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5-(4-Methylbenzoyl)-4-*p*-tolyl-1-(1-*p*-tolylethylideneamino)pyrimidin-2(1*H*)-one

Muharrem Dinçer,[a] Namık Özdemir,[a]* Zülbiye Önal[b] and Elif Korkusuz[b]

[a]Department of Physics, Arts and Sciences Faculty, Ondokuz Mayıs University, 55139 Samsun, Turkey, and [b]Department of Chemistry, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey
Correspondence e-mail: namiko@omu.edu.tr

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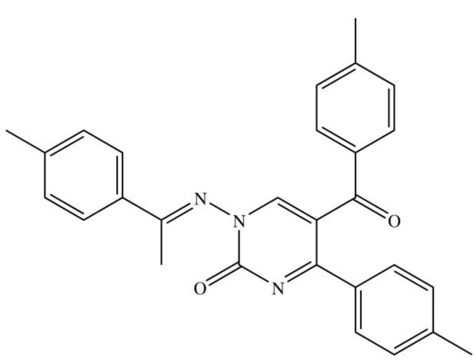
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.127; data-to-parameter ratio = 18.2.

The title compound, $C_{28}H_{25}N_3O_2$, contains four rings that are not coplanar. The pyrimidine ring is slightly distorted from planarity, with a maximum deviation of 0.1032 (9) Å, and adopts the half-chair conformation. The molecules are linked to each other by two C—H···O interactions.

Related literature

For related literature, see: Altural *et al.* (1989); Bernstein *et al.* (1995); Brown (1984, 1985); Burdge (2000); Chakaravorty *et al.* (1992); Hökelek *et al.* (2002); Kleemann & Engel (1982); Kollenz *et al.* (1991); Sarıpınar *et al.* (2000); Shishoo & Jain (1992); Vega *et al.* (1990); Yıldırım *et al.* (2002); Ziegler *et al.* (1967).



Experimental

Crystal data

$C_{28}H_{25}N_3O_2$
M_r = 435.51
Triclinic, $P\overline{1}$
a = 8.0337 (6) Å
b = 10.5159 (8) Å
c = 14.6372 (11) Å
α = 90.814 (6)°
β = 103.780 (5)°
γ = 102.235 (6)°
V = 1170.97 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.75 × 0.57 × 0.29 mm

Data collection

Stoe IPDS2 diffractometer
Absorption correction: integration *X-RED32* (Stoe & Cie, 2002)
T_{min} = 0.951, T_{max} = 0.980
17054 measured reflections
5518 independent reflections
4001 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 1.05
5518 reflections
303 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C53—H53···O2^{i}	0.93	2.50	3.4289 (17)	177
C19—H19C···O2^{ii}	0.96	2.53	3.421 (2)	155

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, y-1, z$.

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: HG2349).

References

Altural, B., Akçamur, Y., Sarıpınar, E., Yıldırım, İ. & Kollenz, G. (1989). *Monatsh. Chem.* **120**, 1015–1020.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Brown, D. J. (1984). *Comprehensive Heterocyclic Chemistry*, edited by A. R. Katritzky & C. W. Rees, Vol. 3, pp. 57–61. Oxford: Pergamon Press.
Brown, D. J. (1985). *The Chemistry of Heterocyclic Compounds, The Pyrimidines*, Suppl. II, edited by A. Weissberger & E. C. Taylor. New York: Interscience.
Burdge, E. L. (2000). *Pest Manag. Sci.* **56**, 245–248.
Chakaravorty, P. K., Grelnlee, W. J., Dooseap, K., Mantlo, N. B. & Patchett, A. A. (1992). APCT Int. Appl. WO 92 20 687 156.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hökelek, T., Sarıpınar, E., Yıldırım, İ., Akkurt, M. & Akçamur, Y. (2002). *Acta Cryst.* E**58**, o30–o32.
Kleemann, A. & Engel, J. (1982). *Pharmazeutische Wirkstoffe*, 2 Aufl., pp. 25, 225, 375, 478, 641. Stuttgart: Georg Thieme Verlag.
Kollenz, G., Kappe, C. O. & El-Nabi, H. A. A. (1991). *Heterocycles*, **32**, 669–674.
Sarıpınar, E., Güzel, Y., Önal, Z., İlhan, İ. Ö. & Akçamur, Y. (2000). *J. Chem. Soc. Pak.* **22**, 308–317.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shishoo, C. J. & Jain, K. S. (1992). *J. Heterocycl. Chem.* **29**, 883–893.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Vega, S., Alonso, J., Diaz, J. A. & Junquera, F. (1990). *J. Heterocycl. Chem.* **27**, 269–273.
Yıldırım, İ., Akçamur, Y., Sarıpınar, E. & Kollenz, G. (2002). *Kuwait J. Sci. Eng.* **29**, 57–65.
Ziegler, E., Eder, M., Belegratis, C. & Prewedourakis, E. (1967). *Monatsh. Chem.* **98**, 2249–2251.

