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4-Benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

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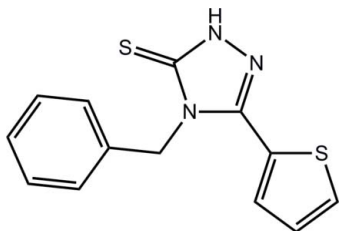
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.045; wR factor = 0.109; data-to-parameter ratio = 17.6.

In the title compound, $\text{C}_{13}\text{H}_{11}\text{N}_3\text{S}_2$, the triazole and thiophene rings are coplanar [dihedral angle = $6.22(13)^\circ$]. By contrast, the phenyl ring is perpendicular to the triazole ring [dihedral angle = $85.58(13)^\circ$], so that the molecule has an L-shape. The thiophene S atom is *syn* with the ring imine N atom. In the crystal, eight-membered $\{\cdots\text{HNCS}\}_2$ synthons form between centrosymmetrically related molecules, leading to dimeric aggregates that are connected into a supramolecular layer parallel to (101) by π - π interactions between centrosymmetrically related triazole rings [centroid-centroid distance = $3.6091(15)$ Å] and C-H $\cdots\pi$ interactions.

Related literature

For the pharmacological properties (anti-inflammatory, antimicrobial and anti-cancer) of 1,2,4-triazole derivatives, see: El-Emam & Ibrahim (1991); Navidpour *et al.* (2006); Kumar *et al.* (2010); Wang *et al.* (2011). For a related structure, see: Zareef *et al.* (2008).



Experimental

Crystal data

$\text{C}_{13}\text{H}_{11}\text{N}_3\text{S}_2$	$a = 13.422(2)$ Å
$M_r = 273.37$	$b = 6.1670(7)$ Å
Monoclinic, $P2_1/n$	$c = 16.596(2)$ Å

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$\beta = 111.972(15)^\circ$
 $V = 1273.9(3)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.40$ mm⁻¹
 $T = 295$ K
 $0.30 \times 0.05 \times 0.05$ mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
 $T_{\min} = 0.806$, $T_{\max} = 1.000$

6460 measured reflections
 2937 independent reflections
 2088 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.109$
 $S = 1.02$
 2937 reflections
 167 parameters
 1 restraint

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C8–C13 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{S2}^{\text{i}}$	0.88 (1)	2.43 (1)	3.297 (2)	169 (2)
$\text{C13}-\text{H13}\cdots\text{Cg1}^{\text{ii}}$	0.93	2.94	3.636 (3)	133

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5308).

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supporting information

Acta Cryst. (2013). E69, o697 [https://doi.org/10.1107/S1600536813009501]

4-Benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

Mona M. Al-Shehri, Ali A. El-Emam, Nasser R. El-Brollosy, Seik Weng Ng and Edward R. T. Tiekink

S1. Comment

In continuation of research into the chemical and pharmacological properties of 1,2,4-triazole derivatives (El-Emam & Ibrahim, 1991; Navidpour *et al.*, 2006; Kumar *et al.*, 2010; Wang *et al.*, 2011), we describe herein the X-ray crystal structure determination of the title compound, (I).

In (I), Fig. 1, the triazole ring is plane (r.m.s. deviation = 0.008 Å) and the thione-S2 atom lies 0.030 (1) Å out of the plane. The thiophene ring is co-planar with the triazole ring [dihedral angle = 6.22 (13)°] and the latter forms a dihedral of 85.58 (13)° with the phenyl ring. The thiophene-S1 atom is *syn* with the ring imine-N2 atom. Overall, the molecule has the shape of the letter *L*. A similar conformation was found in the analogous furanyl compound for which two molecules comprise the asymmetric unit and which was characterized as an hydrate (Zareef *et al.*, 2008).

