

2-Chloro-3-(4-chlorobenzamido)-1,4-naphthoquinone

Yakini Brandy, Ray J. Butcher,* Tolulope A. Adesiyun, Solomon Berhe and Oladapo Bakare

Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA

Correspondence e-mail: rbutcher99@yahoo.com

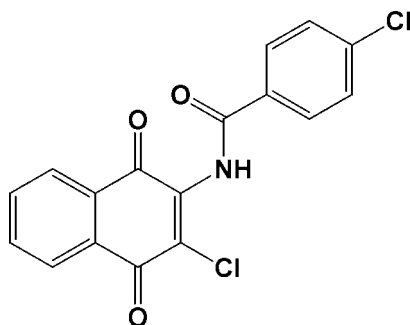
Received 3 December 2008; accepted 4 December 2008

Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.038; wR factor = 0.086; data-to-parameter ratio = 23.3.

The naphthoquinone ring is almost perpendicular [dihedral angle $71.02(3)^\circ$] to the phenyl group of the title compound, $\text{C}_{17}\text{H}_9\text{Cl}_2\text{NO}_3$, while the dihedral angle between the amide group and the 4-chlorophenyl ring is $21.9(2)^\circ$. The conformation of the $\text{N}-\text{H}$ and $\text{C}=\text{O}$ bonds are *anti* to each other. $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds link the molecules into chains in the a -axis direction. In addition, these chains are linked by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions.

Related literature

For similar structures see: Lien *et al.* (1997); Huang *et al.* (2005); Bakare *et al.* (2003); Copeland *et al.* (2007); Win *et al.* (2005); Rubin-Preminger *et al.* (2004). For related literature, see: Gowda, Kožíšek *et al.* (2008); Gowda, Tokarčík *et al.* (2008); van Oosten *et al.* (2008); Shen *et al.* (2008).



Experimental

Crystal data

$\text{C}_{17}\text{H}_9\text{Cl}_2\text{NO}_3$
 $M_r = 346.15$
 Monoclinic, $P2_1/c$
 $a = 5.6011(2)$ Å

$b = 8.7237(3)$ Å
 $c = 29.7957(9)$ Å
 $\beta = 93.504(3)^\circ$
 $V = 1453.16(8)$ Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.46$ mm⁻¹

$T = 200(2)$ K
 $0.49 \times 0.41 \times 0.12$ mm

Data collection

Oxford Diffraction Gemini R diffractometer
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)

$T_{\min} = 0.887$, $T_{\max} = 1.000$
 (expected range = 0.839–0.946)
 13882 measured reflections
 4842 independent reflections
 2832 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.086$
 $S = 0.93$
 4842 reflections

208 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N}-\text{H}0\text{A}\cdots\text{Cl}1^i$	0.88	2.89	3.6491 (12)	145
$\text{C}14-\text{H}14\text{A}\cdots\text{O}2^{ii}$	0.95	2.40	3.2517 (19)	149

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

RJB acknowledges the Laboratory for the Structure of Matter at the Naval Research Laboratory for access to their diffractometers.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2690).

References

- Bakare, O., Ashendel, C. L., Peng, H., Zalkow, L. H. & Burgess, E. M. (2003). *Bioorg. Med. Chem.* **11**, 3165–3170.
- Copeland, R. L., Das, J. R., Bakare, O., Enwerem, N. M., Berhe, S., Hillaire, K., White, D., Beyene, D., Kassim, O. O. & Kanaan, Y. M. (2007). *Anticancer Res.* **27**, 1537–1546.
- Gowda, B. T., Kožíšek, J., Tokarčík, M. & Fuess, H. (2008). *Acta Cryst.* **E64**, o987.
- Gowda, B. T., Tokarčík, M., Kožíšek, J., Sowmya, B. P. & Fuess, H. (2008). *Acta Cryst.* **E64**, o950.
- Huang, L., Chang, F., Lee, K., Wang, J., Teng, C. & Kuo, S. (2005). *Bioorg. Med. Chem.* **6**, 2261–2269.
- Lien, J., Huang, L., Wang, J., Teng, C., Lee, K. & Kuo, S. (1997). *Bioorg. Med. Chem.* **5**, 2111–2120.
- Oosten, E. M. van, Lough, A. J. & Vasdev, N. (2008). *Acta Cryst.* **E64**, o1005. Oxford Diffraction (2007). *CrysAlis CCD* and *CrysAlis RED* (including *SCALE3 ABSPACK*). Oxford Diffraction Ltd, Abingdon, England.
- Rubin-Preminger, J. M., Win, T., Granot, Y. & Bittner, S. (2004). *Z. Kristallogr. New Cryst. Struct.* **219**, 323–324.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Shen, Q., Yu, S.-Q., Hu, B.-B. & Lu, P. (2008). *Acta Cryst.* **E64**, o996.
- Win, T., Yerushalmi, S. & Bittner, S. (2005). *Synthesis*, pp. 1631–1634.

