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Methyl 2-(2-{1-[3-(4-bromophenyl)-1,2,4-oxadiazol-5-yl]-2-(dimethylamino)vinyloxy}phenyl)-3-(dimethylamino)acrylate

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Key indicators

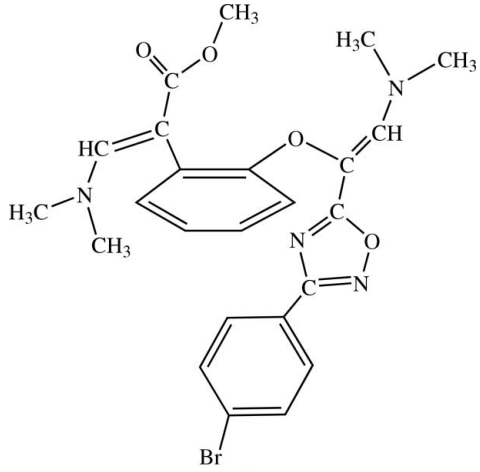
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.069
wR factor = 0.172
Data-to-parameter ratio = 15.2

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

The title compound, $C_{24}H_{25}ClN_4O_4$, was obtained from the reaction of methyl 2-{[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]methoxy}phenylacetate with *N*,*N*-dimethylformamide dimethyl acetal. The molecules interact through weak C—H···O intermolecular hydrogen bonds to form a zigzag chain parallel to the *bc* plane.

Comment

1,2,4-Oxadiazoles represent an important class of five-membered heterocycles. Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties and also may function as agonists [*e.g.* for angiotensin (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 shown in Fig. 1. The most interesting feature is the occurrence of a weak C—H···O hydrogen-bonding interaction (Table 1), leading to the formation of a zigzag chain parallel to the *bc* plane (Fig. 2).

Experimental

Methyl 2-{[3-(2-bromophenyl)-1,2,4-oxadiazol-5-yl]methoxy}phenylacetate (14 mmol) was dissolved in dimethylformamide (20 ml) and *N*,*N*-dimethylformamide dimethyl acetal (8 ml) was added in one portion. The resulting mixture was refluxed for 6 h, then concentrated under reduced pressure to afford crude compound (I). Pure compound (I) was obtained by recrystallization from ethyl acetate and petroleum ether (2:1). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{24}H_{25}BrN_4O_4$
M_r = 513.39
Monoclinic, $P2_1/n$
a = 15.479 (3) Å
b = 8.5690 (17) Å
c = 17.919 (4) Å
β = 98.37 (3)°
V = 2351.5 (9) Å^3
Z = 4
D_x = 1.450 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.79 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.535, T_{max} = 0.842
4779 measured reflections
4603 independent reflections
1956 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.172
S = 1.00
4603 reflections
303 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.032
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.43	3.274 (7)	152
C17—H17···O3^{ii}	0.93	2.51	3.327 (7)	147

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

All H atoms were treated as riding on their parent C atoms with distances of 0.96 (CH_3) and 0.93 Å (CH), with U_{iso}(H) = 1.2U_{eq}(CH) or 1.5U_{eq}(CH_3).

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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

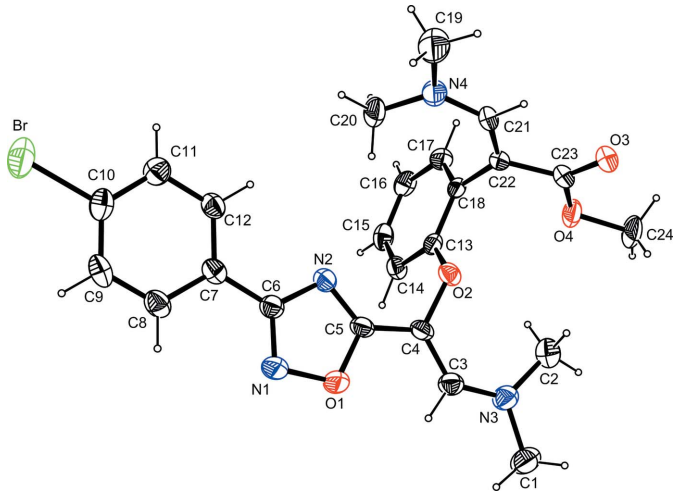


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii.

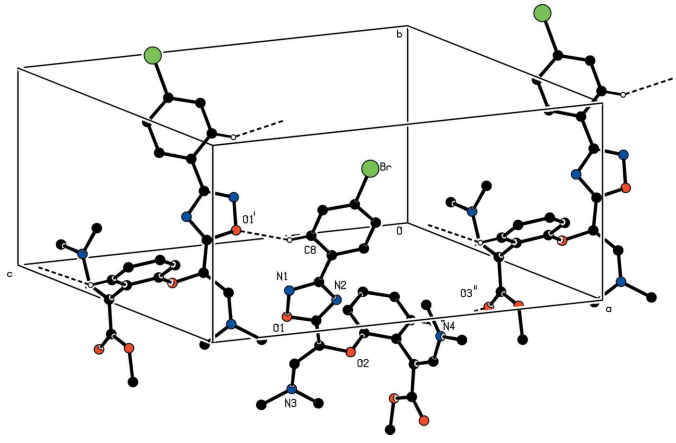


Figure 2
Partial packing view showing the C—H···O hydrogen-bonding interactions. Hydrogen bonds are represented by dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (ii) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$].

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