supplementary materials

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5-(4-Methylbenzoyl)-4-*p*-tolyl-1-(1-*p*-tolylethylideneamino)pyrimidin-2(1*H*)-one

M. Dinçer, N. Özdemir, Z. Önal and E. Korkusuz

Comment

4-Aroyl-5-aryl-2,3-dihydro-2,3-furandiones represent easily accessible building blocks for the synthesis of heterocyclic systems (Altural *et al.*, 1989; Kollenz *et al.*, 1991; Sarıpınar *et al.*, 2000; Hökelek *et al.*, 2002; Yıldırım *et al.*, 2002). In general, pyrimidines have been 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). Some of them are frequently encountered in many drugs used for the treatment of hypothyroidism, hypertension, cancer chemotherapy or HIV infection (Burdge, 2000). Furthermore many condensed heterocyclic systems, especially when linked to a pyrimidine ring, play an important role as analgesic, antipyretic and anti-inflammatory drugs (Vega *et al.*, 1990), and also as 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, (I).

The structure of the title compound, (I), is shown in Fig. 1. The structure of (I) contains one central pyrimidine ring (N1/N3/C2/C4—C6) with a *p*-tolylethylideneamino group (N11/C11—C19) substituted at N1, an O atom substituted at C2, a *p*-tolyl group (C41—C47) substituted at C4 and a methylbenzoyl group substituted at C5. The plane of the pyrimidine ring makes dihedral angles of 35.86 (6), 41.57 (4) and 52.18 (4)° with the (C13—C18), (C41—C46) and (C52—C57) phenyl rings, respectively·The pyrimidine ring is not planar with a maximum deviation of −0.1032 (9) Å for atom C2. The interatomic distances and angles show no anomalies.

In the molecular structure, there is a π—π stacking interaction between the (C41—C46) and (C52—C57) phenyl rings with a distance of 3.749Å between the ring centroids, and a perpendicular distance between the rings of 3.483 Å. In the crystal structure of (I), atom C53 in the molecule at (*x*, *y*, *z*) acts as hydrogen-bond donor to the O2 atom in the molecule at (1 − *x*, 1 − *y*, 2 − *z*), so generating by inversion a dimeric unit characterized by an $R_2^2(18)$ motif (Bernstein *et al.*, 1995). The dimers are connected to one another *via* another C—H···O interactions in which atom C19 in the molecule at (*x*, *y*, *z*) acts as hydrogen-bond donor to the O2 atom in the molecule at (*x*, *y* − 1, *z*), forming one dimensional dimeric chain along the [010] direction.

