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1-Anilino-2-hexylsulfanyl-4,4-dimethyl-1*H*-imidazol-5(4*H*)-one

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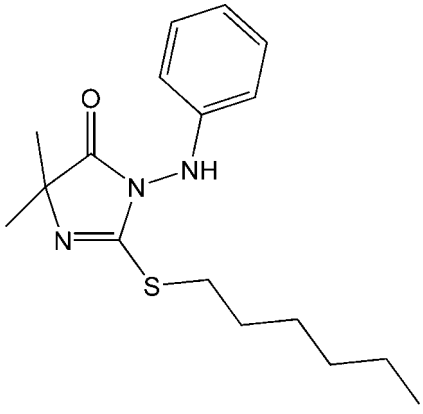
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.053; wR factor = 0.157; data-to-parameter ratio = 18.2.

In the title compound, $C_{17}H_{25}N_3OS$, the mean plane of the imidazolinone system makes a dihedral angle of 83.07 (1)° with the phenyl ring. The crystal packing is stabilized by intermolecular N—H···N and C—H···O hydrogen-bonding interactions. The hexyl group is disordered over two sites with approximate occupancy factors 0.7:0.3.

Related literature

Imidazolinones have been prepared and their biological activities, especially their fungicidal activities, have been studied by Khodair *et al.* (1998) and Bruhn *et al.* (1998). For related literature, see: Yuan *et al.*, 2006.



Experimental

Crystal data

$C_{17}H_{25}N_3OS$
M_r = 319.46
Monoclinic, $P2_1/n$
a = 6.2528 (5) Å
b = 14.8770 (11) Å
c = 19.1740 (15) Å
β = 93.806 (1)°
V = 1779.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 292 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.982
10984 measured reflections
4037 independent reflections
3099 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.157
S = 1.06
4037 reflections
222 parameters
16 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13B···O1^{i}	0.97	2.57	3.430 (2)	148
N1—H1···N3^{ii}	0.86	2.60	3.189 (2)	126
C11—H11A···O1^{iii}	0.96	2.34	3.299 (3)	173

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

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: AT2411).

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supplementary materials

Acta Cryst. (2007). E**63**, o4219 [**doi:10.1107/S1600536807047228**]

1-Anilino-2-hexylsulfanyl-4,4-dimethyl-1*H*-imidazol-5(4*H*)-one

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Comment

Imidazolinones are important heterocycles exhibiting remarkable biological activities, especially fungicidal activities (Khodair *et al.*, 1998). Since a novel mitochondrial respiratory inhibitor (Fenamidone) was found to show high fungicidal activities, many other 2-alkylthio imidazolinones have been synthesized to evaluate their fungicidal activities (Bruhn *et al.*, 1998). We obtained the title compound, (I), which may be used as a new precursor for obtaining bioactive molecules. The crystal structure of (I) is presented here.

Atom S1, N1 and the five-membered imidazolone ring are essentially planar. The C16 and C17 atoms, and the hydrogen atoms attached to C15, C16 and C17 are disordered over two sites, with refined occupancies of 0.309 (7) and 0.691 (7) (Fig. 1). The bond lengths involving atom C9 indicate a degree of electron delocalization (Yuan *et al.*, 2006). As can be seen from the packing diagram (Fig. 2), intermolecular N—H···N and C—H···O hydrogen bondings (Table 1) link the molecules.

Experimental

A mixture of 5,5-dimethyl-3-phenylamino-2-thioxo-4-imidazolidione (0.71 g, 3 mmol), hexyl bromide (0.50 g, 3 mmol) and solid potassium carbonate (0.83 g, 6 mmol) in CH_3CN (15 ml) was stirred for 5 h at 323 K and was filtered. The filtrate was condensed, and the residue was recrystallized from diethyl ether and petroleum ether (1:3) to give the title compound (I) in yield of 83% (m.p. 355 K). Suitable crystals were obtained by slow evaporation of a solution of (I) in dichloromethane and petroleum ether at room temperature.

Refinement

All H atoms were located in difference maps and treated as riding atoms, except those at N1, with the following distance restraints: 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, N—H = 0.86 Å, U_{iso} = 1.2U_{eq}(N) for NH_2, C—H = 0.96 Å, U_{iso} = 1.5U_{eq}(C) for CH_3.

