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

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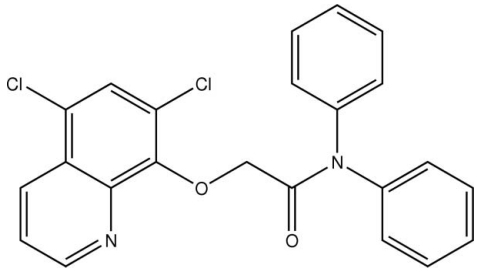
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.130; data-to-parameter ratio = 14.6.

In the title compound, $C_{23}H_{16}Cl_2N_2O_2$, intramolecular C—H···Cl and C—H···N hydrogen bonds from the quinoline fragment form five- and six-membered rings, respectively. The quinoline ring system makes dihedral angles of 30.42 (1) and 81.17 (1)° 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 related literature on unsubstituted 8-hydroxyquinolinate amide compounds, see: Li *et al.* (2005); Wen *et al.* (2005). For applications of 8-hydroxyquinoline derivatives, see: Bratzel *et al.* (1972); Patel & Patel (1999). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{23}H_{16}Cl_2N_2O_2$
M_r = 423.28
Monoclinic, $P2_1/n$
a = 9.8942 (13) Å
b = 9.6703 (13) Å
c = 21.152 (3) Å
β = 93.107 (2)°
V = 2020.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 293 (2) K
0.26 × 0.12 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.916, T_{max} = 0.970
10737 measured reflections
3827 independent reflections
3035 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.04
3827 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···Cl2	0.93	2.70	3.087 (3)	106
C10—H10A···N1	0.97	2.29	2.812 (3)	113
C13—H13A···O2^{i}	0.93	2.42	3.342 (3)	169
C20—H20A···O2^{ii}	0.93	2.56	3.293 (4)	136

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2216).

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supplementary materials

Acta Cryst. (2007). E**63**, o4598 [**doi:10.1107/S1600536807055055**]

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

X.-F. Tang and Y.-H. Wen

Comment

8-Hydroxyquinoline and its derivatives have found extensive application as analytical reagents, *e.g.* in absorption spectrophotometry, 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, the structures of unsubstituted 8-hydroxyquinolinate amide-type compounds, namely, *N*-phenyl-2-(quinolin-8-yloxy)acetamide (Li *et al.*, 2005) and *N*,*N*-diphenyl-2-(quinolin-8-yloxy)acetamide (Wen *et al.*, 2005) have been reported. In continuation of our search for good extractants of metal ions, fluorescent materials and analytical reagents, we obtained the title compound (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 group is essentially planar, with a dihedral angle of 2.25 (1)° between the benzene ring (C1—C4/C8/C9) and pyridine ring (N1/C4—C8). The quinoline mean plane makes dihedral angles of 30.42 (1)° and 81.17 (1)° with the C12—C17 and C18—C23 phenyl rings of the diphenylacetamide fragment, respectively; the dihedral angle between the latter two aromatic rings is 82.77 (1)°.

There are two intramolecular hydrogen bonds from the quinoline fragment, *viz*. C15—H15A···Cl2 and C10—H10A···N1 (Fig. 1 and Table 1), forming a five- and a six-membered ring, respectively; these affect the conformation of the molecule. In the crystal structure, molecules are linked into chains along the *b* axis by C13—H13A···O2^{i} and C20—H20A···O2^{ii} (Fig. 2 and Table 1; symmetry codes as in Table 1) intermolecular hydrogen bonds.

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-dichloro-8-hydroxyquinoline (2.14 g, 10 mmol) in acetone (60 ml) were added 2-chloro-*N*,*N*-diphenylacetamide (2.45 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 4 h. After cooling to room temperature, the mixture was washed three times with water and filtered. Colourless single crystals of the title compound 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 12 d.

Refinement

All H atoms were located in difference Fourier maps, then positioned geometrically 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

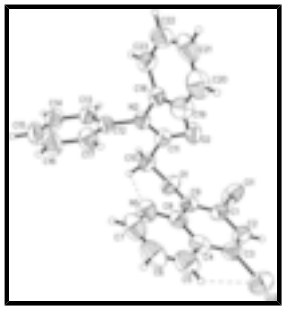

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme. Intramolecular hydrogen bonds are drawn as dashed lines.

