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1-[5-Methyl-1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl]ethanone

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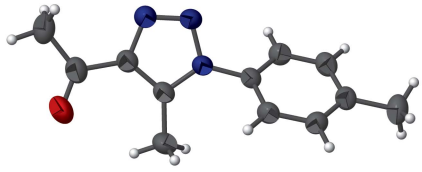
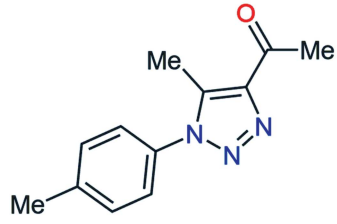
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{12}H_{13}N_3O$, the *p*-tolyl ring is twisted away from the mean plane (r.m.s. deviation = 0.044 Å) of the rest of the molecule by 50.84 (6)°. In the crystal, molecules are linked by C—H···π interactions, forming zigzag chains propagating in the *b*-axis direction.

3D view



Chemical scheme



Structure description

1,2,3-Triazole derivatives can be synthesized using a variety of simple and efficient procedures. The most common one involves cycloaddition of azides and alkynes in the presence of a catalyst (Rostovtsev *et al.*, 2002; Himo *et al.*, 2005; Boren *et al.*, 2008; Quan *et al.*, 2014; Banday & Hruby, 2014; Kolarovič *et al.*, 2011; Shao *et al.*, 2011; Liu & Reiser, 2011). A number of heterocycles containing the 1,2,3-triazole moiety show various medicinal applications (Bock *et al.*, 2006, 2007; Agalave *et al.*, 2011).

The molecule of the title compound, illustrated in Fig. 1, is not planar as the *p*-toly ring (C2–C7) is twisted by 50.84 (6)° away from the mean plane of the rest of the molecule (O1/N1—N3/C8—C12; r.m.s. deviation = 0.044 Å).

In the crystal, zigzag chains, propagating along the *b*-axis direction (Fig. 2), are formed *via* molecules being linked by C—H···π interaction (Table 1).

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

Cg is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*C*···*Cg*^{i}	0.96	2.82	3.729 (3)	159

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

Synthesis and crystallization

The title compound was synthesized from the reaction of 1-azido-4-methylbenzene (10 mmol, 1.33 g) and pentane-2,4-dione (10 mmol, 1.00 g) in anhydrous ethanol (10 mL) in the presence of anhydrous potassium carbonate (15 mmol, 2.07 g). The reaction was heated under reflux for 2 h. The solid obtained on cooling was filtered, washed with ethanol and recrystallized from dimethylformamide solution, to give colourless block-like crystals of the title compound (m.p. 378–380 K; *cf.* data reported by Pokhodylo *et al.*, 2009).

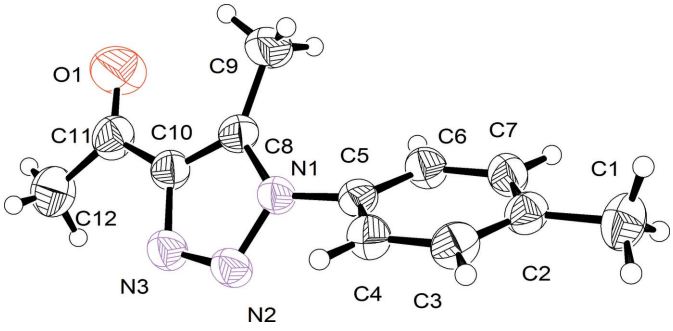


Figure 1
A view of the molecular structure of the title molecule, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

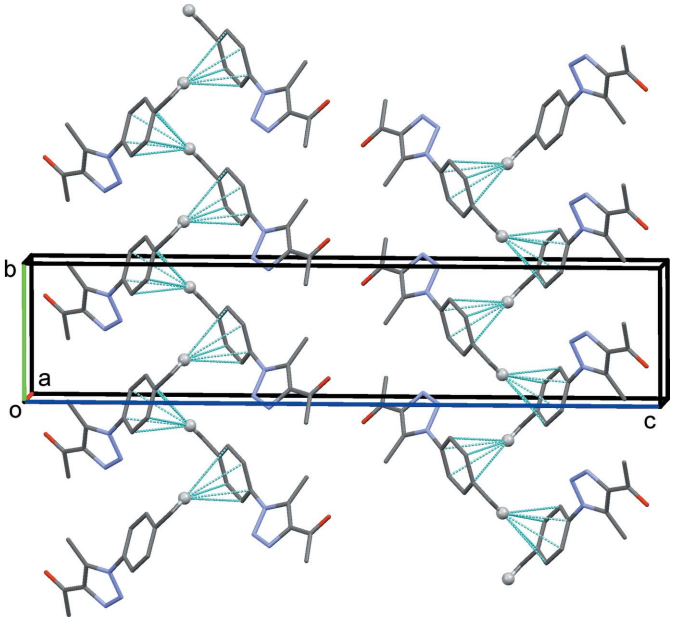


Figure 2
A view along the *a* axis of the crystal packing of the title compound. The C—H···π interactions are represented by dashed lines [see Table 1; only H atom H1*C* (grey ball) has been included].

