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4-[(*Z*)-(2,5-Dimethylphenylamino)-phenylmethylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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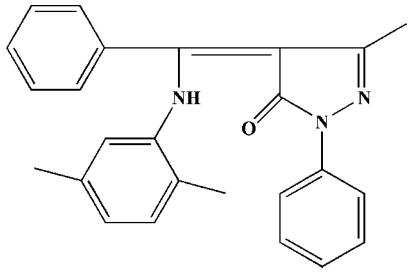
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.063; wR factor = 0.144; data-to-parameter ratio = 13.8.

There are two molecules in the asymmetric unit of the title compound, $C_{25}H_{23}N_3O$, both of which are stabilized by an intramolecular N—H···O hydrogen bond. The dihedral angles between the pyrazole plane and the attached phenyl ring in the two molecules are 19.9 (2) and 17.7 (2)°.

Related literature

For related literature, see: Bao *et al.* (2004); Ma (2005); Ma *et al.* (2006*a*,*b*).



Experimental

Crystal data

$C_{25}H_{23}N_3O$
M_r = 381.46
Monoclinic, $P2_1/c$
a = 24.011 (3) Å
b = 14.2004 (16) Å
c = 12.5487 (15) Å
β = 104.601 (2)°
V = 4140.5 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.982, T_{max} = 0.992
26490 measured reflections
7291 independent reflections
3103 reflections with $I > 2\sigma(I)$
R_{int} = 0.139

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.144
S = 0.85
7291 reflections
530 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	1.94	2.683 (4)	143
N4—H4*A*···O2	0.86	1.94	2.674 (4)	142

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2585).

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supplementary materials

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4-[(*Z*)-(2,5-Dimethylphenylamino)phenylmethylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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Comment

The title compound, (I) (Fig. 1) has two methyl substituents in the 2,5-dimethylphenylamino portion of the molecule; the general features are similar to those found in the analogous 2-tolylamino (Bao *et al.*, 2004), 2,4-dimethylphenylamino(Ma *et al.*, 2006*b*) and 4-tolylamino (Ma, 2005) derivatives. Compound (I) can be used to chelate to a divalent transition metal (Ma *et al.*, 2006*a*). In both asymmetric molecules of (I), an intramolecular N—H···O hydrogen bond occurs (Table 1).

Experimental

1-Phenyl-3-methyl-4-benzoyl-5-pyrazolone (1.60 g, 5.8 mm mol) and 2,4-dimethylaniline (0.73 g, 6.0 mm mol) were dissolved in ethanol (35 ml); formic acid (0.5 ml) was added to catalyse the reaction. The solution was heated under reflux for 8 h. The solvent was removed and the pure product obtained upon recrystallization from a 1:1 ethanol/n-heptane mixture in 80% yield. Yellow blocks of (I) were grown from an ethanol solution of the compound. Elemental analysis calculated for $C_{25}H_{23}N_3O$: C 79.29, H 9.15, N 11.56%; found: C 79.40, H 9.32, N 11.35%.

Refinement

The H atoms were placed in calculated positions (C—H = 0.93–0.96 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

Figures

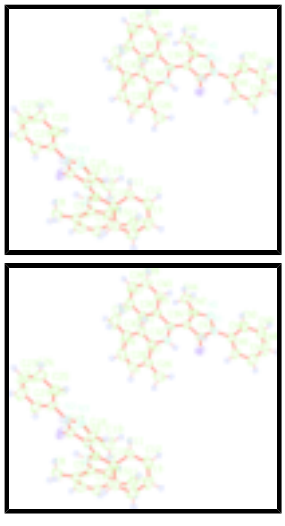


Fig. 1. Vew of the molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

4-[(*Z*)-(2,5-Dimethylphenylamino)phenylmethylene]-3-methyl-1-phenyl-1*H*-pyrazol-\ 5(4*H*)-one

Crystal data

$C_{25}H_{23}N_3O$	F_{000} = 1616
M_r = 381.46	D_x = 1.224 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1791 reflections
a = 24.011 (3) Å	θ = 2.5–17.0º
b = 14.2004 (16) Å	μ = 0.08 mm^{-1}
c = 12.5487 (15) Å	T = 293 (2) K
β = 104.601 (2)º	Block, yellow
V = 4140.5 (9) Å^3	0.30 × 0.20 × 0.10 mm
Z = 8	

