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Ethyl 1-[(6-chloropyridin-3-yl)methyl]-3-phenyl-1*H*-pyrazole-5-carboxylate

Yong Xia,[a] Xiao-Ling Ding,[a] Yan-Qing Ge,[a] Lian-Dong Liu[b] and Bao-Xiang Zhao[a]*

[a]School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China, and [b]College of Chemistry, Chemical Engineering and Materials Science, Shandong Normal University, Jinan 250014, People's Republic of China

Correspondence e-mail: baoxiang_zhao@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.115
Data-to-parameter ratio = 13.6

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

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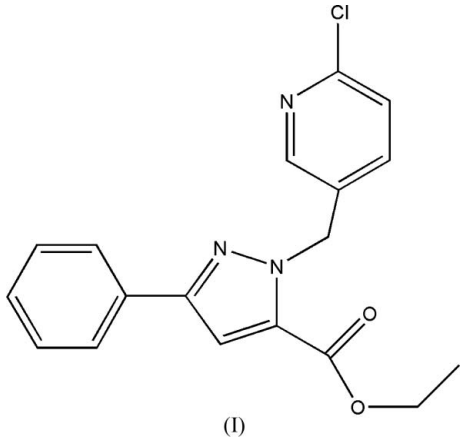
In the title compound, $C_{18}H_{16}ClN_3O_2$, the dihedral angles made by the pyrazole ring with the pyridine and phenyl rings are 82.43 (2) and 8.16 (3)°, respectively. The crystal packing is stabilized mainly by van der Waals forces.

Comment

The pyrazole unit is one of the core structures in a number of natural products. Many pyrazole derivatives are known to exhibit a wide range of biological properties such as anti-hyperglycaemic, analgesic, anti-inflammatory, antipyretic, antibacterial, hypoglycaemic, sedative–hypnotic (Cottineau *et al.*, 2002; Lee *et al.*, 2003), anticoagulant (Jia *et al.*, 2004) and antitumour (Wei *et al.*, 2006) activities. We report here the crystal structure of the title compound, (I).



(I)

All bond lengths and angles in the molecule of (I) are normal (Allen *et al.*, 1987). The C10–C15/N3/Cl1 and C1–C6 planes make angles of 82.43 (2) and 8.16 (3)°, respectively, with the C6–C9/C16/C17/N1/N2/O1/O2 plane.

The crystal packing of (I) is stabilized mainly by van der Waals forces.

Experimental

A mixture of ethyl 3-phenyl-1*H*-pyrazole-5-carboxylate (0.01 mol), 2-chloro-5-(chloromethyl)pyridine (0.01 mol) and potassium carbonate (0.01 mol) in acetonitrile (20 ml) was heated to reflux for 4 h. The solvent was removed under reduced pressure and the residue extracted with ethyl acetate (30 ml). The organic phase was washed with brine and dried over anhydrous magnesium sulfate. After evaporation of the solvent under pressure, a solid was obtained (yield 82%). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid in ethyl acetate and petroleum ether (1:1 *v*/*v*) at room temperature for 3 d.

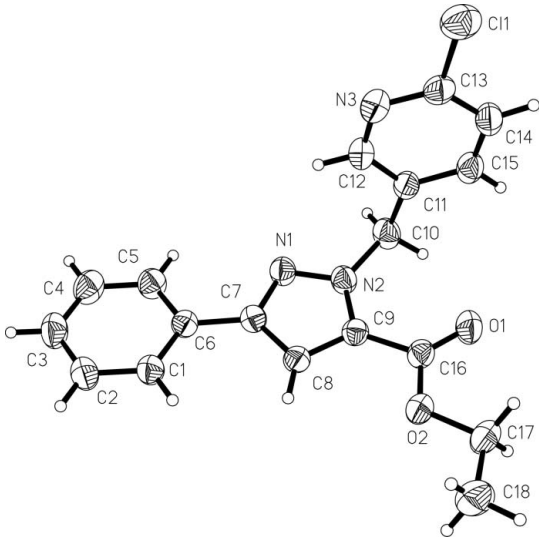


Figure 1
The molecular structure of compound (I), with displacement ellipsoids drawn at the 40% probability level.

Crystal data

$C_{18}H_{16}ClN_3O_2$	V = 843.68 (17) Å^3
M_r = 341.79	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.345 Mg m^{-3}
a = 7.9796 (9) Å	Mo $K\alpha$ radiation
b = 9.9882 (11) Å	μ = 0.24 mm^{-1}
c = 11.0724 (13) Å	T = 298 (2) K
α = 78.696 (2)°	Block, colourless
β = 88.823 (2)°	0.56 × 0.50 × 0.20 mm
γ = 77.216 (2)°	

Data collection

Bruker SMART CCD area-detector diffractometer	4207 measured reflections
φ and ω scans	2947 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2590 reflections with $I > 2\sigma(I)$
T_{min} = 0.877, T_{max} = 0.953	R_{int} = 0.013
	θ_{max} = 25.0°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.1876P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.115	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
S = 1.07	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
2947 reflections	
217 parameters	
H-atom parameters constrained	

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) for aryl and methylene H atoms or 1.5U_{eq}(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL*(Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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