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Crystal structure of 1,3-bis(1*H*-benzotriazol-1-ylmethyl)benzene

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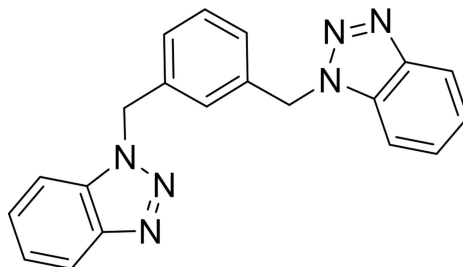
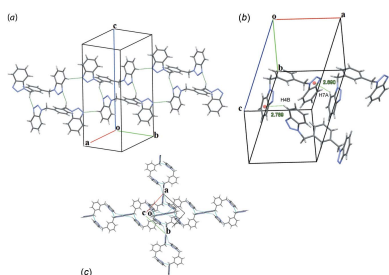
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The molecular structure of the title compound, C₂₀H₁₆N₆, contains two benzotriazole units bonded to a benzene nucleus in a *meta* configuration, forming dihedral angles of 88.74 (11) and 85.83 (10)° with the central aromatic ring and 57.08 (9)° with each other. The three-dimensional structure is controlled mainly by weak C—H···N and C—H···π interactions. The molecules are connected in inversion-related pairs, forming the slabs of infinite chains that run along the $[\bar{1}10]$ and $[110]$ directions.

1. Chemical context

Bis(1*H*-benzotriazol-1-ylmethyl)arene compounds are used as precursors for the synthesis of benzotriazolophanes, a class of positively charged cyclophanes that have the potential ability to trap anions and guest molecules with high electron density (Rajakumar & Murali, 2000). On the other hand, the study of the self-assembly of helicates from the reaction of metal ions with bis(1*H*-benzotriazol-1-ylmethyl)arene ligands has been of great interest. In these complexes, the metal center coordinates through the N3-nitrogen of the benzotriazole ring (O'Keefe & Steel, 2000). We have been interested in the synthesis of metal complexes with ligands derived from benzotriazole, which show high activity as catalysts for oxidative amination of allyl butyl ether (Hurtado *et al.*, 2013). The crystal structures for a number of bis(1*H*-benzotriazol-1-ylmethyl)arene ligands have been determined: 2,6-bis(1*H*-benzotriazol-1-ylmethyl)pyridine (Selvanayagam *et al.*, 2002), 1,4-bis(1*H*-benzotriazol-1-ylmethyl)benzene tetrahydrate (Cai *et al.*, 2004) and benzyl 3,5-bis(1*H*-benzotriazol-1-ylmethyl)phenyl ether (Selvanayagam *et al.*, 2004). As part of structural studies of the self-assembly process of metal ions with ligands derived from benzotriazole, we report here the crystal structure of the ligand 1,3-bis(1*H*-benzotriazol-1-ylmethyl)benzene.



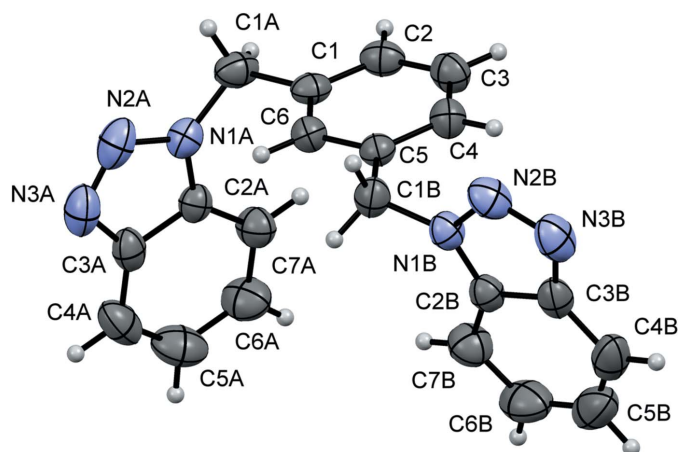


Figure 1
The molecular structure of the title compound, showing anisotropic displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

Fig. 1 shows the molecule of the title compound. The molecular structure is built by two benzotriazole groups describing a *meta* substitution of the central benzene ring. The dihedral angle between the two benzotriazole units is 57.08 (9)° and those between each benzotriazole moiety (N1–N3/C2–C7) and the central benzene ring are 88.74 (11) and 85.83 (10)° for the *A* and *B* groups, respectively. These values differ from the related structures 2,6-bis(*N,N'*-benzotriazol-1-

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

*Cg*1 and *Cg*2 are the centroids of the N1B–N3B/C2B/C3B C2A–C7A rings, respectively.