Figures

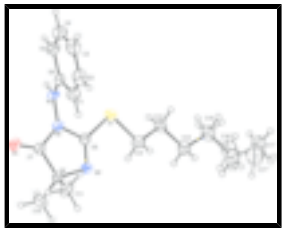


Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme. Only the major disorder component is shown.

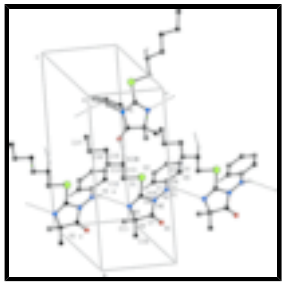


Fig. 2. The packing in the crystal structure, showing the N—H···N and C—H···O hydrogen bonds as dashed lines.

1-Anilino-2-hexylsulfanyl-4,4-dimethyl-1*H*-imidazol-5(4*H*)-one

Crystal data

$C_{17}H_{25}N_3OS$	F_{000} = 688
M_r = 319.46	D_x = 1.192 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3820 reflections
a = 6.2528 (5) Å	θ = 2.5–27.4º
b = 14.8770 (11) Å	μ = 0.19 mm^{-1}
c = 19.1740 (15) Å	T = 292 (2) K
β = 93.8060 (10)º	Block, colourless
V = 1779.7 (2) Å^3	0.20 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4037 independent reflections
Radiation source: fine-focus sealed tube	3099 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 292(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→5
T_{min} = 0.964, T_{max} = 0.982	k = −19→17
10984 measured reflections	l = −21→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.157	$w = 1/[\sigma^2(F_o^2) + (0.0936P)^2 + 0.0291P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$

4037 reflections	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
222 parameters	$\Delta\rho_{min}$ = −0.44 e Å^{-3}
16 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
N1	1.0843 (2)	0.63981 (9)	0.23056 (7)	0.0404 (3)	
H1	1.1701	0.6276	0.1986	0.049*	
N2	0.8961 (2)	0.68754 (9)	0.21568 (8)	0.0401 (3)	
N3	0.5428 (2)	0.70044 (9)	0.18400 (8)	0.0444 (4)	
O1	0.9892 (2)	0.82995 (9)	0.25323 (9)	0.0652 (4)	
S1	0.72154 (8)	0.53663 (3)	0.16269 (3)	0.04854 (19)	
C1	0.9848 (3)	0.62221 (14)	0.35171 (11)	0.0550 (5)	
H1A	0.8532	0.6499	0.3412	0.066*	
C2	1.0374 (4)	0.59096 (16)	0.41849 (12)	0.0708 (7)	
H2	0.9403	0.5982	0.4528	0.085*	
C3	1.2297 (4)	0.54941 (17)	0.43532 (12)	0.0732 (7)	
H3	1.2634	0.5287	0.4805	0.088*	
C4	1.3712 (4)	0.53891 (16)	0.38448 (13)	0.0697 (7)	
H4	1.5020	0.5107	0.3953	0.084*	
C5	1.3226 (3)	0.56953 (14)	0.31739 (11)	0.0543 (5)	
H5	1.4202	0.5615	0.2834	0.065*	
C6	1.1288 (3)	0.61219 (11)	0.30042 (9)	0.0408 (4)	
C7	0.8579 (3)	0.77681 (11)	0.23033 (10)	0.0449 (4)	
C8	0.6195 (3)	0.78913 (11)	0.21235 (11)	0.0498 (5)	
C9	0.7054 (3)	0.64835 (11)	0.18752 (8)	0.0374 (4)	
C10	0.5790 (4)	0.86296 (15)	0.15830 (15)	0.0820 (8)	
H10A	0.6386	0.8457	0.1154	0.123*	
H10B	0.6453	0.9177	0.1752	0.123*	
H10C	0.4274	0.8722	0.1501	0.123*	
C11	0.5136 (3)	0.80949 (17)	0.28010 (15)	0.0739 (7)	
H11A	0.3634	0.8203	0.2699	0.111*	
H11B	0.5787	0.8618	0.3018	0.111*	

