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N,*N*-Dicyclohexyl-2-(5,7-dibromoquinolin-8-yloxy)acetamide

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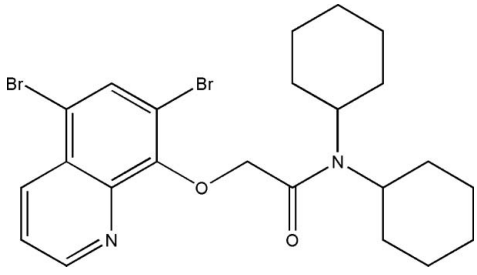
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.044; wR factor = 0.107; data-to-parameter ratio = 17.6.

In the title compound, $C_{23}H_{28}Br_2N_2O_2$, all bond lengths and angles are within normal ranges. The two cyclohexyl groups adopt the normal chair conformation. The sum of the angles around the amide N and C atoms are both 360°, implying a planar configuration. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds.

Related literature

For related literature, see: Allen *et al.* (1987); Bratzel *et al.* (1972); Li *et al.* (2005); Patel & Patel (1999); Wen *et al.* (2005).



Experimental

Crystal data

$C_{23}H_{28}Br_2N_2O_2$
M_r = 524.29
Triclinic, $P\overline{1}$
a = 9.9579 (19) Å
b = 10.811 (2) Å
c = 11.294 (2) Å
α = 72.064 (3)°
β = 86.885 (4)°
γ = 81.366 (3)°
V = 1143.6 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.57 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.482, T_{max} = 0.566
(expected range = 0.448–0.526)
6611 measured reflections
4612 independent reflections
3053 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
S = 1.00
4612 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O2^{i}	0.93	2.49	3.420 (5)	173
C10—H10B···O2^{ii}	0.97	2.47	3.409 (4)	162

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

Data collection: *SMART* (Bruker 2001); cell refinement: *SAINT* (Bruker 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2315).

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supplementary materials

Acta Cryst. (2007). E**63**, o4458 [**doi:10.1107/S1600536807052117**]

N,*N*-Dicyclohexyl-2-(5,7-dibromoquinolin-8-yloxy)acetamide

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Comment

8-Hydroxyquinoline and its derivatives have found extensive application as analytical reagents, *e.g.* in absorption spectrophotometry, fluorimetry, solvent extraction and partition chromatography (Bratzel *et al.*, 1972). Some 8-hydroxyquinoline derivatives and their complexes with transition metals demonstrate antibacterial activity (Patel & Patel,1999). Recently, the structures of the 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. Here, we have synthesized and carried out the structure determination of the title compound, (I) (Fig. 1), a new amide-based 5,7-dibrom-8-hydroxyquinoline derivative.

All bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987) and comparable with those in the related compounds (II) and (III). The geometry of two cyclohexyl groups is the normal chair conformation·The sum of the angles around atoms N2 and C11 are 359.99° and 360.0°, respectively, implying the planar configuration. The crystal packing is stabilized by intermolecular C6—H6···O2 and C10—H10···O2 hydrogen bonds (Fig. 2).

Experimental

2-Chloro-*N*,*N*-dicyclohexylacetamide was prepared by the reaction of dicyclohexylamine and chloroacetyl chloride in the presence of triethylamine, according to the literature method of Wen *et al.* (2005). To a solution of 5,7-dibrom-8-hydroxyquinoline (3.02 g, 10 mmol) in acetone (60 ml) were added 2-chloro-*N*,*N*-dicyclohexylacetamide (2.58 g,10 mmol), K_2CO_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 X-ray diffraction study were obtained by slow evaporation of an ethanol solution over a period of 10 d.

Refinement

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H = 0.95–0.99 Å and with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

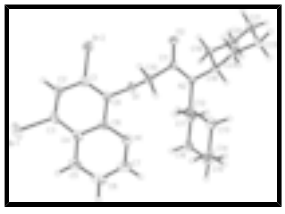

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids.

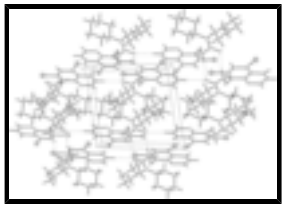

Fig. 2. The packing diagram of (I), viewed down the *c* axis, showing the intermolecular hydrogen bonds (dashed lines).