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C1B–H1B ^A ···N3A ⁱ	0.97	2.59	3.409 (4)	142
C4A–H4A···N3B ⁱⁱ	0.93	2.66	3.443 (4)	143
C7A–H7A··· <i>Cg</i> 1 ⁱⁱⁱ	0.93	2.69	3.423 (3)	136
C4B–H4B··· <i>Cg</i> 2 ^{iv}	0.93	2.89	3.481 (3)	132

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x - 1, y + 1, z$; (iii) $x - 1, y, z$; (iv) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

ylmethyl)pyridine, with a pyridine central ring, where the angle between the two benzotriazole units is 72.49 (6)° and those between the pyridine ring and the two benzotriazole units are 70.26 (6) and 57.70 (7)° (Selvanayagam *et al.*, 2002), and from the 1,4-bis(1*H*-benzotriazol-1-ylmethyl)benzene tetrahydrate, with *para* substitution, where the two benzotriazole units are parallel and the dihedral angle between each benzotriazole unit and the central benzene ring is 74.95 (9)° (Cai *et al.*, 2004).

3. Supramolecular features

The packing is directed by weak C–H···N and C–H··· π interactions as shown in Table 1. Pairs of inversion-related molecules, connected by two equivalent weak C1B–

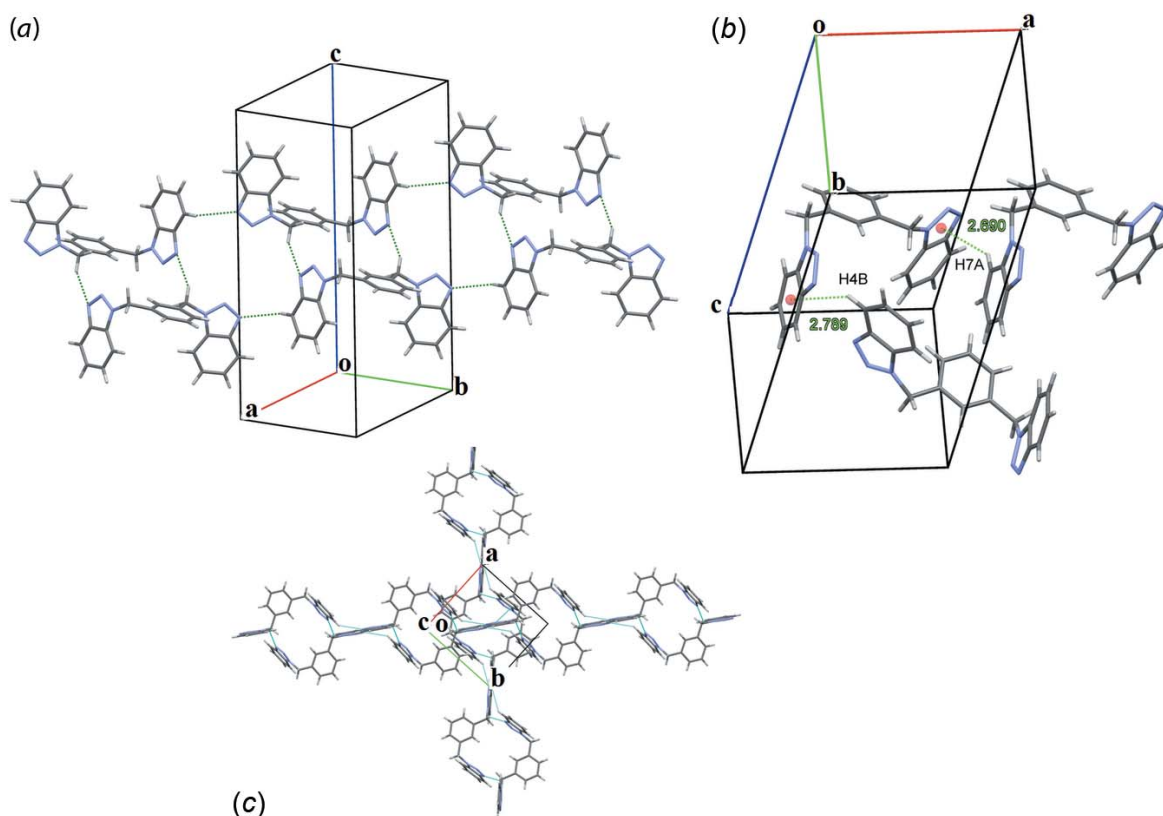


Figure 2
The crystal structure of the title compound showing the hydrogen-bond interactions: (a) C–H···N along $[\bar{1}10]$, (b) C–H··· π and (c) orthogonal chains viewed along $[001]$.

$H1BA \cdots N3A^i$ [symmetry code: (i) $-x + 1, -y + 1, -z + 1$] interactions form slabs of infinite chains of molecules running along $[\bar{1}10]$. Each molecule in a slab connects to two translation-equivalent molecules through $C4A-H4A \cdots N3B^{ii}$ [symmetry code: (ii) $x - 1, y + 1, z$] interactions (Fig. 2a). Parallel chains interact through $C7A-H7A \cdots Cg1^{iii}$ [$Cg1$ is the centroid of the $N2B-N1B-C2B-C3B-N3B$ ring; symmetry code: (iii) $1 - x, y, z$] (Fig. 2b). Since the chains run along the diagonal of the ab plane and $a \approx b$, the 2_1 screw axis parallel to b transforms each chain into an orthogonal one, running along $[110]$ (Fig. 2c). This orthogonal chain interacts with the initial one through $C4B-H4B \cdots Cg2^{iv}$ [$Cg2$ is the centroid of the $C4A-C3A-C2A-C7A-C6A-C5A$ ring; symmetry code: (iv) $\frac{3}{2} - x, -\frac{1}{2} + y, \frac{3}{2} - z$] (Fig. 2b). In this way, each molecule displays four pairs of interactions with seven neighbouring molecules. This crystallographic three-dimensional organization differs from the related 1,4-bis(1*H*-benzotriazol-1-ylmethyl)benzene tetrahydrate where a two-dimensional network is observed (Cai *et al.*, 2004).

