Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

# Crystal structure and Hirshfeld surface analysis of triazatriborinotris[1,3,2]benzodiazaborole acetone disolvate

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Received 9 October 2023
Accepted 24 October 2023

Edited by J. Ellena, Universidade de São Paulo, Brazil

**Keywords:** crystal structure; Hirshfeld surface analysis; borazine; benzodiazaborole.

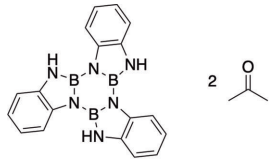
**CCDC reference:** 2303332

**Supporting information:** this article has supporting information at journals.iucr.org/e

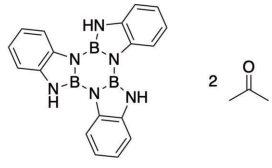
The title compound, alternatively known as benzodiazaborole trimer, $C_{18}H_{15}B_3N_6{\cdot}2C_3H_6O$, at 100 K crystallizes in the triclinic system, space group $P\overline{1}$. The structure displays N—H···O hydrogen bonding connecting the main molecule with the crystallization solvent. Disorder of the main molecule is observed with occupancy factors refined to 0.8922 (14):0.1078 (14). The packing of the crystal shows a parallel-displaced atom-centered orientation with 3.30 (2) Å between the planes of the rings. In the solid state, the title compound is linked with weak C—H···$\pi$ interactions, which is supported by Hirshfeld surface analysis.

## 1. Chemical context

Benzodiazaborole trimer was discovered over 60 years ago, with the first synthesis reported by Brotherton & Steinberg (1961). The formation of the borazine ring from three benzodiazaboroles is thermodynamically favorable and is found to be the major product (Niedenzu *et al.*, 1962). There has been research into the physical characteristics, such as IR (Harris & Rudner, 1962). As a film, the title compound is highly reflective, adherent, hard, and behaves as a narrow-band semiconductor, which is susceptible to modifications by chemical treatment (Maya, 1988). Additionally, its reactivity and synthesis have been studied by several groups (Kreutzberger & Ferris, 1962, Ryschkewitsch, 1964; Trofimenko, 1967; Dandegaonker & Mane, 1974; Maras & Kocevar, 2012). To date, there are no reports on the solid-state structure of the compound. Herein we report on the crystalline structure of the title compound synthesized by the condensation of boron trichloride and *o*-phenylenediamine and recrystallized in acetone.



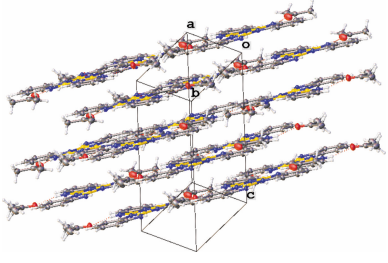

I




Ia

## 2. Structural commentary

The title compound crystallizes with two equivalents of acetone as the crystallization solvent. The structure is disordered, with the acetone molecules remaining stationary while the benzodiazaborle is inverted by 180° (Fig. 1). In each case, the acetone forms hydrogen bonds with a nearby NH group;



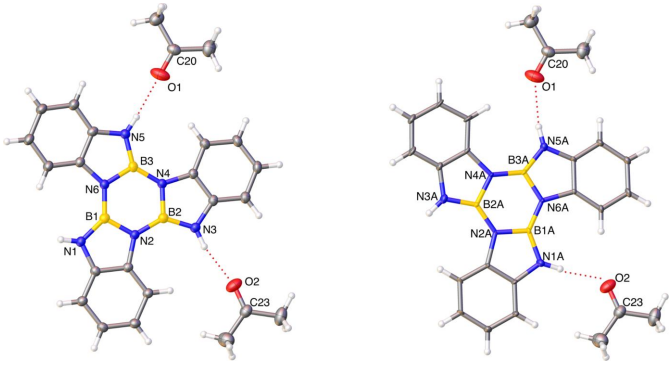



**Figure 1**
The molecular structure of the disordered title compounds, (**I** and **Ia**), with displacements ellipsoids drawn at the 50% probability level.

these bonds range from 2.086 (13) to 2.133 (13) Å. A comparison of between the two molecular orientations, **I** and **Ia**, is given in Table 1. The C1═O20 double bond of acetone is 1.2110 (15) Å and the O2═C23 double bond is 1.2122 (16) Å. The boron nitrogen bonds of the borazine ring vary slightly between the disordered structures, **Ia** has slightly shorter bond lengths, see Table 2. The B—NH bond lengths are similar between the title compounds and vary between 1.4191 (18) and 1.459 (2) Å.

## 3. Supramolecular features

In the crystal (Fig. 2), molecules of (I) adopt a parallel-displaced atom-centered orientation. The structure packs with 3.30 (2) Å between adjacent aromatic compounds. The weak intermolecular interactions of **I** and **Ia** were explored by Hirshfeld surface analysis. The properties ($d_{norm}$, shape-index and $d_e$) are mapped over the Hirshfeld surfaces and two-dimensional fingerprint plots of the title compound were generated using *CrystalExplorer* (Version 17.5; Spackman *et al.*, 2021). The $d_{norm}$ values illustrate whether the intermolecular contact is shorter or longer than the van der Waals radii. Red areas of the Hirshfeld surface indicate negative

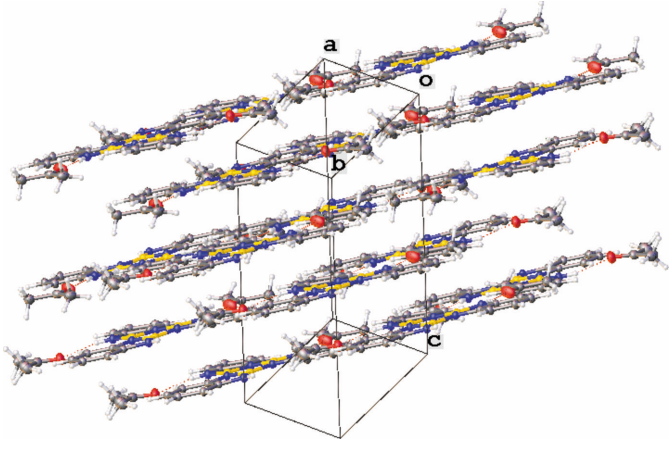



**Figure 2**
Packing diagram.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···O2 | 0.89 (1) | 2.13 (1) | 2.9817 (14) | 160 (1) |
| N5—H5···O1 | 0.87 (1) | 2.09 (1) | 2.9544 (15) | 175 (1) |
| N1*A*—H1*A*···O2 | 0.88 (2) | 2.27 (4) | 3.133 (8) | 165 (11) |
| N5*A*—H5*AA*···O1 | 0.88 (2) | 2.19 (5) | 3.026 (8) | 158 (11) |

**Table 2**
Comparison of borazine bond lengths (Å) in **I** and **Ia**.

| **I** | | **Ia** | |
|---|---|---|---|
| N2—B1 | 1.459 (2) | N2*A*—B1*A* | 1.433 (12) |
| N2—B2 | 1.429 (2) | N2*A*—B2*A* | 1.433 (12) |
| N4—B2 | 1.459 (2) | N4*A*—B2*A* | 1.433 (13) |
| N4—B3 | 1.433 (2) | N4*A*—B3*A* | 1.429 (12) |
| N6—B1 | 1.428 (2) | N6*A*—B1*A* | 1.409 (12) |
| N6—B3 | 1.459 (2) | N6*A*—B3*A* | 1.435 (12) |

$d_{norm}$ values, which in turn represents contacts closer than the van der Waals radii (Fig. 3).

