



Crystal structure and Hirshfeld surface analysis of 4-(naphthalen-2-yl)-*N*-[(*Z*)-4-propoxybenzylidene]-1,3-thiazol-2-amine

Ropak A. Sheakh Mohamad,^{a*} Wali M. Hamad^{b*} and Hashim J. Aziz^c

Received 28 April 2020

Accepted 17 May 2020

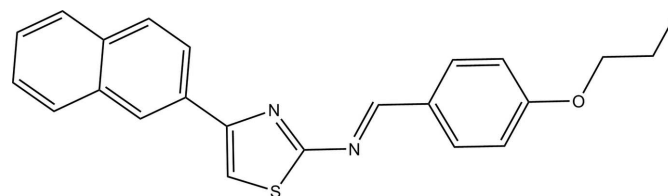
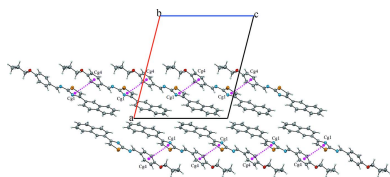
Edited by M. Weil, Vienna University of Technology, Austria

Keywords: Crystal structure; heterocyclic compound; thiazole; Schiff base; Hirshfeld surface analysis; crystal structure.**CCDC reference:** 2004309**Supporting information:** this article has supporting information at journals.iucr.org/e^aSalahaddin University, College of Science, Department of Chemistry, Erbil, Iraq, ^bKoya University, Faculty of Science and Health, Department of Chemistry, Koya, Iraq, and ^cSalahaddin University, College of Education, Department of Chemistry, Erbil, Iraq. *Correspondence e-mail: ropak.shekhmohamad@su.edu.krd, wali.hmd@koyauniversity.org

The asymmetric unit of the title compound, C₂₃H₂₀N₂OS, contains one slightly bent molecule. The naphthalene ring system and the thiazole ring are twisted with respect to each other, making a dihedral angle of 13.69 (10)°; the anisole ring is inclined to the plane of the naphthalene ring system, the dihedral angle being 14.22 (12)°. In the crystal structure, molecules are linked by C—H···π interactions, resulting in the formation of sheets parallel to (100). Within the sheets, very weak π–π stacking interactions lead to additional stabilization. Hirshfeld surface analysis and fingerprint plots reveal that the cohesion in the crystal structure is dominated by H···H (42.5%) and C···H/H···C (37.2%) contacts.

1. Chemical context

A Schiff base (Schiff, 1864) is a compound having the general formula RN=CR₂ (*R* = H, hydrocarbyl) and thus belongs to the family of imines (McNaught & Wilkinson, 1997). The chemistry of Schiff bases and their derivatives has been an interesting field of research since their discovery. Subsequently, Schiff bases have constituted a significant class of compounds for new drug development, exhibiting biological activities including antimicrobial, anti-tuberculosis, antioxidant, anti-inflammatory, anticonvulsant, antidepressant, anxiolytic, antihypertensive, anticancer and antifungal properties. The search for Schiff base-containing compounds with more selective activity and lower side effects continues to be an active area in medicinal chemistry (Kumar *et al.*, 2017). Likewise, heterocyclic compounds play an essential role in medicinal chemistry, or as key templates for the development of various therapeutic agents. As part of this family, thiazoles (Ghawla Amit *et al.*, 2014) and their derivatives have been found to possess anticonvulsant, antimicrobial, anti-inflammatory, anticancer, anti-HIV, antidiabetic, anti-Alzheimer, antihypertensive, and antioxidant activities. As a result of their potent and significant biological activities, they have excellent pharmaceutical importance (Kaur & Goyal, 2018).



OPEN ACCESS

Table 1
 Selected bond lengths (Å).

S1—C12	1.690 (3)	N1—C13	1.304 (3)
S1—C13	1.713 (3)	N1—C11	1.380 (3)
O1—C18	1.362 (3)	N2—C14	1.284 (3)
O1—C21	1.431 (3)	N2—C13	1.393 (3)

Here we report on the synthesis, structure determination and Hirshfeld analysis of a Schiff base, $C_{23}H_{20}N_2OS$, (**I**), comprising a thiazole entity.