Data collection

Bruker SMART CCD diffractometer	7291 independent reflections
Radiation source: fine-focus sealed tube	3103 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.139
T = 292(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 0.9º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −28→28
T_{min} = 0.982, T_{max} = 0.992	k = −14→16
26490 measured reflections	l = −14→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.063	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.144	$(\Delta/\sigma)_{max} < 0.001$
S = 0.85	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
7291 reflections	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
530 parameters	Extinction correction: SHELXTL (Bruker, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0020 (3)
Secondary atom site location: difference Fourier map	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.67019 (10)	0.51803 (16)	0.0567 (2)	0.0646 (8)
N1	0.63486 (11)	0.34429 (19)	−0.0131 (2)	0.0504 (8)
H1	0.6535	0.3959	−0.0142	0.061*
N2	0.60746 (12)	0.5833 (2)	0.1519 (2)	0.0510 (8)
N3	0.55672 (12)	0.5571 (2)	0.1796 (2)	0.0546 (8)
C1	0.67171 (18)	0.0015 (3)	−0.0476 (4)	0.0890 (14)
H1A	0.6670	0.0004	0.0261	0.133*
H1B	0.7068	−0.0300	−0.0495	0.133*
H1C	0.6398	−0.0299	−0.0961	0.133*
C2	0.67414 (15)	0.1026 (3)	−0.0846 (3)	0.0576 (11)
C3	0.69913 (15)	0.1257 (3)	−0.1693 (3)	0.0629 (12)
H3	0.7136	0.0782	−0.2058	0.075*
C4	0.70298 (15)	0.2191 (3)	−0.2008 (3)	0.0635 (11)
H4	0.7208	0.2328	−0.2567	0.076*
C5	0.68098 (14)	0.2915 (3)	−0.1508 (3)	0.0479 (9)
C6	0.65489 (14)	0.2684 (2)	−0.0663 (3)	0.0443 (9)
C7	0.65241 (14)	0.1753 (2)	−0.0341 (3)	0.0512 (10)
H7	0.6356	0.1614	0.0231	0.061*
C8	0.68520 (16)	0.3915 (3)	−0.1861 (3)	0.0683 (12)
H8A	0.7030	0.3931	−0.2465	0.102*
H8B	0.7079	0.4272	−0.1256	0.102*
H8C	0.6473	0.4183	−0.2088	0.102*
C9	0.59229 (13)	0.3519 (2)	0.0385 (3)	0.0400 (8)
C10	0.55344 (14)	0.2711 (2)	0.0405 (3)	0.0389 (8)
C11	0.55606 (14)	0.2278 (2)	0.1404 (3)	0.0481 (9)
H11	0.5809	0.2507	0.2045	0.058*
C12	0.52173 (17)	0.1507 (3)	0.1446 (3)	0.0642 (11)
H12	0.5236	0.1212	0.2117	0.077*
C13	0.48491 (17)	0.1174 (3)	0.0506 (4)	0.0640 (12)
H13	0.4622	0.0649	0.0540	0.077*
C14	0.48122 (16)	0.1607 (3)	−0.0481 (3)	0.0641 (11)
H14	0.4552	0.1387	−0.1112	0.077*
C15	0.51585 (15)	0.2367 (3)	−0.0544 (3)	0.0536 (10)