Contributions by individual elements to intermolecular interactions were analyzed through fingerprint plots generated by *CrystalExplorer* (McKinnon *et al.*, 2004). The significant

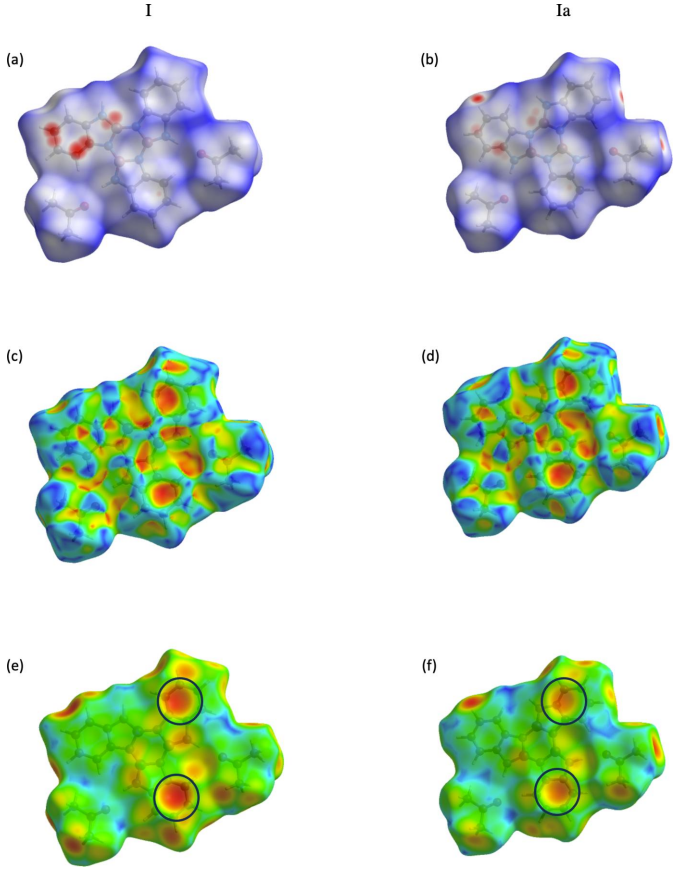



**Figure 3**
Hirshfeld surface interacting molecules mapped over $d_{norm}$. Red areas highlight intermolecular contacts shorter than the sum of the van der Waals radii for **I** (*a*) and **Ia** (*b*), the shape index for **I** (*c*) and **Ia** (*d*), and $d_e$ where the circled areas indicate the C—H···$\pi$ interactions in **I** (*e*) and **Ia** (*f*).

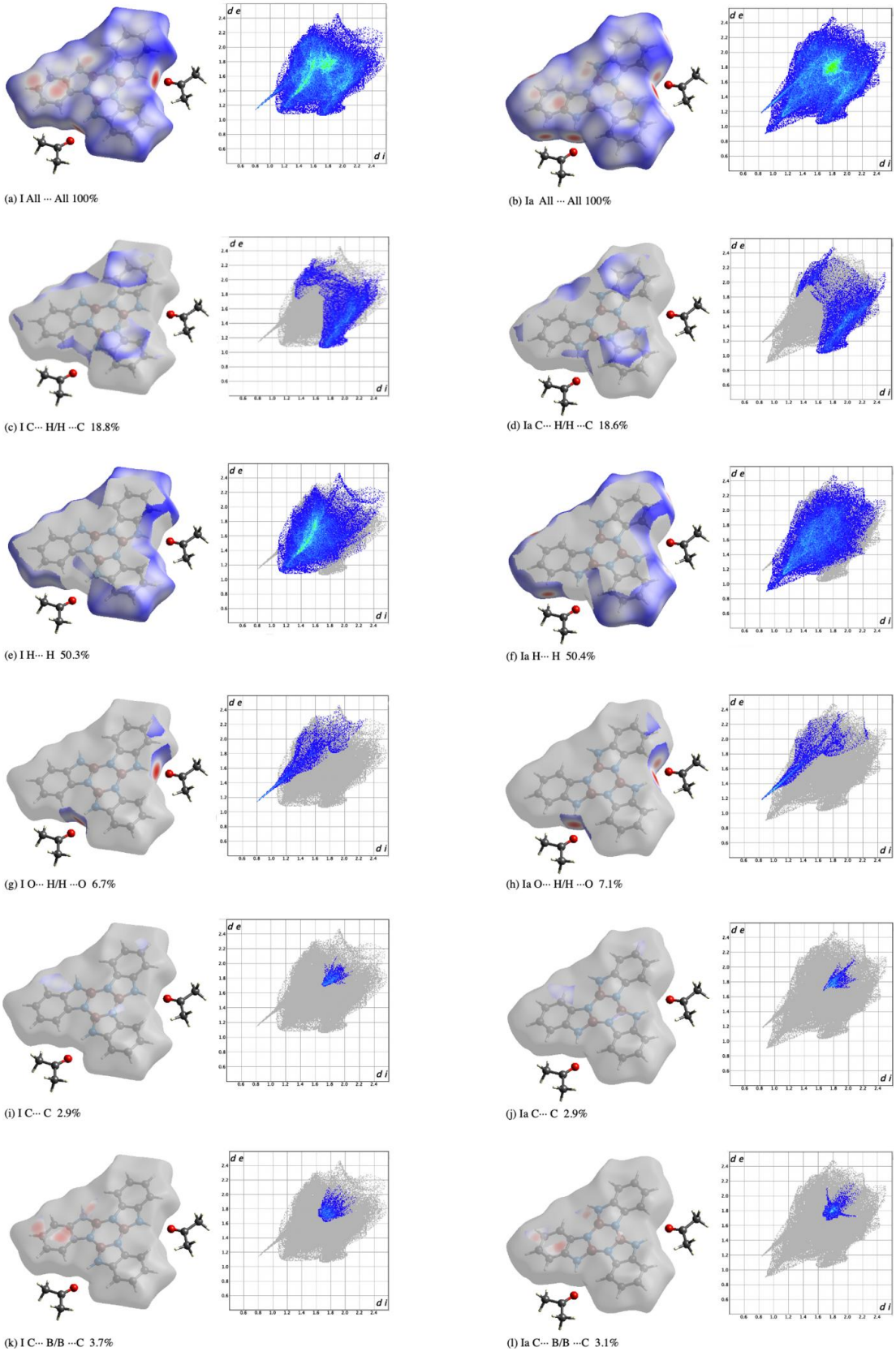



**Figure 4**
Hirshfeld surfaces and fingerprint plots showing percentage of contacts of all interactions for both **I** (*a*) and **Ia** (*b*), C···H/ H···C interactions for **I** (*c*) and **Ia** (*d*), H···H interactions for **I** (*e*) and **Ia** (*f*), O···H/ H···O interactions for **I** (*g*) and **Ia** (*h*), C···C interactions for **I** (*i*) and **Ia** (*j*),and C···B/ B···C interactions for **I** (*k*) and **Ia** (*l*)

interactions for each conformer are shown in Fig. 4(*a*)–(*l*). The dominating interactions are H···H interactions [Fig. 4(*e*) and (*f*)], followed by C···H/ C···H interactions [Fig. 4(*c*) and (*d*)], and few C···C interactions [Fig. 4(*i*) and (*j*)], which suggests C—H···$\pi$ interactions. The hydrogen-bonding interactions between O···H/O···H are very strong [Fig. 4(*g*) and (*h*)]. Interestingly, there are also strong C···B/B···C interactions [Fig. 4(*k*) and (*l*)]. The negligible contributions from other contacts not included in Fig. 4 are as follows: N···H (**I**, 8.0%; **Ia**, 7.1%), B···H (**I**, 3.4%; **Ia** 4.1%),, C···O (**I**, 1.0%; **Ia**, 1.1%), N···O (**I**, 0.6%; **Ia**, 0.6%), B···O (**I**, 0.4%; Ia, 0.3%), C···N (**I**, 3.6%; **Ia**, 4.0%), N···N (**I**, 0.7%; **Ia** 0.5%), N···B (**I**, 0%; **Ia**, 0.4%) with O···O, and B···B contacts not observed.

## 4. Database survey

A survey of the Cambridge Structural Database (CSD version 2023.2.0; Groom *et al.*, 2016) showed there are no examples of the benzodiazaborole trimer structure and very few examples of similar compounds available in the literature. Crystal structures that contain borazine are usually not fused with five-membered rings except for borazatruxenes, where the NH groups are replaced with $CH_2$ groups. These materials are being explored as stable polycyclic aromatic hydrocarbons for material applications (Limberti *et al.*, 2019). Additionally, the synthesis of oxazaborolidine trimers has been studied (Stepanenko *et al.*, 2006).

## 5. Synthesis and crystallization

A solution of *o*-phenylenediamine (1.00 g, 9.247 mmol) in 30 mL of toluene with triethylamine (3.866 mL, 27.7 mmol) was degassed and boron trichloride (9.247 mL, 9.24 mmol) was slowly added. This mixture was refluxed for 2 h. The cooled solution was filtered through celite and purified by column chromatography with acetone/pentane (1:1) solution. Clear needles were isolated from recrystallization in acetone and were suitable for X-ray diffraction.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All non-hydrogen atoms were located in a series of difference-Fourier electron-density maps and refined using anisotropic displacement parameters. All C—H hydrogen atoms were placed in calculated positions with $U_{iso}$(H) = 1.2$U_{eq}$ of the connected C atoms (1.5$U_{eq}$ for methyl groups). Those H atoms attached to nitrogen were located in difference-Fourier maps. A RIGU command was applied to the less occupied component and ISOR to N2*A*, N4*A*, and N6*A*. The N—H bonds were restrained with the SADI command. The benzodiazaborole molecule was modeled with two-part disorder with occupancy factors refined to 0.8922 (14):0.1078 (14). The minor component was restrained using the SAME and RIGU commands.

