

# Crystal structure and Hirshfeld surface analysis of (*E*)-*N*-(4-propoxybenzylidene)benzo[*d*]thiazol-2-amine

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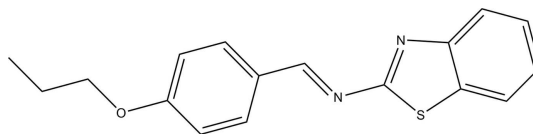
**Supporting information:** this article has supporting information at journals.iucr.org/e

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The title compound, C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>OS, was synthesized by a condensation reaction between 2-amino benzothiazole and 4-*N*-propoxybenzaldehyde. The benzo[*d*]thiazole ring system is nearly planar (r.m.s. deviation 0.0088 Å) and makes a dihedral angle of 3.804 (12)° with the phenyl ring. The configuration about the C=N double bond is *E*. In the crystal structure, pairs of C—H···N hydrogen bonds and C—H···π interactions link the molecules into inversion dimers with an R<sub>2</sub><sup>2</sup>(16) ring motif. These dimers are additionally linked by weak π–π stacking interactions between the phenyl rings, leading to a layered arrangement parallel to (010). Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the packing arrangement are from H···H (47.9%) and C···H/H···C (25.6%) interactions.

## 1. Chemical context

Benzothiazole is one of the most important heterocyclic compounds, comprising of a sulfur and a nitrogen atom that constitute the core structure of thiazole. Benzothiazole is a weak base, and is widely found in bioorganic and medicinal chemistry with application in drug discovery as a pharmacologically and biologically active compound (Quin & Tyrell, 2010). Benzothiazole and its derivatives show numerous biological activities such as antimicrobial, anticancer, anthelmintic or anti-diabetic. They have also found application in industry as antioxidants and vulcanization accelerators (Achaiah *et al.*, 2016).



Schiff bases (Schiff, 1864) are nitrogen analogues of aldehydes or ketones in which the corresponding functional group has been replaced by an imine or azomethine group. They can be synthesized from the reaction of primary amines with an aldehyde or a ketone under particular conditions. Schiff bases are some of the most widely used organic compounds, utilized, for example, as catalysts, pigments and dyes, intermediates in organic synthesis, or as polymer stabilizers. Moreover, Schiff bases exhibit a broad range of biological activities such as antiviral, antibacterial, anti-inflammatory, antimalarial, anti-

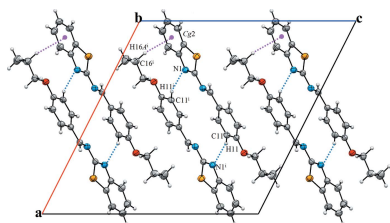


Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the C1–C6 phenyl ring.

D–H...A	D–H	H...A	D...A	D–H...A
C11–H11...N1 <sup>i</sup>	0.93	2.49	3.362 (3)	157
C16–H16A...Cg2 <sup>ii</sup>	0.97	2.91 (2)	3.765 (3)	147

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

fungal, anti-proliferative and antipyretic properties (Bhoi *et al.*, 2015).

In the context given above, we report here the synthesis, molecular and crystal structure of the Schiff base C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>OS, comprising a benzothiazole moiety.

## 2. Structural commentary

The asymmetric unit of the title compound is comprised of one molecule (Fig. 1), which exhibits an *E* configuration for the imine functionality. The benzo[*d*]thiazole ring system is nearly planar [r.m.s. deviation 0.0088 Å, with the largest deviation being 0.0127 (18) Å for atom C4]. The benzo[*d*]thiazole ring system and the phenyl ring (C9–C14) are slightly twisted with respect to each other, making a dihedral angle of 3.804 (12)°. In the thiazole ring, the C6–N1 [1.379 (3) Å] and C7–N1 [1.288 (3) Å] distances indicate substantial electronic delocalization. The C8=N2 double bond has a length of 1.272 (3) Å, and thus is slightly longer than comparable bonds found in other Schiff base structures (Sen *et al.*, 2018; Kansiz *et al.*, 2018), which are in the range of 1.262 (3)–1.270 (3) Å. The methyl group of the propyl chain is moved out by 59.2 (3)° from the mean plane of the rest of the molecule.

