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Crystal structures of (*E*)-4-[1-(2-carbamothioylhydrazinylidene)ethyl]phenyl acetate and (*E*)-4-[1-(2-carbamothioylhydrazinylidene)ethyl]phenyl benzoate

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CCDC references: 1519492; 1519491

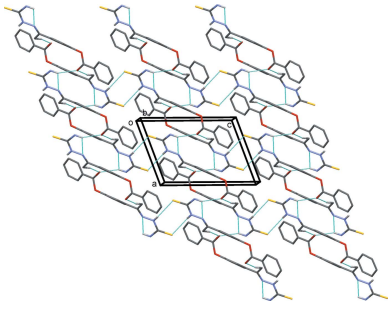
Supporting information: this article has supporting information at journals.iucr.org/e

In the title compounds, $C_{11}H_{13}N_3O_2S$, (I), and $C_{16}H_{15}N_3O_2S$, (II), the thiosemicarbazone group adopts an extended conformation. The acetate ester (I) crystallizes with two independent molecules in the asymmetric unit. In the benzoate ester (II), the planes of the two aryl rings are inclined to one another by 46.70 (7)°. In both compounds, there is a short intramolecular N—H···N contact present, forming an $S(5)$ ring motif. In the crystals of both compounds, molecules are linked *via* pairs of N—H···S hydrogen bonds, forming dimers with $R_2^2(8)$ ring motifs. The dimers are linked by N—H···S and N—H···O hydrogen bonds, forming slabs parallel to $(01\bar{1})$. In (I), there are N—H···π and C—H···π interactions present within the slabs, while in (II), there are only N—H···π interactions present.

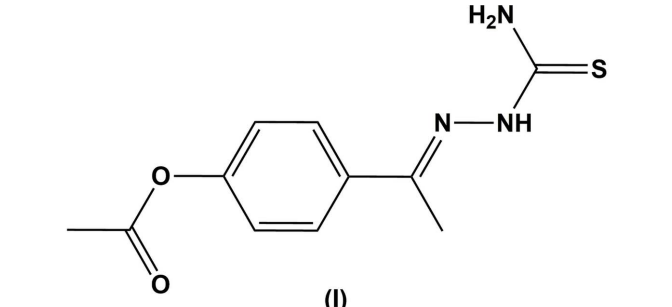
1. Chemical context

Thiosemicarbazones are potent intermediates for the synthesis of pharmaceutical and bioactive materials and they are used extensively in the field of medicinal chemistry. The biological activity of these ligands is related to their ability to coordinate to metal centres in enzymes (Seena *et al.*, 2006). These derivatives possess an additional functional group that is not coordinated to their 'primary' metal ion, thereby suggesting that the biological activity may also depend on the non-coordinating groups (Venkatesh *et al.*, 2016). Thiosemicarbazones in their neutral or deprotonated form behave as *N,N,S*-thiodentate chelates towards metal ions. They display antiproliferative activity on different tumors cell lines and have been a common feature of all compounds with carcinogenic potency. A strong correlation has been found between tumor growth rate and the ribonucleoside diphosphate reductase (RDR) enzyme (Arora *et al.*, 2014).

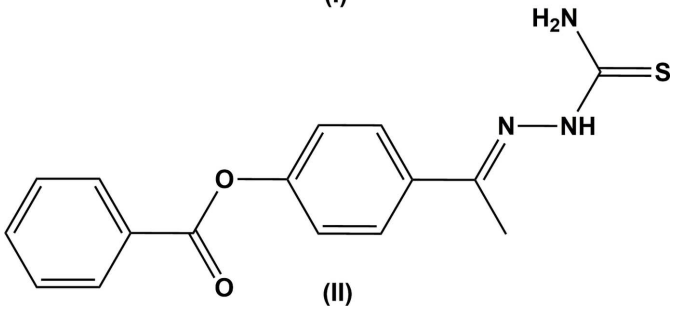
Thiosemicarbazone derivatives have found applications in drug development for the treatment of central nervous system disorders and bacterial infection as well as being analgesic and anti-allergic agents. They are inhibitors of DNA replication and also of many proteases. This inhibitory activity explains the level of interest given to them in the fight against microbial and parasitic diseases (Mani *et al.*, 2015). Thiosemicarbazones have many biological activities such as antiviral, antibacterial, antitumor, anti African trypanosome (Fatondji *et al.*, 2013), antimicrobial, sodium channel blocker, anticancer, antitubercular, antiviral (Venkatesh *et al.*, 2016), antifungal,



locomotor activity (Singh *et al.*, 2011), antimalarial, anticancer and they are used as a cure for leprosy, rheumatism and trypanosomiasis (Parul *et al.*, 2012). As part of our studies in this area, we now describe the syntheses and structures of the title compounds (I) and (II).



(I)



(II)

2. Structural commentary

The molecular structure of compounds (I) and (II) are shown in Figs. 1 and 2, respectively. Compound (I) crystallizes with two independent molecules in the asymmetric unit. In both the compounds, there is a short N—H···N contact, forming an *S*(5) ring motif (Figs. 1 and 2, and Tables 1 and 2). In both compounds, the thiosemicarbazone group adopts an extended conformation, as can be seen from the torsion angle S1—C11—N2—N1 [−173.1 (1)° in molecule *A* and −174.9 (1)° in molecule *B* of compound (I)] and S1—C16—N2—N1 [172.2 (1)° in compound (II)]. In compound (I), the acetate group adopts an extended conformation, which is evidenced by the torsion angle C1—C2—O2—C3 [−173.2 (2) and 179.9 (2)° in molecules *A* and *B*, respectively]. The bond lengths C11*A*—S1*A* [1.692 (2) Å] and C11*B*—S1*B* [1.680 (2) Å] in (I) and C16—S1 [1.679 (1) Å] in (II) are comparable with the values reported in the literature (CSD; Groom *et al.*, 2016). In compound (II), the benzoate and acetophenone thiosemicarbazone groups lie in a plane [C6—C7—O2—C8 = 175.9 (1)°]. The carbonyl group is oriented *syn*-periplanar to C5 [C5—C6—C7—O1 = −15.8 (2) °] and *anti*-periplanar to C1 [C1—C6—C7—O1 = 160.7 (1) °]. The dihedral angle between the benzene rings in compound (II) is 46.70 (7)°.