**Table 3**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{18}H_{15}B_3N_6{\cdot}2C_3H_6O$ |
| $M_r$ | 463.94 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 100 |
| *a*, *b*, *c* (Å) | 5.8357 (4), 13.6362 (9), 15.4653 (10) |
| $\alpha$, $\beta$, $\gamma$ (°) | 97.595 (3), 96.957 (3), 99.771 (3) |
| *V* (Å$^3$) | 1189.13 (14) |
| *Z* | 2 |
| Radiation type | Cu *K*$\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.66 |
| Crystal size (mm) | 0.41 × 0.13 × 0.13 |
| Data collection | |
| Diffractometer | Bruker D8 Venture |
| Absorption correction | Multi-scan (*SADABS*; Krause *et al.*, 2015) |
| $T_{min}$, $T_{max}$ | 0.699, 0.754 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 47276, 4853, 4226 |
| $R_{int}$ | 0.040 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.625 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.039, 0.095, 1.08 |
| No. of reflections | 4853 |
| No. of parameters | 579 |
| No. of restraints | 369 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.22, −0.23 |

Computer programs: *APEX4* (Bruker, 2022), *SAINT-Plus* (Bruker, 2020), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL209/1* (Sheldrick, 2015*b*), and *OLEX2* (Dolomanov *et al.*, 2009).


## Acknowledgements

The authors are grateful for the support from EWU's Faculty Grant for Research and Creative Works.

## Funding information

Funding for this research was provided by: National Science Foundation, MRI (award No. CHE 1827313).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# supporting information

*Acta Cryst.* (2023). E**79**, 1104-1108 [https://doi.org/10.1107/S2056989023009337]

## Crystal structure and Hirshfeld surface analysis of triazatriborinotris[1,3,2]benzodiazaborole acetone disolvate

**Cole Streeter, Kraig A. Wheeler and Ashley N. Lamm**

### Computing details

Data collection: *APEX4* Ver. 8.38A (Bruker, 2022); cell refinement: *SAINT-Plus* V8.40B (Bruker, 2020); data reduction: *SAINT-Plus* Ve8.40B (Bruker, 2020); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL209/1* (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

### Triazatriborinotris[1,3,2]benzodiazaborole acetone disolvate

*Crystal data*

$C_{18}H_{15}B_3N_6 \cdot 2C_3H_6O$
$M_r = 463.94$
Triclinic, $P\overline{1}$
$a = 5.8357$ (4) Å
$b = 13.6362$ (9) Å
$c = 15.4653$ (10) Å
$\alpha = 97.595$ (3)°
$\beta = 96.957$ (3)°
$\gamma = 99.771$ (3)°
$V = 1189.13$ (14) Å$^3$
$Z = 2$
$F(000) = 488$
$D_x = 1.296$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9824 reflections
$\theta = 3.3$–74.3°
$\mu = 0.66$ mm$^{-1}$
$T = 100$ K
Rod, colourless
0.41 × 0.13 × 0.13 mm

*Data collection*

Bruker D8 Venture diffractometer
Radiation source: microfocus sealed X-ray tube, Incoatec I$\mu$S 3.0
Multilayer mirror monochromator
Detector resolution: 7.9 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.699$, $T_{max} = 0.754$
47276 measured reflections
4853 independent reflections
4226 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 74.6°$, $\theta_{min} = 2.9°$
$h = -7 \rightarrow 7$
$k = -17 \rightarrow 17$
$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.095$
$S = 1.08$
4853 reflections
579 parameters
369 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 0.3978P]$ 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.

**Refinement**. All nonhydrogen atoms were located in a series of difference Fourier electron density maps and refined using anisotropic displacement parameters. All C-H hydrogen atoms were placed in calculated positions with Uiso = 1.2xUeqiv of the connected C atoms 1.5xUeqiv for methyl groups). Those H atoms attached to nitrogen were located in Fourier diff maps. A RIGU command was applied to the minor component and ISOR to N2A, N4A, and N6A. The N-H bonds were restrained with the SADI command. The benzodiazaborole molecule was modeled with two-part disorder with occupancy factors refined to 89:11. The minor restrained using the SAME and RIGU commands. N2A, N4A, N6A were also restrained with an ISOR comand. The locations NH hydrogen atoms of the minor componenent were were fixed using AFIX 43 commands.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 1.06089 (19) | 0.80696 (9) | 0.44502 (7) | 0.0509 (3) | |
| C19 | 1.4443 (2) | 0.84484 (11) | 0.52511 (9) | 0.0394 (3) | |
| H19A | 1.465884 | 0.900588 | 0.491055 | 0.059* | |
| H19B | 1.566486 | 0.804633 | 0.517058 | 0.059* | |
| H19C | 1.455742 | 0.871885 | 0.587746 | 0.059* | |
| C20 | 1.2081 (2) | 0.78000 (10) | 0.49384 (8) | 0.0292 (3) | |
| C21 | 1.1621 (3) | 0.68044 (11) | 0.52471 (10) | 0.0414 (3) | |
| H21A | 0.992312 | 0.654847 | 0.516480 | 0.062* | |
| H21B | 1.225795 | 0.688200 | 0.587362 | 0.062* | |
| H21C | 1.238069 | 0.632812 | 0.490587 | 0.062* | |
| O2 | −0.42413 (17) | 0.45535 (8) | 0.15098 (7) | 0.0438 (3) | |
| C22 | −0.7168 (3) | 0.31164 (10) | 0.15045 (10) | 0.0444 (4) | |
| H22A | −0.746614 | 0.260253 | 0.097682 | 0.067* | |
| H22B | −0.863479 | 0.314031 | 0.174805 | 0.067* | |
| H22C | −0.600541 | 0.294781 | 0.194562 | 0.067* | |
| C23 | −0.6251 (2) | 0.41159 (9) | 0.12665 (8) | 0.0307 (3) | |
| C24 | −0.7921 (3) | 0.45521 (12) | 0.06874 (11) | 0.0502 (4) | |
| H24A | −0.911786 | 0.476703 | 0.102329 | 0.075* | |
| H24B | −0.868343 | 0.404166 | 0.018179 | 0.075* | |
| H24C | −0.705855 | 0.513364 | 0.047717 | 0.075* | |
| N1 | 0.05231 (18) | 0.94365 (8) | 0.12177 (7) | 0.0213 (2) | 0.8922 (14) |
| H1 | 0.087 (3) | 1.0065 (10) | 0.1141 (10) | 0.026* | 0.8922 (14) |
| N2 | 0.0215 (2) | 0.79057 (11) | 0.17389 (8) | 0.0199 (3) | 0.8922 (14) |
| N3 | −0.01420 (19) | 0.61709 (8) | 0.23107 (7) | 0.0223 (2) | 0.8922 (14) |
| H3 | −0.155 (2) | 0.5811 (11) | 0.2091 (10) | 0.027* | 0.8922 (14) |
| N4 | 0.3305 (3) | 0.73686 (10) | 0.27224 (7) | 0.0199 (3) | 0.8922 (14) |
| N5 | 0.70842 (18) | 0.87612 (8) | 0.32562 (7) | 0.0217 (2) | 0.8922 (14) |
| H5 | 0.808 (2) | 0.8516 (11) | 0.3595 (9) | 0.026* | 0.8922 (14) |
| N6 | 0.3973 (2) | 0.90929 (9) | 0.23233 (8) | 0.0194 (2) | 0.8922 (14) |
| C1 | −0.1652 (3) | 0.88371 (13) | 0.08577 (11) | 0.0198 (3) | 0.8922 (14) |