supplementary materials

Acta Cryst. (2009). E65, o64 [doi:10.1107/S1600536808040993]

2-Chloro-3-(4-chlorobenzamido)-1,4-naphthoquinone

Y. Brandy, R. J. Butcher, T. A. Adesiyun, S. Berhe and O. Bakare

Comment

The amido and imido derivatives of 3-chloro-1,4-naphthoquinone are well known for their anti-inflammatory, antiplatelet, antiallergic and anticancer activities (Lien *et al.*, 1997; Huang *et al.*, 2005; Bakare *et al.*, 2003; Copeland *et al.*, 2007). The title compound, 2-chloro-3-(*p*-chlorobenzamido)-1,4-naphthoquinone was obtained as an intermediate in the synthesis of some oxazolo-1,4-naphthoquinone and imido-substituted-1,4-naphthoquinone analogs.

The naphthoquinone ring is almost perpendicular to the phenyl group of the title compound $C_{17}H_9Cl_2NO_3$, while the dihedral angle between the amide group and the 4-chlorophenyl ring is $21.9(2)^\circ$ (Fig. 1). The conformation of the N—H and C=O bonds are anti to each other (Gowda, Kožišek *et al.*, 2008; Gowda, Tokarčík *et al.*, 2008). N—H \cdots Cl hydrogen bonds link the molecules into chains in the *a* direction. In addition, these chains are linked by weak intermolecular Ar—H \cdots O interactions (Fig. 2, Table 1).

Experimental

A mixture of 2-amino-3-chloro-1,4-naphthoquinone (213 mg, 1.03 mmol) and 4-chloro-benzoylchloride (2 ml) was refluxed for 2 1/2 h (powerstat setting at 70). The reaction mixture was cooled to room temperature. The precipitate was isolated by vacuum filtration and the yellow-grey solid was washed with diethyl ether. The crude was recrystallized from ethanol (20 ml) to obtain a yellow solid (67 mg, 18.8%). Crystals for *x*-ray study were obtained by recrystallization from methanol.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.95 Å, N—H = 0.88 Å and $U_{iso}(H) = 1.2U_{eq}(C, N)$.

Figures

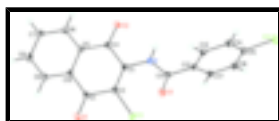


Fig. 1. View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 20% probability level.

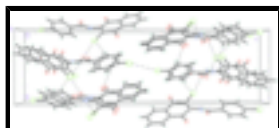


Fig. 2. View of the packing viewed down the *a* axis. Dashed bonds show weak C—H \cdots O interactions.

2-Chloro-3-(4-chlorobenzamido)-1,4-naphthoquinone

Crystal data

$C_{17}H_9Cl_2NO_3$	$F_{000} = 704$
$M_r = 346.15$	$D_x = 1.582 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 5.6011 (2) \text{ \AA}$	Cell parameters from 4629 reflections
$b = 8.7237 (3) \text{ \AA}$	$\theta = 4.6\text{--}32.5^\circ$
$c = 29.7957 (9) \text{ \AA}$	$\mu = 0.46 \text{ mm}^{-1}$
$\beta = 93.504 (3)^\circ$	$T = 200 (2) \text{ K}$
$V = 1453.16 (8) \text{ \AA}^3$	Plate, pale yellow
$Z = 4$	$0.49 \times 0.41 \times 0.12 \text{ mm}$

Data collection

Oxford Diffraction Gemini R diffractometer	4842 independent reflections
Radiation source: fine-focus sealed tube	2832 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.035$
Detector resolution: $10.5081 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 32.6^\circ$
$T = 200(2) \text{ K}$	$\theta_{\text{min}} = 4.6^\circ$
φ and ω scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$k = -12 \rightarrow 12$
$T_{\text{min}} = 0.887$, $T_{\text{max}} = 1.000$	$l = -44 \rightarrow 44$
13882 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
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.086$	$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2]$
$S = 0.93$	where $P = (F_o^2 + 2F_c^2)/3$
4842 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
208 parameters	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.36 \text{ e \AA}^{-3}$
	Extinction correction: none

