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2-Anilino-3-benzoyl-4-(2,5-dichlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-benzo[*b*]pyran

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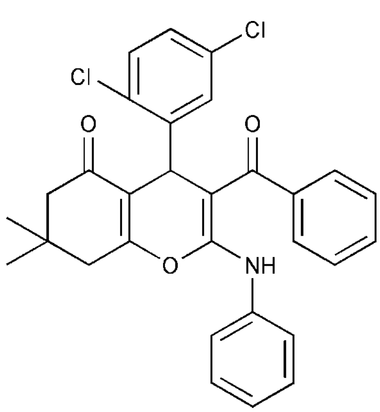
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.124; data-to-parameter ratio = 16.1.

The title compound, $C_{30}H_{25}Cl_2NO_3$, was prepared by the reaction of 3-oxo-*N*,3-diphenylpropanethioamide, 2,5-dichlorobenzaldehyde and 5,5-dimethyl-1,3-cyclohexanedione (1:1:1) in ethanol. The cyclohexene ring adopts a half-chair conformation. The crystal structure exhibits intramolecular N—H···O and C—H···O, and intermolecular C—H···O interactions.

Related literature

For various biological activities, see: Hassanien *et al.* (1999); Jiang *et al.* (2001); Hamann *et al.* (1998). For other aspects of our research, see: Li *et al.* (2006).



Experimental

Crystal data

$C_{30}H_{25}Cl_2NO_3$
M_r = 518.41
Monoclinic, $P2_1/n$
a = 12.844 (3) Å
b = 9.256 (2) Å
c = 22.557 (5) Å
β = 103.365 (4)°
V = 2609.1 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 294 (2) K
0.20 × 0.14 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.946, T_{max} = 0.967
14359 measured reflections
5336 independent reflections
2754 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.123
S = 1.02
5336 reflections
331 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.95 (3)	1.74 (3)	2.565 (3)	144 (3)
C4—H4B···O1^{i}	0.97	2.36	3.308 (3)	164
C13—H13···O2	0.93	2.50	2.915 (3)	108
C28—H28···O3^{ii}	0.93	2.49	3.329 (4)	150

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Bruker, 1999); 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: OB2103).

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supplementary materials

Acta Cryst. (2008). E**64**, o407 [doi:10.1107/S1600536807068377]

2-Anilino-3-benzoyl-4-(2,5-dichlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-benzo[*b*]pyran

L.-R. Wen, J.-H. Sun, C. Ji and H.-Y. Xie

Comment

Many 4*H*-benzo[*b*]pyran derivatives have been reported to show various biological activities (Hassanien *et al.*,1999), such as the cure of lower blood sugar (Jiang *et al.*, 2001), mammary cancer and ovarian cancer (Hamann *et al.*,1998). In the course of our systematic studies aimed at the synthesis of new bioactive compounds (Li *et al.*, 2006), the title compound, (I), was synthesized and its structure is reported here.

In (I), (Fig. 1), the six-membered ring C1—C5/C9 adopts a half-chair conformation with the largest derivation of C3 by 0.369 (3) Å. The phenyl ring C25—C30 is approximately perpendicular to the pyran ring O2/C5—C9, their dihedral angle being 88.51 (8)°. The dihedral angle between the phenyl ring C19—C24 and pyran ring is 67.70 (8) °. In the crystal structure, there are intramolecular N1—H1···O3 and C13—H13···O2 interactions (Table 1). Molecules are linked into chains along the *b* axis by intermolecular C28—H28···O3^{ii} interactions (Fig. 2). Then the other intermolecular interactions C4—H4B···O1 ^{i} connect the chains to a two-dimensional network.