H15	0.5140	0.2650	−0.1220	0.064*
C16	0.58641 (13)	0.4375 (2)	0.0878 (3)	0.0415 (9)
C17	0.62622 (15)	0.5138 (2)	0.0943 (3)	0.0470 (9)
C18	0.54434 (14)	0.4717 (2)	0.1421 (3)	0.0448 (9)
C19	0.49001 (14)	0.4262 (2)	0.1543 (3)	0.0632 (11)
H19A	0.4990	0.3811	0.2132	0.095*
H19B	0.4714	0.3948	0.0870	0.095*
H19C	0.4648	0.4734	0.1707	0.095*
C20	0.63215 (15)	0.6723 (2)	0.1862 (3)	0.0500 (10)
C21	0.67085 (16)	0.7118 (3)	0.1349 (3)	0.0685 (12)
H21	0.6816	0.6793	0.0789	0.082*
C22	0.69358 (19)	0.7996 (3)	0.1665 (4)	0.0880 (15)
H22	0.7191	0.8270	0.1308	0.106*
C23	0.67845 (18)	0.8466 (3)	0.2510 (4)	0.0817 (14)
H23	0.6942	0.9055	0.2729	0.098*
C24	0.64080 (19)	0.8076 (3)	0.3025 (3)	0.0741 (13)
H24	0.6307	0.8400	0.3592	0.089*
C25	0.61707 (15)	0.7188 (3)	0.2709 (3)	0.0564 (10)
H25	0.5915	0.6917	0.3066	0.068*
O2	0.82990 (11)	−0.02049 (16)	0.8951 (2)	0.0628 (7)
N4	0.86655 (12)	0.1502 (2)	0.8538 (2)	0.0522 (8)
H4A	0.8474	0.0989	0.8351	0.063*
N5	0.89146 (12)	−0.0833 (2)	1.0548 (2)	0.0500 (8)
N6	0.94280 (13)	−0.0567 (2)	1.1309 (2)	0.0553 (8)
C26	0.81578 (17)	0.1054 (3)	0.6290 (3)	0.0744 (12)
H26A	0.8017	0.1058	0.5503	0.112*
H26B	0.7893	0.0717	0.6610	0.112*
H26C	0.8527	0.0751	0.6489	0.112*
C27	0.82146 (15)	0.2048 (3)	0.6711 (3)	0.0528 (10)
C28	0.80112 (16)	0.2794 (4)	0.6015 (3)	0.0674 (12)
H28	0.7840	0.2668	0.5278	0.081*
C29	0.80515 (16)	0.3718 (3)	0.6370 (4)	0.0669 (12)
H29	0.7915	0.4200	0.5871	0.080*
C30	0.82946 (15)	0.3925 (3)	0.7463 (4)	0.0592 (11)
C31	0.84949 (14)	0.3184 (3)	0.8175 (3)	0.0532 (10)
H31	0.8652	0.3310	0.8917	0.064*
C32	0.84670 (14)	0.2270 (3)	0.7812 (3)	0.0466 (9)
C33	0.83310 (18)	0.4922 (3)	0.7875 (4)	0.0928 (15)
H33A	0.8315	0.4926	0.8632	0.139*
H33B	0.8014	0.5278	0.7442	0.139*
H33C	0.8687	0.5198	0.7815	0.139*
C34	0.90941 (15)	0.1428 (2)	0.9461 (3)	0.0433 (9)
C35	0.94845 (13)	0.2243 (2)	0.9825 (3)	0.0400 (8)
C36	0.98698 (15)	0.2547 (3)	0.9240 (3)	0.0545 (10)
H36	0.9895	0.2228	0.8606	0.065*
C37	1.02148 (16)	0.3316 (3)	0.9590 (3)	0.0680 (12)
H37	1.0474	0.3516	0.9198	0.082*
C38	1.01742 (18)	0.3792 (3)	1.0532 (4)	0.0708 (12)
H38	1.0401	0.4321	1.0763	0.085*

C39	0.98041 (18)	0.3490 (3)	1.1119 (3)	0.0659 (11)
H39	0.9781	0.3810	1.1753	0.079*
C40	0.94632 (15)	0.2714 (3)	1.0781 (3)	0.0508 (10)
H40	0.9217	0.2504	1.1195	0.061*
C41	0.91444 (14)	0.0598 (2)	1.0050 (3)	0.0418 (9)
