Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

2-(4-Fluorophenyl)-4-(4-methoxyphenyl)-5-(piperidin-1-ylmethyl)thiazole

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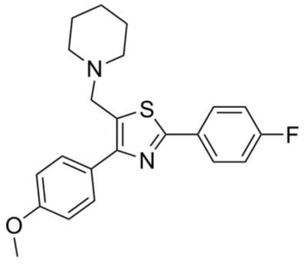
Received 25 November 2010; accepted 24 December 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.110; data-to-parameter ratio = 19.1.

In the title compound, $C_{22}H_{23}FN_2OS$, the piperidine ring shows chair confirmation and the two benzene rings make a dihedral angle of 17.0 (6)°. The thiazole fragment is essentially planar with an r.m.s. deviation of 0.004 (2) Å and a maximum deviation of 0.006 (2) Å.. In the crystal, intermolecular C—H⋯π interactions lead to the formation of a layer structure.

Related literature

For the biological activity of thiazole derivatives, see: Guo *et al.* (2006); Karegoudar *et al.* (2008) Reddy *et al.* (1999);. For related structures, see: Mitsutaka *et al.* (2006); Takayuki *et al.* (2009).



Experimental

Crystal data

$C_{22}H_{23}FN_2OS$
M_r = 382.48
Triclinic, $P\overline{1}$
a = 10.7565 (2) Å
b = 10.8846 (2) Å
c = 11.0179 (2) Å
α = 67.035 (1)°
β = 63.881 (1)°
γ = 60.768 (1)°
V = 985.16 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 296 K
0.26 × 0.26 × 0.24 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.659, T_{max} = 0.746
26568 measured reflections
4674 independent reflections
3614 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.05
4674 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C1—H1A⋯$Cg1_{C10-C15}{}^{i}$	0.96	2.98	3.781 (2)	142
C1—H1C⋯$Cg2_{C2-C7}{}^{ii}$	0.96	2.74	3.595 (2)	149

Symmetry codes: (i) $x, y+1, z$; (ii) $-x, -y+3, -z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (project No. 30873140), the Program for Excellent Talents of Beijing City (project No. 20071D0501600227) and the Beijing Municipal Commission of Education (project No. KM201010028011).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2365).

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supplementary materials

Acta Cryst. (2011). E**67**, o361 [**doi:10.1107/S1600536810054103**]

2-(4-Fluorophenyl)-4-(4-methoxyphenyl)-5-(piperidin-1-ylmethyl)thiazole

C.-B. Guo, C. Lv, W. Wei and H. Zhou

Comment

Thiazole derivatives have a varity of physiological effects, such as antiinflammatory (Guo *et al.*, 2006) and antimicrobial (Karegoudar *et al.*, 2008). Herein, we report the crystal structure of a new thiazole compound.

In the title compound (Fig. 1), the piperidine ring shows a chair confirmation. The thiazole fragment (S1/C9/N1/C8/C16) is essentially planar and it's mean plane makes dihedral angles of 29.2 (6) and 19.8 (1)°, with benzene rings C2—C7 and C10—C15, respectively, while the dihedral angle between the two phenyl rings is 17.0 (6)°.

The molecular packing is stabilized by C—H···π interactions (Fig. 2). The C1—H1*A*···*Cg1* distances are 3.781 (2) Å and C1—H1*C*···*Cg2* 3.595 (2) Å, respectively (*Cg* 1 and 2 are is the centroids of the aromatic rings C10–C15 and C2–C7, respectively. All the C—H···π interactions have been listed in Table 1 and presented in Fig. 2.

For related literature, see: Mitsutaka *et al.* (2006);

Experimental

To a solution of piperidine (0.5 ml) in tetrahydrofuran (THF, 15 ml) was added a solution of 5-(bromomethyl)-2-(4-fluorophenyl)-4-(4-methoxyphenyl)thiazole (0.35 g, 0.92 mmol) in THF (10 ml), and the resulting mixture was stirred at 296 K for 1 h. The precipitate was filtered, the solvent was removed by rotary evaporation, the residue was dissolved in ethyl acetate, washed the organic phase with water and brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure to yield the title compound as a white powder (0.11 g, 32%). Crystals suitable for X-ray analysis were prepared by slow evaporation of a solution of the title compound in dichloromethane and methanol (*v*/*v* = 2:1) at room temperature in three days.