Experimental

The title compound (I) was obtained as follows: 3-oxo-N,3- diphenylpropanethioamide (1 mmol, 0.255 g), 2,5-dichlorobenzaldehyde (1 mmol, 0.161 g), and 5,5-dimethyl-1,3-cyclohexanedione (1 mmol, 0.140 g) were dissolved in ethanol (10 ml), and the solution was refluxed for 10 h in the presence of triethylamine (1 mmol, 0.101 g). Upon cooling, the product was collected by filtration and recrystallized from ethanol and tetrahydrofuran (4:1) (; yield 33%, m.p. 467 K).

Refinement

The H atom attached to N1 was located in a difference Fourier map and refined isotropically with N—H = 0.95 (3) Å. All other H atoms were placed in calculated positions, with C—H = 0.93–0.98 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(CH, CH_2) or 1.5U_{eq}(C) for methyl H atoms.

Figures

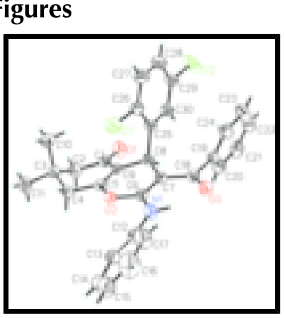

Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 35% probability level.

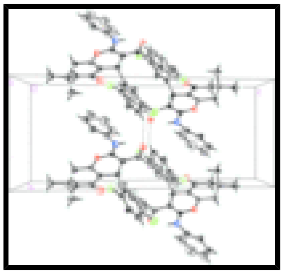

Fig. 2. A packing diagram of (I), viewed down the *a* axis. The C—H···O interactions are shown as dashed lines.

2-Anilino-3-benzoyl-4-(2,5-dichlorophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-\ tetrahydro-4*H*-benzo[*b*]pyran

Crystal data

$C_{30}H_{25}Cl_2NO_3$	F_{000} = 1080
M_r = 518.41	D_x = 1.320 Mg m^{-3} D_m = 1.320 Mg m^{-3} D_m measured by not measured
Monoclinic, $P2_1/n$	Melting point: 467 K
Hall symbol: -P 2yn	Mo *K*α radiation λ = 0.71073 Å
a = 12.844 (3) Å	Cell parameters from 2650 reflections
b = 9.256 (2) Å	θ = 2.4–23.6º
c = 22.557 (5) Å	μ = 0.28 mm^{-1}
β = 103.365 (4)º	T = 294 (2) K
V = 2609.1 (10) Å^3	Block, colorless
Z = 4	0.20 × 0.14 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	5336 independent reflections
Radiation source: fine-focus sealed tube	2754 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -16 \rightarrow 15$
T_{min} = 0.946, T_{max} = 0.967	$k = -10 \rightarrow 11$
14359 measured reflections	$l = -28 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.123	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 0.4267P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.004$
5336 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
331 parameters	$\Delta\rho_{min} = -0.23$ 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}
Cl1	1.02394 (6)	0.53547 (9)	0.14792 (4)	0.0680 (3)
Cl2	0.63077 (9)	0.80839 (10)	−0.03029 (4)	0.1032 (4)
N1	1.01125 (19)	0.1076 (3)	0.12728 (11)	0.0550 (7)
O1	0.65405 (15)	0.5247 (2)	0.17605 (9)	0.0658 (6)
O2	0.96352 (13)	0.23945 (17)	0.20044 (7)	0.0447 (5)
O3	0.91053 (15)	0.1391 (2)	0.01577 (8)	0.0587 (5)
C1	0.7347 (2)	0.4727 (3)	0.20864 (12)	0.0452 (7)
C2	0.7538 (2)	0.4781 (3)	0.27707 (12)	0.0560 (8)
H2A	0.7192	0.3954	0.2907	0.067*
H2B	0.7202	0.5644	0.2884	0.067*
C3	0.8716 (2)	0.4783 (3)	0.31028 (12)	0.0502 (7)
C4	0.9243 (2)	0.3467 (3)	0.28778 (11)	0.0463 (7)
H4A	1.0015	0.3561	0.3008	0.056*
H4B	0.9036	0.2601	0.3063	0.056*
C5	0.89396 (19)	0.3311 (2)	0.22046 (11)	0.0383 (6)
C6	0.9429 (2)	0.2043 (3)	0.13997 (12)	0.0416 (6)
C7	0.86258 (19)	0.2673 (3)	0.09639 (11)	0.0398 (6)
C8	0.79466 (19)	0.3875 (3)	0.11449 (11)	0.0392 (6)
H8	0.7195	0.3616	0.0982	0.047*
C9	0.81208 (19)	0.3949 (2)	0.18249 (11)	0.0369 (6)
C10	0.9257 (2)	0.6182 (3)	0.29677 (15)	0.0734 (10)
H10A	0.8928	0.6992	0.3118	0.110*
H10B	0.9177	0.6278	0.2536	0.110*
H10C	1.0003	0.6152	0.3165	0.110*
C11	0.8814 (3)	0.4667 (4)	0.37879 (13)	0.0771 (10)
H11A	0.8455	0.3810	0.3875	0.116*

