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1-(2,6-Dimethylphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea

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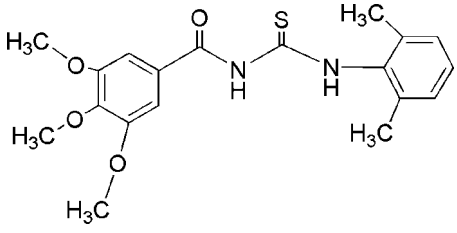
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.107; data-to-parameter ratio = 15.4.

In the molecule of the title compound, $C_{19}H_{22}N_2O_4S$, the rings are oriented at a dihedral angle of 62.83 (3)°. In the crystal structure, intermolecular N—H···S hydrogen bonds link the molecules into centrosymmetric dimers; an intramolecular N—H···O hydrogen bond is also present.

Related literature

For related structures, see: Saeed & Flörke (2007); Wang *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{19}H_{22}N_2O_4S$
M_r = 374.45
Monoclinic, $P2_1/c$
a = 11.610 (3) Å
b = 7.4556 (17) Å
c = 22.085 (5) Å
β = 102.753 (4)°
V = 1864.5 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.980
10230 measured reflections
3809 independent reflections
2496 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.01
3809 reflections
248 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···S1^{i}	0.87 (2)	2.59 (2)	3.4434 (18)	165.3 (18)
N2—H2A···O4	0.86 (2)	1.92 (2)	2.622 (2)	138 (2)

Symmetry code: (i) $-x, -y+1, -z$.

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2387).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1997). *SHELXTL* (Version 5.10), *SMART* (Version 5.611) and *SAINT* (Version 6.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Saeed, A. & Flörke, U. (2007). *Acta Cryst.* E**63**, o3695.
Sheldrick, G. M. (1996). *SADABS*. Version 2.03. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, J., Tian, L. & Liu, S.-Y. (2007). *Acta Cryst.* E**63**, o3667.

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supplementary materials

Acta Cryst. (2007). E**63**, o4827 [**doi:10.1107/S1600536807059892**]

1-(2,6-Dimethylphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea

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Comment

As part of our ongoing studies on thiourea derivatives, we report herein the synthesis and crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and they are in good agrement with the corresponding values in 1-(2,2-Dimethylcyclopropylcarbonyl)-3-(2-pyridyl)thiourea, (II), (Wang *et al.*, 2007) and 1-(3-Methoxyphenyl)-3-(4-methylbenzoyl)thiourea, (III), (Saeed & Flörke, 2007). In (I), rings A (C1–C6) and B (C12–C17) are, of course, planar and the dihedral angle between them is A/B = 62.83 (3)°. It is reported as 48.30 (8)°, in (III).

In the crystal structure, intermolecular N—H···S hydrogen bonds (Table 1, Fig. 2) link the molecules into centrosymmetric dimers; an intramolecular N—H···O hydrogen bond (Table 1) is also present.

Experimental

For the preparation of the title compound, powdered ammonium thiocyanate (15 mmol), 3,4,5-trimethoxylbenzoyl chloride (10 mmol), PEG-400 (0.15 mmol) and acetone (25 ml) were placed in a dried round-bottomed flask containing a magnetic stirrer bar and stirred at room temperature for 1 h. Then, 2,6-methylbenzenamine (9.5 mmol) was added and the mixture was stirred for 4 h. The mixture was poured into water (20 ml). The resulting solid was filtered, dried and recrystallized from DMF–EtOH to give the title compound. Single crystals of the title compound were obtained by slow evaporation of a solution in DMF–EtOH (1:1,*v*/*v*).

Refinement

H atom (for NH) was located in difference syntheses and refined isotropically [N—H = 0.87 (2) Å and U_{iso}(H) = 0.086 (2) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H, and x = 1.2 for aromatic H atoms.

Figures

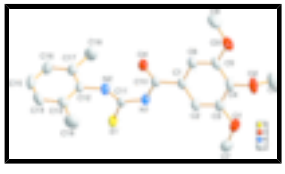

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

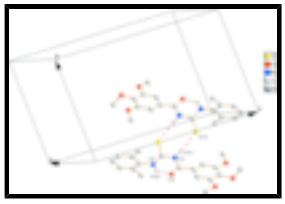

Fig. 2. A partial packing diagram of (I) [symmetry code A: −*x*, 1 − *y*, −*z*]. Hydrogen bonds are shown as dashed lines.

