organic compounds

2-(5,7-Dibromoquinolin-8-yloxy)-N,N-diphenylacetamide

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In the title compound, $C_{23}H_{16}Br_2N_2O_2$, intramolecular C—H···Br and C—H···N hydrogen bonds from the quinoline fragment form two five-membered rings. The quinoline ring system makes dihedral angles of 81.6 (2) and 31.2 (2)° with the phenyl rings of the diphenylacetamide fragment. In the crystal structure, molecules are linked into chains along the b axis by intermolecular C—H···O hydrogen bonds.

Related literature

For background to the applications of 8-hydroxyquinoline and its derivatives, see: Bratzel *et al.* (1972); Patel & Patel (1999). For structures of unsubstituted 8-hydroxyquinolinate amide compounds, see: Li *et al.* (2005); Wen *et al.* (2005). For reference structural data, see: Allen *et al.* (1987).
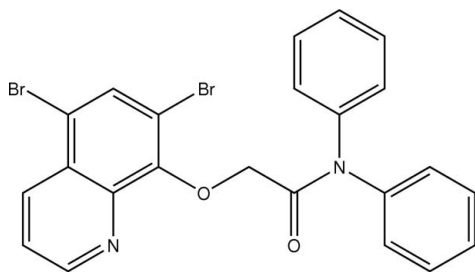
Experimental

Crystal data

$C_{23}H_{16}Br_2N_2O_2$	$V = 2036.7$ (4) Å³
$M_r = 512.18$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 10.1223$ (12) Å	$\mu = 4.00$ mm⁻¹
$b = 9.6013$ (11) Å	$T = 293$ (2) K
$c = 21.003$ (3) Å	$0.17 \times 0.13 \times 0.10$ mm
$\beta = 93.826$ (2)°	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	10474 measured reflections
	3731 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2346 reflections with $I > 2\sigma(I)$
$T_{min} = 0.549$, $T_{max} = 0.690$	$R_{int} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$	262 parameters
$wR(F^2) = 0.110$	H-atom parameters constrained
$S = 0.96$	$\Delta\rho_{max} = 0.92$ e Å⁻³
3731 reflections	$\Delta\rho_{min} = -0.57$ e Å⁻³

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···Br2	0.93	2.80	3.216 (6)	108
C10—H10A···N1	0.97	2.29	2.809 (7)	113
C16—H16A···O2ⁱ	0.93	2.58	3.269 (7)	132
C19—H19A···O2ⁱⁱ	0.93	2.38	3.303 (6)	171

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bratzel, M. P., Aaron, J. J., Winefordner, J. D., Schulman, S. G. & Gershon, H. (1972). *Anal. Chem.* **44**, 1240–1245.

Li, X.-M., Wen, Y.-H., Li, M.-J. & Zhang, S.-S. (2005). *Acta Cryst.* E**61**, o2389–o2390.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

Patel, A. K. & Patel, V. M. (1999). *Synth. React. Inorg. Met.-Org. Chem.* **29**, 193–197.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Wen, Y.-H., Zhang, S.-S., Li, M.-J. & Li, X.-M. (2005). *Acta Cryst.* E**61**, o1807–o1809.

supplementary materials

2-(5,7-Dibromoquinolin-8-yloxy)-*N*,*N*-diphenylacetamide

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Comment

8-Hydroxyquinoline and its derivatives have found extensive applications as analytical reagents, *e.g.* in absorption spectro-photometry, fluorimetry, solvent extraction and partition chromatography, due to their ability to form stable complexes with many metallic ions (Bratzel *et al.*, 1972). Some 8-hydroxyquinoline derivatives and their complexes with transition metals demonstrate antibacterial activity (Patel & Patel, 1999). Recently, structures of unsubstituted 8-hydroxyquinolinate amide-type compounds, namely, *N*-phenyl-2-(quinolin-8-yloxy)acetamide, (II) (Li *et al.*, 2005) and *N*,*N*-diphenyl-2-(quinolin-8-yloxy)acetamide, (III) (Wen *et al.*, 2005) have been reported. In a continuation of our search for suitable reagents to use in the extraction of metal ions, fluorescent materials and analytical reagents, we prepared the title compound, (I) (Fig. 1), a new amide-based 5,7-dibromo-8-hydroxyquinoline derivative, and we report its crystal structure here.

