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3-Phenyl-2-(pyrrolidin-1-yl)-6,7-dihydro-5*H*-cyclopenta[*b*]thieno[5,4-*d*]pyrimidin-4(3*H*)-one

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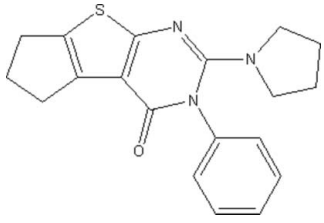
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.153; data-to-parameter ratio = 15.3.

The title compound, $C_{19}H_{19}N_3OS$, was synthesized by base catalytic reaction of ethyl 2-(phenyliminomethyleneamino)-5,6-dihydro-4*H*-cyclopenta[*b*]thiophene-2-carboxylate with pyrrolidine. In the molecule, the fused thienopyrimidinone ring system is essentially planar, making a dihedral angle of 68.64 (9)° with the phenyl ring. The conformations of the cyclopentene and pyrrolidine rings are both distorted half-chair. The crystal packing is mainly stabilized by C—H···O and C—H···π interactions.

Related literature

Many derivatives of pyrimidinone have been prepared and their biological and pharmaceutical activities have been studied by Modica *et al.* (2004) and Panico *et al.* (2001). For related literature, see: Cremer & Pople (1975); Ding *et al.* (2004); Xu *et al.* (2005); Zheng *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{19}N_3OS$
M_r = 337.43
Monoclinic, $C2/c$
a = 23.094 (3) Å
b = 8.5709 (10) Å
c = 17.271 (2) Å
β = 94.503 (2)°
V = 3408.1 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 299 (2) K
0.30 × 0.20 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
12733 measured reflections
3323 independent reflections
2613 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.153
S = 1.05
3323 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

*Cg*1, *Cg*4 and *Cg*5 are the centroids of the S1/C5/C1/C6/C7, N1/C8/C6/C7/N2/C9 and C14–C19 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O1^{i}	0.97	2.45	3.309 (3)	148
C10—H10B···Cg5	0.97	2.90	3.429 (2)	115
C12—H12A···Cg5^{ii}	0.97	2.89	3.630 (2)	134
C12—H12B···Cg1^{iii}	0.97	2.93	3.790 (3)	148
C13—H13A···Cg4^{iii}	0.97	2.67	3.542 (3)	150

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

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: IS2190).

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Zheng, A., Xu, J. & Hu, Y.-G. (2006). *Acta Cryst.* E**62**, o3710–o3711.

supplementary materials

Acta Cryst. (2007). E**63**, o3474-o3475 [**doi:10.1107/S160053680703365X**]

3-Phenyl-2-(pyrrolidin-1-yl)-6,7-dihydro-5*H*-cyclopenta[*b*]thieno[5,4-*d*]pyrimidin-4(3*H*)-one

Y.-G. Hu, Y.-L. Chen, T. Xie and M.-G. Liu

Comment

Derivatives of pyrimidinone are attracting increasing attention in the synthetic chemistry community because of the important role played by such systems in many natural products, also in antibiotics and drugs (Modica *et al.*, 2004; Panico *et al.*, 2001; Ding *et al.*, 2004). Recently, we have been interested in the synthesis of new thieno[3,2-*d*]pyrimidone derivatives. Some related X-ray crystal structure reports for pyrimidinone derivatives have been published (Zheng *et al.*, 2006; Xu *et al.*, 2005). Here, the structure of the title compound, which may be used as a new precursor for obtaining bioactive molecules, is reported (Fig. 1). In the molecule, the bond lengths and angles are unexceptional. The fused ring of the thieno[3,2-*d*]pyrimidone system is essentially planar, making a dihedral angle of 68.64 (9)° with the pnenyl C14—C19 ring. C1—C5 and C10/C11/C12/C13/N3 rings have a total puckering amplitude of 0.118 (4) and 0.418 (3) Å, respectively (Cremer & Pople, 1975) and a distorted half-chair form [φ = 80.0 (2) and 93.2 (3)°]. The crystal packing is mainly stabilized by C—H···O and C—H···π interactions (Table 1 and Fig. 2). There are no π-π interactions.

