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6,7-Dibromo-2-methyl-3-phenylquinoxaline

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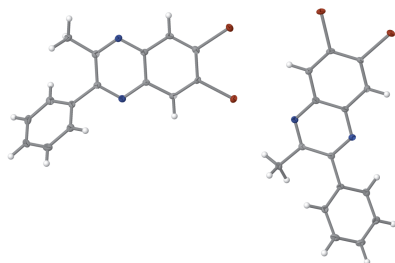
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Keywords: crystal structure; quinoxaline.**CCDC reference:** 2593016

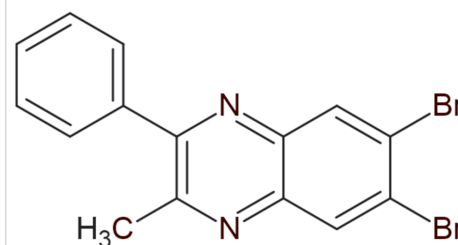
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, C₁₅H₁₀Br₂N₂, was synthesized using the acid catalyst NH₄HF₂ in a water/methanol solution. There are two molecules per asymmetric unit where the quinoxaline moieties make dihedral angles of 48.05 (4) and 40.83 (5)° with respect to their phenyl rings. In the extended structure, molecules form layers stacked along (001) that are held together by hydrogen and halogen bonds.

3D view



Chemical scheme



Structure description

In general, quinoxalines are of interest as potential antibacterial (Parhi *et al.*, 2013), antimicrobial (Singh *et al.*, 2010), and antifungal medicines (Tang *et al.*, 2022); therefore, exploring their synthesis and structures is of interest. The title compound was synthesized *via* a condensation reaction of a diamine and diketone using a water/methanol solution containing a catalytic amount of NH₄HF₂ catalyst (Lassagne *et al.*, 2015).

There are two molecules per asymmetric unit (Fig. 1) where the quinoxaline moieties make dihedral angles of 48.05 (4) and 40.83 (5)° with respect to their phenyl rings. Molecules pack in a herringbone pattern where quinoxalines form planes (Fig. 2). There are two types of intermolecular interactions – halogen bonds and hydrogen bonds. Fig. 3 shows the halogen and hydrogen bonds between molecules that lie normal to the (001) direction of the unit cell. The hydrogen bonds in this layer are between C6–H6···Br3ⁱ, C6–H6···Br4ⁱ, C13–H13···N3ⁱⁱⁱ, C21–H21···Br1, and C28–H28···N1^v (see Table 1 for symmetry codes and metrics). The halogen bonds involve Br1···N4 [3.0230 (19) Å, with C1–Br1···N4 = 171.29 (8)°] and Br4···N2^{vi} [3.2270 (18) Å, with C4–Br4···N2^{vi} = 160.96 (8)°; symmetry code: (vi) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$]. The hydrogen bonds in Table 2 that have not been specifically mentioned involve methyl groups and connect molecules between layers.



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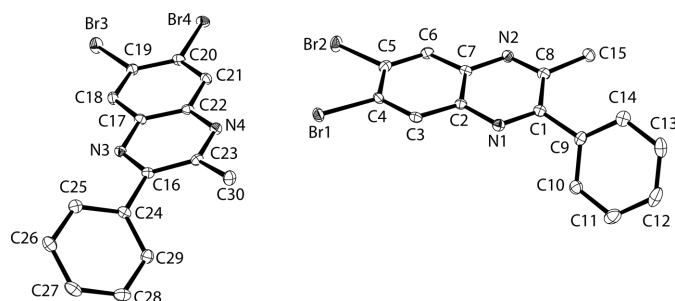
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Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C6-H6\cdots Br3^i$	0.95	2.91	3.784 (2)	154
$C6-H6\cdots Br4^i$	0.95	3.09	3.834 (2)	136
$C15-H15B\cdots Br1^{ii}$	0.98	3.13	4.044 (2)	155
$C21-H21\cdots Br1$	0.95	3.05	3.741 (2)	131
$C13-H13\cdots N3^{iii}$	0.95	2.62	3.495 (3)	152
$C28-H28\cdots N1^v$	0.95	2.68	3.568 (3)	156

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

**Figure 1**

A view of the molecules of the title compound, with displacement ellipsoids drawn at the 50% probability level and H atoms omitted for clarity.

