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ISSN 2414-3146

4-Bromo-*N*,*N*′-diphenylbenzimidamide *N*′-oxide

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Received 27 September 2024
Accepted 1 October 2024

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

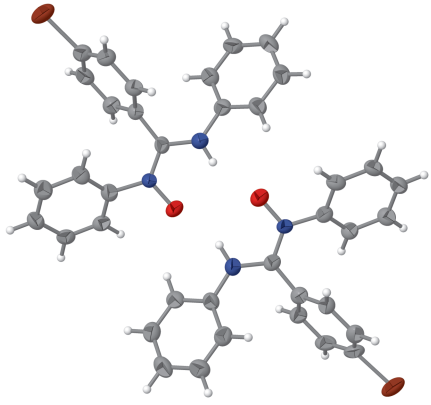
Keywords: amidine *N*-oxides; ligand synthesis; crystal structure.

CCDC reference: 2388273

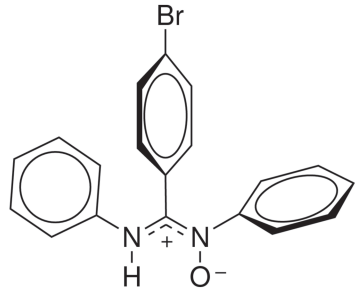
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{19}H_{15}BrN_2O$, crystallizes with two similar molecules in the asymmetric unit. The extended structure features dimers linked by pairs of N—H···O and C—H···O hydrogen bonds. The HNCNO moiety of the title compound shows delocalization over the N—C—N part, as evidenced by the similar C—N bond distances.

3D view



Chemical scheme



Structure description

The title compound $C_{19}H_{15}BrN_2O$ (AMOX-Br) is a symmetrically *N*,*N*′-disubstituted arylamidine *N*′-oxide. Its crystal structure was determined as part of a research project involving the synthesis of AMOX ligands and their coordination complexes with transition-metal ions for assessing their photophysical and electrochemical properties (Patel *et al.*, 1979; Verma *et al.*, 1995; Cibian *et al.*, 2018). The asymmetric unit contains two molecules (labelled with suffixes *A* and *B*) in the orthorhombic $Pna2_1$ space group. Each molecule contains an O—N—C—N bridge bearing a central *C*-aryl ring with 4-bromo substitution and two side *N*-phenyl rings (Fig. 1).

The N—C—N moieties in both molecules display electronic delocalization since the bond lengths are shorter than classical C—N single bonds (1.45 Å) and longer than localized C═N double bonds (1.27 Å) (Filgueiras de Athayde-Filho *et al.*, 2003). This observation is evident from the similar N—C bond distances [C1*A*—N1*A* = 1.321 (11) Å, C1*A*—N2*A* = 1.338 (12) Å and C1*B*—N1*B* = 1.325 (11) Å, C1*B*—N2*B* = 1.366 (11) Å] for the two molecules of the asymmetric unit. Furthermore, these values are comparable to those reported for the N—C—N bond lengths in 4-bromo-*N*-phenylbenzamidoxime (Cibian *et al.*, 2009). The N—C—N—O moiety is slightly twisted with a torsion angle of 3.9 (11)° for N2*B*—C1*B*—N1*B*—O1*B* and −3.9 (12)° for O1*A*—N1*A*—C1*A*—N2*A*. Considering the central and side phenyl rings, if rings C3*A*–C8*A*, C9*A*–C14*A* and C15*A*–C20*A* from molecule *A* are labelled 1, 2 and 3, respectively (4, 5 and 6, respectively, for

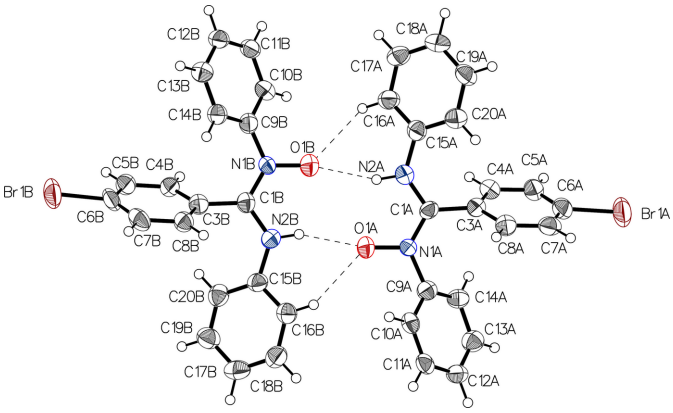


Figure 1
View of the asymmetric unit containing two independent molecules with displacement ellipsoids drawn at the 50% probability level.

the rings of molecule *B*, Fig. 2), the angle between planes 1 and 3 is 68.9 (3)° while the angle between planes 1 and 2 is 57.1 (3)°, with the corresponding angles for molecule *B* being 69.6 (3) and 56.9 (3)°, respectively. The angles between the planes of the side *N*-phenyl rings (2/3 & 5/6 for molecules *A* and *B*, respectively) are 73.6 (3) and 72.6 (3)°, respectively.

Hydrogen bonds are reported in Table 1. The extended structure displays cyclic dimers linked by pairs of N—H···O and C—H···O hydrogen bonds. No notable intermolecular π–π stacking interactions are observed but there are several C—H···π contacts that complement the conventional hydrogen bonds (Fig. 3).

