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3-[4-(Methylsulfanyl)benzyl]-4-{(1*E*)-[4-(methylsulfanyl)phenyl]methyleneamino}-4,5-dihydro-1*H*-1,2,4-triazole-5-thione

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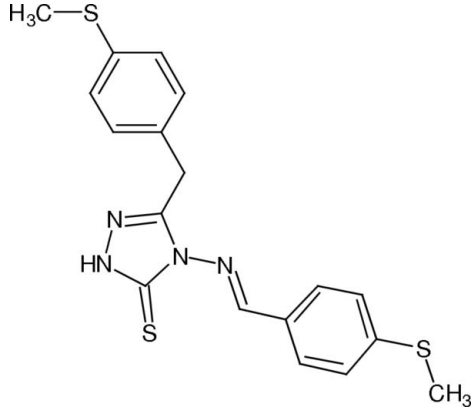
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.077; data-to-parameter ratio = 15.3.

Geometric parameters of the title compound, $C_{18}H_{18}N_4S_3$, are in the usual ranges. The triazole ring makes dihedral angles of 75.00 (5) and 38.51 (7)° with the two aromatic rings. The molecules crystallize as centrosymmetric dimers connected by N—H···S hydrogen bonds.

Related literature

For related literature, see: Agarwal *et al.* (1983); Butcher *et al.* (2007); Büyükgüngör *et al.* (2007); El-Masry, Fahmy & Abdelwahed (2000); Hodnett & Dunn (1970); Misra *et al.* (1981); Narayana *et al.* (2007); Odabaşoğlu *et al.* (2007); Pandey *et al.* (1999); Samadhiya & Halve (2001); Sarojini *et al.* (2007); Siddiqui *et al.* (2006); Singh & Dash (1988); Varma *et al.* (1986); Yathirajan *et al.* (2005); Yathirajan, Sarojini *et al.* (2007); Yathirajan, Vijesh *et al.* (2007).



Experimental

Crystal data

$C_{18}H_{18}N_4S_3$
M_r = 386.54
Triclinic, $P\overline{1}$
a = 7.3269 (7) Å
b = 9.8280 (10) Å
c = 13.6139 (12) Å
α = 91.093 (7)°
β = 98.068 (8)°
γ = 99.789 (8)°
V = 955.56 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 173 (2) K
0.28 × 0.26 × 0.21 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.897, T_{max} = 0.921
12044 measured reflections
3555 independent reflections
3191 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.077
S = 1.05
3555 reflections
233 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···S1^{i}	0.91 (2)	2.43 (2)	3.3307 (13)	169.7 (17)

Symmetry code: (i) $-x+2, -y+2, -z+1$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2474).

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supplementary materials

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3-[4-(Methylsulfanyl)benzyl]-4-{(1*E*)-[4-(methylsulfanyl)phenyl]methyleneamino}-4,5-dihydro-1*H*-1,2,4-triazole-5-thione

