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6-Ethyl-2-(piperidin-1-yl)-3-*p*-tolylthieno[2,3-*d*]pyrimidin-4(3*H*)-one

Hai Xie,[a] Xin-min Peng[b] and Yang-gen Hu[c,d]*

[a]College of Chemistry & Chemical Engineering, ShanXi Datong University, Shanxi 037009, People's Republic of China, [b]Taihe Hospital, Yunyang Medical College, Shiyan 442000, People's Republic of China, [c]Key Laboratory of Pesticides & Chemical Biology, Ministry of Education, Central China Normal University, Wuhan 430079, People's Republic of China, and [d]Department of Medicinal Chemistry, Yunyang Medical College, Shiyan 442000, People's Republic of China
Correspondence e-mail: huyangg111@yahoo.com.cn

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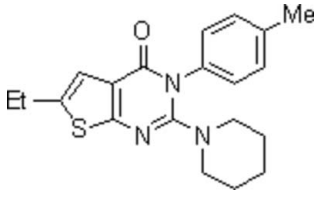
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.069; wR factor = 0.168; data-to-parameter ratio = 16.2.

The crystal structure of the title compound, $C_{20}H_{23}N_3OS$, is stabilized by intermolecular C—H···O hydrogen bonds. The molecule contains a planar heterocyclic ring system, which forms a dihedral angle of 65.87 (1)° with the adjacent tolyl ring. The piperidinyl ring has a distored chair conformation.

Related literature

For preparation and biological activity, see: Walter (1999*a*,*b*). For related literature, see: Ding *et al.* (2004); Hu *et al.* (2006, 2007).



Experimental

Crystal data

$C_{20}H_{23}N_3OS$
M_r = 353.47
Monoclinic, $P2_1/n$
a = 6.5376 (4) Å
b = 18.6415 (12) Å
c = 15.5507 (10) Å
β = 94.967 (1)°
V = 1888.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 296 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.947, T_{max} = 0.964
16199 measured reflections
3683 independent reflections
2714 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.168
S = 1.09
3683 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O1^{i}	0.97	2.58	3.456 (4)	150
C19—H19B···O1^{ii}	0.97	2.59	3.439 (4)	146

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+2, -y+2, -z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2600).

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supplementary materials

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6-Ethyl-2-(piperidin-1-yl)-3-*p*-tolylthieno[2,3-*d*]pyrimidin-4(3*H*)-one

H. Xie, X. Peng and Y. Hu

Comment

The derivatives of heterocycles containing the thienopyrimidine system, which are well known bioisosteres of quinazolines, are of great importance because of their remarkable biological properties (Walter, 1999*a*; Walter, 1999*b*; Ding *et al.*, 2004). Recently, we have focused on the synthesis of fused heterocyclic systems containing thienopyrimidine *via* aza-Wittig reaction at room temperature. Some X-ray crystal structures of fused pyrimidinone derivatives have been reported (Hu *et al.*, 2006; Hu *et al.*, 2007). The title compound (Fig. 1) may be used as a new precursor for obtaining bioactive molecules. In the molecule, the bond lengths and angles are unexceptional. The thienopyrimidine ring system is almost planar, with a maximum deviation of 0.046Å for atom N3. The tolyl ring is twisted with respect to it [dihedral angle 65.87 (1)°]. The piperidinyl ring in shows a distored chair conformation [φ =187 (9)° and θ = 180.0 (3)°, puckering amplitude = 0.571 (3) Å]. Intermolecular C—H···O hydrogen bonds (Fig. 2 and Table 2) are effective in stabilizing the crystal structure.