| | | | | | |
|---|---|---|---|---|---|
| C2 | −0.3450 (4) | 0.90431 (14) | 0.02761 (13) | 0.0224 (4) | 0.8922 (14) |
| H2 | −0.329678 | 0.966365 | 0.005266 | 0.027* | 0.8922 (14) |
| C3 | −0.5501 (3) | 0.83056 (16) | 0.00289 (13) | 0.0229 (4) | 0.8922 (14) |
| H3A | −0.676721 | 0.843184 | −0.036131 | 0.027* | 0.8922 (14) |
| C4 | −0.5705 (3) | 0.73916 (13) | 0.03476 (11) | 0.0229 (4) | 0.8922 (14) |
| H4 | −0.710825 | 0.690246 | 0.017142 | 0.027* | 0.8922 (14) |
| C5 | −0.3876 (3) | 0.71828 (12) | 0.09227 (10) | 0.0212 (3) | 0.8922 (14) |
| H5A | −0.401702 | 0.655786 | 0.113858 | 0.025* | 0.8922 (14) |
| C6 | −0.1858 (3) | 0.79089 (14) | 0.11696 (8) | 0.0191 (3) | 0.8922 (14) |
| C7 | 0.1469 (3) | 0.57793 (15) | 0.28473 (8) | 0.0208 (3) | 0.8922 (14) |
| C8 | 0.1229 (3) | 0.48537 (15) | 0.31331 (13) | 0.0244 (4) | 0.8922 (14) |
| H8 | −0.020650 | 0.438014 | 0.298263 | 0.029* | 0.8922 (14) |
| C9 | 0.3158 (4) | 0.46330 (17) | 0.36499 (18) | 0.0260 (5) | 0.8922 (14) |
| H9 | 0.303614 | 0.400122 | 0.385324 | 0.031* | 0.8922 (14) |
| C10 | 0.5261 (3) | 0.53338 (15) | 0.38692 (12) | 0.0251 (4) | 0.8922 (14) |
| H10 | 0.656080 | 0.516669 | 0.421237 | 0.030* | 0.8922 (14) |
| C11 | 0.5489 (3) | 0.62773 (11) | 0.35930 (10) | 0.0227 (3) | 0.8922 (14) |
| H11 | 0.691815 | 0.675431 | 0.374747 | 0.027* | 0.8922 (14) |
| C12 | 0.3572 (3) | 0.64948 (10) | 0.30890 (10) | 0.0199 (3) | 0.8922 (14) |
| C13 | 0.7668 (4) | 0.97371 (11) | 0.30686 (11) | 0.0215 (3) | 0.8922 (14) |
| C14 | 0.9721 (4) | 1.04497 (16) | 0.33531 (14) | 0.0244 (4) | 0.8922 (14) |
| H14 | 1.097907 | 1.031074 | 0.373927 | 0.029* | 0.8922 (14) |
| C15 | 0.9867 (4) | 1.13764 (18) | 0.30511 (17) | 0.0262 (5) | 0.8922 (14) |
| H15 | 1.125364 | 1.187461 | 0.322980 | 0.031* | 0.8922 (14) |
| C16 | 0.8000 (3) | 1.15820 (13) | 0.24893 (11) | 0.0266 (4) | 0.8922 (14) |
| H16 | 0.813959 | 1.221762 | 0.229232 | 0.032* | 0.8922 (14) |
| C17 | 0.5933 (3) | 1.08661 (14) | 0.22134 (9) | 0.0240 (3) | 0.8922 (14) |
| H17 | 0.466136 | 1.100974 | 0.183733 | 0.029* | 0.8922 (14) |
| C18 | 0.5792 (2) | 0.99461 (14) | 0.25019 (10) | 0.0200 (3) | 0.8922 (14) |
| B1 | 0.1734 (3) | 0.88827 (13) | 0.17792 (10) | 0.0203 (3) | 0.8922 (14) |
| B2 | 0.0951 (3) | 0.71571 (12) | 0.22164 (12) | 0.0206 (3) | 0.8922 (14) |
| B3 | 0.4808 (3) | 0.83321 (14) | 0.27939 (10) | 0.0202 (3) | 0.8922 (14) |
| N1A | −0.1999 (13) | 0.6816 (6) | 0.1539 (5) | 0.0194 (17) | 0.1078 (14) |
| H1A | −0.282 (18) | 0.623 (4) | 0.158 (8) | 0.023* | 0.1078 (14) |
| N2A | 0.0651 (16) | 0.8336 (8) | 0.1694 (6) | 0.0115 (18) | 0.1078 (14) |
| N3A | 0.3577 (13) | 1.0072 (6) | 0.1865 (5) | 0.0199 (17) | 0.1078 (14) |
| H3AA | 0.282922 | 1.041925 | 0.152282 | 0.024* | 0.1078 (14) |
| N4A | 0.4546 (15) | 0.8803 (7) | 0.2592 (6) | 0.0101 (16) | 0.1078 (14) |
| N5A | 0.5854 (14) | 0.7321 (6) | 0.3329 (6) | 0.0202 (18) | 0.1078 (14) |
| H5AA | 0.722 (10) | 0.736 (9) | 0.366 (7) | 0.024* | 0.1078 (14) |
| N6A | 0.2152 (19) | 0.7135 (6) | 0.2538 (6) | 0.0106 (17) | 0.1078 (14) |
| C1A | −0.290 (2) | 0.7472 (10) | 0.1031 (7) | 0.014 (2) | 0.1078 (14) |
| C2A | −0.506 (3) | 0.7254 (10) | 0.0533 (11) | 0.022 (3) | 0.1078 (14) |
| H2A | −0.609929 | 0.663375 | 0.052168 | 0.026* | 0.1078 (14) |
| C3A | −0.568 (3) | 0.7960 (12) | 0.0050 (13) | 0.022 (3) | 0.1078 (14) |
| H3AB | −0.715553 | 0.783290 | −0.031800 | 0.026* | 0.1078 (14) |
| C4A | −0.417 (3) | 0.8847 (12) | 0.0099 (11) | 0.017 (3) | 0.1078 (14) |
| H4A | −0.463478 | 0.933462 | −0.023647 | 0.021* | 0.1078 (14) |