B. Narayana, D. Jagadeesh Prasad, B. K. Sarojini, H. S. Yathirajan and M. Bolte

Comment

Schiff bases are synthesized from a primary amine and a carbonyl compound by a nucleophilic addition reaction. They are used as substrates in the preparation of number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. They are also used as substrates in the preparation of number of biologically active compounds (Siddiqui *et al.*2006). Some Schiff base derivatives are also known to have activities such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh *et al.*, 1988; Varma *et al.*, 1986), antitumor (Hodnett *et al.*, 1970; Misra *et al.* 1981; Agarwal *et al.*, 1983) and as herbicides (Samadhiya & Halve, 2001). Condensed 1,2,4-triazoles are biologically important compounds and are used as strating materials for the synthesis of many heterocycles. The crystal structures of 4-[(1E)-benzylideneamino]-3-methyl-2,4-dihydro-1*H*-1,2,4-triazole-5-thione (Yathirajan, Sarojini *et al.*, 2007), 4-amino-3-(4'-chlorophenyl)-4-*H*-[1,2,4]-tirazolo-5-thiol (Yathirajan *et al.*, 2005), (*E*)-2-hydroxy-5-methyl-3-[(4-methyl-2 pyridyl)iminomethyl] benzaldehyde (Büyükgüngör, *et al.*, 2007); (*E*)-2-hydroxy-5-methyl-3-[(2-pyridylimino) methyl]benzaldehyde (Odabaşoğlu *et al.*, 2007); 1-(4-{[(*E*)-(4-diethylamino-2-hydroxy phenyl)methylene]amino}phenyl)ethanone (Yathirajan, Vijesh *et al.*, (2007), 2-{(*E*)-[(2-chloro-5-nitrophenyl)imino]methyl}-5-(diethylamino)phenol (Butcher *et al.*, 2007), 2-bromo-*N*'-[(*E*)-(4-fluorophenyl)methylene]-5-methoxybenzohydrazide monohydrate (Narayana *et al.*, 2007), 2-bromo-*N*'-isopropylidene-5-methoxybenzohydrazide (Sarojini *et al.*, 2007) have been reported. A new Schiff base, $C_{18}H_{18}N_4S_3$ is prepared and its crystal structure is reported.

Geometric parameters of the title compound are in the usual ranges. The triazole makes dihedral angles of 75.00 (5)Å and 38.51 (7)° with the two aromatic rings. The molecules crystallize as centrosymmetric dimers connected by N—H···S hydrogen bonds.

Experimental

A mixture of 4-amino-5-[4-(methylthio)benzyl]-2,4-dihydro-3*H*-1,2,4-triazole-3-thione (2.52 g, 0.01 mol) and 4-(methylthio)benzaldehyde (1.52 g, 0.01 mol) in 30 ml of ethanol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 5 h. On cooling, the solid separated was filtered and recrystallized from acetone (m.p.: 420–424 K). Analysis found: C 55.84, H 4.66, N 14.43, S 24.82%; $C_{18}H_{18}N_4S_3$ requires: C 55.93, H 4.69, N 14.49, S 24.89%.

Refinement

H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2 U_{eq}(C) or U_{iso}(H) = 1.5 U_{eq}(C_{methyl})] using a riding model with C—H ranging from 0.95Å to 1.0 Å. The methyl groups were allowed to rotate but not to tip. The amino H atom was freely refined.

Figures

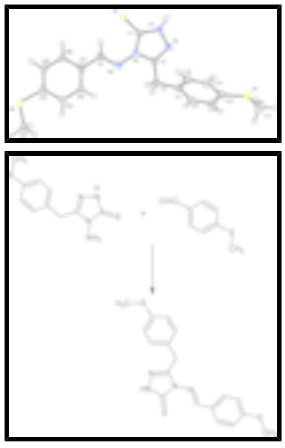

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. The minor occupied site of the disordered ethyl chain is drawn with open bonds. The intramolecular hydrogen bond is shown as a dashed line.

3-[4-(Methylsulfanyl)benzyl]-4-{(1E)-[4-(methylsulfanyl)phenyl]methyleneamino}- 4,5-dihydro-1*H*-1,2,4-triazole-5-thione

Crystal data

$C_{18}H_{18}N_4S_3$	$Z = 2$
$M_r = 386.54$	$F_{000} = 404$
Triclinic, $P\overline{1}$	$D_x = 1.343$ Mg m^{-3}
Hall symbol: P -1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.3269$ (7) Å	Cell parameters from 11444 reflections
$b = 9.8280$ (10) Å	$\theta = 3.8$–$25.7°$
$c = 13.6139$ (12) Å	$\mu = 0.40$ mm^{-1}
$\alpha = 91.093$ (7)°	$T = 173$ (2) K
$\beta = 98.068$ (8)°	Block, yellow
$\gamma = 99.789$ (8)°	0.28 × 0.26 × 0.21 mm
$V = 955.56$ (16) Å^3	

Data collection

STOE IPDS II two-circle-diffractometer	3555 independent reflections
Radiation source: fine-focus sealed tube	3191 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
$T = 173(2)$ K	$\theta_{max} = 25.6°$
ω scans	$\theta_{min} = 3.6°$
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -8 \rightarrow 8$
$T_{min} = 0.897$, $T_{max} = 0.921$	$k = -11 \rightarrow 11$
12044 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.077$