1-(2,6-Dimethylphenyl)-3-(3,4,5-tirmethoxybenzoyl)thiourea

Crystal data

$C_{19}H_{22}N_2O_4S$	F_{000} = 792
M_r = 374.45	D_x = 1.334 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 495 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.610 (3) Å	Cell parameters from 2743 reflections
b = 7.4556 (17) Å	θ = 2.9–25.2º
c = 22.085 (5) Å	μ = 0.20 mm^{-1}
β = 102.753 (4)º	*T* = 294 (2) K
V = 1864.5 (8) Å^3	Prism, colourless
Z = 4	0.20 × 0.18 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	3809 independent reflections
Radiation source: fine-focus sealed tube	2496 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −14→7
T_{min} = 0.961, T_{max} = 0.980	*k* = −9→8
10230 measured reflections	*l* = −18→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.107	$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.3608P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
3809 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}

248 parameters	$\Delta\rho_{min} = -0.20$ 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}
S1	0.00655 (4)	0.61330 (7)	0.08568 (2)	0.04199 (17)
O1	0.32004 (13)	0.1186 (2)	−0.11312 (7)	0.0542 (4)
O2	0.48745 (13)	0.2805 (2)	−0.15944 (7)	0.0544 (4)
O3	0.55058 (13)	0.6217 (2)	−0.13188 (7)	0.0582 (4)
O4	0.34482 (12)	0.79516 (19)	0.03668 (7)	0.0454 (4)
N1	0.18920 (14)	0.6048 (2)	0.03092 (8)	0.0348 (4)
N2	0.20952 (15)	0.7879 (2)	0.11730 (8)	0.0385 (4)
C1	0.33074 (15)	0.5591 (3)	−0.03605 (8)	0.0321 (4)
C2	0.29566 (16)	0.3836 (3)	−0.05213 (9)	0.0357 (5)
H2	0.2389	0.3282	−0.0347	0.043*
C3	0.34643 (17)	0.2921 (3)	−0.09450 (9)	0.0381 (5)
C4	0.43217 (16)	0.3750 (3)	−0.12032 (9)	0.0399 (5)
C5	0.46579 (16)	0.5509 (3)	−0.10428 (9)	0.0398 (5)
C6	0.41557 (16)	0.6430 (3)	−0.06225 (9)	0.0379 (5)
H6	0.4383	0.7604	−0.0515	0.045*
C7	0.2210 (2)	0.0371 (3)	−0.09612 (12)	0.0574 (6)
H7A	0.2360	0.0253	−0.0518	0.086*
H7B	0.2078	−0.0793	−0.1149	0.086*
H7C	0.1523	0.1104	−0.1102	0.086*
C8	0.4273 (2)	0.2828 (4)	−0.22275 (11)	0.0619 (7)
H8A	0.3487	0.2371	−0.2266	0.093*
H8B	0.4690	0.2093	−0.2465	0.093*
H8C	0.4235	0.4036	−0.2381	0.093*
C9	0.5850 (2)	0.8031 (4)	−0.11726 (12)	0.0680 (8)
H9A	0.5175	0.8800	−0.1291	0.102*
H9B	0.6440	0.8374	−0.1394	0.102*
H9C	0.6167	0.8139	−0.0734	0.102*
C10	0.29023 (16)	0.6634 (3)	0.01298 (9)	0.0329 (4)
C11	0.14171 (15)	0.6746 (2)	0.07862 (9)	0.0303 (4)
C12	0.16991 (16)	0.8875 (3)	0.16473 (9)	0.0340 (5)