Experimental

To a solution of ethyl 2-(phenyliminomethyleneamino)-5,6-dihydro-4*H*- cyclopenta[*b*]thiophene-2-carboxylate (3 mmol) in anhydrous dichloromethane (15 ml) was added pyrrolidine (3 mmol). After stirring the reaction mixture for 2 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%. Single crystals suitable for 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 (C—H = 0.93 or 0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

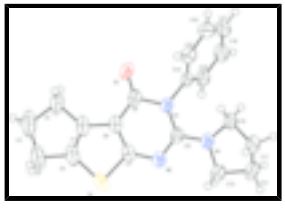

Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme and 50% probability displacement ellipsoids.

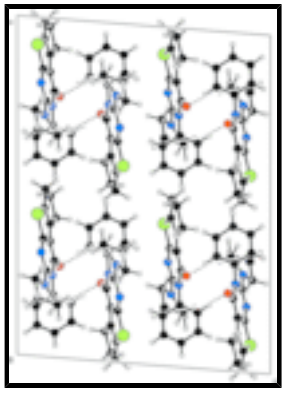

Fig. 2. The packing diagram viewed along the *b* axis, showing the C—H···O hydrogen bonds as dashed lines.

3-Phenyl-2-(pyrrolidin-1-yl)-6,7-dihydro- 5*H*-cyclopenta[*b*]thieno[5,4-*d*]pyrimidin-4(3*H*)-one

Crystal data

$C_{19}H_{19}N_3OS$	F_{000} = 1424
M_r = 337.43	D_x = 1.315 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3147 reflections
a = 23.094 (3) Å	θ = 2.4–25.8º
b = 8.5709 (10) Å	μ = 0.20 mm^{-1}
c = 17.271 (2) Å	*T* = 299 (2) K
β = 94.503 (2)º	Plate, colourless
V = 3408.1 (7) Å^3	0.30 × 0.20 × 0.06 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	2613 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.044
Monochromator: graphite	θ_{max} = 26.0º
T = 299(2) K	θ_{min} = 1.8º
φ and ω scans	*h* = −27→28
Absorption correction: none	*k* = −10→10
12733 measured reflections	*l* = −21→21
3323 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.054	H-atom parameters constrained
$wR(F^2)$ = 0.153	$w = 1/[\sigma^2(F_o^2) + 2.2147P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3323 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
217 parameters	$\Delta\rho_{min} = -0.29$ 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	0.39367 (11)	−0.0658 (3)	0.13067 (14)	0.0543 (6)
C2	0.41197 (13)	−0.2289 (4)	0.15237 (19)	0.0809 (9)
H2A	0.3879	−0.3051	0.1235	0.097*
H2B	0.4099	−0.2471	0.2075	0.097*
C3	0.47452 (15)	−0.2359 (5)	0.1303 (2)	0.1023 (12)
H3A	0.4770	−0.3026	0.0853	0.123*
H3B	0.4994	−0.2790	0.1729	0.123*
C4	0.49430 (14)	−0.0708 (5)	0.1119 (2)	0.1030 (13)
H4A	0.5214	−0.0306	0.1528	0.124*
H4B	0.5121	−0.0673	0.0629	0.124*
C5	0.43829 (11)	0.0173 (3)	0.10746 (16)	0.0630 (7)
C6	0.34115 (9)	0.0224 (2)	0.12941 (13)	0.0442 (5)
C7	0.34809 (9)	0.1721 (3)	0.10331 (13)	0.0442 (5)
C8	0.28480 (9)	−0.0255 (2)	0.14761 (13)	0.0420 (5)
C9	0.25506 (9)	0.2454 (2)	0.11414 (12)	0.0380 (5)
C10	0.16339 (9)	0.3712 (2)	0.15540 (14)	0.0477 (6)
H10A	0.1720	0.3276	0.2068	0.057*
H10B	0.1291	0.3206	0.1309	0.057*
C11	0.15533 (11)	0.5480 (2)	0.15893 (16)	0.0573 (7)
H11A	0.1152	0.5750	0.1656	0.069*
H11B	0.1801	0.5934	0.2010	0.069*
C12	0.17302 (11)	0.6016 (2)	0.08106 (16)	0.0559 (6)
H12A	0.1814	0.7125	0.0813	0.067*
H12B	0.1431	0.5791	0.0400	0.067*
C13	0.22717 (10)	0.5061 (2)	0.07185 (14)	0.0498 (6)
H13A	0.2340	0.4931	0.0175	0.060*