In the crystal packing, centrosymmetrically related molecules aggregate into dimers *via* N—H⋯S hydrogen bonds that lead to eight-membered {⋯HNCS}₂ synthons, Table 1. The dimers are connected into rows along the *b* axis by π — π interactions between centrosymmetrically related triazole rings [inter-centroid distance = 3.6091 (15) Å for symmetry operation: 1 - *x*, 1 - *y*, 1 - *z*]. Projecting out on either side of the row are the phenyl groups that inter-digitate with translationally related rows to enable the formation of edge-to-face C—H⋯ π interactions, Table 1, that result in a supramolecular layer parallel to (1 0 1), Fig. 2. Layers stack with no specific interactions between them, Fig. 3.

S2. Experimental

A mixture of thiophene-2-carbohydrazide (1.42 g, 0.01 mol), benzyl isothiocyanate (1.49 g, 0.01 mol), in ethanol (10 ml) was heated under reflux with stirring for 1 h after which the solvent was distilled off *in vacuo*. Aqueous sodium hydroxide solution (10%, 15 ml) was added to the residue and the mixture was heated under reflux for 2 h then filtered hot. On cooling, the mixture was acidified with hydrochloric acid and the precipitated crude product was filtered, washed with water, dried and crystallized from aqueous ethanol to yield 2.32 g (85%) of the title compound as colourless crystals. *M.pt*: 515–517 K. Single crystals suitable for X-ray analysis were obtained by slow evaporation of its CHCl₃:EtOH (1:1; 10 ml) solution at room temperature. ¹H NMR (DMSO-*d*₆, 500.13 MHz): δ 5.51 (s, 2H, CH₂), 7.13–7.14 (m, 3H, Ar—H), 7.27–7.40 (m, 4H, Ar—H & thiophene-H), 7.77 (d, 1H, thiophene-H, *J* = 4.0 Hz), 14.21 (s, 1H, SH, thiol tautomer). ¹³C NMR (DMSO-*d*₆, 125.76 MHz): δ 46.74 (CH₂), 126.15, 126.33, 127.51, 128.19, 128.72, 128.86, 129.90, 135.40 (Ar—C & thiophene-C), 146.31 (triazole C-3), 168.31 (triazole C-5).

S3. Refinement

The C-bound H-atoms were placed in calculated positions [C—H = 0.93 to 0.97 Å, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding model approximation. The N-bound H-atom was refined with the distance restraint N—H = 0.88±0.01 Å.

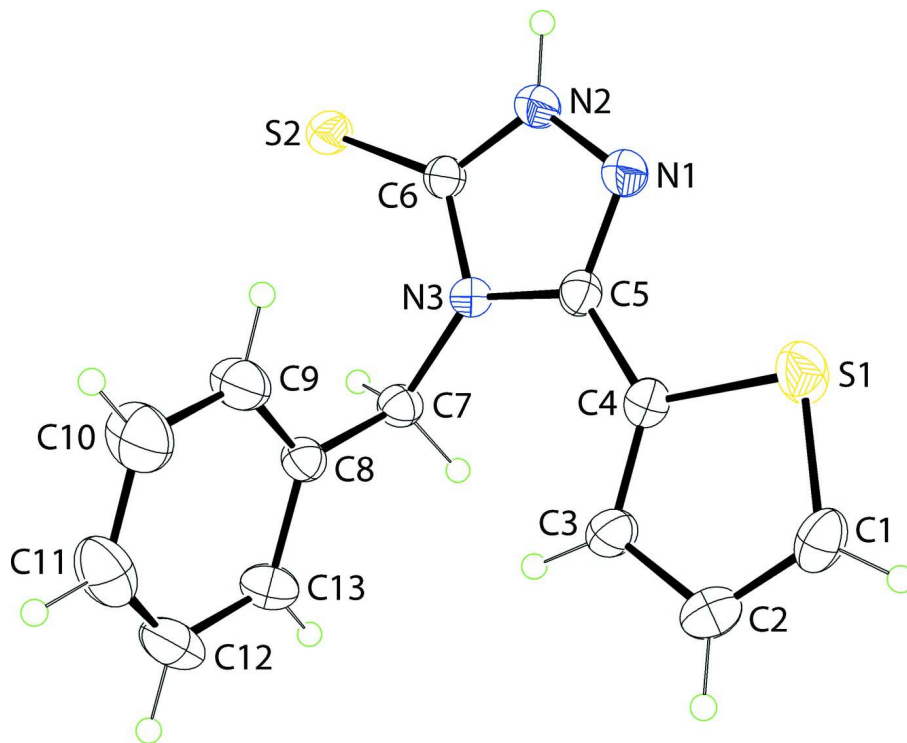


Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 35% probability level.