2. Structural commentary

The asymmetric unit of (**I**) contains one molecule (Fig. 1). The molecule is slightly bent, with the naphthalene ring system and the thiazole ring inclined to each other, subtending a dihedral angle of $13.69 (10)^\circ$; the anisole moiety is inclined to the plane of the naphthalene ring system, the dihedral angle being $14.22 (12)^\circ$. The C18—O1 and C21—O1 bond lengths are typical of single bonds (Table 1). The bond-length distribution in the thiazole ring is normal. The C11—N1 bond has single-bond character and the C13—N1 bond double-bond character, with bond lengths of $1.380 (3)$ and $1.304 (3)$ Å, respectively.

3. Supramolecular features

In the crystal structure, molecules are connected into sheets extending along (100) by C4—H4...Cg3ⁱ and C16—H16...Cg3ⁱⁱ interactions (Table 2; Fig. 2), where Cg3 is the centroid of the C5—C10 ring. Within the sheets, very weak π — π stacking interactions are observed with a centroid-to-centroid distance $Cg1 \cdots Cg4 = 4.494 (2)$ Å, where Cg1 and Cg4 are the

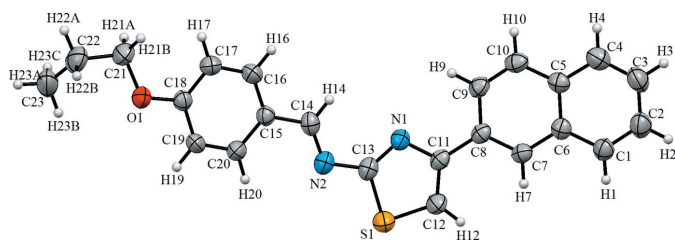


Figure 1
 The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 40% probability level.

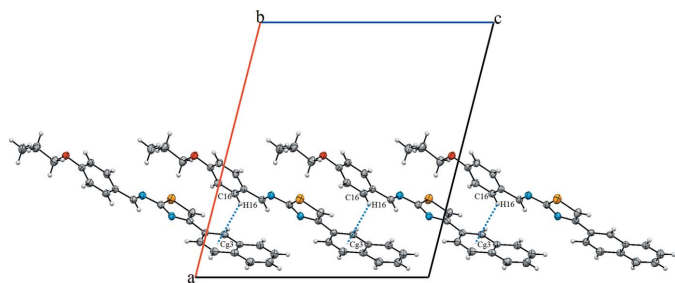


Figure 2
 A view of the crystal packing of the title compound in a view along the *b* axis. C—H... π (ring) interactions are indicated by dashed lines.

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

Cg3 is the centroid of the C5—C10 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>
C4—H4...Cg3 ⁱ	0.93	2.83	3.496	130
C16—H16...Cg3 ⁱⁱ	0.93	3.00	3.607	125

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

centroids of the S1/C12/C11/N1/C13 and the C15—C20 phenyl ring, respectively (Fig. 3).

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update November 2018; Groom *et al.*, 2016) for the 4-(4,6-dihydronaphthalen-1-yl)thiazol-2-amine moiety revealed two hits, *viz.* 4-(pyren-1-yl)-1,3-thiazol-2-amine (pyrene thiazole conjugate, PTC), $C_{19}H_{12}N_2S$ (SOPREW; Mahapatra *et al.*, 2014), and (*E*)-4-(4-chlorophenyl)-*N*-(1,3-benzodioxol-5-ylmethylene)-5-(1*H*-1,2,4-triazol-1-yl)-1,3-thiazol-2-amine, $C_{19}H_{12}ClN_5O_2S$ (XAZJUE; Shao *et al.*, 2006). In the crystal packing of PTC, the two molecules are connected into symmetrical dimers by pairs of N—H...N hydrogen bonds at a distance of 2.49 Å and are stacked along the *a* axis by weak aromatic π — π stacking interactions between the benzene rings in adjacent molecules [centroid-to-centroid distances of $3.5741 (10)$ Å]. Distinctive bond lengths (*e.g.* N1—C11, N—C13, S1—C12, S1—C13) in (**I**) are the same within standard deviations as the corresponding bond lengths in the structure of XAZJUE. In XAZJUE, the molecules are linked by weak C—H...O hydrogen bonds into a three-dimensional network.

