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3-(4-Methylphenyl)-5-[4-(methylthio)-phenyl]-4,5-dihydro-1*H*-pyrazole-1-carbaldehyde

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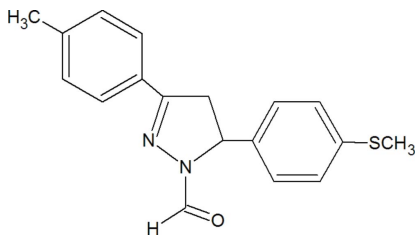
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.141; data-to-parameter ratio = 25.5.

The title molecule, $C_{18}H_{18}N_2OS$, exists as an L-shaped structure with the mean plane of the 4-methylphenyl group twisted slightly about the mean plane of the pyrazole-1-carbaldehyde group by 4.7 (2)°, which in turn makes an angle of 82.4 (7)° with the mean plane of the thiophenyl group. The S-methyl group is slightly twisted out of plane, probably due to steric repulsion between the methyl H and the phenyl H atoms. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between a thiophenyl H atom and the carbaldehyde O atom, which links the molecules into chains in an alternate inverted pattern parallel oblique to the *bc* face and along the *a* axis of the unit cell.

Related literature

For related structures, see: Trilleras *et al.* (2005); Shanmuga Sundara Raj *et al.* (1999). For related literature see: Elguero (1984); El-Emary & Bakhite (1999); Rathelot *et al.* (2002); Mithun & Holla (2006); Holla *et al.* (2000, 2006); Cottineau *et al.* (2002); Om Prakash *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{18}N_2OS$
M_r = 310.40
Triclinic, $P\overline{1}$
a = 6.3751 (17) Å
b = 6.9998 (17) Å
c = 19.791 (5) Å
α = 83.57 (2)°
β = 81.70 (2)°
γ = 64.16 (2)°
V = 785.3 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.51 × 0.22 × 0.17 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.858, T_{max} = 1.000 (expected range = 0.828–0.965)
14289 measured reflections
5145 independent reflections
2591 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.141
S = 0.98
5145 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2A—H2AA···O^{i}	0.93	2.53	3.390 (2)	154

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: BT2481).

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supplementary materials

Acta Cryst. (2007). E**63**, o4005-o4006 [**doi:10.1107/S1600536807043000**]

3-(4-Methylphenyl)-5-[4-(methylthio)phenyl]-4,5-dihydro-1*H*-pyrazole-1-carbaldehyde

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Comment

Pyrazolines have been reported to exhibit a broad spectrum of biological activities such as antibacterial, antifungal, anti-inflammatory, anti-depressent, anti viral activities (Elguero, 1984) and analgesic activities (El-Emary & Bakhite, 1999). Large numbers of pyrazoles are used as antibacterial (Rathelot *et al.* 2002), anti-inflammatory (Mithun & Holla, 2006; Holla *et al.* 2000; 2006), antiparasitic (Cottineau *et al.* 2002) and antidiabetic drugs (Om Prakash *et al.* 2006). The crystal structures of the following pyrazole aldehydes *viz*., 5-Chloro-3-methyl-1-phenyl-1*H*-pyrazole-4-carbaldehyde (Trilleras *et al.* 2005) and 1-(2,4-dinitrophenyl)-3-(2-hydroxyphenyl)-1*H*-pyrazole-4-carbaldehyde (Shanmuga Sundara Raj *et al.* 1999) have been reported. The newly synthesized pyrazolecarbaldehyde, (I), $C_{18}H_{18}N_2OS$, is found to possess good antibacterial activity and its crystal structure is reported.

The title molecule exists as an *L*-shaped structure with the mean plane of the 4-methylphenyl group twisted slightly about the mean plane of the pyrazole-1-carbaldehyde by 4.7 (2)° which in turn makes an angle of 82.4 (7)° with the mean plane of the thiophenyl group (Fig. 1). The *S*-methyl group is twisted slightly out of plane with the phenyl group [C7A–S–C4A–C3A torsion angle = 17.81 (16)°] probably due to steric repulsion between the methyl-H and the phenyl-H atoms. The methyl hydrogen atoms on C7B are disordered [H7BA, H7BB, H7BC (0.49 (4) & H7BD, H7BE, H7BF (0.51 (4)].

Crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between a thiophenyl hydrogen [H2AA] and the carbaldehyde oxygen [O] which link the molecules into chains in an alternate inverted pattern parallel and oblique to the *bc* face and along the *a* axis of the unit cell (Fig. 2).

Experimental

A mixture of (2E)-1-(4-methylphenyl)-3-[4-(methylthio)phenyl]prop-2-en-1-one (2.68 g, 0.01 mol) and a molar equivalent of hydrazine hydrate (5 ml, 80%) in formic acid (15 ml) was heated on an oil bath at 373 K for 3–5 hrs (Fig.3). The reaction mass was then poured into ice cold water and neutralized with sodium bicarbonate solution. The solid obtained was filtered, washed with water, dried, and recrystallized from methanol. (yield: 70%; m.p.: 431–433 K). Analysis found: C 69.56, H 5.79, N 8.94, S 10.25%; $C_{18}H_{18}N_2OS$ requires: C 69.65, H 5.84, N 9.02, S 10.33%.

Refinement

All H atoms were placed in their calculated places and all H atoms were refined using a riding model with C—H = 0.93 to 0.98 Å, and with U_{iso}(H) = 1.19–1.49U_{eq}(C).

Figures

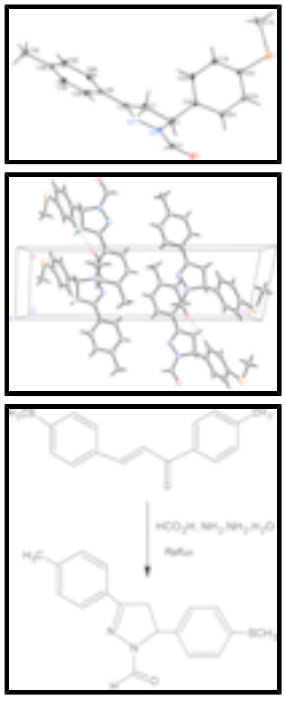

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids. Only the major component of the methyl H atoms on C7B are displayed.
Fig. 2. Packing diagram of the title compound, viewed down the *b* axis. Dashed lines indicate intermolecular C—H···O hydrogen bonds. Only the major component of the methyl H atoms on C7B are displayed.

3-(4-methylphenyl)-5-[4-(methylthio)phenyl]-4, 5-dihydro-1*H*-pyrazole-1-carbaldehyde

Crystal data

$C_{18}H_{18}N_2OS$	$Z = 2$
$M_r = 310.40$	$F_{000} = 328$
Triclinic, $P\overline{1}$	$D_x = 1.313$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.3751$ (17) Å	Cell parameters from 4927 reflections
$b = 6.9998$ (17) Å	$\theta = 5.0$–32.5°
$c = 19.791$ (5) Å	$\mu = 0.21$ mm^{-1}
$\alpha = 83.57$ (2)°	$T = 296$ K
$\beta = 81.70$ (2)°	Needle, colourless
$\gamma = 64.16$ (2)°	0.51 × 0.22 × 0.17 mm
$V = 785.3$ (4) Å^3	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	5145 independent reflections
Radiation source: fine-focus sealed tube	2591 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{max} = 32.5^\circ$

T = 296 K	θ_{min} = 5.0º
φ and ω scans	h = −9→8
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	k = −10→10
T_{min} = 0.858, T_{max} = 1.000	l = −29→28
14289 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.141	$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.98	$(\Delta/\sigma)_{max} < 0.001$
5145 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
202 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. IR(KBr, cm^{-1}): 3058 (Ar—H), 2891 (C—H OF CH_3),1651(CHO) 1592, 1495 and 1428 (C=C, C=N); ^{1}H NMR (DMSO-d6): δ 2.39 (s, 3H, CH_3), 2.44 (s, 3H, SCH_3), 3.14–3.93(dd, 2H, J = 4.8 Hz, J=4.8 Hz), 3.74–3.78(dd, 2H, J = 11.6 Hz, J = 11.6 Hz), 5.45–5.48(dd, 1H, J = 4.8 Hz), 7.24–7.22(d, 2H, J=8 Hz, 4-methylthiophenyl),7.63–7.61(d, 2H, J=8 Hz, 4-methylthiophenyl), 7.17–7.15(d, 2H, J=8.4 Hz 4-methylphenyl),7.22–7.20(d, 2H, J=8.4 Hz -methylphenyl), 8.93(S, 1H, CHO); FAB MS (m/z, %): 310 (M^+, 89), 289 (70), 225 (39), 165 (26).