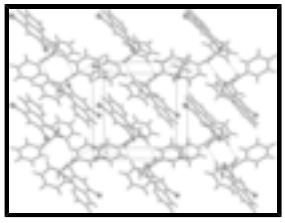

Fig. 2. A packing diagram of the title compound, viewed down the *c* axis. Hydrogen bonds are indicated by dashed lines.

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

Crystal data

$C_{23}H_{16}Cl_2N_2O_2$	F_{000} = 872
M_r = 423.28	D_x = 1.391 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.8942 (13) Å	Cell parameters from 3686 reflections
b = 9.6703 (13) Å	θ = 2.3–25.3º
c = 21.152 (3) Å	μ = 0.34 mm^{-1}
β = 93.107 (2)º	T = 293 (2) K
V = 2020.8 (5) Å^3	Column, colourless
Z = 4	0.26 × 0.12 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3827 independent reflections
Radiation source: fine-focus sealed tube	3035 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 25.7º
T = 293(2) K	θ_{min} = 1.9º
ω scans	h = −8→12
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	k = −11→11
T_{min} = 0.916, T_{max} = 0.970	l = −25→25
10737 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
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.9055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3827 reflections	$\Delta\rho_{max} = 0.52$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.51$ 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 $F^2 > 2$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}
Cl1	0.31549 (8)	0.08217 (8)	0.19801 (3)	0.0807 (3)
Cl2	−0.05972 (8)	0.47583 (9)	0.18328 (4)	0.0938 (3)
O1	0.23409 (17)	0.01537 (15)	0.06956 (7)	0.0565 (4)
N2	0.37018 (18)	0.14865 (17)	−0.07488 (8)	0.0461 (4)
C18	0.4430 (2)	0.2695 (2)	−0.09362 (9)	0.0453 (5)
O2	0.42174 (17)	0.18848 (17)	0.02889 (7)	0.0622 (4)
C9	0.1686 (2)	0.1303 (2)	0.08933 (10)	0.0476 (5)
C11	0.3616 (2)	0.1206 (2)	−0.01194 (10)	0.0471 (5)
C8	0.0703 (2)	0.2077 (2)	0.05243 (10)	0.0516 (5)
C12	0.3029 (2)	0.0664 (2)	−0.12406 (9)	0.0474 (5)
C1	0.1929 (2)	0.1677 (2)	0.15136 (10)	0.0527 (5)
C4	−0.0021 (2)	0.3153 (2)	0.08161 (12)	0.0582 (6)
C2	0.1245 (2)	0.2756 (2)	0.17999 (11)	0.0568 (6)
H2A	0.1451	0.2983	0.2221	0.068*
C10	0.2737 (2)	−0.0002 (2)	0.00576 (10)	0.0538 (5)
H10A	0.1938	−0.0043	−0.0229	0.065*
H10B	0.3235	−0.0859	0.0018	0.065*
N1	0.0480 (2)	0.1756 (2)	−0.01003 (10)	0.0667 (6)