H13B	0.2610	0.5541	0.0988	0.060*
C14	0.18283 (9)	0.0414 (2)	0.14200 (13)	0.0399 (5)
C15	0.16433 (11)	−0.0078 (3)	0.21238 (15)	0.0542 (6)
H15	0.1890	−0.0014	0.2575	0.065*
C16	0.10902 (13)	−0.0664 (3)	0.2147 (2)	0.0689 (8)
H16	0.0962	−0.0998	0.2616	0.083*
C17	0.07258 (12)	−0.0756 (3)	0.1479 (2)	0.0726 (9)
H17	0.0353	−0.1159	0.1496	0.087*
C18	0.09132 (11)	−0.0254 (3)	0.07868 (19)	0.0634 (7)
H18	0.0663	−0.0298	0.0338	0.076*
C19	0.14687 (10)	0.0317 (2)	0.07496 (15)	0.0482 (6)
H19	0.1598	0.0632	0.0277	0.058*
N1	0.24184 (7)	0.09507 (17)	0.13812 (10)	0.0381 (4)
N2	0.30734 (8)	0.28498 (19)	0.09507 (11)	0.0443 (4)
N3	0.21341 (7)	0.35543 (18)	0.10766 (10)	0.0402 (4)
O1	0.27071 (7)	−0.15575 (17)	0.16791 (11)	0.0606 (5)
S1	0.41935 (3)	0.20650 (8)	0.08088 (5)	0.0691 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0435 (14)	0.0687 (14)	0.0502 (14)	0.0220 (11)	0.0003 (11)	−0.0011 (11)
C2	0.0651 (19)	0.0815 (19)	0.097 (2)	0.0427 (16)	0.0127 (17)	0.0180 (16)
C3	0.071 (2)	0.114 (3)	0.123 (3)	0.055 (2)	0.015 (2)	0.006 (2)
C4	0.055 (2)	0.137 (3)	0.121 (3)	0.048 (2)	0.027 (2)	0.028 (2)
C5	0.0397 (14)	0.0848 (18)	0.0645 (17)	0.0224 (13)	0.0047 (12)	0.0015 (13)
C6	0.0369 (12)	0.0485 (11)	0.0468 (13)	0.0123 (9)	0.0009 (9)	−0.0022 (9)
C7	0.0336 (11)	0.0512 (11)	0.0479 (13)	0.0046 (9)	0.0026 (9)	−0.0035 (10)
C8	0.0382 (12)	0.0386 (10)	0.0480 (13)	0.0091 (8)	−0.0043 (9)	−0.0017 (9)
C9	0.0387 (12)	0.0329 (9)	0.0421 (12)	0.0034 (8)	0.0010 (9)	−0.0054 (8)
C10	0.0371 (12)	0.0395 (10)	0.0671 (15)	0.0074 (9)	0.0089 (11)	−0.0094 (10)
C11	0.0547 (15)	0.0385 (11)	0.0794 (18)	0.0105 (10)	0.0107 (13)	−0.0122 (11)
C12	0.0560 (15)	0.0366 (11)	0.0728 (17)	0.0117 (10)	−0.0089 (12)	−0.0043 (10)
C13	0.0568 (15)	0.0346 (10)	0.0576 (15)	0.0055 (9)	0.0028 (11)	0.0014 (9)
C14	0.0336 (11)	0.0279 (9)	0.0584 (13)	0.0053 (8)	0.0048 (10)	−0.0011 (8)
C15	0.0542 (15)	0.0460 (12)	0.0632 (16)	0.0041 (10)	0.0101 (12)	0.0042 (11)
C16	0.0641 (18)	0.0481 (13)	0.099 (2)	0.0045 (12)	0.0351 (18)	0.0120 (13)
C17	0.0427 (15)	0.0408 (12)	0.136 (3)	−0.0017 (10)	0.0174 (18)	0.0003 (15)
C18	0.0404 (14)	0.0461 (12)	0.101 (2)	0.0009 (10)	−0.0098 (14)	−0.0076 (13)
C19	0.0428 (13)	0.0361 (10)	0.0653 (15)	0.0062 (9)	0.0009 (11)	−0.0031 (10)
N1	0.0322 (9)	0.0332 (8)	0.0486 (10)	0.0055 (7)	0.0018 (8)	−0.0009 (7)
N2	0.0362 (10)	0.0399 (9)	0.0573 (12)	0.0035 (7)	0.0064 (8)	−0.0003 (8)
N3	0.0376 (10)	0.0333 (8)	0.0498 (10)	0.0060 (7)	0.0038 (8)	−0.0018 (7)
O1	0.0515 (10)	0.0365 (8)	0.0931 (14)	0.0106 (7)	−0.0001 (9)	0.0087 (8)
S1	0.0379 (4)	0.0785 (5)	0.0927 (6)	0.0067 (3)	0.0174 (4)	0.0095 (4)