Refinement

The H atoms were positioned in calculated positions with C—H = 0.93, 0.96 and 0.97 Å for aryl, methyl and methylene type H-atoms and were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.5\,U_{\text{eq}}(\text{C})$ for methyl H atoms and $U_{\text{iso}} = 1.2U_{\text{eq}}$ for others.

Figures

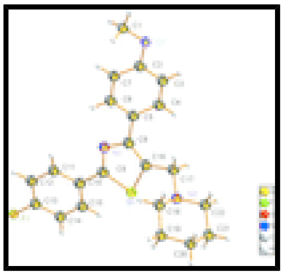

Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoid and the atom numbering scheme.

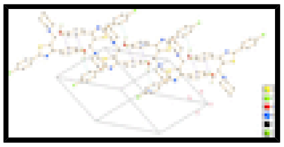

Fig. 2. The three-dimensional structure of the title compound, formed through C—H···π interactions; the dashed lines represent C—H···π interactions.

2-(4-Fluorophenyl)-4-(4-methoxyphenyl)-5-(piperidin-1-ylmethyl)thiazole

Crystal data

$C_{22}H_{23}FN_2OS$	$Z = 2$
$M_r = 382.48$	$F(000) = 404$
Triclinic, $P\overline{1}$	$D_x = 1.289$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.7565$ (2) Å	Cell parameters from 7061 reflections
$b = 10.8846$ (2) Å	$\theta = 2.3–27.9°$
$c = 11.0179$ (2) Å	$\mu = 0.19$ mm^{-1}
$\alpha = 67.035$ (1)°	$T = 296$ K
$\beta = 63.881$ (1)°	Block, colourless
$\gamma = 60.768$ (1)°	0.26 × 0.26 × 0.24 mm
$V = 985.16$ (3) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	4674 independent reflections
Radiation source: fine-focus sealed tube	3614 reflections with $I > 2.0\sigma(I)$
graphite	$R_{int} = 0.035$
φ & ω scans	$\theta_{max} = 27.9°$, $\theta_{min} = 2.1°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)	$h = -14 \rightarrow 14$
$T_{min} = 0.659$, $T_{max} = 0.746$	$k = -14 \rightarrow 14$
26568 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.110$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 0.1593P]$ where $P = (F_o^2 + 2F_c^2)/3$
4674 reflections	$(\Delta/\sigma)_{max} = 0.001$
245 parameters	$\Delta\rho_{max} = 0.16$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.22$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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.

All hydrogen atoms were located in the calculated sites and included in the final refinement in the riding model approximation with displacement parameters derived from the parent atoms to which they were bonded.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.33888 (5)	0.75870 (4)	0.04214 (4)	0.05238 (13)
F1	0.59060 (15)	0.58770 (13)	−0.56262 (10)	0.0869 (4)
O1	0.17330 (14)	1.58657 (12)	−0.00821 (13)	0.0640 (3)
N1	0.36970 (13)	0.98214 (12)	−0.14604 (12)	0.0442 (3)
C17	0.22778 (19)	0.90522 (17)	0.24743 (15)	0.0535 (4)
H17A	0.3087	0.8712	0.2844	0.064*
H17B	0.1614	1.0019	0.2622	0.064*
C1	0.1157 (2)	1.70549 (18)	−0.1103 (2)	0.0711 (5)
H1A	0.1916	1.7013	−0.1992	0.107*
H1B	0.0863	1.7941	−0.0869	0.107*
H1C	0.0302	1.7014	−0.1139	0.107*
C2	0.20949 (16)	1.45111 (16)	−0.01833 (16)	0.0479 (3)
C3	0.25260 (17)	1.33858 (17)	0.08932 (15)	0.0503 (3)
H3	0.2557	1.3581	0.1627	0.060*
C4	0.29100 (16)	1.19791 (16)	0.08885 (15)	0.0471 (3)
H4	0.3210	1.1236	0.1614	0.056*
C5	0.28547 (15)	1.16533 (15)	−0.01895 (14)	0.0428 (3)
C6	0.24580 (18)	1.27941 (16)	−0.12758 (15)	0.0527 (4)
H6	0.2446	1.2603	−0.2022	0.063*
C7	0.20801 (19)	1.42074 (17)	−0.12818 (16)	0.0552 (4)
H7	0.1817	1.4950	−0.2023	0.066*

