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1-{[3-(4-Bromophenyl)-1,2,4-oxadiazol-5-yl]-methyl}-4-[(2,6-dimethylphenyl)aminocarbonyl-methyl]piperazine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.014 Å
R factor = 0.090
wR factor = 0.264
Data-to-parameter ratio = 14.1

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

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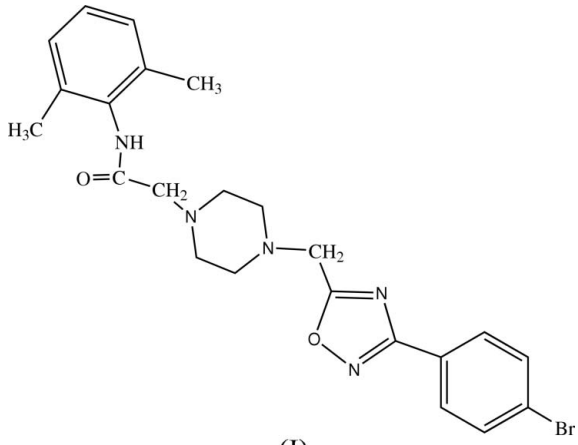
The title compound, $C_{23}H_{26}BrN_5O_2$, was synthesized by the reaction of 4-[(2,6-dimethylphenyl)aminocarbonylmethyl]-piperazine and 3-(3-nitrophenyl)-5-chloromethyl-1,2,4-oxadiazole. There are intramolecular C—H···N and intermolecular N—H···O and C—H···O hydrogen bonds in the crystal structure.

Comment

Piperazine derivatives are of great interest because of their biological properties. Some derivatives of piperazine have antifilarial, anti-amoebic and spermicidal properties (Sonurlikar *et al.*, 1977). Some show high efficacy in preventing neuronal damage or stimulating nerve growth (Tomlinson *et al.*, 2004). Some are used to treat psychosis and bipolar disorders (Aicher *et al.*, 2004) or are neurokinin antagonists (Janssens *et al.*, 2004).



(I)

The molecular structure of the title compound, (I), is shown in Fig. 1. The crystal packing is stabilized by C—H···N, N—H···O and C—H···O hydrogen bonds (Table 1).

Experimental

4-[(2,6-Dimethylphenyl)aminocarbonylmethyl]piperazine (20 mmol) and 3-phenyl-5-chloromethyl-1,2,4-oxadiazole (20 mmol) were dissolved in anhydrous ethanol (80 ml). The resulting mixture was refluxed for 6 h. Subsequent concentration of the mixture under reduced pressure afforded the crude compound. Pure compound (I) was obtained by recrystallization from ethyl acetate. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{23}H_{26}BrN_5O_2$
M_r = 484.40
Monoclinic, $P2_1/c$
a = 7.2000 (14) Å
b = 9.5300 (19) Å
c = 33.089 (7) Å
β = 94.71 (3)°
V = 2262.8 (8) Å^3
Z = 4
D_x = 1.422 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.85 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 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} = 0.607, T_{max} = 0.837
4309 measured reflections
3966 independent reflections
2155 reflections with $I > 2\sigma(I)$
R_{int} = 0.105
θ_{max} = 25.0°
3 standard reflections
every 200 reflections
intensity decay: 3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.090
$wR(F^2)$ = 0.264
S = 0.97
3966 reflections
281 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 21P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.015 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.21	3.047 (9)	163
C7—H7A···N1	0.96	2.45	2.909 (12)	109
C8—H8A···N1	0.96	2.33	2.825 (12)	111
C10—H10B···O1^{i}	0.97	2.55	3.309 (10)	135
C23—H23A···N5	0.93	2.49	2.816 (13)	101

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

All H atoms bonded to the C atoms were positioned geometrically, with C—H distances in the range 0.93–0.96 Å, and they were included in the refinement in a riding-model approximation, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). The N-bound H atom was also positioned geometrically and refined as riding, with N—H = 0.86 Å and with U_{iso}(H) = 1.2U_{eq}(N).

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*.

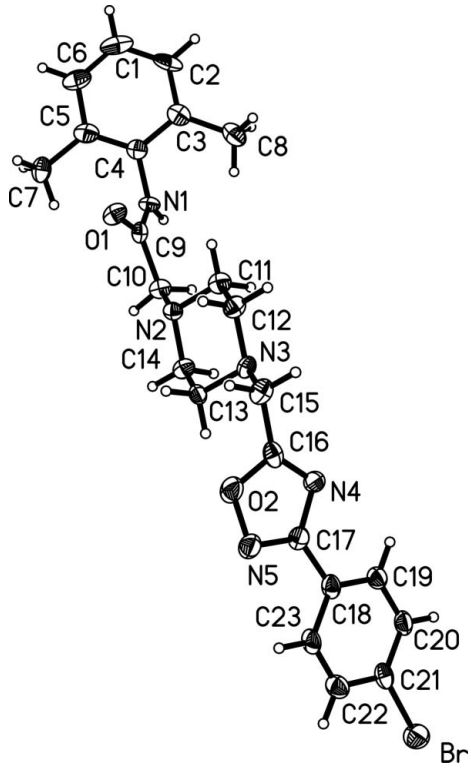


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

References

Aicher, T. D., Chen, Z., Le Huerou, Y., Martin, F. M., Pineiro-Nunez, M. M., Rocco, V. P., Ruley, K. M., Schaus, J. M., Spinazze, P. G. & Tupper, D. (2004). World Patent WO 2004014895.

Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.

Janssens, F. E., Sommen, F. M., De Boeck, B. C. A. G., Leenaerts, J. E., Van Roosbroeck, Y. E. M. & Diels, G. S. M. (2004). World Patent WO 2004033428.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

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.

Sonurlikar, U. A., Shanker, B., Kirke, P. A. & Bhide, M. B. (1977). *Bull. Haffkine Inst.* **5**, 94–96.

Tomlinson, R., Lauffer, D. & Mulican, M. (2004). US Patent 2004034019.