radiation type	Mo $K\alpha$	Cu $K\alpha$	Mo $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.09	1.13	0.20	1.41
Crystal size (mm)	0.30 × 0.15 × 0.12	0.19 × 0.15 × 0.01	0.35 × 0.24 × 0.05	0.28 × 0.27 × 0.02
Data collection				
T_{min}, T_{max}	0.685, 0.746	0.629, 0.753	0.713, 0.746	0.633, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	49333, 5530, 4050	57016, 4230, 2990	75917, 11711, 7793	12819, 12819, 10107
R_{int}	0.071	0.127	0.073	0.091
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.608	0.650	0.594
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.095, 1.03	0.054, 0.123, 1.05	0.043, 0.102, 1.02	0.098, 0.242, 1.09
No. of reflections	5530	4230	11711	12819
No. of parameters	361	326	775	1059
No. of restraints	0	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.24	0.31, −0.24	0.39, −0.31	0.89, −0.57

	PhMeN-BsubPc (**16-I**)	PhMeN-BsubPc (**16-II**)
CCDC Deposition No.	2363938	2363939
Crystallization method	Recrystallization – THF/pentane	Recrystallization – THF/pentane
Crystal data		
Chemical formula	$C_{31}H_{20}BN_7{\cdot}0.14H_2O$	$C_{31}H_{20}BN_7$
M_r	503.87	501.35
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$
a, *b*, *c* (Å)	11.4897 (5), 11.7489 (5), 19.3046 (8)	10.3502 (4), 20.7509 (8), 12.2816 (5)
α, β, γ (°)	73.348 (2), 81.941 (2), 76.167 (2)	90, 114.734 (2), 90
V (Å^3)	2417.05 (18)	2395.80 (17)
Z	4	4

Table 1 (continued)

	PhMeN-BsubPc (**16-I**)	PhMeN-BsubPc (**16-II**)
Radiation type	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.68	0.68
Crystal size (mm)	0.20 × 0.15 × 0.08	0.19 × 0.14 × 0.09
Data collection		
T_{min}, T_{max}	0.657, 0.753	0.462, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	60606, 8275, 7193	41606, 4159, 3432
R_{int}	0.046	0.111
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.592	0.595
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.093, 1.06	0.055, 0.165, 1.06
No. of reflections	8275	4159
No. of parameters	713	354
No. of restraints	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.29	0.28, −0.35

Computer programs: *APEX4* (Bruker, 2021), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2019* (Sheldrick, 2015*b*), *PLATON* (Spek, 2020) and *SHELXTL* (Sheldrick, 2008).

the intermolecular interactions, bowl depths and axial bond lengths was analysed and is discussed below.

3.1. Intermolecular interactions

The previously established method for describing the intermolecular π–π interactions of BsubPcs uses some unique terminology for the side of the BsubPc bowl being considered and the alignment of isoindole units between adjacent BsubPcs (Morse *et al.*, 2014; Virdo *et al.*, 2016; Claessens *et al.*, 2014; Farac *et al.*, 2024). First, the terms concave and convex are used to describe the side of the BsubPc bowl being considered, with concave being the 'inside' of the bowl and convex being the outer surface of the bowl [Fig. 1(*c*)]. Furthermore, the three outermost six-membered carbon rings of the BsubPc are called 'heads', while the six-membered rings containing the boron centre, one imine N atom and two pyrrole N atoms are called 'tails' [Fig. 1(*b*)] (Virdo *et al.*, 2016). With these terms, the intermolecular π–π interactions of BsubPcs can be described as concave–concave, convex–convex, concave–convex, head-to-head, tail-to-tail and head-to-tail (Morse *et al.*, 2010, 2014). Interactions between the axial ligand and BsubPc π-system are also sometimes observed and are described as concave-to-axial ligand and convex-to-axial ligand (Morse *et al.*, 2010, 2014). Distances less than 4 Å are considered significant intermolecular π–π interactions (Fulford *et al.*, 2012). All interactions involving a π-group are measured to the centroid of that group. Other interactions are considered significant if the intermolecular distance between the two atoms is less than the sum of the van der Waals radii of the two atoms (Virdo *et al.*, 2013). For example, weak hydrogen bonds with C—H···O, C—H···F and C—H···N contacts are characterized by H···O, H···F and H···N distances less than 2.72, 2.67 and 2.75 Å, respectively. Furthermore, C—H···halogen bonds are characterized by H···Cl and H···Br distances that are less than 2.95 and 3.05 Å, respectively.

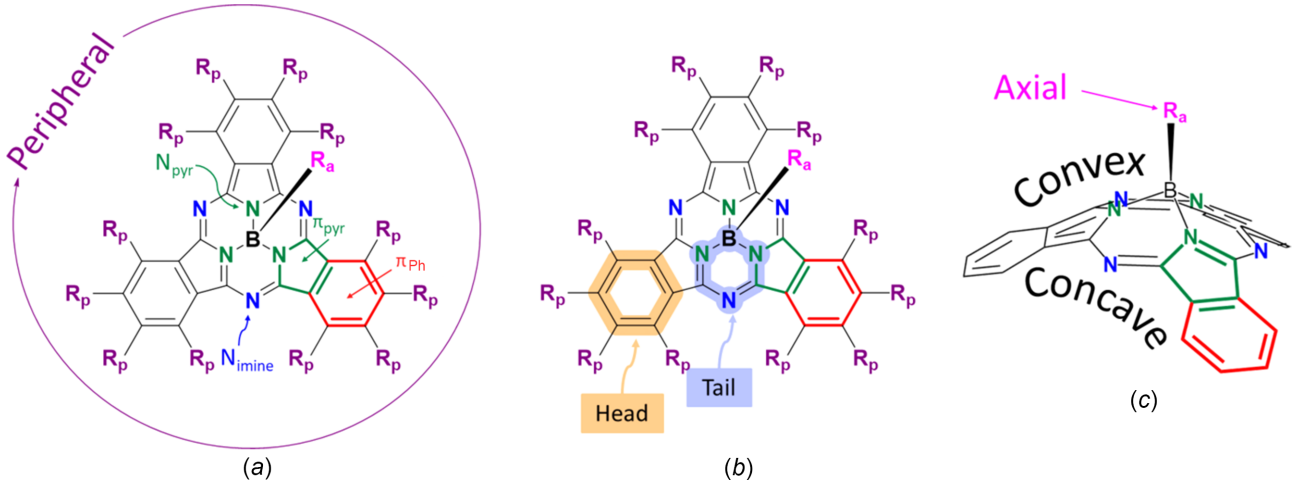


Figure 1
(*a*) General 2D structure of the BsubPc unit with key terms labelled, including the peripheral substituents (R_p), imine (N_{imine}) and pyrrole (N_{pyr}) N atoms, and different π units (π_{Ph} in red and π_{pyr} in green). (*b*) General 2D structure of the BsubPc unit with 'head' (orange highlight) and 'tail' (purple highlight) labelled. (*c*) General 3D structure of the BsubPc unit with the axial substituent (R_a) and concave/convex sides of the bowl labelled. The peripheral substituents have been omitted from the 3D structure for clarity.

3.1.1. Axially halogenated BsubPcs. The crystal structure of Cl-BsubPc [**1**; Fig. 3(*a*)] from train sublimation grown in this study shows good agreement with the previously reported structure (Virdo *et al.*, 2016). It arranges in the orthorhombic *Pnma* space group, with four molecules in the unit cell [Fig. 3(*b*)] **[see Note 2]**. There are significant convex–convex head-to-head interactions, with a π_{pyr}–π_{Ph} distance (pyr is pyrrole and Ph is phenyl) of 3.615 Å, and less significant concave–concave head-to-tail interactions, with an intermolecular distance of 4.150 Å. There are also C—H···halogen interactions between the axial Cl and a π_{Ph} H atom of an adjacent molecule (C—H_{Ph}···Cl—B) at an intermolecular distance of 2.893 Å. Upon extension of the unit cell, there are convex-to-axial ligand halogen–π (B—Cl···π_{Ph}) interactions, with an intermolecular distance of 3.548 Å. The intermolecular interactions of Cl-BsubPc (**1**) are shown in Fig. 3(*c*).

It has been reported previously that a Br-BsubPc [**2**; Fig. 4(*a*)] crystal cannot be grown by train sublimation because the boron–bromine axial bond (B—Br) is not thermally stable at its sublimation temperature (Fulford *et al.*, 2012; Hildebrand *et al.*, 2022). However, within this study, we were able to obtain a sublimed crystal of Br-BsubPc during the attempted purification of TMSO-BsubPc (**13**) by train sublimation (350 °C), as there was some unreacted Br-BsubPc remaining in the crude product from the TMSO-BsubPc axial exchange reaction, and therefore was separated and crystallized during train sublimation. Like Cl-BsubPc, Br-BsubPc arranges in the orthorhombic *Pnma* space group, with four molecules in the unit cell [Fig. 4(*b*)], which is consistent with the previously reported Br-BsubPc crystal structure using solvent-based crystal growth methods (Fulford *et al.*, 2012). The intermolecular interactions observed in the Br-BsubPc crystal

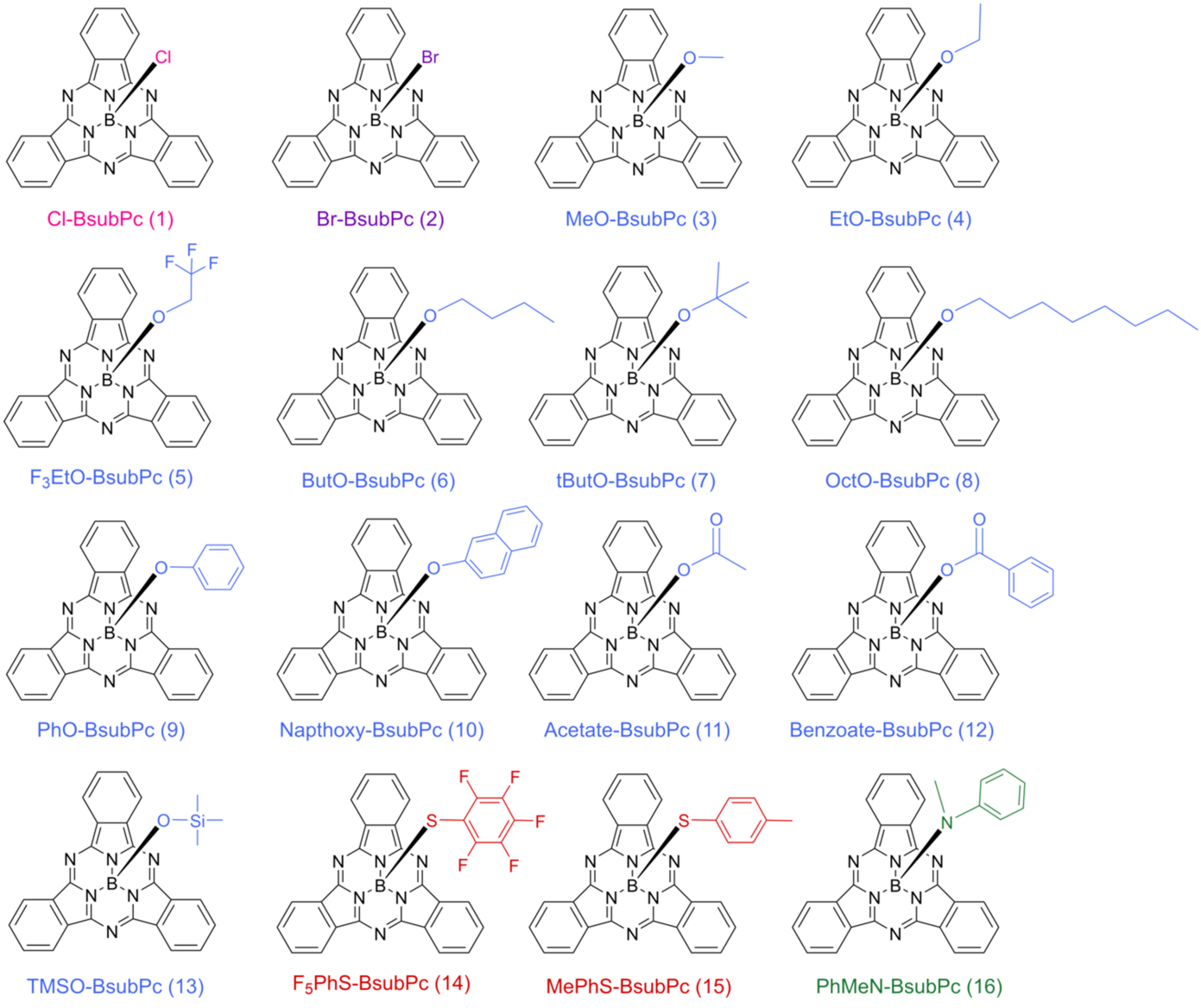


Figure 2
2D structures of investigated axially substituted BsubPcs with the colour of the axial group representing the heteroatom bonded to boron, *i.e.* chlorine – pink, bromine – purple, oxygen – blue, sulfur – red and nitrogen – green.

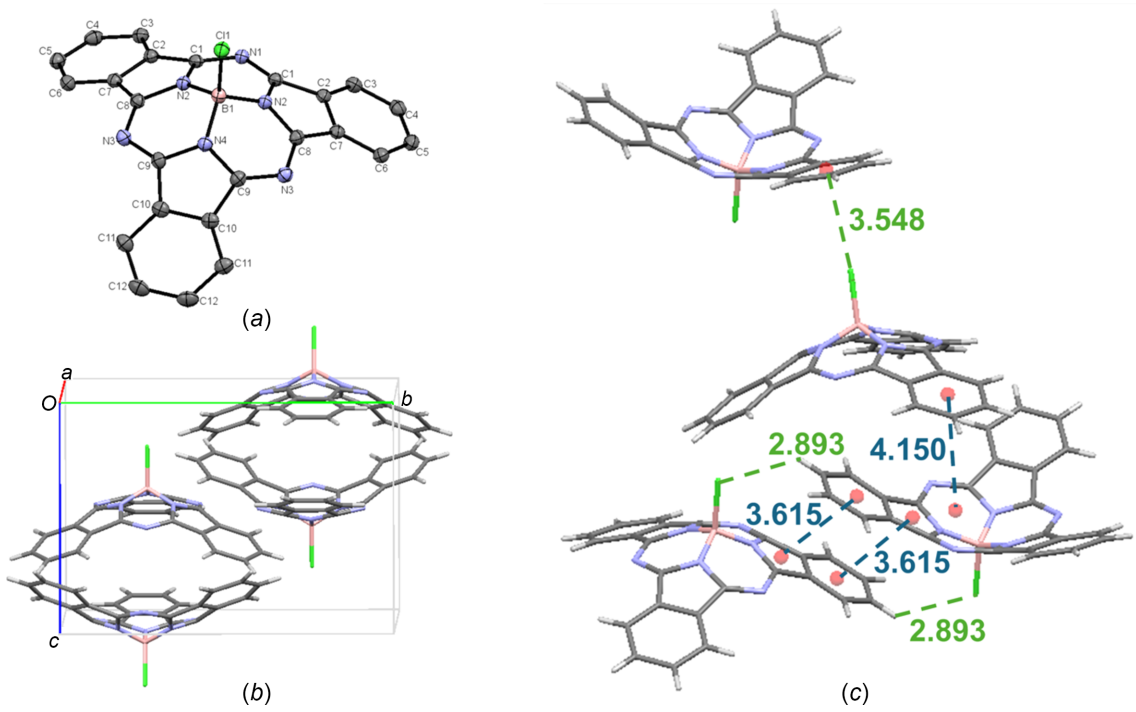


Figure 3
(*a*) The molecular structure of Cl-BsubPc (**1**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and chlorine – green.

structure are very similar to those of the Cl-BsubPc crystal structure. Within the unit cell, Br-BsubPc displays concave–concave head-to-tail packing, with an intermolecular distance of 4.151 Å, which is nearly identical to the distance observed for Cl-BsubPc. Upon extension outside the unit cell, more significant π–π interactions are seen, with convex–convex head-to-head interactions between adjacent molecules at a π_{pyr}–π_{Ph} distance of 3.661 Å. There are also C—H···halogen

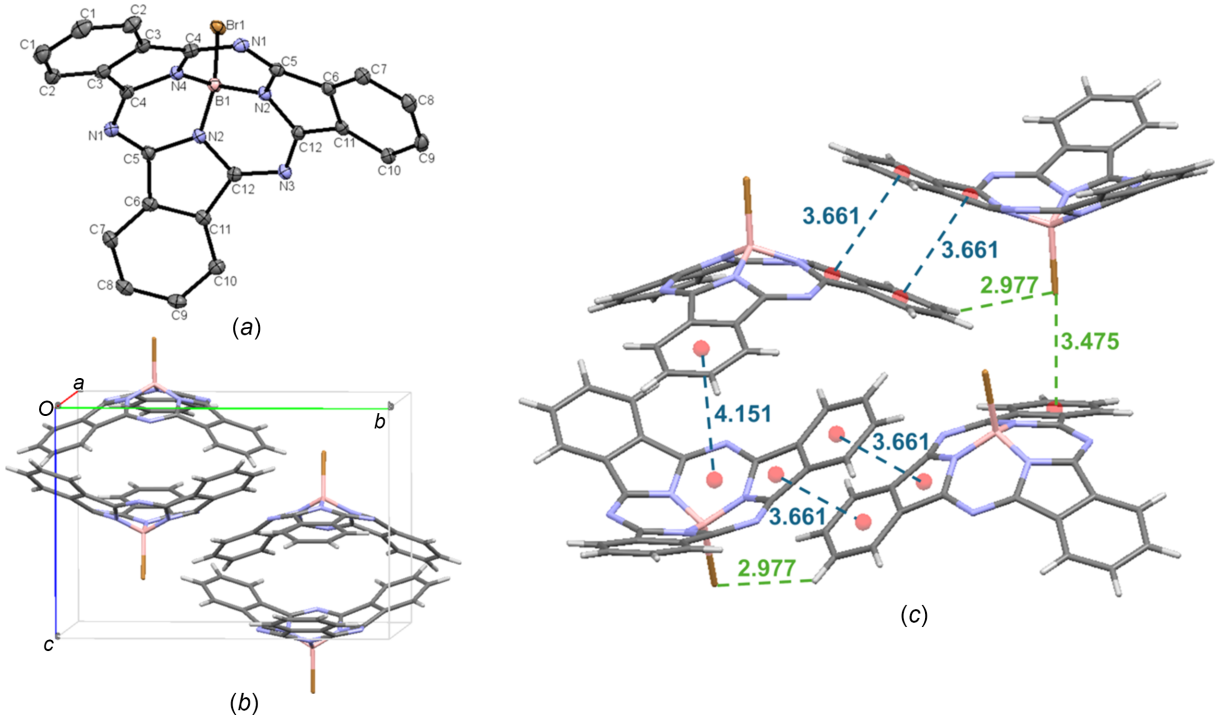


Figure 4
(*a*) The molecular structure of Br-BsubPc (**2**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and bromine – bronze.

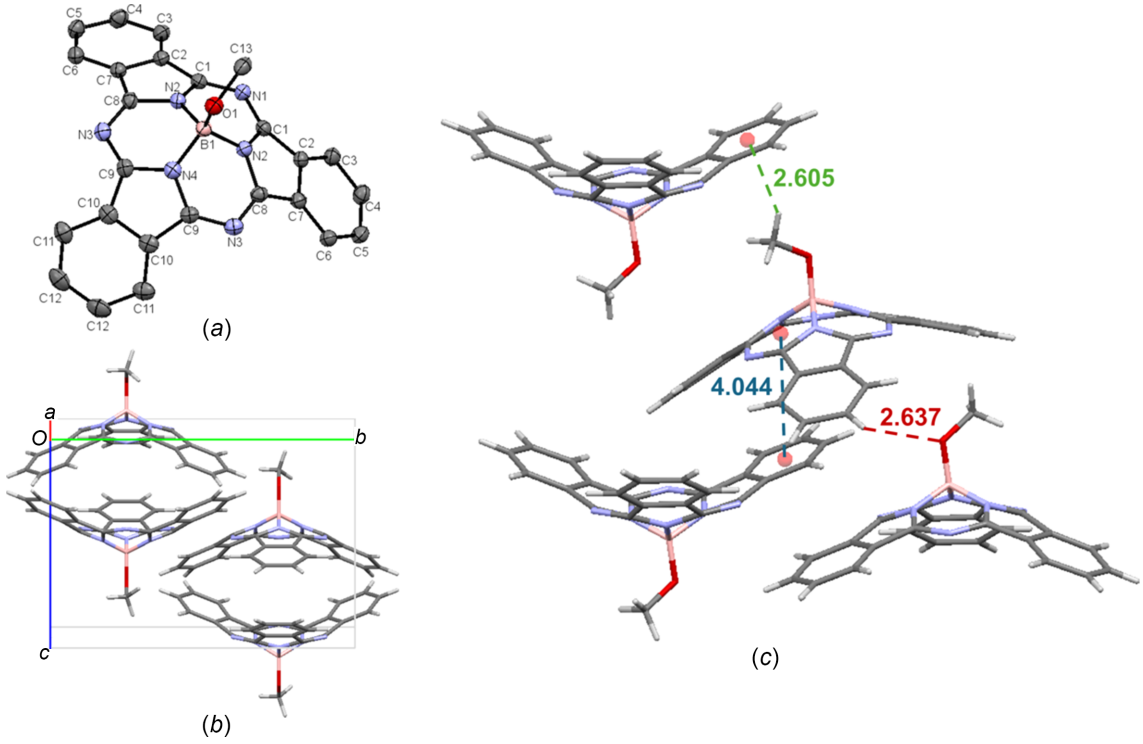


Figure 5
(*a*) The molecular structure of MeO-BsubPc (**3**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue, weak hydrogen bonds are shown in red and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

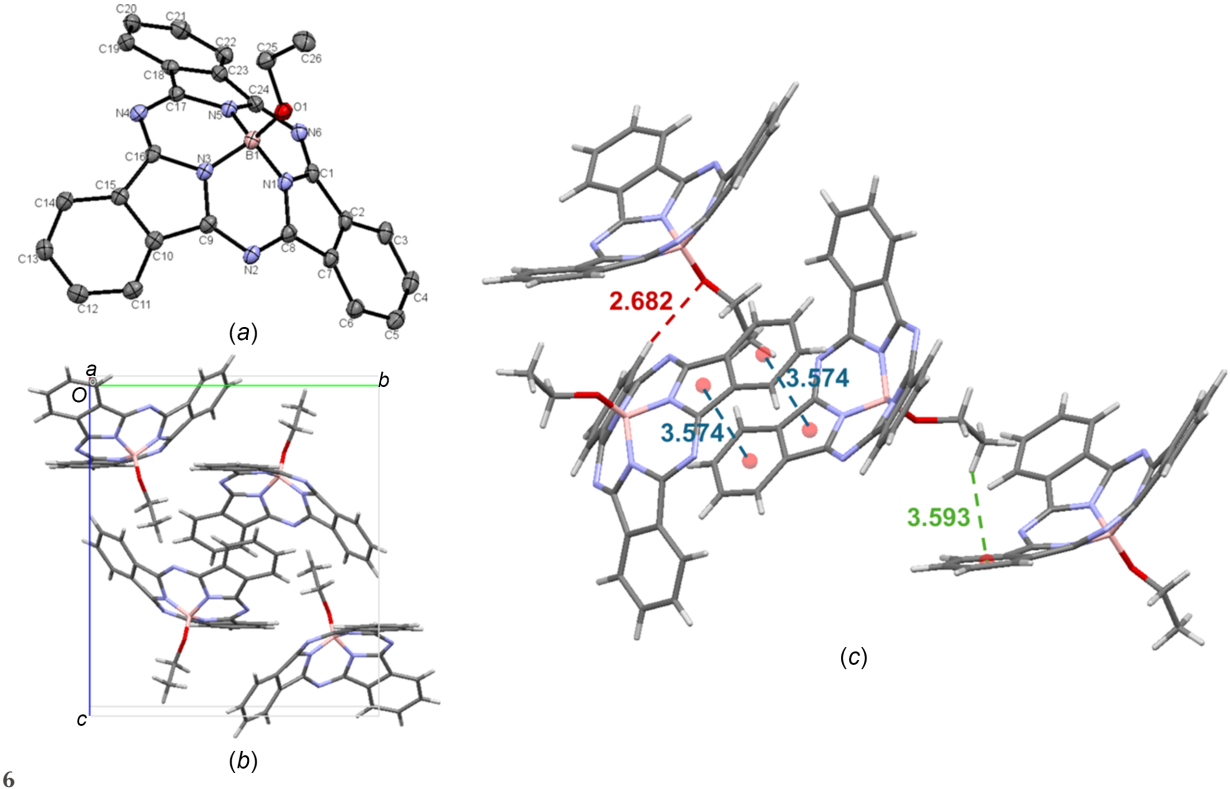


Figure 6
(*a*) The molecular structure of EtO-BsubPc (**4-I**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue, weak hydrogen bonds are shown in red and all other interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

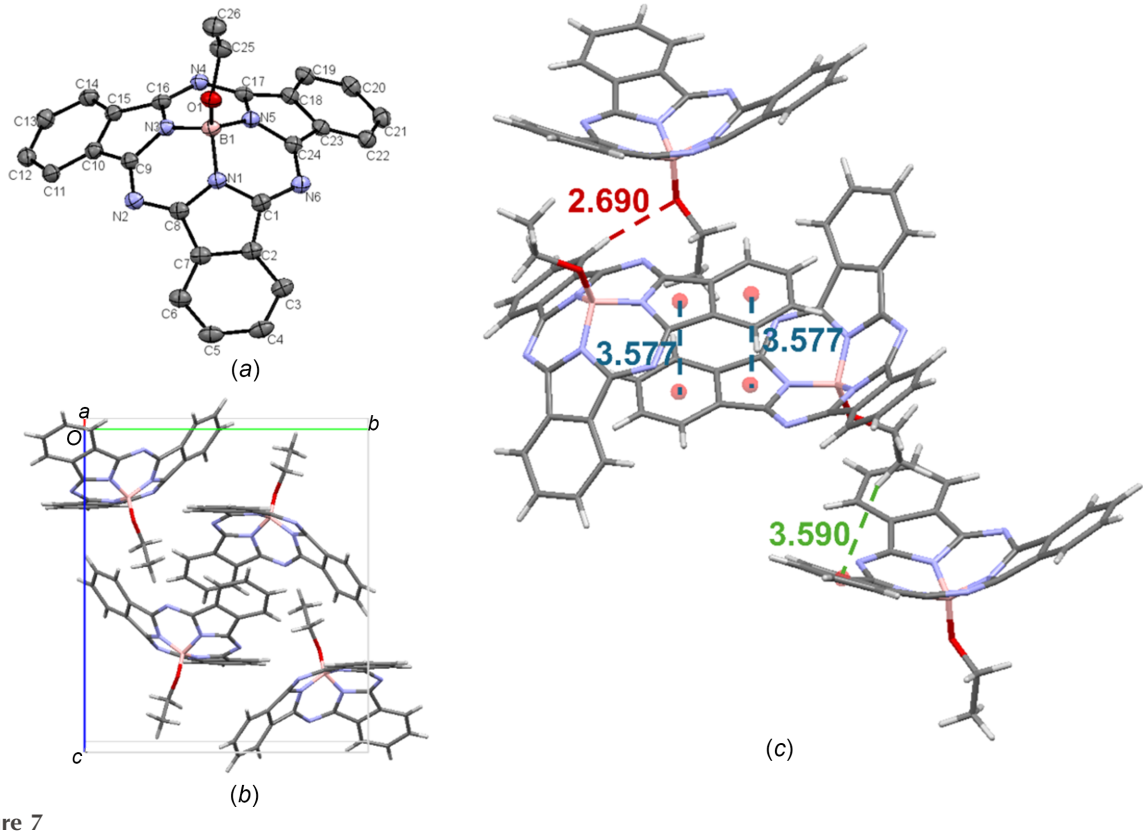


Figure 7
(*a*) The molecular structure of EtO-BsubPc (**4-II**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue, weak hydrogen bonds are shown in red and all other interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

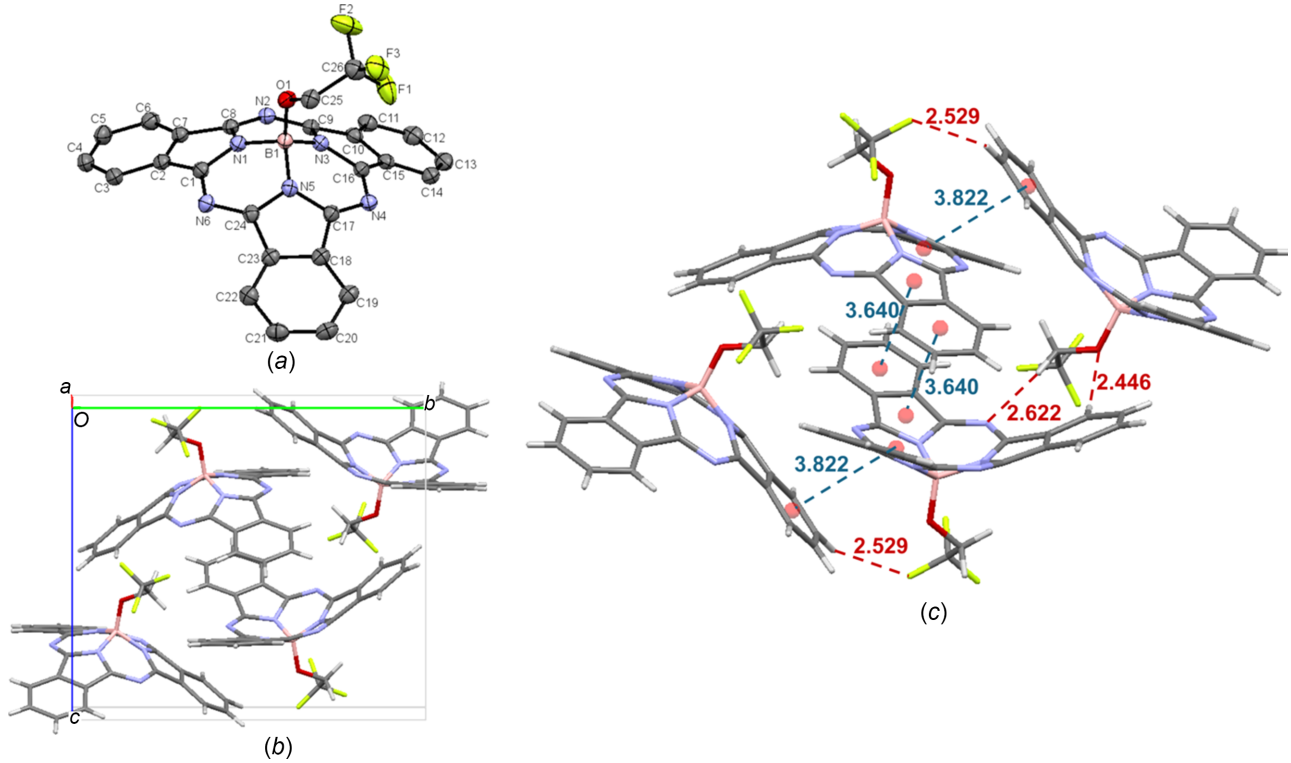


Figure 8
(*a*) The molecular structure of F_3EtO-BsubPc (**5**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue and weak hydrogen bonds are shown in red. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink, oxygen – red and fluorine – green.

interactions between the axial Br atom and an adjacent π_{Ph} H atom (C—H_{Ph}···Br—B), with an intermolecular distance of 2.977 Å, which is slightly longer than what is seen in the Cl-BsubPc crystal structure due to the larger size of bromine compared to chlorine. Convex-to-axial ligand halogen–π (B—Br···π_{Ph}) interactions are also observed, with an intermolecular distance of 3.475 Å. This is shorter than the distance observed for the analogous interaction for Cl-BsubPc. The intermolecular interactions of Br-BsubPc (**2**) are shown in Fig. 4(*c*).

3.1.2. Axial boron–oxygen-bonded BsubPcs. Crystals of MeO-BsubPc [**3**; Fig. 5(*a*)] were grown by train sublimation and arranged in the orthorhombic *Pnma* space group, with four molecules in the unit cell [Fig. 5(*b*)]. The only π–π interactions are weak concave–concave head-to-tail interactions, with an intermolecular distance of 4.044 Å. There is weak hydrogen bonding between the axial O atom and an adjacent π_{Ph} H atom (C—H_{Ph}···O—B), with an intermolecular distance of 2.637 Å. Extending beyond the unit cell, there is a convex-to-axial ligand C—H_{ax}···π_{Ph} interaction, with an intermolecular distance of 2.605 Å. The intermolecular interactions of MeO-BsubPc (**3**) are shown in Fig. 5(*c*).

Crystals of EtO-BsubPc (**4**) were grown in two ways: train sublimation [**4-I**; Fig. 6(*a*)] and slow evaporation of acetone (**4-II**). The crystal structure was the same by both crystal growth methods. EtO-BsubPc is the only compound in the array that crystallizes in the monoclinic $P2_1/n$ space group. Starting with **4-I**, there are four molecules in the unit cell [Fig. 6(*b*)] and the only π–π interactions are concave–concave head-to-head interactions, with a π_{pyr}–π_{Ph} distance of 3.574 Å. There is weak hydrogen bonding between the axial O atom and an adjacent π_{Ph} H atom (C—H_{Ph}···O—B), with an intermolecular distance of 2.682 Å, which is slightly longer than the analogous distance for MeO-BsubPc. Extending beyond the unit cell, there is a concave-to-axial ligand C_{26}—H_{ax}···π_{Ph} interaction, with an intermolecular distance of 3.593 Å. EtO-BsubPc is the only compound in the array with this type of interaction. The intermolecular interactions of EtO-BsubPc (**4-I**) are shown in Fig. 6(*c*).

As mentioned above, the crystal structure of EtO-BsubPc from slow evaporation of acetone [**4-II**; Fig. 7(*a*)] was the same as the crystal structure from train sublimation (**4-I**), arranging in the monoclinic $P2_1/n$ space group, with four molecules in the unit cell [Fig. 7(*b*)]. Identical intermolecular interactions were seen for **4-I** and **4-II**, with very modest differences in the intermolecular distances. The concave–concave head-to-head π_{pyr}–π_{Ph} distance for **4-II** (3.577 Å) was slightly longer than for **4-I** (3.574 Å), whereas the concave-to-axial ligand C_{26}—H_{ax}···π_{Ph} intermolecular distance for **4-II** (3.590 Å) was slightly shorter than for **4-I** (3.593 Å). Lastly, the weak hydrogen bonding between the axial O atom and an adjacent π_{Ph} H atom (C—H_{Ph}···O—B) for **4-II** (2.690 Å) was at a slightly longer intermolecular distance than for **4-I** (2.682 Å). The intermolecular interactions of EtO-BsubPc (**4-II**) are shown in Fig. 7(*c*).

F_3EtO-BsubPc [**5**; Fig. 8(*a*)] crystals were grown by train sublimation, organizing in the monoclinic $P2_1/c$ space group, with four molecules in the unit cell [Fig. 8(*b*)]. Similar to EtO-

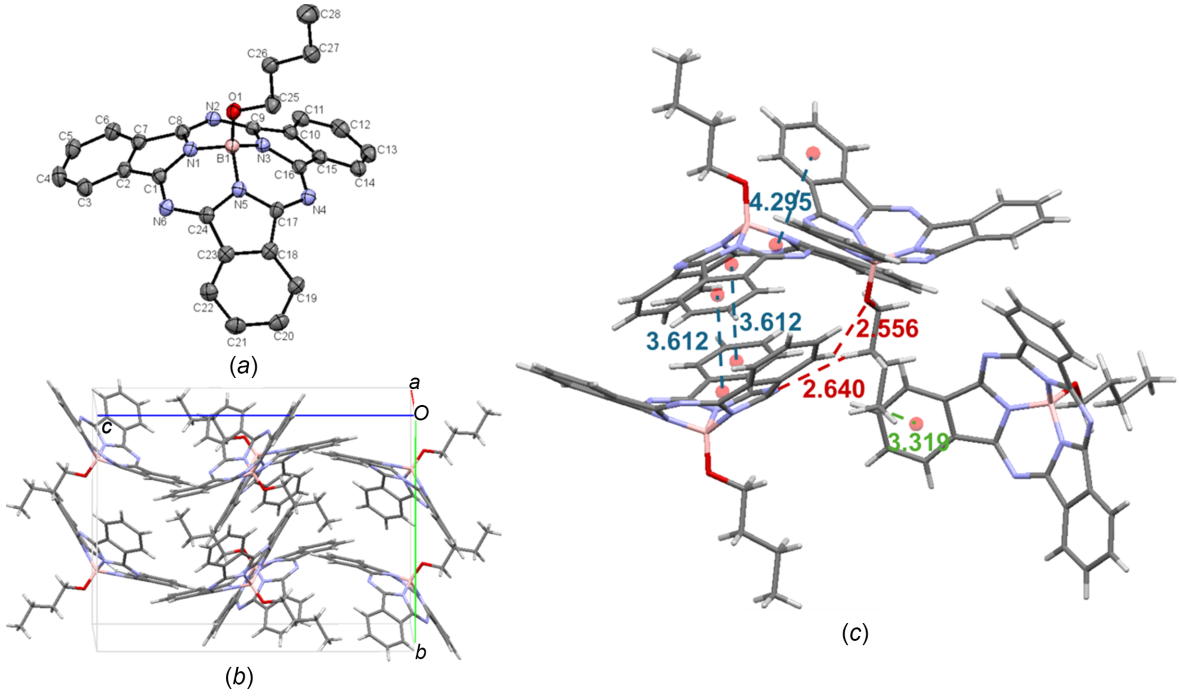


Figure 9
(*a*) The molecular structure of ButO-BsubPc (**6**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue, weak hydrogen bonds are shown in red and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

BsubPc, the most significant π–π interactions are concave–concave head-to-head interactions, although the π_{pyr}–π_{Ph} distance is slightly longer at 3.640 Å. Unlike EtO-BsubPc, convex–convex head-to-tail interactions are observed, with an intermolecular distance of 3.822 Å. The axial group also has significant interactions, with weak hydrogen bonding between the axial O atom and an adjacent π_{Ph} H atom ($C-H_{Ph}\cdots O-B$ = 2.446 Å), an axial F atom with an adjacent π_{Ph} H atom ($C-H_{Ph}\cdots F-C$ = 2.529 Å) and an axial methylene H atom with an adjacent imine N atom ($C_{25}-H_{ax}\cdots N_{imine}$ = 2.622 Å). F_3EtO-BsubPc is the only alkoxy derivative that does not contain any concave- or convex-to-axial ligand interactions, indicating that when H atoms are replaced with F atoms, weak hydrogen bonding dominates over axial–π interactions. The intermolecular interactions of F_3EtO-BsubPc (**5**) are shown in Fig. 8(*c*).

ButO-BsubPc [**6**; Fig. 9(*a*)] is the only compound in the array to crystallize in the orthorhombic *Pbca* space group, with eight molecules in the unit cell [Fig. 9(*b*)]. There are significant concave–concave head-to-head interactions, with a π_{pyr}–π_{Ph} distance of 3.612 Å, and less significant convex–convex head-to-tail interactions, with an intermolecular distance of 4.295 Å. There are also significant interactions involving the axial group, including weak hydrogen bonding between the axial O atom and a neighbouring π_{Ph} H atom ($C-H_{Ph}\cdots O-B$ = 2.556 Å), and between an axial methylene H atom and an adjacent imine N atom ($C_{26}-H_{ax}\cdots N_{imine}$ = 2.640 Å). There is also a convex-to-axial ligand $C_{28}-H_{ax}\cdots\pi_{Ph}$ interaction between an axial methyl H atom and the π_{Ph} group of a neighbouring molecule (3.319 Å). The intermolecular interactions of ButO-BsubPc (**6**) are shown in Fig. 9(*c*).

tButO-BsubPc [**7**; Fig. 10(*a*)] arranges in the monoclinic $P2_1/c$ space group, with four molecules in the unit cell [Fig. 10(*b*)]. Within the unit cell, the only significant π–π interaction is a concave–concave head-to-head interaction, with a π_{pyr}–π_{Ph} distance of 3.564 Å, which is shorter than the distance observed for EtO-BsubPc (**4**), F_3EtO-BsubPc (**5**) and ButO-BsubPc (**6**). Upon extension of the unit cell, there is a convex-to-axial ligand $C_{27}-H_{ax}\cdots\pi_{Ph}$ interaction between an axial H atom and an adjacent π_{Ph} group (3.057 Å). No hydrogen bonding is observed for tButO-BsubPc. The intermolecular interactions of tButO-BsubPc (**7**) are shown in Fig. 10(*c*).

A diffraction-quality crystal of OctO-BsubPc (**8**) was difficult to obtain, likely due to the length of the axial alkyl chain preventing close packing of neighbouring molecules. After several unsuccessful attempts to grow crystals by train sublimation and solvent-based methods, such as slow evaporation and slow vapour diffusion, diffraction-quality crystals of OctO-BsubPc were successfully grown by slow evaporation of methanol, arranging in the triclinic $P\overline{1}$ space group. There are three independent OctO-BsubPc molecules in the asymmetric unit, which are referred to as **8-A** [Fig. 11(*a*)], **8-B** [Fig. 11(*b*)] and **8-C** [Fig. 11(*c*)], and 0.5 molecules of water for every three molecules of OctO-BsubPc [Fig. 11(*d*)]. **8-B** and **8-C** have disorder in the octyl chains. Within the unit cell, there appears to be concave–convex head-to-head packing between **8-A** and **8-B**, although the alignment is not perfect. The two π_{pyr}–π_{Ph} distances between adjacent molecules are not the same, at 3.628 and 3.673 Å. There also appears to be a concave–convex head-to-tail interaction between **8-A** and **8-C**, with an intermolecular distance of 3.890 Å, but again, the alignment is not

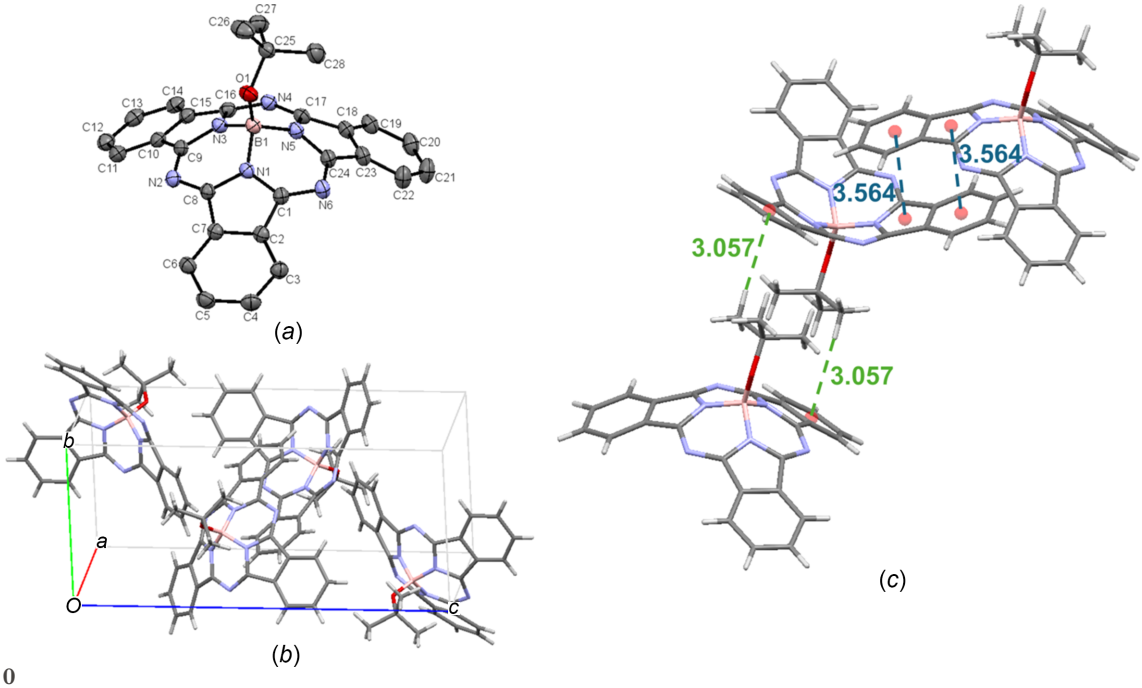


Figure 10
(*a*) The molecular structure of tButO-BsubPc (**7**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

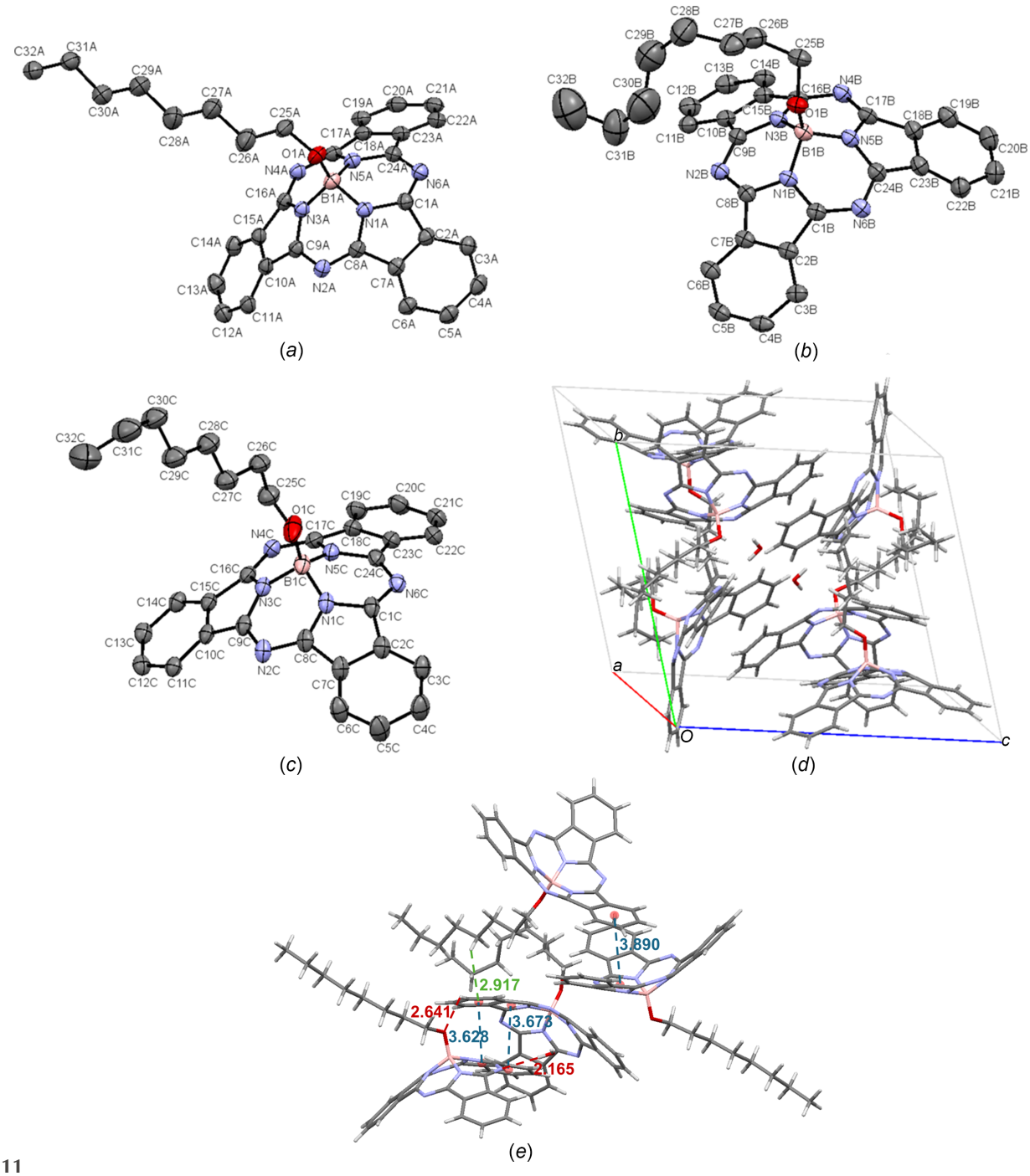


Figure 11
The molecular structures of (*a*) OctO-BsubPc molecule *A* (**8-A**), (*b*) OctO-BsubPc molecule *B* (**8-B**) and (*c*) OctO-BsubPc molecule *C* (**8-C**), with displacement ellipsoids drawn at the 50% probability and H atoms removed for clarity. (*d*) The unit-cell packing of **8** and (*e*) significant intermolecular interactions in the crystal structure of **8**. π–π interactions are shown in blue, strong and weak hydrogen bonds are shown in red, and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

perfect between the two adjacent molecules. The length of the axial octyl chain is likely responsible for the lack of perfect alignment. There is weak hydrogen bond between the axial O atom of **8-A** and a π_{Ph} H atom of the adjacent **8-B** molecule (C—H_{Ph}···O—B), with an intermolecular distance of 2.641 Å. There is also hydrogen bonding between a water molecule and the imine N atom of an adjacent **8-A** molecule (2.165 Å). Lastly, convex-to-axial ligand C—H···π interactions are observed between an axial H atom of **8-C** and the π_{Ph} group of **8-B**, with a C—H_{ax}···π_{Ph} distance of 2.971 Å. The intermolecular interactions of OctO-BsubPc (**8**) are shown in Fig. 11(*e*).

Crystals of PhO-BsubPc [**9**; Fig. 12(*a*)] were grown by slow vapour diffusion of heptane into toluene, arranging in the triclinic $P\overline{1}$ space group, with two molecules in the unit cell [Fig. 12(*b*)], as was reported previously (Paton *et al.*, 2011). While there are no π–π interactions within the unit cell, upon

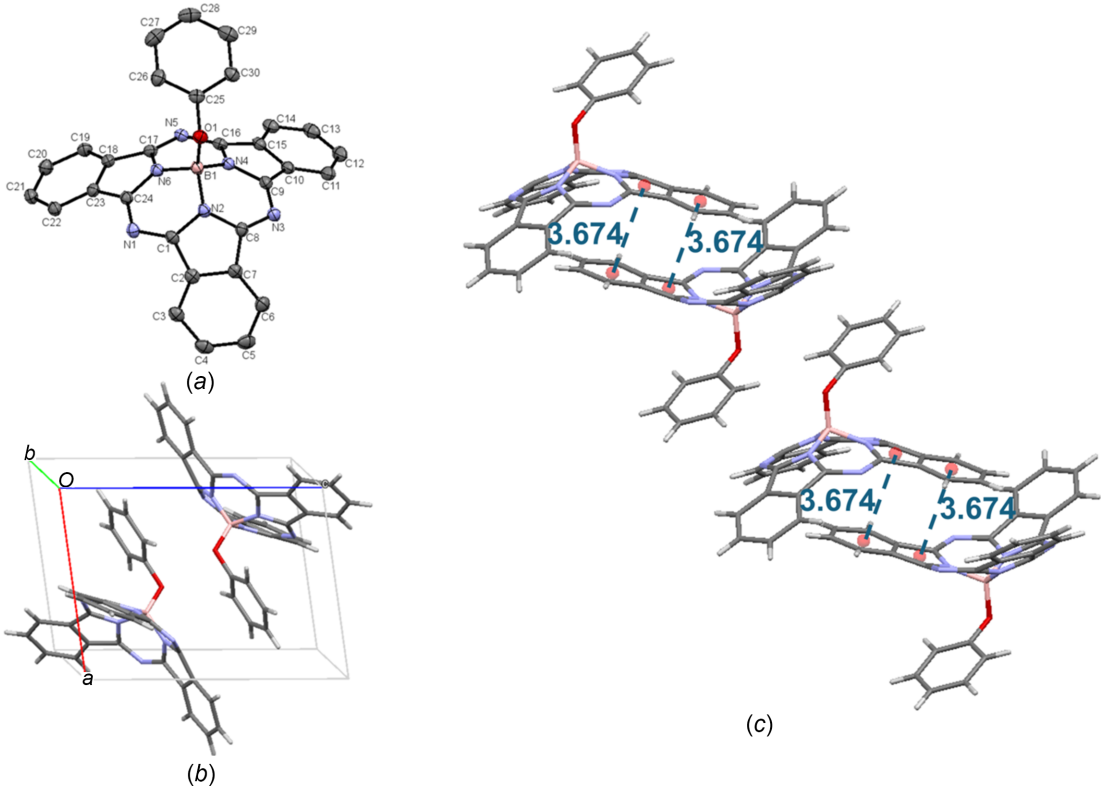


Figure 12
(*a*) The molecular structure of PhO-BsubPc (**9**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

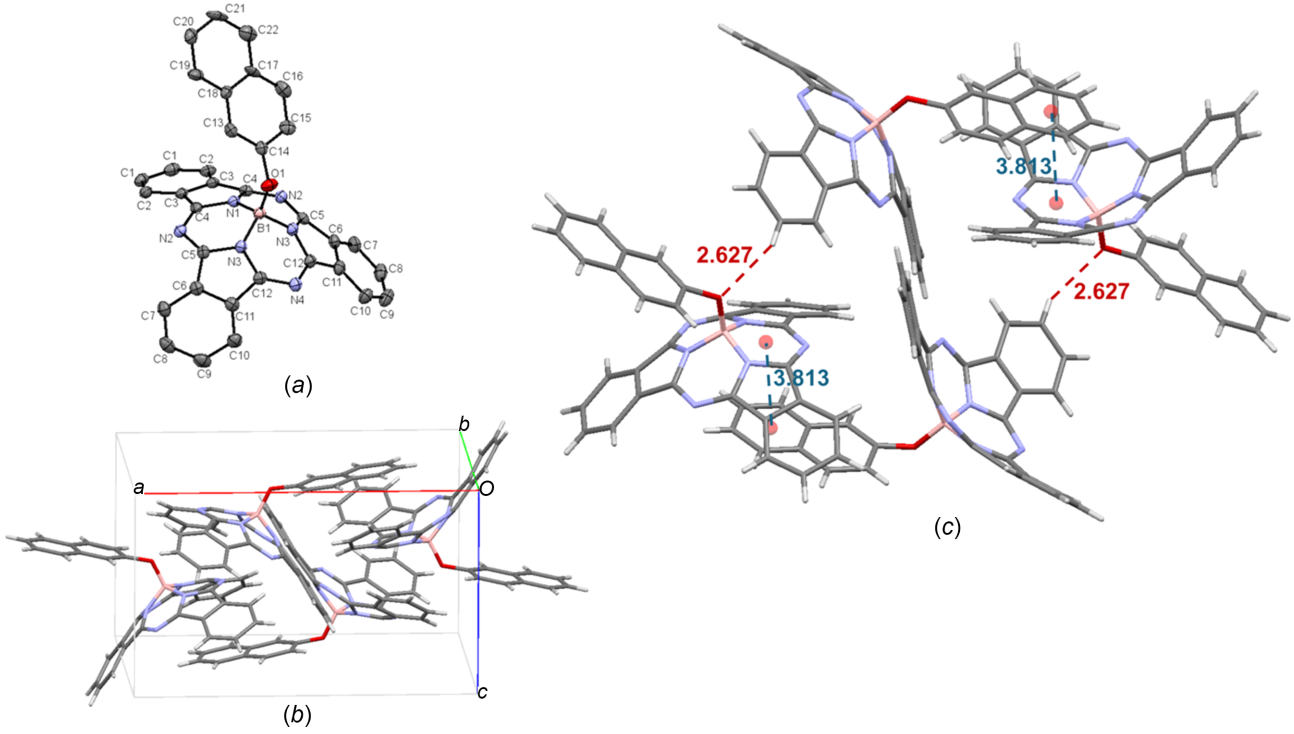


Figure 13
(*a*) The molecular structure of naphthoxy-BsubPc (**10**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue and weak hydrogen bonds are shown in red. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

extension, concave–concave head-to-head packing is observed, with a π_{pyr}–π_{Ph} distance of 3.674 Å. There do not appear to be any π–π interactions between the axial group and the isoindole groups of adjacent molecules, or any other interactions involving the axial group. The intermolecular interactions of PhO-BsubPc (**9**) are shown in Fig. 12(*c*).

Crystals of naphthoxy-BsubPc [**10**; Fig. 13(*a*)] were grown by train sublimation and the resulting crystal structure is identical to a previous report from our group (Paton *et al.*, 2013). Naphthoxy-BsubPc arranges in the orthorhombic *Pnma* space group, with four molecules in the unit cell [Fig. 13(*b*)]. The naphthoxy axial group causes a disruption in the π–π interactions of the isoindole units of neighbouring BsubPcs, instead containing concave-to-axial ligand π–π interactions between the centroid of the outer ring of the naphthoxy unit and the tail of the BsubPc, with an intermolecular distance of 3.813 Å. There is also weak hydrogen bonding between the axial O atom and a neighbouring π_{Ph} H atom (2.627 Å). The intermolecular interactions of naphthoxy-BsubPc (**10**) are shown in Fig. 13(*c*).

Moving on to the carboxylate derivatives (**11** and **12**), crystals of acetate-BsubPc [**11**; Fig. 14(*a*)] were grown by train sublimation, showing good agreement with the previously reported structure from slow vapour diffusion of heptane into toluene (Lessard & Bender, 2013). Acetate-BsubPc crystallizes in the triclinic $P\overline{1}$ space group, with two molecules in the unit cell [Fig. 14(*b*)]. Packing within the unit cell appears to be largely dictated by the axial-group interactions, with weak hydrogen bonding between the axial O atom and an adjacent π_{Ph} H atom (C—H_{Ph}···O—B = 2.581 Å), the axial carbonyl O atom and an adjacent π_{Ph} H atom (C—H_{Ph}···O═C = 2.628 Å), and an axial H atom and an adjacent imine N atom (C—H_{ax}···N_{imine} = 2.635 Å). The only π–π interactions observed in the unit cell are convex–convex tail-to-tail interactions, with an intermolecular distance of 3.897 Å. Looking beyond the unit cell, there are concave–concave head-to-head interactions, with a π_{pyr}–π_{Ph} distance of 3.620 Å. The intermolecular interactions of acetate-BsubPc (**11**) are shown in Fig. 14(*c*).

Crystals of benzoate-BsubPc [**12**; Fig. 15(*a*)] were grown by train sublimation, again showing good agreement with the previously reported structure from slow vapour diffusion of heptane into toluene (Lessard & Bender, 2013). Benzoate-BsubPc arranges in the monoclinic $P2_1/c$ space group, with four molecules in the unit cell [Fig. 15(*b*)], which is different from acetate-BsubPc. The benzoate axial group seems to disrupt the BsubPc π–π interactions, as only weak convex–convex head-to-tail interactions are observed, with an intermolecular distance of 4.163 Å. As with acetate-BsubPc, the most significant intermolecular interactions for benzoate-BsubPc involve the axial group. First, C—H_{Ph}···π_{ax} interactions are observed, with the closest intermolecular distances being 2.726 or 3.612 Å, depending on which molecules in the unit cell are being considered. Weak hydrogen bonding between the axial carbonyl O atom and adjacent π_{Ph} H atoms (C—H_{Ph}···O═C) is also observed, with intermolecular distances of 2.510 or 2.536 Å, depending on the molecules in the unit cell being considered. The intermolecular interactions of benzoate-BsubPc (**12**) are shown in Fig. 15(*c*).

The packing of the crystal of TMSO-BsubPc [**13**; Fig. 16(*a*)] is analogous to that of tButO-BsubPc (**7**), with the only

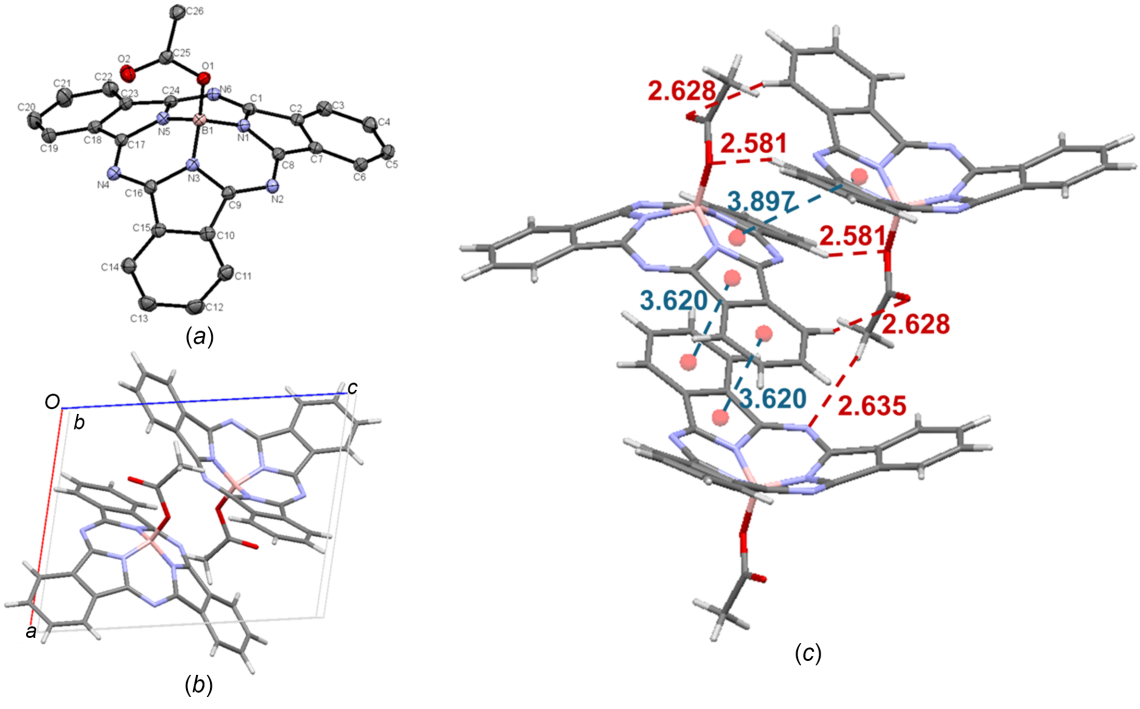


Figure 14
(*a*) The molecular structure of acetate-BsubPc (**11**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue and weak hydrogen bonds are shown in red. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

structural difference between the two compounds being the replacement of the quaternary C atom of the axial *tert*-butyl group in tButO-BsubPc with an Si atom in TMSO-BsubPc. The crystals of both compounds were grown serendipitously during rotary evaporation of DCM/hexanes following purification by column chromatography. Both arrange in the monoclinic $P2_1/c$ space group, with four molecules in the unit cell [Fig. 16(*b*)], and display concave–concave head-to-head packing. The intermolecular π_{pyr}–π_{Ph} distance for TMSO-BsubPc (3.543 Å) is slightly shorter than for tButO-BsubPc, while the convex-to-axial ligand $C_{26}—H_{ax}\cdots\pi_{Ph}$ interaction has a slightly longer intermolecular distance (3.070 Å) for TMSO-BsubPc than for tButO-BsubPc. There is also weak hydrogen bonding observed between an axial H atom and an adjacent π_{Ph} H atom ($C—H_{Ph}\cdots O—B$ = 2.478 Å), which is not observed for tButO-BsubPc. This may result from the longer bond length between oxygen and silicon (1.638 Å) in TMSO-BsubPc compared to oxygen and carbon (1.440 Å) in tButO-BsubPc, allowing for closer interactions with the axial O atom due to less steric hindrance directly around the O atom. The intermolecular interactions of TMSO-BsubPc (**13**) are shown in Fig. 16(*c*).

3.1.3. Axial boron–sulfur- and boron–nitrogen-bonded BsubPcs. Crystals of F_5PhS-BsubPc (**14**) were grown by slow vapour diffusion of heptane into toluene. There are two crystallographically independent molecules in the asymmetric unit, which are referred to as **14-A** [Fig. 17(*a*)] and **14-B** [Fig. 17(*b*)]. F_5PhS-BsubPc arranges in the triclinic $P\overline{1}$ space group, with four molecules in the unit cell [Fig. 17(*c*)]. Within the unit cell, there is concave–convex head-to-tail packing between **14-A** and **14-B**, with an intermolecular distance of 3.958 Å. Upon extension of the unit cell, significant concave-to-axial ligand π–π interactions are observed between the π_{Ph} group and the π_{ax} group, with an intermolecular distance of 3.525 Å. There is also an interaction between the axial S atom and the π_{ax} group of an adjacent molecule ($\pi_{ax}\cdots S—B$), at a distance of 3.560 Å. Finally, weak hydrogen bonding is observed between an axial F atom and an adjacent π_{Ph} H atom ($C—F_{ax}\cdots\pi_{Ph}$), at a distance of 2.546 Å. The intermolecular interactions of F_5PhS-BsubPc (**14**) are shown in Fig. 17(*d*).

MePhS-BsubPc (**15**) crystals were grown by slow vapour diffusion of heptane into toluene. There are three independent molecules in the asymmetric unit that are referred to as **15-A** [Fig. 18(*a*)], **15-B** [Fig. 18(*b*)] and **15-C** [Fig. 18(*c*)]. MePhS-BsubPc arranges in the monoclinic $C2/c$ space group, with 24 molecules in the unit cell [Fig. 18(*d*)]. This is a different polymorph than the previously reported crystal structure of MePhS-BsubPc (Morse & Bender, 2012*b*). With 24 molecules in the unit cell, many interactions are observed. First, there are concave–concave head-to-head interactions between two adjacent **15-A** molecules, with a π_{pyr}–π_{Ph} distance of 3.659 Å. Next, there are less significant concave–concave head-to-tail

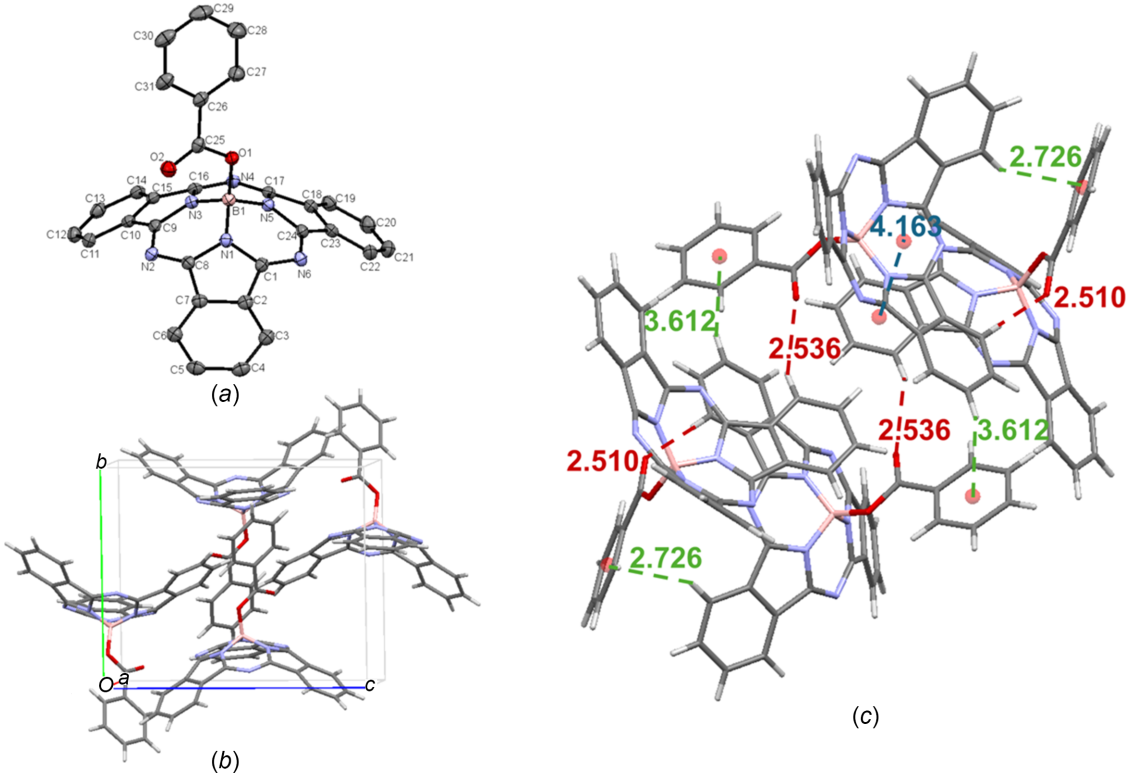


Figure 15
(*a*) The molecular structure of benzoate-BsubPc (**12**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue, weak hydrogen bonds are shown in red and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and oxygen – red.

Table 2
Summary of π–π interactions (Å), not including any axial-group interactions.

Axial group	Concave–concave		Convex–convex			Concave–convex	
	Head-to-head	Head-to-tail	Head-to-head	Head-to-tail	Tail-to-tail	Head-to-head	Head-to-tail
Cl (**1**)	–	4.150	3.615[a]	–	–	–	–
Br (**2**)	–	4.151	3.661[a]	–	–	–	–
MeO (**3**)	–	4.044	–	–	–	–	–
EtO (**4-I**)	3.574[a]	–	–	–	–	–	–
EtO (**4-II**)	3.577[a]	–	–	–	–	–	–
F_3EtO (**5**)	3.640[a]	–	–	3.822	–	–	–
ButO (**6**)	3.612[a]	–	–	4.295	–	–	–
tButO (**7**)	3.564[a]	–	–	–	–	–	–
OctO (**8**)	–	–	–	–	–	3.628[a], 3.673[a]	3.890
PhO (**9**)	3.674[a]	–	–	–	–	–	–
Naphthoxy (**10**)	–	–	–	–	–	–	–
Acetate (**11**)	3.620[a]	–	–	–	3.897	–	–
Benzoate (**12**)	–	–	–	4.163	–	–	–
TMSO (**13**)	3.543[a]	–	–	–	–	–	–
F_5PhS (**14**)	–	–	–	–	–	–	3.958
MePhS (**15**)	3.659[a]	4.040	3.577[a] 3.691[a] 3.537[b] 3.861[a] 3.934[a] 3.911[b]	–	–	–	–
PhMeN (**16-I**)	3.705[a]	–	–	–	–	–	–
PhMeN (**16-II**)	3.790[a]	–	–	–	–	–	–

Notes: (*a*) π_{pyr}–π_{Ph} distance; (*b*) π_{Ph}–π_{Ph} distance.

interactions between two adjacent **15-B** molecules at an intermolecular distance of 4.040 Å. There is also a slightly offset convex–convex head-to-head interaction between molecules **15-B** and **15-C**, with inconsistent π_{pyr}–π_{Ph} distances of 3.577 and 3.691 Å. The most significant overlap between isoindole groups in this interaction is between the adjacent π_{Ph} groups at a distance of 3.537 Å. A similar offset convex–convex head-to-head interaction is seen between **15-A** and **15-B**, with π_{pyr}–π_{Ph} distances of 3.861 and 3.934 Å, and a π_{Ph}–π_{Ph} distance of 3.911 Å. There are also some significant interactions with the axial group. First, there is a concave-to-axial ligand interaction between **15-B** and **15-C**, with a π–π interaction observed between the axial arene group of **15-B** and the 'tail' of **15-C** at a distance of 3.895 Å. There is also a convex-to-axial ligand interaction between the axial S atom of **15-A** and the π_{Ph} group of an adjacent **15-C** molecule ($\pi_{Ph}\cdots$S—B) at a distance of 3.786 Å. Finally, there is a C_{31}—$H_{ax}\cdots\pi_{ax}$ interaction between two adjacent **15-A** molecules involving an axial methyl H atom and an axial arene group at a distance of 2.876 Å. The intermolecular interactions of MePhS-BsubPc (**15**) are shown in Fig. 18(*e*).

On two separate occasions, crystals of PhMeN-BsubPc were grown during a two-solvent recrystallization with THF and pentane, resulting in two different polymorphs. The first polymorph [**16-I**; Fig. 19(*a*)] crystallized in the triclinic $P\overline{1}$ space group, with two molecules in the asymmetric unit [**16-I** (mol 1) and **16-I** (mol 2)] and a partial occupancy water solvent molecule [Fig. 19(*b*)], which is aligned with a previous report (Morse & Bender, 2012*b*). The second polymorph [**16-II**; Fig. 20(*a*)] crystallized in the monoclinic $P2_1/c$ space group, with only one molecule in the asymmetric unit and no water [Fig. 20(*b*)]. Both **16-I** and **16-II** have four molecules in the unit cell. Concave–concave head-to-head interactions were seen within the unit cell for **16-I**, with a π_{pyr}–π_{Ph} distance of 3.705 Å. There is also hydrogen bonding between the water molecule and the imine N atoms of two adjacent BsubPc molecules. Upon extension of the unit cell, there is a C—$H_{Ph,ax}\cdots\pi_{ax}$ interaction between adjacent axial groups, with an intermolecular distance of 3.048 Å. The intermolecular interactions of **16-I** are shown in Fig. 19(*c*).

For another crystal of PhMeN-BsubPc (**16-II**), there are no significant π–π interactions between adjacent isoindole units within the unit cell. The axial group appears to have a strong influence on the packing within the unit cell, with the most significant interactions being a convex-to-axial ligand C_{31}—$H_{ax}\cdots\pi_{Ph}$ interaction between an axial methyl H atom and the adjacent π_{Ph} group (2.816 Å). Upon extension of the unit cell, there are concave–concave head-to-head interactions, with a π_{Ph}–π_{pyr} distance of 3.790 Å, which is slightly longer than the analogous distance observed for **16-I**. The intermolecular interactions of **16-II** are shown in Fig. 20(*c*).

3.1.4. Intermolecular interactions summary. The π–π interactions observed in the crystal structures of the investigated BsubPcs are summarized in Table 2, and all intermolecular interactions involving the axial group are summarized in Table 3. Concave–concave head-to-head interactions were the most common π–π interactions in the analyzed BsubPcs, observed in 10 of the 17 crystal structures (Table 2). Head-to-head interactions, whether concave–concave, convex–convex or concave–convex, tend to display closer packing than head-to-tail interactions. Only MeO- (**3**), naphthoxy- (**10**), benzoate- (**12**) and F_5PhS-BsubPc (**14**) didn't display any head-to-head packing. Concave–convex interactions were rare, appearing only in the crystal structures of OctO- (**8**) and F_5PhS-BsubPc (**14**).

Table 3
Summary of intermolecular interactions (Å) involving the axial group.

Axial group	Convex-to-axial ligand		Concave-to-axial ligand			Hydrogen/halogen bonding				π_{ax} interactions		
	B—*A*···π_{Ph}	C—H_{ax}···π_{Ph}	π_{ax}–π_{tail}	π_{ax}–π_{Ph}	C—H_{ax}···π_{Ph}	B—*A*···H_{Ph}—C	C—H_{ax}···N_{imine}	C—F_{ax}···H_{Ph}—C	C=O_{ax}···H_{Ph}—C	C—H_{Ph}···π_{ax}	B—*A*···π_{ax}	C—H_{ax}···π_{ax}
Cl (**1**)	3.548	–	–	–	–	2.893[b]	–	–	–	–	–	–
Br (**2**)	3.475	–	–	–	–	2.977[b]	–	–	–	–	–	–
MeO (**3**)	–	2.605	–	–	–	2.637[a]	–	–	–	–	–	–
EtO (**4-I**)	–	–	–	–	3.593	2.682[a]	–	–	–	–	–	–
EtO (**4-II**)	–	–	–	–	3.590	2.690[a]	–	–	–	–	–	–
F_3EtO (**5**)	–	–	–	–	–	2.446[a]	2.622[a]	2.529[a]	–	–	–	–
ButO (**6**)	–	3.319	–	–	–	2.556[a]	2.640[a]	–	–	–	–	–
tButO (**7**)	–	3.057	–	–	–	–	–	–	–	–	–	–
OctO (**8**)	–	2.971	–	–	–	2.641[a]	–	–	–	–	–	–
PhO (**9**)	–	–	–	–	–	–	–	–	–	–	–	–
Naphthoxy (**10**)	–	–	3.813	–	–	2.627[a]	–	–	–	–	–	–
Acetate (**11**)	–	–	–	–	–	2.581[a]	2.635[a]	–	2.628[a]	–	–	–
Benzoate (**12**)	–	–	–	–	–	–	–	–	2.510[a], 2.536[a]	2.726, 3.612	–	–
TMSO (**13**)	–	3.070	–	–	–	2.478[a]	–	–	–	–	–	–
F_5PhS (**14**)	–	–	–	3.525	–	–	–	2.546[a]	–	–	3.560	–
MePhS (**15**)	3.786	–	3.895	–	–	–	–	–	–	–	–	2.876
PhMeN (**16-I**)	–	–	–	–	–	–	–	–	–	–	–	3.048
PhMeN (**16-II**)	–	2.816	–	–	–	–	–	–	–	–	–	–

Notes: (*a*) weak hydrogen bond; (*b*) halogen bond.

Regarding intermolecular interactions involving the axial group, convex-to-axial ligand interactions were quite common, appearing in nine of the investigated crystal structures. These interactions always involved a π_{Ph} group and either an axial H atom, which was common among the axial alkoxy derivatives (**3**–**8**), or the axial heteroatom bonded to boron, in the cases of

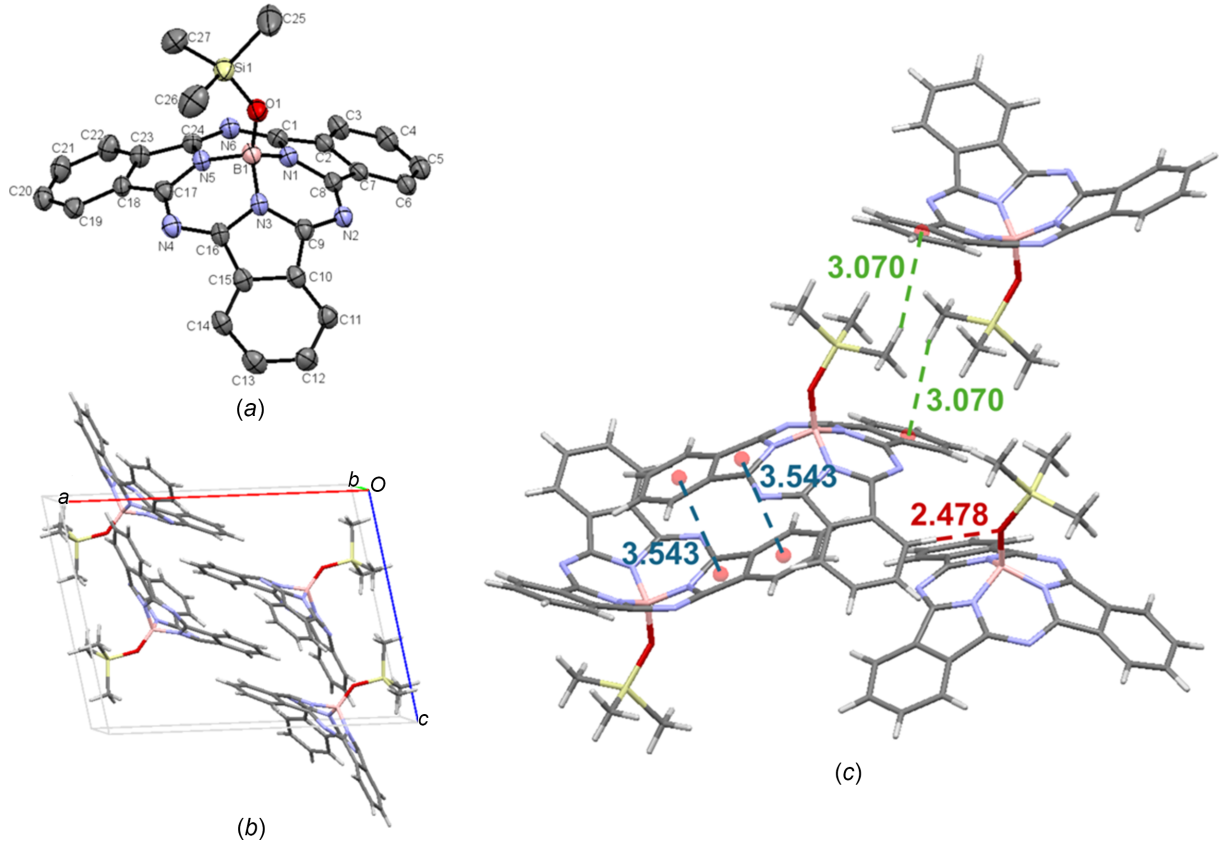


Figure 16
(*a*) The molecular structure of TMSO-BsubPc (**13**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue, weak hydrogen bonds are shown in red and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink, oxygen – red and silicon – yellow.

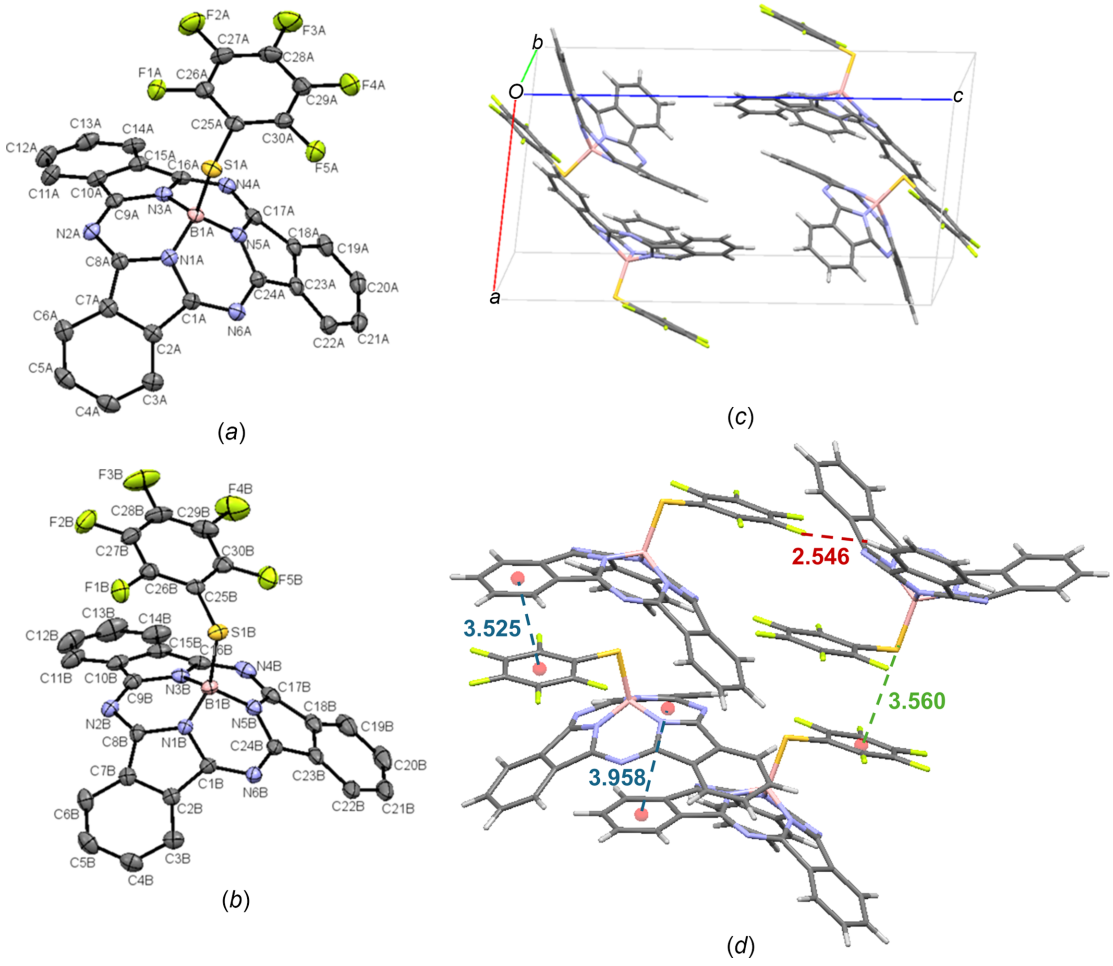


Figure 17
The molecular structures of (*a*) F_5PhS-BsubPc molecule *A* (**14-A**) and (*b*) F_5PhS-BsubPc molecule *B* (**14-B**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity. (*c*) The unit-cell packing and (*d*) significant intermolecular interactions in the crystal structure of **14**. π–π interactions are shown in blue, weak hydrogen bonds are shown in red and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink, sulfur – orange and fluorine – green.