5. Hirshfeld surface analysis

Hirshfeld surface analysis (Spackman & Jayatilaka, 2009; McKinnon *et al.*, 2007) was carried out using *Crystal-Explorer17.5* (Turner *et al.*, 2017). The Hirshfeld surface and their associated two-dimensional fingerprint plots were used to quantify the various intermolecular interactions in (**I**). Hirshfeld surface analysis was performed using a standard

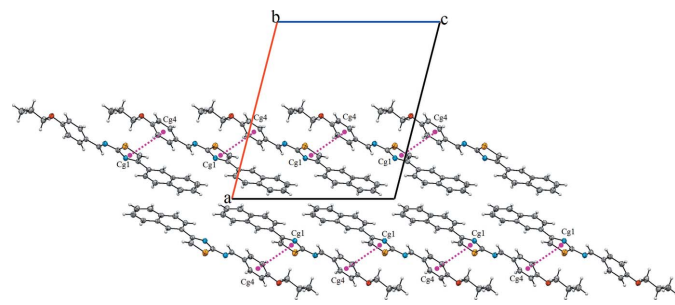


Figure 3
 A view of the crystal packing of the title compound along the *b* axis. $\pi(Cg1) \cdots \pi(Cg4)$ interactions are indicated by dashed lines.

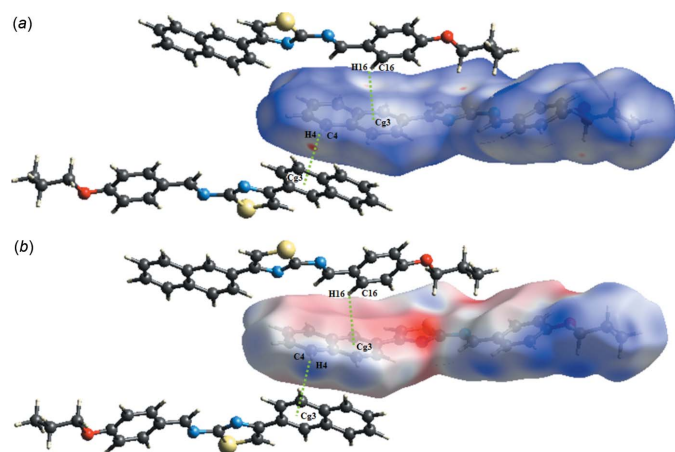


Figure 4
(a) Hirshfeld surfaces of the title compound mapped over d_{norm} with a fixed colour scale of -0.0638 (red) to 1.3242 (blue) a.u., and (b) the molecular electrostatic potential surface of the title compound obtained over Hirshfeld surface containing $\text{C}-\text{H}\cdots\pi$ interactions, with a fixed colour scale of -0.049 (red) to 0.034 (blue) a.u..

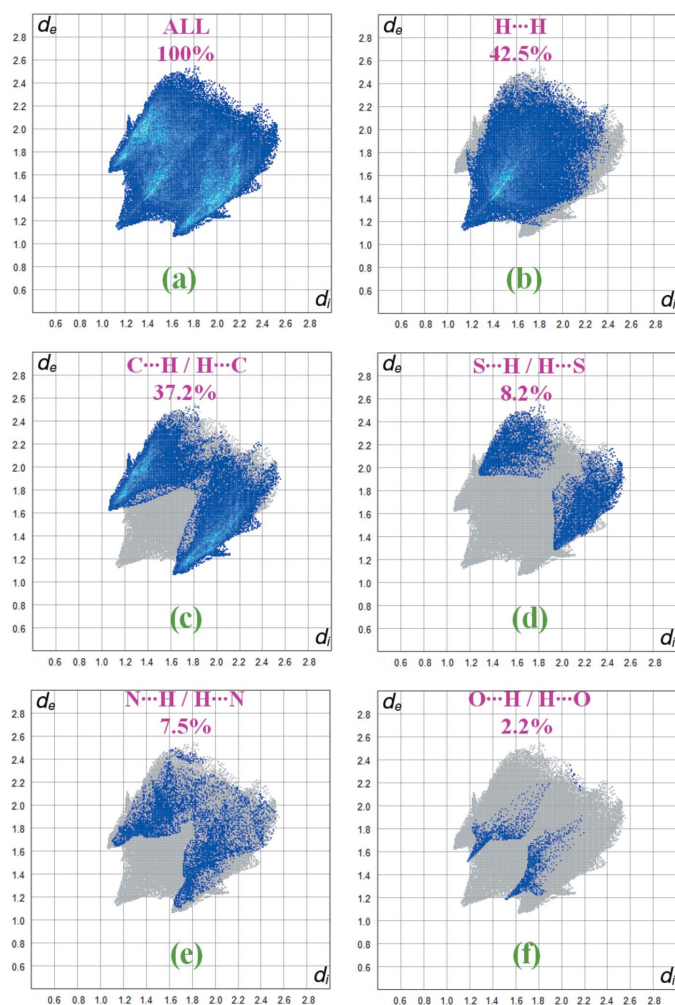


Figure 5
Two-dimensional fingerprint plots for the title compound, with a d_{norm} view (a), and delineated into relative contributions of the atom pairs to the Hirshfeld surface (b–f).