Synthesis and crystallization

The compound was synthesized with some modification to the procedure reported in the literature (Cibian *et al.*, 2018): 4-bromo-*N*,*N*′-diphenylbenzimidamide, AM–Br (0.84 g, 2.4 mmol, 1.0 eq.) was dissolved in dichloromethane in the presence of $NaHCO_3$ (1.19 g, 14.2 mmol, 5.0 eq.) and stirred for 10 minutes. Then, *m*-chloro-peroxibenzoic acid, *m*-CPBA, 70% (0.76 g, 3.1 mmol, 1.1 eq.) was added in small aliquotes to the AM–Br solution. The reaction mixture turned brown instantly and darkened within a minute of stirring. The reaction mixture was stirred at room temperature for 2 h and filtered under vacuum. The filtrate was washed with 2 *M* NaOH solution (2 × 80 ml), distilled water (2 × 80 ml) and brine (3 × 50 ml). The collected dichloromethane layer was dried with anhydrous Na_2SO_4 and the solvent was removed under vacuum. The sticky brown solid obtained was sonicated in a minimum volume of ethyl acetate/hexanes. The precipitate thus formed was filtered and washed with ethyl acetate/hexanes to give a pale-yellow amorphous powder (yield 76%) of the title compound. Bright-yellow needles suitable for X-ray diffraction measurements were grown over a period of 5 d at room temperature by the hexane anti-solvent layering technique with a dichloromethane solution of the compound (1:1 *v*/*v*).

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

*Cg*2, *Cg*3, *Cg*5 and *Cg*6 are the centroids of the C9*A*–C14*A*, C15*A*–C20*A*, C9*B*–C14*B* and C15*B*–C20*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H2*A*···O1*B*	0.88	2.20	3.005 (11)	152
C10*A*—H10*A*···O1*B*^{i}	0.95	2.32	3.249 (12)	167
C16*A*—H16*A*···O1*B*	0.95	2.41	3.191 (12)	139
N2*B*—H2*B*···O1*A*	0.88	2.19	2.999 (10)	152
C10*B*—H10*B*···O1*A*^{ii}	0.95	2.28	3.214 (12)	167
C16*B*—H16*B*···O1*A*	0.95	2.40	3.188 (12)	140
C4*A*—H4*A*···*Cg*2^{ii}	0.95	2.77	3.614 (10)	149
C4*B*—H4*B*···*Cg*6^{ii}	0.95	2.64	3.534 (10)	157
C8*A*—H8*A*···*Cg*3^{i}	0.95	2.71	3.591 (10)	154
C8*B*—H8*B*···*Cg*5^{i}	0.95	2.85	3.688 (10)	148

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

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was refined as a two-component inversion twin.

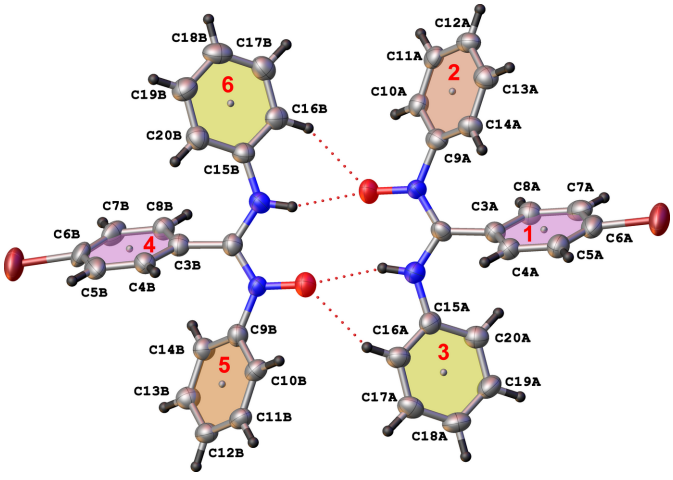


Figure 2
View of planes 1, 2, 3, 4, 5, and 6 for the phenyl rings of the molecules in the asymmetric unit and hydrogen bonds (dotted lines).

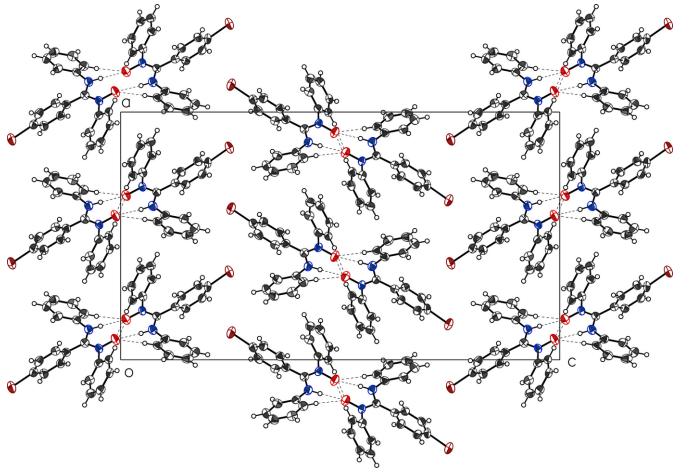


Figure 3
View of the packing of the title compound in the unit cell.