Cl- (**1**), Br- (**2**) and MePhS-BsubPc (**15**). F_3EtO-BsubPc (**5**) was the only alkoxy derivative that did not have any concave- or convex-to-axial ligand interactions. Its nonfluorinated analogue, EtO-BsubPc (**4**), displayed concave-to-axial ligand interactions between one of its axial methyl H atoms and an adjacent π_{Ph} group, but in the case of F_3EtO-BsubPc (**5**), the axial methyl H atoms are all replaced by F atoms. The F atoms instead interacted with adjacent π_{Ph} H atoms through weak hydrogen bonding. Furthermore, neither carboxylate derivative (**11** and **12**) had any concave- or convex-to-axial ligand interactions. Both compounds have two O atoms in the axial group capable of weak hydrogen bonding, which appeared to dictate the axial-group interactions.

Weak hydrogen-bonding interactions were prevalent in compounds with boron–oxygen axial bonds (**3**–**13**). Of the alkoxy derivatives (**3**–**8**), only tButO-BsubPc (**7**) did not display any hydrogen bonding, likely due to steric effects. PhO-BsubPc (**9**) was the only other boron–oxygen-bonded compound that did not display any hydrogen bonding. It looked like there may have been weak hydrogen bonding between the axial O atom and an adjacent axial π_{Ph} H atom in the crystal structure of **9**, but the intermolecular O···H distance (2.766 Å) was slightly greater than the sum of the van der Waals radii of oxygen and hydrogen (2.72 Å). For the carboxylate derivatives, acetate-BsubPc (**11**) had weak hydrogen bonding involving both the axial O atom bonded to boron and the carbonyl O atom, whereas hydrogen bonding was only seen with the carbonyl O atom of benzoate-BsubPc (**12**). Hydrogen bonding involving the axial N atom of PhMeN-BsubPc (**16**) was not observed for either polymorph.

Among the six compounds containing an arene group within the axial moiety (**9**, **10**, **12**, **14**, **15** and **16**), three had π–π interactions involving the axial group. Most significantly, the only π–π interactions seen for naphthoxy-BsubPc (**10**) were concave-to-axial ligand π_{ax}–π_{tail} interactions. The two thiophenoxy derivatives were the only other compounds to display π–π interactions involving the π_{ax} group. Interestingly, PhO-BsubPc (**9**) was the only investigated compound that didn't have any interactions involving the axial group. Finally, the two polymorphs of PhMeN-BsubPc (**16**) have different intermolecular interactions involving the axial group. Both have C—H_{ax}···π interactions, but for **16-I** this interaction is

between an axial phenyl H atom and an adjacent π_{ax} group, while for **16-II** this interaction is between an axial methyl H atom and an adjacent π_{Ph} group.

3.2. Axial bond length and BsubPc bowl depth

The influence of the axial group on the axial bond length was also of interest in this study. The axial bond length is the distance between boron and the heteroatom to which it is bonded. As expected, the axial bond length increased linearly as the atomic radius of the heteroatom bonded to boron increased (Fig. 21). In cases where multiple compounds had the same heteroatom, the average bond length was used to generate Fig. 21. The average axial bond length was 1.430 ± 0.020 Å for boron–oxygen bonds, 1.512 ± 0.002 Å for boron–nitrogen bonds, 1.884 Å for the boron–chlorine bond, 1.931 ± 0.021 Å for boron–sulfur bonds and 2.052 Å for the boron–bromine bond.

Additional trends were observed when comparing the axial bond lengths of compounds with the same heteroatom. Within the compounds with boron–oxygen bonds (Fig. 22), the two carboxylate derivatives [acetate- (**11**) and benzoate-BsubPc (**12**)] had the longest axial bond lengths at 1.473 Å for both compounds. The two phenoxy derivatives [PhO- (**9**) and naphthoxy-BsubPc (**10**)] had the next highest axial bond lengths at 1.441 Å for both compounds. For the axial alkoxy derivatives (**3**–**8**), there was a general slight decrease in axial bond length as the length of the carbon chain increases. The exception was F_3EtO-BsubPc (**5**), which had the longest axial bond length of the alkoxy derivatives at 1.437 Å. The axial bond lengths of the three OctO-BsubPc (**8**) molecules in the asymmetric unit showed some variation, resulting in an average bond length of 1.414 ± 0.006 Å. The bond length of TMSO-BsubPc (**13**) was most closely aligned with ButO-BsubPc (**6**), with both compounds having an axial bond length of 1.415 Å.

For the two compounds with axial boron–sulfur bonds, the axial bond length of F_5PhS-BsubPc (**14**) was longer than that of MePhS-BsubPc (**15**) (Fig. 23). This is similar to what was seen with the alkoxy derivatives (**3**–**8**), with the fluorine-containing axial group (**5**) having the longest axial bond length. These results indicate that F atoms in the axial group cause a slight lengthening of the axial bond. F_5PhS-BsubPc (**14**) has two molecules in its asymmetric unit, with an average bond length of 1.957 ± 0.001 Å, and MePhS-BsubPc (**15**) has three molecules in its asymmetric unit, with an average bond length of 1.915 ± 0.006 Å.

Bowl depth is a measure of the degree of nonplanarity of the BsubPc macrocycle. The greater the bowl depth, the less planar the molecule. Three bowl depths were calculated for

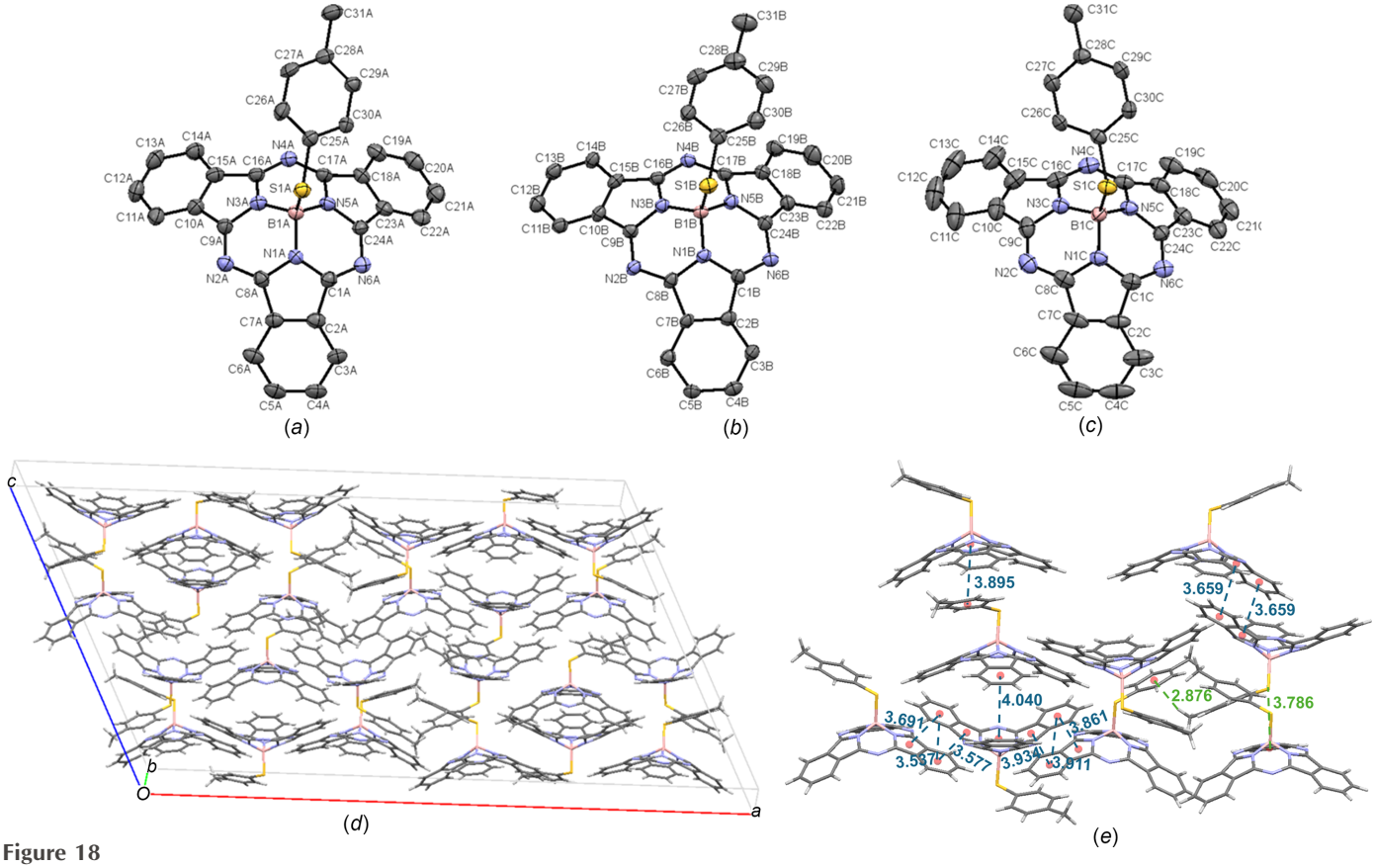


Figure 18
The molecular structures of (*a*) MePhS-BsubPc molecule *A* (**15-A**), (*b*) MePhS-BsubPc molecule *B* (**15-B**) and (*c*) MePhS-BsubPc molecule C (**15-C**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity. (*d*) The unit-cell packing and (*e*) significant intermolecular interactions in the crystal structure of **15**. π–π interactions are shown in blue and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue, boron – light pink and sulfur – orange.

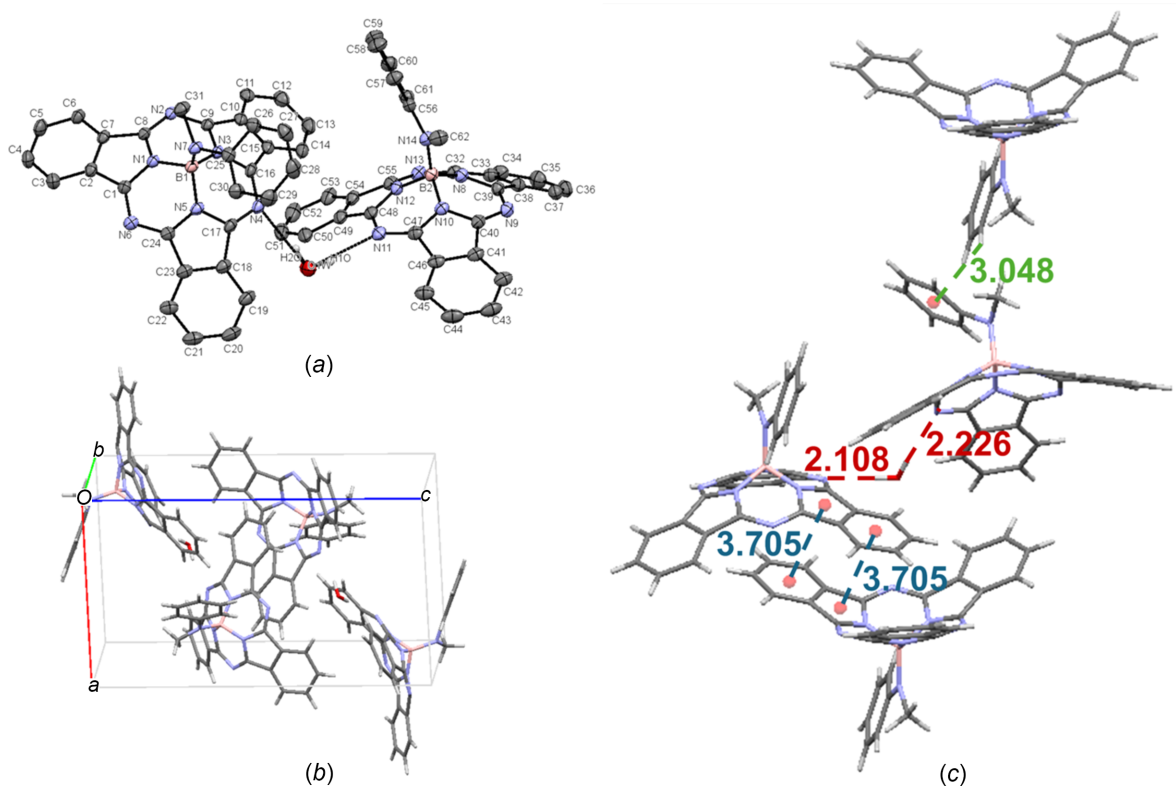


Figure 19
(*a*) The molecular structure of PhMeN-BsubPc (**16-I**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue, hydrogen bonding is shown in red and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue and boron – light pink.

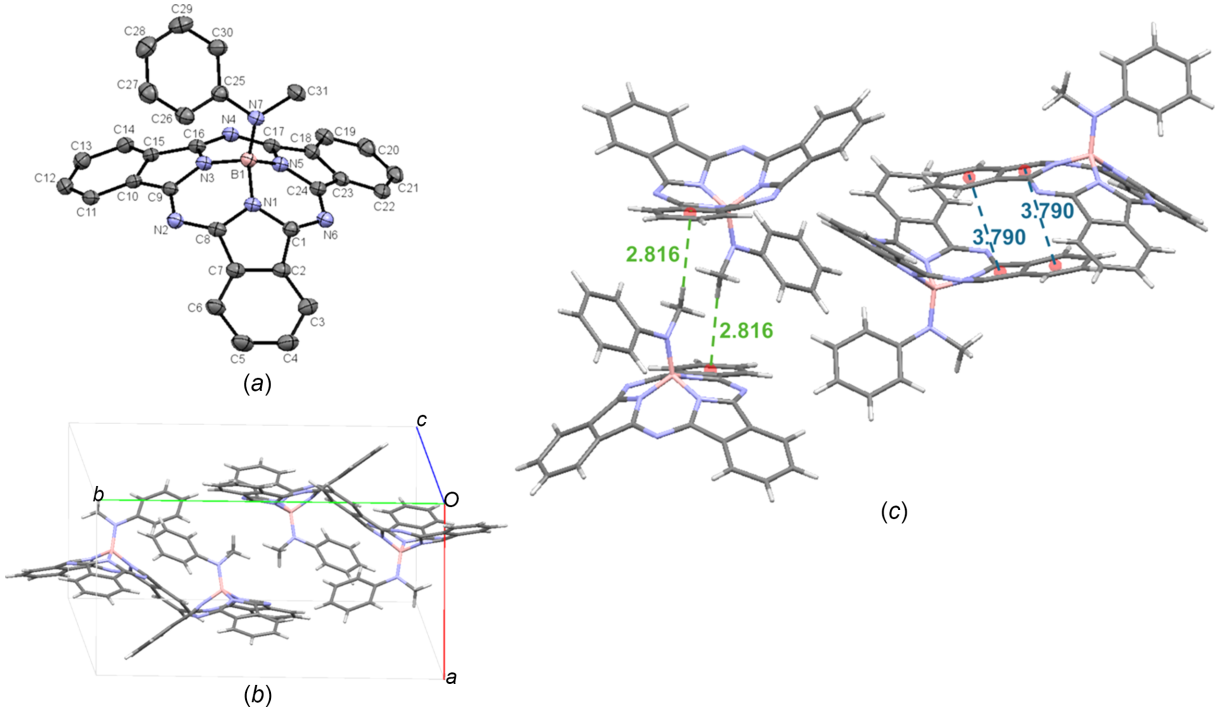


Figure 20
(*a*) The molecular structure of PhMeN-BsubPc (**16-II**), with displacement ellipsoids drawn at the 50% probability level and H atoms removed for clarity, (*b*) the unit-cell packing and (*c*) significant intermolecular interactions in the crystal structure. π–π interactions are shown in blue and all other intermolecular interactions are shown in green. Atom colours: carbon – gray, hydrogen – white, nitrogen – blue and boron – light pink.

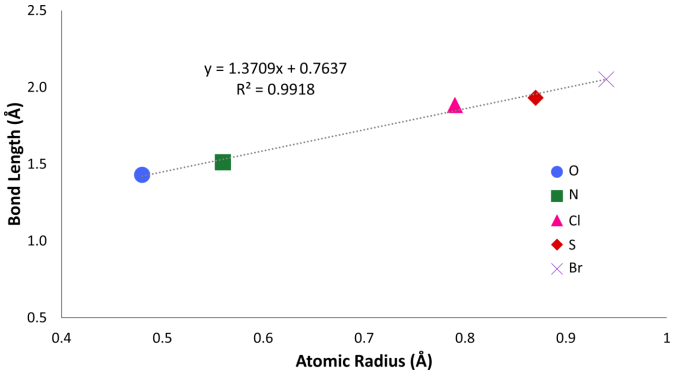


Figure 21
Atomic radius of the heteroatom bonded to boron (oxygen – blue circle, nitrogen – green square, chlorine – pink triangle, sulfur – red diamond and bromine – purple X) *versus* the axial bond length. The boron–oxygen bond length is the average axial bond length of compounds **3**–**13** and the boron–sulfur bond length is the average axial bond length of compounds **14** and **15**.

each BsubPc (Fig. 24) by measuring the distance between the B atom and (i) the plane defined by the three pyrrole N atoms (plane *a*, green), (ii) the plane defined by the three imine N atoms (plane *b*, blue), and (iii) the plane defined by the six outermost C atoms (plane *c*, red). The greatest variation in bowl depth across the axially substituted BsubPcs was seen when considering the distance between boron and plane *c* (Fig. 24). Very little variation was seen in bowl depth when considering the distance between boron and planes *a* and *b* (Fig. 24). Therefore, this discussion will focus on the bowl depth that is measured between boron and plane *c*.

Unlike for the axial bond length, the nature of the heteroatom bonded to boron did not have a clear influence on the BsubPc bowl depth. The axially halogenated derivatives [Cl- (**1**) and Br-BsubPc (**2**)] had two of the smallest bowl depths of the investigated compounds, although the nature of the halogen atom had an almost negligible impact. Acetate-BsubPc (**11**) was the only compound with a smaller bowl depth than the halogens and had the smallest bowl depth of all investigated compounds. Interestingly, the other investigated carboxylate derivative, benzoate-BsubPc (**12**), had the second largest bowl depth of all investigated BsubPcs, behind only naphthoxy-BsubPc (**10**). It appears that adding arenes to

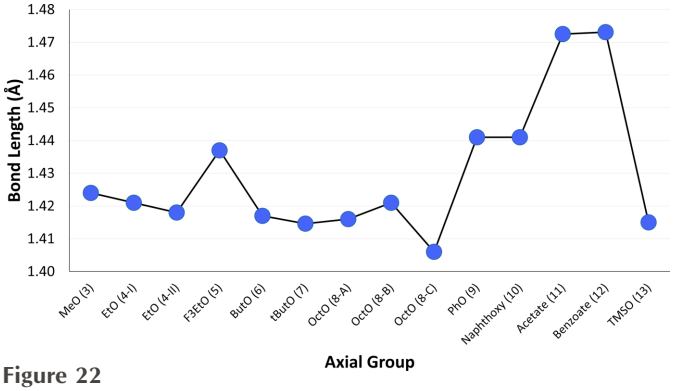


Figure 22
Axial bond lengths of the investigated BsubPcs with boron–oxygen axial bonds.

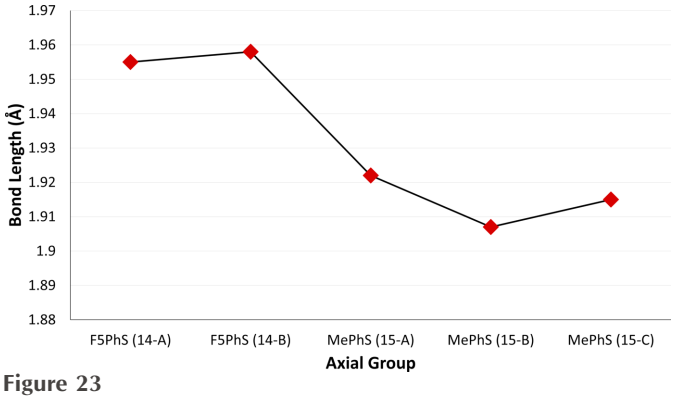


Figure 23
Axial bond lengths of the investigated BsubPcs with boron–sulfur axial bonds.

otherwise identical axial substituents increases the bowl depth. For instance, naphthoxy-BsubPc (**10**), which has two arene sites in the axial position, has a larger bowl depth than PhO-BsubPc (**9**), which has one arene site in the axial position. Furthermore, benzoate-BsubPc (**12**) has a larger bowl depth than acetate-BsubPc (**11**), with the only difference being an arene in place of a methyl group.

While F_3EtO-BsubPc (**5**) stuck out from the other alkoxy-BsubPc derivatives (**3**–**8**) with the longest bond length, it stuck out again here with the smallest bowl depth. Among the nonfluorinated alkoxy derivatives, there does not appear to be a clear correlation between the bowl depth and the length of the axial carbon chain. Furthermore, there was a minimal difference in the bowl depths of ButO- (**6**) and tButO-BsubPc (**7**), indicating that branching does not impact the bowl depth. However, the bowl depth of TMSO-BsubPc (**13**) was smaller than that of its structural analogue, tButO-BsubPc (**7**), indicating that the presence of an Si atom in place of a C atom has a modest impact on the planarity of the BsubPc.

The thiophenoxy derivatives (**14** and **15**) both have multiple molecules in their asymmetric units with varying bowl depths. For F_5PhS-BsubPc (**14**), there are two independent molecules in the asymmetric unit, with an average bowl depth of 2.620 ± 0.131 Å. For MePhS-BsubPc (**15**), the average bowl depth of the three molecules is 2.553 ± 0.019 Å. Therefore, adding F atoms to the thiophenoxy axial group increases both the BsubPc bowl depth and the axial bond length, in contrast to what was seen when adding F atoms to the axial alkoxy group, whereby the bond length increased and the bowl depth decreased.

Finally, the two PhMeN-BsubPc (**16**) polymorphs have very similar bowl depths when comparing the average bowl depth of the two molecules in **16-I** (2.586 ± 0.45 Å) to the bowl depth of **16-II** (2.595 Å).

The axial bond lengths and BsubPc bowl depths are tabulated in Table 4.

4. Conclusions

Overall, the axial-group interactions play a significant role in the crystal packing of BsubPcs, influencing the crystal system/space group and intermolecular interactions. Concave–

Table 4
Axial bond lengths (Å) and bowl depths (Å) of the investigated BsubPcs.

Plane *a* is defined by the three pyrrole N atoms, plane *b* by the three imine N atoms and plane *c* by the six outermost C atoms.

Axial group	Axial bond length	Bowl depth to plane *a*	Bowl depth to plane *b*	Bowl depth to plane *c*
Cl (**1**)	1.884	0.580	1.116	2.456
Br (**2**)	2.052	0.568	1.101	2.457
MeO (**3**)	1.424	0.632	1.191	2.618
EtO (**4-I**)	1.421	0.641	1.193	2.598
EtO (**4-II**)	1.418	0.642	1.192	2.590
F_3EtO (**5**)	1.437	0.631	1.188	2.468
ButO (**6**)	1.417	0.643	1.210	2.718
tButO (**7**)	1.415	0.660	1.225	2.711
OctO (**8-A**)	1.416	0.643	1.230	2.867
OctO (**8-B**)	1.421	0.646	1.209	2.652
OctO (**8-C**)	1.406	0.640	1.195	2.493
PhO (**9**)	1.441	0.624	1.181	2.607
Naphthoxy (**10**)	1.441	0.620	1.202	2.881
Acetate (**11**)	1.473	0.603	1.158	2.389
Benzoate (**12**)	1.473	0.602	1.192	2.835
TMSO (**13**)	1.415	0.649	1.207	2.630
F_5PhS (**14-A**)	1.955	0.587	1.183	2.751
F_5PhS (**14-B**)	1.958	0.587	1.119	2.489
MePhS (**15-A**)	1.922	0.615	1.180	2.580
MePhS (**15-A**)	1.907	0.625	1.173	2.541
MePhS (**15-A**)	1.915	0.619	1.165	2.537
PhMeN (**16–1**, mol 1)	1.509	0.650	1.205	2.541
PhMeN (**16–1**, mol 2)	1.513	0.667	1.250	2.631
PhMeN (**16–2**)	1.513	0.659	1.217	2.595

concave head-to-head interactions were the most common π–π interactions in the crystal structures of the investigated BsubPcs, whereas axial-group interactions with adjacent isoindoline units tended to favour the convex side of the bowl. Weak hydrogen-bonding interactions are prevalent when the axial group contains O and/or F atoms, but the axial N atom in PhMeN-BsubPc did not participate in hydrogen bonding. This may be a result of steric hindrance, as other investigated compounds with bulky axial groups, such as tButO-BsubPc and OctO-BsubPc, also disrupted some of the intermolecular interactions. The bulkiness of tButO-BsubPc disrupted hydrogen bonding with the axial O atom, while OctO-BsubPc disrupted the intermolecular π–π interactions. The presence of arenes in the axial moiety can also have a significant impact, as π–π interactions involving the axial group are now possible. In particular, naphthoxy-, F_5PhS- and MePhS-BsubPc all have concave-to-axial π–π interactions. Furthermore, the axial bond length increases linearly with the atomic radius of the heteroatom bonded to boron, and the presence of F atoms in the axial group tended to lengthen the axial bond. However,

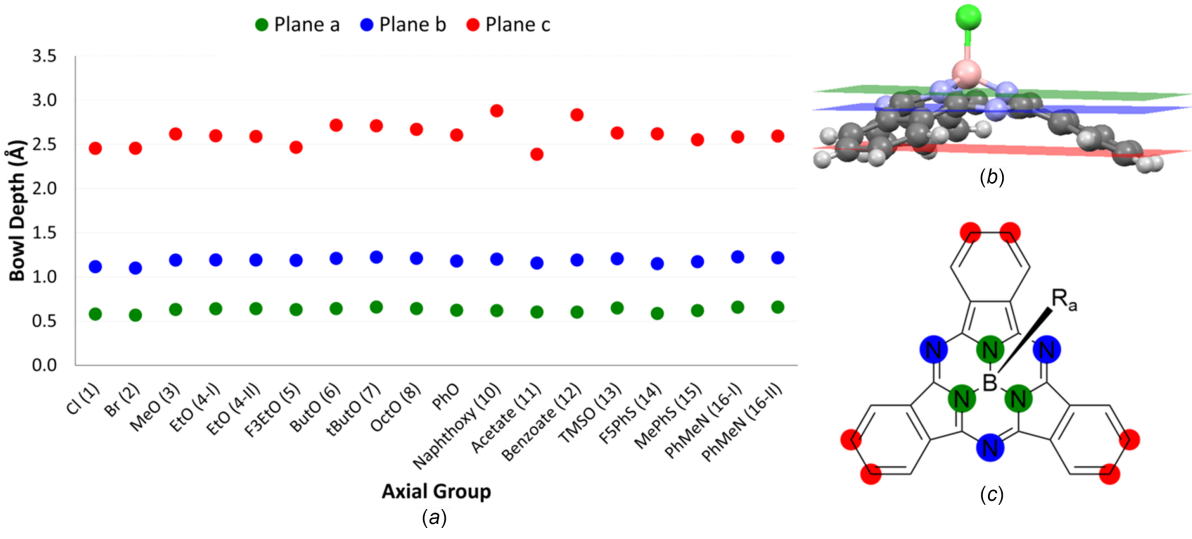


Figure 24
(*a*) Bowl depth variation with different axial substituents. Three bowl depths are reported as the shortest distance between boron and plane *a* (green), boron and plane *b* (blue), and boron and plane *c* (red). (*b*) 3D structure of Cl-BsubPc defining planes *a*, *b* and *c*, and (*c*) 2D general BsubPc structure highlighting the atoms that define planes *a*, *b* and *c*. For compounds with multiple molecules in the asymmetric unit (**8**, **14**, **15** and **16-I**), the reported bowl depths are an average of all the molecules in the asymmetric unit.

there is no clear trend in BsubPc bowl depth related to the axial group, with only a modest impact being observed. There were also no clear trends observed based on some of the crystal growth methods. The crystal structures of EtO-BsubPc from train sublimation (**4-I**) and slow evaporation of acetone (**4-II**) were identical, as were the crystal structures of acetate- (**11**) and benzoate-BsubPc (**12**) grown from train sublimation in this study compared to a previous report of the crystal structures from solvent-based crystal growth methods. Train sublimation is often the preferred crystal growth method, as it most closely mimics the vacuum deposition conditions used for the thin film fabrication in organic electronic applicants. However, in this case, the solvent-based crystal growth methods appeared to produce the same results as train sublimation. The only observed solvent effects were when hygroscopic solvents methanol and THF were used to grow crystals of OctO- (**8**) and PhMeN-BsubPc (**16-I**), respectively, with water molecules incorporated into the crystal structures and hydrogen bonding with imine N atoms. Overall, the results of this study are useful for the nanoengineering of thin films of BsubPcs for their application in organic electronics.

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The influence of the axial group on the crystal structures of boron subphthalocyanines

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Computing details

Chlorido(subphthalocyaninato)boron (d2344a_a)

Crystal data

$C_{24}H_{12}BClN_6$
M_r = 430.66
Orthorhombic, *Pnma*
a = 12.0315 (10) Å
b = 14.8174 (13) Å
c = 10.3002 (8) Å
V = 1836.3 (3) Å^3
Z = 4
F(000) = 880
D_x = 1.558 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 5394 reflections
θ = 5.7–65.5°
μ = 2.07 mm^{-1}
T = 150 K
Shard, pink
0.15 × 0.06 × 0.02 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.646, T_{max} = 0.753
19930 measured reflections
1647 independent reflections
1416 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 66.2°, θ_{min} = 5.2°
h = −14→14
k = −17→16
l = −12→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.097
S = 1.06
1647 reflections
151 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 1.2852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.18664 (5)	0.250000	1.23875 (6)	0.0214 (2)
N1	0.00611 (17)	0.250000	0.9063 (2)	0.0187 (5)
N2	0.16179 (12)	0.32926 (10)	0.99200 (14)	0.0175 (4)
N3	0.33419 (12)	0.40660 (11)	0.97328 (15)	0.0203 (4)
N4	0.32869 (17)	0.250000	1.0229 (2)	0.0189 (5)
C1	0.06079 (14)	0.32723 (13)	0.93070 (17)	0.0182 (4)
C2	0.04565 (15)	0.41770 (12)	0.87898 (18)	0.0184 (4)
C3	−0.04130 (16)	0.45728 (13)	0.80994 (18)	0.0209 (4)
H3A	−0.107253	0.424477	0.791349	0.025*
C4	−0.02881 (17)	0.54552 (14)	0.76936 (18)	0.0237 (4)
H4A	−0.087720	0.574001	0.723614	0.028*
C5	0.06875 (16)	0.59383 (14)	0.79419 (19)	0.0233 (4)
H5A	0.074040	0.654917	0.766882	0.028*
C6	0.15769 (16)	0.55449 (13)	0.85768 (18)	0.0216 (4)
H6A	0.224841	0.586872	0.871258	0.026*
C7	0.14594 (15)	0.46613 (13)	0.90106 (17)	0.0186 (4)
C8	0.22237 (15)	0.40490 (13)	0.96506 (17)	0.0189 (4)
C9	0.38573 (15)	0.32726 (13)	0.99400 (17)	0.0195 (4)
C10	0.49870 (15)	0.29805 (13)	0.96453 (16)	0.0199 (4)
C11	0.59444 (16)	0.34628 (14)	0.93356 (18)	0.0243 (4)
H11	0.594751	0.410391	0.932401	0.029*
C12	0.68919 (16)	0.29719 (15)	0.9045 (2)	0.0286 (5)
H12	0.755883	0.328435	0.884055	0.034*
B1	0.2098 (3)	0.250000	1.0579 (3)	0.0193 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0256 (4)	0.0190 (3)	0.0195 (3)	0.000	0.0007 (2)	0.000
N1	0.0177 (11)	0.0165 (11)	0.0218 (11)	0.000	0.0024 (9)	0.000
N2	0.0171 (7)	0.0156 (8)	0.0196 (8)	0.0000 (6)	0.0003 (6)	0.0002 (6)
N3	0.0194 (8)	0.0205 (8)	0.0211 (8)	−0.0013 (6)	−0.0006 (6)	0.0005 (7)
N4	0.0181 (11)	0.0180 (12)	0.0205 (11)	0.000	−0.0003 (9)	0.000
C1	0.0166 (9)	0.0201 (9)	0.0180 (9)	−0.0003 (8)	0.0030 (7)	−0.0012 (8)
C2	0.0200 (9)	0.0178 (10)	0.0175 (9)	0.0013 (8)	0.0029 (7)	−0.0004 (7)
C3	0.0187 (9)	0.0228 (10)	0.0212 (10)	0.0007 (8)	0.0009 (8)	−0.0010 (8)
C4	0.0235 (10)	0.0258 (11)	0.0218 (10)	0.0065 (8)	0.0009 (8)	0.0016 (8)
C5	0.0273 (10)	0.0196 (10)	0.0230 (10)	0.0027 (8)	0.0039 (8)	0.0027 (8)
C6	0.0229 (9)	0.0199 (10)	0.0220 (10)	−0.0007 (8)	0.0035 (8)	0.0010 (8)

C7	0.0207 (9)	0.0188 (9)	0.0164 (9)	0.0010 (8)	0.0022 (7)	−0.0001 (7)
C8	0.0200 (9)	0.0188 (9)	0.0180 (9)	−0.0018 (7)	0.0003 (7)	−0.0010 (8)
C9	0.0199 (9)	0.0200 (10)	0.0187 (9)	−0.0021 (8)	−0.0022 (7)	−0.0008 (8)
C10	0.0173 (9)	0.0249 (10)	0.0176 (9)	−0.0002 (8)	−0.0037 (7)	0.0008 (8)
C11	0.0215 (9)	0.0278 (11)	0.0234 (10)	−0.0035 (8)	−0.0030 (8)	0.0021 (9)
C12	0.0178 (9)	0.0383 (12)	0.0296 (11)	−0.0039 (9)	0.0003 (8)	0.0015 (10)
B1	0.0199 (15)	0.0176 (15)	0.0205 (15)	0.000	−0.0009 (12)	0.000

Geometric parameters (Å, º)

Cl1—B1	1.884 (3)	C3—H3A	0.9500
N1—C1	1.344 (2)	C4—C5	1.398 (3)
N1—C1^{i}	1.344 (2)	C4—H4A	0.9500
N2—C8	1.365 (2)	C5—C6	1.383 (3)
N2—C1	1.370 (2)	C5—H5A	0.9500
N2—B1	1.474 (2)	C6—C7	1.391 (3)
N3—C9	1.346 (2)	C6—H6A	0.9500
N3—C8	1.348 (2)	C7—C8	1.450 (3)
N4—C9	1.367 (2)	C9—C10	1.458 (3)
N4—C9^{i}	1.367 (2)	C10—C11	1.393 (3)
N4—B1	1.475 (4)	C10—C10^{i}	1.424 (4)
C1—C2	1.454 (3)	C11—C12	1.385 (3)
C2—C3	1.394 (3)	C11—H11	0.9500
C2—C7	1.422 (3)	C12—C12^{i}	1.399 (4)
C3—C4	1.381 (3)	C12—H12	0.9500
C1—N1—C1^{i}	116.8 (2)	C7—C6—H6A	121.0
C8—N2—C1	113.45 (15)	C6—C7—C2	120.65 (17)
C8—N2—B1	122.57 (17)	C6—C7—C8	132.11 (18)
C1—N2—B1	122.83 (17)	C2—C7—C8	107.16 (16)
C9—N3—C8	116.95 (16)	N3—C8—N2	122.36 (17)
C9—N4—C9^{i}	113.7 (2)	N3—C8—C7	130.51 (17)
C9—N4—B1	122.66 (11)	N2—C8—C7	105.51 (15)
C9^{i}—N4—B1	122.67 (11)	N3—C9—N4	122.31 (16)
N1—C1—N2	122.64 (17)	N3—C9—C10	130.96 (17)
N1—C1—C2	130.93 (17)	N4—C9—C10	105.34 (16)
N2—C1—C2	105.06 (15)	C11—C10—C10^{i}	120.87 (12)
C3—C2—C7	120.40 (17)	C11—C10—C9	131.78 (18)
C3—C2—C1	131.96 (17)	C10^{i}—C10—C9	107.26 (11)
C7—C2—C1	107.47 (15)	C12—C11—C10	117.44 (19)
C4—C3—C2	118.09 (18)	C12—C11—H11	121.3
C4—C3—H3A	121.0	C10—C11—H11	121.3
C2—C3—H3A	121.0	C11—C12—C12^{i}	121.68 (12)
C3—C4—C5	121.38 (18)	C11—C12—H12	119.2
C3—C4—H4A	119.3	C12^{i}—C12—H12	119.2
C5—C4—H4A	119.3	N2—B1—N2^{i}	105.6 (2)
C6—C5—C4	121.35 (19)	N2—B1—N4	105.51 (16)
C6—C5—H5A	119.3	N2^{i}—B1—N4	105.52 (16)

C4—C5—H5A	119.3	N2—B1—Cl1	113.41 (14)
C5—C6—C7	118.04 (18)	N2^{i}—B1—Cl1	113.41 (14)
C5—C6—H6A	121.0	N4—B1—Cl1	112.64 (19)
C1^{i}—N1—C1—N2	−7.7 (3)	C2—C7—C8—N3	158.19 (19)
C1^{i}—N1—C1—C2	156.82 (14)	C6—C7—C8—N2	175.97 (19)
C8—N2—C1—N1	156.35 (18)	C2—C7—C8—N2	−7.20 (19)
B1—N2—C1—N1	−11.7 (3)	C8—N3—C9—N4	−8.6 (3)
C8—N2—C1—C2	−11.6 (2)	C8—N3—C9—C10	155.84 (18)
B1—N2—C1—C2	−179.66 (18)	C9^{i}—N4—C9—N3	157.11 (13)
N1—C1—C2—C3	14.9 (3)	B1—N4—C9—N3	−11.8 (3)
N2—C1—C2—C3	−178.50 (19)	C9^{i}—N4—C9—C10	−10.7 (3)
N1—C1—C2—C7	−160.3 (2)	B1—N4—C9—C10	−179.7 (2)
N2—C1—C2—C7	6.32 (19)	N3—C9—C10—C11	16.4 (3)
C7—C2—C3—C4	−2.9 (3)	N4—C9—C10—C11	−177.2 (2)
C1—C2—C3—C4	−177.54 (19)	N3—C9—C10—C10^{i}	−160.25 (17)
C2—C3—C4—C5	1.2 (3)	N4—C9—C10—C10^{i}	6.13 (16)
C3—C4—C5—C6	1.6 (3)	C10^{i}—C10—C11—C12	−0.7 (2)
C4—C5—C6—C7	−2.5 (3)	C9—C10—C11—C12	−177.04 (18)
C5—C6—C7—C2	0.8 (3)	C10—C11—C12—C12^{i}	0.7 (2)
C5—C6—C7—C8	177.25 (19)	C8—N2—B1—N2^{i}	−140.31 (15)
C3—C2—C7—C6	1.9 (3)	C1—N2—B1—N2^{i}	26.6 (3)
C1—C2—C7—C6	177.79 (16)	C8—N2—B1—N4	−28.8 (3)
C3—C2—C7—C8	−175.32 (17)	C1—N2—B1—N4	138.10 (17)
C1—C2—C7—C8	0.52 (19)	C8—N2—B1—Cl1	94.9 (2)
C9—N3—C8—N2	7.9 (3)	C1—N2—B1—Cl1	−98.15 (19)
C9—N3—C8—C7	−155.37 (19)	C9—N4—B1—N2	28.2 (3)
C1—N2—C8—N3	−154.88 (17)	C9^{i}—N4—B1—N2	−139.74 (19)
B1—N2—C8—N3	13.2 (3)	C9—N4—B1—N2^{i}	139.74 (19)
C1—N2—C8—C7	12.0 (2)	C9^{i}—N4—B1—N2^{i}	−28.2 (3)
B1—N2—C8—C7	−179.94 (18)	C9—N4—B1—Cl1	−96.0 (2)
C6—C7—C8—N3	−18.6 (3)	C9^{i}—N4—B1—Cl1	96.0 (2)

Symmetry code: (i) x, $-y+1/2$, z.

Bromido(subphthalocyaninato)boron (d23119a_a)

Crystal data

$C_{24}H_{12}BBrN_6$
M_r = 475.12
Orthorhombic, *Pnma*
a = 12.0010 (6) Å
b = 15.0617 (8) Å
c = 10.3879 (5) Å
V = 1877.67 (16) Å^3
Z = 4
F(000) = 952

D_x = 1.681 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9878 reflections
θ = 2.4–27.5°
μ = 2.22 mm^{-1}
T = 150 K
Shard, purple
0.27 × 0.16 × 0.14 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: sealed tube with Bruker Triumph monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.688, T_{max} = 0.746
23127 measured reflections
2243 independent reflections
1955 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 2.4°
h = −15→13
k = −18→19
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.057
S = 1.09
2243 reflections
151 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0231P)^2 + 1.4706P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-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.

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

	x	y	z	U_{iso}*/U_{eq}
Br1	0.81550 (2)	0.750000	0.24958 (2)	0.01614 (7)
N1	0.66674 (10)	0.59579 (8)	0.52765 (12)	0.0161 (3)
N2	0.83966 (10)	0.67206 (8)	0.50914 (12)	0.0138 (2)
N3	0.99565 (14)	0.750000	0.59384 (17)	0.0146 (3)
N4	0.67202 (14)	0.750000	0.47898 (17)	0.0144 (4)
C1	0.31111 (13)	0.70352 (12)	0.59788 (17)	0.0258 (4)
H1	0.244319	0.672743	0.618348	0.031*
C2	0.40596 (13)	0.65542 (11)	0.56881 (15)	0.0216 (3)
H2	0.405645	0.592354	0.570221	0.026*
C3	0.50217 (12)	0.70269 (10)	0.53733 (14)	0.0172 (3)
C4	0.61501 (12)	0.67384 (10)	0.50787 (14)	0.0157 (3)
C5	0.77859 (12)	0.59742 (10)	0.53537 (14)	0.0147 (3)
C6	0.85558 (12)	0.53724 (10)	0.59867 (14)	0.0152 (3)
C7	0.84333 (13)	0.45010 (10)	0.64201 (14)	0.0175 (3)
H7A	0.776162	0.418167	0.627899	0.021*
C8	0.93209 (13)	0.41167 (10)	0.70617 (16)	0.0197 (3)
H8A	0.926535	0.351706	0.733810	0.024*
C9	1.02985 (13)	0.45920 (11)	0.73121 (14)	0.0196 (3)
H9A	1.088591	0.431358	0.777344	0.023*
C10	1.04267 (12)	0.54609 (10)	0.69005 (14)	0.0171 (3)

H10A	1.108779	0.578365	0.708496	0.021*
C11	0.95604 (12)	0.58479 (10)	0.62094 (14)	0.0146 (3)
C12	0.94074 (11)	0.67398 (10)	0.56982 (14)	0.0141 (3)
B1	0.79108 (19)	0.750000	0.4451 (2)	0.0139 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02272 (12)	0.01261 (11)	0.01311 (11)	0.000	0.00090 (8)	0.000
N1	0.0169 (6)	0.0158 (6)	0.0158 (6)	−0.0018 (5)	−0.0013 (5)	0.0010 (5)
N2	0.0145 (6)	0.0120 (6)	0.0148 (6)	−0.0004 (5)	0.0008 (5)	0.0001 (5)
N3	0.0149 (8)	0.0132 (8)	0.0158 (8)	0.000	0.0018 (7)	0.000
N4	0.0149 (8)	0.0134 (8)	0.0148 (8)	0.000	−0.0004 (7)	0.000
C1	0.0164 (7)	0.0365 (10)	0.0245 (8)	−0.0051 (7)	0.0008 (6)	0.0034 (7)
C2	0.0174 (7)	0.0268 (8)	0.0207 (8)	−0.0036 (6)	−0.0022 (6)	0.0046 (7)
C3	0.0153 (7)	0.0220 (8)	0.0143 (7)	0.0003 (6)	−0.0024 (6)	0.0000 (6)
C4	0.0156 (7)	0.0172 (7)	0.0142 (7)	−0.0023 (6)	−0.0014 (5)	0.0004 (6)
C5	0.0175 (7)	0.0131 (7)	0.0136 (7)	−0.0012 (5)	0.0002 (5)	0.0000 (5)
C6	0.0171 (7)	0.0147 (7)	0.0137 (6)	0.0008 (6)	0.0012 (6)	−0.0003 (5)
C7	0.0190 (7)	0.0150 (7)	0.0184 (7)	−0.0013 (6)	0.0029 (6)	0.0010 (6)
C8	0.0250 (8)	0.0144 (7)	0.0196 (7)	0.0018 (6)	0.0034 (6)	0.0038 (6)
C9	0.0214 (7)	0.0192 (7)	0.0181 (7)	0.0056 (6)	−0.0002 (6)	0.0029 (6)
C10	0.0167 (7)	0.0170 (7)	0.0175 (7)	0.0014 (6)	0.0002 (6)	−0.0009 (6)
C11	0.0171 (6)	0.0130 (7)	0.0136 (7)	0.0015 (5)	0.0029 (5)	−0.0008 (5)
C12	0.0135 (6)	0.0152 (7)	0.0135 (7)	0.0013 (5)	0.0017 (5)	−0.0001 (6)
B1	0.0157 (10)	0.0128 (10)	0.0134 (11)	0.000	−0.0001 (9)	0.000

Geometric parameters (Å, º)

Br1—B1	2.052 (2)	C2—H2	0.9500
N1—C5	1.3449 (18)	C3—C3^{i}	1.425 (3)
N1—C4	1.3452 (19)	C3—C4	1.455 (2)
N2—C12	1.3674 (18)	C5—C6	1.452 (2)
N2—C5	1.3693 (18)	C6—C7	1.395 (2)
N2—B1	1.4698 (18)	C6—C11	1.421 (2)
N3—C12^{i}	1.3444 (17)	C7—C8	1.384 (2)
N3—C12	1.3444 (17)	C7—H7A	0.9500
N4—C4^{i}	1.3689 (17)	C8—C9	1.399 (2)
N4—C4	1.3689 (17)	C8—H8A	0.9500
N4—B1	1.471 (3)	C9—C10	1.385 (2)
C1—C2	1.383 (2)	C9—H9A	0.9500
C1—C1^{i}	1.400 (4)	C10—C11	1.391 (2)
C1—H1	0.9500	C10—H10A	0.9500
C2—C3	1.395 (2)	C11—C12	1.456 (2)
C5—N1—C4	116.99 (13)	C11—C6—C5	107.39 (12)
C12—N2—C5	113.61 (12)	C8—C7—C6	117.89 (14)
C12—N2—B1	122.92 (13)	C8—C7—H7A	121.1

C5—N2—B1	122.24 (13)	C6—C7—H7A	121.1
C12^{i}—N3—C12	116.79 (17)	C7—C8—C9	121.42 (14)
C4^{i}—N4—C4	113.85 (17)	C7—C8—H8A	119.3
C4^{i}—N4—B1	122.53 (9)	C9—C8—H8A	119.3
C4—N4—B1	122.53 (9)	C10—C9—C8	121.28 (14)
C2—C1—C1^{i}	121.60 (10)	C10—C9—H9A	119.4
C2—C1—H1	119.2	C8—C9—H9A	119.4
C1^{i}—C1—H1	119.2	C9—C10—C11	118.17 (14)
C1—C2—C3	117.72 (16)	C9—C10—H10A	120.9
C1—C2—H2	121.1	C11—C10—H10A	120.9
C3—C2—H2	121.1	C10—C11—C6	120.44 (13)
C2—C3—C3^{i}	120.68 (10)	C10—C11—C12	131.98 (14)
C2—C3—C4	131.85 (15)	C6—C11—C12	107.38 (12)
C3^{i}—C3—C4	107.38 (9)	N3—C12—N2	122.58 (13)
N1—C4—N4	122.35 (13)	N3—C12—C11	131.01 (14)
N1—C4—C3	131.18 (14)	N2—C12—C11	105.09 (12)
N4—C4—C3	105.13 (13)	N2^{i}—B1—N2	106.01 (17)
N1—C5—N2	122.50 (13)	N2^{i}—B1—N4	106.08 (12)
N1—C5—C6	130.60 (13)	N2—B1—N4	106.08 (12)
N2—C5—C6	105.19 (12)	N2^{i}—B1—Br1	113.03 (11)
C7—C6—C11	120.73 (14)	N2—B1—Br1	113.03 (11)
C7—C6—C5	131.79 (14)	N4—B1—Br1	112.04 (15)

C1^{i}—C1—C2—C3	−0.93 (18)	C9—C10—C11—C6	2.7 (2)
C1—C2—C3—C3^{i}	0.92 (18)	C9—C10—C11—C12	176.81 (15)
C1—C2—C3—C4	176.97 (16)	C7—C6—C11—C10	−2.1 (2)
C5—N1—C4—N4	8.8 (2)	C5—C6—C11—C10	174.79 (13)
C5—N1—C4—C3	−155.92 (15)	C7—C6—C11—C12	−177.45 (13)
C4^{i}—N4—C4—N1	−157.35 (11)	C5—C6—C11—C12	−0.60 (16)
B1—N4—C4—N1	10.9 (3)	C12^{i}—N3—C12—N2	8.0 (3)
C4^{i}—N4—C4—C3	10.8 (2)	C12^{i}—N3—C12—C11	−156.87 (11)
B1—N4—C4—C3	179.12 (17)	C5—N2—C12—N3	−156.66 (15)
C2—C3—C4—N1	−15.9 (3)	B1—N2—C12—N3	10.9 (2)
C3^{i}—C3—C4—N1	160.54 (14)	C5—N2—C12—C11	11.56 (16)
C2—C3—C4—N4	177.39 (17)	B1—N2—C12—C11	179.14 (15)
C3^{i}—C3—C4—N4	−6.17 (13)	C10—C11—C12—N3	−14.1 (3)
C4—N1—C5—N2	−7.8 (2)	C6—C11—C12—N3	160.59 (16)
C4—N1—C5—C6	155.00 (15)	C10—C11—C12—N2	179.12 (15)
C12—N2—C5—N1	154.60 (14)	C6—C11—C12—N2	−6.23 (15)
B1—N2—C5—N1	−13.1 (2)	C12—N2—B1—N2^{i}	−25.6 (2)
C12—N2—C5—C6	−11.95 (16)	C5—N2—B1—N2^{i}	140.89 (12)
B1—N2—C5—C6	−179.63 (14)	C12—N2—B1—N4	−138.14 (14)
N1—C5—C6—C7	18.5 (3)	C5—N2—B1—N4	28.4 (2)
N2—C5—C6—C7	−176.44 (15)	C12—N2—B1—Br1	98.71 (15)
N1—C5—C6—C11	−157.83 (15)	C5—N2—B1—Br1	−94.76 (16)
N2—C5—C6—C11	7.19 (15)	C4^{i}—N4—B1—N2^{i}	27.4 (2)
C11—C6—C7—C8	−0.4 (2)	C4—N4—B1—N2^{i}	−139.86 (15)
C5—C6—C7—C8	−176.41 (15)	C4^{i}—N4—B1—N2	139.86 (15)

C6—C7—C8—C9	2.2 (2)	C4—N4—B1—N2	−27.4 (2)
C7—C8—C9—C10	−1.5 (2)	C4^{i}—N4—B1—Br1	−96.36 (16)
C8—C9—C10—C11	−1.0 (2)	C4—N4—B1—Br1	96.36 (16)

Symmetry code: (i) x, $-y+3/2$, z.

(Methanolato)(subphthalocyaninato)boron (d2368_a)

Crystal data

$C_{25}H_{15}BN_6O$
M_r = 426.24
Orthorhombic, *Pnma*
a = 12.3162 (11) Å
b = 15.2325 (19) Å
c = 10.4151 (10) Å
V = 1953.9 (4) Å^3
Z = 4
$F(000)$ = 880
D_x = 1.449 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8333 reflections
θ = 5.1–65.5°
μ = 0.75 mm^{-1}
T = 150 K
Shard, pink
0.10 × 0.04 × 0.02 mm

Data collection

Bruker Kappa APEX-DUO CMOs PHOTON II diffractometer
Radiation source: Icoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.659, T_{max} = 0.753
27808 measured reflections
1762 independent reflections
1570 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 66.0°, θ_{min} = 5.1°
h = −14→14
k = −17→17
l = −12→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.078
S = 1.08
1762 reflections
159 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2 + 0.6842P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: SHELXL2019 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0026 (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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.74991 (10)	0.750000	0.29681 (12)	0.0284 (3)	
N1	0.96403 (12)	0.750000	0.56717 (14)	0.0249 (3)	
N2	0.80691 (8)	0.67267 (7)	0.49738 (10)	0.0235 (3)	

N3	0.64054 (8)	0.59780 (7)	0.53777 (10)	0.0266 (3)	
N4	0.64148 (12)	0.750000	0.48741 (14)	0.0248 (3)	
C1	0.90890 (10)	0.67473 (8)	0.54862 (12)	0.0235 (3)	
C2	0.92753 (10)	0.58766 (8)	0.60186 (12)	0.0240 (3)	
C3	1.01583 (10)	0.55147 (8)	0.66539 (13)	0.0281 (3)	
H3A	1.081703	0.583335	0.674325	0.034*	
C4	1.00543 (11)	0.46789 (9)	0.71533 (13)	0.0316 (3)	
H4A	1.065143	0.442124	0.759076	0.038*	
C5	0.90876 (11)	0.42036 (9)	0.70283 (13)	0.0306 (3)	
H5A	0.904612	0.362429	0.736277	0.037*	
C6	0.81926 (10)	0.45637 (8)	0.64260 (13)	0.0276 (3)	
H6A	0.753201	0.424472	0.636119	0.033*	
C7	0.82830 (10)	0.54053 (8)	0.59167 (12)	0.0245 (3)	
C8	0.74954 (10)	0.59952 (8)	0.53308 (12)	0.0246 (3)	
C9	0.58841 (10)	0.67493 (8)	0.52199 (12)	0.0251 (3)	
C10	0.48053 (10)	0.70324 (9)	0.56126 (12)	0.0274 (3)	
C11	0.38841 (10)	0.65651 (10)	0.59870 (13)	0.0332 (3)	
H11	0.388003	0.594147	0.599794	0.040*	
C12	0.29788 (11)	0.70410 (11)	0.63409 (15)	0.0406 (4)	
H12	0.233924	0.673711	0.659092	0.049*	
C13	0.84839 (16)	0.750000	0.23075 (18)	0.0316 (4)	
H13A	0.836530	0.729920	0.142465	0.047*	0.5
H13B	0.899536	0.710471	0.273802	0.047*	0.5
H13C	0.878312	0.809608	0.229560	0.047*	0.5
B1	0.75398 (16)	0.750000	0.43343 (19)	0.0240 (4)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0324 (7)	0.0282 (7)	0.0246 (7)	0.000	−0.0006 (5)	0.000
N1	0.0245 (7)	0.0217 (8)	0.0284 (8)	0.000	0.0037 (6)	0.000
N2	0.0247 (6)	0.0216 (6)	0.0242 (6)	−0.0011 (4)	0.0021 (4)	−0.0001 (4)
N3	0.0263 (6)	0.0280 (6)	0.0255 (6)	−0.0025 (4)	−0.0020 (4)	0.0002 (5)
N4	0.0248 (8)	0.0265 (8)	0.0231 (8)	0.000	−0.0009 (6)	0.000
C1	0.0226 (6)	0.0236 (7)	0.0241 (6)	−0.0004 (5)	0.0042 (5)	−0.0011 (5)
C2	0.0261 (6)	0.0207 (6)	0.0252 (6)	0.0010 (5)	0.0037 (5)	−0.0015 (5)
C3	0.0261 (6)	0.0241 (7)	0.0342 (7)	0.0008 (5)	0.0005 (5)	−0.0026 (5)
C4	0.0317 (7)	0.0273 (7)	0.0359 (8)	0.0046 (6)	−0.0029 (6)	0.0018 (6)
C5	0.0362 (7)	0.0224 (7)	0.0332 (7)	0.0016 (6)	0.0031 (6)	0.0040 (5)
C6	0.0292 (7)	0.0243 (7)	0.0293 (7)	−0.0028 (5)	0.0041 (5)	0.0003 (5)
C7	0.0273 (6)	0.0227 (7)	0.0235 (6)	−0.0002 (5)	0.0030 (5)	−0.0015 (5)
C8	0.0277 (6)	0.0232 (6)	0.0228 (6)	−0.0036 (5)	0.0012 (5)	−0.0014 (5)
C9	0.0255 (6)	0.0272 (7)	0.0227 (6)	−0.0031 (5)	−0.0022 (5)	0.0010 (5)
C10	0.0245 (6)	0.0355 (7)	0.0221 (6)	−0.0013 (5)	−0.0052 (5)	0.0010 (5)
C11	0.0261 (7)	0.0413 (8)	0.0323 (7)	−0.0044 (6)	−0.0049 (6)	0.0046 (6)
C12	0.0236 (7)	0.0557 (9)	0.0426 (8)	−0.0047 (6)	0.0002 (6)	0.0040 (7)
C13	0.0465 (12)	0.0223 (9)	0.0261 (10)	0.000	0.0043 (9)	0.000
B1	0.0265 (10)	0.0228 (10)	0.0228 (10)	0.000	0.0012 (8)	0.000

Geometric parameters (Å, º)

O1—C13	1.394 (2)	C5—C6	1.3819 (19)
O1—B1	1.424 (2)	C5—H5A	0.9500
N1—C1^{i}	1.3465 (14)	C6—C7	1.3920 (18)
N1—C1	1.3466 (14)	C6—H6A	0.9500
N2—C1	1.3651 (16)	C7—C8	1.4563 (18)
N2—C8	1.3708 (16)	C9—C10	1.4555 (18)
N2—B1	1.5020 (16)	C10—C11	1.3950 (18)
N3—C8	1.3435 (16)	C10—C10^{i}	1.425 (3)
N3—C9	1.3489 (17)	C11—C12	1.380 (2)
N4—C9	1.3655 (15)	C11—H11	0.9500
N4—C9^{i}	1.3656 (15)	C12—C12^{i}	1.398 (3)
N4—B1	1.495 (2)	C12—H12	0.9500
C1—C2	1.4556 (17)	C13—H13A	0.9800
C2—C3	1.3872 (18)	C13—H13B	0.9800
C2—C7	1.4213 (17)	C13—H13C	0.9800
C3—C4	1.3813 (19)	C13—H13A^{i}	0.980 (9)
C3—H3A	0.9500	C13—H13B^{i}	0.980 (15)
C4—C5	1.3995 (19)	C13—H13C^{i}	0.980 (5)
C4—H4A	0.9500		

C13—O1—B1	117.55 (15)	C11—C10—C10^{i}	120.68 (8)
C1^{i}—N1—C1	116.76 (15)	C11—C10—C9	132.06 (13)
C1—N2—C8	112.76 (10)	C10^{i}—C10—C9	107.23 (7)
C1—N2—B1	123.69 (11)	C12—C11—C10	117.63 (14)
C8—N2—B1	122.28 (11)	C12—C11—H11	121.2
C8—N3—C9	117.01 (11)	C10—C11—H11	121.2
C9—N4—C9^{i}	113.74 (15)	C11—C12—C12^{i}	121.69 (9)
C9—N4—B1	122.87 (7)	C11—C12—H12	119.2
C9^{i}—N4—B1	122.87 (7)	C12^{i}—C12—H12	119.2
N1—C1—N2	122.66 (11)	O1—C13—H13A	109.5
N1—C1—C2	129.92 (12)	O1—C13—H13B	109.5
N2—C1—C2	105.85 (10)	H13A—C13—H13B	109.5
C3—C2—C7	120.59 (11)	O1—C13—H13C	109.5
C3—C2—C1	131.86 (12)	H13A—C13—H13C	109.5
C7—C2—C1	107.23 (11)	H13B—C13—H13C	109.5
C4—C3—C2	118.24 (12)	O1—C13—H13A^{i}	109.5 (2)
C4—C3—H3A	120.9	H13A—C13—H13A^{i}	36.4
C2—C3—H3A	120.9	H13B—C13—H13A^{i}	135.8
C3—C4—C5	121.38 (12)	H13C—C13—H13A^{i}	75.8
C3—C4—H4A	119.3	O1—C13—H13B^{i}	109.5 (3)
C5—C4—H4A	119.3	H13A—C13—H13B^{i}	135.8
C6—C5—C4	121.03 (12)	H13B—C13—H13B^{i}	75.8
C6—C5—H5A	119.5	H13C—C13—H13B^{i}	36.4
C4—C5—H5A	119.5	H13A^{i}—C13—H13B^{i}	109.5
C5—C6—C7	118.34 (12)	O1—C13—H13C^{i}	109.47 (12)
C5—C6—H6A	120.8	H13A—C13—H13C^{i}	75.8

C7—C6—H6A	120.8	H13B—C13—H13C^{i}	36.4
C6—C7—C2	120.37 (12)	H13C—C13—H13C^{i}	135.8
C6—C7—C8	132.43 (12)	H13A^{i}—C13—H13C^{i}	109.5
C2—C7—C8	107.00 (11)	H13B^{i}—C13—H13C^{i}	109.5
N3—C8—N2	122.73 (11)	O1—B1—N4	110.07 (15)
N3—C8—C7	129.67 (11)	O1—B1—N2	117.29 (10)
N2—C8—C7	105.77 (10)	N4—B1—N2	103.62 (11)
N3—C9—N4	122.25 (11)	O1—B1—N2^{i}	117.28 (10)
N3—C9—C10	131.17 (12)	N4—B1—N2^{i}	103.62 (11)
N4—C9—C10	105.25 (11)	N2—B1—N2^{i}	103.30 (14)

C1^{i}—N1—C1—N2	8.5 (2)	C2—C7—C8—N2	7.22 (13)
C1^{i}—N1—C1—C2	−155.07 (10)	C8—N3—C9—N4	7.75 (18)
C8—N2—C1—N1	−155.14 (13)	C8—N3—C9—C10	−157.04 (13)
B1—N2—C1—N1	12.2 (2)	C9^{i}—N4—C9—N3	−156.56 (9)
C8—N2—C1—C2	11.82 (13)	B1—N4—C9—N3	15.4 (2)
B1—N2—C1—C2	179.17 (12)	C9^{i}—N4—C9—C10	11.64 (19)
N1—C1—C2—C3	−14.3 (2)	B1—N4—C9—C10	−176.44 (14)
N2—C1—C2—C3	−179.94 (13)	N3—C9—C10—C11	−17.8 (2)
N1—C1—C2—C7	159.10 (13)	N4—C9—C10—C11	175.53 (14)
N2—C1—C2—C7	−6.56 (13)	N3—C9—C10—C10^{i}	160.09 (12)
C7—C2—C3—C4	1.61 (18)	N4—C9—C10—C10^{i}	−6.63 (11)
C1—C2—C3—C4	174.26 (13)	C10^{i}—C10—C11—C12	0.65 (15)
C2—C3—C4—C5	−0.04 (19)	C9—C10—C11—C12	178.25 (13)
C3—C4—C5—C6	−1.6 (2)	C10—C11—C12—C12^{i}	−0.66 (15)
C4—C5—C6—C7	1.55 (19)	C13—O1—B1—N4	180.000 (1)
C5—C6—C7—C2	0.02 (18)	C13—O1—B1—N2	−61.93 (13)
C5—C6—C7—C8	−174.12 (13)	C13—O1—B1—N2^{i}	61.93 (13)
C3—C2—C7—C6	−1.63 (18)	C9—N4—B1—O1	94.40 (13)
C1—C2—C7—C6	−175.90 (11)	C9^{i}—N4—B1—O1	−94.40 (13)
C3—C2—C7—C8	173.85 (11)	C9—N4—B1—N2	−31.80 (19)
C1—C2—C7—C8	−0.42 (13)	C9^{i}—N4—B1—N2	139.39 (12)
C9—N3—C8—N2	−8.48 (17)	C9—N4—B1—N2^{i}	−139.39 (12)
C9—N3—C8—C7	153.85 (13)	C9^{i}—N4—B1—N2^{i}	31.80 (19)
C1—N2—C8—N3	153.87 (11)	C1—N2—B1—O1	103.19 (15)
B1—N2—C8—N3	−13.69 (18)	C8—N2—B1—O1	−90.62 (17)
C1—N2—C8—C7	−12.08 (13)	C1—N2—B1—N4	−135.32 (12)
B1—N2—C8—C7	−179.64 (12)	C8—N2—B1—N4	30.86 (16)
C6—C7—C8—N3	17.3 (2)	C1—N2—B1—N2^{i}	−27.49 (19)
C2—C7—C8—N3	−157.40 (13)	C8—N2—B1—N2^{i}	138.69 (10)
C6—C7—C8—N2	−178.07 (13)		

Symmetry code: (i) x, $-y+3/2$, z.

(Ethanolato)(subphthalocyaninato)boron (d22127_a)

Crystal data

$C_{26}H_{17}BN_6O$
$M_r = 440.26$
Monoclinic, $P2_1/n$
$a = 9.0313$ (14) Å
$b = 14.220$ (2) Å
$c = 16.474$ (2) Å
$\beta = 102.667$ (4)°
$V = 2064.3$ (5) Å^3
$Z = 4$
$F(000) = 912$
$D_x = 1.417$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6076 reflections
$\theta = 2.5$–$26.0°$
$\mu = 0.09$ mm^{-1}
$T = 150$ K
Plate, purple
0.21 × 0.12 × 0.03 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: sealed tube with Bruker Triumph Monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.684$, $T_{max} = 0.746$
49575 measured reflections
4744 independent reflections
3311 reflections with $I > 2\sigma(I)$
$R_{int} = 0.101$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -11 \rightarrow 11$
$k = -18 \rightarrow 18$
$l = -21 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.098$
$S = 1.04$
4744 reflections
308 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.5512P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.43092 (12)	0.67237 (8)	0.21540 (6)	0.0226 (3)
N1	0.45908 (14)	0.58982 (9)	0.34451 (8)	0.0197 (3)
N2	0.56828 (14)	0.70834 (9)	0.43968 (8)	0.0209 (3)
N3	0.34169 (14)	0.73791 (9)	0.33712 (8)	0.0185 (3)
N4	0.07319 (14)	0.74430 (9)	0.29173 (8)	0.0200 (3)
N5	0.20976 (14)	0.60783 (9)	0.26680 (8)	0.0186 (3)
N6	0.30979 (14)	0.45416 (9)	0.30217 (8)	0.0211 (3)
C1	0.43968 (17)	0.49460 (11)	0.34219 (10)	0.0196 (3)
C2	0.56971 (17)	0.45745 (11)	0.40263 (10)	0.0212 (3)

C3	0.62097 (18)	0.36620 (12)	0.42212 (10)	0.0238 (4)
H3A	0.567321	0.313513	0.394840	0.029*
C4	0.75308 (18)	0.35475 (12)	0.48276 (10)	0.0262 (4)
H4A	0.792134	0.293223	0.495709	0.031*
C5	0.82990 (19)	0.43142 (12)	0.52514 (10)	0.0266 (4)
H5A	0.919487	0.420909	0.566683	0.032*
C6	0.77830 (18)	0.52271 (12)	0.50793 (10)	0.0247 (4)
H6A	0.829356	0.574522	0.538144	0.030*
C7	0.64924 (17)	0.53599 (11)	0.44495 (10)	0.0208 (3)
C8	0.56794 (17)	0.62028 (11)	0.41016 (10)	0.0202 (3)
C9	0.44772 (17)	0.76266 (11)	0.40651 (10)	0.0197 (3)
C10	0.38257 (17)	0.84138 (11)	0.44307 (10)	0.0192 (3)
C11	0.43401 (18)	0.89251 (11)	0.51574 (10)	0.0220 (4)
H11A	0.532128	0.881631	0.549515	0.026*
C12	0.33899 (18)	0.95956 (12)	0.53769 (10)	0.0241 (4)
H12A	0.373533	0.996338	0.586292	0.029*
C13	0.19304 (18)	0.97406 (11)	0.48953 (10)	0.0240 (4)
H13A	0.130921	1.021538	0.505329	0.029*
C14	0.13725 (18)	0.92083 (11)	0.41948 (10)	0.0224 (4)
H14A	0.036495	0.929469	0.388239	0.027*
C15	0.23215 (17)	0.85429 (11)	0.39580 (9)	0.0191 (3)
C16	0.20517 (17)	0.78150 (11)	0.33235 (9)	0.0192 (3)
C17	0.07709 (17)	0.65512 (11)	0.26457 (9)	0.0194 (3)
C18	−0.04156 (18)	0.58441 (11)	0.25035 (9)	0.0197 (3)
C19	−0.19862 (18)	0.59144 (12)	0.24018 (9)	0.0220 (4)
H19A	−0.246991	0.650926	0.238807	0.026*
C20	−0.28115 (18)	0.50930 (12)	0.23222 (10)	0.0250 (4)
H20A	−0.388527	0.512614	0.223660	0.030*
C21	−0.21131 (19)	0.42095 (12)	0.23637 (10)	0.0255 (4)
H21A	−0.271955	0.365765	0.231144	0.031*
C22	−0.05506 (19)	0.41275 (12)	0.24797 (10)	0.0232 (4)
H22A	−0.007700	0.352779	0.251650	0.028*
C23	0.03053 (17)	0.49511 (11)	0.25409 (9)	0.0202 (3)
C24	0.19339 (17)	0.51235 (11)	0.27071 (9)	0.0196 (3)
C25	0.34167 (18)	0.70717 (12)	0.13924 (10)	0.0260 (4)
H25A	0.289154	0.765629	0.149550	0.031*
H25B	0.263941	0.660151	0.114554	0.031*
C26	0.4441 (2)	0.72668 (13)	0.08048 (11)	0.0318 (4)
H26A	0.382777	0.745504	0.026213	0.048*
H26B	0.501630	0.669782	0.074011	0.048*
H26C	0.514583	0.777464	0.102930	0.048*
B1	0.3627 (2)	0.65482 (13)	0.28386 (11)	0.0196 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0180 (6)	0.0296 (6)	0.0206 (6)	0.0021 (5)	0.0052 (5)	0.0034 (5)
N1	0.0163 (7)	0.0219 (7)	0.0220 (7)	0.0023 (5)	0.0068 (5)	0.0016 (6)

N2	0.0160 (7)	0.0228 (7)	0.0243 (7)	0.0015 (6)	0.0053 (6)	0.0027 (6)
N3	0.0153 (6)	0.0183 (7)	0.0219 (7)	0.0013 (5)	0.0044 (5)	0.0027 (5)
N4	0.0186 (7)	0.0201 (7)	0.0203 (7)	0.0019 (5)	0.0022 (5)	0.0020 (5)
N5	0.0168 (7)	0.0193 (7)	0.0199 (7)	0.0018 (5)	0.0046 (5)	0.0012 (5)
N6	0.0208 (7)	0.0222 (7)	0.0217 (7)	0.0021 (6)	0.0076 (6)	−0.0009 (6)
C1	0.0198 (8)	0.0205 (8)	0.0212 (8)	0.0025 (6)	0.0101 (6)	0.0008 (6)
C2	0.0182 (8)	0.0244 (9)	0.0237 (8)	0.0045 (7)	0.0106 (7)	0.0033 (7)
C3	0.0218 (9)	0.0239 (9)	0.0292 (9)	0.0028 (7)	0.0129 (7)	0.0044 (7)
C4	0.0238 (9)	0.0266 (9)	0.0315 (9)	0.0083 (7)	0.0132 (7)	0.0106 (7)
C5	0.0205 (9)	0.0350 (10)	0.0250 (9)	0.0058 (7)	0.0063 (7)	0.0090 (7)
C6	0.0200 (8)	0.0301 (10)	0.0249 (9)	0.0038 (7)	0.0068 (7)	0.0024 (7)
C7	0.0174 (8)	0.0243 (9)	0.0225 (8)	0.0024 (7)	0.0082 (6)	0.0032 (7)
C8	0.0149 (8)	0.0251 (9)	0.0218 (8)	−0.0002 (7)	0.0067 (6)	0.0016 (7)
C9	0.0159 (8)	0.0204 (8)	0.0228 (8)	−0.0017 (6)	0.0045 (6)	0.0026 (7)
C10	0.0179 (8)	0.0182 (8)	0.0223 (8)	−0.0013 (6)	0.0057 (6)	0.0043 (6)
C11	0.0196 (8)	0.0220 (9)	0.0235 (8)	−0.0029 (7)	0.0029 (7)	0.0030 (7)
C12	0.0263 (9)	0.0242 (9)	0.0223 (8)	−0.0048 (7)	0.0061 (7)	−0.0005 (7)
C13	0.0249 (9)	0.0218 (9)	0.0275 (9)	0.0030 (7)	0.0103 (7)	0.0008 (7)
C14	0.0193 (8)	0.0231 (9)	0.0248 (8)	0.0028 (7)	0.0046 (7)	0.0041 (7)
C15	0.0198 (8)	0.0179 (8)	0.0199 (8)	−0.0001 (6)	0.0052 (6)	0.0037 (6)
C16	0.0187 (8)	0.0183 (8)	0.0208 (8)	0.0032 (6)	0.0050 (6)	0.0057 (6)
C17	0.0179 (8)	0.0238 (9)	0.0165 (8)	0.0032 (6)	0.0038 (6)	0.0022 (6)
C18	0.0208 (8)	0.0228 (8)	0.0150 (7)	0.0006 (7)	0.0025 (6)	0.0003 (6)
C19	0.0199 (8)	0.0262 (9)	0.0198 (8)	0.0018 (7)	0.0043 (7)	−0.0024 (7)
C20	0.0187 (8)	0.0343 (10)	0.0231 (9)	−0.0014 (7)	0.0071 (7)	−0.0045 (7)
C21	0.0256 (9)	0.0278 (9)	0.0246 (9)	−0.0065 (7)	0.0087 (7)	−0.0019 (7)
C22	0.0257 (9)	0.0234 (9)	0.0208 (8)	0.0005 (7)	0.0061 (7)	−0.0010 (7)
C23	0.0202 (8)	0.0235 (9)	0.0174 (8)	0.0014 (7)	0.0050 (6)	−0.0008 (7)
C24	0.0210 (8)	0.0203 (8)	0.0181 (8)	0.0024 (7)	0.0053 (6)	−0.0018 (6)
C25	0.0224 (9)	0.0326 (10)	0.0224 (9)	0.0013 (7)	0.0037 (7)	0.0035 (7)
C26	0.0366 (10)	0.0362 (10)	0.0247 (9)	0.0009 (8)	0.0111 (8)	0.0047 (8)
B1	0.0161 (9)	0.0199 (9)	0.0230 (9)	0.0021 (7)	0.0051 (7)	0.0018 (7)

Geometric parameters (Å, º)

O1—B1	1.421 (2)	C10—C11	1.391 (2)
O1—C25	1.4231 (18)	C10—C15	1.422 (2)
N1—C8	1.363 (2)	C11—C12	1.383 (2)
N1—C1	1.365 (2)	C11—H11A	0.9500
N1—B1	1.493 (2)	C12—C13	1.397 (2)
N2—C8	1.343 (2)	C12—H12A	0.9500
N2—C9	1.349 (2)	C13—C14	1.380 (2)
N3—C9	1.3665 (19)	C13—H13A	0.9500
N3—C16	1.3667 (19)	C14—C15	1.389 (2)
N3—B1	1.508 (2)	C14—H14A	0.9500
N4—C16	1.341 (2)	C15—C16	1.453 (2)
N4—C17	1.348 (2)	C17—C18	1.451 (2)
N5—C17	1.3675 (19)	C18—C19	1.395 (2)

N5—C24	1.369 (2)	C18—C23	1.422 (2)
N5—B1	1.504 (2)	C19—C20	1.376 (2)
N6—C1	1.342 (2)	C19—H19A	0.9500
N6—C24	1.349 (2)	C20—C21	1.401 (2)
C1—C2	1.462 (2)	C20—H20A	0.9500
C2—C3	1.392 (2)	C21—C22	1.387 (2)
C2—C7	1.425 (2)	C21—H21A	0.9500
C3—C4	1.387 (2)	C22—C23	1.395 (2)
C3—H3A	0.9500	C22—H22A	0.9500
C4—C5	1.395 (2)	C23—C24	1.457 (2)
C4—H4A	0.9500	C25—C26	1.504 (2)
C5—C6	1.387 (2)	C25—H25A	0.9900
C5—H5A	0.9500	C25—H25B	0.9900
C6—C7	1.393 (2)	C26—H26A	0.9800
C6—H6A	0.9500	C26—H26B	0.9800
C7—C8	1.456 (2)	C26—H26C	0.9800
C9—C10	1.455 (2)		

B1—O1—C25	120.02 (12)	C13—C14—C15	118.29 (15)
C8—N1—C1	113.79 (13)	C13—C14—H14A	120.9
C8—N1—B1	123.21 (13)	C15—C14—H14A	120.9
C1—N1—B1	122.88 (13)	C14—C15—C10	120.57 (14)
C8—N2—C9	116.72 (13)	C14—C15—C16	132.13 (14)
C9—N3—C16	112.90 (13)	C10—C15—C16	106.94 (13)
C9—N3—B1	122.28 (13)	N4—C16—N3	122.79 (14)
C16—N3—B1	123.28 (13)	N4—C16—C15	129.08 (14)
C16—N4—C17	116.85 (13)	N3—C16—C15	105.95 (13)
C17—N5—C24	112.70 (13)	N4—C17—N5	122.71 (14)
C17—N5—B1	123.34 (13)	N4—C17—C18	129.32 (14)
C24—N5—B1	122.42 (13)	N5—C17—C18	105.98 (13)
C1—N6—C24	116.70 (13)	C19—C18—C23	120.87 (14)
N6—C1—N1	122.12 (14)	C19—C18—C17	131.71 (15)
N6—C1—C2	131.66 (14)	C23—C18—C17	107.27 (13)
N1—C1—C2	105.09 (13)	C20—C19—C18	117.76 (15)
C3—C2—C7	120.77 (14)	C20—C19—H19A	121.1
C3—C2—C1	132.15 (15)	C18—C19—H19A	121.1
C7—C2—C1	107.07 (13)	C19—C20—C21	121.87 (15)
C4—C3—C2	117.75 (16)	C19—C20—H20A	119.1
C4—C3—H3A	121.1	C21—C20—H20A	119.1
C2—C3—H3A	121.1	C22—C21—C20	121.05 (15)
C3—C4—C5	121.57 (16)	C22—C21—H21A	119.5
C3—C4—H4A	119.2	C20—C21—H21A	119.5
C5—C4—H4A	119.2	C21—C22—C23	118.06 (15)
C6—C5—C4	121.42 (15)	C21—C22—H22A	121.0
C6—C5—H5A	119.3	C23—C22—H22A	121.0
C4—C5—H5A	119.3	C22—C23—C18	120.36 (14)
C5—C6—C7	117.89 (16)	C22—C23—C24	132.50 (15)
C5—C6—H6A	121.1	C18—C23—C24	106.96 (13)

C7—C6—H6A	121.1	N6—C24—N5	122.92 (14)
C6—C7—C2	120.53 (15)	N6—C24—C23	129.70 (14)
C6—C7—C8	132.24 (15)	N5—C24—C23	105.85 (13)
C2—C7—C8	107.22 (13)	O1—C25—C26	108.79 (13)
N2—C8—N1	121.84 (14)	O1—C25—H25A	109.9
N2—C8—C7	131.61 (14)	C26—C25—H25A	109.9
N1—C8—C7	105.34 (13)	O1—C25—H25B	109.9
N2—C9—N3	123.14 (14)	C26—C25—H25B	109.9
N2—C9—C10	129.53 (14)	H25A—C25—H25B	108.3
N3—C9—C10	105.76 (13)	C25—C26—H26A	109.5
C11—C10—C15	120.18 (14)	C25—C26—H26B	109.5
C11—C10—C9	132.03 (14)	H26A—C26—H26B	109.5
C15—C10—C9	107.28 (13)	C25—C26—H26C	109.5
C12—C11—C10	118.44 (15)	H26A—C26—H26C	109.5
C12—C11—H11A	120.8	H26B—C26—H26C	109.5
C10—C11—H11A	120.8	O1—B1—N1	110.43 (13)
C11—C12—C13	121.05 (15)	O1—B1—N5	118.04 (14)
C11—C12—H12A	119.5	N1—B1—N5	103.11 (13)
C13—C12—H12A	119.5	O1—B1—N3	117.12 (14)
C14—C13—C12	121.35 (16)	N1—B1—N3	102.99 (13)
C14—C13—H13A	119.3	N5—B1—N3	103.27 (12)
C12—C13—H13A	119.3		

C24—N6—C1—N1	−6.1 (2)	C14—C15—C16—N4	−17.3 (3)
C24—N6—C1—C2	159.88 (16)	C10—C15—C16—N4	155.65 (15)
C8—N1—C1—N6	156.73 (14)	C14—C15—C16—N3	179.45 (16)
B1—N1—C1—N6	−19.4 (2)	C10—C15—C16—N3	−7.64 (16)
C8—N1—C1—C2	−12.44 (17)	C16—N4—C17—N5	−9.2 (2)
B1—N1—C1—C2	171.41 (13)	C16—N4—C17—C18	152.47 (16)
N6—C1—C2—C3	19.7 (3)	C24—N5—C17—N4	154.08 (14)
N1—C1—C2—C3	−172.63 (16)	B1—N5—C17—N4	−12.1 (2)
N6—C1—C2—C7	−160.56 (16)	C24—N5—C17—C18	−11.23 (17)
N1—C1—C2—C7	7.15 (16)	B1—N5—C17—C18	−177.40 (13)
C7—C2—C3—C4	−1.2 (2)	N4—C17—C18—C19	18.0 (3)
C1—C2—C3—C4	178.56 (16)	N5—C17—C18—C19	−178.01 (16)
C2—C3—C4—C5	2.2 (2)	N4—C17—C18—C23	−157.53 (15)
C3—C4—C5—C6	−0.6 (3)	N5—C17—C18—C23	6.46 (17)
C4—C5—C6—C7	−1.9 (2)	C23—C18—C19—C20	−1.3 (2)
C5—C6—C7—C2	2.8 (2)	C17—C18—C19—C20	−176.34 (16)
C5—C6—C7—C8	−178.47 (16)	C18—C19—C20—C21	1.8 (2)
C3—C2—C7—C6	−1.3 (2)	C19—C20—C21—C22	−0.6 (2)
C1—C2—C7—C6	178.86 (14)	C20—C21—C22—C23	−1.0 (2)
C3—C2—C7—C8	179.69 (14)	C21—C22—C23—C18	1.4 (2)
C1—C2—C7—C8	−0.12 (17)	C21—C22—C23—C24	175.98 (16)
C9—N2—C8—N1	6.2 (2)	C19—C18—C23—C22	−0.3 (2)
C9—N2—C8—C7	−159.34 (16)	C17—C18—C23—C22	175.85 (14)
C1—N1—C8—N2	−156.42 (14)	C19—C18—C23—C24	−176.08 (14)
B1—N1—C8—N2	19.7 (2)	C17—C18—C23—C24	0.04 (17)