H11B	0.8493	0.5499	0.3927	0.116*
H11C	0.9556	0.4619	0.3994	0.116*
C12	1.0879 (2)	0.0194 (3)	0.16614 (13)	0.0485 (7)
C13	1.0736 (2)	−0.0379 (3)	0.21985 (14)	0.0609 (8)
H13	1.0137	−0.0131	0.2342	0.073*
C14	1.1488 (3)	−0.1329 (3)	0.25254 (15)	0.0770 (11)
H14	1.1393	−0.1719	0.2889	0.092*
C15	1.2367 (3)	−0.1695 (4)	0.2314 (2)	0.0991 (15)
H15	1.2879	−0.2316	0.2538	0.119*
C16	1.2491 (3)	−0.1147 (5)	0.1776 (2)	0.1075 (15)
H16	1.3078	−0.1423	0.1627	0.129*
C17	1.1760 (2)	−0.0190 (4)	0.14480 (16)	0.0781 (10)
H17	1.1861	0.0194	0.1085	0.094*
C18	0.8497 (2)	0.2257 (3)	0.03393 (12)	0.0457 (7)
C19	0.7627 (2)	0.2933 (3)	−0.01376 (12)	0.0455 (7)
C20	0.6553 (2)	0.2647 (3)	−0.01880 (14)	0.0599 (8)
H20	0.6343	0.2005	0.0079	0.072*
C21	0.5790 (2)	0.3324 (4)	−0.06390 (15)	0.0722 (10)
H21	0.5068	0.3133	−0.0672	0.087*
C22	0.6089 (3)	0.4266 (4)	−0.10348 (15)	0.0785 (11)
H22	0.5572	0.4719	−0.1334	0.094*
C23	0.7149 (3)	0.4542 (4)	−0.09893 (14)	0.0781 (10)
H23	0.7354	0.5180	−0.1260	0.094*
C24	0.7915 (2)	0.3877 (3)	−0.05430 (13)	0.0639 (9)
H24	0.8636	0.4068	−0.0516	0.077*
C25	0.8126 (2)	0.5352 (3)	0.08756 (11)	0.0428 (6)
C26	0.9106 (2)	0.6062 (3)	0.09834 (13)	0.0530 (7)
C27	0.9232 (3)	0.7360 (3)	0.07054 (15)	0.0687 (9)
H27	0.9896	0.7812	0.0788	0.082*
C28	0.8378 (3)	0.7983 (3)	0.03080 (16)	0.0782 (10)
H28	0.8461	0.8849	0.0115	0.094*
C29	0.7397 (3)	0.7304 (3)	0.01996 (14)	0.0666 (9)
C30	0.7271 (2)	0.6016 (3)	0.04800 (12)	0.0542 (8)
H30	0.6600	0.5582	0.0403	0.065*
H1	0.998 (2)	0.096 (3)	0.0845 (13)	0.073 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0498 (4)	0.0769 (6)	0.0765 (6)	−0.0138 (4)	0.0127 (4)	0.0079 (4)
Cl2	0.1407 (9)	0.0856 (7)	0.0772 (6)	0.0470 (6)	0.0125 (6)	0.0360 (5)
N1	0.0586 (15)	0.0595 (16)	0.0444 (15)	0.0226 (13)	0.0066 (13)	−0.0016 (13)
O1	0.0536 (12)	0.0750 (14)	0.0651 (14)	0.0274 (11)	0.0058 (11)	−0.0011 (11)
O2	0.0443 (11)	0.0443 (11)	0.0423 (11)	0.0114 (9)	0.0037 (9)	−0.0008 (9)
O3	0.0700 (13)	0.0590 (13)	0.0473 (12)	0.0196 (11)	0.0141 (10)	−0.0010 (10)
C1	0.0425 (16)	0.0382 (15)	0.0537 (18)	0.0032 (13)	0.0086 (14)	0.0007 (13)
C2	0.0557 (18)	0.0582 (19)	0.0551 (19)	0.0103 (15)	0.0147 (15)	−0.0021 (15)
C3	0.0611 (18)	0.0421 (16)	0.0461 (17)	0.0019 (14)	0.0100 (14)	−0.0056 (13)

