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Methyl 2-[3-(2-chlorophenyl)-1,2,4-oxadiazol-5-ylmethoxy]phenylacetate

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Key indicators

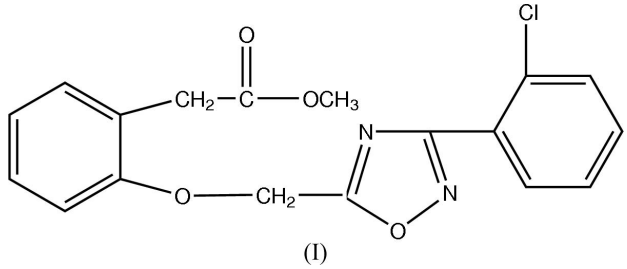
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.060
wR factor = 0.150
Data-to-parameter ratio = 13.3

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

The title compound, $C_{18}H_{15}ClN_2O_4$, was synthesized by the reaction of methyl (2-hydroxyphenyl)acetate and 5-chloromethyl-3-(2-chlorophenyl)1,2,4-oxadiazole. In the crystal structure, there are a weak intramolecular C—H···N hydrogen bond and intermolecular C—H···O and C—H···π interactions.

Comment

1,2,4-Oxadiazole derivatives are of great interest because of their biological properties. Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and anti-picornaviral (Romero, 2001) properties and show high efficacy as agonists [*e.g.* for formuscarinic (Macor *et al.*, 1996), adrenergic (Quagliato & Andrae, 2002), and 5-hydroxytryptamine (Gur *et al.*, 2001)] and antagonists [*e.g.* for forangiotensin (Naka & Kubo (1999) and adhesion (Juraszyk *et al.*, 1997)] for different receptors. We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is stabilized by a weak intramolecular C—H···N hydrogen bond. The molecular packing in the crystal structure is stabilized by intermolecular C—H···O and C—H···π interactions (Table 2 and Fig. 2).

Experimental

Methyl (2-hydroxyphenyl)acetate (20 mmol) was dissolved in acetone (20 ml) and potassium carbonate (30 mmol) was added in one portion. 5-Chloromethyl-3-(2-chlorophenyl)1,2,4-oxadiazole (20 mmol) in acetone (20 ml) was added to this mixture. The resulting mixture was refluxed for 6 h, then concentrated under reduced pressure to afford crude compound (I). Pure (I) was obtained by crystallization from ethyl acetate (m.p. 341–343 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. ^{1}H NMR ($CDCl_3$): δ 7.92–7.94 (*m*, 1H), 7.53–7.54 (*m*, 1H), 7.42–7.45 (*m*, 1H), 7.37–7.40 (*m*, 1H), 7.23–7.29 (*m*, 2H), 6.99–7.03 (*m*, 2H), 5.39 (*s*, 2H), 3.73 (*s*, 2H), 3.69 (*s*, 3H).

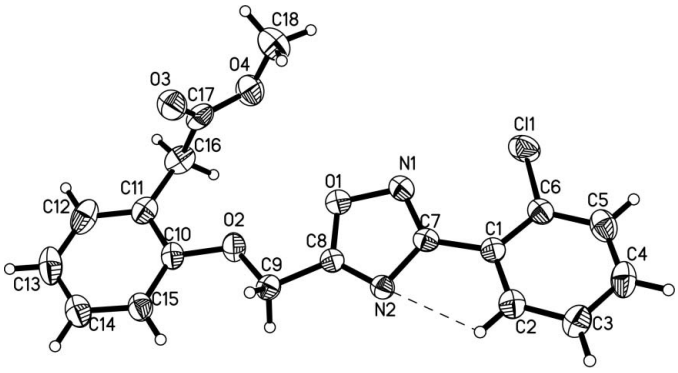


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates a hydrogen bond.