4. Database survey

A search of the Cambridge Structural Database (CSD Version 5.36 with one update; Groom *et al.*, 2016) for the 1,3-bis(1*H*-benzotriazol-1-ylmethyl)benzene molecular structure with the possibility of any group replacing the 2,4,5,6-H atoms in the central benzene ring gave four hits, from which two have one additional arene substituent (Br, $-OCH_2Ph$), one has the bis(1*H*-benzotriazole-1-ylmethanone) moiety instead of bis(1*H*-benzotriazol-1-ylmethyl) and the last one corresponds to a more complex molecular structure. When the search also considers heterocyclic compounds, two new hits (in addition to the first four structures) appear, one cyclic bipyridine and the related molecular structure 2,6-bis(1*H*-benzotriazol-1-ylmethyl)pyridine. A search for the 1,4-bis(1*H*-benzotriazol-1-ylmethyl)-substituted benzene ring gave four hits, one of which corresponds to a ligand with additional methyl groups at the 1,3,5,6-sites of the central benzene ring and the other to its corresponding palladium complex. The remaining two relate to the same compound, *viz.* 1,4-bis(1*H*-benzotriazol-1-ylmethyl)benzene tetrahydrate, a related molecular structure.

5. Synthesis and crystallization

m-Xylylene dibromide (1.16 g, 4.4 mmol) was added to a solution of 1*H*-benzotriazole (1.04 g, 8.7 mmol) in toluene (60 mL), and the mixture was heated at reflux for 72 h. The resulting mixture was filtered, and the toluene solution was concentrated and cooled to give a white solid. Single crystals suitable for X-ray structure analysis were obtained by dissolving the compound in the minimum volume of dichloromethane, adding diethyl ether and cooling the solution to 277 K. The title compound formed colorless parallelepipeds. Yield: 668 mg (45%). M.p. 423–424 K. IR (KBr, cm^{-1}): ν 3058 (*w*), 3031 (*w*), 2979 (*w*), 2944 (*w*), 1613 (*m*), 1494 (*m*), 1452 (*s*), 1228 (*s*), 1159 (*m*), 1080 (*s*), 781 (*s*), 754 (*s*), 743 (*s*). 1H NMR (400 MHz, DMSO-*d*₆): δ (p.p.m.) 8.04 (*d*, $J = 8.3$ Hz,