## 3. Supramolecular features

In the crystal structure, molecules are linked by C–H... $\pi$  hydrogen bonds (Table 1) between one of the methylene C atoms of the propyl group (C16–H16A) and the centroid of the C1–C6 phenyl ring (Cg2) of an adjacent molecule (Fig. 2). Pairs of additional C–H...N hydrogen bonds form inversion dimers with an *R*<sub>2</sub><sup>2</sup>(16) ring motif (Fig. 2). The dimers are additionally linked by weak  $\pi$ – $\pi$  interactions, with a centroid-to-centroid distance of 4.695 (2) Å between Cg3 and Cg3<sup>i</sup> [Symmetry code: (i):  $-x + 1, -y + 2, -z$ ] where Cg3 is the

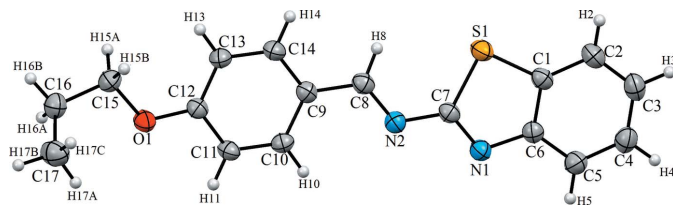


Figure 1

The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 40% probability level.

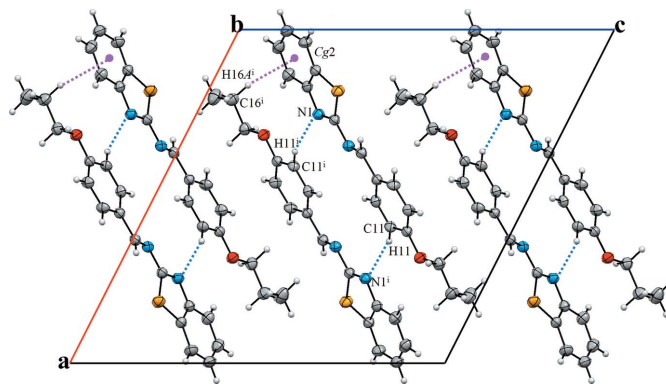


Figure 2

A view of the crystal packing of the title compound. Intermolecular interactions are displayed by dotted lines. The symmetry code refers to Table 1.

centroid of the C9–C14 phenyl ring. The resulting supramolecular network is layered and expands parallel to (010).

## 4. Hirshfeld surface analysis

Hirshfeld surface analysis together with two-dimensional fingerprint plots are a powerful tool for the visualization and interpretation of intermolecular contacts in molecular crystals (Spackman & Jayatilaka, 2009). The corresponding surfaces and fingerprint plots were obtained using *CrystalExplorer* (Turner *et al.*, 2017). The  $d_{\text{norm}}$  and molecular electrostatic potential maps for the title compound are shown in Fig. 3a and