Synthesis and crystallization

In a 50 ml Erlenmeyer flask, 1.48 g of 1-phenylpropane-1,2-dione (10.0 mmol) was added to 2 ml of H_2O and 20 ml of a 2.5×10^{-3} M methanol solution of NH_4HF_2 (Lassagne *et al.*, 2015). To this mixture, 2.66 g of 4,5-dibromo-1,2-phenylenediamine (10.0 mmol) was added. The solution was stirred

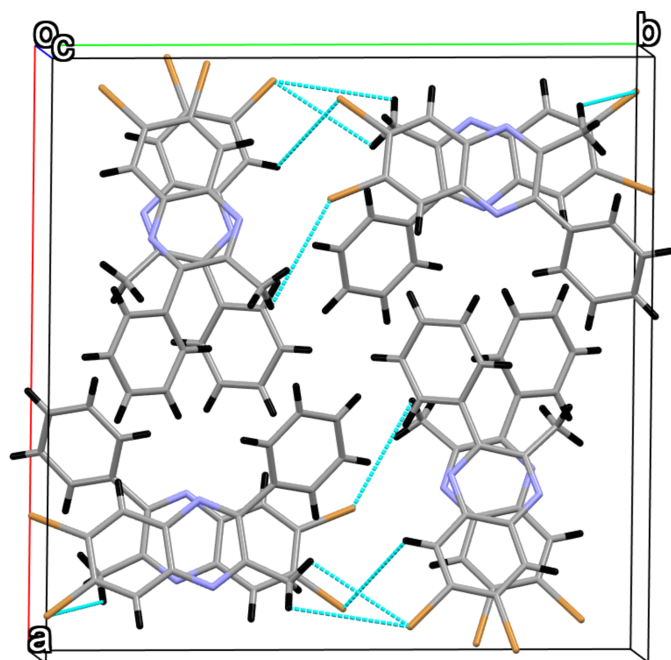
Table 2

Experimental details.

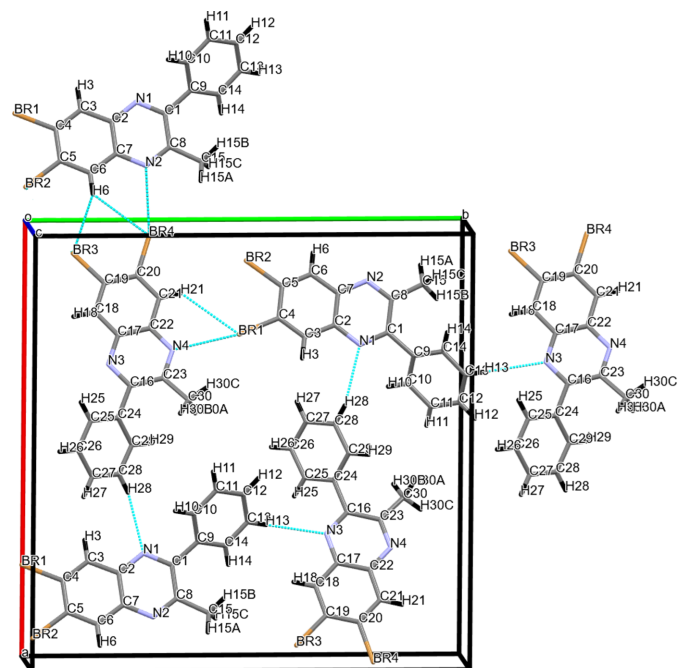
Crystal data	$C_{15}H_{10}Br_2N_2$
Chemical formula	378.07
M_r	Monoclinic, $P2_1/c$
Crystal system, space group	100
Temperature (K)	19.0464 (3), 18.6850 (4), 7.5964 (2)
a, b, c (Å)	97.495 (2)
β (°)	2680.32 (10)
V (Å ³)	8
Z	Mo $K\alpha$
Radiation type	6.03
μ (mm ⁻¹)	$0.28 \times 0.21 \times 0.12 \times 0.09$ (radius)
Crystal size (mm)	
Data collection	Rigaku XtaLAB Synergy Single source diffractometer with a HyPix-Arc 100 detector
Diffractometer	For a sphere (<i>CrysAlis PRO</i> ; Rigaku OD, 2024)
Absorption correction	T_{min}, T_{max}
	0.420, 0.436
	No. of measured, independent and observed [$I > 2\sigma(I)$] reflections
	44577, 9561, 7295
	R_{int}
	($\sin \theta/\lambda$) _{max} (Å ⁻¹)
	0.047
	0.784
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.043, 0.065, 1.05
No. of reflections	9561
No. of parameters	345
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.68, -0.54