Experimental

An equimolar mixture of 4-(4-methylbenzoyl)-5-(4-methylphenyl)furan-2,3-dione (0.50 g), easily obtained from oxalyl dichloride and 4,4'-dimethyldibenzoylmethan, as described by Ziegler *et al.* (1967), and 4-methylacetophenone semicarbazone (0.34 g) (molar ratio 1:1) were refluxed in 30 ml boiling toluene for 4 h. After evaporation of the solvent, the oily residue was treated with dry diethyl ether to give a yellow precipitate, which was filtered off and recrystallized from ethanol (yield: 0.35 g, 50%; m.p. 488 K). IR (KBr, ν, cm^{-1}): 3050, 3044, 2920 (aromatic and aliphatic C—H), 1690, 1645 (s, C═O), 1602–1473 (m, C═C and C═N aromatic rings); ^{1}H NMR (200 MHz, DMSO, p.p.m.): δ 8.47 (s, 1H at C-6), 7.94–7.13 (m, 12H, Ar—H), 2.39, 2.33, 2.31, 2.27 (s, 12H, 4xCH_3). Analysis Calculated for $C_{28}H_{25}N_3O_2$: C 77.21, H 5.78, N 9.64%; found: C 77.40, H 5.57, N 9.50%.

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

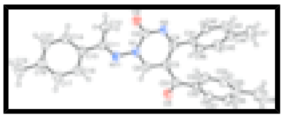

Fig. 1. An *ORTEP-3* (Farrugia, 1997) drawing of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

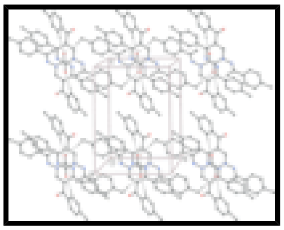

Fig. 2. A projection of the crystal structure of (I) along the *a* axis. Dashed lines show the C—H···O intermolecular interactions. For the sake of clarity, H atoms have been omitted unless they are involved in hydrogen bonding.

5-(4-Methylbenzoyl)-4-*p*-tolyl-1-(1-*p*-tolylethylideneamino)pyrimidin-2(1*H*)-one

Crystal data

$C_{28}H_{25}N_3O_2$	Z = 2
M_r = 435.51	F_{000} = 460
Triclinic, $P\bar{1}$	D_x = 1.235 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.0337 (6) Å	Cell parameters from 18925 reflections
b = 10.5159 (8) Å	θ = 2.4–27.9°
c = 14.6372 (11) Å	μ = 0.08 mm^{-1}
α = 90.814 (6)°	T = 296 K
β = 103.780 (5)°	Prism, yellow
γ = 102.235 (6)°	0.75 × 0.57 × 0.29 mm
V = 1170.97 (15) Å^3	

Data collection

Stoe IPDS2 diffractometer	5518 independent reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	4001 reflections with $I > 2\sigma(I)$
Monochromator: plane graphite	R_{int} = 0.059
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 27.9°
T = 296 K	θ_{min} = 2.4°

ω scans	$h = -10 \rightarrow 10$
Absorption correction: integration X-RED32 (Stoe & Cie, 2002)	$k = -13 \rightarrow 13$
$T_{min} = 0.951$, $T_{max} = 0.980$	$l = -19 \rightarrow 19$
17054 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.1024P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.127$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
5518 reflections	$\Delta\rho_{min} = -0.13$ e Å^{-3}
303 parameters	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.018 (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}
O2	0.36136 (14)	0.45935 (11)	1.07609 (7)	0.0605 (3)
O5	0.1090 (2)	0.29263 (11)	0.65039 (8)	0.0858 (4)
N1	0.25410 (15)	0.32241 (11)	0.94305 (8)	0.0485 (3)
N3	0.26204 (15)	0.54801 (11)	0.93782 (7)	0.0478 (3)
N11	0.27934 (16)	0.20825 (11)	0.98928 (8)	0.0517 (3)
C2	0.29839 (17)	0.44711 (14)	0.99159 (9)	0.0481 (3)
C4	0.22738 (16)	0.53503 (13)	0.84561 (9)	0.0446 (3)
C5	0.21944 (18)	0.41521 (13)	0.79567 (9)	0.0483 (3)
C6	0.22964 (19)	0.31113 (13)	0.84897 (9)	0.0511 (3)
H6	0.2194	0.2299	0.8196	0.061*
C11	0.19358 (16)	0.17533 (13)	1.05206 (9)	0.0460 (3)