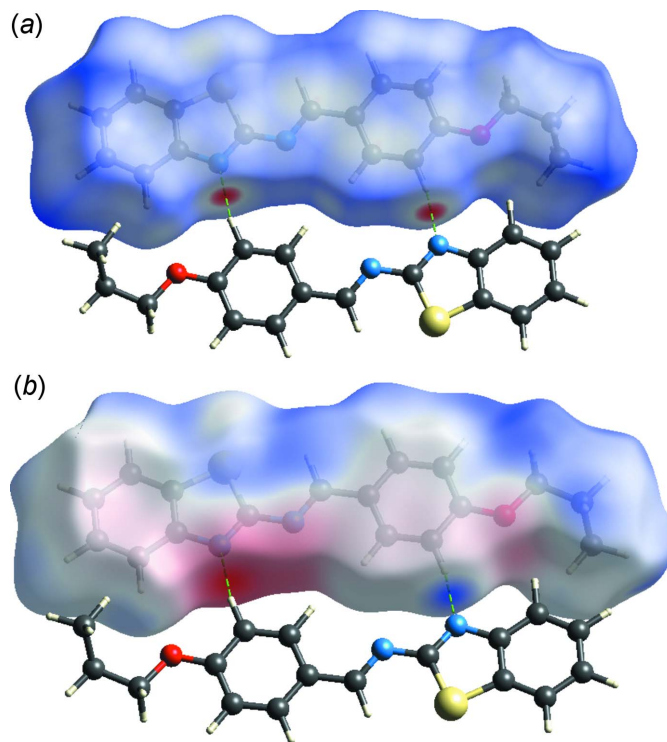
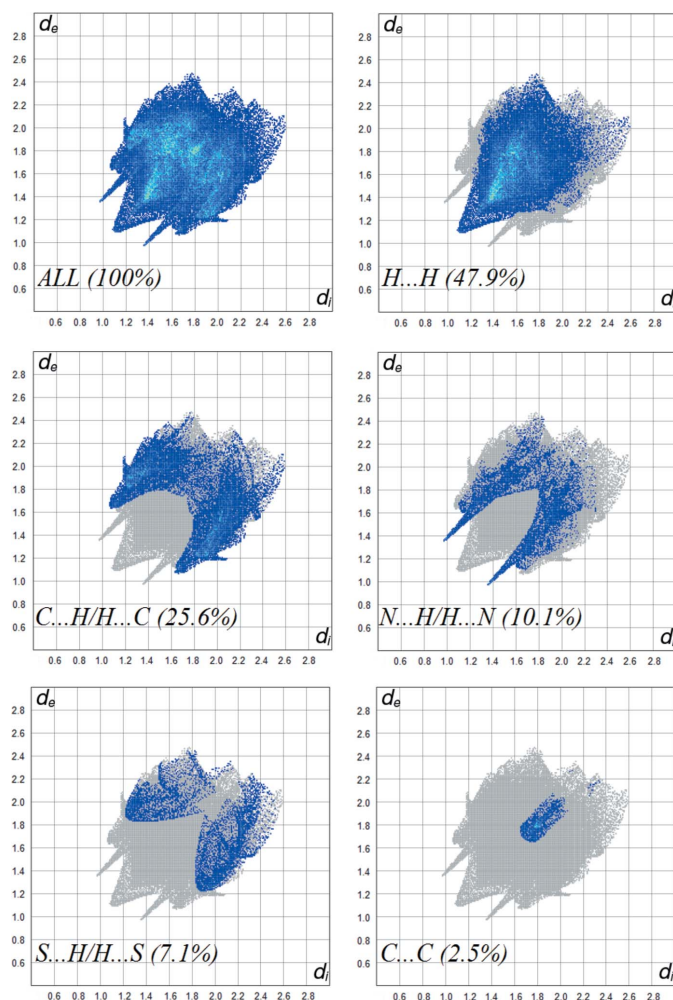


Figure 3

The Hirshfeld surface of the title compound mapped over (a)  $d_{\text{norm}}$  and (b) electrostatic potential, showing the C–H...N hydrogen bond.



**Figure 4**  
Two-dimensional fingerprint plots, showing the relative contribution of the atom-pair interactions to the Hirshfeld surface.

3*b*, respectively, with the prominent hydrogen-bonding interactions shown as red spots. The red spots identified in Fig. 3*a* correspond to the H $\cdots$ N contacts resulting from hydrogen bond C—H $\cdots$ N (Table 1). The most important contribution to the Hirshfeld surface comes from H $\cdots$ H contacts with 47.9%. C $\cdots$ H and N $\cdots$ H interactions follow with 25.6% and 10.1% contributions, respectively (Fig. 4). Other minor contributors are S $\cdots$ H/H $\cdots$ S (7.1%), C $\cdots$ C (2.5%), O $\cdots$ H/H $\cdots$ O (2.1%), C $\cdots$ N/N $\cdots$ C (1.8%), C $\cdots$ S/S $\cdots$ C (1.1%) and C $\cdots$ O/O $\cdots$ C (0.8%).