C8	0.31552 (15)	1.01781 (15)	−0.01896 (14)	0.0431 (3)
C9	0.38848 (16)	0.84914 (15)	−0.12873 (14)	0.0438 (3)
C10	0.44413 (15)	0.77917 (15)	−0.24329 (14)	0.0438 (3)
C11	0.43754 (18)	0.86279 (17)	−0.37501 (15)	0.0524 (4)
H11	0.3992	0.9629	−0.3906	0.063*
C12	0.4874 (2)	0.79865 (19)	−0.48320 (16)	0.0595 (4)
H12	0.4839	0.8544	−0.5715	0.071*
C13	0.5419 (2)	0.65120 (19)	−0.45685 (16)	0.0584 (4)
C14	0.5508 (2)	0.56486 (18)	−0.32943 (17)	0.0613 (4)
H14	0.5890	0.4648	−0.3150	0.074*
C15	0.50171 (18)	0.63000 (16)	−0.22271 (16)	0.0539 (4)
H15	0.5073	0.5729	−0.1353	0.065*
C16	0.29129 (17)	0.90992 (15)	0.09436 (14)	0.0470 (3)
N2	0.14491 (14)	0.80983 (13)	0.32118 (12)	0.0468 (3)
C18	0.00257 (19)	0.87436 (18)	0.29190 (16)	0.0571 (4)
H18A	0.0214	0.9003	0.1924	0.068*
H18B	−0.0614	0.9618	0.3268	0.068*
C19	−0.0763 (2)	0.7702 (2)	0.35887 (19)	0.0665 (5)
H19A	−0.0150	0.6851	0.3199	0.080*
H19B	−0.1707	0.8155	0.3394	0.080*
C20	−0.1053 (2)	0.7259 (2)	0.51460 (19)	0.0736 (5)
H20A	−0.1780	0.8084	0.5555	0.088*
H20B	−0.1464	0.6517	0.5548	0.088*
C21	0.0389 (2)	0.6692 (2)	0.54608 (18)	0.0677 (5)
H21A	0.1047	0.5777	0.5188	0.081*
H21B	0.0171	0.6521	0.6452	0.081*
C22	0.11816 (19)	0.77385 (18)	0.47077 (15)	0.0545 (4)
H22A	0.0575	0.8615	0.5057	0.065*
H22B	0.2131	0.7310	0.4888	0.065*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0689 (3)	0.0436 (2)	0.0398 (2)	−0.02424 (18)	−0.00998 (17)	−0.00904 (15)
F1	0.1297 (10)	0.0886 (8)	0.0513 (6)	−0.0570 (7)	−0.0035 (6)	−0.0326 (5)
O1	0.0744 (8)	0.0491 (6)	0.0779 (8)	−0.0251 (6)	−0.0247 (6)	−0.0200 (6)
N1	0.0470 (7)	0.0405 (6)	0.0400 (6)	−0.0140 (5)	−0.0111 (5)	−0.0106 (5)
C17	0.0668 (10)	0.0557 (9)	0.0420 (8)	−0.0297 (8)	−0.0106 (7)	−0.0136 (7)
C1	0.0652 (11)	0.0448 (9)	0.1013 (15)	−0.0165 (8)	−0.0290 (10)	−0.0170 (9)
C2	0.0450 (8)	0.0455 (8)	0.0561 (8)	−0.0192 (6)	−0.0107 (6)	−0.0172 (7)
C3	0.0542 (9)	0.0615 (9)	0.0483 (8)	−0.0292 (7)	−0.0146 (7)	−0.0171 (7)
C4	0.0491 (8)	0.0509 (8)	0.0458 (7)	−0.0220 (7)	−0.0186 (6)	−0.0069 (6)
C5	0.0397 (7)	0.0436 (7)	0.0421 (7)	−0.0150 (6)	−0.0086 (6)	−0.0126 (6)
C6	0.0681 (10)	0.0468 (8)	0.0445 (8)	−0.0185 (7)	−0.0199 (7)	−0.0134 (6)
C7	0.0687 (10)	0.0442 (8)	0.0498 (8)	−0.0172 (7)	−0.0239 (8)	−0.0072 (6)
C8	0.0427 (7)	0.0434 (7)	0.0406 (7)	−0.0150 (6)	−0.0111 (6)	−0.0109 (6)
C9	0.0446 (7)	0.0411 (7)	0.0401 (7)	−0.0141 (6)	−0.0106 (6)	−0.0097 (6)
C10	0.0440 (7)	0.0438 (7)	0.0405 (7)	−0.0172 (6)	−0.0083 (6)	−0.0115 (6)