C13	0.3431 (3)	−0.0680 (2)	−0.13415 (11)	0.0578 (6)
H13A	0.4143	−0.1064	−0.1095	0.069*
C3	0.0288 (2)	0.3460 (2)	0.14595 (12)	0.0598 (6)
C17	0.1987 (3)	0.1239 (3)	−0.16139 (11)	0.0643 (6)
H17A	0.1723	0.2149	−0.1550	0.077*
C23	0.5474 (3)	0.2569 (3)	−0.13324 (11)	0.0627 (6)
H23A	0.5727	0.1704	−0.1477	0.075*
C19	0.4078 (3)	0.3976 (2)	−0.07156 (13)	0.0665 (7)
H19A	0.3375	0.4056	−0.0444	0.080*
C16	0.1338 (3)	0.0448 (4)	−0.20847 (13)	0.0800 (8)
H16A	0.0633	0.0829	−0.2336	0.096*
C22	0.6151 (3)	0.3750 (4)	−0.15141 (13)	0.0823 (9)
H22A	0.6856	0.3677	−0.1785	0.099*
C21	0.5784 (3)	0.5024 (3)	−0.12956 (15)	0.0843 (10)
H21A	0.6235	0.5812	−0.1421	0.101*
C15	0.1729 (3)	−0.0892 (4)	−0.21829 (13)	0.0802 (9)
H15A	0.1291	−0.1418	−0.2500	0.096*
C20	0.4756 (4)	0.5133 (3)	−0.08937 (16)	0.0831 (9)
H20A	0.4516	0.5996	−0.0741	0.100*
C5	−0.1036 (3)	0.3830 (3)	0.04406 (16)	0.0816 (8)
H5A	−0.1553	0.4520	0.0616	0.098*
C7	−0.0466 (3)	0.2445 (3)	−0.04277 (15)	0.0824 (9)
H7A	−0.0616	0.2233	−0.0855	0.099*
C6	−0.1259 (3)	0.3477 (4)	−0.01708 (17)	0.0917 (10)
H6A	−0.1933	0.3916	−0.0420	0.110*
C14	0.2762 (3)	−0.1450 (3)	−0.18139 (12)	0.0751 (8)
H14A	0.3021	−0.2361	−0.1880	0.090*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0928 (5)	0.0995 (6)	0.0494 (3)	0.0435 (4)	0.0019 (3)	0.0035 (3)
Cl2	0.0833 (5)	0.0809 (5)	0.1175 (7)	0.0296 (4)	0.0073 (4)	−0.0241 (4)
O1	0.0766 (11)	0.0482 (9)	0.0459 (8)	0.0082 (8)	0.0136 (7)	0.0055 (7)
N2	0.0539 (10)	0.0423 (9)	0.0420 (9)	−0.0053 (8)	0.0021 (7)	0.0003 (7)
C18	0.0489 (12)	0.0446 (11)	0.0416 (10)	−0.0019 (9)	−0.0039 (9)	0.0041 (9)
O2	0.0768 (11)	0.0612 (10)	0.0477 (9)	−0.0133 (9)	−0.0042 (8)	−0.0025 (7)
C9	0.0499 (12)	0.0446 (11)	0.0491 (11)	0.0001 (9)	0.0110 (9)	0.0070 (9)
C11	0.0530 (12)	0.0445 (11)	0.0437 (11)	0.0014 (9)	0.0024 (9)	−0.0014 (9)
C8	0.0488 (12)	0.0506 (12)	0.0555 (13)	−0.0078 (10)	0.0031 (10)	0.0080 (10)
C12	0.0514 (12)	0.0504 (12)	0.0404 (10)	−0.0086 (10)	0.0038 (9)	0.0017 (9)
C1	0.0537 (13)	0.0577 (13)	0.0474 (12)	0.0076 (11)	0.0100 (9)	0.0078 (10)
C4	0.0436 (12)	0.0525 (14)	0.0783 (16)	−0.0015 (10)	0.0012 (11)	0.0091 (12)
C2	0.0564 (14)	0.0616 (14)	0.0532 (12)	0.0052 (11)	0.0109 (10)	−0.0037 (11)
C10	0.0673 (15)	0.0499 (13)	0.0451 (12)	−0.0035 (11)	0.0116 (10)	−0.0028 (9)
N1	0.0731 (14)	0.0689 (14)	0.0571 (12)	−0.0063 (11)	−0.0070 (10)	0.0086 (10)
C13	0.0677 (15)	0.0535 (13)	0.0525 (12)	−0.0026 (11)	0.0046 (11)	−0.0060 (10)
C3	0.0511 (13)	0.0534 (14)	0.0755 (16)	0.0043 (11)	0.0104 (11)	−0.0044 (12)