## 5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.41, update of November 2019; Groom *et al.*, 2016) for an (*E*)-*N*-benzylidenebenzo[*d*]thiazol-2-amine skeleton gave 20 hits. Of these 20, the most similar to the title compound are 2-[(6-methoxy-1,3-benzothiazol-2-yl)carboimidoyl]phenol (SUFFEG; Hijji *et al.*, 2015), (*E*)-2-[(6-ethoxybenzothiazol-2-yl)iminomethyl]-6-methoxyphenol (VOQKAO; Kong, 2009) and 2-[(1,3-benzothiazol-2-ylimino)methyl]phenol

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub>
<i>M<sub>r</sub></i>	296.38
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	17.251 (1), 5.6849 (3), 17.3101 (11)
$\beta$ (°)	116.958 (4)
<i>V</i> (Å <sup>3</sup> )	1513.14 (16)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.21
Crystal size (mm)	0.67 $\times$ 0.34 $\times$ 0.04
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration ( <i>X-RED32</i> ; Stoe & Cie, 2002)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.896, 0.983
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	10315, 2962, 1950
<i>R<sub>int</sub></i>	0.048
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.617
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.045, 0.099, 0.98
No. of reflections	2962
No. of parameters	191
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.14, -0.13

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXT2017/1* (Sheldrick, 2015*a*), *SHELXL2017/1* (Sheldrick, 2015*b*), *PLATON* (Spek, 2020) and *WinGX* (Farrugia, 2012).

(VOQQOP01; Asiri *et al.*, 2010). All these compounds have an *E* configuration about the C=N imine bond, and have similar bond lengths and angles as mentioned above for the title compound.

## 6. Synthesis and crystallization

2-Amino benzothiazole (0.3 g, 2 mmol) was dissolved in 10 ml of 1-propanol in a 50 ml borosilicate glass beaker. 4-*N*-Propoxybenzaldehyde (0.328 g, 2 mmol) was then added dropwise into the mixture under stirring, in the presence of a catalytic amount of glacial acetic acid. The reaction mixture was then placed inside an unmodified household microwave oven and was irradiated for 32 min (eight pulses each of 4 min) at 540 W power, with short interruptions of one minute. The progress of the reaction was monitored by thin-layer chromatography using ethyl acetate and *n*-hexane (3:7 *v:v*) as eluent (*R<sub>f</sub>* = 0.69). The formed precipitate was filtered off, washed with 1-propanol, and dried. The resulting solid was further purified by recrystallization from *n*-hexane to give the pure imine as a crystalline solid (yield: 72.4%, m.p. 357–358 K).

## 7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were placed in idealized positions and refined using a riding model with C—H

= 0.93–0.97 Å with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$  and  $1.2U_{\text{eq}}(\text{C})$  for other C-bound H atoms.

### Funding information

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## supporting information

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## Crystal structure and Hirshfeld surface analysis of (*E*)-*N*-(4-propyloxybenzylidene)benzo[*d*]thiazol-2-amine

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### Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXT2017/1* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2020); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

### (*E*)-*N*-(4-Propyloxybenzylidene)benzo[*d*]thiazol-2-amine

#### Crystal data

C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>OS

*M<sub>r</sub>* = 296.38

Monoclinic, *P2<sub>1</sub>/c*

*a* = 17.251 (1) Å

*b* = 5.6849 (3) Å

*c* = 17.3101 (11) Å

β = 116.958 (4)°

*V* = 1513.14 (16) Å<sup>3</sup>

*Z* = 4

*F*(000) = 624

*D<sub>x</sub>* = 1.301 Mg m<sup>-3</sup>

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 9824 reflections

θ = 2.4–28.1°

μ = 0.21 mm<sup>-1</sup>

*T* = 296 K

Plate, yellow

0.67 × 0.34 × 0.04 mm

#### Data collection

Stoe IPDS 2

diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus

Detector resolution: 6.67 pixels mm<sup>-1</sup>

rotation method scans

Absorption correction: integration

(*X-RED32*; Stoe & Cie, 2002)

*T<sub>min</sub>* = 0.896, *T<sub>max</sub>* = 0.983

10315 measured reflections

2962 independent reflections

1950 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.048

θ<sub>max</sub> = 26.0°, θ<sub>min</sub> = 2.4°

*h* = -21 → 21

*k* = -7 → 7

*l* = -21 → 19

#### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.045

*wR*(*F*<sup>2</sup>) = 0.099

*S* = 0.98

2962 reflections

191 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0451*P*)<sup>2</sup>]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> < 0.001