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{16}N_6$
M_r	340.39
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	9.3050 (5), 9.4479 (5), 19.5429 (9)
β (°)	99.205 (2)
V (Å ³)	1695.94 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.40 × 0.39 × 0.18
Data collection	
Diffractometer	Bruker D8 Venture/Photon 100 CMOS
Absorption correction	Multi-scan (SADABS; Bruker, 2013)
T_{min}, T_{max}	0.666, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28764, 3480, 2830
R_{int}	0.035
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.067, 0.160, 1.42
No. of reflections	3480
No. of parameters	236
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.24, -0.27

Computer programs: APEX2 and SAINT (Bruker, 2013), SHELXS2014 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015) and Mercury (Macrae *et al.*, 2008).

2H), 7.72 (*d*, $J = 8.3$ Hz, 2H), 7.47 (*t*, $J = 8.1$ Hz, 2H), 7.38 (*t*, $J = 8.2$ Hz, 2H), 7.36 (*s*, 1H), 7.32 (*dd*, $J = 8.5, 6.6$ Hz, 1H), 7.25 (*d*, $J = 8.2$ Hz, 2H), 5.95 (*s*, 4H). ^{13}C NMR (100 MHz, DMSO-*d*₆): δ (p.p.m.) 145.3 (C), 136.5 (C), 132.6 (C), 129.3 (CH), 127.5 (CH), 127.4 (CH), 127.2 (CH), 124.0 (CH), 119.2 (CH), 110.6 (CH), 50.7 (CH₂). HRMS m/z (ESI) calculated for $[C_{20}H_{16}N_6+H]^+$: 341.1509; found 341.1532 $[M+H]^+$.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in calculated positions (C–H: 0.93–0.97 Å) and included as riding contributions with isotropic displacement parameters set at 1.2–1.5 times the U_{eq} value of the parent atom.

Acknowledgements

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Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

1,3-Bis(1*H*-benzotriazol-1-ylmethyl)benzene

Crystal data

C₂₀H₁₆N₆

$M_r = 340.39$

Monoclinic, *P2₁/n*

$a = 9.3050$ (5) Å

$b = 9.4479$ (5) Å

$c = 19.5429$ (9) Å

$\beta = 99.205$ (2)°

$V = 1695.94$ (15) Å³

$Z = 4$

$F(000) = 712$

$D_x = 1.333$ Mg m⁻³

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 9846 reflections

$\theta = 3.0$ – 27.1 °

$\mu = 0.08$ mm⁻¹

$T = 293$ K

Parallelepiped, colorless

$0.40 \times 0.39 \times 0.18$ mm

Data collection

Bruker D8 Venture/Photon 100 CMOS diffractometer

Radiation source: Mo sealed tube

Detector resolution: 10.4167 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2013)

$T_{\min} = 0.666$, $T_{\max} = 0.746$

28764 measured reflections

3480 independent reflections

2830 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 3.0$ °

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -24 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.067$

$wR(F^2) = 0.160$

$S = 1.42$

3480 reflections

236 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.9412P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.24$ e Å⁻³