Acknowledgements

We gratefully acknowledge all the personnel from the XRD facilities of Université de Montréal. Professor Frank Schaper is acknowledged for the crystallographic course and training of AS.

Funding information

Funding for this research was provided by: Natural Sciences and Engineering Research Council of Canada (NSERC); Centre in Green Chemistry and Catalysis (CGCC); Quebec Centre for Advanced Materials (CQMF); Université de Montréal ESP excellence scholarship (scholarship to A. Saha).

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{15}BrN_2O$
M_r	367.24
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	150
a, b, c (Å)	17.7036 (16), 5.8468 (6), 31.418 (3)
V (Å^3)	3252.0 (5)
Z	8
Radiation type	Ga $K\alpha$, λ = 1.34139 Å
μ (mm^{-1})	2.30
Crystal size (mm)	0.19 × 0.03 × 0.03
Data collection	
Diffractometer	Bruker Venture Metaljet
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.079, 0.201
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	100504, 6071, 4793
R_{int}	0.090
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.610
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.158, 1.07
No. of reflections	6071
No. of parameters	416
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.13, −0.64
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.23 (6)

Computer programs: *APEX4* (Bruker, 2022), *SAINT* (Bruker, 2020), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *FinalCIF* (Kratzert, 2024) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2024). **9**, x240968 [https://doi.org/10.1107/S2414314624009684]

4-Bromo-*N*,*N*′-diphenylbenzimidamide *N*′-oxide

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4-Bromo-*N*,*N*′-diphenylbenzimidamide *N*′-oxide

Crystal data

$C_{19}H_{15}BrN_2O$
M_r = 367.24
Orthorhombic, $Pna2_1$
a = 17.7036 (16) Å
b = 5.8468 (6) Å
c = 31.418 (3) Å
V = 3252.0 (5) Å^3
Z = 8
$F(000)$ = 1488
D_x = 1.500 Mg m^{-3}
Ga $K\alpha$ radiation, λ = 1.34139 Å
Cell parameters from 9781 reflections
θ = 4.5–54.4°
μ = 2.30 mm^{-1}
T = 150 K
Needle, clear light colourless
0.19 × 0.03 × 0.03 mm

Data collection

Bruker Venture Metaljet diffractometer
Radiation source: Metal Jet, Gallium Liquid Metal Jet Source
Helios MX Mirror Optics monochromator
Detector resolution: 10.42 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.079, T_{max} = 0.201
100504 measured reflections
6071 independent reflections
4793 reflections with $I > 2\sigma(I)$
R_{int} = 0.090
θ_{max} = 54.9°, θ_{min} = 2.5°
h = −21→21
k = −6→7
l = −38→37

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.158
S = 1.07
6071 reflections
416 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2 + 6.1028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.23 (6)

Special details

Experimental. X-ray crystallographic data for I were collected from a single crystal sample, which was mounted on a loop fiber. Data were collected using a Bruker Venture diffractometer equipped with a Photon III CMOS Detector, a Helios MX optics and a Kappa goniometer. The crystal-to-detector distance was 4.0 cm, and the data collection was carried out in 1024 x 1024 pixel mode.

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 inversion twin.

Hydrogen atoms attached to nitrogen were first located from Fourier difference map then refined using the equivalent calculated positions. The C-bound H atoms were geometrically placed and refined as riding atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1A	0.61038 (7)	0.6881 (3)	0.25148 (3)	0.0760 (4)
O1A	0.4180 (4)	0.7299 (11)	0.4878 (2)	0.0500 (18)
N1A	0.4538 (4)	0.7506 (11)	0.4507 (3)	0.0344 (17)
C1A	0.4319 (4)	0.6209 (13)	0.4185 (3)	0.0351 (18)
N2A	0.3778 (4)	0.4681 (13)	0.4271 (2)	0.0417 (17)
H2A	0.363970	0.461329	0.453973	0.050*
C3A	0.4695 (4)	0.6315 (15)	0.3761 (3)	0.0369 (18)
C4A	0.5143 (5)	0.4453 (15)	0.3630 (3)	0.0402 (19)
H4A	0.516330	0.310580	0.379883	0.048*
C5A	0.5558 (5)	0.4585 (18)	0.3253 (3)	0.047 (2)
H5A	0.586546	0.334943	0.315994	0.057*
C6A	0.5504 (6)	0.6599 (19)	0.3018 (3)	0.051 (2)
C7A	0.5056 (6)	0.8449 (17)	0.3136 (3)	0.047 (2)
H7A	0.503148	0.978161	0.296394	0.057*
C8A	0.4644 (5)	0.8303 (17)	0.3516 (3)	0.043 (2)
H8A	0.433335	0.953821	0.360476	0.051*
C9A	0.5134 (5)	0.9239 (15)	0.4500 (3)	0.0396 (19)
C10A	0.4990 (5)	1.1212 (15)	0.4729 (3)	0.0380 (19)
H10A	0.451900	1.142036	0.486832	0.046*
C11A	0.5530 (5)	1.2838 (15)	0.4752 (3)	0.040 (2)
H11A	0.543730	1.417141	0.491620	0.048*
C12A	0.6217 (5)	1.2623 (15)	0.4542 (4)	0.042 (2)
H12A	0.658205	1.381271	0.455257	0.051*
C13A	0.6354 (5)	1.0632 (17)	0.4319 (3)	0.048 (2)
H13A	0.682490	1.045000	0.417789	0.057*
C14A	0.5821 (5)	0.8882 (14)	0.4296 (3)	0.0409 (19)
H14A	0.592282	0.750290	0.414638	0.049*
C15A	0.3389 (5)	0.3147 (16)	0.3995 (3)	0.041 (2)
C16A	0.3139 (5)	0.1128 (15)	0.4159 (3)	0.044 (2)
H16A	0.323975	0.076505	0.444787	0.053*
C17A	0.2739 (5)	−0.0410 (16)	0.3908 (3)	0.047 (2)
H17A	0.256372	−0.180680	0.402644	0.056*
C18A	0.2594 (5)	0.0097 (19)	0.3481 (3)	0.052 (3)
H18A	0.233473	−0.096676	0.330491	0.062*
C19A	0.2838 (6)	0.2216 (18)	0.3316 (4)	0.051 (3)
H19A	0.272754	0.260575	0.302911	0.061*
C20A	0.3238 (5)	0.3733 (16)	0.3568 (3)	0.045 (2)