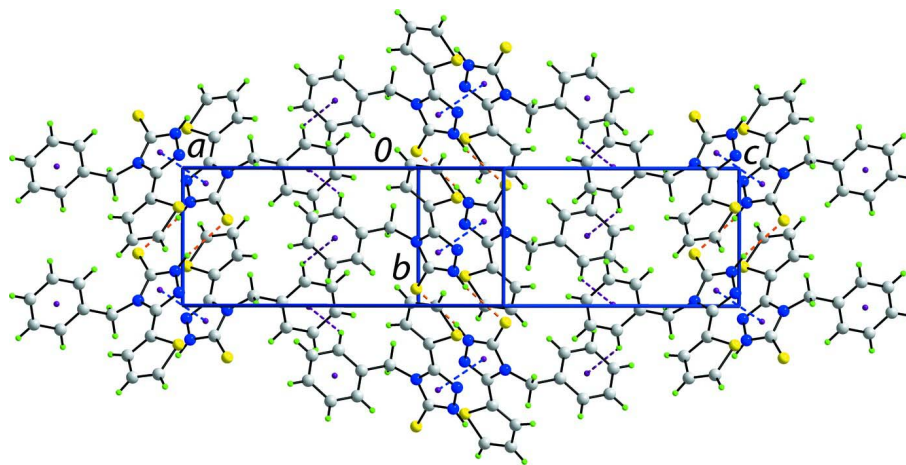


Figure 2

A view of the supramolecular layer in (I), which is sustained by N—H...S hydrogen bonds as well as by π — π and C—H... π interactions shown as orange, blue and purple dashed lines, respectively.

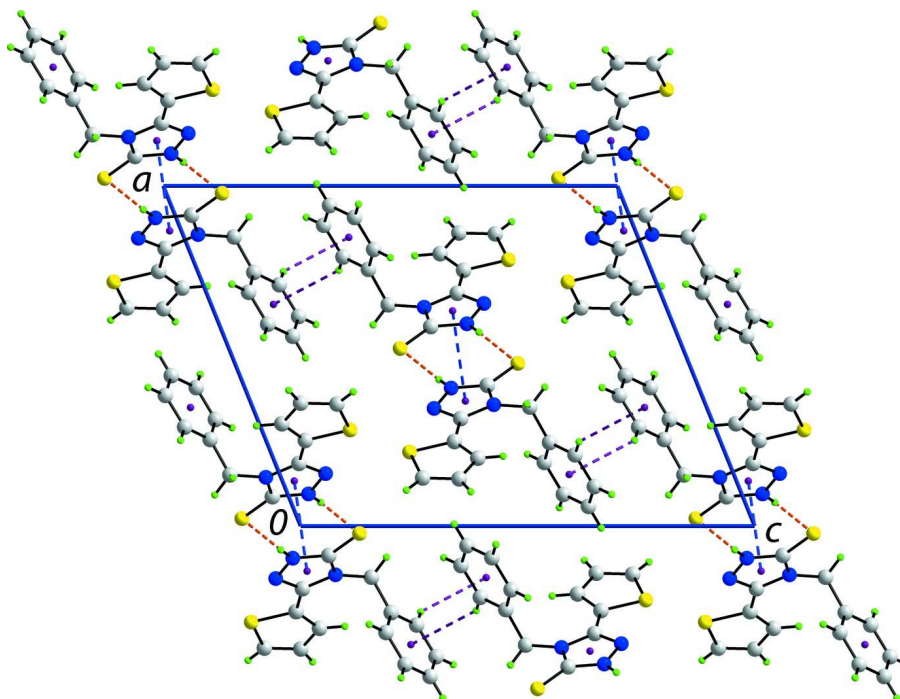


Figure 3

View of the unit-cell contents in projection down the b axis of (I), highlighting the stacking of layers. The N—H \cdots S hydrogen bonds as well as by π — π and C—H \cdots π interactions shown as orange, blue and purple dashed lines, respectively.