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

*Cg*1 and *Cg*2 are the centroids of the C3*A*–C8*A* and C3*B*–C8*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3*A*—H3*A*1···N1*A*	0.86	2.26	2.617 (2)	105
N3*B*—H3*B*1···N1*B*	0.86	2.28	2.633 (2)	105
N2*A*—H2*A*···S1*B*	0.86	2.63	3.4724 (15)	167
N2*B*—H2*B*···S1*A*	0.86	2.71	3.4228 (16)	141
N3*A*—H3*A*1···O1*B*^{i}	0.86	2.44	3.164 (2)	142
N3*B*—H3*B*2···S1*A*^{ii}	0.86	2.57	3.4262 (17)	176
N3*A*—H3*A*2···*Cg*2^{iii}	0.86	2.62	3.4763 (19)	130
C1*B*—H1*B*3···*Cg*1^{iv}	0.96	2.73	3.691 (3)	154

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $-x, -y+1, -z$; (iv) $-x+1, -y+1, -z$.

Table 2
Hydrogen-bond geometry (Å, °) for (II).

*Cg*2 is the centroid of the C8–C13 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1	0.86	2.24	2.5953 (18)	105
N2—H2*A*···S1^{i}	0.86	2.68	3.4697 (12)	153
N3—H3*A*···O1^{ii}	0.86	2.27	3.0653 (15)	153
C15—H15*B*···O1^{iii}	0.96	2.55	3.454 (2)	156
N3—H3*B*···*Cg*2^{ii}	0.86	2.47	3.3385 (15)	122

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

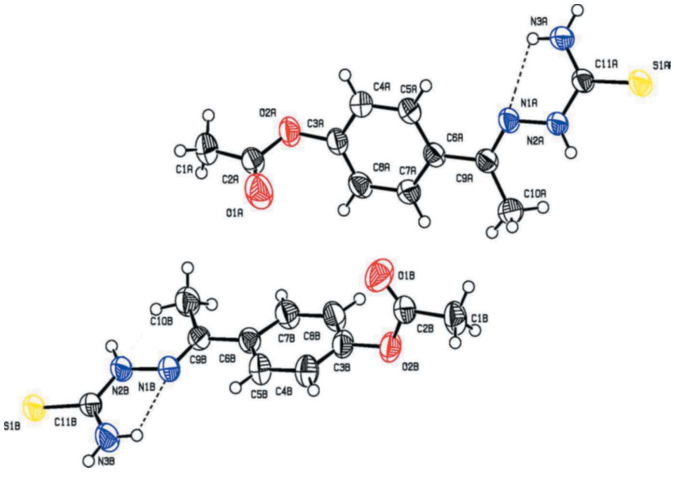


Figure 1
The molecular structure of the compound (I), showing the atom labelling and displacement ellipsoids drawn at the 30% probability level. The short intramolecular N—H···N contact is shown as a dashed line (see Table 1).

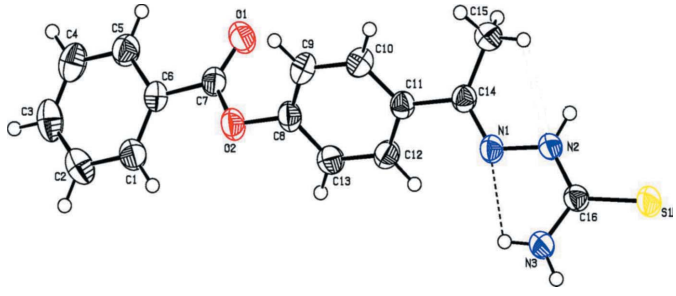


Figure 2
The molecular structure of the compound (II), showing the atom labelling and displacement ellipsoids drawn at the 40% probability level. The short intramolecular N—H···N contact is shown as a dashed line (see Table 2).

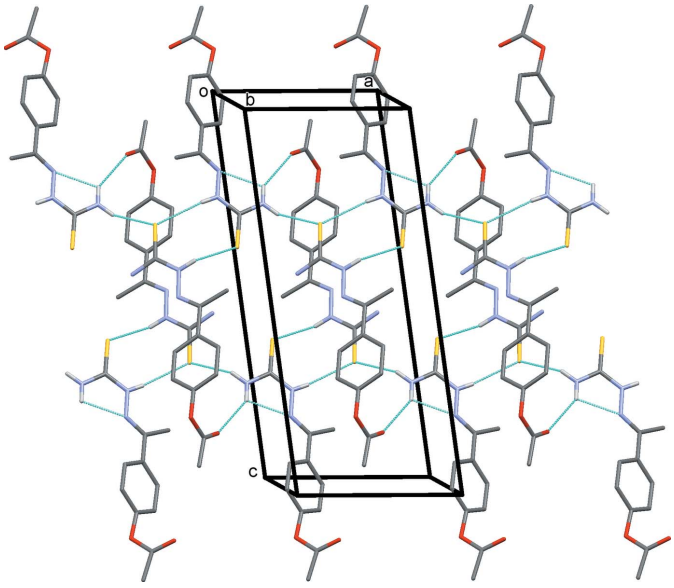


Figure 3
A view along the *b* axis of the crystal packing of compound (I). Hydrogen bonds are shown as dashed lines (see Table 1) and H atoms not involved in hydrogen bonds have been excluded for clarity.

3. Supramolecular features

In the crystal of (I), the two molecules are linked by a pair of N—H···S hydrogen bonds forming *A*–*B* dimers with an $R_2^2(8)$ ring motif. The dimers are linked by N—H···S and N—H···O hydrogen bonds, forming slabs lying parallel to $(01\bar{1})$, as shown in Table 1 and Fig. 3. Within the slabs there are N—H···π and C—H···π interactions present (Table 1).

In the crystal of (II), molecules are linked by pairs of N—H···S hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif (Table 2 and Fig. 4). As in the crystal of compound (I), the dimers are linked by N—H···S and N—H···O hydrogen bonds, forming slabs lying parallel to plane $(01\bar{1})$; see Table 2 and Fig. 4. Within the slabs, there are only N—H···π interactions present (Table 2).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.37, last update May 2016; Groom *et al.*, 2016) for the substructure 2-(1-phenylethylidene)hydrazine-1-carbothioamide yielded 100 hits. One of the compounds, (*E*)-4-(*N*-carbamothioylethanehydrazonoyl)phenyl 4-methylbenzoate (NOVFOV; Mani *et al.*, 2015) is the 4-methylbenzoate analogue of compound (II). Like compound (I), it crystallizes with two independent molecules in the asymmetric unit. The two molecules differ essentially in the orientation of the hydrazinecarbothioamide unit with respect to the central benzene ring. This dihedral angle is 5.95 (8)° in the first molecule and 42.56 (9)° in the second. The benzoate groups are relatively planar and are inclined to the central benzene ring by 72.23 (7) and 53.10 (9)°, respectively, in the first and second molecules. Hence, the conformation of the second molecule resembles that of compound (II).

