

Crystal structure of a tetrakis-substituted pyrazine compound: 2,3,5,6-tetrakis(bromomethyl)pyrazine

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Keywords: crystal structure; tetrakis-substituted; pyrazine; chiral

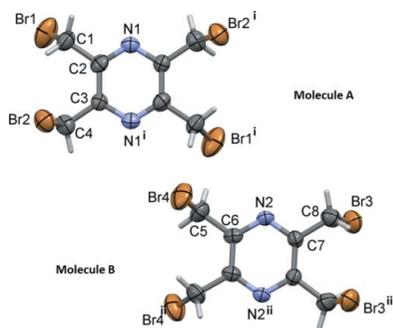
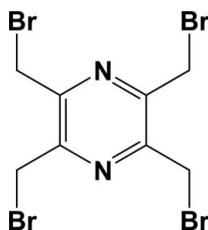
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The title compound, C₈H₈Br₄N₂, crystallizes in the enantiomorphic-defining space group *P*4₁2₁2 and has a refined Flack *x* parameter of 0.04 (4). In the asymmetric unit, there are two half-molecules; the whole molecules (*A* and *B*) are generated by twofold rotation symmetry. In molecule *A*, the twofold axis is normal to the pyrazine ring passing through the centre of the ring, while in molecule *B*, the twofold rotation axis lies in the plane of the pyrazine ring bisecting the C—C aromatic bonds. The two molecules are pseudo-mirror images of one another, and the best fit of the two molecules was obtained for inverted molecule *B* on molecule *A*, with an r.m.s. deviation of 0.1048 Å and a maximum deviation of any two equivalent atoms of 0.2246 Å. In the crystal, the *A* molecules are linked by weak C—H···Br hydrogen bonds and Br···Br interactions [3.524 (3) Å], forming a three-dimensional framework. The *B* molecules are also linked by weak C—H···Br hydrogen bonds and Br···Br interactions [3.548 (3) Å], forming a three-dimensional network that interpenetrates the network of *A* molecules.

1. Chemical context

The title compound is the starting material used for the synthesis of a number of 2,3,5,6-tetrakis-substituted pyrazine compounds (Ferigo *et al.*, 1994; Assoumatine, 1999). For example, 2,3,5,6-tetrakis(aminomethyl)pyrazine has been used as a ligand to prepare copper(II), zinc(II) and manganese(II) binuclear and polymeric complexes (Ferigo *et al.*, 1994).



2. Structural commentary

The title compound, Fig. 1, crystallizes with two half-molecules per asymmetric unit. The whole molecules (*A* and *B*) are generated by twofold rotation symmetry. In molecule *A*, the twofold axis is normal to the pyrazine ring passing through the centre of the ring. In molecule *B*, the twofold rotation axis lies in the plane of the pyrazine ring bisecting the C6—C6ⁱⁱ and C7—C7ⁱⁱ bonds [symmetry code: (ii) *y*, *x*, *-z*]. Placed side by side, it can be seen that the two molecules are almost perfect mirror images of each other (Fig. 1). The best fit of the two molecules,

Table 1
Selected torsion angles ($^{\circ}$).

Br1—C1—C2—N1	91.3 (13)	Br4—C5—C6—N2	-93.3 (12)
Br1—C1—C2—C3	-92.6 (15)	Br4—C5—C6—C6 ⁱⁱ	84.8 (17)
N1 ⁱ —C3—C4—Br2	103.1 (11)	N2—C7—C8—Br3	-101.0 (12)
C2—C3—C4—Br2	-78.6 (15)	C7 ⁱⁱ —C7—C8—Br3	77.4 (18)

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

Table 2
Hydrogen-bond geometry ($\text{\AA}, ^{\circ}$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1A \cdots Br2 ⁱⁱⁱ	0.97	3.02	3.863 (14)	146
C1—H1B \cdots Br2	0.97	2.86	3.617 (16)	135
C5—H5A \cdots Br4 ⁱⁱ	0.97	3.04	3.748 (16)	131
C5—H5B \cdots Br3 ^{iv}	0.97	3.03	3.864 (14)	145
C8—H8A \cdots Br3 ⁱⁱ	0.97	2.96	3.654 (15)	130

Symmetry codes: (ii) $y, x, -z$; (iii) $-y + \frac{3}{2}, x - \frac{1}{2}, z + \frac{1}{4}$; (iv) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{4}$.

calculated using the Molecular Overlay routine in *Mercury* (Macrae *et al.*, 2008), was obtained for inverted molecule *B* on molecule *A* with an r.m.s. deviation of 0.1048 \AA and a maximum deviation of any two equivalent atoms of 0.2246 \AA .