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015a), *SHELXL2025* (Sheldrick, 2015b), *ORTEP-3* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020), and *ShelXle* (Hübschle *et al.*, 2011).

for 24 h, during which time the product precipitated as a pink-white product. 3.48 g of crude product was isolated and

**Figure 2**

A view of unit-cell packing along [001], with some of the $C-H\cdots Br$ hydrogen-bonding interactions shown.

**Figure 3**

A view of the intermolecular interactions (halogen and hydrogen bonds) in layers along the (001) direction.

recrystallized from methanol solution, yielding 1.60 g of white purified powder (42%). The yield was low due to loss of material during recrystallization. Crystals for diffraction study were isolated from the slow evaporation of a CH₂Cl₂ solution (m.p. 416 K). ¹H NMR (CDCl₃, 300 MHz): δ 2.72 (s, 3H), 7.50 (m, 3H), 7.61 (m, 2H), 8.30 (s, 1H), 8.35 (s, 1H); ¹³C NMR (CDCl₃, 300 MHz): δ 24.54, 125.65, 126.20, 128.65, 128.90, 129.48, 132.42, 133.17, 138.18, 140.21, 140.34, 154.14, 155.99.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms on *sp*² and *sp*³ C atoms were placed at calculated positions with C—H distances of 0.95 and 0.98 Å, respectively, and were included in the refinement in riding motion approximation with *U*_{iso}(H) = 1.2*U*_{eq} or 1.5*U*_{eq} of the carrier atom, respectively.

Acknowledgements

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full crystallographic data

IUCrData (2026). **11**, x261027 [<https://doi.org/10.1107/S2414314626010278>]

6,7-Dibromo-2-methyl-3-phenylquinoxaline

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Crystal data

$C_{15}H_{10}Br_2N_2$

$M_r = 378.07$

Monoclinic, $P2_1/c$

$a = 19.0464(3) \text{ \AA}$

$b = 18.6850(4) \text{ \AA}$

$c = 7.5964(2) \text{ \AA}$

$\beta = 97.495(2)^\circ$

$V = 2680.32(10) \text{ \AA}^3$

$Z = 8$

$F(000) = 1472$

$D_x = 1.874 \text{ Mg m}^{-3}$

Melting point: 416 K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 15741 reflections

$\theta = 2.9\text{--}32.9^\circ$

$\mu = 6.03 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Block, colorless

$0.28 \times 0.21 \times 0.12 \times 0.09$ (radius) mm

Data collection

Rigaku XtaLAB Synergy Single source
diffractometer with a HyPix-Arc 100 detector

Radiation source: fine-focus sealed X-ray tube,
Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: $10.0000 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: for a sphere
(CrysAlis PRO; Rigaku OD, 2024)

$T_{\min} = 0.420$, $T_{\max} = 0.436$

44577 measured reflections

9561 independent reflections

7295 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 33.9^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -29 \rightarrow 27$

$k = -29 \rightarrow 24$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.065$

$S = 1.05$

9561 reflections

345 parameters

0 restraints

Primary atom site location: SHELXT
(Sheldrick, 2015a)

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0185P)^2 + 2.9293P]$

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

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

$\Delta\rho_{\max} = 0.68 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.54 \text{ e \AA}^{-3}$