C13	0.19512 (17)	0.8244 (3)	0.22532 (10)	0.0421 (5)
C14	0.1593 (2)	0.9309 (4)	0.26999 (11)	0.0543 (6)
H14	0.1750	0.8929	0.3111	0.065*
C15	0.1012 (2)	1.0906 (4)	0.25423 (12)	0.0589 (7)
H15	0.0776	1.1589	0.2846	0.071*
C16	0.0780 (2)	1.1497 (3)	0.19418 (12)	0.0535 (6)
H16	0.0390	1.2584	0.1842	0.064*
C17	0.11159 (17)	1.0501 (3)	0.14765 (10)	0.0417 (5)
C18	0.0834 (2)	1.1136 (3)	0.08123 (11)	0.0603 (7)
H18A	0.1549	1.1208	0.0663	0.091*
H18B	0.0472	1.2299	0.0789	0.091*
H18C	0.0301	1.0305	0.0561	0.091*
C19	0.2545 (2)	0.6459 (3)	0.24182 (12)	0.0673 (7)
H19A	0.1958	0.5533	0.2373	0.101*
H19B	0.2988	0.6488	0.2840	0.101*
H19C	0.3069	0.6218	0.2147	0.101*
H1A	0.1415 (17)	0.532 (3)	0.0064 (10)	0.044 (6)*
H2A	0.276 (2)	0.808 (3)	0.1082 (11)	0.059 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0365 (3)	0.0504 (3)	0.0432 (3)	−0.0081 (2)	0.0179 (2)	−0.0152 (3)
O1	0.0579 (9)	0.0465 (9)	0.0660 (11)	−0.0007 (8)	0.0303 (8)	−0.0193 (8)
O2	0.0493 (9)	0.0779 (11)	0.0405 (9)	0.0143 (8)	0.0200 (7)	−0.0142 (8)
O3	0.0538 (9)	0.0779 (12)	0.0525 (10)	−0.0131 (9)	0.0326 (8)	−0.0089 (9)
O4	0.0476 (8)	0.0499 (9)	0.0437 (9)	−0.0135 (7)	0.0204 (7)	−0.0149 (7)
N1	0.0340 (9)	0.0382 (10)	0.0346 (10)	−0.0049 (8)	0.0129 (7)	−0.0118 (8)
N2	0.0349 (9)	0.0478 (11)	0.0364 (10)	−0.0072 (8)	0.0156 (8)	−0.0134 (8)
C1	0.0293 (10)	0.0405 (12)	0.0269 (11)	0.0048 (8)	0.0072 (8)	−0.0018 (9)
C2	0.0306 (10)	0.0443 (12)	0.0341 (11)	0.0040 (9)	0.0115 (8)	−0.0031 (10)
C3	0.0372 (11)	0.0409 (12)	0.0365 (12)	0.0062 (9)	0.0086 (9)	−0.0058 (10)
C4	0.0335 (10)	0.0570 (14)	0.0312 (11)	0.0095 (10)	0.0114 (9)	−0.0070 (10)
C5	0.0327 (10)	0.0575 (14)	0.0316 (11)	−0.0001 (10)	0.0123 (9)	−0.0020 (10)
C6	0.0350 (10)	0.0447 (12)	0.0350 (11)	−0.0025 (9)	0.0097 (9)	−0.0041 (9)
C7	0.0659 (15)	0.0414 (13)	0.0700 (18)	−0.0004 (12)	0.0263 (13)	−0.0077 (12)
C8	0.0703 (16)	0.0791 (18)	0.0397 (14)	0.0027 (14)	0.0193 (12)	−0.0174 (13)
C9	0.0659 (16)	0.089 (2)	0.0544 (16)	−0.0345 (15)	0.0253 (13)	−0.0064 (14)
C10	0.0328 (10)	0.0358 (11)	0.0314 (11)	0.0028 (9)	0.0099 (8)	−0.0013 (9)
C11	0.0339 (10)	0.0299 (10)	0.0285 (10)	0.0018 (8)	0.0098 (8)	−0.0022 (8)
C12	0.0351 (10)	0.0383 (11)	0.0318 (11)	−0.0097 (9)	0.0142 (8)	−0.0116 (9)
C13	0.0408 (11)	0.0498 (13)	0.0373 (12)	−0.0130 (10)	0.0124 (9)	−0.0060 (10)
C14	0.0598 (14)	0.0751 (18)	0.0319 (13)	−0.0232 (13)	0.0187 (11)	−0.0107 (12)
C15	0.0637 (15)	0.0671 (17)	0.0542 (16)	−0.0156 (13)	0.0310 (13)	−0.0322 (14)
C16	0.0551 (14)	0.0472 (14)	0.0612 (17)	−0.0009 (11)	0.0191 (12)	−0.0190 (12)
C17	0.0438 (12)	0.0415 (12)	0.0413 (13)	−0.0065 (10)	0.0124 (10)	−0.0089 (10)
C18	0.0764 (17)	0.0549 (15)	0.0488 (15)	0.0037 (13)	0.0118 (12)	0.0039 (12)
C19	0.0725 (17)	0.0720 (18)	0.0560 (17)	0.0029 (14)	0.0109 (13)	0.0136 (14)

Geometric parameters (Å, °)