C4	0.0510 (17)	0.0405 (16)	0.0440 (16)	0.0019 (13)	0.0042 (13)	0.0015 (13)
C5	0.0401 (15)	0.0287 (14)	0.0458 (16)	−0.0009 (12)	0.0094 (13)	−0.0019 (12)
C6	0.0412 (15)	0.0384 (15)	0.0443 (16)	0.0036 (13)	0.0080 (13)	−0.0006 (13)
C7	0.0403 (15)	0.0366 (14)	0.0406 (15)	0.0029 (12)	0.0055 (12)	0.0016 (12)
C8	0.0368 (14)	0.0372 (14)	0.0414 (15)	0.0022 (12)	0.0042 (12)	0.0033 (12)
C9	0.0350 (14)	0.0319 (14)	0.0423 (15)	0.0018 (11)	0.0057 (12)	0.0014 (12)
C10	0.089 (2)	0.0463 (18)	0.080 (2)	−0.0088 (17)	0.0093 (19)	−0.0055 (17)
C11	0.099 (3)	0.081 (2)	0.0485 (19)	0.012 (2)	0.0121 (18)	−0.0085 (17)
C12	0.0424 (16)	0.0452 (16)	0.0513 (18)	0.0116 (13)	−0.0026 (14)	−0.0085 (14)
C13	0.063 (2)	0.0516 (18)	0.062 (2)	0.0130 (16)	0.0028 (17)	0.0004 (16)
C14	0.098 (3)	0.053 (2)	0.064 (2)	0.017 (2)	−0.013 (2)	−0.0009 (17)
C15	0.091 (3)	0.093 (3)	0.090 (3)	0.049 (2)	−0.026 (3)	−0.016 (2)
C16	0.064 (2)	0.142 (4)	0.108 (4)	0.052 (3)	0.003 (3)	−0.019 (3)
C17	0.059 (2)	0.101 (3)	0.072 (2)	0.031 (2)	0.0102 (18)	−0.003 (2)
C18	0.0461 (16)	0.0393 (16)	0.0509 (17)	0.0018 (13)	0.0092 (14)	0.0022 (14)
C19	0.0503 (17)	0.0451 (16)	0.0396 (16)	0.0039 (13)	0.0071 (14)	−0.0016 (13)
C20	0.0542 (19)	0.063 (2)	0.059 (2)	−0.0079 (16)	0.0060 (16)	−0.0017 (16)
C21	0.0470 (19)	0.093 (3)	0.068 (2)	−0.0026 (18)	−0.0047 (18)	−0.015 (2)
C22	0.070 (2)	0.104 (3)	0.052 (2)	0.024 (2)	−0.0052 (19)	0.003 (2)
C23	0.073 (2)	0.104 (3)	0.057 (2)	0.023 (2)	0.0143 (18)	0.0295 (19)
C24	0.0537 (19)	0.082 (2)	0.0557 (19)	0.0118 (17)	0.0119 (16)	0.0130 (17)
C25	0.0522 (17)	0.0346 (14)	0.0424 (16)	0.0066 (13)	0.0129 (13)	0.0047 (12)
C26	0.0608 (19)	0.0441 (17)	0.0558 (18)	−0.0024 (15)	0.0170 (15)	0.0015 (14)
C27	0.086 (2)	0.050 (2)	0.077 (2)	−0.0123 (18)	0.032 (2)	0.0047 (18)
C28	0.129 (3)	0.0416 (19)	0.073 (2)	0.005 (2)	0.041 (2)	0.0112 (17)
C29	0.099 (3)	0.0466 (19)	0.0545 (19)	0.0207 (19)	0.0191 (19)	0.0126 (16)
C30	0.0639 (19)	0.0459 (17)	0.0520 (18)	0.0113 (15)	0.0119 (15)	0.0059 (14)