Δρ<sub>max</sub> = 0.14 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.13 e Å<sup>-3</sup>

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.18402 (4)	0.57314 (11)	0.34622 (4)	0.0693 (2)
O1	0.68408 (9)	0.4674 (3)	0.79162 (9)	0.0670 (4)
N2	0.34892 (11)	0.7538 (3)	0.44924 (11)	0.0594 (4)
N1	0.25411 (11)	0.9575 (3)	0.32624 (11)	0.0605 (4)
C7	0.27040 (13)	0.7771 (4)	0.37623 (13)	0.0548 (5)
C9	0.44990 (12)	0.5343 (4)	0.57024 (12)	0.0536 (5)
C12	0.60529 (13)	0.4773 (4)	0.72070 (12)	0.0543 (5)
C8	0.36920 (13)	0.5628 (4)	0.49215 (13)	0.0594 (5)
H8	0.330649	0.436935	0.472533	0.071*
C6	0.17124 (13)	0.9462 (4)	0.25862 (13)	0.0574 (5)
C1	0.12228 (13)	0.7506 (4)	0.25832 (13)	0.0591 (5)
C10	0.51498 (13)	0.7056 (4)	0.59654 (12)	0.0570 (5)
H10	0.506190	0.841213	0.563558	0.068*
C11	0.59124 (13)	0.6761 (4)	0.67003 (13)	0.0581 (5)
H11	0.634211	0.790845	0.686230	0.070*
C14	0.46538 (14)	0.3363 (4)	0.62163 (14)	0.0635 (6)
H14	0.422987	0.219895	0.604920	0.076*
C15	0.70221 (14)	0.2747 (4)	0.85021 (13)	0.0671 (6)
H15A	0.700893	0.127967	0.821055	0.081*
H15B	0.658921	0.266962	0.871337	0.081*
C13	0.54145 (14)	0.3061 (4)	0.69666 (13)	0.0619 (5)
H13	0.549857	0.172823	0.730695	0.074*
C5	0.13532 (15)	1.1122 (4)	0.19285 (14)	0.0718 (6)
H5	0.167215	1.243665	0.192412	0.086*
C16	0.79051 (15)	0.3130 (5)	0.92404 (15)	0.0773 (7)
H16A	0.832723	0.320157	0.901537	0.093*
H16B	0.805157	0.179131	0.962854	0.093*
C2	0.03805 (15)	0.7197 (5)	0.19350 (15)	0.0742 (6)
H2	0.005409	0.589611	0.193574	0.089*
C3	0.00415 (16)	0.8855 (5)	0.12943 (16)	0.0789 (7)
H3	-0.052292	0.867632	0.085531	0.095*
C4	0.05246 (17)	1.0798 (5)	0.12880 (15)	0.0777 (7)
H4	0.028216	1.189367	0.084265	0.093*
C17	0.7977 (2)	0.5324 (5)	0.97463 (17)	0.0988 (9)
H17A	0.790480	0.667237	0.938607	0.148*