H11C	0.5320	0.7591	0.3112	0.111*	
C12	0.4533 (3)	0.51978 (13)	0.12390 (11)	0.0532 (5)	
H12A	0.3519	0.5205	0.1600	0.064*	
H12B	0.4164	0.5681	0.0913	0.064*	
C13	0.4406 (3)	0.43057 (12)	0.08595 (10)	0.0483 (5)	
H13A	0.5435	0.4302	0.0503	0.058*	
H13B	0.4789	0.3827	0.1188	0.058*	
C14	0.2194 (3)	0.41275 (14)	0.05226 (11)	0.0574 (5)	
H14A	0.1164	0.4183	0.0877	0.069*	
H14B	0.1864	0.4589	0.0175	0.069*	
C15	0.1907 (4)	0.32247 (14)	0.01789 (13)	0.0706 (7)	
H15A	0.2309	0.2754	0.0512	0.085*	0.691 (7)
H15B	0.2826	0.3179	−0.0208	0.085*	0.691 (7)
H15C	0.1875	0.2791	0.0556	0.085*	0.309 (7)
H15D	0.3216	0.3110	−0.0050	0.085*	0.309 (7)
C16	−0.0461 (7)	0.3103 (3)	−0.0092 (3)	0.0754 (15)	0.691 (7)
H16A	−0.1365	0.3178	0.0296	0.091*	0.691 (7)
H16B	−0.0834	0.3571	−0.0431	0.091*	0.691 (7)
C17	−0.0929 (7)	0.2202 (3)	−0.0426 (3)	0.0909 (17)	0.691 (7)
H17A	0.0061	0.2093	−0.0779	0.136*	0.691 (7)
H17B	−0.2366	0.2198	−0.0636	0.136*	0.691 (7)
H17C	−0.0778	0.1740	−0.0077	0.136*	0.691 (7)
C16'	0.0146 (17)	0.2957 (9)	−0.0348 (5)	0.081 (4)	0.309 (7)
H16C	−0.0410	0.3465	−0.0620	0.097*	0.309 (7)
H16D	0.0589	0.2487	−0.0658	0.097*	0.309 (7)
C17'	−0.141 (2)	0.2625 (10)	0.0151 (7)	0.120 (5)	0.309 (7)
H17D	−0.0639	0.2387	0.0561	0.179*	0.309 (7)
H17E	−0.2283	0.2161	−0.0068	0.179*	0.309 (7)
H17F	−0.2304	0.3112	0.0283	0.179*	0.309 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0312 (7)	0.0454 (8)	0.0447 (8)	0.0094 (6)	0.0031 (6)	−0.0019 (6)
N2	0.0296 (7)	0.0379 (7)	0.0524 (9)	0.0038 (6)	−0.0010 (6)	−0.0040 (6)
N3	0.0350 (8)	0.0358 (7)	0.0613 (9)	0.0019 (6)	−0.0054 (7)	−0.0079 (6)
O1	0.0362 (8)	0.0492 (8)	0.1091 (12)	−0.0066 (6)	−0.0028 (7)	−0.0211 (8)
S1	0.0460 (3)	0.0359 (3)	0.0621 (3)	0.00756 (19)	−0.0089 (2)	−0.00951 (19)
C1	0.0502 (12)	0.0572 (12)	0.0587 (12)	0.0017 (9)	0.0111 (9)	−0.0004 (9)
C2	0.0889 (19)	0.0719 (15)	0.0536 (13)	−0.0121 (13)	0.0192 (12)	0.0029 (11)
C3	0.0871 (19)	0.0748 (15)	0.0557 (13)	−0.0169 (13)	−0.0106 (13)	0.0155 (11)
C4	0.0591 (14)	0.0749 (15)	0.0725 (15)	−0.0030 (11)	−0.0150 (11)	0.0225 (11)
C5	0.0407 (11)	0.0651 (12)	0.0566 (11)	0.0042 (9)	−0.0002 (9)	0.0090 (9)
C6	0.0364 (9)	0.0386 (9)	0.0470 (10)	−0.0065 (7)	−0.0007 (7)	−0.0020 (7)
C7	0.0344 (9)	0.0395 (9)	0.0608 (11)	−0.0001 (7)	0.0028 (8)	−0.0047 (8)
C8	0.0337 (9)	0.0358 (9)	0.0786 (13)	0.0024 (7)	−0.0053 (9)	−0.0123 (8)
C9	0.0362 (9)	0.0354 (8)	0.0401 (9)	0.0006 (7)	−0.0005 (7)	−0.0026 (7)
C10	0.0710 (16)	0.0419 (11)	0.129 (2)	0.0058 (11)	−0.0260 (15)	0.0086 (12)