C12	0.0720 (2)	0.24654 (16)	1.08184 (12)	0.0612 (4)
H12A	0.0269	0.2975	1.0318	0.092*
H12B	0.1342	0.3031	1.1369	0.092*
H12C	−0.0237	0.1851	1.0961	0.092*
C13	0.22176 (16)	0.05315 (13)	1.09645 (9)	0.0464 (3)
C14	0.1693 (2)	0.01848 (16)	1.17784 (11)	0.0605 (4)
H14	0.1162	0.0733	1.2060	0.073*
C15	0.1946 (2)	−0.09636 (17)	1.21779 (11)	0.0679 (4)
H15	0.1600	−0.1167	1.2731	0.081*
C16	0.2702 (2)	−0.18145 (15)	1.17752 (11)	0.0599 (4)
C17	0.3223 (2)	−0.14700 (15)	1.09630 (11)	0.0602 (4)
H17	0.3739	−0.2026	1.0679	0.072*
C18	0.2995 (2)	−0.03240 (15)	1.05655 (10)	0.0555 (3)
H18	0.3367	−0.0116	1.0020	0.067*
C19	0.2925 (3)	−0.30805 (19)	1.21997 (15)	0.0899 (6)
H19A	0.2090	−0.3333	1.2572	0.135*
H19B	0.4095	−0.2972	1.2593	0.135*
H19C	0.2735	−0.3744	1.1705	0.135*
C41	0.19553 (16)	0.65154 (12)	0.79447 (9)	0.0440 (3)
C42	0.30585 (18)	0.77205 (14)	0.82568 (10)	0.0509 (3)
H42	0.3928	0.7808	0.8816	0.061*
C43	0.2875 (2)	0.87876 (15)	0.77436 (11)	0.0609 (4)
H43	0.3638	0.9588	0.7956	0.073*
C44	0.1573 (2)	0.86939 (16)	0.69154 (11)	0.0630 (4)
C45	0.0431 (2)	0.74996 (16)	0.66348 (11)	0.0624 (4)
H45	−0.0480	0.7423	0.6094	0.075*
C46	0.06107 (19)	0.64227 (15)	0.71359 (10)	0.0544 (3)
H46	−0.0173	0.5628	0.6932	0.065*
C47	0.1430 (4)	0.9854 (2)	0.63299 (17)	0.1050 (8)
H47A	0.1624	0.9671	0.5724	0.158*
H47B	0.2296	1.0603	0.6644	0.158*
H47C	0.0278	1.0025	0.6249	0.158*
C51	0.2031 (2)	0.39281 (14)	0.69258 (10)	0.0561 (4)
C52	0.3062 (2)	0.49146 (14)	0.64407 (9)	0.0517 (3)
C53	0.4596 (2)	0.57584 (16)	0.69096 (10)	0.0582 (4)
H53	0.5064	0.5687	0.7547	0.070*
C54	0.5438 (2)	0.67092 (18)	0.64341 (11)	0.0679 (4)
H54	0.6482	0.7268	0.6756	0.081*
C55	0.4767 (2)	0.68502 (18)	0.54924 (12)	0.0698 (4)
C56	0.3253 (3)	0.59822 (19)	0.50232 (11)	0.0762 (5)
H56	0.2794	0.6052	0.4384	0.091*
C57	0.2411 (2)	0.50158 (17)	0.54816 (10)	0.0661 (4)
H57	0.1403	0.4428	0.5150	0.079*
C58	0.5664 (3)	0.7934 (2)	0.49902 (17)	0.1040 (7)
H58A	0.6373	0.8624	0.5443	0.156*
H58B	0.4792	0.8265	0.4550	0.156*
H58C	0.6395	0.7602	0.4659	0.156*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0677 (6)	0.0647 (7)	0.0429 (5)	0.0096 (5)	0.0062 (4)	0.0063 (4)
O5	0.1368 (12)	0.0523 (7)	0.0549 (6)	−0.0028 (7)	0.0193 (7)	−0.0048 (5)