H17B	0.853871	0.538215	1.024129	0.148*
H17C	0.753332	0.532467	0.993616	0.148*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0643 (3)	0.0685 (4)	0.0671 (3)	-0.0171 (3)	0.0228 (3)	0.0012 (3)
O1	0.0604 (9)	0.0715 (10)	0.0616 (8)	-0.0100 (7)	0.0210 (7)	0.0101 (8)
N2	0.0560 (10)	0.0623 (12)	0.0584 (10)	-0.0022 (9)	0.0246 (9)	-0.0007 (9)
N1	0.0549 (10)	0.0621 (11)	0.0612 (10)	-0.0054 (9)	0.0236 (9)	0.0008 (9)
C7	0.0539 (12)	0.0579 (13)	0.0551 (11)	-0.0053 (10)	0.0271 (10)	-0.0050 (11)
C9	0.0524 (11)	0.0560 (13)	0.0557 (11)	-0.0021 (10)	0.0274 (10)	-0.0045 (10)
C12	0.0536 (11)	0.0575 (13)	0.0550 (11)	-0.0029 (10)	0.0275 (10)	-0.0014 (10)
C8	0.0570 (12)	0.0614 (14)	0.0635 (12)	-0.0044 (11)	0.0305 (11)	-0.0050 (12)
C6	0.0565 (12)	0.0599 (13)	0.0550 (11)	0.0021 (11)	0.0246 (10)	-0.0044 (11)
C1	0.0572 (12)	0.0614 (13)	0.0594 (12)	-0.0056 (10)	0.0270 (10)	-0.0093 (10)
C10	0.0651 (13)	0.0516 (12)	0.0592 (12)	-0.0013 (10)	0.0325 (11)	0.0027 (10)
C11	0.0584 (12)	0.0552 (12)	0.0616 (12)	-0.0137 (10)	0.0282 (11)	-0.0034 (11)
C14	0.0579 (13)	0.0548 (13)	0.0759 (14)	-0.0098 (10)	0.0286 (12)	0.0004 (12)
C15	0.0700 (15)	0.0647 (14)	0.0652 (13)	0.0009 (12)	0.0294 (12)	0.0079 (12)
C13	0.0603 (13)	0.0539 (12)	0.0696 (13)	-0.0032 (11)	0.0278 (11)	0.0088 (11)
C5	0.0758 (16)	0.0652 (15)	0.0683 (14)	-0.0010 (12)	0.0273 (13)	0.0016 (12)
C16	0.0734 (16)	0.0823 (17)	0.0662 (14)	0.0032 (13)	0.0230 (12)	0.0061 (13)
C2	0.0589 (14)	0.0809 (17)	0.0744 (15)	-0.0115 (13)	0.0229 (12)	-0.0076 (14)
C3	0.0581 (13)	0.096 (2)	0.0686 (15)	0.0044 (14)	0.0160 (12)	-0.0107 (15)
C4	0.0792 (16)	0.0786 (17)	0.0643 (13)	0.0142 (15)	0.0229 (13)	0.0020 (13)
C17	0.117 (2)	0.093 (2)	0.0732 (15)	-0.0224 (17)	0.0309 (16)	-0.0068 (15)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

