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1-Methyl-5-(4-methylbenzoyl)-4-(4-methylphenyl)pyrimidine-2(1*H*)-thione

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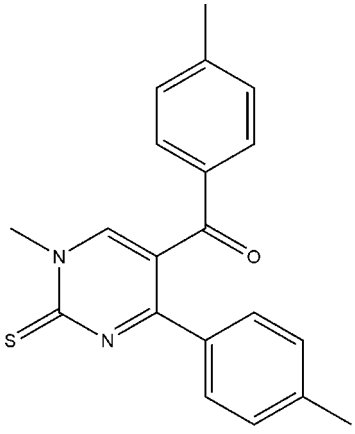
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.107; data-to-parameter ratio = 15.0.

The title compound, $C_{20}H_{18}N_2OS$, contains three rings that are not coplanar. The benzene rings make dihedral angles of 31.37 (8) and 68.84 (5)° with the pyrimidine ring, while the dihedral angle between the two benzene rings is 76.70 (5)°. The structure is stabilized by intermolecular C—H···O hydrogen bonds, resulting in the formation of molecular chains along the [010] direction.

Related literature

The starting material was prepared in a manner similar to that described by Ziegler *et al.* (1967). Biological activities of pyrimidines and pyrimidinethiones are described by Brown (1984, 1985), Cannito *et al.* (1990), Chakaravorty *et al.* (1992), De Clerq & Walker (1985), Kleemann & Engel (1982), Lomis *et al.* (1988), Perrissin *et al.* (1988), Shishoo & Jain (1992), Smith & Kan (1964), Tetsuo *et al.* (1987) and Vega *et al.* (1990).



Experimental

Crystal data

$C_{20}H_{18}N_2OS$
M_r = 334.42
Monoclinic, $P2_1/c$
a = 5.8203 (5) Å
b = 15.6178 (10) Å
c = 19.4161 (16) Å
β = 104.466 (6)°
V = 1709.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 296 K
0.61 × 0.35 × 0.20 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.923, T_{max} = 0.978
14819 measured reflections
3294 independent reflections
2225 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.01
3294 reflections
220 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C47—H47B···O5^{i}	0.96	2.47	3.393 (3)	162

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

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, 1997); 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) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2088).

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supplementary materials

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1-Methyl-5-(4-methylbenzoyl)-4-(4-methylphenyl)pyrimidine-2(1*H*)-thione

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Comment

In general, pyrimidines have found much interest for their widespread potential biological activities (Kleemann & Engel, 1982) and medicinal applications, thus their chemistry has been investigated extensively (Brown, 1984, 1985; Lomis *et al.*, 1988). In particular, various analogues of pyrimidine-thiones possess effective antibacterial, antifungal, antiviral, anti-AIDS, insecticidal and miticidal activities (De Clerq & Walker, 1985). Furthermore many condensed heterocyclic systems, especially when linked to a pyrimidine ring, play an important role as analgesic (Perrissin *et al.*, 1988), antihypertensive (Cannito *et al.*, 1990), antipyretic (Smith & Kan, 1964), and antiinflammatory drugs (Vega *et al.*, 1990), also as pesticides (Tetsuo *et al.*, 1987), herbicides (Chakaravorty *et al.*, 1992), and plant growth regulators (Shishoo & Jain, 1992). In view of these important properties, we have undertaken the X-ray diffraction study of the title compound.

The structure of the title compound is shown in Fig. 1. The structure contains one central pyrimidine ring (N1/N3/C2/C4—C6) with a methyl substituent at N1, an S substituent at C2, a *p*-tolyl group (C41—C47) at C4 and a methylbenzoyl group (O5/C51—C58) at C5. The plane of the pyrimidine ring makes dihedral angles of 31.37 (8) and 68.84 (5)° with the (C41—C46) and (C52—C57) phenyl rings, respectively. The pyrimidine ring is planar with a maximum deviation of 0.0776 (12) Å for atom C2. The interatomic distances and angles show no anomalies.

The molecular structure of the title compound contains no significant intramolecular interactions. In the construction of the intermolecular connections, 2_1 screw symmetry-related molecules, which form pairs of neighbouring molecules translated linearly along the *b* axis of the unit cell, play an active bridging role. Atom C47 acts as a hydrogen-bond donor, *via* atom H47B, to atom O5 at $(2 - x, -1/2 + y, 1/2 - z)$. Extension of this hydrogen-bonding interaction along b results in the formation of molecular chains along the [010] direction (Fig. 2).