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 $F^2 > 2$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)
S	0.83477 (8)	0.72163 (8)	0.04968 (3)	0.0731 (2)	
O	0.97536 (16)	1.20267 (18)	0.28726 (6)	0.0595 (3)	
N1	0.37522 (17)	1.42564 (18)	0.34594 (6)	0.0388 (3)	
N2	0.57960 (17)	1.37435 (18)	0.30170 (6)	0.0398 (3)	
C1	0.5374 (2)	1.4618 (2)	0.23080 (7)	0.0406 (3)	
H1A	0.6321	1.5403	0.2149	0.049*	

C2	0.2761 (2)	1.6180 (2)	0.24187 (8)	0.0444 (4)	
H2A	0.2561	1.7642	0.2380	0.053*	
H2B	0.1873	1.5999	0.2092	0.053*	
C3	0.2027 (2)	1.5570 (2)	0.31349 (7)	0.0350 (3)	
C4	0.7900 (2)	1.2526 (2)	0.32355 (8)	0.0462 (4)	
H4A	0.7947	1.2034	0.3692	0.055*	
C1A	0.5975 (2)	1.2842 (2)	0.18385 (7)	0.0364 (3)	
C2A	0.4479 (2)	1.1897 (2)	0.18079 (7)	0.0415 (3)	
H2AA	0.3019	1.2417	0.2064	0.050*	
C3A	0.5116 (2)	1.0197 (2)	0.14046 (8)	0.0446 (3)	
H3AA	0.4090	0.9582	0.1394	0.054*	
C4A	0.7287 (2)	0.9408 (2)	0.10156 (7)	0.0425 (3)	
C5A	0.8778 (2)	1.0362 (2)	0.10358 (8)	0.0461 (4)	
H5AA	1.0224	0.9861	0.0772	0.055*	
C6A	0.8144 (2)	1.2047 (2)	0.14428 (8)	0.0434 (3)	
H6AA	0.9172	1.2659	0.1453	0.052*	
C7A	0.5825 (3)	0.6886 (3)	0.03797 (10)	0.0661 (5)	
H7AA	0.6239	0.5827	0.0054	0.099*	
H7AB	0.4661	0.8211	0.0213	0.099*	
H7AC	0.5209	0.6442	0.0808	0.099*	
C1B	−0.0388 (2)	1.6430 (2)	0.34630 (7)	0.0350 (3)	
C2B	−0.0923 (2)	1.5813 (2)	0.41334 (7)	0.0460 (4)	
H2BA	0.0269	1.4804	0.4374	0.055*	
C3B	−0.3186 (2)	1.6667 (3)	0.44475 (8)	0.0492 (4)	
H3BA	−0.3492	1.6236	0.4898	0.059*	
C4B	−0.5018 (2)	1.8162 (2)	0.41031 (8)	0.0435 (3)	
C5B	−0.4506 (2)	1.8747 (2)	0.34345 (8)	0.0455 (4)	
H5BA	−0.5711	1.9731	0.3192	0.055*	
C6B	−0.2231 (2)	1.7901 (2)	0.31140 (7)	0.0414 (3)	
H6BA	−0.1934	1.8321	0.2661	0.050*	
C7B	−0.7478 (2)	1.9114 (3)	0.44524 (10)	0.0628 (5)	
H7BA	−0.8105	2.0637	0.4402	0.094*	0.49 (4)
H7BB	−0.7466	1.8675	0.4930	0.094*	0.49 (4)
H7BC	−0.8435	1.8640	0.4249	0.094*	0.49 (4)
H7BD	−0.7995	1.8013	0.4583	0.094*	0.51 (4)
H7BE	−0.8498	2.0146	0.4145	0.094*	0.51 (4)
H7BF	−0.7512	1.9791	0.4852	0.094*	0.51 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0565 (3)	0.0700 (3)	0.0936 (4)	−0.0259 (2)	0.0137 (2)	−0.0406 (3)
O	0.0292 (5)	0.0737 (8)	0.0696 (8)	−0.0156 (5)	0.0024 (5)	−0.0179 (6)
N1	0.0286 (5)	0.0460 (7)	0.0386 (6)	−0.0128 (5)	0.0013 (4)	−0.0091 (5)
N2	0.0276 (5)	0.0483 (7)	0.0388 (7)	−0.0118 (5)	0.0014 (4)	−0.0093 (5)
C1	0.0330 (7)	0.0414 (8)	0.0446 (8)	−0.0159 (5)	0.0056 (6)	−0.0041 (6)
C2	0.0381 (7)	0.0382 (7)	0.0437 (9)	−0.0069 (6)	0.0048 (6)	−0.0026 (6)
C3	0.0307 (6)	0.0361 (7)	0.0362 (7)	−0.0124 (5)	0.0000 (5)	−0.0068 (5)