Special details

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

Refinement. 1. Fixed Uiso At 1.2 times of: All C(H) groups At 1.5 times of: All C(H,H,H) groups 2.a Aromatic/amide H refined with riding coordinates: C3(H3), C6(H6), C10(H10), C11(H11), C12(H12), C13(H13), C14(H14), C18(H18), C21(H21), C25(H25), C26(H26), C27(H27), C28(H28), C29(H29) 2.b Idealised Me refined as rotating group: C15(H15a,H15b,H15c), C30(H30a,H30b,H30c)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.24220 (2)	0.47648 (2)	0.59870 (3)	0.01589 (5)
Br2	0.08173 (2)	0.49698 (2)	0.36507 (3)	0.02061 (6)
N1	0.26864 (10)	0.75369 (10)	0.5630 (2)	0.0127 (4)
N2	0.12777 (10)	0.77270 (10)	0.4032 (2)	0.0130 (4)
C1	0.24242 (11)	0.81804 (12)	0.5236 (3)	0.0118 (4)
C2	0.22464 (11)	0.69655 (12)	0.5254 (3)	0.0108 (4)
C3	0.25015 (11)	0.62685 (12)	0.5712 (3)	0.0123 (4)
H3	0.296657	0.620597	0.631582	0.015*
C4	0.20793 (11)	0.56870 (12)	0.5287 (3)	0.0120 (4)
C5	0.13873 (12)	0.57774 (13)	0.4358 (3)	0.0145 (4)
C6	0.11233 (11)	0.64483 (12)	0.3933 (3)	0.0137 (4)
H6	0.065779	0.650351	0.332637	0.016*
C7	0.15481 (11)	0.70558 (12)	0.4404 (3)	0.0120 (4)
C8	0.16899 (11)	0.82787 (12)	0.4477 (3)	0.0129 (4)
C9	0.29498 (11)	0.87743 (12)	0.5513 (3)	0.0130 (4)
C10	0.36089 (12)	0.86606 (13)	0.4938 (3)	0.0156 (5)
H10	0.369780	0.822506	0.436123	0.019*
C11	0.41331 (13)	0.91774 (14)	0.5203 (3)	0.0218 (5)
H11	0.457800	0.909752	0.479885	0.026*
C12	0.40080 (13)	0.98142 (13)	0.6062 (3)	0.0225 (5)
H12	0.436954	1.016625	0.625970	0.027*
C13	0.33547 (13)	0.99332 (13)	0.6627 (3)	0.0200 (5)
H13	0.326855	1.036866	0.720752	0.024*
C14	0.28258 (13)	0.94190 (13)	0.6348 (3)	0.0161 (5)
H14	0.237760	0.950631	0.672709	0.019*
C15	0.13594 (12)	0.90040 (12)	0.4132 (3)	0.0157 (5)
H15A	0.095392	0.896590	0.319925	0.024*
H15B	0.170950	0.933389	0.374788	0.024*
H15C	0.119921	0.918504	0.522263	0.024*
Br3	0.06220 (2)	0.10061 (2)	0.38293 (3)	0.02061 (6)
Br4	0.02408 (2)	0.27571 (2)	0.34126 (3)	0.01466 (5)
N3	0.30515 (9)	0.17557 (10)	0.7234 (2)	0.0121 (4)
N4	0.27362 (9)	0.32225 (10)	0.7003 (2)	0.0120 (4)
C16	0.35225 (11)	0.22414 (12)	0.7863 (3)	0.0103 (4)
C17	0.24113 (11)	0.19876 (12)	0.6434 (3)	0.0115 (4)
C18	0.19038 (11)	0.14799 (12)	0.5711 (3)	0.0137 (4)
H18	0.200116	0.098282	0.584403	0.016*
C19	0.12717 (11)	0.17060 (12)	0.4820 (3)	0.0127 (4)
C20	0.11180 (11)	0.24510 (13)	0.4634 (3)	0.0129 (4)
C21	0.16011 (11)	0.29493 (12)	0.5334 (3)	0.0123 (4)