Table 3
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{23}\text{H}_{20}\text{N}_2\text{O}_5$
M_r	372.47
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	19.1636 (11), 6.0482 (3), 17.023 (1)
β (°)	104.370 (5)
V (Å ³)	1911.32 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.18
Crystal size (mm)	$0.68 \times 0.29 \times 0.05$
Data collection	
Diffractometer	STOE <i>IPDS 2</i>
Absorption correction	Integration (<i>X-RED32</i> ; Stoe & Cie, 2002)
$T_{\text{min}}, T_{\text{max}}$	0.919, 0.989
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12341, 3770, 1951
R_{int}	0.078
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.056, 0.087, 0.96
No. of reflections	3770
No. of parameters	245
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.12, -0.16

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

(high) surface resolution with the three-dimensional d_{norm} surfaces mapped over a fixed colour scale of -0.0638 (red) to 1.3242 (blue) a.u., and the results are illustrated in Fig. 4a. The red spots identified in Fig. 4a correspond to the near-type $\text{H}\cdots\pi$ contacts resulting from hydrogen bonds of the type $\text{C}-\text{H}\cdots\pi(\text{ring})$ (Table 2). The view of the three-dimensional Hirshfeld surface of the title compound plotted over electrostatic potentials with a fixed colour scale of -0.049 (red) to 0.034 (blue) a.u. is given in Fig. 4b, emphasizing on $\text{C}-\text{H}\cdots\pi(\text{ring})$ contacts.

Fig. 5a shows the two-dimensional fingerprint as the sum of all contacts contributing to the Hirshfeld surface indicated in normal mode. Fig. 5b illustrates the two-dimensional fingerprint of (d_i, d_e) points related to $\text{H}\cdots\text{H}$ contacts that represent a 42.5% contribution in the title structure. In Fig. 5c, two symmetrical wings on the left and right sides indicate $\text{C}\cdots\text{H}/\text{H}\cdots\text{C}$ interactions with a contribution of 37.2%. Furthermore, there are $\text{S}\cdots\text{H}/\text{H}\cdots\text{S}$ (8.2%; Fig. 5d), $\text{N}\cdots\text{H}/\text{H}\cdots\text{N}$ (7.5%; Fig. 5e) and $\text{O}\cdots\text{H}/\text{H}\cdots\text{O}$ (2.2%; Fig. 5f) contacts contributing to the overall crystal packing of (**I**).

6. Synthesis and crystallization

Compound (**I**) was prepared by adding 4-*N*-propoxybenzaldehyde (0.145 g, 0.885 mmol) dropwise under constant stirring to a solution of 2-amino-4-(2-naphthyl)thiazole (0.2 g, 0.885 mmol) in 1-propanol (10 ml). The reaction was catalysed by NaOH (0.1 g), and the mixture stirred for 1 h in a water

bath at approximately 278–283 K. The reaction was monitored by thin-layer chromatography (TLC) using ethyl acetate and *n*-hexane (3:7 *v:v*), and had an R_f of 0.675. The formed precipitate was filtered off, washed with 1-propanol, and dried. The resulting solid was further purified by washing with ethanol and diethyl ether. Single crystals of (**I**) for X-ray analysis were obtained by slow evaporation of an acetone solution (yield 60%, m.p. 411–413 K).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bound H atoms were placed in idealized positions and refined using a riding model with C–H = 0.93–0.97 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ or $1.2U_{\text{eq}}(\text{C})$ for other C-bound H atoms.

Acknowledgements

This study was supported by Ondokuz Mayıs University under project No. PYO-FEN.1906.19.001.

Funding information

Funding for this research was provided by: Ondokuz Mayıs University (award No. PYO.FEN.1906.19.001).