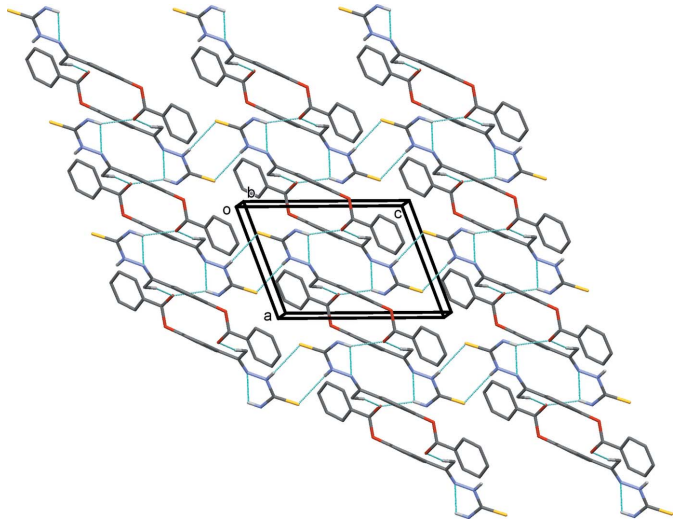


Figure 4
A view along the *b* axis of the crystal packing of compound (II). Hydrogen bonds are shown as dashed lines (see Table 2) and H atoms not involved in hydrogen bonds have been excluded for clarity.

5. Synthesis and crystallization

Compounds (I) and (II): Thiosemicarbazide (0.91g, 0.01 mol) was added to 50 ml of an ethanolic solution of the 4-acetyl phenyl acetate (0.01 mol) for (I), and to an ethanolic solution of the 4-acetylphenyl benzoate (0.01 mol) for (II), with continuous stirring for 4–5 h. The resulting mixtures were refluxed at 333 K and the purity of the products as well as composition of the reaction mixtures was monitored by TLC using ethyl acetate: hexane (3:7). The reaction mixtures were cooled to room temperature and the separated products were filtered, dried and finally recrystallized from chloroform, solution, yielding block-like yellow crystals of (I) and pale-yellow crystals of (II).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were placed in calculated positions and refined as riding atoms: C—H = 0.93–0.96 Å and N—H = 0.86 Å, with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C,N) for other H atoms.

Acknowledgements

The authors thank the TBI X-ray facility, CAS in Crystallography and Biophysics, University of Madras, India, for the data collection. VV thanks the DBT, Government of India, for a fellowship.

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{11}H_{13}N_3O_2S$	$C_{16}H_{15}N_3O_2S$
M_r	251.30	313.37
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	293	293
a, b, c (Å)	7.8783 (2), 8.9254 (3), 18.7372 (5)	7.8145 (4), 9.7538 (5), 10.9050 (7)
α, β, γ (°)	77.243 (2), 82.423 (2), 78.856 (2)	78.855 (4), 69.031 (2), 84.200 (3)
V (Å^3)	1255.30 (6)	761.05 (8)
Z	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.25	0.22
Crystal size (mm)	0.20 × 0.15 × 0.10	0.25 × 0.18 × 0.14
Data collection		
Diffractometer	Bruker SMART APEXII area-detector	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.785, 0.854	0.745, 0.865
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18970, 5128, 4104	11596, 3154, 2857
R_{int}	0.023	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.628
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.109, 1.03	0.034, 0.099, 1.05
No. of reflections	5128	3154
No. of parameters	311	201
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.31	0.26, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

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supporting information

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Crystal structures of (*E*)-4-[1-(2-carbamothioylhydrazinylidene)ethyl]phenyl acetate and (*E*)-4-[1-(2-carbamothioylhydrazinylidene)ethyl]phenyl benzoate

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Computing details

For both compounds, data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008). Software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009) for (I); *SHELXL2014* (Sheldrick, 2008) and *PLATON* (Spek, 2009) for (II).

(I) (*E*)-4-[1-(2-Carbamothioylhydrazinylidene)ethyl]phenyl acetate

Crystal data

$C_{11}H_{13}N_3O_2S$
$M_r = 251.30$
Triclinic, $P\overline{1}$
$a = 7.8783$ (2) Å
$b = 8.9254$ (3) Å
$c = 18.7372$ (5) Å
$\alpha = 77.243$ (2)°
$\beta = 82.423$ (2)°
$\gamma = 78.856$ (2)°
$V = 1255.30$ (6) Å^3
$Z = 4$
$F(000) = 528$
$D_x = 1.330$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5128 reflections
$\theta = 1.1$–$26.4°$
$\mu = 0.25$ mm^{-1}
$T = 293$ K
Block, yellow
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
$T_{min} = 0.785$, $T_{max} = 0.854$
18970 measured reflections
5128 independent reflections
4104 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.4°$, $\theta_{min} = 1.1°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.109$
$S = 1.03$
5128 reflections
311 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.3822P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C10B	0.2271 (3)	0.1728 (3)	0.52308 (11)	0.0616 (5)
H10A	0.1335	0.2449	0.5001	0.092*
H10B	0.2263	0.1858	0.5726	0.092*
H10C	0.2129	0.0681	0.5235	0.092*
C1A	0.0183 (3)	0.8835 (3)	1.22191 (11)	0.0706 (6)
H1A1	0.0436	0.9807	1.2279	0.106*
H1A2	0.0630	0.8015	1.2607	0.106*
H1A3	−0.1051	0.8899	1.2236	0.106*
C1B	0.5549 (3)	0.0841 (3)	0.07427 (10)	0.0632 (5)
H1B1	0.4721	0.1283	0.0388	0.095*
H1B2	0.5685	−0.0275	0.0835	0.095*
H1B3	0.6646	0.1158	0.0556	0.095*
C2A	0.1010 (3)	0.8500 (2)	1.15003 (10)	0.0506 (4)
C2B	0.4920 (3)	0.1395 (2)	0.14379 (9)	0.0515 (4)
C3A	0.0618 (2)	0.7263 (2)	1.05471 (9)	0.0438 (4)
C3B	0.5256 (3)	0.0862 (2)	0.27010 (9)	0.0501 (4)
C4A	−0.0202 (2)	0.7922 (2)	0.99205 (10)	0.0497 (4)
H4A	−0.1086	0.8781	0.9916	0.060*
C4B	0.6282 (3)	0.1679 (2)	0.29458 (10)	0.0564 (5)
H4B	0.7253	0.1982	0.2652	0.068*
C5A	0.0297 (2)	0.7298 (2)	0.92993 (9)	0.0476 (4)
H5A	−0.0266	0.7738	0.8877	0.057*
C5B	0.5867 (3)	0.2050 (2)	0.36322 (9)	0.0533 (5)
H5B	0.6566	0.2603	0.3800	0.064*
C6A	0.1629 (2)	0.60209 (19)	0.92929 (8)	0.0396 (4)
C6B	0.4412 (2)	0.16043 (19)	0.40777 (9)	0.0438 (4)
C7A	0.2445 (2)	0.5402 (2)	0.99344 (9)	0.0459 (4)
H7A	0.3351	0.4559	0.9942	0.055*
C7B	0.3427 (3)	0.0750 (2)	0.38147 (10)	0.0548 (5)
H7B	0.2464	0.0423	0.4106	0.066*
C8A	0.1934 (2)	0.6015 (2)	1.05617 (9)	0.0481 (4)
H8A	0.2482	0.5581	1.0988	0.058*
C8B	0.3850 (3)	0.0372 (2)	0.31264 (10)	0.0588 (5)
H8B	0.3182	−0.0207	0.2958	0.071*
C9A	0.2116 (2)	0.5324 (2)	0.86296 (8)	0.0412 (4)
C9B	0.3961 (2)	0.20310 (19)	0.48111 (9)	0.0427 (4)