N1	0.0577 (6)	0.0464 (6)	0.0450 (6)	0.0151 (5)	0.0156 (5)	0.0111 (5)
N3	0.0536 (6)	0.0450 (6)	0.0444 (6)	0.0104 (5)	0.0119 (5)	0.0043 (4)
N11	0.0622 (7)	0.0493 (7)	0.0496 (6)	0.0184 (5)	0.0197 (5)	0.0149 (5)
C2	0.0483 (7)	0.0513 (8)	0.0447 (7)	0.0093 (6)	0.0129 (5)	0.0051 (6)
C4	0.0435 (6)	0.0440 (7)	0.0457 (6)	0.0082 (5)	0.0113 (5)	0.0049 (5)
C5	0.0573 (8)	0.0446 (7)	0.0438 (6)	0.0124 (6)	0.0131 (6)	0.0069 (5)
C6	0.0638 (8)	0.0452 (8)	0.0461 (7)	0.0133 (6)	0.0155 (6)	0.0039 (6)
C11	0.0437 (6)	0.0490 (7)	0.0437 (6)	0.0074 (5)	0.0102 (5)	0.0055 (5)
C12	0.0541 (8)	0.0634 (9)	0.0752 (10)	0.0186 (7)	0.0278 (7)	0.0163 (8)
C13	0.0461 (7)	0.0478 (7)	0.0442 (6)	0.0062 (6)	0.0126 (5)	0.0069 (5)
C14	0.0769 (10)	0.0570 (9)	0.0570 (8)	0.0179 (7)	0.0314 (7)	0.0120 (7)
C15	0.0916 (12)	0.0647 (10)	0.0566 (8)	0.0180 (9)	0.0348 (8)	0.0197 (7)
C16	0.0709 (9)	0.0518 (8)	0.0544 (8)	0.0112 (7)	0.0120 (7)	0.0116 (6)
C17	0.0736 (10)	0.0563 (9)	0.0567 (8)	0.0218 (7)	0.0209 (7)	0.0077 (7)
C18	0.0651 (9)	0.0570 (9)	0.0495 (7)	0.0154 (7)	0.0217 (6)	0.0100 (6)
C19	0.1304 (18)	0.0670 (12)	0.0829 (13)	0.0356 (12)	0.0336 (12)	0.0292 (10)
C41	0.0472 (7)	0.0426 (7)	0.0446 (6)	0.0122 (5)	0.0140 (5)	0.0044 (5)
C42	0.0514 (7)	0.0489 (8)	0.0505 (7)	0.0080 (6)	0.0113 (6)	0.0039 (6)
C43	0.0679 (9)	0.0448 (8)	0.0688 (9)	0.0062 (7)	0.0201 (7)	0.0082 (7)
C44	0.0821 (11)	0.0539 (9)	0.0612 (9)	0.0259 (8)	0.0228 (8)	0.0166 (7)
C45	0.0720 (10)	0.0600 (10)	0.0536 (8)	0.0256 (8)	0.0021 (7)	0.0065 (7)
C46	0.0554 (8)	0.0494 (8)	0.0548 (8)	0.0133 (6)	0.0055 (6)	0.0023 (6)
C47	0.152 (2)	0.0719 (13)	0.0965 (15)	0.0379 (14)	0.0266 (15)	0.0392 (12)
C51	0.0787 (10)	0.0454 (8)	0.0450 (7)	0.0182 (7)	0.0127 (7)	0.0044 (6)
C52	0.0691 (9)	0.0507 (8)	0.0393 (6)	0.0216 (7)	0.0137 (6)	0.0052 (5)
C53	0.0596 (8)	0.0765 (10)	0.0418 (7)	0.0217 (7)	0.0125 (6)	0.0102 (7)
C54	0.0619 (9)	0.0845 (12)	0.0567 (9)	0.0100 (8)	0.0189 (7)	0.0079 (8)
C55	0.0836 (11)	0.0732 (11)	0.0582 (9)	0.0176 (9)	0.0275 (8)	0.0168 (8)
C56	0.0997 (13)	0.0848 (12)	0.0402 (7)	0.0163 (11)	0.0125 (8)	0.0165 (8)
C57	0.0854 (11)	0.0652 (10)	0.0409 (7)	0.0101 (8)	0.0081 (7)	0.0036 (7)
C58	0.1195 (18)	0.1058 (18)	0.0881 (14)	0.0085 (14)	0.0414 (13)	0.0367 (13)