| | | | | | |
|---|---|---|---|---|---|
| C5A | −0.201 (2) | 0.9069 (10) | 0.0609 (9) | 0.014 (2) | 0.1078 (14) |
| H5AB | −0.096661 | 0.968971 | 0.062466 | 0.017* | 0.1078 (14) |
| C6A | −0.1419 (18) | 0.8371 (10) | 0.1089 (7) | 0.013 (2) | 0.1078 (14) |
| C7A | 0.5800 (17) | 1.0397 (11) | 0.2354 (8) | 0.018 (2) | 0.1078 (14) |
| C8A | 0.720 (3) | 1.1301 (10) | 0.2390 (10) | 0.025 (3) | 0.1078 (14) |
| H8A | 0.670904 | 1.178949 | 0.206266 | 0.030* | 0.1078 (14) |
| C9A | 0.935 (3) | 1.1498 (14) | 0.2911 (15) | 0.020 (3) | 0.1078 (14) |
| H9A | 1.036852 | 1.213402 | 0.296635 | 0.025* | 0.1078 (14) |
| C10A | 1.000 (3) | 1.0759 (13) | 0.3346 (15) | 0.025 (4) | 0.1078 (14) |
| H10A | 1.151947 | 1.089307 | 0.368572 | 0.030* | 0.1078 (14) |
| C11A | 0.860 (2) | 0.9829 (10) | 0.3327 (9) | 0.020 (3) | 0.1078 (14) |
| H11A | 0.908625 | 0.933801 | 0.365401 | 0.024* | 0.1078 (14) |
| C12A | 0.647 (2) | 0.9667 (8) | 0.2801 (8) | 0.012 (2) | 0.1078 (14) |
| C13A | 0.462 (2) | 0.6377 (8) | 0.3348 (8) | 0.015 (2) | 0.1078 (14) |
| C14A | 0.542 (2) | 0.5652 (11) | 0.3771 (11) | 0.018 (3) | 0.1078 (14) |
| H14A | 0.697182 | 0.574882 | 0.407814 | 0.022* | 0.1078 (14) |
| C15A | 0.382 (3) | 0.4774 (15) | 0.3719 (16) | 0.019 (3) | 0.1078 (14) |
| H15A | 0.429636 | 0.425514 | 0.400910 | 0.022* | 0.1078 (14) |
| C16A | 0.156 (3) | 0.4599 (12) | 0.3273 (13) | 0.020 (3) | 0.1078 (14) |
| H16A | 0.053894 | 0.397267 | 0.325790 | 0.023* | 0.1078 (14) |
| C17A | 0.077 (2) | 0.5340 (10) | 0.2846 (8) | 0.016 (2) | 0.1078 (14) |
| H17A | −0.077468 | 0.524471 | 0.253539 | 0.019* | 0.1078 (14) |
| C18A | 0.236 (2) | 0.6213 (8) | 0.2900 (6) | 0.0082 (18) | 0.1078 (14) |
| B1A | 0.0310 (19) | 0.7366 (9) | 0.1970 (8) | 0.011 (2) | 0.1078 (14) |
| B2A | 0.273 (2) | 0.9081 (8) | 0.2018 (8) | 0.010 (2) | 0.1078 (14) |
| B3A | 0.434 (2) | 0.7822 (9) | 0.2840 (7) | 0.012 (2) | 0.1078 (14) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0489 (6) | 0.0642 (7) | 0.0388 (6) | 0.0269 (5) | −0.0118 (5) | 0.0005 (5) |
| C19 | 0.0371 (7) | 0.0432 (8) | 0.0344 (7) | 0.0001 (6) | 0.0072 (6) | 0.0006 (6) |
| C20 | 0.0295 (6) | 0.0356 (7) | 0.0227 (6) | 0.0107 (5) | 0.0019 (5) | 0.0010 (5) |
| C21 | 0.0511 (9) | 0.0364 (8) | 0.0373 (7) | 0.0044 (6) | 0.0156 (6) | 0.0045 (6) |
| O2 | 0.0341 (5) | 0.0417 (6) | 0.0466 (6) | −0.0080 (4) | 0.0031 (4) | −0.0040 (5) |
| C22 | 0.0566 (9) | 0.0283 (7) | 0.0492 (9) | 0.0015 (6) | 0.0233 (7) | 0.0035 (6) |
| C23 | 0.0324 (7) | 0.0251 (6) | 0.0322 (6) | 0.0013 (5) | 0.0069 (5) | −0.0012 (5) |
| C24 | 0.0539 (9) | 0.0412 (8) | 0.0520 (9) | 0.0131 (7) | −0.0053 (7) | 0.0006 (7) |
| N1 | 0.0204 (5) | 0.0182 (5) | 0.0245 (5) | 0.0017 (4) | 0.0015 (4) | 0.0043 (4) |
| N2 | 0.0173 (6) | 0.0192 (7) | 0.0226 (6) | 0.0017 (5) | 0.0019 (4) | 0.0048 (6) |
| N3 | 0.0193 (5) | 0.0217 (5) | 0.0252 (5) | 0.0017 (4) | 0.0012 (4) | 0.0053 (4) |
| N4 | 0.0181 (7) | 0.0201 (6) | 0.0214 (6) | 0.0023 (5) | 0.0016 (5) | 0.0060 (5) |
| N5 | 0.0202 (5) | 0.0221 (5) | 0.0223 (5) | 0.0028 (4) | 0.0002 (4) | 0.0059 (4) |
| N6 | 0.0192 (6) | 0.0189 (6) | 0.0199 (6) | 0.0024 (5) | 0.0020 (5) | 0.0046 (5) |
| C1 | 0.0204 (7) | 0.0201 (9) | 0.0195 (8) | 0.0055 (6) | 0.0033 (6) | 0.0026 (6) |
| C2 | 0.0201 (10) | 0.0215 (8) | 0.0243 (9) | 0.0029 (7) | 0.0014 (8) | 0.0020 (7) |
| C3 | 0.0217 (8) | 0.0249 (10) | 0.0222 (7) | 0.0059 (8) | 0.0005 (6) | 0.0044 (8) |
| C4 | 0.0214 (8) | 0.0254 (9) | 0.0202 (8) | 0.0029 (6) | 0.0002 (6) | 0.0021 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0205 (8) | 0.0208 (7) | 0.0211 (7) | 0.0023 (6) | 0.0015 (6) | 0.0019 (6) |
| C6 | 0.0182 (7) | 0.0195 (8) | 0.0194 (6) | 0.0035 (6) | 0.0032 (5) | 0.0018 (6) |
| C7 | 0.0237 (8) | 0.0186 (8) | 0.0204 (7) | 0.0028 (7) | 0.0057 (6) | 0.0030 (7) |
| C8 | 0.0270 (8) | 0.0225 (10) | 0.0244 (10) | 0.0037 (7) | 0.0053 (7) | 0.0055 (7) |
| C9 | 0.0331 (13) | 0.0193 (9) | 0.0262 (10) | 0.0025 (8) | 0.0060 (10) | 0.0074 (8) |
| C10 | 0.0303 (9) | 0.0230 (10) | 0.0238 (8) | 0.0078 (8) | 0.0024 (6) | 0.0078 (7) |
| C11 | 0.0245 (7) | 0.0227 (8) | 0.0216 (7) | 0.0056 (6) | 0.0029 (6) | 0.0053 (6) |
| C12 | 0.0209 (8) | 0.0202 (7) | 0.0190 (7) | 0.0038 (6) | 0.0039 (6) | 0.0042 (5) |
| C13 | 0.0191 (9) | 0.0231 (7) | 0.0203 (8) | 0.0005 (7) | 0.0031 (7) | 0.0006 (6) |
| C14 | 0.0232 (9) | 0.0224 (10) | 0.0262 (8) | 0.0010 (8) | 0.0030 (7) | 0.0038 (9) |
| C15 | 0.0234 (10) | 0.0245 (10) | 0.0272 (11) | −0.0020 (7) | 0.0003 (7) | 0.0029 (7) |
| C16 | 0.0271 (9) | 0.0217 (8) | 0.0276 (8) | −0.0034 (7) | 0.0022 (7) | 0.0036 (6) |
| C17 | 0.0250 (8) | 0.0213 (8) | 0.0235 (7) | −0.0003 (6) | 0.0013 (5) | 0.0035 (6) |
| C18 | 0.0205 (7) | 0.0196 (8) | 0.0194 (7) | 0.0022 (6) | 0.0035 (5) | 0.0024 (6) |
| B1 | 0.0207 (8) | 0.0208 (8) | 0.0192 (7) | 0.0031 (7) | 0.0041 (6) | 0.0017 (6) |
| B2 | 0.0195 (9) | 0.0227 (8) | 0.0200 (8) | 0.0040 (6) | 0.0038 (7) | 0.0037 (6) |
| B3 | 0.0225 (7) | 0.0204 (9) | 0.0190 (7) | 0.0049 (7) | 0.0056 (5) | 0.0049 (7) |
| N1A | 0.018 (3) | 0.016 (3) | 0.022 (3) | 0.001 (2) | −0.006 (2) | 0.007 (3) |
| N2A | 0.011 (3) | 0.007 (3) | 0.015 (3) | −0.001 (2) | −0.007 (2) | 0.008 (2) |
| N3A | 0.019 (3) | 0.014 (3) | 0.024 (4) | −0.002 (2) | 0.000 (3) | 0.006 (2) |
| N4A | 0.007 (3) | 0.008 (3) | 0.013 (3) | −0.0032 (19) | −0.004 (2) | 0.005 (2) |
| N5A | 0.016 (3) | 0.018 (3) | 0.026 (4) | 0.001 (2) | −0.002 (2) | 0.010 (3) |
| N6A | 0.008 (3) | 0.007 (3) | 0.015 (3) | −0.002 (2) | −0.005 (2) | 0.005 (2) |
| C1A | 0.010 (3) | 0.010 (4) | 0.017 (4) | −0.004 (2) | −0.007 (3) | 0.005 (3) |
| C2A | 0.016 (4) | 0.014 (4) | 0.029 (6) | −0.006 (3) | −0.014 (3) | 0.011 (4) |
| C3A | 0.014 (4) | 0.020 (5) | 0.028 (6) | −0.002 (4) | −0.008 (3) | 0.012 (5) |
| C4A | 0.009 (4) | 0.016 (5) | 0.027 (6) | 0.004 (3) | −0.007 (3) | 0.012 (4) |
| C5A | 0.009 (4) | 0.014 (4) | 0.020 (5) | 0.005 (3) | −0.003 (3) | 0.010 (3) |
| C6A | 0.010 (3) | 0.007 (4) | 0.020 (4) | −0.002 (2) | −0.009 (3) | 0.007 (3) |
| C7A | 0.015 (3) | 0.011 (3) | 0.024 (5) | −0.004 (3) | −0.003 (3) | 0.007 (3) |
| C8A | 0.020 (4) | 0.014 (4) | 0.034 (6) | −0.009 (3) | −0.005 (4) | 0.007 (3) |
| C9A | 0.019 (5) | 0.014 (5) | 0.025 (6) | −0.008 (3) | 0.000 (4) | 0.004 (4) |
| C10A | 0.015 (4) | 0.017 (5) | 0.036 (7) | −0.012 (3) | −0.005 (4) | 0.008 (5) |
| C11A | 0.010 (4) | 0.018 (4) | 0.026 (5) | −0.008 (3) | −0.005 (3) | 0.005 (4) |
| C12A | 0.008 (3) | 0.010 (3) | 0.016 (4) | −0.004 (2) | −0.001 (3) | 0.003 (3) |
| C13A | 0.009 (4) | 0.016 (3) | 0.021 (5) | 0.001 (2) | −0.005 (3) | 0.011 (3) |
| C14A | 0.016 (4) | 0.015 (4) | 0.022 (5) | 0.001 (3) | −0.007 (3) | 0.010 (4) |
| C15A | 0.018 (5) | 0.016 (4) | 0.022 (6) | 0.003 (3) | −0.004 (4) | 0.010 (4) |
| C16A | 0.021 (5) | 0.014 (4) | 0.024 (6) | 0.003 (3) | −0.003 (4) | 0.012 (4) |
| C17A | 0.016 (4) | 0.011 (4) | 0.020 (5) | 0.000 (3) | −0.001 (3) | 0.010 (3) |
| C18A | 0.008 (3) | 0.008 (3) | 0.009 (4) | 0.001 (2) | −0.001 (3) | 0.004 (3) |
| B1A | 0.011 (3) | 0.008 (3) | 0.013 (4) | 0.001 (2) | −0.003 (3) | 0.006 (3) |
| B2A | 0.008 (3) | 0.008 (3) | 0.013 (4) | −0.001 (2) | −0.003 (3) | 0.004 (2) |
| B3A | 0.009 (3) | 0.009 (3) | 0.016 (4) | −0.003 (2) | −0.004 (3) | 0.005 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C20 | 1.2110 (15) | C13—C18 | 1.410 (2) |
| C19—H19A | 0.9800 | C14—H14 | 0.9500 |
| C19—H19B | 0.9800 | C14—C15 | 1.397 (2) |
| C19—H19C | 0.9800 | C15—H15 | 0.9500 |
| C19—C20 | 1.4927 (18) | C15—C16 | 1.400 (2) |
| C20—C21 | 1.4906 (19) | C16—H16 | 0.9500 |
| C21—H21A | 0.9800 | C16—C17 | 1.398 (2) |
| C21—H21B | 0.9800 | C17—H17 | 0.9500 |
| C21—H21C | 0.9800 | C17—C18 | 1.379 (2) |
| O2—C23 | 1.2122 (16) | N1A—H1A | 0.880 (18) |
| C22—H22A | 0.9800 | N1A—C1A | 1.391 (11) |
| C22—H22B | 0.9800 | N1A—B1A | 1.460 (12) |
| C22—H22C | 0.9800 | N2A—C6A | 1.447 (11) |
| C22—C23 | 1.4873 (18) | N2A—B1A | 1.433 (12) |
| C23—C24 | 1.494 (2) | N2A—B2A | 1.433 (12) |
| C24—H24A | 0.9800 | N3A—H3AA | 0.8800 |
| C24—H24B | 0.9800 | N3A—C7A | 1.389 (11) |
| C24—H24C | 0.9800 | N3A—B2A | 1.419 (11) |
| N1—H1 | 0.874 (12) | N4A—C12A | 1.454 (11) |
| N1—C1 | 1.3948 (18) | N4A—B2A | 1.433 (13) |
| N1—B1 | 1.4247 (19) | N4A—B3A | 1.429 (12) |
| N2—C6 | 1.4082 (17) | N5A—H5AA | 0.883 (18) |
| N2—B1 | 1.459 (2) | N5A—C13A | 1.370 (11) |
| N2—B2 | 1.429 (2) | N5A—B3A | 1.414 (11) |
| N3—H3 | 0.886 (12) | N6A—C18A | 1.459 (11) |
| N3—C7 | 1.3985 (17) | N6A—B1A | 1.409 (12) |
| N3—B2 | 1.4212 (19) | N6A—B3A | 1.435 (12) |
| N4—C12 | 1.4091 (18) | C1A—C2A | 1.362 (13) |
| N4—B2 | 1.459 (2) | C1A—C6A | 1.359 (13) |
| N4—B3 | 1.433 (2) | C2A—H2A | 0.9500 |
| N5—H5 | 0.871 (12) | C2A—C3A | 1.363 (14) |
| N5—C13 | 1.3941 (17) | C3A—H3AB | 0.9500 |
| N5—B3 | 1.4191 (18) | C3A—C4A | 1.356 (14) |
| N6—C18 | 1.4077 (18) | C4A—H4A | 0.9500 |
| N6—B1 | 1.428 (2) | C4A—C5A | 1.369 (13) |
| N6—B3 | 1.459 (2) | C5A—H5AB | 0.9500 |
| C1—C2 | 1.388 (2) | C5A—C6A | 1.346 (12) |
| C1—C6 | 1.405 (2) | C7A—C8A | 1.349 (13) |
| C2—H2 | 0.9500 | C7A—C12A | 1.367 (13) |
| C2—C3 | 1.403 (2) | C8A—H8A | 0.9500 |
| C3—H3A | 0.9500 | C8A—C9A | 1.371 (15) |
| C3—C4 | 1.392 (2) | C9A—H9A | 0.9500 |
| C4—H4 | 0.9500 | C9A—C10A | 1.363 (15) |
| C4—C5 | 1.397 (2) | C10A—H10A | 0.9500 |
| C5—H5A | 0.9500 | C10A—C11A | 1.382 (13) |
| C5—C6 | 1.382 (2) | C11A—H11A | 0.9500 |