Experimental

To a solution of the ethyl 2-((*p*-tolylimino)methyleneamino)-5-ethylthiophene-3-carboxylate(II) (3 mmol) in dichloromethane (5 ml) was added piperidine(3 mmol). After stirring the reaction mixture for 1 h, the solvent was removed and anhydrous ethanol (10 ml) with several drops of EtONa in EtOH was added. The mixture was stirred for 4 h at room temperature. The solution was concentrated under reduced pressure and the residue was recrystallized from ethanol to give the title compound in a yield of 86%. Crystals suitable for single-crystal X-ray diffraction were obtained by recrystallization from a mixed solvent of ethanol and dichloromethane (1:1 *v*/*v*) at room temperature.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å, U_{iso} = 1.2U_{eq}(C) for Csp^2, C—H = 0.97 Å, U_{iso} = 1.2U_{eq}(C) for CH_2, C—H = 0.96 Å, U_{iso} = 1.5U_{eq}(C) for CH_3.

Figures

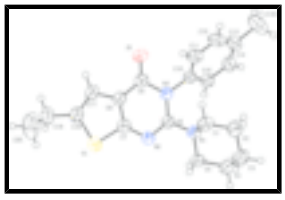

Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme.

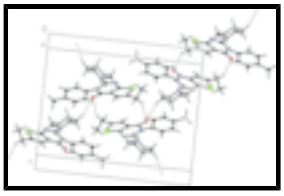

Fig. 2. The packing in the crystal structure, showing the C—H···O hydrogen bonds as dashed lines.

6-Ethyl-2-(piperidin-1-yl)-3-*p*-tolylthieno[2,3-*d*]pyrimidin-4(3*H*)-one

Crystal data

$C_{20}H_{23}N_3OS$	F_{000} = 752
M_r = 353.47	D_x = 1.244 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2891 reflections
a = 6.5376 (4) Å	θ = 2.6–22.9º
b = 18.6415 (12) Å	μ = 0.18 mm^{-1}
c = 15.5507 (10) Å	T = 296 (2) K
β = 94.967 (1)º	Block, colorless
V = 1888.1 (2) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	3683 independent reflections
Radiation source: fine-focus sealed tube	2714 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 296(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −8→8
T_{min} = 0.947, T_{max} = 0.964	k = −22→22
16199 measured reflections	l = −18→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.069	H-atom parameters constrained
$wR(F^2)$ = 0.168	$w = 1/[\sigma^2(F_o^2) + (0.072P)^2 + 0.7436P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max} < 0.001$
3683 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
228 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Primary atom site location: structure-invariant direct methods

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}
C1	0.6795 (5)	0.80842 (15)	0.33985 (18)	0.0534 (7)
H1A	0.7609	0.8283	0.3893	0.064*
H1B	0.7646	0.7747	0.3116	0.064*
C2	0.4956 (5)	0.76995 (16)	0.3697 (2)	0.0663 (9)
H2A	0.5412	0.7332	0.4112	0.080*
H2B	0.4209	0.7466	0.3208	0.080*
C3	0.3549 (5)	0.82198 (17)	0.4107 (2)	0.0698 (9)
H3A	0.4230	0.8405	0.4640	0.084*
H3B	0.2311	0.7973	0.4244	0.084*
C4	0.2989 (5)	0.88368 (17)	0.3490 (2)	0.0667 (9)
H4A	0.2149	0.8656	0.2992	0.080*
H4B	0.2186	0.9187	0.3776	0.080*
C5	0.4870 (5)	0.91967 (14)	0.3192 (2)	0.0578 (8)
H5A	0.4461	0.9570	0.2778	0.069*
H5B	0.5654	0.9417	0.3681	0.069*
C6	0.7593 (4)	0.89267 (13)	0.22814 (16)	0.0416 (6)
C7	0.9598 (4)	0.97979 (14)	0.18017 (17)	0.0474 (7)
C8	1.0504 (4)	0.93702 (14)	0.12372 (17)	0.0456 (6)
C9	0.9877 (4)	0.86358 (14)	0.11460 (16)	0.0438 (6)
C10	0.7312 (4)	0.77628 (13)	0.15011 (16)	0.0419 (6)
C11	0.8398 (5)	0.71284 (14)	0.16331 (18)	0.0539 (7)
H11	0.9759	0.7135	0.1863	0.065*
C12	0.7433 (6)	0.64854 (15)	0.14186 (19)	0.0632 (9)
H12	0.8157	0.6059	0.1513	0.076*
C13	0.5423 (6)	0.64604 (15)	0.10678 (18)	0.0607 (9)
C14	0.4362 (5)	0.70978 (15)	0.09467 (18)	0.0551 (7)
H14	0.2997	0.7090	0.0722	0.066*
C15	0.5298 (4)	0.77485 (14)	0.11540 (17)	0.0468 (7)
H15	0.4572	0.8174	0.1060	0.056*
C16	0.4395 (8)	0.57519 (17)	0.0815 (3)	0.0977 (14)
H16A	0.3044	0.5742	0.1013	0.147*