C4	0.0324 (7)	0.0550 (9)	0.0502 (9)	−0.0150 (6)	−0.0063 (6)	−0.0115 (7)
C1A	0.0297 (6)	0.0405 (7)	0.0334 (7)	−0.0121 (5)	0.0018 (5)	0.0012 (5)
C2A	0.0325 (6)	0.0533 (9)	0.0362 (8)	−0.0185 (6)	0.0040 (5)	−0.0011 (6)
C3A	0.0385 (7)	0.0569 (9)	0.0429 (8)	−0.0259 (6)	−0.0003 (6)	−0.0013 (7)
C4A	0.0373 (7)	0.0432 (8)	0.0428 (8)	−0.0139 (6)	−0.0017 (6)	−0.0030 (6)
C5A	0.0301 (6)	0.0533 (9)	0.0490 (9)	−0.0144 (6)	0.0084 (6)	−0.0107 (7)
C6A	0.0312 (6)	0.0516 (8)	0.0463 (8)	−0.0190 (6)	0.0060 (6)	−0.0061 (6)
C7A	0.0727 (12)	0.0660 (11)	0.0649 (12)	−0.0320 (9)	−0.0084 (9)	−0.0127 (9)
C1B	0.0290 (6)	0.0352 (7)	0.0391 (8)	−0.0112 (5)	−0.0014 (5)	−0.0089 (5)
C2B	0.0304 (6)	0.0595 (9)	0.0397 (8)	−0.0114 (6)	−0.0051 (6)	−0.0007 (7)
C3B	0.0364 (7)	0.0679 (10)	0.0382 (8)	−0.0193 (7)	0.0017 (6)	−0.0031 (7)
C4B	0.0290 (6)	0.0465 (8)	0.0524 (9)	−0.0131 (6)	0.0017 (6)	−0.0143 (6)
C5B	0.0303 (6)	0.0402 (8)	0.0565 (10)	−0.0059 (5)	−0.0069 (6)	−0.0010 (6)
C6B	0.0360 (7)	0.0399 (7)	0.0411 (8)	−0.0102 (6)	−0.0030 (6)	−0.0008 (6)
C7B	0.0317 (7)	0.0752 (12)	0.0686 (12)	−0.0121 (7)	0.0076 (7)	−0.0155 (9)

Geometric parameters (Å, °)