Experimental

An equimolar mixture of 4-(4-methylbenzoyl)-5-(4-methylphenyl)-2,3-dihydro-2,3-furandione (0.50 g, 1.63 mmol), easily obtained from oxalyl chloride and 1,3-bis(4-methylphenyl)propane-1,3-dione, in a similar way as described by Ziegler *et al.* (1967), and *N*-methylthiourea (0.15 g, 1.63 mmol) were refluxed in 30 ml boiling benzene for 3 h. After the evaporation of the solvent, the oily residue was treated with dry diethylether to give a yellow precipitate, which was filtered off and recrystallized from acetic acid (yield: 0.35 g, 64%; m.p. 483 K). IR (KBr, ν, cm^{-1}): 3040–2840 (w, aromatic and aliphatic C—H), 1650 (s, C═O), 1603 s, 1567 w, 1514 s, 1492 m (C⋯C, C⋯N, phenyl and aromatic rings), 1185 (m, C═S); ^{1}H NMR (300 MHz, $CDCl_3$, p.p.m.): δ 8.16 (s, 1H at C-6), 7.56–6.99 (m, 8H, Ar—H), 3.97 (s, 3H, N—CH_3), 2.31, 2.24 (two s, 6H, Ar—CH_3). Analysis calculated for $C_{20}H_{18}N2OS$: C 71.83, H 5.42, N 8.38, S 9.59%; found: C 71.80, H 5.47, N 8.18, S 9.60%.

Refinement

H atoms were positioned geometrically and treated using a riding model, fixing the bond lengths at 0.96 and 0.93 Å for CH_3 and CH(aromatic), respectively. The displacement parameters of the H atoms were constrained as U_{iso}(H)= 1.2U_{eq}(1.5U_{eq} for methyl groups). Riding methyl H atoms were allowed to rotate freely during refinement using the AFIX 137 command of *SHELXL97* (Sheldrick, 1997).

Figures

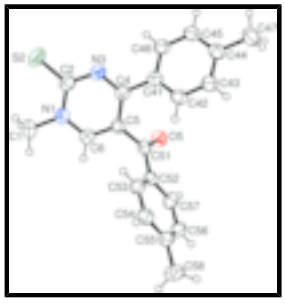

Fig. 1. : An *ORTEP-3* (Farrugia, 1997) drawing of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

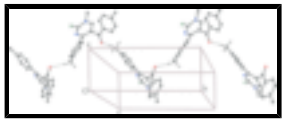

Fig. 2. : The molecular packing of the title compound, viewed along the *c* axis. Dashed lines show the C—H···O interactions.

1-Methyl-5-(4-methylbenzoyl)-4-(4-methylphenyl)pyrimidine-2(1*H*)-thione

Crystal data

$C_{20}H_{18}N_2OS$	F_{000} = 704
M_r = 334.42	D_x = 1.300 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 20480 reflections
a = 5.8203 (5) Å	θ = 1.7–27.9º
b = 15.6178 (10) Å	μ = 0.20 mm^{-1}
c = 19.4161 (16) Å	T = 296 K
β = 104.466 (6)º	Prismatic rod, colorless
V = 1709.0 (2) Å^3	0.61 × 0.35 × 0.20 mm
Z = 4	

Data collection

Stoe IPDSII diffractometer	3294 independent reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	2225 reflections with $I > 2\sigma(I)$
Monochromator: plane graphite	R_{int} = 0.043
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 26.0º

T = 296 K

w scans

Absorption correction: integration (X-RED32; Stoe & Cie, 2002)

T_{min} = 0.923, T_{max} = 0.978

14819 measured reflections

θ_{min} = 1.7º

h = −7→6

k = −19→19

l = −23→23

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.039

$wR(F^2)$ = 0.107

S = 1.01

3294 reflections

220 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.17 e Å^{-3}

$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Extinction correction: none

