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(*E*)-Methyl 2-[2-(6-chloropyrimidin-4-yloxy)-phenyl]-3-methoxyacrylate

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In the molecule of the title compound, $C_{15}H_{13}ClN_2O_4$, the pyrimidine and benzene rings form a dihedral angle of 69.3 (3)°. No π–π stacking interactions are observed in the crystal structure.

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.050
wR factor = 0.136
Data-to-parameter ratio = 14.4

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

Comment

The title compound, (I), can be used as an intermediate in the preparation of fungicides (Jones *et al.*, 1998). We report here the crystal structure of (I)

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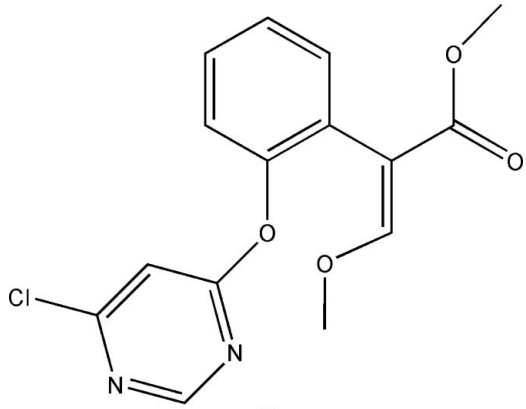

(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the pyrimidine and benzene rings is 69.3 (3)°. The O2–O4/C13–C17 and C7–C12 planes are inclined at an angle of 71.0 (1)°. An intramolecular C—H···O hydrogen bond (Table 1) is observed in the molecular structure.

Experimental

Compound (I) was prepared according to the literature method of Jones *et al.* (1998). Single crystals were obtained by dissolving compound (I) (0.5 g) in ethanol (50 ml) and evaporating the solvent slowly at room temperature for about 10 d.

Crystal data

$C_{15}H_{13}ClN_2O_4$
M_r = 320.72
Monoclinic, $P2_1/n$
a = 13.2642 (11) Å
b = 7.7971 (7) Å
c = 14.2757 (12) Å
β = 96.88 (3)°
V = 1465.8 (2) Å^3
Z = 4
D_x = 1.453 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 298 (2) K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.896, T_{max} = 0.946
2861 measured reflections
2861 independent reflections
2003 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.136
S = 1.00
2861 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 0.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17A···O3	0.93	2.45	2.776 (3)	101

H atoms were positioned geometrically [C—H = 0.93 (Csp^2) or 0.96 Å (methyl)] and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.2 for Csp^2 and x = 1.5 for other H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); 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* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

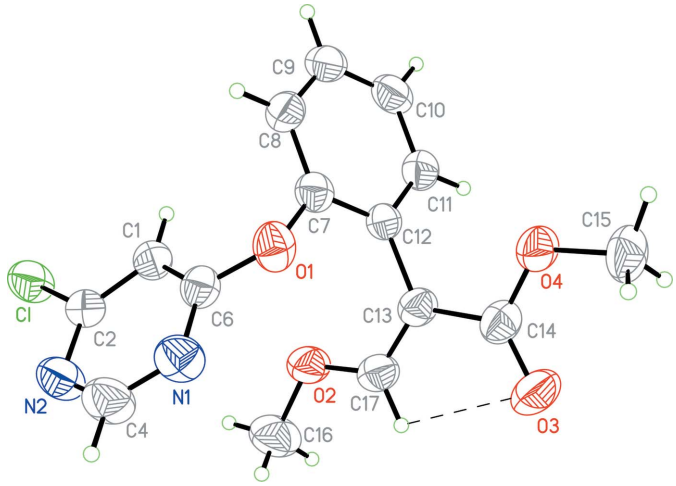

Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

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