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2-(2-Nitrophenyl)-4,5-benz-1,3-oxazin-6-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.105
Data-to-parameter ratio = 11.7

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

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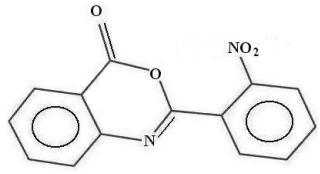
In the title compound, $C_{14}H_8N_2O_4$, the planar benzoxazinone moiety forms a dihedral angle of 54.54 (8)° with the phenyl ring. The crystal structure is stabilized by weak C—H···O hydrogen bonds and van der Waals interactions.

Comment

The preparation of several new 2-phenyl substituted phenyl benzoxazinones and evaluation of their biological activity against some pathogenic fungi and bacteria have been reported (Kumar *et al.*, 1977). A project has been undertaken by us to study the crystal structures of some of these benzoxazinones to establish their stereochemistry. The present paper reports the structure of the title compound, $C_{14}H_8N_2O_4$ (I), a benzoxazinone derivative.



(I)

A displacement ellipsoid plot of the molecule is shown in Fig. 1. The benzoxazinone moiety is essentially planar, with O2 deviating by a maximum of 0.037 (1) Å, and it forms a dihedral angle of 54.54 (8)° with the phenyl ring. The nitro group is twisted out of the phenyl ring plane by 19.63 (11)°. Although there is no —NH or —OH group available in the structure to form strong hydrogen bonds, the C atoms are involved in the formation of weak C—H···O hydrogen bonds with the O atoms O3 and O4 of the nitro group (Table 2 and Fig. 2). Some other short intermolecular contacts are listed in Table 3.

Experimental

The title compound was obtained by the reaction of *o*-nitrobenzoyl chloride with anthranilic acid at 273 K (Kumar *et al.*, 1977). The precipitate was recrystallized from EtOH/H_2O (4:1) as pale-yellow crystals.

Crystal data

$C_{14}H_8N_2O_4$
M_r = 268.22
Monoclinic, $P2_1/c$
a = 4.1824 (6) Å
b = 22.191 (2) Å
c = 12.767 (1) Å
β = 93.26 (1)°
V = 1183.0 (2) Å^3
Z = 4
D_x = 1.506 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 11.2–35.2°
μ = 0.96 mm^{-1}
T = 293 (2) K
Needle, light yellow
0.36 × 0.24 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.968, T_{max} = 0.999
2438 measured reflections
2130 independent reflections
1739 reflections with $I > 2\sigma(I)$

R_{int} = 0.014
θ_{max} = 67.7°
$h = 0 \rightarrow 5$
$k = 0 \rightarrow 26$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
S = 1.06
2130 reflections
182 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.4728P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0048 (6)

Table 1
Selected geometric parameters (Å, °).

C5—N1	1.401 (2)	C8—O2	1.366 (2)
C7—O1	1.193 (2)	C14—N2	1.469 (2)
C7—O2	1.392 (2)	N2—O3	1.213 (2)
C8—N1	1.265 (2)	N2—O4	1.216 (2)
O1—C7—O2	117.08 (17)	O2—C8—C9	112.39 (14)
O1—C7—C6	127.93 (17)	O3—N2—O4	123.76 (17)
N1—C8—O2	126.33 (15)	O3—N2—C14	118.43 (15)
N1—C8—C9—C10	−54.3 (2)	C13—C14—N2—O3	158.17 (18)
O2—C8—C9—C10	121.85 (18)	C9—C14—N2—O3	−18.0 (3)
N1—C8—C9—C14	127.61 (19)	C13—C14—N2—O4	−20.3 (3)
O2—C8—C9—C14	−56.3 (2)	C9—C14—N2—O4	163.51 (19)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{iv}	0.93	2.75	3.434 (2)	131
C12—H12···O1^{v}	0.93	2.91	3.470 (3)	120
C13—H13···O1^{v}	0.93	2.68	3.353 (2)	130
C12—H12···O3^{vi}	0.93	2.61	3.386 (2)	141
C11—H11···O4^{vi}	0.93	2.79	3.633 (3)	151
C2—H2···O4^{vii}	0.93	2.84	3.342 (3)	115
C3—H3···O4^{vii}	0.93	2.53	3.189 (2)	129

Symmetry codes: (iv) $-x, -y, -z$; (v) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (vi) $x-1, \frac{1}{2}-y, \frac{1}{2}+z$; (vii) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$.

Table 3
Some short inter-molecular contacts shorter than 3.5 Å.

N1···C10^{i}	3.353 (3)	O3···C9^{i}	3.200 (3)
O2···O3^{ii}	3.045 (3)	O3···C14^{i}	3.103 (3)
O2···C5^{ii}	3.485 (3)	O4···C11^{iii}	3.245 (3)

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

After checking their presence in a difference map, all the H atoms were positioned geometrically and were treated as riding on their aromatic parent C atoms, with C—H = 0.93 Å.

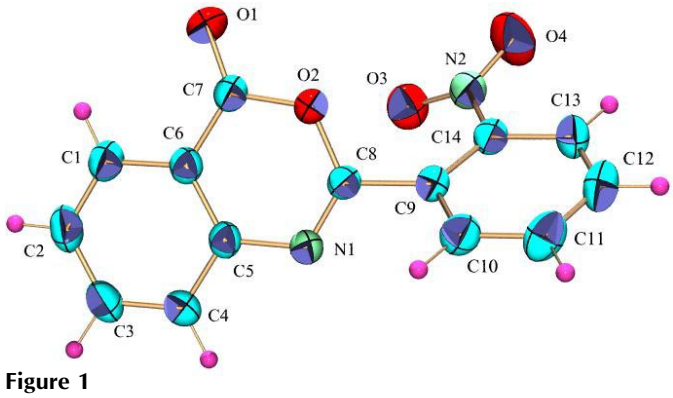


Figure 1
An *ORTEP*-3 plot (Farrugia, 1997) of the molecule, with 50% probability displacement ellipsoids for non-H atoms.

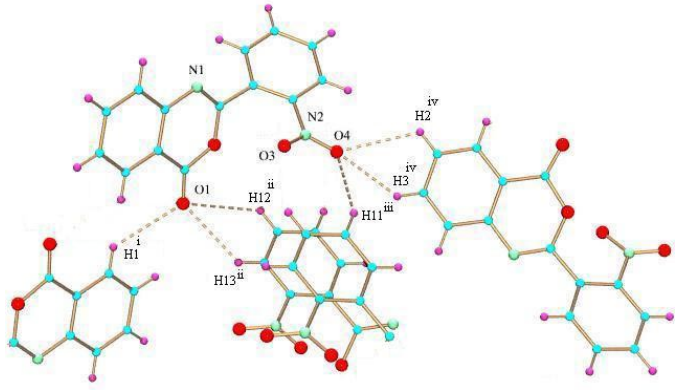


Figure 2
A view of the weak C—H···O hydrogen bonds in the title compound. Symmetry codes: (i) $-x, -y, -z$, (ii) $x, \frac{1}{2}-y, \frac{1}{2}+z$ (iii) $= 1+x, \frac{1}{2}-y, \frac{1}{2}+z$ and (iv) $= 1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MoLEN* (Fair,1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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