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4-(2-Chloro-4-nitrophenoxy)-*N*-[2-(4,6-dimethoxypyrimidin-2-yloxy)benzyl]aniline

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Key indicators

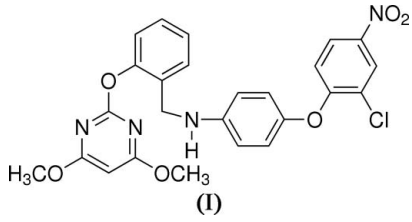
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.140
Data-to-parameter ratio = 16.7

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

In the title molecule, $C_{25}H_{21}Cl_1N_4O_6$, all bond lengths and angles show normal values. Weak intermolecular C—H···Cl hydrogen bonds link the molecules into chains extending along the crystallographic *c* axis. The crystal packing is further stabilized by van der Waals forces.

Comment

The derivatives of diphenyl ether show high herbicidal activities (Motoo *et al.*, 1995; Arnould *et al.*, 1998). The title compound, (I), has been prepared as a new herbicide. We report here its crystal structure.



(I)

In (I) (Fig. 1), the bond lengths and angles show normal values. The benzene C1–C6 (*A*), C7–C12 (*B*), C14–C19 (*C*) and pyrimidine (*D*) rings make the following dihedral angles: *A*/*B* = 80.93 (6)°, *B*/*C* = 82.73 (7)° and *C*/*D* = 85.70 (7)°.

Weak intermolecular C—H···Cl hydrogen bonds (Table 1) link the molecules into chains extending along the *c* axis. The crystal structure is further stabilized by van der Waals forces.

Experimental

A mixture of 2-((4-(2-chloro-4-nitrophenoxy)phenylamino)methyl)phenol (0.20 g, 0.5 mmol), 2-methanesulfonyl-4,6-dimethoxypyrimidine (0.13 g, 0.5 mmol), and K_2CO_3 (0.14 g, 1.0 mmol) in THF (40 ml) was refluxed for 8 h. After the insoluble substance had been removed from the mixture by filtration, the organic layer was evaporated *in vacuo* to give the crude product. Recrystallization of the crude product from ethanol gave yellow crystals (m.p. 391.3–392.2 K).

Crystal data

$C_{25}H_{21}ClN_4O_6$
M_r = 508.91
Triclinic, $P\overline{1}$
a = 9.524 (4) Å
b = 11.064 (4) Å
c = 12.334 (7) Å
α = 88.869 (17)°
β = 70.14 (2)°
γ = 83.410 (19)°
V = 1214.0 (10) Å^3
Z = 2
D_x = 1.392 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8448 reflections
θ = 3.1–27.5°
μ = 0.21 mm^{-1}
T = 298 (1) K
Chunk, yellow
0.32 × 0.20 × 0.18 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
ω scans
Absorption correction: multi-scan *ABSCOR* (Higashi, 1995)
T_{min} = 0.928, T_{max} = 0.964
11829 measured reflections
5464 independent reflections
3282 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°
$h = -10 \rightarrow 12$
$k = -14 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.140
S = 1.05
5464 reflections
327 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13A···Cl1^{i}	0.97	2.69	3.600 (3)	156

Symmetry code: (i) $x, y, z + 1$.

Atom H1, attached to N1, was located in a difference Fourier map and refined as riding in its as-found relative position, with a fixed U_{iso} of 0.08 Å^2. The C-bound H atoms were placed in calculated positions, with C—H = 0.93 Å (aromatic), 0.96 Å (methyl group) and 0.97 Å (methylene group), and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) for aromatic and methylene H atoms or 1.5U_{eq}(C) for methyl.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC and Rigaku Corporation, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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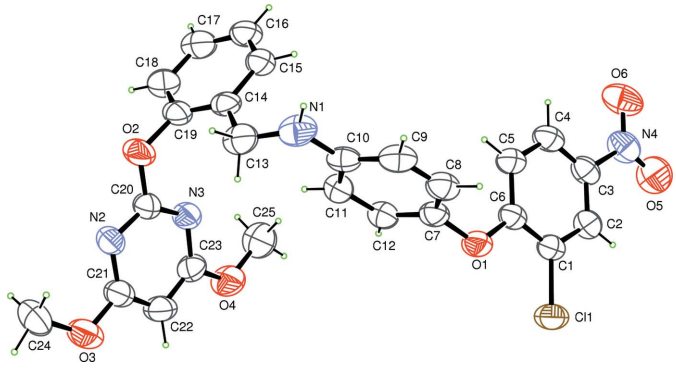

Figure 1
The molecular structure of (I), with 40% probability displacement ellipsoids.

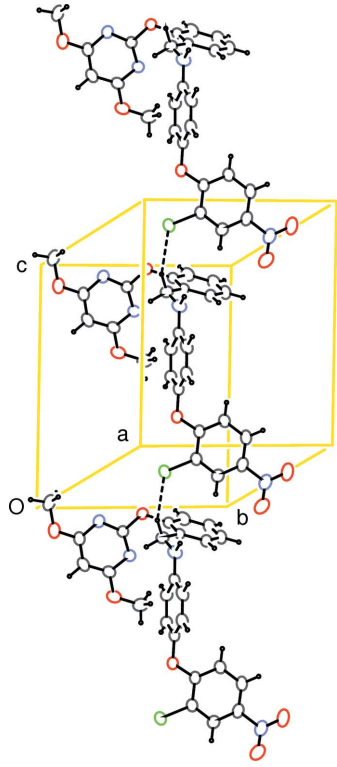

Figure 2
The packing of (I), showing the weak intermolecular C—H···Cl hydrogen bonds as dashed lines.

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