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N-(2,6-Dimethylphenyl)-2-{2-[3-(3-methoxyphenyl)-1,2,4-oxadiazol-5-yl]phenoxy}acetamide

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In the title compound, $C_{25}H_{23}N_3O_4$, a bifurcated intramolecular N—H···(O,N) hydrogen bond helps to establish the molecular conformation.

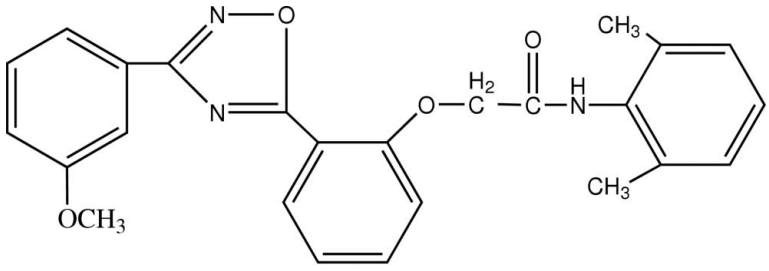
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.059
wR factor = 0.169
Data-to-parameter ratio = 14.8

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

Comment

1,2,4-Oxadiazole derivatives possess biological properties, such as intrinsic analgesic (Terashita *et al.*, 2002) and anti-picornaviral (Romero, 2001) effects. As part of our studies in this area, we report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).



(I)

The dihedral angles between the N1/O2/C9/N2/C8 ring and the attached benzene rings are 7.40 (19) and 4.10 (18)° for the C10–C15 and C2–C7 rings, respectively.

An intramolecular bifurcated N—H···(N,O) hydrogen bond (Table 2) helps to establish the molecular conformation of (I). Three short acute intramolecular C—H···O,N close contacts also occur.

Experimental

2-Chloro-*N*-(2,6-dimethylphenyl)acetamide (10 mmol) was dissolved in acetone (100 ml) and potassium carbonate (15 mmol) was added, followed by 5-(2-hydroxyphenyl)-3-(3-methoxyphenyl)-1,2,4-oxadiazole (10 mmol). The resulting mixture was refluxed for 12 h. After cooling and filtration, the crude title compound was obtained; it was purified by recrystallization from ethyl acetate. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{25}H_{23}N_3O_4$
M_r = 429.46
Triclinic, $P\overline{1}$
a = 8.0360 (16) Å
b = 11.692 (2) Å
c = 12.780 (3) Å
α = 66.93 (3)°
β = 85.56 (3)°
γ = 81.18 (3)°
V = 1091.5 (4) Å^3
Z = 2
D_x = 1.307 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.974, T_{max} = 0.991
4271 measured reflections
4271 independent reflections
2740 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.169
S = 1.07
4271 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0809P)^2 + 0.1494P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19A···N3	0.96	2.42	2.893 (4)	110
C18—H18A···N3	0.96	2.40	2.873 (4)	110
C11—H11A···O2	0.93	2.41	2.741 (3)	101
N3—H3A···N2	0.86	2.53	3.385 (3)	179
N3—H3A···O3	0.86	2.12	2.543 (3)	110

All H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C).

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: *PLATON* (Spek, 2003).

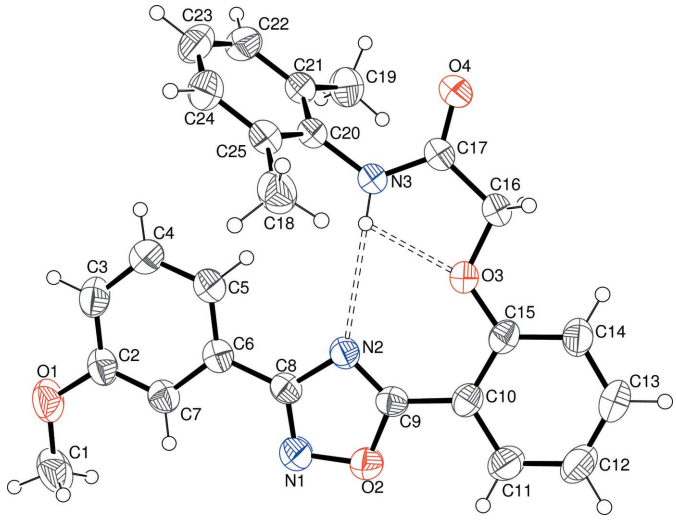


Figure 1
A view of the molecular structure of (I), showing 40% displacement ellipsoids (arbitrary spheres for the H atoms). Dashed lines indicate hydrogen bonds.

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