H16B	0.5194	0.5364	0.1075	0.147*
H16C	0.4297	0.5701	0.0199	0.147*
C17	1.1956 (5)	0.97442 (16)	0.07732 (19)	0.0571 (8)
H17	1.2713	0.9526	0.0366	0.068*
C18	1.2124 (5)	1.04385 (16)	0.09795 (19)	0.0572 (8)
C19	1.3451 (5)	1.10055 (18)	0.0615 (2)	0.0711 (9)
H19A	1.4076	1.0805	0.0125	0.085*
H19B	1.2584	1.1402	0.0405	0.085*
C20	1.5056 (7)	1.1280 (3)	0.1226 (3)	0.1155 (16)
H20A	1.4451	1.1510	0.1694	0.173*
H20B	1.5872	1.1621	0.0943	0.173*
H20C	1.5911	1.0891	0.1445	0.173*
N1	0.6137 (3)	0.86650 (10)	0.27945 (13)	0.0433 (5)
N2	0.8165 (4)	0.95937 (11)	0.23473 (14)	0.0489 (6)
N3	0.8313 (3)	0.84460 (10)	0.16904 (13)	0.0412 (5)
O1	1.0499 (3)	0.82006 (10)	0.06466 (13)	0.0585 (5)
S1	1.05291 (14)	1.06658 (4)	0.17733 (6)	0.0656 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0629 (19)	0.0562 (17)	0.0420 (15)	0.0139 (14)	0.0093 (14)	0.0072 (13)
C2	0.090 (2)	0.0512 (17)	0.0617 (19)	0.0066 (16)	0.0285 (18)	0.0191 (14)
C3	0.074 (2)	0.076 (2)	0.065 (2)	0.0014 (17)	0.0359 (18)	0.0127 (16)
C4	0.064 (2)	0.0637 (19)	0.077 (2)	0.0125 (16)	0.0345 (17)	0.0083 (16)
C5	0.069 (2)	0.0400 (15)	0.069 (2)	0.0081 (13)	0.0288 (16)	−0.0006 (13)
C6	0.0447 (15)	0.0396 (14)	0.0414 (14)	0.0035 (11)	0.0091 (12)	0.0025 (11)
C7	0.0486 (17)	0.0454 (15)	0.0491 (16)	−0.0027 (12)	0.0098 (13)	0.0015 (12)
C8	0.0426 (16)	0.0502 (15)	0.0448 (15)	−0.0008 (12)	0.0087 (13)	0.0002 (12)
C9	0.0403 (15)	0.0491 (15)	0.0422 (14)	0.0042 (12)	0.0048 (12)	−0.0008 (12)
C10	0.0521 (17)	0.0357 (13)	0.0393 (14)	0.0015 (11)	0.0127 (12)	−0.0002 (10)
C11	0.066 (2)	0.0466 (16)	0.0494 (16)	0.0115 (14)	0.0086 (14)	0.0011 (12)
C12	0.098 (3)	0.0391 (16)	0.0536 (18)	0.0144 (16)	0.0148 (18)	0.0015 (13)
C13	0.098 (3)	0.0426 (16)	0.0426 (16)	−0.0129 (16)	0.0137 (17)	−0.0034 (12)
C14	0.062 (2)	0.0535 (17)	0.0499 (17)	−0.0109 (14)	0.0076 (14)	−0.0033 (13)
C15	0.0536 (18)	0.0393 (14)	0.0487 (16)	0.0024 (12)	0.0108 (13)	0.0020 (11)
C16	0.157 (4)	0.052 (2)	0.082 (3)	−0.024 (2)	−0.001 (3)	−0.0102 (18)
C17	0.0532 (19)	0.0645 (19)	0.0559 (18)	−0.0077 (14)	0.0190 (15)	−0.0054 (14)
C18	0.0542 (19)	0.0625 (18)	0.0564 (18)	−0.0115 (14)	0.0141 (15)	0.0009 (14)
C19	0.064 (2)	0.075 (2)	0.076 (2)	−0.0196 (17)	0.0196 (18)	0.0002 (18)
C20	0.092 (3)	0.134 (4)	0.118 (3)	−0.052 (3)	−0.009 (3)	0.006 (3)
N1	0.0529 (14)	0.0338 (11)	0.0455 (12)	0.0061 (9)	0.0179 (10)	0.0031 (9)
N2	0.0575 (15)	0.0391 (12)	0.0526 (13)	−0.0017 (10)	0.0191 (11)	−0.0034 (10)
N3	0.0429 (13)	0.0393 (11)	0.0425 (12)	0.0025 (9)	0.0097 (10)	−0.0003 (9)
O1	0.0608 (13)	0.0567 (12)	0.0613 (12)	0.0000 (10)	0.0251 (10)	−0.0141 (10)
S1	0.0775 (6)	0.0468 (4)	0.0768 (6)	−0.0131 (4)	0.0311 (5)	−0.0058 (4)