Geometric parameters (Å, °)

O2—C2	1.2133 (16)	C19—H19C	0.9600
O5—C51	1.2185 (19)	C41—C42	1.3837 (19)
N1—C6	1.3437 (16)	C41—C46	1.3859 (19)
N1—N11	1.4146 (15)	C42—C43	1.374 (2)
N1—C2	1.4165 (18)	C42—H42	0.9300
N3—C4	1.3105 (16)	C43—C44	1.386 (2)
N3—C2	1.3696 (17)	C43—H43	0.9300
N11—C11	1.2840 (16)	C44—C45	1.380 (2)
C4—C5	1.4295 (18)	C44—C47	1.509 (2)

C4—C41	1.4815 (17)	C45—C46	1.373 (2)
C5—C6	1.3583 (18)	C45—H45	0.9300
C5—C51	1.4941 (18)	C46—H46	0.9300
C6—H6	0.9300	C47—H47A	0.9600
C11—C13	1.4836 (18)	C47—H47B	0.9600
C11—C12	1.4863 (19)	C47—H47C	0.9600
C12—H12A	0.9600	C51—C52	1.484 (2)
C12—H12B	0.9600	C52—C53	1.376 (2)
C12—H12C	0.9600	C52—C57	1.3907 (19)
C13—C14	1.3844 (18)	C53—C54	1.378 (2)
C13—C18	1.392 (2)	C53—H53	0.9300
C14—C15	1.382 (2)	C54—C55	1.378 (2)
C14—H14	0.9300	C54—H54	0.9300
C15—C16	1.379 (2)	C55—C56	1.377 (3)
C15—H15	0.9300	C55—C58	1.512 (2)
C16—C17	1.380 (2)	C56—C57	1.373 (2)
C16—C19	1.504 (2)	C56—H56	0.9300
C17—C18	1.374 (2)	C57—H57	0.9300
C17—H17	0.9300	C58—H58A	0.9600
C18—H18	0.9300	C58—H58B	0.9600
C19—H19A	0.9600	C58—H58C	0.9600
C19—H19B	0.9600		