4-Benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thione

Crystal data

$C_{13}H_{11}N_3S_2$

$M_r = 273.37$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 13.422\ (2)\ \text{\AA}$

$b = 6.1670\ (7)\ \text{\AA}$

$c = 16.596\ (2)\ \text{\AA}$

$\beta = 111.972\ (15)^\circ$

$V = 1273.9\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 568$

$D_x = 1.425\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1615 reflections

$\theta = 3.0\text{--}27.5^\circ$

$\mu = 0.40\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Prism, colourless

$0.30 \times 0.05 \times 0.05\ \text{mm}$

Data collection

Agilent SuperNova Dual

diffractometer with an Atlas detector

Radiation source: SuperNova (Mo) X-ray

Source

Mirror monochromator

Detector resolution: $10.4041\ \text{pixels mm}^{-1}$

ω scan

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2011)

$T_{\min} = 0.806$, $T_{\max} = 1.000$

6460 measured reflections

2937 independent reflections

2088 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 27.6^\circ$, $\theta_{\min} = 3.3^\circ$

$h = -12 \rightarrow 17$

$k = -8 \rightarrow 5$

$l = -21 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.109$
 $S = 1.02$
 2937 reflections
 167 parameters
 1 restraint
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.2539P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.21756 (5)	0.78528 (13)	0.30574 (4)	0.0548 (2)
S2	0.47823 (5)	0.12218 (10)	0.62298 (3)	0.03891 (18)
N1	0.34574 (15)	0.4060 (3)	0.39839 (11)	0.0395 (5)
N2	0.40554 (15)	0.2515 (3)	0.45408 (12)	0.0383 (5)
H2	0.4302 (18)	0.138 (3)	0.4349 (15)	0.052 (8)*
N3	0.35676 (13)	0.4651 (3)	0.53331 (10)	0.0304 (4)
C1	0.14130 (18)	0.9997 (4)	0.31144 (16)	0.0475 (6)
H1	0.1054	1.0904	0.2648	0.057*
C2	0.1387 (2)	1.0233 (4)	0.39097 (16)	0.0492 (6)
H2A	0.1008	1.1330	0.4054	0.059*
C3	0.19944 (19)	0.8647 (4)	0.45051 (14)	0.0426 (6)
H3	0.2054	0.8574	0.5081	0.051*
C4	0.24840 (16)	0.7233 (4)	0.41373 (13)	0.0346 (5)
C5	0.31583 (17)	0.5357 (4)	0.44809 (13)	0.0323 (5)
C6	0.41379 (16)	0.2783 (3)	0.53621 (13)	0.0315 (5)
C7	0.34971 (17)	0.5686 (4)	0.61041 (13)	0.0344 (5)
H7A	0.3586	0.7238	0.6065	0.041*
H7B	0.4085	0.5168	0.6614	0.041*
C8	0.24552 (17)	0.5271 (4)	0.62246 (12)	0.0344 (5)
C9	0.1871 (2)	0.3419 (5)	0.59316 (17)	0.0534 (7)
H9	0.2110	0.2391	0.5635	0.064*
C10	0.0931 (2)	0.3049 (5)	0.6069 (2)	0.0708 (9)
H10	0.0540	0.1787	0.5863	0.085*
C11	0.0579 (2)	0.4550 (6)	0.65120 (19)	0.0665 (8)