N,*N*-Dicyclohexyl-2-(5,7-dibromoquinolin-8-yloxy)acetamide

Crystal data

$C_{23}H_{28}Br_2N_2O_2$	$Z = 2$
$M_r = 524.29$	$F_{000} = 532$
Triclinic, $P\overline{1}$	$D_x = 1.523$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.9579$ (19) Å	Cell parameters from 1863 reflections
$b = 10.811$ (2) Å	$\theta = 2.3$–24.0º
$c = 11.294$ (2) Å	$\mu = 3.57$ mm^{-1}
$\alpha = 72.064$ (3)º	$T = 294$ (2) K
$\beta = 86.885$ (4)º	Column, colourless
$\gamma = 81.366$ (3)º	0.24 × 0.20 × 0.18 mm
$V = 1143.6$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4612 independent reflections
Radiation source: fine-focus sealed tube	3053 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 294$(2) K	$\theta_{max} = 26.4$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.482$, $T_{max} = 0.566$	$k = -13 \rightarrow 13$
6611 measured reflections	$l = -9 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.3567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
4612 reflections	$\Delta\rho_{max} = 0.69$ e Å^{-3}

262 parameters	$\Delta\rho_{min} = -0.68$ 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	−0.03290 (7)	0.89977 (6)	0.91083 (5)	0.0925 (2)
Br2	0.10028 (4)	0.42835 (4)	0.79360 (4)	0.04862 (15)
O1	0.2236 (2)	0.6051 (2)	0.5599 (2)	0.0358 (6)
O2	0.1713 (2)	0.4081 (2)	0.4135 (2)	0.0410 (6)
N1	0.2223 (3)	0.8703 (3)	0.4919 (3)	0.0474 (8)
N2	0.3227 (3)	0.5463 (3)	0.3177 (2)	0.0295 (6)
C1	0.1047 (4)	0.6110 (4)	0.7471 (3)	0.0365 (8)
C2	0.0481 (4)	0.6795 (4)	0.8296 (3)	0.0473 (10)
H2	0.0107	0.6350	0.9051	0.057*
C3	0.0485 (4)	0.8106 (4)	0.7980 (4)	0.0473 (10)
C4	0.1048 (4)	0.8829 (4)	0.6840 (4)	0.0428 (9)
C5	0.1102 (4)	1.0194 (4)	0.6452 (4)	0.0556 (11)
H5	0.0738	1.0697	0.6959	0.067*
C6	0.1677 (5)	1.0771 (4)	0.5353 (5)	0.0618 (13)
H6	0.1710	1.1671	0.5090	0.074*
C7	0.2225 (5)	0.9988 (4)	0.4616 (4)	0.0591 (12)
H7	0.2618	1.0399	0.3858	0.071*
C8	0.1632 (3)	0.8124 (3)	0.6027 (3)	0.0355 (8)
C9	0.1617 (3)	0.6746 (3)	0.6354 (3)	0.0333 (8)
C10	0.1437 (3)	0.6126 (3)	0.4542 (3)	0.0331 (8)
H10A	0.1358	0.7003	0.3955	0.040*
H10B	0.0531	0.5925	0.4811	0.040*
C11	0.2157 (3)	0.5133 (3)	0.3934 (3)	0.0297 (8)
C12	0.3800 (3)	0.6695 (3)	0.2997 (3)	0.0296 (8)
H12A	0.3322	0.7124	0.3579	0.036*
C13	0.3550 (4)	0.7651 (3)	0.1691 (3)	0.0418 (9)
H13A	0.3973	0.7244	0.1083	0.050*
H13B	0.2581	0.7849	0.1534	0.050*
C14	0.4123 (4)	0.8913 (4)	0.1546 (4)	0.0498 (10)
H14A	0.3619	0.9373	0.2081	0.060*