Geometric parameters (Å, °)

C1—N1	1.473 (3)	C10—C15	1.379 (4)
C1—C2	1.507 (4)	C10—C11	1.385 (4)
C1—H1A	0.9700	C10—N3	1.450 (3)
C1—H1B	0.9700	C11—C12	1.382 (4)
C2—C3	1.516 (4)	C11—H11	0.9300
C2—H2A	0.9700	C12—C13	1.379 (5)
C2—H2B	0.9700	C12—H12	0.9300
C3—C4	1.522 (4)	C13—C14	1.380 (4)
C3—H3A	0.9700	C13—C16	1.518 (4)
C3—H3B	0.9700	C14—C15	1.384 (4)
C4—C5	1.508 (4)	C14—H14	0.9300
C4—H4A	0.9700	C15—H15	0.9300
C4—H4B	0.9700	C16—H16A	0.9600
C5—N1	1.463 (3)	C16—H16B	0.9600
C5—H5A	0.9700	C16—H16C	0.9600
C5—H5B	0.9700	C17—C18	1.336 (4)
C6—N2	1.300 (3)	C17—H17	0.9300
C6—N1	1.383 (3)	C18—C19	1.509 (4)
C6—N3	1.394 (3)	C18—S1	1.736 (3)
C7—C8	1.359 (4)	C19—C20	1.447 (5)
C7—N2	1.371 (3)	C19—H19A	0.9700
C7—S1	1.731 (3)	C19—H19B	0.9700
C8—C17	1.424 (4)	C20—H20A	0.9600
C8—C9	1.433 (4)	C20—H20B	0.9600
C9—O1	1.217 (3)	C20—H20C	0.9600
C9—N3	1.427 (3)		
N1—C1—C2	110.4 (2)	C12—C11—H11	120.4
N1—C1—H1A	109.6	C10—C11—H11	120.4
C2—C1—H1A	109.6	C13—C12—C11	121.6 (3)
N1—C1—H1B	109.6	C13—C12—H12	119.2
C2—C1—H1B	109.6	C11—C12—H12	119.2
H1A—C1—H1B	108.1	C12—C13—C14	118.4 (3)
C1—C2—C3	110.8 (3)	C12—C13—C16	121.1 (3)
C1—C2—H2A	109.5	C14—C13—C16	120.5 (4)
C3—C2—H2A	109.5	C13—C14—C15	121.1 (3)
C1—C2—H2B	109.5	C13—C14—H14	119.5
C3—C2—H2B	109.5	C15—C14—H14	119.5
H2A—C2—H2B	108.1	C10—C15—C14	119.7 (3)
C2—C3—C4	109.8 (2)	C10—C15—H15	120.1
C2—C3—H3A	109.7	C14—C15—H15	120.1
C4—C3—H3A	109.7	C13—C16—H16A	109.5
C2—C3—H3B	109.7	C13—C16—H16B	109.5
C4—C3—H3B	109.7	H16A—C16—H16B	109.5
H3A—C3—H3B	108.2	C13—C16—H16C	109.5
C5—C4—C3	111.8 (3)	H16A—C16—H16C	109.5
C5—C4—H4A	109.2	H16B—C16—H16C	109.5