C1—N1—C8—C7	12.39 (17)	C1—N6—C24—N5	10.3 (2)
B1—N1—C8—C7	−171.47 (14)	C1—N6—C24—C23	−153.46 (16)
C6—C7—C8—N2	−18.5 (3)	C17—N5—C24—N6	−155.86 (14)
C2—C7—C8—N2	160.30 (16)	B1—N5—C24—N6	10.5 (2)
C6—C7—C8—N1	174.22 (17)	C17—N5—C24—C23	11.24 (17)
C2—C7—C8—N1	−6.97 (17)	B1—N5—C24—C23	177.55 (13)
C8—N2—C9—N3	−11.0 (2)	C22—C23—C24—N6	−15.7 (3)
C8—N2—C9—C10	152.64 (16)	C18—C23—C24—N6	159.39 (16)
C16—N3—C9—N2	156.63 (14)	C22—C23—C24—N5	178.39 (16)
B1—N3—C9—N2	−9.6 (2)	C18—C23—C24—N5	−6.51 (16)
C16—N3—C9—C10	−10.29 (17)	B1—O1—C25—C26	175.44 (14)
B1—N3—C9—C10	−176.52 (13)	C25—O1—B1—N1	160.56 (13)
N2—C9—C10—C11	10.6 (3)	C25—O1—B1—N5	42.4 (2)
N3—C9—C10—C11	176.42 (16)	C25—O1—B1—N3	−82.04 (18)
N2—C9—C10—C15	−160.93 (15)	C8—N1—B1—O1	91.45 (17)
N3—C9—C10—C15	4.84 (17)	C1—N1—B1—O1	−92.76 (17)
C15—C10—C11—C12	−3.8 (2)	C8—N1—B1—N5	−141.56 (14)
C9—C10—C11—C12	−174.54 (16)	C1—N1—B1—N5	34.24 (19)
C10—C11—C12—C13	1.8 (2)	C8—N1—B1—N3	−34.36 (19)
C11—C12—C13—C14	1.4 (2)	C1—N1—B1—N3	141.43 (14)
C12—C13—C14—C15	−2.4 (2)	C17—N5—B1—O1	−102.86 (17)
C13—C14—C15—C10	0.3 (2)	C24—N5—B1—O1	92.29 (18)
C13—C14—C15—C16	172.45 (16)	C17—N5—B1—N1	135.14 (14)
C11—C10—C15—C14	2.8 (2)	C24—N5—B1—N1	−29.72 (18)
C9—C10—C15—C14	175.61 (14)	C17—N5—B1—N3	28.15 (19)
C11—C10—C15—C16	−171.05 (14)	C24—N5—B1—N3	−136.70 (14)
C9—C10—C15—C16	1.71 (17)	C9—N3—B1—O1	−92.20 (17)
C17—N4—C16—N3	8.8 (2)	C16—N3—B1—O1	103.01 (17)
C17—N4—C16—C15	−152.04 (15)	C9—N3—B1—N1	29.17 (19)
C9—N3—C16—N4	−153.22 (14)	C16—N3—B1—N1	−135.62 (14)
B1—N3—C16—N4	12.8 (2)	C9—N3—B1—N5	136.25 (14)
C9—N3—C16—C15	11.38 (17)	C16—N3—B1—N5	−28.55 (19)
B1—N3—C16—C15	177.45 (13)		

(Ethanolato)(subphthalocyaninato)boron (d22128_a)

Crystal data

$C_{26}H_{17}BN_6O$
M_r = 440.26
Monoclinic, $P2_1/n$
a = 9.0304 (5) Å
b = 14.2423 (8) Å
c = 16.4452 (9) Å
β = 102.476 (3)°
V = 2065.1 (2) Å^3
Z = 4
$F(000)$ = 912
D_x = 1.416 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9939 reflections
θ = 4.2–65.7°
μ = 0.72 mm^{-1}
T = 150 K
Block, purple
0.15 × 0.15 × 0.10 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.654, T_{max} = 0.753
46104 measured reflections
3555 independent reflections
3148 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 66.1°, θ_{min} = 4.2°
h = −10→10
k = −16→16
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.102
S = 1.05
3555 reflections
308 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.8523P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.43100 (11)	0.67170 (7)	0.21518 (6)	0.0284 (3)
N1	0.45941 (13)	0.58926 (9)	0.34451 (8)	0.0247 (3)
N2	0.56875 (13)	0.70791 (9)	0.43942 (8)	0.0270 (3)
N3	0.34174 (13)	0.73692 (8)	0.33710 (8)	0.0243 (3)
N4	0.07299 (13)	0.74350 (9)	0.29183 (8)	0.0253 (3)
N5	0.20962 (13)	0.60716 (9)	0.26691 (7)	0.0241 (3)
N6	0.31011 (14)	0.45375 (9)	0.30233 (8)	0.0264 (3)
C1	0.44029 (16)	0.49430 (10)	0.34227 (9)	0.0253 (3)
C2	0.57050 (16)	0.45711 (11)	0.40250 (9)	0.0264 (3)
C3	0.62145 (17)	0.36615 (11)	0.42205 (10)	0.0300 (4)
H3A	0.567517	0.313576	0.394978	0.036*
C4	0.75388 (18)	0.35451 (12)	0.48250 (10)	0.0331 (4)
H4A	0.793009	0.293066	0.495193	0.040*
C5	0.83088 (18)	0.43129 (12)	0.52509 (10)	0.0339 (4)
H5A	0.920282	0.420810	0.566635	0.041*
C6	0.77923 (17)	0.52228 (12)	0.50784 (10)	0.0305 (4)
H6A	0.830297	0.574069	0.537896	0.037*
C7	0.64952 (16)	0.53554 (11)	0.44475 (9)	0.0271 (3)
C8	0.56827 (15)	0.61983 (11)	0.40996 (9)	0.0255 (3)
C9	0.44810 (16)	0.76202 (10)	0.40642 (9)	0.0252 (3)

C10	0.38312 (16)	0.84085 (10)	0.44303 (9)	0.0260 (3)
C11	0.43452 (17)	0.89237 (11)	0.51549 (10)	0.0292 (3)
H11A	0.532775	0.881930	0.549059	0.035*
C12	0.33929 (18)	0.95902 (11)	0.53744 (10)	0.0304 (4)
H12A	0.373671	0.995742	0.586086	0.036*
C13	0.19338 (18)	0.97357 (11)	0.48956 (10)	0.0310 (4)
H13A	0.131530	1.021163	0.505424	0.037*
C14	0.13711 (17)	0.92004 (11)	0.41949 (10)	0.0288 (3)
H14A	0.036258	0.928440	0.388532	0.035*
C15	0.23225 (16)	0.85365 (10)	0.39565 (9)	0.0252 (3)
C16	0.20527 (16)	0.78083 (10)	0.33249 (9)	0.0245 (3)
C17	0.07694 (16)	0.65457 (10)	0.26476 (9)	0.0241 (3)
C18	−0.04180 (16)	0.58398 (10)	0.25038 (9)	0.0250 (3)
C19	−0.19910 (16)	0.59083 (11)	0.24007 (9)	0.0276 (3)
H19A	−0.247657	0.650166	0.238637	0.033*
C20	−0.28149 (17)	0.50859 (12)	0.23204 (10)	0.0305 (4)
H20A	−0.388824	0.511746	0.223543	0.037*
C21	−0.21143 (18)	0.42064 (12)	0.23607 (10)	0.0310 (4)
H21A	−0.272034	0.365522	0.230474	0.037*
C22	−0.05515 (17)	0.41233 (11)	0.24806 (9)	0.0287 (3)
H22A	−0.007766	0.352455	0.251932	0.034*
C23	0.03028 (17)	0.49473 (11)	0.25427 (9)	0.0254 (3)
C24	0.19340 (16)	0.51184 (10)	0.27080 (9)	0.0248 (3)
C25	0.34110 (18)	0.70714 (12)	0.13931 (10)	0.0342 (4)
H25A	0.289660	0.765756	0.150133	0.041*
H25B	0.262630	0.660635	0.114787	0.041*
C26	0.4432 (2)	0.72616 (13)	0.08009 (11)	0.0404 (4)
H26A	0.381919	0.745375	0.025975	0.061*
H26B	0.499809	0.669051	0.073209	0.061*
H26C	0.514504	0.776445	0.102470	0.061*
B1	0.36277 (18)	0.65409 (12)	0.28368 (11)	0.0248 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0225 (5)	0.0359 (6)	0.0268 (5)	0.0022 (4)	0.0054 (4)	0.0042 (5)
N1	0.0205 (6)	0.0268 (7)	0.0269 (7)	0.0030 (5)	0.0054 (5)	0.0020 (5)
N2	0.0208 (6)	0.0287 (7)	0.0310 (7)	0.0007 (5)	0.0048 (5)	0.0029 (5)
N3	0.0212 (6)	0.0247 (6)	0.0265 (7)	0.0010 (5)	0.0041 (5)	0.0032 (5)
N4	0.0235 (6)	0.0265 (7)	0.0250 (6)	0.0020 (5)	0.0029 (5)	0.0022 (5)
N5	0.0215 (6)	0.0253 (6)	0.0254 (6)	0.0021 (5)	0.0049 (5)	0.0007 (5)
N6	0.0239 (6)	0.0280 (7)	0.0279 (7)	0.0039 (5)	0.0071 (5)	0.0005 (5)
C1	0.0236 (7)	0.0267 (8)	0.0272 (8)	0.0033 (6)	0.0090 (6)	0.0009 (6)
C2	0.0230 (7)	0.0305 (8)	0.0275 (8)	0.0047 (6)	0.0096 (6)	0.0045 (6)
C3	0.0282 (8)	0.0308 (8)	0.0334 (9)	0.0044 (6)	0.0122 (7)	0.0058 (7)
C4	0.0296 (8)	0.0351 (9)	0.0376 (9)	0.0098 (7)	0.0137 (7)	0.0131 (7)
C5	0.0259 (8)	0.0441 (10)	0.0322 (9)	0.0078 (7)	0.0076 (7)	0.0114 (7)
C6	0.0241 (8)	0.0376 (9)	0.0304 (8)	0.0039 (7)	0.0068 (6)	0.0043 (7)

C7	0.0217 (7)	0.0332 (8)	0.0281 (8)	0.0035 (6)	0.0088 (6)	0.0043 (6)
C8	0.0192 (7)	0.0302 (8)	0.0278 (8)	0.0009 (6)	0.0066 (6)	0.0031 (6)
C9	0.0200 (7)	0.0275 (8)	0.0276 (8)	−0.0018 (6)	0.0039 (6)	0.0028 (6)
C10	0.0236 (7)	0.0252 (8)	0.0290 (8)	−0.0017 (6)	0.0052 (6)	0.0043 (6)
C11	0.0259 (8)	0.0292 (8)	0.0308 (8)	−0.0038 (6)	0.0019 (6)	0.0025 (7)
C12	0.0332 (8)	0.0297 (8)	0.0284 (8)	−0.0039 (7)	0.0068 (7)	−0.0012 (6)
C13	0.0314 (8)	0.0288 (8)	0.0340 (9)	0.0018 (6)	0.0097 (7)	−0.0012 (7)
C14	0.0260 (8)	0.0291 (8)	0.0307 (8)	0.0025 (6)	0.0049 (6)	0.0036 (6)
C15	0.0245 (7)	0.0240 (7)	0.0265 (8)	0.0001 (6)	0.0043 (6)	0.0037 (6)
C16	0.0219 (7)	0.0261 (8)	0.0252 (8)	0.0031 (6)	0.0043 (6)	0.0053 (6)
C17	0.0224 (7)	0.0269 (8)	0.0224 (7)	0.0039 (6)	0.0034 (6)	0.0020 (6)
C18	0.0242 (7)	0.0294 (8)	0.0207 (7)	0.0014 (6)	0.0036 (6)	−0.0007 (6)
C19	0.0243 (8)	0.0339 (9)	0.0242 (8)	0.0025 (6)	0.0046 (6)	−0.0025 (6)
C20	0.0226 (7)	0.0409 (9)	0.0284 (8)	−0.0022 (7)	0.0067 (6)	−0.0046 (7)
C21	0.0292 (8)	0.0350 (9)	0.0292 (8)	−0.0062 (7)	0.0074 (7)	−0.0030 (7)
C22	0.0303 (8)	0.0290 (8)	0.0271 (8)	−0.0002 (6)	0.0069 (6)	−0.0009 (6)
C23	0.0249 (7)	0.0295 (8)	0.0218 (7)	0.0007 (6)	0.0050 (6)	−0.0008 (6)
C24	0.0249 (7)	0.0261 (8)	0.0241 (7)	0.0016 (6)	0.0067 (6)	−0.0008 (6)
C25	0.0297 (8)	0.0415 (9)	0.0301 (9)	0.0015 (7)	0.0034 (7)	0.0041 (7)
C26	0.0434 (10)	0.0456 (10)	0.0333 (9)	0.0007 (8)	0.0105 (8)	0.0046 (8)
B1	0.0201 (8)	0.0270 (9)	0.0270 (9)	0.0022 (7)	0.0046 (7)	0.0028 (7)

Geometric parameters (Å, º)

O1—B1	1.418 (2)	C10—C11	1.391 (2)
O1—C25	1.4257 (19)	C10—C15	1.428 (2)
N1—C8	1.3628 (19)	C11—C12	1.380 (2)
N1—C1	1.363 (2)	C11—H11A	0.9500
N1—B1	1.496 (2)	C12—C13	1.397 (2)
N2—C8	1.344 (2)	C12—H12A	0.9500
N2—C9	1.3491 (19)	C13—C14	1.384 (2)
N3—C16	1.3694 (18)	C13—H13A	0.9500
N3—C9	1.3700 (19)	C14—C15	1.390 (2)
N3—B1	1.507 (2)	C14—H14A	0.9500
N4—C17	1.3456 (19)	C15—C16	1.451 (2)
N4—C16	1.3460 (19)	C17—C18	1.452 (2)
N5—C24	1.368 (2)	C18—C19	1.397 (2)
N5—C17	1.3691 (18)	C18—C23	1.423 (2)
N5—B1	1.507 (2)	C19—C20	1.379 (2)
N6—C1	1.3466 (19)	C19—H19A	0.9500
N6—C24	1.3520 (19)	C20—C21	1.398 (2)
C1—C2	1.463 (2)	C20—H20A	0.9500
C2—C3	1.389 (2)	C21—C22	1.387 (2)
C2—C7	1.423 (2)	C21—H21A	0.9500
C3—C4	1.390 (2)	C22—C23	1.396 (2)
C3—H3A	0.9500	C22—H22A	0.9500
C4—C5	1.400 (3)	C23—C24	1.459 (2)
C4—H4A	0.9500	C25—C26	1.504 (2)

C5—C6	1.386 (2)	C25—H25A	0.9900
C5—H5A	0.9500	C25—H25B	0.9900
C6—C7	1.400 (2)	C26—H26A	0.9800
C6—H6A	0.9500	C26—H26B	0.9800
C7—C8	1.458 (2)	C26—H26C	0.9800
C9—C10	1.456 (2)		

B1—O1—C25	119.65 (11)	C13—C14—C15	118.14 (14)
C8—N1—C1	113.82 (12)	C13—C14—H14A	120.9
C8—N1—B1	123.23 (13)	C15—C14—H14A	120.9
C1—N1—B1	122.84 (13)	C14—C15—C10	120.55 (14)
C8—N2—C9	116.65 (13)	C14—C15—C16	132.06 (14)
C16—N3—C9	112.81 (12)	C10—C15—C16	107.00 (13)
C16—N3—B1	123.39 (12)	N4—C16—N3	122.59 (13)
C9—N3—B1	122.37 (12)	N4—C16—C15	129.18 (13)
C17—N4—C16	116.87 (12)	N3—C16—C15	106.08 (12)
C24—N5—C17	112.87 (12)	N4—C17—N5	122.77 (13)
C24—N5—B1	122.33 (12)	N4—C17—C18	129.38 (13)
C17—N5—B1	123.32 (13)	N5—C17—C18	105.91 (12)
C1—N6—C24	116.79 (13)	C19—C18—C23	120.73 (14)
N6—C1—N1	122.06 (13)	C19—C18—C17	131.86 (14)
N6—C1—C2	131.62 (14)	C23—C18—C17	107.26 (12)
N1—C1—C2	105.21 (13)	C20—C19—C18	117.76 (14)
C3—C2—C7	120.86 (14)	C20—C19—H19A	121.1
C3—C2—C1	132.21 (15)	C18—C19—H19A	121.1
C7—C2—C1	106.94 (13)	C19—C20—C21	121.82 (14)
C2—C3—C4	117.87 (15)	C19—C20—H20A	119.1
C2—C3—H3A	121.1	C21—C20—H20A	119.1
C4—C3—H3A	121.1	C22—C21—C20	121.28 (15)
C3—C4—C5	121.49 (15)	C22—C21—H21A	119.4
C3—C4—H4A	119.3	C20—C21—H21A	119.4
C5—C4—H4A	119.3	C21—C22—C23	117.89 (14)
C6—C5—C4	121.28 (15)	C21—C22—H22A	121.1
C6—C5—H5A	119.4	C23—C22—H22A	121.1
C4—C5—H5A	119.4	C22—C23—C18	120.49 (14)
C5—C6—C7	117.95 (16)	C22—C23—C24	132.34 (14)
C5—C6—H6A	121.0	C18—C23—C24	107.02 (13)
C7—C6—H6A	121.0	N6—C24—N5	122.86 (13)
C6—C7—C2	120.47 (14)	N6—C24—C23	129.87 (14)
C6—C7—C8	132.19 (15)	N5—C24—C23	105.71 (12)
C2—C7—C8	107.33 (13)	O1—C25—C26	108.53 (13)
N2—C8—N1	121.90 (13)	O1—C25—H25A	110.0
N2—C8—C7	131.66 (14)	C26—C25—H25A	110.0
N1—C8—C7	105.24 (13)	O1—C25—H25B	110.0
N2—C9—N3	123.08 (13)	C26—C25—H25B	110.0
N2—C9—C10	129.55 (14)	H25A—C25—H25B	108.4
N3—C9—C10	105.82 (12)	C25—C26—H26A	109.5
C11—C10—C15	120.18 (14)	C25—C26—H26B	109.5

C11—C10—C9	132.17 (14)	H26A—C26—H26B	109.5
C15—C10—C9	107.17 (13)	C25—C26—H26C	109.5
C12—C11—C10	118.38 (14)	H26A—C26—H26C	109.5
C12—C11—H11A	120.8	H26B—C26—H26C	109.5
C10—C11—H11A	120.8	O1—B1—N1	110.46 (12)
C11—C12—C13	121.31 (15)	O1—B1—N5	118.17 (13)
C11—C12—H12A	119.3	N1—B1—N5	103.20 (12)
C13—C12—H12A	119.3	O1—B1—N3	117.11 (13)
C14—C13—C12	121.33 (15)	N1—B1—N3	102.83 (12)
C14—C13—H13A	119.3	N5—B1—N3	103.16 (12)
C12—C13—H13A	119.3		

C24—N6—C1—N1	−6.0 (2)	C14—C15—C16—N4	−16.8 (3)
C24—N6—C1—C2	160.12 (15)	C10—C15—C16—N4	155.77 (14)
C8—N1—C1—N6	156.80 (13)	C14—C15—C16—N3	179.82 (15)
B1—N1—C1—N6	−19.5 (2)	C10—C15—C16—N3	−7.59 (16)
C8—N1—C1—C2	−12.45 (16)	C16—N4—C17—N5	−9.1 (2)
B1—N1—C1—C2	171.22 (13)	C16—N4—C17—C18	152.72 (15)
N6—C1—C2—C3	19.3 (3)	C24—N5—C17—N4	154.15 (13)
N1—C1—C2—C3	−172.91 (15)	B1—N5—C17—N4	−12.2 (2)
N6—C1—C2—C7	−160.49 (15)	C24—N5—C17—C18	−11.34 (16)
N1—C1—C2—C7	7.31 (15)	B1—N5—C17—C18	−177.72 (13)
C7—C2—C3—C4	−1.6 (2)	N4—C17—C18—C19	17.9 (3)
C1—C2—C3—C4	178.61 (15)	N5—C17—C18—C19	−177.93 (15)
C2—C3—C4—C5	2.6 (2)	N4—C17—C18—C23	−157.53 (14)
C3—C4—C5—C6	−0.9 (2)	N5—C17—C18—C23	6.65 (16)
C4—C5—C6—C7	−1.7 (2)	C23—C18—C19—C20	−1.4 (2)
C5—C6—C7—C2	2.6 (2)	C17—C18—C19—C20	−176.29 (15)
C5—C6—C7—C8	−178.40 (15)	C18—C19—C20—C21	1.6 (2)
C3—C2—C7—C6	−0.9 (2)	C19—C20—C21—C22	−0.2 (2)
C1—C2—C7—C6	178.88 (13)	C20—C21—C22—C23	−1.3 (2)
C3—C2—C7—C8	179.82 (13)	C21—C22—C23—C18	1.5 (2)
C1—C2—C7—C8	−0.37 (16)	C21—C22—C23—C24	176.41 (15)
C9—N2—C8—N1	6.3 (2)	C19—C18—C23—C22	−0.2 (2)
C9—N2—C8—C7	−159.23 (15)	C17—C18—C23—C22	175.85 (13)
C1—N1—C8—N2	−156.59 (13)	C19—C18—C23—C24	−176.23 (13)
B1—N1—C8—N2	19.7 (2)	C17—C18—C23—C24	−0.19 (16)
C1—N1—C8—C7	12.23 (16)	C1—N6—C24—N5	10.1 (2)
B1—N1—C8—C7	−171.46 (13)	C1—N6—C24—C23	−153.51 (15)
C6—C7—C8—N2	−18.6 (3)	C17—N5—C24—N6	−155.84 (13)
C2—C7—C8—N2	160.55 (15)	B1—N5—C24—N6	10.7 (2)
C6—C7—C8—N1	174.17 (15)	C17—N5—C24—C23	11.19 (16)
C2—C7—C8—N1	−6.71 (16)	B1—N5—C24—C23	177.73 (13)
C8—N2—C9—N3	−10.9 (2)	C22—C23—C24—N6	−15.9 (3)
C8—N2—C9—C10	152.75 (15)	C18—C23—C24—N6	159.45 (15)
C16—N3—C9—N2	156.91 (14)	C22—C23—C24—N5	178.28 (15)
B1—N3—C9—N2	−9.9 (2)	C18—C23—C24—N5	−6.33 (16)
C16—N3—C9—C10	−10.08 (16)	B1—O1—C25—C26	175.74 (14)

B1—N3—C9—C10	−176.86 (12)	C25—O1—B1—N1	161.12 (13)
N2—C9—C10—C11	10.6 (3)	C25—O1—B1—N5	42.67 (19)
N3—C9—C10—C11	176.44 (15)	C25—O1—B1—N3	−81.67 (17)
N2—C9—C10—C15	−161.15 (15)	C8—N1—B1—O1	91.19 (16)
N3—C9—C10—C15	4.69 (16)	C1—N1—B1—O1	−92.82 (16)
C15—C10—C11—C12	−3.4 (2)	C8—N1—B1—N5	−141.58 (13)
C9—C10—C11—C12	−174.31 (15)	C1—N1—B1—N5	34.41 (18)
C10—C11—C12—C13	1.4 (2)	C8—N1—B1—N3	−34.53 (17)
C11—C12—C13—C14	1.7 (2)	C1—N1—B1—N3	141.46 (13)
C12—C13—C14—C15	−2.7 (2)	C24—N5—B1—O1	92.26 (17)
C13—C14—C15—C10	0.6 (2)	C17—N5—B1—O1	−102.61 (16)
C13—C14—C15—C16	172.42 (15)	C24—N5—B1—N1	−29.94 (18)
C11—C10—C15—C14	2.5 (2)	C17—N5—B1—N1	135.19 (13)
C9—C10—C15—C14	175.39 (13)	C24—N5—B1—N3	−136.74 (13)
C11—C10—C15—C16	−171.16 (13)	C17—N5—B1—N3	28.39 (18)
C9—C10—C15—C16	1.77 (16)	C16—N3—B1—O1	102.80 (16)
C17—N4—C16—N3	8.7 (2)	C9—N3—B1—O1	−91.83 (17)
C17—N4—C16—C15	−152.26 (15)	C16—N3—B1—N1	−135.91 (13)
C9—N3—C16—N4	−153.51 (14)	C9—N3—B1—N1	29.45 (17)
B1—N3—C16—N4	13.1 (2)	C16—N3—B1—N5	−28.83 (18)
C9—N3—C16—C15	11.22 (16)	C9—N3—B1—N5	136.53 (13)
B1—N3—C16—C15	177.83 (13)		

(Subphthalocyaninato)(2,2,2-trifluoroethanolato)boron (d22126_a)

Crystal data

$C_{26}H_{14}BF_3N_6O$
M_r = 494.24
Monoclinic, $P2_1/c$
a = 10.4664 (6) Å
b = 15.4986 (8) Å
c = 14.3171 (8) Å
β = 110.221 (3)°
V = 2179.3 (2) Å^3
Z = 4
$F(000)$ = 1008
D_x = 1.506 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8597 reflections
θ = 4.4–65.2°
μ = 0.96 mm^{-1}
T = 150 K
Needle, purple
0.14 × 0.09 × 0.04 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.624, T_{max} = 0.753
39716 measured reflections
3759 independent reflections
3043 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 66.3°, θ_{min} = 4.4°
h = −12→12
k = −18→18
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.04
3759 reflections
335 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.5694P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: SHELXL2019 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0077 (6)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.14828 (12)	0.32579 (9)	0.15721 (11)	0.0619 (4)
F2	0.12876 (12)	0.35980 (8)	0.00694 (10)	0.0642 (4)
F3	0.10380 (11)	0.22880 (7)	0.04406 (9)	0.0493 (3)
O1	0.40052 (12)	0.36016 (7)	0.13347 (8)	0.0281 (3)
N1	0.60948 (13)	0.42611 (8)	0.23935 (10)	0.0240 (3)
N2	0.53157 (13)	0.55917 (9)	0.28127 (10)	0.0253 (3)
N3	0.42606 (13)	0.42704 (8)	0.29839 (10)	0.0236 (3)
N4	0.39573 (13)	0.30705 (9)	0.39199 (10)	0.0249 (3)
N5	0.54216 (13)	0.29777 (9)	0.29696 (10)	0.0238 (3)
N6	0.75795 (14)	0.30516 (9)	0.27647 (10)	0.0267 (3)
C1	0.73096 (16)	0.38769 (11)	0.24857 (11)	0.0247 (4)
C2	0.82193 (17)	0.45773 (11)	0.24592 (12)	0.0261 (4)
C3	0.95492 (17)	0.45794 (12)	0.24534 (13)	0.0299 (4)
H3A	1.002880	0.405582	0.247105	0.036*
C4	1.01423 (19)	0.53653 (12)	0.24214 (14)	0.0337 (4)
H4A	1.104046	0.538081	0.240258	0.040*
C5	0.94627 (18)	0.61398 (12)	0.24159 (13)	0.0339 (4)
H5A	0.990399	0.667082	0.239219	0.041*
C6	0.81507 (18)	0.61465 (11)	0.24444 (12)	0.0303 (4)
H6A	0.769392	0.667474	0.245174	0.036*
C7	0.75239 (17)	0.53604 (11)	0.24620 (12)	0.0258 (4)
C8	0.61905 (16)	0.51318 (10)	0.25096 (11)	0.0240 (4)
C9	0.44168 (16)	0.51425 (10)	0.31008 (11)	0.0239 (4)
C10	0.36737 (16)	0.53890 (11)	0.37553 (12)	0.0254 (4)
C11	0.33740 (17)	0.61856 (11)	0.40721 (12)	0.0291 (4)
H11A	0.368751	0.670501	0.387225	0.035*
C12	0.26033 (18)	0.62009 (12)	0.46888 (13)	0.0325 (4)
H12A	0.235136	0.673985	0.488973	0.039*
C13	0.21908 (18)	0.54373 (12)	0.50201 (13)	0.0322 (4)
H13A	0.166915	0.546880	0.544601	0.039*
C14	0.25226 (17)	0.46388 (11)	0.47436 (12)	0.0285 (4)
H14A	0.226622	0.412318	0.499143	0.034*
C15	0.32478 (16)	0.46125 (11)	0.40874 (12)	0.0252 (4)

C16	0.37397 (16)	0.39014 (11)	0.36432 (12)	0.0243 (4)
C17	0.48759 (16)	0.26371 (11)	0.36294 (11)	0.0244 (4)
C18	0.57039 (17)	0.18891 (10)	0.40590 (12)	0.0248 (4)
C19	0.56054 (18)	0.12527 (11)	0.47146 (12)	0.0287 (4)
H19A	0.486998	0.124697	0.495976	0.034*
C20	0.66076 (19)	0.06292 (11)	0.49991 (12)	0.0320 (4)
H20A	0.653186	0.017315	0.542023	0.038*
C21	0.77307 (19)	0.06506 (11)	0.46843 (13)	0.0342 (4)
H21A	0.841187	0.021796	0.490708	0.041*
C22	0.78658 (18)	0.12919 (11)	0.40537 (13)	0.0301 (4)
H22A	0.864497	0.131765	0.385839	0.036*
C23	0.68316 (17)	0.18960 (10)	0.37145 (12)	0.0256 (4)
C24	0.66641 (16)	0.26342 (10)	0.30644 (12)	0.0248 (4)
C25	0.32578 (17)	0.28402 (11)	0.10139 (13)	0.0285 (4)
H25A	0.356760	0.239782	0.154346	0.034*
H25B	0.342072	0.261682	0.041700	0.034*
C26	0.17718 (19)	0.30021 (12)	0.07709 (14)	0.0354 (4)
B1	0.48581 (19)	0.37544 (12)	0.23485 (13)	0.0237 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0388 (7)	0.0799 (9)	0.0757 (9)	−0.0018 (6)	0.0309 (6)	−0.0268 (7)
F2	0.0441 (7)	0.0473 (7)	0.0741 (9)	−0.0030 (6)	−0.0144 (6)	0.0187 (6)
F3	0.0363 (6)	0.0454 (7)	0.0586 (7)	−0.0149 (5)	0.0067 (5)	−0.0029 (6)
O1	0.0299 (6)	0.0294 (6)	0.0235 (6)	−0.0066 (5)	0.0071 (5)	0.0005 (5)
N1	0.0236 (7)	0.0262 (7)	0.0229 (7)	−0.0005 (5)	0.0089 (6)	0.0004 (5)
N2	0.0240 (7)	0.0275 (7)	0.0233 (7)	0.0005 (6)	0.0068 (6)	0.0031 (6)
N3	0.0204 (7)	0.0264 (7)	0.0231 (7)	0.0006 (5)	0.0066 (6)	0.0020 (6)
N4	0.0230 (7)	0.0279 (7)	0.0239 (7)	−0.0006 (6)	0.0083 (6)	−0.0001 (6)
N5	0.0239 (7)	0.0247 (7)	0.0240 (7)	−0.0008 (5)	0.0096 (6)	−0.0006 (6)
N6	0.0280 (8)	0.0283 (7)	0.0255 (7)	0.0002 (6)	0.0114 (6)	−0.0008 (6)
C1	0.0257 (9)	0.0282 (9)	0.0213 (8)	0.0006 (7)	0.0094 (7)	−0.0013 (7)
C2	0.0258 (9)	0.0327 (9)	0.0196 (8)	−0.0014 (7)	0.0077 (7)	0.0012 (7)
C3	0.0246 (9)	0.0384 (10)	0.0269 (9)	0.0021 (7)	0.0093 (7)	0.0048 (7)
C4	0.0242 (9)	0.0448 (11)	0.0313 (9)	−0.0038 (8)	0.0086 (7)	0.0057 (8)
C5	0.0295 (10)	0.0373 (10)	0.0339 (9)	−0.0088 (7)	0.0098 (8)	0.0052 (8)
C6	0.0311 (9)	0.0305 (9)	0.0284 (9)	−0.0025 (7)	0.0091 (7)	0.0014 (7)
C7	0.0252 (9)	0.0306 (9)	0.0216 (8)	−0.0017 (7)	0.0080 (7)	0.0001 (7)
C8	0.0240 (8)	0.0262 (8)	0.0205 (8)	−0.0006 (7)	0.0061 (7)	0.0022 (6)
C9	0.0223 (8)	0.0264 (8)	0.0219 (8)	0.0011 (6)	0.0062 (7)	0.0019 (7)
C10	0.0204 (8)	0.0306 (9)	0.0225 (8)	0.0013 (6)	0.0039 (7)	−0.0005 (7)
C11	0.0271 (9)	0.0300 (9)	0.0273 (9)	−0.0001 (7)	0.0057 (7)	−0.0012 (7)
C12	0.0332 (10)	0.0345 (10)	0.0280 (9)	0.0026 (7)	0.0085 (8)	−0.0065 (7)
C13	0.0300 (9)	0.0428 (11)	0.0242 (9)	0.0038 (8)	0.0099 (7)	−0.0029 (7)
C14	0.0274 (9)	0.0341 (9)	0.0242 (8)	0.0015 (7)	0.0091 (7)	0.0021 (7)
C15	0.0207 (8)	0.0309 (9)	0.0223 (8)	0.0018 (6)	0.0052 (7)	0.0007 (7)
C16	0.0214 (8)	0.0285 (9)	0.0222 (8)	−0.0023 (6)	0.0064 (7)	0.0017 (7)

C17	0.0238 (8)	0.0271 (8)	0.0222 (8)	−0.0037 (7)	0.0076 (7)	−0.0011 (7)
C18	0.0290 (9)	0.0226 (8)	0.0224 (8)	−0.0033 (7)	0.0083 (7)	−0.0029 (6)
C19	0.0349 (9)	0.0267 (9)	0.0245 (8)	−0.0042 (7)	0.0104 (7)	−0.0032 (7)
C20	0.0433 (11)	0.0259 (9)	0.0257 (9)	−0.0015 (8)	0.0105 (8)	0.0014 (7)
C21	0.0390 (10)	0.0284 (9)	0.0325 (9)	0.0049 (8)	0.0088 (8)	−0.0001 (8)
C22	0.0311 (9)	0.0292 (9)	0.0295 (9)	0.0013 (7)	0.0099 (7)	−0.0036 (7)
C23	0.0290 (9)	0.0252 (8)	0.0225 (8)	−0.0009 (7)	0.0090 (7)	−0.0040 (6)
C24	0.0255 (9)	0.0263 (8)	0.0241 (8)	−0.0005 (7)	0.0103 (7)	−0.0028 (7)
C25	0.0311 (9)	0.0282 (9)	0.0272 (8)	−0.0034 (7)	0.0114 (7)	−0.0041 (7)
C26	0.0326 (10)	0.0325 (10)	0.0378 (10)	−0.0037 (8)	0.0081 (8)	−0.0031 (8)
B1	0.0223 (9)	0.0266 (10)	0.0233 (9)	−0.0015 (7)	0.0092 (8)	0.0004 (7)

Geometric parameters (Å, º)

F1—C26	1.343 (2)	C6—H6A	0.9500
F2—C26	1.329 (2)	C7—C8	1.464 (2)
F3—C26	1.337 (2)	C9—C10	1.461 (2)
O1—C25	1.403 (2)	C10—C11	1.388 (2)
O1—B1	1.437 (2)	C10—C15	1.421 (2)
N1—C8	1.359 (2)	C11—C12	1.387 (3)
N1—C1	1.368 (2)	C11—H11A	0.9500
N1—B1	1.496 (2)	C12—C13	1.398 (3)
N2—C9	1.345 (2)	C12—H12A	0.9500
N2—C8	1.345 (2)	C13—C14	1.380 (3)
N3—C9	1.365 (2)	C13—H13A	0.9500
N3—C16	1.368 (2)	C14—C15	1.398 (2)
N3—B1	1.500 (2)	C14—H14A	0.9500
N4—C16	1.343 (2)	C15—C16	1.453 (2)
N4—C17	1.351 (2)	C17—C18	1.451 (2)
N5—C17	1.367 (2)	C18—C19	1.390 (2)
N5—C24	1.368 (2)	C18—C23	1.428 (2)
N5—B1	1.492 (2)	C19—C20	1.380 (3)
N6—C1	1.341 (2)	C19—H19A	0.9500
N6—C24	1.343 (2)	C20—C21	1.397 (3)
C1—C2	1.453 (2)	C20—H20A	0.9500
C2—C3	1.395 (3)	C21—C22	1.382 (3)
C2—C7	1.416 (2)	C21—H21A	0.9500
C3—C4	1.375 (2)	C22—C23	1.386 (2)
C3—H3A	0.9500	C22—H22A	0.9500
C4—C5	1.394 (3)	C23—C24	1.447 (2)
C4—H4A	0.9500	C25—C26	1.493 (3)
C5—C6	1.388 (3)	C25—H25A	0.9900
C5—H5A	0.9500	C25—H25B	0.9900
C6—C7	1.388 (2)		

C25—O1—B1	123.44 (13)	C13—C14—C15	117.91 (16)
C8—N1—C1	113.17 (13)	C13—C14—H14A	121.0
C8—N1—B1	123.54 (14)	C15—C14—H14A	121.0

C1—N1—B1	122.48 (14)	C14—C15—C10	120.41 (15)
C9—N2—C8	116.80 (14)	C14—C15—C16	132.33 (16)
C9—N3—C16	112.89 (13)	C10—C15—C16	107.25 (14)
C9—N3—B1	123.02 (14)	N4—C16—N3	122.48 (15)
C16—N3—B1	122.99 (14)	N4—C16—C15	130.37 (15)
C16—N4—C17	116.86 (14)	N3—C16—C15	105.72 (14)
C17—N5—C24	113.02 (13)	N4—C17—N5	122.17 (14)
C17—N5—B1	123.35 (14)	N4—C17—C18	130.62 (15)
C24—N5—B1	122.66 (13)	N5—C17—C18	105.69 (14)
C1—N6—C24	117.03 (14)	C19—C18—C23	120.12 (15)
N6—C1—N1	122.48 (15)	C19—C18—C17	132.90 (16)
N6—C1—C2	130.39 (15)	C23—C18—C17	106.94 (14)
N1—C1—C2	105.53 (14)	C20—C19—C18	118.04 (17)
C3—C2—C7	120.86 (15)	C20—C19—H19A	121.0
C3—C2—C1	131.77 (16)	C18—C19—H19A	121.0
C7—C2—C1	107.35 (14)	C19—C20—C21	121.77 (17)
C4—C3—C2	117.73 (16)	C19—C20—H20A	119.1
C4—C3—H3A	121.1	C21—C20—H20A	119.1
C2—C3—H3A	121.1	C22—C21—C20	121.00 (17)
C3—C4—C5	121.85 (17)	C22—C21—H21A	119.5
C3—C4—H4A	119.1	C20—C21—H21A	119.5
C5—C4—H4A	119.1	C21—C22—C23	118.08 (17)
C6—C5—C4	120.95 (17)	C21—C22—H22A	121.0
C6—C5—H5A	119.5	C23—C22—H22A	121.0
C4—C5—H5A	119.5	C22—C23—C18	120.83 (16)
C7—C6—C5	118.21 (17)	C22—C23—C24	131.76 (16)
C7—C6—H6A	120.9	C18—C23—C24	107.30 (14)
C5—C6—H6A	120.9	N6—C24—N5	122.65 (14)
C6—C7—C2	120.38 (16)	N6—C24—C23	130.17 (15)
C6—C7—C8	132.64 (16)	N5—C24—C23	105.74 (14)
C2—C7—C8	106.97 (14)	O1—C25—C26	110.68 (14)
N2—C8—N1	122.41 (14)	O1—C25—H25A	109.5
N2—C8—C7	130.75 (15)	C26—C25—H25A	109.5
N1—C8—C7	105.41 (14)	O1—C25—H25B	109.5
N2—C9—N3	122.82 (15)	C26—C25—H25B	109.5
N2—C9—C10	130.21 (15)	H25A—C25—H25B	108.1
N3—C9—C10	105.66 (14)	F2—C26—F3	106.60 (14)
C11—C10—C15	120.77 (16)	F2—C26—F1	107.49 (16)
C11—C10—C9	132.30 (16)	F3—C26—F1	105.96 (16)
C15—C10—C9	106.93 (14)	F2—C26—C25	112.78 (16)
C12—C11—C10	118.04 (16)	F3—C26—C25	111.61 (15)
C12—C11—H11A	121.0	F1—C26—C25	111.99 (15)
C10—C11—H11A	121.0	O1—B1—N5	116.67 (14)
C11—C12—C13	121.16 (16)	O1—B1—N1	110.87 (14)
C11—C12—H12A	119.4	N5—B1—N1	103.88 (13)
C13—C12—H12A	119.4	O1—B1—N3	117.18 (14)
C14—C13—C12	121.61 (17)	N5—B1—N3	103.33 (13)
C14—C13—H13A	119.2	N1—B1—N3	103.28 (13)

C12—C13—H13A	119.2

C24—N6—C1—N1	−7.4 (2)	C10—C15—C16—N4	158.64 (16)
C24—N6—C1—C2	155.98 (16)	C14—C15—C16—N3	174.03 (17)
C8—N1—C1—N6	154.59 (15)	C10—C15—C16—N3	−7.64 (17)
B1—N1—C1—N6	−15.4 (2)	C16—N4—C17—N5	−9.1 (2)
C8—N1—C1—C2	−12.37 (17)	C16—N4—C17—C18	154.73 (16)
B1—N1—C1—C2	177.64 (14)	C24—N5—C17—N4	155.36 (14)
N6—C1—C2—C3	19.4 (3)	B1—N5—C17—N4	−13.6 (2)
N1—C1—C2—C3	−175.05 (17)	C24—N5—C17—C18	−11.96 (17)
N6—C1—C2—C7	−159.14 (16)	B1—N5—C17—C18	179.06 (14)
N1—C1—C2—C7	6.39 (17)	N4—C17—C18—C19	19.2 (3)
C7—C2—C3—C4	−1.8 (2)	N5—C17—C18—C19	−174.95 (17)
C1—C2—C3—C4	179.75 (17)	N4—C17—C18—C23	−158.20 (16)
C2—C3—C4—C5	1.3 (3)	N5—C17—C18—C23	7.64 (17)
C3—C4—C5—C6	0.1 (3)	C23—C18—C19—C20	−1.2 (2)
C4—C5—C6—C7	−1.1 (3)	C17—C18—C19—C20	−178.37 (16)
C5—C6—C7—C2	0.5 (2)	C18—C19—C20—C21	3.1 (2)
C5—C6—C7—C8	178.76 (17)	C19—C20—C21—C22	−1.4 (3)
C3—C2—C7—C6	0.9 (2)	C20—C21—C22—C23	−2.2 (3)
C1—C2—C7—C6	179.70 (15)	C21—C22—C23—C18	4.1 (2)
C3—C2—C7—C8	−177.70 (15)	C21—C22—C23—C24	179.74 (16)
C1—C2—C7—C8	1.05 (17)	C19—C18—C23—C22	−2.4 (2)
C9—N2—C8—N1	6.9 (2)	C17—C18—C23—C22	175.42 (15)
C9—N2—C8—C7	−157.45 (16)	C19—C18—C23—C24	−179.02 (14)
C1—N1—C8—N2	−154.74 (14)	C17—C18—C23—C24	−1.21 (17)
B1—N1—C8—N2	15.1 (2)	C1—N6—C24—N5	8.8 (2)
C1—N1—C8—C7	12.99 (17)	C1—N6—C24—C23	−155.46 (16)
B1—N1—C8—C7	−177.14 (14)	C17—N5—C24—N6	−156.34 (15)
C6—C7—C8—N2	−20.3 (3)	B1—N5—C24—N6	12.7 (2)
C2—C7—C8—N2	158.15 (16)	C17—N5—C24—C23	11.21 (17)
C6—C7—C8—N1	173.44 (17)	B1—N5—C24—C23	−179.72 (14)
C2—C7—C8—N1	−8.15 (17)	C22—C23—C24—N6	−15.5 (3)
C8—N2—C9—N3	−8.0 (2)	C18—C23—C24—N6	160.58 (16)
C8—N2—C9—C10	156.98 (16)	C22—C23—C24—N5	178.20 (17)
C16—N3—C9—N2	155.65 (14)	C18—C23—C24—N5	−5.68 (17)
B1—N3—C9—N2	−12.6 (2)	B1—O1—C25—C26	108.42 (17)
C16—N3—C9—C10	−12.50 (17)	O1—C25—C26—F2	58.5 (2)
B1—N3—C9—C10	179.23 (13)	O1—C25—C26—F3	178.51 (14)
N2—C9—C10—C11	19.1 (3)	O1—C25—C26—F1	−62.88 (19)
N3—C9—C10—C11	−173.93 (17)	C25—O1—B1—N5	26.0 (2)
N2—C9—C10—C15	−160.02 (16)	C25—O1—B1—N1	144.61 (14)
N3—C9—C10—C15	6.91 (16)	C25—O1—B1—N3	−97.22 (18)
C15—C10—C11—C12	−2.5 (2)	C17—N5—B1—O1	−99.68 (18)
C9—C10—C11—C12	178.46 (16)	C24—N5—B1—O1	92.39 (18)
C10—C11—C12—C13	2.9 (3)	C17—N5—B1—N1	137.99 (14)
C11—C12—C13—C14	−0.5 (3)	C24—N5—B1—N1	−29.94 (19)
C12—C13—C14—C15	−2.3 (3)	C17—N5—B1—N3	30.43 (19)

C13—C14—C15—C10	2.6 (2)	C24—N5—B1—N3	−137.50 (14)
C13—C14—C15—C16	−179.22 (16)	C8—N1—B1—O1	96.21 (18)
C11—C10—C15—C14	−0.3 (2)	C1—N1—B1—O1	−94.85 (17)
C9—C10—C15—C14	179.02 (14)	C8—N1—B1—N5	−137.70 (14)
C11—C10—C15—C16	−178.82 (14)	C1—N1—B1—N5	31.24 (19)
C9—C10—C15—C16	0.46 (17)	C8—N1—B1—N3	−30.11 (19)
C17—N4—C16—N3	9.1 (2)	C1—N1—B1—N3	138.84 (14)
C17—N4—C16—C15	−155.18 (16)	C9—N3—B1—O1	−93.42 (18)
C9—N3—C16—N4	−154.83 (14)	C16—N3—B1—O1	99.48 (17)
B1—N3—C16—N4	13.4 (2)	C9—N3—B1—N5	136.78 (14)
C9—N3—C16—C15	12.79 (17)	C16—N3—B1—N5	−30.32 (19)
B1—N3—C16—C15	−178.93 (13)	C9—N3—B1—N1	28.76 (19)
C14—C15—C16—N4	−19.7 (3)	C16—N3—B1—N1	−138.34 (14)

(Butanolato)(subphthalocyaninato)boron (d2365_a)

Crystal data

$C_{28}H_{21}BN_6O$
M_r = 468.32
Orthorhombic, *Pbca*
a = 14.6398 (8) Å
b = 15.2842 (9) Å
c = 20.5313 (12) Å
V = 4594.0 (5) Å^3
Z = 8
$F(000)$ = 1952
D_x = 1.354 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 7196 reflections
θ = 4.7–63.5°
μ = 0.68 mm^{-1}
T = 150 K
Shard, red
0.15 × 0.07 × 0.06 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.661, T_{max} = 0.753
45733 measured reflections
3951 independent reflections
3295 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 66.3°, θ_{min} = 4.7°
h = −17→16
k = −16→17
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.095
S = 1.07
3951 reflections
326 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 1.7934P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.65454 (7)	0.16749 (7)	0.52754 (5)	0.0285 (3)
N1	0.58690 (8)	0.22126 (8)	0.42800 (6)	0.0248 (3)
N2	0.44187 (9)	0.26949 (8)	0.46684 (6)	0.0263 (3)
N3	0.57903 (9)	0.31323 (8)	0.51964 (6)	0.0250 (3)
N4	0.70172 (8)	0.41129 (8)	0.54038 (6)	0.0267 (3)
N5	0.71948 (8)	0.29367 (8)	0.46566 (6)	0.0252 (3)
N6	0.71634 (9)	0.23507 (8)	0.35842 (6)	0.0275 (3)
C1	0.62896 (10)	0.21061 (10)	0.36922 (7)	0.0259 (3)
C2	0.55680 (11)	0.19102 (10)	0.32311 (7)	0.0269 (3)
C3	0.55809 (11)	0.17229 (10)	0.25676 (8)	0.0322 (4)
H3A	0.614156	0.167151	0.233781	0.039*
C4	0.47546 (12)	0.16141 (11)	0.22530 (8)	0.0363 (4)
H4A	0.475089	0.147802	0.180154	0.044*
C5	0.39223 (12)	0.16993 (11)	0.25832 (8)	0.0342 (4)
H5A	0.336628	0.162068	0.235187	0.041*
C6	0.38963 (11)	0.18955 (10)	0.32386 (8)	0.0300 (4)
H6A	0.333032	0.195459	0.346052	0.036*
C7	0.47213 (11)	0.20048 (10)	0.35668 (7)	0.0263 (3)
C8	0.49379 (10)	0.22703 (10)	0.42291 (7)	0.0253 (3)
C9	0.48618 (10)	0.31643 (10)	0.51220 (7)	0.0251 (3)
C10	0.45570 (10)	0.39165 (10)	0.55014 (7)	0.0264 (3)
C11	0.36938 (11)	0.42489 (11)	0.56440 (7)	0.0303 (4)
H11A	0.315704	0.397116	0.548633	0.036*
C12	0.36428 (12)	0.49964 (11)	0.60225 (8)	0.0343 (4)
H12A	0.306052	0.521543	0.614558	0.041*
C13	0.44299 (12)	0.54373 (11)	0.62283 (8)	0.0343 (4)
H13A	0.436989	0.595398	0.648198	0.041*
C14	0.52909 (11)	0.51372 (10)	0.60704 (8)	0.0306 (4)
H14A	0.582202	0.545163	0.619654	0.037*
C15	0.53575 (10)	0.43579 (10)	0.57201 (7)	0.0260 (3)
C16	0.61408 (11)	0.38657 (10)	0.54796 (7)	0.0257 (3)
C17	0.75094 (10)	0.36772 (10)	0.49558 (7)	0.0256 (3)
C18	0.82841 (10)	0.39771 (10)	0.45701 (8)	0.0270 (4)
C19	0.88477 (11)	0.47080 (10)	0.46284 (8)	0.0304 (4)
H19A	0.881078	0.508072	0.499773	0.036*
C20	0.94620 (11)	0.48738 (11)	0.41319 (9)	0.0355 (4)
H20A	0.986726	0.535668	0.416917	0.043*
C21	0.94995 (11)	0.43464 (12)	0.35767 (9)	0.0372 (4)
H21A	0.992352	0.448279	0.324149	0.045*

C22	0.89308 (11)	0.36290 (11)	0.35053 (8)	0.0327 (4)
H22A	0.895339	0.327776	0.312391	0.039*
C23	0.83258 (10)	0.34367 (10)	0.40074 (8)	0.0275 (3)
C24	0.75772 (10)	0.28113 (10)	0.40558 (7)	0.0264 (3)
C25	0.69849 (13)	0.18122 (11)	0.58877 (8)	0.0371 (4)
H25A	0.663075	0.223900	0.614799	0.045*
H25B	0.760334	0.205582	0.581576	0.045*
C26	0.70553 (11)	0.09683 (11)	0.62503 (8)	0.0327 (4)
H26A	0.742726	0.055377	0.599157	0.039*
H26B	0.643656	0.071458	0.629674	0.039*
C27	0.74800 (13)	0.10629 (12)	0.69235 (8)	0.0405 (4)
H27A	0.810516	0.130236	0.687871	0.049*
H27B	0.711594	0.148443	0.718175	0.049*
C28	0.75238 (17)	0.02032 (14)	0.72826 (10)	0.0595 (6)
H28A	0.785888	0.028192	0.769166	0.089*
H28B	0.783825	−0.023103	0.701230	0.089*
H28C	0.690291	0.000015	0.737717	0.089*
B1	0.63728 (12)	0.24284 (11)	0.48926 (8)	0.0254 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0352 (6)	0.0240 (6)	0.0262 (6)	−0.0006 (5)	−0.0076 (5)	−0.0007 (4)
N1	0.0262 (7)	0.0232 (7)	0.0248 (7)	0.0000 (5)	−0.0014 (5)	−0.0011 (5)
N2	0.0288 (7)	0.0253 (7)	0.0248 (7)	−0.0025 (5)	−0.0003 (5)	0.0021 (5)
N3	0.0276 (7)	0.0243 (7)	0.0232 (6)	−0.0011 (5)	−0.0012 (5)	−0.0007 (5)
N4	0.0278 (7)	0.0262 (7)	0.0261 (7)	0.0006 (5)	−0.0029 (5)	−0.0013 (5)
N5	0.0256 (7)	0.0243 (7)	0.0257 (7)	0.0013 (5)	−0.0017 (5)	−0.0016 (5)
N6	0.0268 (7)	0.0255 (7)	0.0302 (7)	0.0020 (5)	−0.0003 (5)	−0.0036 (6)
C1	0.0290 (8)	0.0231 (8)	0.0258 (8)	0.0028 (6)	0.0003 (6)	−0.0016 (6)
C2	0.0318 (9)	0.0214 (8)	0.0274 (8)	0.0016 (6)	−0.0027 (7)	−0.0021 (6)
C3	0.0372 (9)	0.0301 (9)	0.0292 (8)	0.0032 (7)	0.0015 (7)	−0.0052 (7)
C4	0.0449 (10)	0.0371 (10)	0.0268 (8)	0.0045 (8)	−0.0070 (8)	−0.0073 (7)
C5	0.0372 (9)	0.0320 (9)	0.0334 (9)	0.0013 (7)	−0.0102 (7)	−0.0046 (7)
C6	0.0302 (9)	0.0275 (8)	0.0323 (9)	0.0006 (7)	−0.0041 (7)	−0.0024 (7)
C7	0.0302 (8)	0.0213 (8)	0.0275 (8)	0.0007 (6)	−0.0022 (6)	−0.0007 (6)
C8	0.0266 (8)	0.0234 (8)	0.0260 (8)	−0.0010 (6)	−0.0011 (6)	0.0014 (6)
C9	0.0263 (8)	0.0257 (8)	0.0233 (8)	−0.0017 (6)	0.0007 (6)	0.0032 (6)
C10	0.0318 (8)	0.0272 (8)	0.0202 (7)	0.0014 (7)	0.0011 (6)	0.0035 (6)
C11	0.0313 (9)	0.0335 (9)	0.0261 (8)	0.0029 (7)	0.0004 (7)	0.0049 (7)
C12	0.0364 (9)	0.0364 (9)	0.0301 (9)	0.0108 (7)	0.0038 (7)	0.0041 (7)
C13	0.0444 (10)	0.0286 (9)	0.0299 (9)	0.0070 (7)	0.0021 (7)	−0.0011 (7)
C14	0.0376 (9)	0.0273 (8)	0.0269 (8)	0.0012 (7)	0.0001 (7)	−0.0003 (7)
C15	0.0306 (8)	0.0251 (8)	0.0222 (8)	0.0008 (6)	0.0017 (6)	0.0031 (6)
C16	0.0312 (8)	0.0238 (8)	0.0222 (8)	−0.0008 (6)	−0.0021 (6)	0.0003 (6)
C17	0.0274 (8)	0.0234 (8)	0.0261 (8)	0.0005 (6)	−0.0053 (7)	−0.0019 (6)
C18	0.0235 (8)	0.0249 (8)	0.0327 (9)	0.0035 (6)	−0.0035 (6)	0.0003 (7)
C19	0.0276 (8)	0.0270 (8)	0.0364 (9)	0.0004 (6)	−0.0040 (7)	−0.0005 (7)

C20	0.0294 (9)	0.0327 (9)	0.0445 (10)	−0.0035 (7)	−0.0032 (8)	0.0038 (8)
C21	0.0279 (9)	0.0421 (10)	0.0416 (10)	−0.0018 (7)	0.0031 (7)	0.0050 (8)
C22	0.0272 (9)	0.0361 (9)	0.0348 (9)	0.0035 (7)	0.0019 (7)	−0.0021 (7)
C23	0.0240 (8)	0.0257 (8)	0.0330 (8)	0.0038 (6)	−0.0016 (6)	0.0000 (7)
C24	0.0258 (8)	0.0247 (8)	0.0287 (8)	0.0046 (6)	−0.0004 (7)	−0.0019 (7)
C25	0.0501 (11)	0.0324 (9)	0.0288 (9)	0.0005 (8)	−0.0114 (8)	−0.0004 (7)
C26	0.0339 (9)	0.0319 (9)	0.0325 (9)	−0.0025 (7)	−0.0037 (7)	0.0028 (7)
C27	0.0484 (11)	0.0415 (10)	0.0318 (9)	−0.0047 (8)	−0.0061 (8)	0.0034 (8)
C28	0.0765 (15)	0.0565 (13)	0.0457 (12)	−0.0175 (11)	−0.0181 (11)	0.0175 (10)
B1	0.0277 (9)	0.0244 (9)	0.0241 (9)	−0.0005 (7)	−0.0010 (7)	−0.0020 (7)

Geometric parameters (Å, º)

O1—B1	1.417 (2)	C11—H11A	0.9500
O1—C25	1.4277 (19)	C12—C13	1.400 (2)
N1—C1	1.3646 (19)	C12—H12A	0.9500
N1—C8	1.3700 (19)	C13—C14	1.380 (2)
N1—B1	1.495 (2)	C13—H13A	0.9500
N2—C9	1.343 (2)	C14—C15	1.395 (2)
N2—C8	1.346 (2)	C14—H14A	0.9500
N3—C16	1.3630 (19)	C15—C16	1.458 (2)
N3—C9	1.369 (2)	C17—C18	1.457 (2)
N3—B1	1.508 (2)	C18—C19	1.394 (2)
N4—C17	1.345 (2)	C18—C23	1.421 (2)
N4—C16	1.346 (2)	C19—C20	1.383 (2)
N5—C17	1.3676 (19)	C19—H19A	0.9500
N5—C24	1.3680 (19)	C20—C21	1.397 (3)
N5—B1	1.512 (2)	C20—H20A	0.9500
N6—C24	1.342 (2)	C21—C22	1.385 (2)
N6—C1	1.351 (2)	C21—H21A	0.9500
C1—C2	1.450 (2)	C22—C23	1.391 (2)
C2—C3	1.392 (2)	C22—H22A	0.9500
C2—C7	1.426 (2)	C23—C24	1.458 (2)
C3—C4	1.381 (2)	C25—C26	1.493 (2)
C3—H3A	0.9500	C25—H25A	0.9900
C4—C5	1.401 (2)	C25—H25B	0.9900
C4—H4A	0.9500	C26—C27	1.523 (2)
C5—C6	1.379 (2)	C26—H26A	0.9900
C5—H5A	0.9500	C26—H26B	0.9900
C6—C7	1.393 (2)	C27—C28	1.508 (3)
C6—H6A	0.9500	C27—H27A	0.9900
C7—C8	1.454 (2)	C27—H27B	0.9900
C9—C10	1.459 (2)	C28—H28A	0.9800
C10—C11	1.393 (2)	C28—H28B	0.9800
C10—C15	1.425 (2)	C28—H28C	0.9800
C11—C12	1.384 (2)		
B1—O1—C25	116.69 (12)	N4—C16—N3	122.69 (14)

C1—N1—C8	112.90 (12)	N4—C16—C15	130.09 (14)
C1—N1—B1	123.22 (13)	N3—C16—C15	105.83 (13)
C8—N1—B1	122.74 (13)	N4—C17—N5	122.45 (14)
C9—N2—C8	116.71 (13)	N4—C17—C18	129.27 (14)
C16—N3—C9	113.09 (13)	N5—C17—C18	106.15 (13)
C16—N3—B1	123.39 (13)	C19—C18—C23	120.67 (15)
C9—N3—B1	122.74 (13)	C19—C18—C17	131.76 (15)
C17—N4—C16	116.79 (13)	C23—C18—C17	106.99 (13)
C17—N5—C24	112.53 (13)	C20—C19—C18	117.94 (15)
C17—N5—B1	123.31 (12)	C20—C19—H19A	121.0
C24—N5—B1	122.86 (12)	C18—C19—H19A	121.0
C24—N6—C1	117.02 (13)	C19—C20—C21	121.41 (16)
N6—C1—N1	122.64 (14)	C19—C20—H20A	119.3
N6—C1—C2	129.79 (14)	C21—C20—H20A	119.3
N1—C1—C2	105.86 (13)	C22—C21—C20	121.31 (16)
C3—C2—C7	120.38 (14)	C22—C21—H21A	119.3
C3—C2—C1	132.19 (15)	C20—C21—H21A	119.3
C7—C2—C1	107.27 (13)	C21—C22—C23	118.16 (15)
C4—C3—C2	118.07 (15)	C21—C22—H22A	120.9
C4—C3—H3A	121.0	C23—C22—H22A	120.9
C2—C3—H3A	121.0	C22—C23—C18	120.46 (14)
C3—C4—C5	121.63 (15)	C22—C23—C24	131.92 (15)
C3—C4—H4A	119.2	C18—C23—C24	107.07 (13)
C5—C4—H4A	119.2	N6—C24—N5	122.65 (14)
C6—C5—C4	121.09 (15)	N6—C24—C23	129.38 (14)
C6—C5—H5A	119.5	N5—C24—C23	106.09 (13)
C4—C5—H5A	119.5	O1—C25—C26	110.07 (13)
C5—C6—C7	118.31 (15)	O1—C25—H25A	109.6
C5—C6—H6A	120.8	C26—C25—H25A	109.6
C7—C6—H6A	120.8	O1—C25—H25B	109.6
C6—C7—C2	120.51 (14)	C26—C25—H25B	109.6
C6—C7—C8	132.45 (15)	H25A—C25—H25B	108.2
C2—C7—C8	106.90 (13)	C25—C26—C27	113.51 (14)
N2—C8—N1	122.80 (13)	C25—C26—H26A	108.9
N2—C8—C7	129.64 (14)	C27—C26—H26A	108.9
N1—C8—C7	105.69 (13)	C25—C26—H26B	108.9
N2—C9—N3	122.56 (14)	C27—C26—H26B	108.9
N2—C9—C10	130.07 (14)	H26A—C26—H26B	107.7
N3—C9—C10	105.80 (13)	C28—C27—C26	112.24 (15)
C11—C10—C15	120.48 (14)	C28—C27—H27A	109.2
C11—C10—C9	132.62 (15)	C26—C27—H27A	109.2
C15—C10—C9	106.85 (13)	C28—C27—H27B	109.2
C12—C11—C10	117.91 (15)	C26—C27—H27B	109.2
C12—C11—H11A	121.0	H27A—C27—H27B	107.9
C10—C11—H11A	121.0	C27—C28—H28A	109.5
C11—C12—C13	121.50 (15)	C27—C28—H28B	109.5
C11—C12—H12A	119.3	H28A—C28—H28B	109.5
C13—C12—H12A	119.3	C27—C28—H28C	109.5

C14—C13—C12	121.39 (15)	H28A—C28—H28C	109.5
C14—C13—H13A	119.3	H28B—C28—H28C	109.5
C12—C13—H13A	119.3	O1—B1—N1	112.04 (13)
C13—C14—C15	117.95 (15)	O1—B1—N3	116.83 (13)
C13—C14—H14A	121.0	N1—B1—N3	103.09 (12)
C15—C14—H14A	121.0	O1—B1—N5	116.97 (13)
C14—C15—C10	120.62 (14)	N1—B1—N5	103.67 (12)
C14—C15—C16	132.09 (14)	N3—B1—N5	102.47 (12)
C10—C15—C16	107.22 (13)		

C24—N6—C1—N1	−8.4 (2)	C10—C15—C16—N4	160.67 (15)
C24—N6—C1—C2	154.51 (15)	C14—C15—C16—N3	177.24 (15)
C8—N1—C1—N6	154.80 (14)	C10—C15—C16—N3	−5.86 (16)
B1—N1—C1—N6	−13.3 (2)	C16—N4—C17—N5	−9.5 (2)
C8—N1—C1—C2	−11.62 (16)	C16—N4—C17—C18	151.51 (15)
B1—N1—C1—C2	−179.71 (13)	C24—N5—C17—N4	153.85 (14)
N6—C1—C2—C3	16.4 (3)	B1—N5—C17—N4	−13.5 (2)
N1—C1—C2—C3	−178.53 (16)	C24—N5—C17—C18	−10.97 (16)
N6—C1—C2—C7	−158.88 (15)	B1—N5—C17—C18	−178.28 (13)
N1—C1—C2—C7	6.20 (16)	N4—C17—C18—C19	14.1 (3)
C7—C2—C3—C4	−1.4 (2)	N5—C17—C18—C19	177.53 (16)
C1—C2—C3—C4	−176.16 (16)	N4—C17—C18—C23	−157.01 (15)
C2—C3—C4—C5	0.9 (2)	N5—C17—C18—C23	6.41 (16)
C3—C4—C5—C6	−0.1 (3)	C23—C18—C19—C20	−1.8 (2)
C4—C5—C6—C7	−0.2 (2)	C17—C18—C19—C20	−171.89 (16)
C5—C6—C7—C2	−0.3 (2)	C18—C19—C20—C21	2.2 (2)
C5—C6—C7—C8	174.89 (16)	C19—C20—C21—C22	−0.9 (3)
C3—C2—C7—C6	1.2 (2)	C20—C21—C22—C23	−0.9 (2)
C1—C2—C7—C6	177.11 (14)	C21—C22—C23—C18	1.3 (2)
C3—C2—C7—C8	−175.16 (14)	C21—C22—C23—C24	171.58 (16)
C1—C2—C7—C8	0.78 (16)	C19—C18—C23—C22	0.0 (2)
C9—N2—C8—N1	8.5 (2)	C17—C18—C23—C22	172.32 (14)
C9—N2—C8—C7	−153.64 (15)	C19—C18—C23—C24	−172.41 (14)
C1—N1—C8—N2	−153.67 (14)	C17—C18—C23—C24	−0.10 (16)
B1—N1—C8—N2	14.5 (2)	C1—N6—C24—N5	8.6 (2)
C1—N1—C8—C7	12.10 (17)	C1—N6—C24—C23	−153.51 (15)
B1—N1—C8—C7	−179.74 (13)	C17—N5—C24—N6	−154.79 (14)
C6—C7—C8—N2	−18.7 (3)	B1—N5—C24—N6	12.6 (2)
C2—C7—C8—N2	156.99 (15)	C17—N5—C24—C23	10.90 (16)
C6—C7—C8—N1	176.85 (16)	B1—N5—C24—C23	178.27 (13)
C2—C7—C8—N1	−7.44 (16)	C22—C23—C24—N6	−13.1 (3)
C8—N2—C9—N3	−8.3 (2)	C18—C23—C24—N6	158.15 (15)
C8—N2—C9—C10	155.31 (15)	C22—C23—C24—N5	−177.46 (16)
C16—N3—C9—N2	155.60 (14)	C18—C23—C24—N5	−6.24 (16)
B1—N3—C9—N2	−14.6 (2)	B1—O1—C25—C26	175.87 (14)
C16—N3—C9—C10	−11.42 (17)	O1—C25—C26—C27	−177.48 (14)
B1—N3—C9—C10	178.37 (13)	C25—C26—C27—C28	178.82 (17)
N2—C9—C10—C11	18.6 (3)	C25—O1—B1—N1	−177.06 (13)

N3—C9—C10—C11	−175.67 (16)	C25—O1—B1—N3	−58.47 (19)
N2—C9—C10—C15	−158.69 (15)	C25—O1—B1—N5	63.47 (18)
N3—C9—C10—C15	6.99 (16)	C1—N1—B1—O1	−97.97 (16)
C15—C10—C11—C12	−2.4 (2)	C8—N1—B1—O1	95.08 (17)
C9—C10—C11—C12	−179.44 (15)	C1—N1—B1—N3	135.58 (14)
C10—C11—C12—C13	3.5 (2)	C8—N1—B1—N3	−31.36 (18)
C11—C12—C13—C14	−1.0 (2)	C1—N1—B1—N5	29.03 (18)
C12—C13—C14—C15	−2.5 (2)	C8—N1—B1—N5	−137.91 (13)
C13—C14—C15—C10	3.5 (2)	C16—N3—B1—O1	98.99 (17)
C13—C14—C15—C16	−179.89 (16)	C9—N3—B1—O1	−91.81 (17)
C11—C10—C15—C14	−1.1 (2)	C16—N3—B1—N1	−137.69 (13)
C9—C10—C15—C14	176.62 (13)	C9—N3—B1—N1	31.50 (18)
C11—C10—C15—C16	−178.43 (14)	C16—N3—B1—N5	−30.24 (18)
C9—C10—C15—C16	−0.71 (16)	C9—N3—B1—N5	138.96 (14)
C17—N4—C16—N3	9.7 (2)	C17—N5—B1—O1	−98.84 (17)
C17—N4—C16—C15	−154.90 (15)	C24—N5—B1—O1	95.14 (17)
C9—N3—C16—N4	−156.81 (14)	C17—N5—B1—N1	137.31 (13)
B1—N3—C16—N4	13.3 (2)	C24—N5—B1—N1	−28.71 (18)
C9—N3—C16—C15	10.97 (17)	C17—N5—B1—N3	30.30 (18)
B1—N3—C16—C15	−178.90 (13)	C24—N5—B1—N3	−135.72 (13)
C14—C15—C16—N4	−16.2 (3)		

(*tert*-Butanolato)(subphthalocyaninato)boron (d23115_a)

Crystal data

$C_{28}H_{21}BN_6O$
M_r = 468.32
Monoclinic, $P2_1/c$
a = 14.3815 (7) Å
b = 8.2702 (4) Å
c = 19.8660 (9) Å
β = 102.074 (2)°
V = 2310.55 (19) Å^3
Z = 4
$F(000)$ = 976
D_x = 1.346 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9907 reflections
θ = 3.1–65.6°
μ = 0.68 mm^{-1}
T = 150 K
Shard, pink
0.17 × 0.09 × 0.02 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.673, T_{max} = 0.753
41764 measured reflections
3994 independent reflections
3363 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 66.4°, θ_{min} = 3.1°
h = −17→16
k = −9→9
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.089
S = 1.05
3994 reflections
329 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.6555P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: SHELXL2019 (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0027 (2)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.13233 (7)	0.45659 (12)	0.34123 (5)	0.0322 (2)
N1	0.25586 (8)	0.26134 (13)	0.35481 (6)	0.0257 (3)
N2	0.38286 (8)	0.42521 (14)	0.33597 (6)	0.0273 (3)
N3	0.29197 (8)	0.50116 (14)	0.41822 (6)	0.0261 (3)
N4	0.26678 (8)	0.50795 (14)	0.53271 (6)	0.0282 (3)
N5	0.19298 (8)	0.30535 (14)	0.45350 (6)	0.0269 (3)
N6	0.18897 (8)	0.04134 (15)	0.40441 (6)	0.0295 (3)
C1	0.23293 (10)	0.10185 (17)	0.35669 (7)	0.0264 (3)
C2	0.28511 (10)	0.02031 (17)	0.31120 (7)	0.0269 (3)
C3	0.28641 (11)	−0.13979 (18)	0.28963 (7)	0.0313 (3)
H3A	0.246279	−0.218727	0.303556	0.038*
C4	0.34791 (11)	−0.18023 (19)	0.24732 (8)	0.0358 (4)
H4A	0.348608	−0.287988	0.230871	0.043*
C5	0.40911 (11)	−0.06566 (19)	0.22827 (8)	0.0347 (4)
H5A	0.450767	−0.097125	0.199282	0.042*
C6	0.41009 (10)	0.09253 (18)	0.25084 (7)	0.0301 (3)
H6A	0.453337	0.168813	0.238916	0.036*
C7	0.34651 (10)	0.13761 (17)	0.29132 (7)	0.0263 (3)
C8	0.32972 (10)	0.28996 (17)	0.32361 (7)	0.0253 (3)
C9	0.36722 (10)	0.52164 (16)	0.38687 (7)	0.0264 (3)
C10	0.43102 (10)	0.63519 (16)	0.42978 (7)	0.0277 (3)
C11	0.51788 (10)	0.70194 (17)	0.42372 (8)	0.0314 (3)
H11A	0.544142	0.680471	0.384550	0.038*
C12	0.56482 (11)	0.80038 (17)	0.47634 (8)	0.0337 (3)
H12A	0.623371	0.849009	0.472596	0.040*
C13	0.52780 (11)	0.82968 (17)	0.53489 (8)	0.0335 (4)
H13A	0.561216	0.898917	0.569887	0.040*
C14	0.44356 (11)	0.75980 (17)	0.54275 (8)	0.0313 (3)
H14A	0.419707	0.777328	0.583280	0.038*
C15	0.39448 (10)	0.66299 (16)	0.48975 (7)	0.0283 (3)
C16	0.30911 (10)	0.56455 (16)	0.48327 (7)	0.0272 (3)
C17	0.21516 (10)	0.37185 (17)	0.51812 (7)	0.0275 (3)
C18	0.19411 (10)	0.24788 (18)	0.56463 (7)	0.0282 (3)
C19	0.20229 (10)	0.24625 (19)	0.63576 (7)	0.0315 (3)

H19A	0.220049	0.340896	0.662455	0.038*
C20	0.18385 (11)	0.1032 (2)	0.66637 (8)	0.0376 (4)
H20A	0.186793	0.100649	0.714580	0.045*
C21	0.16091 (12)	−0.0380 (2)	0.62762 (8)	0.0423 (4)
H21A	0.149430	−0.134835	0.650270	0.051*
C22	0.15452 (12)	−0.0400 (2)	0.55722 (8)	0.0383 (4)
H22A	0.140249	−0.136935	0.531472	0.046*
C23	0.16970 (10)	0.10470 (18)	0.52524 (7)	0.0305 (3)
C24	0.17644 (10)	0.14261 (17)	0.45474 (7)	0.0281 (3)
C25	0.04743 (10)	0.53426 (18)	0.35279 (8)	0.0307 (3)
C26	0.00330 (13)	0.6075 (2)	0.28332 (9)	0.0488 (4)
H26A	−0.056878	0.660087	0.286012	0.073*
H26B	−0.008593	0.522026	0.248406	0.073*
H26C	0.046902	0.687616	0.270735	0.073*
C27	0.07026 (11)	0.66450 (19)	0.40753 (9)	0.0396 (4)
H27A	0.011984	0.723032	0.410430	0.059*
H27B	0.116618	0.740102	0.395416	0.059*
H27C	0.096944	0.614488	0.452109	0.059*
C28	−0.01812 (11)	0.4078 (2)	0.37321 (9)	0.0433 (4)
H28A	−0.080008	0.456834	0.373695	0.065*
H28B	0.009899	0.366219	0.419177	0.065*
H28C	−0.026529	0.318737	0.339947	0.065*
B1	0.20919 (11)	0.3904 (2)	0.38962 (8)	0.0270 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0296 (5)	0.0411 (6)	0.0274 (5)	0.0076 (4)	0.0091 (4)	0.0016 (4)
N1	0.0276 (6)	0.0273 (6)	0.0234 (6)	0.0002 (5)	0.0083 (5)	−0.0003 (5)
N2	0.0309 (6)	0.0273 (6)	0.0249 (6)	0.0010 (5)	0.0085 (5)	0.0025 (5)
N3	0.0294 (6)	0.0253 (6)	0.0250 (6)	0.0011 (5)	0.0084 (5)	−0.0006 (5)
N4	0.0313 (6)	0.0278 (6)	0.0271 (6)	0.0023 (5)	0.0095 (5)	−0.0010 (5)
N5	0.0281 (6)	0.0298 (6)	0.0245 (6)	−0.0007 (5)	0.0092 (5)	−0.0011 (5)
N6	0.0302 (6)	0.0329 (7)	0.0273 (6)	−0.0052 (5)	0.0101 (5)	−0.0023 (5)
C1	0.0269 (7)	0.0274 (7)	0.0251 (7)	−0.0023 (6)	0.0062 (6)	−0.0003 (6)
C2	0.0290 (7)	0.0303 (7)	0.0215 (7)	0.0008 (6)	0.0057 (6)	−0.0001 (6)
C3	0.0342 (8)	0.0295 (8)	0.0311 (8)	−0.0011 (6)	0.0089 (6)	−0.0013 (6)
C4	0.0398 (9)	0.0309 (8)	0.0380 (9)	0.0029 (7)	0.0110 (7)	−0.0053 (7)
C5	0.0353 (8)	0.0371 (8)	0.0345 (8)	0.0048 (7)	0.0137 (7)	−0.0032 (6)
C6	0.0300 (7)	0.0337 (8)	0.0283 (8)	0.0008 (6)	0.0100 (6)	−0.0002 (6)
C7	0.0274 (7)	0.0289 (7)	0.0227 (7)	0.0013 (6)	0.0052 (6)	0.0008 (6)
C8	0.0268 (7)	0.0279 (7)	0.0222 (7)	0.0009 (6)	0.0078 (6)	0.0025 (6)
C9	0.0291 (7)	0.0254 (7)	0.0268 (7)	0.0021 (6)	0.0104 (6)	0.0043 (6)
C10	0.0317 (8)	0.0223 (7)	0.0296 (8)	0.0018 (6)	0.0076 (6)	0.0030 (6)
C11	0.0336 (8)	0.0270 (7)	0.0351 (8)	0.0022 (6)	0.0106 (7)	0.0025 (6)
C12	0.0297 (8)	0.0284 (8)	0.0418 (9)	0.0006 (6)	0.0047 (7)	0.0035 (6)
C13	0.0373 (8)	0.0247 (7)	0.0349 (8)	0.0010 (6)	−0.0011 (7)	0.0022 (6)
C14	0.0396 (8)	0.0245 (7)	0.0291 (8)	0.0036 (6)	0.0054 (6)	0.0030 (6)

C15	0.0333 (8)	0.0230 (7)	0.0286 (8)	0.0025 (6)	0.0065 (6)	0.0029 (6)
C16	0.0314 (8)	0.0253 (7)	0.0255 (7)	0.0032 (6)	0.0076 (6)	−0.0002 (6)
C17	0.0279 (7)	0.0311 (8)	0.0254 (7)	0.0018 (6)	0.0098 (6)	−0.0024 (6)
C18	0.0252 (7)	0.0344 (8)	0.0269 (7)	−0.0008 (6)	0.0101 (6)	−0.0002 (6)
C19	0.0285 (7)	0.0403 (9)	0.0268 (8)	−0.0026 (6)	0.0082 (6)	−0.0013 (6)
C20	0.0378 (9)	0.0502 (10)	0.0262 (8)	−0.0074 (7)	0.0099 (7)	0.0025 (7)
C21	0.0507 (10)	0.0447 (9)	0.0334 (9)	−0.0138 (8)	0.0134 (8)	0.0048 (7)
C22	0.0448 (9)	0.0382 (9)	0.0341 (9)	−0.0124 (7)	0.0130 (7)	−0.0005 (7)
C23	0.0291 (8)	0.0371 (8)	0.0277 (8)	−0.0052 (6)	0.0113 (6)	−0.0004 (6)
C24	0.0277 (7)	0.0312 (8)	0.0269 (7)	−0.0037 (6)	0.0089 (6)	−0.0010 (6)
C25	0.0266 (7)	0.0333 (8)	0.0331 (8)	0.0027 (6)	0.0089 (6)	0.0001 (6)
C26	0.0429 (10)	0.0640 (12)	0.0395 (9)	0.0200 (9)	0.0086 (8)	0.0086 (9)
C27	0.0355 (9)	0.0340 (8)	0.0497 (10)	0.0012 (7)	0.0096 (7)	−0.0071 (7)
C28	0.0351 (9)	0.0407 (9)	0.0568 (11)	−0.0060 (7)	0.0160 (8)	−0.0049 (8)
B1	0.0285 (8)	0.0287 (8)	0.0254 (8)	0.0011 (7)	0.0096 (7)	−0.0004 (7)

Geometric parameters (Å, º)

O1—B1	1.4146 (19)	C11—H11A	0.9500
O1—C25	1.4399 (17)	C12—C13	1.398 (2)
N1—C8	1.3578 (17)	C12—H12A	0.9500
N1—C1	1.3620 (18)	C13—C14	1.380 (2)
N1—B1	1.5040 (19)	C13—H13A	0.9500
N2—C9	1.3432 (18)	C14—C15	1.392 (2)
N2—C8	1.3480 (18)	C14—H14A	0.9500
N3—C9	1.3675 (17)	C15—C16	1.456 (2)
N3—C16	1.3684 (18)	C17—C18	1.454 (2)
N3—B1	1.515 (2)	C18—C19	1.393 (2)
N4—C16	1.3434 (18)	C18—C23	1.422 (2)
N4—C17	1.3461 (19)	C19—C20	1.381 (2)
N5—C24	1.3679 (18)	C19—H19A	0.9500
N5—C17	1.3715 (18)	C20—C21	1.400 (2)
N5—B1	1.5110 (19)	C20—H20A	0.9500
N6—C1	1.3416 (18)	C21—C22	1.382 (2)
N6—C24	1.3450 (18)	C21—H21A	0.9500
C1—C2	1.4554 (19)	C22—C23	1.393 (2)
C2—C3	1.393 (2)	C22—H22A	0.9500
C2—C7	1.4222 (19)	C23—C24	1.4581 (19)
C3—C4	1.383 (2)	C25—C27	1.517 (2)
C3—H3A	0.9500	C25—C28	1.519 (2)
C4—C5	1.398 (2)	C25—C26	1.519 (2)
C4—H4A	0.9500	C26—H26A	0.9800
C5—C6	1.382 (2)	C26—H26B	0.9800
C5—H5A	0.9500	C26—H26C	0.9800
C6—C7	1.389 (2)	C27—H27A	0.9800
C6—H6A	0.9500	C27—H27B	0.9800
C7—C8	1.4568 (19)	C27—H27C	0.9800
C9—C10	1.457 (2)	C28—H28A	0.9800

C10—C11	1.394 (2)	C28—H28B	0.9800
C10—C15	1.418 (2)	C28—H28C	0.9800
C11—C12	1.384 (2)		

B1—O1—C25	129.23 (11)	N4—C16—N3	122.50 (13)
C8—N1—C1	113.47 (11)	N4—C16—C15	129.27 (13)
C8—N1—B1	123.58 (12)	N3—C16—C15	106.24 (11)
C1—N1—B1	122.73 (12)	N4—C17—N5	123.14 (12)
C9—N2—C8	116.87 (11)	N4—C17—C18	129.16 (13)
C9—N3—C16	112.29 (12)	N5—C17—C18	105.88 (12)
C9—N3—B1	122.59 (11)	C19—C18—C23	120.58 (13)
C16—N3—B1	123.92 (11)	C19—C18—C17	131.82 (13)
C16—N4—C17	116.60 (12)	C23—C18—C17	107.32 (12)
C24—N5—C17	112.64 (12)	C20—C19—C18	118.15 (14)
C24—N5—B1	122.08 (12)	C20—C19—H19A	120.9
C17—N5—B1	123.57 (12)	C18—C19—H19A	120.9
C1—N6—C24	116.70 (12)	C19—C20—C21	121.16 (14)
N6—C1—N1	122.22 (12)	C19—C20—H20A	119.4
N6—C1—C2	130.26 (13)	C21—C20—H20A	119.4
N1—C1—C2	105.81 (11)	C22—C21—C20	121.65 (15)
C3—C2—C7	120.92 (13)	C22—C21—H21A	119.2
C3—C2—C1	132.32 (13)	C20—C21—H21A	119.2
C7—C2—C1	106.68 (12)	C21—C22—C23	117.85 (15)
C4—C3—C2	117.92 (14)	C21—C22—H22A	121.1
C4—C3—H3A	121.0	C23—C22—H22A	121.1
C2—C3—H3A	121.0	C22—C23—C18	120.56 (13)
C3—C4—C5	121.31 (14)	C22—C23—C24	132.13 (14)
C3—C4—H4A	119.3	C18—C23—C24	106.93 (12)
C5—C4—H4A	119.3	N6—C24—N5	123.26 (12)
C6—C5—C4	121.19 (14)	N6—C24—C23	128.78 (13)
C6—C5—H5A	119.4	N5—C24—C23	106.00 (12)
C4—C5—H5A	119.4	O1—C25—C27	111.56 (12)
C5—C6—C7	118.59 (14)	O1—C25—C28	109.25 (12)
C5—C6—H6A	120.7	C27—C25—C28	110.53 (13)
C7—C6—H6A	120.7	O1—C25—C26	103.89 (11)
C6—C7—C2	119.99 (13)	C27—C25—C26	110.78 (14)
C6—C7—C8	132.61 (13)	C28—C25—C26	110.64 (14)
C2—C7—C8	107.33 (11)	C25—C26—H26A	109.5
N2—C8—N1	121.96 (12)	C25—C26—H26B	109.5
N2—C8—C7	131.15 (12)	H26A—C26—H26B	109.5
N1—C8—C7	105.54 (11)	C25—C26—H26C	109.5
N2—C9—N3	122.85 (13)	H26A—C26—H26C	109.5
N2—C9—C10	129.72 (12)	H26B—C26—H26C	109.5
N3—C9—C10	105.95 (12)	C25—C27—H27A	109.5
C11—C10—C15	120.32 (13)	C25—C27—H27B	109.5
C11—C10—C9	132.12 (13)	H27A—C27—H27B	109.5
C15—C10—C9	107.31 (12)	C25—C27—H27C	109.5
C12—C11—C10	118.16 (14)	H27A—C27—H27C	109.5