In the title compound, the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The quinoline fragment is essentially planar, with a dihedral angle of 2.0 (3)° between the benzene (C1–C4/C8/C9) ring and pyridine (N1/C4–C8) ring. The quinoline mean plane makes dihedral angles of 81.6 (2)° and 31.2 (2)°, with C12–C17 and C18–C23 benzene rings, respectively, while the dihedral angle between the latter two aromatic rings is 82.4 (3)°. Intramolecular C5—H5A···Br2 and C10—H10A···N1 hydrogen bonds (Fig.1 and Table 1), form two five-numbered rings and affect the conformation of the molecule.

In the crystal structure, molecules are linked into chains along the *b* axis (Fig. 2) by intermolecular C16—H16A···O2 and C19—H19A···O2 hydrogen bonds(Fig. 2 and Table 1).

Experimental

2-Chloro-*N*,*N*-diphenylacetamide was prepared by the reaction of diphenylamine and chloroacetyl chloride in the presence of triethylamine, according to the literature method of Wen *et al.* (2005). To a solution of 5,7-dibromo-8-hydroxyquinoline (3.02 g, 10 mmol) in acetone (60 ml) were added 2-chloro-*N*,*N*-diphenylacetamide (2.45 g,10 mmol), K$_2$CO$_3$ (1.52 g, 11 mmol) and KI (0.5 g), and the resulting mixture was stirred at 333 K for 5 h. After cooling to room temperature, the mixture was washed three times with water and filtered. Colourless single crystals of (I) suitable for an X-ray diffraction study were obtained by slow evaporation of an ethanol-DMF (1:1 *v*/*v*) solution over a period of 15 d.

Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C).
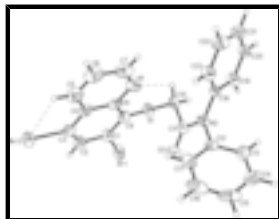
Figures

Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme. Intramolecular hydrogen bonds are drawn as dashed lines.
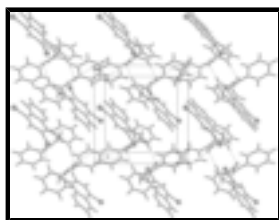

Fig. 2. A packing diagram of (I), viewed down the *c* axis. Hydrogen bonds are indicated by dashed lines.