| | | | |
|---|---|---|---|
| C7—C8 | 1.382 (3) | C11A—C12A | 1.370 (13) |
| C7—C12 | 1.409 (2) | C13A—C14A | 1.369 (14) |
| C8—H8 | 0.9500 | C13A—C18A | 1.382 (13) |
| C8—C9 | 1.399 (3) | C14A—H14A | 0.9500 |
| C9—H9 | 0.9500 | C14A—C15A | 1.375 (15) |
| C9—C10 | 1.396 (2) | C15A—H15A | 0.9500 |
| C10—H10 | 0.9500 | C15A—C16A | 1.378 (15) |
| C10—C11 | 1.399 (2) | C16A—H16A | 0.9500 |
| C11—H11 | 0.9500 | C16A—C17A | 1.387 (12) |
| C11—C12 | 1.382 (2) | C17A—H17A | 0.9500 |
| C13—C14 | 1.392 (3) | C17A—C18A | 1.365 (13) |

| | | | |
|---|---|---|---|
| H19A—C19—H19B | 109.5 | C16—C17—H17 | 120.9 |
| H19A—C19—H19C | 109.5 | C18—C17—C16 | 118.20 (14) |
| H19B—C19—H19C | 109.5 | C18—C17—H17 | 120.9 |
| C20—C19—H19A | 109.5 | N6—C18—C13 | 108.64 (17) |
| C20—C19—H19B | 109.5 | C17—C18—N6 | 130.44 (16) |
| C20—C19—H19C | 109.5 | C17—C18—C13 | 120.92 (13) |
| O1—C20—C19 | 121.34 (13) | N1—B1—N2 | 107.25 (15) |
| O1—C20—C21 | 121.53 (13) | N1—B1—N6 | 133.95 (16) |
| C21—C20—C19 | 117.12 (12) | N6—B1—N2 | 118.79 (13) |
| C20—C21—H21A | 109.5 | N2—B2—N4 | 118.80 (13) |
| C20—C21—H21B | 109.5 | N3—B2—N2 | 133.35 (16) |
| C20—C21—H21C | 109.5 | N3—B2—N4 | 107.85 (15) |
| H21A—C21—H21B | 109.5 | N4—B3—N6 | 118.71 (12) |
| H21A—C21—H21C | 109.5 | N5—B3—N4 | 133.60 (16) |
| H21B—C21—H21C | 109.5 | N5—B3—N6 | 107.68 (14) |
| H22A—C22—H22B | 109.5 | C1A—N1A—H1A | 122 (8) |
| H22A—C22—H22C | 109.5 | C1A—N1A—B1A | 105.0 (9) |
| H22B—C22—H22C | 109.5 | B1A—N1A—H1A | 133 (8) |
| C23—C22—H22A | 109.5 | B1A—N2A—C6A | 107.3 (9) |
| C23—C22—H22B | 109.5 | B1A—N2A—B2A | 121.9 (9) |
| C23—C22—H22C | 109.5 | B2A—N2A—C6A | 130.8 (9) |
| O2—C23—C22 | 122.38 (13) | C7A—N3A—H3AA | 126.2 |
| O2—C23—C24 | 120.99 (13) | C7A—N3A—B2A | 107.6 (10) |
| C22—C23—C24 | 116.61 (13) | B2A—N3A—H3AA | 126.2 |
| C23—C24—H24A | 109.5 | B2A—N4A—C12A | 106.9 (9) |
| C23—C24—H24B | 109.5 | B3A—N4A—C12A | 130.8 (10) |
| C23—C24—H24C | 109.5 | B3A—N4A—B2A | 122.2 (8) |
| H24A—C24—H24B | 109.5 | C13A—N5A—H5AA | 106 (8) |
| H24A—C24—H24C | 109.5 | C13A—N5A—B3A | 107.1 (9) |
| H24B—C24—H24C | 109.5 | B3A—N5A—H5AA | 147 (8) |
| C1—N1—H1 | 121.2 (10) | B1A—N6A—C18A | 130.6 (10) |
| C1—N1—B1 | 107.84 (14) | B1A—N6A—B3A | 122.9 (9) |
| B1—N1—H1 | 130.4 (10) | B3A—N6A—C18A | 106.5 (9) |
| C6—N2—B1 | 106.69 (14) | C2A—C1A—N1A | 123.9 (12) |
| C6—N2—B2 | 132.10 (15) | C6A—C1A—N1A | 113.6 (10) |
| B2—N2—B1 | 121.21 (13) | C6A—C1A—C2A | 122.5 (10) |