H20A	0.340832	0.514948	0.345548	0.055*
C1B	0.3236 (4)	0.3768 (15)	0.5820 (3)	0.0370 (18)
Br1B	0.14367 (7)	0.2681 (2)	0.74742 (3)	0.0701 (4)
N1B	0.3017 (4)	0.2490 (11)	0.5494 (3)	0.0336 (17)
O1B	0.3366 (4)	0.2703 (11)	0.5123 (2)	0.0478 (17)
N2B	0.3789 (4)	0.5326 (12)	0.5731 (2)	0.0417 (17)
H2B	0.393219	0.539951	0.546301	0.050*
C3B	0.2863 (5)	0.3580 (16)	0.6241 (3)	0.0387 (19)
C4B	0.2924 (5)	0.1630 (16)	0.6482 (3)	0.0391 (19)
H4B	0.325401	0.044035	0.639406	0.047*
C5B	0.2506 (5)	0.1381 (18)	0.6856 (3)	0.048 (2)
H5B	0.254569	0.001873	0.701917	0.058*
C6B	0.2046 (6)	0.3074 (19)	0.6984 (3)	0.048 (2)
C7B	0.1990 (5)	0.5162 (18)	0.6760 (3)	0.050 (2)
H7B	0.167883	0.637004	0.686058	0.060*
C8B	0.2411 (5)	0.5390 (16)	0.6382 (3)	0.041 (2)
H8B	0.238858	0.677153	0.622357	0.049*
C9B	0.2439 (5)	0.0776 (15)	0.5503 (3)	0.0393 (19)
C10B	0.2578 (5)	−0.1214 (15)	0.5272 (3)	0.040 (2)
H10B	0.304907	−0.142167	0.513284	0.049*
C11B	0.2031 (6)	−0.2875 (16)	0.5248 (3)	0.042 (2)
H11B	0.212594	−0.422652	0.508851	0.051*
C12B	0.1340 (5)	−0.2606 (14)	0.5453 (4)	0.041 (2)
H12B	0.096363	−0.376087	0.543340	0.049*
C13B	0.1207 (5)	−0.0633 (17)	0.5685 (3)	0.042 (2)
H13B	0.074096	−0.045649	0.583136	0.051*
C14B	0.1746 (5)	0.1094 (15)	0.5707 (3)	0.0401 (19)
H14B	0.164413	0.246787	0.585759	0.048*
C15B	0.4160 (5)	0.6836 (15)	0.6013 (3)	0.040 (2)
C16B	0.4421 (4)	0.8874 (15)	0.5840 (3)	0.041 (2)
H16B	0.433158	0.921877	0.554880	0.050*
C17B	0.4814 (5)	1.0404 (17)	0.6097 (3)	0.049 (2)
H17B	0.498950	1.180375	0.597936	0.059*
C18B	0.4953 (5)	0.9913 (18)	0.6523 (4)	0.054 (3)
H18B	0.521577	1.097190	0.669808	0.065*
C19B	0.4695 (6)	0.7814 (18)	0.6691 (5)	0.053 (3)
H19B	0.479286	0.744164	0.698056	0.063*
C20B	0.4308 (5)	0.6319 (17)	0.6440 (3)	0.046 (2)
H20B	0.413583	0.491091	0.655569	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.0716 (8)	0.1182 (10)	0.0382 (7)	−0.0140 (7)	0.0150 (7)	0.0000 (9)
O1A	0.060 (4)	0.053 (4)	0.038 (4)	−0.010 (3)	0.018 (3)	−0.007 (3)
N1A	0.040 (4)	0.032 (4)	0.031 (5)	−0.006 (3)	0.006 (4)	−0.006 (3)
C1A	0.039 (4)	0.026 (4)	0.040 (5)	−0.002 (3)	0.003 (3)	0.002 (3)
N2A	0.045 (4)	0.044 (4)	0.036 (4)	−0.005 (3)	0.004 (3)	−0.004 (3)