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}
S2	0.46693 (13)	0.34236 (4)	0.50064 (3)	0.0795 (2)
O5	0.6981 (3)	0.54459 (8)	0.24409 (7)	0.0582 (3)
N1	0.2814 (3)	0.44445 (10)	0.39131 (7)	0.0513 (4)
N3	0.5736 (3)	0.34751 (9)	0.37627 (8)	0.0522 (4)
C1	0.1086 (4)	0.47291 (14)	0.43011 (11)	0.0665 (6)
H1A	0.1881	0.5061	0.4707	0.100*
H1B	0.0355	0.4239	0.4456	0.100*
H1C	−0.0108	0.5074	0.3994	0.100*
C2	0.4422 (3)	0.37950 (12)	0.41885 (9)	0.0518 (4)
C4	0.5771 (3)	0.38456 (11)	0.31569 (9)	0.0450 (4)
C5	0.4461 (3)	0.46083 (11)	0.29287 (8)	0.0447 (4)
C6	0.2926 (3)	0.48546 (12)	0.33108 (9)	0.0502 (4)

H6	0.1924	0.5317	0.3155	0.060*
C41	0.7127 (3)	0.34048 (10)	0.27081 (9)	0.0464 (4)
C42	0.6388 (4)	0.34305 (11)	0.19719 (9)	0.0525 (5)
H42	0.5051	0.3747	0.1754	0.063*
C43	0.7608 (4)	0.29933 (12)	0.15594 (10)	0.0555 (5)
H43	0.7066	0.3014	0.1067	0.067*
C44	0.9619 (4)	0.25246 (11)	0.18617 (10)	0.0531 (4)
C45	1.0344 (4)	0.24938 (12)	0.25993 (10)	0.0598 (5)
H45	1.1682	0.2176	0.2815	0.072*
C46	0.9127 (3)	0.29225 (12)	0.30189 (10)	0.0539 (5)
H46	0.9646	0.2889	0.3512	0.065*
C47	1.0966 (4)	0.20643 (14)	0.14034 (12)	0.0702 (6)
H47A	0.9894	0.1908	0.0960	0.105*
H47B	1.1683	0.1558	0.1644	0.105*
H47C	1.2177	0.2434	0.1314	0.105*
C51	0.4959 (3)	0.51927 (10)	0.23664 (9)	0.0450 (4)
C52	0.2996 (3)	0.54438 (10)	0.17599 (8)	0.0447 (4)
C53	0.0838 (4)	0.50202 (11)	0.16035 (9)	0.0514 (4)
H53	0.0575	0.4584	0.1901	0.062*
C54	−0.0921 (4)	0.52392 (13)	0.10124 (10)	0.0581 (5)
H54	−0.2355	0.4945	0.0914	0.070*
C55	−0.0594 (4)	0.58882 (13)	0.05625 (9)	0.0566 (5)
C56	0.1566 (4)	0.63170 (13)	0.07211 (10)	0.0624 (5)
H56	0.1813	0.6759	0.0427	0.075*
C57	0.3338 (4)	0.60988 (12)	0.13040 (10)	0.0559 (5)
H57	0.4780	0.6388	0.1397	0.067*
C58	−0.2554 (5)	0.61164 (16)	−0.00808 (11)	0.0796 (7)
H58A	−0.3507	0.6566	0.0041	0.119*
H58B	−0.3525	0.5622	−0.0235	0.119*
H58C	−0.1875	0.6307	−0.0457	0.119*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S2	0.0944 (5)	0.0918 (4)	0.0535 (3)	−0.0007 (3)	0.0208 (3)	0.0217 (3)
O5	0.0490 (9)	0.0646 (8)	0.0613 (8)	−0.0083 (7)	0.0141 (6)	0.0010 (6)
N1	0.0519 (10)	0.0569 (9)	0.0478 (8)	−0.0017 (7)	0.0174 (7)	−0.0001 (6)
N3	0.0521 (10)	0.0539 (9)	0.0485 (8)	0.0008 (7)	0.0087 (7)	0.0058 (6)
C1	0.0691 (16)	0.0777 (14)	0.0615 (11)	0.0007 (11)	0.0330 (10)	−0.0042 (10)
C2	0.0502 (12)	0.0544 (10)	0.0494 (9)	−0.0073 (9)	0.0100 (8)	0.0030 (8)
C4	0.0392 (11)	0.0486 (9)	0.0444 (8)	−0.0035 (7)	0.0048 (7)	0.0002 (7)
C5	0.0430 (11)	0.0472 (9)	0.0428 (8)	0.0001 (8)	0.0088 (7)	0.0012 (7)
C6	0.0512 (12)	0.0528 (10)	0.0468 (9)	0.0026 (8)	0.0124 (8)	0.0034 (7)
C41	0.0449 (11)	0.0437 (9)	0.0494 (9)	−0.0019 (8)	0.0095 (7)	0.0007 (7)
C42	0.0497 (12)	0.0505 (10)	0.0518 (9)	0.0060 (8)	0.0020 (8)	−0.0040 (8)
C43	0.0617 (14)	0.0518 (10)	0.0500 (9)	0.0036 (9)	0.0084 (9)	−0.0049 (8)
C44	0.0531 (12)	0.0418 (9)	0.0668 (11)	−0.0025 (8)	0.0193 (9)	−0.0019 (8)
C45	0.0528 (13)	0.0585 (11)	0.0672 (12)	0.0133 (9)	0.0135 (9)	0.0079 (9)