S1—C1	1.731 (2)	C14—C13	1.376 (3)
S1—C7	1.770 (2)	C14—H14	0.9300
O1—C12	1.358 (2)	C15—C16	1.495 (3)
O1—C15	1.428 (2)	C15—H15A	0.9700
N2—C8	1.272 (3)	C15—H15B	0.9700
N2—C7	1.378 (2)	C13—H13	0.9300
N1—C7	1.288 (3)	C5—C4	1.367 (3)
N1—C6	1.379 (3)	C5—H5	0.9300
C9—C14	1.384 (3)	C16—C17	1.496 (3)
C9—C10	1.397 (3)	C16—H16A	0.9700
C9—C8	1.444 (3)	C16—H16B	0.9700
C12—C11	1.383 (3)	C2—C3	1.368 (3)
C12—C13	1.385 (3)	C2—H2	0.9300
C8—H8	0.9300	C3—C4	1.387 (4)
C6—C5	1.390 (3)	C3—H3	0.9300
C6—C1	1.395 (3)	C4—H4	0.9300
C1—C2	1.387 (3)	C17—H17A	0.9600
C10—C11	1.364 (3)	C17—H17B	0.9600
C10—H10	0.9300	C17—H17C	0.9600
C11—H11	0.9300		

C1—S1—C7	88.68 (10)	O1—C15—H15A	110.1
C12—O1—C15	118.74 (16)	C16—C15—H15A	110.1
C8—N2—C7	120.89 (19)	O1—C15—H15B	110.1
C7—N1—C6	111.07 (18)	C16—C15—H15B	110.1
N1—C7—N2	121.13 (18)	H15A—C15—H15B	108.5
N1—C7—S1	115.23 (15)	C14—C13—C12	119.0 (2)
N2—C7—S1	123.60 (16)	C14—C13—H13	120.5
C14—C9—C10	117.71 (18)	C12—C13—H13	120.5
C14—C9—C8	121.1 (2)	C4—C5—C6	119.1 (2)
C10—C9—C8	121.2 (2)	C4—C5—H5	120.4
O1—C12—C11	115.01 (17)	C6—C5—H5	120.4
O1—C12—C13	125.19 (19)	C15—C16—C17	113.8 (2)
C11—C12—C13	119.79 (19)	C15—C16—H16A	108.8
N2—C8—C9	122.4 (2)	C17—C16—H16A	108.8
N2—C8—H8	118.8	C15—C16—H16B	108.8
C9—C8—H8	118.8	C17—C16—H16B	108.8
N1—C6—C5	124.7 (2)	H16A—C16—H16B	107.7
N1—C6—C1	115.69 (19)	C3—C2—C1	118.3 (2)
C5—C6—C1	119.6 (2)	C3—C2—H2	120.8
C2—C1—C6	121.0 (2)	C1—C2—H2	120.8
C2—C1—S1	129.72 (19)	C2—C3—C4	121.2 (2)
C6—C1—S1	109.32 (15)	C2—C3—H3	119.4
C11—C10—C9	120.7 (2)	C4—C3—H3	119.4
C11—C10—H10	119.6	C5—C4—C3	120.8 (2)
C9—C10—H10	119.6	C5—C4—H4	119.6
C10—C11—C12	120.63 (19)	C3—C4—H4	119.6
C10—C11—H11	119.7	C16—C17—H17A	109.5
C12—C11—H11	119.7	C16—C17—H17B	109.5
C13—C14—C9	122.1 (2)	H17A—C17—H17B	109.5
C13—C14—H14	118.9	C16—C17—H17C	109.5
C9—C14—H14	118.9	H17A—C17—H17C	109.5
O1—C15—C16	107.79 (18)	H17B—C17—H17C	109.5
C6—N1—C7—N2	-178.59 (17)	C14—C9—C10—C11	0.6 (3)
C6—N1—C7—S1	-0.9 (2)	C8—C9—C10—C11	-179.48 (19)
C8—N2—C7—N1	-170.83 (19)	C9—C10—C11—C12	-0.8 (3)
C8—N2—C7—S1	11.7 (3)	O1—C12—C11—C10	179.34 (18)
C1—S1—C7—N1	0.44 (17)	C13—C12—C11—C10	0.1 (3)
C1—S1—C7—N2	178.05 (17)	C10—C9—C14—C13	0.5 (3)
C15—O1—C12—C11	176.51 (18)	C8—C9—C14—C13	-179.47 (19)
C15—O1—C12—C13	-4.3 (3)	C12—O1—C15—C16	-177.16 (18)
C7—N2—C8—C9	-178.31 (17)	C9—C14—C13—C12	-1.2 (3)
C14—C9—C8—N2	171.56 (19)	O1—C12—C13—C14	-178.23 (19)
C10—C9—C8—N2	-8.4 (3)	C11—C12—C13—C14	1.0 (3)
C7—N1—C6—C5	-178.5 (2)	N1—C6—C5—C4	179.4 (2)
C7—N1—C6—C1	1.1 (2)	C1—C6—C5—C4	-0.2 (3)
N1—C6—C1—C2	-179.90 (19)	O1—C15—C16—C17	61.6 (3)
C5—C6—C1—C2	-0.3 (3)	C6—C1—C2—C3	0.3 (3)



N1—C6—C1—S1	-0.7 (2)	S1—C1—C2—C3	-178.68 (18)
C5—C6—C1—S1	178.91 (16)	C1—C2—C3—C4	0.1 (4)
C7—S1—C1—C2	179.3 (2)	C6—C5—C4—C3	0.6 (4)
C7—S1—C1—C6	0.16 (15)	C2—C3—C4—C5	-0.6 (4)

*Hydrogen-bond geometry (Å, °)*

*Cg2* is the centroid of the C1–C6 phenyl ring.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C11—H11 $\cdots$ N1 <sup>i</sup>	0.93	2.49	3.362 (3)	157
C16—H16 <i>A</i> $\cdots$ Cg2 <sup>ii</sup>	0.97	2.91 (2)	3.765 (3)	147

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