C11	0.0382 (11)	0.0704 (14)	0.1143 (19)	−0.0057 (10)	0.0140 (11)	−0.0458 (13)
C12	0.0461 (11)	0.0480 (10)	0.0640 (12)	0.0049 (8)	−0.0088 (9)	−0.0175 (9)
C13	0.0530 (12)	0.0397 (9)	0.0513 (11)	0.0012 (8)	−0.0042 (8)	−0.0066 (8)
C14	0.0524 (12)	0.0529 (11)	0.0658 (13)	−0.0040 (9)	−0.0058 (10)	−0.0104 (9)
C15	0.0780 (17)	0.0515 (12)	0.0792 (16)	−0.0100 (11)	−0.0187 (12)	−0.0076 (10)
C16	0.066 (3)	0.068 (3)	0.090 (4)	−0.005 (2)	−0.009 (2)	−0.028 (3)
C17	0.085 (3)	0.078 (3)	0.106 (3)	−0.025 (2)	−0.023 (2)	−0.018 (2)
C16'	0.103 (7)	0.081 (6)	0.059 (5)	−0.016 (5)	0.006 (5)	−0.018 (4)
C17'	0.116 (9)	0.102 (9)	0.144 (10)	−0.019 (7)	0.035 (8)	−0.007 (8)

Geometric parameters (Å, °)

N1—N2	1.3878 (18)	C11—H11C	0.9600
N1—C6	1.411 (2)	C12—C13	1.513 (2)
N1—H1	0.8600	C12—H12A	0.9700
N2—C7	1.382 (2)	C12—H12B	0.9700
N2—C9	1.403 (2)	C13—C14	1.510 (3)
N3—C9	1.276 (2)	C13—H13A	0.9700
N3—C8	1.494 (2)	C13—H13B	0.9700
O1—C7	1.202 (2)	C14—C15	1.502 (3)
S1—C9	1.7337 (16)	C14—H14A	0.9700
S1—C12	1.8063 (19)	C14—H14B	0.9700
C1—C2	1.381 (3)	C15—C16'	1.497 (7)
C1—C6	1.385 (2)	C15—C16	1.547 (4)
C1—H1A	0.9300	C15—H15A	0.9700
C2—C3	1.372 (3)	C15—H15B	0.9700
C2—H2	0.9300	C15—H15C	0.9700
C3—C4	1.368 (4)	C15—H15D	0.9700
C3—H3	0.9300	C16—C17	1.506 (5)
C4—C5	1.379 (3)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C5—C6	1.388 (3)	C17—H17A	0.9600
C5—H5	0.9300	C17—H17B	0.9600
C7—C8	1.519 (2)	C17—H17C	0.9600
C8—C10	1.520 (3)	C16'—C17'	1.493 (8)
C8—C11	1.527 (3)	C16'—H16C	0.9700
C10—H10A	0.9600	C16'—H16D	0.9700
C10—H10B	0.9600	C17'—H17D	0.9600
C10—H10C	0.9600	C17'—H17E	0.9600
C11—H11A	0.9600	C17'—H17F	0.9600
C11—H11B	0.9600		
N2—N1—C6	117.06 (13)	S1—C12—H12B	109.7
N2—N1—H1	121.5	H12A—C12—H12B	108.2
C6—N1—H1	121.5	C14—C13—C12	112.16 (15)
C7—N2—N1	127.29 (14)	C14—C13—H13A	109.2
C7—N2—C9	108.89 (14)	C12—C13—H13A	109.2
N1—N2—C9	123.64 (13)	C14—C13—H13B	109.2
C9—N3—C8	106.38 (14)	C12—C13—H13B	109.2
C9—S1—C12	100.18 (8)	H13A—C13—H13B	107.9