H14B	0.4010	0.9474	0.0693	0.060*
C15	0.5617 (4)	0.8651 (4)	0.1877 (4)	0.0515 (11)
H15A	0.6136	0.8272	0.1290	0.062*
H15B	0.5937	0.9473	0.1817	0.062*
C16	0.5843 (4)	0.7722 (4)	0.3184 (4)	0.0460 (10)
H16A	0.5388	0.8132	0.3777	0.055*
H16B	0.6807	0.7539	0.3365	0.055*
C17	0.5297 (4)	0.6444 (3)	0.3319 (3)	0.0381 (9)
H17A	0.5804	0.6000	0.2773	0.046*
H17B	0.5422	0.5874	0.4169	0.046*
C18	0.3855 (3)	0.4595 (3)	0.2438 (3)	0.0308 (8)
H18	0.4571	0.5041	0.1929	0.037*
C19	0.4553 (4)	0.3268 (3)	0.3240 (3)	0.0372 (9)
H19A	0.3885	0.2784	0.3769	0.045*
H19B	0.5216	0.3402	0.3770	0.045*
C20	0.5256 (4)	0.2481 (4)	0.2411 (4)	0.0504 (10)
H20A	0.5990	0.2922	0.1952	0.060*
H20B	0.5647	0.1619	0.2928	0.060*
C21	0.4273 (4)	0.2328 (4)	0.1499 (4)	0.0515 (11)
H21A	0.4764	0.1870	0.0957	0.062*
H21B	0.3597	0.1800	0.1956	0.062*
C22	0.3571 (4)	0.3641 (4)	0.0722 (3)	0.0475 (10)
H22A	0.2909	0.3505	0.0193	0.057*
H22B	0.4235	0.4127	0.0190	0.057*
C23	0.2861 (4)	0.4444 (4)	0.1531 (3)	0.0433 (9)
H23A	0.2478	0.5304	0.1006	0.052*
H23B	0.2123	0.4011	0.1992	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1217 (5)	0.0965 (4)	0.0829 (4)	−0.0135 (4)	0.0330 (3)	−0.0680 (4)
Br2	0.0544 (3)	0.0414 (2)	0.0444 (2)	−0.00424 (18)	0.00150 (18)	−0.00636 (18)
O1	0.0381 (14)	0.0396 (14)	0.0294 (12)	0.0032 (11)	0.0026 (11)	−0.0149 (11)
O2	0.0440 (15)	0.0339 (14)	0.0500 (15)	−0.0169 (12)	0.0162 (12)	−0.0171 (12)
N1	0.052 (2)	0.043 (2)	0.047 (2)	−0.0115 (16)	0.0074 (16)	−0.0130 (16)
N2	0.0311 (16)	0.0291 (15)	0.0309 (15)	−0.0071 (12)	0.0090 (12)	−0.0130 (12)
C1	0.036 (2)	0.039 (2)	0.035 (2)	−0.0027 (17)	−0.0009 (16)	−0.0137 (17)
C2	0.053 (3)	0.060 (3)	0.035 (2)	−0.008 (2)	0.0054 (19)	−0.023 (2)
C3	0.048 (2)	0.060 (3)	0.046 (2)	−0.005 (2)	0.0061 (19)	−0.036 (2)
C4	0.042 (2)	0.041 (2)	0.052 (2)	−0.0027 (18)	−0.0025 (19)	−0.026 (2)
C5	0.062 (3)	0.049 (3)	0.068 (3)	−0.010 (2)	−0.003 (2)	−0.035 (2)
C6	0.070 (3)	0.033 (2)	0.086 (4)	−0.011 (2)	−0.008 (3)	−0.020 (2)
C7	0.071 (3)	0.042 (3)	0.064 (3)	−0.021 (2)	0.005 (2)	−0.012 (2)
C8	0.034 (2)	0.038 (2)	0.037 (2)	−0.0056 (16)	−0.0016 (16)	−0.0137 (17)
C9	0.0311 (19)	0.039 (2)	0.0314 (19)	−0.0004 (16)	0.0014 (15)	−0.0160 (16)
C10	0.0305 (19)	0.037 (2)	0.0338 (19)	−0.0063 (16)	0.0031 (15)	−0.0131 (16)
C11	0.0309 (19)	0.0314 (19)	0.0258 (17)	−0.0033 (16)	0.0026 (15)	−0.0080 (15)