The main difference appears for the torsion angles Br1—C1—C2—C3 = -92.6 (15) $^{\circ}$ in molecule *A* and Br4—C5—C6—C6ⁱⁱ = 84.8 (17) $^{\circ}$ in molecule *B* [Table 1; symmetry code: (ii) $y, x, -z$]. The other torsion angles involving the Br—C—C_{ar}—C_{ar} (ar = aromatic) arms do not differ significantly (Table 2).

3. Supramolecular features

In the crystal, there are two interpenetrating three-dimensional networks composed of a network of *A* molecules, linked by weak C—H \cdots Br hydrogen bonds and Br1 \cdots Br2ⁱⁱⁱ interactions [3.524 (3) \AA ; symmetry code: (iii) $-y + 2, -x + 1, -z + \frac{1}{2}$], and a network of *B* molecules, are also linked by weak C—H \cdots Br hydrogen bonds and Br3 \cdots Br4^{iv} interactions

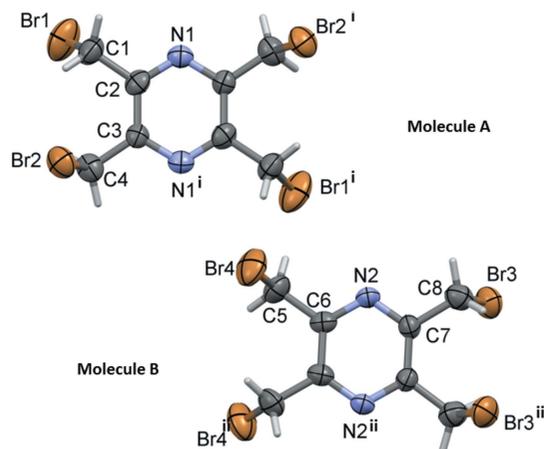


Figure 1
A view of the molecular structure of the two independent molecules (*A* and *B*) of the title compound, with atom labelling [symmetry codes: (i) $-y + 1, -x + 1, -z + \frac{1}{2}$; (ii) $y, x, -z$]. The displacement ellipsoids are drawn at the 50% probability level.

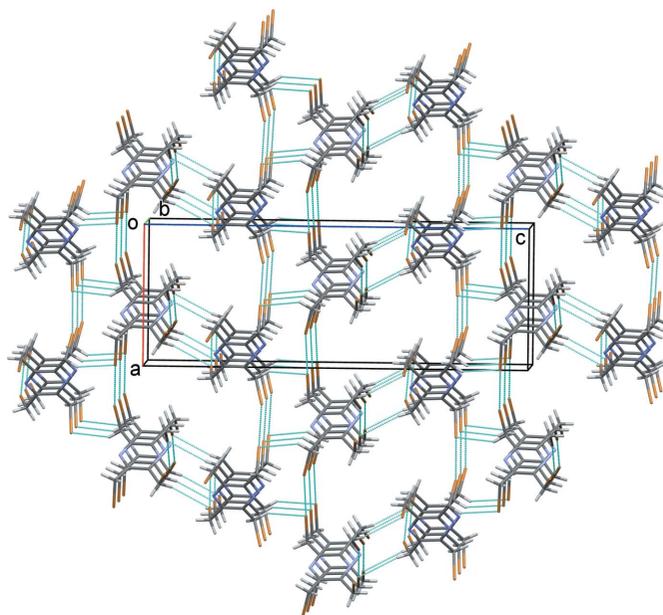


Figure 2
A view along the *b* axis of the crystal packing of the *A* molecules of the title compound. The weak C—H \cdots Br hydrogen bonds and Br \cdots Br interactions are shown as dashed lines (see Table 2 for details).