C2—C1—C6	119.7 (2)	C15—C14—C13	115.09 (18)
C2—C1—H1A	120.1	C15—C14—H14A	108.5
C6—C1—H1A	120.1	C13—C14—H14A	108.5
C3—C2—C1	121.4 (2)	C15—C14—H14B	108.5
C3—C2—H2	119.3	C13—C14—H14B	108.5
C1—C2—H2	119.3	H14A—C14—H14B	107.5
C4—C3—C2	118.8 (2)	C16'—C15—C14	126.5 (6)
C4—C3—H3	120.6	C16'—C15—C16	25.6 (4)
C2—C3—H3	120.6	C14—C15—C16	109.6 (2)
C3—C4—C5	120.9 (2)	C16'—C15—H15A	113.6
C3—C4—H4	119.5	C14—C15—H15A	109.7
C5—C4—H4	119.5	C16—C15—H15A	109.7
C4—C5—C6	120.3 (2)	C16'—C15—H15B	85.0
C4—C5—H5	119.8	C14—C15—H15B	109.7
C6—C5—H5	119.8	C16—C15—H15B	109.7
C1—C6—C5	118.79 (18)	H15A—C15—H15B	108.2
C1—C6—N1	123.13 (17)	C16'—C15—H15C	106.0
C5—C6—N1	118.02 (16)	C14—C15—H15C	106.0
O1—C7—N2	125.69 (16)	C16—C15—H15C	96.1
O1—C7—C8	129.81 (16)	H15A—C15—H15C	17.5
N2—C7—C8	104.49 (14)	H15B—C15—H15C	124.4
N3—C8—C7	105.20 (13)	C16'—C15—H15D	104.6
N3—C8—C10	110.81 (17)	C14—C15—H15D	106.0
C7—C8—C10	111.01 (17)	C16—C15—H15D	130.2
N3—C8—C11	109.76 (16)	H15A—C15—H15D	88.9
C7—C8—C11	107.78 (17)	H15B—C15—H15D	23.2
C10—C8—C11	112.01 (19)	H15C—C15—H15D	106.3
N3—C9—N2	114.94 (14)	C17—C16—C15	113.7 (3)
N3—C9—S1	128.92 (13)	C17—C16—H16A	108.8
N2—C9—S1	116.14 (12)	C15—C16—H16A	108.8
C8—C10—H10A	109.5	C17—C16—H16B	108.8
C8—C10—H10B	109.5	C15—C16—H16B	108.8
H10A—C10—H10B	109.5	H16A—C16—H16B	107.7
C8—C10—H10C	109.5	C17'—C16'—C15	97.8 (8)
H10A—C10—H10C	109.5	C17'—C16'—H16C	112.2
H10B—C10—H10C	109.5	C15—C16'—H16C	112.2
C8—C11—H11A	109.5	C17'—C16'—H16D	112.2
C8—C11—H11B	109.5	C15—C16'—H16D	112.2
H11A—C11—H11B	109.5	H16C—C16'—H16D	109.8
C8—C11—H11C	109.5	C16'—C17'—H17D	109.5
H11A—C11—H11C	109.5	C16'—C17'—H17E	109.5
H11B—C11—H11C	109.5	H17D—C17'—H17E	109.5
C13—C12—S1	109.73 (13)	C16'—C17'—H17F	109.5
C13—C12—H12A	109.7	H17D—C17'—H17F	109.5
S1—C12—H12A	109.7	H17E—C17'—H17F	109.5
C13—C12—H12B	109.7		
C6—N1—N2—C7	76.7 (2)	O1—C7—C8—C10	58.3 (3)
C6—N1—N2—C9	−97.85 (18)	N2—C7—C8—C10	−122.80 (18)
C6—C1—C2—C3	−0.4 (3)	O1—C7—C8—C11	−64.7 (3)