H21	0.149460	0.344479	0.520711	0.015*
C22	0.22615 (11)	0.27262 (12)	0.6252 (3)	0.0114 (4)
C23	0.33522 (11)	0.29920 (12)	0.7821 (3)	0.0111 (4)
C24	0.42317 (11)	0.19515 (12)	0.8601 (3)	0.0114 (4)
C25	0.42573 (12)	0.13067 (12)	0.9540 (3)	0.0132 (4)
H25	0.382968	0.107428	0.972814	0.016*
C26	0.49055 (12)	0.10032 (13)	1.0202 (3)	0.0155 (5)
H26	0.491937	0.056718	1.084880	0.019*
C27	0.55319 (12)	0.13373 (13)	0.9918 (3)	0.0181 (5)
H27	0.597436	0.113425	1.038665	0.022*
C28	0.55113 (12)	0.19686 (13)	0.8948 (3)	0.0172 (5)
H28	0.594027	0.218994	0.872762	0.021*
C29	0.48638 (11)	0.22790 (12)	0.8297 (3)	0.0138 (4)
H29	0.485254	0.271393	0.764633	0.017*
C30	0.38241 (12)	0.35517 (12)	0.8767 (3)	0.0141 (4)
H30A	0.415288	0.372920	0.797704	0.021*
H30B	0.409292	0.334255	0.983132	0.021*
H30C	0.353484	0.394892	0.911121	0.021*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01469 (10)	0.01104 (11)	0.02134 (12)	0.00220 (8)	0.00010 (8)	0.00060 (9)
Br2	0.01600 (11)	0.01336 (11)	0.03052 (14)	−0.00353 (9)	−0.00431 (9)	0.00033 (10)
N1	0.0122 (9)	0.0133 (9)	0.0125 (9)	−0.0003 (7)	0.0011 (7)	−0.0007 (7)
N2	0.0124 (9)	0.0125 (9)	0.0139 (9)	0.0013 (7)	0.0008 (7)	0.0013 (7)
C1	0.0123 (10)	0.0140 (11)	0.0091 (10)	0.0009 (8)	0.0015 (8)	−0.0006 (8)
C2	0.0107 (9)	0.0133 (11)	0.0087 (10)	0.0006 (8)	0.0022 (7)	0.0001 (8)
C3	0.0093 (10)	0.0146 (11)	0.0130 (11)	0.0022 (8)	0.0013 (8)	0.0003 (8)
C4	0.0125 (10)	0.0105 (11)	0.0134 (11)	0.0031 (8)	0.0032 (8)	0.0009 (8)
C5	0.0139 (10)	0.0150 (11)	0.0147 (11)	−0.0033 (8)	0.0025 (8)	−0.0007 (9)
C6	0.0101 (10)	0.0167 (12)	0.0138 (11)	−0.0008 (8)	−0.0007 (8)	0.0004 (9)
C7	0.0110 (10)	0.0140 (11)	0.0112 (10)	0.0016 (8)	0.0018 (8)	−0.0003 (8)
C8	0.0143 (10)	0.0145 (11)	0.0100 (10)	0.0010 (8)	0.0022 (8)	0.0016 (8)
C9	0.0140 (10)	0.0124 (11)	0.0118 (11)	−0.0018 (8)	−0.0016 (8)	0.0029 (8)
C10	0.0155 (11)	0.0142 (12)	0.0168 (12)	0.0009 (9)	0.0013 (9)	0.0021 (9)
C11	0.0141 (11)	0.0240 (14)	0.0265 (14)	−0.0015 (10)	−0.0010 (9)	0.0084 (10)
C12	0.0206 (12)	0.0162 (12)	0.0276 (14)	−0.0068 (9)	−0.0081 (10)	0.0085 (10)
C13	0.0276 (13)	0.0118 (12)	0.0186 (12)	0.0006 (10)	−0.0049 (10)	0.0007 (9)
C14	0.0186 (11)	0.0173 (12)	0.0117 (11)	−0.0007 (9)	−0.0008 (9)	0.0009 (9)
C15	0.0136 (10)	0.0135 (11)	0.0196 (12)	0.0031 (9)	0.0001 (8)	0.0025 (9)
Br3	0.01343 (11)	0.01599 (12)	0.02968 (14)	−0.00320 (9)	−0.00745 (9)	−0.00083 (10)
Br4	0.00940 (9)	0.01911 (12)	0.01489 (11)	0.00257 (8)	−0.00061 (7)	0.00171 (9)
N3	0.0095 (8)	0.0123 (9)	0.0144 (9)	0.0008 (7)	0.0009 (7)	0.0002 (7)
N4	0.0118 (8)	0.0124 (9)	0.0115 (9)	−0.0006 (7)	0.0006 (7)	−0.0003 (7)
C16	0.0103 (9)	0.0123 (11)	0.0086 (10)	−0.0001 (8)	0.0014 (7)	−0.0022 (8)
C17	0.0093 (9)	0.0130 (11)	0.0118 (10)	0.0001 (8)	−0.0001 (8)	−0.0011 (8)
C18	0.0129 (10)	0.0097 (11)	0.0181 (11)	0.0004 (8)	0.0005 (8)	0.0005 (8)