C11	0.0627 (9)	0.0457 (8)	0.0460 (8)	−0.0214 (7)	−0.0145 (7)	−0.0096 (6)
C12	0.0754 (11)	0.0637 (10)	0.0414 (8)	−0.0331 (9)	−0.0155 (8)	−0.0082 (7)
C13	0.0689 (10)	0.0670 (10)	0.0452 (8)	−0.0350 (9)	−0.0023 (7)	−0.0243 (7)
C14	0.0758 (11)	0.0476 (9)	0.0529 (9)	−0.0231 (8)	−0.0083 (8)	−0.0181 (7)
C15	0.0654 (10)	0.0451 (8)	0.0428 (8)	−0.0184 (7)	−0.0124 (7)	−0.0106 (6)
C16	0.0524 (8)	0.0456 (8)	0.0412 (7)	−0.0198 (7)	−0.0102 (6)	−0.0118 (6)
N2	0.0540 (7)	0.0492 (7)	0.0366 (6)	−0.0219 (6)	−0.0106 (5)	−0.0102 (5)
C18	0.0599 (9)	0.0585 (9)	0.0471 (8)	−0.0178 (8)	−0.0179 (7)	−0.0113 (7)
C19	0.0593 (10)	0.0815 (12)	0.0655 (11)	−0.0297 (9)	−0.0174 (8)	−0.0216 (9)
C20	0.0693 (12)	0.0880 (14)	0.0620 (11)	−0.0436 (10)	−0.0075 (9)	−0.0123 (10)
C21	0.0751 (12)	0.0708 (11)	0.0480 (9)	−0.0359 (10)	−0.0140 (8)	0.0002 (8)
C22	0.0633 (9)	0.0591 (9)	0.0391 (7)	−0.0242 (8)	−0.0135 (7)	−0.0110 (7)

Geometric parameters (Å, °)

S1—C16	1.7201 (15)	C10—C15	1.388 (2)
S1—C9	1.7264 (14)	C10—C11	1.392 (2)
F1—C13	1.3593 (17)	C11—C12	1.385 (2)
O1—C2	1.3665 (17)	C11—H11	0.9300
O1—C1	1.421 (2)	C12—C13	1.368 (2)
N1—C9	1.3060 (18)	C12—H12	0.9300
N1—C8	1.3912 (17)	C13—C14	1.365 (2)
C17—N2	1.4632 (19)	C14—C15	1.379 (2)
C17—C16	1.5054 (19)	C14—H14	0.9300
C17—H17A	0.9700	C15—H15	0.9300
C17—H17B	0.9700	N2—C22	1.4634 (18)
C1—H1A	0.9600	N2—C18	1.466 (2)
C1—H1B	0.9600	C18—C19	1.512 (2)
C1—H1C	0.9600	C18—H18A	0.9700
C2—C7	1.382 (2)	C18—H18B	0.9700
C2—C3	1.385 (2)	C19—C20	1.518 (3)
C3—C4	1.379 (2)	C19—H19A	0.9700
C3—H3	0.9300	C19—H19B	0.9700
C4—C5	1.3970 (19)	C20—C21	1.510 (3)
C4—H4	0.9300	C20—H20A	0.9700
C5—C6	1.389 (2)	C20—H20B	0.9700
C5—C8	1.4751 (19)	C21—C22	1.517 (2)
C6—C7	1.384 (2)	C21—H21A	0.9700
C6—H6	0.9300	C21—H21B	0.9700
C7—H7	0.9300	C22—H22A	0.9700
C8—C16	1.369 (2)	C22—H22B	0.9700
C9—C10	1.4734 (19)		
C16—S1—C9	89.65 (7)	C11—C12—H12	120.9
C2—O1—C1	117.72 (13)	F1—C13—C14	118.51 (15)
C9—N1—C8	110.92 (11)	F1—C13—C12	118.50 (15)
N2—C17—C16	111.16 (12)	C14—C13—C12	122.99 (14)
N2—C17—H17A	109.4	C13—C14—C15	118.20 (15)
C16—C17—H17A	109.4	C13—C14—H14	120.9
N2—C17—H17B	109.4	C15—C14—H14	120.9