$\Delta\rho_{\min} = -0.27$ e Å⁻³

Extinction correction: *SHELXL2014* (Sheldrick, 2015), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0162 (17)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2899 (2)	0.1606 (3)	0.54469 (11)	0.0400 (5)
C2	0.2736 (3)	0.0198 (3)	0.56154 (13)	0.0475 (6)
H2	0.1814	-0.0207	0.5552	0.057*
C3	0.3936 (3)	-0.0607 (3)	0.58775 (13)	0.0499 (6)
H3	0.3820	-0.1554	0.5985	0.060*
C4	0.5308 (3)	-0.0010 (3)	0.59803 (13)	0.0454 (6)
H4	0.6109	-0.0560	0.6159	0.054*
C5	0.5505 (2)	0.1396 (2)	0.58204 (11)	0.0366 (5)
C6	0.4286 (2)	0.2197 (3)	0.55500 (12)	0.0401 (5)
H6	0.4403	0.3141	0.5437	0.048*
C1A	0.1582 (3)	0.2463 (3)	0.51371 (14)	0.0516 (7)
H1AA	0.1547	0.2522	0.4639	0.062*
H1AB	0.0708	0.1981	0.5223	0.062*
N1A	0.1601 (2)	0.3890 (2)	0.54221 (10)	0.0433 (5)
C2A	0.1399 (2)	0.4294 (2)	0.60655 (12)	0.0380 (5)
N2A	0.1856 (3)	0.5036 (3)	0.50437 (13)	0.0606 (6)
C1B	0.6995 (3)	0.2062 (3)	0.59004 (13)	0.0457 (6)
H1BA	0.7311	0.2092	0.5451	0.055*
H1BB	0.6932	0.3030	0.6059	0.055*
N1B	0.8073 (2)	0.1311 (2)	0.63824 (10)	0.0408 (5)
C3A	0.1528 (3)	0.5760 (3)	0.60636 (14)	0.0458 (6)
N3A	0.1814 (3)	0.6171 (3)	0.54235 (14)	0.0621 (7)
C2B	0.8262 (2)	0.1272 (2)	0.70871 (12)	0.0400 (5)
N2B	0.9063 (2)	0.0455 (2)	0.61519 (12)	0.0530 (6)
C4A	0.1384 (3)	0.6549 (3)	0.66532 (18)	0.0633 (8)
H4A	0.1454	0.7531	0.6658	0.076*
C3B	0.9426 (3)	0.0367 (3)	0.72765 (14)	0.0455 (6)
N3B	0.9888 (2)	-0.0122 (2)	0.66848 (14)	0.0589 (6)
C5A	0.1133 (4)	0.5806 (4)	0.72234 (18)	0.0716 (9)
H5A	0.1039	0.6297	0.7626	0.086*
C4B	0.9949 (3)	0.0093 (3)	0.79741 (17)	0.0656 (9)
H4B	1.0748	-0.0492	0.8108	0.079*
C6A	0.1013 (4)	0.4324 (4)	0.72188 (15)	0.0654 (8)
H6A	0.0840	0.3864	0.7618	0.078*
C5B	0.9239 (4)	0.0719 (4)	0.84490 (18)	0.0782 (11)
H5B	0.9553	0.0550	0.8918	0.094*
C7A	0.1143 (3)	0.3539 (3)	0.66457 (13)	0.0504 (6)
H7A	0.1065	0.2557	0.6643	0.060*
C7B	0.7529 (3)	0.1924 (3)	0.75700 (15)	0.0589 (7)