2-(5,7-Dibromoquinolin-8-yloxy)-*N*,*N*-diphenylacetamide

Crystal data

$C_{23}H_{16}Br_2N_2O_2$	$F_{000} = 1016$
$M_r = 512.18$	$D_x = 1.670$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1172 reflections
$a = 10.1223$ (12) Å	$\theta = 2.9$–20.3º
$b = 9.6013$ (11) Å	$\mu = 4.00$ mm^{-1}
$c = 21.003$ (3) Å	$T = 293$ (2) K
$\beta = 93.826$ (2)º	Block, colourless
$V = 2036.7$ (4) Å^3	$0.17 \times 0.13 \times 0.10$ mm
$Z = 4$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3731 independent reflections
Radiation source: fine-focus sealed tube	2346 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.066$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 25.4$º
$T = 293(2)$ K	$\theta_{min} = 1.9$º
ω scans	$h = -12 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -7 \rightarrow 11$
$T_{min} = 0.549$, $T_{max} = 0.690$	$l = -25 \rightarrow 25$
10474 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{max} < 0.001$
3731 reflections	$\Delta\rho_{max} = 0.92$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.57$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Br1	0.32777 (6)	0.08638 (7)	0.20333 (3)	0.0431 (2)
Br2	−0.07694 (6)	0.48192 (6)	0.17923 (3)	0.0484 (2)
O1	0.2377 (3)	0.0119 (4)	0.06982 (16)	0.0322 (9)
N2	0.3683 (4)	0.1452 (4)	−0.07504 (19)	0.0279 (10)
C11	0.3618 (5)	0.1175 (6)	−0.0113 (2)	0.0292 (13)
C9	0.1699 (5)	0.1282 (6)	0.0876 (2)	0.0297 (13)
C19	0.3447 (5)	−0.0735 (6)	−0.1338 (2)	0.0352 (14)
H19A	0.4155	−0.1102	−0.1087	0.042*
C10	0.2784 (5)	−0.0065 (5)	0.0065 (2)	0.0308 (13)
H10A	0.2012	−0.0144	−0.0232	0.037*
H10B	0.3297	−0.0915	0.0042	0.037*
O2	0.4198 (4)	0.1870 (4)	0.03023 (17)	0.0381 (10)
C2	0.1211 (5)	0.2776 (5)	0.1766 (3)	0.0344 (14)
H2A	0.1388	0.3034	0.2190	0.041*
C1	0.1932 (5)	0.1694 (5)	0.1497 (2)	0.0295 (13)
C18	0.3034 (5)	0.0620 (6)	−0.1244 (2)	0.0274 (13)
C12	0.4366 (5)	0.2706 (5)	−0.0935 (2)	0.0267 (12)
C8	0.0732 (5)	0.2001 (6)	0.0481 (3)	0.0296 (13)

C4	−0.0027 (5)	0.3077 (6)	0.0750 (3)	0.0339 (13)
N1	0.0543 (5)	0.1642 (5)	−0.0144 (2)	0.0392 (12)
C3	0.0256 (5)	0.3436 (5)	0.1397 (3)	0.0350 (14)
C23	0.1990 (5)	0.1175 (6)	−0.1627 (3)	0.0372 (14)
H23A	0.1719	0.2088	−0.1567	0.045*
C20	0.2799 (6)	−0.1541 (6)	−0.1809 (3)	0.0414 (15)
H20A	0.3070	−0.2454	−0.1873	0.050*
C13	0.5378 (5)	0.2598 (6)	−0.1340 (3)	0.0381 (15)
H13A	0.5625	0.1734	−0.1493	0.046*
C16	0.4666 (7)	0.5170 (6)	−0.0880 (3)	0.0561 (19)
H16A	0.4421	0.6035	−0.0727	0.067*
C5	−0.1016 (5)	0.3726 (6)	0.0342 (3)	0.0451 (16)
H5A	−0.1544	0.4420	0.0501	0.054*
C7	−0.0373 (6)	0.2291 (7)	−0.0504 (3)	0.0487 (17)
H7A	−0.0486	0.2046	−0.0932	0.058*
C17	0.4011 (6)	0.3991 (6)	−0.0702 (3)	0.0418 (15)
H17A	0.3333	0.4058	−0.0426	0.050*
C6	−0.1195 (6)	0.3344 (7)	−0.0274 (3)	0.0497 (17)
H6A	−0.1846	0.3764	−0.0543	0.060*
C14	0.6021 (6)	0.3799 (8)	−0.1516 (3)	0.0540 (19)
H14A	0.6695	0.3743	−0.1795	0.065*
C15	0.5668 (7)	0.5078 (7)	−0.1280 (3)	0.0539 (19)
H15A	0.6115	0.5877	−0.1393	0.065*
C21	0.1755 (6)	−0.0993 (7)	−0.2184 (3)	0.0440 (16)
H21A	0.1318	−0.1542	−0.2496	0.053*
C22	0.1357 (6)	0.0358 (7)	−0.2099 (3)	0.0438 (16)
H22A	0.0661	0.0725	−0.2358	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0501 (4)	0.0464 (4)	0.0326 (3)	0.0204 (3)	0.0024 (3)	0.0026 (3)
Br2	0.0444 (4)	0.0339 (4)	0.0667 (5)	0.0125 (3)	0.0013 (3)	−0.0111 (3)
O1	0.044 (2)	0.022 (2)	0.031 (2)	0.0046 (18)	0.0090 (18)	0.0023 (17)
N2	0.038 (3)	0.020 (2)	0.025 (2)	−0.003 (2)	0.000 (2)	0.000 (2)
C11	0.034 (3)	0.027 (3)	0.026 (3)	0.002 (3)	0.001 (3)	0.002 (3)
C9	0.032 (3)	0.025 (3)	0.033 (3)	0.000 (3)	0.005 (3)	0.003 (3)
C19	0.043 (3)	0.026 (3)	0.037 (3)	0.003 (3)	0.005 (3)	0.002 (3)
C10	0.042 (3)	0.024 (3)	0.027 (3)	−0.002 (3)	0.010 (3)	0.000 (2)
O2	0.051 (2)	0.032 (2)	0.031 (2)	−0.009 (2)	−0.0028 (19)	−0.0022 (19)
C2	0.039 (3)	0.025 (3)	0.041 (3)	0.000 (3)	0.008 (3)	0.002 (3)
C1	0.036 (3)	0.022 (3)	0.031 (3)	0.003 (3)	0.003 (2)	0.008 (2)
C18	0.033 (3)	0.027 (3)	0.022 (3)	−0.006 (3)	0.003 (2)	−0.002 (2)
C12	0.028 (3)	0.021 (3)	0.030 (3)	−0.006 (3)	−0.004 (2)	0.003 (2)
C8	0.025 (3)	0.026 (3)	0.037 (3)	−0.009 (3)	−0.001 (2)	0.007 (3)
C4	0.028 (3)	0.028 (3)	0.046 (4)	−0.002 (3)	0.000 (3)	0.002 (3)
N1	0.046 (3)	0.034 (3)	0.036 (3)	−0.002 (3)	−0.006 (2)	0.002 (2)
C3	0.030 (3)	0.020 (3)	0.055 (4)	−0.001 (3)	0.008 (3)	−0.002 (3)

