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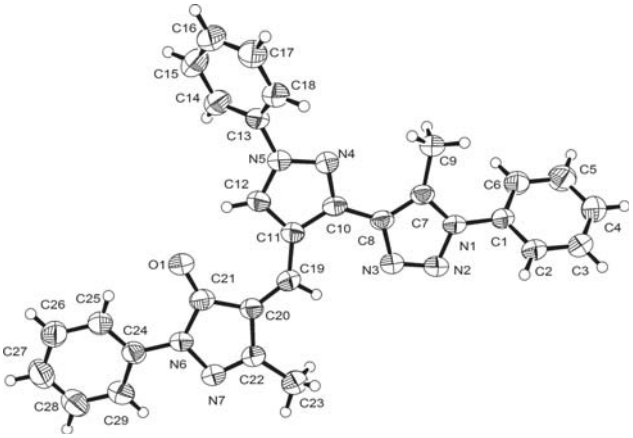
Crystal structure of (*E*)-3-methyl-4-((3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazol-4-yl)methylene)-1-phenyl-1*H*-pyrazol-5(4*H*)-one, $C_{29}H_{23}N_7O$



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Abstract

$C_{29}H_{23}N_7O$, triclinic, $P\bar{1}$ (no. 2), $a = 8.2785(12)$ Å, $b = 12.1750(18)$ Å, $c = 13.8122(16)$ Å, $\alpha = 114.401(13)°$, $\beta = 103.083(11)°$, $\gamma = 93.384(12)°$, $V = 1216.5(3)$Å^3, $Z = 2$, $R_{gt}(F) = 0.0713$, $wR_{ref}(F^2) = 0.1880$, $T = 293(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless needle
Size:	0.39 × 0.05 × 0.03 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.9 cm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
$2\theta_{max}$, completeness:	60°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11194, 5684, 0.059
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2627
$N(param)_{refined}$:	336
Programs:	CrysAlis^{PRO} [1], SHELX [2], PLATON [3], ChemDraw [4]

Source of material

The title compound was prepared from the reaction of 3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazole-4-carbaldehyde with 3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one in ethanol in the presence of few drops of piperidine as catalyst under reflux for 1.5 h. The solid obtained on cooling was recrystallized from dimethylformamide to give colorless crystals of the title compound (Mp 267-268 °C) [5].

Experimental details

All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with $U_{iso} = 1.5\ U_{eq}$(C), and were allowed to spin about the C—C bond. Aromatic C—H distances were set to 0.93 Å and U_{iso} of the H atoms set to 1.2 U_{eq}(C).

Comment

Some triazolylpyrazoles [6, 7] are at the center of attention due to their useful applications as antibacterial, antiviral

