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1-(3-Nitrophenyl)-3-(1*H*-1,2,4-triazol-1-yl)-propan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.092
Data-to-parameter ratio = 7.5

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

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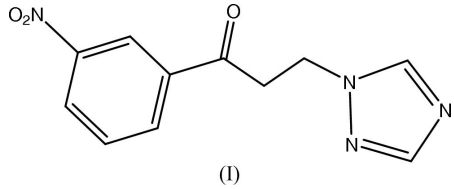
In the title compound, $C_{11}H_{10}N_4O_3$, the substituted phenyl ring and the triazole ring make a dihedral angle of 59.7 (2)°. The molecules are linked into zigzag chains by intermolecular C—H···O hydrogen bonds. These chains are further connected through C—H···N hydrogen bonds to build up a three-dimensional network.

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 for related compounds (Wan, Li, Li & Zhang, 2005; Wan, Li, Li, Zhang *et al.*, 2005). The molecule of (I) is non-planar, with the substituted phenyl ring and the triazole ring making a dihedral angle of 59.7 (2)°.



(I)

In the crystal structure, the molecules of (I) are linked into zigzag chains by C—H···O hydrogen bonds (Fig. 2, Table 1). Further C—H···N hydrogen bonds connect these chains to build up a three-dimensional network which stabilizes the packing.

Experimental

To a solution of 3-(dimethylamino)-1-(3-nitrophenyl)propan-1-one hydrochloride (18 g, 0.07 mol) in water (20 ml) was added triazole (5.5 g, 0.08 mol). The mixture was heated under reflux for 5 h,

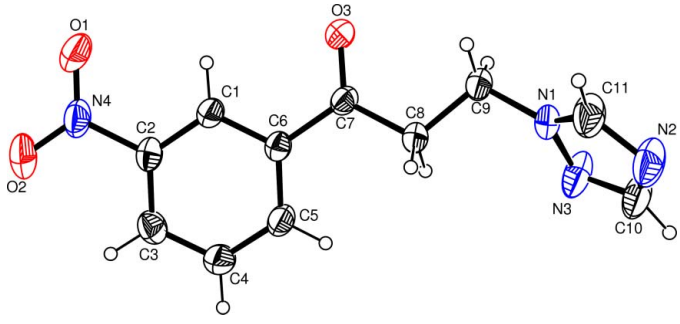


Figure 1
A view of compound (I), with the atom-labelling scheme. Ellipsoids are drawn at the 30% probability level.

yielding a copious precipitate. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of an ethyl acetate–petroleum ether (1:1 (*v*/*v*) solution over a period of two weeks.

Crystal data

$C_{11}H_{10}N_4O_3$
M_r = 246.23
Orthorhombic, $Pca2_1$
a = 26.334 (8) Å
b = 4.5962 (13) Å
c = 9.570 (3) Å
V = 1158.4 (6) Å^3
Z = 4
D_x = 1.412 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1871 reflections
θ = 2.6–22.3°
μ = 0.11 mm^{-1}
T = 293 (2) K
Thick plate, colourless
0.26 × 0.24 × 0.13 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.973, T_{max} = 0.986
5794 measured reflections
1215 independent reflections
1093 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.0°
$h = -31 \rightarrow 32$
$k = -5 \rightarrow 5$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.092
S = 1.14
1215 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.1225P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3B···O3^{i}	0.93	2.48	3.400 (4)	172
C4—H4A···O1^{i}	0.93	2.55	3.481 (5)	175
C5—H5A···N2^{ii}	0.93	2.53	3.449 (4)	169

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C). The Friedel reflections were merged before the final refinement because of the absence of any significant anomalous scattering effects.

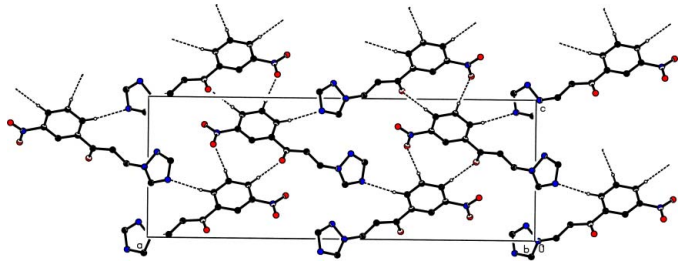


Figure 2
A view down the *b* axis, showing the C—H···O and C—H···N hydrogen bonds (dashed lines) leading to a three-dimensional network. H atoms not involved in hydrogen-bond interactions have been omitted for clarity.

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: *ORTEP3* (Farrugia, 1997), *PLATON* (Spek, 2003) and *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON*.

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