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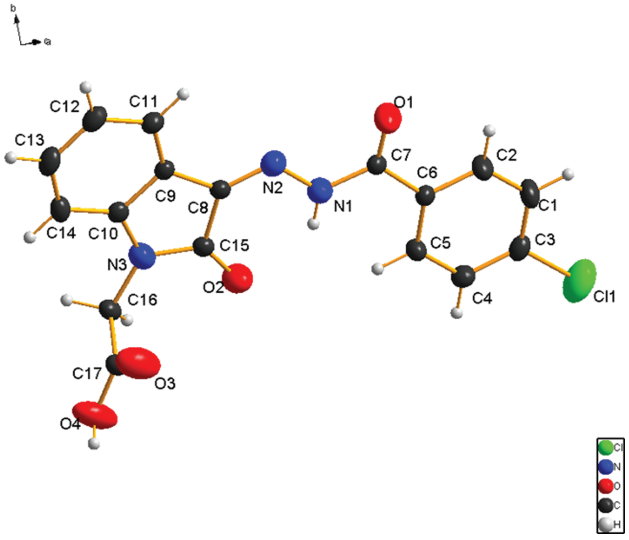
The crystal structure of (*Z*)-2-(3-(2-(4-chlorobenzoyl)hydrazono)-2-oxoindolin-1-yl) acetic acid, $C_{17}H_{12}ClN_3O_4$



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Abstract

$C_{17}H_{12}ClN_3O_4$, monoclinic, $P2_1/c$ (no. 14), $a = 6.8425(7)$ Å, $b = 14.1931(16)$ Å, $c = 17.0132(17)$ Å, $\beta = 101.044(3)°$, $V = 1621.1(3)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0522$, $wR_{ref}(F^2) = 0.1171$, $T = 296$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Firstly, the intermediates obtained by condensation reaction between indigo and bromoacetic acid, was proceeded by adding 1.5 times of potassium carbonate in ethanol.

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Table 1: Data collection and handling.

Crystal:	Colourless, block
Size:	0.35 × 0.28 × 0.25 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.26 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
$2\theta_{max}$, completeness:	28°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	17955, 4016, 0.048
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2688
$N(param)_{refined}$:	227
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.28395(9)	0.00012(5)	0.43180(4)	0.0721(2)
N1	0.3818(2)	0.20241(11)	0.32385(10)	0.0402(4)
N2	0.2120(2)	0.25468(11)	0.31215(9)	0.0392(4)
N3	−0.0960(2)	0.15407(11)	0.14138(10)	0.0405(4)
C1	1.0517(3)	0.14175(18)	0.46310(14)	0.0603(6)
C2	0.8770(3)	0.19258(17)	0.45154(13)	0.0554(6)
C3	1.0647(3)	0.06428(16)	0.41666(13)	0.0469(5)
C4	0.9090(3)	0.03775(16)	0.35745(13)	0.0502(5)
C5	0.7347(3)	0.08918(15)	0.34606(12)	0.0453(5)
C6	0.7156(3)	0.16680(13)	0.39347(11)	0.0372(4)
C7	0.5326(3)	0.22531(13)	0.38477(11)	0.0386(4)
C8	0.0763(3)	0.23082(13)	0.25198(11)	0.0370(4)
C9	−0.1187(3)	0.27454(13)	0.22948(11)	0.0367(4)
C10	−0.2217(3)	0.22477(13)	0.16341(11)	0.0378(4)
C11	−0.2103(3)	0.34700(14)	0.26253(13)	0.0455(5)
C12	−0.4060(3)	0.36814(16)	0.22934(14)	0.0531(6)
C13	−0.5054(3)	0.31775(18)	0.16452(14)	0.0559(6)
C14	−0.4168(3)	0.24494(16)	0.13005(12)	0.0487(5)
C15	0.0817(3)	0.15154(14)	0.19373(12)	0.0403(5)
C16	−0.1504(3)	0.08332(14)	0.07943(11)	0.0429(5)
C17	−0.2412(3)	−0.00254(14)	0.11004(12)	0.0433(5)
H1	0.3932	0.1555	0.2930	0.048*
H1A	1.1597	0.1600	0.5021	0.072*
H2	0.8676	0.2451	0.4833	0.067*
H4	−0.3259	−0.1140	0.0706	0.105*
H4A	0.9207	−0.0142	0.3254	0.060*
H5	0.6284	0.0715	0.3060	0.054*
H11	−0.1420	0.3808	0.3061	0.055*
H12	−0.4709	0.4165	0.2508	0.064*
H13	−0.6369	0.3333	0.1431	0.067*

Table 2 continued

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
H14	−0.4858	0.2113	0.0865	0.058*
H16A	−0.0327	0.0648	0.0593	0.051*
H16B	−0.2448	0.1102	0.0352	0.051*
O1	0.5192(2)	0.29076(10)	0.43043(9)	0.0537(4)
O2	0.2173(2)	0.09554(10)	0.19296(9)	0.0536(4)
O3	−0.2863(3)	−0.00781(12)	0.17362(10)	0.0692(5)
O4	−0.2618(3)	−0.07061(11)	0.05616(10)	0.0699(5)

Secondly, reduction of the intermediate with hydrazide in dichloromethane leads to the title compound. Yellow block-shaped crystals were obtained by slow evaporation of the solution containing the compound in air.

Experimental details

All hydrogen atoms were identified in difference Fourier syntheses and refined using the standard riding models of the SHELX system [2].

Discussion

Isatin derivatives possess a wide spectrum of biological activities like including anti-angiogenic, antineoplastic, anticonvulsant, antimicrobial, antituberculosis, antiviral and antimalarial activities [3–5]. Structure-activity relationships showed that isatin is an important regional center where α receptors combine with drugs basic center, and these compounds have α receptor blocking activity in different degrees. In addition, isatin connects with aromatic heterocyclic moieties or other carriers, it has nerve regulation and antiviral pharmacological activity [6, 7]. The molecular structure of the title compound shows a value of 2.2° for the dihedral angle between isatin and phenyl rings. The molecular conformation is stabilized by an intramolecular N—H···O hydrogen bond (N(1)–H(1)···O(2); *cf*. the figure).

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