C17	0.0674 (15)	0.0657 (15)	0.0586 (14)	−0.0044 (12)	−0.0076 (12)	0.0075 (12)
C23	0.0717 (16)	0.0672 (16)	0.0500 (12)	−0.0094 (13)	0.0092 (11)	−0.0045 (11)
C19	0.0704 (16)	0.0476 (14)	0.0820 (17)	0.0062 (12)	0.0076 (13)	0.0059 (12)
C16	0.0717 (18)	0.105 (2)	0.0613 (16)	−0.0189 (17)	−0.0157 (13)	0.0106 (16)
C22	0.0786 (19)	0.111 (3)	0.0574 (15)	−0.0345 (18)	0.0097 (13)	0.0081 (16)
C21	0.101 (2)	0.074 (2)	0.0752 (19)	−0.0414 (18)	−0.0233 (17)	0.0226 (16)
C15	0.089 (2)	0.097 (2)	0.0545 (15)	−0.0423 (18)	−0.0001 (14)	−0.0113 (15)
C20	0.108 (2)	0.0459 (15)	0.094 (2)	−0.0075 (15)	−0.0082 (19)	0.0082 (14)
C5	0.0627 (17)	0.0745 (19)	0.105 (2)	0.0110 (14)	−0.0162 (16)	0.0080 (16)
C7	0.084 (2)	0.086 (2)	0.0741 (18)	−0.0126 (17)	−0.0209 (15)	0.0188 (16)
C6	0.0714 (19)	0.090 (2)	0.110 (3)	0.0054 (17)	−0.0320 (18)	0.021 (2)
C14	0.099 (2)	0.0640 (17)	0.0629 (16)	−0.0192 (15)	0.0112 (15)	−0.0164 (13)

Geometric parameters (Å, °)

Cl1—C1	1.732 (2)	N1—C7	1.315 (3)
Cl2—C3	1.744 (2)	C13—C14	1.386 (3)
O1—C9	1.363 (2)	C13—H13A	0.9300
O1—C10	1.433 (2)	C17—C16	1.385 (4)
N2—C11	1.366 (3)	C17—H17A	0.9300
N2—C18	1.440 (3)	C23—C22	1.388 (4)
N2—C12	1.443 (3)	C23—H23A	0.9300
C18—C23	1.371 (3)	C19—C20	1.368 (4)
C18—C19	1.375 (3)	C19—H19A	0.9300
O2—C11	1.214 (2)	C16—C15	1.371 (4)
C9—C1	1.370 (3)	C16—H16A	0.9300
C9—C8	1.426 (3)	C22—C21	1.371 (5)
C11—C10	1.515 (3)	C22—H22A	0.9300
C8—N1	1.364 (3)	C21—C20	1.365 (5)
C8—C4	1.422 (3)	C21—H21A	0.9300
C12—C13	1.379 (3)	C15—C14	1.363 (4)
C12—C17	1.381 (3)	C15—H15A	0.9300
C1—C2	1.399 (3)	C20—H20A	0.9300
C4—C5	1.408 (3)	C5—C6	1.344 (5)
C4—C3	1.410 (4)	C5—H5A	0.9300
C2—C3	1.344 (3)	C7—C6	1.398 (5)
C2—H2A	0.9300	C7—H7A	0.9300
C10—H10A	0.9700	C6—H6A	0.9300
C10—H10B	0.9700	C14—H14A	0.9300
C9—O1—C10	122.21 (16)	C2—C3—Cl2	118.6 (2)
C11—N2—C18	119.20 (17)	C4—C3—Cl2	120.07 (19)
C11—N2—C12	122.87 (17)	C12—C17—C16	119.5 (3)
C18—N2—C12	117.84 (16)	C12—C17—H17A	120.3
C23—C18—C19	120.1 (2)	C16—C17—H17A	120.3
C23—C18—N2	120.1 (2)	C18—C23—C22	119.1 (3)
C19—C18—N2	119.9 (2)	C18—C23—H23A	120.4
O1—C9—C1	116.58 (19)	C22—C23—H23A	120.4
O1—C9—C8	125.56 (19)	C20—C19—C18	120.4 (3)
C1—C9—C8	117.7 (2)	C20—C19—H19A	119.8