C12	0.037 (2)	0.0240 (17)	0.0281 (17)	−0.0081 (15)	0.0092 (15)	−0.0073 (14)
C13	0.048 (2)	0.035 (2)	0.039 (2)	−0.0059 (18)	−0.0013 (18)	−0.0057 (17)
C14	0.066 (3)	0.031 (2)	0.044 (2)	−0.010 (2)	0.005 (2)	0.0021 (18)
C15	0.068 (3)	0.039 (2)	0.051 (2)	−0.026 (2)	0.017 (2)	−0.013 (2)
C16	0.054 (3)	0.043 (2)	0.045 (2)	−0.019 (2)	0.0032 (19)	−0.0134 (19)
C17	0.047 (2)	0.032 (2)	0.034 (2)	−0.0097 (17)	0.0016 (17)	−0.0065 (16)
C18	0.0334 (19)	0.0321 (19)	0.0295 (18)	−0.0074 (15)	0.0065 (15)	−0.0128 (15)
C19	0.042 (2)	0.037 (2)	0.035 (2)	−0.0034 (17)	0.0000 (17)	−0.0164 (17)
C20	0.057 (3)	0.044 (2)	0.051 (2)	0.006 (2)	0.000 (2)	−0.022 (2)
C21	0.076 (3)	0.040 (2)	0.046 (2)	−0.008 (2)	0.009 (2)	−0.024 (2)
C22	0.062 (3)	0.053 (3)	0.037 (2)	−0.015 (2)	0.0023 (19)	−0.0244 (19)
C23	0.049 (2)	0.046 (2)	0.036 (2)	0.0011 (19)	−0.0055 (18)	−0.0176 (18)

Geometric parameters (Å, °)

Br1—C3	1.902 (4)	C13—H13A	0.9700
Br2—C1	1.888 (4)	C13—H13B	0.9700
O1—C9	1.367 (4)	C14—C15	1.517 (6)
O1—C10	1.446 (4)	C14—H14A	0.9700
O2—C11	1.234 (4)	C14—H14B	0.9700
N1—C7	1.325 (5)	C15—C16	1.514 (5)
N1—C8	1.361 (4)	C15—H15A	0.9700
N2—C11	1.349 (4)	C15—H15B	0.9700
N2—C12	1.480 (4)	C16—C17	1.522 (5)
N2—C18	1.489 (4)	C16—H16A	0.9700
C1—C9	1.376 (5)	C16—H16B	0.9700
C1—C2	1.405 (5)	C17—H17A	0.9700
C2—C3	1.352 (5)	C17—H17B	0.9700
C2—H2	0.9300	C18—C23	1.523 (5)
C3—C4	1.419 (5)	C18—C19	1.526 (5)
C4—C5	1.413 (5)	C18—H18	0.9800
C4—C8	1.416 (5)	C19—C20	1.527 (5)
C5—C6	1.346 (6)	C19—H19A	0.9700
C5—H5	0.9300	C19—H19B	0.9700
C6—C7	1.398 (6)	C20—C21	1.520 (5)
C6—H6	0.9300	C20—H20A	0.9700
C7—H7	0.9300	C20—H20B	0.9700
C8—C9	1.422 (5)	C21—C22	1.509 (5)
C10—C11	1.519 (5)	C21—H21A	0.9700
C10—H10A	0.9700	C21—H21B	0.9700
C10—H10B	0.9700	C22—C23	1.524 (5)
C12—C17	1.518 (5)	C22—H22A	0.9700
C12—C13	1.526 (5)	C22—H22B	0.9700
C12—H12A	0.9800	C23—H23A	0.9700
C13—C14	1.517 (5)	C23—H23B	0.9700
C9—O1—C10	114.4 (3)	C15—C14—H14B	109.3
C7—N1—C8	116.7 (4)	H14A—C14—H14B	107.9
C11—N2—C12	123.1 (3)	C16—C15—C14	110.8 (3)
C11—N2—C18	120.0 (3)	C16—C15—H15A	109.5