C12—C11—H11A	120.9	H27B—C27—H27C	109.5
C10—C11—H11A	120.9	C25—C28—H28A	109.5
C11—C12—C13	121.32 (14)	C25—C28—H28B	109.5
C11—C12—H12A	119.3	H28A—C28—H28B	109.5
C13—C12—H12A	119.3	C25—C28—H28C	109.5
C14—C13—C12	121.18 (14)	H28A—C28—H28C	109.5
C14—C13—H13A	119.4	H28B—C28—H28C	109.5
C12—C13—H13A	119.4	O1—B1—N1	108.82 (12)
C13—C14—C15	118.26 (14)	O1—B1—N5	120.99 (12)
C13—C14—H14A	120.9	N1—B1—N5	102.59 (11)
C15—C14—H14A	120.9	O1—B1—N3	117.50 (12)
C14—C15—C10	120.70 (13)	N1—B1—N3	102.13 (11)
C14—C15—C16	132.32 (13)	N5—B1—N3	102.33 (11)
C10—C15—C16	106.79 (12)		

C24—N6—C1—N1	−6.2 (2)	C10—C15—C16—N4	156.41 (14)
C24—N6—C1—C2	156.75 (14)	C14—C15—C16—N3	177.62 (14)
C8—N1—C1—N6	155.21 (13)	C10—C15—C16—N3	−7.51 (15)
B1—N1—C1—N6	−19.7 (2)	C16—N4—C17—N5	−10.1 (2)
C8—N1—C1—C2	−11.33 (16)	C16—N4—C17—C18	152.35 (14)
B1—N1—C1—C2	173.79 (12)	C24—N5—C17—N4	154.67 (13)
N6—C1—C2—C3	18.9 (3)	B1—N5—C17—N4	−10.7 (2)
N1—C1—C2—C3	−176.02 (15)	C24—N5—C17—C18	−11.22 (15)
N6—C1—C2—C7	−157.83 (14)	B1—N5—C17—C18	−176.55 (12)
N1—C1—C2—C7	7.22 (15)	N4—C17—C18—C19	15.4 (3)
C7—C2—C3—C4	−1.2 (2)	N5—C17—C18—C19	−179.91 (15)
C1—C2—C3—C4	−177.55 (14)	N4—C17—C18—C23	−158.39 (14)
C2—C3—C4—C5	1.9 (2)	N5—C17—C18—C23	6.35 (15)
C3—C4—C5—C6	−0.3 (2)	C23—C18—C19—C20	−1.5 (2)
C4—C5—C6—C7	−2.1 (2)	C17—C18—C19—C20	−174.57 (15)
C5—C6—C7—C2	2.7 (2)	C18—C19—C20—C21	2.3 (2)
C5—C6—C7—C8	179.19 (15)	C19—C20—C21—C22	−0.8 (3)
C3—C2—C7—C6	−1.1 (2)	C20—C21—C22—C23	−1.4 (3)
C1—C2—C7—C6	176.06 (13)	C21—C22—C23—C18	2.1 (2)
C3—C2—C7—C8	−178.40 (13)	C21—C22—C23—C24	173.96 (16)
C1—C2—C7—C8	−1.19 (15)	C19—C18—C23—C22	−0.7 (2)
C9—N2—C8—N1	7.97 (19)	C17—C18—C23—C22	173.92 (14)
C9—N2—C8—C7	−156.70 (14)	C19—C18—C23—C24	−174.38 (13)
C1—N1—C8—N2	−157.53 (13)	C17—C18—C23—C24	0.21 (16)
B1—N1—C8—N2	17.3 (2)	C1—N6—C24—N5	10.0 (2)
C1—N1—C8—C7	10.55 (15)	C1—N6—C24—C23	−151.74 (14)
B1—N1—C8—C7	−174.62 (12)	C17—N5—C24—N6	−153.95 (13)
C6—C7—C8—N2	−15.5 (3)	B1—N5—C24—N6	11.6 (2)
C2—C7—C8—N2	161.26 (14)	C17—N5—C24—C23	11.36 (16)
C6—C7—C8—N1	177.95 (15)	B1—N5—C24—C23	176.94 (12)
C2—C7—C8—N1	−5.28 (15)	C22—C23—C24—N6	−15.2 (3)
C8—N2—C9—N3	−10.19 (19)	C18—C23—C24—N6	157.52 (14)
C8—N2—C9—C10	153.89 (14)	C22—C23—C24—N5	−179.40 (16)

C16—N3—C9—N2	155.48 (13)	C18—C23—C24—N5	−6.70 (16)
B1—N3—C9—N2	−12.4 (2)	B1—O1—C25—C27	49.70 (19)
C16—N3—C9—C10	−11.85 (15)	B1—O1—C25—C28	−72.81 (18)
B1—N3—C9—C10	−179.74 (12)	B1—O1—C25—C26	169.09 (15)
N2—C9—C10—C11	14.4 (3)	C25—O1—B1—N1	154.31 (12)
N3—C9—C10—C11	−179.50 (14)	C25—O1—B1—N5	36.1 (2)
N2—C9—C10—C15	−159.66 (14)	C25—O1—B1—N3	−90.36 (17)
N3—C9—C10—C15	6.47 (15)	C8—N1—B1—O1	91.35 (16)
C15—C10—C11—C12	−2.5 (2)	C1—N1—B1—O1	−94.29 (15)
C9—C10—C11—C12	−175.92 (14)	C8—N1—B1—N5	−139.34 (13)
C10—C11—C12—C13	1.5 (2)	C1—N1—B1—N5	35.02 (17)
C11—C12—C13—C14	0.8 (2)	C8—N1—B1—N3	−33.56 (17)
C12—C13—C14—C15	−2.0 (2)	C1—N1—B1—N3	140.79 (12)
C13—C14—C15—C10	0.9 (2)	C24—N5—B1—O1	90.43 (17)
C13—C14—C15—C16	175.22 (14)	C17—N5—B1—O1	−105.58 (16)
C11—C10—C15—C14	1.4 (2)	C24—N5—B1—N1	−30.88 (17)
C9—C10—C15—C14	176.22 (12)	C17—N5—B1—N1	133.10 (13)
C11—C10—C15—C16	−174.24 (12)	C24—N5—B1—N3	−136.51 (13)
C9—C10—C15—C16	0.63 (15)	C17—N5—B1—N3	27.48 (17)
C17—N4—C16—N3	8.1 (2)	C9—N3—B1—O1	−88.02 (16)
C17—N4—C16—C15	−153.56 (14)	C16—N3—B1—O1	105.50 (15)
C9—N3—C16—N4	−153.00 (13)	C9—N3—B1—N1	30.93 (16)
B1—N3—C16—N4	14.7 (2)	C16—N3—B1—N1	−135.55 (13)
C9—N3—C16—C15	12.28 (15)	C9—N3—B1—N5	136.90 (12)
B1—N3—C16—C15	179.99 (12)	C16—N3—B1—N5	−29.58 (17)
C14—C15—C16—N4	−18.5 (3)		

(Octanolato)(subphthalocyaninato)boron (d23123_a)

Crystal data

$6C_{32}H_{29}BN_6O{\cdot}2H_2O_{0.50}$
M_r = 3166.55
Triclinic, $P\overline{1}$
a = 15.3028 (7) Å
b = 16.2278 (7) Å
c = 17.3604 (7) Å
α = 103.045 (3)°
β = 105.716 (3)°
γ = 94.022 (3)°
V = 4003.0 (3) Å^3
Z = 1
$F(000)$ = 1668
D_x = 1.314 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6400 reflections
θ = 2.7–63.9°
μ = 0.65 mm^{-1}
T = 150 K
Shard, pink
0.24 × 0.16 × 0.06 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.622, T_{max} = 0.753
110436 measured reflections
13816 independent reflections
10618 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 66.4°, θ_{min} = 2.7°
h = −17→18
k = −19→19
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.149$
$S = 1.05$
13816 reflections
1201 parameters
499 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 2.1766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}
Extinction correction: SHELXL2019 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00223 (15)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1A	0.77624 (11)	0.36183 (10)	0.70390 (9)	0.0390 (4)	
N1A	0.65242 (12)	0.26603 (12)	0.59626 (10)	0.0316 (4)	
N2A	0.71668 (12)	0.13671 (12)	0.57327 (10)	0.0326 (4)	
N3A	0.72729 (12)	0.21399 (12)	0.71030 (10)	0.0303 (4)	
N4A	0.67121 (12)	0.23869 (12)	0.82811 (10)	0.0332 (4)	
N5A	0.62832 (12)	0.31692 (12)	0.72638 (11)	0.0332 (4)	
N6A	0.52633 (13)	0.34070 (12)	0.60570 (11)	0.0380 (5)	
C1A	0.57428 (15)	0.29578 (14)	0.56100 (13)	0.0337 (5)	
C2A	0.54488 (15)	0.24989 (15)	0.47383 (13)	0.0345 (5)	
C3A	0.46960 (17)	0.25264 (16)	0.40831 (14)	0.0395 (6)	
H3AA	0.430692	0.295265	0.414304	0.047*	
C4A	0.45320 (17)	0.19143 (17)	0.33424 (14)	0.0426 (6)	
H4AA	0.402382	0.192387	0.288788	0.051*	
C5A	0.50962 (17)	0.12849 (17)	0.32495 (14)	0.0406 (6)	
H5AA	0.496195	0.087195	0.273400	0.049*	
C6A	0.58470 (16)	0.12477 (16)	0.38906 (13)	0.0370 (5)	
H6AA	0.622853	0.081622	0.382273	0.044*	
C7A	0.60278 (15)	0.18617 (15)	0.46395 (13)	0.0328 (5)	
C8A	0.66774 (14)	0.19482 (14)	0.54496 (13)	0.0313 (5)	
C9A	0.74113 (14)	0.14480 (14)	0.65553 (13)	0.0309 (5)	
C10A	0.75977 (14)	0.07926 (15)	0.70003 (13)	0.0321 (5)	
C11A	0.77972 (15)	−0.00374 (16)	0.67651 (14)	0.0376 (5)	
H11A	0.789968	−0.024741	0.624462	0.045*	
C12A	0.78409 (17)	−0.05425 (17)	0.73115 (15)	0.0442 (6)	
H12A	0.798119	−0.110721	0.716502	0.053*	
C13A	0.76830 (18)	−0.02420 (17)	0.80787 (16)	0.0458 (6)	
H13A	0.771315	−0.060867	0.843862	0.055*	
C14A	0.74848 (16)	0.05751 (16)	0.83205 (14)	0.0390 (5)	

H14A	0.737483	0.077359	0.883948	0.047*
C15A	0.74499 (14)	0.11037 (15)	0.77825 (13)	0.0319 (5)
C16A	0.71809 (14)	0.19458 (15)	0.78081 (12)	0.0321 (5)
C17A	0.62236 (15)	0.29559 (14)	0.79709 (13)	0.0333 (5)
C18A	0.54126 (15)	0.32801 (14)	0.81356 (13)	0.0347 (5)
C19A	0.50171 (16)	0.32619 (15)	0.87688 (14)	0.0375 (5)
H19A	0.531442	0.305859	0.923105	0.045*
C20A	0.41774 (16)	0.35503 (15)	0.86993 (15)	0.0414 (6)
H20A	0.389700	0.354774	0.912483	0.050*
C21A	0.37301 (17)	0.38452 (15)	0.80207 (16)	0.0439 (6)
H21A	0.315361	0.403837	0.799509	0.053*
C22A	0.41091 (17)	0.38620 (15)	0.73843 (15)	0.0425 (6)
H22A	0.379886	0.405570	0.691973	0.051*
C23A	0.49608 (16)	0.35851 (15)	0.74487 (14)	0.0366 (5)
C24A	0.55087 (16)	0.34516 (14)	0.68727 (14)	0.0357 (5)
C25A	0.83225 (17)	0.39292 (17)	0.78780 (15)	0.0457 (6)
H25A	0.802926	0.369796	0.824250	0.055*
H25B	0.837113	0.455978	0.804270	0.055*
C26A	0.92488 (19)	0.3681 (2)	0.79900 (18)	0.0624 (8)
H26A	0.951904	0.386498	0.758791	0.075*
H26B	0.920434	0.305150	0.787606	0.075*
C27A	0.98796 (19)	0.4084 (2)	0.88718 (18)	0.0583 (7)
H27A	0.988059	0.471077	0.899872	0.070*
H27B	0.962854	0.386659	0.926818	0.070*
C28A	1.0846 (2)	0.3902 (2)	0.8993 (2)	0.0710 (9)
H28A	1.108246	0.408854	0.857407	0.085*
H28B	1.084609	0.327667	0.889598	0.085*
C29A	1.1493 (2)	0.4336 (2)	0.98479 (18)	0.0581 (7)
H29A	1.145916	0.495693	0.996609	0.070*
H29B	1.128971	0.411305	1.026644	0.070*
C30A	1.24692 (19)	0.41957 (19)	0.99252 (17)	0.0532 (7)
H30A	1.264479	0.435496	0.946411	0.064*
H30B	1.251065	0.357980	0.986755	0.064*
C31A	1.31477 (19)	0.46988 (17)	1.07356 (15)	0.0486 (6)
H31A	1.310528	0.531503	1.079745	0.058*
H31B	1.297984	0.453492	1.119810	0.058*
C32A	1.41249 (18)	0.45535 (17)	1.07933 (16)	0.0484 (6)
H32A	1.453270	0.489286	1.132747	0.073*
H32B	1.417524	0.394647	1.074539	0.073*
H32C	1.430073	0.472690	1.034459	0.073*
B1A	0.70321 (18)	0.29553 (17)	0.68701 (15)	0.0340 (6)
N1B	0.54418 (12)	0.17729 (11)	0.14279 (10)	0.0290 (4)
N2B	0.68560 (12)	0.15591 (11)	0.22919 (11)	0.0318 (4)
N3B	0.63544 (12)	0.29256 (11)	0.25022 (11)	0.0304 (4)
N4B	0.55947 (13)	0.39765 (12)	0.31570 (11)	0.0339 (4)
N5B	0.48129 (12)	0.30104 (11)	0.18579 (10)	0.0309 (4)
N6B	0.38246 (12)	0.17359 (11)	0.10262 (10)	0.0318 (4)
C1B	0.45758 (15)	0.13443 (14)	0.10575 (12)	0.0292 (5)

C2B	0.46782 (15)	0.04419 (14)	0.09085 (12)	0.0297 (5)	
C3B	0.40548 (16)	−0.03011 (14)	0.05101 (13)	0.0330 (5)	
H3BA	0.342689	−0.027384	0.025991	0.040*	
C4B	0.43778 (17)	−0.10798 (15)	0.04899 (13)	0.0372 (5)	
H4BA	0.396667	−0.159300	0.021258	0.045*	
C5B	0.52956 (17)	−0.11243 (15)	0.08691 (14)	0.0375 (5)	
H5BA	0.549824	−0.166753	0.083954	0.045*	
C6B	0.59174 (16)	−0.03945 (14)	0.12875 (13)	0.0341 (5)	
H6BA	0.653637	−0.042992	0.156134	0.041*	
C7B	0.56093 (15)	0.03915 (14)	0.12949 (12)	0.0300 (5)	
C8B	0.60736 (15)	0.12615 (14)	0.16756 (13)	0.0297 (5)	
C9B	0.69478 (14)	0.23733 (14)	0.27341 (13)	0.0311 (5)	
C10B	0.74647 (15)	0.27666 (14)	0.35949 (13)	0.0322 (5)	
C11B	0.81553 (15)	0.24968 (15)	0.41503 (14)	0.0362 (5)	
H11C	0.842541	0.200634	0.397411	0.043*	
C12B	0.84344 (17)	0.29682 (16)	0.49675 (14)	0.0408 (6)	
H12C	0.890512	0.279686	0.535696	0.049*	
C13B	0.80404 (17)	0.36904 (16)	0.52340 (14)	0.0407 (6)	
H13C	0.824908	0.399989	0.579932	0.049*	
C14B	0.73544 (16)	0.39605 (15)	0.46901 (14)	0.0371 (5)	
H14C	0.708348	0.444746	0.487447	0.045*	
C15B	0.70689 (15)	0.35006 (14)	0.38632 (13)	0.0322 (5)	
C16B	0.63209 (15)	0.35593 (14)	0.31657 (13)	0.0322 (5)	
C17B	0.48290 (15)	0.36609 (14)	0.25208 (13)	0.0321 (5)	
C18B	0.38776 (15)	0.37471 (15)	0.24656 (13)	0.0346 (5)	
C19B	0.34798 (17)	0.43257 (16)	0.29397 (15)	0.0415 (6)	
H19C	0.384550	0.477172	0.339221	0.050*	
C20B	0.25313 (18)	0.42293 (17)	0.27291 (16)	0.0471 (6)	
H20C	0.224098	0.462690	0.303123	0.057*	
C21B	0.19961 (18)	0.35591 (18)	0.20819 (16)	0.0474 (6)	
H21C	0.134749	0.351248	0.195306	0.057*	
C22B	0.23781 (16)	0.29607 (16)	0.16222 (15)	0.0411 (6)	
H22C	0.200487	0.249811	0.119247	0.049*	
C23B	0.33295 (16)	0.30587 (15)	0.18100 (13)	0.0353 (5)	
C24B	0.39575 (15)	0.25567 (14)	0.14705 (13)	0.0317 (5)	
O1B	0.59133 (11)	0.30152 (9)	0.10243 (9)	0.0359 (4)	
C25B	0.63545 (18)	0.38710 (15)	0.12029 (16)	0.0435 (6)	0.735 (5)
H25C	0.627306	0.421193	0.172233	0.052*	0.735 (5)
H25D	0.606933	0.413429	0.075114	0.052*	0.735 (5)
C26B	0.7365 (2)	0.3880 (2)	0.1291 (2)	0.0626 (7)	0.735 (5)
H26C	0.767364	0.447762	0.148176	0.075*	0.735 (5)
H26D	0.763897	0.357832	0.171537	0.075*	0.735 (5)
C27B	0.7525 (3)	0.3457 (3)	0.0487 (3)	0.0637 (12)	0.735 (5)
H27C	0.732392	0.381163	0.009393	0.076*	0.735 (5)
H27D	0.712649	0.289832	0.025785	0.076*	0.735 (5)
C28B	0.8512 (3)	0.3304 (4)	0.0517 (4)	0.0877 (16)	0.735 (5)
H28C	0.851797	0.303487	−0.005252	0.105*	0.735 (5)
H28D	0.889985	0.386726	0.069637	0.105*	0.735 (5)

C29B	0.8957 (4)	0.2757 (4)	0.1074 (4)	0.1024 (17)	0.735 (5)
H29C	0.888217	0.297551	0.162934	0.123*	0.735 (5)
H29D	0.962232	0.281643	0.113476	0.123*	0.735 (5)
C30B	0.8554 (4)	0.1785 (3)	0.0748 (3)	0.1314 (16)	0.735 (5)
H30C	0.787696	0.171374	0.060540	0.158*	0.735 (5)
H30D	0.872783	0.152406	0.024752	0.158*	0.735 (5)
C31B	0.8961 (3)	0.1354 (4)	0.1454 (3)	0.0941 (17)	0.735 (5)
H31C	0.886617	0.167521	0.197569	0.113*	0.735 (5)
H31D	0.864446	0.076314	0.131499	0.113*	0.735 (5)
C32B	0.9955 (4)	0.1343 (4)	0.1564 (4)	0.144 (2)	0.735 (5)
H32D	1.021209	0.107092	0.200944	0.217*	0.735 (5)
H32E	1.004480	0.101969	0.104803	0.217*	0.735 (5)
H32F	1.026597	0.192952	0.170710	0.217*	0.735 (5)
C25D	0.63545 (18)	0.38710 (15)	0.12029 (16)	0.0435 (6)	0.265 (5)
H25E	0.627306	0.421193	0.172233	0.052*	0.265 (5)
H25F	0.606933	0.413429	0.075114	0.052*	0.265 (5)
C26D	0.7365 (2)	0.3880 (2)	0.1291 (2)	0.0626 (7)	0.265 (5)
H26E	0.759478	0.443635	0.122305	0.075*	0.265 (5)
H26F	0.767371	0.386839	0.186856	0.075*	0.265 (5)
C27D	0.7678 (8)	0.3223 (8)	0.0756 (9)	0.075 (3)	0.265 (5)
H27E	0.738522	0.322925	0.017478	0.090*	0.265 (5)
H27F	0.746795	0.266020	0.082469	0.090*	0.265 (5)
C28D	0.8736 (8)	0.3314 (8)	0.0916 (10)	0.084 (3)	0.265 (5)
H28E	0.905607	0.337598	0.150758	0.100*	0.265 (5)
H28F	0.895531	0.381663	0.075013	0.100*	0.265 (5)
C29D	0.8904 (10)	0.2463 (7)	0.0364 (9)	0.098 (3)	0.265 (5)
H29E	0.854867	0.237375	−0.022358	0.118*	0.265 (5)
H29F	0.956241	0.246088	0.040819	0.118*	0.265 (5)
C30D	0.8554 (4)	0.1785 (3)	0.0748 (3)	0.1314 (16)	0.265 (5)
H30E	0.852391	0.206273	0.130823	0.158*	0.265 (5)
H30F	0.792896	0.151282	0.040352	0.158*	0.265 (5)
C31D	0.9189 (10)	0.1114 (9)	0.0803 (9)	0.124 (3)	0.265 (5)
H31E	0.883335	0.056693	0.077173	0.149*	0.265 (5)
H31F	0.943316	0.102492	0.032204	0.149*	0.265 (5)
C32D	0.9955 (4)	0.1343 (4)	0.1564 (4)	0.144 (2)	0.265 (5)
H32M	1.034230	0.088641	0.156635	0.217*	0.265 (5)
H32N	1.031882	0.187663	0.159298	0.217*	0.265 (5)
H32O	0.971874	0.141843	0.204287	0.217*	0.265 (5)
B1B	0.56605 (17)	0.27289 (16)	0.16599 (15)	0.0312 (5)	
N1C	0.13334 (12)	0.19929 (11)	0.72603 (10)	0.0318 (4)	
N2C	−0.02401 (12)	0.14414 (12)	0.65772 (10)	0.0339 (4)	
N3C	0.07636 (12)	0.17606 (11)	0.58153 (10)	0.0306 (4)	
N4C	0.17635 (12)	0.14168 (12)	0.49917 (11)	0.0344 (4)	
N5C	0.23513 (12)	0.19534 (12)	0.64534 (11)	0.0325 (4)	
N6C	0.28824 (12)	0.17955 (11)	0.78215 (11)	0.0324 (4)	
C1C	0.20267 (15)	0.18497 (14)	0.78823 (13)	0.0316 (5)	
C2C	0.15901 (15)	0.15785 (14)	0.84433 (13)	0.0337 (5)	
C3C	0.19425 (17)	0.13847 (16)	0.92022 (13)	0.0397 (6)	

H3CA	0.258476	0.144692	0.945766	0.048*	
C4C	0.13259 (18)	0.10997 (19)	0.95682 (15)	0.0497 (7)	
H4CA	0.155069	0.097960	1.009178	0.060*	
C5C	0.03801 (19)	0.0983 (2)	0.91901 (15)	0.0540 (7)	
H5CA	−0.002178	0.078135	0.946022	0.065*	
C6C	0.00154 (17)	0.11549 (18)	0.84299 (14)	0.0464 (6)	
H6CA	−0.062778	0.106536	0.817119	0.056*	
C7C	0.06235 (15)	0.14635 (15)	0.80580 (13)	0.0359 (5)	
C8C	0.04847 (15)	0.16719 (14)	0.72637 (13)	0.0336 (5)	
C9C	−0.00699 (15)	0.14378 (14)	0.58546 (13)	0.0308 (5)	
C10C	−0.05796 (14)	0.09803 (13)	0.50040 (12)	0.0293 (5)	
C11C	−0.14766 (15)	0.05620 (14)	0.46462 (13)	0.0316 (5)	
H11B	−0.187949	0.052352	0.497165	0.038*	
C12C	−0.17588 (15)	0.02045 (14)	0.37984 (13)	0.0336 (5)	
H12B	−0.237360	−0.006420	0.353825	0.040*	
C13C	−0.11654 (15)	0.02286 (14)	0.33174 (13)	0.0346 (5)	
H13B	−0.138655	−0.001474	0.273703	0.042*	
C14C	−0.02592 (16)	0.06010 (14)	0.36707 (13)	0.0344 (5)	
H14B	0.015165	0.059095	0.334596	0.041*	
C15C	0.00316 (15)	0.09905 (14)	0.45160 (13)	0.0302 (5)	
C16C	0.09146 (15)	0.14334 (14)	0.50739 (13)	0.0315 (5)	
C17C	0.24669 (15)	0.16291 (14)	0.56954 (13)	0.0344 (5)	
C18C	0.33898 (15)	0.13995 (15)	0.58579 (14)	0.0359 (5)	
C19C	0.39147 (16)	0.11047 (17)	0.53419 (15)	0.0416 (6)	
H19B	0.369209	0.104444	0.476250	0.050*	
C20C	0.47704 (16)	0.09008 (17)	0.56928 (15)	0.0441 (6)	
H20B	0.514745	0.071477	0.535220	0.053*	
C21C	0.50874 (16)	0.09647 (16)	0.65411 (15)	0.0407 (6)	
H21B	0.566956	0.080349	0.676264	0.049*	
C22C	0.45746 (15)	0.12573 (15)	0.70684 (14)	0.0364 (5)	
H22B	0.479547	0.129540	0.764395	0.044*	
C23C	0.37277 (15)	0.14928 (14)	0.67285 (13)	0.0335 (5)	
C24C	0.30167 (15)	0.18014 (14)	0.70868 (13)	0.0325 (5)	
O1C	0.15664 (14)	0.31964 (11)	0.66693 (12)	0.0652 (6)	0.513 (4)
C25C	0.1609 (4)	0.3589 (3)	0.6120 (3)	0.0466 (12)	0.513 (4)
H25G	0.109155	0.332983	0.561700	0.056*	0.513 (4)
H25H	0.218272	0.349317	0.597403	0.056*	0.513 (4)
C26C	0.1585 (4)	0.4530 (3)	0.6350 (4)	0.0455 (13)	0.513 (4)
H26G	0.179991	0.478739	0.595716	0.055*	0.513 (4)
H26H	0.201974	0.477728	0.690846	0.055*	0.513 (4)
C27C	0.0651 (4)	0.4774 (4)	0.6353 (5)	0.0505 (14)	0.513 (4)
H27G	0.051034	0.466293	0.684721	0.061*	0.513 (4)
H27H	0.018538	0.440629	0.585768	0.061*	0.513 (4)
C28C	0.0579 (5)	0.5704 (5)	0.6357 (9)	0.0539 (19)	0.513 (4)
H28G	0.105235	0.606437	0.685079	0.065*	0.513 (4)
H28H	0.072989	0.580869	0.586412	0.065*	0.513 (4)
C29C	−0.0339 (4)	0.6006 (4)	0.6358 (4)	0.0590 (14)	0.513 (4)
H29G	−0.046559	0.596393	0.687862	0.071*	0.513 (4)

H29H	−0.082615	0.561947	0.589354	0.071*	0.513 (4)
C30C	−0.0384 (4)	0.6921 (4)	0.6279 (5)	0.0636 (14)	0.513 (4)
H30G	0.017105	0.728830	0.667853	0.076*	0.513 (4)
H30H	−0.036516	0.693653	0.571705	0.076*	0.513 (4)
C31C	−0.1219 (5)	0.7304 (5)	0.6426 (6)	0.0804 (19)	0.513 (4)
H31G	−0.115212	0.791062	0.640814	0.096*	0.513 (4)
H31H	−0.124484	0.728956	0.698623	0.096*	0.513 (4)
C32C	−0.2115 (8)	0.6844 (8)	0.5797 (9)	0.123 (4)	0.513 (4)
H32G	−0.262620	0.712114	0.592532	0.185*	0.513 (4)
H32H	−0.210267	0.686825	0.524148	0.185*	0.513 (4)
H32I	−0.219547	0.624666	0.582006	0.185*	0.513 (4)
O1E	0.15664 (14)	0.31964 (11)	0.66693 (12)	0.0652 (6)	0.487 (4)
C25E	0.0916 (3)	0.3650 (3)	0.6582 (3)	0.0408 (11)	0.487 (4)
H25J	0.064748	0.366466	0.704246	0.049*	0.487 (4)
H25K	0.043259	0.336133	0.606179	0.049*	0.487 (4)
C26E	0.1162 (5)	0.4543 (3)	0.6559 (4)	0.0387 (12)	0.487 (4)
H26J	0.133138	0.453758	0.604625	0.046*	0.487 (4)
H26K	0.170502	0.481387	0.703488	0.046*	0.487 (4)
C27E	0.0390 (4)	0.5076 (4)	0.6587 (4)	0.0457 (14)	0.487 (4)
H27J	0.027900	0.515021	0.713227	0.055*	0.487 (4)
H27K	−0.017703	0.476710	0.615781	0.055*	0.487 (4)
C28E	0.0598 (6)	0.5949 (5)	0.6446 (8)	0.0510 (18)	0.487 (4)
H28J	0.063627	0.586915	0.587408	0.061*	0.487 (4)
H28K	0.120840	0.622048	0.682711	0.061*	0.487 (4)
C29E	−0.0093 (4)	0.6559 (5)	0.6569 (4)	0.0615 (15)	0.487 (4)
H29J	−0.016984	0.660866	0.712551	0.074*	0.487 (4)
H29K	0.015268	0.713194	0.654933	0.074*	0.487 (4)
C30E	−0.1017 (4)	0.6279 (4)	0.5931 (5)	0.0760 (17)	0.487 (4)
H30J	−0.130677	0.574861	0.600377	0.091*	0.487 (4)
H30K	−0.093551	0.615192	0.537181	0.091*	0.487 (4)
C31E	−0.1651 (7)	0.6971 (6)	0.6003 (7)	0.075 (2)	0.487 (4)
H31J	−0.135608	0.751899	0.596813	0.090*	0.487 (4)
H31K	−0.179780	0.706188	0.653416	0.090*	0.487 (4)
C32E	−0.2526 (8)	0.6626 (8)	0.5266 (8)	0.120 (4)	0.487 (4)
H32J	−0.296217	0.704047	0.527533	0.180*	0.487 (4)
H32K	−0.236666	0.653725	0.474601	0.180*	0.487 (4)
H32L	−0.280579	0.608281	0.530872	0.180*	0.487 (4)
B1C	0.15010 (18)	0.23063 (16)	0.65562 (16)	0.0352 (6)	
O1W	0.4156 (8)	0.4621 (6)	0.5274 (6)	0.233 (7)	0.5
H1WB	0.446348	0.427861	0.548992	0.350*	
H1WA	0.422128	0.500970	0.570542	0.350*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0391 (9)	0.0421 (9)	0.0293 (8)	−0.0029 (7)	0.0034 (7)	0.0068 (7)
N1A	0.0339 (10)	0.0331 (10)	0.0263 (9)	0.0033 (8)	0.0075 (7)	0.0065 (8)
N2A	0.0289 (9)	0.0430 (11)	0.0268 (9)	0.0059 (8)	0.0097 (7)	0.0084 (8)

N3A	0.0286 (9)	0.0367 (10)	0.0244 (9)	0.0050 (8)	0.0076 (7)	0.0058 (8)
N4A	0.0331 (10)	0.0386 (11)	0.0252 (9)	0.0063 (8)	0.0075 (7)	0.0037 (8)
N5A	0.0362 (10)	0.0338 (10)	0.0271 (9)	0.0057 (8)	0.0079 (8)	0.0041 (8)
N6A	0.0445 (11)	0.0343 (11)	0.0326 (10)	0.0085 (9)	0.0070 (8)	0.0075 (8)
C1A	0.0355 (12)	0.0333 (12)	0.0317 (11)	0.0055 (10)	0.0075 (9)	0.0099 (10)
C2A	0.0391 (12)	0.0349 (13)	0.0290 (11)	0.0024 (10)	0.0076 (9)	0.0110 (9)
C3A	0.0448 (13)	0.0422 (14)	0.0328 (12)	0.0086 (11)	0.0085 (10)	0.0147 (10)
C4A	0.0454 (14)	0.0510 (15)	0.0277 (12)	0.0017 (12)	0.0024 (10)	0.0149 (11)
C5A	0.0476 (14)	0.0467 (15)	0.0264 (11)	0.0025 (11)	0.0107 (10)	0.0089 (10)
C6A	0.0419 (13)	0.0415 (14)	0.0281 (11)	0.0035 (10)	0.0121 (10)	0.0082 (10)
C7A	0.0339 (11)	0.0385 (13)	0.0272 (11)	0.0011 (10)	0.0098 (9)	0.0109 (9)
C8A	0.0296 (11)	0.0376 (13)	0.0275 (11)	0.0026 (9)	0.0097 (9)	0.0086 (9)
C9A	0.0254 (10)	0.0391 (13)	0.0273 (11)	0.0043 (9)	0.0081 (8)	0.0063 (9)
C10A	0.0259 (11)	0.0409 (13)	0.0282 (11)	0.0073 (9)	0.0068 (8)	0.0071 (9)
C11A	0.0315 (12)	0.0448 (14)	0.0343 (12)	0.0109 (10)	0.0081 (9)	0.0061 (10)
C12A	0.0440 (14)	0.0437 (15)	0.0459 (14)	0.0162 (11)	0.0111 (11)	0.0131 (11)
C13A	0.0501 (15)	0.0488 (16)	0.0442 (14)	0.0140 (12)	0.0139 (11)	0.0213 (12)
C14A	0.0371 (12)	0.0502 (15)	0.0313 (11)	0.0100 (11)	0.0091 (10)	0.0136 (11)
C15A	0.0266 (11)	0.0401 (13)	0.0288 (11)	0.0076 (9)	0.0071 (9)	0.0086 (9)
C16A	0.0280 (11)	0.0413 (13)	0.0250 (10)	0.0042 (9)	0.0064 (9)	0.0066 (9)
C17A	0.0366 (12)	0.0337 (12)	0.0257 (11)	0.0035 (10)	0.0077 (9)	0.0023 (9)
C18A	0.0376 (12)	0.0291 (12)	0.0323 (11)	0.0033 (9)	0.0097 (9)	−0.0011 (9)
C19A	0.0420 (13)	0.0306 (12)	0.0361 (12)	0.0022 (10)	0.0129 (10)	−0.0001 (10)
C20A	0.0409 (13)	0.0341 (13)	0.0448 (13)	0.0019 (10)	0.0172 (11)	−0.0036 (10)
C21A	0.0366 (13)	0.0345 (14)	0.0530 (15)	0.0048 (10)	0.0139 (11)	−0.0044 (11)
C22A	0.0426 (13)	0.0329 (13)	0.0433 (13)	0.0090 (10)	0.0065 (11)	−0.0011 (10)
C23A	0.0381 (12)	0.0311 (12)	0.0347 (12)	0.0052 (10)	0.0084 (10)	−0.0005 (10)
C24A	0.0385 (12)	0.0295 (12)	0.0344 (12)	0.0075 (10)	0.0054 (10)	0.0048 (9)
C25A	0.0462 (14)	0.0421 (15)	0.0363 (13)	−0.0023 (11)	−0.0013 (11)	0.0042 (11)
C26A	0.0450 (16)	0.074 (2)	0.0550 (17)	0.0027 (14)	0.0019 (13)	0.0070 (15)
C27A	0.0467 (15)	0.0650 (19)	0.0505 (16)	0.0056 (14)	0.0041 (12)	0.0026 (14)
C28A	0.0510 (17)	0.079 (2)	0.0650 (19)	0.0185 (16)	0.0009 (14)	−0.0013 (16)
C29A	0.0570 (17)	0.0544 (18)	0.0496 (16)	0.0091 (14)	0.0032 (13)	0.0014 (13)
C30A	0.0557 (16)	0.0491 (16)	0.0465 (15)	0.0113 (13)	0.0056 (12)	0.0058 (12)
C31A	0.0606 (17)	0.0399 (15)	0.0387 (13)	0.0072 (12)	0.0065 (12)	0.0071 (11)
C32A	0.0542 (16)	0.0409 (15)	0.0439 (14)	0.0072 (12)	0.0080 (12)	0.0064 (11)
B1A	0.0360 (14)	0.0372 (15)	0.0268 (12)	0.0032 (11)	0.0071 (10)	0.0072 (11)
N1B	0.0358 (10)	0.0241 (9)	0.0266 (9)	0.0043 (8)	0.0087 (7)	0.0058 (7)
N2B	0.0347 (10)	0.0282 (10)	0.0326 (9)	0.0052 (8)	0.0109 (8)	0.0067 (8)
N3B	0.0341 (10)	0.0252 (9)	0.0301 (9)	0.0036 (8)	0.0082 (8)	0.0052 (7)
N4B	0.0396 (10)	0.0274 (10)	0.0323 (10)	0.0063 (8)	0.0085 (8)	0.0049 (8)
N5B	0.0363 (10)	0.0270 (10)	0.0279 (9)	0.0062 (8)	0.0072 (8)	0.0060 (7)
N6B	0.0374 (10)	0.0300 (10)	0.0256 (9)	0.0059 (8)	0.0060 (7)	0.0059 (8)
C1B	0.0352 (11)	0.0295 (12)	0.0232 (10)	0.0033 (9)	0.0086 (9)	0.0077 (9)
C2B	0.0396 (12)	0.0278 (11)	0.0233 (10)	0.0035 (9)	0.0127 (9)	0.0059 (9)
C3B	0.0409 (12)	0.0323 (12)	0.0258 (10)	0.0001 (10)	0.0128 (9)	0.0058 (9)
C4B	0.0543 (15)	0.0279 (12)	0.0305 (11)	−0.0023 (10)	0.0184 (10)	0.0047 (9)
C5B	0.0551 (15)	0.0268 (12)	0.0348 (12)	0.0085 (10)	0.0186 (11)	0.0092 (10)

C6B	0.0452 (13)	0.0307 (12)	0.0301 (11)	0.0089 (10)	0.0146 (10)	0.0100 (9)
C7B	0.0409 (12)	0.0275 (11)	0.0238 (10)	0.0051 (9)	0.0132 (9)	0.0067 (9)
C8B	0.0340 (11)	0.0297 (12)	0.0282 (10)	0.0068 (9)	0.0120 (9)	0.0092 (9)
C9B	0.0314 (11)	0.0285 (12)	0.0343 (11)	0.0041 (9)	0.0096 (9)	0.0100 (9)
C10B	0.0335 (11)	0.0285 (12)	0.0331 (11)	−0.0010 (9)	0.0084 (9)	0.0082 (9)
C11B	0.0350 (12)	0.0323 (12)	0.0399 (13)	0.0007 (10)	0.0079 (10)	0.0117 (10)
C12B	0.0424 (13)	0.0386 (14)	0.0374 (13)	0.0005 (11)	0.0031 (10)	0.0141 (11)
C13B	0.0469 (14)	0.0400 (14)	0.0304 (12)	−0.0037 (11)	0.0059 (10)	0.0091 (10)
C14B	0.0407 (13)	0.0320 (12)	0.0358 (12)	0.0002 (10)	0.0096 (10)	0.0063 (10)
C15B	0.0340 (11)	0.0287 (12)	0.0322 (11)	−0.0008 (9)	0.0086 (9)	0.0075 (9)
C16B	0.0374 (12)	0.0244 (11)	0.0329 (11)	0.0009 (9)	0.0098 (9)	0.0051 (9)
C17B	0.0407 (12)	0.0242 (11)	0.0298 (11)	0.0056 (9)	0.0094 (9)	0.0048 (9)
C18B	0.0383 (12)	0.0326 (12)	0.0324 (11)	0.0106 (10)	0.0083 (9)	0.0083 (10)
C19B	0.0495 (14)	0.0365 (13)	0.0377 (12)	0.0120 (11)	0.0125 (11)	0.0063 (10)
C20B	0.0495 (15)	0.0481 (16)	0.0481 (14)	0.0190 (12)	0.0206 (12)	0.0099 (12)
C21B	0.0398 (13)	0.0523 (16)	0.0523 (15)	0.0140 (12)	0.0153 (12)	0.0133 (13)
C22B	0.0389 (13)	0.0408 (14)	0.0414 (13)	0.0085 (11)	0.0093 (10)	0.0084 (11)
C23B	0.0384 (12)	0.0347 (13)	0.0335 (11)	0.0108 (10)	0.0089 (10)	0.0104 (10)
C24B	0.0360 (12)	0.0310 (12)	0.0266 (10)	0.0064 (9)	0.0063 (9)	0.0072 (9)
O1B	0.0454 (9)	0.0290 (8)	0.0345 (8)	0.0013 (7)	0.0139 (7)	0.0089 (6)
C25B	0.0540 (14)	0.0303 (12)	0.0479 (13)	0.0027 (11)	0.0158 (11)	0.0133 (10)
C26B	0.0606 (16)	0.0530 (16)	0.0702 (17)	−0.0051 (13)	0.0128 (14)	0.0197 (14)
C27B	0.062 (2)	0.067 (3)	0.069 (2)	0.001 (2)	0.021 (2)	0.031 (2)
C28B	0.064 (3)	0.096 (3)	0.105 (4)	0.006 (2)	0.023 (3)	0.032 (3)
C29B	0.080 (3)	0.105 (4)	0.114 (4)	0.005 (3)	0.017 (3)	0.027 (3)
C30B	0.089 (3)	0.136 (3)	0.136 (3)	0.002 (2)	−0.004 (2)	0.019 (3)
C31B	0.078 (3)	0.111 (4)	0.084 (3)	0.033 (3)	0.020 (3)	0.004 (3)
C32B	0.150 (5)	0.150 (5)	0.130 (4)	0.052 (4)	0.028 (4)	0.037 (4)
C25D	0.0540 (14)	0.0303 (12)	0.0479 (13)	0.0027 (11)	0.0158 (11)	0.0133 (10)
C26D	0.0606 (16)	0.0530 (16)	0.0702 (17)	−0.0051 (13)	0.0128 (14)	0.0197 (14)
C27D	0.064 (4)	0.076 (4)	0.089 (5)	0.008 (4)	0.026 (4)	0.025 (4)
C28D	0.065 (4)	0.093 (5)	0.092 (5)	0.009 (4)	0.012 (4)	0.037 (5)
C29D	0.074 (4)	0.116 (5)	0.099 (5)	0.017 (4)	0.013 (4)	0.030 (4)
C30D	0.089 (3)	0.136 (3)	0.136 (3)	0.002 (2)	−0.004 (2)	0.019 (3)
C31D	0.109 (5)	0.133 (6)	0.119 (6)	0.017 (5)	0.018 (5)	0.027 (5)
C32D	0.150 (5)	0.150 (5)	0.130 (4)	0.052 (4)	0.028 (4)	0.037 (4)
B1B	0.0367 (13)	0.0266 (13)	0.0294 (12)	0.0051 (10)	0.0087 (10)	0.0065 (10)
N1C	0.0340 (10)	0.0291 (10)	0.0269 (9)	0.0103 (8)	0.0019 (7)	0.0030 (7)
N2C	0.0341 (10)	0.0388 (11)	0.0258 (9)	0.0145 (8)	0.0049 (8)	0.0042 (8)
N3C	0.0338 (10)	0.0286 (10)	0.0270 (9)	0.0084 (8)	0.0032 (7)	0.0079 (7)
N4C	0.0350 (10)	0.0379 (11)	0.0307 (9)	0.0020 (8)	0.0062 (8)	0.0149 (8)
N5C	0.0336 (10)	0.0303 (10)	0.0299 (9)	0.0011 (8)	0.0020 (8)	0.0099 (8)
N6C	0.0330 (10)	0.0283 (10)	0.0300 (9)	0.0028 (8)	0.0024 (7)	0.0048 (8)
C1C	0.0333 (12)	0.0276 (11)	0.0270 (11)	0.0075 (9)	0.0016 (9)	0.0010 (9)
C2C	0.0368 (12)	0.0338 (12)	0.0256 (10)	0.0104 (10)	0.0059 (9)	0.0006 (9)
C3C	0.0412 (13)	0.0464 (14)	0.0254 (11)	0.0109 (11)	0.0039 (10)	0.0031 (10)
C4C	0.0506 (15)	0.0702 (19)	0.0267 (12)	0.0122 (13)	0.0080 (11)	0.0119 (12)
C5C	0.0474 (15)	0.083 (2)	0.0323 (13)	0.0091 (14)	0.0138 (11)	0.0140 (13)

C6C	0.0380 (13)	0.0658 (18)	0.0301 (12)	0.0106 (12)	0.0071 (10)	0.0040 (11)
C7C	0.0357 (12)	0.0433 (14)	0.0250 (11)	0.0141 (10)	0.0067 (9)	0.0014 (10)
C8C	0.0341 (12)	0.0346 (12)	0.0286 (11)	0.0142 (10)	0.0061 (9)	0.0024 (9)
C9C	0.0330 (12)	0.0282 (11)	0.0297 (11)	0.0125 (9)	0.0055 (9)	0.0064 (9)
C10C	0.0335 (11)	0.0264 (11)	0.0270 (10)	0.0115 (9)	0.0048 (9)	0.0078 (9)
C11C	0.0335 (11)	0.0307 (12)	0.0306 (11)	0.0100 (9)	0.0078 (9)	0.0080 (9)
C12C	0.0338 (12)	0.0297 (12)	0.0319 (11)	0.0068 (9)	0.0047 (9)	0.0028 (9)
C13C	0.0401 (12)	0.0299 (12)	0.0285 (11)	0.0068 (10)	0.0053 (9)	0.0021 (9)
C14C	0.0401 (13)	0.0351 (13)	0.0278 (11)	0.0095 (10)	0.0088 (9)	0.0080 (9)
C15C	0.0350 (11)	0.0271 (11)	0.0278 (11)	0.0078 (9)	0.0056 (9)	0.0092 (9)
C16C	0.0377 (12)	0.0283 (12)	0.0284 (11)	0.0054 (9)	0.0057 (9)	0.0116 (9)
C17C	0.0372 (12)	0.0329 (12)	0.0326 (12)	−0.0007 (10)	0.0068 (9)	0.0134 (10)
C18C	0.0312 (12)	0.0389 (13)	0.0360 (12)	−0.0033 (10)	0.0063 (9)	0.0137 (10)
C19C	0.0370 (13)	0.0514 (15)	0.0350 (12)	−0.0059 (11)	0.0094 (10)	0.0131 (11)
C20C	0.0346 (13)	0.0526 (16)	0.0435 (14)	−0.0029 (11)	0.0130 (11)	0.0104 (12)
C21C	0.0292 (12)	0.0470 (15)	0.0444 (13)	−0.0006 (10)	0.0085 (10)	0.0135 (11)
C22C	0.0304 (11)	0.0377 (13)	0.0364 (12)	−0.0019 (10)	0.0034 (9)	0.0102 (10)
C23C	0.0313 (11)	0.0332 (12)	0.0330 (11)	−0.0021 (9)	0.0048 (9)	0.0104 (9)
C24C	0.0322 (11)	0.0276 (12)	0.0312 (11)	−0.0002 (9)	0.0008 (9)	0.0064 (9)
O1C	0.0783 (13)	0.0281 (9)	0.0611 (11)	0.0053 (9)	−0.0238 (10)	0.0099 (8)
C25C	0.048 (2)	0.039 (2)	0.054 (3)	0.007 (2)	0.014 (2)	0.015 (2)
C26C	0.044 (3)	0.035 (2)	0.060 (3)	0.005 (2)	0.014 (2)	0.020 (2)
C27C	0.049 (3)	0.040 (3)	0.065 (3)	0.005 (2)	0.017 (2)	0.020 (2)
C28C	0.055 (3)	0.044 (4)	0.068 (3)	0.010 (3)	0.017 (3)	0.025 (4)
C29C	0.059 (3)	0.047 (3)	0.079 (3)	0.010 (2)	0.024 (2)	0.029 (3)
C30C	0.064 (3)	0.056 (3)	0.088 (3)	0.018 (3)	0.031 (3)	0.039 (3)
C31C	0.076 (4)	0.070 (4)	0.118 (5)	0.023 (3)	0.042 (4)	0.050 (4)
C32C	0.097 (8)	0.106 (7)	0.158 (9)	−0.020 (6)	0.004 (7)	0.068 (7)
O1E	0.0783 (13)	0.0281 (9)	0.0611 (11)	0.0053 (9)	−0.0238 (10)	0.0099 (8)
C25E	0.041 (2)	0.031 (2)	0.053 (2)	0.0106 (19)	0.016 (2)	0.0133 (19)
C26E	0.035 (3)	0.033 (2)	0.052 (3)	0.011 (2)	0.014 (2)	0.015 (2)
C27E	0.047 (3)	0.035 (3)	0.061 (3)	0.012 (2)	0.021 (2)	0.017 (2)
C28E	0.059 (3)	0.040 (3)	0.065 (4)	0.014 (3)	0.021 (3)	0.029 (3)
C29E	0.072 (3)	0.050 (3)	0.073 (3)	0.018 (3)	0.029 (3)	0.025 (3)
C30E	0.068 (3)	0.066 (3)	0.104 (4)	0.020 (3)	0.023 (3)	0.040 (3)
C31E	0.076 (5)	0.065 (4)	0.101 (5)	0.027 (4)	0.027 (4)	0.050 (4)
C32E	0.143 (11)	0.093 (8)	0.135 (10)	0.036 (8)	0.039 (8)	0.047 (7)
B1C	0.0384 (14)	0.0281 (14)	0.0323 (13)	0.0072 (11)	−0.0004 (11)	0.0065 (11)
O1W	0.269 (12)	0.168 (9)	0.182 (9)	0.155 (9)	−0.043 (8)	−0.022 (7)

Geometric parameters (Å, º)

O1A—B1A	1.416 (3)	C28B—H28D	0.9900
O1A—C25A	1.429 (3)	C29B—C30B	1.568 (6)
N1A—C1A	1.362 (3)	C29B—H29C	0.9900
N1A—C8A	1.367 (3)	C29B—H29D	0.9900
N1A—B1A	1.503 (3)	C30B—C31B	1.553 (6)
N2A—C8A	1.342 (3)	C30B—H30C	0.9900

N2A—C9A	1.347 (3)	C30B—H30D	0.9900
N3A—C9A	1.368 (3)	C31B—C32B	1.484 (6)
N3A—C16A	1.371 (3)	C31B—H31C	0.9900
N3A—B1A	1.510 (3)	C31B—H31D	0.9900
N4A—C17A	1.343 (3)	C32B—H32D	0.9800
N4A—C16A	1.352 (3)	C32B—H32E	0.9800
N5A—C24A	1.362 (3)	C32B—H32F	0.9800
N5A—C17A	1.372 (3)	C25D—C26D	1.511 (4)
N5A—B1A	1.508 (3)	C25D—H25E	0.9900
N6A—C1A	1.342 (3)	C25D—H25F	0.9900
N6A—C24A	1.347 (3)	C26D—C27D	1.447 (9)
C1A—C2A	1.457 (3)	C26D—H26E	0.9900
C2A—C3A	1.394 (3)	C26D—H26F	0.9900
C2A—C7A	1.419 (3)	C27D—C28D	1.557 (10)
C3A—C4A	1.384 (4)	C27D—H27E	0.9900
C3A—H3AA	0.9500	C27D—H27F	0.9900
C4A—C5A	1.393 (4)	C28D—C29D	1.573 (10)
C4A—H4AA	0.9500	C28D—H28E	0.9900
C5A—C6A	1.382 (3)	C28D—H28F	0.9900
C5A—H5AA	0.9500	C29D—C30D	1.544 (10)
C6A—C7A	1.393 (3)	C29D—H29E	0.9900
C6A—H6AA	0.9500	C29D—H29F	0.9900
C7A—C8A	1.456 (3)	C30D—C31D	1.511 (10)
C9A—C10A	1.450 (3)	C30D—H30E	0.9900
C10A—C11A	1.397 (3)	C30D—H30F	0.9900
C10A—C15A	1.422 (3)	C31D—C32D	1.462 (10)
C11A—C12A	1.378 (4)	C31D—H31E	0.9900
C11A—H11A	0.9500	C31D—H31F	0.9900
C12A—C13A	1.403 (4)	C32D—H32M	0.9800
C12A—H12A	0.9500	C32D—H32N	0.9800
C13A—C14A	1.379 (4)	C32D—H32O	0.9800
C13A—H13A	0.9500	N1C—C8C	1.367 (3)
C14A—C15A	1.397 (3)	N1C—C1C	1.369 (3)
C14A—H14A	0.9500	N1C—B1C	1.500 (3)
C15A—C16A	1.449 (3)	N2C—C8C	1.347 (3)
C17A—C18A	1.454 (3)	N2C—C9C	1.347 (3)
C18A—C19A	1.396 (3)	N3C—C16C	1.365 (3)
C18A—C23A	1.419 (3)	N3C—C9C	1.369 (3)
C19A—C20A	1.382 (3)	N3C—B1C	1.507 (3)
C19A—H19A	0.9500	N4C—C16C	1.346 (3)
C20A—C21A	1.396 (4)	N4C—C17C	1.347 (3)
C20A—H20A	0.9500	N5C—C24C	1.363 (3)
C21A—C22A	1.384 (4)	N5C—C17C	1.366 (3)
C21A—H21A	0.9500	N5C—B1C	1.496 (3)
C22A—C23A	1.393 (3)	N6C—C24C	1.348 (3)
C22A—H22A	0.9500	N6C—C1C	1.349 (3)
C23A—C24A	1.460 (3)	C1C—C2C	1.447 (3)
C25A—C26A	1.475 (4)	C2C—C3C	1.397 (3)

C25A—H25A	0.9900	C2C—C7C	1.428 (3)
C25A—H25B	0.9900	C3C—C4C	1.380 (4)
C26A—C27A	1.537 (4)	C3C—H3CA	0.9500
C26A—H26A	0.9900	C4C—C5C	1.397 (4)
C26A—H26B	0.9900	C4C—H4CA	0.9500
C27A—C28A	1.497 (4)	C5C—C6C	1.386 (4)
C27A—H27A	0.9900	C5C—H5CA	0.9500
C27A—H27B	0.9900	C6C—C7C	1.393 (4)
C28A—C29A	1.520 (4)	C6C—H6CA	0.9500
C28A—H28A	0.9900	C7C—C8C	1.457 (3)
C28A—H28B	0.9900	C9C—C10C	1.463 (3)
C29A—C30A	1.502 (4)	C10C—C11C	1.396 (3)
C29A—H29A	0.9900	C10C—C15C	1.424 (3)
C29A—H29B	0.9900	C11C—C12C	1.387 (3)
C30A—C31A	1.515 (4)	C11C—H11B	0.9500
C30A—H30A	0.9900	C12C—C13C	1.394 (3)
C30A—H30B	0.9900	C12C—H12B	0.9500
C31A—C32A	1.510 (4)	C13C—C14C	1.385 (3)
C31A—H31A	0.9900	C13C—H13B	0.9500
C31A—H31B	0.9900	C14C—C15C	1.393 (3)
C32A—H32A	0.9800	C14C—H14B	0.9500
C32A—H32B	0.9800	C15C—C16C	1.456 (3)
C32A—H32C	0.9800	C17C—C18C	1.456 (3)
N1B—C8B	1.363 (3)	C18C—C19C	1.388 (4)
N1B—C1B	1.364 (3)	C18C—C23C	1.427 (3)
N1B—B1B	1.501 (3)	C19C—C20C	1.384 (3)
N2B—C8B	1.343 (3)	C19C—H19B	0.9500
N2B—C9B	1.346 (3)	C20C—C21C	1.397 (3)
N3B—C9B	1.367 (3)	C20C—H20B	0.9500
N3B—C16B	1.375 (3)	C21C—C22C	1.387 (3)
N3B—B1B	1.506 (3)	C21C—H21B	0.9500
N4B—C16B	1.340 (3)	C22C—C23C	1.390 (3)
N4B—C17B	1.347 (3)	C22C—H22B	0.9500
N5B—C17B	1.368 (3)	C23C—C24C	1.457 (3)
N5B—C24B	1.368 (3)	O1C—C25C	1.274 (4)
N5B—B1B	1.504 (3)	O1C—B1C	1.406 (3)
N6B—C1B	1.346 (3)	C25C—C26C	1.494 (5)
N6B—C24B	1.350 (3)	C25C—H25G	0.9900
C1B—C2B	1.456 (3)	C25C—H25H	0.9900
C2B—C3B	1.395 (3)	C26C—C27C	1.510 (6)
C2B—C7B	1.418 (3)	C26C—H26G	0.9900
C3B—C4B	1.385 (3)	C26C—H26H	0.9900
C3B—H3BA	0.9500	C27C—C28C	1.520 (6)
C4B—C5B	1.395 (3)	C27C—H27G	0.9900
C4B—H4BA	0.9500	C27C—H27H	0.9900
C5B—C6B	1.384 (3)	C28C—C29C	1.520 (6)
C5B—H5BA	0.9500	C28C—H28G	0.9900
C6B—C7B	1.389 (3)	C28C—H28H	0.9900

C6B—H6BA	0.9500	C29C—C30C	1.527 (6)
C7B—C8B	1.455 (3)	C29C—H29G	0.9900
C9B—C10B	1.458 (3)	C29C—H29H	0.9900
C10B—C11B	1.393 (3)	C30C—C31C	1.517 (6)
C10B—C15B	1.416 (3)	C30C—H30G	0.9900
C11B—C12B	1.384 (3)	C30C—H30H	0.9900
C11B—H11C	0.9500	C31C—C32C	1.518 (8)
C12B—C13B	1.399 (4)	C31C—H31G	0.9900
C12B—H12C	0.9500	C31C—H31H	0.9900
C13B—C14B	1.378 (3)	C32C—H32G	0.9800
C13B—H13C	0.9500	C32C—H32H	0.9800
C14B—C15B	1.393 (3)	C32C—H32I	0.9800
C14B—H14C	0.9500	O1E—C25E	1.276 (4)
C15B—C16B	1.450 (3)	O1E—B1C	1.406 (3)
C17B—C18B	1.452 (3)	C25E—C26E	1.484 (6)
C18B—C19B	1.390 (3)	C25E—H25J	0.9900
C18B—C23B	1.423 (3)	C25E—H25K	0.9900
C19B—C20B	1.386 (4)	C26E—C27E	1.516 (7)
C19B—H19C	0.9500	C26E—H26J	0.9900
C20B—C21B	1.393 (4)	C26E—H26K	0.9900
C20B—H20C	0.9500	C27E—C28E	1.517 (8)
C21B—C22B	1.380 (4)	C27E—H27J	0.9900
C21B—H21C	0.9500	C27E—H27K	0.9900
C22B—C23B	1.392 (3)	C28E—C29E	1.523 (8)
C22B—H22C	0.9500	C28E—H28J	0.9900
C23B—C24B	1.461 (3)	C28E—H28K	0.9900
O1B—B1B	1.421 (3)	C29E—C30E	1.505 (7)
O1B—C25B	1.429 (3)	C29E—H29J	0.9900
O1B—C25D	1.429 (3)	C29E—H29K	0.9900
C25B—C26B	1.511 (4)	C30E—C31E	1.540 (8)
C25B—H25C	0.9900	C30E—H30J	0.9900
C25B—H25D	0.9900	C30E—H30K	0.9900
C26B—C27B	1.503 (5)	C31E—C32E	1.545 (10)
C26B—H26C	0.9900	C31E—H31J	0.9900
C26B—H26D	0.9900	C31E—H31K	0.9900
C27B—C28B	1.536 (5)	C32E—H32J	0.9800
C27B—H27C	0.9900	C32E—H32K	0.9800
C27B—H27D	0.9900	C32E—H32L	0.9800
C28B—C29B	1.516 (6)	O1W—H1WB	0.8400
C28B—H28C	0.9900	O1W—H1WA	0.8400

B1A—O1A—C25A	117.29 (18)	H30C—C30B—H30D	108.6
C1A—N1A—C8A	112.41 (17)	C32B—C31B—C30B	109.4 (5)
C1A—N1A—B1A	123.00 (19)	C32B—C31B—H31C	109.8
C8A—N1A—B1A	123.16 (18)	C30B—C31B—H31C	109.8
C8A—N2A—C9A	117.18 (19)	C32B—C31B—H31D	109.8
C9A—N3A—C16A	112.27 (18)	C30B—C31B—H31D	109.8
C9A—N3A—B1A	122.79 (18)	H31C—C31B—H31D	108.2

C16A—N3A—B1A	123.52 (18)	C31B—C32B—H32D	109.5
C17A—N4A—C16A	116.72 (18)	C31B—C32B—H32E	109.5
C24A—N5A—C17A	112.40 (19)	H32D—C32B—H32E	109.5
C24A—N5A—B1A	122.71 (18)	C31B—C32B—H32F	109.5
C17A—N5A—B1A	123.86 (18)	H32D—C32B—H32F	109.5
C1A—N6A—C24A	116.90 (19)	H32E—C32B—H32F	109.5
N6A—C1A—N1A	122.66 (19)	O1B—C25D—C26D	110.4 (2)
N6A—C1A—C2A	129.0 (2)	O1B—C25D—H25E	109.6
N1A—C1A—C2A	106.23 (19)	C26D—C25D—H25E	109.6
C3A—C2A—C7A	120.4 (2)	O1B—C25D—H25F	109.6
C3A—C2A—C1A	132.1 (2)	C26D—C25D—H25F	109.6
C7A—C2A—C1A	107.01 (18)	H25E—C25D—H25F	108.1
C4A—C3A—C2A	118.0 (2)	C27D—C26D—C25D	120.4 (5)
C4A—C3A—H3AA	121.0	C27D—C26D—H26E	107.2
C2A—C3A—H3AA	121.0	C25D—C26D—H26E	107.2
C3A—C4A—C5A	121.4 (2)	C27D—C26D—H26F	107.2
C3A—C4A—H4AA	119.3	C25D—C26D—H26F	107.2
C5A—C4A—H4AA	119.3	H26E—C26D—H26F	106.9
C6A—C5A—C4A	121.5 (2)	C26D—C27D—C28D	114.8 (9)
C6A—C5A—H5AA	119.3	C26D—C27D—H27E	108.6
C4A—C5A—H5AA	119.3	C28D—C27D—H27E	108.6
C5A—C6A—C7A	118.0 (2)	C26D—C27D—H27F	108.6
C5A—C6A—H6AA	121.0	C28D—C27D—H27F	108.6
C7A—C6A—H6AA	121.0	H27E—C27D—H27F	107.5
C6A—C7A—C2A	120.6 (2)	C27D—C28D—C29D	104.7 (8)
C6A—C7A—C8A	132.0 (2)	C27D—C28D—H28E	110.8
C2A—C7A—C8A	106.88 (19)	C29D—C28D—H28E	110.8
N2A—C8A—N1A	122.72 (18)	C27D—C28D—H28F	110.8
N2A—C8A—C7A	128.9 (2)	C29D—C28D—H28F	110.8
N1A—C8A—C7A	106.27 (18)	H28E—C28D—H28F	108.9
N2A—C9A—N3A	122.64 (19)	C30D—C29D—C28D	101.8 (9)
N2A—C9A—C10A	128.9 (2)	C30D—C29D—H29E	111.4
N3A—C9A—C10A	106.25 (18)	C28D—C29D—H29E	111.4
C11A—C10A—C15A	120.7 (2)	C30D—C29D—H29F	111.4
C11A—C10A—C9A	132.1 (2)	C28D—C29D—H29F	111.4
C15A—C10A—C9A	106.94 (19)	H29E—C29D—H29F	109.3
C12A—C11A—C10A	118.0 (2)	C31D—C30D—C29D	110.1 (9)
C12A—C11A—H11A	121.0	C31D—C30D—H30E	109.6
C10A—C11A—H11A	121.0	C29D—C30D—H30E	109.6
C11A—C12A—C13A	121.5 (2)	C31D—C30D—H30F	109.6
C11A—C12A—H12A	119.2	C29D—C30D—H30F	109.6
C13A—C12A—H12A	119.2	H30E—C30D—H30F	108.1
C14A—C13A—C12A	121.3 (2)	C32D—C31D—C30D	113.0 (8)
C14A—C13A—H13A	119.4	C32D—C31D—H31E	109.0
C12A—C13A—H13A	119.4	C30D—C31D—H31E	109.0
C13A—C14A—C15A	118.3 (2)	C32D—C31D—H31F	109.0
C13A—C14A—H14A	120.9	C30D—C31D—H31F	109.0
C15A—C14A—H14A	120.9	H31E—C31D—H31F	107.8

C14A—C15A—C10A	120.3 (2)	C31D—C32D—H32M	109.5
C14A—C15A—C16A	132.1 (2)	C31D—C32D—H32N	109.5
C10A—C15A—C16A	107.21 (18)	H32M—C32D—H32N	109.5
N4A—C16A—N3A	122.7 (2)	C31D—C32D—H32O	109.5
N4A—C16A—C15A	129.2 (2)	H32M—C32D—H32O	109.5
N3A—C16A—C15A	106.07 (18)	H32N—C32D—H32O	109.5
N4A—C17A—N5A	122.4 (2)	O1B—B1B—N1B	110.72 (18)
N4A—C17A—C18A	129.7 (2)	O1B—B1B—N5B	117.42 (19)
N5A—C17A—C18A	106.05 (18)	N1B—B1B—N5B	102.59 (18)
C19A—C18A—C23A	120.6 (2)	O1B—B1B—N3B	118.1 (2)
C19A—C18A—C17A	132.0 (2)	N1B—B1B—N3B	103.49 (17)
C23A—C18A—C17A	107.2 (2)	N5B—B1B—N3B	102.61 (18)
C20A—C19A—C18A	117.6 (2)	C8C—N1C—C1C	112.88 (19)
C20A—C19A—H19A	121.2	C8C—N1C—B1C	123.24 (18)
C18A—C19A—H19A	121.2	C1C—N1C—B1C	122.78 (19)
C19A—C20A—C21A	121.8 (2)	C8C—N2C—C9C	116.7 (2)
C19A—C20A—H20A	119.1	C16C—N3C—C9C	113.21 (18)
C21A—C20A—H20A	119.1	C16C—N3C—B1C	122.8 (2)
C22A—C21A—C20A	121.4 (2)	C9C—N3C—B1C	123.29 (19)
C22A—C21A—H21A	119.3	C16C—N4C—C17C	116.72 (19)
C20A—C21A—H21A	119.3	C24C—N5C—C17C	113.03 (19)
C21A—C22A—C23A	117.7 (2)	C24C—N5C—B1C	123.58 (19)
C21A—C22A—H22A	121.2	C17C—N5C—B1C	122.65 (18)
C23A—C22A—H22A	121.2	C24C—N6C—C1C	117.39 (17)
C22A—C23A—C18A	120.9 (2)	N6C—C1C—N1C	122.3 (2)
C22A—C23A—C24A	131.8 (2)	N6C—C1C—C2C	130.14 (19)
C18A—C23A—C24A	106.92 (19)	N1C—C1C—C2C	105.85 (19)
N6A—C24A—N5A	122.7 (2)	C3C—C2C—C7C	120.5 (2)
N6A—C24A—C23A	129.5 (2)	C3C—C2C—C1C	132.3 (2)
N5A—C24A—C23A	106.23 (19)	C7C—C2C—C1C	107.12 (18)
O1A—C25A—C26A	111.6 (2)	C4C—C3C—C2C	117.7 (2)
O1A—C25A—H25A	109.3	C4C—C3C—H3CA	121.1
C26A—C25A—H25A	109.3	C2C—C3C—H3CA	121.1
O1A—C25A—H25B	109.3	C3C—C4C—C5C	121.8 (2)
C26A—C25A—H25B	109.3	C3C—C4C—H4CA	119.1
H25A—C25A—H25B	108.0	C5C—C4C—H4CA	119.1
C25A—C26A—C27A	111.7 (2)	C6C—C5C—C4C	121.5 (3)
C25A—C26A—H26A	109.3	C6C—C5C—H5CA	119.3
C27A—C26A—H26A	109.3	C4C—C5C—H5CA	119.3
C25A—C26A—H26B	109.3	C5C—C6C—C7C	117.8 (2)
C27A—C26A—H26B	109.3	C5C—C6C—H6CA	121.1
H26A—C26A—H26B	107.9	C7C—C6C—H6CA	121.1
C28A—C27A—C26A	113.4 (3)	C6C—C7C—C2C	120.7 (2)
C28A—C27A—H27A	108.9	C6C—C7C—C8C	132.2 (2)
C26A—C27A—H27A	108.9	C2C—C7C—C8C	107.0 (2)
C28A—C27A—H27B	108.9	N2C—C8C—N1C	122.8 (2)
C26A—C27A—H27B	108.9	N2C—C8C—C7C	130.1 (2)
H27A—C27A—H27B	107.7	N1C—C8C—C7C	105.51 (18)

C27A—C28A—C29A	114.1 (3)	N2C—C9C—N3C	122.52 (18)
C27A—C28A—H28A	108.7	N2C—C9C—C10C	131.0 (2)
C29A—C28A—H28A	108.7	N3C—C9C—C10C	105.31 (18)
C27A—C28A—H28B	108.7	C11C—C10C—C15C	120.49 (19)
C29A—C28A—H28B	108.7	C11C—C10C—C9C	132.2 (2)
H28A—C28A—H28B	107.6	C15C—C10C—C9C	107.25 (19)
C30A—C29A—C28A	112.6 (2)	C12C—C11C—C10C	117.6 (2)
C30A—C29A—H29A	109.1	C12C—C11C—H11B	121.2
C28A—C29A—H29A	109.1	C10C—C11C—H11B	121.2
C30A—C29A—H29B	109.1	C11C—C12C—C13C	121.8 (2)
C28A—C29A—H29B	109.1	C11C—C12C—H12B	119.1
H29A—C29A—H29B	107.8	C13C—C12C—H12B	119.1
C29A—C30A—C31A	114.0 (2)	C14C—C13C—C12C	121.2 (2)
C29A—C30A—H30A	108.7	C14C—C13C—H13B	119.4
C31A—C30A—H30A	108.7	C12C—C13C—H13B	119.4
C29A—C30A—H30B	108.7	C13C—C14C—C15C	118.0 (2)
C31A—C30A—H30B	108.7	C13C—C14C—H14B	121.0
H30A—C30A—H30B	107.6	C15C—C14C—H14B	121.0
C32A—C31A—C30A	112.9 (2)	C14C—C15C—C10C	120.7 (2)
C32A—C31A—H31A	109.0	C14C—C15C—C16C	132.3 (2)
C30A—C31A—H31A	109.0	C10C—C15C—C16C	106.97 (18)
C32A—C31A—H31B	109.0	N4C—C16C—N3C	122.39 (19)
C30A—C31A—H31B	109.0	N4C—C16C—C15C	130.6 (2)
H31A—C31A—H31B	107.8	N3C—C16C—C15C	105.83 (19)
C31A—C32A—H32A	109.5	N4C—C17C—N5C	122.6 (2)
C31A—C32A—H32B	109.5	N4C—C17C—C18C	130.0 (2)
H32A—C32A—H32B	109.5	N5C—C17C—C18C	105.88 (18)
C31A—C32A—H32C	109.5	C19C—C18C—C23C	120.7 (2)
H32A—C32A—H32C	109.5	C19C—C18C—C17C	132.5 (2)
H32B—C32A—H32C	109.5	C23C—C18C—C17C	106.8 (2)
O1A—B1A—N1A	111.98 (19)	C20C—C19C—C18C	118.3 (2)
O1A—B1A—N5A	116.5 (2)	C20C—C19C—H19B	120.8
N1A—B1A—N5A	103.26 (18)	C18C—C19C—H19B	120.8
O1A—B1A—N3A	117.28 (19)	C19C—C20C—C21C	120.9 (2)
N1A—B1A—N3A	103.62 (18)	C19C—C20C—H20B	119.5
N5A—B1A—N3A	102.45 (18)	C21C—C20C—H20B	119.5
C8B—N1B—C1B	113.48 (18)	C22C—C21C—C20C	121.7 (2)
C8B—N1B—B1B	122.40 (18)	C22C—C21C—H21B	119.1
C1B—N1B—B1B	123.49 (18)	C20C—C21C—H21B	119.1
C8B—N2B—C9B	116.97 (18)	C21C—C22C—C23C	117.9 (2)
C9B—N3B—C16B	112.23 (17)	C21C—C22C—H22B	121.0
C9B—N3B—B1B	122.45 (18)	C23C—C22C—H22B	121.0
C16B—N3B—B1B	123.70 (18)	C22C—C23C—C18C	120.3 (2)
C16B—N4B—C17B	116.94 (18)	C22C—C23C—C24C	132.4 (2)
C17B—N5B—C24B	112.65 (18)	C18C—C23C—C24C	107.14 (19)
C17B—N5B—B1B	123.72 (18)	N6C—C24C—N5C	122.1 (2)
C24B—N5B—B1B	122.88 (18)	N6C—C24C—C23C	130.92 (19)
C1B—N6B—C24B	116.74 (18)	N5C—C24C—C23C	105.76 (19)

N6B—C1B—N1B	122.37 (19)	C25C—O1C—B1C	125.3 (3)
N6B—C1B—C2B	130.8 (2)	O1C—C25C—C26C	116.1 (4)
N1B—C1B—C2B	105.49 (18)	O1C—C25C—H25G	108.3
C3B—C2B—C7B	120.3 (2)	C26C—C25C—H25G	108.3
C3B—C2B—C1B	132.6 (2)	O1C—C25C—H25H	108.3
C7B—C2B—C1B	107.05 (18)	C26C—C25C—H25H	108.3
C4B—C3B—C2B	118.1 (2)	H25G—C25C—H25H	107.4
C4B—C3B—H3BA	121.0	C25C—C26C—C27C	114.4 (5)
C2B—C3B—H3BA	121.0	C25C—C26C—H26G	108.7
C3B—C4B—C5B	121.2 (2)	C27C—C26C—H26G	108.7
C3B—C4B—H4BA	119.4	C25C—C26C—H26H	108.7
C5B—C4B—H4BA	119.4	C27C—C26C—H26H	108.7
C6B—C5B—C4B	121.5 (2)	H26G—C26C—H26H	107.6
C6B—C5B—H5BA	119.3	C26C—C27C—C28C	113.4 (4)
C4B—C5B—H5BA	119.3	C26C—C27C—H27G	108.9
C5B—C6B—C7B	118.0 (2)	C28C—C27C—H27G	108.9
C5B—C6B—H6BA	121.0	C26C—C27C—H27H	108.9
C7B—C6B—H6BA	121.0	C28C—C27C—H27H	108.9
C6B—C7B—C2B	120.8 (2)	H27G—C27C—H27H	107.7
C6B—C7B—C8B	131.7 (2)	C29C—C28C—C27C	117.0 (6)
C2B—C7B—C8B	107.41 (18)	C29C—C28C—H28G	108.0
N2B—C8B—N1B	122.66 (19)	C27C—C28C—H28G	108.0
N2B—C8B—C7B	130.29 (19)	C29C—C28C—H28H	108.0
N1B—C8B—C7B	105.32 (18)	C27C—C28C—H28H	108.0
N2B—C9B—N3B	122.60 (19)	H28G—C28C—H28H	107.3
N2B—C9B—C10B	129.37 (19)	C28C—C29C—C30C	113.8 (5)
N3B—C9B—C10B	105.95 (18)	C28C—C29C—H29G	108.8
C11B—C10B—C15B	120.7 (2)	C30C—C29C—H29G	108.8
C11B—C10B—C9B	131.6 (2)	C28C—C29C—H29H	108.8
C15B—C10B—C9B	107.33 (18)	C30C—C29C—H29H	108.8
C12B—C11B—C10B	117.7 (2)	H29G—C29C—H29H	107.7
C12B—C11B—H11C	121.2	C31C—C30C—C29C	115.7 (5)
C10B—C11B—H11C	121.2	C31C—C30C—H30G	108.4
C11B—C12B—C13B	121.6 (2)	C29C—C30C—H30G	108.4
C11B—C12B—H12C	119.2	C31C—C30C—H30H	108.4
C13B—C12B—H12C	119.2	C29C—C30C—H30H	108.4
C14B—C13B—C12B	121.1 (2)	H30G—C30C—H30H	107.4
C14B—C13B—H13C	119.5	C30C—C31C—C32C	113.5 (8)
C12B—C13B—H13C	119.5	C30C—C31C—H31G	108.9
C13B—C14B—C15B	118.2 (2)	C32C—C31C—H31G	108.9
C13B—C14B—H14C	120.9	C30C—C31C—H31H	108.9
C15B—C14B—H14C	120.9	C32C—C31C—H31H	108.9
C14B—C15B—C10B	120.6 (2)	H31G—C31C—H31H	107.7
C14B—C15B—C16B	131.9 (2)	C31C—C32C—H32G	109.5
C10B—C15B—C16B	107.10 (19)	C31C—C32C—H32H	109.5
N4B—C16B—N3B	122.59 (19)	H32G—C32C—H32H	109.5
N4B—C16B—C15B	129.4 (2)	C31C—C32C—H32I	109.5
N3B—C16B—C15B	106.27 (19)	H32G—C32C—H32I	109.5

N4B—C17B—N5B	122.3 (2)	H32H—C32C—H32I	109.5
N4B—C17B—C18B	130.0 (2)	C25E—O1E—B1C	128.0 (3)
N5B—C17B—C18B	106.08 (18)	O1E—C25E—C26E	116.4 (4)
C19B—C18B—C23B	121.0 (2)	O1E—C25E—H25J	108.2
C19B—C18B—C17B	131.7 (2)	C26E—C25E—H25J	108.2
C23B—C18B—C17B	107.16 (19)	O1E—C25E—H25K	108.2
C20B—C19B—C18B	117.7 (2)	C26E—C25E—H25K	108.2
C20B—C19B—H19C	121.2	H25J—C25E—H25K	107.3
C18B—C19B—H19C	121.2	C25E—C26E—C27E	113.0 (5)
C19B—C20B—C21B	121.1 (2)	C25E—C26E—H26J	109.0
C19B—C20B—H20C	119.4	C27E—C26E—H26J	109.0
C21B—C20B—H20C	119.4	C25E—C26E—H26K	109.0
C22B—C21B—C20B	122.1 (2)	C27E—C26E—H26K	109.0
C22B—C21B—H21C	119.0	H26J—C26E—H26K	107.8
C20B—C21B—H21C	119.0	C26E—C27E—C28E	112.6 (5)
C21B—C22B—C23B	117.7 (2)	C26E—C27E—H27J	109.1
C21B—C22B—H22C	121.2	C28E—C27E—H27J	109.1
C23B—C22B—H22C	121.2	C26E—C27E—H27K	109.1
C22B—C23B—C18B	120.3 (2)	C28E—C27E—H27K	109.1
C22B—C23B—C24B	132.7 (2)	H27J—C27E—H27K	107.8
C18B—C23B—C24B	106.97 (19)	C27E—C28E—C29E	115.5 (7)
N6B—C24B—N5B	122.46 (19)	C27E—C28E—H28J	108.4
N6B—C24B—C23B	130.1 (2)	C29E—C28E—H28J	108.4
N5B—C24B—C23B	105.75 (18)	C27E—C28E—H28K	108.4
B1B—O1B—C25B	119.09 (18)	C29E—C28E—H28K	108.4
B1B—O1B—C25D	119.09 (18)	H28J—C28E—H28K	107.5
O1B—C25B—C26B	110.4 (2)	C30E—C29E—C28E	113.3 (7)
O1B—C25B—H25C	109.6	C30E—C29E—H29J	108.9
C26B—C25B—H25C	109.6	C28E—C29E—H29J	108.9
O1B—C25B—H25D	109.6	C30E—C29E—H29K	108.9
C26B—C25B—H25D	109.6	C28E—C29E—H29K	108.9
H25C—C25B—H25D	108.1	H29J—C29E—H29K	107.7
C27B—C26B—C25B	111.5 (3)	C29E—C30E—C31E	111.6 (6)
C27B—C26B—H26C	109.3	C29E—C30E—H30J	109.3
C25B—C26B—H26C	109.3	C31E—C30E—H30J	109.3
C27B—C26B—H26D	109.3	C29E—C30E—H30K	109.3
C25B—C26B—H26D	109.3	C31E—C30E—H30K	109.3
H26C—C26B—H26D	108.0	H30J—C30E—H30K	108.0
C26B—C27B—C28B	116.8 (4)	C30E—C31E—C32E	105.4 (8)
C26B—C27B—H27C	108.1	C30E—C31E—H31J	110.7
C28B—C27B—H27C	108.1	C32E—C31E—H31J	110.7
C26B—C27B—H27D	108.1	C30E—C31E—H31K	110.7
C28B—C27B—H27D	108.1	C32E—C31E—H31K	110.7
H27C—C27B—H27D	107.3	H31J—C31E—H31K	108.8
C29B—C28B—C27B	117.2 (5)	C31E—C32E—H32J	109.5
C29B—C28B—H28C	108.0	C31E—C32E—H32K	109.5
C27B—C28B—H28C	108.0	H32J—C32E—H32K	109.5
C29B—C28B—H28D	108.0	C31E—C32E—H32L	109.5

C27B—C28B—H28D	108.0	H32J—C32E—H32L	109.5
H28C—C28B—H28D	107.2	H32K—C32E—H32L	109.5
C28B—C29B—C30B	114.0 (5)	O1E—B1C—N5C	113.6 (2)
C28B—C29B—H29C	108.8	O1C—B1C—N5C	113.6 (2)
C30B—C29B—H29C	108.8	O1E—B1C—N1C	114.8 (2)
C28B—C29B—H29D	108.8	O1C—B1C—N1C	114.8 (2)
C30B—C29B—H29D	108.8	N5C—B1C—N1C	103.66 (17)
H29C—C29B—H29D	107.6	O1E—B1C—N3C	117.28 (18)
C31B—C30B—C29B	107.0 (4)	O1C—B1C—N3C	117.28 (18)
C31B—C30B—H30C	110.3	N5C—B1C—N3C	102.80 (18)
C29B—C30B—H30C	110.3	N1C—B1C—N3C	102.97 (19)
C31B—C30B—H30D	110.3	H1WB—O1W—H1WA	98.6
C29B—C30B—H30D	110.3		