O2—C11—N2	122.1 (2)	C18—C19—H19A	119.8
O2—C11—C10	120.43 (19)	C15—C16—C17	120.5 (3)
N2—C11—C10	117.43 (18)	C15—C16—H16A	119.8
N1—C8—C4	121.9 (2)	C17—C16—H16A	119.8
N1—C8—C9	118.7 (2)	C21—C22—C23	120.4 (3)
C4—C8—C9	119.4 (2)	C21—C22—H22A	119.8
C13—C12—C17	120.2 (2)	C23—C22—H22A	119.8
C13—C12—N2	120.3 (2)	C20—C21—C22	120.0 (3)
C17—C12—N2	119.5 (2)	C20—C21—H21A	120.0
C9—C1—C2	123.2 (2)	C22—C21—H21A	120.0
C9—C1—Cl1	120.06 (17)	C14—C15—C16	119.7 (3)
C2—C1—Cl1	116.74 (17)	C14—C15—H15A	120.1
C5—C4—C3	123.8 (2)	C16—C15—H15A	120.1
C5—C4—C8	117.1 (2)	C21—C20—C19	120.1 (3)
C3—C4—C8	119.0 (2)	C21—C20—H20A	120.0
C3—C2—C1	119.3 (2)	C19—C20—H20A	120.0
C3—C2—H2A	120.3	C6—C5—C4	120.0 (3)
C1—C2—H2A	120.3	C6—C5—H5A	120.0
O1—C10—C11	109.98 (17)	C4—C5—H5A	120.0
O1—C10—H10A	109.7	N1—C7—C6	123.8 (3)
C11—C10—H10A	109.7	N1—C7—H7A	118.1
O1—C10—H10B	109.7	C6—C7—H7A	118.1
C11—C10—H10B	109.7	C5—C6—C7	119.3 (3)
H10A—C10—H10B	108.2	C5—C6—H6A	120.4
C7—N1—C8	117.9 (3)	C7—C6—H6A	120.4
C12—C13—C14	119.2 (2)	C15—C14—C13	121.0 (3)
C12—C13—H13A	120.4	C15—C14—H14A	119.5
C14—C13—H13A	120.4	C13—C14—H14A	119.5
C2—C3—C4	121.3 (2)		

C11—N2—C18—C23	124.0 (2)	N2—C11—C10—O1	−158.10 (19)
C12—N2—C18—C23	−59.4 (3)	C4—C8—N1—C7	−2.1 (3)
C11—N2—C18—C19	−55.8 (3)	C9—C8—N1—C7	177.5 (2)
C12—N2—C18—C19	120.8 (2)	C17—C12—C13—C14	−1.1 (3)
C10—O1—C9—C1	−148.9 (2)	N2—C12—C13—C14	179.5 (2)
C10—O1—C9—C8	36.0 (3)	C1—C2—C3—C4	−1.3 (4)
C18—N2—C11—O2	−5.5 (3)	C1—C2—C3—Cl2	177.64 (18)
C12—N2—C11—O2	178.0 (2)	C5—C4—C3—C2	178.3 (3)
C18—N2—C11—C10	174.66 (18)	C8—C4—C3—C2	−0.2 (4)
C12—N2—C11—C10	−1.8 (3)	C5—C4—C3—Cl2	−0.7 (4)
O1—C9—C8—N1	−7.4 (3)	C8—C4—C3—Cl2	−179.18 (17)
C1—C9—C8—N1	177.6 (2)	C13—C12—C17—C16	0.8 (4)
O1—C9—C8—C4	172.27 (19)	N2—C12—C17—C16	−179.8 (2)
C1—C9—C8—C4	−2.7 (3)	C19—C18—C23—C22	−1.1 (4)
C11—N2—C12—C13	−67.6 (3)	N2—C18—C23—C22	179.1 (2)
C18—N2—C12—C13	115.9 (2)	C23—C18—C19—C20	0.6 (4)
C11—N2—C12—C17	113.1 (2)	N2—C18—C19—C20	−179.5 (2)
C18—N2—C12—C17	−63.4 (3)	C12—C17—C16—C15	−0.3 (4)
O1—C9—C1—C2	−174.2 (2)	C18—C23—C22—C21	0.5 (4)
C8—C9—C1—C2	1.2 (3)	C23—C22—C21—C20	0.5 (4)

