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

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In the title compound, $C_{24}H_{20}FN_3O_3$, a bifurcated intramolecular N—H···(O,N) hydrogen bond helps to establish the molecular conformation.

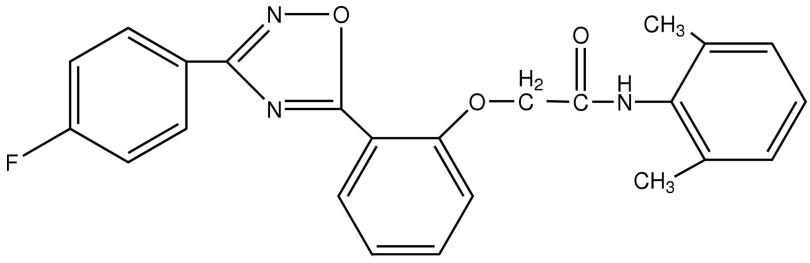
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.062
wR factor = 0.182
Data-to-parameter ratio = 14.9

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 N2/C18/N3/C17/O4 ring in (I) and its adjacent benzene rings are 10.50 (19) and 12.30 (18)° for the C19 and C11 rings, respectively.

An intramolecular bifurcated N—H···(N,O) hydrogen bond (Table 2) helps to establish the molecular conformation of (I). Some short intra- and intermolecular C—H···O contacts are also present.

Experimental

2-Chloro-*N*-(2,6-dimethylphenyl)acetamide (10 mmol) was dissolved in acetone (100 ml) and potassium carbonate (15 mmol) was added. 5-(2-Hydroxyphenyl)-3-(4-fluorophenyl)phenyl-1,2,4-oxadiazole (10 mmol) was then added to the reaction and the resulting mixture was refluxed for 12 h. After cooling and filtration, the crude title compound was obtained and 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

$C_{24}H_{20}FN_3O_3$
M_r = 417.43
Monoclinic, $P2_1/n$
a = 12.143 (2) Å
b = 8.1850 (16) Å
c = 20.942 (4) Å
β = 90.52 (3)°
V = 2081.3 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.962, T_{max} = 0.981
4269 measured reflections
4071 independent reflections
2335 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.182
S = 1.10
4071 reflections
274 parameters
29 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10B···O1^{i}	0.97	2.50	3.166 (4)	126
C8—H8C···O1	0.96	2.56	3.265 (5)	130
C1—H1B···N1	0.96	2.36	2.838 (4)	110
N1—H1A···N3	0.86	2.37	3.223 (4)	171
N1—H1A···O2	0.86	2.12	2.557 (3)	111

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

All H atoms were positioned geometrically, with 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}(C) for methyl H.

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).

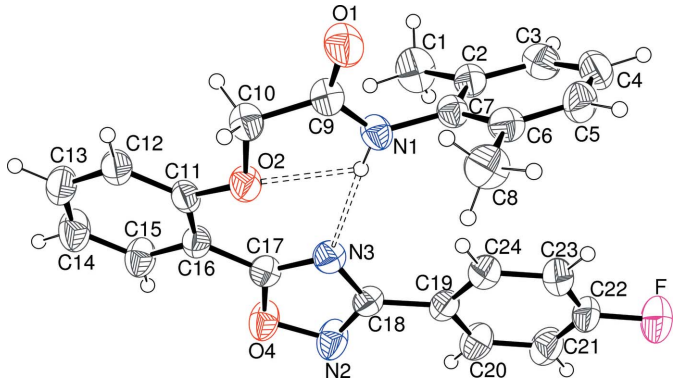


Figure 1
A view of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level (arbitrary spheres for H atoms). Double dashed lines indicate the bifurcated N—H···(O,N) hydrogen bond.

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