S—C4A	1.7641 (16)	C5A—H5AA	0.9300
S—C7A	1.7710 (19)	C6A—H6AA	0.9300
O—C4	1.2186 (17)	C7A—H7AA	0.9600
N1—C3	1.2874 (17)	C7A—H7AB	0.9600
N1—N2	1.3879 (15)	C7A—H7AC	0.9600
N2—C4	1.3422 (17)	C1B—C2B	1.390 (2)
N2—C1	1.4795 (19)	C1B—C6B	1.3919 (18)
C1—C1A	1.516 (2)	C2B—C3B	1.3774 (19)
C1—C2	1.5424 (19)	C2B—H2BA	0.9300
C1—H1A	0.9800	C3B—C4B	1.389 (2)
C2—C3	1.5024 (19)	C3B—H3BA	0.9300
C2—H2A	0.9700	C4B—C5B	1.377 (2)
C2—H2B	0.9700	C4B—C7B	1.504 (2)
C3—C1B	1.4648 (18)	C5B—C6B	1.3881 (19)
C4—H4A	0.9300	C5B—H5BA	0.9300
C1A—C2A	1.388 (2)	C6B—H6BA	0.9300
C1A—C6A	1.3959 (18)	C7B—H7BA	0.9600
C2A—C3A	1.384 (2)	C7B—H7BB	0.9600
C2A—H2AA	0.9300	C7B—H7BC	0.9600
C3A—C4A	1.391 (2)	C7B—H7BD	0.9600
C3A—H3AA	0.9300	C7B—H7BE	0.9600
C4A—C5A	1.386 (2)	C7B—H7BF	0.9600
C5A—C6A	1.380 (2)		
C4A—S—C7A	104.73 (8)	C4A—C5A—H5AA	119.6
C3—N1—N2	108.01 (11)	C5A—C6A—C1A	120.74 (14)
C4—N2—N1	120.99 (12)	C5A—C6A—H6AA	119.6
C4—N2—C1	125.62 (11)	C1A—C6A—H6AA	119.6
N1—N2—C1	113.37 (10)	S—C7A—H7AA	109.5
N2—C1—C1A	110.28 (11)	S—C7A—H7AB	109.5
N2—C1—C2	100.34 (10)	H7AA—C7A—H7AB	109.5
C1A—C1—C2	116.00 (12)	S—C7A—H7AC	109.5