C3—C4—H4A	109.2	C18—C17—C8	113.4 (3)
C5—C4—H4B	109.2	C18—C17—H17	123.3
C3—C4—H4B	109.2	C8—C17—H17	123.3
H4A—C4—H4B	107.9	C17—C18—C19	128.8 (3)
N1—C5—C4	109.6 (2)	C17—C18—S1	111.4 (2)
N1—C5—H5A	109.8	C19—C18—S1	119.8 (2)
C4—C5—H5A	109.8	C20—C19—C18	114.1 (3)
N1—C5—H5B	109.8	C20—C19—H19A	108.7
C4—C5—H5B	109.8	C18—C19—H19A	108.7
H5A—C5—H5B	108.2	C20—C19—H19B	108.7
N2—C6—N1	120.0 (2)	C18—C19—H19B	108.7
N2—C6—N3	123.7 (2)	H19A—C19—H19B	107.6
N1—C6—N3	116.2 (2)	C19—C20—H20A	109.5
C8—C7—N2	126.6 (2)	C19—C20—H20B	109.5
C8—C7—S1	111.0 (2)	H20A—C20—H20B	109.5
N2—C7—S1	122.4 (2)	C19—C20—H20C	109.5
C7—C8—C17	112.8 (2)	H20A—C20—H20C	109.5
C7—C8—C9	119.2 (2)	H20B—C20—H20C	109.5
C17—C8—C9	128.0 (2)	C6—N1—C5	116.6 (2)
O1—C9—N3	120.6 (2)	C6—N1—C1	116.7 (2)
O1—C9—C8	126.3 (2)	C5—N1—C1	111.9 (2)
N3—C9—C8	113.1 (2)	C6—N2—C7	115.1 (2)
C15—C10—C11	120.1 (2)	C6—N3—C9	122.1 (2)
C15—C10—N3	119.7 (2)	C6—N3—C10	121.7 (2)
C11—C10—N3	120.2 (3)	C9—N3—C10	115.55 (19)
C12—C11—C10	119.2 (3)	C7—S1—C18	91.39 (14)
N1—C1—C2—C3	−56.8 (3)	N2—C6—N1—C5	18.2 (4)
C1—C2—C3—C4	53.8 (4)	N3—C6—N1—C5	−159.7 (2)
C2—C3—C4—C5	−54.1 (4)	N2—C6—N1—C1	−117.9 (3)
C3—C4—C5—N1	56.4 (4)	N3—C6—N1—C1	64.3 (3)
N2—C7—C8—C17	−179.0 (3)	C4—C5—N1—C6	162.7 (2)
S1—C7—C8—C17	−0.3 (3)	C4—C5—N1—C1	−59.3 (3)
N2—C7—C8—C9	3.5 (4)	C2—C1—N1—C6	−161.9 (2)
S1—C7—C8—C9	−177.8 (2)	C2—C1—N1—C5	60.0 (3)
C7—C8—C9—O1	177.2 (3)	N1—C6—N2—C7	−179.3 (2)
C17—C8—C9—O1	0.1 (5)	N3—C6—N2—C7	−1.6 (4)
C7—C8—C9—N3	−0.2 (4)	C8—C7—N2—C6	−2.6 (4)
C17—C8—C9—N3	−177.3 (3)	S1—C7—N2—C6	178.8 (2)
C15—C10—C11—C12	−0.4 (4)	N2—C6—N3—C9	4.9 (4)
N3—C10—C11—C12	−177.6 (2)	N1—C6—N3—C9	−177.4 (2)
C10—C11—C12—C13	0.7 (4)	N2—C6—N3—C10	−165.7 (2)
C11—C12—C13—C14	−1.1 (4)	N1—C6—N3—C10	12.0 (3)
C11—C12—C13—C16	178.6 (3)	O1—C9—N3—C6	178.8 (2)
C12—C13—C14—C15	1.3 (4)	C8—C9—N3—C6	−3.7 (3)
C16—C13—C14—C15	−178.4 (3)	O1—C9—N3—C10	−10.1 (3)
C11—C10—C15—C14	0.7 (4)	C8—C9—N3—C10	167.5 (2)
N3—C10—C15—C14	177.9 (2)	C15—C10—N3—C6	61.3 (3)
C13—C14—C15—C10	−1.1 (4)	C11—C10—N3—C6	−121.5 (3)
C7—C8—C17—C18	−0.5 (4)	C15—C10—N3—C9	−110.0 (3)