References

- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Ghawla Amit, C. P., Sunaina, Singh Mansimran, Kaur Kuldeep & Dhawan, R. K. (2014). *Int. J. Pharmacol. Pharm. Sci.* **2**, 1–8.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Kaur, H. & Goyal, A. (2018). *Int. J. Pharm. Drug. Anal.* **6**, 509–522.
- Kumar, J., Rai, A. & Raj, V. (2017). *Org. Med. Chem. J.* **1**, 555–564.
- Mahapatra, A. K., Mondal, S., Maiti, K., Manna, S. K., Maji, R., Mandal, D., Mandal, S., Goswami, S., Quah, C. K. & Fun, H.-K. (2014). *RSC Adv.* **4**, 56605–56614.
- McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.
- McNaught, A. D. & Wilkinson, A. (1997). *Compendium of Chemical Terminology*. Blackwell Science Oxford.
- Schiff, H. (1864). *Ann. Chem. Pharm.* **131**, 118–119.
- Shao, L., Zhang, Q., Zhou, X. & Fang, J.-X. (2006). *Acta Cryst.* **E62**, o334–o335.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.
- Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.
- Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie GmbH, Darmstadt, Germany.
- Turner, M. J., MacKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *Crystal Explorer 17.5*. University of Western Australia. <http://hirshfeldsurface.net>.

supporting information

Acta Cryst. (2020). E76, 920-923 [https://doi.org/10.1107/S2056989020006611]

Crystal structure and Hirshfeld surface analysis of 4-(naphthalen-2-yl)-*N*-[(*Z*)-4-propoxybenzylidene]-1,3-thiazol-2-amine

Ropak A. Sheakh Mohamad, Wali M. Hamad and Hashim J. Aziz

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).

4-(Naphthalen-2-yl)-*N*-[(*Z*)-4-propoxybenzylidene]-1,3-thiazol-2-amine

Crystal data

$C_{23}H_{20}N_2OS$	$F(000) = 784$
$M_r = 372.47$	$D_x = 1.294 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 19.1636 (11) \text{ \AA}$	Cell parameters from 9076 reflections
$b = 6.0482 (3) \text{ \AA}$	$\theta = 1.8\text{--}31.6^\circ$
$c = 17.023 (1) \text{ \AA}$	$\mu = 0.18 \text{ mm}^{-1}$
$\beta = 104.370 (5)^\circ$	$T = 296 \text{ K}$
$V = 1911.32 (19) \text{ \AA}^3$	Stick, yellow
$Z = 4$	$0.68 \times 0.29 \times 0.05 \text{ mm}$

Data collection

STOE IPDS 2	12341 measured reflections
diffractometer	3770 independent reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	1951 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{\text{int}} = 0.078$
rotation method scans	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -19 \rightarrow 23$
$T_{\text{min}} = 0.919$, $T_{\text{max}} = 0.989$	$k = -7 \rightarrow 7$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2]$
$wR(F^2) = 0.087$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3770 reflections	$\Delta\rho_{\text{max}} = 0.12 \text{ e \AA}^{-3}$
245 parameters	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$
0 restraints	

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.72771 (5)	0.01821 (13)	0.45111 (4)	0.0700 (2)
O1	0.57359 (10)	0.7728 (3)	−0.00225 (10)	0.0614 (5)
N1	0.78855 (12)	0.3982 (3)	0.46984 (12)	0.0518 (6)
N2	0.71496 (12)	0.3175 (4)	0.33523 (12)	0.0574 (6)
C15	0.69256 (14)	0.5693 (4)	0.22324 (14)	0.0471 (6)
C6	0.88892 (13)	0.4646 (4)	0.76167 (14)	0.0486 (6)
C8	0.84752 (13)	0.4163 (4)	0.61580 (15)	0.0467 (6)
C11	0.80536 (13)	0.2954 (4)	0.54458 (15)	0.0481 (6)
C7	0.85390 (13)	0.3407 (4)	0.69324 (15)	0.0497 (7)
H7	0.834523	0.203683	0.700743	0.060*
C20	0.63762 (14)	0.4417 (4)	0.17593 (14)	0.0552 (7)
H20	0.626787	0.304989	0.194986	0.066*
C18	0.61554 (13)	0.7170 (4)	0.07205 (14)	0.0494 (7)
C13	0.74782 (15)	0.2697 (4)	0.41597 (15)	0.0526 (7)
C5	0.91907 (14)	0.6724 (4)	0.75068 (16)	0.0520 (7)
C9	0.87997 (14)	0.6206 (4)	0.60570 (16)	0.0542 (7)
H9	0.877676	0.671926	0.553618	0.065*
C19	0.59913 (14)	0.5150 (5)	0.10142 (14)	0.0557 (7)
H19	0.562053	0.428985	0.070646	0.067*
C10	0.91444 (14)	0.7434 (5)	0.67047 (16)	0.0581 (7)
H10	0.935420	0.876963	0.661879	0.070*
C17	0.67016 (15)	0.8446 (5)	0.11727 (16)	0.0570 (7)
H17	0.681829	0.979223	0.097421	0.068*
C14	0.72982 (13)	0.5003 (5)	0.30469 (13)	0.0548 (7)
H14	0.765398	0.591233	0.335507	0.066*
C16	0.70766 (14)	0.7699 (5)	0.19294 (15)	0.0574 (7)
H16	0.744007	0.857655	0.224102	0.069*
C1	0.89269 (14)	0.3919 (5)	0.84200 (16)	0.0592 (7)
H1	0.873907	0.254632	0.850405	0.071*
C12	0.77718 (16)	0.0891 (4)	0.54435 (16)	0.0617 (7)
H12	0.784240	−0.001549	0.589769	0.074*
C2	0.92348 (16)	0.5211 (6)	0.90667 (17)	0.0732 (9)
H2	0.924833	0.472661	0.958877	0.088*
C21	0.59299 (17)	0.9645 (5)	−0.04130 (15)	0.0699 (8)
H21A	0.642670	0.953582	−0.044645	0.084*
H21B	0.587991	1.096221	−0.010673	0.084*
C4	0.95124 (16)	0.7990 (5)	0.81968 (18)	0.0696 (8)
H4	0.971585	0.935292	0.813145	0.084*
C3	0.95304 (17)	0.7257 (6)	0.89530 (18)	0.0761 (9)