C23	0.044 (3)	0.027 (3)	0.041 (3)	0.001 (3)	0.006 (3)	0.003 (3)
C20	0.053 (4)	0.028 (3)	0.044 (4)	−0.008 (3)	0.012 (3)	−0.014 (3)
C13	0.034 (3)	0.045 (4)	0.036 (3)	−0.001 (3)	0.005 (3)	−0.003 (3)
C16	0.086 (5)	0.018 (3)	0.062 (5)	−0.008 (4)	−0.013 (4)	0.003 (3)
C5	0.040 (4)	0.037 (4)	0.057 (4)	0.004 (3)	−0.008 (3)	0.006 (3)
C7	0.048 (4)	0.046 (4)	0.050 (4)	−0.015 (4)	−0.007 (3)	0.008 (3)
C17	0.047 (4)	0.028 (3)	0.051 (4)	0.006 (3)	0.005 (3)	−0.003 (3)
C6	0.044 (4)	0.047 (4)	0.055 (4)	0.001 (3)	−0.014 (3)	0.015 (4)
C14	0.048 (4)	0.072 (5)	0.043 (4)	−0.027 (4)	0.006 (3)	0.007 (4)
C15	0.072 (5)	0.042 (4)	0.045 (4)	−0.030 (4)	−0.023 (4)	0.018 (3)
C21	0.048 (4)	0.045 (4)	0.040 (4)	−0.017 (3)	0.005 (3)	−0.004 (3)
C22	0.039 (4)	0.049 (4)	0.041 (4)	−0.001 (3)	−0.012 (3)	0.015 (3)

Geometric parameters (Å, °)