C9—C8—C17—C18	176.7 (3)	C11—C10—N3—C9	67.3 (3)
C8—C17—C18—C19	−178.5 (3)	C8—C7—S1—C18	0.7 (2)
C8—C17—C18—S1	1.1 (4)	N2—C7—S1—C18	179.5 (2)
C17—C18—C19—C20	−113.6 (4)	C17—C18—S1—C7	−1.0 (3)
S1—C18—C19—C20	67.0 (4)	C19—C18—S1—C7	178.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···O1^{i}	0.97	2.58	3.456 (4)	150
C19—H19B···O1^{ii}	0.97	2.59	3.439 (4)	146

Symmetry codes: (i) *x*−1/2, −*y*+3/2, *z*+1/2; (ii) −*x*+2, −*y*+2, −*z*.

Fig. 1

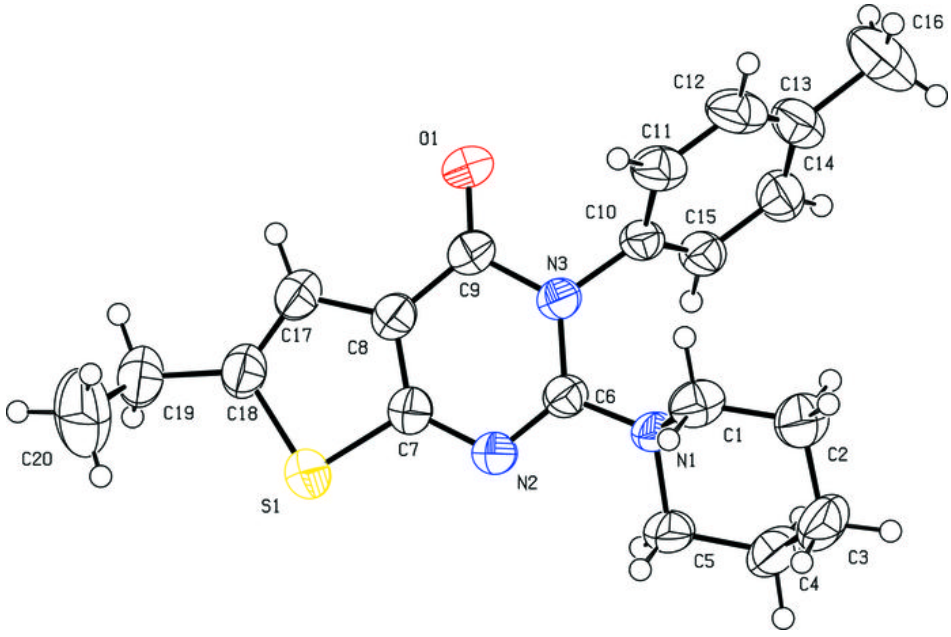
C16
C12
C13
C11
O1
C14
C10
C15
N3
C9
C17
C8
C6
C19
C18
C1
C7
C2
C20
N1
N2
S1
C5
C3
C4

Fig. 2