H3	0.974148	0.812465	0.939997	0.091*
C22	0.54367 (17)	0.9770 (6)	-0.12479 (17)	0.0846 (10)
H22A	0.554784	1.109652	-0.151339	0.102*
H22B	0.494394	0.989504	-0.120138	0.102*
C23	0.54931 (19)	0.7806 (7)	-0.17675 (18)	0.0990 (12)
H23A	0.518100	0.801144	-0.229840	0.149*
H23B	0.535317	0.649628	-0.152709	0.149*
H23C	0.598123	0.765472	-0.180940	0.149*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0868 (6)	0.0596 (5)	0.0589 (4)	-0.0121 (5)	0.0092 (4)	0.0028 (4)
O1	0.0618 (12)	0.0702 (13)	0.0472 (10)	-0.0091 (10)	0.0041 (9)	0.0089 (9)
N1	0.0573 (14)	0.0520 (13)	0.0459 (13)	0.0032 (12)	0.0128 (11)	0.0038 (11)
N2	0.0621 (15)	0.0622 (15)	0.0476 (13)	0.0043 (13)	0.0130 (11)	0.0051 (12)
C15	0.0488 (16)	0.0527 (17)	0.0402 (13)	-0.0014 (14)	0.0117 (12)	-0.0031 (12)
C6	0.0387 (14)	0.0577 (17)	0.0493 (14)	0.0052 (14)	0.0107 (12)	0.0021 (14)
C8	0.0437 (15)	0.0471 (15)	0.0496 (16)	0.0062 (13)	0.0123 (12)	0.0080 (12)
C11	0.0460 (15)	0.0497 (16)	0.0494 (15)	0.0075 (13)	0.0134 (13)	0.0084 (13)
C7	0.0462 (16)	0.0480 (16)	0.0553 (16)	-0.0014 (13)	0.0136 (13)	0.0053 (13)
C20	0.0679 (19)	0.0524 (17)	0.0463 (15)	-0.0097 (15)	0.0159 (14)	0.0010 (13)
C18	0.0457 (15)	0.0578 (18)	0.0437 (15)	-0.0019 (14)	0.0093 (12)	-0.0005 (13)
C13	0.0562 (17)	0.0571 (18)	0.0452 (15)	0.0088 (15)	0.0140 (13)	0.0041 (14)
C5	0.0432 (16)	0.0509 (17)	0.0607 (18)	0.0018 (14)	0.0103 (13)	0.0005 (14)
C9	0.0556 (17)	0.0562 (17)	0.0497 (16)	0.0031 (15)	0.0107 (14)	0.0123 (13)
C19	0.0610 (17)	0.0587 (18)	0.0450 (14)	-0.0186 (16)	0.0085 (13)	-0.0065 (14)
C10	0.0540 (17)	0.0513 (17)	0.0680 (19)	0.0011 (15)	0.0135 (15)	0.0109 (15)
C17	0.0616 (18)	0.0525 (17)	0.0563 (17)	-0.0101 (15)	0.0135 (14)	0.0033 (13)
C14	0.0522 (17)	0.0664 (19)	0.0446 (14)	0.0054 (16)	0.0101 (12)	-0.0054 (15)
C16	0.0545 (17)	0.0619 (19)	0.0534 (17)	-0.0124 (15)	0.0085 (14)	-0.0033 (14)
C1	0.0509 (17)	0.073 (2)	0.0528 (17)	-0.0034 (15)	0.0119 (14)	0.0007 (15)
C12	0.0750 (19)	0.0530 (18)	0.0530 (16)	-0.0017 (17)	0.0079 (14)	0.0076 (14)
C2	0.072 (2)	0.094 (2)	0.0542 (17)	-0.005 (2)	0.0168 (15)	-0.0041 (18)
C21	0.085 (2)	0.0626 (19)	0.0587 (17)	-0.0039 (18)	0.0113 (16)	0.0097 (16)
C4	0.066 (2)	0.067 (2)	0.075 (2)	-0.0083 (17)	0.0159 (17)	-0.0091 (17)
C3	0.076 (2)	0.087 (3)	0.062 (2)	-0.012 (2)	0.0097 (17)	-0.0188 (18)
C22	0.084 (2)	0.099 (3)	0.0621 (19)	-0.002 (2)	0.0013 (17)	0.028 (2)
C23	0.100 (3)	0.139 (3)	0.0546 (19)	-0.035 (3)	0.0144 (19)	-0.005 (2)