C10A	0.3766 (3)	0.4199 (3)	0.85640 (11)	0.0705 (6)
H10D	0.4646	0.4736	0.8273	0.106*
H10E	0.3581	0.3395	0.8332	0.106*
H10F	0.4132	0.3743	0.9045	0.106*
C11A	0.0194 (2)	0.5408 (2)	0.70414 (9)	0.0428 (4)
C11B	0.6013 (2)	0.3524 (2)	0.59815 (9)	0.0448 (4)
N1A	0.10302 (18)	0.57512 (17)	0.81405 (7)	0.0423 (3)
N1B	0.50947 (19)	0.26330 (17)	0.50292 (7)	0.0460 (3)
N2A	0.14402 (18)	0.52010 (17)	0.74940 (7)	0.0444 (3)
H2A	0.2473	0.4736	0.7384	0.053*
N2B	0.47614 (19)	0.30636 (18)	0.57038 (7)	0.0483 (4)
H2B	0.3756	0.3037	0.5945	0.058*
N3A	−0.1399 (2)	0.5972 (2)	0.72772 (8)	0.0602 (4)
H3A1	−0.1609	0.6193	0.7708	0.072*
H3A2	−0.2229	0.6120	0.7001	0.072*
N3B	0.7503 (2)	0.3608 (2)	0.55723 (9)	0.0641 (5)
H3B1	0.7642	0.3371	0.5145	0.077*
H3B2	0.8335	0.3898	0.5733	0.077*
O1A	0.2381 (2)	0.8767 (2)	1.12093 (9)	0.0800 (5)
O1B	0.3862 (2)	0.2510 (2)	0.15026 (8)	0.0863 (5)
O2A	−0.00302 (17)	0.78178 (16)	1.11913 (7)	0.0555 (3)
O2B	0.57246 (19)	0.04701 (15)	0.20057 (7)	0.0607 (4)
S1A	0.07063 (6)	0.49355 (7)	0.62043 (2)	0.05713 (16)
S1B	0.56754 (6)	0.39051 (7)	0.68325 (2)	0.05582 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C10B	0.0553 (12)	0.0813 (14)	0.0553 (11)	−0.0165 (11)	0.0010 (9)	−0.0283 (10)
C1A	0.0818 (15)	0.0834 (15)	0.0541 (11)	−0.0020 (12)	−0.0163 (11)	−0.0344 (11)
C1B	0.0750 (14)	0.0799 (14)	0.0428 (10)	−0.0222 (11)	0.0034 (9)	−0.0265 (9)
C2A	0.0566 (12)	0.0518 (10)	0.0477 (10)	−0.0062 (9)	−0.0142 (9)	−0.0161 (8)
C2B	0.0558 (11)	0.0610 (11)	0.0406 (9)	−0.0078 (10)	−0.0053 (8)	−0.0179 (8)
C3A	0.0435 (9)	0.0564 (10)	0.0378 (8)	−0.0175 (8)	0.0009 (7)	−0.0177 (7)
C3B	0.0664 (12)	0.0445 (9)	0.0384 (9)	0.0034 (9)	−0.0108 (8)	−0.0140 (7)
C4A	0.0490 (10)	0.0543 (10)	0.0488 (10)	−0.0039 (8)	−0.0074 (8)	−0.0192 (8)
C4B	0.0699 (13)	0.0590 (11)	0.0427 (9)	−0.0163 (10)	0.0035 (9)	−0.0158 (8)
C5A	0.0514 (10)	0.0539 (10)	0.0396 (9)	−0.0061 (8)	−0.0110 (7)	−0.0126 (7)
C5B	0.0665 (12)	0.0565 (10)	0.0428 (9)	−0.0181 (9)	−0.0010 (8)	−0.0181 (8)
C6A	0.0379 (9)	0.0493 (9)	0.0352 (8)	−0.0144 (7)	−0.0021 (6)	−0.0106 (7)
C6B	0.0530 (10)	0.0417 (9)	0.0364 (8)	−0.0031 (8)	−0.0094 (7)	−0.0086 (7)
C7A	0.0440 (10)	0.0544 (10)	0.0394 (8)	−0.0043 (8)	−0.0064 (7)	−0.0118 (7)
C7B	0.0580 (12)	0.0644 (11)	0.0464 (10)	−0.0153 (9)	−0.0054 (8)	−0.0157 (8)
C8A	0.0500 (10)	0.0623 (11)	0.0340 (8)	−0.0116 (9)	−0.0081 (7)	−0.0095 (7)
C8B	0.0694 (13)	0.0628 (12)	0.0530 (11)	−0.0124 (10)	−0.0154 (10)	−0.0235 (9)
C9A	0.0368 (9)	0.0536 (10)	0.0352 (8)	−0.0112 (7)	−0.0013 (7)	−0.0113 (7)
C9B	0.0452 (9)	0.0456 (9)	0.0365 (8)	−0.0022 (7)	−0.0078 (7)	−0.0093 (7)
C10A	0.0578 (13)	0.1042 (17)	0.0488 (11)	0.0159 (12)	−0.0143 (9)	−0.0341 (11)