$S = 1.05$

3555 reflections

233 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.3204P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.24$ e Å^{-3}

$\Delta\rho_{min} = -0.30$ e Å^{-3}

Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.015 (2)

Special details

Experimental. ;

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}
S1	1.01643 (5)	0.94490 (4)	0.66117 (3)	0.02266 (11)
S2	−0.09236 (6)	0.51351 (5)	0.14774 (3)	0.03943 (14)
S3	0.57354 (6)	0.82097 (4)	1.22497 (3)	0.03008 (12)
C1	0.8033 (2)	0.87947 (14)	0.59765 (10)	0.0205 (3)
C2	0.5085 (2)	0.76653 (15)	0.55282 (10)	0.0212 (3)
C3	0.3210 (2)	0.68345 (16)	0.56391 (11)	0.0259 (3)
H3A	0.2506	0.7408	0.5997	0.031*
H3B	0.3393	0.6026	0.6040	0.031*
C4	0.6811 (2)	0.87988 (15)	0.79592 (11)	0.0230 (3)
H4	0.7434	0.9660	0.7769	0.028*
N1	0.74922 (17)	0.87201 (13)	0.49904 (9)	0.0246 (3)
H1	0.817 (3)	0.911 (2)	0.4520 (15)	0.039 (5)*
N2	0.56841 (17)	0.80276 (14)	0.46955 (9)	0.0259 (3)
N3	0.64388 (16)	0.81443 (12)	0.63284 (8)	0.0199 (3)

N4	0.61541 (17)	0.78174 (13)	0.73026 (9)	0.0230 (3)
C11	0.20827 (19)	0.63422 (16)	0.46387 (11)	0.0237 (3)
C12	0.1275 (2)	0.72730 (16)	0.40330 (13)	0.0308 (4)
H12	0.1374	0.8201	0.4272	0.037*
C13	0.0329 (2)	0.68735 (17)	0.30888 (13)	0.0334 (4)
H13	−0.0205	0.7527	0.2688	0.040*
C14	0.0160 (2)	0.55068 (16)	0.27268 (12)	0.0266 (3)
C15	0.0897 (2)	0.45557 (15)	0.33402 (12)	0.0266 (3)
H15	0.0748	0.3617	0.3115	0.032*
C16	0.1855 (2)	0.49790 (16)	0.42849 (11)	0.0258 (3)
H16	0.2361	0.4322	0.4695	0.031*
C17	−0.0465 (3)	0.3443 (2)	0.12139 (16)	0.0547 (6)
H17A	0.0883	0.3442	0.1364	0.082*
H17B	−0.0894	0.3183	0.0510	0.082*
H17C	−0.1133	0.2777	0.1623	0.082*
C21	0.6600 (2)	0.85875 (16)	0.90013 (11)	0.0232 (3)
C22	0.5609 (2)	0.73536 (16)	0.93015 (11)	0.0280 (3)
H22	0.5106	0.6619	0.8825	0.034*
C23	0.5354 (2)	0.71928 (16)	1.02835 (11)	0.0285 (3)
H23	0.4674	0.6353	1.0475	0.034*
C24	0.6095 (2)	0.82651 (16)	1.09967 (11)	0.0240 (3)
C25	0.7133 (2)	0.94843 (17)	1.07040 (11)	0.0295 (3)
H25	0.7678	1.0206	1.1184	0.035*
C26	0.7368 (2)	0.96429 (16)	0.97167 (11)	0.0282 (3)
H26	0.8058	1.0479	0.9525	0.034*
C27	0.4774 (3)	0.64210 (19)	1.23845 (13)	0.0392 (4)
H27A	0.3585	0.6170	1.1939	0.059*
H27B	0.4558	0.6282	1.3073	0.059*
H27C	0.5655	0.5838	1.2216	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02176 (19)	0.02459 (19)	0.01955 (18)	−0.00150 (14)	0.00242 (13)	0.00275 (13)
S2	0.0392 (2)	0.0359 (2)	0.0385 (3)	0.00935 (18)	−0.01336 (18)	−0.00501 (18)
S3	0.0344 (2)	0.0375 (2)	0.01671 (19)	0.00034 (17)	0.00564 (15)	−0.00206 (15)
C1	0.0236 (7)	0.0190 (7)	0.0189 (7)	0.0010 (5)	0.0061 (5)	0.0018 (5)
C2	0.0215 (7)	0.0233 (7)	0.0185 (7)	0.0018 (6)	0.0042 (5)	−0.0011 (5)
C3	0.0211 (7)	0.0317 (8)	0.0242 (7)	−0.0009 (6)	0.0080 (6)	0.0019 (6)
C4	0.0241 (7)	0.0245 (7)	0.0218 (7)	0.0046 (6)	0.0077 (6)	0.0017 (6)
N1	0.0217 (6)	0.0319 (7)	0.0173 (6)	−0.0053 (5)	0.0046 (5)	0.0021 (5)
N2	0.0216 (6)	0.0336 (7)	0.0196 (6)	−0.0037 (5)	0.0037 (5)	0.0004 (5)
N3	0.0218 (6)	0.0222 (6)	0.0157 (6)	0.0009 (5)	0.0058 (5)	0.0016 (4)
N4	0.0256 (6)	0.0283 (7)	0.0155 (6)	0.0024 (5)	0.0073 (5)	0.0032 (5)
C11	0.0159 (6)	0.0281 (8)	0.0270 (8)	−0.0002 (5)	0.0077 (6)	0.0005 (6)
C12	0.0273 (8)	0.0234 (8)	0.0406 (9)	0.0062 (6)	−0.0003 (7)	−0.0045 (6)
C13	0.0290 (8)	0.0267 (8)	0.0428 (10)	0.0094 (6)	−0.0064 (7)	0.0006 (7)
C14	0.0173 (7)	0.0277 (8)	0.0329 (8)	0.0019 (6)	−0.0001 (6)	−0.0012 (6)