H11	-0.0056	0.4316	0.6602	0.080*
C12	0.1160 (2)	0.6383 (5)	0.68195 (17)	0.0595 (8)
H12	0.0928	0.7387	0.7129	0.071*
C13	0.2092 (2)	0.6763 (4)	0.66753 (15)	0.0474 (6)
H13	0.2479	0.8029	0.6882	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0569 (4)	0.0694 (5)	0.0403 (3)	0.0206 (4)	0.0206 (3)	0.0166 (3)
S2	0.0448 (3)	0.0349 (3)	0.0365 (3)	0.0064 (3)	0.0146 (2)	0.0030 (3)
N1	0.0467 (11)	0.0384 (11)	0.0365 (10)	0.0075 (9)	0.0190 (8)	0.0045 (9)
N2	0.0453 (11)	0.0369 (11)	0.0369 (10)	0.0088 (9)	0.0204 (9)	0.0021 (9)
N3	0.0335 (9)	0.0279 (9)	0.0318 (9)	0.0017 (8)	0.0145 (7)	-0.0002 (8)
C1	0.0385 (13)	0.0476 (15)	0.0501 (14)	0.0047 (12)	0.0095 (10)	0.0177 (12)
C2	0.0478 (14)	0.0404 (14)	0.0561 (15)	0.0098 (12)	0.0155 (12)	0.0040 (12)
C3	0.0500 (14)	0.0378 (13)	0.0386 (12)	0.0104 (12)	0.0148 (10)	0.0046 (11)
C4	0.0328 (11)	0.0346 (12)	0.0355 (11)	-0.0007 (10)	0.0117 (9)	0.0036 (10)
C5	0.0345 (11)	0.0308 (11)	0.0313 (10)	-0.0024 (10)	0.0120 (9)	0.0009 (10)
C6	0.0309 (11)	0.0301 (11)	0.0355 (11)	-0.0029 (9)	0.0148 (9)	-0.0015 (9)
C7	0.0371 (12)	0.0337 (12)	0.0314 (10)	0.0001 (10)	0.0116 (9)	-0.0031 (9)
C8	0.0371 (12)	0.0363 (12)	0.0307 (10)	0.0035 (10)	0.0137 (9)	0.0008 (10)
C9	0.0547 (16)	0.0503 (16)	0.0651 (16)	-0.0097 (13)	0.0339 (13)	-0.0164 (13)
C10	0.0595 (18)	0.073 (2)	0.092 (2)	-0.0239 (17)	0.0418 (17)	-0.0182 (19)
C11	0.0493 (16)	0.089 (2)	0.0722 (18)	0.0006 (17)	0.0350 (14)	0.0030 (18)
C12	0.0588 (17)	0.073 (2)	0.0550 (15)	0.0159 (16)	0.0313 (13)	-0.0069 (15)
C13	0.0531 (15)	0.0455 (15)	0.0458 (13)	0.0023 (12)	0.0211 (11)	-0.0120 (12)

Geometric parameters (Å, °)

S1—C1	1.696 (3)	C4—C5	1.448 (3)
S1—C4	1.725 (2)	C7—C8	1.507 (3)
S2—C6	1.678 (2)	C7—H7A	0.9700
N1—C5	1.315 (3)	C7—H7B	0.9700
N1—N2	1.361 (3)	C8—C9	1.368 (3)
N2—C6	1.336 (3)	C8—C13	1.384 (3)
N2—H2	0.881 (10)	C9—C10	1.382 (4)
N3—C6	1.374 (3)	C9—H9	0.9300
N3—C5	1.382 (2)	C10—C11	1.372 (4)
N3—C7	1.464 (2)	C10—H10	0.9300
C1—C2	1.341 (3)	C11—C12	1.359 (4)
C1—H1	0.9300	C11—H11	0.9300
C2—C3	1.412 (3)	C12—C13	1.379 (4)
C2—H2A	0.9300	C12—H12	0.9300
C3—C4	1.366 (3)	C13—H13	0.9300
C3—H3	0.9300		
C1—S1—C4	91.71 (11)	N3—C6—S2	127.78 (15)