Special details

Experimental. (CrysAlis RED; Oxford Diffraction, 2007) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.42210 (6)	0.13331 (4)	0.298854 (11)	0.02796 (10)
C12	-0.42944 (7)	-0.05032 (6)	0.057164 (13)	0.04852 (14)
O1	0.54644 (18)	0.07511 (14)	0.39281 (4)	0.0401 (3)
O2	-0.26101 (17)	-0.20745 (14)	0.33569 (3)	0.0378 (3)
O3	0.31583 (17)	-0.12832 (14)	0.24103 (3)	0.0364 (3)
N	-0.02512 (19)	-0.06128 (15)	0.27365 (4)	0.0273 (3)
H0A	-0.1786	-0.0415	0.2689	0.033*
C1	0.3653 (2)	0.00688 (18)	0.38026 (5)	0.0275 (3)
C2	0.2705 (2)	0.01309 (17)	0.33244 (4)	0.0251 (3)
C3	0.0712 (2)	-0.06238 (17)	0.31773 (4)	0.0240 (3)
C4	-0.0749 (2)	-0.14777 (18)	0.34975 (5)	0.0264 (3)
C5	0.0144 (2)	-0.15604 (18)	0.39758 (5)	0.0272 (3)
C6	-0.1138 (3)	-0.2369 (2)	0.42817 (5)	0.0391 (4)
H6A	-0.2591	-0.2864	0.4186	0.047*
C7	-0.0289 (3)	-0.2451 (3)	0.47288 (5)	0.0477 (5)
H7A	-0.1169	-0.3002	0.4939	0.057*
C8	0.1823 (3)	-0.1737 (2)	0.48705 (5)	0.0477 (5)
H8A	0.2390	-0.1794	0.5177	0.057*
C9	0.3111 (3)	-0.0940 (2)	0.45660 (5)	0.0391 (4)
H9A	0.4574	-0.0459	0.4663	0.047*
C10	0.2273 (2)	-0.08383 (18)	0.41170 (5)	0.0287 (3)
C11	0.1070 (3)	-0.08964 (17)	0.23680 (5)	0.0263 (3)
C12	-0.0252 (2)	-0.07098 (17)	0.19218 (4)	0.0245 (3)
C13	-0.2316 (2)	0.01736 (18)	0.18635 (5)	0.0277 (3)
H13A	-0.2882	0.0726	0.2110	0.033*
C14	-0.3550 (3)	0.02492 (19)	0.14462 (5)	0.0315 (3)
H14A	-0.4966	0.0846	0.1406	0.038*
C15	-0.2697 (3)	-0.05531 (19)	0.10907 (5)	0.0307 (3)
C16	-0.0608 (3)	-0.1395 (2)	0.11357 (5)	0.0319 (3)
H16A	-0.0020	-0.1913	0.0885	0.038*

supplementary materials

C17	0.0618 (3)	-0.14706 (19)	0.15551 (5)	0.0295 (3)
H17A	0.2058	-0.2045	0.1592	0.035*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.02827 (17)	0.0286 (2)	0.02758 (17)	-0.00541 (15)	0.00608 (13)	0.00212 (15)
C12	0.0514 (2)	0.0680 (4)	0.02503 (18)	0.0176 (2)	-0.00744 (17)	-0.0029 (2)
O1	0.0364 (6)	0.0500 (8)	0.0334 (6)	-0.0141 (6)	-0.0034 (5)	-0.0042 (5)
O2	0.0321 (5)	0.0490 (8)	0.0318 (6)	-0.0152 (5)	-0.0010 (5)	0.0023 (5)
O3	0.0328 (6)	0.0476 (8)	0.0288 (5)	0.0120 (5)	0.0007 (4)	-0.0072 (5)
N	0.0240 (6)	0.0383 (8)	0.0196 (5)	0.0012 (5)	0.0019 (5)	0.0013 (5)
C1	0.0266 (7)	0.0307 (9)	0.0253 (7)	-0.0004 (6)	0.0021 (6)	-0.0031 (6)
C2	0.0272 (7)	0.0247 (8)	0.0239 (7)	0.0006 (6)	0.0058 (6)	-0.0012 (6)
C3	0.0252 (6)	0.0278 (8)	0.0192 (6)	0.0026 (6)	0.0028 (5)	-0.0013 (6)
C4	0.0278 (7)	0.0268 (8)	0.0248 (7)	-0.0014 (6)	0.0030 (6)	-0.0008 (6)
C5	0.0294 (7)	0.0302 (9)	0.0220 (6)	0.0000 (6)	0.0023 (6)	0.0005 (6)
C6	0.0374 (8)	0.0517 (12)	0.0286 (7)	-0.0087 (8)	0.0041 (7)	0.0049 (8)
C7	0.0502 (10)	0.0654 (14)	0.0282 (8)	-0.0078 (9)	0.0083 (7)	0.0117 (9)
C8	0.0532 (10)	0.0680 (15)	0.0214 (7)	0.0003 (10)	-0.0008 (7)	0.0049 (8)
C9	0.0374 (8)	0.0562 (12)	0.0232 (7)	-0.0047 (8)	-0.0026 (6)	-0.0018 (7)
C10	0.0296 (7)	0.0348 (9)	0.0218 (6)	0.0004 (6)	0.0023 (6)	-0.0028 (6)
C11	0.0306 (7)	0.0258 (8)	0.0228 (7)	0.0018 (6)	0.0033 (6)	-0.0012 (6)
C12	0.0275 (7)	0.0260 (8)	0.0201 (6)	-0.0020 (6)	0.0034 (5)	0.0002 (6)
C13	0.0321 (7)	0.0282 (8)	0.0233 (7)	0.0034 (6)	0.0060 (6)	-0.0017 (6)
C14	0.0293 (7)	0.0361 (9)	0.0291 (7)	0.0071 (7)	0.0022 (6)	0.0014 (7)
C15	0.0359 (8)	0.0359 (9)	0.0202 (6)	0.0015 (7)	-0.0008 (6)	0.0018 (7)
C16	0.0347 (8)	0.0400 (10)	0.0215 (7)	0.0064 (7)	0.0051 (6)	-0.0032 (7)
C17	0.0292 (7)	0.0348 (9)	0.0246 (7)	0.0052 (6)	0.0035 (6)	-0.0009 (6)