C24A—N6A—C1A—N1A	−9.4 (3)	C18B—C19B—C20B—C21B	2.1 (4)
C24A—N6A—C1A—C2A	151.6 (2)	C19B—C20B—C21B—C22B	0.1 (4)
C8A—N1A—C1A—N6A	153.4 (2)	C20B—C21B—C22B—C23B	−1.8 (4)
B1A—N1A—C1A—N6A	−13.3 (3)	C21B—C22B—C23B—C18B	1.1 (3)
C8A—N1A—C1A—C2A	−11.3 (2)	C21B—C22B—C23B—C24B	179.1 (2)
B1A—N1A—C1A—C2A	−178.0 (2)	C19B—C18B—C23B—C22B	1.1 (3)
N6A—C1A—C2A—C3A	15.6 (4)	C17B—C18B—C23B—C22B	178.4 (2)
N1A—C1A—C2A—C3A	179.0 (2)	C19B—C18B—C23B—C24B	−177.3 (2)
N6A—C1A—C2A—C7A	−156.3 (2)	C17B—C18B—C23B—C24B	0.0 (2)
N1A—C1A—C2A—C7A	7.1 (2)	C1B—N6B—C24B—N5B	7.5 (3)
C7A—C2A—C3A—C4A	0.3 (3)	C1B—N6B—C24B—C23B	−155.6 (2)
C1A—C2A—C3A—C4A	−170.6 (2)	C17B—N5B—C24B—N6B	−154.7 (2)
C2A—C3A—C4A—C5A	0.3 (4)	B1B—N5B—C24B—N6B	15.7 (3)
C3A—C4A—C5A—C6A	−0.4 (4)	C17B—N5B—C24B—C23B	12.0 (2)
C4A—C5A—C6A—C7A	0.0 (4)	B1B—N5B—C24B—C23B	−177.59 (18)
C5A—C6A—C7A—C2A	0.6 (3)	C22B—C23B—C24B—N6B	−19.8 (4)
C5A—C6A—C7A—C8A	171.7 (2)	C18B—C23B—C24B—N6B	158.4 (2)
C3A—C2A—C7A—C6A	−0.8 (3)	C22B—C23B—C24B—N5B	174.9 (2)
C1A—C2A—C7A—C6A	172.2 (2)	C18B—C23B—C24B—N5B	−6.9 (2)
C3A—C2A—C7A—C8A	−173.9 (2)	B1B—O1B—C25B—C26B	105.0 (2)
C1A—C2A—C7A—C8A	−0.9 (2)	O1B—C25B—C26B—C27B	65.9 (3)
C9A—N2A—C8A—N1A	8.4 (3)	C25B—C26B—C27B—C28B	−171.3 (4)
C9A—N2A—C8A—C7A	−152.9 (2)	C26B—C27B—C28B—C29B	59.0 (7)
C1A—N1A—C8A—N2A	−154.2 (2)	C27B—C28B—C29B—C30B	71.1 (7)
B1A—N1A—C8A—N2A	12.5 (3)	C28B—C29B—C30B—C31B	−170.4 (5)
C1A—N1A—C8A—C7A	10.8 (2)	C29B—C30B—C31B—C32B	−69.2 (6)
B1A—N1A—C8A—C7A	177.5 (2)	B1B—O1B—C25D—C26D	105.0 (2)
C6A—C7A—C8A—N2A	−13.9 (4)	O1B—C25D—C26D—C27D	38.3 (9)
C2A—C7A—C8A—N2A	158.0 (2)	C25D—C26D—C27D—C28D	179.8 (10)
C6A—C7A—C8A—N1A	−177.6 (2)	C26D—C27D—C28D—C29D	171.4 (12)
C2A—C7A—C8A—N1A	−5.7 (2)	C27D—C28D—C29D—C30D	−62.7 (14)
C8A—N2A—C9A—N3A	−7.7 (3)	C28D—C29D—C30D—C31D	−139.0 (9)
C8A—N2A—C9A—C10A	153.0 (2)	C29D—C30D—C31D—C32D	87.0 (15)
C16A—N3A—C9A—N2A	153.0 (2)	C25B—O1B—B1B—N1B	−165.08 (18)

B1A—N3A—C9A—N2A	−13.8 (3)	C25D—O1B—B1B—N1B	−165.08 (18)
C16A—N3A—C9A—C10A	−11.5 (2)	C25B—O1B—B1B—N5B	77.6 (3)
B1A—N3A—C9A—C10A	−178.27 (19)	C25D—O1B—B1B—N5B	77.6 (3)
N2A—C9A—C10A—C11A	17.6 (4)	C25B—O1B—B1B—N3B	−46.1 (3)
N3A—C9A—C10A—C11A	−179.3 (2)	C25D—O1B—B1B—N3B	−46.1 (3)
N2A—C9A—C10A—C15A	−156.2 (2)	C8B—N1B—B1B—O1B	95.1 (2)
N3A—C9A—C10A—C15A	6.9 (2)	C1B—N1B—B1B—O1B	−94.6 (2)
C15A—C10A—C11A—C12A	0.3 (3)	C8B—N1B—B1B—N5B	−138.82 (19)
C9A—C10A—C11A—C12A	−172.8 (2)	C1B—N1B—B1B—N5B	31.5 (2)
C10A—C11A—C12A—C13A	0.6 (4)	C8B—N1B—B1B—N3B	−32.3 (3)
C11A—C12A—C13A—C14A	−0.6 (4)	C1B—N1B—B1B—N3B	137.99 (19)
C12A—C13A—C14A—C15A	−0.4 (4)	C17B—N5B—B1B—O1B	−101.0 (2)
C13A—C14A—C15A—C10A	1.3 (3)	C24B—N5B—B1B—O1B	89.7 (3)
C13A—C14A—C15A—C16A	173.2 (2)	C17B—N5B—B1B—N1B	137.43 (19)
C11A—C10A—C15A—C14A	−1.3 (3)	C24B—N5B—B1B—N1B	−32.0 (2)
C9A—C10A—C15A—C14A	173.4 (2)	C17B—N5B—B1B—N3B	30.3 (3)
C11A—C10A—C15A—C16A	−175.02 (19)	C24B—N5B—B1B—N3B	−139.10 (19)
C9A—C10A—C15A—C16A	−0.3 (2)	C9B—N3B—B1B—O1B	−92.4 (3)
C17A—N4A—C16A—N3A	9.2 (3)	C16B—N3B—B1B—O1B	103.3 (2)
C17A—N4A—C16A—C15A	−152.6 (2)	C9B—N3B—B1B—N1B	30.3 (3)
C9A—N3A—C16A—N4A	−154.1 (2)	C16B—N3B—B1B—N1B	−134.0 (2)
B1A—N3A—C16A—N4A	12.5 (3)	C9B—N3B—B1B—N5B	136.8 (2)
C9A—N3A—C16A—C15A	11.3 (2)	C16B—N3B—B1B—N5B	−27.6 (3)
B1A—N3A—C16A—C15A	177.93 (19)	C24C—N6C—C1C—N1C	−6.6 (3)
C14A—C15A—C16A—N4A	−14.9 (4)	C24C—N6C—C1C—C2C	156.4 (2)
C10A—C15A—C16A—N4A	157.8 (2)	C8C—N1C—C1C—N6C	153.4 (2)
C14A—C15A—C16A—N3A	−179.0 (2)	B1C—N1C—C1C—N6C	−15.0 (3)
C10A—C15A—C16A—N3A	−6.3 (2)	C8C—N1C—C1C—C2C	−13.1 (2)
C16A—N4A—C17A—N5A	−8.4 (3)	B1C—N1C—C1C—C2C	178.50 (19)
C16A—N4A—C17A—C18A	154.0 (2)	N6C—C1C—C2C—C3C	18.6 (4)
C24A—N5A—C17A—N4A	154.4 (2)	N1C—C1C—C2C—C3C	−176.4 (2)
B1A—N5A—C17A—N4A	−14.2 (3)	N6C—C1C—C2C—C7C	−157.4 (2)
C24A—N5A—C17A—C18A	−11.6 (2)	N1C—C1C—C2C—C7C	7.7 (2)
B1A—N5A—C17A—C18A	179.84 (19)	C7C—C2C—C3C—C4C	−1.4 (3)
N4A—C17A—C18A—C19A	16.3 (4)	C1C—C2C—C3C—C4C	−176.9 (2)
N5A—C17A—C18A—C19A	−179.2 (2)	C2C—C3C—C4C—C5C	1.7 (4)
N4A—C17A—C18A—C23A	−157.5 (2)	C3C—C4C—C5C—C6C	−0.5 (5)
N5A—C17A—C18A—C23A	7.0 (2)	C4C—C5C—C6C—C7C	−1.1 (4)
C23A—C18A—C19A—C20A	0.0 (3)	C5C—C6C—C7C—C2C	1.4 (4)
C17A—C18A—C19A—C20A	−173.1 (2)	C5C—C6C—C7C—C8C	177.0 (3)
C18A—C19A—C20A—C21A	0.4 (3)	C3C—C2C—C7C—C6C	−0.1 (3)
C19A—C20A—C21A—C22A	0.0 (4)	C1C—C2C—C7C—C6C	176.3 (2)
C20A—C21A—C22A—C23A	−0.9 (3)	C3C—C2C—C7C—C8C	−176.7 (2)
C21A—C22A—C23A—C18A	1.3 (3)	C1C—C2C—C7C—C8C	−0.3 (2)
C21A—C22A—C23A—C24A	174.0 (2)	C9C—N2C—C8C—N1C	8.2 (3)
C19A—C18A—C23A—C22A	−0.9 (3)	C9C—N2C—C8C—C7C	−155.2 (2)
C17A—C18A—C23A—C22A	173.7 (2)	C1C—N1C—C8C—N2C	−154.0 (2)
C19A—C18A—C23A—C24A	−175.2 (2)	B1C—N1C—C8C—N2C	14.3 (3)

C17A—C18A—C23A—C24A	−0.6 (2)
C1A—N6A—C24A—N5A	9.4 (3)
C1A—N6A—C24A—C23A	−154.0 (2)
C17A—N5A—C24A—N6A	−155.6 (2)
B1A—N5A—C24A—N6A	13.2 (3)
C17A—N5A—C24A—C23A	11.2 (2)
B1A—N5A—C24A—C23A	179.9 (2)
C22A—C23A—C24A—N6A	−14.1 (4)
C18A—C23A—C24A—N6A	159.4 (2)
C22A—C23A—C24A—N5A	−179.6 (2)
C18A—C23A—C24A—N5A	−6.1 (2)
B1A—O1A—C25A—C26A	110.0 (3)
O1A—C25A—C26A—C27A	174.7 (2)
C25A—C26A—C27A—C28A	−175.7 (3)
C26A—C27A—C28A—C29A	176.8 (3)
C27A—C28A—C29A—C30A	−175.4 (3)
C28A—C29A—C30A—C31A	173.6 (3)
C29A—C30A—C31A—C32A	−179.4 (2)
C25A—O1A—B1A—N1A	−177.44 (19)
C25A—O1A—B1A—N5A	64.0 (3)
C25A—O1A—B1A—N3A	−57.8 (3)
C1A—N1A—B1A—O1A	−95.9 (3)
C8A—N1A—B1A—O1A	98.8 (2)
C1A—N1A—B1A—N5A	30.2 (3)
C8A—N1A—B1A—N5A	−135.1 (2)
C1A—N1A—B1A—N3A	136.8 (2)
C8A—N1A—B1A—N3A	−28.5 (3)
C24A—N5A—B1A—O1A	93.1 (2)
C17A—N5A—B1A—O1A	−99.5 (3)
C24A—N5A—B1A—N1A	−30.1 (3)
C17A—N5A—B1A—N1A	137.4 (2)
C24A—N5A—B1A—N3A	−137.5 (2)
C17A—N5A—B1A—N3A	29.9 (3)
C9A—N3A—B1A—O1A	−94.8 (2)
C16A—N3A—B1A—O1A	99.9 (2)
C9A—N3A—B1A—N1A	29.1 (3)
C16A—N3A—B1A—N1A	−136.2 (2)
C9A—N3A—B1A—N5A	136.29 (19)
C16A—N3A—B1A—N5A	−29.0 (3)
C24B—N6B—C1B—N1B	−8.2 (3)
C24B—N6B—C1B—C2B	156.6 (2)
C8B—N1B—C1B—N6B	156.63 (19)
B1B—N1B—C1B—N6B	−14.5 (3)
C8B—N1B—C1B—C2B	−11.5 (2)
B1B—N1B—C1B—C2B	177.39 (18)
N6B—C1B—C2B—C3B	17.5 (4)
N1B—C1B—C2B—C3B	−175.8 (2)
N6B—C1B—C2B—C7B	−160.0 (2)
C1C—N1C—C8C—C7C	12.9 (2)
B1C—N1C—C8C—C7C	−178.77 (19)
C6C—C7C—C8C—N2C	−17.8 (4)
C2C—C7C—C8C—N2C	158.3 (2)
C6C—C7C—C8C—N1C	176.7 (3)
C2C—C7C—C8C—N1C	−7.3 (2)
C8C—N2C—C9C—N3C	−8.8 (3)
C8C—N2C—C9C—C10C	157.1 (2)
C16C—N3C—C9C—N2C	157.42 (19)
B1C—N3C—C9C—N2C	−13.0 (3)
C16C—N3C—C9C—C10C	−11.6 (2)
B1C—N3C—C9C—C10C	177.97 (18)
N2C—C9C—C10C—C11C	16.3 (4)
N3C—C9C—C10C—C11C	−176.0 (2)
N2C—C9C—C10C—C15C	−162.0 (2)
N3C—C9C—C10C—C15C	5.7 (2)
C15C—C10C—C11C—C12C	−3.6 (3)
C9C—C10C—C11C—C12C	178.3 (2)
C10C—C11C—C12C—C13C	2.4 (3)
C11C—C12C—C13C—C14C	1.1 (3)
C12C—C13C—C14C—C15C	−3.2 (3)
C13C—C14C—C15C—C10C	2.0 (3)
C13C—C14C—C15C—C16C	−179.9 (2)
C11C—C10C—C15C—C14C	1.5 (3)
C9C—C10C—C15C—C14C	180.00 (19)
C11C—C10C—C15C—C16C	−177.09 (19)
C9C—C10C—C15C—C16C	1.4 (2)
C17C—N4C—C16C—N3C	9.0 (3)
C17C—N4C—C16C—C15C	−156.6 (2)
C9C—N3C—C16C—N4C	−156.07 (19)
B1C—N3C—C16C—N4C	14.4 (3)
C9C—N3C—C16C—C15C	12.6 (2)
B1C—N3C—C16C—C15C	−176.95 (18)
C14C—C15C—C16C—N4C	−19.1 (4)
C10C—C15C—C16C—N4C	159.2 (2)
C14C—C15C—C16C—N3C	173.5 (2)
C10C—C15C—C16C—N3C	−8.1 (2)
C16C—N4C—C17C—N5C	−8.3 (3)
C16C—N4C—C17C—C18C	155.5 (2)
C24C—N5C—C17C—N4C	154.6 (2)
B1C—N5C—C17C—N4C	−15.9 (3)
C24C—N5C—C17C—C18C	−12.6 (2)
B1C—N5C—C17C—C18C	176.9 (2)
N4C—C17C—C18C—C19C	19.7 (4)
N5C—C17C—C18C—C19C	−174.4 (2)
N4C—C17C—C18C—C23C	−157.6 (2)
N5C—C17C—C18C—C23C	8.3 (2)
C23C—C18C—C19C—C20C	0.3 (4)

N1B—C1B—C2B—C7B	6.7 (2)	C17C—C18C—C19C—C20C	−176.8 (2)
C7B—C2B—C3B—C4B	−1.4 (3)	C18C—C19C—C20C—C21C	1.9 (4)
C1B—C2B—C3B—C4B	−178.6 (2)	C19C—C20C—C21C—C22C	−2.0 (4)
C2B—C3B—C4B—C5B	1.2 (3)	C20C—C21C—C22C—C23C	−0.3 (4)
C3B—C4B—C5B—C6B	0.7 (3)	C21C—C22C—C23C—C18C	2.5 (3)
C4B—C5B—C6B—C7B	−2.3 (3)	C21C—C22C—C23C—C24C	178.4 (2)
C5B—C6B—C7B—C2B	2.1 (3)	C19C—C18C—C23C—C22C	−2.5 (3)
C5B—C6B—C7B—C8B	179.3 (2)	C17C—C18C—C23C—C22C	175.2 (2)
C3B—C2B—C7B—C6B	−0.2 (3)	C19C—C18C—C23C—C24C	−179.4 (2)
C1B—C2B—C7B—C6B	177.64 (19)	C17C—C18C—C23C—C24C	−1.6 (2)
C3B—C2B—C7B—C8B	−178.10 (19)	C1C—N6C—C24C—N5C	7.4 (3)
C1B—C2B—C7B—C8B	−0.2 (2)	C1C—N6C—C24C—C23C	−157.9 (2)
C9B—N2B—C8B—N1B	8.1 (3)	C17C—N5C—C24C—N6C	−156.9 (2)
C9B—N2B—C8B—C7B	−154.6 (2)	B1C—N5C—C24C—N6C	13.5 (3)
C1B—N1B—C8B—N2B	−155.1 (2)	C17C—N5C—C24C—C23C	11.6 (2)
B1B—N1B—C8B—N2B	16.1 (3)	B1C—N5C—C24C—C23C	−178.02 (19)
C1B—N1B—C8B—C7B	11.3 (2)	C22C—C23C—C24C—N6C	−14.9 (4)
B1B—N1B—C8B—C7B	−177.44 (18)	C18C—C23C—C24C—N6C	161.4 (2)
C6B—C7B—C8B—N2B	−18.9 (4)	C22C—C23C—C24C—N5C	178.1 (2)
C2B—C7B—C8B—N2B	158.6 (2)	C18C—C23C—C24C—N5C	−5.6 (2)
C6B—C7B—C8B—N1B	176.1 (2)	B1C—O1C—C25C—C26C	174.3 (4)
C2B—C7B—C8B—N1B	−6.4 (2)	O1C—C25C—C26C—C27C	−74.6 (6)
C8B—N2B—C9B—N3B	−10.1 (3)	C25C—C26C—C27C—C28C	−164.4 (7)
C8B—N2B—C9B—C10B	151.0 (2)	C26C—C27C—C28C—C29C	179.9 (8)
C16B—N3B—C9B—N2B	154.0 (2)	C27C—C28C—C29C—C30C	−174.5 (8)
B1B—N3B—C9B—N2B	−11.9 (3)	C28C—C29C—C30C—C31C	−169.9 (8)
C16B—N3B—C9B—C10B	−10.9 (2)	C29C—C30C—C31C—C32C	−63.5 (10)
B1B—N3B—C9B—C10B	−176.88 (19)	B1C—O1E—C25E—C26E	−166.9 (4)
N2B—C9B—C10B—C11B	16.2 (4)	O1E—C25E—C26E—C27E	−171.1 (5)
N3B—C9B—C10B—C11B	179.7 (2)	C25E—C26E—C27E—C28E	−172.2 (7)
N2B—C9B—C10B—C15B	−156.8 (2)	C26E—C27E—C28E—C29E	−172.9 (7)
N3B—C9B—C10B—C15B	6.8 (2)	C27E—C28E—C29E—C30E	−67.4 (11)
C15B—C10B—C11B—C12B	0.2 (3)	C28E—C29E—C30E—C31E	−172.0 (8)
C9B—C10B—C11B—C12B	−171.9 (2)	C29E—C30E—C31E—C32E	175.0 (8)
C10B—C11B—C12B—C13B	0.1 (4)	C25E—O1E—B1C—N5C	162.1 (4)
C11B—C12B—C13B—C14B	0.1 (4)	C25E—O1E—B1C—N1C	−78.8 (4)
C12B—C13B—C14B—C15B	−0.7 (4)	C25E—O1E—B1C—N3C	42.3 (5)
C13B—C14B—C15B—C10B	1.1 (3)	C25C—O1C—B1C—N5C	68.8 (4)
C13B—C14B—C15B—C16B	172.9 (2)	C25C—O1C—B1C—N1C	−172.2 (3)
C11B—C10B—C15B—C14B	−0.9 (3)	C25C—O1C—B1C—N3C	−51.0 (4)
C9B—C10B—C15B—C14B	173.0 (2)	C24C—N5C—B1C—O1E	95.8 (3)
C11B—C10B—C15B—C16B	−174.5 (2)	C17C—N5C—B1C—O1E	−94.7 (2)
C9B—C10B—C15B—C16B	−0.6 (2)	C24C—N5C—B1C—O1C	95.8 (3)
C17B—N4B—C16B—N3B	10.4 (3)	C17C—N5C—B1C—O1C	−94.7 (2)
C17B—N4B—C16B—C15B	−152.4 (2)	C24C—N5C—B1C—N1C	−29.5 (3)
C9B—N3B—C16B—N4B	−155.7 (2)	C17C—N5C—B1C—N1C	140.0 (2)
B1B—N3B—C16B—N4B	10.1 (3)	C24C—N5C—B1C—N3C	−136.5 (2)
C9B—N3B—C16B—C15B	10.6 (2)	C17C—N5C—B1C—N3C	33.0 (3)

B1B—N3B—C16B—C15B	176.33 (19)	C8C—N1C—B1C—O1E	98.4 (3)
C14B—C15B—C16B—N4B	−13.4 (4)	C1C—N1C—B1C—O1E	−94.4 (3)
C10B—C15B—C16B—N4B	159.3 (2)	C8C—N1C—B1C—O1C	98.4 (3)
C14B—C15B—C16B—N3B	−178.4 (2)	C1C—N1C—B1C—O1C	−94.4 (3)
C10B—C15B—C16B—N3B	−5.7 (2)	C8C—N1C—B1C—N5C	−137.1 (2)
C16B—N4B—C17B—N5B	−7.8 (3)	C1C—N1C—B1C—N5C	30.0 (3)
C16B—N4B—C17B—C18B	155.4 (2)	C8C—N1C—B1C—N3C	−30.3 (3)
C24B—N5B—C17B—N4B	154.7 (2)	C1C—N1C—B1C—N3C	136.90 (19)
B1B—N5B—C17B—N4B	−15.6 (3)	C16C—N3C—B1C—O1E	93.0 (3)
C24B—N5B—C17B—C18B	−12.0 (2)	C9C—N3C—B1C—O1E	−97.5 (3)
B1B—N5B—C17B—C18B	177.66 (19)	C16C—N3C—B1C—O1C	93.0 (3)
N4B—C17B—C18B—C19B	18.6 (4)	C9C—N3C—B1C—O1C	−97.5 (3)
N5B—C17B—C18B—C19B	−176.1 (2)	C16C—N3C—B1C—N5C	−32.4 (3)
N4B—C17B—C18B—C23B	−158.4 (2)	C9C—N3C—B1C—N5C	137.2 (2)
N5B—C17B—C18B—C23B	6.9 (2)	C16C—N3C—B1C—N1C	−139.87 (19)
C23B—C18B—C19B—C20B	−2.6 (3)	C9C—N3C—B1C—N1C	29.6 (3)
C17B—C18B—C19B—C20B	−179.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WB*···N6*A*	0.84	2.16	3.005 (8)	179
O1*W*—H1*WA*···N4*B*^{i}	0.84	2.20	3.043 (9)	179

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

(Phenolato)(subphthalocyaninato)boron (d2335_a)

Crystal data

$C_{30}H_{17}BN_6O$
M_r = 488.30
Triclinic, $P\overline{1}$
a = 10.0268 (10) Å
b = 10.7263 (12) Å
c = 11.8090 (13) Å
α = 85.879 (4)°
β = 77.440 (3)°
γ = 66.151 (3)°
V = 1133.6 (2) Å^3

Z = 2
F(000) = 504
D_x = 1.431 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 6094 reflections
θ = 2.3–27.2°
μ = 0.09 mm^{-1}
T = 150 K
Shard, pink
0.28 × 0.15 × 0.09 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: sealed tube with Bruker Triumph monochromator
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.687, T_{max} = 0.746

26461 measured reflections
5137 independent reflections
3795 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −12→11
k = −13→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.095$
$S = 1.03$
5137 reflections
343 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.1591P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.60836 (9)	0.58360 (9)	0.39809 (7)	0.0225 (2)
N1	0.82829 (12)	0.20316 (11)	0.37311 (9)	0.0217 (2)
N2	0.86304 (11)	0.41087 (11)	0.36391 (9)	0.0200 (2)
N3	0.99417 (12)	0.54932 (11)	0.28170 (10)	0.0229 (2)
N4	0.78717 (11)	0.55805 (10)	0.21103 (9)	0.0194 (2)
N5	0.66845 (11)	0.50195 (10)	0.08169 (9)	0.0216 (2)
N6	0.69756 (11)	0.38657 (10)	0.26052 (9)	0.0200 (2)
C1	0.89779 (14)	0.27856 (13)	0.39799 (11)	0.0209 (3)
C2	1.03999 (14)	0.23562 (13)	0.43385 (11)	0.0219 (3)
C3	1.13027 (15)	0.11419 (14)	0.47752 (11)	0.0249 (3)
H3A	1.097207	0.042659	0.498462	0.030*
C4	1.26953 (15)	0.10072 (14)	0.48954 (12)	0.0282 (3)
H4A	1.332206	0.018810	0.519985	0.034*
C5	1.32060 (15)	0.20416 (15)	0.45819 (12)	0.0301 (3)
H5A	1.417158	0.191245	0.467242	0.036*
C6	1.23264 (15)	0.32495 (14)	0.41420 (12)	0.0279 (3)
H6A	1.267864	0.394918	0.392013	0.033*
C7	1.09155 (14)	0.34156 (13)	0.40321 (11)	0.0222 (3)
C8	0.97963 (14)	0.44909 (13)	0.35198 (11)	0.0213 (3)
C9	0.90088 (14)	0.59754 (13)	0.20773 (11)	0.0216 (3)
C10	0.91289 (14)	0.66902 (13)	0.09880 (11)	0.0221 (3)
C11	1.00034 (14)	0.74072 (13)	0.05127 (12)	0.0266 (3)
H11A	1.069321	0.748820	0.091051	0.032*
C12	0.98350 (15)	0.79963 (14)	−0.05555 (13)	0.0295 (3)
H12A	1.038160	0.852913	−0.087655	0.035*
C13	0.88785 (15)	0.78252 (14)	−0.11731 (12)	0.0284 (3)
H13A	0.879883	0.823482	−0.190946	0.034*
C14	0.80442 (14)	0.70726 (13)	−0.07371 (12)	0.0250 (3)
H14A	0.742488	0.693035	−0.117405	0.030*

C15	0.81440 (14)	0.65294 (13)	0.03674 (11)	0.0217 (3)
C16	0.74174 (13)	0.57282 (12)	0.10831 (11)	0.0204 (3)
C17	0.65606 (13)	0.40411 (13)	0.15564 (11)	0.0206 (3)
C18	0.63636 (13)	0.28129 (13)	0.13500 (11)	0.0206 (3)
C19	0.59450 (14)	0.24229 (14)	0.04296 (12)	0.0244 (3)
H19A	0.563656	0.303407	−0.017647	0.029*
C20	0.59931 (15)	0.11185 (14)	0.04268 (12)	0.0273 (3)
H20A	0.568344	0.083898	−0.017991	0.033*
C21	0.64868 (15)	0.02013 (14)	0.12962 (12)	0.0258 (3)
H21A	0.650520	−0.068858	0.126791	0.031*
C22	0.69491 (14)	0.05581 (13)	0.21967 (12)	0.0230 (3)
H22A	0.731545	−0.008265	0.276977	0.028*
C23	0.68631 (13)	0.18853 (13)	0.22413 (11)	0.0208 (3)
C24	0.73460 (14)	0.25611 (13)	0.29959 (11)	0.0202 (3)
C25	0.48406 (14)	0.66715 (13)	0.35606 (11)	0.0213 (3)
C26	0.37130 (15)	0.62436 (15)	0.35710 (12)	0.0287 (3)
H26A	0.378545	0.538020	0.387713	0.034*
C27	0.24733 (16)	0.70750 (17)	0.31343 (13)	0.0359 (4)
H27A	0.170203	0.677554	0.313346	0.043*
C28	0.23567 (16)	0.83366 (17)	0.27007 (13)	0.0373 (4)
H28A	0.150759	0.890544	0.240092	0.045*
C29	0.34800 (16)	0.87679 (15)	0.27049 (13)	0.0330 (3)
H29A	0.339533	0.963989	0.241377	0.040*
C30	0.47267 (15)	0.79420 (14)	0.31288 (12)	0.0256 (3)
H30A	0.549959	0.824095	0.312488	0.031*
B1	0.72912 (16)	0.49125 (15)	0.31433 (13)	0.0202 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0238 (5)	0.0221 (5)	0.0209 (5)	−0.0078 (4)	−0.0059 (4)	0.0012 (4)
N1	0.0255 (6)	0.0218 (6)	0.0196 (6)	−0.0112 (5)	−0.0053 (5)	0.0021 (4)
N2	0.0231 (5)	0.0187 (6)	0.0196 (6)	−0.0091 (4)	−0.0061 (4)	0.0021 (4)
N3	0.0251 (6)	0.0196 (6)	0.0262 (6)	−0.0096 (5)	−0.0087 (5)	0.0019 (5)
N4	0.0204 (5)	0.0162 (5)	0.0212 (6)	−0.0066 (4)	−0.0053 (4)	0.0012 (4)
N5	0.0214 (5)	0.0176 (6)	0.0246 (6)	−0.0059 (4)	−0.0067 (4)	0.0023 (5)
N6	0.0212 (5)	0.0184 (5)	0.0208 (6)	−0.0079 (4)	−0.0059 (4)	0.0020 (4)
C1	0.0252 (6)	0.0190 (6)	0.0177 (7)	−0.0081 (5)	−0.0051 (5)	0.0026 (5)
C2	0.0263 (7)	0.0227 (7)	0.0167 (7)	−0.0090 (5)	−0.0058 (5)	−0.0007 (5)
C3	0.0315 (7)	0.0223 (7)	0.0208 (7)	−0.0091 (6)	−0.0092 (6)	0.0022 (5)
C4	0.0329 (7)	0.0247 (7)	0.0231 (7)	−0.0042 (6)	−0.0127 (6)	0.0016 (6)
C5	0.0261 (7)	0.0338 (8)	0.0303 (8)	−0.0078 (6)	−0.0135 (6)	−0.0014 (6)
C6	0.0294 (7)	0.0277 (8)	0.0309 (8)	−0.0130 (6)	−0.0122 (6)	0.0006 (6)
C7	0.0268 (7)	0.0214 (7)	0.0196 (7)	−0.0085 (5)	−0.0091 (5)	0.0001 (5)
C8	0.0234 (6)	0.0201 (7)	0.0220 (7)	−0.0093 (5)	−0.0063 (5)	−0.0017 (5)
C9	0.0219 (6)	0.0171 (6)	0.0257 (7)	−0.0080 (5)	−0.0039 (5)	−0.0012 (5)
C10	0.0203 (6)	0.0162 (6)	0.0257 (7)	−0.0045 (5)	−0.0026 (5)	0.0010 (5)
C11	0.0224 (6)	0.0216 (7)	0.0326 (8)	−0.0070 (5)	−0.0029 (6)	0.0017 (6)

C12	0.0249 (7)	0.0248 (7)	0.0329 (8)	−0.0090 (6)	0.0029 (6)	0.0053 (6)
C13	0.0287 (7)	0.0239 (7)	0.0235 (7)	−0.0052 (6)	0.0010 (6)	0.0045 (6)
C14	0.0243 (7)	0.0214 (7)	0.0235 (7)	−0.0044 (5)	−0.0027 (5)	0.0001 (5)
C15	0.0220 (6)	0.0154 (6)	0.0231 (7)	−0.0040 (5)	−0.0022 (5)	0.0007 (5)
C16	0.0194 (6)	0.0166 (6)	0.0215 (7)	−0.0035 (5)	−0.0047 (5)	0.0009 (5)
C17	0.0183 (6)	0.0204 (7)	0.0218 (7)	−0.0056 (5)	−0.0059 (5)	0.0003 (5)
C18	0.0177 (6)	0.0194 (7)	0.0245 (7)	−0.0072 (5)	−0.0045 (5)	0.0009 (5)
C19	0.0239 (7)	0.0240 (7)	0.0267 (7)	−0.0088 (6)	−0.0105 (6)	0.0032 (6)
C20	0.0286 (7)	0.0282 (7)	0.0286 (8)	−0.0125 (6)	−0.0097 (6)	−0.0029 (6)
C21	0.0280 (7)	0.0204 (7)	0.0306 (8)	−0.0112 (6)	−0.0056 (6)	−0.0012 (6)
C22	0.0248 (6)	0.0200 (7)	0.0245 (7)	−0.0098 (5)	−0.0046 (5)	0.0025 (5)
C23	0.0186 (6)	0.0216 (7)	0.0220 (7)	−0.0087 (5)	−0.0031 (5)	0.0020 (5)
C24	0.0211 (6)	0.0188 (6)	0.0204 (7)	−0.0085 (5)	−0.0030 (5)	0.0021 (5)
C25	0.0216 (6)	0.0229 (7)	0.0164 (6)	−0.0059 (5)	−0.0028 (5)	−0.0019 (5)
C26	0.0280 (7)	0.0329 (8)	0.0273 (8)	−0.0157 (6)	−0.0026 (6)	−0.0002 (6)
C27	0.0254 (7)	0.0519 (10)	0.0325 (9)	−0.0170 (7)	−0.0052 (6)	−0.0053 (7)
C28	0.0279 (7)	0.0438 (10)	0.0307 (8)	−0.0017 (7)	−0.0101 (6)	−0.0044 (7)
C29	0.0380 (8)	0.0249 (8)	0.0287 (8)	−0.0040 (6)	−0.0086 (6)	−0.0005 (6)
C30	0.0284 (7)	0.0225 (7)	0.0248 (7)	−0.0087 (6)	−0.0057 (6)	−0.0015 (6)
B1	0.0233 (7)	0.0177 (7)	0.0213 (8)	−0.0092 (6)	−0.0068 (6)	0.0025 (6)

Geometric parameters (Å, º)

O1—C25	1.3801 (15)	C11—C12	1.382 (2)
O1—B1	1.4407 (17)	C11—H11A	0.9500
N1—C1	1.3435 (17)	C12—C13	1.397 (2)
N1—C24	1.3459 (16)	C12—H12A	0.9500
N2—C8	1.3646 (16)	C13—C14	1.3840 (19)
N2—C1	1.3699 (16)	C13—H13A	0.9500
N2—B1	1.4907 (17)	C14—C15	1.3968 (18)
N3—C9	1.3434 (16)	C14—H14A	0.9500
N3—C8	1.3460 (17)	C15—C16	1.4553 (18)
N4—C9	1.3601 (16)	C17—C18	1.4531 (18)
N4—C16	1.3632 (16)	C18—C19	1.3922 (18)
N4—B1	1.4977 (18)	C18—C23	1.4229 (18)
N5—C16	1.3428 (16)	C19—C20	1.3806 (19)
N5—C17	1.3438 (16)	C19—H19A	0.9500
N6—C17	1.3673 (16)	C20—C21	1.3961 (19)
N6—C24	1.3677 (16)	C20—H20A	0.9500
N6—B1	1.4974 (18)	C21—C22	1.3815 (19)
C1—C2	1.4587 (18)	C21—H21A	0.9500
C2—C3	1.3910 (18)	C22—C23	1.3952 (18)
C2—C7	1.4227 (18)	C22—H22A	0.9500
C3—C4	1.3824 (19)	C23—C24	1.4553 (18)
C3—H3A	0.9500	C25—C26	1.3791 (19)
C4—C5	1.396 (2)	C25—C30	1.3892 (19)
C4—H4A	0.9500	C26—C27	1.387 (2)
C5—C6	1.3802 (19)	C26—H26A	0.9500

C5—H5A	0.9500	C27—C28	1.380 (2)
C6—C7	1.3866 (19)	C27—H27A	0.9500
C6—H6A	0.9500	C28—C29	1.381 (2)
C7—C8	1.4504 (18)	C28—H28A	0.9500
C9—C10	1.4569 (18)	C29—C30	1.3824 (19)
C10—C11	1.3945 (18)	C29—H29A	0.9500
C10—C15	1.4187 (19)	C30—H30A	0.9500

C25—O1—B1	115.60 (10)	C14—C15—C10	120.64 (12)
C1—N1—C24	117.24 (11)	C14—C15—C16	132.10 (12)
C8—N2—C1	112.86 (10)	C10—C15—C16	107.24 (11)
C8—N2—B1	122.15 (11)	N5—C16—N4	122.23 (11)
C1—N2—B1	123.00 (10)	N5—C16—C15	131.32 (12)
C9—N3—C8	116.66 (11)	N4—C16—C15	105.34 (11)
C9—N4—C16	113.67 (11)	N5—C17—N6	122.99 (11)
C9—N4—B1	122.62 (11)	N5—C17—C18	129.76 (12)
C16—N4—B1	123.41 (11)	N6—C17—C18	105.53 (11)
C16—N5—C17	116.65 (11)	C19—C18—C23	121.07 (12)
C17—N6—C24	113.19 (11)	C19—C18—C17	131.30 (12)
C17—N6—B1	122.71 (11)	C23—C18—C17	107.27 (11)
C24—N6—B1	122.97 (11)	C20—C19—C18	117.79 (12)
N1—C1—N2	122.77 (11)	C20—C19—H19A	121.1
N1—C1—C2	129.71 (12)	C18—C19—H19A	121.1
N2—C1—C2	105.62 (11)	C19—C20—C21	121.44 (13)
C3—C2—C7	120.10 (12)	C19—C20—H20A	119.3
C3—C2—C1	132.70 (12)	C21—C20—H20A	119.3
C7—C2—C1	106.84 (11)	C22—C21—C20	121.50 (13)
C4—C3—C2	118.01 (13)	C22—C21—H21A	119.2
C4—C3—H3A	121.0	C20—C21—H21A	119.2
C2—C3—H3A	121.0	C21—C22—C23	118.18 (12)
C3—C4—C5	121.81 (13)	C21—C22—H22A	120.9
C3—C4—H4A	119.1	C23—C22—H22A	120.9
C5—C4—H4A	119.1	C22—C23—C18	119.95 (12)
C6—C5—C4	120.86 (13)	C22—C23—C24	132.56 (12)
C6—C5—H5A	119.6	C18—C23—C24	107.14 (11)
C4—C5—H5A	119.6	N1—C24—N6	122.38 (11)
C5—C6—C7	118.30 (13)	N1—C24—C23	130.16 (12)
C5—C6—H6A	120.9	N6—C24—C23	105.55 (10)
C7—C6—H6A	120.9	C26—C25—O1	119.91 (12)
C6—C7—C2	120.90 (12)	C26—C25—C30	120.12 (12)
C6—C7—C8	131.41 (13)	O1—C25—C30	119.97 (11)
C2—C7—C8	107.37 (11)	C25—C26—C27	119.92 (14)
N3—C8—N2	123.34 (11)	C25—C26—H26A	120.0
N3—C8—C7	128.92 (12)	C27—C26—H26A	120.0
N2—C8—C7	105.94 (11)	C28—C27—C26	120.19 (14)
N3—C9—N4	122.13 (11)	C28—C27—H27A	119.9
N3—C9—C10	131.07 (11)	C26—C27—H27A	119.9
N4—C9—C10	105.36 (11)	C27—C28—C29	119.69 (14)

C11—C10—C15	120.64 (12)	C27—C28—H28A	120.2
C11—C10—C9	132.19 (12)	C29—C28—H28A	120.2
C15—C10—C9	107.16 (11)	C28—C29—C30	120.59 (14)
C12—C11—C10	117.91 (13)	C28—C29—H29A	119.7
C12—C11—H11A	121.0	C30—C29—H29A	119.7
C10—C11—H11A	121.0	C29—C30—C25	119.48 (13)
C11—C12—C13	121.42 (13)	C29—C30—H30A	120.3
C11—C12—H12A	119.3	C25—C30—H30A	120.3
C13—C12—H12A	119.3	O1—B1—N2	112.61 (11)
C14—C13—C12	121.53 (13)	O1—B1—N6	116.43 (11)
C14—C13—H13A	119.2	N2—B1—N6	104.58 (10)
C12—C13—H13A	119.2	O1—B1—N4	114.90 (11)
C13—C14—C15	117.72 (13)	N2—B1—N4	104.01 (10)
C13—C14—H14A	121.1	N6—B1—N4	102.89 (11)
C15—C14—H14A	121.1		

C24—N1—C1—N2	8.44 (18)	C16—N5—C17—N6	8.23 (17)
C24—N1—C1—C2	−153.51 (13)	C16—N5—C17—C18	−154.60 (13)
C8—N2—C1—N1	−153.46 (12)	C24—N6—C17—N5	−154.54 (12)
B1—N2—C1—N1	10.81 (19)	B1—N6—C17—N5	13.66 (18)
C8—N2—C1—C2	12.21 (14)	C24—N6—C17—C18	11.84 (14)
B1—N2—C1—C2	176.49 (11)	B1—N6—C17—C18	−179.96 (11)
N1—C1—C2—C3	−16.5 (2)	N5—C17—C18—C19	−15.1 (2)
N2—C1—C2—C3	179.24 (14)	N6—C17—C18—C19	179.80 (13)
N1—C1—C2—C7	156.39 (13)	N5—C17—C18—C23	157.89 (12)
N2—C1—C2—C7	−7.92 (14)	N6—C17—C18—C23	−7.22 (13)
C7—C2—C3—C4	−0.11 (19)	C23—C18—C19—C20	1.68 (19)
C1—C2—C3—C4	171.97 (13)	C17—C18—C19—C20	173.85 (13)
C2—C3—C4—C5	−0.6 (2)	C18—C19—C20—C21	−1.9 (2)
C3—C4—C5—C6	0.3 (2)	C19—C20—C21—C22	0.0 (2)
C4—C5—C6—C7	0.7 (2)	C20—C21—C22—C23	2.18 (19)
C5—C6—C7—C2	−1.5 (2)	C21—C22—C23—C18	−2.36 (19)
C5—C6—C7—C8	−174.04 (14)	C21—C22—C23—C24	−174.66 (13)
C3—C2—C7—C6	1.2 (2)	C19—C18—C23—C22	0.45 (19)
C1—C2—C7—C6	−172.74 (12)	C17—C18—C23—C22	−173.39 (11)
C3—C2—C7—C8	175.34 (12)	C19—C18—C23—C24	174.52 (11)
C1—C2—C7—C8	1.42 (14)	C17—C18—C23—C24	0.68 (14)
C9—N3—C8—N2	−10.55 (18)	C1—N1—C24—N6	−6.90 (18)
C9—N3—C8—C7	151.96 (13)	C1—N1—C24—C23	154.97 (13)
C1—N2—C8—N3	154.57 (12)	C17—N6—C24—N1	154.29 (12)
B1—N2—C8—N3	−9.85 (19)	B1—N6—C24—N1	−13.87 (19)
C1—N2—C8—C7	−11.36 (15)	C17—N6—C24—C23	−11.42 (14)
B1—N2—C8—C7	−175.78 (11)	B1—N6—C24—C23	−179.58 (11)
C6—C7—C8—N3	14.1 (2)	C22—C23—C24—N1	15.0 (2)
C2—C7—C8—N3	−159.22 (13)	C18—C23—C24—N1	−158.06 (13)
C6—C7—C8—N2	178.95 (14)	C22—C23—C24—N6	179.14 (13)
C2—C7—C8—N2	5.64 (14)	C18—C23—C24—N6	6.12 (13)
C8—N3—C9—N4	6.63 (18)	B1—O1—C25—C26	89.71 (15)

C8—N3—C9—C10	−157.56 (13)	B1—O1—C25—C30	−90.34 (14)
C16—N4—C9—N3	−156.21 (12)	O1—C25—C26—C27	−179.12 (12)
B1—N4—C9—N3	17.75 (18)	C30—C25—C26—C27	0.9 (2)
C16—N4—C9—C10	11.49 (14)	C25—C26—C27—C28	−0.7 (2)
B1—N4—C9—C10	−174.55 (11)	C26—C27—C28—C29	−0.1 (2)
N3—C9—C10—C11	−19.3 (2)	C27—C28—C29—C30	0.6 (2)
N4—C9—C10—C11	174.53 (13)	C28—C29—C30—C25	−0.4 (2)
N3—C9—C10—C15	159.29 (13)	C26—C25—C30—C29	−0.4 (2)
N4—C9—C10—C15	−6.87 (14)	O1—C25—C30—C29	179.69 (12)
C15—C10—C11—C12	2.48 (19)	C25—O1—B1—N2	176.22 (10)
C9—C10—C11—C12	−179.08 (13)	C25—O1—B1—N6	−63.00 (14)
C10—C11—C12—C13	−3.3 (2)	C25—O1—B1—N4	57.36 (15)
C11—C12—C13—C14	0.8 (2)	C8—N2—B1—O1	−96.40 (14)
C12—C13—C14—C15	2.46 (19)	C1—N2—B1—O1	100.76 (14)
C13—C14—C15—C10	−3.18 (18)	C8—N2—B1—N6	136.25 (12)
C13—C14—C15—C16	178.71 (13)	C1—N2—B1—N6	−26.59 (16)
C11—C10—C15—C14	0.75 (19)	C8—N2—B1—N4	28.64 (16)
C9—C10—C15—C14	−178.05 (11)	C1—N2—B1—N4	−134.20 (12)
C11—C10—C15—C16	179.28 (11)	C17—N6—B1—O1	96.10 (14)
C9—C10—C15—C16	0.48 (14)	C24—N6—B1—O1	−96.85 (14)
C17—N5—C16—N4	−7.18 (17)	C17—N6—B1—N2	−138.93 (11)
C17—N5—C16—C15	158.90 (13)	C24—N6—B1—N2	28.12 (15)
C9—N4—C16—N5	158.01 (11)	C17—N6—B1—N4	−30.50 (15)
B1—N4—C16—N5	−15.89 (18)	C24—N6—B1—N4	136.55 (11)
C9—N4—C16—C15	−11.20 (14)	C9—N4—B1—O1	90.86 (14)
B1—N4—C16—C15	174.90 (11)	C16—N4—B1—O1	−95.77 (14)
C14—C15—C16—N5	16.5 (2)	C9—N4—B1—N2	−32.70 (15)
C10—C15—C16—N5	−161.76 (13)	C16—N4—B1—N2	140.67 (11)
C14—C15—C16—N4	−175.64 (13)	C9—N4—B1—N6	−141.56 (11)
C10—C15—C16—N4	6.07 (13)	C16—N4—B1—N6	31.80 (15)

(Naphthalen-2-olato)(subphthalocyaninato)boron (d23108a_a)

Crystal data

$C_{34}H_{19}BN_6O$
M_r = 538.36
Orthorhombic, *Pnma*
a = 17.133 (3) Å
b = 13.929 (2) Å
c = 10.3669 (16) Å
V = 2474.0 (7) Å^3
Z = 4
$F(000)$ = 1112
D_x = 1.445 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2369 reflections
θ = 2.4–25.5°
μ = 0.09 mm^{-1}
T = 150 K
Shard, pink
0.26 × 0.15 × 0.08 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: sealed tube with Bruker Triumph monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.609, T_{max} = 0.746
17347 measured reflections
2963 independent reflections

1878 reflections with $I > 2\sigma(I)$
$R_{int} = 0.092$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -21 \rightarrow 22$
$k = -12 \rightarrow 18$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.119$
$S = 1.05$
2963 reflections
217 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 0.9945P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.59212 (11)	0.250000	0.05723 (17)	0.0314 (5)	
N1	0.57797 (12)	0.250000	0.2966 (2)	0.0192 (5)	
N2	0.59624 (9)	0.08455 (11)	0.34594 (14)	0.0225 (4)	
N3	0.68267 (9)	0.16555 (10)	0.20190 (14)	0.0206 (4)	
N4	0.80024 (13)	0.250000	0.1556 (2)	0.0235 (5)	
C1	0.43709 (11)	0.19995 (15)	0.66531 (18)	0.0280 (5)	
H1	0.411493	0.166663	0.733194	0.034*	
C2	0.47342 (10)	0.14803 (15)	0.56894 (18)	0.0252 (4)	
H2	0.473573	0.079829	0.569892	0.030*	
C3	0.50988 (10)	0.19921 (13)	0.47016 (17)	0.0204 (4)	
C4	0.55865 (11)	0.16829 (13)	0.36331 (17)	0.0206 (4)	
C5	0.66114 (11)	0.08664 (13)	0.27245 (17)	0.0210 (4)	
C6	0.72892 (11)	0.02434 (13)	0.27627 (17)	0.0233 (4)	
C7	0.74262 (12)	−0.06215 (14)	0.34004 (19)	0.0287 (5)	
H7A	0.701759	−0.094351	0.384388	0.034*	
C8	0.81729 (13)	−0.09982 (15)	0.3370 (2)	0.0335 (5)	
H8A	0.827620	−0.158970	0.379338	0.040*	
C9	0.87772 (13)	−0.05256 (16)	0.2730 (2)	0.0359 (5)	
H9A	0.928086	−0.081037	0.270487	0.043*	
C10	0.86578 (12)	0.03504 (15)	0.2129 (2)	0.0308 (5)	
H10A	0.907557	0.067706	0.171646	0.037*	
C11	0.79093 (11)	0.07398 (14)	0.21471 (18)	0.0249 (4)	
C12	0.76111 (11)	0.16782 (13)	0.17731 (16)	0.0223 (4)	
C13	0.45932 (13)	0.30777 (14)	0.0242 (2)	0.0255 (9)	0.5
H13	0.474810	0.373095	0.030414	0.031*	0.5
C14	0.51433 (10)	0.23520 (18)	0.03849 (18)	0.0211 (10)	0.5

C15	0.49167 (12)	0.13962 (16)	0.0294 (2)	0.0296 (10)	0.5
H15	0.529267	0.090016	0.039168	0.036*	0.5
C16	0.41400 (14)	0.11661 (13)	0.0060 (2)	0.0324 (10)	0.5
H16	0.398511	0.051288	−0.000158	0.039*	0.5
C17	0.35899 (10)	0.18919 (16)	−0.00823 (14)	0.0240 (11)	0.5
C18	0.38165 (11)	0.28477 (15)	0.00085 (13)	0.0221 (12)	0.5
C19	0.32664 (16)	0.35734 (19)	−0.0134 (2)	0.0326 (12)	0.5
H19	0.342132	0.422667	−0.007226	0.039*	0.5
C20	0.24897 (15)	0.3343 (3)	−0.0368 (2)	0.0317 (15)	0.5
H20	0.211375	0.383944	−0.046552	0.038*	0.5
C21	0.22631 (10)	0.2388 (3)	−0.04587 (19)	0.0407 (14)	0.5
H21	0.173223	0.223042	−0.061839	0.049*	0.5
C22	0.28132 (11)	0.1662 (2)	−0.0316 (2)	0.0388 (17)	0.5
H22	0.265826	0.100863	−0.037800	0.047*	0.5
B1	0.63003 (17)	0.250000	0.1813 (3)	0.0205 (7)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0203 (11)	0.0549 (13)	0.0189 (9)	0.000	0.0012 (8)	0.000
N1	0.0167 (12)	0.0221 (11)	0.0189 (11)	0.000	0.0000 (9)	0.000
N2	0.0212 (8)	0.0235 (9)	0.0227 (8)	−0.0005 (7)	0.0014 (7)	−0.0016 (7)
N3	0.0211 (9)	0.0222 (8)	0.0186 (8)	−0.0002 (7)	0.0031 (7)	−0.0005 (6)
N4	0.0249 (12)	0.0259 (12)	0.0196 (11)	0.000	0.0023 (10)	0.000
C1	0.0210 (10)	0.0447 (12)	0.0184 (9)	−0.0031 (9)	0.0023 (8)	0.0035 (9)
C2	0.0183 (10)	0.0331 (11)	0.0243 (10)	−0.0023 (9)	−0.0001 (8)	0.0046 (9)
C3	0.0148 (9)	0.0282 (10)	0.0183 (9)	−0.0010 (8)	−0.0008 (7)	0.0009 (7)
C4	0.0188 (10)	0.0225 (10)	0.0206 (9)	−0.0026 (8)	−0.0021 (8)	0.0010 (8)
C5	0.0246 (10)	0.0202 (9)	0.0182 (9)	−0.0017 (8)	−0.0008 (8)	−0.0023 (8)
C6	0.0270 (11)	0.0227 (10)	0.0202 (10)	0.0014 (8)	0.0026 (8)	−0.0030 (8)
C7	0.0356 (12)	0.0235 (10)	0.0269 (10)	0.0012 (9)	0.0030 (9)	−0.0004 (8)
C8	0.0435 (14)	0.0271 (11)	0.0298 (11)	0.0114 (10)	0.0003 (10)	0.0018 (9)
C9	0.0339 (13)	0.0426 (13)	0.0311 (12)	0.0160 (10)	0.0050 (10)	0.0018 (10)
C10	0.0264 (11)	0.0361 (12)	0.0299 (11)	0.0045 (9)	0.0060 (9)	0.0006 (9)
C11	0.0278 (11)	0.0278 (10)	0.0192 (9)	0.0040 (9)	0.0028 (9)	−0.0017 (8)
C12	0.0224 (11)	0.0282 (11)	0.0163 (9)	0.0014 (8)	0.0032 (8)	−0.0021 (7)
C13	0.031 (2)	0.022 (2)	0.023 (2)	−0.0020 (18)	−0.0011 (18)	−0.0026 (17)
C14	0.0255 (17)	0.024 (3)	0.0142 (14)	0.0002 (18)	0.0016 (12)	0.0006 (17)
C15	0.033 (3)	0.035 (3)	0.020 (2)	−0.001 (2)	−0.0028 (18)	0.0035 (19)
C16	0.045 (3)	0.028 (2)	0.025 (2)	−0.010 (2)	0.003 (2)	0.0016 (17)
C17	0.025 (3)	0.026 (3)	0.021 (2)	−0.018 (2)	0.0038 (19)	−0.0007 (19)
C18	0.022 (2)	0.027 (3)	0.0172 (19)	0.0052 (18)	0.0000 (17)	−0.0003 (14)
C19	0.024 (3)	0.049 (3)	0.025 (2)	−0.008 (3)	−0.002 (2)	−0.010 (2)
C20	0.034 (4)	0.044 (3)	0.018 (2)	0.006 (3)	0.0035 (19)	−0.008 (2)
C21	0.0253 (19)	0.074 (4)	0.0224 (16)	−0.030 (4)	0.0011 (14)	−0.008 (4)
C22	0.037 (5)	0.057 (4)	0.022 (3)	−0.012 (3)	0.007 (2)	−0.005 (3)
B1	0.0187 (16)	0.0232 (16)	0.0195 (15)	0.000	0.0022 (12)	0.000

Geometric parameters (Å, º)

O1—C14	1.362 (2)	C8—H8A	0.9500
O1—B1	1.441 (3)	C9—C10	1.385 (3)
N1—C4	1.372 (2)	C9—H9A	0.9500
N1—C4^{i}	1.372 (2)	C10—C11	1.393 (3)
N1—B1	1.491 (4)	C10—H10A	0.9500
N2—C4	1.345 (2)	C11—C12	1.456 (3)
N2—C5	1.348 (2)	C13—C14	1.3900
N3—C12	1.368 (2)	C13—C18	1.3900
N3—C5	1.371 (2)	C13—H13	0.9500
N3—B1	1.498 (2)	C14—C15	1.3900
N4—C12^{i}	1.345 (2)	C15—C16	1.3900
N4—C12	1.345 (2)	C15—H15	0.9500
C1—C2	1.382 (3)	C16—C17	1.3900
C1—C1^{i}	1.394 (4)	C16—H16	0.9500
C1—H1	0.9500	C17—C18	1.3900
C2—C3	1.395 (3)	C17—C22	1.3900
C2—H2	0.9500	C18—C19	1.3900
C3—C3^{i}	1.415 (4)	C19—C20	1.3900
C3—C4	1.453 (3)	C19—H19	0.9500
C5—C6	1.450 (3)	C20—C21	1.3900
C6—C7	1.394 (3)	C20—H20	0.9500
C6—C11	1.419 (3)	C21—C22	1.3900
C7—C8	1.383 (3)	C21—H21	0.9500
C7—H7A	0.9500	C22—H22	0.9500
C8—C9	1.395 (3)		

C14—O1—B1	124.61 (19)	C6—C11—C12	107.13 (16)
C4—N1—C4^{i}	112.1 (2)	N4—C12—N3	122.70 (17)
C4—N1—B1	123.23 (11)	N4—C12—C11	129.31 (18)
C4^{i}—N1—B1	123.24 (11)	N3—C12—C11	105.91 (16)
C4—N2—C5	116.88 (15)	C14—C13—C18	120.0
C12—N3—C5	112.48 (15)	C14—C13—H13	120.0
C12—N3—B1	123.15 (16)	C18—C13—H13	120.0
C5—N3—B1	122.93 (16)	O1—C14—C13	124.63 (16)
C12^{i}—N4—C12	116.6 (2)	O1—C14—C15	115.33 (16)
C2—C1—C1^{i}	121.57 (12)	C13—C14—C15	120.0
C2—C1—H1	119.2	C14—C15—C16	120.0
C1^{i}—C1—H1	119.2	C14—C15—H15	120.0
C1—C2—C3	117.70 (19)	C16—C15—H15	120.0
C1—C2—H2	121.1	C15—C16—C17	120.0
C3—C2—H2	121.1	C15—C16—H16	120.0
C2—C3—C3^{i}	120.73 (11)	C17—C16—H16	120.0
C2—C3—C4	131.72 (18)	C18—C17—C16	120.0
C3^{i}—C3—C4	107.25 (10)	C18—C17—C22	120.0
N2—C4—N1	122.45 (17)	C16—C17—C22	120.0
N2—C4—C3	129.41 (17)	C17—C18—C19	120.0

N1—C4—C3	106.08 (16)	C17—C18—C13	120.0
N2—C5—N3	122.73 (16)	C19—C18—C13	120.0
N2—C5—C6	129.21 (16)	C20—C19—C18	120.0
N3—C5—C6	106.19 (16)	C20—C19—H19	120.0
C7—C6—C11	120.55 (18)	C18—C19—H19	120.0
C7—C6—C5	131.67 (18)	C19—C20—C21	120.0
C11—C6—C5	107.19 (16)	C19—C20—H20	120.0
C8—C7—C6	118.21 (19)	C21—C20—H20	120.0
C8—C7—H7A	120.9	C20—C21—C22	120.0
C6—C7—H7A	120.9	C20—C21—H21	120.0
C7—C8—C9	121.21 (19)	C22—C21—H21	120.0
C7—C8—H8A	119.4	C21—C22—C17	120.0
C9—C8—H8A	119.4	C21—C22—H22	120.0
C10—C9—C8	121.34 (19)	C17—C22—H22	120.0
C10—C9—H9A	119.3	O1—B1—N1	116.5 (2)
C8—C9—H9A	119.3	O1—B1—N3^{i}	113.48 (15)
C9—C10—C11	118.25 (19)	N1—B1—N3^{i}	104.25 (15)
C9—C10—H10A	120.9	O1—B1—N3	113.48 (15)
C11—C10—H10A	120.9	N1—B1—N3	104.25 (15)
C10—C11—C6	120.37 (18)	N3^{i}—B1—N3	103.5 (2)
C10—C11—C12	132.01 (19)		

C1^{i}—C1—C2—C3	−0.5 (2)	C6—C11—C12—N4	156.1 (2)
C1—C2—C3—C3^{i}	0.5 (2)	C10—C11—C12—N3	−179.3 (2)
C1—C2—C3—C4	173.30 (19)	C6—C11—C12—N3	−7.52 (19)
C5—N2—C4—N1	8.7 (3)	B1—O1—C14—C13	96.59 (13)
C5—N2—C4—C3	−152.58 (18)	B1—O1—C14—C15	−85.63 (15)
C4^{i}—N1—C4—N2	−153.68 (13)	C18—C13—C14—O1	177.68 (17)
B1—N1—C4—N2	13.0 (3)	C18—C13—C14—C15	0.0
C4^{i}—N1—C4—C3	11.4 (3)	O1—C14—C15—C16	−177.89 (16)
B1—N1—C4—C3	178.0 (2)	C13—C14—C15—C16	0.0
C2—C3—C4—N2	−16.5 (3)	C14—C15—C16—C17	0.0
C3^{i}—C3—C4—N2	157.01 (17)	C15—C16—C17—C18	0.0
C2—C3—C4—N1	179.88 (19)	C15—C16—C17—C22	180.0
C3^{i}—C3—C4—N1	−6.62 (16)	C16—C17—C18—C19	180.0
C4—N2—C5—N3	−9.7 (3)	C22—C17—C18—C19	0.0
C4—N2—C5—C6	152.53 (18)	C16—C17—C18—C13	0.0
C12—N3—C5—N2	155.83 (17)	C22—C17—C18—C13	180.0
B1—N3—C5—N2	−10.9 (3)	C14—C13—C18—C17	0.0
C12—N3—C5—C6	−9.90 (19)	C14—C13—C18—C19	180.0
B1—N3—C5—C6	−176.59 (17)	C17—C18—C19—C20	0.0
N2—C5—C6—C7	11.1 (3)	C13—C18—C19—C20	180.0
N3—C5—C6—C7	175.57 (19)	C18—C19—C20—C21	0.0
N2—C5—C6—C11	−159.89 (18)	C19—C20—C21—C22	0.0
N3—C5—C6—C11	4.58 (19)	C20—C21—C22—C17	0.0
C11—C6—C7—C8	−2.6 (3)	C18—C17—C22—C21	0.0
C5—C6—C7—C8	−172.59 (19)	C16—C17—C22—C21	180.0
C6—C7—C8—C9	0.5 (3)	C14—O1—B1—N1	−10.60 (13)

C7—C8—C9—C10	1.7 (3)	C14—O1—B1—N3^{i}	−131.68 (19)
C8—C9—C10—C11	−1.8 (3)	C14—O1—B1—N3	110.5 (2)
C9—C10—C11—C6	−0.2 (3)	C4—N1—B1—O1	97.41 (19)
C9—C10—C11—C12	170.6 (2)	C4^{i}—N1—B1—O1	−97.41 (19)
C7—C6—C11—C10	2.5 (3)	C4—N1—B1—N3^{i}	−136.73 (18)
C5—C6—C11—C10	174.69 (17)	C4^{i}—N1—B1—N3^{i}	28.5 (3)
C7—C6—C11—C12	−170.40 (17)	C4—N1—B1—N3	−28.5 (3)
C5—C6—C11—C12	1.8 (2)	C4^{i}—N1—B1—N3	136.72 (18)
C12^{i}—N4—C12—N3	9.3 (3)	C12—N3—B1—O1	94.4 (2)
C12^{i}—N4—C12—C11	−151.92 (15)	C5—N3—B1—O1	−100.4 (2)
C5—N3—C12—N4	−154.01 (18)	C12—N3—B1—N1	−137.90 (17)
B1—N3—C12—N4	12.6 (3)	C5—N3—B1—N1	27.4 (2)
C5—N3—C12—C11	10.98 (19)	C12—N3—B1—N3^{i}	−29.1 (3)
B1—N3—C12—C11	177.64 (18)	C5—N3—B1—N3^{i}	136.18 (15)
C10—C11—C12—N4	−15.6 (3)		

Symmetry code: (i) x, $-y+1/2$, z.

(Acetato)(subphthalocyaninato)boron (d22121a_a)

Crystal data

$C_{26}H_{15}BN_6O_2$
$M_r = 454.25$
Triclinic, $P\overline{1}$
$a = 9.3432$ (9) Å
$b = 9.3548$ (7) Å
$c = 12.3322$ (12) Å
$\alpha = 104.203$ (2)°
$\beta = 100.751$ (3)°
$\gamma = 90.701$ (2)°
$V = 1024.69$ (16) Å^3
$Z = 2$
$F(000) = 468$
$D_x = 1.472$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6060 reflections
$\theta = 2.5$–$26.8°$
$\mu = 0.10$ mm^{-1}
$T = 150$ K
Shard, purple
0.24 × 0.22 × 0.13 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: sealed tube with Bruker Triumph monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.710$, $T_{max} = 0.746$
21123 measured reflections
4670 independent reflections
3665 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 11$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.096$
$S = 1.03$
4670 reflections
317 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.293P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.51457 (9)	0.16222 (10)	0.42428 (8)	0.0180 (2)
O2	0.33335 (11)	0.11501 (11)	0.27076 (8)	0.0266 (2)
N1	0.73832 (11)	0.31198 (12)	0.46314 (9)	0.0164 (2)
N2	0.90693 (12)	0.12760 (12)	0.42234 (9)	0.0181 (2)
N3	0.68811 (12)	0.13099 (12)	0.28825 (9)	0.0171 (2)
N4	0.55469 (12)	0.20043 (12)	0.12679 (9)	0.0185 (2)
N5	0.55739 (11)	0.34670 (11)	0.31392 (9)	0.0161 (2)
N6	0.64703 (12)	0.54978 (12)	0.47176 (9)	0.0175 (2)
C1	0.73959 (14)	0.45890 (14)	0.51425 (11)	0.0171 (3)
C2	0.87244 (14)	0.49059 (14)	0.60151 (11)	0.0178 (3)
C3	0.92841 (15)	0.61748 (15)	0.68630 (11)	0.0210 (3)
H3A	0.877122	0.705362	0.695344	0.025*
C4	1.06085 (15)	0.61146 (16)	0.75680 (12)	0.0232 (3)
H4A	1.099424	0.695948	0.816275	0.028*
C5	1.13944 (15)	0.48379 (16)	0.74260 (12)	0.0230 (3)
H5A	1.229956	0.483405	0.792646	0.028*
C6	1.08749 (14)	0.35795 (15)	0.65680 (11)	0.0202 (3)
H6A	1.142441	0.272578	0.646052	0.024*
C7	0.95253 (14)	0.36032 (14)	0.58689 (11)	0.0176 (3)
C8	0.86760 (14)	0.25015 (14)	0.49070 (11)	0.0172 (3)
C9	0.82094 (14)	0.07573 (14)	0.31928 (11)	0.0179 (3)
C10	0.85492 (14)	−0.01303 (14)	0.21341 (11)	0.0188 (3)
C11	0.96888 (15)	−0.10341 (15)	0.18993 (12)	0.0233 (3)
H11A	1.042170	−0.119308	0.249708	0.028*
C12	0.97183 (16)	−0.16921 (16)	0.07677 (13)	0.0285 (3)
H12A	1.046424	−0.234067	0.059297	0.034*
C13	0.86795 (16)	−0.14265 (16)	−0.01232 (13)	0.0280 (3)
H13A	0.873896	−0.188946	−0.088928	0.034*
C14	0.75651 (15)	−0.05006 (15)	0.00910 (12)	0.0220 (3)
H14A	0.688062	−0.029366	−0.051605	0.026*
C15	0.74784 (14)	0.01171 (14)	0.12215 (11)	0.0186 (3)
C16	0.64749 (14)	0.11331 (14)	0.17299 (11)	0.0177 (3)
C17	0.51454 (14)	0.31884 (14)	0.19836 (11)	0.0173 (3)
C18	0.45372 (14)	0.45407 (14)	0.17736 (11)	0.0187 (3)
C19	0.38252 (15)	0.48801 (16)	0.07794 (12)	0.0224 (3)
H19A	0.361657	0.414911	0.007488	0.027*
C20	0.34312 (17)	0.63161 (17)	0.08506 (13)	0.0283 (3)
H20A	0.294024	0.657104	0.018336	0.034*
C21	0.37395 (17)	0.73993 (17)	0.18817 (13)	0.0297 (3)

H21A	0.345795	0.837585	0.189952	0.036*
C22	0.44477 (15)	0.70809 (15)	0.28805 (12)	0.0241 (3)
H22A	0.465685	0.782615	0.357717	0.029*
C23	0.48448 (14)	0.56374 (14)	0.28350 (11)	0.0186 (3)
C24	0.56196 (14)	0.49317 (14)	0.36891 (11)	0.0171 (3)
C25	0.37765 (14)	0.11811 (14)	0.37020 (11)	0.0181 (3)
C26	0.28623 (15)	0.07167 (16)	0.44437 (13)	0.0241 (3)
H26A	0.183080	0.082274	0.414825	0.036*
H26B	0.314413	0.134049	0.522317	0.036*
H26C	0.301221	−0.031754	0.444617	0.036*
B1	0.61638 (15)	0.23270 (16)	0.37237 (12)	0.0162 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0147 (4)	0.0206 (5)	0.0201 (5)	0.0018 (4)	0.0038 (4)	0.0073 (4)
O2	0.0264 (5)	0.0315 (5)	0.0198 (5)	−0.0057 (4)	0.0001 (4)	0.0064 (4)
N1	0.0158 (5)	0.0186 (5)	0.0159 (5)	0.0029 (4)	0.0041 (4)	0.0053 (4)
N2	0.0183 (5)	0.0189 (5)	0.0182 (6)	0.0025 (4)	0.0041 (4)	0.0063 (4)
N3	0.0152 (5)	0.0180 (5)	0.0181 (6)	0.0017 (4)	0.0029 (4)	0.0048 (4)
N4	0.0157 (5)	0.0204 (6)	0.0191 (6)	0.0010 (4)	0.0030 (4)	0.0046 (4)
N5	0.0143 (5)	0.0180 (5)	0.0159 (5)	0.0014 (4)	0.0029 (4)	0.0042 (4)
N6	0.0163 (5)	0.0206 (6)	0.0165 (6)	0.0031 (4)	0.0048 (4)	0.0049 (4)
C1	0.0172 (6)	0.0190 (6)	0.0166 (6)	0.0014 (5)	0.0061 (5)	0.0049 (5)
C2	0.0158 (6)	0.0230 (7)	0.0165 (6)	0.0014 (5)	0.0047 (5)	0.0075 (5)
C3	0.0227 (7)	0.0209 (7)	0.0198 (7)	0.0010 (5)	0.0051 (5)	0.0049 (5)
C4	0.0228 (7)	0.0247 (7)	0.0198 (7)	−0.0035 (5)	0.0028 (6)	0.0025 (6)
C5	0.0159 (6)	0.0326 (8)	0.0201 (7)	−0.0009 (5)	0.0009 (5)	0.0076 (6)
C6	0.0166 (6)	0.0257 (7)	0.0196 (7)	0.0035 (5)	0.0043 (5)	0.0077 (5)
C7	0.0170 (6)	0.0220 (6)	0.0159 (6)	0.0009 (5)	0.0058 (5)	0.0067 (5)
C8	0.0158 (6)	0.0198 (6)	0.0179 (6)	0.0020 (5)	0.0039 (5)	0.0080 (5)
C9	0.0168 (6)	0.0179 (6)	0.0209 (7)	0.0024 (5)	0.0052 (5)	0.0073 (5)
C10	0.0188 (6)	0.0167 (6)	0.0205 (7)	−0.0003 (5)	0.0043 (5)	0.0038 (5)
C11	0.0207 (7)	0.0222 (7)	0.0261 (7)	0.0036 (5)	0.0048 (6)	0.0040 (6)
C12	0.0235 (7)	0.0284 (8)	0.0311 (8)	0.0065 (6)	0.0090 (6)	−0.0001 (6)
C13	0.0281 (8)	0.0294 (8)	0.0229 (7)	0.0013 (6)	0.0084 (6)	−0.0029 (6)
C14	0.0212 (7)	0.0228 (7)	0.0195 (7)	−0.0020 (5)	0.0033 (5)	0.0014 (5)
C15	0.0174 (6)	0.0175 (6)	0.0200 (7)	−0.0013 (5)	0.0037 (5)	0.0032 (5)
C16	0.0161 (6)	0.0194 (6)	0.0164 (6)	−0.0017 (5)	0.0017 (5)	0.0033 (5)
C17	0.0137 (6)	0.0212 (6)	0.0172 (6)	0.0000 (5)	0.0022 (5)	0.0060 (5)
C18	0.0150 (6)	0.0226 (7)	0.0196 (7)	0.0030 (5)	0.0047 (5)	0.0064 (5)
C19	0.0215 (7)	0.0277 (7)	0.0180 (7)	0.0050 (6)	0.0035 (5)	0.0060 (6)
C20	0.0308 (8)	0.0338 (8)	0.0224 (7)	0.0124 (6)	0.0034 (6)	0.0121 (6)
C21	0.0364 (9)	0.0261 (8)	0.0282 (8)	0.0129 (6)	0.0046 (7)	0.0105 (6)
C22	0.0264 (7)	0.0230 (7)	0.0221 (7)	0.0057 (6)	0.0044 (6)	0.0043 (6)
C23	0.0152 (6)	0.0234 (7)	0.0186 (7)	0.0038 (5)	0.0044 (5)	0.0066 (5)
C24	0.0156 (6)	0.0190 (6)	0.0185 (6)	0.0031 (5)	0.0065 (5)	0.0058 (5)
C25	0.0172 (6)	0.0147 (6)	0.0217 (7)	0.0024 (5)	0.0033 (5)	0.0033 (5)

C26	0.0189 (7)	0.0282 (7)	0.0267 (8)	0.0004 (5)	0.0048 (6)	0.0098 (6)
B1	0.0148 (7)	0.0183 (7)	0.0158 (7)	0.0021 (5)	0.0031 (6)	0.0046 (6)

Geometric parameters (Å, º)

O1—C25	1.3362 (15)	C7—C8	1.4587 (18)
O1—B1	1.4725 (17)	C9—C10	1.4573 (18)
O2—C25	1.2120 (16)	C10—C11	1.3962 (18)
N1—C1	1.3631 (17)	C10—C15	1.4264 (19)
N1—C8	1.3673 (16)	C11—C12	1.386 (2)
N1—B1	1.4823 (18)	C11—H11A	0.9500
N2—C9	1.3428 (17)	C12—C13	1.397 (2)
N2—C8	1.3460 (17)	C12—H12A	0.9500
N3—C16	1.3689 (17)	C13—C14	1.384 (2)
N3—C9	1.3746 (16)	C13—H13A	0.9500
N3—B1	1.4904 (17)	C14—C15	1.3900 (19)
N4—C17	1.3419 (17)	C14—H14A	0.9500
N4—C16	1.3421 (17)	C15—C16	1.4574 (18)
N5—C17	1.3644 (17)	C17—C18	1.4539 (18)
N5—C24	1.3678 (17)	C18—C19	1.3923 (18)
N5—B1	1.4846 (17)	C18—C23	1.4290 (19)
N6—C24	1.3435 (17)	C19—C20	1.384 (2)
N6—C1	1.3465 (17)	C19—H19A	0.9500
C1—C2	1.4569 (18)	C20—C21	1.397 (2)
C2—C3	1.3956 (19)	C20—H20A	0.9500
C2—C7	1.4292 (18)	C21—C22	1.387 (2)
C3—C4	1.3837 (19)	C21—H21A	0.9500
C3—H3A	0.9500	C22—C23	1.3954 (19)
C4—C5	1.401 (2)	C22—H22A	0.9500
C4—H4A	0.9500	C23—C24	1.4621 (18)
C5—C6	1.387 (2)	C25—C26	1.4941 (19)
C5—H5A	0.9500	C26—H26A	0.9800
C6—C7	1.3922 (18)	C26—H26B	0.9800
C6—H6A	0.9500	C26—H26C	0.9800
C25—O1—B1	121.85 (10)	C14—C13—H13A	119.4
C1—N1—C8	113.88 (11)	C12—C13—H13A	119.4
C1—N1—B1	122.67 (11)	C13—C14—C15	117.97 (13)
C8—N1—B1	122.78 (11)	C13—C14—H14A	121.0
C9—N2—C8	117.21 (11)	C15—C14—H14A	121.0
C16—N3—C9	113.09 (11)	C14—C15—C10	121.07 (12)
C16—N3—B1	122.79 (11)	C14—C15—C16	131.64 (13)
C9—N3—B1	122.33 (11)	C10—C15—C16	107.17 (11)
C17—N4—C16	117.15 (11)	N4—C16—N3	122.87 (12)
C17—N5—C24	113.67 (11)	N4—C16—C15	130.06 (12)
C17—N5—B1	122.88 (11)	N3—C16—C15	105.63 (11)
C24—N5—B1	122.73 (11)	N4—C17—N5	122.44 (11)
C24—N6—C1	116.91 (11)	N4—C17—C18	130.67 (12)

N6—C1—N1	122.65 (12)	N5—C17—C18	105.39 (11)
N6—C1—C2	130.98 (12)	C19—C18—C23	121.12 (12)
N1—C1—C2	105.26 (11)	C19—C18—C17	131.76 (12)
C3—C2—C7	120.43 (12)	C23—C18—C17	107.07 (11)
C3—C2—C1	132.35 (12)	C20—C19—C18	117.86 (13)
C7—C2—C1	107.20 (11)	C20—C19—H19A	121.1
C4—C3—C2	118.01 (13)	C18—C19—H19A	121.1
C4—C3—H3A	121.0	C19—C20—C21	121.45 (13)
C2—C3—H3A	121.0	C19—C20—H20A	119.3
C3—C4—C5	121.61 (13)	C21—C20—H20A	119.3
C3—C4—H4A	119.2	C22—C21—C20	121.47 (13)
C5—C4—H4A	119.2	C22—C21—H21A	119.3
C6—C5—C4	121.19 (13)	C20—C21—H21A	119.3
C6—C5—H5A	119.4	C21—C22—C23	118.26 (13)
C4—C5—H5A	119.4	C21—C22—H22A	120.9
C5—C6—C7	118.11 (12)	C23—C22—H22A	120.9
C5—C6—H6A	120.9	C22—C23—C18	119.83 (12)
C7—C6—H6A	120.9	C22—C23—C24	132.97 (13)
C6—C7—C2	120.60 (12)	C18—C23—C24	107.15 (11)
C6—C7—C8	132.30 (12)	N6—C24—N5	122.26 (11)
C2—C7—C8	107.08 (11)	N6—C24—C23	131.61 (12)
N2—C8—N1	122.27 (12)	N5—C24—C23	104.94 (11)
N2—C8—C7	131.19 (12)	O2—C25—O1	123.07 (12)
N1—C8—C7	105.13 (11)	O2—C25—C26	123.79 (12)
N2—C9—N3	122.59 (12)	O1—C25—C26	113.13 (11)
N2—C9—C10	130.32 (12)	C25—C26—H26A	109.5
N3—C9—C10	105.35 (11)	C25—C26—H26B	109.5
C11—C10—C15	120.00 (12)	H26A—C26—H26B	109.5
C11—C10—C9	132.66 (12)	C25—C26—H26C	109.5
C15—C10—C9	107.25 (11)	H26A—C26—H26C	109.5
C12—C11—C10	117.98 (13)	H26B—C26—H26C	109.5
C12—C11—H11A	121.0	O1—B1—N1	109.01 (11)
C10—C11—H11A	121.0	O1—B1—N5	116.59 (11)
C11—C12—C13	121.72 (13)	N1—B1—N5	104.40 (10)
C11—C12—H12A	119.1	O1—B1—N3	116.01 (11)
C13—C12—H12A	119.1	N1—B1—N3	104.83 (10)
C14—C13—C12	121.15 (13)	N5—B1—N3	104.79 (11)

C24—N6—C1—N1	−6.98 (18)	C14—C15—C16—N4	−16.1 (2)
C24—N6—C1—C2	159.13 (13)	C10—C15—C16—N4	159.94 (13)
C8—N1—C1—N6	156.87 (12)	C14—C15—C16—N3	177.61 (14)
B1—N1—C1—N6	−13.95 (19)	C10—C15—C16—N3	−6.33 (14)
C8—N1—C1—C2	−12.30 (14)	C16—N4—C17—N5	−4.05 (18)
B1—N1—C1—C2	176.88 (11)	C16—N4—C17—C18	159.85 (13)
N6—C1—C2—C3	17.4 (2)	C24—N5—C17—N4	153.53 (12)
N1—C1—C2—C3	−174.73 (14)	B1—N5—C17—N4	−17.04 (19)
N6—C1—C2—C7	−160.90 (13)	C24—N5—C17—C18	−13.86 (14)
N1—C1—C2—C7	7.01 (14)	B1—N5—C17—C18	175.56 (11)

C7—C2—C3—C4	−1.65 (19)	N4—C17—C18—C19	20.0 (2)
C1—C2—C3—C4	−179.73 (13)	N5—C17—C18—C19	−174.03 (14)
C2—C3—C4—C5	1.6 (2)	N4—C17—C18—C23	−157.47 (13)
C3—C4—C5—C6	0.1 (2)	N5—C17—C18—C23	8.48 (14)
C4—C5—C6—C7	−1.9 (2)	C23—C18—C19—C20	0.3 (2)
C5—C6—C7—C2	1.80 (19)	C17—C18—C19—C20	−176.87 (14)
C5—C6—C7—C8	179.83 (13)	C18—C19—C20—C21	0.3 (2)
C3—C2—C7—C6	−0.06 (19)	C19—C20—C21—C22	−0.3 (2)
C1—C2—C7—C6	178.45 (12)	C20—C21—C22—C23	−0.3 (2)
C3—C2—C7—C8	−178.53 (12)	C21—C22—C23—C18	0.9 (2)
C1—C2—C7—C8	−0.02 (14)	C21—C22—C23—C24	178.05 (14)
C9—N2—C8—N1	6.77 (18)	C19—C18—C23—C22	−0.9 (2)
C9—N2—C8—C7	−157.61 (13)	C17—C18—C23—C22	176.87 (12)
C1—N1—C8—N2	−155.60 (12)	C19—C18—C23—C24	−178.75 (12)
B1—N1—C8—N2	15.20 (19)	C17—C18—C23—C24	−0.94 (14)
C1—N1—C8—C7	12.28 (14)	C1—N6—C24—N5	6.48 (18)
B1—N1—C8—C7	−176.91 (11)	C1—N6—C24—C23	−159.10 (13)
C6—C7—C8—N2	−18.8 (2)	C17—N5—C24—N6	−155.67 (12)
C2—C7—C8—N2	159.41 (13)	B1—N5—C24—N6	14.92 (19)
C6—C7—C8—N1	174.83 (13)	C17—N5—C24—C23	13.22 (14)
C2—C7—C8—N1	−6.95 (13)	B1—N5—C24—C23	−176.19 (11)
C8—N2—C9—N3	−8.47 (18)	C22—C23—C24—N6	−16.9 (2)
C8—N2—C9—C10	154.20 (13)	C18—C23—C24—N6	160.49 (13)
C16—N3—C9—N2	153.58 (12)	C22—C23—C24—N5	175.67 (14)
B1—N3—C9—N2	−11.54 (19)	C18—C23—C24—N5	−6.92 (14)
C16—N3—C9—C10	−12.79 (14)	B1—O1—C25—O2	9.79 (18)
B1—N3—C9—C10	−177.91 (11)	B1—O1—C25—C26	−170.89 (11)
N2—C9—C10—C11	19.6 (2)	C25—O1—B1—N1	161.53 (10)
N3—C9—C10—C11	−175.47 (14)	C25—O1—B1—N5	43.71 (16)
N2—C9—C10—C15	−156.92 (13)	C25—O1—B1—N3	−80.48 (14)
N3—C9—C10—C15	8.00 (14)	C1—N1—B1—O1	−95.33 (13)
C15—C10—C11—C12	−1.3 (2)	C8—N1—B1—O1	94.66 (13)
C9—C10—C11—C12	−177.50 (14)	C1—N1—B1—N5	29.92 (16)
C10—C11—C12—C13	2.4 (2)	C8—N1—B1—N5	−140.08 (12)
C11—C12—C13—C14	−0.6 (2)	C1—N1—B1—N3	139.84 (12)
C12—C13—C14—C15	−2.3 (2)	C8—N1—B1—N3	−30.16 (15)
C13—C14—C15—C10	3.3 (2)	C17—N5—B1—O1	−100.40 (14)
C13—C14—C15—C16	178.92 (14)	C24—N5—B1—O1	89.87 (15)
C11—C10—C15—C14	−1.5 (2)	C17—N5—B1—N1	139.29 (12)
C9—C10—C15—C14	175.51 (12)	C24—N5—B1—N1	−30.43 (15)
C11—C10—C15—C16	−178.11 (12)	C17—N5—B1—N3	29.34 (16)
C9—C10—C15—C16	−1.05 (14)	C24—N5—B1—N3	−140.38 (11)
C17—N4—C16—N3	7.59 (18)	C16—N3—B1—O1	104.34 (14)
C17—N4—C16—C15	−156.62 (13)	C9—N3—B1—O1	−91.99 (14)
C9—N3—C16—N4	−155.35 (12)	C16—N3—B1—N1	−135.39 (12)
B1—N3—C16—N4	9.69 (19)	C9—N3—B1—N1	28.29 (15)
C9—N3—C16—C15	12.16 (14)	C16—N3—B1—N5	−25.75 (16)
B1—N3—C16—C15	177.20 (11)	C9—N3—B1—N5	137.92 (12)