Br1—C1	1.885 (5)	C4—C3	1.413 (7)
Br2—C3	1.909 (5)	C4—C5	1.419 (7)
O1—C9	1.376 (6)	N1—C7	1.314 (7)
O1—C10	1.429 (5)	C23—C22	1.387 (8)
N2—C11	1.370 (6)	C23—H23A	0.9300
N2—C18	1.433 (6)	C20—C21	1.379 (8)
N2—C12	1.453 (6)	C20—H20A	0.9300
C11—O2	1.218 (6)	C13—C14	1.386 (8)
C11—C10	1.521 (7)	C13—H13A	0.9300
C9—C1	1.369 (7)	C16—C15	1.362 (9)
C9—C8	1.420 (7)	C16—C17	1.376 (8)
C19—C18	1.385 (7)	C16—H16A	0.9300
C19—C20	1.386 (7)	C5—C6	1.345 (8)
C19—H19A	0.9300	C5—H5A	0.9300
C10—H10A	0.9700	C7—C6	1.415 (8)
C10—H10B	0.9700	C7—H7A	0.9300
C2—C3	1.355 (7)	C17—H17A	0.9300
C2—C1	1.410 (7)	C6—H6A	0.9300
C2—H2A	0.9300	C14—C15	1.380 (9)
C18—C23	1.391 (7)	C14—H14A	0.9300
C12—C13	1.379 (7)	C15—H15A	0.9300
C12—C17	1.383 (7)	C21—C22	1.373 (8)
C8—N1	1.358 (6)	C21—H21A	0.9300
C8—C4	1.426 (7)	C22—H22A	0.9300
C9—O1—C10	122.2 (4)	C2—C3—Br2	117.7 (4)
C11—N2—C18	123.3 (4)	C4—C3—Br2	120.5 (4)
C11—N2—C12	118.4 (4)	C22—C23—C18	119.6 (5)
C18—N2—C12	118.2 (4)	C22—C23—H23A	120.2
O2—C11—N2	122.8 (5)	C18—C23—H23A	120.2
O2—C11—C10	120.1 (5)	C21—C20—C19	120.1 (6)
N2—C11—C10	117.1 (5)	C21—C20—H20A	119.9
C1—C9—O1	115.8 (5)	C19—C20—H20A	119.9
C1—C9—C8	119.0 (5)	C12—C13—C14	119.0 (6)
O1—C9—C8	125.0 (5)	C12—C13—H13A	120.5