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{13}N_3O$
M_r	215.25
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	5.7747 (4), 6.5171 (5), 30.234 (2)
β (°)	95.342 (7)
V (Å^3)	1132.88 (14)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.28 × 0.20 × 0.11
Data collection	
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.978, 0.989
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6757, 2745, 1930
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.698
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.060, 0.152, 1.07
No. of reflections	2745
No. of parameters	149
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.16

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS2013* (Sheldrick, 2008), *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *SHELXL2013* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

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Crystal data

$C_{12}H_{13}N_3O$
M_r = 215.25
Monoclinic, $P2_1/c$
a = 5.7747 (4) Å
b = 6.5171 (5) Å
c = 30.234 (2) Å
β = 95.342 (7)°
V = 1132.88 (14) Å^3
Z = 4
$F(000)$ = 456
D_x = 1.262 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2318 reflections
θ = 4.2–28.9°
μ = 0.08 mm^{-1}
T = 296 K
Block, colourless
0.28 × 0.20 × 0.11 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
ω scans
Absorption correction: gaussian (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.978, T_{max} = 0.989
6757 measured reflections
2745 independent reflections
1930 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 29.8°, θ_{min} = 3.4°
h = −8→7
k = −7→8
l = −39→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.152
S = 1.07
2745 reflections
149 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.4633P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL2013 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.009 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8118 (4)	0.7032 (4)	0.27023 (8)	0.0618 (6)
H1A	0.8921	0.6129	0.2517	0.093*
H1B	0.9230	0.7810	0.2889	0.093*
H1C	0.7147	0.7950	0.2519	0.093*
C2	0.6633 (3)	0.5785 (3)	0.29871 (6)	0.0451 (5)
C3	0.7163 (3)	0.3765 (3)	0.30953 (7)	0.0489 (5)
H3	0.8467	0.3163	0.2991	0.059*
C4	0.5796 (3)	0.2620 (3)	0.33559 (6)	0.0446 (5)
H4	0.6178	0.1265	0.3426	0.054*
C5	0.3860 (3)	0.3514 (3)	0.35103 (6)	0.0397 (4)
C6	0.3286 (3)	0.5524 (3)	0.34067 (6)	0.0457 (5)
H6	0.1977	0.6121	0.3510	0.055*
C7	0.4684 (4)	0.6643 (3)	0.31467 (7)	0.0476 (5)
H7	0.4303	0.8000	0.3078	0.057*
C8	0.1361 (3)	0.2725 (3)	0.41319 (6)	0.0447 (5)
C9	0.1918 (5)	0.4577 (4)	0.44114 (8)	0.0720 (7)
H9A	0.3572	0.4774	0.4448	0.108*
H9B	0.1350	0.4389	0.4697	0.108*
H9C	0.1190	0.5759	0.4269	0.108*
C10	−0.0073 (3)	0.1067 (3)	0.41849 (6)	0.0451 (5)
C11	−0.1760 (4)	0.0730 (4)	0.45140 (7)	0.0567 (6)
C12	−0.3247 (4)	−0.1147 (4)	0.44668 (9)	0.0703 (7)
H12A	−0.4442	−0.1063	0.4667	0.105*
H12B	−0.2306	−0.2339	0.4537	0.105*
H12C	−0.3948	−0.1246	0.4167	0.105*
N1	0.2356 (3)	0.2300 (2)	0.37565 (5)	0.0408 (4)
N2	0.1592 (3)	0.0449 (2)	0.35832 (5)	0.0474 (4)
N3	0.0134 (3)	−0.0285 (2)	0.38449 (6)	0.0487 (4)
O1	−0.1958 (4)	0.1974 (3)	0.48064 (7)	0.0915 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0540 (12)	0.0736 (15)	0.0592 (14)	−0.0061 (12)	0.0137 (10)	0.0128 (11)
C2	0.0411 (10)	0.0536 (12)	0.0409 (10)	−0.0041 (9)	0.0049 (8)	−0.0008 (8)
C3	0.0393 (10)	0.0578 (12)	0.0505 (11)	0.0045 (9)	0.0100 (8)	−0.0026 (9)
C4	0.0420 (10)	0.0432 (10)	0.0488 (11)	0.0058 (9)	0.0050 (8)	0.0009 (8)
C5	0.0412 (10)	0.0405 (10)	0.0380 (9)	0.0003 (8)	0.0075 (7)	−0.0028 (7)
C6	0.0463 (11)	0.0408 (10)	0.0517 (11)	0.0044 (9)	0.0138 (9)	−0.0041 (8)