(Benzoato)(subphthalocyaninato)boron (d22123a_a)

Crystal data

$C_{31}H_{17}BN_6O_2$
$M_r = 516.31$
Monoclinic, $P2_1/c$
$a = 15.671$ (2) Å
$b = 11.1920$ (13) Å
$c = 15.2363$ (19) Å
$\beta = 115.386$ (4)°
$V = 2414.3$ (5) Å^3
$Z = 4$
$F(000) = 1064$
$D_x = 1.420$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7016 reflections
$\theta = 2.4$–$26.5°$
$\mu = 0.09$ mm^{-1}
$T = 150$ K
Shard, purple
0.30 × 0.15 × 0.12 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: sealed tube with Bruker Triumph monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.685$, $T_{max} = 0.746$
49333 measured reflections
5530 independent reflections
4050 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -20 \rightarrow 19$
$k = -14 \rightarrow 14$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.095$
$S = 1.03$
5530 reflections
361 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.5643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.23861 (7)	0.35273 (8)	0.50040 (7)	0.0209 (2)
O2	0.37184 (7)	0.41722 (9)	0.62313 (7)	0.0277 (2)
N1	0.36297 (8)	0.20804 (10)	0.49803 (8)	0.0187 (3)
N2	0.46030 (8)	0.17010 (10)	0.66567 (8)	0.0197 (3)
N3	0.29257 (8)	0.17210 (10)	0.60497 (8)	0.0185 (2)
N4	0.14395 (8)	0.07323 (10)	0.54412 (8)	0.0207 (3)
N5	0.20195 (8)	0.15311 (10)	0.43511 (8)	0.0183 (3)
N6	0.28428 (8)	0.13708 (10)	0.33543 (8)	0.0204 (3)
C1	0.36234 (10)	0.17422 (12)	0.41122 (9)	0.0192 (3)

C2	0.46093 (10)	0.15779 (12)	0.43022 (10)	0.0200 (3)
C3	0.50344 (10)	0.12818 (13)	0.36951 (10)	0.0232 (3)
H3A	0.467163	0.118337	0.301563	0.028*
C4	0.60064 (11)	0.11359 (13)	0.41186 (11)	0.0255 (3)
H4A	0.631602	0.096427	0.371656	0.031*
C5	0.65433 (10)	0.12346 (13)	0.51222 (11)	0.0265 (3)
H5A	0.720884	0.113456	0.538597	0.032*
C6	0.61234 (10)	0.14755 (13)	0.57398 (11)	0.0232 (3)
H6A	0.648565	0.150503	0.642391	0.028*
C7	0.51517 (10)	0.16730 (12)	0.53225 (10)	0.0202 (3)
C8	0.44935 (10)	0.18976 (12)	0.57478 (10)	0.0195 (3)
C9	0.38098 (10)	0.15422 (12)	0.67778 (9)	0.0192 (3)
C10	0.36703 (10)	0.08998 (12)	0.75356 (10)	0.0197 (3)
C11	0.43129 (10)	0.04217 (13)	0.84154 (10)	0.0232 (3)
H11A	0.496991	0.058001	0.865532	0.028*
C12	0.39635 (11)	−0.02920 (14)	0.89293 (10)	0.0264 (3)
H12A	0.438988	−0.062705	0.953114	0.032*
C13	0.29967 (11)	−0.05309 (13)	0.85826 (10)	0.0258 (3)
H13A	0.277954	−0.100885	0.896093	0.031*
C14	0.23526 (10)	−0.00862 (13)	0.77021 (10)	0.0226 (3)
H14A	0.169858	−0.026252	0.746470	0.027*
C15	0.26911 (10)	0.06298 (12)	0.71715 (9)	0.0199 (3)
C16	0.22426 (10)	0.10886 (12)	0.61832 (10)	0.0192 (3)
C17	0.13748 (9)	0.08822 (12)	0.45387 (10)	0.0192 (3)
C18	0.08486 (10)	0.01871 (13)	0.36687 (10)	0.0209 (3)
C19	0.01279 (10)	−0.06518 (13)	0.34499 (11)	0.0250 (3)
H19A	−0.016278	−0.077976	0.387578	0.030*
C20	−0.01502 (11)	−0.12889 (14)	0.25987 (11)	0.0299 (4)
H20A	−0.064764	−0.185408	0.243152	0.036*
C21	0.02850 (11)	−0.11216 (15)	0.19734 (11)	0.0298 (4)
H21A	0.008053	−0.158124	0.139473	0.036*
C22	0.10047 (10)	−0.03027 (14)	0.21811 (10)	0.0256 (3)
H22A	0.130006	−0.019926	0.175671	0.031*
C23	0.12866 (9)	0.03695 (13)	0.30318 (10)	0.0207 (3)
C24	0.20710 (10)	0.11861 (12)	0.35138 (9)	0.0192 (3)
C25	0.29049 (10)	0.43418 (13)	0.56571 (10)	0.0206 (3)
C26	0.23874 (10)	0.54689 (12)	0.56255 (10)	0.0224 (3)
C27	0.14812 (11)	0.56741 (14)	0.49178 (11)	0.0305 (4)
H27A	0.117876	0.509561	0.442499	0.037*
C28	0.10142 (13)	0.67269 (15)	0.49288 (13)	0.0388 (4)
H28A	0.039559	0.687250	0.443944	0.047*
C29	0.14523 (14)	0.75613 (15)	0.56536 (13)	0.0396 (4)
H29A	0.113295	0.827864	0.566469	0.048*
C30	0.23529 (13)	0.73522 (14)	0.63603 (12)	0.0350 (4)
H30A	0.264859	0.792507	0.685975	0.042*
C31	0.28302 (12)	0.63147 (14)	0.63486 (11)	0.0280 (3)
H31A	0.345463	0.618190	0.683025	0.034*
B1	0.27495 (11)	0.22967 (14)	0.51035 (11)	0.0189 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0230 (5)	0.0174 (5)	0.0202 (5)	0.0011 (4)	0.0072 (4)	−0.0009 (4)
O2	0.0232 (6)	0.0271 (6)	0.0286 (5)	−0.0011 (4)	0.0073 (5)	−0.0031 (4)
N1	0.0193 (6)	0.0184 (6)	0.0180 (6)	−0.0005 (5)	0.0077 (5)	0.0003 (5)
N2	0.0206 (6)	0.0190 (6)	0.0195 (6)	−0.0012 (5)	0.0086 (5)	−0.0014 (5)
N3	0.0187 (6)	0.0188 (6)	0.0180 (6)	0.0013 (5)	0.0079 (5)	−0.0006 (5)
N4	0.0190 (6)	0.0236 (6)	0.0198 (6)	0.0020 (5)	0.0087 (5)	−0.0004 (5)
N5	0.0181 (6)	0.0189 (6)	0.0179 (6)	0.0014 (5)	0.0078 (5)	0.0011 (5)
N6	0.0209 (6)	0.0213 (6)	0.0184 (6)	0.0001 (5)	0.0078 (5)	0.0025 (5)
C1	0.0250 (8)	0.0165 (7)	0.0176 (7)	−0.0001 (5)	0.0103 (6)	0.0018 (5)
C2	0.0228 (7)	0.0154 (7)	0.0232 (7)	−0.0018 (5)	0.0111 (6)	0.0012 (6)
C3	0.0289 (8)	0.0196 (7)	0.0237 (7)	−0.0025 (6)	0.0137 (6)	−0.0001 (6)
C4	0.0291 (8)	0.0215 (8)	0.0325 (8)	−0.0010 (6)	0.0195 (7)	−0.0016 (6)
C5	0.0216 (8)	0.0227 (8)	0.0362 (8)	0.0005 (6)	0.0135 (7)	0.0006 (6)
C6	0.0221 (8)	0.0215 (8)	0.0254 (7)	−0.0009 (6)	0.0097 (6)	0.0007 (6)
C7	0.0221 (7)	0.0163 (7)	0.0234 (7)	−0.0010 (5)	0.0108 (6)	0.0008 (6)
C8	0.0191 (7)	0.0167 (7)	0.0210 (7)	−0.0011 (5)	0.0070 (6)	−0.0009 (5)
C9	0.0213 (7)	0.0171 (7)	0.0171 (6)	0.0001 (5)	0.0062 (6)	−0.0030 (5)
C10	0.0224 (7)	0.0190 (7)	0.0190 (6)	0.0023 (6)	0.0101 (6)	−0.0026 (6)
C11	0.0247 (8)	0.0248 (8)	0.0182 (7)	0.0021 (6)	0.0073 (6)	−0.0028 (6)
C12	0.0325 (9)	0.0262 (8)	0.0192 (7)	0.0042 (6)	0.0099 (6)	0.0023 (6)
C13	0.0369 (9)	0.0237 (8)	0.0218 (7)	0.0012 (6)	0.0172 (7)	0.0008 (6)
C14	0.0250 (8)	0.0233 (8)	0.0229 (7)	0.0019 (6)	0.0135 (6)	−0.0019 (6)
C15	0.0238 (7)	0.0190 (7)	0.0186 (6)	0.0035 (6)	0.0107 (6)	−0.0020 (5)
C16	0.0208 (7)	0.0192 (7)	0.0205 (7)	0.0015 (6)	0.0117 (6)	−0.0013 (6)
C17	0.0168 (7)	0.0198 (7)	0.0209 (7)	0.0025 (5)	0.0081 (6)	0.0001 (6)
C18	0.0174 (7)	0.0232 (8)	0.0198 (7)	0.0039 (6)	0.0058 (6)	0.0010 (6)
C19	0.0187 (7)	0.0286 (8)	0.0258 (7)	−0.0003 (6)	0.0078 (6)	0.0004 (6)
C20	0.0215 (8)	0.0310 (9)	0.0316 (8)	−0.0045 (6)	0.0062 (7)	−0.0053 (7)
C21	0.0255 (8)	0.0334 (9)	0.0254 (7)	−0.0014 (7)	0.0062 (7)	−0.0095 (7)
C22	0.0219 (8)	0.0321 (9)	0.0205 (7)	0.0019 (6)	0.0070 (6)	−0.0026 (6)
C23	0.0172 (7)	0.0226 (7)	0.0197 (7)	0.0040 (5)	0.0053 (6)	0.0014 (6)
C24	0.0207 (7)	0.0193 (7)	0.0164 (6)	0.0028 (5)	0.0069 (6)	0.0017 (5)
C25	0.0247 (8)	0.0215 (7)	0.0185 (7)	−0.0029 (6)	0.0120 (6)	0.0012 (5)
C26	0.0309 (8)	0.0186 (7)	0.0231 (7)	−0.0004 (6)	0.0165 (6)	0.0010 (6)
C27	0.0379 (9)	0.0253 (8)	0.0272 (8)	0.0054 (7)	0.0129 (7)	0.0011 (6)
C28	0.0466 (11)	0.0305 (9)	0.0390 (9)	0.0142 (8)	0.0179 (8)	0.0069 (8)
C29	0.0607 (12)	0.0217 (9)	0.0521 (11)	0.0098 (8)	0.0390 (10)	0.0054 (8)
C30	0.0509 (11)	0.0238 (8)	0.0436 (10)	−0.0077 (7)	0.0330 (9)	−0.0080 (7)
C31	0.0349 (9)	0.0253 (8)	0.0311 (8)	−0.0068 (7)	0.0210 (7)	−0.0049 (6)
B1	0.0192 (8)	0.0187 (8)	0.0178 (7)	0.0011 (6)	0.0070 (6)	0.0003 (6)

Geometric parameters (Å, º)

O1—C25	1.3374 (16)	C11—C12	1.385 (2)
O1—B1	1.4731 (18)	C11—H11A	0.9500

O2—C25	1.2126 (17)	C12—C13	1.400 (2)
N1—C1	1.3718 (17)	C12—H12A	0.9500
N1—C8	1.3728 (17)	C13—C14	1.380 (2)
N1—B1	1.489 (2)	C13—H13A	0.9500
N2—C8	1.3385 (17)	C14—C15	1.394 (2)
N2—C9	1.3444 (18)	C14—H14A	0.9500
N3—C9	1.3684 (17)	C15—C16	1.4552 (19)
N3—C16	1.3693 (18)	C17—C18	1.4509 (19)
N3—B1	1.4928 (19)	C18—C19	1.395 (2)
N4—C16	1.3421 (18)	C18—C23	1.423 (2)
N4—C17	1.3453 (17)	C19—C20	1.377 (2)
N5—C24	1.3680 (17)	C19—H19A	0.9500
N5—C17	1.3702 (17)	C20—C21	1.402 (2)
N5—B1	1.4942 (19)	C20—H20A	0.9500
N6—C1	1.3385 (18)	C21—C22	1.381 (2)
N6—C24	1.3477 (18)	C21—H21A	0.9500
C1—C2	1.457 (2)	C22—C23	1.3964 (19)
C2—C3	1.392 (2)	C22—H22A	0.9500
C2—C7	1.4204 (19)	C23—C24	1.453 (2)
C3—C4	1.386 (2)	C25—C26	1.489 (2)
C3—H3A	0.9500	C26—C27	1.385 (2)
C4—C5	1.398 (2)	C26—C31	1.391 (2)
C4—H4A	0.9500	C27—C28	1.391 (2)
C5—C6	1.386 (2)	C27—H27A	0.9500
C5—H5A	0.9500	C28—C29	1.383 (2)
C6—C7	1.393 (2)	C28—H28A	0.9500
C6—H6A	0.9500	C29—C30	1.380 (3)
C7—C8	1.456 (2)	C29—H29A	0.9500
C9—C10	1.4541 (19)	C30—C31	1.386 (2)
C10—C11	1.3928 (19)	C30—H30A	0.9500
C10—C15	1.423 (2)	C31—H31A	0.9500

C25—O1—B1	118.41 (11)	C14—C15—C16	131.88 (13)
C1—N1—C8	112.15 (11)	C10—C15—C16	106.87 (12)
C1—N1—B1	122.83 (11)	N4—C16—N3	122.61 (12)
C8—N1—B1	123.04 (11)	N4—C16—C15	129.00 (13)
C8—N2—C9	116.60 (12)	N3—C16—C15	105.94 (11)
C9—N3—C16	112.85 (11)	N4—C17—N5	122.69 (12)
C9—N3—B1	123.36 (12)	N4—C17—C18	129.14 (13)
C16—N3—B1	122.27 (11)	N5—C17—C18	105.95 (11)
C16—N4—C17	117.16 (12)	C19—C18—C23	120.76 (13)
C24—N5—C17	112.86 (11)	C19—C18—C17	131.61 (13)
C24—N5—B1	123.06 (12)	C23—C18—C17	107.14 (12)
C17—N5—B1	122.30 (11)	C20—C19—C18	118.07 (14)
C1—N6—C24	116.81 (12)	C20—C19—H19A	121.0
N6—C1—N1	122.93 (12)	C18—C19—H19A	121.0
N6—C1—C2	129.17 (13)	C19—C20—C21	121.42 (14)
N1—C1—C2	105.95 (11)	C19—C20—H20A	119.3

C3—C2—C7	120.86 (13)	C21—C20—H20A	119.3
C3—C2—C1	131.84 (13)	C22—C21—C20	121.37 (14)
C7—C2—C1	107.10 (12)	C22—C21—H21A	119.3
C4—C3—C2	117.53 (13)	C20—C21—H21A	119.3
C4—C3—H3A	121.2	C21—C22—C23	118.21 (14)
C2—C3—H3A	121.2	C21—C22—H22A	120.9
C3—C4—C5	121.73 (14)	C23—C22—H22A	120.9
C3—C4—H4A	119.1	C22—C23—C18	120.16 (13)
C5—C4—H4A	119.1	C22—C23—C24	132.10 (13)
C6—C5—C4	121.29 (14)	C18—C23—C24	107.24 (11)
C6—C5—H5A	119.4	N6—C24—N5	122.76 (12)
C4—C5—H5A	119.4	N6—C24—C23	129.45 (12)
C5—C6—C7	117.71 (13)	N5—C24—C23	105.87 (11)
C5—C6—H6A	121.1	O2—C25—O1	123.09 (13)
C7—C6—H6A	121.1	O2—C25—C26	123.05 (13)
C6—C7—C2	120.77 (13)	O1—C25—C26	113.85 (12)
C6—C7—C8	131.94 (13)	C27—C26—C31	120.03 (14)
C2—C7—C8	107.12 (12)	C27—C26—C25	121.86 (13)
N2—C8—N1	123.23 (13)	C31—C26—C25	118.09 (13)
N2—C8—C7	129.12 (13)	C26—C27—C28	120.01 (15)
N1—C8—C7	105.94 (11)	C26—C27—H27A	120.0
N2—C9—N3	122.94 (12)	C28—C27—H27A	120.0
N2—C9—C10	129.56 (12)	C29—C28—C27	119.86 (16)
N3—C9—C10	105.75 (12)	C29—C28—H28A	120.1
C11—C10—C15	120.51 (13)	C27—C28—H28A	120.1
C11—C10—C9	131.41 (13)	C30—C29—C28	120.01 (16)
C15—C10—C9	107.44 (12)	C30—C29—H29A	120.0
C12—C11—C10	117.89 (14)	C28—C29—H29A	120.0
C12—C11—H11A	121.1	C29—C30—C31	120.63 (15)
C10—C11—H11A	121.1	C29—C30—H30A	119.7
C11—C12—C13	121.53 (13)	C31—C30—H30A	119.7
C11—C12—H12A	119.2	C30—C31—C26	119.45 (15)
C13—C12—H12A	119.2	C30—C31—H31A	120.3
C14—C13—C12	121.34 (14)	C26—C31—H31A	120.3
C14—C13—H13A	119.3	O1—B1—N1	118.49 (12)
C12—C13—H13A	119.3	O1—B1—N3	113.97 (12)
C13—C14—C15	117.99 (14)	N1—B1—N3	104.69 (11)
C13—C14—H14A	121.0	O1—B1—N5	108.79 (11)
C15—C14—H14A	121.0	N1—B1—N5	104.83 (11)
C14—C15—C10	120.72 (13)	N3—B1—N5	104.91 (11)

C24—N6—C1—N1	−8.6 (2)	C24—N5—C17—N4	154.42 (13)
C24—N6—C1—C2	153.16 (14)	B1—N5—C17—N4	−10.8 (2)
C8—N1—C1—N6	152.01 (13)	C24—N5—C17—C18	−10.04 (15)
B1—N1—C1—N6	−12.4 (2)	B1—N5—C17—C18	−175.26 (12)
C8—N1—C1—C2	−13.38 (15)	N4—C17—C18—C19	14.9 (3)
B1—N1—C1—C2	−177.79 (12)	N5—C17—C18—C19	177.99 (14)
N6—C1—C2—C3	18.5 (2)	N4—C17—C18—C23	−156.91 (14)

N1—C1—C2—C3	−177.36 (14)	N5—C17—C18—C23	6.19 (15)
N6—C1—C2—C7	−156.29 (14)	C23—C18—C19—C20	−0.5 (2)
N1—C1—C2—C7	7.86 (15)	C17—C18—C19—C20	−171.33 (15)
C7—C2—C3—C4	−2.7 (2)	C18—C19—C20—C21	1.1 (2)
C1—C2—C3—C4	−176.90 (14)	C19—C20—C21—C22	−0.6 (2)
C2—C3—C4—C5	2.4 (2)	C20—C21—C22—C23	−0.6 (2)
C3—C4—C5—C6	0.5 (2)	C21—C22—C23—C18	1.2 (2)
C4—C5—C6—C7	−3.0 (2)	C21—C22—C23—C24	171.92 (15)
C5—C6—C7—C2	2.7 (2)	C19—C18—C23—C22	−0.7 (2)
C5—C6—C7—C8	177.27 (14)	C17—C18—C23—C22	172.17 (12)
C3—C2—C7—C6	0.2 (2)	C19—C18—C23—C24	−173.51 (13)
C1—C2—C7—C6	175.67 (13)	C17—C18—C23—C24	−0.64 (15)
C3—C2—C7—C8	−175.61 (12)	C1—N6—C24—N5	10.2 (2)
C1—C2—C7—C8	−0.14 (15)	C1—N6—C24—C23	−151.73 (14)
C9—N2—C8—N1	7.90 (19)	C17—N5—C24—N6	−155.94 (13)
C9—N2—C8—C7	−155.02 (14)	B1—N5—C24—N6	9.2 (2)
C1—N1—C8—N2	−152.99 (13)	C17—N5—C24—C23	9.63 (15)
B1—N1—C8—N2	11.4 (2)	B1—N5—C24—C23	174.72 (12)
C1—N1—C8—C7	13.30 (15)	C22—C23—C24—N6	−12.5 (3)
B1—N1—C8—C7	177.66 (12)	C18—C23—C24—N6	159.10 (14)
C6—C7—C8—N2	−17.6 (3)	C22—C23—C24—N5	−176.77 (15)
C2—C7—C8—N2	157.57 (14)	C18—C23—C24—N5	−5.16 (15)
C6—C7—C8—N1	177.22 (14)	B1—O1—C25—O2	12.02 (19)
C2—C7—C8—N1	−7.62 (15)	B1—O1—C25—C26	−167.05 (11)
C8—N2—C9—N3	−8.38 (19)	O2—C25—C26—C27	175.26 (14)
C8—N2—C9—C10	154.34 (14)	O1—C25—C26—C27	−5.67 (19)
C16—N3—C9—N2	155.77 (13)	O2—C25—C26—C31	−6.4 (2)
B1—N3—C9—N2	−10.4 (2)	O1—C25—C26—C31	172.67 (12)
C16—N3—C9—C10	−10.47 (15)	C31—C26—C27—C28	0.1 (2)
B1—N3—C9—C10	−176.62 (12)	C25—C26—C27—C28	178.42 (14)
N2—C9—C10—C11	10.8 (2)	C26—C27—C28—C29	−0.7 (2)
N3—C9—C10—C11	175.80 (14)	C27—C28—C29—C30	0.4 (3)
N2—C9—C10—C15	−159.73 (14)	C28—C29—C30—C31	0.5 (2)
N3—C9—C10—C15	5.26 (15)	C29—C30—C31—C26	−1.1 (2)
C15—C10—C11—C12	−1.7 (2)	C27—C26—C31—C30	0.8 (2)
C9—C10—C11—C12	−171.21 (14)	C25—C26—C31—C30	−177.55 (13)
C10—C11—C12—C13	0.0 (2)	C25—O1—B1—N1	−65.32 (16)
C11—C12—C13—C14	1.5 (2)	C25—O1—B1—N3	58.54 (16)
C12—C13—C14—C15	−1.1 (2)	C25—O1—B1—N5	175.20 (11)
C13—C14—C15—C10	−0.6 (2)	C1—N1—B1—O1	−94.46 (16)
C13—C14—C15—C16	169.87 (14)	C8—N1—B1—O1	102.82 (15)
C11—C10—C15—C14	2.1 (2)	C1—N1—B1—N3	137.21 (12)
C9—C10—C15—C14	173.82 (12)	C8—N1—B1—N3	−25.51 (17)
C11—C10—C15—C16	−170.55 (12)	C1—N1—B1—N5	27.06 (17)
C9—C10—C15—C16	1.22 (15)	C8—N1—B1—N5	−135.66 (12)
C17—N4—C16—N3	8.50 (19)	C9—N3—B1—O1	−105.91 (15)
C17—N4—C16—C15	−151.17 (14)	C16—N3—B1—O1	89.21 (15)
C9—N3—C16—N4	−152.44 (13)	C9—N3—B1—N1	25.11 (17)

B1—N3—C16—N4	13.9 (2)	C16—N3—B1—N1	−139.77 (12)
C9—N3—C16—C15	11.25 (15)	C9—N3—B1—N5	135.20 (12)
B1—N3—C16—C15	177.58 (12)	C16—N3—B1—N5	−29.68 (17)
C14—C15—C16—N4	−16.4 (3)	C24—N5—B1—O1	102.14 (14)
C10—C15—C16—N4	155.03 (14)	C17—N5—B1—O1	−94.15 (14)
C14—C15—C16—N3	−178.70 (14)	C24—N5—B1—N1	−25.54 (17)
C10—C15—C16—N3	−7.25 (15)	C17—N5—B1—N1	138.17 (12)
C16—N4—C17—N5	−10.01 (19)	C24—N5—B1—N3	−135.53 (13)
C16—N4—C17—C18	150.60 (14)	C17—N5—B1—N3	28.18 (16)

(Subphthalocyaninato)(trimethylsilanolato)boron (d23117_a)

Crystal data

$C_{27}H_{21}BN_6OSi$
M_r = 484.40
Monoclinic, $P2_1/c$
a = 16.343 (3) Å
b = 11.9655 (16) Å
c = 12.5059 (19) Å
β = 99.996 (11)°
V = 2408.4 (6) Å^3
Z = 4
$F(000)$ = 1008
D_x = 1.336 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 6743 reflections
θ = 2.8–62.7°
μ = 1.13 mm^{-1}
T = 150 K
Plate, pink
0.19 × 0.15 × 0.01 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.629, T_{max} = 0.753
57016 measured reflections
4230 independent reflections
2990 reflections with $I > 2\sigma(I)$
R_{int} = 0.127
θ_{max} = 69.6°, θ_{min} = 2.8°
h = −19→18
k = −14→14
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.123
S = 1.05
4230 reflections
326 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 2.7611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: SHELXL2019 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00173 (18)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Si1	0.92196 (5)	0.56589 (8)	0.69390 (6)	0.0419 (3)
O1	0.82133 (11)	0.58527 (17)	0.66502 (14)	0.0404 (5)
N1	0.67572 (14)	0.54454 (19)	0.59336 (16)	0.0315 (5)
N2	0.61079 (13)	0.7152 (2)	0.62674 (16)	0.0324 (5)
N3	0.73048 (13)	0.71287 (19)	0.54058 (16)	0.0311 (5)
N4	0.79269 (13)	0.7113 (2)	0.38153 (17)	0.0337 (5)
N5	0.76928 (13)	0.54202 (19)	0.47089 (16)	0.0315 (5)
N6	0.69104 (15)	0.37895 (19)	0.49431 (17)	0.0362 (6)
C1	0.65420 (17)	0.4375 (2)	0.5652 (2)	0.0339 (6)
C2	0.57669 (17)	0.4167 (2)	0.6060 (2)	0.0341 (7)
C3	0.52886 (18)	0.3214 (3)	0.6107 (2)	0.0383 (7)
H3A	0.544905	0.251917	0.584005	0.046*
C4	0.45704 (19)	0.3303 (3)	0.6553 (2)	0.0411 (7)
H4A	0.424840	0.265383	0.662027	0.049*
C5	0.43160 (18)	0.4327 (3)	0.6903 (2)	0.0396 (7)
H5A	0.381451	0.436591	0.718769	0.047*
C6	0.47703 (17)	0.5288 (3)	0.6848 (2)	0.0353 (7)
H6A	0.458409	0.598563	0.707774	0.042*
C7	0.55133 (17)	0.5207 (2)	0.6443 (2)	0.0321 (6)
C8	0.61404 (16)	0.6031 (2)	0.62890 (19)	0.0314 (6)
C9	0.66603 (16)	0.7676 (2)	0.5752 (2)	0.0317 (6)
C10	0.65924 (17)	0.8756 (2)	0.5218 (2)	0.0326 (6)
C11	0.60688 (18)	0.9665 (2)	0.5262 (2)	0.0365 (7)
H11A	0.568910	0.967777	0.575691	0.044*
C12	0.61161 (19)	1.0550 (2)	0.4565 (2)	0.0401 (7)
H12A	0.577332	1.118639	0.459568	0.048*
C13	0.66574 (19)	1.0526 (3)	0.3817 (2)	0.0413 (7)
H13A	0.667074	1.114729	0.334729	0.050*
C14	0.71758 (18)	0.9627 (2)	0.3739 (2)	0.0362 (7)
H14A	0.753403	0.961298	0.321717	0.043*
C15	0.71516 (17)	0.8744 (2)	0.4455 (2)	0.0324 (6)
C16	0.75527 (16)	0.7655 (2)	0.4544 (2)	0.0313 (6)
C17	0.79452 (16)	0.5993 (2)	0.3877 (2)	0.0323 (6)
C18	0.80059 (16)	0.5173 (2)	0.3038 (2)	0.0317 (6)
C19	0.82400 (17)	0.5265 (3)	0.2025 (2)	0.0356 (7)
H19A	0.844024	0.595257	0.179144	0.043*
C20	0.81744 (17)	0.4334 (3)	0.1369 (2)	0.0388 (7)
H20A	0.834223	0.437620	0.067973	0.047*
C21	0.78666 (19)	0.3333 (3)	0.1699 (2)	0.0445 (8)
H21A	0.782564	0.270531	0.122721	0.053*
C22	0.76184 (19)	0.3225 (3)	0.2695 (2)	0.0436 (8)
H22A	0.740326	0.253783	0.290727	0.052*
C23	0.76918 (17)	0.4151 (2)	0.3380 (2)	0.0355 (7)
C24	0.74429 (17)	0.4358 (2)	0.4426 (2)	0.0341 (6)
C25	0.9463 (2)	0.5487 (4)	0.8434 (3)	0.0847 (15)

H25A	1.006156	0.536694	0.865852	0.127*
H25B	0.929659	0.616126	0.878614	0.127*
H25C	0.915995	0.484114	0.864899	0.127*
C26	0.9766 (2)	0.6865 (3)	0.6480 (3)	0.0651 (10)
H26A	1.036749	0.674094	0.665679	0.098*
H26B	0.960095	0.695330	0.569359	0.098*
H26C	0.962191	0.754221	0.684696	0.098*
C27	0.9503 (2)	0.4385 (3)	0.6252 (3)	0.0544 (9)
H27A	1.010494	0.427158	0.642697	0.082*
H27B	0.921838	0.373842	0.650062	0.082*
H27C	0.933464	0.446856	0.546533	0.082*
B1	0.7561 (2)	0.5960 (3)	0.5750 (2)	0.0331 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0324 (4)	0.0598 (6)	0.0333 (4)	0.0051 (4)	0.0054 (3)	−0.0022 (4)
O1	0.0334 (11)	0.0576 (14)	0.0303 (10)	0.0052 (9)	0.0057 (8)	−0.0006 (9)
N1	0.0350 (13)	0.0335 (14)	0.0271 (11)	0.0026 (10)	0.0087 (9)	0.0015 (10)
N2	0.0349 (13)	0.0374 (15)	0.0259 (11)	−0.0005 (11)	0.0081 (9)	−0.0009 (10)
N3	0.0335 (12)	0.0363 (14)	0.0256 (11)	−0.0018 (11)	0.0107 (9)	−0.0024 (10)
N4	0.0321 (13)	0.0387 (15)	0.0309 (12)	−0.0056 (11)	0.0075 (10)	−0.0026 (10)
N5	0.0330 (12)	0.0370 (14)	0.0262 (11)	0.0019 (10)	0.0103 (9)	0.0007 (10)
N6	0.0417 (14)	0.0355 (14)	0.0335 (12)	0.0050 (11)	0.0129 (10)	0.0027 (10)
C1	0.0389 (16)	0.0339 (17)	0.0295 (14)	0.0029 (13)	0.0077 (12)	0.0060 (12)
C2	0.0365 (15)	0.0395 (18)	0.0268 (13)	−0.0001 (13)	0.0071 (11)	0.0063 (12)
C3	0.0463 (18)	0.0412 (18)	0.0290 (14)	−0.0059 (14)	0.0109 (13)	0.0017 (12)
C4	0.0462 (18)	0.047 (2)	0.0307 (15)	−0.0111 (15)	0.0087 (13)	0.0020 (13)
C5	0.0350 (16)	0.054 (2)	0.0306 (14)	−0.0046 (15)	0.0076 (12)	0.0016 (14)
C6	0.0374 (16)	0.0428 (18)	0.0266 (13)	−0.0004 (14)	0.0080 (12)	0.0025 (12)
C7	0.0331 (15)	0.0392 (17)	0.0240 (13)	−0.0006 (13)	0.0053 (11)	0.0050 (12)
C8	0.0336 (15)	0.0386 (18)	0.0231 (12)	0.0026 (13)	0.0079 (11)	0.0014 (12)
C9	0.0312 (14)	0.0393 (17)	0.0248 (13)	−0.0019 (13)	0.0054 (11)	−0.0046 (12)
C10	0.0379 (16)	0.0341 (17)	0.0264 (13)	−0.0054 (13)	0.0070 (11)	−0.0034 (11)
C11	0.0420 (17)	0.0374 (18)	0.0313 (14)	−0.0001 (14)	0.0093 (12)	−0.0042 (12)
C12	0.0514 (18)	0.0325 (17)	0.0365 (15)	0.0016 (14)	0.0080 (13)	−0.0044 (13)
C13	0.0546 (19)	0.0342 (18)	0.0351 (15)	−0.0077 (15)	0.0081 (14)	−0.0007 (13)
C14	0.0458 (17)	0.0363 (17)	0.0277 (14)	−0.0092 (14)	0.0100 (12)	−0.0032 (12)
C15	0.0376 (16)	0.0319 (16)	0.0286 (14)	−0.0076 (13)	0.0078 (12)	−0.0054 (12)
C16	0.0313 (15)	0.0379 (17)	0.0264 (13)	−0.0060 (12)	0.0096 (11)	−0.0044 (12)
C17	0.0277 (14)	0.0382 (18)	0.0314 (14)	−0.0018 (12)	0.0059 (11)	0.0004 (12)
C18	0.0296 (14)	0.0407 (17)	0.0257 (13)	0.0029 (12)	0.0078 (11)	−0.0018 (12)
C19	0.0308 (15)	0.0437 (18)	0.0327 (14)	0.0023 (13)	0.0063 (12)	0.0006 (13)
C20	0.0370 (16)	0.050 (2)	0.0303 (14)	0.0008 (14)	0.0071 (12)	−0.0061 (13)
C21	0.0472 (19)	0.048 (2)	0.0400 (16)	0.0010 (15)	0.0128 (14)	−0.0132 (14)
C22	0.0446 (18)	0.0393 (19)	0.0496 (18)	−0.0023 (14)	0.0154 (15)	−0.0062 (14)
C23	0.0349 (15)	0.0380 (18)	0.0351 (14)	0.0018 (13)	0.0108 (12)	0.0002 (12)
C24	0.0363 (15)	0.0345 (17)	0.0336 (14)	0.0047 (13)	0.0121 (12)	0.0030 (12)

C25	0.047 (2)	0.162 (5)	0.044 (2)	0.030 (3)	0.0036 (16)	−0.001 (2)
C26	0.048 (2)	0.063 (3)	0.083 (3)	−0.0077 (18)	0.0090 (19)	−0.014 (2)
C27	0.0458 (19)	0.058 (2)	0.059 (2)	0.0088 (17)	0.0087 (16)	0.0019 (17)
B1	0.0326 (17)	0.040 (2)	0.0282 (15)	−0.0019 (15)	0.0078 (13)	0.0004 (14)

Geometric parameters (Å, º)

Si1—O1	1.638 (2)	C10—C11	1.391 (4)
Si1—C26	1.840 (4)	C10—C15	1.431 (4)
Si1—C27	1.847 (3)	C11—C12	1.382 (4)
Si1—C25	1.855 (3)	C11—H11A	0.9500
O1—B1	1.415 (4)	C12—C13	1.394 (4)
N1—C1	1.358 (3)	C12—H12A	0.9500
N1—C8	1.364 (3)	C13—C14	1.384 (4)
N1—B1	1.504 (4)	C13—H13A	0.9500
N2—C8	1.342 (3)	C14—C15	1.389 (4)
N2—C9	1.351 (3)	C14—H14A	0.9500
N3—C16	1.368 (3)	C15—C16	1.455 (4)
N3—C9	1.372 (3)	C17—C18	1.452 (4)
N3—B1	1.502 (4)	C18—C19	1.390 (4)
N4—C17	1.343 (3)	C18—C23	1.422 (4)
N4—C16	1.348 (3)	C19—C20	1.377 (4)
N5—C24	1.363 (4)	C19—H19A	0.9500
N5—C17	1.368 (3)	C20—C21	1.389 (4)
N5—B1	1.502 (4)	C20—H20A	0.9500
N6—C1	1.351 (3)	C21—C22	1.381 (4)
N6—C24	1.354 (3)	C21—H21A	0.9500
C1—C2	1.466 (4)	C22—C23	1.393 (4)
C2—C3	1.390 (4)	C22—H22A	0.9500
C2—C7	1.420 (4)	C23—C24	1.457 (4)
C3—C4	1.388 (4)	C25—H25A	0.9800
C3—H3A	0.9500	C25—H25B	0.9800
C4—C5	1.389 (4)	C25—H25C	0.9800
C4—H4A	0.9500	C26—H26A	0.9800
C5—C6	1.377 (4)	C26—H26B	0.9800
C5—H5A	0.9500	C26—H26C	0.9800
C6—C7	1.397 (4)	C27—H27A	0.9800
C6—H6A	0.9500	C27—H27B	0.9800
C7—C8	1.459 (4)	C27—H27C	0.9800
C9—C10	1.451 (4)		

O1—Si1—C26	110.09 (15)	C13—C14—C15	117.4 (3)
O1—Si1—C27	109.70 (14)	C13—C14—H14A	121.3
C26—Si1—C27	109.14 (17)	C15—C14—H14A	121.3
O1—Si1—C25	105.64 (14)	C14—C15—C10	121.0 (3)
C26—Si1—C25	111.7 (2)	C14—C15—C16	131.9 (2)
C27—Si1—C25	110.48 (19)	C10—C15—C16	106.8 (2)
B1—O1—Si1	141.00 (18)	N4—C16—N3	122.9 (2)

C1—N1—C8	113.3 (2)	N4—C16—C15	129.0 (2)
C1—N1—B1	122.7 (2)	N3—C16—C15	106.4 (2)
C8—N1—B1	123.6 (2)	N4—C17—N5	122.5 (2)
C8—N2—C9	116.5 (2)	N4—C17—C18	129.5 (2)
C16—N3—C9	112.2 (2)	N5—C17—C18	106.2 (2)
C16—N3—B1	123.3 (2)	C19—C18—C23	120.9 (3)
C9—N3—B1	123.0 (2)	C19—C18—C17	132.0 (3)
C17—N4—C16	116.7 (2)	C23—C18—C17	106.9 (2)
C24—N5—C17	112.7 (2)	C20—C19—C18	118.3 (3)
C24—N5—B1	123.0 (2)	C20—C19—H19A	120.8
C17—N5—B1	123.5 (2)	C18—C19—H19A	120.8
C1—N6—C24	116.7 (2)	C19—C20—C21	121.0 (3)
N6—C1—N1	122.3 (2)	C19—C20—H20A	119.5
N6—C1—C2	130.6 (3)	C21—C20—H20A	119.5
N1—C1—C2	105.7 (2)	C22—C21—C20	121.8 (3)
C3—C2—C7	120.3 (2)	C22—C21—H21A	119.1
C3—C2—C1	132.8 (3)	C20—C21—H21A	119.1
C7—C2—C1	106.8 (2)	C21—C22—C23	118.2 (3)
C4—C3—C2	118.4 (3)	C21—C22—H22A	120.9
C4—C3—H3A	120.8	C23—C22—H22A	120.9
C2—C3—H3A	120.8	C22—C23—C18	119.8 (2)
C3—C4—C5	120.9 (3)	C22—C23—C24	132.8 (3)
C3—C4—H4A	119.5	C18—C23—C24	107.2 (2)
C5—C4—H4A	119.5	N6—C24—N5	122.2 (2)
C6—C5—C4	121.9 (3)	N6—C24—C23	130.3 (3)
C6—C5—H5A	119.1	N5—C24—C23	105.9 (2)
C4—C5—H5A	119.1	Si1—C25—H25A	109.5
C5—C6—C7	118.0 (3)	Si1—C25—H25B	109.5
C5—C6—H6A	121.0	H25A—C25—H25B	109.5
C7—C6—H6A	121.0	Si1—C25—H25C	109.5
C6—C7—C2	120.4 (3)	H25A—C25—H25C	109.5
C6—C7—C8	132.5 (3)	H25B—C25—H25C	109.5
C2—C7—C8	107.1 (2)	Si1—C26—H26A	109.5
N2—C8—N1	122.4 (2)	Si1—C26—H26B	109.5
N2—C8—C7	130.7 (2)	H26A—C26—H26B	109.5
N1—C8—C7	105.7 (2)	Si1—C26—H26C	109.5
N2—C9—N3	122.8 (2)	H26A—C26—H26C	109.5
N2—C9—C10	129.0 (2)	H26B—C26—H26C	109.5
N3—C9—C10	106.3 (2)	Si1—C27—H27A	109.5
C11—C10—C15	120.1 (3)	Si1—C27—H27B	109.5
C11—C10—C9	132.6 (2)	H27A—C27—H27B	109.5
C15—C10—C9	106.9 (2)	Si1—C27—H27C	109.5
C12—C11—C10	118.2 (3)	H27A—C27—H27C	109.5
C12—C11—H11A	120.9	H27B—C27—H27C	109.5
C10—C11—H11A	120.9	O1—B1—N3	116.5 (2)
C11—C12—C13	121.2 (3)	O1—B1—N5	116.7 (2)
C11—C12—H12A	119.4	N3—B1—N5	103.1 (2)
C13—C12—H12A	119.4	O1—B1—N1	113.5 (2)

C14—C13—C12	122.0 (3)	N3—B1—N1	102.6 (2)
C14—C13—H13A	119.0	N5—B1—N1	102.5 (2)
C12—C13—H13A	119.0		
C26—Si1—O1—B1	65.4 (4)	C9—N3—C16—C15	11.8 (3)
C27—Si1—O1—B1	−54.7 (4)	B1—N3—C16—C15	177.9 (2)
C25—Si1—O1—B1	−173.8 (3)	C14—C15—C16—N4	−15.2 (5)
C24—N6—C1—N1	−7.2 (4)	C10—C15—C16—N4	158.2 (3)
C24—N6—C1—C2	156.9 (3)	C14—C15—C16—N3	179.9 (3)
C8—N1—C1—N6	155.7 (2)	C10—C15—C16—N3	−6.7 (3)
B1—N1—C1—N6	−17.9 (4)	C16—N4—C17—N5	−7.8 (4)
C8—N1—C1—C2	−11.9 (3)	C16—N4—C17—C18	154.7 (3)
B1—N1—C1—C2	174.5 (2)	C24—N5—C17—N4	155.2 (2)
N6—C1—C2—C3	20.3 (5)	B1—N5—C17—N4	−14.6 (4)
N1—C1—C2—C3	−173.5 (3)	C24—N5—C17—C18	−10.9 (3)
N6—C1—C2—C7	−158.6 (3)	B1—N5—C17—C18	179.3 (2)
N1—C1—C2—C7	7.6 (3)	N4—C17—C18—C19	16.2 (5)
C7—C2—C3—C4	−1.1 (4)	N5—C17—C18—C19	−179.1 (3)
C1—C2—C3—C4	−179.9 (3)	N4—C17—C18—C23	−158.4 (3)
C2—C3—C4—C5	2.7 (4)	N5—C17—C18—C23	6.3 (3)
C3—C4—C5—C6	−1.6 (4)	C23—C18—C19—C20	−1.2 (4)
C4—C5—C6—C7	−1.1 (4)	C17—C18—C19—C20	−175.2 (3)
C5—C6—C7—C2	2.6 (4)	C18—C19—C20—C21	1.3 (4)
C5—C6—C7—C8	−179.0 (3)	C19—C20—C21—C22	−0.3 (5)
C3—C2—C7—C6	−1.5 (4)	C20—C21—C22—C23	−0.7 (5)
C1—C2—C7—C6	177.6 (2)	C21—C22—C23—C18	0.8 (4)
C3—C2—C7—C8	179.8 (2)	C21—C22—C23—C24	174.9 (3)
C1—C2—C7—C8	−1.2 (3)	C19—C18—C23—C22	0.2 (4)
C9—N2—C8—N1	7.9 (4)	C17—C18—C23—C22	175.5 (3)
C9—N2—C8—C7	−157.9 (3)	C19—C18—C23—C24	−175.4 (2)
C1—N1—C8—N2	−157.7 (2)	C17—C18—C23—C24	0.0 (3)
B1—N1—C8—N2	15.9 (4)	C1—N6—C24—N5	9.2 (4)
C1—N1—C8—C7	11.2 (3)	C1—N6—C24—C23	−154.0 (3)
B1—N1—C8—C7	−175.3 (2)	C17—N5—C24—N6	−155.9 (2)
C6—C7—C8—N2	−16.6 (5)	B1—N5—C24—N6	13.9 (4)
C2—C7—C8—N2	161.9 (3)	C17—N5—C24—C23	10.8 (3)
C6—C7—C8—N1	175.9 (3)	B1—N5—C24—C23	−179.3 (2)
C2—C7—C8—N1	−5.6 (3)	C22—C23—C24—N6	−15.7 (5)
C8—N2—C9—N3	−9.5 (4)	C18—C23—C24—N6	159.0 (3)
C8—N2—C9—C10	152.8 (3)	C22—C23—C24—N5	179.1 (3)
C16—N3—C9—N2	153.8 (2)	C18—C23—C24—N5	−6.2 (3)
B1—N3—C9—N2	−12.4 (4)	Si1—O1—B1—N3	−96.9 (3)
C16—N3—C9—C10	−12.0 (3)	Si1—O1—B1—N5	25.4 (5)
B1—N3—C9—C10	−178.2 (2)	Si1—O1—B1—N1	144.3 (2)
N2—C9—C10—C11	16.4 (5)	C16—N3—B1—O1	100.6 (3)
N3—C9—C10—C11	−179.0 (3)	C9—N3—B1—O1	−94.8 (3)
N2—C9—C10—C15	−157.5 (3)	C16—N3—B1—N5	−28.5 (3)
N3—C9—C10—C15	7.1 (3)	C9—N3—B1—N5	136.1 (2)

C15—C10—C11—C12	−1.0 (4)	C16—N3—B1—N1	−134.8 (2)
C9—C10—C11—C12	−174.2 (3)	C9—N3—B1—N1	29.9 (3)
C10—C11—C12—C13	1.6 (4)	C24—N5—B1—O1	92.2 (3)
C11—C12—C13—C14	−0.4 (4)	C17—N5—B1—O1	−99.1 (3)
C12—C13—C14—C15	−1.3 (4)	C24—N5—B1—N3	−138.8 (2)
C13—C14—C15—C10	1.9 (4)	C17—N5—B1—N3	30.0 (3)
C13—C14—C15—C16	174.5 (3)	C24—N5—B1—N1	−32.6 (3)
C11—C10—C15—C14	−0.8 (4)	C17—N5—B1—N1	136.2 (2)
C9—C10—C15—C14	174.0 (2)	C1—N1—B1—O1	−92.3 (3)
C11—C10—C15—C16	−175.1 (2)	C8—N1—B1—O1	94.8 (3)
C9—C10—C15—C16	−0.3 (3)	C1—N1—B1—N3	141.2 (2)
C17—N4—C16—N3	9.2 (4)	C8—N1—B1—N3	−31.8 (3)
C17—N4—C16—C15	−153.6 (3)	C1—N1—B1—N5	34.5 (3)
C9—N3—C16—N4	−154.2 (2)	C8—N1—B1—N5	−138.5 (2)
B1—N3—C16—N4	11.9 (4)		

(2,3,4,5,6-Pentafluorobenzenethiolato)(subphthalocyaninato)boron (d23110_a)

Crystal data

$C_{30}H_{12}BF_5N_6S$
M_r = 594.33
Triclinic, $P\overline{1}$
a = 10.7010 (5) Å
b = 11.8651 (6) Å
c = 22.4968 (13) Å
α = 95.863 (2)°
β = 92.861 (2)°
γ = 115.433 (2)°
V = 2552.1 (2) Å^3
Z = 4
$F(000)$ = 1200
D_x = 1.547 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9956 reflections
θ = 2.7–27.4°
μ = 0.20 mm^{-1}
T = 150 K
Shard, pink
0.35 × 0.24 × 0.05 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: sealed tube with Bruker Triumph monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.713, T_{max} = 0.746
75917 measured reflections
11711 independent reflections
7793 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −13→13
k = −15→15
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.102
S = 1.02
11711 reflections
775 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.8213P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.49981 (5)	0.53057 (5)	0.88589 (2)	0.02616 (12)
F1A	0.70408 (13)	0.72707 (11)	0.98271 (5)	0.0396 (3)
F2A	0.87347 (15)	0.69748 (13)	1.06595 (6)	0.0555 (4)
F3A	0.86448 (16)	0.46768 (15)	1.07207 (6)	0.0605 (4)
F4A	0.68146 (16)	0.26465 (13)	0.99579 (6)	0.0546 (4)
F5A	0.51425 (13)	0.29185 (11)	0.91116 (6)	0.0408 (3)
N1A	0.59322 (15)	0.61609 (14)	0.77505 (7)	0.0215 (3)
N2A	0.73161 (16)	0.83583 (15)	0.80554 (7)	0.0242 (4)
N3A	0.77455 (15)	0.68489 (14)	0.85414 (7)	0.0215 (3)
N4A	0.89447 (16)	0.55887 (15)	0.86719 (7)	0.0243 (4)
N5A	0.67759 (15)	0.47455 (14)	0.80606 (7)	0.0215 (3)
N6A	0.54706 (15)	0.42765 (14)	0.71034 (7)	0.0239 (4)
C1A	0.53955 (18)	0.53801 (17)	0.72171 (8)	0.0222 (4)
C2A	0.51256 (18)	0.61359 (18)	0.68042 (9)	0.0232 (4)
C3A	0.45649 (19)	0.5861 (2)	0.62048 (9)	0.0279 (4)
H3AA	0.420030	0.502772	0.599805	0.034*
C4A	0.4556 (2)	0.6839 (2)	0.59199 (10)	0.0322 (5)
H4AA	0.417881	0.667264	0.551164	0.039*
C5A	0.5091 (2)	0.8069 (2)	0.62219 (10)	0.0322 (5)
H5AA	0.506186	0.871727	0.601473	0.039*
C6A	0.56586 (19)	0.83616 (19)	0.68124 (9)	0.0278 (4)
H6AA	0.602715	0.920053	0.701251	0.033*
C7A	0.56762 (18)	0.73904 (18)	0.71074 (9)	0.0241 (4)
C8A	0.63000 (19)	0.73977 (17)	0.76930 (8)	0.0226 (4)
C9A	0.80774 (19)	0.80627 (18)	0.84451 (8)	0.0233 (4)
C10A	0.9500 (2)	0.88135 (18)	0.87186 (8)	0.0261 (4)
C11A	1.0384 (2)	1.00860 (19)	0.87489 (9)	0.0320 (5)
H11A	1.005876	1.065382	0.861224	0.038*
C12A	1.1753 (2)	1.0506 (2)	0.89839 (10)	0.0370 (5)
H12A	1.237145	1.137540	0.901278	0.044*
C13A	1.2244 (2)	0.9674 (2)	0.91794 (9)	0.0347 (5)
H13A	1.318807	0.999044	0.934015	0.042*
C14A	1.1379 (2)	0.8396 (2)	0.91432 (9)	0.0298 (5)
H14A	1.172164	0.783299	0.927093	0.036*
C15A	0.99935 (19)	0.79625 (18)	0.89140 (8)	0.0252 (4)
C16A	0.88793 (19)	0.66983 (18)	0.87543 (8)	0.0226 (4)
C17A	0.79314 (19)	0.46576 (18)	0.82956 (8)	0.0227 (4)
C18A	0.79684 (19)	0.35882 (17)	0.79304 (9)	0.0242 (4)
C19A	0.8868 (2)	0.30175 (18)	0.79667 (10)	0.0292 (5)

H19A	0.957599	0.327545	0.829189	0.035*
C20A	0.8695 (2)	0.20672 (19)	0.75150 (10)	0.0327 (5)
H20A	0.927164	0.164496	0.753782	0.039*
C21A	0.7686 (2)	0.17136 (19)	0.70237 (10)	0.0328 (5)
H21A	0.761129	0.107275	0.671469	0.039*
C22A	0.6794 (2)	0.22745 (18)	0.69774 (9)	0.0291 (5)
H22A	0.611713	0.203445	0.664093	0.035*
C23A	0.69218 (19)	0.32043 (17)	0.74412 (9)	0.0244 (4)
C24A	0.62320 (18)	0.40202 (17)	0.75149 (8)	0.0226 (4)
C25A	0.60524 (19)	0.51087 (18)	0.94308 (8)	0.0245 (4)
C26A	0.6973 (2)	0.61149 (19)	0.98424 (9)	0.0285 (4)
C27A	0.7847 (2)	0.5979 (2)	1.02709 (9)	0.0352 (5)
C28A	0.7799 (2)	0.4815 (2)	1.03038 (9)	0.0375 (5)
C29A	0.6884 (2)	0.3795 (2)	0.99165 (9)	0.0353 (5)
C30A	0.6022 (2)	0.39450 (19)	0.94868 (9)	0.0275 (4)
B1A	0.6405 (2)	0.5772 (2)	0.82919 (10)	0.0219 (5)
S1B	0.05882 (5)	0.33569 (5)	0.26516 (2)	0.02715 (12)
F1B	0.04317 (13)	0.09077 (11)	0.29706 (6)	0.0424 (3)
F2B	0.14031 (15)	0.04637 (13)	0.39967 (7)	0.0585 (4)
F3B	0.26808 (17)	0.23581 (17)	0.49192 (6)	0.0701 (5)
F4B	0.30082 (17)	0.47153 (16)	0.47987 (7)	0.0698 (5)
F5B	0.20496 (13)	0.51909 (11)	0.37741 (6)	0.0433 (3)
N1B	−0.23801 (15)	0.23867 (14)	0.23854 (7)	0.0207 (3)
N2B	−0.30813 (16)	0.06499 (15)	0.29462 (7)	0.0254 (4)
N3B	−0.15998 (15)	0.27250 (15)	0.34106 (7)	0.0228 (3)
N4B	−0.10216 (16)	0.47125 (16)	0.39815 (8)	0.0307 (4)
N5B	−0.13423 (15)	0.44460 (14)	0.29154 (7)	0.0237 (4)
N6B	−0.27014 (16)	0.40254 (14)	0.19762 (7)	0.0249 (4)
C1B	−0.29694 (19)	0.28062 (18)	0.19606 (8)	0.0221 (4)
C2B	−0.40868 (19)	0.16806 (18)	0.16220 (8)	0.0237 (4)
C3B	−0.5002 (2)	0.1510 (2)	0.11228 (9)	0.0285 (4)
H3BA	−0.492009	0.219762	0.091914	0.034*
C4B	−0.6034 (2)	0.0308 (2)	0.09323 (9)	0.0344 (5)
H4BA	−0.665957	0.016571	0.058757	0.041*
C5B	−0.6174 (2)	−0.0702 (2)	0.12372 (10)	0.0364 (5)
H5BA	−0.690252	−0.151387	0.109873	0.044*
C6B	−0.5279 (2)	−0.05479 (19)	0.17342 (9)	0.0310 (5)
H6BA	−0.538709	−0.123884	0.194044	0.037*
C7B	−0.42164 (19)	0.06468 (18)	0.19246 (8)	0.0243 (4)
C8B	−0.31642 (19)	0.11382 (17)	0.24397 (9)	0.0228 (4)
C9B	−0.23438 (19)	0.14713 (19)	0.34350 (9)	0.0251 (4)
C10B	−0.2379 (2)	0.1365 (2)	0.40754 (9)	0.0300 (5)
C11B	−0.2983 (2)	0.0321 (2)	0.43806 (10)	0.0400 (6)
H11B	−0.342530	−0.051183	0.417192	0.048*
C12B	−0.2910 (3)	0.0554 (3)	0.50023 (11)	0.0526 (7)
H12B	−0.330177	−0.013614	0.522317	0.063*
C13B	−0.2278 (3)	0.1772 (3)	0.53090 (11)	0.0561 (7)
H13B	−0.224288	0.188703	0.573469	0.067*

C14B	−0.1697 (2)	0.2822 (3)	0.50167 (10)	0.0437 (6)
H14B	−0.128543	0.364963	0.523142	0.052*
C15B	−0.1743 (2)	0.2611 (2)	0.43919 (9)	0.0318 (5)
C16B	−0.13312 (19)	0.3478 (2)	0.39478 (9)	0.0274 (4)
C17B	−0.11308 (19)	0.51507 (19)	0.34637 (9)	0.0280 (4)
C18B	−0.13774 (19)	0.62262 (19)	0.33445 (10)	0.0320 (5)
C19B	−0.1270 (2)	0.7287 (2)	0.37161 (12)	0.0426 (6)
H19B	−0.094618	0.743089	0.413044	0.051*
C20B	−0.1650 (2)	0.8119 (2)	0.34621 (14)	0.0501 (7)
H20B	−0.156079	0.885709	0.370620	0.060*
C21B	−0.2161 (2)	0.7912 (2)	0.28592 (13)	0.0461 (6)
H21B	−0.241384	0.850687	0.270219	0.055*
C22B	−0.2304 (2)	0.68553 (19)	0.24864 (12)	0.0376 (5)
H22B	−0.266527	0.670671	0.207679	0.045*
C23B	−0.19008 (19)	0.60121 (18)	0.27311 (10)	0.0295 (5)
C24B	−0.19621 (19)	0.48072 (18)	0.24739 (9)	0.0247 (4)
C25B	0.12095 (18)	0.30688 (18)	0.33317 (9)	0.0241 (4)
C26B	0.1063 (2)	0.18742 (19)	0.34126 (9)	0.0292 (5)
C27B	0.1549 (2)	0.1632 (2)	0.39406 (11)	0.0367 (5)
C28B	0.2192 (2)	0.2582 (3)	0.44062 (10)	0.0426 (6)
C29B	0.2361 (2)	0.3779 (2)	0.43455 (10)	0.0408 (6)
C30B	0.1874 (2)	0.4015 (2)	0.38137 (9)	0.0303 (5)
B1B	−0.1227 (2)	0.3236 (2)	0.28434 (10)	0.0218 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0222 (2)	0.0340 (3)	0.0249 (3)	0.0136 (2)	0.0059 (2)	0.0076 (2)
F1A	0.0545 (8)	0.0296 (7)	0.0365 (7)	0.0221 (6)	−0.0012 (6)	−0.0010 (5)
F2A	0.0630 (9)	0.0541 (9)	0.0418 (8)	0.0258 (8)	−0.0208 (7)	−0.0145 (7)
F3A	0.0809 (11)	0.0797 (11)	0.0376 (8)	0.0549 (9)	−0.0187 (7)	0.0003 (7)
F4A	0.0915 (11)	0.0470 (8)	0.0410 (8)	0.0453 (8)	−0.0020 (7)	0.0093 (7)
F5A	0.0473 (8)	0.0287 (7)	0.0396 (8)	0.0117 (6)	−0.0016 (6)	0.0015 (6)
N1A	0.0187 (8)	0.0230 (9)	0.0233 (9)	0.0094 (7)	0.0035 (7)	0.0040 (7)
N2A	0.0221 (8)	0.0252 (9)	0.0260 (9)	0.0118 (7)	0.0035 (7)	−0.0001 (7)
N3A	0.0220 (8)	0.0253 (9)	0.0182 (8)	0.0114 (7)	0.0028 (6)	0.0025 (7)
N4A	0.0260 (8)	0.0287 (9)	0.0202 (9)	0.0128 (8)	0.0046 (7)	0.0070 (7)
N5A	0.0195 (8)	0.0230 (8)	0.0213 (9)	0.0078 (7)	0.0044 (6)	0.0064 (7)
N6A	0.0191 (8)	0.0237 (9)	0.0251 (9)	0.0054 (7)	0.0024 (7)	0.0048 (7)
C1A	0.0166 (9)	0.0242 (10)	0.0225 (10)	0.0057 (8)	0.0019 (8)	0.0038 (8)
C2A	0.0167 (9)	0.0290 (11)	0.0257 (11)	0.0106 (8)	0.0045 (8)	0.0071 (8)
C3A	0.0203 (10)	0.0346 (12)	0.0283 (11)	0.0116 (9)	0.0006 (8)	0.0042 (9)
C4A	0.0252 (10)	0.0464 (14)	0.0285 (12)	0.0176 (10)	0.0019 (9)	0.0113 (10)
C5A	0.0262 (11)	0.0423 (13)	0.0371 (13)	0.0202 (10)	0.0080 (9)	0.0186 (10)
C6A	0.0205 (10)	0.0288 (11)	0.0372 (12)	0.0124 (9)	0.0062 (9)	0.0098 (9)
C7A	0.0168 (9)	0.0293 (11)	0.0291 (11)	0.0117 (8)	0.0059 (8)	0.0068 (9)
C8A	0.0214 (9)	0.0243 (10)	0.0250 (10)	0.0119 (8)	0.0068 (8)	0.0056 (8)
C9A	0.0243 (10)	0.0260 (11)	0.0210 (10)	0.0129 (9)	0.0051 (8)	−0.0005 (8)

C10A	0.0265 (10)	0.0287 (11)	0.0216 (10)	0.0122 (9)	0.0017 (8)	−0.0036 (8)
C11A	0.0316 (11)	0.0261 (11)	0.0347 (12)	0.0117 (9)	0.0005 (9)	−0.0051 (9)
C12A	0.0317 (11)	0.0299 (12)	0.0404 (13)	0.0078 (10)	0.0008 (10)	−0.0070 (10)
C13A	0.0225 (10)	0.0408 (13)	0.0313 (12)	0.0087 (10)	−0.0023 (9)	−0.0097 (10)
C14A	0.0275 (10)	0.0397 (13)	0.0209 (11)	0.0153 (10)	−0.0007 (8)	−0.0024 (9)
C15A	0.0245 (10)	0.0302 (11)	0.0187 (10)	0.0108 (9)	0.0028 (8)	−0.0006 (8)
C16A	0.0226 (10)	0.0303 (11)	0.0155 (9)	0.0118 (9)	0.0031 (7)	0.0041 (8)
C17A	0.0224 (10)	0.0253 (10)	0.0225 (10)	0.0104 (9)	0.0067 (8)	0.0100 (8)
C18A	0.0243 (10)	0.0216 (10)	0.0271 (11)	0.0084 (8)	0.0083 (8)	0.0095 (8)
C19A	0.0256 (10)	0.0257 (11)	0.0385 (12)	0.0108 (9)	0.0091 (9)	0.0130 (9)
C20A	0.0339 (11)	0.0255 (11)	0.0456 (14)	0.0163 (10)	0.0158 (10)	0.0130 (10)
C21A	0.0398 (12)	0.0214 (11)	0.0374 (13)	0.0120 (10)	0.0152 (10)	0.0058 (9)
C22A	0.0320 (11)	0.0221 (11)	0.0302 (12)	0.0080 (9)	0.0069 (9)	0.0058 (9)
C23A	0.0243 (10)	0.0199 (10)	0.0281 (11)	0.0069 (8)	0.0086 (8)	0.0095 (8)
C24A	0.0198 (9)	0.0204 (10)	0.0223 (10)	0.0036 (8)	0.0042 (8)	0.0032 (8)
C25A	0.0232 (10)	0.0317 (11)	0.0214 (10)	0.0137 (9)	0.0088 (8)	0.0060 (8)
C26A	0.0326 (11)	0.0299 (11)	0.0256 (11)	0.0160 (10)	0.0071 (9)	0.0027 (9)
C27A	0.0387 (12)	0.0423 (13)	0.0235 (11)	0.0192 (11)	−0.0020 (9)	−0.0040 (10)
C28A	0.0458 (13)	0.0540 (15)	0.0215 (11)	0.0312 (12)	−0.0026 (10)	0.0038 (10)
C29A	0.0528 (14)	0.0373 (13)	0.0273 (12)	0.0293 (12)	0.0070 (10)	0.0081 (10)
C30A	0.0313 (11)	0.0292 (11)	0.0209 (10)	0.0121 (9)	0.0060 (9)	0.0020 (9)
B1A	0.0209 (10)	0.0234 (12)	0.0215 (11)	0.0089 (9)	0.0050 (9)	0.0048 (9)
S1B	0.0247 (2)	0.0386 (3)	0.0241 (3)	0.0174 (2)	0.0081 (2)	0.0107 (2)
F1B	0.0457 (8)	0.0275 (7)	0.0490 (8)	0.0130 (6)	−0.0004 (6)	−0.0006 (6)
F2B	0.0599 (9)	0.0552 (9)	0.0758 (11)	0.0336 (8)	0.0095 (8)	0.0360 (8)
F3B	0.0752 (11)	0.1215 (15)	0.0381 (9)	0.0635 (11)	−0.0019 (7)	0.0260 (9)
F4B	0.0746 (11)	0.0881 (12)	0.0421 (9)	0.0411 (10)	−0.0204 (8)	−0.0242 (8)
F5B	0.0436 (7)	0.0329 (7)	0.0528 (9)	0.0185 (6)	0.0031 (6)	−0.0045 (6)
N1B	0.0220 (8)	0.0198 (8)	0.0217 (8)	0.0099 (7)	0.0039 (6)	0.0043 (7)
N2B	0.0285 (9)	0.0272 (9)	0.0258 (9)	0.0157 (8)	0.0071 (7)	0.0081 (7)
N3B	0.0198 (8)	0.0287 (9)	0.0209 (9)	0.0113 (7)	0.0035 (7)	0.0034 (7)
N4B	0.0208 (8)	0.0373 (11)	0.0298 (10)	0.0109 (8)	0.0018 (7)	−0.0047 (8)
N5B	0.0204 (8)	0.0239 (9)	0.0257 (9)	0.0092 (7)	0.0024 (7)	0.0010 (7)
N6B	0.0235 (8)	0.0233 (9)	0.0294 (9)	0.0106 (7)	0.0047 (7)	0.0075 (7)
C1B	0.0224 (9)	0.0254 (10)	0.0217 (10)	0.0124 (8)	0.0057 (8)	0.0063 (8)
C2B	0.0245 (10)	0.0259 (10)	0.0221 (10)	0.0121 (9)	0.0059 (8)	0.0023 (8)
C3B	0.0291 (11)	0.0353 (12)	0.0233 (11)	0.0165 (10)	0.0040 (8)	0.0015 (9)
C4B	0.0314 (11)	0.0428 (13)	0.0243 (11)	0.0141 (10)	−0.0003 (9)	−0.0046 (10)
C5B	0.0330 (12)	0.0331 (12)	0.0296 (12)	0.0043 (10)	0.0043 (9)	−0.0082 (10)
C6B	0.0360 (12)	0.0228 (11)	0.0286 (12)	0.0077 (9)	0.0101 (9)	0.0001 (9)
C7B	0.0269 (10)	0.0244 (10)	0.0226 (10)	0.0121 (9)	0.0067 (8)	0.0014 (8)
C8B	0.0250 (10)	0.0207 (10)	0.0259 (11)	0.0121 (8)	0.0075 (8)	0.0038 (8)
C9B	0.0241 (10)	0.0323 (11)	0.0254 (11)	0.0167 (9)	0.0081 (8)	0.0097 (9)
C10B	0.0269 (10)	0.0475 (13)	0.0272 (11)	0.0245 (10)	0.0087 (9)	0.0146 (10)
C11B	0.0436 (13)	0.0567 (15)	0.0385 (14)	0.0341 (12)	0.0157 (11)	0.0250 (11)
C12B	0.0626 (17)	0.080 (2)	0.0411 (15)	0.0474 (16)	0.0236 (13)	0.0373 (15)
C13B	0.0678 (18)	0.096 (2)	0.0279 (14)	0.0536 (18)	0.0158 (13)	0.0234 (15)
C14B	0.0447 (13)	0.0743 (18)	0.0239 (12)	0.0368 (13)	0.0045 (10)	0.0069 (12)

C15B	0.0256 (10)	0.0527 (14)	0.0252 (11)	0.0243 (11)	0.0032 (9)	0.0068 (10)
C16B	0.0186 (9)	0.0428 (13)	0.0211 (11)	0.0145 (9)	0.0017 (8)	0.0006 (9)
C17B	0.0186 (9)	0.0293 (11)	0.0316 (12)	0.0080 (9)	0.0033 (8)	−0.0035 (9)
C18B	0.0192 (10)	0.0246 (11)	0.0476 (14)	0.0063 (9)	0.0079 (9)	−0.0025 (10)
C19B	0.0286 (11)	0.0307 (12)	0.0604 (16)	0.0084 (10)	0.0090 (11)	−0.0096 (11)
C20B	0.0322 (12)	0.0245 (12)	0.089 (2)	0.0108 (10)	0.0141 (13)	−0.0098 (13)
C21B	0.0287 (12)	0.0230 (12)	0.086 (2)	0.0117 (10)	0.0064 (13)	0.0039 (12)
C22B	0.0230 (10)	0.0259 (11)	0.0642 (16)	0.0105 (9)	0.0062 (10)	0.0076 (11)
C23B	0.0175 (9)	0.0205 (10)	0.0476 (14)	0.0056 (8)	0.0075 (9)	0.0033 (9)
C24B	0.0193 (9)	0.0227 (10)	0.0330 (12)	0.0090 (8)	0.0061 (8)	0.0065 (9)
C25B	0.0192 (9)	0.0314 (11)	0.0247 (11)	0.0129 (9)	0.0064 (8)	0.0054 (9)
C26B	0.0256 (10)	0.0330 (12)	0.0311 (12)	0.0141 (9)	0.0049 (9)	0.0061 (9)
C27B	0.0325 (12)	0.0432 (14)	0.0441 (14)	0.0226 (11)	0.0075 (10)	0.0188 (11)
C28B	0.0382 (13)	0.0706 (18)	0.0314 (13)	0.0335 (13)	0.0032 (10)	0.0161 (12)
C29B	0.0352 (12)	0.0589 (16)	0.0273 (12)	0.0238 (12)	−0.0037 (10)	−0.0102 (11)
C30B	0.0253 (10)	0.0339 (12)	0.0348 (12)	0.0165 (10)	0.0041 (9)	0.0003 (10)
B1B	0.0207 (10)	0.0252 (12)	0.0217 (11)	0.0120 (9)	0.0027 (9)	0.0037 (9)

Geometric parameters (Å, º)

S1A—C25A	1.7679 (19)	S1B—C25B	1.7608 (19)
S1A—B1A	1.955 (2)	S1B—B1B	1.958 (2)
F1A—C26A	1.346 (2)	F1B—C26B	1.340 (2)
F2A—C27A	1.344 (2)	F2B—C27B	1.347 (2)
F3A—C28A	1.341 (2)	F3B—C28B	1.341 (2)
F4A—C29A	1.346 (2)	F4B—C29B	1.338 (3)
F5A—C30A	1.344 (2)	F5B—C30B	1.339 (2)
N1A—C8A	1.369 (2)	N1B—C1B	1.366 (2)
N1A—C1A	1.369 (2)	N1B—C8B	1.376 (2)
N1A—B1A	1.486 (3)	N1B—B1B	1.481 (3)
N2A—C9A	1.339 (2)	N2B—C8B	1.346 (2)
N2A—C8A	1.343 (2)	N2B—C9B	1.347 (3)
N3A—C16A	1.371 (2)	N3B—C9B	1.361 (2)
N3A—C9A	1.371 (2)	N3B—C16B	1.366 (2)
N3A—B1A	1.484 (3)	N3B—B1B	1.468 (3)
N4A—C17A	1.342 (2)	N4B—C17B	1.343 (3)
N4A—C16A	1.343 (2)	N4B—C16B	1.349 (3)
N5A—C24A	1.367 (2)	N5B—C17B	1.368 (2)
N5A—C17A	1.370 (2)	N5B—C24B	1.369 (2)
N5A—B1A	1.489 (3)	N5B—B1B	1.487 (3)
N6A—C24A	1.345 (2)	N6B—C1B	1.345 (2)
N6A—C1A	1.346 (2)	N6B—C24B	1.345 (2)
C1A—C2A	1.455 (3)	C1B—C2B	1.457 (3)
C2A—C3A	1.395 (3)	C2B—C3B	1.391 (3)
C2A—C7A	1.424 (3)	C2B—C7B	1.422 (3)
C3A—C4A	1.386 (3)	C3B—C4B	1.383 (3)
C3A—H3AA	0.9500	C3B—H3BA	0.9500
C4A—C5A	1.399 (3)	C4B—C5B	1.397 (3)

C4A—H4AA	0.9500	C4B—H4BA	0.9500
C5A—C6A	1.378 (3)	C5B—C6B	1.379 (3)
C5A—H5AA	0.9500	C5B—H5BA	0.9500
C6A—C7A	1.394 (3)	C6B—C7B	1.389 (3)
C6A—H6AA	0.9500	C6B—H6BA	0.9500
C7A—C8A	1.444 (3)	C7B—C8B	1.456 (3)
C9A—C10A	1.456 (3)	C9B—C10B	1.460 (3)
C10A—C11A	1.387 (3)	C10B—C11B	1.397 (3)
C10A—C15A	1.421 (3)	C10B—C15B	1.424 (3)
C11A—C12A	1.385 (3)	C11B—C12B	1.389 (3)
C11A—H11A	0.9500	C11B—H11B	0.9500
C12A—C13A	1.397 (3)	C12B—C13B	1.390 (4)
C12A—H12A	0.9500	C12B—H12B	0.9500
C13A—C14A	1.387 (3)	C13B—C14B	1.383 (4)
C13A—H13A	0.9500	C13B—H13B	0.9500
C14A—C15A	1.394 (3)	C14B—C15B	1.397 (3)
C14A—H14A	0.9500	C14B—H14B	0.9500
C15A—C16A	1.453 (3)	C15B—C16B	1.455 (3)
C17A—C18A	1.456 (3)	C17B—C18B	1.457 (3)
C18A—C19A	1.398 (3)	C18B—C19B	1.395 (3)
C18A—C23A	1.417 (3)	C18B—C23B	1.418 (3)
C19A—C20A	1.381 (3)	C19B—C20B	1.380 (3)
C19A—H19A	0.9500	C19B—H19B	0.9500
C20A—C21A	1.400 (3)	C20B—C21B	1.393 (4)
C20A—H20A	0.9500	C20B—H20B	0.9500
C21A—C22A	1.383 (3)	C21B—C22B	1.380 (3)
C21A—H21A	0.9500	C21B—H21B	0.9500
C22A—C23A	1.395 (3)	C22B—C23B	1.396 (3)
C22A—H22A	0.9500	C22B—H22B	0.9500
C23A—C24A	1.450 (3)	C23B—C24B	1.459 (3)
C25A—C30A	1.386 (3)	C25B—C30B	1.389 (3)
C25A—C26A	1.388 (3)	C25B—C26B	1.390 (3)
C26A—C27A	1.378 (3)	C26B—C27B	1.379 (3)
C27A—C28A	1.369 (3)	C27B—C28B	1.364 (3)
C28A—C29A	1.366 (3)	C28B—C29B	1.376 (3)
C29A—C30A	1.380 (3)	C29B—C30B	1.382 (3)

C25A—S1A—B1A	95.25 (9)	C25B—S1B—B1B	100.93 (9)
C8A—N1A—C1A	112.74 (15)	C1B—N1B—C8B	112.98 (15)
C8A—N1A—B1A	122.29 (16)	C1B—N1B—B1B	123.47 (15)
C1A—N1A—B1A	123.18 (15)	C8B—N1B—B1B	121.84 (15)
C9A—N2A—C8A	116.86 (16)	C8B—N2B—C9B	116.87 (16)
C16A—N3A—C9A	112.63 (15)	C9B—N3B—C16B	114.69 (16)
C16A—N3A—B1A	122.86 (16)	C9B—N3B—B1B	122.56 (16)
C9A—N3A—B1A	122.64 (15)	C16B—N3B—B1B	122.52 (17)
C17A—N4A—C16A	116.84 (15)	C17B—N4B—C16B	117.07 (17)
C24A—N5A—C17A	112.72 (15)	C17B—N5B—C24B	113.19 (16)
C24A—N5A—B1A	123.01 (15)	C17B—N5B—B1B	122.36 (16)

C17A—N5A—B1A	122.26 (16)	C24B—N5B—B1B	122.91 (16)
C24A—N6A—C1A	116.87 (16)	C1B—N6B—C24B	116.82 (16)
N6A—C1A—N1A	122.72 (16)	N6B—C1B—N1B	122.63 (17)
N6A—C1A—C2A	129.83 (17)	N6B—C1B—C2B	130.16 (16)
N1A—C1A—C2A	105.55 (16)	N1B—C1B—C2B	105.71 (15)
C3A—C2A—C7A	120.40 (18)	C3B—C2B—C7B	120.70 (18)
C3A—C2A—C1A	132.43 (18)	C3B—C2B—C1B	132.07 (18)
C7A—C2A—C1A	106.97 (16)	C7B—C2B—C1B	107.08 (16)
C4A—C3A—C2A	118.01 (19)	C4B—C3B—C2B	117.91 (19)
C4A—C3A—H3AA	121.0	C4B—C3B—H3BA	121.0
C2A—C3A—H3AA	121.0	C2B—C3B—H3BA	121.0
C3A—C4A—C5A	121.27 (19)	C3B—C4B—C5B	121.2 (2)
C3A—C4A—H4AA	119.4	C3B—C4B—H4BA	119.4
C5A—C4A—H4AA	119.4	C5B—C4B—H4BA	119.4
C6A—C5A—C4A	121.61 (19)	C6B—C5B—C4B	121.6 (2)
C6A—C5A—H5AA	119.2	C6B—C5B—H5BA	119.2
C4A—C5A—H5AA	119.2	C4B—C5B—H5BA	119.2
C5A—C6A—C7A	118.01 (19)	C5B—C6B—C7B	118.1 (2)
C5A—C6A—H6AA	121.0	C5B—C6B—H6BA	121.0
C7A—C6A—H6AA	121.0	C7B—C6B—H6BA	121.0
C6A—C7A—C2A	120.69 (18)	C6B—C7B—C2B	120.49 (18)
C6A—C7A—C8A	131.67 (19)	C6B—C7B—C8B	131.90 (18)
C2A—C7A—C8A	107.36 (16)	C2B—C7B—C8B	107.43 (16)
N2A—C8A—N1A	123.01 (16)	N2B—C8B—N1B	122.60 (17)
N2A—C8A—C7A	129.21 (17)	N2B—C8B—C7B	130.50 (17)
N1A—C8A—C7A	105.73 (16)	N1B—C8B—C7B	105.37 (15)
N2A—C9A—N3A	123.00 (17)	N2B—C9B—N3B	122.19 (17)
N2A—C9A—C10A	129.34 (18)	N2B—C9B—C10B	131.59 (18)
N3A—C9A—C10A	105.93 (16)	N3B—C9B—C10B	104.77 (17)
C11A—C10A—C15A	120.83 (18)	C11B—C10B—C15B	120.9 (2)
C11A—C10A—C9A	131.68 (18)	C11B—C10B—C9B	131.6 (2)
C15A—C10A—C9A	107.07 (17)	C15B—C10B—C9B	107.30 (18)
C12A—C11A—C10A	118.2 (2)	C12B—C11B—C10B	117.1 (2)
C12A—C11A—H11A	120.9	C12B—C11B—H11B	121.4
C10A—C11A—H11A	120.9	C10B—C11B—H11B	121.4
C11A—C12A—C13A	121.3 (2)	C11B—C12B—C13B	121.6 (2)
C11A—C12A—H12A	119.4	C11B—C12B—H12B	119.2
C13A—C12A—H12A	119.4	C13B—C12B—H12B	119.2
C14A—C13A—C12A	121.29 (19)	C14B—C13B—C12B	122.4 (2)
C14A—C13A—H13A	119.4	C14B—C13B—H13B	118.8
C12A—C13A—H13A	119.4	C12B—C13B—H13B	118.8
C13A—C14A—C15A	118.08 (19)	C13B—C14B—C15B	117.0 (2)
C13A—C14A—H14A	121.0	C13B—C14B—H14B	121.5
C15A—C14A—H14A	121.0	C15B—C14B—H14B	121.5
C14A—C15A—C10A	120.35 (19)	C14B—C15B—C10B	120.9 (2)
C14A—C15A—C16A	131.84 (18)	C14B—C15B—C16B	131.4 (2)
C10A—C15A—C16A	107.36 (16)	C10B—C15B—C16B	107.52 (17)
N4A—C16A—N3A	122.66 (17)	N4B—C16B—N3B	122.09 (18)

N4A—C16A—C15A	129.55 (16)	N4B—C16B—C15B	131.92 (18)
N3A—C16A—C15A	105.83 (16)	N3B—C16B—C15B	104.74 (18)
N4A—C17A—N5A	123.08 (16)	N4B—C17B—N5B	122.35 (18)
N4A—C17A—C18A	129.28 (16)	N4B—C17B—C18B	130.83 (18)
N5A—C17A—C18A	105.48 (16)	N5B—C17B—C18B	105.38 (17)
C19A—C18A—C23A	120.70 (18)	C19B—C18B—C23B	120.1 (2)
C19A—C18A—C17A	131.89 (18)	C19B—C18B—C17B	132.3 (2)
C23A—C18A—C17A	107.21 (16)	C23B—C18B—C17B	107.44 (17)
C20A—C19A—C18A	117.88 (19)	C20B—C19B—C18B	117.8 (2)
C20A—C19A—H19A	121.1	C20B—C19B—H19B	121.1
C18A—C19A—H19A	121.1	C18B—C19B—H19B	121.1
C19A—C20A—C21A	121.30 (19)	C19B—C20B—C21B	122.1 (2)
C19A—C20A—H20A	119.4	C19B—C20B—H20B	118.9
C21A—C20A—H20A	119.4	C21B—C20B—H20B	118.9
C22A—C21A—C20A	121.62 (19)	C22B—C21B—C20B	121.0 (2)
C22A—C21A—H21A	119.2	C22B—C21B—H21B	119.5
C20A—C21A—H21A	119.2	C20B—C21B—H21B	119.5
C21A—C22A—C23A	117.76 (19)	C21B—C22B—C23B	117.8 (2)
C21A—C22A—H22A	121.1	C21B—C22B—H22B	121.1
C23A—C22A—H22A	121.1	C23B—C22B—H22B	121.1
C22A—C23A—C18A	120.67 (17)	C22B—C23B—C18B	121.08 (19)
C22A—C23A—C24A	131.79 (18)	C22B—C23B—C24B	131.7 (2)
C18A—C23A—C24A	107.26 (16)	C18B—C23B—C24B	107.14 (17)
N6A—C24A—N5A	123.10 (16)	N6B—C24B—N5B	122.85 (16)
N6A—C24A—C23A	129.36 (17)	N6B—C24B—C23B	130.29 (17)
N5A—C24A—C23A	105.87 (15)	N5B—C24B—C23B	105.43 (17)
C30A—C25A—C26A	116.31 (18)	C30B—C25B—C26B	116.38 (18)
C30A—C25A—S1A	121.85 (15)	C30B—C25B—S1B	122.24 (15)
C26A—C25A—S1A	121.84 (15)	C26B—C25B—S1B	121.38 (15)
F1A—C26A—C27A	117.95 (18)	F1B—C26B—C27B	117.55 (19)
F1A—C26A—C25A	119.92 (17)	F1B—C26B—C25B	120.24 (18)
C27A—C26A—C25A	122.12 (19)	C27B—C26B—C25B	122.2 (2)
F2A—C27A—C28A	119.74 (19)	F2B—C27B—C28B	119.8 (2)
F2A—C27A—C26A	120.62 (19)	F2B—C27B—C26B	120.3 (2)
C28A—C27A—C26A	119.6 (2)	C28B—C27B—C26B	119.9 (2)
F3A—C28A—C29A	120.0 (2)	F3B—C28B—C27B	120.3 (2)
F3A—C28A—C27A	119.9 (2)	F3B—C28B—C29B	119.8 (2)
C29A—C28A—C27A	120.07 (19)	C27B—C28B—C29B	119.8 (2)
F4A—C29A—C28A	120.06 (19)	F4B—C29B—C28B	119.9 (2)
F4A—C29A—C30A	120.2 (2)	F4B—C29B—C30B	120.2 (2)
C28A—C29A—C30A	119.73 (19)	C28B—C29B—C30B	119.9 (2)
F5A—C30A—C29A	117.86 (18)	F5B—C30B—C29B	118.04 (19)
F5A—C30A—C25A	120.04 (17)	F5B—C30B—C25B	120.16 (18)
C29A—C30A—C25A	122.10 (19)	C29B—C30B—C25B	121.8 (2)
N3A—B1A—N1A	105.58 (15)	N3B—B1B—N1B	105.47 (16)
N3A—B1A—N5A	105.31 (15)	N3B—B1B—N5B	105.02 (15)
N1A—B1A—N5A	105.43 (15)	N1B—B1B—N5B	105.31 (15)
N3A—B1A—S1A	113.72 (14)	N3B—B1B—S1B	111.66 (13)

