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1-(4-Chlorophenyl)-3-(1*H*-imidazol-1-yl)-propan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.112
Data-to-parameter ratio = 15.3

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

The molecule of the title compound, $C_{12}H_{11}ClN_2O$, is non-planar, the benzene and imidazole rings making a dihedral angle of 72.5 (1)°. Molecules are linked into a three-dimensional framework by weak intermolecular C—H···O and C—H···N hydrogen bonds.

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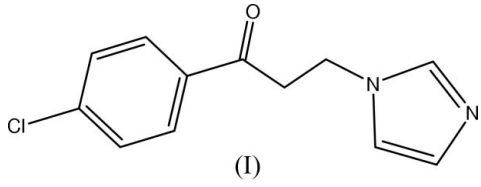
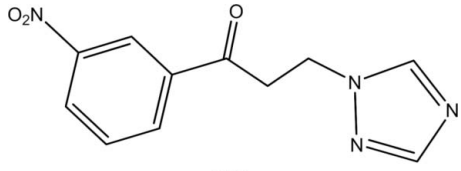
Comment

A molecular view of the title compound, (I), is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and compare well with those reported in the related compound, (II) (Wan *et al.*, 2005). In contrast to the planar conformation of (II), compound (I) is non-planar, with the substituted benzene ring and the imidazole ring making a dihedral angle of 72.5 (1)°.



(I)



(II)

In the crystal structure, molecules are linked into a three-dimensional framework by weak intermolecular C—H···O and C—H···N hydrogen bonds (Fig. 2 and Table 1).

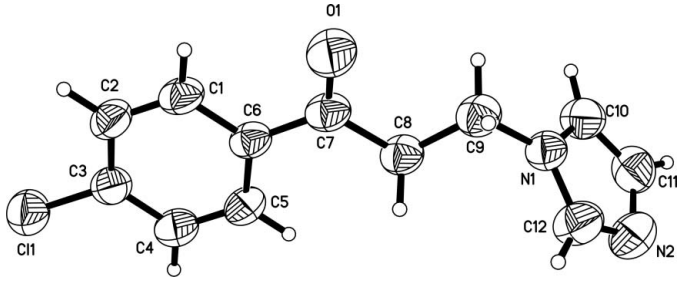


Figure 1
The structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

To a solution of 1-(4-chlorophenyl)-3-(dimethylamino)propan-1-one (10.6 g, 0.05 mol) in water (25 ml) was added imidazole (4.4 g, 0.06 mol). The mixture was heated under reflux for 5 h, yielding a copious precipitate. Colorless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a dichloromethane–cyclohexane (1:2, *v*/*v*) solution over a period of 5 d.

Crystal data

$C_{12}H_{11}ClN_2O$
$M_r = 234.68$
Monoclinic, $P2_1/n$
$a = 10.4902$ (9) Å
$b = 8.1611$ (7) Å
$c = 13.8691$ (12) Å
$\beta = 107.252$ (1)°
$V = 1133.94$ (17) Å^3
$Z = 4$
$D_x = 1.375$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2278 reflections
$\theta = 2.9$–25.9°
$\mu = 0.32$ mm^{-1}
$T = 293$ (2) K
Plate, colorless
0.49 × 0.26 × 0.06 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.861$, $T_{max} = 0.981$
6176 measured reflections
2218 independent reflections
1860 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 26.0°$
$h = -12 \rightarrow 12$
$k = -10 \rightarrow 9$
$l = -17 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.112$
$S = 1.05$
2218 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.2452P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.51	3.353 (2)	151
C8—H8A···N2^{ii}	0.97	2.57	3.499 (2)	160

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

All H atoms were located in difference Fourier maps but they were treated as riding on their parent atoms [C—H = 0.93 and 0.97 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

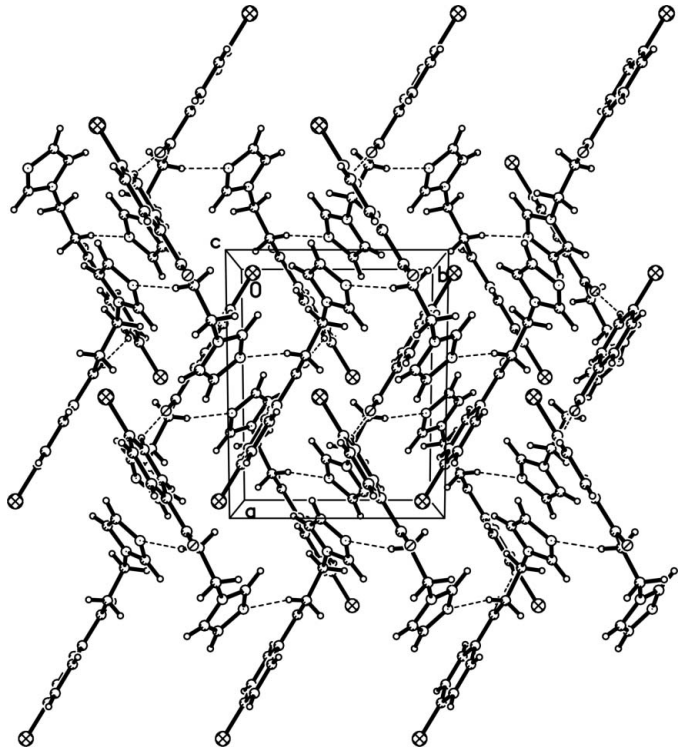


Figure 2
A view down the *c* axis. Hydrogen bonds are indicated by dashed lines.

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