Geometric parameters (Å, °)

C1—C5	1.340 (4)	C10—H10A	0.9700

C1—C6	1.428 (3)	C10—H10B	0.9700
C1—C2	1.499 (3)	C11—C12	1.507 (4)
C2—C3	1.524 (4)	C11—H11A	0.9700
C2—H2A	0.9700	C11—H11B	0.9700
C2—H2B	0.9700	C12—C13	1.514 (3)
C3—C4	1.528 (5)	C12—H12A	0.9700
C3—H3A	0.9700	C12—H12B	0.9700
C3—H3B	0.9700	C13—N3	1.477 (3)
C4—C5	1.495 (3)	C13—H13A	0.9700
C4—H4A	0.9700	C13—H13B	0.9700
C4—H4B	0.9700	C14—C19	1.373 (3)
C5—S1	1.732 (3)	C14—C15	1.385 (3)
C6—C7	1.373 (3)	C14—N1	1.445 (3)
C6—C8	1.423 (3)	C15—C16	1.376 (4)
C7—N2	1.350 (3)	C15—H15	0.9300
C7—S1	1.745 (2)	C16—C17	1.376 (4)
C8—O1	1.222 (3)	C16—H16	0.9300
C8—N1	1.433 (2)	C17—C18	1.372 (4)
C9—N2	1.321 (3)	C17—H17	0.9300
C9—N3	1.345 (2)	C18—C19	1.379 (3)
C9—N1	1.395 (2)	C18—H18	0.9300
C10—N3	1.477 (3)	C19—H19	0.9300
C10—C11	1.528 (3)		
C5—C1—C6	112.7 (2)	C12—C11—H11A	111.2
C5—C1—C2	111.2 (2)	C10—C11—H11A	111.2
C6—C1—C2	136.0 (2)	C12—C11—H11B	111.2
C1—C2—C3	103.2 (3)	C10—C11—H11B	111.2
C1—C2—H2A	111.1	H11A—C11—H11B	109.1
C3—C2—H2A	111.1	C11—C12—C13	102.31 (18)
C1—C2—H2B	111.1	C11—C12—H12A	111.3
C3—C2—H2B	111.1	C13—C12—H12A	111.3
H2A—C2—H2B	109.1	C11—C12—H12B	111.3
C2—C3—C4	108.7 (2)	C13—C12—H12B	111.3
C2—C3—H3A	110.0	H12A—C12—H12B	109.2
C4—C3—H3A	110.0	N3—C13—C12	102.83 (18)
C2—C3—H3B	110.0	N3—C13—H13A	111.2
C4—C3—H3B	110.0	C12—C13—H13A	111.2
H3A—C3—H3B	108.3	N3—C13—H13B	111.2
C5—C4—C3	102.0 (3)	C12—C13—H13B	111.2
C5—C4—H4A	111.4	H13A—C13—H13B	109.1
C3—C4—H4A	111.4	C19—C14—C15	120.9 (2)
C5—C4—H4B	111.4	C19—C14—N1	119.35 (19)
C3—C4—H4B	111.4	C15—C14—N1	119.6 (2)
H4A—C4—H4B	109.2	C16—C15—C14	119.2 (3)
C1—C5—C4	113.5 (3)	C16—C15—H15	120.4
C1—C5—S1	113.14 (18)	C14—C15—H15	120.4
C4—C5—S1	133.3 (2)	C15—C16—C17	120.3 (3)
C7—C6—C8	118.32 (18)	C15—C16—H16	119.8
C7—C6—C1	112.3 (2)	C17—C16—H16	119.8