C16—C17—H17B	109.4	C14—C15—C10	121.25 (15)
H17A—C17—H17B	108.0	C14—C15—H15	119.4
O1—C1—H1A	109.5	C10—C15—H15	119.4
O1—C1—H1B	109.5	C8—C16—C17	131.87 (13)
H1A—C1—H1B	109.5	C8—C16—S1	110.02 (10)
O1—C1—H1C	109.5	C17—C16—S1	118.06 (11)
H1A—C1—H1C	109.5	C17—N2—C22	111.27 (12)
H1B—C1—H1C	109.5	C17—N2—C18	111.22 (12)
O1—C2—C7	124.48 (14)	C22—N2—C18	110.21 (12)
O1—C2—C3	116.31 (13)	N2—C18—C19	110.86 (13)
C7—C2—C3	119.20 (14)	N2—C18—H18A	109.5
C4—C3—C2	120.72 (13)	C19—C18—H18A	109.5
C4—C3—H3	119.6	N2—C18—H18B	109.5
C2—C3—H3	119.6	C19—C18—H18B	109.5
C3—C4—C5	120.99 (13)	H18A—C18—H18B	108.1
C3—C4—H4	119.5	C18—C19—C20	110.67 (15)
C5—C4—H4	119.5	C18—C19—H19A	109.5
C6—C5—C4	117.27 (13)	C20—C19—H19A	109.5
C6—C5—C8	119.91 (12)	C18—C19—H19B	109.5
C4—C5—C8	122.80 (13)	C20—C19—H19B	109.5
C7—C6—C5	121.99 (14)	H19A—C19—H19B	108.1
C7—C6—H6	119.0	C21—C20—C19	109.97 (15)
C5—C6—H6	119.0	C21—C20—H20A	109.7
C2—C7—C6	119.77 (14)	C19—C20—H20A	109.7
C2—C7—H7	120.1	C21—C20—H20B	109.7
C6—C7—H7	120.1	C19—C20—H20B	109.7
C16—C8—N1	114.69 (12)	H20A—C20—H20B	108.2
C16—C8—C5	127.01 (13)	C20—C21—C22	111.94 (15)
N1—C8—C5	118.26 (12)	C20—C21—H21A	109.2
N1—C9—C10	124.09 (12)	C22—C21—H21A	109.2
N1—C9—S1	114.71 (10)	C20—C21—H21B	109.2
C10—C9—S1	121.19 (10)	C22—C21—H21B	109.2
C15—C10—C11	118.52 (13)	H21A—C21—H21B	107.9
C15—C10—C9	121.36 (13)	N2—C22—C21	111.09 (13)
C11—C10—C9	120.11 (13)	N2—C22—H22A	109.4
C12—C11—C10	120.77 (14)	C21—C22—H22A	109.4
C12—C11—H11	119.6	N2—C22—H22B	109.4
C10—C11—H11	119.6	C21—C22—H22B	109.4
C13—C12—C11	118.27 (15)	H22A—C22—H22B	108.0
C13—C12—H12	120.9		

C1—O1—C2—C7	6.7 (2)	C9—C10—C11—C12	−179.05 (14)
C1—O1—C2—C3	−174.43 (14)	C10—C11—C12—C13	0.6 (3)
O1—C2—C3—C4	179.86 (13)	C11—C12—C13—F1	179.83 (15)
C7—C2—C3—C4	−1.2 (2)	C11—C12—C13—C14	−0.8 (3)
C2—C3—C4—C5	−0.9 (2)	F1—C13—C14—C15	179.78 (15)
C3—C4—C5—C6	2.5 (2)	C12—C13—C14—C15	0.4 (3)
C3—C4—C5—C8	−175.70 (13)	C13—C14—C15—C10	0.2 (3)
C4—C5—C6—C7	−2.2 (2)	C11—C10—C15—C14	−0.4 (2)
C8—C5—C6—C7	176.13 (14)	C9—C10—C15—C14	178.63 (15)