[3.548 (3) \AA , symmetry code: (iv) $x, y - 1, z$] (Table 2 and Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (Version 5.33, last update November 2013; Allen, 2002) indicated the presence of a large number of tetrasubstituted pyrazine derivatives and their metal complexes, mainly involving

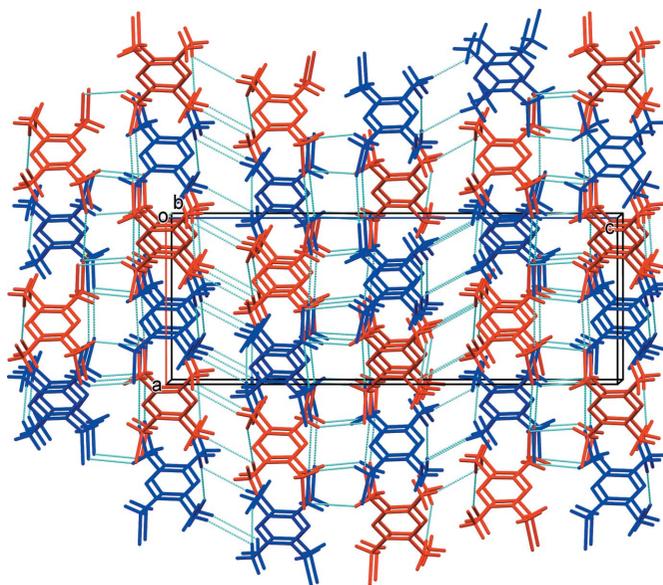


Figure 3
A view along the *b* axis of the crystal packing of the title compound. The C—H \cdots Br hydrogen bonds and Br \cdots Br interactions are shown as dashed lines (see Table 2 for details; *A* molecules blue, *B* molecules red).

Table 3
Experimental details.

Crystal data	
Chemical formula	C ₈ H ₈ Br ₄ N ₂
<i>M_r</i>	451.80
Crystal system, space group	Tetragonal, <i>P</i> 4 ₁ 2 ₁ 2
Temperature (K)	293
<i>a</i> , <i>c</i> (Å)	9.6858 (4), 26.5116 (17)
<i>V</i> (Å ³)	2487.2 (3)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
<i>μ</i> (mm ⁻¹)	12.91
Crystal size (mm)	0.50 × 0.40 × 0.30
Data collection	
Diffractometer	Stoe <i>IPDS</i> 1
Absorption correction	Multi-scan (<i>MULscanABS</i> in <i>PLATON</i> ; Spek, 2009)
<i>T_{min}</i> , <i>T_{max}</i>	0.430, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	19463, 2417, 1276
<i>R_{int}</i>	0.113
(sin θ/λ) _{max} (Å ⁻¹)	0.616
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.043, 0.096, 0.84
No. of reflections	2417
No. of parameters	127
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.69, -0.54
Absolute structure	Flack <i>x</i> determined using 419 quotients [(<i>I</i> ⁺ - <i>I</i> ⁻)] / [(<i>I</i> ⁺ + <i>I</i> ⁻)] (Parsons & Flack, 2004)
Absolute structure parameter	0.04 (4)

Computer programs: *EXPOSE*, *CELL* and *INTEGRATE* in *IPDS-1* (Stoe & Cie, 2004), *SHELXS97* and *SHELXL2013* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

tetramethylpyrazine. A small number of them involve 2,3,5,6-tetrakis(aminomethyl)pyrazine (tampyz), which was used to prepare transition metal binuclear complexes, for example [Cl₂Zn(tampyz)ZnCl₂], and a quasi-linear one-dimensional coordination polymer, {Mn(tampyz)Cl₂·2H₂O}_{*n*} (Ferigo *et al.*, 1994). The title compound has also been used in the synthesis of two triclinic polymorphs of 2,3,5,6-tetrakis(naphthalen-2-ylsulfanylmethyl)pyrazine (Pacífico & Stoeckli-Evans, 2004), 2,3,5,6-tetrakis((naphthalen-2-yloxy)methyl)pyrazine (Gasser & Stoeckli-Evans, 2007), 2,3,5,6-tetrakis(phenoxy)methylpyrazine and 2,3,5,6-tetrakis(phenylsulfanylmethyl)pyrazine (Assoumatine *et al.*, 2007). All five structures possess inversion symmetry. The sulfanyl derivatives crystallize in the triclinic space group *P* $\bar{1}$, while the oxy derivatives crystallize in the monoclinic space group *P*2₁/*c*.