C3A	0.037 (4)	0.036 (4)	0.037 (5)	−0.002 (4)	0.002 (4)	0.000 (4)
C4A	0.042 (5)	0.040 (5)	0.038 (4)	0.000 (4)	−0.001 (4)	−0.004 (4)
C5A	0.048 (5)	0.055 (6)	0.039 (5)	−0.005 (4)	0.003 (4)	−0.004 (4)
C6A	0.046 (5)	0.069 (7)	0.037 (5)	−0.012 (5)	−0.003 (4)	−0.003 (5)
C7A	0.057 (6)	0.040 (5)	0.046 (6)	−0.007 (5)	−0.015 (5)	0.001 (4)
C8A	0.038 (4)	0.047 (5)	0.043 (6)	0.001 (4)	−0.001 (4)	0.001 (4)
C9A	0.038 (4)	0.041 (5)	0.039 (4)	−0.002 (4)	−0.007 (4)	0.005 (4)
C10A	0.039 (4)	0.045 (5)	0.031 (4)	0.004 (4)	−0.002 (3)	0.001 (4)
C11A	0.049 (5)	0.043 (5)	0.028 (5)	0.002 (4)	−0.007 (4)	0.002 (4)
C12A	0.047 (5)	0.036 (5)	0.045 (6)	−0.005 (4)	−0.008 (4)	0.001 (4)
C13A	0.042 (5)	0.051 (6)	0.050 (6)	−0.002 (4)	−0.003 (4)	0.002 (5)
C14A	0.043 (5)	0.032 (4)	0.048 (5)	0.001 (4)	−0.003 (4)	−0.002 (4)
C15A	0.034 (4)	0.050 (5)	0.039 (5)	−0.001 (4)	0.005 (4)	−0.005 (4)
C16A	0.046 (5)	0.039 (5)	0.048 (5)	−0.004 (4)	−0.001 (4)	−0.005 (4)
C17A	0.050 (5)	0.032 (5)	0.059 (6)	−0.003 (4)	0.003 (4)	−0.002 (4)
C18A	0.049 (5)	0.049 (6)	0.057 (6)	−0.008 (5)	−0.010 (4)	−0.012 (5)
C19A	0.052 (6)	0.063 (7)	0.037 (7)	−0.005 (5)	−0.008 (4)	−0.007 (5)
C20A	0.043 (5)	0.045 (5)	0.049 (5)	−0.002 (4)	−0.003 (4)	−0.001 (4)
C1B	0.036 (4)	0.041 (5)	0.034 (4)	0.002 (4)	0.003 (3)	0.000 (4)
Br1B	0.0672 (7)	0.1061 (9)	0.0369 (6)	−0.0024 (6)	0.0184 (6)	0.0002 (7)
N1B	0.041 (4)	0.032 (4)	0.028 (5)	−0.001 (3)	0.004 (3)	−0.004 (3)
O1B	0.053 (4)	0.051 (4)	0.040 (4)	−0.004 (3)	0.010 (3)	−0.002 (3)
N2B	0.046 (4)	0.038 (4)	0.041 (4)	−0.007 (3)	0.006 (3)	−0.001 (3)
C3B	0.033 (4)	0.045 (5)	0.037 (5)	0.001 (4)	−0.001 (3)	0.001 (4)
C4B	0.038 (4)	0.041 (5)	0.038 (5)	−0.003 (4)	0.001 (4)	0.001 (4)
C5B	0.046 (5)	0.061 (6)	0.036 (5)	−0.013 (5)	−0.010 (4)	0.008 (4)
C6B	0.057 (6)	0.063 (6)	0.024 (5)	−0.002 (5)	−0.001 (4)	−0.007 (4)
C7B	0.041 (5)	0.066 (6)	0.043 (5)	0.006 (4)	0.005 (4)	−0.021 (5)
C8B	0.043 (5)	0.039 (5)	0.040 (5)	0.002 (4)	0.004 (4)	−0.002 (4)
C9B	0.043 (5)	0.039 (5)	0.035 (4)	0.000 (4)	0.004 (4)	0.000 (4)
C10B	0.046 (5)	0.040 (5)	0.036 (4)	0.003 (4)	−0.004 (4)	−0.005 (4)
C11B	0.053 (6)	0.037 (5)	0.037 (6)	−0.004 (4)	−0.005 (4)	−0.004 (4)
C12B	0.043 (5)	0.040 (5)	0.040 (6)	−0.005 (4)	−0.005 (4)	−0.002 (4)
C13B	0.036 (4)	0.044 (6)	0.047 (5)	0.003 (4)	−0.003 (4)	−0.003 (4)
C14B	0.037 (4)	0.042 (5)	0.041 (4)	0.001 (4)	0.004 (4)	−0.003 (4)
C15B	0.037 (5)	0.041 (5)	0.042 (5)	−0.005 (4)	−0.003 (4)	0.000 (4)
C16B	0.036 (4)	0.044 (5)	0.044 (5)	0.003 (4)	0.006 (4)	−0.007 (4)
C17B	0.048 (5)	0.044 (5)	0.054 (6)	−0.002 (4)	0.009 (4)	0.001 (5)
C18B	0.042 (5)	0.051 (6)	0.070 (7)	−0.008 (4)	−0.004 (5)	−0.011 (5)
C19B	0.052 (6)	0.057 (7)	0.048 (7)	−0.004 (5)	−0.007 (5)	−0.005 (5)
C20B	0.039 (5)	0.052 (6)	0.046 (5)	−0.001 (4)	0.002 (4)	0.004 (4)