Geometric parameters (Å, °)

Cl1—C26	1.745 (3)	C12—C13	1.373 (4)
Cl2—C29	1.741 (3)	C12—C17	1.374 (4)
N1—C6	1.330 (3)	C13—C14	1.386 (4)
N1—C12	1.417 (3)	C13—H13	0.9300
N1—H1	0.95 (3)	C14—C15	1.366 (5)
O1—C1	1.222 (3)	C14—H14	0.9300
O2—C6	1.367 (3)	C15—C16	1.359 (5)
O2—C5	1.381 (3)	C15—H15	0.9300
O3—C18	1.252 (3)	C16—C17	1.376 (5)
C1—C9	1.458 (3)	C16—H16	0.9300
C1—C2	1.507 (4)	C17—H17	0.9300
C2—C3	1.525 (4)	C18—C19	1.498 (3)
C2—H2A	0.9700	C19—C24	1.376 (4)
C2—H2B	0.9700	C19—C20	1.383 (4)
C3—C11	1.525 (4)	C20—C21	1.388 (4)
C3—C10	1.533 (4)	C20—H20	0.9300
C3—C4	1.536 (4)	C21—C22	1.366 (4)
C4—C5	1.485 (3)	C21—H21	0.9300
C4—H4A	0.9700	C22—C23	1.365 (4)

C4—H4B	0.9700	C22—H22	0.9300
C5—C9	1.331 (3)	C23—C24	1.380 (4)
C6—C7	1.379 (3)	C23—H23	0.9300
C7—C18	1.433 (4)	C24—H24	0.9300
C7—C8	1.527 (3)	C25—C30	1.388 (3)
C8—C9	1.499 (3)	C25—C26	1.391 (3)
C8—C25	1.535 (3)	C26—C27	1.382 (4)
C8—H8	0.9800	C27—C28	1.373 (4)
C10—H10A	0.9600	C27—H27	0.9300
C10—H10B	0.9600	C28—C29	1.379 (4)
C10—H10C	0.9600	C28—H28	0.9300
C11—H11A	0.9600	C29—C30	1.377 (4)
C11—H11B	0.9600	C30—H30	0.9300
C11—H11C	0.9600		