C42	0.95604 (14)	0.0279 (3)	1.1014 (3)	0.0451 (9)
C43	0.87312 (16)	−0.0160 (2)	0.9754 (3)	0.0483 (9)
C44	1.01056 (14)	0.0730 (2)	1.1639 (3)	0.0617 (11)
H44A	1.0335	0.0276	1.2127	0.093*
H44B	1.0018	0.1248	1.2060	0.093*
H44C	1.0316	0.0955	1.1133	0.093*
C45	0.86489 (16)	−0.1701 (3)	1.0705 (3)	0.0504 (10)
C46	0.82352 (18)	−0.2102 (3)	0.9886 (3)	0.0704 (12)
H46	0.8125	−0.1809	0.9202	0.084*
C47	0.79789 (19)	−0.2935 (3)	1.0058 (4)	0.0866 (14)
H47	0.7699	−0.3207	0.9492	0.104*
C48	0.8140 (2)	−0.3363 (3)	1.1072 (5)	0.0890 (15)
H48	0.7966	−0.3923	1.1194	0.107*
C49	0.8553 (2)	−0.2972 (3)	1.1897 (4)	0.0750 (13)
H49	0.8665	−0.3270	1.2577	0.090*
C50	0.88070 (15)	−0.2128 (3)	1.1725 (3)	0.0566 (10)
H50	0.9083	−0.1852	1.2294	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0691 (18)	0.0505 (17)	0.088 (2)	−0.0123 (14)	0.0454 (16)	−0.0124 (14)
N1	0.0615 (19)	0.0379 (18)	0.061 (2)	−0.0102 (16)	0.0330 (16)	−0.0075 (15)
N2	0.058 (2)	0.043 (2)	0.059 (2)	−0.0052 (16)	0.0281 (16)	−0.0092 (16)
N3	0.062 (2)	0.050 (2)	0.060 (2)	−0.0035 (17)	0.0301 (17)	−0.0097 (16)
C1	0.087 (3)	0.053 (3)	0.131 (4)	−0.008 (2)	0.033 (3)	−0.014 (3)
C2	0.043 (2)	0.049 (3)	0.079 (3)	−0.003 (2)	0.013 (2)	−0.017 (2)
C3	0.053 (3)	0.068 (3)	0.070 (3)	0.007 (2)	0.020 (2)	−0.031 (2)
C4	0.049 (2)	0.090 (4)	0.054 (3)	0.005 (2)	0.017 (2)	−0.013 (3)
C5	0.048 (2)	0.056 (3)	0.044 (2)	0.000 (2)	0.0192 (18)	−0.001 (2)
C6	0.048 (2)	0.042 (2)	0.046 (2)	−0.0021 (19)	0.0170 (18)	−0.0108 (19)
C7	0.053 (2)	0.043 (3)	0.060 (3)	−0.005 (2)	0.0197 (19)	−0.009 (2)
C8	0.072 (3)	0.075 (3)	0.067 (3)	−0.007 (2)	0.035 (2)	0.006 (2)
C9	0.041 (2)	0.044 (2)	0.037 (2)	−0.0027 (18)	0.0140 (17)	0.0034 (18)
C10	0.043 (2)	0.041 (2)	0.035 (2)	0.0013 (18)	0.0147 (17)	−0.0015 (17)
C11	0.057 (2)	0.048 (2)	0.038 (2)	−0.005 (2)	0.0100 (18)	0.0047 (19)
C12	0.078 (3)	0.064 (3)	0.059 (3)	−0.006 (2)	0.032 (2)	0.012 (2)
C13	0.072 (3)	0.041 (3)	0.088 (3)	−0.016 (2)	0.037 (3)	−0.005 (2)
C14	0.061 (3)	0.063 (3)	0.065 (3)	−0.019 (2)	0.011 (2)	−0.018 (2)
C15	0.059 (3)	0.055 (3)	0.046 (2)	−0.006 (2)	0.013 (2)	0.002 (2)
C16	0.044 (2)	0.042 (2)	0.042 (2)	−0.0031 (19)	0.0165 (17)	0.0012 (18)
C17	0.051 (2)	0.043 (2)	0.052 (2)	−0.0003 (19)	0.0220 (19)	−0.0030 (19)
C18	0.054 (2)	0.037 (2)	0.047 (2)	−0.0014 (19)	0.0189 (19)	−0.0022 (18)