C6—N1—N11	114.84 (11)	C42—C41—C4	119.64 (12)
C6—N1—C2	120.41 (11)	C46—C41—C4	121.51 (12)
N11—N1—C2	122.59 (11)	C43—C42—C41	120.26 (13)
C4—N3—C2	121.04 (11)	C43—C42—H42	119.9
C11—N11—N1	116.95 (11)	C41—C42—H42	119.9
O2—C2—N3	123.89 (13)	C42—C43—C44	121.28 (15)
O2—C2—N1	120.12 (12)	C42—C43—H43	119.4
N3—C2—N1	115.97 (11)	C44—C43—H43	119.4
N3—C4—C5	122.47 (12)	C45—C44—C43	117.86 (14)
N3—C4—C41	116.60 (11)	C45—C44—C47	121.05 (17)
C5—C4—C41	120.93 (11)	C43—C44—C47	121.08 (17)
C6—C5—C4	115.61 (12)	C46—C45—C44	121.42 (14)
C6—C5—C51	117.06 (12)	C46—C45—H45	119.3
C4—C5—C51	127.32 (12)	C44—C45—H45	119.3
N1—C6—C5	121.76 (12)	C45—C46—C41	120.26 (14)
N1—C6—H6	119.1	C45—C46—H46	119.9
C5—C6—H6	119.1	C41—C46—H46	119.9
N11—C11—C13	114.57 (11)	C44—C47—H47A	109.5
N11—C11—C12	126.30 (13)	C44—C47—H47B	109.5
C13—C11—C12	119.13 (11)	H47A—C47—H47B	109.5
C11—C12—H12A	109.5	C44—C47—H47C	109.5
C11—C12—H12B	109.5	H47A—C47—H47C	109.5
H12A—C12—H12B	109.5	H47B—C47—H47C	109.5
C11—C12—H12C	109.5	O5—C51—C52	121.22 (13)
H12A—C12—H12C	109.5	O5—C51—C5	119.49 (13)
H12B—C12—H12C	109.5	C52—C51—C5	119.26 (13)
C14—C13—C18	117.41 (13)	C53—C52—C57	119.04 (14)

C14—C13—C11	121.58 (12)	C53—C52—C51	122.56 (12)
C18—C13—C11	121.00 (11)	C57—C52—C51	118.35 (14)
C15—C14—C13	120.92 (14)	C52—C53—C54	119.99 (14)
C15—C14—H14	119.5	C52—C53—H53	120.0
C13—C14—H14	119.5	C54—C53—H53	120.0
C16—C15—C14	121.47 (13)	C55—C54—C53	121.40 (17)
C16—C15—H15	119.3	C55—C54—H54	119.3
C14—C15—H15	119.3	C53—C54—H54	119.3
C15—C16—C17	117.60 (14)	C56—C55—C54	118.22 (15)
C15—C16—C19	121.10 (15)	C56—C55—C58	120.97 (17)
C17—C16—C19	121.30 (15)	C54—C55—C58	120.81 (19)
C18—C17—C16	121.42 (14)	C57—C56—C55	121.18 (15)
C18—C17—H17	119.3	C57—C56—H56	119.4
C16—C17—H17	119.3	C55—C56—H56	119.4
C17—C18—C13	121.17 (13)	C56—C57—C52	120.10 (16)
C17—C18—H18	119.4	C56—C57—H57	120.0
C13—C18—H18	119.4	C52—C57—H57	120.0
C16—C19—H19A	109.5	C55—C58—H58A	109.5
C16—C19—H19B	109.5	C55—C58—H58B	109.5
H19A—C19—H19B	109.5	H58A—C58—H58B	109.5
C16—C19—H19C	109.5	C55—C58—H58C	109.5
H19A—C19—H19C	109.5	H58A—C58—H58C	109.5
H19B—C19—H19C	109.5	H58B—C58—H58C	109.5
C42—C41—C46	118.80 (12)		