Geometric parameters (Å, º)

Br1A—C6A	1.911 (10)	C1B—N1B	1.325 (11)
O1A—N1A	1.333 (11)	C1B—N2B	1.366 (11)
N1A—C1A	1.321 (11)	C1B—C3B	1.485 (12)
N1A—C9A	1.463 (11)	Br1B—C6B	1.894 (10)

C1A—N2A	1.338 (11)	N1B—O1B	1.326 (10)
C1A—C3A	1.491 (12)	N1B—C9B	1.433 (11)
N2A—H2A	0.8800	N2B—H2B	0.8800
N2A—C15A	1.423 (12)	N2B—C15B	1.415 (12)
C3A—C4A	1.408 (12)	C3B—C4B	1.373 (14)
C3A—C8A	1.398 (14)	C3B—C8B	1.398 (13)
C4A—H4A	0.9500	C4B—H4B	0.9500
C4A—C5A	1.397 (13)	C4B—C5B	1.396 (13)
C5A—H5A	0.9500	C5B—H5B	0.9500
C5A—C6A	1.393 (15)	C5B—C6B	1.343 (15)
C6A—C7A	1.392 (15)	C6B—C7B	1.413 (15)
C7A—H7A	0.9500	C7B—H7B	0.9500
C7A—C8A	1.400 (14)	C7B—C8B	1.407 (13)
C8A—H8A	0.9500	C8B—H8B	0.9500
C9A—C10A	1.383 (12)	C9B—C10B	1.393 (12)
C9A—C14A	1.391 (12)	C9B—C14B	1.396 (12)
C10A—H10A	0.9500	C10B—H10B	0.9500
C10A—C11A	1.350 (13)	C10B—C11B	1.374 (13)
C11A—H11A	0.9500	C11B—H11B	0.9500
C11A—C12A	1.387 (14)	C11B—C12B	1.392 (14)
C12A—H12A	0.9500	C12B—H12B	0.9500
C12A—C13A	1.381 (14)	C12B—C13B	1.385 (14)
C13A—H13A	0.9500	C13B—H13B	0.9500
C13A—C14A	1.394 (13)	C13B—C14B	1.391 (13)
C14A—H14A	0.9500	C14B—H14B	0.9500
C15A—C16A	1.361 (13)	C15B—C16B	1.389 (13)
C15A—C20A	1.410 (13)	C15B—C20B	1.398 (13)
C16A—H16A	0.9500	C16B—H16B	0.9500
C16A—C17A	1.391 (13)	C16B—C17B	1.391 (13)
C17A—H17A	0.9500	C17B—H17B	0.9500
C17A—C18A	1.397 (15)	C17B—C18B	1.393 (15)
C18A—H18A	0.9500	C18B—H18B	0.9500
C18A—C19A	1.412 (16)	C18B—C19B	1.411 (15)
C19A—H19A	0.9500	C19B—H19B	0.9500
C19A—C20A	1.384 (14)	C19B—C20B	1.364 (15)
C20A—H20A	0.9500	C20B—H20B	0.9500

O1A—N1A—C9A	114.7 (7)	N1B—C1B—N2B	115.3 (7)
C1A—N1A—O1A	118.6 (7)	N1B—C1B—C3B	121.2 (8)
C1A—N1A—C9A	126.7 (8)	N2B—C1B—C3B	123.4 (7)
N1A—C1A—N2A	116.1 (7)	C1B—N1B—O1B	119.3 (7)
N1A—C1A—C3A	121.9 (7)	C1B—N1B—C9B	126.0 (8)
N2A—C1A—C3A	121.8 (7)	O1B—N1B—C9B	114.6 (7)
C1A—N2A—H2A	114.9	C1B—N2B—H2B	115.8
C1A—N2A—C15A	130.1 (8)	C1B—N2B—C15B	128.4 (7)
C15A—N2A—H2A	114.9	C15B—N2B—H2B	115.8
C4A—C3A—C1A	118.7 (8)	C4B—C3B—C1B	121.2 (8)
C8A—C3A—C1A	119.9 (8)	C4B—C3B—C8B	119.9 (9)