C19	0.065 (3)	0.056 (3)	0.081 (3)	−0.003 (2)	0.040 (2)	−0.007 (2)
C20	0.056 (2)	0.036 (2)	0.057 (3)	−0.0055 (19)	0.012 (2)	−0.0115 (19)
C21	0.085 (3)	0.042 (3)	0.087 (3)	−0.016 (2)	0.039 (3)	−0.015 (2)
C22	0.103 (4)	0.053 (3)	0.120 (4)	−0.020 (3)	0.051 (3)	−0.015 (3)
C23	0.070 (3)	0.053 (3)	0.118 (4)	−0.008 (3)	0.017 (3)	−0.016 (3)
C24	0.081 (3)	0.057 (3)	0.075 (3)	0.009 (3)	0.003 (3)	−0.025 (2)
C25	0.061 (3)	0.050 (3)	0.057 (3)	0.002 (2)	0.013 (2)	−0.008 (2)
O2	0.0699 (18)	0.0556 (18)	0.0517 (16)	−0.0130 (14)	−0.0052 (14)	0.0022 (14)
N4	0.064 (2)	0.042 (2)	0.0416 (19)	−0.0072 (17)	−0.0027 (16)	0.0000 (16)
N5	0.055 (2)	0.044 (2)	0.0463 (19)	−0.0075 (17)	0.0047 (16)	0.0042 (16)
N6	0.061 (2)	0.049 (2)	0.048 (2)	−0.0061 (17)	−0.0022 (16)	0.0074 (16)
C26	0.077 (3)	0.094 (4)	0.050 (3)	−0.004 (3)	0.011 (2)	−0.009 (2)
C27	0.045 (2)	0.071 (3)	0.040 (2)	−0.003 (2)	0.0070 (18)	0.006 (2)
C28	0.052 (3)	0.106 (4)	0.043 (3)	−0.001 (3)	0.010 (2)	0.016 (3)
C29	0.051 (3)	0.078 (4)	0.067 (3)	0.008 (2)	0.007 (2)	0.038 (3)
C30	0.039 (2)	0.054 (3)	0.083 (3)	−0.002 (2)	0.013 (2)	0.018 (3)
C31	0.052 (2)	0.051 (3)	0.052 (2)	−0.001 (2)	0.0031 (19)	0.010 (2)
C32	0.047 (2)	0.047 (3)	0.044 (2)	−0.003 (2)	0.0084 (18)	0.011 (2)
C33	0.085 (3)	0.052 (3)	0.131 (4)	−0.001 (3)	0.007 (3)	0.023 (3)
C34	0.053 (2)	0.041 (2)	0.036 (2)	−0.0023 (19)	0.0106 (18)	−0.0080 (19)
C35	0.044 (2)	0.037 (2)	0.037 (2)	0.0039 (18)	0.0072 (17)	−0.0008 (17)
C36	0.058 (3)	0.057 (3)	0.051 (2)	−0.005 (2)	0.018 (2)	−0.004 (2)
C37	0.066 (3)	0.070 (3)	0.068 (3)	−0.019 (2)	0.018 (2)	0.012 (2)
C38	0.079 (3)	0.047 (3)	0.075 (3)	−0.015 (2)	−0.003 (3)	0.001 (2)
C39	0.084 (3)	0.055 (3)	0.057 (3)	−0.010 (2)	0.013 (2)	−0.015 (2)
C40	0.061 (2)	0.049 (3)	0.041 (2)	−0.006 (2)	0.0116 (18)	−0.0087 (19)
C41	0.047 (2)	0.038 (2)	0.040 (2)	−0.0021 (19)	0.0093 (17)	−0.0017 (18)
C42	0.048 (2)	0.046 (2)	0.039 (2)	0.000 (2)	0.0072 (18)	−0.0006 (19)
C43	0.055 (3)	0.043 (2)	0.043 (2)	0.000 (2)	0.005 (2)	0.001 (2)
C44	0.059 (3)	0.055 (3)	0.060 (3)	−0.003 (2)	−0.006 (2)	0.004 (2)
C45	0.055 (2)	0.043 (2)	0.056 (3)	−0.004 (2)	0.021 (2)	0.007 (2)
C46	0.088 (3)	0.048 (3)	0.070 (3)	−0.023 (3)	0.010 (3)	0.004 (2)
C47	0.092 (4)	0.061 (3)	0.100 (4)	−0.025 (3)	0.013 (3)	0.002 (3)
C48	0.075 (3)	0.054 (3)	0.140 (5)	−0.012 (3)	0.032 (3)	0.027 (3)
C49	0.078 (3)	0.057 (3)	0.097 (4)	0.009 (3)	0.036 (3)	0.031 (3)
C50	0.065 (3)	0.047 (3)	0.060 (3)	0.003 (2)	0.018 (2)	0.007 (2)