Geometric parameters (Å, °)

S1—C12	1.690 (3)	C9—C10	1.357 (4)
S1—C13	1.713 (3)	C9—H9	0.9300
O1—C18	1.362 (3)	C19—H19	0.9300
O1—C21	1.431 (3)	C10—H10	0.9300
N1—C13	1.304 (3)	C17—C16	1.386 (3)
N1—C11	1.380 (3)	C17—H17	0.9300

N2—C14	1.284 (3)	C14—H14	0.9300
N2—C13	1.393 (3)	C16—H16	0.9300
C15—C16	1.377 (3)	C1—C2	1.360 (4)
C15—C20	1.390 (3)	C1—H1	0.9300
C15—C14	1.454 (3)	C12—H12	0.9300
C6—C7	1.407 (3)	C2—C3	1.394 (4)
C6—C5	1.415 (3)	C2—H2	0.9300
C6—C1	1.421 (3)	C21—C22	1.501 (3)
C8—C7	1.372 (3)	C21—H21A	0.9700
C8—C9	1.413 (3)	C21—H21B	0.9700
C8—C11	1.473 (3)	C4—C3	1.354 (4)
C11—C12	1.359 (3)	C4—H4	0.9300
C7—H7	0.9300	C3—H3	0.9300
C20—C19	1.373 (3)	C22—C23	1.501 (4)
C20—H20	0.9300	C22—H22A	0.9700
C18—C17	1.372 (3)	C22—H22B	0.9700
C18—C19	1.386 (3)	C23—H23A	0.9600
C5—C4	1.409 (4)	C23—H23B	0.9600
C5—C10	1.413 (3)	C23—H23C	0.9600
C12—S1—C13	88.87 (14)	C18—C17—H17	120.5
C18—O1—C21	118.1 (2)	C16—C17—H17	120.5
C13—N1—C11	110.0 (2)	N2—C14—C15	121.8 (3)
C14—N2—C13	119.1 (2)	N2—C14—H14	119.1
C16—C15—C20	118.1 (2)	C15—C14—H14	119.1
C16—C15—C14	120.7 (3)	C15—C16—C17	121.8 (3)
C20—C15—C14	121.0 (2)	C15—C16—H16	119.1
C7—C6—C5	119.3 (2)	C17—C16—H16	119.1
C7—C6—C1	122.1 (3)	C2—C1—C6	120.6 (3)
C5—C6—C1	118.5 (2)	C2—C1—H1	119.7
C7—C8—C9	118.1 (2)	C6—C1—H1	119.7
C7—C8—C11	121.7 (2)	C11—C12—S1	111.4 (2)
C9—C8—C11	120.1 (2)	C11—C12—H12	124.3
C12—C11—N1	114.2 (2)	S1—C12—H12	124.3
C12—C11—C8	126.4 (2)	C1—C2—C3	120.5 (3)
N1—C11—C8	119.3 (2)	C1—C2—H2	119.8
C8—C7—C6	121.9 (2)	C3—C2—H2	119.8
C8—C7—H7	119.0	O1—C21—C22	107.8 (2)
C6—C7—H7	119.0	O1—C21—H21A	110.1
C19—C20—C15	120.8 (2)	C22—C21—H21A	110.1
C19—C20—H20	119.6	O1—C21—H21B	110.1
C15—C20—H20	119.6	C22—C21—H21B	110.1
O1—C18—C17	125.0 (2)	H21A—C21—H21B	108.5
O1—C18—C19	114.8 (2)	C3—C4—C5	121.1 (3)
C17—C18—C19	120.2 (2)	C3—C4—H4	119.4
N1—C13—N2	128.0 (2)	C5—C4—H4	119.4
N1—C13—S1	115.54 (19)	C4—C3—C2	120.5 (3)
N2—C13—S1	116.3 (2)	C4—C3—H3	119.8