C12—N2—C18	116.9 (2)	C14—C15—H15A	109.5
C9—C1—C2	121.3 (3)	C16—C15—H15B	109.5
C9—C1—Br2	120.6 (3)	C14—C15—H15B	109.5
C2—C1—Br2	118.1 (3)	H15A—C15—H15B	108.1
C3—C2—C1	119.4 (4)	C15—C16—C17	110.6 (3)
C3—C2—H2	120.3	C15—C16—H16A	109.5
C1—C2—H2	120.3	C17—C16—H16A	109.5
C2—C3—C4	122.4 (3)	C15—C16—H16B	109.5
C2—C3—Br1	117.9 (3)	C17—C16—H16B	109.5
C4—C3—Br1	119.6 (3)	H16A—C16—H16B	108.1
C5—C4—C8	116.7 (4)	C12—C17—C16	111.1 (3)
C5—C4—C3	125.7 (4)	C12—C17—H17A	109.4
C8—C4—C3	117.6 (3)	C16—C17—H17A	109.4
C6—C5—C4	120.4 (4)	C12—C17—H17B	109.4
C6—C5—H5	119.8	C16—C17—H17B	109.4
C4—C5—H5	119.8	H17A—C17—H17B	108.0
C5—C6—C7	118.5 (4)	N2—C18—C23	112.3 (3)
C5—C6—H6	120.8	N2—C18—C19	113.3 (3)
C7—C6—H6	120.8	C23—C18—C19	111.8 (3)
N1—C7—C6	124.7 (4)	N2—C18—H18	106.2
N1—C7—H7	117.7	C23—C18—H18	106.2
C6—C7—H7	117.7	C19—C18—H18	106.2
N1—C8—C4	123.0 (3)	C18—C19—C20	110.0 (3)
N1—C8—C9	117.0 (3)	C18—C19—H19A	109.7
C4—C8—C9	120.0 (3)	C20—C19—H19A	109.7
O1—C9—C1	120.4 (3)	C18—C19—H19B	109.7
O1—C9—C8	120.2 (3)	C20—C19—H19B	109.7
C1—C9—C8	119.3 (3)	H19A—C19—H19B	108.2
O1—C10—C11	107.5 (3)	C21—C20—C19	111.6 (3)
O1—C10—H10A	110.2	C21—C20—H20A	109.3
C11—C10—H10A	110.2	C19—C20—H20A	109.3
O1—C10—H10B	110.2	C21—C20—H20B	109.3
C11—C10—H10B	110.2	C19—C20—H20B	109.3
H10A—C10—H10B	108.5	H20A—C20—H20B	108.0
O2—C11—N2	123.5 (3)	C22—C21—C20	111.5 (3)
O2—C11—C10	118.3 (3)	C22—C21—H21A	109.3
N2—C11—C10	118.2 (3)	C20—C21—H21A	109.3
N2—C12—C17	112.2 (3)	C22—C21—H21B	109.3
N2—C12—C13	112.3 (3)	C20—C21—H21B	109.3
C17—C12—C13	111.1 (3)	H21A—C21—H21B	108.0
N2—C12—H12A	106.9	C21—C22—C23	111.6 (3)
C17—C12—H12A	106.9	C21—C22—H22A	109.3
C13—C12—H12A	106.9	C23—C22—H22A	109.3
C14—C13—C12	111.0 (3)	C21—C22—H22B	109.3
C14—C13—H13A	109.4	C23—C22—H22B	109.3
C12—C13—H13A	109.4	H22A—C22—H22B	108.0
C14—C13—H13B	109.4	C18—C23—C22	110.7 (3)
C12—C13—H13B	109.4	C18—C23—H23A	109.5
H13A—C13—H13B	108.0	C22—C23—H23A	109.5