H7B	0.6744	0.2529	0.7439	0.071*
C6B	0.8042 (4)	0.1616 (4)	0.82488 (16)	0.0756 (10)
H6B	0.7580	0.2015	0.8591	0.091*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0383 (12)	0.0479 (14)	0.0339 (11)	0.0014 (10)	0.0059 (9)	-0.0096 (10)
C2	0.0445 (13)	0.0528 (15)	0.0460 (14)	-0.0082 (12)	0.0102 (11)	-0.0078 (11)
C3	0.0537 (15)	0.0423 (14)	0.0545 (15)	-0.0078 (12)	0.0106 (12)	0.0013 (12)
C4	0.0477 (13)	0.0418 (13)	0.0466 (13)	0.0024 (11)	0.0074 (11)	0.0043 (11)
C5	0.0393 (12)	0.0386 (12)	0.0324 (11)	0.0002 (10)	0.0067 (9)	-0.0014 (9)
C6	0.0422 (12)	0.0378 (12)	0.0396 (12)	0.0009 (10)	0.0048 (10)	-0.0001 (10)
C1A	0.0419 (13)	0.0631 (17)	0.0472 (14)	0.0063 (12)	-0.0009 (11)	-0.0123 (12)
N1A	0.0405 (11)	0.0486 (12)	0.0407 (11)	0.0041 (9)	0.0059 (9)	0.0062 (9)
C2A	0.0316 (11)	0.0408 (12)	0.0414 (12)	0.0029 (9)	0.0052 (9)	0.0043 (10)
N2A	0.0552 (14)	0.0708 (17)	0.0561 (14)	0.0028 (12)	0.0096 (11)	0.0247 (13)
C1B	0.0420 (13)	0.0432 (13)	0.0502 (14)	-0.0009 (11)	0.0027 (11)	0.0070 (11)
N1B	0.0351 (10)	0.0399 (11)	0.0474 (11)	0.0040 (8)	0.0071 (8)	-0.0005 (9)
C3A	0.0370 (12)	0.0391 (13)	0.0600 (16)	0.0051 (10)	0.0041 (11)	0.0074 (11)
N3A	0.0586 (14)	0.0537 (14)	0.0725 (16)	0.0015 (12)	0.0062 (12)	0.0232 (13)
C2B	0.0373 (12)	0.0360 (12)	0.0466 (13)	-0.0016 (10)	0.0061 (10)	-0.0005 (10)
N2B	0.0445 (12)	0.0517 (13)	0.0651 (14)	0.0055 (10)	0.0155 (11)	-0.0103 (11)
C4A	0.0559 (17)	0.0421 (15)	0.091 (2)	0.0059 (13)	0.0083 (16)	-0.0118 (15)
C3B	0.0354 (12)	0.0368 (12)	0.0615 (16)	-0.0022 (10)	-0.0006 (11)	0.0035 (11)
N3B	0.0445 (12)	0.0496 (13)	0.0823 (17)	0.0103 (10)	0.0087 (12)	-0.0032 (12)
C5A	0.067 (2)	0.078 (2)	0.073 (2)	0.0010 (17)	0.0205 (16)	-0.0281 (18)
C4B	0.0582 (17)	0.0525 (17)	0.077 (2)	-0.0098 (14)	-0.0182 (15)	0.0150 (16)
C6A	0.077 (2)	0.072 (2)	0.0515 (16)	-0.0086 (17)	0.0232 (15)	-0.0035 (15)
C5B	0.100 (3)	0.071 (2)	0.0560 (19)	-0.028 (2)	-0.0110 (18)	0.0139 (17)
C7A	0.0571 (15)	0.0460 (14)	0.0490 (14)	-0.0057 (12)	0.0119 (12)	0.0020 (11)
C7B	0.0622 (17)	0.0583 (17)	0.0587 (17)	0.0045 (14)	0.0176 (14)	-0.0055 (14)
C6B	0.102 (3)	0.076 (2)	0.0519 (18)	-0.012 (2)	0.0221 (18)	-0.0090 (16)

Geometric parameters (Å, °)

C1—C2	1.384 (4)	N1B—N2B	1.355 (3)
C1—C6	1.391 (3)	N1B—C2B	1.361 (3)
C1—C1A	1.513 (3)	C3A—N3A	1.376 (3)
C2—C3	1.380 (4)	C3A—C4A	1.397 (4)
C2—H2	0.9300	C2B—C3B	1.383 (3)
C3—C4	1.380 (4)	C2B—C7B	1.394 (4)
C3—H3	0.9300	N2B—N3B	1.310 (3)
C4—C5	1.384 (3)	C4A—C5A	1.369 (5)
C4—H4	0.9300	C4A—H4A	0.9300
C5—C6	1.395 (3)	C3B—N3B	1.376 (4)
C5—C1B	1.507 (3)	C3B—C4B	1.396 (4)
C6—H6	0.9300	C5A—C6A	1.404 (5)