Geometric parameters (Å, °)

O1—C17	1.261 (4)	O2—C43	1.253 (4)
N1—C9	1.345 (4)	N4—C34	1.346 (4)
N1—C6	1.413 (4)	N4—C32	1.424 (4)
N1—H1	0.8609	N4—H4A	0.8615
N2—C17	1.365 (4)	N5—C43	1.370 (4)
N2—N3	1.399 (3)	N5—N6	1.407 (3)
N2—C20	1.415 (4)	N5—C45	1.425 (4)
N3—C18	1.308 (4)	N6—C42	1.320 (4)
C1—C2	1.514 (5)	C26—C27	1.501 (5)
C1—H1A	0.9600	C26—H26A	0.9600

C1—H1B	0.9600	C26—H26B	0.9600
C1—H1C	0.9600	C26—H26C	0.9600
C2—C7	1.380 (4)	C27—C28	1.381 (5)
C2—C3	1.386 (5)	C27—C32	1.398 (4)
C3—C4	1.393 (5)	C28—C29	1.381 (5)
C3—H3	0.9300	C28—H28	0.9300
C4—C5	1.378 (5)	C29—C30	1.381 (5)
C4—H4	0.9300	C29—H29	0.9300
C5—C6	1.400 (4)	C30—C31	1.385 (5)
C5—C8	1.498 (5)	C30—C33	1.501 (5)
C6—C7	1.389 (4)	C31—C32	1.372 (5)
C7—H7	0.9300	C31—H31	0.9300
C8—H8A	0.9600	C33—H33A	0.9600
C8—H8B	0.9600	C33—H33B	0.9600
C8—H8C	0.9600	C33—H33C	0.9600
C9—C16	1.389 (4)	C34—C41	1.382 (4)
C9—C10	1.483 (4)	C34—C35	1.486 (4)
C10—C11	1.383 (4)	C35—C40	1.386 (4)
C10—C15	1.388 (4)	C35—C36	1.387 (4)
C11—C12	1.380 (4)	C36—C37	1.374 (5)
C11—H11	0.9300	C36—H36	0.9300
C12—C13	1.368 (5)	C37—C38	1.386 (5)
C12—H12	0.9300	C37—H37	0.9300
C13—C14	1.366 (5)	C38—C39	1.359 (5)
C13—H13	0.9300	C38—H38	0.9300
C14—C15	1.378 (5)	C39—C40	1.375 (5)
C14—H14	0.9300	C39—H39	0.9300
C15—H15	0.9300	C40—H40	0.9300
C16—C17	1.433 (4)	C41—C42	1.434 (4)
C16—C18	1.437 (4)	C41—C43	1.447 (4)
C18—C19	1.498 (4)	C42—C44	1.490 (4)
C19—H19A	0.9600	C44—H44A	0.9600
C19—H19B	0.9600	C44—H44B	0.9600
C19—H19C	0.9600	C44—H44C	0.9600
C20—C25	1.375 (4)	C45—C46	1.362 (5)
C20—C21	1.377 (5)	C45—C50	1.380 (4)
C21—C22	1.379 (5)	C46—C47	1.375 (5)
C21—H21	0.9300	C46—H46	0.9300
C22—C23	1.378 (5)	C47—C48	1.375 (6)
C22—H22	0.9300	C47—H47	0.9300
C23—C24	1.355 (5)	C48—C49	1.358 (5)
C23—H23	0.9300	C48—H48	0.9300
C24—C25	1.399 (5)	C49—C50	1.386 (5)
C24—H24	0.9300	C49—H49	0.9300
C25—H25	0.9300	C50—H50	0.9300
C9—N1—C6	132.7 (3)	C34—N4—C32	132.1 (3)
C9—N1—H1	113.7	C34—N4—H4A	114.1
C6—N1—H1	113.6	C32—N4—H4A	113.8
C17—N2—N3	111.3 (3)	C43—N5—N6	111.9 (3)