5. Synthesis and crystallization

The title compound was prepared by a modification of the procedure described by Ferigo *et al.* (1994). To 2,3,5,6-tetramethylpyrazine (28 g, 0.28 mol) in CCl₄ (1 l) was added well-ground *N*-bromosuccinimide (150 g, 0.84 mol). The mixture

was stirred vigorously and heated to reflux. As soon as the reflux set in, the mixture was irradiated for 5 h with two 200 W lamps fitted at least 10 cm at opposite sides of the flask. After the mixture was then cooled firstly to room temperature and the floating succinimide filtered off. The orange filtrate was cooled overnight to 278 K to crystallize the remaining traces of succinimide, which was filtered off. The filtrate was evaporated and the residual orange oil dissolved in 50 ml of diethyl ether. This solution was maintained at 278 K for at least one week, whereupon a white crystalline material deposited. The solid was filtered off, then recrystallized in ethanol to give colourless rod-like crystals of the title compound: Yield 7.87 g (8%); m.p. 401–405 K; *R_F* 0.54 (toluene/light petroleum, 10/1 *v/v*). Analysis for C₈H₈Br₄N₂ (*M_r* = 451.78 g/mol); Calculated (%): C 21.27; H 1.79; N 6.20. Found (%): C 21.41; H 1.72; N 6.10. Spectroscopic data: ¹H-RMN (CDCl₃, 400 MHz): δ = 4.69 (*s*, 8H, Pz-CH₂-S) p.p.m.; ¹³C-RMN (CDCl₃, 100 MHz): δ = 150.41, 28.75 p.p.m. MS (EI, 70 eV), *m/z* (%): 452 ([*M*⁺], 11.9), 371 (100), 292 (13.2), 211 (20.7), 131 (32.7), 92 (20.4), 65 (18.8); IR (KBr disc, cm⁻¹): 3030 *w*, 2977 *w*, 1438 *s*, 1405 *s*, 1220 *s*, 1096 *m*, 923 *w*, 787 *s*, 731 *m*, 629 *m*, 596 *w*, 543 *m*, 445 *m*.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bound H atoms were included in calculated positions and treated as riding atoms: C–H = 0.97 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Acknowledgements

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supporting information

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Computing details

Data collection: *EXPOSE* in *IPDS-I* (Stoe & Cie, 2004); cell refinement: *CELL* in *IPDS-I* (Stoe & Cie, 2004); data reduction: *INTEGRATE* in *IPDS-I* (Stoe & Cie, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

2,3,5,6-Tetrakis(bromomethyl)pyrazine

Crystal data

$C_8H_8Br_4N_2$

$M_r = 451.80$

Tetragonal, $P4_12_12$

Hall symbol: P 4abw 2nw

$a = 9.6858$ (4) Å

$c = 26.5116$ (17) Å

$V = 2487.2$ (3) Å³

$Z = 8$

$F(000) = 1680$

$D_x = 2.413$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5000 reflections

$\theta = 2.2$ – 26.0°

$\mu = 12.91$ mm⁻¹

$T = 293$ K

Rod, colourless

$0.50 \times 0.40 \times 0.30$ mm

Data collection

Stoe IPDS 1

diffractometer

Radiation source: fine-focus sealed tube

Plane graphite monochromator

ϕ rotation scans

Absorption correction: multi-scan

(*MULscanABS* in *PLATON*; Spek, 2009)

$T_{\min} = 0.430$, $T_{\max} = 1.000$

19463 measured reflections

2417 independent reflections

1276 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.113$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -32 \rightarrow 32$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.096$

$S = 0.84$

2417 reflections

127 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$

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

$(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.69 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$