O1—C2—C7—C6	−179.58 (14)	N1—C8—C16—C17	−176.66 (15)
C3—C2—C7—C6	1.6 (2)	C5—C8—C16—C17	1.1 (3)
C5—C6—C7—C2	0.1 (3)	N1—C8—C16—S1	0.64 (16)
C9—N1—C8—C16	−1.13 (18)	C5—C8—C16—S1	178.38 (12)
C9—N1—C8—C5	−179.08 (12)	N2—C17—C16—C8	146.91 (16)
C6—C5—C8—C16	−148.99 (16)	N2—C17—C16—S1	−30.21 (18)
C4—C5—C8—C16	29.2 (2)	C9—S1—C16—C8	−0.01 (12)
C6—C5—C8—N1	28.7 (2)	C9—S1—C16—C17	177.71 (13)
C4—C5—C8—N1	−153.12 (13)	C16—C17—N2—C22	164.61 (13)
C8—N1—C9—C10	179.82 (13)	C16—C17—N2—C18	−72.10 (16)
C8—N1—C9—S1	1.11 (16)	C17—N2—C18—C19	175.32 (13)
C16—S1—C9—N1	−0.66 (12)	C22—N2—C18—C19	−60.79 (17)
C16—S1—C9—C10	−179.41 (12)	N2—C18—C19—C20	58.33 (19)
N1—C9—C10—C15	161.52 (15)	C18—C19—C20—C21	−53.4 (2)
S1—C9—C10—C15	−19.8 (2)	C19—C20—C21—C22	52.2 (2)
N1—C9—C10—C11	−19.5 (2)	C17—N2—C22—C21	−177.25 (14)
S1—C9—C10—C11	159.13 (12)	C18—N2—C22—C21	58.89 (17)
C15—C10—C11—C12	0.0 (2)	C20—C21—C22—N2	−55.4 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1A···$\mathrm{Cg1}_{\mathrm{C10\text{-}C15}}^{\mathrm{i}}$	0.96	2.98	3.781 (2)	142
C1—H1C···$\mathrm{Cg2}_{\mathrm{C2\text{-}C7}}^{\mathrm{ii}}$	0.96	2.74	3.595 (2)	149

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

Fig. 1

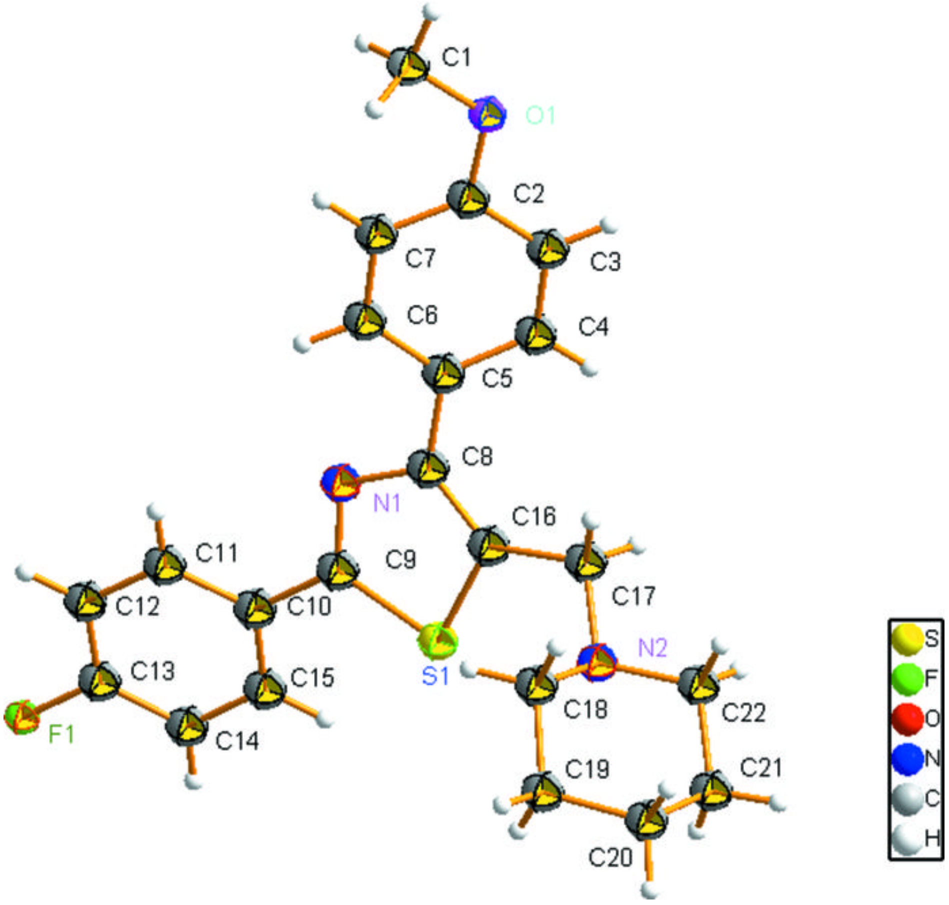
C1
O1
C2
C7
C3
C6
C4
C5
C8
N1
C16
C11
C9
C17
C12
C10
N2
S1
C13
C15
C18
C22
F1
C14
C19
C21
C20
S
F
O
N
C
H

Fig. 2