Geometric parameters (\AA , $^\circ$)

C11—C2	1.7105 (15)	C7—C8	1.380 (2)
C12—C15	1.7394 (14)	C7—H7A	0.9500
O1—C1	1.2154 (17)	C8—C9	1.381 (2)
O2—C4	1.2166 (16)	C8—H8A	0.9500
O3—C11	1.2167 (16)	C9—C10	1.3932 (19)
N—C11	1.3834 (18)	C9—H9A	0.9500
N—C3	1.3890 (15)	C11—C12	1.4905 (19)
N—H0A	0.8800	C12—C17	1.392 (2)
C1—C10	1.480 (2)	C12—C13	1.392 (2)
C1—C2	1.4907 (18)	C13—C14	1.3867 (19)
C2—C3	1.3461 (19)	C13—H13A	0.9500
C3—C4	1.494 (2)	C14—C15	1.379 (2)
C4—C5	1.4829 (19)	C14—H14A	0.9500
C5—C6	1.387 (2)	C15—C16	1.381 (2)
C5—C10	1.391 (2)	C16—C17	1.3903 (19)
C6—C7	1.389 (2)	C16—H16A	0.9500
C6—H6A	0.9500	C17—H17A	0.9500

C11—N—C3	123.62 (11)	C8—C9—C10	120.27 (15)
C11—N—H0A	118.2	C8—C9—H9A	119.9
C3—N—H0A	118.2	C10—C9—H9A	119.9
O1—C1—C10	121.71 (13)	C5—C10—C9	119.60 (14)
O1—C1—C2	121.20 (14)	C5—C10—C1	121.47 (12)
C10—C1—C2	117.08 (12)	C9—C10—C1	118.91 (13)
C3—C2—C1	122.21 (13)	O3—C11—N	121.65 (12)
C3—C2—C11	122.74 (11)	O3—C11—C12	123.01 (13)
C1—C2—C11	114.90 (10)	N—C11—C12	115.34 (12)
C2—C3—N	124.82 (13)	C17—C12—C13	119.63 (12)
C2—C3—C4	120.79 (12)	C17—C12—C11	118.00 (12)
N—C3—C4	114.27 (12)	C13—C12—C11	122.36 (12)
O2—C4—C5	122.80 (13)	C14—C13—C12	120.19 (13)
O2—C4—C3	119.01 (12)	C14—C13—H13A	119.9
C5—C4—C3	118.19 (12)	C12—C13—H13A	119.9
C6—C5—C10	120.03 (13)	C15—C14—C13	119.16 (13)
C6—C5—C4	119.89 (13)	C15—C14—H14A	120.4
C10—C5—C4	120.08 (13)	C13—C14—H14A	120.4
C5—C6—C7	119.71 (15)	C14—C15—C16	121.78 (13)
C5—C6—H6A	120.1	C14—C15—C12	119.11 (11)
C7—C6—H6A	120.1	C16—C15—C12	119.11 (11)
C8—C7—C6	120.49 (16)	C15—C16—C17	118.79 (14)
C8—C7—H7A	119.8	C15—C16—H16A	120.6