C46	0.0517 (12)	0.0552 (11)	0.0521 (10)	0.0057 (9)	0.0078 (8)	0.0062 (8)
C47	0.0744 (17)	0.0586 (13)	0.0851 (14)	0.0067 (11)	0.0342 (12)	−0.0048 (10)
C51	0.0461 (12)	0.0441 (9)	0.0466 (9)	−0.0016 (8)	0.0151 (7)	−0.0043 (7)
C52	0.0495 (12)	0.0422 (9)	0.0442 (9)	0.0031 (8)	0.0151 (7)	0.0009 (7)
C53	0.0505 (13)	0.0534 (10)	0.0508 (9)	−0.0005 (8)	0.0138 (8)	0.0097 (8)
C54	0.0477 (13)	0.0680 (12)	0.0568 (10)	0.0016 (9)	0.0094 (8)	0.0054 (9)
C55	0.0635 (14)	0.0570 (11)	0.0481 (9)	0.0169 (10)	0.0118 (9)	0.0028 (8)
C56	0.0816 (17)	0.0527 (11)	0.0536 (11)	0.0070 (11)	0.0181 (10)	0.0144 (8)
C57	0.0636 (14)	0.0494 (10)	0.0560 (10)	−0.0073 (9)	0.0174 (9)	0.0033 (8)
C58	0.0835 (18)	0.0877 (16)	0.0610 (12)	0.0265 (13)	0.0054 (11)	0.0140 (11)

Geometric parameters (Å, °)

S2—C2	1.6628 (18)	C44—C47	1.507 (3)
O5—C51	1.215 (2)	C45—C46	1.379 (3)
N1—C6	1.349 (2)	C45—H45	0.9300
N1—C2	1.393 (2)	C46—H46	0.9300
N1—C1	1.468 (2)	C47—H47A	0.9600
N3—C4	1.316 (2)	C47—H47B	0.9600
N3—C2	1.354 (2)	C47—H47C	0.9600
C1—H1A	0.9600	C51—C52	1.474 (2)
C1—H1B	0.9600	C52—C53	1.384 (3)
C1—H1C	0.9600	C52—C57	1.399 (2)
C4—C5	1.424 (2)	C53—C54	1.377 (3)
C4—C41	1.483 (2)	C53—H53	0.9300
C5—C6	1.352 (2)	C54—C55	1.382 (3)
C5—C51	1.506 (2)	C54—H54	0.9300
C6—H6	0.9300	C55—C56	1.390 (3)
C41—C42	1.387 (2)	C55—C58	1.509 (3)
C41—C46	1.391 (3)	C56—C57	1.370 (3)
C42—C43	1.377 (3)	C56—H56	0.9300
C42—H42	0.9300	C57—H57	0.9300
C43—C44	1.381 (3)	C58—H58A	0.9600
C43—H43	0.9300	C58—H58B	0.9600
C44—C45	1.389 (3)	C58—H58C	0.9600
C6—N1—C2	120.33 (16)	C45—C46—C41	120.27 (17)
C6—N1—C1	119.26 (16)	C45—C46—H46	119.9
C2—N1—C1	120.28 (15)	C41—C46—H46	119.9
C4—N3—C2	121.39 (16)	C44—C47—H47A	109.5
N1—C1—H1A	109.5	C44—C47—H47B	109.5
N1—C1—H1B	109.5	H47A—C47—H47B	109.5
H1A—C1—H1B	109.5	C44—C47—H47C	109.5
N1—C1—H1C	109.5	H47A—C47—H47C	109.5
H1A—C1—H1C	109.5	H47B—C47—H47C	109.5
H1B—C1—H1C	109.5	O5—C51—C52	122.87 (16)
N3—C2—N1	117.52 (15)	O5—C51—C5	117.83 (16)
N3—C2—S2	121.80 (15)	C52—C51—C5	119.29 (16)
N1—C2—S2	120.67 (14)	C53—C52—C57	118.39 (16)
N3—C4—C5	121.29 (16)	C53—C52—C51	121.85 (15)