C11A	0.0387 (9)	0.0554 (10)	0.0362 (8)	−0.0082 (8)	−0.0039 (7)	−0.0130 (7)
C11B	0.0403 (9)	0.0559 (10)	0.0388 (8)	−0.0021 (8)	−0.0052 (7)	−0.0153 (7)
N1A	0.0410 (8)	0.0560 (8)	0.0335 (7)	−0.0104 (6)	−0.0013 (6)	−0.0158 (6)
N1B	0.0477 (8)	0.0579 (9)	0.0338 (7)	−0.0041 (7)	−0.0047 (6)	−0.0156 (6)
N2A	0.0355 (7)	0.0657 (9)	0.0349 (7)	−0.0049 (7)	−0.0024 (6)	−0.0202 (6)
N2B	0.0397 (8)	0.0720 (10)	0.0371 (7)	−0.0072 (7)	−0.0011 (6)	−0.0228 (7)
N3A	0.0410 (9)	0.0971 (13)	0.0450 (8)	0.0060 (8)	−0.0084 (7)	−0.0322 (8)
N3B	0.0451 (9)	0.1090 (14)	0.0489 (9)	−0.0192 (9)	0.0046 (7)	−0.0384 (9)
O1A	0.0727 (11)	0.1024 (12)	0.0834 (11)	−0.0401 (10)	0.0012 (8)	−0.0408 (9)
O1B	0.1032 (13)	0.0907 (11)	0.0507 (8)	0.0349 (10)	−0.0177 (8)	−0.0223 (8)
O2A	0.0525 (8)	0.0791 (9)	0.0448 (7)	−0.0190 (7)	0.0029 (6)	−0.0311 (6)
O2B	0.0776 (9)	0.0599 (8)	0.0442 (7)	0.0098 (7)	−0.0114 (6)	−0.0246 (6)
S1A	0.0422 (3)	0.0971 (4)	0.0381 (2)	−0.0090 (2)	−0.00201 (18)	−0.0298 (2)
S1B	0.0444 (3)	0.0874 (4)	0.0418 (2)	−0.0056 (2)	−0.00359 (19)	−0.0310 (2)

Geometric parameters (Å, º)

C10B—C9B	1.494 (3)	C6A—C7A	1.392 (2)
C10B—H10A	0.9600	C6A—C9A	1.484 (2)
C10B—H10B	0.9600	C6B—C7B	1.387 (2)
C10B—H10C	0.9600	C6B—C9B	1.487 (2)
C1A—C2A	1.483 (3)	C7A—C8A	1.385 (2)
C1A—H1A1	0.9600	C7A—H7A	0.9300
C1A—H1A2	0.9600	C7B—C8B	1.387 (2)
C1A—H1A3	0.9600	C7B—H7B	0.9300
C1B—C2B	1.485 (2)	C8A—H8A	0.9300
C1B—H1B1	0.9600	C8B—H8B	0.9300
C1B—H1B2	0.9600	C9A—N1A	1.282 (2)
C1B—H1B3	0.9600	C9A—C10A	1.490 (3)
C2A—O1A	1.186 (2)	C9B—N1B	1.278 (2)
C2A—O2A	1.361 (2)	C10A—H10D	0.9600
C2B—O1B	1.186 (2)	C10A—H10E	0.9600
C2B—O2B	1.343 (2)	C10A—H10F	0.9600
C3A—C8A	1.366 (3)	C11A—N3A	1.315 (2)
C3A—C4A	1.375 (2)	C11A—N2A	1.341 (2)
C3A—O2A	1.4023 (19)	C11A—S1A	1.6915 (16)
C3B—C8B	1.361 (3)	C11B—N3B	1.320 (2)
C3B—C4B	1.367 (3)	C11B—N2B	1.341 (2)
C3B—O2B	1.4074 (19)	C11B—S1B	1.6799 (16)
C4A—C5A	1.379 (2)	N1A—N2A	1.3825 (17)
C4A—H4A	0.9300	N1B—N2B	1.3792 (18)
C4B—C5B	1.381 (2)	N2A—H2A	0.8600
C4B—H4B	0.9300	N2B—H2B	0.8600
C5A—C6A	1.394 (2)	N3A—H3A1	0.8600
C5A—H5A	0.9300	N3A—H3A2	0.8600
C5B—C6B	1.395 (3)	N3B—H3B1	0.8600
C5B—H5B	0.9300	N3B—H3B2	0.8600