C13—C14—C15	111.7 (3)	C18—C23—H23B	109.5
C13—C14—H14A	109.3	C22—C23—H23B	109.5
C15—C14—H14A	109.3	H23A—C23—H23B	108.1
C13—C14—H14B	109.3		
C9—C1—C2—C3	0.6 (6)	C12—N2—C11—O2	−176.4 (3)
Br2—C1—C2—C3	−179.3 (3)	C18—N2—C11—O2	5.9 (5)
C1—C2—C3—C4	−0.2 (6)	C12—N2—C11—C10	5.4 (5)
C1—C2—C3—Br1	178.6 (3)	C18—N2—C11—C10	−172.4 (3)
C2—C3—C4—C5	−179.3 (4)	O1—C10—C11—O2	101.8 (3)
Br1—C3—C4—C5	1.9 (5)	O1—C10—C11—N2	−79.8 (4)
C2—C3—C4—C8	−0.7 (6)	C11—N2—C12—C17	122.6 (3)
Br1—C3—C4—C8	−179.5 (3)	C18—N2—C12—C17	−59.6 (4)
C8—C4—C5—C6	0.5 (6)	C11—N2—C12—C13	−111.4 (3)
C3—C4—C5—C6	179.2 (4)	C18—N2—C12—C13	66.4 (4)
C4—C5—C6—C7	−0.5 (6)	N2—C12—C13—C14	178.8 (3)
C8—N1—C7—C6	0.6 (6)	C17—C12—C13—C14	−54.6 (4)
C5—C6—C7—N1	−0.1 (7)	C12—C13—C14—C15	54.8 (4)
C7—N1—C8—C4	−0.5 (5)	C13—C14—C15—C16	−56.1 (4)
C7—N1—C8—C9	179.5 (3)	C14—C15—C16—C17	56.8 (4)
C5—C4—C8—N1	0.0 (5)	N2—C12—C17—C16	−177.4 (3)
C3—C4—C8—N1	−178.8 (3)	C13—C12—C17—C16	56.0 (4)
C5—C4—C8—C9	179.9 (3)	C15—C16—C17—C12	−57.1 (4)
C3—C4—C8—C9	1.1 (5)	C11—N2—C18—C23	61.3 (4)
C10—O1—C9—C1	103.1 (3)	C12—N2—C18—C23	−116.6 (3)
C10—O1—C9—C8	−80.8 (4)	C11—N2—C18—C19	−66.6 (4)
C2—C1—C9—O1	176.0 (3)	C12—N2—C18—C19	115.5 (3)
Br2—C1—C9—O1	−4.1 (4)	N2—C18—C19—C20	−175.9 (3)
C2—C1—C9—C8	−0.1 (5)	C23—C18—C19—C20	55.9 (4)
Br2—C1—C9—C8	179.8 (3)	C18—C19—C20—C21	−55.4 (4)
N1—C8—C9—O1	3.0 (5)	C19—C20—C21—C22	55.6 (4)
C4—C8—C9—O1	−177.0 (3)	C20—C21—C22—C23	−55.1 (5)
N1—C8—C9—C1	179.2 (3)	N2—C18—C23—C22	175.4 (3)
C4—C8—C9—C1	−0.8 (5)	C19—C18—C23—C22	−55.9 (4)
C9—O1—C10—C11	−170.7 (3)	C21—C22—C23—C18	55.0 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O2^{i}	0.93	2.49	3.420 (5)	173
C10—H10B···O2^{ii}	0.97	2.47	3.409 (4)	162

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

Fig. 1

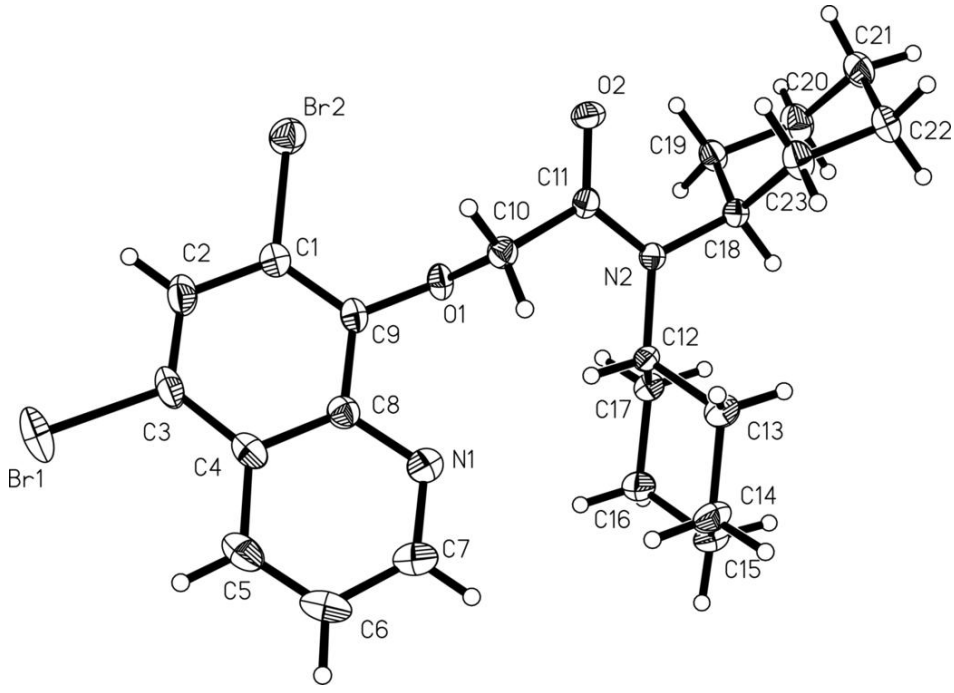
C21
C20
O2
Br2
C22
C19
C11
C23
C10
C18
C2
C1
N2
O1
C9
C12
C8
C17
C13
C3
N1
Br1
C4
C14
C16
C7
C15
C5
C6

Fig. 2