Absolute structure: Flack x determined using
 419 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons &
 Flack, 2004)
 Absolute structure parameter: 0.04 (4)

Special details

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

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	1.2259 (2)	0.2336 (2)	0.31902 (9)	0.0928 (7)
Br2	0.97546 (18)	0.47643 (17)	0.18421 (6)	0.0654 (5)
N1	0.8843 (11)	0.1271 (10)	0.3022 (5)	0.043 (3)
C1	1.0492 (15)	0.3062 (16)	0.3026 (6)	0.058 (4)
H1A	1.0016	0.3313	0.3335	0.069*
H1B	1.0608	0.3893	0.2827	0.069*
C2	0.9639 (14)	0.2070 (12)	0.2742 (5)	0.045 (3)
C3	0.9590 (13)	0.2017 (12)	0.2214 (4)	0.038 (3)
C4	1.0501 (16)	0.2865 (14)	0.1876 (5)	0.053 (4)
H4A	1.0525	0.2463	0.1541	0.063*
H4B	1.1435	0.2883	0.2008	0.063*
Br3	0.02090 (19)	-0.23131 (16)	0.06101 (6)	0.0663 (5)
Br4	0.2379 (2)	0.4746 (2)	0.07000 (7)	0.0854 (6)
N2	0.1293 (10)	0.1274 (11)	0.0529 (5)	0.042 (4)
C5	0.3130 (15)	0.2938 (15)	0.0568 (6)	0.060 (4)
H5A	0.3995	0.3030	0.0387	0.072*
H5B	0.3317	0.2476	0.0885	0.072*
C6	0.2145 (13)	0.2082 (13)	0.0262 (4)	0.041 (3)
C7	0.0442 (13)	0.0470 (13)	0.0261 (4)	0.039 (3)
C8	-0.0509 (16)	-0.0420 (17)	0.0578 (5)	0.056 (4)
H8A	-0.1426	-0.0425	0.0432	0.068*
H8B	-0.0575	-0.0041	0.0916	0.068*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0587 (12)	0.0884 (15)	0.1313 (15)	0.0040 (9)	-0.0371 (11)	-0.0122 (14)
Br2	0.0729 (11)	0.0512 (9)	0.0719 (10)	0.0017 (7)	0.0043 (10)	0.0119 (9)
N1	0.046 (9)	0.046 (9)	0.037 (7)	0.002 (5)	-0.002 (5)	0.002 (5)
C1	0.056 (9)	0.059 (9)	0.058 (9)	-0.009 (8)	-0.009 (8)	-0.011 (8)
C2	0.051 (8)	0.035 (7)	0.050 (7)	0.004 (6)	-0.003 (7)	-0.008 (6)
C3	0.034 (7)	0.037 (7)	0.043 (7)	0.003 (6)	0.001 (6)	-0.003 (6)
C4	0.053 (9)	0.047 (8)	0.059 (8)	0.004 (6)	0.007 (8)	0.002 (7)
Br3	0.0813 (12)	0.0468 (9)	0.0710 (9)	-0.0060 (8)	-0.0011 (10)	0.0101 (8)
Br4	0.0862 (13)	0.0616 (11)	0.1086 (15)	-0.0065 (9)	0.0033 (12)	-0.0330 (11)

N2	0.046 (9)	0.050 (9)	0.030 (6)	-0.006 (5)	-0.007 (5)	0.003 (5)
C5	0.053 (9)	0.073 (10)	0.054 (9)	-0.009 (8)	-0.015 (8)	-0.006 (8)
C6	0.047 (8)	0.043 (7)	0.033 (6)	0.007 (6)	-0.002 (6)	-0.002 (6)
C7	0.036 (7)	0.040 (7)	0.042 (6)	-0.003 (6)	0.000 (6)	0.005 (6)
C8	0.060 (9)	0.062 (9)	0.047 (7)	0.001 (8)	0.000 (8)	0.007 (8)

Geometric parameters (Å, °)