C15	0.0255 (7)	0.0203 (7)	0.0332 (8)	0.0002 (6)	0.0069 (6)	0.0008 (6)
C16	0.0254 (7)	0.0247 (7)	0.0281 (8)	0.0030 (6)	0.0081 (6)	0.0061 (6)
C17	0.0704 (14)	0.0471 (12)	0.0437 (12)	0.0224 (10)	−0.0146 (10)	−0.0157 (9)
C21	0.0216 (7)	0.0284 (8)	0.0202 (7)	0.0039 (6)	0.0056 (5)	0.0003 (6)
C22	0.0333 (8)	0.0281 (8)	0.0199 (7)	−0.0022 (6)	0.0045 (6)	−0.0044 (6)
C23	0.0318 (8)	0.0292 (8)	0.0224 (8)	−0.0035 (6)	0.0069 (6)	0.0010 (6)
C24	0.0214 (7)	0.0326 (8)	0.0176 (7)	0.0040 (6)	0.0030 (5)	−0.0003 (6)
C25	0.0311 (8)	0.0317 (8)	0.0222 (8)	−0.0030 (6)	0.0033 (6)	−0.0062 (6)
C26	0.0294 (8)	0.0283 (8)	0.0249 (8)	−0.0030 (6)	0.0075 (6)	−0.0011 (6)
C27	0.0449 (10)	0.0436 (10)	0.0262 (8)	−0.0085 (8)	0.0149 (7)	−0.0012 (7)

Geometric parameters (Å, °)