N2—C1—H1A	109.9	H7AA—C7A—H7AC	109.5
C1A—C1—H1A	109.9	H7AB—C7A—H7AC	109.5
C2—C1—H1A	109.9	C2B—C1B—C6B	117.62 (12)
C3—C2—C1	102.89 (11)	C2B—C1B—C3	121.29 (11)
C3—C2—H2A	111.2	C6B—C1B—C3	121.09 (12)
C1—C2—H2A	111.2	C3B—C2B—C1B	121.22 (13)
C3—C2—H2B	111.2	C3B—C2B—H2BA	119.4
C1—C2—H2B	111.2	C1B—C2B—H2BA	119.4
H2A—C2—H2B	109.1	C2B—C3B—C4B	121.14 (14)
N1—C3—C1B	121.57 (12)	C2B—C3B—H3BA	119.4
N1—C3—C2	113.67 (11)	C4B—C3B—H3BA	119.4
C1B—C3—C2	124.69 (11)	C5B—C4B—C3B	117.89 (12)
O—C4—N2	124.02 (15)	C5B—C4B—C7B	121.23 (13)
O—C4—H4A	118.0	C3B—C4B—C7B	120.88 (14)
N2—C4—H4A	118.0	C4B—C5B—C6B	121.41 (12)
C2A—C1A—C6A	118.11 (14)	C4B—C5B—H5BA	119.3
C2A—C1A—C1	122.22 (11)	C6B—C5B—H5BA	119.3
C6A—C1A—C1	119.61 (13)	C5B—C6B—C1B	120.69 (13)
C3A—C2A—C1A	121.36 (13)	C5B—C6B—H6BA	119.7
C3A—C2A—H2AA	119.3	C1B—C6B—H6BA	119.7
C1A—C2A—H2AA	119.3	C4B—C7B—H7BA	109.5
C2A—C3A—C4A	120.07 (14)	C4B—C7B—H7BB	109.5
C2A—C3A—H3AA	120.0	C4B—C7B—H7BC	109.5
C4A—C3A—H3AA	120.0	C4B—C7B—H7BD	109.5
C5A—C4A—C3A	118.92 (14)	C4B—C7B—H7BE	109.5
C5A—C4A—S	116.27 (10)	H7BD—C7B—H7BE	109.5
C3A—C4A—S	124.80 (12)	C4B—C7B—H7BF	109.5
C6A—C5A—C4A	120.79 (13)	H7BD—C7B—H7BF	109.5
C6A—C5A—H5AA	119.6	H7BE—C7B—H7BF	109.5
C3—N1—N2—C4	174.68 (13)	C2A—C3A—C4A—S	178.40 (11)
C3—N1—N2—C1	−6.72 (15)	C7A—S—C4A—C5A	−163.29 (12)
C4—N2—C1—C1A	67.84 (17)	C7A—S—C4A—C3A	17.76 (15)
N1—N2—C1—C1A	−110.69 (12)	C3A—C4A—C5A—C6A	1.0 (2)
C4—N2—C1—C2	−169.31 (14)	S—C4A—C5A—C6A	−177.99 (12)
N1—N2—C1—C2	12.16 (14)	C4A—C5A—C6A—C1A	−0.6 (2)
N2—C1—C2—C3	−12.10 (14)	C2A—C1A—C6A—C5A	−0.3 (2)
C1A—C1—C2—C3	106.65 (13)	C1—C1A—C6A—C5A	176.90 (13)
N2—N1—C3—C1B	−179.75 (12)	N1—C3—C1B—C2B	−1.9 (2)
N2—N1—C3—C2	−2.50 (16)	C2—C3—C1B—C2B	−178.86 (14)
C1—C2—C3—N1	9.91 (16)	N1—C3—C1B—C6B	177.97 (13)
C1—C2—C3—C1B	−172.94 (13)	C2—C3—C1B—C6B	1.0 (2)
N1—N2—C4—O	−179.83 (13)	C6B—C1B—C2B—C3B	−1.7 (2)
C1—N2—C4—O	1.7 (2)	C3—C1B—C2B—C3B	178.17 (15)
N2—C1—C1A—C2A	78.51 (15)	C1B—C2B—C3B—C4B	0.7 (2)
C2—C1—C1A—C2A	−34.64 (18)	C2B—C3B—C4B—C5B	0.7 (2)
N2—C1—C1A—C6A	−98.57 (14)	C2B—C3B—C4B—C7B	−179.02 (16)
C2—C1—C1A—C6A	148.29 (13)	C3B—C4B—C5B—C6B	−0.9 (2)
C6A—C1A—C2A—C3A	0.8 (2)	C7B—C4B—C5B—C6B	178.80 (16)
C1—C1A—C2A—C3A	−176.32 (12)	C4B—C5B—C6B—C1B	−0.2 (2)

C1A—C2A—C3A—C4A	−0.4 (2)	C2B—C1B—C6B—C5B	1.5 (2)
C2A—C3A—C4A—C5A	−0.5 (2)	C3—C1B—C6B—C5B	−178.40 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2A—H2AA···O^{i}	0.93	2.53	3.390 (2)	154