C7	0.0534 (11)	0.0392 (10)	0.0513 (11)	−0.0008 (9)	0.0103 (9)	0.0008 (8)
C8	0.0521 (11)	0.0433 (10)	0.0399 (10)	0.0026 (9)	0.0109 (8)	−0.0037 (8)
C9	0.102 (2)	0.0596 (14)	0.0586 (14)	−0.0184 (14)	0.0299 (13)	−0.0191 (11)
C10	0.0484 (11)	0.0439 (10)	0.0440 (10)	0.0030 (9)	0.0096 (8)	0.0001 (8)
C11	0.0587 (13)	0.0601 (13)	0.0535 (12)	0.0004 (11)	0.0180 (10)	0.0019 (10)
C12	0.0670 (15)	0.0763 (16)	0.0711 (15)	−0.0135 (13)	0.0260 (12)	0.0055 (13)
N1	0.0463 (9)	0.0358 (8)	0.0415 (8)	0.0012 (7)	0.0101 (7)	−0.0028 (6)
N2	0.0530 (10)	0.0393 (9)	0.0518 (10)	−0.0018 (8)	0.0153 (8)	−0.0075 (7)
N3	0.0535 (10)	0.0429 (9)	0.0517 (10)	−0.0016 (8)	0.0144 (8)	−0.0032 (7)
O1	0.1084 (15)	0.0912 (13)	0.0840 (13)	−0.0220 (12)	0.0574 (11)	−0.0271 (11)

Geometric parameters (Å, º)

C1—C2	1.508 (3)	C8—N1	1.348 (2)
C1—H1A	0.9600	C8—C10	1.380 (3)
C1—H1B	0.9600	C8—C9	1.491 (3)
C1—H1C	0.9600	C9—H9A	0.9600
C2—C7	1.383 (3)	C9—H9B	0.9600
C2—C3	1.384 (3)	C9—H9C	0.9600
C3—C4	1.384 (3)	C10—N3	1.368 (2)
C3—H3	0.9300	C10—C11	1.472 (3)
C4—C5	1.380 (3)	C11—O1	1.212 (3)
C4—H4	0.9300	C11—C12	1.494 (3)
C5—C6	1.380 (3)	C12—H12A	0.9600
C5—N1	1.434 (2)	C12—H12B	0.9600
C6—C7	1.385 (3)	C12—H12C	0.9600
C6—H6	0.9300	N1—N2	1.372 (2)
C7—H7	0.9300	N2—N3	1.299 (2)
C2—C1—H1A	109.5	N1—C8—C9	123.86 (19)
C2—C1—H1B	109.5	C10—C8—C9	131.93 (18)
H1A—C1—H1B	109.5	C8—C9—H9A	109.5
C2—C1—H1C	109.5	C8—C9—H9B	109.5
H1A—C1—H1C	109.5	H9A—C9—H9B	109.5
H1B—C1—H1C	109.5	C8—C9—H9C	109.5
C7—C2—C3	118.11 (18)	H9A—C9—H9C	109.5
C7—C2—C1	120.38 (19)	H9B—C9—H9C	109.5
C3—C2—C1	121.51 (19)	N3—C10—C8	108.77 (16)
C2—C3—C4	121.47 (18)	N3—C10—C11	121.45 (18)
C2—C3—H3	119.3	C8—C10—C11	129.58 (18)
C4—C3—H3	119.3	O1—C11—C10	120.4 (2)
C5—C4—C3	119.20 (18)	O1—C11—C12	121.7 (2)
C5—C4—H4	120.4	C10—C11—C12	117.9 (2)
C3—C4—H4	120.4	C11—C12—H12A	109.5
C4—C5—C6	120.60 (18)	C11—C12—H12B	109.5
C4—C5—N1	119.44 (16)	H12A—C12—H12B	109.5
C6—C5—N1	119.84 (16)	C11—C12—H12C	109.5
C5—C6—C7	119.21 (18)	H12A—C12—H12C	109.5

C5—C6—H6	120.4	H12B—C12—H12C	109.5
C7—C6—H6	120.4	C8—N1—N2	110.80 (15)
C2—C7—C6	121.42 (18)	C8—N1—C5	130.56 (16)
C2—C7—H7	119.3	N2—N1—C5	118.44 (14)
C6—C7—H7	119.3	N3—N2—N1	107.14 (14)
N1—C8—C10	104.15 (16)	N2—N3—C10	109.14 (16)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*C*···*Cg*^{i}	0.96	2.82	3.729 (3)	159

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+1/2.