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| C7—N3—H3 | 121.0 (10) | C1A—C2A—H2A | 121.3 |
| C7—N3—B2 | 107.62 (14) | C1A—C2A—C3A | 117.3 (12) |
| B2—N3—H3 | 131.4 (10) | C3A—C2A—H2A | 121.3 |
| C12—N4—B2 | 106.30 (14) | C2A—C3A—H3AB | 120.2 |
| C12—N4—B3 | 132.59 (15) | C4A—C3A—C2A | 119.7 (13) |
| B3—N4—B2 | 121.07 (12) | C4A—C3A—H3AB | 120.2 |
| C13—N5—H5 | 120.5 (10) | C3A—C4A—H4A | 118.6 |
| C13—N5—B3 | 107.76 (14) | C3A—C4A—C5A | 122.8 (14) |
| B3—N5—H5 | 131.7 (10) | C5A—C4A—H4A | 118.6 |
| C18—N6—B1 | 132.24 (15) | C4A—C5A—H5AB | 121.4 |
| C18—N6—B3 | 106.46 (14) | C6A—C5A—C4A | 117.2 (13) |
| B1—N6—B3 | 121.25 (12) | C6A—C5A—H5AB | 121.4 |
| N1—C1—C6 | 109.50 (16) | C1A—C6A—N2A | 106.6 (10) |
| C2—C1—N1 | 129.53 (19) | C5A—C6A—N2A | 132.9 (12) |
| C2—C1—C6 | 120.97 (15) | C5A—C6A—C1A | 120.4 (10) |
| C1—C2—H2 | 121.1 | C8A—C7A—N3A | 126.1 (13) |
| C1—C2—C3 | 117.88 (17) | C8A—C7A—C12A | 122.4 (10) |
| C3—C2—H2 | 121.1 | C12A—C7A—N3A | 111.4 (11) |
| C2—C3—H3A | 119.6 | C7A—C8A—H8A | 120.7 |
| C4—C3—C2 | 120.88 (17) | C7A—C8A—C9A | 118.5 (12) |
| C4—C3—H3A | 119.6 | C9A—C8A—H8A | 120.7 |
| C3—C4—H4 | 119.5 | C8A—C9A—H9A | 120.9 |
| C3—C4—C5 | 120.98 (16) | C10A—C9A—C8A | 118.3 (15) |
| C5—C4—H4 | 119.5 | C10A—C9A—H9A | 120.9 |
| C4—C5—H5A | 120.9 | C9A—C10A—H10A | 117.7 |
| C6—C5—C4 | 118.26 (14) | C9A—C10A—C11A | 124.6 (16) |
| C6—C5—H5A | 120.9 | C11A—C10A—H10A | 117.7 |
| C1—C6—N2 | 108.71 (16) | C10A—C11A—H11A | 122.5 |
| C5—C6—N2 | 130.27 (16) | C12A—C11A—C10A | 115.0 (13) |
| C5—C6—C1 | 121.01 (13) | C12A—C11A—H11A | 122.5 |
| N3—C7—C12 | 109.33 (17) | C7A—C12A—N4A | 106.8 (11) |
| C8—C7—N3 | 129.57 (19) | C7A—C12A—C11A | 121.1 (10) |
| C8—C7—C12 | 121.10 (15) | C11A—C12A—N4A | 132.1 (12) |
| C7—C8—H8 | 120.9 | N5A—C13A—C18A | 112.6 (11) |
| C7—C8—C9 | 118.21 (18) | C14A—C13A—N5A | 126.2 (13) |
| C9—C8—H8 | 120.9 | C14A—C13A—C18A | 121.1 (9) |
| C8—C9—H9 | 119.7 | C13A—C14A—H14A | 122.4 |
| C10—C9—C8 | 120.5 (2) | C13A—C14A—C15A | 115.3 (12) |
| C10—C9—H9 | 119.7 | C15A—C14A—H14A | 122.4 |
| C9—C10—H10 | 119.4 | C14A—C15A—H15A | 117.9 |
| C9—C10—C11 | 121.24 (18) | C14A—C15A—C16A | 124.2 (16) |
| C11—C10—H10 | 119.4 | C16A—C15A—H15A | 117.9 |
| C10—C11—H11 | 121.0 | C15A—C16A—H16A | 120.1 |
| C12—C11—C10 | 118.00 (15) | C15A—C16A—C17A | 119.9 (15) |
| C12—C11—H11 | 121.0 | C17A—C16A—H16A | 120.1 |
| C7—C12—N4 | 108.88 (17) | C16A—C17A—H17A | 122.0 |
| C11—C12—N4 | 130.22 (16) | C18A—C17A—C16A | 116.0 (12) |
| C11—C12—C7 | 120.88 (13) | C18A—C17A—H17A | 122.0 |

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| N5—C13—C18 | 109.44 (17) | C13A—C18A—N6A | 105.6 (10) |
| C14—C13—N5 | 129.36 (19) | C17A—C18A—N6A | 130.9 (12) |
| C14—C13—C18 | 121.20 (15) | C17A—C18A—C13A | 123.5 (9) |
| C13—C14—H14 | 121.2 | N2A—B1A—N1A | 107.4 (9) |
| C13—C14—C15 | 117.67 (18) | N6A—B1A—N1A | 134.6 (11) |
| C15—C14—H14 | 121.2 | N6A—B1A—N2A | 118.0 (9) |
| C14—C15—H15 | 119.5 | N2A—B2A—N4A | 117.6 (8) |
| C14—C15—C16 | 121.0 (2) | N3A—B2A—N2A | 135.0 (11) |
| C16—C15—H15 | 119.5 | N3A—B2A—N4A | 107.2 (9) |
| C15—C16—H16 | 119.5 | N4A—B3A—N6A | 117.2 (8) |
| C17—C16—C15 | 121.01 (17) | N5A—B3A—N4A | 134.7 (10) |
| C17—C16—H16 | 119.5 | N5A—B3A—N6A | 108.1 (9) |

