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5,7-Dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.062
wR factor = 0.186
Data-to-parameter ratio = 14.5

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

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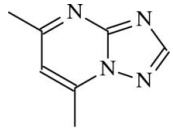
The molecules in the title compound, $C_7H_8N_4$, are linked into sheets by a combination of C—H···N hydrogen bonds and π–π interactions. The hydrogen bonds generate two-dimensional networks with a *C*(6) chain motif. There are two planar symmetry-independent molecules in the asymmetric unit, with a dihedral angle of 4.29 (8)° between their least-squares mean planes.

Comment

Many triazolo[1,5-*a*]pyrimidine derivatives have been reported, showing a range of biological activities (Hess *et al.*, 2004; Nam *et al.*, 2002; Gilligan *et al.*, 2000; Wong *et al.*, 2000; Yang & Yang, 1999). In this paper, we report the synthesis and crystal structure of 5,7-dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine, (I).



(I)

There are two symmetry-independent molecules in the asymmetric unit (Fig. 1). Selected bond distances and angles are listed in Table 1. All ring atoms in the triazolopyrimidine system are almost coplanar, the largest deviations from the mean planes being 0.008 (2) Å for atoms C4. The dihedral angles between the five-membered rings and the fused six-membered rings are 3.57 (14) (*P*1/*P*2) and 4.68 (11)° (*P*3/*P*4) (*P*1 is N2–N4/C4/C5, *P*2 is N1/N2/C1–C4, *P*3 is N12–N14/C14/C15 and *P*4 is N11/N12/C11–C14); the dihedral angle between the mean planes of the two independent molecules is 4.29 (8)°. The geometry of the triazolopyrimidine system is very similar to that reported for the related compounds 7-ethoxycarbonylmethyl-5-methyl-1,2,4-triazolo[1,5-*a*]pyrimidine (Fettouhi *et al.*, 1996) and 5,7-diphenyl-1,2,4-triazolo[1,5-*a*]-pyrimidine[1,5-*a*]pyrimidine (Surdykowski *et al.*, 1999).

In (I), there are intermolecular C—H···N hydrogen bonds (Table 2) and π–π intermolecular interactions (Fig. 2). The latter are $Cg2\cdots Cg3^{iii}$ [3.437 (1) Å; symmetry code: (iii) $x-1$, y, z; perpendicular distance = 3.445 (1) Å] and $Cg4\cdots Cg1$ [3.458 (1) Å; perpendicular distance = 3.375 (1) Å] (*Cg*i are the centroids of planes *P*i).

Experimental

The title compound was prepared as described by Petrova *et al.* (2003), using acetylacetone and 1*H*-1,2,4-triazol-3-amine as starting materials. Well shaped crystals of (I) were obtained by slow evaporation of an ethyl acetate solution (yield 75%; m.p. 423–424 K).

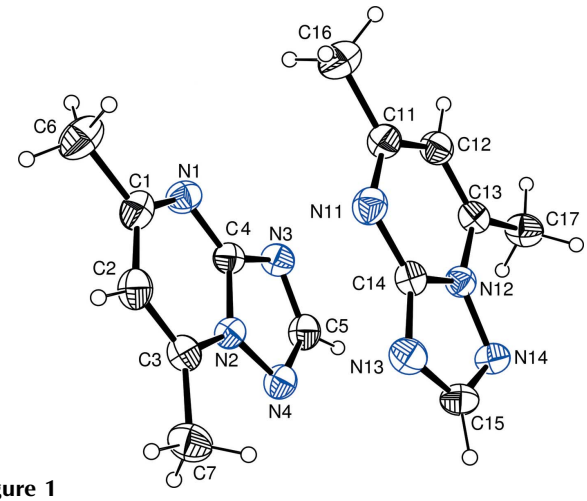


Figure 1
The asymmetric unit of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

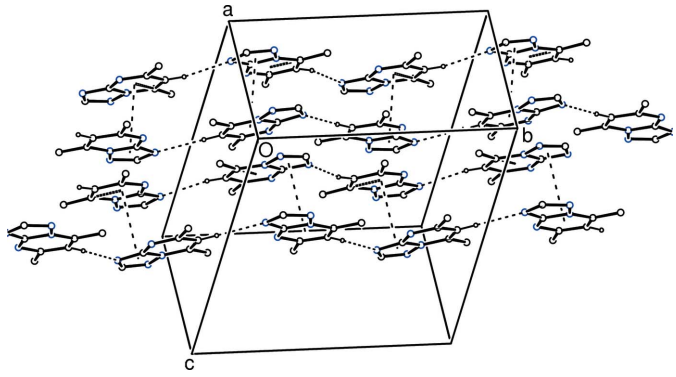


Figure 2
A packing diagram of the title compound, showing the hydrogen-bonding and π–π stacking (dashed lines). H atoms not involved in hydrogen bonding have been omitted. /p>

Crystal data

$C_7H_8N_4$	D_x = 1.306 Mg m^{-3}
M_r = 148.17	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 15967 reflections
a = 7.0872 (8) Å	θ = 2.0–28.0°
b = 12.8239 (13) Å	μ = 0.09 mm^{-1}
c = 16.527 (2) Å	T = 296 K
β = 90.303 (9)°	Prism, colorless
V = 1502.0 (3) Å^3	0.46 × 0.37 × 0.28 mm
Z = 8	

Data collection

Stoe IPDS-2 diffractometer	1890 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.056
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	θ_{max} = 26.0°
T_{min} = 0.972, T_{max} = 0.984	$h = -8 \rightarrow 8$
9749 measured reflections	$k = -15 \rightarrow 15$
2946 independent reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1069P)^2 + 0.0599P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.062	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.186	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
2946 reflections	
203 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.323 (3)	C11—C12	1.415 (4)
C1—C2	1.409 (4)	C12—C13	1.351 (3)
C2—C3	1.349 (3)	C13—N12	1.373 (3)
C3—N2	1.372 (3)	C14—N13	1.335 (3)
C4—N3	1.334 (3)	C14—N11	1.345 (3)
C4—N1	1.335 (3)	C14—N12	1.375 (3)
C4—N2	1.385 (3)	C15—N14	1.319 (3)
C5—N4	1.325 (3)	C15—N13	1.336 (3)
C5—N3	1.337 (3)	N2—N4	1.362 (3)
C11—N11	1.326 (3)	N12—N14	1.368 (3)
N4—C5—N3	117.6 (2)	N4—N2—C3	127.70 (19)
N13—C14—N11	128.9 (2)	C13—N12—C14	123.07 (19)
N14—C15—N13	118.5 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N3^{i}	0.93	2.54	3.439 (3)	162
C12—H12···N13^{ii}	0.93	2.52	3.445 (3)	172

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

All H atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic and 0.96 Å for methyl H atoms, and with U_{iso}(H) = 1.2U_{eq}(aromatic C) and 1.5U_{eq}(methyl C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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