C8—C6—C1	129.4 (2)	C18—C17—C16	119.9 (2)
N2—C7—C6	127.3 (2)	C18—C17—H17	120.1
N2—C7—S1	121.15 (17)	C16—C17—H17	120.1
C6—C7—S1	111.55 (16)	C17—C18—C19	120.7 (3)
O1—C8—C6	126.57 (19)	C17—C18—H18	119.7
O1—C8—N1	119.61 (19)	C19—C18—H18	119.7
C6—C8—N1	113.80 (17)	C14—C19—C18	119.0 (2)
N2—C9—N3	117.44 (18)	C14—C19—H19	120.5
N2—C9—N1	122.49 (17)	C18—C19—H19	120.5
N3—C9—N1	120.04 (18)	C9—N1—C8	122.32 (17)
N3—C10—C11	102.49 (17)	C9—N1—C14	122.50 (16)
N3—C10—H10A	111.3	C8—N1—C14	114.33 (15)
C11—C10—H10A	111.3	C9—N2—C7	115.67 (18)
N3—C10—H10B	111.3	C9—N3—C13	118.14 (17)
C11—C10—H10B	111.3	C9—N3—C10	127.09 (18)
H10A—C10—H10B	109.2	C13—N3—C10	110.91 (15)
C12—C11—C10	102.94 (18)	C5—S1—C7	90.33 (11)
C5—C1—C2—C3	−5.6 (3)	N1—C14—C19—C18	177.51 (18)
C6—C1—C2—C3	175.2 (3)	C17—C18—C19—C14	−1.7 (3)
C1—C2—C3—C4	10.9 (4)	N2—C9—N1—C8	3.2 (3)
C2—C3—C4—C5	−11.9 (4)	N3—C9—N1—C8	−178.62 (18)
C6—C1—C5—C4	177.3 (3)	N2—C9—N1—C14	−165.56 (19)
C2—C1—C5—C4	−2.1 (4)	N3—C9—N1—C14	12.6 (3)
C6—C1—C5—S1	−1.1 (3)	O1—C8—N1—C9	−179.2 (2)
C2—C1—C5—S1	179.5 (2)	C6—C8—N1—C9	−0.8 (3)
C3—C4—C5—C1	8.7 (4)	O1—C8—N1—C14	−9.5 (3)
C3—C4—C5—S1	−173.2 (3)	C6—C8—N1—C14	168.88 (18)
C5—C1—C6—C7	1.1 (3)	C19—C14—N1—C9	63.7 (2)
C2—C1—C6—C7	−179.7 (3)	C15—C14—N1—C9	−119.9 (2)
C5—C1—C6—C8	178.0 (2)	C19—C14—N1—C8	−106.0 (2)
C2—C1—C6—C8	−2.8 (5)	C15—C14—N1—C8	70.4 (2)
C8—C6—C7—N2	2.7 (4)	N3—C9—N2—C7	179.18 (19)
C1—C6—C7—N2	180.0 (2)	N1—C9—N2—C7	−2.6 (3)
C8—C6—C7—S1	−177.87 (16)	C6—C7—N2—C9	−0.3 (3)
C1—C6—C7—S1	−0.5 (3)	S1—C7—N2—C9	−179.74 (15)
C7—C6—C8—O1	176.4 (2)	N2—C9—N3—C13	6.6 (3)
C1—C6—C8—O1	−0.4 (4)	N1—C9—N3—C13	−171.66 (18)
C7—C6—C8—N1	−1.9 (3)	N2—C9—N3—C10	−149.2 (2)
C1—C6—C8—N1	−178.7 (2)	N1—C9—N3—C10	32.6 (3)
N3—C10—C11—C12	33.1 (2)	C12—C13—N3—C9	−175.30 (18)
C10—C11—C12—C13	−43.4 (2)	C12—C13—N3—C10	−15.8 (2)
C11—C12—C13—N3	36.1 (2)	C11—C10—N3—C9	146.5 (2)
C19—C14—C15—C16	−0.3 (3)	C11—C10—N3—C13	−10.7 (2)
N1—C14—C15—C16	−176.64 (19)	C1—C5—S1—C7	0.7 (2)
C14—C15—C16—C17	−0.1 (3)	C4—C5—S1—C7	−177.4 (3)
C15—C16—C17—C18	−0.4 (4)	N2—C7—S1—C5	179.4 (2)
C16—C17—C18—C19	1.3 (4)	C6—C7—S1—C5	−0.06 (19)
C15—C14—C19—C18	1.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10A···O1^{i}	0.97	2.45	3.309 (3)	148
C10—H10B···Cg5	0.97	2.90	3.429 (2)	115
C12—H12A···Cg5^{ii}	0.97	2.89	3.630 (2)	134
C12—H12B···Cg1^{iii}	0.97	2.93	3.790 (3)	148
C13—H13A···Cg4^{iii}	0.97	2.67	3.542 (3)	150