S1—C11	1.6743 (19)	C7—H7C	0.9600
O1—C3	1.371 (2)	C8—H8A	0.9600
O1—C7	1.422 (3)	C8—H8B	0.9600
O2—C4	1.378 (2)	C8—H8C	0.9600
O2—C8	1.418 (3)	C9—H9A	0.9600
O3—C5	1.373 (2)	C9—H9B	0.9600
O3—C9	1.427 (3)	C9—H9C	0.9600
O4—C10	1.223 (2)	C12—C13	1.387 (3)
N1—C10	1.389 (2)	C12—C17	1.399 (3)
N1—C11	1.393 (2)	C13—C14	1.399 (3)
N1—H1A	0.87 (2)	C13—C19	1.506 (3)
N2—C11	1.329 (2)	C14—C15	1.375 (3)
N2—C12	1.439 (2)	C14—H14	0.9300
N2—H2A	0.86 (2)	C15—C16	1.367 (3)
C1—C2	1.393 (3)	C15—H15	0.9300
C1—C6	1.395 (3)	C16—C17	1.392 (3)
C1—C10	1.491 (3)	C16—H16	0.9300
C2—C3	1.390 (3)	C17—C18	1.507 (3)
C2—H2	0.9300	C18—H18A	0.9600
C3—C4	1.396 (3)	C18—H18B	0.9600
C4—C5	1.391 (3)	C18—H18C	0.9600
C5—C6	1.383 (3)	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—H7A	0.9600	C19—H19C	0.9600
C7—H7B	0.9600		
C3—O1—C7	117.64 (16)	H9A—C9—H9B	109.5
C4—O2—C8	114.56 (16)	O3—C9—H9C	109.5
C5—O3—C9	117.16 (17)	H9A—C9—H9C	109.5
C10—N1—C11	126.75 (16)	H9B—C9—H9C	109.5
C10—N1—H1A	118.5 (14)	O4—C10—N1	121.42 (17)
C11—N1—H1A	113.5 (14)	O4—C10—C1	120.87 (17)
C11—N2—C12	123.81 (16)	N1—C10—C1	117.71 (17)
C11—N2—H2A	113.6 (16)	N2—C11—N1	116.51 (16)
C12—N2—H2A	122.1 (16)	N2—C11—S1	123.22 (14)
C2—C1—C6	120.57 (17)	N1—C11—S1	120.27 (14)
C2—C1—C10	123.61 (17)	C13—C12—C17	122.69 (18)
C6—C1—C10	115.60 (17)	C13—C12—N2	119.59 (18)
C3—C2—C1	119.29 (18)	C17—C12—N2	117.65 (18)
C3—C2—H2	120.4	C12—C13—C14	117.1 (2)
C1—C2—H2	120.4	C12—C13—C19	121.4 (2)
O1—C3—C2	124.40 (18)	C14—C13—C19	121.5 (2)
O1—C3—C4	115.31 (17)	C15—C14—C13	121.2 (2)
C2—C3—C4	120.28 (19)	C15—C14—H14	119.4
O2—C4—C5	119.88 (18)	C13—C14—H14	119.4
O2—C4—C3	120.15 (19)	C16—C15—C14	120.4 (2)
C5—C4—C3	119.90 (18)	C16—C15—H15	119.8