O1—C9—C1—Cl1	6.9 (3)	C17—C16—C15—C14	0.1 (4)
C8—C9—C1—Cl1	−177.62 (16)	C22—C21—C20—C19	−0.9 (5)
N1—C8—C4—C5	3.3 (3)	C18—C19—C20—C21	0.4 (4)
C9—C8—C4—C5	−176.3 (2)	C3—C4—C5—C6	179.6 (3)
N1—C8—C4—C3	−178.1 (2)	C8—C4—C5—C6	−1.9 (4)
C9—C8—C4—C3	2.3 (3)	C8—N1—C7—C6	−0.5 (4)
C9—C1—C2—C3	0.8 (4)	C4—C5—C6—C7	−0.5 (5)
Cl1—C1—C2—C3	179.71 (19)	N1—C7—C6—C5	1.9 (5)
C9—O1—C10—C11	55.9 (3)	C16—C15—C14—C13	−0.4 (4)
O2—C11—C10—O1	22.1 (3)	C12—C13—C14—C15	0.9 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···Cl2	0.93	2.70	3.087 (3)	106
C10—H10A···N1	0.97	2.29	2.812 (3)	113
C13—H13A···O2^{i}	0.93	2.42	3.342 (3)	169
C20—H20A···O2^{ii}	0.93	2.56	3.293 (4)	136

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

Fig. 1

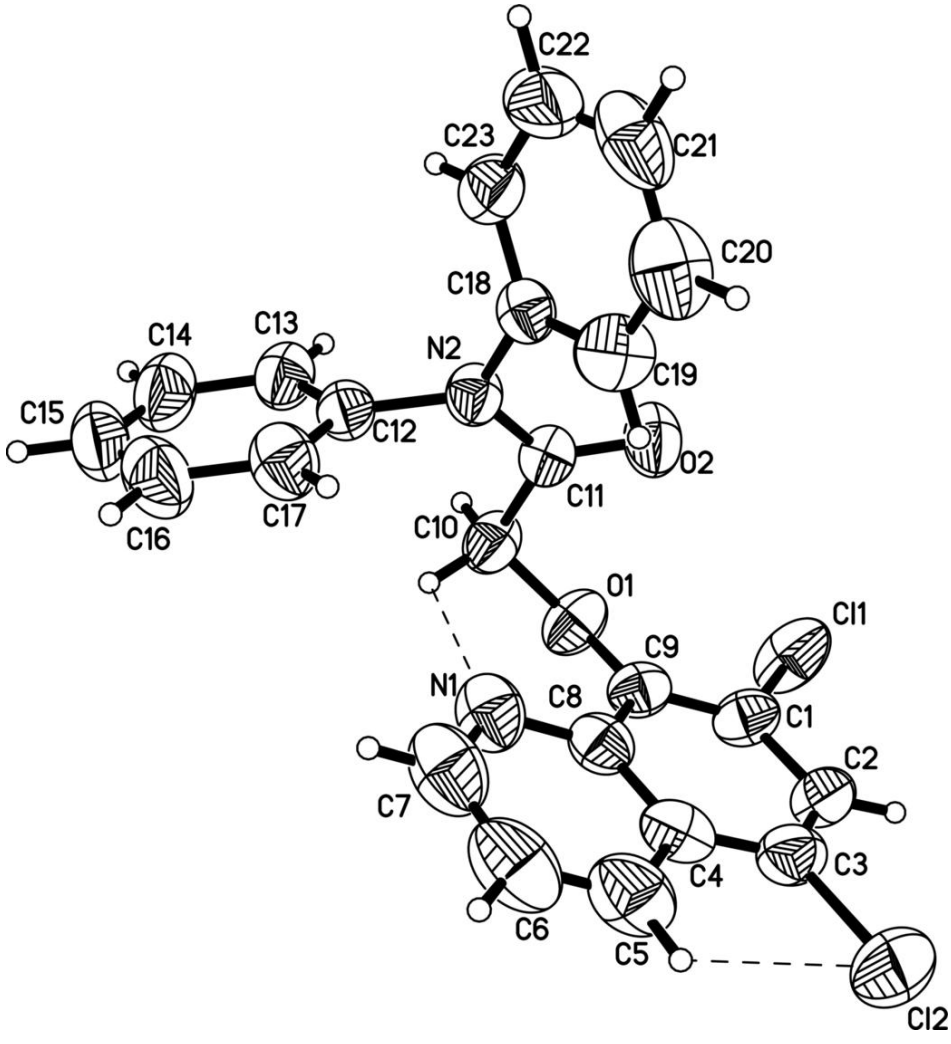
C22
C23
C21
C20
C18
C14
C13
N2
C19
C15
C12
O2
C11
C17
C16
C10
O1
Cl1
C9
N1
C8
C1
C2
C7
C4
C3
C6
C5
Cl2

Fig. 2