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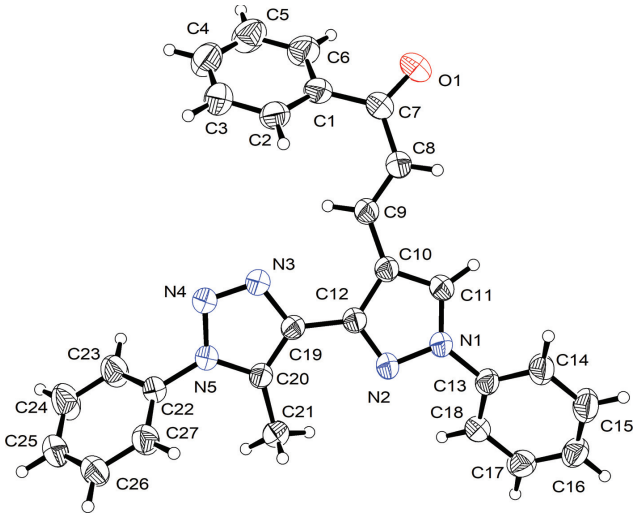
Crystal structure of (*E*)-3-(3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazol-4-yl)-1-phenylprop-2-en-1-one, $C_{27}H_{21}N_5O$



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Abstract

$C_{27}H_{21}N_5O$, triclinic, $P\bar{1}$ (no. 2), $a = 8.1464(7)$ Å, $b = 10.3861(8)$ Å, $c = 13.2507(9)$ Å, $\alpha = 84.898(6)°$, $\beta = 89.413(6)°$, $\gamma = 80.351(7)°$, $V = 1100.88(15)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0648$, $wR_{ref}(F_2) = 0.1726$, $T = 296(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.31 × 0.18 × 0.08 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	29.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8540, 5164, 0.035
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2801
$N(param)_{refined}$:	300
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], WinGX/ORTEP [4]

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was synthesized from the reaction of equimolar quantities of 3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazole-4-carbaldehyde and acetophenone in ethanol in presence of sodium hydroxide (10%) for 2 h at room temperature. The crude product was collected by filtration, washed with water and recrystallized from dimethylformamide to give colourless crystals (90%).

Experimental details

All hydrogen atoms were placed in calculated positions using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with $U(H) = 1.5\ U_{eq}(C)$. C—H distances for sp^2 hybridized groups were set to 0.93 Å and their $U_{iso}(H)$ set to 1.2 times the $U_{eq}(C)$. The high R1 value for all reflections is attributable to the weakness of data, particularly above 0.9 Å resolution.

Comment

Chalcones are an important class of compounds found in various natural products [5]. The synthetic methods for chalcone-containing compounds are simple, efficient, convenient, and high yielding [6]. Synthetic and natural chalcones show various interesting medicinal activities [7, 8]. They act as