Crystal data

$C_{18}H_{15}ClN_2O_4$
M_r = 358.77
Monoclinic, $P2_1/c$
a = 11.314 (2) Å
b = 7.9510 (16) Å
c = 19.598 (4) Å
β = 103.08 (3)°
V = 1717.2 (6) Å^3
Z = 4
D_x = 1.388 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–13°
μ = 0.25 mm^{-1}
T = 293 (2) K
Block, colourless
0.3 × 0.2 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
3191 measured reflections
3028 independent reflections
1559 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.0°
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 9$
$l = -23 \rightarrow 22$
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.06
$wR(F^2)$ = 0.15
S = 0.98
3028 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.455 (5)	C10—O2	1.381 (4)
C6—Cl1	1.719 (4)	C11—C16	1.495 (5)
C7—N1	1.303 (4)	C16—C17	1.501 (5)
C7—N2	1.390 (4)	C17—O3	1.211 (4)
C8—N2	1.274 (4)	C17—O4	1.322 (5)
C8—O1	1.327 (4)	C18—O4	1.439 (5)
C8—C9	1.498 (4)	N1—O1	1.420 (4)
C9—O2	1.401 (4)		
C2—C1—C7	118.0 (3)	O2—C10—C15	124.2 (3)
C6—C1—C7	125.2 (3)	O2—C10—C11	114.4 (3)
C5—C6—Cl1	117.4 (3)	C12—C11—C16	123.7 (4)
C1—C6—Cl1	122.4 (3)	C10—C11—C16	119.4 (3)
N1—C7—N2	113.2 (3)	C11—C16—C17	113.8 (3)
N1—C7—C1	125.4 (3)	O3—C17—O4	123.2 (4)
N2—C7—C1	121.3 (3)	C7—N1—O1	103.8 (3)
N2—C8—O1	114.9 (3)	C8—N2—C7	102.7 (3)
N2—C8—C9	127.6 (3)	C8—O1—N1	105.3 (2)
O1—C8—C9	117.4 (3)	C10—O2—C9	119.6 (3)
O2—C9—C8	107.1 (3)	C17—O4—C18	116.5 (4)

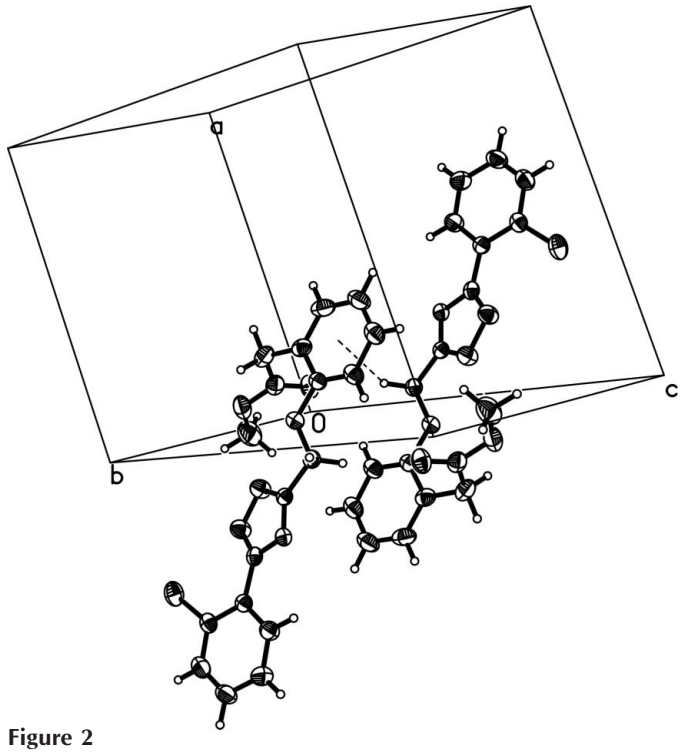


Figure 2
The C—H···π interaction in (I), shown as a dashed line.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N2	0.93	2.47	2.838 (4)	104
C9—H9B···*Cg*1^{i}	0.97	2.82	3.588 (4)	137
C15—H15···O3^{i}	0.93	2.54	3.349 (5)	146
C18—H18*B*···O3^{ii}	0.96	2.59	3.541 (6)	172

Symmetry codes: (i) $2-x, 1-y, 1-z$; (ii) $2-x, \frac{1}{2}+y, \frac{1}{2}-z$. Note: *Cg*1 is the centroid of ring C10–C15

All H atoms were positioned geometrically, with C—H distances of 0.93–0.97 Å, and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2 or 1.5U_{eq} of the carrier atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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