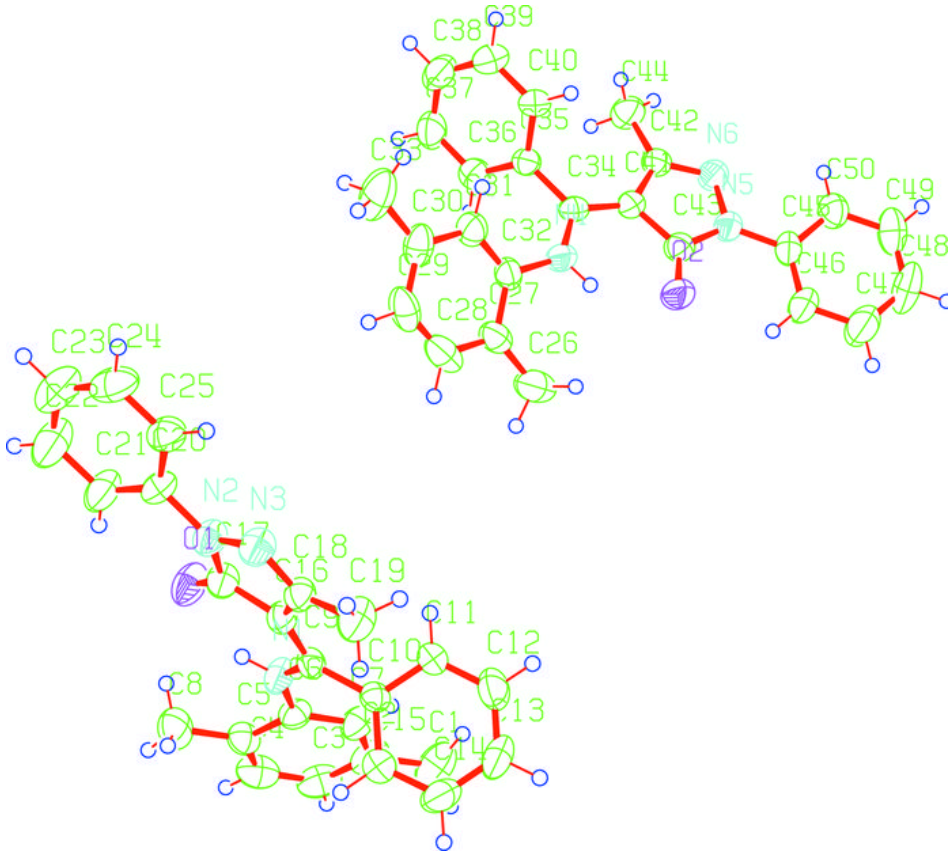
C17—N2—C20	129.6 (3)	C43—N5—C45	129.1 (3)
N3—N2—C20	119.1 (3)	N6—N5—C45	118.9 (3)
C18—N3—N2	106.9 (3)	C42—N6—N5	106.6 (3)
C2—C1—H1A	109.5	C27—C26—H26A	109.5
C2—C1—H1B	109.5	C27—C26—H26B	109.5
H1A—C1—H1B	109.5	H26A—C26—H26B	109.5
C2—C1—H1C	109.5	C27—C26—H26C	109.5
H1A—C1—H1C	109.5	H26A—C26—H26C	109.5
H1B—C1—H1C	109.5	H26B—C26—H26C	109.5
C7—C2—C3	117.5 (4)	C28—C27—C32	116.6 (4)
C7—C2—C1	121.4 (4)	C28—C27—C26	120.8 (4)
C3—C2—C1	121.2 (4)	C32—C27—C26	122.6 (4)
C2—C3—C4	121.0 (3)	C29—C28—C27	122.7 (4)
C2—C3—H3	119.5	C29—C28—H28	118.7
C4—C3—H3	119.5	C27—C28—H28	118.7
C5—C4—C3	121.4 (4)	C28—C29—C30	120.1 (4)
C5—C4—H4	119.3	C28—C29—H29	120.0
C3—C4—H4	119.3	C30—C29—H29	120.0
C4—C5—C6	117.8 (4)	C29—C30—C31	118.0 (4)
C4—C5—C8	120.7 (3)	C29—C30—C33	121.1 (4)
C6—C5—C8	121.5 (3)	C31—C30—C33	120.9 (4)
C7—C6—C5	120.2 (3)	C32—C31—C30	121.7 (4)
C7—C6—N1	123.0 (3)	C32—C31—H31	119.2
C5—C6—N1	116.7 (3)	C30—C31—H31	119.2
C2—C7—C6	122.0 (3)	C31—C32—C27	120.9 (3)
C2—C7—H7	119.0	C31—C32—N4	122.2 (3)
C6—C7—H7	119.0	C27—C32—N4	116.8 (3)
C5—C8—H8A	109.5	C30—C33—H33A	109.5
C5—C8—H8B	109.5	C30—C33—H33B	109.5
H8A—C8—H8B	109.5	H33A—C33—H33B	109.5
C5—C8—H8C	109.5	C30—C33—H33C	109.5
H8A—C8—H8C	109.5	H33A—C33—H33C	109.5
H8B—C8—H8C	109.5	H33B—C33—H33C	109.5
N1—C9—C16	117.4 (3)	N4—C34—C41	118.2 (3)
N1—C9—C10	120.3 (3)	N4—C34—C35	119.4 (3)
C16—C9—C10	122.4 (3)	C41—C34—C35	122.5 (3)
C11—C10—C15	119.5 (3)	C40—C35—C36	118.9 (3)
C11—C10—C9	118.3 (3)	C40—C35—C34	118.9 (3)
C15—C10—C9	122.2 (3)	C36—C35—C34	122.2 (3)
C12—C11—C10	119.7 (3)	C37—C36—C35	120.5 (3)
C12—C11—H11	120.1	C37—C36—H36	119.8
C10—C11—H11	120.1	C35—C36—H36	119.8
C13—C12—C11	120.3 (4)	C36—C37—C38	119.6 (4)
C13—C12—H12	119.9	C36—C37—H37	120.2
C11—C12—H12	119.9	C38—C37—H37	120.2
C14—C13—C12	120.4 (4)	C39—C38—C37	120.3 (4)
C14—C13—H13	119.8	C39—C38—H38	119.8
C12—C13—H13	119.8	C37—C38—H38	119.8
C13—C14—C15	120.2 (4)	C38—C39—C40	120.3 (4)