C1—C2—C3—C4	−0.1 (4)	N2—C7—C8—C11	114.19 (17)
C2—C3—C4—C5	0.1 (4)	C8—N3—C9—N2	0.3 (2)
C3—C4—C5—C6	0.4 (4)	C8—N3—C9—S1	−179.96 (14)
C2—C1—C6—C5	0.9 (3)	C7—N2—C9—N3	−2.3 (2)
C2—C1—C6—N1	178.00 (18)	N1—N2—C9—N3	173.08 (15)
C4—C5—C6—C1	−0.9 (3)	C7—N2—C9—S1	177.90 (12)
C4—C5—C6—N1	−178.14 (18)	N1—N2—C9—S1	−6.7 (2)
N2—N1—C6—C1	7.0 (2)	C12—S1—C9—N3	5.03 (19)
N2—N1—C6—C5	−175.88 (15)	C12—S1—C9—N2	−175.25 (13)
N1—N2—C7—O1	6.9 (3)	C9—S1—C12—C13	169.55 (14)
C9—N2—C7—O1	−177.93 (19)	S1—C12—C13—C14	−179.94 (14)
N1—N2—C7—C8	−172.10 (15)	C12—C13—C14—C15	−175.90 (19)
C9—N2—C7—C8	3.10 (19)	C13—C14—C15—C16'	−162.4 (5)
C9—N3—C8—C7	1.6 (2)	C13—C14—C15—C16	175.6 (3)
C9—N3—C8—C10	121.66 (19)	C16'—C15—C16—C17	46.1 (12)
C9—N3—C8—C11	−114.11 (18)	C14—C15—C16—C17	−178.1 (4)
O1—C7—C8—N3	178.2 (2)	C14—C15—C16'—C17'	−89.9 (9)
N2—C7—C8—N3	−2.88 (19)	C16—C15—C16'—C17'	−35.1 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13B···O1^{i}	0.97	2.57	3.430 (2)	148
N1—H1···N3^{ii}	0.86	2.60	3.189 (2)	126
C11—H11A···O1^{iii}	0.96	2.34	3.299 (3)	173