C6—N1—C12	130.8 (3)	C13—C12—N1	123.5 (3)
C6—N1—H1	108.8 (17)	C17—C12—N1	116.3 (3)
C12—N1—H1	120.2 (17)	C12—C13—C14	119.7 (3)
C6—O2—C5	118.79 (18)	C12—C13—H13	120.2
O1—C1—C9	120.9 (2)	C14—C13—H13	120.2
O1—C1—C2	121.2 (2)	C15—C14—C13	120.2 (4)
C9—C1—C2	117.8 (2)	C15—C14—H14	119.9
C1—C2—C3	114.3 (2)	C13—C14—H14	119.9
C1—C2—H2A	108.7	C16—C15—C14	119.7 (4)
C3—C2—H2A	108.7	C16—C15—H15	120.1
C1—C2—H2B	108.7	C14—C15—H15	120.1
C3—C2—H2B	108.7	C15—C16—C17	121.0 (4)
H2A—C2—H2B	107.6	C15—C16—H16	119.5
C11—C3—C2	109.7 (2)	C17—C16—H16	119.5
C11—C3—C10	109.0 (2)	C12—C17—C16	119.5 (4)
C2—C3—C10	110.3 (2)	C12—C17—H17	120.2
C11—C3—C4	109.9 (2)	C16—C17—H17	120.2
C2—C3—C4	107.5 (2)	O3—C18—C7	123.7 (2)
C10—C3—C4	110.5 (2)	O3—C18—C19	116.8 (2)
C5—C4—C3	112.6 (2)	C7—C18—C19	119.4 (2)
C5—C4—H4A	109.1	C24—C19—C20	118.9 (3)
C3—C4—H4A	109.1	C24—C19—C18	118.1 (3)
C5—C4—H4B	109.1	C20—C19—C18	123.0 (3)
C3—C4—H4B	109.1	C19—C20—C21	119.7 (3)
H4A—C4—H4B	107.8	C19—C20—H20	120.1
C9—C5—O2	122.5 (2)	C21—C20—H20	120.1
C9—C5—C4	126.6 (2)	C22—C21—C20	120.6 (3)
O2—C5—C4	110.9 (2)	C22—C21—H21	119.7
N1—C6—O2	112.9 (2)	C20—C21—H21	119.7
N1—C6—C7	123.6 (3)	C23—C22—C21	119.8 (3)
O2—C6—C7	123.4 (2)	C23—C22—H22	120.1
C6—C7—C18	119.0 (2)	C21—C22—H22	120.1
C6—C7—C8	119.8 (2)	C22—C23—C24	120.2 (3)
C18—C7—C8	121.1 (2)	C22—C23—H23	119.9
C9—C8—C7	110.32 (19)	C24—C23—H23	119.9

C9—C8—C25	111.3 (2)	C19—C24—C23	120.8 (3)
C7—C8—C25	113.3 (2)	C19—C24—H24	119.6
C9—C8—H8	107.2	C23—C24—H24	119.6
C7—C8—H8	107.2	C30—C25—C26	116.9 (2)
C25—C8—H8	107.2	C30—C25—C8	118.7 (2)
C5—C9—C1	118.0 (2)	C26—C25—C8	124.3 (2)
C5—C9—C8	123.1 (2)	C27—C26—C25	121.8 (3)
C1—C9—C8	118.8 (2)	C27—C26—Cl1	116.7 (2)
C3—C10—H10A	109.5	C25—C26—Cl1	121.5 (2)
C3—C10—H10B	109.5	C28—C27—C26	120.2 (3)
H10A—C10—H10B	109.5	C28—C27—H27	119.9
C3—C10—H10C	109.5	C26—C27—H27	119.9
H10A—C10—H10C	109.5	C27—C28—C29	118.9 (3)
H10B—C10—H10C	109.5	C27—C28—H28	120.5
C3—C11—H11A	109.5	C29—C28—H28	120.5
C3—C11—H11B	109.5	C30—C29—C28	120.9 (3)
H11A—C11—H11B	109.5	C30—C29—Cl2	119.7 (3)
C3—C11—H11C	109.5	C28—C29—Cl2	119.4 (3)
H11A—C11—H11C	109.5	C29—C30—C25	121.3 (3)
H11B—C11—H11C	109.5	C29—C30—H30	119.4
C13—C12—C17	119.9 (3)	C25—C30—H30	119.4