N1A—B1A—S1A	111.33 (13)	N1B—B1B—S1B	113.09 (13)
N5A—B1A—S1A	114.69 (14)	N5B—B1B—S1B	115.45 (14)
C24A—N6A—C1A—N1A	−6.8 (3)	C24B—N6B—C1B—N1B	−8.5 (3)
C24A—N6A—C1A—C2A	155.10 (18)	C24B—N6B—C1B—C2B	155.41 (19)
C8A—N1A—C1A—N6A	153.15 (17)	C8B—N1B—C1B—N6B	154.90 (17)
B1A—N1A—C1A—N6A	−11.9 (3)	B1B—N1B—C1B—N6B	−10.4 (3)
C8A—N1A—C1A—C2A	−12.54 (19)	C8B—N1B—C1B—C2B	−12.4 (2)
B1A—N1A—C1A—C2A	−177.56 (15)	B1B—N1B—C1B—C2B	−177.74 (16)
N6A—C1A—C2A—C3A	16.9 (3)	N6B—C1B—C2B—C3B	17.3 (3)
N1A—C1A—C2A—C3A	−178.82 (19)	N1B—C1B—C2B—C3B	−176.70 (19)
N6A—C1A—C2A—C7A	−157.83 (18)	N6B—C1B—C2B—C7B	−158.19 (19)
N1A—C1A—C2A—C7A	6.46 (19)	N1B—C1B—C2B—C7B	7.80 (19)
C7A—C2A—C3A—C4A	−0.4 (3)	C7B—C2B—C3B—C4B	0.0 (3)
C1A—C2A—C3A—C4A	−174.53 (19)	C1B—C2B—C3B—C4B	−175.04 (19)
C2A—C3A—C4A—C5A	0.0 (3)	C2B—C3B—C4B—C5B	1.2 (3)
C3A—C4A—C5A—C6A	0.5 (3)	C3B—C4B—C5B—C6B	−1.0 (3)
C4A—C5A—C6A—C7A	−0.6 (3)	C4B—C5B—C6B—C7B	−0.5 (3)
C5A—C6A—C7A—C2A	0.2 (3)	C5B—C6B—C7B—C2B	1.6 (3)
C5A—C6A—C7A—C8A	173.23 (19)	C5B—C6B—C7B—C8B	176.15 (19)
C3A—C2A—C7A—C6A	0.3 (3)	C3B—C2B—C7B—C6B	−1.4 (3)
C1A—C2A—C7A—C6A	175.80 (16)	C1B—C2B—C7B—C6B	174.71 (17)
C3A—C2A—C7A—C8A	−174.25 (16)	C3B—C2B—C7B—C8B	−177.13 (16)
C1A—C2A—C7A—C8A	1.23 (19)	C1B—C2B—C7B—C8B	−1.0 (2)
C9A—N2A—C8A—N1A	7.0 (3)	C9B—N2B—C8B—N1B	9.5 (2)
C9A—N2A—C8A—C7A	−154.32 (18)	C9B—N2B—C8B—C7B	−154.26 (18)
C1A—N1A—C8A—N2A	−151.72 (17)	C1B—N1B—C8B—N2B	−155.48 (16)
B1A—N1A—C8A—N2A	13.5 (3)	B1B—N1B—C8B—N2B	10.1 (3)
C1A—N1A—C8A—C7A	13.34 (19)	C1B—N1B—C8B—C7B	11.7 (2)
B1A—N1A—C8A—C7A	178.51 (15)	B1B—N1B—C8B—C7B	177.36 (15)
C6A—C7A—C8A—N2A	−18.4 (3)	C6B—C7B—C8B—N2B	−15.3 (3)
C2A—C7A—C8A—N2A	155.33 (18)	C2B—C7B—C8B—N2B	159.74 (18)
C6A—C7A—C8A—N1A	177.79 (18)	C6B—C7B—C8B—N1B	178.87 (19)
C2A—C7A—C8A—N1A	−8.47 (19)	C2B—C7B—C8B—N1B	−6.09 (19)
C8A—N2A—C9A—N3A	−9.0 (3)	C8B—N2B—C9B—N3B	−6.3 (2)
C8A—N2A—C9A—C10A	153.80 (19)	C8B—N2B—C9B—C10B	157.78 (18)
C16A—N3A—C9A—N2A	155.46 (17)	C16B—N3B—C9B—N2B	157.76 (16)
B1A—N3A—C9A—N2A	−9.4 (3)	B1B—N3B—C9B—N2B	−16.9 (3)
C16A—N3A—C9A—C10A	−10.8 (2)	C16B—N3B—C9B—C10B	−10.0 (2)
B1A—N3A—C9A—C10A	−175.61 (16)	B1B—N3B—C9B—C10B	175.33 (15)
N2A—C9A—C10A—C11A	13.2 (3)	N2B—C9B—C10B—C11B	14.0 (3)
N3A—C9A—C10A—C11A	178.3 (2)	N3B—C9B—C10B—C11B	−179.86 (19)
N2A—C9A—C10A—C15A	−159.18 (19)	N2B—C9B—C10B—C15B	−160.80 (19)
N3A—C9A—C10A—C15A	5.9 (2)	N3B—C9B—C10B—C15B	5.31 (19)
C15A—C10A—C11A—C12A	−1.1 (3)	C15B—C10B—C11B—C12B	−1.2 (3)
C9A—C10A—C11A—C12A	−172.6 (2)	C9B—C10B—C11B—C12B	−175.47 (19)
C10A—C11A—C12A—C13A	0.8 (3)	C10B—C11B—C12B—C13B	0.7 (3)
C11A—C12A—C13A—C14A	0.3 (3)	C11B—C12B—C13B—C14B	0.6 (4)

C12A—C13A—C14A—C15A	−1.0 (3)	C12B—C13B—C14B—C15B	−1.4 (3)
C13A—C14A—C15A—C10A	0.7 (3)	C13B—C14B—C15B—C10B	0.8 (3)
C13A—C14A—C15A—C16A	171.95 (19)	C13B—C14B—C15B—C16B	175.0 (2)
C11A—C10A—C15A—C14A	0.3 (3)	C11B—C10B—C15B—C14B	0.5 (3)
C9A—C10A—C15A—C14A	173.74 (17)	C9B—C10B—C15B—C14B	175.99 (17)
C11A—C10A—C15A—C16A	−172.86 (17)	C11B—C10B—C15B—C16B	−174.97 (17)
C9A—C10A—C15A—C16A	0.5 (2)	C9B—C10B—C15B—C16B	0.5 (2)
C17A—N4A—C16A—N3A	9.3 (3)	C17B—N4B—C16B—N3B	6.9 (3)
C17A—N4A—C16A—C15A	−152.40 (19)	C17B—N4B—C16B—C15B	−158.25 (19)
C9A—N3A—C16A—N4A	−154.32 (17)	C9B—N3B—C16B—N4B	−158.29 (17)
B1A—N3A—C16A—N4A	10.5 (3)	B1B—N3B—C16B—N4B	16.4 (3)
C9A—N3A—C16A—C15A	11.1 (2)	C9B—N3B—C16B—C15B	10.3 (2)
B1A—N3A—C16A—C15A	175.90 (16)	B1B—N3B—C16B—C15B	−175.01 (15)
C14A—C15A—C16A—N4A	−14.8 (3)	C14B—C15B—C16B—N4B	−13.9 (4)
C10A—C15A—C16A—N4A	157.29 (19)	C10B—C15B—C16B—N4B	160.87 (19)
C14A—C15A—C16A—N3A	−178.9 (2)	C14B—C15B—C16B—N3B	179.1 (2)
C10A—C15A—C16A—N3A	−6.8 (2)	C10B—C15B—C16B—N3B	−6.1 (2)
C16A—N4A—C17A—N5A	−8.4 (3)	C16B—N4B—C17B—N5B	−9.5 (3)
C16A—N4A—C17A—C18A	152.33 (18)	C16B—N4B—C17B—C18B	154.72 (19)
C24A—N5A—C17A—N4A	152.10 (17)	C24B—N5B—C17B—N4B	155.44 (17)
B1A—N5A—C17A—N4A	−12.2 (3)	B1B—N5B—C17B—N4B	−10.7 (3)
C24A—N5A—C17A—C18A	−12.5 (2)	C24B—N5B—C17B—C18B	−12.2 (2)
B1A—N5A—C17A—C18A	−176.86 (16)	B1B—N5B—C17B—C18B	−178.41 (16)
N4A—C17A—C18A—C19A	19.3 (3)	N4B—C17B—C18B—C19B	16.7 (4)
N5A—C17A—C18A—C19A	−177.40 (19)	N5B—C17B—C18B—C19B	−177.1 (2)
N4A—C17A—C18A—C23A	−155.39 (19)	N4B—C17B—C18B—C23B	−158.9 (2)
N5A—C17A—C18A—C23A	7.9 (2)	N5B—C17B—C18B—C23B	7.3 (2)
C23A—C18A—C19A—C20A	−0.5 (3)	C23B—C18B—C19B—C20B	−1.8 (3)
C17A—C18A—C19A—C20A	−174.55 (19)	C17B—C18B—C19B—C20B	−176.9 (2)
C18A—C19A—C20A—C21A	2.3 (3)	C18B—C19B—C20B—C21B	1.6 (3)
C19A—C20A—C21A—C22A	−1.8 (3)	C19B—C20B—C21B—C22B	−0.2 (4)
C20A—C21A—C22A—C23A	−0.6 (3)	C20B—C21B—C22B—C23B	−1.0 (3)
C21A—C22A—C23A—C18A	2.3 (3)	C21B—C22B—C23B—C18B	0.8 (3)
C21A—C22A—C23A—C24A	175.47 (19)	C21B—C22B—C23B—C24B	177.4 (2)
C19A—C18A—C23A—C22A	−1.9 (3)	C19B—C18B—C23B—C22B	0.6 (3)
C17A—C18A—C23A—C22A	173.52 (17)	C17B—C18B—C23B—C22B	176.85 (17)
C19A—C18A—C23A—C24A	−176.50 (17)	C19B—C18B—C23B—C24B	−176.74 (18)
C17A—C18A—C23A—C24A	−1.1 (2)	C17B—C18B—C23B—C24B	−0.5 (2)
C1A—N6A—C24A—N5A	7.9 (3)	C1B—N6B—C24B—N5B	8.5 (3)
C1A—N6A—C24A—C23A	−155.16 (18)	C1B—N6B—C24B—C23B	−155.83 (19)
C17A—N5A—C24A—N6A	−154.60 (17)	C17B—N5B—C24B—N6B	−155.70 (17)
B1A—N5A—C24A—N6A	9.6 (3)	B1B—N5B—C24B—N6B	10.4 (3)
C17A—N5A—C24A—C23A	11.9 (2)	C17B—N5B—C24B—C23B	11.9 (2)
B1A—N5A—C24A—C23A	176.07 (16)	B1B—N5B—C24B—C23B	178.02 (16)
C22A—C23A—C24A—N6A	−14.6 (3)	C22B—C23B—C24B—N6B	−17.1 (4)
C18A—C23A—C24A—N6A	159.18 (18)	C18B—C23B—C24B—N6B	159.83 (19)
C22A—C23A—C24A—N5A	−179.97 (19)	C22B—C23B—C24B—N5B	176.5 (2)
C18A—C23A—C24A—N5A	−6.1 (2)	C18B—C23B—C24B—N5B	−6.5 (2)

B1A—S1A—C25A—C30A	−93.53 (17)	B1B—S1B—C25B—C30B	−84.01 (17)
B1A—S1A—C25A—C26A	85.40 (17)	B1B—S1B—C25B—C26B	96.28 (17)
C30A—C25A—C26A—F1A	−178.39 (17)	C30B—C25B—C26B—F1B	179.89 (17)
S1A—C25A—C26A—F1A	2.6 (3)	S1B—C25B—C26B—F1B	−0.4 (3)
C30A—C25A—C26A—C27A	2.2 (3)	C30B—C25B—C26B—C27B	−0.1 (3)
S1A—C25A—C26A—C27A	−176.77 (16)	S1B—C25B—C26B—C27B	179.64 (16)
F1A—C26A—C27A—F2A	0.0 (3)	F1B—C26B—C27B—F2B	1.0 (3)
C25A—C26A—C27A—F2A	179.41 (18)	C25B—C26B—C27B—F2B	−179.01 (18)
F1A—C26A—C27A—C28A	179.43 (19)	F1B—C26B—C27B—C28B	−179.61 (19)
C25A—C26A—C27A—C28A	−1.2 (3)	C25B—C26B—C27B—C28B	0.4 (3)
F2A—C27A—C28A—F3A	−0.4 (3)	F2B—C27B—C28B—F3B	0.1 (3)
C26A—C27A—C28A—F3A	−179.9 (2)	C26B—C27B—C28B—F3B	−179.34 (19)
F2A—C27A—C28A—C29A	179.0 (2)	F2B—C27B—C28B—C29B	179.0 (2)
C26A—C27A—C28A—C29A	−0.5 (3)	C26B—C27B—C28B—C29B	−0.4 (3)
F3A—C28A—C29A—F4A	0.9 (3)	F3B—C28B—C29B—F4B	−0.1 (3)
C27A—C28A—C29A—F4A	−178.5 (2)	C27B—C28B—C29B—F4B	−179.1 (2)
F3A—C28A—C29A—C30A	−179.7 (2)	F3B—C28B—C29B—C30B	179.10 (19)
C27A—C28A—C29A—C30A	0.9 (3)	C27B—C28B—C29B—C30B	0.2 (3)
F4A—C29A—C30A—F5A	−1.1 (3)	F4B—C29B—C30B—F5B	−1.2 (3)
C28A—C29A—C30A—F5A	179.53 (19)	C28B—C29B—C30B—F5B	179.53 (19)
F4A—C29A—C30A—C25A	179.61 (18)	F4B—C29B—C30B—C25B	179.37 (19)
C28A—C29A—C30A—C25A	0.2 (3)	C28B—C29B—C30B—C25B	0.1 (3)
C26A—C25A—C30A—F5A	178.96 (17)	C26B—C25B—C30B—F5B	−179.54 (17)
S1A—C25A—C30A—F5A	−2.0 (3)	S1B—C25B—C30B—F5B	0.7 (3)
C26A—C25A—C30A—C29A	−1.7 (3)	C26B—C25B—C30B—C29B	−0.2 (3)
S1A—C25A—C30A—C29A	177.24 (16)	S1B—C25B—C30B—C29B	−179.89 (16)
C16A—N3A—B1A—N1A	−137.85 (16)	C9B—N3B—B1B—N1B	31.7 (2)
C9A—N3A—B1A—N1A	25.4 (2)	C16B—N3B—B1B—N1B	−142.52 (16)
C16A—N3A—B1A—N5A	−26.6 (2)	C9B—N3B—B1B—N5B	142.72 (16)
C9A—N3A—B1A—N5A	136.68 (16)	C16B—N3B—B1B—N5B	−31.5 (2)
C16A—N3A—B1A—S1A	99.80 (18)	C9B—N3B—B1B—S1B	−91.46 (18)
C9A—N3A—B1A—S1A	−96.93 (18)	C16B—N3B—B1B—S1B	94.28 (18)
C8A—N1A—B1A—N3A	−27.3 (2)	C1B—N1B—B1B—N3B	135.81 (17)
C1A—N1A—B1A—N3A	136.30 (16)	C8B—N1B—B1B—N3B	−28.3 (2)
C8A—N1A—B1A—N5A	−138.50 (16)	C1B—N1B—B1B—N5B	25.0 (2)
C1A—N1A—B1A—N5A	25.1 (2)	C8B—N1B—B1B—N5B	−139.04 (16)
C8A—N1A—B1A—S1A	96.55 (17)	C1B—N1B—B1B—S1B	−101.90 (17)
C1A—N1A—B1A—S1A	−99.83 (17)	C8B—N1B—B1B—S1B	94.02 (18)
C24A—N5A—B1A—N3A	−135.37 (17)	C17B—N5B—B1B—N3B	28.8 (2)
C17A—N5A—B1A—N3A	27.3 (2)	C24B—N5B—B1B—N3B	−136.01 (17)
C24A—N5A—B1A—N1A	−24.0 (2)	C17B—N5B—B1B—N1B	139.91 (17)
C17A—N5A—B1A—N1A	138.70 (16)	C24B—N5B—B1B—N1B	−24.9 (2)
C24A—N5A—B1A—S1A	98.83 (18)	C17B—N5B—B1B—S1B	−94.60 (19)
C17A—N5A—B1A—S1A	−98.46 (18)	C24B—N5B—B1B—S1B	100.57 (18)

(4-Methylbenzenethiolato)(subphthalocyaninato)boron (d23112_a_tw_sq)

Crystal data

$C_{31}H_{19}BN_6S$
$M_r = 518.39$
Monoclinic, $C2/c$
$a = 49.653$ (4) Å
$b = 12.1268$ (10) Å
$c = 27.559$ (2) Å
$\beta = 114.838$ (4)°
$V = 15059$ (2) Å^3
$Z = 24$
$F(000) = 6432$
$D_x = 1.372$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 6283 reflections
$\theta = 3.5$–$62.5°$
$\mu = 1.41$ mm^{-1}
$T = 150$ K
Plate, pink
0.28 × 0.27 × 0.02 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.633$, $T_{max} = 0.753$
12819 measured reflections
12819 independent reflections
10107 reflections with $I > 2\sigma(I)$
$R_{int} = 0.091$
$\theta_{max} = 66.3°$, $\theta_{min} = 2.0°$
$h = -58 \rightarrow 58$
$k = -14 \rightarrow 14$
$l = -21 \rightarrow 32$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.098$
$wR(F^2) = 0.242$
$S = 1.09$
12819 reflections
1059 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 145.1404P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}
Extinction correction: SHELXL2019 (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00058 (4)

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. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.59339 (3)	0.51753 (12)	0.73057 (6)	0.0332 (4)
N1A	0.59808 (10)	0.5166 (4)	0.63321 (19)	0.0319 (11)
N2A	0.56798 (11)	0.3623 (4)	0.5883 (2)	0.0362 (12)
N3A	0.54799 (10)	0.5100 (4)	0.62041 (19)	0.0340 (11)
N4A	0.52161 (10)	0.6784 (4)	0.60952 (19)	0.0345 (11)
N5A	0.57430 (10)	0.6766 (4)	0.64365 (19)	0.0308 (11)

N6A	0.61955 (10)	0.6927 (4)	0.63371 (19)	0.0335 (11)
C1A	0.61884 (12)	0.5823 (5)	0.6276 (2)	0.0334 (13)
C2A	0.63308 (13)	0.5140 (5)	0.6021 (2)	0.0363 (14)
C3A	0.65616 (13)	0.5368 (6)	0.5868 (3)	0.0401 (15)
H3AA	0.666057	0.605947	0.594543	0.048*
C4A	0.66399 (14)	0.4552 (6)	0.5603 (3)	0.0452 (16)
H4AA	0.679585	0.468532	0.549612	0.054*
C5A	0.64946 (14)	0.3538 (6)	0.5487 (3)	0.0446 (16)
H5AA	0.655837	0.298714	0.531338	0.053*
C6A	0.62604 (14)	0.3308 (6)	0.5618 (2)	0.0413 (15)
H6AA	0.615838	0.262355	0.552509	0.050*
C7A	0.61790 (13)	0.4118 (5)	0.5892 (2)	0.0349 (14)
C8A	0.59385 (13)	0.4191 (5)	0.6056 (2)	0.0325 (13)
C9A	0.54495 (13)	0.4124 (5)	0.5934 (2)	0.0338 (13)
C10A	0.51306 (13)	0.3972 (5)	0.5631 (2)	0.0365 (14)
C11A	0.49668 (14)	0.3119 (6)	0.5302 (2)	0.0403 (15)
H11A	0.506026	0.247966	0.524520	0.048*
C12A	0.46574 (14)	0.3245 (6)	0.5058 (3)	0.0453 (16)
H12A	0.453893	0.266894	0.483772	0.054*
C13A	0.45193 (14)	0.4187 (6)	0.5129 (3)	0.0466 (17)
H13A	0.430901	0.423987	0.495932	0.056*
C14A	0.46833 (13)	0.5054 (6)	0.5444 (3)	0.0414 (15)
H14A	0.458900	0.570878	0.548139	0.050*
C15A	0.49906 (13)	0.4934 (6)	0.5703 (2)	0.0362 (14)
C16A	0.52231 (12)	0.5687 (5)	0.6040 (2)	0.0323 (13)
C17A	0.54772 (12)	0.7320 (5)	0.6269 (2)	0.0317 (13)
C18A	0.55452 (13)	0.8458 (5)	0.6203 (2)	0.0333 (13)
C19A	0.53729 (14)	0.9420 (6)	0.6065 (2)	0.0402 (15)
H19A	0.517001	0.939765	0.600476	0.048*
C20A	0.55014 (16)	1.0400 (6)	0.6019 (3)	0.0444 (16)
H20A	0.538811	1.106064	0.593581	0.053*
C21A	0.57980 (16)	1.0422 (6)	0.6095 (3)	0.0468 (16)
H21A	0.588281	1.110399	0.606119	0.056*
C22A	0.59720 (14)	0.9482 (5)	0.6217 (2)	0.0384 (14)
H22A	0.617209	0.950849	0.626024	0.046*
C23A	0.58454 (13)	0.8503 (5)	0.6274 (2)	0.0344 (13)
C24A	0.59621 (12)	0.7387 (5)	0.6388 (2)	0.0320 (13)
C25A	0.57037 (12)	0.5904 (5)	0.7551 (2)	0.0327 (13)
C26A	0.55151 (14)	0.5325 (6)	0.7712 (3)	0.0409 (15)
H26A	0.549561	0.454854	0.766458	0.049*
C27A	0.53520 (14)	0.5895 (6)	0.7946 (3)	0.0423 (16)
H27A	0.522325	0.549187	0.805590	0.051*
C28A	0.53746 (13)	0.7018 (6)	0.8019 (2)	0.0372 (14)
C29A	0.55642 (12)	0.7579 (5)	0.7854 (2)	0.0342 (13)
H29A	0.558272	0.835583	0.789992	0.041*
C30A	0.57274 (12)	0.7044 (5)	0.7623 (2)	0.0320 (13)
H30A	0.585579	0.745279	0.751451	0.038*
C31A	0.51886 (14)	0.7624 (7)	0.8245 (3)	0.0503 (18)

H31A	0.522446	0.841826	0.824314	0.075*
H31B	0.524201	0.737849	0.861285	0.075*
H31C	0.497821	0.746979	0.802649	0.075*
B1A	0.57748 (14)	0.5575 (6)	0.6563 (3)	0.0310 (14)
S1B	0.70480 (3)	0.12941 (13)	0.54527 (5)	0.0330 (4)
N1B	0.75052 (9)	0.1664 (4)	0.64832 (18)	0.0259 (10)
N2B	0.73408 (9)	0.3260 (4)	0.67907 (18)	0.0285 (10)
N3B	0.70331 (9)	0.1666 (4)	0.64869 (18)	0.0263 (10)
N4B	0.68356 (10)	−0.0029 (4)	0.66323 (18)	0.0282 (10)
N5B	0.72493 (9)	−0.0007 (4)	0.64095 (18)	0.0273 (10)
N6B	0.77646 (10)	−0.0037 (4)	0.66115 (18)	0.0293 (10)
C1B	0.77611 (12)	0.1075 (5)	0.6624 (2)	0.0276 (12)
C2B	0.80016 (12)	0.1853 (5)	0.6884 (2)	0.0288 (12)
C3B	0.83085 (12)	0.1732 (5)	0.7092 (2)	0.0303 (12)
H3BA	0.839539	0.105418	0.705949	0.036*
C4B	0.84822 (12)	0.2619 (5)	0.7346 (2)	0.0337 (13)
H4BA	0.869198	0.255873	0.748314	0.040*
C5B	0.83550 (12)	0.3618 (5)	0.7408 (2)	0.0323 (13)
H5BA	0.848048	0.421961	0.758434	0.039*
C6B	0.80492 (12)	0.3738 (5)	0.7216 (2)	0.0311 (13)
H6BA	0.796367	0.440026	0.727068	0.037*
C7B	0.78730 (11)	0.2855 (5)	0.6941 (2)	0.0271 (12)
C8B	0.75513 (12)	0.2692 (5)	0.6715 (2)	0.0275 (12)
C9B	0.70903 (12)	0.2702 (5)	0.6704 (2)	0.0267 (12)
C10B	0.68695 (12)	0.2891 (5)	0.6915 (2)	0.0287 (12)
C11B	0.68130 (12)	0.3792 (5)	0.7165 (2)	0.0317 (13)
H11B	0.692027	0.446073	0.720578	0.038*
C12B	0.65958 (13)	0.3696 (5)	0.7354 (2)	0.0366 (14)
H12B	0.654985	0.431143	0.751909	0.044*
C13B	0.64448 (12)	0.2709 (5)	0.7306 (2)	0.0356 (14)
H13B	0.629667	0.266694	0.743884	0.043*
C14B	0.65024 (12)	0.1797 (5)	0.7074 (2)	0.0302 (13)
H14B	0.640028	0.112341	0.705296	0.036*
C15B	0.67155 (11)	0.1880 (5)	0.6868 (2)	0.0286 (12)
C16B	0.68418 (11)	0.1081 (5)	0.6630 (2)	0.0274 (12)
C17B	0.70515 (12)	−0.0555 (5)	0.6548 (2)	0.0278 (12)
C18B	0.71713 (12)	−0.1672 (5)	0.6689 (2)	0.0336 (13)
C19B	0.70641 (14)	−0.2611 (5)	0.6833 (2)	0.0358 (14)
H19B	0.687557	−0.261993	0.684404	0.043*
C20B	0.72429 (15)	−0.3530 (6)	0.6958 (3)	0.0478 (17)
H20B	0.717224	−0.418854	0.705152	0.057*
C21B	0.75224 (15)	−0.3540 (5)	0.6956 (3)	0.0441 (16)
H21B	0.763789	−0.419539	0.704640	0.053*
C22B	0.76322 (13)	−0.2598 (5)	0.6821 (2)	0.0370 (14)
H22B	0.782448	−0.259470	0.682484	0.044*
C23B	0.74577 (13)	−0.1664 (5)	0.6680 (2)	0.0312 (13)
C24B	0.75077 (12)	−0.0554 (5)	0.6532 (2)	0.0300 (12)
C25B	0.67610 (12)	0.0277 (5)	0.5266 (2)	0.0323 (13)

C26B	0.65046 (12)	0.0452 (5)	0.5346 (2)	0.0354 (14)
H26B	0.647228	0.114717	0.547077	0.042*
C27B	0.62986 (13)	−0.0375 (6)	0.5245 (2)	0.0397 (15)
H27B	0.612757	−0.023714	0.530755	0.048*
C28B	0.63306 (14)	−0.1393 (6)	0.5056 (2)	0.0414 (15)
C29B	0.65804 (15)	−0.1544 (6)	0.4943 (3)	0.0473 (17)
H29B	0.660582	−0.222266	0.479532	0.057*
C30B	0.67888 (14)	−0.0714 (6)	0.5044 (2)	0.0412 (15)
H30B	0.695360	−0.082835	0.495964	0.049*
C31B	0.61155 (16)	−0.2325 (6)	0.4988 (3)	0.0531 (19)
H31D	0.611549	−0.250304	0.533455	0.080*
H31E	0.617600	−0.297530	0.484722	0.080*
H31F	0.591564	−0.209982	0.473728	0.080*
B1B	0.72051 (13)	0.1155 (5)	0.6211 (2)	0.0263 (13)
S1C	0.59674 (3)	0.00520 (14)	0.75499 (6)	0.0351 (4)
N1C	0.64464 (10)	−0.0089 (4)	0.85662 (19)	0.0343 (11)
N2C	0.66937 (12)	0.1610 (5)	0.8589 (2)	0.0444 (13)
N3C	0.61870 (10)	0.1582 (4)	0.84376 (19)	0.0350 (11)
N4C	0.57961 (12)	0.1708 (5)	0.8714 (2)	0.0413 (13)
N5C	0.59878 (10)	−0.0031 (4)	0.86186 (19)	0.0329 (11)
N6C	0.63067 (11)	−0.1585 (4)	0.89589 (19)	0.0381 (12)
C1C	0.65042 (13)	−0.1077 (5)	0.8820 (2)	0.0366 (14)
C2C	0.68224 (13)	−0.1231 (6)	0.9004 (2)	0.0433 (17)
C3C	0.70084 (16)	−0.2118 (7)	0.9261 (2)	0.055 (2)
H3C	0.693213	−0.277165	0.934668	0.066*
C4C	0.73082 (18)	−0.2007 (10)	0.9385 (3)	0.071 (3)
H4CA	0.743743	−0.261659	0.952994	0.085*
C5C	0.74220 (17)	−0.1016 (10)	0.9301 (3)	0.076 (3)
H5CA	0.763031	−0.095861	0.941152	0.091*
C6C	0.72503 (15)	−0.0121 (8)	0.9068 (3)	0.057 (2)
H6CA	0.733431	0.055046	0.901987	0.069*
C7C	0.69402 (13)	−0.0241 (7)	0.8902 (2)	0.0459 (18)
C8C	0.66960 (13)	0.0509 (6)	0.8652 (2)	0.0394 (15)
C9C	0.64407 (15)	0.2138 (6)	0.8515 (2)	0.0404 (15)
C10C	0.63896 (17)	0.3269 (6)	0.8620 (3)	0.0507 (18)
C11C	0.6560 (2)	0.4232 (7)	0.8700 (3)	0.066 (2)
H11C	0.674481	0.422407	0.867333	0.079*
C12C	0.6449 (3)	0.5191 (8)	0.8818 (3)	0.079 (3)
H12C	0.655796	0.585541	0.885750	0.095*
C13C	0.6183 (3)	0.5225 (7)	0.8882 (3)	0.079 (3)
H13C	0.611761	0.589764	0.897216	0.094*
C14C	0.6016 (2)	0.4263 (6)	0.8813 (3)	0.060 (2)
H14C	0.583765	0.426662	0.886015	0.072*
C15C	0.61181 (17)	0.3300 (6)	0.8672 (3)	0.0492 (17)
C16C	0.60011 (14)	0.2183 (6)	0.8584 (2)	0.0405 (15)
C17C	0.58067 (12)	0.0604 (6)	0.8761 (2)	0.0355 (14)
C18C	0.57047 (13)	−0.0113 (6)	0.9071 (2)	0.0382 (15)
C19C	0.55125 (14)	0.0084 (7)	0.9316 (3)	0.0495 (18)

H19C	0.540768	0.076079	0.926546	0.059*
C20C	0.54811 (14)	−0.0745 (8)	0.9634 (3)	0.054 (2)
H20C	0.535243	−0.063491	0.980550	0.064*
C21C	0.56364 (16)	−0.1745 (7)	0.9708 (3)	0.0526 (19)
H21C	0.560742	−0.230226	0.992365	0.063*
C22C	0.58285 (15)	−0.1937 (6)	0.9477 (2)	0.0454 (16)
H22C	0.593796	−0.260483	0.953975	0.055*
C23C	0.58581 (13)	−0.1113 (6)	0.9145 (2)	0.0371 (14)
C24C	0.60596 (13)	−0.1025 (5)	0.8889 (2)	0.0332 (13)
C25C	0.56426 (12)	0.0896 (5)	0.7315 (2)	0.0308 (13)
C26C	0.56611 (13)	0.2000 (5)	0.7208 (3)	0.0379 (14)
H26C	0.584909	0.231148	0.727599	0.045*
C27C	0.54095 (13)	0.2661 (6)	0.7002 (3)	0.0402 (15)
H27C	0.542897	0.341742	0.693317	0.048*
C28C	0.51321 (13)	0.2243 (5)	0.6896 (2)	0.0353 (14)
C29C	0.51136 (13)	0.1125 (5)	0.6996 (3)	0.0388 (15)
H29C	0.492510	0.080992	0.692196	0.047*
C30C	0.53641 (13)	0.0463 (5)	0.7202 (2)	0.0356 (14)
H30C	0.534470	−0.029607	0.726607	0.043*
C31C	0.48627 (15)	0.2975 (6)	0.6687 (3)	0.0513 (18)
H31I	0.492169	0.372800	0.664658	0.077*
H31J	0.477036	0.297331	0.693911	0.077*
H31G	0.472036	0.269956	0.633913	0.077*
B1C	0.61421 (14)	0.0393 (6)	0.8298 (3)	0.0312 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0307 (7)	0.0330 (8)	0.0379 (8)	0.0026 (6)	0.0165 (6)	0.0009 (6)
N1A	0.032 (2)	0.027 (3)	0.039 (3)	−0.001 (2)	0.017 (2)	−0.006 (2)
N2A	0.035 (3)	0.031 (3)	0.045 (3)	0.003 (2)	0.020 (2)	0.000 (2)
N3A	0.029 (2)	0.036 (3)	0.040 (3)	0.002 (2)	0.017 (2)	−0.003 (2)
N4A	0.031 (3)	0.037 (3)	0.037 (3)	−0.001 (2)	0.017 (2)	−0.005 (2)
N5A	0.029 (2)	0.029 (3)	0.036 (3)	0.004 (2)	0.015 (2)	−0.004 (2)
N6A	0.032 (3)	0.037 (3)	0.032 (3)	0.001 (2)	0.014 (2)	0.000 (2)
C1A	0.026 (3)	0.040 (4)	0.031 (3)	0.000 (3)	0.010 (2)	−0.003 (3)
C2A	0.031 (3)	0.043 (4)	0.033 (3)	0.006 (3)	0.012 (3)	0.000 (3)
C3A	0.032 (3)	0.046 (4)	0.046 (4)	0.004 (3)	0.021 (3)	0.000 (3)
C4A	0.039 (4)	0.051 (4)	0.053 (4)	0.010 (3)	0.027 (3)	−0.002 (3)
C5A	0.044 (4)	0.044 (4)	0.050 (4)	0.017 (3)	0.024 (3)	−0.002 (3)
C6A	0.043 (4)	0.040 (4)	0.042 (3)	0.014 (3)	0.019 (3)	0.000 (3)
C7A	0.033 (3)	0.036 (4)	0.038 (3)	0.007 (3)	0.017 (3)	0.002 (3)
C8A	0.033 (3)	0.028 (3)	0.034 (3)	0.003 (3)	0.012 (2)	−0.001 (2)
C9A	0.032 (3)	0.029 (3)	0.042 (3)	−0.001 (3)	0.018 (3)	−0.001 (3)
C10A	0.033 (3)	0.037 (4)	0.041 (3)	−0.002 (3)	0.017 (3)	−0.001 (3)
C11A	0.042 (4)	0.039 (4)	0.041 (3)	−0.007 (3)	0.019 (3)	−0.002 (3)
C12A	0.036 (3)	0.042 (4)	0.052 (4)	−0.010 (3)	0.013 (3)	0.000 (3)
C13A	0.029 (3)	0.059 (5)	0.048 (4)	−0.009 (3)	0.013 (3)	0.000 (3)

C14A	0.034 (3)	0.041 (4)	0.050 (4)	0.002 (3)	0.019 (3)	0.000 (3)
C15A	0.030 (3)	0.043 (4)	0.039 (3)	0.003 (3)	0.017 (3)	0.000 (3)
C16A	0.030 (3)	0.031 (3)	0.041 (3)	0.004 (3)	0.020 (3)	0.001 (3)
C17A	0.030 (3)	0.030 (3)	0.037 (3)	0.006 (3)	0.017 (3)	−0.001 (3)
C18A	0.039 (3)	0.028 (3)	0.033 (3)	0.005 (3)	0.015 (3)	−0.002 (2)
C19A	0.042 (3)	0.040 (4)	0.036 (3)	0.009 (3)	0.013 (3)	−0.005 (3)
C20A	0.058 (4)	0.033 (4)	0.039 (3)	0.012 (3)	0.018 (3)	0.003 (3)
C21A	0.056 (4)	0.041 (4)	0.044 (4)	−0.002 (3)	0.023 (3)	0.001 (3)
C22A	0.043 (3)	0.043 (4)	0.031 (3)	0.000 (3)	0.017 (3)	−0.002 (3)
C23A	0.040 (3)	0.035 (4)	0.031 (3)	0.002 (3)	0.018 (3)	−0.005 (2)
C24A	0.029 (3)	0.039 (4)	0.030 (3)	−0.003 (3)	0.015 (2)	−0.005 (2)
C25A	0.029 (3)	0.035 (3)	0.035 (3)	0.000 (3)	0.014 (2)	0.001 (3)
C26A	0.038 (3)	0.037 (4)	0.050 (4)	−0.009 (3)	0.021 (3)	0.002 (3)
C27A	0.037 (3)	0.051 (4)	0.050 (4)	−0.004 (3)	0.030 (3)	0.004 (3)
C28A	0.031 (3)	0.049 (4)	0.035 (3)	0.001 (3)	0.017 (3)	0.000 (3)
C29A	0.028 (3)	0.039 (4)	0.035 (3)	0.001 (3)	0.013 (3)	−0.004 (3)
C30A	0.031 (3)	0.029 (3)	0.038 (3)	−0.003 (2)	0.016 (3)	−0.002 (2)
C31A	0.037 (4)	0.069 (5)	0.054 (4)	0.000 (3)	0.027 (3)	−0.006 (4)
B1A	0.029 (3)	0.029 (4)	0.036 (3)	0.002 (3)	0.015 (3)	−0.001 (3)
S1B	0.0310 (7)	0.0384 (9)	0.0311 (7)	−0.0035 (6)	0.0144 (6)	0.0028 (6)
N1B	0.022 (2)	0.027 (3)	0.032 (2)	−0.0017 (19)	0.0153 (19)	0.0033 (19)
N2B	0.022 (2)	0.031 (3)	0.035 (3)	0.001 (2)	0.014 (2)	0.003 (2)
N3B	0.023 (2)	0.026 (3)	0.034 (2)	−0.0008 (19)	0.0153 (19)	0.0023 (19)
N4B	0.026 (2)	0.027 (3)	0.034 (2)	−0.006 (2)	0.015 (2)	−0.004 (2)
N5B	0.025 (2)	0.027 (3)	0.034 (2)	0.000 (2)	0.016 (2)	0.002 (2)
N6B	0.026 (2)	0.029 (3)	0.034 (2)	−0.003 (2)	0.014 (2)	−0.001 (2)
C1B	0.030 (3)	0.021 (3)	0.037 (3)	−0.001 (2)	0.018 (2)	0.002 (2)
C2B	0.026 (3)	0.033 (3)	0.032 (3)	−0.003 (2)	0.017 (2)	0.001 (2)
C3B	0.025 (3)	0.031 (3)	0.036 (3)	0.004 (2)	0.014 (2)	0.004 (2)
C4B	0.025 (3)	0.040 (4)	0.037 (3)	−0.004 (3)	0.015 (2)	0.002 (3)
C5B	0.027 (3)	0.031 (3)	0.040 (3)	−0.007 (2)	0.014 (2)	−0.005 (3)
C6B	0.030 (3)	0.033 (3)	0.035 (3)	0.001 (3)	0.018 (2)	0.002 (3)
C7B	0.022 (3)	0.030 (3)	0.035 (3)	0.000 (2)	0.017 (2)	0.001 (2)
C8B	0.025 (3)	0.027 (3)	0.034 (3)	0.003 (2)	0.017 (2)	0.006 (2)
C9B	0.027 (3)	0.027 (3)	0.029 (3)	−0.004 (2)	0.015 (2)	0.001 (2)
C10B	0.024 (3)	0.032 (3)	0.033 (3)	0.003 (2)	0.015 (2)	0.002 (2)
C11B	0.027 (3)	0.030 (3)	0.039 (3)	−0.001 (2)	0.014 (2)	0.002 (3)
C12B	0.034 (3)	0.039 (4)	0.043 (3)	0.000 (3)	0.023 (3)	−0.003 (3)
C13B	0.027 (3)	0.039 (4)	0.044 (3)	0.000 (3)	0.018 (3)	0.003 (3)
C14B	0.026 (3)	0.028 (3)	0.041 (3)	0.003 (2)	0.018 (2)	0.005 (2)
C15B	0.019 (3)	0.038 (3)	0.029 (3)	0.004 (2)	0.010 (2)	0.004 (2)
C16B	0.022 (3)	0.028 (3)	0.032 (3)	−0.003 (2)	0.011 (2)	0.001 (2)
C17B	0.026 (3)	0.026 (3)	0.032 (3)	−0.007 (2)	0.013 (2)	−0.003 (2)
C18B	0.030 (3)	0.031 (3)	0.040 (3)	−0.004 (3)	0.015 (3)	−0.007 (3)
C19B	0.038 (3)	0.028 (3)	0.045 (3)	−0.008 (3)	0.021 (3)	−0.004 (3)
C20B	0.053 (4)	0.030 (4)	0.066 (5)	−0.001 (3)	0.031 (4)	0.007 (3)
C21B	0.046 (4)	0.021 (3)	0.068 (4)	0.005 (3)	0.027 (3)	0.003 (3)
C22B	0.033 (3)	0.033 (4)	0.045 (4)	0.001 (3)	0.016 (3)	−0.002 (3)

C23B	0.033 (3)	0.027 (3)	0.037 (3)	0.000 (2)	0.018 (3)	−0.002 (2)
C24B	0.028 (3)	0.029 (3)	0.036 (3)	0.000 (2)	0.016 (2)	−0.002 (2)
C25B	0.032 (3)	0.039 (4)	0.026 (3)	0.001 (3)	0.012 (2)	0.001 (2)
C26B	0.029 (3)	0.039 (4)	0.037 (3)	0.004 (3)	0.013 (3)	−0.001 (3)
C27B	0.026 (3)	0.051 (4)	0.040 (3)	−0.001 (3)	0.012 (3)	0.004 (3)
C28B	0.039 (3)	0.047 (4)	0.035 (3)	−0.007 (3)	0.013 (3)	0.006 (3)
C29B	0.051 (4)	0.041 (4)	0.050 (4)	−0.006 (3)	0.022 (3)	−0.012 (3)
C30B	0.038 (3)	0.047 (4)	0.041 (3)	0.000 (3)	0.018 (3)	−0.006 (3)
C31B	0.055 (4)	0.057 (5)	0.047 (4)	−0.018 (4)	0.021 (3)	0.002 (3)
B1B	0.023 (3)	0.026 (3)	0.031 (3)	−0.004 (3)	0.012 (3)	−0.002 (3)
S1C	0.0300 (7)	0.0436 (9)	0.0328 (7)	0.0036 (6)	0.0142 (6)	0.0001 (6)
N1C	0.027 (2)	0.043 (3)	0.036 (3)	0.004 (2)	0.016 (2)	0.003 (2)
N2C	0.041 (3)	0.053 (4)	0.044 (3)	−0.007 (3)	0.022 (3)	−0.003 (3)
N3C	0.032 (3)	0.036 (3)	0.039 (3)	0.001 (2)	0.016 (2)	0.000 (2)
N4C	0.040 (3)	0.047 (4)	0.035 (3)	0.011 (3)	0.015 (2)	0.004 (2)
N5C	0.029 (2)	0.040 (3)	0.032 (3)	0.003 (2)	0.015 (2)	0.002 (2)
N6C	0.040 (3)	0.043 (3)	0.031 (3)	0.004 (2)	0.014 (2)	−0.003 (2)
C1C	0.034 (3)	0.044 (4)	0.032 (3)	0.004 (3)	0.014 (3)	−0.005 (3)
C2C	0.032 (3)	0.066 (5)	0.026 (3)	0.019 (3)	0.007 (3)	−0.008 (3)
C3C	0.050 (4)	0.085 (6)	0.028 (3)	0.032 (4)	0.013 (3)	−0.006 (3)
C4C	0.053 (5)	0.121 (9)	0.033 (4)	0.050 (5)	0.012 (3)	−0.006 (5)
C5C	0.036 (4)	0.134 (10)	0.051 (5)	0.026 (5)	0.013 (4)	−0.016 (5)
C6C	0.034 (4)	0.096 (7)	0.046 (4)	0.006 (4)	0.021 (3)	−0.015 (4)
C7C	0.024 (3)	0.081 (6)	0.032 (3)	0.003 (3)	0.012 (3)	−0.011 (3)
C8C	0.034 (3)	0.057 (5)	0.034 (3)	−0.001 (3)	0.020 (3)	−0.008 (3)
C9C	0.050 (4)	0.042 (4)	0.036 (3)	−0.009 (3)	0.024 (3)	0.000 (3)
C10C	0.067 (5)	0.042 (4)	0.042 (4)	−0.012 (4)	0.022 (3)	0.001 (3)
C11C	0.094 (6)	0.051 (5)	0.060 (5)	−0.019 (5)	0.040 (5)	0.002 (4)
C12C	0.141 (9)	0.047 (5)	0.061 (5)	−0.029 (6)	0.053 (6)	−0.008 (4)
C13C	0.140 (9)	0.038 (5)	0.058 (5)	0.012 (5)	0.042 (6)	0.003 (4)
C14C	0.089 (6)	0.041 (5)	0.046 (4)	0.014 (4)	0.025 (4)	0.005 (3)
C15C	0.064 (5)	0.044 (4)	0.041 (4)	0.015 (4)	0.024 (3)	0.007 (3)
C16C	0.043 (4)	0.042 (4)	0.035 (3)	0.013 (3)	0.014 (3)	0.004 (3)
C17C	0.028 (3)	0.048 (4)	0.029 (3)	0.005 (3)	0.011 (2)	−0.004 (3)
C18C	0.028 (3)	0.055 (4)	0.033 (3)	0.001 (3)	0.015 (3)	0.001 (3)
C19C	0.031 (3)	0.081 (6)	0.039 (3)	−0.001 (3)	0.017 (3)	−0.003 (4)
C20C	0.031 (3)	0.099 (7)	0.036 (3)	−0.014 (4)	0.019 (3)	−0.002 (4)
C21C	0.047 (4)	0.074 (6)	0.035 (3)	−0.017 (4)	0.016 (3)	0.004 (3)
C22C	0.044 (4)	0.053 (4)	0.036 (3)	−0.009 (3)	0.013 (3)	0.005 (3)
C23C	0.034 (3)	0.050 (4)	0.028 (3)	−0.006 (3)	0.014 (3)	−0.001 (3)
C24C	0.034 (3)	0.033 (3)	0.031 (3)	0.001 (3)	0.013 (3)	0.001 (2)
C25C	0.027 (3)	0.039 (4)	0.029 (3)	−0.002 (3)	0.015 (2)	−0.002 (2)
C26C	0.026 (3)	0.039 (4)	0.048 (4)	−0.006 (3)	0.014 (3)	0.005 (3)
C27C	0.034 (3)	0.038 (4)	0.048 (4)	−0.005 (3)	0.017 (3)	0.000 (3)
C28C	0.033 (3)	0.040 (4)	0.034 (3)	0.003 (3)	0.016 (3)	0.002 (3)
C29C	0.030 (3)	0.040 (4)	0.047 (4)	−0.006 (3)	0.017 (3)	0.002 (3)
C30C	0.036 (3)	0.032 (3)	0.040 (3)	−0.005 (3)	0.017 (3)	0.004 (3)
C31C	0.043 (4)	0.049 (5)	0.065 (5)	0.002 (3)	0.025 (4)	0.006 (4)

B1C	0.032 (3)	0.030 (4)	0.033 (3)	0.003 (3)	0.015 (3)	0.004 (3)

Geometric parameters (Å, º)

S1A—C25A	1.786 (6)	C12B—C13B	1.388 (9)
S1A—B1A	1.922 (7)	C12B—H12B	0.9500
N1A—C1A	1.363 (7)	C13B—C14B	1.368 (8)
N1A—C8A	1.374 (7)	C13B—H13B	0.9500
N1A—B1A	1.497 (8)	C14B—C15B	1.399 (7)
N2A—C9A	1.354 (7)	C14B—H14B	0.9500
N2A—C8A	1.355 (8)	C15B—C16B	1.452 (8)
N3A—C16A	1.361 (7)	C17B—C18B	1.465 (8)
N3A—C9A	1.372 (8)	C18B—C19B	1.383 (8)
N3A—B1A	1.495 (8)	C18B—C23B	1.432 (8)
N4A—C16A	1.341 (8)	C19B—C20B	1.376 (9)
N4A—C17A	1.346 (7)	C19B—H19B	0.9500
N5A—C24A	1.375 (7)	C20B—C21B	1.391 (9)
N5A—C17A	1.376 (7)	C20B—H20B	0.9500
N5A—B1A	1.479 (8)	C21B—C22B	1.382 (9)
N6A—C24A	1.346 (7)	C21B—H21B	0.9500
N6A—C1A	1.348 (8)	C22B—C23B	1.379 (8)
C1A—C2A	1.448 (8)	C22B—H22B	0.9500
C2A—C3A	1.404 (8)	C23B—C24B	1.458 (8)
C2A—C7A	1.416 (9)	C25B—C30B	1.381 (9)
C3A—C4A	1.380 (9)	C25B—C26B	1.396 (8)
C3A—H3AA	0.9500	C26B—C27B	1.375 (9)
C4A—C5A	1.394 (10)	C26B—H26B	0.9500
C4A—H4AA	0.9500	C27B—C28B	1.375 (10)
C5A—C6A	1.383 (9)	C27B—H27B	0.9500
C5A—H5AA	0.9500	C28B—C29B	1.412 (9)
C6A—C7A	1.397 (9)	C28B—C31B	1.511 (9)
C6A—H6AA	0.9500	C29B—C30B	1.385 (9)
C7A—C8A	1.447 (8)	C29B—H29B	0.9500
C9A—C10A	1.459 (8)	C30B—H30B	0.9500
C10A—C11A	1.390 (9)	C31B—H31D	0.9800
C10A—C15A	1.414 (9)	C31B—H31E	0.9800
C11A—C12A	1.403 (9)	C31B—H31F	0.9800
C11A—H11A	0.9500	S1C—C25C	1.786 (6)
C12A—C13A	1.388 (10)	S1C—B1C	1.915 (7)
C12A—H12A	0.9500	N1C—C1C	1.357 (8)
C13A—C14A	1.388 (9)	N1C—C8C	1.368 (8)
C13A—H13A	0.9500	N1C—B1C	1.494 (8)
C14A—C15A	1.394 (8)	N2C—C8C	1.345 (9)
C14A—H14A	0.9500	N2C—C9C	1.347 (8)
C15A—C16A	1.459 (9)	N3C—C16C	1.364 (8)
C17A—C18A	1.450 (9)	N3C—C9C	1.364 (8)
C18A—C19A	1.401 (9)	N3C—B1C	1.486 (9)
C18A—C23A	1.421 (8)	N4C—C16C	1.342 (8)

C19A—C20A	1.379 (10)	N4C—C17C	1.344 (8)
C19A—H19A	0.9500	N5C—C17C	1.361 (7)
C20A—C21A	1.399 (10)	N5C—C24C	1.383 (8)
C20A—H20A	0.9500	N5C—B1C	1.484 (8)
C21A—C22A	1.384 (9)	N6C—C1C	1.343 (8)
C21A—H21A	0.9500	N6C—C24C	1.344 (8)
C22A—C23A	1.383 (9)	C1C—C2C	1.454 (8)
C22A—H22A	0.9500	C2C—C3C	1.400 (10)
C23A—C24A	1.453 (9)	C2C—C7C	1.415 (11)
C25A—C26A	1.384 (8)	C3C—C4C	1.387 (11)
C25A—C30A	1.395 (8)	C3C—H3C	0.9500
C26A—C27A	1.410 (9)	C4C—C5C	1.388 (14)
C26A—H26A	0.9500	C4C—H4CA	0.9500
C27A—C28A	1.374 (9)	C5C—C6C	1.362 (13)
C27A—H27A	0.9500	C5C—H5CA	0.9500
C28A—C29A	1.385 (8)	C6C—C7C	1.417 (9)
C28A—C31A	1.505 (8)	C6C—H6CA	0.9500
C29A—C30A	1.384 (8)	C7C—C8C	1.439 (10)
C29A—H29A	0.9500	C9C—C10C	1.446 (10)
C30A—H30A	0.9500	C10C—C11C	1.404 (11)
C31A—H31A	0.9800	C10C—C15C	1.414 (10)
C31A—H31B	0.9800	C11C—C12C	1.382 (13)
C31A—H31C	0.9800	C11C—H11C	0.9500
S1B—C25B	1.789 (6)	C12C—C13C	1.405 (14)
S1B—B1B	1.907 (6)	C12C—H12C	0.9500
N1B—C1B	1.364 (7)	C13C—C14C	1.397 (13)
N1B—C8B	1.376 (7)	C13C—H13C	0.9500
N1B—B1B	1.491 (7)	C14C—C15C	1.390 (10)
N2B—C8B	1.338 (7)	C14C—H14C	0.9500
N2B—C9B	1.346 (7)	C15C—C16C	1.454 (10)
N3B—C16B	1.369 (7)	C17C—C18C	1.451 (9)
N3B—C9B	1.370 (7)	C18C—C23C	1.401 (9)
N3B—B1B	1.495 (7)	C18C—C19C	1.401 (8)
N4B—C16B	1.345 (7)	C19C—C20C	1.385 (11)
N4B—C17B	1.349 (7)	C19C—H19C	0.9500
N5B—C24B	1.355 (7)	C20C—C21C	1.405 (11)
N5B—C17B	1.366 (7)	C20C—H20C	0.9500
N5B—B1B	1.494 (8)	C21C—C22C	1.371 (10)
N6B—C1B	1.349 (7)	C21C—H21C	0.9500
N6B—C24B	1.354 (7)	C22C—C23C	1.403 (9)
C1B—C2B	1.453 (8)	C22C—H22C	0.9500
C2B—C3B	1.392 (7)	C23C—C24C	1.451 (8)
C2B—C7B	1.412 (8)	C25C—C26C	1.383 (9)
C3B—C4B	1.373 (8)	C25C—C30C	1.386 (8)
C3B—H3BA	0.9500	C26C—C27C	1.389 (9)
C4B—C5B	1.409 (9)	C26C—H26C	0.9500
C4B—H4BA	0.9500	C27C—C28C	1.379 (8)
C5B—C6B	1.390 (8)	C27C—H27C	0.9500

C5B—H5BA	0.9500	C28C—C29C	1.394 (9)
C6B—C7B	1.389 (8)	C28C—C31C	1.504 (9)
C6B—H6BA	0.9500	C29C—C30C	1.386 (9)
C7B—C8B	1.464 (7)	C29C—H29C	0.9500
C9B—C10B	1.458 (7)	C30C—H30C	0.9500
C10B—C11B	1.382 (8)	C31C—H31I	0.9800
C10B—C15B	1.422 (8)	C31C—H31J	0.9800
C11B—C12B	1.387 (8)	C31C—H31G	0.9800
C11B—H11B	0.9500		

C25A—S1A—B1A	103.7 (3)	N4B—C16B—N3B	122.7 (5)
C1A—N1A—C8A	112.8 (5)	N4B—C16B—C15B	130.5 (5)
C1A—N1A—B1A	122.6 (5)	N3B—C16B—C15B	105.5 (5)
C8A—N1A—B1A	123.2 (5)	N4B—C17B—N5B	122.3 (5)
C9A—N2A—C8A	117.0 (5)	N4B—C17B—C18B	131.0 (5)
C16A—N3A—C9A	113.4 (5)	N5B—C17B—C18B	105.4 (5)
C16A—N3A—B1A	122.6 (5)	C19B—C18B—C23B	121.0 (6)
C9A—N3A—B1A	123.0 (5)	C19B—C18B—C17B	132.4 (5)
C16A—N4A—C17A	116.9 (5)	C23B—C18B—C17B	106.6 (5)
C24A—N5A—C17A	112.7 (5)	C20B—C19B—C18B	117.0 (6)
C24A—N5A—B1A	123.2 (5)	C20B—C19B—H19B	121.5
C17A—N5A—B1A	123.3 (5)	C18B—C19B—H19B	121.5
C24A—N6A—C1A	116.5 (5)	C19B—C20B—C21B	123.1 (6)
N6A—C1A—N1A	123.2 (5)	C19B—C20B—H20B	118.5
N6A—C1A—C2A	129.5 (6)	C21B—C20B—H20B	118.5
N1A—C1A—C2A	105.5 (5)	C22B—C21B—C20B	120.1 (6)
C3A—C2A—C7A	120.8 (6)	C22B—C21B—H21B	119.9
C3A—C2A—C1A	131.3 (6)	C20B—C21B—H21B	119.9
C7A—C2A—C1A	107.8 (5)	C23B—C22B—C21B	118.8 (6)
C4A—C3A—C2A	117.7 (6)	C23B—C22B—H22B	120.6
C4A—C3A—H3AA	121.1	C21B—C22B—H22B	120.6
C2A—C3A—H3AA	121.1	C22B—C23B—C18B	120.1 (6)
C3A—C4A—C5A	121.3 (6)	C22B—C23B—C24B	132.6 (5)
C3A—C4A—H4AA	119.4	C18B—C23B—C24B	107.3 (5)
C5A—C4A—H4AA	119.4	N6B—C24B—N5B	122.8 (5)
C6A—C5A—C4A	122.0 (6)	N6B—C24B—C23B	129.9 (5)
C6A—C5A—H5AA	119.0	N5B—C24B—C23B	105.6 (5)
C4A—C5A—H5AA	119.0	C30B—C25B—C26B	118.0 (6)
C5A—C6A—C7A	117.7 (7)	C30B—C25B—S1B	120.8 (4)
C5A—C6A—H6AA	121.1	C26B—C25B—S1B	121.3 (5)
C7A—C6A—H6AA	121.1	C27B—C26B—C25B	120.5 (6)
C6A—C7A—C2A	120.4 (6)	C27B—C26B—H26B	119.7
C6A—C7A—C8A	132.5 (6)	C25B—C26B—H26B	119.7
C2A—C7A—C8A	106.9 (5)	C26B—C27B—C28B	122.5 (6)
N2A—C8A—N1A	122.2 (5)	C26B—C27B—H27B	118.8
N2A—C8A—C7A	130.2 (5)	C28B—C27B—H27B	118.8
N1A—C8A—C7A	105.7 (5)	C27B—C28B—C29B	116.8 (6)
N2A—C9A—N3A	122.5 (5)	C27B—C28B—C31B	122.1 (6)

N2A—C9A—C10A	130.1 (5)	C29B—C28B—C31B	121.1 (7)
N3A—C9A—C10A	105.4 (5)	C30B—C29B—C28B	120.9 (6)
C11A—C10A—C15A	121.2 (6)	C30B—C29B—H29B	119.6
C11A—C10A—C9A	131.7 (6)	C28B—C29B—H29B	119.6
C15A—C10A—C9A	107.1 (5)	C25B—C30B—C29B	121.1 (6)
C10A—C11A—C12A	117.0 (6)	C25B—C30B—H30B	119.5
C10A—C11A—H11A	121.5	C29B—C30B—H30B	119.5
C12A—C11A—H11A	121.5	C28B—C31B—H31D	109.5
C13A—C12A—C11A	121.9 (6)	C28B—C31B—H31E	109.5
C13A—C12A—H12A	119.1	H31D—C31B—H31E	109.5
C11A—C12A—H12A	119.1	C28B—C31B—H31F	109.5
C14A—C13A—C12A	121.1 (6)	H31D—C31B—H31F	109.5
C14A—C13A—H13A	119.5	H31E—C31B—H31F	109.5
C12A—C13A—H13A	119.5	N1B—B1B—N5B	104.1 (5)
C13A—C14A—C15A	118.1 (6)	N1B—B1B—N3B	103.7 (4)
C13A—C14A—H14A	121.0	N5B—B1B—N3B	103.4 (4)
C15A—C14A—H14A	121.0	N1B—B1B—S1B	112.1 (4)
C14A—C15A—C10A	120.7 (6)	N5B—B1B—S1B	114.5 (4)
C14A—C15A—C16A	131.6 (6)	N3B—B1B—S1B	117.5 (4)
C10A—C15A—C16A	107.5 (5)	C25C—S1C—B1C	101.4 (3)
N4A—C16A—N3A	123.1 (5)	C1C—N1C—C8C	113.5 (5)
N4A—C16A—C15A	129.9 (5)	C1C—N1C—B1C	123.5 (5)
N3A—C16A—C15A	105.3 (5)	C8C—N1C—B1C	122.2 (5)
N4A—C17A—N5A	121.9 (5)	C8C—N2C—C9C	116.7 (5)
N4A—C17A—C18A	130.9 (5)	C16C—N3C—C9C	112.6 (5)
N5A—C17A—C18A	105.4 (5)	C16C—N3C—B1C	123.3 (5)
C19A—C18A—C23A	119.4 (6)	C9C—N3C—B1C	123.3 (5)
C19A—C18A—C17A	132.7 (6)	C16C—N4C—C17C	116.8 (5)
C23A—C18A—C17A	107.7 (5)	C17C—N5C—C24C	112.9 (5)
C20A—C19A—C18A	119.3 (6)	C17C—N5C—B1C	123.1 (5)
C20A—C19A—H19A	120.4	C24C—N5C—B1C	122.8 (5)
C18A—C19A—H19A	120.4	C1C—N6C—C24C	117.3 (5)
C19A—C20A—C21A	120.1 (6)	N6C—C1C—N1C	122.0 (5)
C19A—C20A—H20A	120.0	N6C—C1C—C2C	131.1 (6)
C21A—C20A—H20A	120.0	N1C—C1C—C2C	104.9 (6)
C22A—C21A—C20A	122.1 (7)	C3C—C2C—C7C	120.8 (6)
C22A—C21A—H21A	119.0	C3C—C2C—C1C	131.7 (7)
C20A—C21A—H21A	119.0	C7C—C2C—C1C	107.5 (6)
C23A—C22A—C21A	117.9 (6)	C4C—C3C—C2C	117.5 (9)
C23A—C22A—H22A	121.0	C4C—C3C—H3C	121.2
C21A—C22A—H22A	121.0	C2C—C3C—H3C	121.2
C22A—C23A—C18A	121.2 (6)	C3C—C4C—C5C	120.9 (8)
C22A—C23A—C24A	131.7 (6)	C3C—C4C—H4CA	119.6
C18A—C23A—C24A	107.1 (5)	C5C—C4C—H4CA	119.6
N6A—C24A—N5A	122.3 (5)	C6C—C5C—C4C	123.3 (8)
N6A—C24A—C23A	130.3 (5)	C6C—C5C—H5CA	118.3
N5A—C24A—C23A	105.7 (5)	C4C—C5C—H5CA	118.3
C26A—C25A—C30A	119.0 (6)	C5C—C6C—C7C	116.8 (9)

C26A—C25A—S1A	119.8 (5)	C5C—C6C—H6CA	121.6
C30A—C25A—S1A	121.0 (4)	C7C—C6C—H6CA	121.6
C25A—C26A—C27A	119.6 (6)	C2C—C7C—C6C	120.4 (7)
C25A—C26A—H26A	120.2	C2C—C7C—C8C	107.3 (5)
C27A—C26A—H26A	120.2	C6C—C7C—C8C	132.2 (8)
C28A—C27A—C26A	121.7 (6)	N2C—C8C—N1C	123.0 (6)
C28A—C27A—H27A	119.1	N2C—C8C—C7C	130.5 (6)
C26A—C27A—H27A	119.1	N1C—C8C—C7C	105.5 (6)
C27A—C28A—C29A	117.6 (6)	N2C—C9C—N3C	122.0 (6)
C27A—C28A—C31A	121.2 (6)	N2C—C9C—C10C	130.7 (6)
C29A—C28A—C31A	121.1 (6)	N3C—C9C—C10C	105.8 (6)
C30A—C29A—C28A	122.1 (6)	C11C—C10C—C15C	120.0 (8)
C30A—C29A—H29A	119.0	C11C—C10C—C9C	132.4 (7)
C28A—C29A—H29A	119.0	C15C—C10C—C9C	107.5 (6)
C29A—C30A—C25A	120.0 (6)	C12C—C11C—C10C	117.6 (9)
C29A—C30A—H30A	120.0	C12C—C11C—H11C	121.2
C25A—C30A—H30A	120.0	C10C—C11C—H11C	121.2
C28A—C31A—H31A	109.5	C11C—C12C—C13C	122.8 (9)
C28A—C31A—H31B	109.5	C11C—C12C—H12C	118.6
H31A—C31A—H31B	109.5	C13C—C12C—H12C	118.6
C28A—C31A—H31C	109.5	C14C—C13C—C12C	119.6 (8)
H31A—C31A—H31C	109.5	C14C—C13C—H13C	120.2
H31B—C31A—H31C	109.5	C12C—C13C—H13C	120.2
N5A—B1A—N3A	104.0 (5)	C15C—C14C—C13C	118.4 (9)
N5A—B1A—N1A	104.4 (5)	C15C—C14C—H14C	120.8
N3A—B1A—N1A	104.2 (5)	C13C—C14C—H14C	120.8
N5A—B1A—S1A	116.9 (4)	C14C—C15C—C10C	121.6 (8)
N3A—B1A—S1A	117.2 (4)	C14C—C15C—C16C	131.5 (7)
N1A—B1A—S1A	108.7 (4)	C10C—C15C—C16C	106.8 (6)
C25B—S1B—B1B	99.4 (3)	N4C—C16C—N3C	122.2 (6)
C1B—N1B—C8B	112.9 (4)	N4C—C16C—C15C	130.6 (6)
C1B—N1B—B1B	122.7 (5)	N3C—C16C—C15C	105.9 (6)
C8B—N1B—B1B	123.0 (4)	N4C—C17C—N5C	122.5 (6)
C8B—N2B—C9B	115.9 (5)	N4C—C17C—C18C	130.2 (6)
C16B—N3B—C9B	113.0 (4)	N5C—C17C—C18C	105.5 (6)
C16B—N3B—B1B	123.0 (5)	C23C—C18C—C19C	121.1 (6)
C9B—N3B—B1B	123.0 (4)	C23C—C18C—C17C	107.5 (5)
C16B—N4B—C17B	116.8 (4)	C19C—C18C—C17C	131.1 (7)
C24B—N5B—C17B	114.0 (5)	C20C—C19C—C18C	117.5 (7)
C24B—N5B—B1B	122.1 (5)	C20C—C19C—H19C	121.3
C17B—N5B—B1B	123.3 (5)	C18C—C19C—H19C	121.3
C1B—N6B—C24B	116.5 (5)	C19C—C20C—C21C	121.2 (6)
N6B—C1B—N1B	122.5 (5)	C19C—C20C—H20C	119.4
N6B—C1B—C2B	130.2 (5)	C21C—C20C—H20C	119.4
N1B—C1B—C2B	105.9 (5)	C22C—C21C—C20C	121.7 (7)
C3B—C2B—C7B	120.8 (5)	C22C—C21C—H21C	119.1
C3B—C2B—C1B	131.7 (6)	C20C—C21C—H21C	119.1
C7B—C2B—C1B	107.3 (5)	C21C—C22C—C23C	117.8 (7)

C4B—C3B—C2B	118.2 (5)	C21C—C22C—H22C	121.1
C4B—C3B—H3BA	120.9	C23C—C22C—H22C	121.1
C2B—C3B—H3BA	120.9	C18C—C23C—C22C	120.7 (6)
C3B—C4B—C5B	121.2 (5)	C18C—C23C—C24C	108.0 (5)
C3B—C4B—H4BA	119.4	C22C—C23C—C24C	130.7 (6)
C5B—C4B—H4BA	119.4	N6C—C24C—N5C	122.1 (5)
C6B—C5B—C4B	121.2 (5)	N6C—C24C—C23C	131.9 (6)
C6B—C5B—H5BA	119.4	N5C—C24C—C23C	104.6 (5)
C4B—C5B—H5BA	119.4	C26C—C25C—C30C	117.9 (5)
C7B—C6B—C5B	117.7 (5)	C26C—C25C—S1C	120.1 (4)
C7B—C6B—H6BA	121.2	C30C—C25C—S1C	121.9 (5)
C5B—C6B—H6BA	121.2	C25C—C26C—C27C	121.1 (6)
C6B—C7B—C2B	120.9 (5)	C25C—C26C—H26C	119.4
C6B—C7B—C8B	131.3 (5)	C27C—C26C—H26C	119.4
C2B—C7B—C8B	107.5 (5)	C28C—C27C—C26C	121.4 (6)
N2B—C8B—N1B	123.4 (5)	C28C—C27C—H27C	119.3
N2B—C8B—C7B	130.4 (5)	C26C—C27C—H27C	119.3
N1B—C8B—C7B	105.0 (4)	C27C—C28C—C29C	117.3 (6)
N2B—C9B—N3B	123.0 (5)	C27C—C28C—C31C	120.8 (6)
N2B—C9B—C10B	130.1 (5)	C29C—C28C—C31C	121.9 (6)
N3B—C9B—C10B	105.4 (5)	C30C—C29C—C28C	121.4 (6)
C11B—C10B—C15B	120.9 (5)	C30C—C29C—H29C	119.3
C11B—C10B—C9B	131.8 (5)	C28C—C29C—H29C	119.3
C15B—C10B—C9B	107.1 (5)	C29C—C30C—C25C	120.8 (6)
C10B—C11B—C12B	118.3 (6)	C29C—C30C—H30C	119.6
C10B—C11B—H11B	120.9	C25C—C30C—H30C	119.6
C12B—C11B—H11B	120.9	C28C—C31C—H31I	109.5
C11B—C12B—C13B	120.7 (6)	C28C—C31C—H31J	109.5
C11B—C12B—H12B	119.6	H31I—C31C—H31J	109.5
C13B—C12B—H12B	119.6	C28C—C31C—H31G	109.5
C14B—C13B—C12B	122.1 (5)	H31I—C31C—H31G	109.5
C14B—C13B—H13B	119.0	H31J—C31C—H31G	109.5
C12B—C13B—H13B	119.0	N5C—B1C—N3C	103.9 (5)
C13B—C14B—C15B	118.3 (6)	N5C—B1C—N1C	103.7 (5)
C13B—C14B—H14B	120.8	N3C—B1C—N1C	103.9 (5)
C15B—C14B—H14B	120.8	N5C—B1C—S1C	116.9 (4)
C14B—C15B—C10B	119.7 (5)	N3C—B1C—S1C	116.1 (4)
C14B—C15B—C16B	132.8 (6)	N1C—B1C—S1C	110.8 (4)
C10B—C15B—C16B	107.4 (4)		

C24A—N6A—C1A—N1A	−8.7 (8)	C16B—N4B—C17B—N5B	−6.8 (8)
C24A—N6A—C1A—C2A	154.1 (6)	C16B—N4B—C17B—C18B	157.5 (6)
C8A—N1A—C1A—N6A	155.5 (5)	C24B—N5B—C17B—N4B	156.6 (5)
B1A—N1A—C1A—N6A	−11.3 (9)	B1B—N5B—C17B—N4B	−15.3 (8)
C8A—N1A—C1A—C2A	−10.8 (6)	C24B—N5B—C17B—C18B	−11.2 (6)
B1A—N1A—C1A—C2A	−177.6 (5)	B1B—N5B—C17B—C18B	176.9 (5)
N6A—C1A—C2A—C3A	15.5 (11)	N4B—C17B—C18B—C19B	17.6 (11)
N1A—C1A—C2A—C3A	−179.3 (6)	N5B—C17B—C18B—C19B	−176.2 (6)

N6A—C1A—C2A—C7A	−159.9 (6)
N1A—C1A—C2A—C7A	5.3 (6)
C7A—C2A—C3A—C4A	−1.7 (9)
C1A—C2A—C3A—C4A	−176.5 (6)
C2A—C3A—C4A—C5A	0.2 (10)
C3A—C4A—C5A—C6A	1.9 (10)
C4A—C5A—C6A—C7A	−2.4 (10)
C5A—C6A—C7A—C2A	0.9 (9)
C5A—C6A—C7A—C8A	175.1 (6)
C3A—C2A—C7A—C6A	1.1 (9)
C1A—C2A—C7A—C6A	177.1 (5)
C3A—C2A—C7A—C8A	−174.4 (6)
C1A—C2A—C7A—C8A	1.6 (7)
C9A—N2A—C8A—N1A	8.1 (8)
C9A—N2A—C8A—C7A	−154.0 (6)
C1A—N1A—C8A—N2A	−154.1 (6)
B1A—N1A—C8A—N2A	12.6 (9)
C1A—N1A—C8A—C7A	11.8 (7)
B1A—N1A—C8A—C7A	178.5 (5)
C6A—C7A—C8A—N2A	−18.2 (11)
C2A—C7A—C8A—N2A	156.6 (6)
C6A—C7A—C8A—N1A	177.5 (6)
C2A—C7A—C8A—N1A	−7.8 (6)
C8A—N2A—C9A—N3A	−7.7 (8)
C8A—N2A—C9A—C10A	154.2 (6)
C16A—N3A—C9A—N2A	155.0 (6)
B1A—N3A—C9A—N2A	−13.6 (9)
C16A—N3A—C9A—C10A	−10.7 (7)
B1A—N3A—C9A—C10A	−179.3 (5)
N2A—C9A—C10A—C11A	18.6 (11)
N3A—C9A—C10A—C11A	−177.2 (6)
N2A—C9A—C10A—C15A	−158.9 (6)
N3A—C9A—C10A—C15A	5.3 (6)
C15A—C10A—C11A—C12A	−1.6 (9)
C9A—C10A—C11A—C12A	−178.9 (6)
C10A—C11A—C12A—C13A	1.5 (10)
C11A—C12A—C13A—C14A	0.5 (10)
C12A—C13A—C14A—C15A	−2.3 (10)
C13A—C14A—C15A—C10A	2.1 (9)
C13A—C14A—C15A—C16A	177.6 (6)
C11A—C10A—C15A—C14A	−0.2 (9)
C9A—C10A—C15A—C14A	177.7 (6)
C11A—C10A—C15A—C16A	−176.6 (6)
C9A—C10A—C15A—C16A	1.3 (7)
C17A—N4A—C16A—N3A	7.3 (8)
C17A—N4A—C16A—C15A	−155.9 (6)
C9A—N3A—C16A—N4A	−155.3 (6)
B1A—N3A—C16A—N4A	13.4 (9)
N4B—C17B—C18B—C23B	−159.7 (6)
N5B—C17B—C18B—C23B	6.5 (6)
C23B—C18B—C19B—C20B	−0.9 (9)
C17B—C18B—C19B—C20B	−177.9 (6)
C18B—C19B—C20B—C21B	1.2 (10)
C19B—C20B—C21B—C22B	−0.2 (11)
C20B—C21B—C22B—C23B	−1.3 (10)
C21B—C22B—C23B—C18B	1.6 (9)
C21B—C22B—C23B—C24B	178.4 (6)
C19B—C18B—C23B—C22B	−0.5 (9)
C17B—C18B—C23B—C22B	177.2 (5)
C19B—C18B—C23B—C24B	−178.0 (5)
C17B—C18B—C23B—C24B	−0.4 (6)
C1B—N6B—C24B—N5B	7.5 (8)
C1B—N6B—C24B—C23B	−155.4 (6)
C17B—N5B—C24B—N6B	−155.5 (5)
B1B—N5B—C24B—N6B	16.5 (8)
C17B—N5B—C24B—C23B	11.0 (6)
B1B—N5B—C24B—C23B	−177.0 (5)
C22B—C23B—C24B—N6B	−17.9 (11)
C18B—C23B—C24B—N6B	159.2 (6)
C22B—C23B—C24B—N5B	176.9 (6)
C18B—C23B—C24B—N5B	−6.0 (6)
B1B—S1B—C25B—C30B	−107.4 (5)
B1B—S1B—C25B—C26B	71.7 (5)
C30B—C25B—C26B—C27B	5.0 (9)
S1B—C25B—C26B—C27B	−174.2 (5)
C25B—C26B—C27B—C28B	−0.9 (9)
C26B—C27B—C28B—C29B	−3.1 (9)
C26B—C27B—C28B—C31B	175.0 (6)
C27B—C28B—C29B—C30B	3.1 (10)
C31B—C28B—C29B—C30B	−175.1 (6)
C26B—C25B—C30B—C29B	−5.0 (9)
S1B—C25B—C30B—C29B	174.2 (5)
C28B—C29B—C30B—C25B	1.0 (10)
C1B—N1B—B1B—N5B	30.1 (6)
C8B—N1B—B1B—N5B	−135.6 (5)
C1B—N1B—B1B—N3B	138.0 (5)
C8B—N1B—B1B—N3B	−27.7 (7)
C1B—N1B—B1B—S1B	−94.2 (5)
C8B—N1B—B1B—S1B	100.1 (5)
C24B—N5B—B1B—N1B	−32.4 (7)
C17B—N5B—B1B—N1B	138.9 (5)
C24B—N5B—B1B—N3B	−140.5 (5)
C17B—N5B—B1B—N3B	30.8 (7)
C24B—N5B—B1B—S1B	90.4 (6)
C17B—N5B—B1B—S1B	−98.3 (5)
C16B—N3B—B1B—N1B	−138.3 (5)

C9A—N3A—C16A—C15A	11.4 (7)
B1A—N3A—C16A—C15A	−179.9 (5)
C14A—C15A—C16A—N4A	−17.8 (11)
C10A—C15A—C16A—N4A	158.1 (6)
C14A—C15A—C16A—N3A	176.7 (6)
C10A—C15A—C16A—N3A	−7.4 (6)
C16A—N4A—C17A—N5A	−6.7 (8)
C16A—N4A—C17A—C18A	155.9 (6)
C24A—N5A—C17A—N4A	154.9 (5)
B1A—N5A—C17A—N4A	−14.8 (8)
C24A—N5A—C17A—C18A	−11.6 (6)
B1A—N5A—C17A—C18A	178.7 (5)
N4A—C17A—C18A—C19A	18.6 (11)
N5A—C17A—C18A—C19A	−176.7 (6)
N4A—C17A—C18A—C23A	−157.8 (6)
N5A—C17A—C18A—C23A	7.0 (6)
C23A—C18A—C19A—C20A	−2.2 (9)
C17A—C18A—C19A—C20A	−178.2 (6)
C18A—C19A—C20A—C21A	1.7 (9)
C19A—C20A—C21A—C22A	0.0 (10)
C20A—C21A—C22A—C23A	−1.2 (9)
C21A—C22A—C23A—C18A	0.7 (9)
C21A—C22A—C23A—C24A	178.6 (6)
C19A—C18A—C23A—C22A	0.9 (9)
C17A—C18A—C23A—C22A	177.9 (5)
C19A—C18A—C23A—C24A	−177.4 (5)
C17A—C18A—C23A—C24A	−0.5 (6)
C1A—N6A—C24A—N5A	7.2 (8)
C1A—N6A—C24A—C23A	−155.6 (6)
C17A—N5A—C24A—N6A	−155.1 (5)
B1A—N5A—C24A—N6A	14.6 (8)
C17A—N5A—C24A—C23A	11.3 (6)
B1A—N5A—C24A—C23A	−179.0 (5)
C22A—C23A—C24A—N6A	−19.4 (11)
C18A—C23A—C24A—N6A	158.7 (6)
C22A—C23A—C24A—N5A	175.7 (6)
C18A—C23A—C24A—N5A	−6.2 (6)
B1A—S1A—C25A—C26A	112.4 (5)
B1A—S1A—C25A—C30A	−72.8 (5)
C30A—C25A—C26A—C27A	−0.1 (9)
S1A—C25A—C26A—C27A	174.8 (5)
C25A—C26A—C27A—C28A	0.1 (10)
C26A—C27A—C28A—C29A	0.0 (10)
C26A—C27A—C28A—C31A	177.0 (6)
C27A—C28A—C29A—C30A	−0.1 (9)
C31A—C28A—C29A—C30A	−177.1 (6)
C28A—C29A—C30A—C25A	0.1 (9)
C26A—C25A—C30A—C29A	0.1 (9)
C9B—N3B—B1B—N1B	29.7 (7)
C16B—N3B—B1B—N5B	−29.8 (6)
C9B—N3B—B1B—N5B	138.1 (5)
C16B—N3B—B1B—S1B	97.4 (6)
C9B—N3B—B1B—S1B	−94.7 (6)
C24C—N6C—C1C—N1C	−7.0 (8)
C24C—N6C—C1C—C2C	154.9 (6)
C8C—N1C—C1C—N6C	154.1 (5)
B1C—N1C—C1C—N6C	−15.8 (9)
C8C—N1C—C1C—C2C	−11.8 (6)
B1C—N1C—C1C—C2C	178.3 (5)
N6C—C1C—C2C—C3C	20.4 (11)
N1C—C1C—C2C—C3C	−175.5 (6)
N6C—C1C—C2C—C7C	−157.0 (6)
N1C—C1C—C2C—C7C	7.1 (6)
C7C—C2C—C3C—C4C	−3.1 (9)
C1C—C2C—C3C—C4C	179.8 (6)
C2C—C3C—C4C—C5C	5.6 (10)
C3C—C4C—C5C—C6C	−3.8 (12)
C4C—C5C—C6C—C7C	−0.9 (11)
C3C—C2C—C7C—C6C	−1.4 (9)
C1C—C2C—C7C—C6C	176.3 (6)
C3C—C2C—C7C—C8C	−178.3 (5)
C1C—C2C—C7C—C8C	−0.6 (7)
C5C—C6C—C7C—C2C	3.4 (9)
C5C—C6C—C7C—C8C	179.3 (7)
C9C—N2C—C8C—N1C	9.8 (9)
C9C—N2C—C8C—C7C	−157.2 (6)
C1C—N1C—C8C—N2C	−158.3 (6)
B1C—N1C—C8C—N2C	11.8 (9)
C1C—N1C—C8C—C7C	11.5 (6)
B1C—N1C—C8C—C7C	−178.4 (5)
C2C—C7C—C8C—N2C	162.5 (6)
C6C—C7C—C8C—N2C	−13.8 (11)
C2C—C7C—C8C—N1C	−6.2 (6)
C6C—C7C—C8C—N1C	177.5 (6)
C8C—N2C—C9C—N3C	−8.3 (9)
C8C—N2C—C9C—C10C	155.3 (7)
C16C—N3C—C9C—N2C	155.0 (6)
B1C—N3C—C9C—N2C	−15.2 (9)
C16C—N3C—C9C—C10C	−12.1 (7)
B1C—N3C—C9C—C10C	177.7 (5)
N2C—C9C—C10C—C11C	18.6 (13)
N3C—C9C—C10C—C11C	−175.9 (8)
N2C—C9C—C10C—C15C	−157.6 (7)
N3C—C9C—C10C—C15C	7.9 (7)
C15C—C10C—C11C—C12C	−1.2 (11)
C9C—C10C—C11C—C12C	−177.1 (8)