C1A—N1A	1.457 (3)	C5A—H5A	0.9300
C1A—H1AA	0.9700	C4B—C5B	1.358 (5)
C1A—H1AB	0.9700	C4B—H4B	0.9300
N1A—N2A	1.354 (3)	C6A—C7A	1.365 (4)
N1A—C2A	1.355 (3)	C6A—H6A	0.9300
C2A—C3A	1.390 (3)	C5B—C6B	1.405 (5)
C2A—C7A	1.392 (3)	C5B—H5B	0.9300
N2A—N3A	1.308 (4)	C7A—H7A	0.9300
C1B—N1B	1.447 (3)	C7B—C6B	1.367 (4)
C1B—H1BA	0.9700	C7B—H7B	0.9300
C1B—H1BB	0.9700	C6B—H6B	0.9300
H1BA…N3A ⁱ	2.59	H7A…Cg1 ⁱⁱⁱ	2.69
H4A…N3B ⁱⁱ	2.66	H4B…Cg2 ^{iv}	2.79
C2—C1—C6	119.1 (2)	N2B—N1B—C1B	120.9 (2)
C2—C1—C1A	119.8 (2)	C2B—N1B—C1B	129.5 (2)
C6—C1—C1A	121.1 (2)	N3A—C3A—C2A	108.2 (2)
C3—C2—C1	120.3 (2)	N3A—C3A—C4A	131.1 (3)
C3—C2—H2	119.8	C2A—C3A—C4A	120.7 (3)
C1—C2—H2	119.8	N2A—N3A—C3A	108.2 (2)
C2—C3—C4	120.2 (2)	N1B—C2B—C3B	104.9 (2)
C2—C3—H3	119.9	N1B—C2B—C7B	132.5 (2)
C4—C3—H3	119.9	C3B—C2B—C7B	122.6 (2)
C3—C4—C5	120.8 (2)	N3B—N2B—N1B	109.1 (2)
C3—C4—H4	119.6	C5A—C4A—C3A	116.7 (3)
C5—C4—H4	119.6	C5A—C4A—H4A	121.7
C4—C5—C6	118.5 (2)	C3A—C4A—H4A	121.7
C4—C5—C1B	122.0 (2)	N3B—C3B—C2B	108.6 (2)
C6—C5—C1B	119.4 (2)	N3B—C3B—C4B	130.7 (3)
C1—C6—C5	121.1 (2)	C2B—C3B—C4B	120.8 (3)
C1—C6—H6	119.4	N2B—N3B—C3B	107.8 (2)
C5—C6—H6	119.4	C4A—C5A—C6A	122.0 (3)
N1A—C1A—C1	112.5 (2)	C4A—C5A—H5A	119.0
N1A—C1A—H1AA	109.1	C6A—C5A—H5A	119.0
C1—C1A—H1AA	109.1	C5B—C4B—C3B	117.1 (3)
N1A—C1A—H1AB	109.1	C5B—C4B—H4B	121.5
C1—C1A—H1AB	109.1	C3B—C4B—H4B	121.5
H1AA—C1A—H1AB	107.8	C7A—C6A—C5A	122.0 (3)
N2A—N1A—C2A	110.1 (2)	C7A—C6A—H6A	119.0
N2A—N1A—C1A	121.6 (2)	C5A—C6A—H6A	119.0
C2A—N1A—C1A	128.3 (2)	C4B—C5B—C6B	121.5 (3)
N1A—C2A—C3A	104.7 (2)	C4B—C5B—H5B	119.2
N1A—C2A—C7A	132.7 (2)	C6B—C5B—H5B	119.2
C3A—C2A—C7A	122.6 (2)	C6A—C7A—C2A	116.0 (3)
N3A—N2A—N1A	108.8 (2)	C6A—C7A—H7A	122.0
N1B—C1B—C5	113.11 (19)	C2A—C7A—H7A	122.0
N1B—C1B—H1BA	109.0	C6B—C7B—C2B	115.5 (3)

C5—C1B—H1BA	109.0	C6B—C7B—H7B	122.3
N1B—C1B—H1BB	109.0	C2B—C7B—H7B	122.3
C5—C1B—H1BB	109.0	C7B—C6B—C5B	122.5 (3)
H1BA—C1B—H1BB	107.8	C7B—C6B—H6B	118.8
N2B—N1B—C2B	109.6 (2)	C5B—C6B—H6B	118.8

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y+1, z$; (iii) $x-1, y, z$; (iv) $-x+3/2, y-1/2, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$Cg1$ and $Cg2$ are the centroids of the N1B–N3B/C2B/C3B C2A–C7A rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1B—H1BA \cdots N3A ⁱ	0.97	2.59	3.409 (4)	142
C4A—H4A \cdots N3B ⁱⁱ	0.93	2.66	3.443 (4)	143
C7A—H7A \cdots Cg1 ⁱⁱⁱ	0.93	2.69	3.423 (3)	136
C4B—H4B \cdots Cg2 ^{iv}	0.93	2.89	3.481 (3)	132

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y+1, z$; (iii) $x-1, y, z$; (iv) $-x+3/2, y-1/2, -z+3/2$.