O1—C1—C2—C3	−152.1 (3)	C12—C13—C14—C15	0.0 (5)
C9—C1—C2—C3	32.0 (3)	C13—C14—C15—C16	−1.4 (6)
C1—C2—C3—C11	−173.7 (2)	C14—C15—C16—C17	2.1 (6)
C1—C2—C3—C10	66.2 (3)	C13—C12—C17—C16	0.0 (5)
C1—C2—C3—C4	−54.2 (3)	N1—C12—C17—C16	−174.3 (3)
C11—C3—C4—C5	165.2 (2)	C15—C16—C17—C12	−1.4 (6)
C2—C3—C4—C5	45.8 (3)	C6—C7—C18—O3	−3.2 (4)
C10—C3—C4—C5	−74.5 (3)	C8—C7—C18—O3	172.1 (2)
C6—O2—C5—C9	−5.1 (3)	C6—C7—C18—C19	179.9 (2)
C6—O2—C5—C4	175.3 (2)	C8—C7—C18—C19	−4.8 (4)
C3—C4—C5—C9	−16.4 (4)	O3—C18—C19—C24	−67.0 (3)
C3—C4—C5—O2	163.2 (2)	C7—C18—C19—C24	110.1 (3)
C12—N1—C6—O2	12.1 (4)	O3—C18—C19—C20	112.9 (3)
C12—N1—C6—C7	−170.6 (3)	C7—C18—C19—C20	−70.0 (4)
C5—O2—C6—N1	−175.5 (2)	C24—C19—C20—C21	−0.7 (4)
C5—O2—C6—C7	7.2 (3)	C18—C19—C20—C21	179.5 (3)
N1—C6—C7—C18	1.1 (4)	C19—C20—C21—C22	0.1 (5)
O2—C6—C7—C18	178.2 (2)	C20—C21—C22—C23	0.3 (5)
N1—C6—C7—C8	−174.3 (2)	C21—C22—C23—C24	−0.3 (5)
O2—C6—C7—C8	2.8 (4)	C20—C19—C24—C23	0.7 (5)
C6—C7—C8—C9	−13.0 (3)	C18—C19—C24—C23	−179.5 (3)
C18—C7—C8—C9	171.7 (2)	C22—C23—C24—C19	−0.2 (5)
C6—C7—C8—C25	112.6 (3)	C9—C8—C25—C30	−117.1 (3)
C18—C7—C8—C25	−62.7 (3)	C7—C8—C25—C30	117.9 (3)
O2—C5—C9—C1	171.3 (2)	C9—C8—C25—C26	65.4 (3)
C4—C5—C9—C1	−9.1 (4)	C7—C8—C25—C26	−59.7 (3)
O2—C5—C9—C8	−7.2 (4)	C30—C25—C26—C27	−0.7 (4)
C4—C5—C9—C8	172.3 (2)	C8—C25—C26—C27	176.9 (3)

O1—C1—C9—C5	−174.8 (2)	C30—C25—C26—Cl1	179.1 (2)
C2—C1—C9—C5	1.2 (3)	C8—C25—C26—Cl1	−3.3 (4)
O1—C1—C9—C8	3.8 (4)	C25—C26—C27—C28	−0.3 (5)
C2—C1—C9—C8	179.8 (2)	Cl1—C26—C27—C28	179.8 (2)
C7—C8—C9—C5	15.5 (3)	C26—C27—C28—C29	1.0 (5)
C25—C8—C9—C5	−111.2 (3)	C27—C28—C29—C30	−0.5 (5)
C7—C8—C9—C1	−163.1 (2)	C27—C28—C29—Cl2	179.9 (3)
C25—C8—C9—C1	70.2 (3)	C28—C29—C30—C25	−0.6 (5)
C6—N1—C12—C13	34.3 (5)	Cl2—C29—C30—C25	179.0 (2)
C6—N1—C12—C17	−151.7 (3)	C26—C25—C30—C29	1.2 (4)
C17—C12—C13—C14	0.7 (4)	C8—C25—C30—C29	−176.6 (3)
N1—C12—C13—C14	174.6 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3	0.95 (3)	1.74 (3)	2.565 (3)	144 (3)
C4—H4B···O1^{i}	0.97	2.36	3.308 (3)	164
C13—H13···O2	0.93	2.50	2.915 (3)	108
C28—H28···O3^{ii}	0.93	2.49	3.329 (4)	150

