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2-Chlorobenzoxazolo[3,2-*b*]isoquinolin-6-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.069
wR factor = 0.173
Data-to-parameter ratio = 11.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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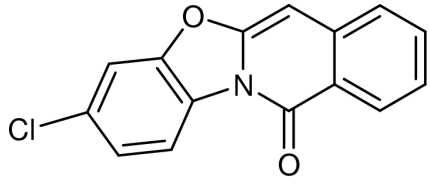
The title molecule, $C_{15}H_8ClNO_2$, is essentially planar. In the solid state, the molecules form sheet-like structures parallel to (011), which are stabilized by weak C—H···O hydrogen bonds and π–π interactions.

Comment

Tetrahydroisoquinoline compounds are of great interest because of their biological and pharmaceutical properties; they are also useful as key intermediates for the synthesis of isoquinoline alkaloids such as cherylline and latifine (Honda *et al.*, 2001). Isoquinoline fused-ring systems, such as pyrroloisoquinoline, show valuable pharmaceutical activities such as antileukemic (Anderson *et al.*, 1998), muscarinic agonistic (Loesel *et al.*, 1998) and antidepressant properties (Elwan *et al.*, 1996). The crystal structure determination of the title compound, (I), was undertaken as part of our studies on isoquinoline compounds.



(I)

The title molecule is essentially planar with the planar benzoxazole and isoquinoline moieties forming a dihedral angle of 3.8 (1)°. In the crystal, the molecules translated along the *a* cell axis are linked by weak C—H···O hydrogen bonds to form an infinite chain so that C5—H5 is 2.52 Å from O2^{i} with C5···O2^{i}, of 3.261 (4) Å, and the angle subtended at H5 is equal to 137° [symmetry code: (i) *x*−1, *y*, *z*]. The molecular chains form a sheet-like structure parallel to (011). Significant π–π interaction is observed between the centrosymmetrically related molecules of adjacent molecular sheets separated by a distance of 3.456 Å.

Experimental

Irradiation of *N*-(2,4-dichlorophenyl)-1,2,3,4-tetrahydroisoquinoline-1,3-dione (0.3 g, 0.00098 *M*) in a multilamp reactor using CH_3CN/NaOH (1 M) for 7 h gave the title compound (yield: 38%, m.p 473–475 K).

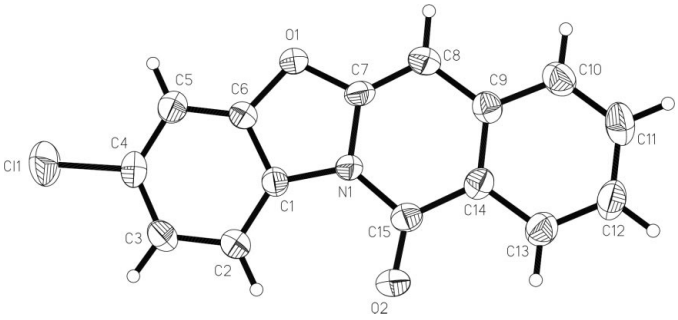


Figure 1
The structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_{15}H_8ClNO_2$
M_r = 269.67
Triclinic, $P\overline{1}$
a = 7.6104 (6) Å
b = 7.8699 (7) Å
c = 9.8571 (9) Å
α = 81.891 (2)°
β = 83.268 (2)°
γ = 85.499 (2)°
V = 579.29 (9) Å^3
Z = 2
D_x = 1.546 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2122 reflections
θ = 2.1–29.6°
μ = 0.33 mm^{-1}
T = 293 (2) K
Slab, yellow
0.28 × 0.20 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.915, T_{max} = 0.968
3273 measured reflections
1976 independent reflections
1244 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 25.0°
$h = -9 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.173
S = 0.93
1976 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.738 (3)	N1—C7	1.386 (4)
O1—C7	1.374 (4)	N1—C1	1.402 (4)
O1—C6	1.384 (4)	N1—C15	1.408 (4)
O2—C15	1.219 (4)	C7—C8	1.333 (5)
C6—O1—C7—C8	−178.6 (3)	O1—C7—C8—C9	177.3 (3)

After checking their presence in a difference map, all the H atoms were placed at geometrically calculated positions and a riding model was used for their refinement. Owing to weak reflections at higher angles, the completeness is only 0.97 even though the 2θ maximum was limited to 50°.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

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References

Anderson, W. K., Heiden, A. R., Raju, N. & Yucht, A. (1998). *J. Med. Chem.* **31**, 2097–2102.
Elwan, N. M., Abdelhadi, H. A., Abdallah, T. A. & Hassaheen, H. M. (1996). *Tetrahedron*, **52**, 3451–3456.
Honda, T., Namiki, H. & Satoh, F. (2001). *Org. Lett.* pp. 631–633.
Loesel, W., Roos, O. & Schnorrenberger, G. V. S. (1998). *Chem. Abstr.* **108**, 204513.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M.(1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and SAINT. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.