C6—C7—H7A	119.8	C17—C16—H16A	120.6
C7—C8—C9	119.89 (14)	C16—C17—C12	120.37 (13)
C7—C8—H8A	120.1	C16—C17—H17A	119.8
C9—C8—H8A	120.1	C12—C17—H17A	119.8
O1—C1—C2—C3	179.54 (14)	C6—C5—C10—C1	-178.31 (15)
C10—C1—C2—C3	-1.3 (2)	C4—C5—C10—C1	2.1 (2)
O1—C1—C2—C11	-4.8 (2)	C8—C9—C10—C5	-0.8 (3)
C10—C1—C2—C11	174.35 (11)	C8—C9—C10—C1	177.93 (16)
C1—C2—C3—N	-179.82 (14)	O1—C1—C10—C5	177.09 (15)
C11—C2—C3—N	4.8 (2)	C2—C1—C10—C5	-2.0 (2)
C1—C2—C3—C4	4.4 (2)	O1—C1—C10—C9	-1.6 (2)
C11—C2—C3—C4	-170.99 (11)	C2—C1—C10—C9	179.29 (14)
C11—N—C3—C2	49.6 (2)	C3—N—C11—O3	5.2 (2)
C11—N—C3—C4	-134.37 (14)	C3—N—C11—C12	-175.37 (13)
C2—C3—C4—O2	175.91 (14)	O3—C11—C12—C17	21.9 (2)
N—C3—C4—O2	-0.3 (2)	N—C11—C12—C17	-157.54 (14)
C2—C3—C4—C5	-4.1 (2)	O3—C11—C12—C13	-159.00 (15)
N—C3—C4—C5	179.64 (12)	N—C11—C12—C13	21.6 (2)
O2—C4—C5—C6	1.2 (2)	C17—C12—C13—C14	2.4 (2)
C3—C4—C5—C6	-178.73 (15)	C11—C12—C13—C14	-176.72 (14)
O2—C4—C5—C10	-179.23 (15)	C12—C13—C14—C15	-0.4 (2)
C3—C4—C5—C10	0.8 (2)	C13—C14—C15—C16	-1.9 (2)
C10—C5—C6—C7	0.1 (3)	C13—C14—C15—C12	178.10 (12)
C4—C5—C6—C7	179.64 (16)	C14—C15—C16—C17	2.1 (2)
C5—C6—C7—C8	-0.2 (3)	C12—C15—C16—C17	-177.92 (13)

supplementary materials

C6—C7—C8—C9	-0.3 (3)	C15—C16—C17—C12	0.0 (2)
C7—C8—C9—C10	0.7 (3)	C13—C12—C17—C16	-2.2 (2)
C6—C5—C10—C9	0.4 (2)	C11—C12—C17—C16	176.94 (14)
C4—C5—C10—C9	-179.17 (15)		

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>
N—H0A \cdots C11 ⁱ	0.88	2.89	3.6491 (12)	145
C14—H14A \cdots O2 ⁱⁱ	0.95	2.40	3.2517 (19)	149

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

Fig. 1

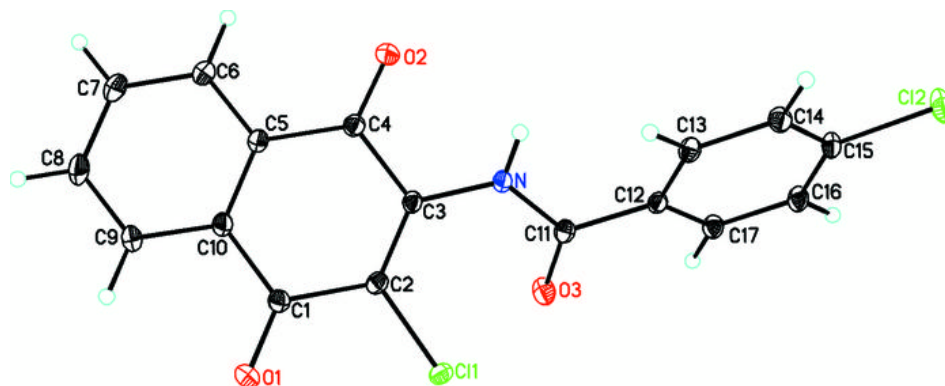


Fig. 2