C5—N1—N2	103.94 (17)	N3—C7—C8	114.11 (17)
C6—N2—N1	114.13 (18)	N3—C7—H7A	108.7
C6—N2—H2	124.6 (16)	C8—C7—H7A	108.7
N1—N2—H2	121.0 (16)	N3—C7—H7B	108.7
C6—N3—C5	107.63 (16)	C8—C7—H7B	108.7
C6—N3—C7	123.51 (17)	H7A—C7—H7B	107.6
C5—N3—C7	128.77 (18)	C9—C8—C13	118.4 (2)
C2—C1—S1	112.20 (18)	C9—C8—C7	122.1 (2)
C2—C1—H1	123.9	C13—C8—C7	119.4 (2)
S1—C1—H1	123.9	C8—C9—C10	121.1 (3)
C1—C2—C3	113.1 (2)	C8—C9—H9	119.5
C1—C2—H2A	123.4	C10—C9—H9	119.5
C3—C2—H2A	123.4	C11—C10—C9	119.7 (3)
C4—C3—C2	112.2 (2)	C11—C10—H10	120.1
C4—C3—H3	123.9	C9—C10—H10	120.1
C2—C3—H3	123.9	C12—C11—C10	119.9 (3)
C3—C4—C5	131.97 (19)	C12—C11—H11	120.1
C3—C4—S1	110.76 (16)	C10—C11—H11	120.1
C5—C4—S1	117.24 (16)	C11—C12—C13	120.4 (3)
N1—C5—N3	110.66 (19)	C11—C12—H12	119.8
N1—C5—C4	122.11 (18)	C13—C12—H12	119.8
N3—C5—C4	127.23 (19)	C12—C13—C8	120.4 (3)
N2—C6—N3	103.62 (17)	C12—C13—H13	119.8
N2—C6—S2	128.59 (17)	C8—C13—H13	119.8
C5—N1—N2—C6	0.3 (3)	N1—N2—C6—N3	-1.0 (2)
C4—S1—C1—C2	-0.2 (2)	N1—N2—C6—S2	178.98 (16)
S1—C1—C2—C3	-0.2 (3)	C5—N3—C6—N2	1.3 (2)
C1—C2—C3—C4	0.7 (3)	C7—N3—C6—N2	-175.41 (18)
C2—C3—C4—C5	-178.7 (2)	C5—N3—C6—S2	-178.73 (16)
C2—C3—C4—S1	-0.8 (3)	C7—N3—C6—S2	4.6 (3)
C1—S1—C4—C3	0.61 (19)	C6—N3—C7—C8	-102.1 (2)
C1—S1—C4—C5	178.87 (18)	C5—N3—C7—C8	81.9 (3)
N2—N1—C5—N3	0.5 (2)	N3—C7—C8—C9	29.0 (3)
N2—N1—C5—C4	-179.08 (19)	N3—C7—C8—C13	-153.6 (2)
C6—N3—C5—N1	-1.2 (2)	C13—C8—C9—C10	0.9 (4)
C7—N3—C5—N1	175.28 (19)	C7—C8—C9—C10	178.3 (2)
C6—N3—C5—C4	178.4 (2)	C8—C9—C10—C11	-0.5 (5)
C7—N3—C5—C4	-5.1 (3)	C9—C10—C11—C12	-0.6 (5)
C3—C4—C5—N1	172.4 (2)	C10—C11—C12—C13	1.2 (5)
S1—C4—C5—N1	-5.4 (3)	C11—C12—C13—C8	-0.8 (4)
C3—C4—C5—N3	-7.2 (4)	C9—C8—C13—C12	-0.3 (3)
S1—C4—C5—N3	175.03 (17)	C7—C8—C13—C12	-177.8 (2)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C8–C13 ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2···S2 ⁱ	0.88 (1)	2.43 (1)	3.297 (2)	169 (2)
C13—H13···Cg1 ⁱⁱ	0.93	2.94	3.636 (3)	133

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1/2, y+1/2, -z+3/2$.