S1—C1	1.6907 (15)	C13—C14	1.401 (2)
S2—C14	1.7763 (16)	C13—H13	0.9500
S2—C17	1.792 (2)	C14—C15	1.392 (2)
S3—C24	1.7628 (15)	C15—C16	1.395 (2)
S3—C27	1.8022 (18)	C15—H15	0.9500
C1—N1	1.3423 (19)	C16—H16	0.9500
C1—N3	1.3845 (18)	C17—H17A	0.9800
C2—N2	1.3064 (18)	C17—H17B	0.9800
C2—N3	1.3822 (18)	C17—H17C	0.9800
C2—C3	1.5029 (19)	C21—C26	1.396 (2)
C3—C11	1.515 (2)	C21—C22	1.403 (2)
C3—H3A	0.9900	C22—C23	1.384 (2)
C3—H3B	0.9900	C22—H22	0.9500
C4—N4	1.2844 (19)	C23—C24	1.402 (2)
C4—C21	1.464 (2)	C23—H23	0.9500
C4—H4	0.9500	C24—C25	1.402 (2)
N1—N2	1.3831 (17)	C25—C26	1.387 (2)
N1—H1	0.91 (2)	C25—H25	0.9500
N3—N4	1.4060 (16)	C26—H26	0.9500
C11—C16	1.390 (2)	C27—H27A	0.9800
C11—C12	1.394 (2)	C27—H27B	0.9800
C12—C13	1.387 (2)	C27—H27C	0.9800
C12—H12	0.9500		
C14—S2—C17	103.29 (9)	C14—C15—C16	120.10 (14)
C24—S3—C27	103.51 (8)	C14—C15—H15	119.9
N1—C1—N3	102.44 (12)	C16—C15—H15	119.9
N1—C1—S1	128.21 (11)	C11—C16—C15	121.32 (14)
N3—C1—S1	129.28 (11)	C11—C16—H16	119.3
N2—C2—N3	110.54 (12)	C15—C16—H16	119.3
N2—C2—C3	126.49 (13)	S2—C17—H17A	109.5
N3—C2—C3	122.97 (12)	S2—C17—H17B	109.5
C2—C3—C11	111.42 (12)	H17A—C17—H17B	109.5
C2—C3—H3A	109.3	S2—C17—H17C	109.5
C11—C3—H3A	109.3	H17A—C17—H17C	109.5
C2—C3—H3B	109.3	H17B—C17—H17C	109.5
C11—C3—H3B	109.3	C26—C21—C22	118.78 (13)