C8A—C3A—C4A	121.2 (9)	C8B—C3B—C1B	118.8 (8)
C3A—C4A—H4A	120.0	C3B—C4B—H4B	119.7
C5A—C4A—C3A	120.1 (9)	C3B—C4B—C5B	120.6 (9)
C5A—C4A—H4A	120.0	C5B—C4B—H4B	119.7
C4A—C5A—H5A	121.3	C4B—C5B—H5B	120.1
C6A—C5A—C4A	117.4 (9)	C6B—C5B—C4B	119.8 (9)
C6A—C5A—H5A	121.3	C6B—C5B—H5B	120.1
C5A—C6A—Br1A	118.2 (8)	C5B—C6B—Br1B	119.9 (8)
C5A—C6A—C7A	123.7 (10)	C5B—C6B—C7B	122.0 (9)
C7A—C6A—Br1A	118.1 (8)	C7B—C6B—Br1B	118.0 (7)
C6A—C7A—H7A	120.7	C6B—C7B—H7B	121.2
C6A—C7A—C8A	118.5 (9)	C8B—C7B—C6B	117.7 (9)
C8A—C7A—H7A	120.7	C8B—C7B—H7B	121.2
C3A—C8A—C7A	119.1 (9)	C3B—C8B—C7B	119.9 (9)
C3A—C8A—H8A	120.4	C3B—C8B—H8B	120.1
C7A—C8A—H8A	120.4	C7B—C8B—H8B	120.1
C10A—C9A—N1A	116.0 (7)	C10B—C9B—N1B	116.6 (7)
C10A—C9A—C14A	121.7 (8)	C10B—C9B—C14B	120.3 (8)
C14A—C9A—N1A	122.2 (8)	C14B—C9B—N1B	122.9 (8)
C9A—C10A—H10A	120.5	C9B—C10B—H10B	120.1
C11A—C10A—C9A	119.0 (8)	C11B—C10B—C9B	119.7 (8)
C11A—C10A—H10A	120.5	C11B—C10B—H10B	120.1
C10A—C11A—H11A	118.9	C10B—C11B—H11B	119.5
C10A—C11A—C12A	122.1 (9)	C10B—C11B—C12B	120.9 (9)
C12A—C11A—H11A	118.9	C12B—C11B—H11B	119.5
C11A—C12A—H12A	120.9	C11B—C12B—H12B	120.4
C13A—C12A—C11A	118.1 (9)	C13B—C12B—C11B	119.1 (8)
C13A—C12A—H12A	120.9	C13B—C12B—H12B	120.4
C12A—C13A—H13A	119.1	C12B—C13B—H13B	119.5
C12A—C13A—C14A	121.8 (9)	C12B—C13B—C14B	120.9 (9)
C14A—C13A—H13A	119.1	C14B—C13B—H13B	119.5
C9A—C14A—C13A	117.2 (8)	C9B—C14B—H14B	120.5
C9A—C14A—H14A	121.4	C13B—C14B—C9B	118.9 (8)
C13A—C14A—H14A	121.4	C13B—C14B—H14B	120.5
C16A—C15A—N2A	118.3 (9)	C16B—C15B—N2B	116.3 (8)
C16A—C15A—C20A	120.5 (9)	C16B—C15B—C20B	120.0 (9)
C20A—C15A—N2A	121.2 (8)	C20B—C15B—N2B	123.6 (8)
C15A—C16A—H16A	119.6	C15B—C16B—H16B	120.3
C15A—C16A—C17A	120.9 (9)	C15B—C16B—C17B	119.4 (9)
C17A—C16A—H16A	119.6	C17B—C16B—H16B	120.3
C16A—C17A—H17A	120.0	C16B—C17B—H17B	119.5
C16A—C17A—C18A	120.1 (9)	C16B—C17B—C18B	120.9 (9)
C18A—C17A—H17A	120.0	C18B—C17B—H17B	119.5
C17A—C18A—H18A	120.6	C17B—C18B—H18B	120.6
C17A—C18A—C19A	118.8 (9)	C17B—C18B—C19B	118.9 (10)
C19A—C18A—H18A	120.6	C19B—C18B—H18B	120.6
C18A—C19A—H19A	119.7	C18B—C19B—H19B	119.9
C20A—C19A—C18A	120.6 (11)	C20B—C19B—C18B	120.2 (12)