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

Fig. 1

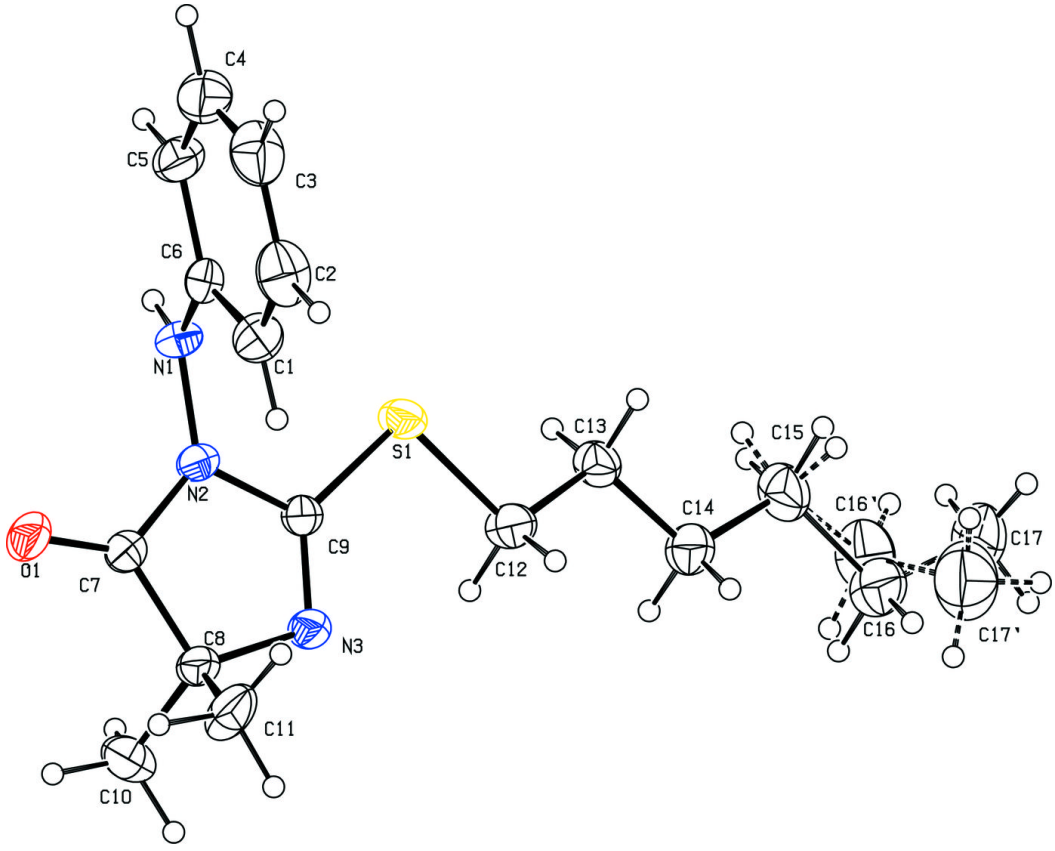
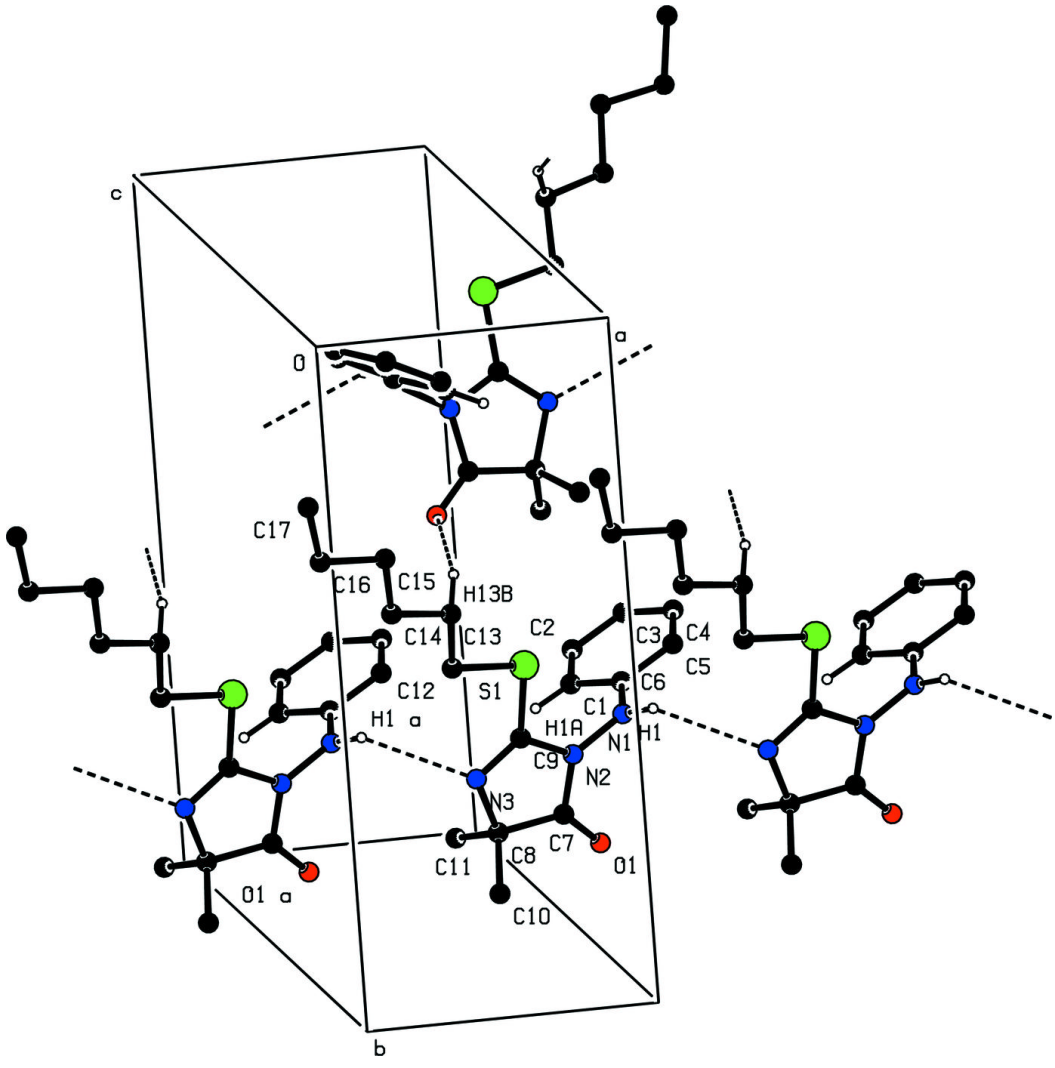

C4
C5
C3
C6
C2
N1
C1
S1
C13
C15
N2
C14
C16'
C17
C9
O1
C7
C12
C16
C17'
C8
N3
C11
C10

Fig. 2


c
a
O
C17
C16
C15
H13B
C14
C13
C2
C3
C4
C5
C6
C12
S1
C1
H1 a
H1A
N1
H1
C9
N2
N3
C7
C11
C8
O1
O1 a
C10
b