C9B—C10B—H10A	109.5	C5B—C6B—C9B	120.40 (15)
C9B—C10B—H10B	109.5	C8A—C7A—C6A	121.27 (17)
H10A—C10B—H10B	109.5	C8A—C7A—H7A	119.4
C9B—C10B—H10C	109.5	C6A—C7A—H7A	119.4
H10A—C10B—H10C	109.5	C8B—C7B—C6B	121.33 (18)
H10B—C10B—H10C	109.5	C8B—C7B—H7B	119.3
C2A—C1A—H1A1	109.5	C6B—C7B—H7B	119.3
C2A—C1A—H1A2	109.5	C3A—C8A—C7A	119.29 (16)
H1A1—C1A—H1A2	109.5	C3A—C8A—H8A	120.4
C2A—C1A—H1A3	109.5	C7A—C8A—H8A	120.4
H1A1—C1A—H1A3	109.5	C3B—C8B—C7B	119.06 (17)
H1A2—C1A—H1A3	109.5	C3B—C8B—H8B	120.5
C2B—C1B—H1B1	109.5	C7B—C8B—H8B	120.5
C2B—C1B—H1B2	109.5	N1A—C9A—C6A	115.51 (15)
H1B1—C1B—H1B2	109.5	N1A—C9A—C10A	124.10 (15)
C2B—C1B—H1B3	109.5	C6A—C9A—C10A	120.39 (14)
H1B1—C1B—H1B3	109.5	N1B—C9B—C6B	115.48 (15)
H1B2—C1B—H1B3	109.5	N1B—C9B—C10B	125.51 (15)
O1A—C2A—O2A	122.19 (17)	C6B—C9B—C10B	119.01 (15)
O1A—C2A—C1A	127.08 (18)	C9A—C10A—H10D	109.5
O2A—C2A—C1A	110.72 (17)	C9A—C10A—H10E	109.5
O1B—C2B—O2B	122.74 (16)	H10D—C10A—H10E	109.5
O1B—C2B—C1B	126.04 (18)	C9A—C10A—H10F	109.5
O2B—C2B—C1B	111.22 (17)	H10D—C10A—H10F	109.5
C8A—C3A—C4A	121.15 (15)	H10E—C10A—H10F	109.5
C8A—C3A—O2A	120.42 (15)	N3A—C11A—N2A	117.60 (14)
C4A—C3A—O2A	118.20 (16)	N3A—C11A—S1A	122.72 (13)
C8B—C3B—C4B	121.45 (16)	N2A—C11A—S1A	119.68 (12)
C8B—C3B—O2B	119.99 (17)	N3B—C11B—N2B	117.47 (15)
C4B—C3B—O2B	118.50 (17)	N3B—C11B—S1B	122.55 (13)
C3A—C4A—C5A	119.40 (17)	N2B—C11B—S1B	119.94 (13)
C3A—C4A—H4A	120.3	C9A—N1A—N2A	118.53 (14)
C5A—C4A—H4A	120.3	C9B—N1B—N2B	118.72 (14)
C3B—C4B—C5B	119.52 (18)	C11A—N2A—N1A	118.60 (13)
C3B—C4B—H4B	120.2	C11A—N2A—H2A	120.7
C5B—C4B—H4B	120.2	N1A—N2A—H2A	120.7
C4A—C5A—C6A	121.19 (16)	C11B—N2B—N1B	119.63 (14)
C4A—C5A—H5A	119.4	C11B—N2B—H2B	120.2
C6A—C5A—H5A	119.4	N1B—N2B—H2B	120.2
C4B—C5B—C6B	120.83 (17)	C11A—N3A—H3A1	120.0
C4B—C5B—H5B	119.6	C11A—N3A—H3A2	120.0
C6B—C5B—H5B	119.6	H3A1—N3A—H3A2	120.0
C7A—C6A—C5A	117.68 (15)	C11B—N3B—H3B1	120.0
C7A—C6A—C9A	121.51 (15)	C11B—N3B—H3B2	120.0
C5A—C6A—C9A	120.79 (14)	H3B1—N3B—H3B2	120.0
C7B—C6B—C5B	117.77 (16)	C2A—O2A—C3A	118.74 (14)
C7B—C6B—C9B	121.82 (16)	C2B—O2B—C3B	117.30 (14)

C8A—C3A—C4A—C5A	0.9 (3)	C5A—C6A—C9A—C10A	166.64 (18)
O2A—C3A—C4A—C5A	−173.63 (15)	C7B—C6B—C9B—N1B	170.96 (17)
C8B—C3B—C4B—C5B	−1.6 (3)	C5B—C6B—C9B—N1B	−8.5 (2)
O2B—C3B—C4B—C5B	−178.73 (17)	C7B—C6B—C9B—C10B	−8.7 (3)
C3A—C4A—C5A—C6A	−0.6 (3)	C5B—C6B—C9B—C10B	171.80 (17)
C3B—C4B—C5B—C6B	−0.1 (3)	C6A—C9A—N1A—N2A	177.13 (13)
C4A—C5A—C6A—C7A	−0.3 (3)	C10A—C9A—N1A—N2A	−3.3 (3)
C4A—C5A—C6A—C9A	177.89 (16)	C6B—C9B—N1B—N2B	179.76 (14)
C4B—C5B—C6B—C7B	1.4 (3)	C10B—C9B—N1B—N2B	−0.6 (3)
C4B—C5B—C6B—C9B	−179.04 (17)	N3A—C11A—N2A—N1A	−7.3 (2)
C5A—C6A—C7A—C8A	1.0 (2)	S1A—C11A—N2A—N1A	173.06 (12)
C9A—C6A—C7A—C8A	−177.17 (15)	C9A—N1A—N2A—C11A	168.09 (16)
C5B—C6B—C7B—C8B	−1.2 (3)	N3B—C11B—N2B—N1B	3.0 (3)
C9B—C6B—C7B—C8B	179.30 (17)	S1B—C11B—N2B—N1B	−174.85 (12)
C4A—C3A—C8A—C7A	−0.2 (3)	C9B—N1B—N2B—C11B	172.12 (16)
O2A—C3A—C8A—C7A	174.20 (15)	O1A—C2A—O2A—C3A	7.0 (3)
C6A—C7A—C8A—C3A	−0.8 (3)	C1A—C2A—O2A—C3A	−173.17 (16)
C4B—C3B—C8B—C7B	1.8 (3)	C8A—C3A—O2A—C2A	67.9 (2)
O2B—C3B—C8B—C7B	178.94 (17)	C4A—C3A—O2A—C2A	−117.52 (19)
C6B—C7B—C8B—C3B	−0.4 (3)	O1B—C2B—O2B—C3B	0.6 (3)
C7A—C6A—C9A—N1A	164.41 (16)	C1B—C2B—O2B—C3B	179.85 (16)
C5A—C6A—C9A—N1A	−13.8 (2)	C8B—C3B—O2B—C2B	84.9 (2)
C7A—C6A—C9A—C10A	−15.2 (3)	C4B—C3B—O2B—C2B	−97.9 (2)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C3*A*–C8*A* and C3*B*–C8*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3*A*—H3*A*1···N1*A*	0.86	2.26	2.617 (2)	105
N3*B*—H3*B*1···N1*B*	0.86	2.28	2.633 (2)	105
N2*A*—H2*A*···S1*B*	0.86	2.63	3.4724 (15)	167
N2*B*—H2*B*···S1*A*	0.86	2.71	3.4228 (16)	141
N3*A*—H3*A*1···O1*B*^{i}	0.86	2.44	3.164 (2)	142
N3*B*—H3*B*2···S1*A*^{ii}	0.86	2.57	3.4262 (17)	176
N3*A*—H3*A*2···*Cg*2^{iii}	0.86	2.62	3.4763 (19)	130
C1*B*—H1*B*3···*Cg*1^{iv}	0.96	2.73	3.691 (3)	154