C19	0.0092 (9)	0.0125 (11)	0.0157 (11)	−0.0023 (8)	−0.0007 (8)	−0.0007 (8)
C20	0.0094 (9)	0.0182 (12)	0.0106 (11)	0.0021 (8)	−0.0009 (8)	0.0026 (8)
C21	0.0126 (10)	0.0126 (11)	0.0116 (10)	0.0027 (8)	0.0018 (8)	0.0012 (8)
C22	0.0108 (9)	0.0135 (11)	0.0105 (10)	−0.0001 (8)	0.0033 (8)	−0.0021 (8)
C23	0.0118 (10)	0.0130 (11)	0.0086 (10)	−0.0018 (8)	0.0020 (8)	−0.0004 (8)
C24	0.0098 (9)	0.0140 (11)	0.0097 (10)	0.0013 (8)	−0.0011 (7)	−0.0027 (8)
C25	0.0145 (10)	0.0133 (11)	0.0119 (11)	−0.0014 (8)	0.0019 (8)	−0.0041 (8)
C26	0.0171 (11)	0.0143 (11)	0.0145 (11)	0.0034 (9)	−0.0001 (8)	−0.0024 (9)
C27	0.0129 (11)	0.0204 (13)	0.0199 (12)	0.0051 (9)	−0.0023 (9)	−0.0043 (10)
C28	0.0117 (10)	0.0217 (13)	0.0182 (12)	−0.0011 (9)	0.0021 (9)	−0.0051 (9)
C29	0.0148 (10)	0.0128 (11)	0.0136 (11)	−0.0014 (8)	0.0008 (8)	−0.0003 (8)
C30	0.0153 (10)	0.0123 (11)	0.0141 (11)	−0.0022 (8)	−0.0007 (8)	−0.0022 (8)

Geometric parameters (Å, °)

Br1—C4	1.894 (2)	Br3—C19	1.888 (2)
Br2—C5	1.895 (2)	Br4—C20	1.891 (2)
N1—C1	1.321 (3)	N3—C16	1.321 (3)
N1—C2	1.364 (3)	N3—C17	1.360 (3)
N2—C8	1.313 (3)	N4—C23	1.326 (3)
N2—C7	1.371 (3)	N4—C22	1.367 (3)
C1—C8	1.453 (3)	C16—C23	1.439 (3)
C1—C9	1.491 (3)	C16—C24	1.495 (3)
C2—C7	1.411 (3)	C17—C22	1.412 (3)
C2—C3	1.418 (3)	C17—C18	1.413 (3)
C3—C4	1.365 (3)	C18—C19	1.369 (3)
C3—H3	0.9500	C18—H18	0.9500
C4—C5	1.422 (3)	C19—C20	1.426 (3)
C5—C6	1.373 (3)	C20—C21	1.367 (3)
C6—C7	1.413 (3)	C21—C22	1.419 (3)
C6—H6	0.9500	C21—H21	0.9500
C8—C15	1.503 (3)	C23—C30	1.500 (3)
C9—C14	1.396 (3)	C24—C29	1.396 (3)
C9—C10	1.398 (3)	C24—C25	1.398 (3)
C10—C11	1.385 (3)	C25—C26	1.392 (3)
C10—H10	0.9500	C25—H25	0.9500
C11—C12	1.392 (4)	C26—C27	1.388 (3)
C11—H11	0.9500	C26—H26	0.9500
C12—C13	1.386 (4)	C27—C28	1.389 (3)
C12—H12	0.9500	C27—H27	0.9500
C13—C14	1.388 (3)	C28—C29	1.394 (3)
C13—H13	0.9500	C28—H28	0.9500
C14—H14	0.9500	C29—H29	0.9500
C15—H15A	0.9800	C30—H30A	0.9800
C15—H15B	0.9800	C30—H30B	0.9800
C15—H15C	0.9800	C30—H30C	0.9800
C1—N1—C2	117.45 (18)	C16—N3—C17	118.01 (19)