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

Fig. 1

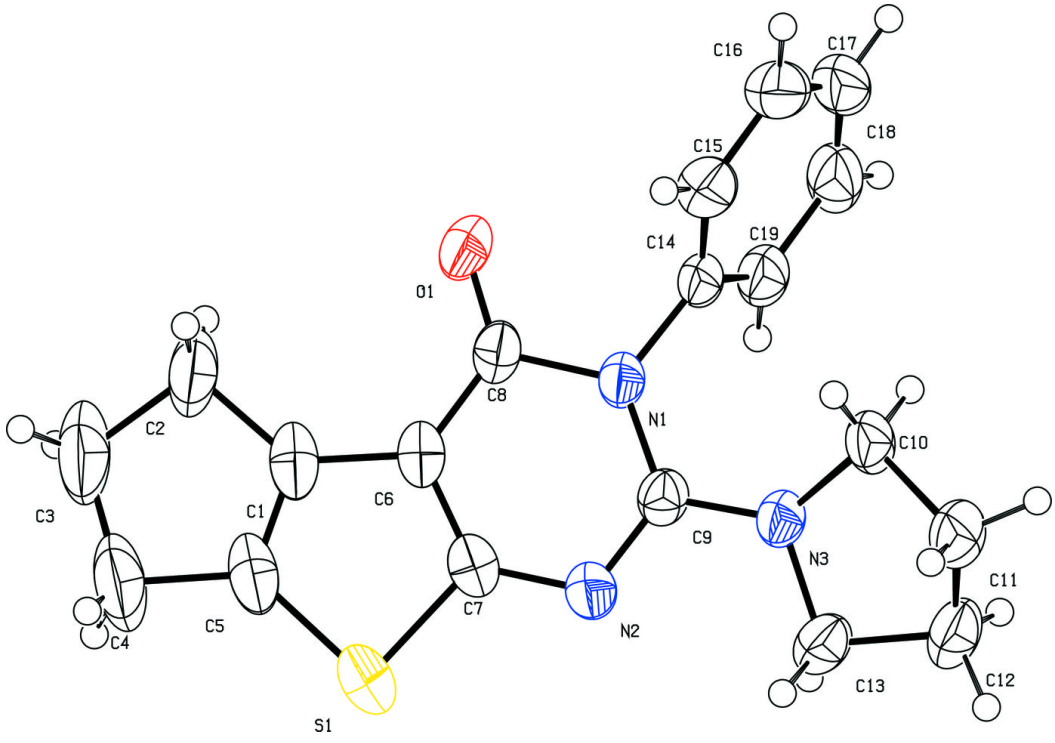
C16
C17
C18
C15
C14
C19
O1
C8
N1
C10
C2
C6
C9
C3
C1
N3
C11
C7
N2
C4
C5
C13
C12
S1

Fig. 2