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

(II) (*E*)-4-[1-(2-Carbamothioylhydrazinylidene)ethyl]phenyl benzoate

Crystal data

$C_{16}H_{15}N_3O_2S$
M_r = 313.37
Triclinic, $P\overline{1}$
a = 7.8145 (4) Å
b = 9.7538 (5) Å
c = 10.9050 (7) Å
α = 78.855 (4)°
β = 69.031 (2)°
γ = 84.200 (3)°
V = 761.05 (8) Å^3
Z = 2
F(000) = 328
D_x = 1.367 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3154 reflections
θ = 2.0–26.5°

μ = 0.22 mm^{-1}
T = 293 K

Block, pale-yellow
0.25 × 0.18 × 0.14 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.745, T_{max} = 0.865
11596 measured reflections

3154 independent reflections
2857 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.5°, θ_{min} = 2.0°
h = −8→9
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.099
S = 1.05
3154 reflections
201 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.1914P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.080 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	−0.0574 (2)	0.60395 (15)	0.12357 (14)	0.0461 (3)
H1	0.0581	0.6165	0.1252	0.055*
C2	−0.1286 (2)	0.69706 (17)	0.03984 (16)	0.0562 (4)
H2	−0.0616	0.7736	−0.0138	0.067*
C3	−0.2978 (3)	0.67730 (18)	0.03519 (16)	0.0596 (4)
H3	−0.3439	0.7398	−0.0223	0.072*
C4	−0.3993 (2)	0.56519 (19)	0.11541 (17)	0.0579 (4)
H4	−0.5134	0.5519	0.1117	0.069*
C5	−0.3315 (2)	0.47264 (16)	0.20141 (15)	0.0483 (3)
H5	−0.4005	0.3977	0.2567	0.058*
C6	−0.15975 (18)	0.49176 (14)	0.20510 (12)	0.0384 (3)
C7	−0.09783 (18)	0.39381 (14)	0.30353 (12)	0.0392 (3)
C8	0.15463 (18)	0.31751 (15)	0.37198 (13)	0.0400 (3)
C9	0.15816 (19)	0.17391 (15)	0.39018 (14)	0.0442 (3)
H9	0.1159	0.1286	0.3395	0.053*
C10	0.22566 (19)	0.09777 (14)	0.48531 (14)	0.0412 (3)
H10	0.2247	0.0006	0.5004	0.049*
C11	0.29489 (16)	0.16457 (13)	0.55862 (12)	0.0346 (3)

C12	0.29666 (19)	0.31025 (14)	0.53336 (14)	0.0406 (3)
H12	0.3466	0.3565	0.5790	0.049*
C13	0.22498 (19)	0.38662 (14)	0.44118 (14)	0.0433 (3)
H13	0.2243	0.4838	0.4260	0.052*
C14	0.36348 (17)	0.08555 (13)	0.66391 (12)	0.0353 (3)
C15	0.2849 (2)	−0.05203 (16)	0.73732 (16)	0.0549 (4)
H15A	0.3642	−0.1019	0.7820	0.082*
H15B	0.2737	−0.1056	0.6755	0.082*
H15C	0.1661	−0.0373	0.8018	0.082*
C16	0.70223 (17)	0.13075 (13)	0.78932 (12)	0.0358 (3)
N1	0.48733 (14)	0.14652 (11)	0.68311 (10)	0.0361 (2)
N2	0.54777 (15)	0.08471 (11)	0.78611 (11)	0.0374 (2)
H2A	0.4883	0.0188	0.8464	0.045*
N3	0.79854 (16)	0.21798 (13)	0.68277 (11)	0.0467 (3)
H3A	0.7611	0.2423	0.6162	0.056*
H3B	0.8984	0.2502	0.6803	0.056*
O1	−0.19599 (15)	0.31803 (12)	0.39711 (10)	0.0550 (3)
O2	0.08423 (13)	0.40017 (11)	0.27880 (9)	0.0477 (3)
S1	0.77088 (5)	0.07598 (4)	0.92056 (4)	0.05405 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0487 (8)	0.0491 (8)	0.0399 (7)	−0.0026 (6)	−0.0165 (6)	−0.0032 (6)
C2	0.0671 (10)	0.0487 (8)	0.0458 (8)	0.0029 (7)	−0.0183 (7)	0.0033 (6)
C3	0.0728 (11)	0.0613 (10)	0.0465 (8)	0.0207 (8)	−0.0300 (8)	−0.0070 (7)
C4	0.0528 (9)	0.0721 (10)	0.0583 (9)	0.0112 (8)	−0.0323 (8)	−0.0149 (8)
C5	0.0451 (8)	0.0555 (8)	0.0467 (8)	−0.0013 (6)	−0.0206 (6)	−0.0055 (6)
C6	0.0423 (7)	0.0432 (7)	0.0315 (6)	0.0014 (5)	−0.0157 (5)	−0.0067 (5)
C7	0.0409 (7)	0.0454 (7)	0.0333 (6)	−0.0030 (5)	−0.0159 (5)	−0.0048 (5)
C8	0.0341 (6)	0.0523 (7)	0.0320 (6)	−0.0008 (5)	−0.0134 (5)	0.0004 (5)
C9	0.0457 (7)	0.0526 (8)	0.0419 (7)	0.0009 (6)	−0.0224 (6)	−0.0131 (6)
C10	0.0426 (7)	0.0409 (7)	0.0447 (7)	0.0023 (5)	−0.0196 (6)	−0.0112 (5)
C11	0.0308 (6)	0.0398 (6)	0.0328 (6)	0.0008 (5)	−0.0115 (5)	−0.0055 (5)
C12	0.0425 (7)	0.0419 (7)	0.0429 (7)	−0.0020 (5)	−0.0211 (6)	−0.0073 (5)
C13	0.0451 (7)	0.0394 (7)	0.0473 (7)	−0.0026 (5)	−0.0214 (6)	−0.0006 (5)
C14	0.0332 (6)	0.0384 (6)	0.0345 (6)	0.0000 (5)	−0.0128 (5)	−0.0054 (5)
C15	0.0616 (10)	0.0520 (8)	0.0568 (9)	−0.0181 (7)	−0.0328 (8)	0.0094 (7)
C16	0.0333 (6)	0.0364 (6)	0.0365 (6)	−0.0022 (5)	−0.0130 (5)	−0.0010 (5)
N1	0.0360 (5)	0.0396 (5)	0.0339 (5)	−0.0005 (4)	−0.0162 (4)	−0.0013 (4)
N2	0.0365 (6)	0.0404 (6)	0.0354 (5)	−0.0073 (4)	−0.0166 (4)	0.0047 (4)
N3	0.0427 (6)	0.0574 (7)	0.0394 (6)	−0.0168 (5)	−0.0187 (5)	0.0098 (5)
O1	0.0480 (6)	0.0675 (7)	0.0456 (6)	−0.0137 (5)	−0.0208 (5)	0.0146 (5)
O2	0.0404 (5)	0.0622 (6)	0.0387 (5)	−0.0055 (4)	−0.0193 (4)	0.0083 (4)
S1	0.0454 (2)	0.0720 (3)	0.0464 (2)	−0.01842 (18)	−0.02749 (17)	0.01713 (18)

