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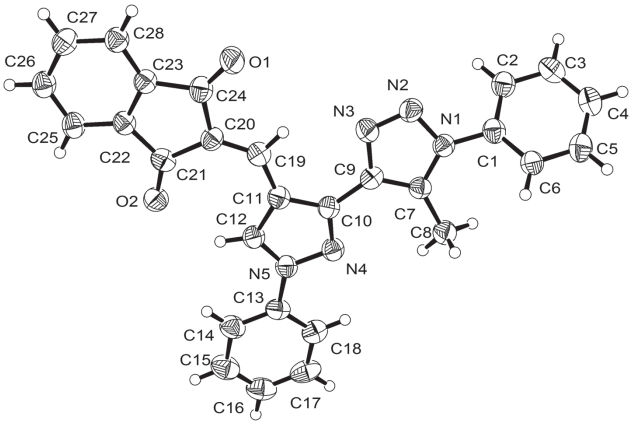
Crystal structure of 2-((3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazol-4-yl) methylene)-1*H*-indene-1,3(2*H*)-dione, $C_{28}H_{19}N_5O_2$



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Abstract

$C_{28}H_{19}N_5O_2$, monoclinic, *Cc* (no. 9), $a = 13.9896(9)$ Å, $b = 21.9561(14)$ Å, $c = 7.1643(5)$ Å, $\beta = 91.782(6)°$, $V = 2199.5(3)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0632$, $wR_{ref}(F^2) = 0.1727$, $T = 150(2)$ K.

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

Table 1: Data collection and handling.

Crystal:	Orange block Size 0.24 × 0.14 × 0.06 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.9 cm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
$2\theta_{max}$, completeness:	59.8°, >87%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10805, 4741, 0.066
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2799
$N(param)_{refined}$:	318
Programs:	CrysAlis^{PRO} [10], SHELX [11], Platon [12], CHEMDRAW [13]

Source of material

The title compound was synthesized from 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 1*H*-indene-1,3(2*H*)-dione in ethanol containing a few drops of piperidine as catalyst under reflux. The crude product was recrystallized from dimethylformamide to give yellow crystals of the title compound (Mp 276–277 °C) [1].

Experimental details

All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C-H bonds were fixed at 0.97 Å, with $U(H) = 1.5\ U_{eq}(C)$, and were allowed to spin about the C—C bond. Aromatic C-H distances were set to 0.95 Å and their U_{iso} set to 1.2 times the U_{eq} of the parent atom.

Discussion

1,2,3-Triazoles [2–6] are known for their biological applications such as antidiabetic, anti-inflammatory, antifungal, antiviral and antibacterial activity [7–9].

In the title crystal structure, the asymmetric unit consists of one molecule of $C_{28}H_{19}N_5O_2$. With the exception of phenyl ring (C1—C6) (A), the rest of the molecule [i.e. the triazole

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0237(4)	0.9349(2)	0.9453(7)	0.0430(12)
C2	−0.1021(4)	0.9607(2)	1.0272(8)	0.0474(13)
H2	−0.0944	0.9933	1.1138	0.057*
C3	−0.1926(4)	0.9380(3)	0.9798(8)	0.0528(14)
H3	−0.2474	0.9561	1.0320	0.063*
C4	−0.2037(4)	0.8899(3)	0.8585(8)	0.0531(14)
H4	−0.2655	0.8737	0.8313	0.064*
C5	−0.1244(4)	0.8652(3)	0.7764(8)	0.0528(14)
H5	−0.1321	0.8325	0.6907	0.063*
C6	−0.0333(4)	0.8880(2)	0.8180(8)	0.0437(12)
H6	0.0211	0.8716	0.7599	0.052*
C7	0.1548(3)	0.9314(2)	1.0301(7)	0.0383(11)
C8	0.1724(4)	0.8652(2)	1.0079(8)	0.0483(14)
H8A	0.1899	0.8568	0.8790	0.072*
H8B	0.1142	0.8425	1.0363	0.072*
H8C	0.2246	0.8525	1.0936	0.072*
C9	0.2144(4)	0.9784(2)	1.0820(7)	0.0387(12)
C10	0.3140(3)	0.9782(2)	1.1439(7)	0.0374(12)
C11	0.3761(3)	1.0284(2)	1.1817(7)	0.0389(12)
C12	0.4621(4)	1.0022(2)	1.2426(8)	0.0399(12)
H12	0.5188	1.0233	1.2805	0.048*
C13	0.5175(4)	0.8961(2)	1.2926(7)	0.0417(12)
C14	0.6096(4)	0.9126(3)	1.3439(8)	0.0502(14)
H14	0.6283	0.9542	1.3431	0.060*
C15	0.6745(4)	0.8678(3)	1.3967(9)	0.0581(16)
H15	0.7385	0.8790	1.4288	0.070*
C16	0.6485(5)	0.8075(3)	1.4036(9)	0.0577(16)
H16	0.6933	0.7773	1.4436	0.069*
C17	0.5561(5)	0.7917(2)	1.3515(8)	0.0561(16)
H17	0.5376	0.7501	1.3533	0.067*
C18	0.4900(4)	0.8354(2)	1.2966(7)	0.0476(13)
H18	0.4263	0.8240	1.2621	0.057*
C19	0.3530(4)	1.0923(2)	1.1649(7)	0.0408(12)
H19	0.2915	1.1003	1.1104	0.049*
C20	0.4026(4)	1.1424(2)	1.2121(7)	0.0394(11)
C21	0.4989(3)	1.1526(2)	1.3031(7)	0.0412(12)
C22	0.5094(4)	1.2192(2)	1.3298(7)	0.0390(11)
C23	0.4292(4)	1.2493(2)	1.2601(7)	0.0390(11)
C24	0.3597(4)	1.2036(2)	1.1826(7)	0.0443(13)
C25	0.5853(4)	1.2511(2)	1.4106(7)	0.0444(13)
H25	0.6409	1.2307	1.4578	0.053*
C26	0.5771(4)	1.3141(2)	1.4199(7)	0.0460(13)
H26	0.6279	1.3372	1.4752	0.055*
C27	0.4954(4)	1.3440(2)	1.3493(8)	0.0469(12)
H27	0.4916	1.3872	1.3573	0.056*
C28	0.4199(4)	1.3117(2)	1.2680(7)	0.0438(12)
H28	0.3642	1.3317	1.2198	0.053*
N1	0.0691(3)	0.95903(17)	0.9929(6)	0.0383(9)
N2	0.0761(3)	1.02063(17)	1.0209(7)	0.0453(11)
N3	0.1639(3)	1.03202(18)	1.0733(6)	0.0449(11)
N4	0.3586(3)	0.92532(19)	1.1781(6)	0.0418(10)
N5	0.4501(3)	0.94175(18)	1.2379(6)	0.0398(10)
O1	0.2820(3)	1.21425(16)	1.1088(6)	0.0586(11)
O2	0.5588(3)	1.11419(15)	1.3481(5)	0.0473(9)

(B), pyrazole (C), phenyl (C13—C18) (D) and indandione (E) groups] is close to planar. The interplanar angles between groups A and B, B and C, C and D, C and E are 38.3(2)°, 9.4(2)°, 5.1(2)° and 9.1(2)°, respectively. In the crystal, the molecules stack along the *c*-axis with a π-π contact distance of 3.6 Å. Within the stack, the molecules are linked by edge-to face interactions between rings A of neighbouring molecules (C . . . centroid distance = 3.86 Å).

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