C8—N2—C7	117.97 (19)	C23—N4—C22	118.16 (19)
N1—C1—C8	121.4 (2)	N3—C16—C23	121.41 (19)
N1—C1—C9	114.73 (19)	N3—C16—C24	115.12 (19)
C8—C1—C9	123.8 (2)	C23—C16—C24	123.47 (19)
N1—C2—C7	121.3 (2)	N3—C17—C22	120.86 (19)
N1—C2—C3	119.08 (19)	N3—C17—C18	119.2 (2)
C7—C2—C3	119.7 (2)	C22—C17—C18	119.91 (19)
C4—C3—C2	120.05 (19)	C19—C18—C17	119.9 (2)
C4—C3—H3	120.0	C19—C18—H18	120.1
C2—C3—H3	120.0	C17—C18—H18	120.1
C3—C4—C5	120.1 (2)	C18—C19—C20	120.4 (2)
C3—C4—Br1	119.14 (16)	C18—C19—Br3	118.16 (17)
C5—C4—Br1	120.71 (17)	C20—C19—Br3	121.42 (16)
C6—C5—C4	120.8 (2)	C21—C20—C19	120.49 (19)
C6—C5—Br2	118.79 (16)	C21—C20—Br4	119.46 (17)
C4—C5—Br2	120.38 (17)	C19—C20—Br4	120.05 (16)
C5—C6—C7	119.6 (2)	C20—C21—C22	120.0 (2)
C5—C6—H6	120.2	C20—C21—H21	120.0
C7—C6—H6	120.2	C22—C21—H21	120.0
N2—C7—C2	120.7 (2)	N4—C22—C17	120.51 (19)
N2—C7—C6	119.68 (19)	N4—C22—C21	120.1 (2)
C2—C7—C6	119.6 (2)	C17—C22—C21	119.3 (2)
N2—C8—C1	121.0 (2)	N4—C23—C16	120.68 (19)
N2—C8—C15	116.12 (19)	N4—C23—C30	115.88 (19)
C1—C8—C15	122.9 (2)	C16—C23—C30	123.34 (19)
C14—C9—C10	119.0 (2)	C29—C24—C25	119.3 (2)
C14—C9—C1	123.8 (2)	C29—C24—C16	122.4 (2)
C10—C9—C1	117.2 (2)	C25—C24—C16	118.25 (19)
C11—C10—C9	120.6 (2)	C26—C25—C24	120.4 (2)
C11—C10—H10	119.7	C26—C25—H25	119.8
C9—C10—H10	119.7	C24—C25—H25	119.8
C10—C11—C12	120.0 (2)	C27—C26—C25	120.0 (2)
C10—C11—H11	120.0	C27—C26—H26	120.0
C12—C11—H11	120.0	C25—C26—H26	120.0
C13—C12—C11	119.8 (2)	C26—C27—C28	119.9 (2)
C13—C12—H12	120.1	C26—C27—H27	120.0
C11—C12—H12	120.1	C28—C27—H27	120.0
C12—C13—C14	120.3 (2)	C27—C28—C29	120.3 (2)
C12—C13—H13	119.8	C27—C28—H28	119.9
C14—C13—H13	119.8	C29—C28—H28	119.9
C13—C14—C9	120.3 (2)	C28—C29—C24	120.1 (2)
C13—C14—H14	119.9	C28—C29—H29	120.0
C9—C14—H14	119.9	C24—C29—H29	120.0
C8—C15—H15A	109.5	C23—C30—H30A	109.5
C8—C15—H15B	109.5	C23—C30—H30B	109.5
H15A—C15—H15B	109.5	H30A—C30—H30B	109.5
C8—C15—H15C	109.5	C23—C30—H30C	109.5
H15A—C15—H15C	109.5	H30A—C30—H30C	109.5