N3—C4—C41	116.78 (15)	C57—C52—C51	119.68 (17)
C5—C4—C41	121.84 (15)	C54—C53—C52	120.61 (17)
C6—C5—C4	116.30 (15)	C54—C53—H53	119.7
C6—C5—C51	119.91 (15)	C52—C53—H53	119.7
C4—C5—C51	123.21 (16)	C53—C54—C55	121.2 (2)
N1—C6—C5	121.48 (17)	C53—C54—H54	119.4
N1—C6—H6	119.3	C55—C54—H54	119.4
C5—C6—H6	119.3	C54—C55—C56	118.24 (17)
C42—C41—C46	118.24 (17)	C54—C55—C58	120.1 (2)
C42—C41—C4	121.24 (16)	C56—C55—C58	121.65 (19)
C46—C41—C4	120.46 (16)	C57—C56—C55	121.07 (18)
C43—C42—C41	120.87 (18)	C57—C56—H56	119.5
C43—C42—H42	119.6	C55—C56—H56	119.5
C41—C42—H42	119.6	C56—C57—C52	120.49 (19)
C42—C43—C44	121.41 (17)	C56—C57—H57	119.8
C42—C43—H43	119.3	C52—C57—H57	119.8
C44—C43—H43	119.3	C55—C58—H58A	109.5
C43—C44—C45	117.60 (18)	C55—C58—H58B	109.5
C43—C44—C47	120.84 (18)	H58A—C58—H58B	109.5
C45—C44—C47	121.56 (19)	C55—C58—H58C	109.5
C46—C45—C44	121.58 (18)	H58A—C58—H58C	109.5
C46—C45—H45	119.2	H58B—C58—H58C	109.5
C44—C45—H45	119.2		
C4—N3—C2—N1	10.2 (3)	C42—C43—C44—C47	−178.71 (19)
C4—N3—C2—S2	−170.65 (14)	C43—C44—C45—C46	−0.8 (3)
C6—N1—C2—N3	−13.5 (3)	C47—C44—C45—C46	179.28 (19)
C1—N1—C2—N3	170.69 (17)	C44—C45—C46—C41	−0.3 (3)
C6—N1—C2—S2	167.39 (14)	C42—C41—C46—C45	0.8 (3)
C1—N1—C2—S2	−8.4 (2)	C4—C41—C46—C45	178.15 (17)
C2—N3—C4—C5	1.1 (3)	C6—C5—C51—O5	118.22 (19)
C2—N3—C4—C41	−175.58 (16)	C4—C5—C51—O5	−52.7 (2)
N3—C4—C5—C6	−9.4 (3)	C6—C5—C51—C52	−60.9 (2)
C41—C4—C5—C6	167.09 (16)	C4—C5—C51—C52	128.16 (18)
N3—C4—C5—C51	161.81 (16)	O5—C51—C52—C53	166.43 (17)
C41—C4—C5—C51	−21.7 (3)	C5—C51—C52—C53	−14.5 (2)
C2—N1—C6—C5	5.2 (3)	O5—C51—C52—C57	−10.3 (2)
C1—N1—C6—C5	−178.97 (18)	C5—C51—C52—C57	168.79 (15)
C4—C5—C6—N1	6.1 (3)	C57—C52—C53—C54	0.1 (3)
C51—C5—C6—N1	−165.48 (16)	C51—C52—C53—C54	−176.60 (17)
N3—C4—C41—C42	145.70 (18)	C52—C53—C54—C55	−0.4 (3)
C5—C4—C41—C42	−31.0 (3)	C53—C54—C55—C56	0.1 (3)
N3—C4—C41—C46	−31.5 (2)	C53—C54—C55—C58	−179.87 (19)
C5—C4—C41—C46	151.79 (18)	C54—C55—C56—C57	0.6 (3)
C46—C41—C42—C43	−0.3 (3)	C58—C55—C56—C57	−179.47 (19)
C4—C41—C42—C43	−177.57 (17)	C55—C56—C57—C52	−0.9 (3)
C41—C42—C43—C44	−0.8 (3)	C53—C52—C57—C56	0.5 (3)
C42—C43—C44—C45	1.4 (3)	C51—C52—C57—C56	177.33 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C47—H47B···O5^{i}	0.96	2.47	3.393 (3)	162