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| N1—C1—C2—C3 | −178.74 (15) | N1A—C1A—C2A—C3A | −178.3 (14) |
| N1—C1—C6—N2 | −0.09 (15) | N1A—C1A—C6A—N2A | −0.7 (14) |
| N1—C1—C6—C5 | 178.83 (11) | N1A—C1A—C6A—C5A | 177.6 (11) |
| N3—C7—C8—C9 | 178.04 (17) | N3A—C7A—C8A—C9A | 179.9 (15) |
| N3—C7—C12—N4 | 1.36 (14) | N3A—C7A—C12A—N4A | −0.1 (13) |
| N3—C7—C12—C11 | −177.48 (11) | N3A—C7A—C12A—C11A | −179.9 (11) |
| N5—C13—C14—C15 | 178.95 (17) | N5A—C13A—C14A—C15A | 177.8 (15) |
| N5—C13—C18—N6 | 0.09 (14) | N5A—C13A—C18A—N6A | 1.8 (12) |
| N5—C13—C18—C17 | −179.75 (11) | N5A—C13A—C18A—C17A | −178.2 (10) |
| C1—N1—B1—N2 | 0.79 (14) | C1A—N1A—B1A—N2A | 0.4 (12) |
| C1—N1—B1—N6 | −179.44 (14) | C1A—N1A—B1A—N6A | −177.3 (13) |
| C1—C2—C3—C4 | −0.9 (2) | C1A—C2A—C3A—C4A | −2 (3) |
| C2—C1—C6—N2 | 179.59 (13) | C2A—C1A—C6A—N2A | 178.1 (12) |
| C2—C1—C6—C5 | −1.5 (2) | C2A—C1A—C6A—C5A | −4 (2) |
| C2—C3—C4—C5 | 0.1 (2) | C2A—C3A—C4A—C5A | 1 (3) |
| C3—C4—C5—C6 | 0.2 (2) | C3A—C4A—C5A—C6A | −1 (2) |
| C4—C5—C6—N2 | 179.21 (13) | C4A—C5A—C6A—N2A | −179.6 (13) |
| C4—C5—C6—C1 | 0.55 (19) | C4A—C5A—C6A—C1A | 3 (2) |
| C6—N2—B1—N1 | −0.83 (14) | C6A—N2A—B1A—N1A | −0.9 (12) |
| C6—N2—B1—N6 | 179.35 (11) | C6A—N2A—B1A—N6A | 177.3 (9) |
| C6—N2—B2—N3 | −2.1 (3) | C6A—N2A—B2A—N3A | −2 (2) |
| C6—N2—B2—N4 | 176.60 (12) | C6A—N2A—B2A—N4A | −177.4 (10) |
| C6—C1—C2—C3 | 1.7 (2) | C6A—C1A—C2A—C3A | 3 (2) |
| C7—N3—B2—N2 | 178.35 (14) | C7A—N3A—B2A—N2A | −177.2 (12) |
| C7—N3—B2—N4 | −0.47 (14) | C7A—N3A—B2A—N4A | −1.9 (12) |
| C7—C8—C9—C10 | 0.1 (3) | C7A—C8A—C9A—C10A | 2 (3) |
| C8—C7—C12—N4 | −178.79 (13) | C8A—C7A—C12A—N4A | −179.0 (12) |
| C8—C7—C12—C11 | 2.4 (2) | C8A—C7A—C12A—C11A | 1 (2) |
| C8—C9—C10—C11 | 1.1 (3) | C8A—C9A—C10A—C11A | −2 (3) |
| C9—C10—C11—C12 | −0.5 (2) | C9A—C10A—C11A—C12A | 2 (3) |
| C10—C11—C12—N4 | −179.74 (14) | C10A—C11A—C12A—N4A | 178.8 (15) |
| C10—C11—C12—C7 | −1.2 (2) | C10A—C11A—C12A—C7A | −2 (2) |
| C12—N4—B2—N2 | −177.75 (11) | C12A—N4A—B2A—N2A | 178.1 (9) |
| C12—N4—B2—N3 | 1.27 (14) | C12A—N4A—B2A—N3A | 1.9 (11) |
| C12—N4—B3—N5 | −0.4 (2) | C12A—N4A—B3A—N5A | −3 (2) |

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| C12—N4—B3—N6 | −179.55 (12) | C12A—N4A—B3A—N6A | 178.5 (9) |
| C12—C7—C8—C9 | −1.8 (2) | C12A—C7A—C8A—C9A | −1 (2) |
| C13—N5—B3—N4 | 179.53 (14) | C13A—N5A—B3A—N4A | 179.4 (12) |
| C13—N5—B3—N6 | −1.21 (14) | C13A—N5A—B3A—N6A | −1.8 (12) |
| C13—C14—C15—C16 | 0.6 (3) | C13A—C14A—C15A—C16A | 1 (3) |
| C14—C13—C18—N6 | 179.70 (14) | C14A—C13A—C18A—N6A | −179.7 (12) |
| C14—C13—C18—C17 | −0.1 (2) | C14A—C13A—C18A—C17A | 0 (2) |
| C14—C15—C16—C17 | 0.0 (3) | C14A—C15A—C16A—C17A | −1 (3) |
| C15—C16—C17—C18 | −0.7 (2) | C15A—C16A—C17A—C18A | 0 (2) |
| C16—C17—C18—N6 | −179.02 (13) | C16A—C17A—C18A—N6A | 179.9 (13) |
| C16—C17—C18—C13 | 0.78 (19) | C16A—C17A—C18A—C13A | −0.1 (19) |
| C18—N6—B1—N1 | 0.6 (2) | C18A—N6A—B1A—N1A | 0 (2) |
| C18—N6—B1—N2 | −179.62 (12) | C18A—N6A—B1A—N2A | −177.5 (9) |
| C18—N6—B3—N4 | −179.36 (11) | C18A—N6A—B3A—N4A | −178.1 (9) |
| C18—N6—B3—N5 | 1.26 (13) | C18A—N6A—B3A—N5A | 2.8 (11) |
| C18—C13—C14—C15 | −0.6 (3) | C18A—C13A—C14A—C15A | −1 (2) |
| B1—N1—C1—C2 | 179.91 (15) | B1A—N1A—C1A—C2A | −178.6 (13) |
| B1—N1—C1—C6 | −0.45 (14) | B1A—N1A—C1A—C6A | 0.2 (13) |
| B1—N2—C6—C1 | 0.57 (14) | B1A—N2A—C6A—C1A | 1.0 (13) |
| B1—N2—C6—C5 | −178.21 (13) | B1A—N2A—C6A—C5A | −177.0 (14) |
| B1—N2—B2—N3 | 178.83 (14) | B1A—N2A—B2A—N3A | 178.8 (12) |
| B1—N2—B2—N4 | −2.45 (18) | B1A—N2A—B2A—N4A | 3.8 (16) |
| B1—N6—C18—C13 | −178.00 (13) | B1A—N6A—C18A—C13A | 174.6 (11) |
| B1—N6—C18—C17 | 1.8 (2) | B1A—N6A—C18A—C17A | −5.4 (19) |
| B1—N6—B3—N4 | −1.81 (18) | B1A—N6A—B3A—N4A | 4.2 (16) |
| B1—N6—B3—N5 | 178.81 (11) | B1A—N6A—B3A—N5A | −174.8 (9) |
| B2—N2—C6—C1 | −178.58 (13) | B2A—N2A—C6A—C1A | −178.0 (11) |
| B2—N2—C6—C5 | 2.6 (2) | B2A—N2A—C6A—C5A | 4 (2) |
| B2—N2—B1—N1 | 178.43 (11) | B2A—N2A—B1A—N1A | 178.2 (9) |
| B2—N2—B1—N6 | −1.38 (18) | B2A—N2A—B1A—N6A | −3.7 (16) |
| B2—N3—C7—C8 | 179.63 (15) | B2A—N3A—C7A—C8A | −179.9 (13) |
| B2—N3—C7—C12 | −0.53 (14) | B2A—N3A—C7A—C12A | 1.3 (13) |
| B2—N4—C12—C7 | −1.60 (13) | B2A—N4A—C12A—C7A | −1.1 (12) |
| B2—N4—C12—C11 | 177.09 (13) | B2A—N4A—C12A—C11A | 178.6 (13) |
| B2—N4—B3—N5 | 177.03 (13) | B2A—N4A—B3A—N5A | 174.7 (11) |
| B2—N4—B3—N6 | −2.16 (18) | B2A—N4A—B3A—N6A | −4.0 (15) |
| B3—N4—C12—C7 | 176.07 (12) | B3A—N4A—C12A—C7A | 176.6 (11) |
| B3—N4—C12—C11 | −5.2 (2) | B3A—N4A—C12A—C11A | −4 (2) |
| B3—N4—B2—N2 | 4.25 (18) | B3A—N4A—B2A—N2A | 0.2 (15) |
| B3—N4—B2—N3 | −176.73 (11) | B3A—N4A—B2A—N3A | −176.1 (9) |
| B3—N5—C13—C14 | −178.86 (16) | B3A—N5A—C13A—C14A | −178.4 (13) |
| B3—N5—C13—C18 | 0.71 (14) | B3A—N5A—C13A—C18A | 0.0 (13) |
| B3—N6—C18—C13 | −0.83 (14) | B3A—N6A—C18A—C13A | −2.8 (11) |
| B3—N6—C18—C17 | 178.99 (13) | B3A—N6A—C18A—C17A | 177.2 (12) |
| B3—N6—B1—N1 | −176.20 (13) | B3A—N6A—B1A—N1A | 177.0 (11) |
| B3—N6—B1—N2 | 3.55 (18) | B3A—N6A—B1A—N2A | −0.5 (16) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···O2 | 0.89 (1) | 2.13 (1) | 2.9817 (14) | 160 (1) |
| N5—H5···O1 | 0.87 (1) | 2.09 (1) | 2.9544 (15) | 175 (1) |
| N1*A*—H1*A*···O2 | 0.88 (2) | 2.27 (4) | 3.133 (8) | 165 (11) |
| N5*A*—H5*AA*···O1 | 0.88 (2) | 2.19 (5) | 3.026 (8) | 158 (11) |