C13—C14—H14	119.9	C38—C39—H39	119.8
C15—C14—H14	119.9	C40—C39—H39	119.8
C14—C15—C10	119.8 (4)	C39—C40—C35	120.4 (3)
C14—C15—H15	120.1	C39—C40—H40	119.8
C10—C15—H15	120.1	C35—C40—H40	119.8
C9—C16—C17	123.1 (3)	C34—C41—C42	132.0 (3)
C9—C16—C18	132.0 (3)	C34—C41—C43	122.4 (3)
C17—C16—C18	104.9 (3)	C42—C41—C43	105.6 (3)
O1—C17—N2	125.6 (3)	N6—C42—C41	111.0 (3)
O1—C17—C16	128.6 (3)	N6—C42—C44	119.0 (3)
N2—C17—C16	105.8 (3)	C41—C42—C44	129.9 (3)
N3—C18—C16	111.1 (3)	O2—C43—N5	126.8 (3)
N3—C18—C19	119.2 (3)	O2—C43—C41	128.3 (3)
C16—C18—C19	129.6 (3)	N5—C43—C41	104.9 (3)
C18—C19—H19A	109.5	C42—C44—H44A	109.5
C18—C19—H19B	109.5	C42—C44—H44B	109.5
H19A—C19—H19B	109.5	H44A—C44—H44B	109.5
C18—C19—H19C	109.5	C42—C44—H44C	109.5
H19A—C19—H19C	109.5	H44A—C44—H44C	109.5
H19B—C19—H19C	109.5	H44B—C44—H44C	109.5
C25—C20—C21	120.4 (3)	C46—C45—C50	119.6 (4)
C25—C20—N2	119.5 (3)	C46—C45—N5	121.6 (3)
C21—C20—N2	120.1 (3)	C50—C45—N5	118.8 (3)
C20—C21—C22	119.9 (4)	C45—C46—C47	120.7 (4)
C20—C21—H21	120.0	C45—C46—H46	119.6
C22—C21—H21	120.0	C47—C46—H46	119.6
C23—C22—C21	119.9 (4)	C48—C47—C46	119.5 (4)
C23—C22—H22	120.1	C48—C47—H47	120.2
C21—C22—H22	120.1	C46—C47—H47	120.2
C24—C23—C22	120.4 (4)	C49—C48—C47	120.4 (4)
C24—C23—H23	119.8	C49—C48—H48	119.8
C22—C23—H23	119.8	C47—C48—H48	119.8
C23—C24—C25	120.5 (4)	C48—C49—C50	120.0 (4)
C23—C24—H24	119.8	C48—C49—H49	120.0
C25—C24—H24	119.8	C50—C49—H49	120.0
C20—C25—C24	119.0 (4)	C45—C50—C49	119.7 (4)
C20—C25—H25	120.5	C45—C50—H50	120.1
C24—C25—H25	120.5	C49—C50—H50	120.1

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86	1.94	2.683 (4)	143
N4—H4A···O2	0.86	1.94	2.674 (4)	142

Fig. 1


C38
C39
C40
C44
C42
N6
C36
C34
N5
C50
C49
C30
C43
C48
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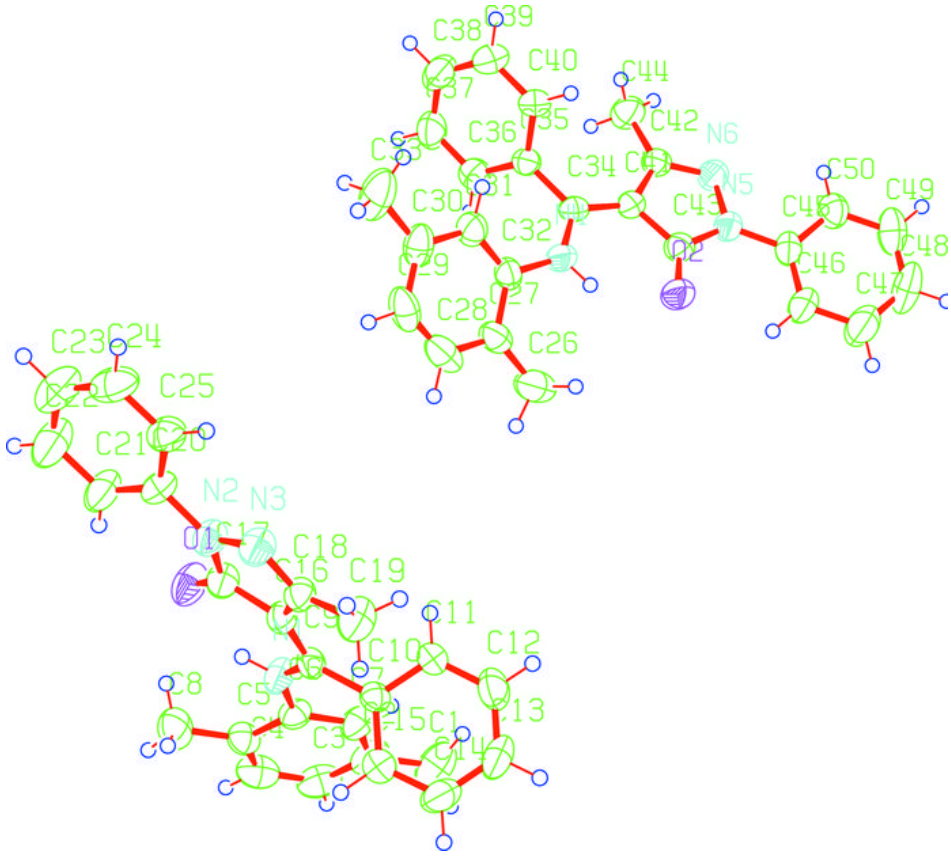
C46
C29
C47
C28
C26
C23
C24
C25
C21
N2
N3
C18
C19
C11
C12
C8
C5
C13
C1

Fig. 2


C38
C39
C40
C44
C42
N6
C36
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N5
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C47
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C13
C1