Br1—C1	1.901 (15)	Br3—C8	1.963 (17)
Br2—C4	1.978 (14)	Br4—C5	1.928 (15)
N1—C2	1.319 (17)	N2—C7	1.337 (15)
N1—C3 ⁱ	1.334 (15)	N2—C6	1.339 (16)
C1—C2	1.474 (18)	C5—C6	1.502 (17)
C1—H1A	0.9700	C5—H5A	0.9700
C1—H1B	0.9700	C5—H5B	0.9700
C2—C3	1.402 (15)	C6—C6 ⁱⁱ	1.39 (2)
C3—N1 ⁱ	1.334 (15)	C7—C7 ⁱⁱ	1.39 (2)
C3—C4	1.504 (17)	C7—C8	1.516 (17)
C4—H4A	0.9700	C8—H8A	0.9700
C4—H4B	0.9700	C8—H8B	0.9700
C2—N1—C3 ⁱ	117.9 (13)	C7—N2—C6	116.1 (12)
C2—C1—Br1	112.4 (10)	C6—C5—Br4	111.1 (9)
C2—C1—H1A	109.1	C6—C5—H5A	109.4
Br1—C1—H1A	109.1	Br4—C5—H5A	109.4
C2—C1—H1B	109.1	C6—C5—H5B	109.4
Br1—C1—H1B	109.1	Br4—C5—H5B	109.4
H1A—C1—H1B	107.9	H5A—C5—H5B	108.0
N1—C2—C3	121.3 (11)	N2—C6—C6 ⁱⁱ	121.7 (7)
N1—C2—C1	115.0 (12)	N2—C6—C5	115.4 (11)
C3—C2—C1	123.6 (12)	C6 ⁱⁱ —C6—C5	122.9 (8)
N1 ⁱ —C3—C2	120.8 (11)	N2—C7—C7 ⁱⁱ	121.9 (7)
N1 ⁱ —C3—C4	115.3 (12)	N2—C7—C8	114.3 (11)
C2—C3—C4	123.8 (11)	C7 ⁱⁱ —C7—C8	123.7 (7)
C3—C4—Br2	108.7 (9)	C7—C8—Br3	109.9 (10)
C3—C4—H4A	109.9	C7—C8—H8A	109.7
Br2—C4—H4A	109.9	Br3—C8—H8A	109.7
C3—C4—H4B	109.9	C7—C8—H8B	109.7
Br2—C4—H4B	109.9	Br3—C8—H8B	109.7
H4A—C4—H4B	108.3	H8A—C8—H8B	108.2
C3 ⁱ —N1—C2—C3	-0.2 (16)	C2—C3—C4—Br2	-78.6 (15)
C3 ⁱ —N1—C2—C1	175.9 (12)	C7—N2—C6—C6 ⁱⁱ	4 (2)
Br1—C1—C2—N1	91.3 (13)	C7—N2—C6—C5	-177.8 (12)
Br1—C1—C2—C3	-92.6 (15)	Br4—C5—C6—N2	-93.3 (12)
N1—C2—C3—N1 ⁱ	0.3 (19)	Br4—C5—C6—C6 ⁱⁱ	84.8 (17)
C1—C2—C3—N1 ⁱ	-175.5 (12)	C6—N2—C7—C7 ⁱⁱ	2 (2)
N1—C2—C3—C4	-177.9 (12)	C6—N2—C7—C8	-179.7 (12)

C1—C2—C3—C4	6 (2)	N2—C7—C8—Br3	-101.0 (12)
N1 ⁱ —C3—C4—Br2	103.1 (11)	C7 ⁱⁱ —C7—C8—Br3	77.4 (18)

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C1—H1A...Br2 ⁱⁱⁱ	0.97	3.02	3.863 (14)	146
C1—H1B...Br2	0.97	2.86	3.617 (16)	135
C5—H5A...Br4 ⁱⁱ	0.97	3.04	3.748 (16)	131
C5—H5B...Br3 ^{iv}	0.97	3.03	3.864 (14)	145
C8—H8A...Br3 ⁱⁱ	0.97	2.96	3.654 (15)	130

Symmetry codes: (ii) $y, x, -z$; (iii) $-y+3/2, x-1/2, z+1/4$; (iv) $-x+1/2, y+1/2, -z+1/4$.