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	1.2591(4)	1.0245(2)	0.9026(2)	0.0458(7)
C2	1.2019(4)	1.0981(2)	0.9899(2)	0.0535(8)
H2	1.0927	1.0783	0.9917	0.064*
C3	1.3069(5)	1.2013(3)	1.0746(2)	0.0621(9)
H3	1.2691	1.2505	1.1341	0.075*
C4	1.4682(5)	1.2315(3)	1.0710(3)	0.0689(10)
H4	1.5387	1.3015	1.1279	0.083*
C5	1.5249(5)	1.1578(3)	0.9830(3)	0.0709(9)
H5	1.6332	1.1785	0.9803	0.085*
C6	1.4206(4)	1.0535(3)	0.8990(2)	0.0594(8)
H6	1.4590	1.0031	0.8402	0.071*
C7	1.1111(4)	0.8699(2)	0.7062(2)	0.0437(7)
C8	1.0037(4)	0.7607(2)	0.6683(2)	0.0432(7)
C9	1.1697(4)	0.9350(2)	0.6471(2)	0.0574(8)
H9A	1.1955	1.0215	0.6943	0.086*
H9B	1.0827	0.9190	0.5813	0.086*
H9C	1.2687	0.9068	0.6273	0.086*
C10	0.9194(3)	0.6706(2)	0.5546(2)	0.0423(7)
C11	0.8095(4)	0.5557(2)	0.5151(2)	0.0430(7)
C12	0.7726(4)	0.5103(2)	0.4016(2)	0.0473(7)
H12	0.7052	0.4360	0.3502	0.057*
C13	0.8326(4)	0.5878(2)	0.2718(2)	0.0492(7)
C14	0.8484(4)	0.4824(3)	0.1864(2)	0.0645(9)
H14	0.8763	0.4154	0.1985	0.077*
C15	0.8219(5)	0.4783(3)	0.0824(3)	0.0816(12)
H15	0.8312	0.4074	0.0238	0.098*
C16	0.7821(5)	0.5775(3)	0.0645(3)	0.0831(12)
H16	0.7640	0.5735	−0.0059	0.100*
C17	0.7689(5)	0.6826(3)	0.1508(3)	0.0747(11)
H17	0.7429	0.7502	0.1389	0.090*
C18	0.7941(4)	0.6882(3)	0.2547(2)	0.0628(9)
H18	0.7853	0.7593	0.3132	0.075*
C19	0.7509(4)	0.5055(2)	0.5808(2)	0.0468(7)
H19	0.7943	0.5526	0.6567	0.056*
C20	0.6432(4)	0.4016(2)	0.5520(2)	0.0466(7)
C21	0.5523(4)	0.3031(2)	0.4425(2)	0.0501(7)
C22	0.5928(4)	0.3646(2)	0.6291(2)	0.0507(8)
C23	0.6488(5)	0.4303(3)	0.7517(2)	0.0745(10)
H23A	0.6025	0.3819	0.7822	0.112*
H23B	0.6105	0.5076	0.7758	0.112*
H23C	0.7695	0.4437	0.7765	0.112*
C24	0.3593(4)	0.1074(2)	0.3923(2)	0.0487(7)
C25	0.3085(4)	0.0720(2)	0.2798(2)	0.0552(8)
H25	0.3374	0.1251	0.2514	0.066*
C26	0.2148(4)	−0.0424(3)	0.2100(3)	0.0666(9)
H26	0.1819	−0.0662	0.1342	0.080*
C27	0.1690(5)	−0.1220(3)	0.2503(3)	0.0737(10)
H27	0.1073	−0.1996	0.2023	0.088*
C28	0.2158(5)	−0.0853(3)	0.3622(3)	0.0757(10)
H28	0.1831	−0.1377	0.3904	0.091*
C29	0.3108(4)	0.0287(3)	0.4337(3)	0.0627(9)
H29	0.3422	0.0525	0.5095	0.075*
N1	1.1509(3)	0.91404(18)	0.81728(17)	0.0459(6)
N2	1.0735(3)	0.8376(2)	0.84837(18)	0.0537(7)
N3	0.9844(3)	0.74405(19)	0.75684(17)	0.0517(6)
N4	0.9417(3)	0.69274(18)	0.47162(17)	0.0487(6)
N5	0.8508(3)	0.59184(18)	0.37836(17)	0.0472(6)
N6	0.4609(3)	0.22280(18)	0.46589(17)	0.0483(6)
N7	0.4894(3)	0.2616(2)	0.58018(17)	0.0537(7)
O1	0.5514(3)	0.28920(17)	0.34902(16)	0.0680(7)

and antitumor reagents, as well as pesticides and herbicides [8–10]. The asymmetric unit comprises one molecule of $C_{29}H_{23}N_7O$. The triazole-pyrazole ring system (apart from the methyl protons) is planar with rms deviation of 0.0385 Å. The three phenyl rings are twisted from the triazole-pyrazole system with interplanar angles of 11.08(11)°, 42.42(9)° and 83.62(12)°. In the crystal structure, the planar segments of the molecules form a π-stack along [100].

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