organic papers

# 2-{2-[3-(4-Chlorophenyl)-1,2,4-oxadiazol-5-yl]-phenoxy}-N-(2,6-dimethylphenyl)acetamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.064
wR factor = 0.160
Data-to-parameter ratio = 15.1

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

In the title compound, $C_{24}H_{20}ClN_3O_3$, a bifurcated intra-molecular N—H···(O,N) hydrogen bond helps to establish the molecular conformation.

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)
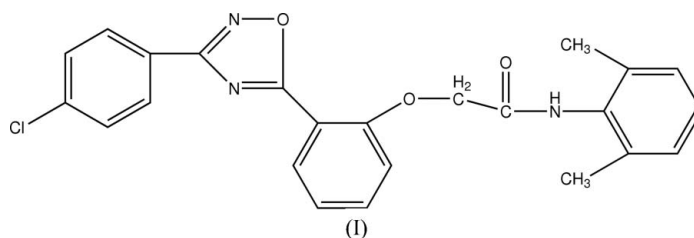
The geometric parameters for (I) are normal. The dihedral angles between the C17/C18/N2/N3/O3 ring and its adjacent benzene rings are 9.78 (19) and 10.77 (18)° for the C11 and C19 rings, respectively.

An intramolecular bifurcated N—H···(O,N) hydrogen bond (Table 1) helps to establish the molecular conformation of (I). A short C—H···O intermolecular contact is 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-chloro)phenyl-1,2,4-oxadiazole (10 mmol) was then added to the reaction. The resulting mixture was refluxed for 10 h. After cooling and filtering, the crude title compound was obtained and this 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

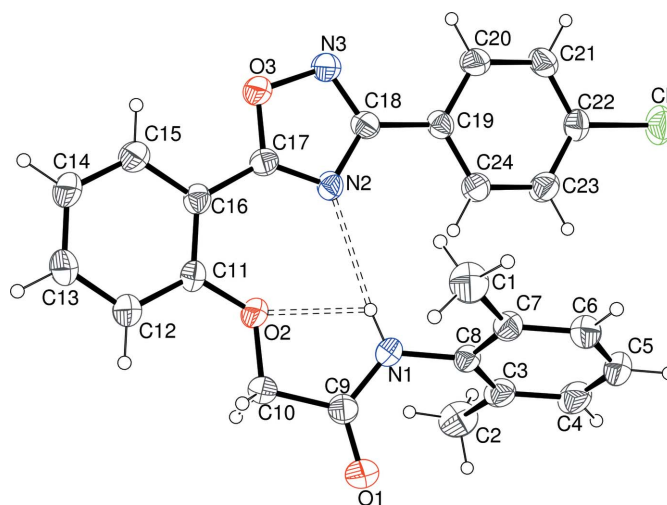|	
$C_{24}H_{20}ClN_3O_3$	$Z = 4$
$M_r = 433.88$	$D_x = 1.335$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 12.498$ (3) Å	$\mu = 0.21$ mm^{-1}
$b = 8.2410$ (16) Å	$T = 293$ (2) K
$c = 20.996$ (4) Å	Block, colourless
$\beta = 93.21$ (3)°	$0.30 \times 0.20 \times 0.10$ mm
$V = 2159.1$ (7) Å^3	

Data collection

Enraf–Nonius CAD-4
  diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan
  (North *et al.*, 1968)
  $T_{min} = 0.940$, $T_{max} = 0.980$
4239 measured reflections

4239 independent reflections
2179 reflections with $I > 2\sigma(I)$
$\theta_{max} = 26.0°$
3 standard reflections
  every 200 reflections
  intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.160$
$S = 1.00$
4239 reflections
280 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots N2$	0.86	2.40	3.254 (4)	170
$N1-H1A\cdots O2$	0.86	2.13	2.558 (3)	111
$C10-H10B\cdots O1^i$	0.97	2.46	3.159 (5)	128

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 and C—H = 0.93–0.96 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}$(carrier) or $1.5U_{eq}$(methyl carrier).

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 30% probability level and H atoms are shown as small spheres of arbitrary radii. Dashed lines indicate the hydrogen bonds.

References

Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Romero, J. R. (2001). *Exp. Opin. Invest. Drugs*, **10**, 369–379.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Terashita, Z., Naruo, K. & Morimoto, S. (2002). PCT Int. Appl. WO 02060439.