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6089(3)	0.1784(2)	−0.2761(2)	0.0612(7)
C2	0.6412(4)	0.3049(2)	−0.2969(2)	0.0660(7)
H2	0.660160	0.353945	−0.244058	0.079*
C3	0.6451(4)	0.3581(3)	−0.3960(2)	0.0796(9)
H3	0.667613	0.442744	−0.409638	0.096*
C4	0.6162(4)	0.2875(3)	−0.4738(2)	0.0856(9)
H4	0.616829	0.324622	−0.540299	0.103*
C5	0.5865(4)	0.1624(3)	−0.4542(2)	0.0895(10)
H5	0.569364	0.113822	−0.507679	0.107*
C6	0.5816(4)	0.1077(3)	−0.3566(2)	0.0807(9)
H6	0.559874	0.022691	−0.344140	0.097*
C7	0.6034(4)	0.1137(2)	−0.1708(2)	0.0652(7)
C8	0.5277(3)	0.1846(2)	−0.08732(19)	0.0585(7)
H8	0.545470	0.142525	−0.022470	0.070*
C9	0.4355(3)	0.3039(2)	−0.09493(17)	0.0501(6)
H9	0.426345	0.349818	−0.158716	0.060*
C10	0.3489(3)	0.3679(2)	−0.01301(16)	0.0467(6)
C11	0.3147(3)	0.3126(2)	0.08149(17)	0.0511(6)
H11	0.346655	0.225166	0.105600	0.061*
C12	0.2738(3)	0.5013(2)	−0.01143(16)	0.0463(6)
C13	0.1591(3)	0.3941(2)	0.23171(17)	0.0495(6)
C14	0.2429(4)	0.3062(2)	0.30552(19)	0.0649(7)
H14	0.345146	0.256278	0.291775	0.078*
C15	0.1718(4)	0.2936(3)	0.4003(2)	0.0737(8)
H15	0.226417	0.233793	0.450413	0.088*
C16	0.0224(4)	0.3678(3)	0.42142(19)	0.0672(8)
H16	−0.023686	0.358802	0.485630	0.081*
C17	−0.0593(4)	0.4558(2)	0.3475(2)	0.0657(7)
H17	−0.161269	0.505861	0.361536	0.079*
C18	0.0098(3)	0.4700(2)	0.25212(18)	0.0562(6)
H18	−0.044530	0.530426	0.202291	0.067*
C19	0.2722(3)	0.6090(2)	−0.09084(16)	0.0456(6)
C20	0.1836(3)	0.7342(2)	−0.09528(16)	0.0464(6)
C21	0.0581(3)	0.8011(2)	−0.02716(19)	0.0603(7)
H21A	0.112761	0.844419	0.020424	0.091*
H21B	0.000916	0.737577	0.008784	0.091*
H21C	−0.020517	0.864517	−0.066555	0.091*
C22	0.1777(3)	0.9212(2)	−0.23063(17)	0.0498(6)
C23	0.1120(4)	0.9394(2)	−0.3261(2)	0.0761(9)
H23	0.102721	0.867816	−0.361756	0.091*
C24	0.0597(5)	1.0649(3)	−0.3689(2)	0.0902(11)
H24	0.014412	1.077883	−0.433927	0.108*
C25	0.0733(4)	1.1702(3)	−0.3176(2)	0.0717(8)
H25	0.037417	1.254620	−0.347327	0.086*
C26	0.1398(4)	1.1517(2)	−0.2224(2)	0.0722(8)
H26	0.149137	1.223692	−0.187122	0.087*
C27	0.1931(4)	1.0268(2)	−0.1782(2)	0.0653(7)
H27	0.239114	1.014022	−0.113464	0.078*
N1	0.2275(3)	0.40624(17)	0.13255(13)	0.0491(5)
N2	0.1999(3)	0.52498(16)	0.07659(14)	0.0511(5)
N3	0.3666(3)	0.59442(17)	−0.17605(14)	0.0529(5)
N4	0.3412(3)	0.70498(18)	−0.23374(14)	0.0546(5)
N5	0.2308(3)	0.79058(17)	−0.18469(13)	0.0487(5)
O1	0.6609(3)	−0.00381(18)	−0.15491(17)	0.1037(8)

antibacterial, antiviral, antiulcer, antihelmintic, antiprotozoal, antioxidative, and insecticidal agents [9–13].

In the crystal structure, the asymmetric unit consists of one molecule (see the figure). The molecule comprises five ring systems, namely: **A**, phenyl (C1—C6); **B**, pyrazolyl (C10—C12,N1,N2); **C**, a second phenyl (C13—C18); **D**, triazolyl (C19—C21,N3—N5) and **E**, a third phenyl (C22—C27) group. The core of the molecule consists of rings **B** and **D**, which are almost coplanar with a twist angle of 10.35(12)°. The phenyl groups deviate from the core plane with interplanar angles **A**/**B**, **B**/**C** and **D**/**E** of 42.24(7)°, 33.54(11)° and 55.72(7)°, respectively.

The molecule displays an intramolecular C—H···N contact with a C21···N2 distance of 3.109(3) Å. An intermolecular C—H···O contact with a C11···O1 distance of 3.241(3) Å is also observed. Some related structures show similar features [14, 15].

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