C20A—C19A—H19A	119.7	C20B—C19B—H19B	119.9
C15A—C20A—H20A	120.4	C15B—C20B—H20B	119.7
C19A—C20A—C15A	119.1 (10)	C19B—C20B—C15B	120.7 (10)
C19A—C20A—H20A	120.4	C19B—C20B—H20B	119.7
Br1A—C6A—C7A—C8A	−176.9 (7)	C1B—N1B—C9B—C10B	−140.5 (9)
O1A—N1A—C1A—N2A	−3.9 (12)	C1B—N1B—C9B—C14B	43.6 (13)
O1A—N1A—C1A—C3A	−179.3 (8)	C1B—N2B—C15B—C16B	−151.1 (8)
O1A—N1A—C9A—C10A	−37.2 (11)	C1B—N2B—C15B—C20B	32.5 (14)
O1A—N1A—C9A—C14A	139.3 (8)	C1B—C3B—C4B—C5B	−173.1 (8)
N1A—C1A—N2A—C15A	175.7 (8)	C1B—C3B—C8B—C7B	173.5 (8)
N1A—C1A—C3A—C4A	109.5 (9)	Br1B—C6B—C7B—C8B	−176.4 (7)
N1A—C1A—C3A—C8A	−65.9 (11)	N1B—C1B—N2B—C15B	−176.6 (8)
N1A—C9A—C10A—C11A	177.1 (8)	N1B—C1B—C3B—C4B	66.9 (11)
N1A—C9A—C14A—C13A	−178.4 (8)	N1B—C1B—C3B—C8B	−109.9 (10)
C1A—N1A—C9A—C10A	141.1 (9)	N1B—C9B—C10B—C11B	−176.4 (8)
C1A—N1A—C9A—C14A	−42.3 (13)	N1B—C9B—C14B—C13B	177.5 (8)
C1A—N2A—C15A—C16A	149.9 (9)	O1B—N1B—C9B—C10B	37.1 (11)
C1A—N2A—C15A—C20A	−32.7 (14)	O1B—N1B—C9B—C14B	−138.8 (8)
C1A—C3A—C4A—C5A	−174.1 (8)	N2B—C1B—N1B—O1B	3.9 (11)
C1A—C3A—C8A—C7A	174.2 (8)	N2B—C1B—N1B—C9B	−178.6 (8)
N2A—C1A—C3A—C4A	−65.7 (11)	N2B—C1B—C3B—C4B	−117.0 (10)
N2A—C1A—C3A—C8A	119.0 (9)	N2B—C1B—C3B—C8B	66.2 (11)
N2A—C15A—C16A—C17A	178.3 (8)	N2B—C15B—C16B—C17B	−177.9 (8)
N2A—C15A—C20A—C19A	−178.0 (9)	N2B—C15B—C20B—C19B	177.4 (9)
C3A—C1A—N2A—C15A	−8.9 (14)	C3B—C1B—N1B—O1B	−179.8 (7)
C3A—C4A—C5A—C6A	−0.3 (13)	C3B—C1B—N1B—C9B	−2.3 (13)
C4A—C3A—C8A—C7A	−1.0 (13)	C3B—C1B—N2B—C15B	7.1 (14)
C4A—C5A—C6A—Br1A	177.0 (7)	C3B—C4B—C5B—C6B	−0.8 (14)
C4A—C5A—C6A—C7A	−0.8 (14)	C4B—C3B—C8B—C7B	−3.3 (13)
C5A—C6A—C7A—C8A	0.9 (14)	C4B—C5B—C6B—Br1B	176.7 (7)
C6A—C7A—C8A—C3A	0.0 (13)	C4B—C5B—C6B—C7B	−2.4 (14)
C8A—C3A—C4A—C5A	1.2 (13)	C5B—C6B—C7B—C8B	2.7 (14)
C9A—N1A—C1A—N2A	177.8 (8)	C6B—C7B—C8B—C3B	0.2 (13)
C9A—N1A—C1A—C3A	2.4 (13)	C8B—C3B—C4B—C5B	3.7 (13)
C9A—C10A—C11A—C12A	1.9 (14)	C9B—C10B—C11B—C12B	−0.4 (15)
C10A—C9A—C14A—C13A	−2.0 (13)	C10B—C9B—C14B—C13B	1.7 (13)
C10A—C11A—C12A—C13A	−2.6 (15)	C10B—C11B—C12B—C13B	−0.2 (16)
C11A—C12A—C13A—C14A	0.9 (15)	C11B—C12B—C13B—C14B	1.6 (15)
C12A—C13A—C14A—C9A	1.3 (14)	C12B—C13B—C14B—C9B	−2.4 (14)
C14A—C9A—C10A—C11A	0.5 (13)	C14B—C9B—C10B—C11B	−0.3 (13)
C15A—C16A—C17A—C18A	0.6 (14)	C15B—C16B—C17B—C18B	0.4 (13)
C16A—C15A—C20A—C19A	−0.6 (14)	C16B—C15B—C20B—C19B	1.1 (14)
C16A—C17A—C18A—C19A	−2.1 (14)	C16B—C17B—C18B—C19B	0.8 (14)
C17A—C18A—C19A—C20A	2.2 (15)	C17B—C18B—C19B—C20B	−1.0 (15)
C18A—C19A—C20A—C15A	−0.9 (15)	C18B—C19B—C20B—C15B	0.1 (15)
C20A—C15A—C16A—C17A	0.8 (14)	C20B—C15B—C16B—C17B	−1.3 (13)

Hydrogen-bond geometry (Å, º)

*Cg*2, *Cg*3, *Cg*5 and *Cg*6 are the centroids of the C9*A*–C14*A*, C15*A*–C20*A*, C9*B*–C14*B* and C15*B*–C20*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H2*A*···O1*B*	0.88	2.20	3.005 (11)	152
C10*A*—H10*A*···O1*B*^{i}	0.95	2.32	3.249 (12)	167
C16*A*—H16*A*···O1*B*	0.95	2.41	3.191 (12)	139
N2*B*—H2*B*···O1*A*	0.88	2.19	2.999 (10)	152
C10*B*—H10*B*···O1*A*^{ii}	0.95	2.28	3.214 (12)	167
C16*B*—H16*B*···O1*A*	0.95	2.40	3.188 (12)	140
C4*A*—H4*A*···*Cg*2^{ii}	0.95	2.77	3.614 (10)	149
C4*B*—H4*B*···*Cg*6^{ii}	0.95	2.64	3.534 (10)	157
C8*A*—H8*A*···*Cg*3^{i}	0.95	2.71	3.591 (10)	154
C8*B*—H8*B*···*Cg*5^{i}	0.95	2.85	3.688 (10)	148

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*, *y*−1, *z*.