H3A—C3—H3B	108.0	C26—C21—C4	119.66 (13)
N4—C4—C21	119.89 (13)	C22—C21—C4	121.55 (13)
N4—C4—H4	120.1	C23—C22—C21	120.82 (14)
C21—C4—H4	120.1	C23—C22—H22	119.6
C1—N1—N2	114.21 (12)	C21—C22—H22	119.6
C1—N1—H1	126.7 (13)	C22—C23—C24	120.25 (14)
N2—N1—H1	118.9 (12)	C22—C23—H23	119.9
C2—N2—N1	103.96 (11)	C24—C23—H23	119.9
C2—N3—C1	108.76 (11)	C25—C24—C23	119.05 (13)
C2—N3—N4	120.95 (11)	C25—C24—S3	116.97 (11)
C1—N3—N4	129.89 (12)	C23—C24—S3	123.94 (11)
C4—N4—N3	114.65 (12)	C26—C25—C24	120.35 (14)
C16—C11—C12	118.03 (14)	C26—C25—H25	119.8
C16—C11—C3	121.93 (14)	C24—C25—H25	119.8
C12—C11—C3	120.03 (14)	C25—C26—C21	120.72 (14)
C13—C12—C11	121.43 (15)	C25—C26—H26	119.6
C13—C12—H12	119.3	C21—C26—H26	119.6
C11—C12—H12	119.3	S3—C27—H27A	109.5
C12—C13—C14	120.05 (15)	S3—C27—H27B	109.5
C12—C13—H13	120.0	H27A—C27—H27B	109.5
C14—C13—H13	120.0	S3—C27—H27C	109.5
C15—C14—C13	118.98 (15)	H27A—C27—H27C	109.5
C15—C14—S2	124.56 (12)	H27B—C27—H27C	109.5
C13—C14—S2	116.41 (12)		
N2—C2—C3—C11	4.5 (2)	C12—C13—C14—C15	2.2 (2)
N3—C2—C3—C11	−174.87 (13)	C12—C13—C14—S2	−175.46 (13)
N3—C1—N1—N2	−1.95 (17)	C17—S2—C14—C15	−8.65 (17)
S1—C1—N1—N2	175.26 (11)	C17—S2—C14—C13	168.82 (14)
N3—C2—N2—N1	1.76 (16)	C13—C14—C15—C16	−2.6 (2)
C3—C2—N2—N1	−177.69 (15)	S2—C14—C15—C16	174.81 (11)
C1—N1—N2—C2	0.17 (18)	C12—C11—C16—C15	1.9 (2)
N2—C2—N3—C1	−3.08 (17)	C3—C11—C16—C15	−176.55 (13)
C3—C2—N3—C1	176.39 (14)	C14—C15—C16—C11	0.5 (2)
N2—C2—N3—N4	−176.48 (13)	N4—C4—C21—C26	178.02 (14)
C3—C2—N3—N4	3.0 (2)	N4—C4—C21—C22	−3.2 (2)
N1—C1—N3—C2	2.92 (15)	C26—C21—C22—C23	1.5 (2)
S1—C1—N3—C2	−174.26 (12)	C4—C21—C22—C23	−177.23 (15)
N1—C1—N3—N4	175.53 (13)	C21—C22—C23—C24	−0.3 (3)
S1—C1—N3—N4	−1.6 (2)	C22—C23—C24—C25	−1.5 (2)
C21—C4—N4—N3	179.85 (12)	C22—C23—C24—S3	176.05 (13)
C2—N3—N4—C4	−142.47 (14)	C27—S3—C24—C25	−169.52 (14)
C1—N3—N4—C4	45.7 (2)	C27—S3—C24—C23	12.87 (17)
C2—C3—C11—C16	104.67 (16)	C23—C24—C25—C26	2.1 (2)
C2—C3—C11—C12	−73.78 (18)	S3—C24—C25—C26	−175.62 (13)
C16—C11—C12—C13	−2.4 (2)	C24—C25—C26—C21	−0.9 (3)
C3—C11—C12—C13	176.13 (14)	C22—C21—C26—C25	−0.9 (2)
C11—C12—C13—C14	0.4 (3)	C4—C21—C26—C25	177.86 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···S1^{i}	0.91 (2)	2.43 (2)	3.3307 (13)	169.7 (17)

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

Fig. 1

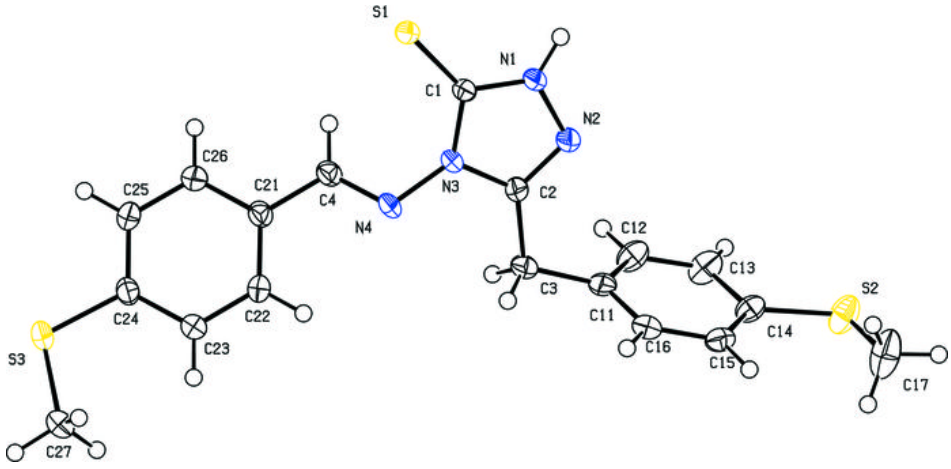
S1
N1
C1
N2
C26
C25
C21
C4
N3
C2
N4
C12
C13
C3
S2
C24
C22
C11
C14
S3
C23
C16
C15
C17
C27

Fig. 2