C4—C5—C10	123.4 (3)	C2—C3—H3	119.8
C4—C5—C6	118.8 (2)	C21—C22—C23	113.4 (3)
C10—C5—C6	117.9 (2)	C21—C22—H22A	108.9
C10—C9—C8	121.3 (2)	C23—C22—H22A	108.9
C10—C9—H9	119.3	C21—C22—H22B	108.9
C8—C9—H9	119.3	C23—C22—H22B	108.9
C20—C19—C18	120.0 (2)	H22A—C22—H22B	107.7
C20—C19—H19	120.0	C22—C23—H23A	109.5
C18—C19—H19	120.0	C22—C23—H23B	109.5
C9—C10—C5	121.3 (3)	H23A—C23—H23B	109.5
C9—C10—H10	119.3	C22—C23—H23C	109.5
C5—C10—H10	119.3	H23A—C23—H23C	109.5
C18—C17—C16	119.0 (2)	H23B—C23—H23C	109.5
C13—N1—C11—C12	0.8 (3)	C15—C20—C19—C18	0.9 (4)
C13—N1—C11—C8	-176.4 (2)	O1—C18—C19—C20	-179.7 (2)
C7—C8—C11—C12	-9.7 (4)	C17—C18—C19—C20	-0.1 (4)
C9—C8—C11—C12	173.2 (3)	C8—C9—C10—C5	-0.2 (4)
C7—C8—C11—N1	167.1 (2)	C4—C5—C10—C9	-176.9 (3)
C9—C8—C11—N1	-10.0 (3)	C6—C5—C10—C9	2.3 (4)
C9—C8—C7—C6	2.6 (4)	O1—C18—C17—C16	178.6 (2)
C11—C8—C7—C6	-174.5 (2)	C19—C18—C17—C16	-1.0 (4)
C5—C6—C7—C8	-0.5 (4)	C13—N2—C14—C15	-174.3 (2)
C1—C6—C7—C8	176.9 (2)	C16—C15—C14—N2	177.6 (3)
C16—C15—C20—C19	-0.6 (4)	C20—C15—C14—N2	1.9 (4)
C14—C15—C20—C19	175.3 (2)	C20—C15—C16—C17	-0.5 (4)
C21—O1—C18—C17	8.3 (4)	C14—C15—C16—C17	-176.4 (2)
C21—O1—C18—C19	-172.1 (2)	C18—C17—C16—C15	1.3 (4)
C11—N1—C13—N2	174.8 (2)	C7—C6—C1—C2	-176.4 (3)
C11—N1—C13—S1	-0.4 (3)	C5—C6—C1—C2	1.1 (4)
C14—N2—C13—N1	7.1 (4)	N1—C11—C12—S1	-0.9 (3)
C14—N2—C13—S1	-177.7 (2)	C8—C11—C12—S1	176.1 (2)
C12—S1—C13—N1	0.0 (2)	C13—S1—C12—C11	0.5 (2)
C12—S1—C13—N2	-175.9 (2)	C6—C1—C2—C3	-1.1 (4)
C7—C6—C5—C4	177.3 (2)	C18—O1—C21—C22	174.3 (2)
C1—C6—C5—C4	-0.3 (4)	C10—C5—C4—C3	178.6 (3)
C7—C6—C5—C10	-1.9 (4)	C6—C5—C4—C3	-0.5 (4)
C1—C6—C5—C10	-179.5 (2)	C5—C4—C3—C2	0.6 (5)
C7—C8—C9—C10	-2.3 (4)	C1—C2—C3—C4	0.3 (5)
C11—C8—C9—C10	174.9 (2)	O1—C21—C22—C23	-61.0 (3)

Hydrogen-bond geometry (Å, °)

Cg3 is the centroid of the C5—C10 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>
C4—H4 \cdots Cg3 ⁱ	0.93	2.83	3.496	130

C16—H16...Cg ³ⁱⁱ	0.93	3.00	3.607	125
-----------------------------	------	------	-------	-----

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