O3—C5—C6	123.9 (2)	C14—C15—H15	119.8
O3—C5—C4	115.96 (18)	C15—C16—C17	121.1 (2)
C6—C5—C4	120.18 (19)	C15—C16—H16	119.4
C5—C6—C1	119.77 (19)	C17—C16—H16	119.4
C5—C6—H6	120.1	C16—C17—C12	117.5 (2)
C1—C6—H6	120.1	C16—C17—C18	121.0 (2)
O1—C7—H7A	109.5	C12—C17—C18	121.50 (19)
O1—C7—H7B	109.5	C17—C18—H18A	109.5
H7A—C7—H7B	109.5	C17—C18—H18B	109.5
O1—C7—H7C	109.5	H18A—C18—H18B	109.5
H7A—C7—H7C	109.5	C17—C18—H18C	109.5
H7B—C7—H7C	109.5	H18A—C18—H18C	109.5
O2—C8—H8A	109.5	H18B—C18—H18C	109.5
O2—C8—H8B	109.5	C13—C19—H19A	109.5
H8A—C8—H8B	109.5	C13—C19—H19B	109.5
O2—C8—H8C	109.5	H19A—C19—H19B	109.5
H8A—C8—H8C	109.5	C13—C19—H19C	109.5
H8B—C8—H8C	109.5	H19A—C19—H19C	109.5
O3—C9—H9A	109.5	H19B—C19—H19C	109.5
O3—C9—H9B	109.5		
C6—C1—C2—C3	0.2 (3)	C2—C1—C10—O4	160.75 (18)
C10—C1—C2—C3	−174.25 (17)	C6—C1—C10—O4	−14.0 (3)
C7—O1—C3—C2	10.9 (3)	C2—C1—C10—N1	−18.8 (3)
C7—O1—C3—C4	−170.38 (18)	C6—C1—C10—N1	166.44 (16)
C1—C2—C3—O1	179.09 (17)	C12—N2—C11—N1	172.86 (18)
C1—C2—C3—C4	0.4 (3)	C12—N2—C11—S1	−7.9 (3)
C8—O2—C4—C5	−95.9 (2)	C10—N1—C11—N2	−12.0 (3)
C8—O2—C4—C3	87.0 (2)	C10—N1—C11—S1	168.76 (15)
O1—C3—C4—O2	−2.7 (3)	C11—N2—C12—C13	97.8 (2)
C2—C3—C4—O2	176.11 (17)	C11—N2—C12—C17	−85.1 (2)
O1—C3—C4—C5	−179.73 (17)	C17—C12—C13—C14	0.2 (3)
C2—C3—C4—C5	−0.9 (3)	N2—C12—C13—C14	177.09 (17)
C9—O3—C5—C6	−2.1 (3)	C17—C12—C13—C19	178.00 (19)
C9—O3—C5—C4	178.74 (19)	N2—C12—C13—C19	−5.1 (3)
O2—C4—C5—O3	3.0 (3)	C12—C13—C14—C15	0.2 (3)
C3—C4—C5—O3	−179.99 (18)	C19—C13—C14—C15	−177.6 (2)
O2—C4—C5—C6	−176.23 (18)	C13—C14—C15—C16	−0.5 (3)
C3—C4—C5—C6	0.8 (3)	C14—C15—C16—C17	0.4 (3)
O3—C5—C6—C1	−179.31 (17)	C15—C16—C17—C12	0.0 (3)
C4—C5—C6—C1	−0.2 (3)	C15—C16—C17—C18	178.6 (2)
C2—C1—C6—C5	−0.3 (3)	C13—C12—C17—C16	−0.3 (3)
C10—C1—C6—C5	174.57 (17)	N2—C12—C17—C16	−177.29 (18)
C11—N1—C10—O4	−4.5 (3)	C13—C12—C17—C18	−178.8 (2)
C11—N1—C10—C1	175.02 (17)	N2—C12—C17—C18	4.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···S1^{i}	0.87 (2)	2.59 (2)	3.4434 (18)	165.3 (18)

N2—H2A···O4	0.86 (2)	1.92 (2)	2.622 (2)	138 (2)

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

Fig. 1

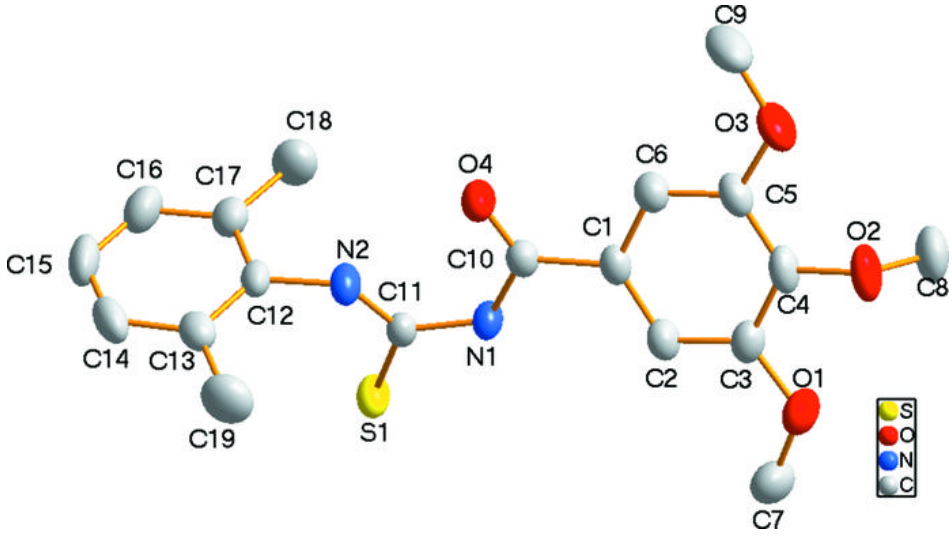

Fig. 2