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

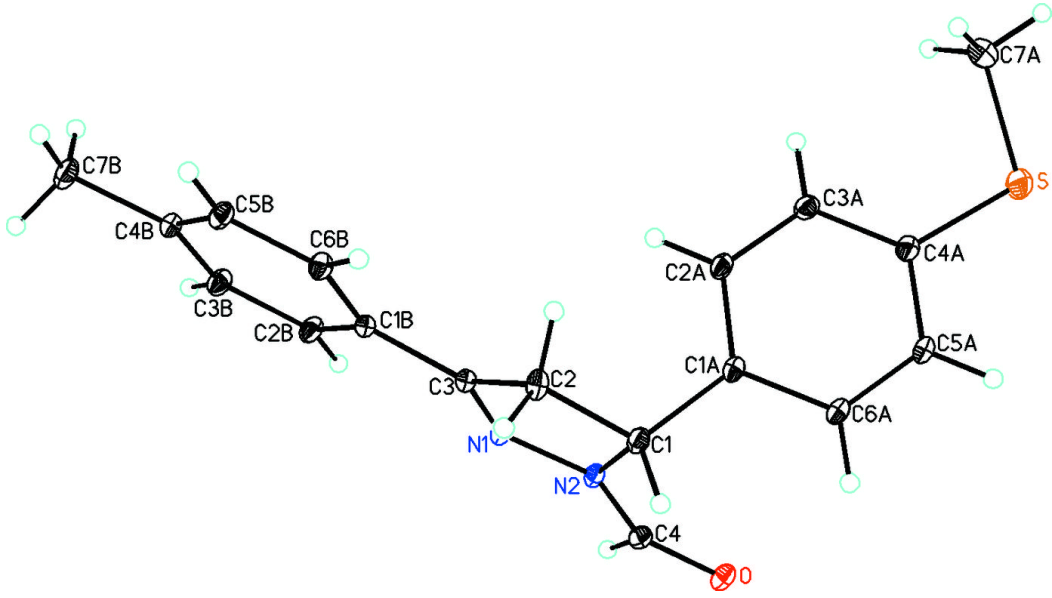
C7A
S
C3A
C4A
C2A
C5A
C1A
C6A
C7B
C5B
C4B
C6B
C3B
C2B
C1B
C3
C2
N1
C1
N2
C4
O

Fig. 2

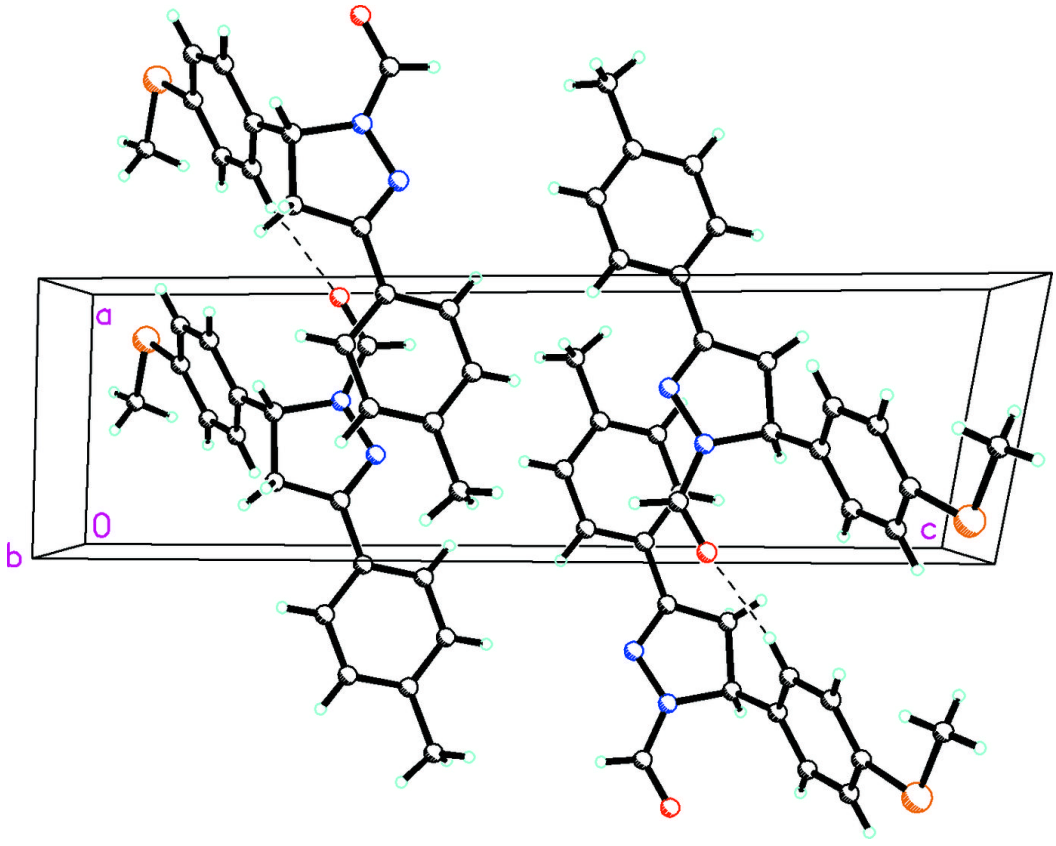

Fig. 3