S1A—C25A—C30A—C29A	−174.8 (4)	C10C—C11C—C12C—C13C	2.7 (13)
C24A—N5A—B1A—N3A	−138.6 (5)	C11C—C12C—C13C—C14C	−1.6 (14)
C17A—N5A—B1A—N3A	30.1 (7)	C12C—C13C—C14C—C15C	−1.1 (12)
C24A—N5A—B1A—N1A	−29.5 (7)	C13C—C14C—C15C—C10C	2.5 (11)
C17A—N5A—B1A—N1A	139.1 (5)	C13C—C14C—C15C—C16C	178.4 (7)
C24A—N5A—B1A—S1A	90.5 (6)	C11C—C10C—C15C—C14C	−1.4 (11)
C17A—N5A—B1A—S1A	−100.8 (6)	C9C—C10C—C15C—C14C	175.4 (6)
C16A—N3A—B1A—N5A	−29.4 (7)	C11C—C10C—C15C—C16C	−178.2 (6)
C9A—N3A—B1A—N5A	138.2 (5)	C9C—C10C—C15C—C16C	−1.4 (8)
C16A—N3A—B1A—N1A	−138.5 (5)	C17C—N4C—C16C—N3C	8.5 (9)
C9A—N3A—B1A—N1A	29.1 (7)	C17C—N4C—C16C—C15C	−156.6 (7)
C16A—N3A—B1A—S1A	101.4 (6)	C9C—N3C—C16C—N4C	−157.1 (6)
C9A—N3A—B1A—S1A	−91.0 (6)	B1C—N3C—C16C—N4C	13.1 (9)
C1A—N1A—B1A—N5A	27.9 (7)	C9C—N3C—C16C—C15C	11.3 (7)
C8A—N1A—B1A—N5A	−137.6 (5)	B1C—N3C—C16C—C15C	−178.5 (5)
C1A—N1A—B1A—N3A	136.8 (5)	C14C—C15C—C16C—N4C	−15.0 (12)
C8A—N1A—B1A—N3A	−28.7 (7)	C10C—C15C—C16C—N4C	161.3 (7)
C1A—N1A—B1A—S1A	−97.5 (6)	C14C—C15C—C16C—N3C	178.0 (7)
C8A—N1A—B1A—S1A	97.0 (6)	C10C—C15C—C16C—N3C	−5.6 (7)
C24B—N6B—C1B—N1B	−10.0 (8)	C16C—N4C—C17C—N5C	−8.6 (9)
C24B—N6B—C1B—C2B	154.2 (6)	C16C—N4C—C17C—C18C	154.3 (6)
C8B—N1B—C1B—N6B	155.5 (5)	C24C—N5C—C17C—N4C	154.8 (6)
B1B—N1B—C1B—N6B	−11.5 (8)	B1C—N5C—C17C—N4C	−13.0 (9)
C8B—N1B—C1B—C2B	−12.0 (6)	C24C—N5C—C17C—C18C	−11.7 (6)
B1B—N1B—C1B—C2B	−179.0 (5)	B1C—N5C—C17C—C18C	−179.5 (5)
N6B—C1B—C2B—C3B	16.3 (10)	N4C—C17C—C18C—C23C	−158.7 (6)
N1B—C1B—C2B—C3B	−177.5 (6)	N5C—C17C—C18C—C23C	6.3 (6)
N6B—C1B—C2B—C7B	−159.3 (6)	N4C—C17C—C18C—C19C	15.6 (11)
N1B—C1B—C2B—C7B	6.9 (6)	N5C—C17C—C18C—C19C	−179.3 (6)
C7B—C2B—C3B—C4B	−1.0 (8)	C23C—C18C—C19C—C20C	0.2 (9)
C1B—C2B—C3B—C4B	−176.2 (6)	C17C—C18C—C19C—C20C	−173.5 (6)
C2B—C3B—C4B—C5B	1.6 (8)	C18C—C19C—C20C—C21C	0.0 (10)
C3B—C4B—C5B—C6B	0.3 (9)	C19C—C20C—C21C—C22C	1.1 (11)
C4B—C5B—C6B—C7B	−2.7 (8)	C20C—C21C—C22C—C23C	−2.3 (10)
C5B—C6B—C7B—C2B	3.2 (8)	C19C—C18C—C23C—C22C	−1.5 (9)
C5B—C6B—C7B—C8B	176.4 (6)	C17C—C18C—C23C—C22C	173.5 (6)
C3B—C2B—C7B—C6B	−1.4 (8)	C19C—C18C—C23C—C24C	−174.3 (6)
C1B—C2B—C7B—C6B	174.8 (5)	C17C—C18C—C23C—C24C	0.8 (7)
C3B—C2B—C7B—C8B	−176.1 (5)	C21C—C22C—C23C—C18C	2.5 (9)
C1B—C2B—C7B—C8B	0.1 (6)	C21C—C22C—C23C—C24C	173.4 (6)
C9B—N2B—C8B—N1B	10.1 (8)	C1C—N6C—C24C—N5C	8.8 (8)
C9B—N2B—C8B—C7B	−155.2 (6)	C1C—N6C—C24C—C23C	−155.5 (6)
C1B—N1B—C8B—N2B	−156.5 (5)	C17C—N5C—C24C—N6C	−155.8 (5)
B1B—N1B—C8B—N2B	10.4 (8)	B1C—N5C—C24C—N6C	12.0 (9)
C1B—N1B—C8B—C7B	12.0 (6)	C17C—N5C—C24C—C23C	12.1 (6)
B1B—N1B—C8B—C7B	178.9 (5)	B1C—N5C—C24C—C23C	180.0 (5)
C6B—C7B—C8B—N2B	−13.4 (10)	C18C—C23C—C24C—N6C	158.8 (6)
C2B—C7B—C8B—N2B	160.4 (6)	C22C—C23C—C24C—N6C	−13.0 (12)

C6B—C7B—C8B—N1B	179.2 (6)	C18C—C23C—C24C—N5C	−7.4 (6)
C2B—C7B—C8B—N1B	−7.0 (6)	C22C—C23C—C24C—N5C	−179.2 (6)
C8B—N2B—C9B—N3B	−8.1 (8)	B1C—S1C—C25C—C26C	82.0 (5)
C8B—N2B—C9B—C10B	155.8 (6)	B1C—S1C—C25C—C30C	−102.3 (5)
C16B—N3B—C9B—N2B	154.6 (5)	C30C—C25C—C26C—C27C	1.2 (9)
B1B—N3B—C9B—N2B	−14.5 (8)	S1C—C25C—C26C—C27C	177.0 (5)
C16B—N3B—C9B—C10B	−12.7 (6)	C25C—C26C—C27C—C28C	−0.2 (10)
B1B—N3B—C9B—C10B	178.2 (5)	C26C—C27C—C28C—C29C	−0.9 (9)
N2B—C9B—C10B—C11B	15.7 (10)	C26C—C27C—C28C—C31C	178.3 (6)
N3B—C9B—C10B—C11B	−178.2 (6)	C27C—C28C—C29C—C30C	0.9 (9)
N2B—C9B—C10B—C15B	−158.7 (6)	C31C—C28C—C29C—C30C	−178.3 (6)
N3B—C9B—C10B—C15B	7.4 (6)	C28C—C29C—C30C—C25C	0.1 (9)
C15B—C10B—C11B—C12B	−2.0 (8)	C26C—C25C—C30C—C29C	−1.1 (9)
C9B—C10B—C11B—C12B	−175.8 (6)	S1C—C25C—C30C—C29C	−176.9 (5)
C10B—C11B—C12B—C13B	1.7 (9)	C17C—N5C—B1C—N3C	29.2 (7)
C11B—C12B—C13B—C14B	0.2 (10)	C24C—N5C—B1C—N3C	−137.4 (5)
C12B—C13B—C14B—C15B	−1.6 (9)	C17C—N5C—B1C—N1C	137.6 (5)
C13B—C14B—C15B—C10B	1.3 (8)	C24C—N5C—B1C—N1C	−29.0 (7)
C13B—C14B—C15B—C16B	175.8 (6)	C17C—N5C—B1C—S1C	−100.0 (6)
C11B—C10B—C15B—C14B	0.5 (8)	C24C—N5C—B1C—S1C	93.4 (6)
C9B—C10B—C15B—C14B	175.7 (5)	C16C—N3C—B1C—N5C	−29.4 (7)
C11B—C10B—C15B—C16B	−175.2 (5)	C9C—N3C—B1C—N5C	139.8 (5)
C9B—C10B—C15B—C16B	−0.1 (6)	C16C—N3C—B1C—N1C	−137.6 (5)
C17B—N4B—C16B—N3B	7.6 (8)	C9C—N3C—B1C—N1C	31.5 (7)
C17B—N4B—C16B—C15B	−157.3 (5)	C16C—N3C—B1C—S1C	100.4 (6)
C9B—N3B—C16B—N4B	−155.5 (5)	C9C—N3C—B1C—S1C	−90.4 (6)
B1B—N3B—C16B—N4B	13.6 (8)	C1C—N1C—B1C—N5C	31.1 (7)
C9B—N3B—C16B—C15B	12.7 (6)	C8C—N1C—B1C—N5C	−138.0 (5)
B1B—N3B—C16B—C15B	−178.3 (5)	C1C—N1C—B1C—N3C	139.5 (5)
C14B—C15B—C16B—N4B	−15.3 (10)	C8C—N1C—B1C—N3C	−29.6 (7)
C10B—C15B—C16B—N4B	159.7 (6)	C1C—N1C—B1C—S1C	−95.2 (6)
C14B—C15B—C16B—N3B	177.8 (6)	C8C—N1C—B1C—S1C	95.7 (6)
C10B—C15B—C16B—N3B	−7.2 (6)		

(*N*-Phenylbenzamido)(subphthalocyaninato)boron (d2339_a)

Crystal data

$C_{31}H_{20}BN_7 \cdot 0.14H_2O$
$M_r = 503.87$
Triclinic, $P\overline{1}$
$a = 11.4897$ (5) Å
$b = 11.7489$ (5) Å
$c = 19.3046$ (8) Å
$\alpha = 73.348$ (2)°
$\beta = 81.941$ (2)°
$\gamma = 76.167$ (2)°
$V = 2417.05$ (18) Å^3
$Z = 4$
$F(000) = 1046$
$D_x = 1.385$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9824 reflections
$\theta = 4.0$–$65.7°$
$\mu = 0.68$ mm^{-1}
$T = 150$ K
Shard, pink
0.20 × 0.15 × 0.08 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Incoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan SADABS (Krause *et al.*, 2015)
T_{min} = 0.657, T_{max} = 0.753
60606 measured reflections
8275 independent reflections
7193 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 66.0°, θ_{min} = 2.4°
h = −13→13
k = −13→13
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 1.06
8275 reflections
713 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.687P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	−0.01647 (9)	0.70429 (10)	0.08430 (6)	0.0216 (2)	
N2	−0.00691 (9)	0.49963 (10)	0.15298 (6)	0.0228 (2)	
N3	0.16519 (9)	0.58812 (10)	0.13041 (6)	0.0229 (2)	
N4	0.29543 (10)	0.68828 (11)	0.16512 (6)	0.0279 (3)	
N5	0.13649 (10)	0.80098 (10)	0.09047 (6)	0.0240 (2)	
N6	−0.06157 (10)	0.91739 (10)	0.06937 (6)	0.0250 (2)	
N7	0.16020 (10)	0.68676 (10)	−0.00712 (6)	0.0251 (2)	
C1	−0.09554 (11)	0.81378 (12)	0.07385 (7)	0.0230 (3)	
C2	−0.21422 (12)	0.78506 (13)	0.08656 (7)	0.0251 (3)	
C3	−0.32857 (13)	0.85814 (14)	0.07843 (8)	0.0332 (3)	
H3A	−0.339567	0.943705	0.059301	0.040*	
C4	−0.42578 (13)	0.80261 (15)	0.09901 (9)	0.0385 (4)	
H4A	−0.504640	0.850486	0.092060	0.046*	
C5	−0.41054 (13)	0.67746 (15)	0.12984 (9)	0.0365 (4)	
H5A	−0.479314	0.642303	0.144975	0.044*	
C6	−0.29758 (12)	0.60402 (13)	0.13871 (8)	0.0280 (3)	
H6A	−0.287886	0.519170	0.160426	0.034*	
C7	−0.19825 (11)	0.65711 (12)	0.11511 (7)	0.0230 (3)	
C8	−0.06908 (11)	0.60808 (12)	0.11715 (7)	0.0218 (3)	
C9	0.10872 (11)	0.49409 (12)	0.16254 (7)	0.0231 (3)	
C10	0.18630 (12)	0.41069 (13)	0.21727 (7)	0.0252 (3)	

C11	0.17561 (13)	0.30096 (13)	0.26734 (8)	0.0291 (3)
H11A	0.110620	0.263722	0.267657	0.035*
C12	0.26251 (14)	0.24755 (14)	0.31676 (8)	0.0355 (3)
H12A	0.257140	0.172320	0.351045	0.043*
C13	0.35778 (14)	0.30231 (15)	0.31706 (9)	0.0383 (4)
H13A	0.416995	0.262606	0.350776	0.046*
C14	0.36757 (13)	0.41301 (14)	0.26931 (8)	0.0329 (3)
H14A	0.431531	0.450678	0.270490	0.039*
C15	0.28107 (12)	0.46783 (13)	0.21940 (8)	0.0272 (3)
C16	0.25890 (11)	0.58633 (13)	0.16753 (7)	0.0259 (3)
C17	0.22837 (11)	0.79456 (13)	0.13026 (7)	0.0264 (3)
C18	0.21547 (12)	0.91685 (13)	0.13773 (8)	0.0286 (3)
C19	0.28483 (13)	0.96887 (15)	0.16923 (8)	0.0352 (4)
H19A	0.356331	0.922151	0.191056	0.042*
C20	0.24601 (15)	1.09026 (15)	0.16757 (9)	0.0388 (4)
H20A	0.293367	1.128054	0.187015	0.047*
C21	0.13861 (15)	1.15892 (15)	0.13793 (8)	0.0374 (4)
H21A	0.114973	1.242308	0.137504	0.045*
C22	0.06604 (14)	1.10814 (13)	0.10922 (8)	0.0322 (3)
H22A	−0.008343	1.154240	0.090895	0.039*
C23	0.10615 (12)	0.98678 (13)	0.10819 (7)	0.0270 (3)
C24	0.05306 (12)	0.90673 (12)	0.08295 (7)	0.0242 (3)
C25	0.28121 (12)	0.69402 (13)	−0.03300 (7)	0.0254 (3)
C26	0.36217 (13)	0.59752 (14)	−0.05290 (8)	0.0315 (3)
H26A	0.336981	0.524086	−0.048062	0.038*
C27	0.47876 (14)	0.60706 (15)	−0.07962 (9)	0.0386 (4)
H27A	0.531879	0.540775	−0.093837	0.046*
C28	0.51855 (14)	0.71100 (15)	−0.08581 (9)	0.0408 (4)
H28A	0.599024	0.716652	−0.103336	0.049*
C29	0.43931 (14)	0.80749 (15)	−0.06607 (9)	0.0384 (4)
H29A	0.466225	0.879469	−0.069503	0.046*
C30	0.32135 (13)	0.80070 (14)	−0.04137 (8)	0.0317 (3)
H30A	0.267394	0.869113	−0.030052	0.038*
C31	0.11511 (13)	0.59755 (14)	−0.02957 (8)	0.0319 (3)
H31A	0.031735	0.598047	−0.009695	0.048*
H31B	0.118520	0.618280	−0.082630	0.048*
H31C	0.164840	0.516517	−0.011427	0.048*
B1	0.11629 (13)	0.69448 (14)	0.06916 (8)	0.0237 (3)
N8	0.80208 (10)	0.22661 (10)	0.44369 (6)	0.0248 (2)
N9	0.97660 (10)	0.31154 (11)	0.40625 (6)	0.0273 (3)
N10	0.79477 (10)	0.40585 (10)	0.34885 (6)	0.0249 (2)
N11	0.60890 (10)	0.54894 (11)	0.33121 (6)	0.0289 (3)
N12	0.61599 (10)	0.34840 (10)	0.40642 (6)	0.0247 (2)
N13	0.62459 (10)	0.20647 (11)	0.52258 (6)	0.0275 (3)
N14	0.74153 (10)	0.23329 (10)	0.31662 (6)	0.0258 (3)
C32	0.74483 (12)	0.17952 (12)	0.50877 (7)	0.0259 (3)
C33	0.83819 (13)	0.12217 (12)	0.55928 (8)	0.0277 (3)
C34	0.83378 (14)	0.05840 (13)	0.63239 (8)	0.0329 (3)

H34A	0.760386	0.041292	0.657945	0.040*
C35	0.93989 (14)	0.02096 (14)	0.66637 (8)	0.0369 (4)
H35A	0.939374	−0.023987	0.715860	0.044*
C36	1.04779 (14)	0.04769 (14)	0.62961 (8)	0.0361 (3)
H36A	1.119249	0.019380	0.654424	0.043*
C37	1.05289 (13)	0.11445 (13)	0.55789 (8)	0.0319 (3)
H37A	1.126004	0.134737	0.533697	0.038*
C38	0.94727 (12)	0.15113 (13)	0.52213 (8)	0.0274 (3)
C39	0.91895 (12)	0.22814 (13)	0.45033 (7)	0.0257 (3)
C40	0.91044 (12)	0.40437 (13)	0.35936 (7)	0.0256 (3)
C41	0.92861 (13)	0.52674 (13)	0.32510 (7)	0.0275 (3)
C42	1.02796 (14)	0.57922 (14)	0.31861 (8)	0.0327 (3)
H42A	1.102593	0.531800	0.335909	0.039*
C43	1.01408 (16)	0.70269 (15)	0.28612 (8)	0.0402 (4)
H43A	1.081017	0.739948	0.279910	0.048*
C44	0.90370 (17)	0.77357 (15)	0.26230 (8)	0.0411 (4)
H44A	0.897586	0.857825	0.239768	0.049*
C45	0.80302 (15)	0.72415 (14)	0.27068 (8)	0.0345 (3)
H45A	0.727590	0.773501	0.255953	0.041*
C46	0.81619 (13)	0.59917 (13)	0.30156 (7)	0.0285 (3)
C47	0.73002 (12)	0.52042 (13)	0.32209 (7)	0.0267 (3)
C48	0.55510 (12)	0.46415 (13)	0.37720 (7)	0.0273 (3)
C49	0.43838 (12)	0.47681 (14)	0.41828 (8)	0.0309 (3)
C50	0.33515 (13)	0.56869 (15)	0.40909 (9)	0.0380 (4)
H50A	0.333399	0.641871	0.371602	0.046*
C51	0.23524 (14)	0.54967 (17)	0.45645 (10)	0.0448 (4)
H51A	0.162836	0.609666	0.450205	0.054*
C52	0.23860 (14)	0.44417 (18)	0.51322 (9)	0.0454 (4)
H52A	0.167837	0.433276	0.544077	0.054*
C53	0.34236 (13)	0.35509 (16)	0.52568 (8)	0.0369 (4)
H53A	0.345181	0.285741	0.566037	0.044*
C54	0.44269 (12)	0.37063 (14)	0.47694 (8)	0.0302 (3)
C55	0.56274 (12)	0.29493 (13)	0.47186 (7)	0.0264 (3)
C56	0.67307 (12)	0.14705 (12)	0.32086 (7)	0.0251 (3)
C57	0.64720 (14)	0.12150 (14)	0.25856 (8)	0.0339 (3)
H57A	0.676114	0.163778	0.212068	0.041*
C58	0.57979 (15)	0.03512 (15)	0.26419 (9)	0.0417 (4)
H58A	0.563730	0.019383	0.221245	0.050*
C59	0.53559 (15)	−0.02839 (15)	0.33041 (9)	0.0400 (4)
H59A	0.488893	−0.086606	0.333504	0.048*
C60	0.56122 (13)	−0.00485 (14)	0.39217 (9)	0.0345 (3)
H60A	0.531533	−0.047420	0.438366	0.041*
C61	0.62956 (12)	0.07987 (13)	0.38775 (8)	0.0290 (3)
H61A	0.647346	0.092735	0.431168	0.035*
C62	0.81233 (14)	0.26659 (14)	0.24757 (8)	0.0348 (3)
H62A	0.857108	0.326886	0.249300	0.052*
H62B	0.868840	0.194126	0.238969	0.052*
H62C	0.758458	0.301048	0.208202	0.052*

B2	0.73887 (14)	0.29648 (14)	0.37514 (8)	0.0247 (3)	
O1W	0.4210 (4)	0.7569 (3)	0.2715 (2)	0.0384 (14)	0.281 (4)
H2O	0.387836	0.725753	0.247583	0.058*	0.281 (4)
H1O	0.485406	0.707403	0.283633	0.058*	0.281 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0188 (5)	0.0265 (6)	0.0220 (5)	−0.0075 (4)	−0.0001 (4)	−0.0087 (4)
N2	0.0196 (5)	0.0282 (6)	0.0233 (6)	−0.0059 (5)	−0.0010 (4)	−0.0106 (5)
N3	0.0171 (5)	0.0301 (6)	0.0251 (6)	−0.0064 (5)	0.0001 (4)	−0.0123 (5)
N4	0.0179 (5)	0.0392 (7)	0.0320 (6)	−0.0086 (5)	0.0017 (5)	−0.0176 (5)
N5	0.0208 (5)	0.0308 (6)	0.0248 (6)	−0.0109 (5)	0.0034 (4)	−0.0124 (5)
N6	0.0264 (6)	0.0283 (6)	0.0218 (6)	−0.0089 (5)	0.0002 (4)	−0.0073 (5)
N7	0.0225 (6)	0.0321 (6)	0.0259 (6)	−0.0114 (5)	0.0034 (4)	−0.0136 (5)
C1	0.0223 (7)	0.0280 (7)	0.0196 (6)	−0.0061 (5)	−0.0009 (5)	−0.0072 (5)
C2	0.0218 (7)	0.0321 (7)	0.0236 (7)	−0.0061 (6)	−0.0014 (5)	−0.0107 (6)
C3	0.0255 (7)	0.0339 (8)	0.0405 (9)	−0.0023 (6)	−0.0054 (6)	−0.0123 (7)
C4	0.0191 (7)	0.0449 (9)	0.0527 (10)	−0.0011 (6)	−0.0036 (6)	−0.0191 (8)
C5	0.0200 (7)	0.0466 (9)	0.0471 (9)	−0.0113 (6)	0.0027 (6)	−0.0178 (7)
C6	0.0220 (7)	0.0352 (8)	0.0297 (7)	−0.0101 (6)	0.0005 (5)	−0.0110 (6)
C7	0.0201 (6)	0.0316 (7)	0.0207 (6)	−0.0072 (5)	−0.0005 (5)	−0.0113 (5)
C8	0.0200 (6)	0.0282 (7)	0.0209 (6)	−0.0088 (5)	0.0002 (5)	−0.0101 (5)
C9	0.0202 (6)	0.0288 (7)	0.0241 (7)	−0.0065 (5)	0.0004 (5)	−0.0128 (6)
C10	0.0222 (7)	0.0305 (7)	0.0261 (7)	−0.0019 (6)	−0.0017 (5)	−0.0154 (6)
C11	0.0291 (7)	0.0304 (8)	0.0295 (7)	−0.0016 (6)	−0.0030 (6)	−0.0138 (6)
C12	0.0400 (9)	0.0331 (8)	0.0323 (8)	0.0004 (7)	−0.0085 (6)	−0.0109 (6)
C13	0.0337 (8)	0.0441 (9)	0.0377 (9)	0.0048 (7)	−0.0145 (7)	−0.0171 (7)
C14	0.0233 (7)	0.0435 (9)	0.0357 (8)	−0.0004 (6)	−0.0073 (6)	−0.0194 (7)
C15	0.0203 (7)	0.0355 (8)	0.0291 (7)	−0.0012 (6)	−0.0012 (5)	−0.0178 (6)
C16	0.0159 (6)	0.0375 (8)	0.0286 (7)	−0.0056 (6)	0.0004 (5)	−0.0166 (6)
C17	0.0181 (6)	0.0393 (8)	0.0279 (7)	−0.0119 (6)	0.0043 (5)	−0.0166 (6)
C18	0.0261 (7)	0.0373 (8)	0.0287 (7)	−0.0153 (6)	0.0075 (6)	−0.0159 (6)
C19	0.0285 (8)	0.0501 (10)	0.0377 (8)	−0.0188 (7)	0.0065 (6)	−0.0241 (7)
C20	0.0427 (9)	0.0500 (10)	0.0384 (9)	−0.0278 (8)	0.0090 (7)	−0.0252 (7)
C21	0.0519 (10)	0.0351 (8)	0.0326 (8)	−0.0208 (7)	0.0064 (7)	−0.0156 (7)
C22	0.0420 (8)	0.0322 (8)	0.0255 (7)	−0.0149 (7)	0.0045 (6)	−0.0102 (6)
C23	0.0299 (7)	0.0331 (8)	0.0225 (7)	−0.0151 (6)	0.0063 (5)	−0.0116 (6)
C24	0.0249 (7)	0.0284 (7)	0.0212 (7)	−0.0094 (6)	0.0034 (5)	−0.0087 (5)
C25	0.0236 (7)	0.0326 (7)	0.0204 (7)	−0.0079 (6)	0.0021 (5)	−0.0078 (6)
C26	0.0307 (8)	0.0319 (8)	0.0314 (8)	−0.0069 (6)	0.0024 (6)	−0.0095 (6)
C27	0.0303 (8)	0.0391 (9)	0.0407 (9)	−0.0014 (7)	0.0075 (7)	−0.0109 (7)
C28	0.0252 (8)	0.0478 (10)	0.0441 (9)	−0.0102 (7)	0.0092 (7)	−0.0073 (7)
C29	0.0322 (8)	0.0405 (9)	0.0440 (9)	−0.0172 (7)	0.0091 (7)	−0.0112 (7)
C30	0.0286 (7)	0.0341 (8)	0.0345 (8)	−0.0117 (6)	0.0084 (6)	−0.0133 (6)
C31	0.0328 (8)	0.0401 (8)	0.0308 (8)	−0.0156 (6)	0.0038 (6)	−0.0185 (7)
B1	0.0198 (7)	0.0294 (8)	0.0254 (8)	−0.0088 (6)	0.0003 (6)	−0.0106 (6)
N8	0.0233 (6)	0.0289 (6)	0.0234 (6)	−0.0076 (5)	0.0000 (4)	−0.0077 (5)

N9	0.0240 (6)	0.0332 (6)	0.0255 (6)	−0.0074 (5)	0.0019 (5)	−0.0097 (5)
N10	0.0263 (6)	0.0281 (6)	0.0218 (6)	−0.0079 (5)	−0.0008 (4)	−0.0077 (5)
N11	0.0318 (6)	0.0318 (6)	0.0260 (6)	−0.0059 (5)	−0.0070 (5)	−0.0103 (5)
N12	0.0220 (6)	0.0306 (6)	0.0236 (6)	−0.0067 (5)	−0.0017 (4)	−0.0097 (5)
N13	0.0264 (6)	0.0346 (7)	0.0250 (6)	−0.0118 (5)	−0.0003 (5)	−0.0096 (5)
N14	0.0267 (6)	0.0294 (6)	0.0231 (6)	−0.0102 (5)	0.0018 (5)	−0.0077 (5)
C32	0.0281 (7)	0.0278 (7)	0.0236 (7)	−0.0106 (6)	−0.0001 (5)	−0.0068 (6)
C33	0.0299 (7)	0.0256 (7)	0.0278 (7)	−0.0069 (6)	−0.0023 (6)	−0.0067 (6)
C34	0.0374 (8)	0.0312 (8)	0.0294 (8)	−0.0102 (6)	−0.0029 (6)	−0.0041 (6)
C35	0.0443 (9)	0.0334 (8)	0.0289 (8)	−0.0047 (7)	−0.0083 (7)	−0.0019 (6)
C36	0.0350 (8)	0.0346 (8)	0.0360 (8)	0.0019 (6)	−0.0107 (7)	−0.0090 (7)
C37	0.0276 (7)	0.0328 (8)	0.0349 (8)	−0.0023 (6)	−0.0043 (6)	−0.0109 (6)
C38	0.0279 (7)	0.0272 (7)	0.0276 (7)	−0.0047 (6)	−0.0018 (6)	−0.0092 (6)
C39	0.0214 (7)	0.0304 (7)	0.0264 (7)	−0.0055 (6)	0.0008 (5)	−0.0104 (6)
C40	0.0240 (7)	0.0331 (8)	0.0225 (7)	−0.0094 (6)	0.0029 (5)	−0.0114 (6)
C41	0.0332 (7)	0.0344 (8)	0.0189 (7)	−0.0136 (6)	0.0042 (5)	−0.0106 (6)
C42	0.0366 (8)	0.0415 (9)	0.0266 (7)	−0.0181 (7)	0.0081 (6)	−0.0161 (6)
C43	0.0512 (10)	0.0451 (9)	0.0339 (8)	−0.0285 (8)	0.0106 (7)	−0.0170 (7)
C44	0.0643 (11)	0.0335 (8)	0.0300 (8)	−0.0227 (8)	0.0044 (7)	−0.0087 (7)
C45	0.0502 (9)	0.0318 (8)	0.0236 (7)	−0.0124 (7)	−0.0015 (6)	−0.0078 (6)
C46	0.0388 (8)	0.0311 (8)	0.0191 (7)	−0.0123 (6)	0.0001 (6)	−0.0089 (6)
C47	0.0319 (7)	0.0299 (7)	0.0200 (7)	−0.0073 (6)	−0.0040 (5)	−0.0077 (6)
C48	0.0274 (7)	0.0318 (8)	0.0265 (7)	−0.0047 (6)	−0.0073 (6)	−0.0123 (6)
C49	0.0260 (7)	0.0404 (8)	0.0332 (8)	−0.0049 (6)	−0.0057 (6)	−0.0203 (7)
C50	0.0317 (8)	0.0450 (9)	0.0448 (9)	0.0003 (7)	−0.0108 (7)	−0.0266 (8)
C51	0.0289 (8)	0.0640 (12)	0.0515 (10)	0.0036 (8)	−0.0078 (7)	−0.0395 (9)
C52	0.0278 (8)	0.0780 (13)	0.0415 (10)	−0.0077 (8)	0.0032 (7)	−0.0387 (10)
C53	0.0280 (8)	0.0594 (10)	0.0320 (8)	−0.0119 (7)	0.0021 (6)	−0.0252 (7)
C54	0.0240 (7)	0.0440 (9)	0.0299 (8)	−0.0085 (6)	−0.0020 (6)	−0.0197 (7)
C55	0.0249 (7)	0.0345 (8)	0.0248 (7)	−0.0115 (6)	0.0004 (5)	−0.0125 (6)
C56	0.0219 (7)	0.0245 (7)	0.0292 (7)	−0.0032 (5)	−0.0021 (5)	−0.0087 (6)
C57	0.0388 (8)	0.0356 (8)	0.0299 (8)	−0.0121 (7)	−0.0039 (6)	−0.0086 (6)
C58	0.0504 (10)	0.0444 (9)	0.0395 (9)	−0.0178 (8)	−0.0089 (7)	−0.0164 (7)
C59	0.0406 (9)	0.0365 (9)	0.0496 (10)	−0.0175 (7)	−0.0039 (7)	−0.0137 (7)
C60	0.0337 (8)	0.0326 (8)	0.0376 (8)	−0.0113 (6)	0.0027 (6)	−0.0089 (7)
C61	0.0290 (7)	0.0298 (7)	0.0301 (8)	−0.0074 (6)	0.0002 (6)	−0.0110 (6)
C62	0.0422 (9)	0.0388 (9)	0.0273 (8)	−0.0176 (7)	0.0069 (6)	−0.0117 (6)
B2	0.0233 (8)	0.0268 (8)	0.0238 (8)	−0.0071 (6)	−0.0001 (6)	−0.0060 (6)
O1W	0.045 (2)	0.032 (2)	0.038 (2)	0.0009 (17)	−0.0176 (17)	−0.0095 (17)

Geometric parameters (Å, º)

N1—C8	1.3616 (17)	N8—C39	1.3714 (17)
N1—C1	1.3655 (17)	N8—B2	1.5213 (19)
N1—B1	1.4952 (18)	N9—C39	1.3408 (18)
N2—C8	1.3455 (17)	N9—C40	1.3481 (18)
N2—C9	1.3505 (17)	N10—C47	1.3648 (18)
N3—C9	1.3651 (17)	N10—C40	1.3676 (17)

N3—C16	1.3675 (16)	N10—B2	1.5002 (19)
N3—B1	1.5096 (19)	N11—C48	1.3404 (19)
N4—C17	1.3451 (19)	N11—C47	1.3498 (18)
N4—C16	1.3475 (18)	N12—C48	1.3687 (18)
N5—C24	1.3601 (18)	N12—C55	1.3701 (18)
N5—C17	1.3661 (17)	N12—B2	1.5134 (19)
N5—B1	1.4997 (19)	N13—C55	1.3425 (18)
N6—C1	1.3413 (17)	N13—C32	1.3475 (18)
N6—C24	1.3484 (17)	N14—C56	1.4026 (17)
N7—C25	1.4238 (17)	N14—C62	1.4632 (18)
N7—C31	1.4622 (17)	N14—B2	1.5128 (19)
N7—B1	1.5093 (18)	C32—C33	1.4583 (19)
C1—C2	1.4533 (18)	C33—C34	1.396 (2)
C2—C3	1.389 (2)	C33—C38	1.419 (2)
C2—C7	1.421 (2)	C34—C35	1.383 (2)
C3—C4	1.381 (2)	C34—H34A	0.9500
C3—H3A	0.9500	C35—C36	1.397 (2)
C4—C5	1.397 (2)	C35—H35A	0.9500
C4—H4A	0.9500	C36—C37	1.383 (2)
C5—C6	1.379 (2)	C36—H36A	0.9500
C5—H5A	0.9500	C37—C38	1.396 (2)
C6—C7	1.3896 (19)	C37—H37A	0.9500
C6—H6A	0.9500	C38—C39	1.4534 (19)
C7—C8	1.4596 (18)	C40—C41	1.452 (2)
C9—C10	1.4573 (19)	C41—C42	1.397 (2)
C10—C11	1.393 (2)	C41—C46	1.420 (2)
C10—C15	1.4199 (19)	C42—C43	1.385 (2)
C11—C12	1.387 (2)	C42—H42A	0.9500
C11—H11A	0.9500	C43—C44	1.397 (3)
C12—C13	1.397 (2)	C43—H43A	0.9500
C12—H12A	0.9500	C44—C45	1.384 (2)
C13—C14	1.381 (2)	C44—H44A	0.9500
C13—H13A	0.9500	C45—C46	1.397 (2)
C14—C15	1.392 (2)	C45—H45A	0.9500
C14—H14A	0.9500	C46—C47	1.453 (2)
C15—C16	1.452 (2)	C48—C49	1.457 (2)
C17—C18	1.455 (2)	C49—C50	1.393 (2)
C18—C19	1.400 (2)	C49—C54	1.420 (2)
C18—C23	1.420 (2)	C50—C51	1.384 (2)
C19—C20	1.381 (2)	C50—H50A	0.9500
C19—H19A	0.9500	C51—C52	1.396 (3)
C20—C21	1.399 (2)	C51—H51A	0.9500
C20—H20A	0.9500	C52—C53	1.383 (2)
C21—C22	1.384 (2)	C52—H52A	0.9500
C21—H21A	0.9500	C53—C54	1.395 (2)
C22—C23	1.395 (2)	C53—H53A	0.9500
C22—H22A	0.9500	C54—C55	1.459 (2)
C23—C24	1.4541 (19)	C56—C61	1.401 (2)

C25—C26	1.394 (2)	C56—C57	1.405 (2)
C25—C30	1.396 (2)	C57—C58	1.389 (2)
C26—C27	1.385 (2)	C57—H57A	0.9500
C26—H26A	0.9500	C58—C59	1.379 (2)
C27—C28	1.372 (2)	C58—H58A	0.9500
C27—H27A	0.9500	C59—C60	1.382 (2)
C28—C29	1.384 (2)	C59—H59A	0.9500
C28—H28A	0.9500	C60—C61	1.386 (2)
C29—C30	1.385 (2)	C60—H60A	0.9500
C29—H29A	0.9500	C61—H61A	0.9500
C30—H30A	0.9500	C62—H62A	0.9800
C31—H31A	0.9800	C62—H62B	0.9800
C31—H31B	0.9800	C62—H62C	0.9800
C31—H31C	0.9800	O1W—H2O	0.8401
N8—C32	1.3642 (17)	O1W—H1O	0.8400

C8—N1—C1	113.38 (10)	C32—N8—B2	124.40 (11)
C8—N1—B1	124.01 (11)	C39—N8—B2	122.09 (11)
C1—N1—B1	122.20 (11)	C39—N9—C40	116.86 (11)
C8—N2—C9	116.50 (11)	C47—N10—C40	112.78 (11)
C9—N3—C16	112.49 (11)	C47—N10—B2	122.91 (11)
C9—N3—B1	123.58 (11)	C40—N10—B2	123.59 (12)
C16—N3—B1	123.03 (11)	C48—N11—C47	116.64 (12)
C17—N4—C16	117.11 (11)	C48—N12—C55	112.39 (11)
C24—N5—C17	113.28 (11)	C48—N12—B2	122.23 (11)
C24—N5—B1	122.27 (11)	C55—N12—B2	124.57 (11)
C17—N5—B1	123.49 (12)	C55—N13—C32	116.47 (12)
C1—N6—C24	116.38 (11)	C56—N14—C62	114.88 (11)
C25—N7—C31	114.43 (11)	C56—N14—B2	124.55 (11)
C25—N7—B1	119.69 (11)	C62—N14—B2	120.43 (11)
C31—N7—B1	113.68 (11)	N13—C32—N8	123.15 (12)
N6—C1—N1	122.43 (11)	N13—C32—C33	129.25 (12)
N6—C1—C2	130.60 (12)	N8—C32—C33	106.29 (11)
N1—C1—C2	105.39 (11)	C34—C33—C38	120.82 (13)
C3—C2—C7	120.80 (12)	C34—C33—C32	132.17 (13)
C3—C2—C1	131.97 (13)	C38—C33—C32	106.80 (12)
C7—C2—C1	107.17 (11)	C35—C34—C33	117.74 (14)
C4—C3—C2	117.96 (14)	C35—C34—H34A	121.1
C4—C3—H3A	121.0	C33—C34—H34A	121.1
C2—C3—H3A	121.0	C34—C35—C36	121.53 (14)
C3—C4—C5	121.35 (14)	C34—C35—H35A	119.2
C3—C4—H4A	119.3	C36—C35—H35A	119.2
C5—C4—H4A	119.3	C37—C36—C35	121.44 (14)
C6—C5—C4	121.23 (13)	C37—C36—H36A	119.3
C6—C5—H5A	119.4	C35—C36—H36A	119.3
C4—C5—H5A	119.4	C36—C37—C38	117.95 (14)
C5—C6—C7	118.40 (14)	C36—C37—H37A	121.0
C5—C6—H6A	120.8	C38—C37—H37A	121.0

C7—C6—H6A	120.8	C37—C38—C33	120.45 (13)
C6—C7—C2	120.12 (12)	C37—C38—C39	132.18 (13)
C6—C7—C8	132.66 (13)	C33—C38—C39	107.11 (12)
C2—C7—C8	107.08 (11)	N9—C39—N8	122.90 (12)
N2—C8—N1	122.62 (11)	N9—C39—C38	128.68 (12)
N2—C8—C7	131.06 (12)	N8—C39—C38	106.02 (11)
N1—C8—C7	105.40 (11)	N9—C40—N10	122.31 (12)
N2—C9—N3	122.39 (12)	N9—C40—C41	130.29 (12)
N2—C9—C10	130.04 (12)	N10—C40—C41	105.90 (12)
N3—C9—C10	106.02 (11)	C42—C41—C46	120.67 (13)
C11—C10—C15	120.29 (12)	C42—C41—C40	131.84 (14)
C11—C10—C9	132.45 (12)	C46—C41—C40	107.24 (12)
C15—C10—C9	106.92 (12)	C43—C42—C41	117.82 (15)
C12—C11—C10	118.15 (14)	C43—C42—H42A	121.1
C12—C11—H11A	120.9	C41—C42—H42A	121.1
C10—C11—H11A	120.9	C42—C43—C44	121.38 (14)
C11—C12—C13	121.26 (15)	C42—C43—H43A	119.3
C11—C12—H12A	119.4	C44—C43—H43A	119.3
C13—C12—H12A	119.4	C45—C44—C43	121.67 (15)
C14—C13—C12	121.31 (14)	C45—C44—H44A	119.2
C14—C13—H13A	119.3	C43—C44—H44A	119.2
C12—C13—H13A	119.3	C44—C45—C46	117.69 (15)
C13—C14—C15	118.13 (14)	C44—C45—H45A	121.2
C13—C14—H14A	120.9	C46—C45—H45A	121.2
C15—C14—H14A	120.9	C45—C46—C41	120.69 (13)
C14—C15—C10	120.79 (14)	C45—C46—C47	132.07 (14)
C14—C15—C16	131.87 (13)	C41—C46—C47	107.03 (12)
C10—C15—C16	107.13 (11)	N11—C47—N10	122.46 (12)
N4—C16—N3	122.16 (13)	N11—C47—C46	129.81 (13)
N4—C16—C15	129.87 (12)	N10—C47—C46	106.02 (12)
N3—C16—C15	105.96 (11)	N11—C48—N12	122.61 (12)
N4—C17—N5	122.55 (12)	N11—C48—C49	130.11 (13)
N4—C17—C18	130.64 (12)	N12—C48—C49	105.88 (12)
N5—C17—C18	105.45 (12)	C50—C49—C54	120.88 (14)
C19—C18—C23	120.20 (14)	C50—C49—C48	132.12 (15)
C19—C18—C17	132.59 (14)	C54—C49—C48	107.00 (12)
C23—C18—C17	107.15 (11)	C51—C50—C49	117.69 (16)
C20—C19—C18	117.89 (15)	C51—C50—H50A	121.2
C20—C19—H19A	121.1	C49—C50—H50A	121.2
C18—C19—H19A	121.1	C50—C51—C52	121.40 (15)
C19—C20—C21	121.59 (14)	C50—C51—H51A	119.3
C19—C20—H20A	119.2	C52—C51—H51A	119.3
C21—C20—H20A	119.2	C53—C52—C51	121.67 (15)
C22—C21—C20	121.52 (15)	C53—C52—H52A	119.2
C22—C21—H21A	119.2	C51—C52—H52A	119.2
C20—C21—H21A	119.2	C52—C53—C54	117.69 (16)
C21—C22—C23	117.53 (15)	C52—C53—H53A	121.2
C21—C22—H22A	121.2	C54—C53—H53A	121.2

C23—C22—H22A	121.2	C53—C54—C49	120.51 (14)
C22—C23—C18	121.17 (13)	C53—C54—C55	132.38 (15)
C22—C23—C24	131.68 (13)	C49—C54—C55	107.10 (12)
C18—C23—C24	107.11 (12)	N13—C55—N12	122.55 (12)
N6—C24—N5	123.03 (12)	N13—C55—C54	130.57 (13)
N6—C24—C23	129.86 (12)	N12—C55—C54	105.60 (12)
N5—C24—C23	105.70 (11)	C61—C56—N14	121.49 (12)
C26—C25—C30	117.79 (13)	C61—C56—C57	116.67 (13)
C26—C25—N7	121.72 (12)	N14—C56—C57	121.82 (12)
C30—C25—N7	120.46 (12)	C58—C57—C56	120.76 (14)
C27—C26—C25	121.02 (14)	C58—C57—H57A	119.6
C27—C26—H26A	119.5	C56—C57—H57A	119.6
C25—C26—H26A	119.5	C59—C58—C57	121.78 (15)
C28—C27—C26	120.85 (15)	C59—C58—H58A	119.1
C28—C27—H27A	119.6	C57—C58—H58A	119.1
C26—C27—H27A	119.6	C58—C59—C60	118.05 (14)
C27—C28—C29	118.79 (14)	C58—C59—H59A	121.0
C27—C28—H28A	120.6	C60—C59—H59A	121.0
C29—C28—H28A	120.6	C59—C60—C61	121.04 (14)
C28—C29—C30	121.02 (15)	C59—C60—H60A	119.5
C28—C29—H29A	119.5	C61—C60—H60A	119.5
C30—C29—H29A	119.5	C60—C61—C56	121.67 (13)
C29—C30—C25	120.46 (14)	C60—C61—H61A	119.2
C29—C30—H30A	119.8	C56—C61—H61A	119.2
C25—C30—H30A	119.8	N14—C62—H62A	109.5
N7—C31—H31A	109.5	N14—C62—H62B	109.5
N7—C31—H31B	109.5	H62A—C62—H62B	109.5
H31A—C31—H31B	109.5	N14—C62—H62C	109.5
N7—C31—H31C	109.5	H62A—C62—H62C	109.5
H31A—C31—H31C	109.5	H62B—C62—H62C	109.5
H31B—C31—H31C	109.5	N10—B2—N14	112.75 (11)
N1—B1—N5	102.87 (11)	N10—B2—N12	102.23 (11)
N1—B1—N7	113.06 (11)	N14—B2—N12	116.53 (11)
N5—B1—N7	116.61 (11)	N10—B2—N8	102.36 (11)
N1—B1—N3	102.27 (11)	N14—B2—N8	119.22 (12)
N5—B1—N3	102.77 (11)	N12—B2—N8	101.40 (11)
N7—B1—N3	117.25 (12)	H2O—O1W—H1O	106.2
C32—N8—C39	112.03 (11)		

C24—N6—C1—N1	−6.41 (18)	C55—N13—C32—N8	−8.12 (19)
C24—N6—C1—C2	157.01 (13)	C55—N13—C32—C33	156.97 (14)
C8—N1—C1—N6	153.70 (12)	C39—N8—C32—N13	155.20 (13)
B1—N1—C1—N6	−19.18 (19)	B2—N8—C32—N13	−11.1 (2)
C8—N1—C1—C2	−13.32 (14)	C39—N8—C32—C33	−12.83 (15)
B1—N1—C1—C2	173.80 (11)	B2—N8—C32—C33	−179.16 (12)
N6—C1—C2—C3	20.4 (2)	N13—C32—C33—C34	14.1 (3)
N1—C1—C2—C3	−174.04 (14)	N8—C32—C33—C34	−178.85 (15)
N6—C1—C2—C7	−156.65 (13)	N13—C32—C33—C38	−160.50 (14)

N1—C1—C2—C7	8.88 (14)	N8—C32—C33—C38	6.53 (15)
C7—C2—C3—C4	0.1 (2)	C38—C33—C34—C35	−2.2 (2)
C1—C2—C3—C4	−176.66 (14)	C32—C33—C34—C35	−176.24 (15)
C2—C3—C4—C5	2.6 (2)	C33—C34—C35—C36	1.2 (2)
C3—C4—C5—C6	−2.2 (2)	C34—C35—C36—C37	1.0 (2)
C4—C5—C6—C7	−1.0 (2)	C35—C36—C37—C38	−2.2 (2)
C5—C6—C7—C2	3.6 (2)	C36—C37—C38—C33	1.2 (2)
C5—C6—C7—C8	178.76 (14)	C36—C37—C38—C39	174.66 (15)
C3—C2—C7—C6	−3.2 (2)	C34—C33—C38—C37	1.1 (2)
C1—C2—C7—C6	174.25 (12)	C32—C33—C38—C37	176.42 (13)
C3—C2—C7—C8	−179.48 (12)	C34—C33—C38—C39	−173.89 (13)
C1—C2—C7—C8	−2.02 (14)	C32—C33—C38—C39	1.47 (15)
C9—N2—C8—N1	7.69 (18)	C40—N9—C39—N8	7.64 (19)
C9—N2—C8—C7	−159.65 (13)	C40—N9—C39—C38	−152.21 (14)
C1—N1—C8—N2	−158.07 (12)	C32—N8—C39—N9	−150.03 (13)
B1—N1—C8—N2	14.66 (19)	B2—N8—C39—N9	16.7 (2)
C1—N1—C8—C7	12.06 (14)	C32—N8—C39—C38	13.73 (15)
B1—N1—C8—C7	−175.21 (11)	B2—N8—C39—C38	−179.58 (12)
C6—C7—C8—N2	−12.3 (2)	C37—C38—C39—N9	−20.5 (3)
C2—C7—C8—N2	163.34 (13)	C33—C38—C39—N9	153.60 (14)
C6—C7—C8—N1	178.77 (14)	C37—C38—C39—N8	176.99 (15)
C2—C7—C8—N1	−5.62 (14)	C33—C38—C39—N8	−8.90 (15)
C8—N2—C9—N3	−7.82 (18)	C39—N9—C40—N10	−9.49 (19)
C8—N2—C9—C10	155.91 (13)	C39—N9—C40—C41	154.45 (14)
C16—N3—C9—N2	155.30 (12)	C47—N10—C40—N9	157.11 (12)
B1—N3—C9—N2	−14.09 (19)	B2—N10—C40—N9	−13.4 (2)
C16—N3—C9—C10	−11.81 (14)	C47—N10—C40—C41	−10.22 (15)
B1—N3—C9—C10	178.80 (11)	B2—N10—C40—C41	179.28 (12)
N2—C9—C10—C11	13.2 (2)	N9—C40—C41—C42	13.8 (2)
N3—C9—C10—C11	178.95 (14)	N10—C40—C41—C42	179.78 (14)
N2—C9—C10—C15	−159.83 (13)	N9—C40—C41—C46	−160.26 (14)
N3—C9—C10—C15	5.93 (14)	N10—C40—C41—C46	5.67 (14)
C15—C10—C11—C12	−2.7 (2)	C46—C41—C42—C43	−2.4 (2)
C9—C10—C11—C12	−174.92 (14)	C40—C41—C42—C43	−175.84 (14)
C10—C11—C12—C13	0.6 (2)	C41—C42—C43—C44	1.7 (2)
C11—C12—C13—C14	1.5 (2)	C42—C43—C44—C45	0.7 (2)
C12—C13—C14—C15	−1.4 (2)	C43—C44—C45—C46	−2.3 (2)
C13—C14—C15—C10	−0.7 (2)	C44—C45—C46—C41	1.6 (2)
C13—C14—C15—C16	173.40 (14)	C44—C45—C46—C47	175.55 (14)
C11—C10—C15—C14	2.8 (2)	C42—C41—C46—C45	0.7 (2)
C9—C10—C15—C14	176.81 (12)	C40—C41—C46—C45	175.62 (12)
C11—C10—C15—C16	−172.62 (12)	C42—C41—C46—C47	−174.55 (12)
C9—C10—C15—C16	1.43 (14)	C40—C41—C46—C47	0.35 (14)
C17—N4—C16—N3	6.41 (19)	C48—N11—C47—N10	9.80 (18)
C17—N4—C16—C15	−155.14 (13)	C48—N11—C47—C46	−153.14 (14)
C9—N3—C16—N4	−152.66 (12)	C40—N10—C47—N11	−155.99 (12)
B1—N3—C16—N4	16.80 (19)	B2—N10—C47—N11	14.58 (19)
C9—N3—C16—C15	12.70 (14)	C40—N10—C47—C46	10.44 (15)

B1—N3—C16—C15	−177.84 (11)	B2—N10—C47—C46	−178.98 (11)
C14—C15—C16—N4	−19.1 (2)	C45—C46—C47—N11	−15.7 (2)
C10—C15—C16—N4	155.57 (13)	C41—C46—C47—N11	158.82 (13)
C14—C15—C16—N3	177.09 (14)	C45—C46—C47—N10	179.22 (14)
C10—C15—C16—N3	−8.24 (14)	C41—C46—C47—N10	−6.25 (14)
C16—N4—C17—N5	−8.54 (19)	C47—N11—C48—N12	−8.67 (18)
C16—N4—C17—C18	156.14 (13)	C47—N11—C48—C49	155.79 (13)
C24—N5—C17—N4	156.40 (12)	C55—N12—C48—N11	153.61 (12)
B1—N5—C17—N4	−12.61 (19)	B2—N12—C48—N11	−16.58 (19)
C24—N5—C17—C18	−11.60 (15)	C55—N12—C48—C49	−14.09 (14)
B1—N5—C17—C18	179.39 (11)	B2—N12—C48—C49	175.73 (11)
N4—C17—C18—C19	17.0 (3)	N11—C48—C49—C50	20.8 (2)
N5—C17—C18—C19	−176.36 (15)	N12—C48—C49—C50	−172.79 (14)
N4—C17—C18—C23	−160.04 (14)	N11—C48—C49—C54	−158.87 (13)
N5—C17—C18—C23	6.61 (14)	N12—C48—C49—C54	7.55 (14)
C23—C18—C19—C20	−2.8 (2)	C54—C49—C50—C51	−3.7 (2)
C17—C18—C19—C20	−179.47 (14)	C48—C49—C50—C51	176.72 (14)
C18—C19—C20—C21	2.3 (2)	C49—C50—C51—C52	2.3 (2)
C19—C20—C21—C22	0.3 (2)	C50—C51—C52—C53	1.4 (2)
C20—C21—C22—C23	−2.5 (2)	C51—C52—C53—C54	−3.6 (2)
C21—C22—C23—C18	2.1 (2)	C52—C53—C54—C49	2.2 (2)
C21—C22—C23—C24	179.51 (14)	C52—C53—C54—C55	−177.52 (14)
C19—C18—C23—C22	0.6 (2)	C50—C49—C54—C53	1.4 (2)
C17—C18—C23—C22	178.05 (12)	C48—C49—C54—C53	−178.85 (12)
C19—C18—C23—C24	−177.44 (12)	C50—C49—C54—C55	−178.78 (12)
C17—C18—C23—C24	0.04 (14)	C48—C49—C54—C55	0.92 (15)
C1—N6—C24—N5	9.36 (18)	C32—N13—C55—N12	5.74 (19)
C1—N6—C24—C23	−155.11 (13)	C32—N13—C55—C54	−159.42 (14)
C17—N5—C24—N6	−156.04 (12)	C48—N12—C55—N13	−153.71 (12)
B1—N5—C24—N6	13.13 (19)	B2—N12—C55—N13	16.2 (2)
C17—N5—C24—C23	11.64 (15)	C48—N12—C55—C54	14.63 (14)
B1—N5—C24—C23	−179.19 (11)	B2—N12—C55—C54	−175.46 (12)
C22—C23—C24—N6	−17.9 (2)	C53—C54—C55—N13	−22.3 (3)
C18—C23—C24—N6	159.82 (13)	C49—C54—C55—N13	158.00 (14)
C22—C23—C24—N5	175.58 (14)	C53—C54—C55—N12	170.69 (14)
C18—C23—C24—N5	−6.70 (14)	C49—C54—C55—N12	−9.04 (14)
C31—N7—C25—C26	−23.22 (18)	C62—N14—C56—C61	160.96 (13)
B1—N7—C25—C26	116.85 (15)	B2—N14—C56—C61	−23.3 (2)
C31—N7—C25—C30	154.75 (13)	C62—N14—C56—C57	−17.44 (19)
B1—N7—C25—C30	−65.19 (18)	B2—N14—C56—C57	158.30 (13)
C30—C25—C26—C27	0.4 (2)	C61—C56—C57—C58	1.1 (2)
N7—C25—C26—C27	178.44 (13)	N14—C56—C57—C58	179.60 (14)
C25—C26—C27—C28	1.4 (2)	C56—C57—C58—C59	0.2 (3)
C26—C27—C28—C29	−1.1 (3)	C57—C58—C59—C60	−0.7 (3)
C27—C28—C29—C30	−0.9 (3)	C58—C59—C60—C61	−0.1 (2)
C28—C29—C30—C25	2.7 (2)	C59—C60—C61—C56	1.5 (2)
C26—C25—C30—C29	−2.4 (2)	N14—C56—C61—C60	179.57 (13)
N7—C25—C30—C29	179.54 (14)	C57—C56—C61—C60	−1.9 (2)

C8—N1—B1—N5	−136.81 (12)	C47—N10—B2—N14	92.61 (15)
C1—N1—B1—N5	35.30 (16)	C40—N10—B2—N14	−97.83 (14)
C8—N1—B1—N7	96.56 (15)	C47—N10—B2—N12	−33.31 (16)
C1—N1—B1—N7	−91.33 (15)	C40—N10—B2—N12	136.26 (12)
C8—N1—B1—N3	−30.44 (16)	C47—N10—B2—N8	−138.06 (12)
C1—N1—B1—N3	141.67 (11)	C40—N10—B2—N8	31.51 (16)
C24—N5—B1—N1	−32.34 (16)	C56—N14—B2—N10	−164.96 (12)
C17—N5—B1—N1	135.72 (12)	C62—N14—B2—N10	10.56 (18)
C24—N5—B1—N7	91.99 (15)	C56—N14—B2—N12	−47.17 (18)
C17—N5—B1—N7	−99.96 (15)	C62—N14—B2—N12	128.35 (14)
C24—N5—B1—N3	−138.32 (12)	C56—N14—B2—N8	75.00 (17)
C17—N5—B1—N3	29.73 (16)	C62—N14—B2—N8	−109.48 (15)
C25—N7—B1—N1	171.31 (11)	C48—N12—B2—N10	34.20 (15)
C31—N7—B1—N1	−48.35 (16)	C55—N12—B2—N10	−134.76 (12)
C25—N7—B1—N5	52.36 (17)	C48—N12—B2—N14	−89.21 (15)
C31—N7—B1—N5	−167.30 (12)	C55—N12—B2—N14	101.83 (15)
C25—N7—B1—N3	−70.06 (16)	C48—N12—B2—N8	139.70 (12)
C31—N7—B1—N3	70.28 (15)	C55—N12—B2—N8	−29.26 (16)
C9—N3—B1—N1	30.12 (16)	C32—N8—B2—N10	132.17 (13)
C16—N3—B1—N1	−138.18 (12)	C39—N8—B2—N10	−32.85 (16)
C9—N3—B1—N5	136.56 (12)	C32—N8—B2—N14	−102.64 (15)
C16—N3—B1—N5	−31.74 (16)	C39—N8—B2—N14	92.34 (16)
C9—N3—B1—N7	−94.14 (15)	C32—N8—B2—N12	26.77 (17)
C16—N3—B1—N7	97.56 (15)	C39—N8—B2—N12	−138.24 (12)

(*N*-Phenylbenzamido)(subphthalocyaninato)boron (d22150_a)

Crystal data

$C_{31}H_{20}BN_7$
M_r = 501.35
Monoclinic, $P2_1/c$
a = 10.3502 (4) Å
b = 20.7509 (8) Å
c = 12.2816 (5) Å
β = 114.734 (2)°
V = 2395.80 (17) Å^3
Z = 4
$F(000)$ = 1040
D_x = 1.390 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9219 reflections
θ = 4.3–65.8°
μ = 0.68 mm^{-1}
T = 150 K
Shard, purple
0.19 × 0.14 × 0.09 mm

Data collection

Bruker Kappa APEX-DUO CMOS PHOTON II diffractometer
Radiation source: Inoatec ImuS with multi-layer optics
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.462, T_{max} = 0.753
41606 measured reflections
4159 independent reflections
3432 reflections with $I > 2\sigma(I)$
R_{int} = 0.111
θ_{max} = 66.4°, θ_{min} = 4.3°
h = −12→12
k = −24→24
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.165$
$S = 1.06$
4159 reflections
354 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1179P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: SHELXL2019 (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0101 (12)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.65532 (16)	0.59175 (7)	0.21413 (13)	0.0257 (4)
N2	0.73697 (17)	0.69317 (7)	0.17604 (13)	0.0281 (4)
N3	0.75068 (16)	0.66827 (7)	0.36934 (13)	0.0258 (4)
N4	0.87250 (17)	0.63159 (8)	0.57049 (13)	0.0286 (4)
N5	0.73686 (17)	0.55959 (7)	0.41500 (13)	0.0268 (4)
N6	0.69933 (16)	0.48035 (7)	0.26647 (13)	0.0287 (4)
N7	0.50830 (17)	0.62224 (7)	0.33581 (14)	0.0295 (4)
B1	0.6507 (2)	0.61169 (10)	0.33133 (18)	0.0260 (5)
C1	0.66648 (19)	0.52872 (9)	0.18618 (16)	0.0274 (4)
C2	0.67281 (19)	0.52945 (9)	0.07061 (16)	0.0279 (5)
C3	0.6813 (2)	0.48015 (10)	−0.00334 (17)	0.0326 (5)
H3A	0.675160	0.436222	0.015789	0.039*
C4	0.6988 (2)	0.49697 (11)	−0.10515 (18)	0.0385 (5)
H4A	0.704486	0.464057	−0.156727	0.046*
C5	0.7083 (2)	0.56135 (11)	−0.13372 (18)	0.0399 (5)
H5A	0.719779	0.571278	−0.204686	0.048*
C6	0.7015 (2)	0.61122 (10)	−0.06111 (16)	0.0335 (5)
H6A	0.709225	0.654920	−0.080673	0.040*
C7	0.68294 (19)	0.59499 (10)	0.04165 (16)	0.0291 (5)
C8	0.68407 (19)	0.63353 (9)	0.14095 (16)	0.0271 (4)
C9	0.7765 (2)	0.70803 (9)	0.29241 (16)	0.0259 (4)
C10	0.8777 (2)	0.75606 (9)	0.36766 (16)	0.0268 (4)
C11	0.9404 (2)	0.80922 (9)	0.34031 (17)	0.0297 (5)
H11A	0.914763	0.821832	0.259550	0.036*
C12	1.0412 (2)	0.84310 (9)	0.43435 (18)	0.0340 (5)
H12A	1.082772	0.880434	0.417544	0.041*
C13	1.0837 (2)	0.82399 (10)	0.55379 (19)	0.0345 (5)

H13A	1.154291	0.848103	0.616179	0.041*
C14	1.0241 (2)	0.77033 (9)	0.58198 (18)	0.0308 (5)
H14A	1.054145	0.756741	0.662766	0.037*
C15	0.9192 (2)	0.73697 (9)	0.48870 (16)	0.0274 (4)
C16	0.8426 (2)	0.67775 (9)	0.48600 (16)	0.0266 (4)
C17	0.8247 (2)	0.57179 (9)	0.53119 (16)	0.0274 (5)
C18	0.8719 (2)	0.50927 (9)	0.58638 (16)	0.0285 (4)
C19	0.9529 (2)	0.49073 (10)	0.70445 (17)	0.0315 (5)
H19A	0.989752	0.521786	0.766778	0.038*
C20	0.9779 (2)	0.42583 (10)	0.72813 (18)	0.0340 (5)
H20A	1.029217	0.411922	0.808573	0.041*
C21	0.9292 (2)	0.38011 (10)	0.63620 (18)	0.0331 (5)
H21A	0.948039	0.335780	0.655653	0.040*
C22	0.8544 (2)	0.39775 (9)	0.51793 (19)	0.0317 (5)
H22A	0.826125	0.366534	0.455678	0.038*
C23	0.8217 (2)	0.46271 (9)	0.49248 (17)	0.0279 (4)
C24	0.7415 (2)	0.49745 (9)	0.38169 (16)	0.0277 (4)
C25	0.4518 (2)	0.68471 (9)	0.32846 (17)	0.0298 (5)
C26	0.4561 (2)	0.72829 (10)	0.24303 (18)	0.0338 (5)
H26A	0.493158	0.714706	0.187913	0.041*
C27	0.4072 (2)	0.79084 (11)	0.2374 (2)	0.0413 (5)
H27A	0.414424	0.820032	0.180682	0.050*
C28	0.3480 (2)	0.81124 (11)	0.3135 (2)	0.0452 (6)
H28A	0.313590	0.854061	0.308949	0.054*
C29	0.3396 (2)	0.76848 (12)	0.3959 (2)	0.0454 (6)
H29A	0.297853	0.781872	0.447959	0.054*
C30	0.3913 (2)	0.70597 (10)	0.40425 (19)	0.0366 (5)
H30A	0.385245	0.677382	0.462364	0.044*
C31	0.4606 (2)	0.57447 (10)	0.3988 (2)	0.0382 (5)
H31A	0.487879	0.531267	0.383831	0.057*
H31B	0.356914	0.576775	0.369558	0.057*
H31C	0.505052	0.583395	0.485013	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0278 (8)	0.0275 (9)	0.0265 (8)	−0.0002 (6)	0.0159 (6)	−0.0006 (6)
N2	0.0313 (9)	0.0293 (9)	0.0274 (8)	0.0018 (7)	0.0159 (7)	0.0015 (6)
N3	0.0302 (8)	0.0260 (8)	0.0266 (8)	0.0006 (6)	0.0172 (7)	0.0000 (6)
N4	0.0369 (9)	0.0273 (9)	0.0279 (8)	0.0006 (7)	0.0200 (7)	−0.0001 (6)
N5	0.0302 (9)	0.0269 (9)	0.0282 (8)	−0.0002 (6)	0.0169 (7)	−0.0006 (6)
N6	0.0292 (8)	0.0303 (9)	0.0303 (9)	−0.0018 (7)	0.0162 (7)	−0.0015 (7)
N7	0.0337 (9)	0.0274 (9)	0.0358 (9)	0.0006 (7)	0.0228 (7)	0.0013 (6)
B1	0.0293 (11)	0.0270 (11)	0.0256 (11)	0.0007 (9)	0.0154 (9)	0.0011 (8)
C1	0.0261 (10)	0.0299 (10)	0.0290 (9)	−0.0022 (8)	0.0144 (8)	−0.0036 (8)
C2	0.0237 (10)	0.0348 (11)	0.0275 (9)	−0.0012 (8)	0.0129 (8)	−0.0027 (8)
C3	0.0283 (10)	0.0368 (11)	0.0321 (10)	0.0004 (8)	0.0120 (8)	−0.0066 (8)
C4	0.0380 (12)	0.0453 (13)	0.0368 (11)	−0.0008 (10)	0.0203 (9)	−0.0099 (9)

C5	0.0437 (13)	0.0520 (14)	0.0300 (11)	−0.0046 (10)	0.0214 (9)	−0.0048 (9)
C6	0.0361 (11)	0.0412 (12)	0.0267 (10)	−0.0040 (9)	0.0167 (8)	−0.0024 (8)
C7	0.0254 (10)	0.0362 (11)	0.0279 (10)	−0.0015 (8)	0.0134 (8)	−0.0020 (8)
C8	0.0269 (10)	0.0328 (11)	0.0250 (9)	0.0014 (8)	0.0142 (8)	0.0014 (7)
C9	0.0293 (10)	0.0270 (10)	0.0266 (9)	0.0039 (8)	0.0168 (8)	0.0027 (7)
C10	0.0329 (10)	0.0247 (10)	0.0305 (10)	0.0032 (8)	0.0207 (8)	−0.0011 (7)
C11	0.0356 (11)	0.0277 (11)	0.0339 (10)	0.0042 (8)	0.0227 (9)	0.0025 (8)
C12	0.0387 (11)	0.0271 (10)	0.0447 (12)	−0.0021 (8)	0.0259 (9)	−0.0011 (8)
C13	0.0371 (11)	0.0307 (11)	0.0398 (11)	−0.0028 (8)	0.0201 (9)	−0.0063 (8)
C14	0.0375 (11)	0.0278 (10)	0.0311 (10)	0.0021 (8)	0.0184 (9)	−0.0020 (8)
C15	0.0353 (10)	0.0242 (10)	0.0307 (10)	0.0025 (8)	0.0217 (8)	−0.0016 (7)
C16	0.0312 (10)	0.0275 (10)	0.0276 (10)	−0.0003 (8)	0.0186 (8)	−0.0016 (7)
C17	0.0329 (10)	0.0291 (10)	0.0259 (10)	0.0005 (8)	0.0179 (8)	0.0005 (7)
C18	0.0315 (10)	0.0280 (10)	0.0324 (10)	−0.0001 (8)	0.0199 (8)	0.0027 (8)
C19	0.0312 (10)	0.0364 (11)	0.0316 (10)	−0.0020 (8)	0.0178 (8)	0.0030 (8)
C20	0.0290 (11)	0.0374 (12)	0.0379 (11)	0.0040 (8)	0.0161 (9)	0.0095 (9)
C21	0.0299 (11)	0.0307 (11)	0.0455 (12)	0.0045 (8)	0.0223 (9)	0.0092 (9)
C22	0.0306 (10)	0.0287 (11)	0.0449 (12)	0.0006 (8)	0.0248 (9)	0.0010 (8)
C23	0.0264 (10)	0.0304 (11)	0.0341 (10)	0.0006 (8)	0.0198 (8)	0.0034 (8)
C24	0.0304 (10)	0.0266 (10)	0.0332 (10)	−0.0001 (8)	0.0203 (8)	−0.0003 (8)
C25	0.0278 (10)	0.0318 (11)	0.0320 (10)	−0.0010 (8)	0.0146 (8)	−0.0019 (8)
C26	0.0309 (10)	0.0387 (12)	0.0343 (11)	0.0033 (9)	0.0163 (8)	0.0042 (8)
C27	0.0389 (12)	0.0407 (13)	0.0450 (13)	0.0040 (9)	0.0182 (10)	0.0096 (10)
C28	0.0449 (13)	0.0367 (12)	0.0522 (14)	0.0098 (10)	0.0184 (11)	−0.0012 (10)
C29	0.0458 (13)	0.0500 (14)	0.0466 (13)	0.0096 (11)	0.0256 (11)	−0.0068 (10)
C30	0.0402 (12)	0.0396 (12)	0.0365 (11)	0.0038 (9)	0.0226 (9)	−0.0007 (9)
C31	0.0401 (12)	0.0386 (12)	0.0470 (13)	−0.0024 (9)	0.0293 (10)	0.0044 (9)

Geometric parameters (Å, º)

N1—C8	1.368 (2)	C11—H11A	0.9500
N1—C1	1.369 (2)	C12—C13	1.401 (3)
N1—B1	1.518 (2)	C12—H12A	0.9500
N2—C9	1.348 (2)	C13—C14	1.385 (3)
N2—C8	1.349 (3)	C13—H13A	0.9500
N3—C16	1.362 (2)	C14—C15	1.389 (3)
N3—C9	1.362 (2)	C14—H14A	0.9500
N3—B1	1.504 (3)	C15—C16	1.456 (3)
N4—C17	1.348 (2)	C17—C18	1.450 (3)
N4—C16	1.350 (2)	C18—C19	1.392 (3)
N5—C17	1.357 (2)	C18—C23	1.425 (3)
N5—C24	1.360 (2)	C19—C20	1.379 (3)
N5—B1	1.501 (3)	C19—H19A	0.9500
N6—C24	1.342 (2)	C20—C21	1.397 (3)
N6—C1	1.347 (2)	C20—H20A	0.9500
N7—C25	1.409 (3)	C21—C22	1.379 (3)
N7—C31	1.464 (3)	C21—H21A	0.9500
N7—B1	1.513 (3)	C22—C23	1.393 (3)

C1—C2	1.448 (3)	C22—H22A	0.9500
C2—C3	1.395 (3)	C23—C24	1.454 (3)
C2—C7	1.421 (3)	C25—C30	1.394 (3)
C3—C4	1.381 (3)	C25—C26	1.400 (3)
C3—H3A	0.9500	C26—C27	1.384 (3)
C4—C5	1.395 (3)	C26—H26A	0.9500
C4—H4A	0.9500	C27—C28	1.380 (3)
C5—C6	1.387 (3)	C27—H27A	0.9500
C5—H5A	0.9500	C28—C29	1.376 (3)
C6—C7	1.395 (3)	C28—H28A	0.9500
C6—H6A	0.9500	C29—C30	1.391 (3)
C7—C8	1.454 (3)	C29—H29A	0.9500
C9—C10	1.461 (3)	C30—H30A	0.9500
C10—C11	1.390 (3)	C31—H31A	0.9800
C10—C15	1.420 (3)	C31—H31B	0.9800
C11—C12	1.381 (3)	C31—H31C	0.9800

C8—N1—C1	112.10 (15)	C12—C13—H13A	119.6
C8—N1—B1	123.51 (16)	C13—C14—C15	118.07 (18)
C1—N1—B1	122.53 (15)	C13—C14—H14A	121.0
C9—N2—C8	116.83 (15)	C15—C14—H14A	121.0
C16—N3—C9	112.88 (15)	C14—C15—C10	120.93 (17)
C16—N3—B1	121.73 (15)	C14—C15—C16	132.07 (17)
C9—N3—B1	124.51 (15)	C10—C15—C16	106.76 (15)
C17—N4—C16	116.49 (16)	N4—C16—N3	122.75 (17)
C17—N5—C24	113.64 (15)	N4—C16—C15	129.35 (17)
C17—N5—B1	122.02 (15)	N3—C16—C15	106.25 (15)
C24—N5—B1	124.24 (15)	N4—C17—N5	122.15 (17)
C24—N6—C1	116.48 (16)	N4—C17—C18	130.88 (17)
C25—N7—C31	115.73 (16)	N5—C17—C18	105.73 (16)
C25—N7—B1	120.98 (15)	C19—C18—C23	120.82 (18)
C31—N7—B1	118.03 (15)	C19—C18—C17	132.26 (18)
N5—B1—N3	102.41 (15)	C23—C18—C17	106.90 (16)
N5—B1—N7	112.84 (16)	C20—C19—C18	117.89 (19)
N3—B1—N7	115.47 (16)	C20—C19—H19A	121.1
N5—B1—N1	101.96 (15)	C18—C19—H19A	121.1
N3—B1—N1	102.49 (15)	C19—C20—C21	121.34 (19)
N7—B1—N1	119.45 (16)	C19—C20—H20A	119.3
N6—C1—N1	123.37 (16)	C21—C20—H20A	119.3
N6—C1—C2	128.62 (17)	C22—C21—C20	121.64 (19)
N1—C1—C2	106.19 (15)	C22—C21—H21A	119.2
C3—C2—C7	120.52 (18)	C20—C21—H21A	119.2
C3—C2—C1	132.17 (18)	C21—C22—C23	118.01 (19)
C7—C2—C1	107.09 (16)	C21—C22—H22A	121.0
C4—C3—C2	118.15 (19)	C23—C22—H22A	121.0
C4—C3—H3A	120.9	C22—C23—C18	120.14 (17)
C2—C3—H3A	120.9	C22—C23—C24	132.81 (18)
C3—C4—C5	121.31 (19)	C18—C23—C24	107.04 (16)

C3—C4—H4A	119.3	N6—C24—N5	122.07 (16)
C5—C4—H4A	119.3	N6—C24—C23	131.43 (17)
C6—C5—C4	121.65 (19)	N5—C24—C23	105.47 (15)
C6—C5—H5A	119.2	C30—C25—C26	117.39 (18)
C4—C5—H5A	119.2	C30—C25—N7	122.60 (18)
C5—C6—C7	117.7 (2)	C26—C25—N7	120.01 (17)
C5—C6—H6A	121.1	C27—C26—C25	121.2 (2)
C7—C6—H6A	121.1	C27—C26—H26A	119.4
C6—C7—C2	120.67 (18)	C25—C26—H26A	119.4
C6—C7—C8	132.07 (19)	C28—C27—C26	120.7 (2)
C2—C7—C8	106.98 (16)	C28—C27—H27A	119.6
N2—C8—N1	122.84 (16)	C26—C27—H27A	119.6
N2—C8—C7	129.21 (17)	C29—C28—C27	118.9 (2)
N1—C8—C7	105.95 (16)	C29—C28—H28A	120.6
N2—C9—N3	122.43 (17)	C27—C28—H28A	120.6
N2—C9—C10	130.26 (16)	C28—C29—C30	121.0 (2)
N3—C9—C10	105.73 (15)	C28—C29—H29A	119.5
C11—C10—C15	120.45 (17)	C30—C29—H29A	119.5
C11—C10—C9	132.22 (17)	C29—C30—C25	120.9 (2)
C15—C10—C9	107.14 (15)	C29—C30—H30A	119.6
C12—C11—C10	117.86 (18)	C25—C30—H30A	119.6
C12—C11—H11A	121.1	N7—C31—H31A	109.5
C10—C11—H11A	121.1	N7—C31—H31B	109.5
C11—C12—C13	121.87 (19)	H31A—C31—H31B	109.5
C11—C12—H12A	119.1	N7—C31—H31C	109.5
C13—C12—H12A	119.1	H31A—C31—H31C	109.5
C14—C13—C12	120.76 (19)	H31B—C31—H31C	109.5
C14—C13—H13A	119.6		

C17—N5—B1—N3	37.5 (2)	C15—C10—C11—C12	−1.3 (3)
C24—N5—B1—N3	−138.68 (17)	C9—C10—C11—C12	−175.58 (19)
C17—N5—B1—N7	−87.3 (2)	C10—C11—C12—C13	2.1 (3)
C24—N5—B1—N7	96.5 (2)	C11—C12—C13—C14	−0.9 (3)
C17—N5—B1—N1	143.34 (16)	C12—C13—C14—C15	−1.3 (3)
C24—N5—B1—N1	−32.8 (2)	C13—C14—C15—C10	2.1 (3)
C16—N3—B1—N5	−34.8 (2)	C13—C14—C15—C16	175.63 (19)
C9—N3—B1—N5	133.72 (17)	C11—C10—C15—C14	−0.8 (3)
C16—N3—B1—N7	88.3 (2)	C9—C10—C15—C14	174.77 (17)
C9—N3—B1—N7	−103.3 (2)	C11—C10—C15—C16	−175.80 (17)
C16—N3—B1—N1	−140.19 (16)	C9—C10—C15—C16	−0.24 (19)
C9—N3—B1—N1	28.3 (2)	C17—N4—C16—N3	10.2 (3)
C25—N7—B1—N5	141.49 (17)	C17—N4—C16—C15	−153.12 (19)
C31—N7—B1—N5	−11.8 (2)	C9—N3—C16—N4	−155.34 (17)
C25—N7—B1—N3	24.2 (2)	B1—N3—C16—N4	14.4 (3)
C31—N7—B1—N3	−129.11 (18)	C9—N3—C16—C15	11.3 (2)
C25—N7—B1—N1	−98.8 (2)	B1—N3—C16—C15	−179.02 (16)
C31—N7—B1—N1	107.9 (2)	C14—C15—C16—N4	−15.1 (3)
C8—N1—B1—N5	−133.49 (17)	C10—C15—C16—N4	159.09 (19)

C1—N1—B1—N5	29.8 (2)	C14—C15—C16—N3	179.45 (19)
C8—N1—B1—N3	−27.7 (2)	C10—C15—C16—N3	−6.32 (19)
C1—N1—B1—N3	135.54 (16)	C16—N4—C17—N5	−7.6 (3)
C8—N1—B1—N7	101.4 (2)	C16—N4—C17—C18	157.72 (19)
C1—N1—B1—N7	−95.3 (2)	C24—N5—C17—N4	156.89 (18)
C24—N6—C1—N1	−9.3 (3)	B1—N5—C17—N4	−19.7 (3)
C24—N6—C1—C2	153.20 (19)	C24—N5—C17—C18	−11.6 (2)
C8—N1—C1—N6	152.83 (17)	B1—N5—C17—C18	171.81 (17)
B1—N1—C1—N6	−12.1 (3)	N4—C17—C18—C19	18.9 (4)
C8—N1—C1—C2	−13.0 (2)	N5—C17—C18—C19	−174.0 (2)
B1—N1—C1—C2	−177.97 (15)	N4—C17—C18—C23	−159.61 (19)
N6—C1—C2—C3	16.8 (3)	N5—C17—C18—C23	7.5 (2)
N1—C1—C2—C3	−178.39 (19)	C23—C18—C19—C20	−2.6 (3)
N6—C1—C2—C7	−157.64 (18)	C17—C18—C19—C20	179.1 (2)
N1—C1—C2—C7	7.2 (2)	C18—C19—C20—C21	2.8 (3)
C7—C2—C3—C4	−0.4 (3)	C19—C20—C21—C22	0.2 (3)
C1—C2—C3—C4	−174.19 (19)	C20—C21—C22—C23	−3.3 (3)
C2—C3—C4—C5	0.2 (3)	C21—C22—C23—C18	3.5 (3)
C3—C4—C5—C6	0.4 (3)	C21—C22—C23—C24	−177.12 (19)
C4—C5—C6—C7	−0.8 (3)	C19—C18—C23—C22	−0.6 (3)
C5—C6—C7—C2	0.6 (3)	C17—C18—C23—C22	178.12 (17)
C5—C6—C7—C8	173.7 (2)	C19—C18—C23—C24	179.91 (17)
C3—C2—C7—C6	0.0 (3)	C17—C18—C23—C24	−1.4 (2)
C1—C2—C7—C6	175.20 (17)	C1—N6—C24—N5	6.9 (3)
C3—C2—C7—C8	−174.65 (16)	C1—N6—C24—C23	−159.73 (19)
C1—C2—C7—C8	0.6 (2)	C17—N5—C24—N6	−158.89 (17)
C9—N2—C8—N1	7.4 (3)	B1—N5—C24—N6	17.6 (3)
C9—N2—C8—C7	−154.15 (19)	C17—N5—C24—C23	10.7 (2)
C1—N1—C8—N2	−151.92 (17)	B1—N5—C24—C23	−172.81 (17)
B1—N1—C8—N2	12.9 (3)	C22—C23—C24—N6	−16.4 (4)
C1—N1—C8—C7	13.3 (2)	C18—C23—C24—N6	163.04 (19)
B1—N1—C8—C7	178.11 (16)	C22—C23—C24—N5	175.3 (2)
C6—C7—C8—N2	−17.9 (3)	C18—C23—C24—N5	−5.2 (2)
C2—C7—C8—N2	155.87 (18)	C31—N7—C25—C30	19.0 (3)
C6—C7—C8—N1	178.1 (2)	B1—N7—C25—C30	−134.9 (2)
C2—C7—C8—N1	−8.09 (19)	C31—N7—C25—C26	−161.42 (18)
C8—N2—C9—N3	−7.2 (3)	B1—N7—C25—C26	44.7 (3)
C8—N2—C9—C10	156.40 (18)	C30—C25—C26—C27	2.5 (3)
C16—N3—C9—N2	155.68 (17)	N7—C25—C26—C27	−177.08 (19)
B1—N3—C9—N2	−13.7 (3)	C25—C26—C27—C28	−2.4 (3)
C16—N3—C9—C10	−11.4 (2)	C26—C27—C28—C29	0.6 (3)
B1—N3—C9—C10	179.27 (16)	C27—C28—C29—C30	0.8 (4)
N2—C9—C10—C11	15.9 (3)	C28—C29—C30—C25	−0.6 (3)
N3—C9—C10—C11	−178.48 (19)	C26—C25—C30—C29	−1.1 (3)
N2—C9—C10—C15	−158.94 (19)	N7—C25—C30—C29	178.54 (19)
N3—C9—C10—C15	6.70 (19)		