H15B—C15—H15C	109.5	H30B—C30—H30C	109.5
C2—N1—C1—C8	1.7 (3)	C17—N3—C16—C23	4.2 (3)
C2—N1—C1—C9	−174.23 (19)	C17—N3—C16—C24	−175.61 (19)
C1—N1—C2—C7	2.7 (3)	C16—N3—C17—C22	1.2 (3)
C1—N1—C2—C3	−177.9 (2)	C16—N3—C17—C18	178.5 (2)
N1—C2—C3—C4	−177.5 (2)	N3—C17—C18—C19	−176.5 (2)
C7—C2—C3—C4	1.8 (3)	C22—C17—C18—C19	0.7 (3)
C2—C3—C4—C5	1.0 (3)	C17—C18—C19—C20	−0.8 (3)
C2—C3—C4—Br1	−177.87 (16)	C17—C18—C19—Br3	178.43 (17)
C3—C4—C5—C6	−2.5 (3)	C18—C19—C20—C21	0.4 (3)
Br1—C4—C5—C6	176.45 (17)	Br3—C19—C20—C21	−178.83 (17)
C3—C4—C5—Br2	176.60 (17)	C18—C19—C20—Br4	−179.61 (17)
Br1—C4—C5—Br2	−4.5 (3)	Br3—C19—C20—Br4	1.2 (3)
C4—C5—C6—C7	0.9 (3)	C19—C20—C21—C22	0.1 (3)
Br2—C5—C6—C7	−178.19 (17)	Br4—C20—C21—C22	−179.92 (16)
C8—N2—C7—C2	0.5 (3)	C23—N4—C22—C17	3.5 (3)
C8—N2—C7—C6	−179.5 (2)	C23—N4—C22—C21	−178.8 (2)
N1—C2—C7—N2	−4.1 (3)	N3—C17—C22—N4	−5.3 (3)
C3—C2—C7—N2	176.6 (2)	C18—C17—C22—N4	177.4 (2)
N1—C2—C7—C6	175.9 (2)	N3—C17—C22—C21	177.0 (2)
C3—C2—C7—C6	−3.4 (3)	C18—C17—C22—C21	−0.3 (3)
C5—C6—C7—N2	−177.9 (2)	C20—C21—C22—N4	−177.9 (2)
C5—C6—C7—C2	2.0 (3)	C20—C21—C22—C17	−0.2 (3)
C7—N2—C8—C1	3.9 (3)	C22—N4—C23—C16	1.9 (3)
C7—N2—C8—C15	−176.87 (19)	C22—N4—C23—C30	−174.46 (19)
N1—C1—C8—N2	−5.3 (3)	N3—C16—C23—N4	−6.1 (3)
C9—C1—C8—N2	170.3 (2)	C24—C16—C23—N4	173.75 (19)
N1—C1—C8—C15	175.5 (2)	N3—C16—C23—C30	170.0 (2)
C9—C1—C8—C15	−8.9 (3)	C24—C16—C23—C30	−10.1 (3)
N1—C1—C9—C14	−134.7 (2)	N3—C16—C24—C29	138.6 (2)
C8—C1—C9—C14	49.4 (3)	C23—C16—C24—C29	−41.3 (3)
N1—C1—C9—C10	43.5 (3)	N3—C16—C24—C25	−37.6 (3)
C8—C1—C9—C10	−132.4 (2)	C23—C16—C24—C25	142.5 (2)
C14—C9—C10—C11	0.4 (3)	C29—C24—C25—C26	1.5 (3)
C1—C9—C10—C11	−177.8 (2)	C16—C24—C25—C26	177.9 (2)
C9—C10—C11—C12	0.6 (4)	C24—C25—C26—C27	−0.6 (3)
C10—C11—C12—C13	−0.9 (4)	C25—C26—C27—C28	−1.0 (3)
C11—C12—C13—C14	0.3 (4)	C26—C27—C28—C29	1.7 (4)
C12—C13—C14—C9	0.7 (4)	C27—C28—C29—C24	−0.7 (3)
C10—C9—C14—C13	−1.1 (3)	C25—C24—C29—C28	−0.9 (3)
C1—C9—C14—C13	177.1 (2)	C16—C24—C29—C28	−177.1 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C6—H6 $\cdots$ Br3 ⁱ	0.95	2.91	3.784 (2)	154
C6—H6 $\cdots$ Br4 ⁱ	0.95	3.09	3.834 (2)	136

C15—H15 <i>B</i> ⋯Br1 ⁱⁱ	0.98	3.13	4.044 (2)	155
C21—H21⋯Br1	0.95	3.05	3.741 (2)	131
C13—H13⋯N3 ⁱⁱⁱ	0.95	2.62	3.495 (3)	152
C30—H30 <i>B</i> ⋯N3 ^{iv}	0.98	2.87	3.231 (3)	103
C28—H28⋯N1 ^v	0.95	2.68	3.568 (3)	156

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