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+1/2.

Fig. 1

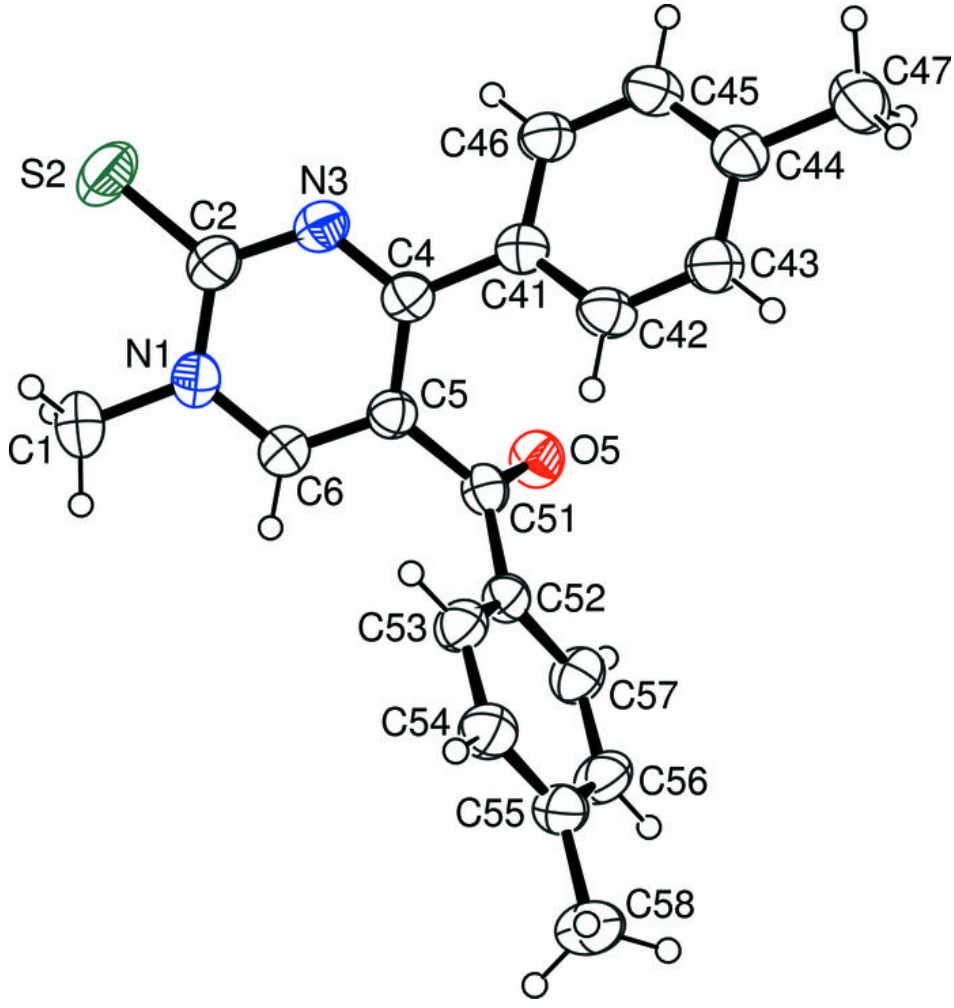
S2
C2
N3
C4
C41
C42
C43
C44
C45
C46
C47
N1
C1
C5
C6
O5
C51
C52
C53
C54
C55
C56
C57
C58

Fig. 2