C6—N1—N11—C11	−134.63 (13)	C11—C13—C18—C17	−178.55 (13)
C2—N1—N11—C11	62.05 (17)	N3—C4—C41—C42	44.96 (17)
C4—N3—C2—O2	166.33 (13)	C5—C4—C41—C42	−135.29 (14)
C4—N3—C2—N1	−15.11 (18)	N3—C4—C41—C46	−137.44 (13)
C6—N1—C2—O2	−162.09 (13)	C5—C4—C41—C46	42.31 (18)
N11—N1—C2—O2	0.33 (19)	C46—C41—C42—C43	−3.4 (2)
C6—N1—C2—N3	19.29 (18)	C4—C41—C42—C43	174.26 (12)
N11—N1—C2—N3	−178.29 (11)	C41—C42—C43—C44	1.1 (2)
C2—N3—C4—C5	2.15 (19)	C42—C43—C44—C45	1.8 (2)
C2—N3—C4—C41	−178.09 (11)	C42—C43—C44—C47	−177.08 (17)
N3—C4—C5—C6	7.43 (19)	C43—C44—C45—C46	−2.5 (2)
C41—C4—C5—C6	−172.32 (12)	C47—C44—C45—C46	176.43 (17)
N3—C4—C5—C51	−171.91 (14)	C44—C45—C46—C41	0.2 (2)
C41—C4—C5—C51	8.3 (2)	C42—C41—C46—C45	2.8 (2)
N11—N1—C6—C5	−173.97 (12)	C4—C41—C46—C45	−174.85 (13)
C2—N1—C6—C5	−10.3 (2)	C6—C5—C51—O5	40.4 (2)
C4—C5—C6—N1	−3.1 (2)	C4—C5—C51—O5	−140.30 (16)
C51—C5—C6—N1	176.34 (13)	C6—C5—C51—C52	−137.87 (14)
N1—N11—C11—C13	178.54 (11)	C4—C5—C51—C52	41.5 (2)
N1—N11—C11—C12	−0.9 (2)	O5—C51—C52—C53	−153.66 (16)
N11—C11—C13—C14	166.44 (14)	C5—C51—C52—C53	24.5 (2)
C12—C11—C13—C14	−14.1 (2)	O5—C51—C52—C57	28.7 (2)
N11—C11—C13—C18	−14.75 (19)	C5—C51—C52—C57	−153.05 (14)
C12—C11—C13—C18	164.70 (14)	C57—C52—C53—C54	1.7 (2)
C18—C13—C14—C15	0.4 (2)	C51—C52—C53—C54	−175.85 (14)

C11—C13—C14—C15	179.27 (15)	C52—C53—C54—C55	0.8 (3)
C13—C14—C15—C16	−1.1 (3)	C53—C54—C55—C56	−2.3 (3)
C14—C15—C16—C17	0.9 (3)	C53—C54—C55—C58	177.37 (19)
C14—C15—C16—C19	−178.23 (18)	C54—C55—C56—C57	1.3 (3)
C15—C16—C17—C18	−0.2 (2)	C58—C55—C56—C57	−178.4 (2)
C19—C16—C17—C18	178.96 (17)	C55—C56—C57—C52	1.3 (3)
C16—C17—C18—C13	−0.4 (2)	C53—C52—C57—C56	−2.8 (3)
C14—C13—C18—C17	0.3 (2)	C51—C52—C57—C56	174.93 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C53—H53···O2^{i}	0.93	2.50	3.4289 (17)	177
C19—H19C···O2^{ii}	0.96	2.53	3.421 (2)	155

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

Fig. 1

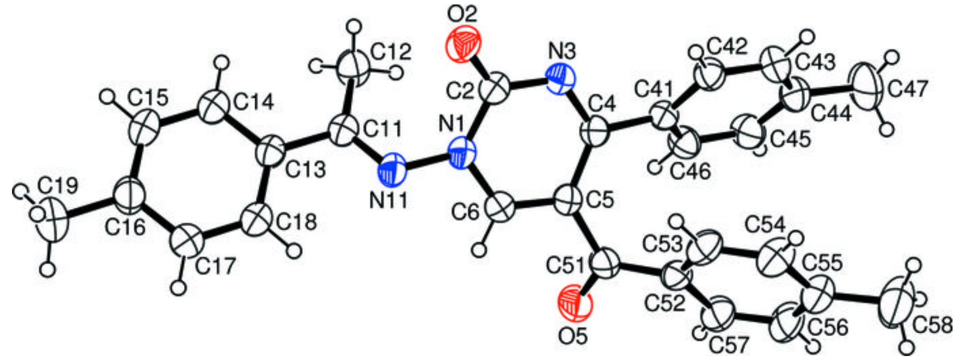
O2
N3
C12
C42
C43
C47
C15
C14
C2
C41
C44
C11
N1
C4
C45
C13
C46
C19
N11
C6
C5
C16
C18
C53
C54
C51
C55
C17
C52
C56
C58
O5
C57

Fig. 2