C18—C19—C20	119.6 (5)	C14—C13—H13A	120.5
C18—C19—H19A	120.2	C15—C16—C17	120.4 (6)
C20—C19—H19A	120.2	C15—C16—H16A	119.8
O1—C10—C11	109.4 (4)	C17—C16—H16A	119.8
O1—C10—H10A	109.8	C6—C5—C4	120.4 (6)
C11—C10—H10A	109.8	C6—C5—H5A	119.8
O1—C10—H10B	109.8	C4—C5—H5A	119.8
C11—C10—H10B	109.8	N1—C7—C6	123.5 (6)
H10A—C10—H10B	108.2	N1—C7—H7A	118.3
C3—C2—C1	119.0 (5)	C6—C7—H7A	118.3
C3—C2—H2A	120.5	C16—C17—C12	119.8 (6)
C1—C2—H2A	120.5	C16—C17—H17A	120.1
C9—C1—C2	122.3 (5)	C12—C17—H17A	120.1
C9—C1—Br1	121.3 (4)	C5—C6—C7	118.5 (6)
C2—C1—Br1	116.4 (4)	C5—C6—H6A	120.7
C19—C18—C23	120.1 (5)	C7—C6—H6A	120.7
C19—C18—N2	120.0 (5)	C15—C14—C13	120.4 (6)
C23—C18—N2	119.9 (5)	C15—C14—H14A	119.8
C13—C12—C17	120.4 (5)	C13—C14—H14A	119.8
C13—C12—N2	119.3 (5)	C16—C15—C14	120.0 (6)
C17—C12—N2	120.3 (5)	C16—C15—H15A	120.0
N1—C8—C9	119.2 (5)	C14—C15—H15A	120.0
N1—C8—C4	121.5 (5)	C22—C21—C20	120.5 (6)
C9—C8—C4	119.3 (5)	C22—C21—H21A	119.8
C3—C4—C5	124.3 (5)	C20—C21—H21A	119.8
C3—C4—C8	118.6 (5)	C21—C22—C23	120.1 (5)
C5—C4—C8	117.1 (5)	C21—C22—H22A	120.0
C7—N1—C8	119.0 (5)	C23—C22—H22A	120.0
C2—C3—C4	121.8 (5)		
C18—N2—C11—O2	178.2 (5)	C9—C8—C4—C3	3.0 (7)
C12—N2—C11—O2	−6.1 (7)	N1—C8—C4—C5	1.9 (8)
C18—N2—C11—C10	−1.4 (7)	C9—C8—C4—C5	−177.6 (5)
C12—N2—C11—C10	174.2 (4)	C9—C8—N1—C7	178.6 (5)
C10—O1—C9—C1	−148.4 (5)	C4—C8—N1—C7	−0.9 (8)
C10—O1—C9—C8	36.2 (7)	C1—C2—C3—C4	−0.6 (8)
C9—O1—C10—C11	55.7 (6)	C1—C2—C3—Br2	176.3 (4)
O2—C11—C10—O1	24.0 (7)	C5—C4—C3—C2	179.8 (5)
N2—C11—C10—O1	−156.3 (4)	C8—C4—C3—C2	−0.8 (8)
O1—C9—C1—C2	−173.3 (4)	C5—C4—C3—Br2	2.9 (7)
C8—C9—C1—C2	2.4 (8)	C8—C4—C3—Br2	−177.7 (4)
O1—C9—C1—Br1	8.4 (7)	C19—C18—C23—C22	0.8 (8)
C8—C9—C1—Br1	−175.9 (4)	N2—C18—C23—C22	−179.2 (5)
C3—C2—C1—C9	−0.2 (8)	C18—C19—C20—C21	0.4 (8)
C3—C2—C1—Br1	178.2 (4)	C17—C12—C13—C14	−0.8 (8)
C20—C19—C18—C23	−1.1 (8)	N2—C12—C13—C14	179.7 (5)
C20—C19—C18—N2	178.9 (5)	C3—C4—C5—C6	178.2 (5)
C11—N2—C18—C19	−67.1 (7)	C8—C4—C5—C6	−1.2 (8)
C12—N2—C18—C19	117.3 (5)	C8—N1—C7—C6	−0.8 (8)
C11—N2—C18—C23	112.9 (6)	C15—C16—C17—C12	−0.6 (9)

C12—N2—C18—C23	−62.7 (6)	C13—C12—C17—C16	0.5 (8)
C11—N2—C12—C13	125.1 (5)	N2—C12—C17—C16	−180.0 (5)
C18—N2—C12—C13	−59.0 (6)	C4—C5—C6—C7	−0.4 (9)
C11—N2—C12—C17	−54.4 (7)	N1—C7—C6—C5	1.5 (9)
C18—N2—C12—C17	121.5 (5)	C12—C13—C14—C15	1.1 (9)
C1—C9—C8—N1	176.8 (5)	C17—C16—C15—C14	1.0 (9)
O1—C9—C8—N1	−8.0 (8)	C13—C14—C15—C16	−1.2 (9)
C1—C9—C8—C4	−3.7 (7)	C19—C20—C21—C22	0.7 (8)
O1—C9—C8—C4	171.5 (5)	C20—C21—C22—C23	−1.0 (9)
N1—C8—C4—C3	−177.5 (5)	C18—C23—C22—C21	0.3 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···Br2	0.93	2.80	3.216 (6)	108
C10—H10A···N1	0.97	2.29	2.809 (7)	113
C16—H16A···O2[i]	0.93	2.58	3.269 (7)	132
C19—H19A···O2[ii]	0.93	2.38	3.303 (6)	171

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

Fig. 1

Fig. 2