Geometric parameters (Å, º)

C1—C2	1.381 (2)	C10—C11	1.3923 (18)
C1—C6	1.3853 (19)	C10—H10	0.9300
C1—H1	0.9300	C11—C12	1.3947 (18)
C2—C3	1.375 (3)	C11—C14	1.4881 (17)
C2—H2	0.9300	C12—C13	1.3815 (18)
C3—C4	1.378 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.381 (2)	C14—N1	1.2820 (16)
C4—H4	0.9300	C14—C15	1.4894 (18)
C5—C6	1.389 (2)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600
C6—C7	1.4767 (17)	C15—H15C	0.9600
C7—O1	1.1995 (16)	C16—N3	1.3273 (16)
C7—O2	1.3555 (16)	C16—N2	1.3437 (16)
C8—C9	1.375 (2)	C16—S1	1.6785 (13)
C8—C13	1.376 (2)	N1—N2	1.3816 (14)
C8—O2	1.4067 (15)	N2—H2A	0.8600
C9—C10	1.3858 (19)	N3—H3A	0.8600
C9—H9	0.9300	N3—H3B	0.8600
C2—C1—C6	119.40 (14)	C10—C11—C12	118.52 (12)
C2—C1—H1	120.3	C10—C11—C14	122.07 (11)
C6—C1—H1	120.3	C12—C11—C14	119.40 (11)
C3—C2—C1	120.47 (15)	C13—C12—C11	120.66 (12)
C3—C2—H2	119.8	C13—C12—H12	119.7
C1—C2—H2	119.8	C11—C12—H12	119.7
C2—C3—C4	120.27 (14)	C8—C13—C12	119.37 (13)
C2—C3—H3	119.9	C8—C13—H13	120.3
C4—C3—H3	119.9	C12—C13—H13	120.3
C3—C4—C5	119.92 (16)	N1—C14—C11	114.67 (11)
C3—C4—H4	120.0	N1—C14—C15	126.07 (12)
C5—C4—H4	120.0	C11—C14—C15	119.26 (11)
C4—C5—C6	119.80 (14)	C14—C15—H15A	109.5
C4—C5—H5	120.1	C14—C15—H15B	109.5
C6—C5—H5	120.1	H15A—C15—H15B	109.5
C1—C6—C5	120.12 (13)	C14—C15—H15C	109.5
C1—C6—C7	122.27 (12)	H15A—C15—H15C	109.5
C5—C6—C7	117.51 (12)	H15B—C15—H15C	109.5
O1—C7—O2	122.72 (12)	N3—C16—N2	116.66 (11)
O1—C7—C6	124.71 (12)	N3—C16—S1	122.30 (10)
O2—C7—C6	112.56 (11)	N2—C16—S1	121.02 (9)
C9—C8—C13	121.44 (12)	C14—N1—N2	118.03 (10)
C9—C8—O2	121.45 (12)	C16—N2—N1	117.98 (10)
C13—C8—O2	117.08 (12)	C16—N2—H2A	121.0
C8—C9—C10	118.95 (12)	N1—N2—H2A	121.0
C8—C9—H9	120.5	C16—N3—H3A	120.0

C10—C9—H9	120.5	C16—N3—H3B	120.0
C9—C10—C11	120.96 (12)	H3A—N3—H3B	120.0
C9—C10—H10	119.5	C7—O2—C8	116.96 (10)
C11—C10—H10	119.5		

C6—C1—C2—C3	−1.3 (2)	C14—C11—C12—C13	−176.57 (12)
C1—C2—C3—C4	0.8 (3)	C9—C8—C13—C12	−1.6 (2)
C2—C3—C4—C5	0.4 (3)	O2—C8—C13—C12	−179.67 (12)
C3—C4—C5—C6	−1.0 (2)	C11—C12—C13—C8	−1.3 (2)
C2—C1—C6—C5	0.7 (2)	C10—C11—C14—N1	152.10 (12)
C2—C1—C6—C7	−175.72 (13)	C12—C11—C14—N1	−28.98 (17)
C4—C5—C6—C1	0.5 (2)	C10—C11—C14—C15	−28.60 (19)
C4—C5—C6—C7	177.06 (13)	C12—C11—C14—C15	150.32 (14)
C1—C6—C7—O1	160.66 (14)	C11—C14—N1—N2	175.16 (10)
C5—C6—C7—O1	−15.8 (2)	C15—C14—N1—N2	−4.1 (2)
C1—C6—C7—O2	−18.01 (18)	N3—C16—N2—N1	−9.43 (18)
C5—C6—C7—O2	165.53 (12)	S1—C16—N2—N1	172.24 (9)
C13—C8—C9—C10	3.3 (2)	C14—N1—N2—C16	166.17 (12)
O2—C8—C9—C10	−178.70 (12)	O1—C7—O2—C8	−2.8 (2)
C8—C9—C10—C11	−2.2 (2)	C6—C7—O2—C8	175.91 (11)
C9—C10—C11—C12	−0.6 (2)	C9—C8—O2—C7	66.31 (17)
C9—C10—C11—C14	178.29 (12)	C13—C8—O2—C7	−115.64 (14)
C10—C11—C12—C13	2.4 (2)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C8–C13 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1	0.86	2.24	2.5953 (18)	105
N2—H2*A*···S1^{i}	0.86	2.68	3.4697 (12)	153
N3—H3*A*···O1^{ii}	0.86	2.27	3.0653 (15)	153
C15—H15*B*···O1^{iii}	0.96	2.55	3.454 (2)	156
N3—H3*B*···*Cg*2^{ii}	0.86	2.47	3.3385 (15)	122

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