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2; (ii) *x*, *y*+1, *z*.

Fig. 1

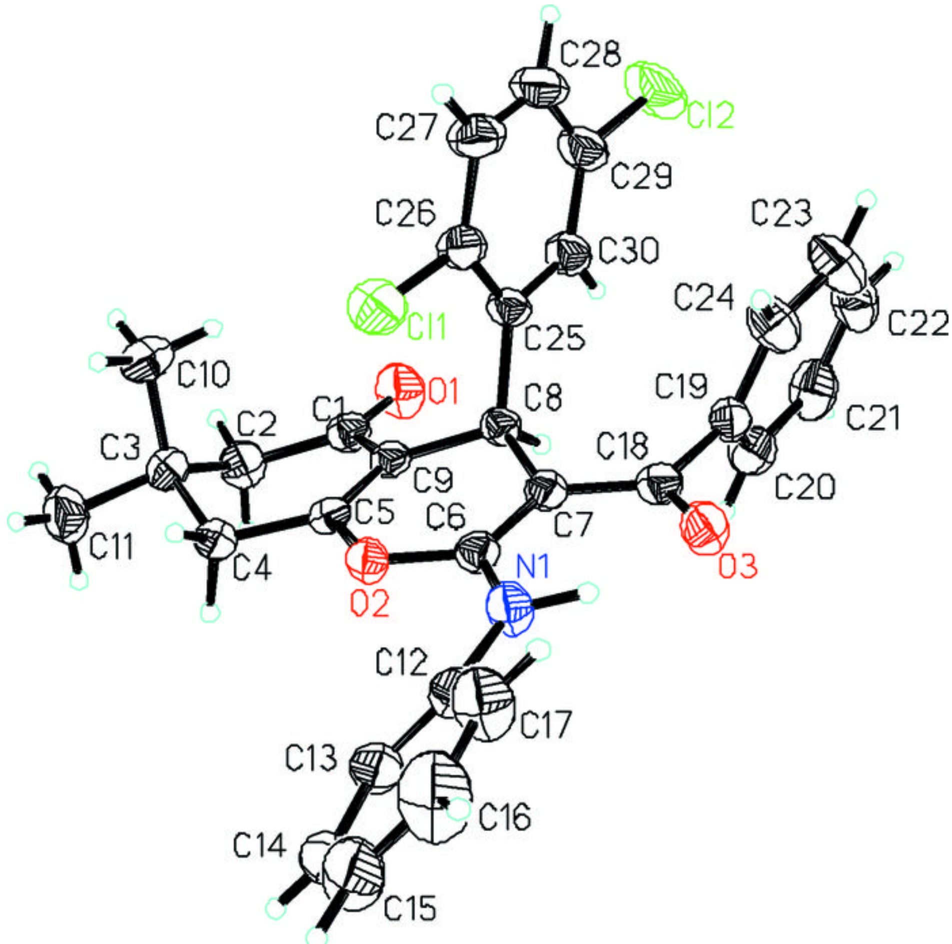
C28
Cl2
C27
C29
C26
C23
C30
C24
C22
Cl1
C25
C10
O1
C19
C21
C2
C1
C8
C3
C18
C9
C20
C11
C5
C6
C7
O3
C4
N1
O2
C12
C17
C13
C16
C14
C15

Fig. 2