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Crystal structure and Hirshfeld surface analysis of 4-{[(*E*)-4-(heptyloxy)benzylidene]amino}-*N*-(naphthalen-2-yl)-1,3-thiazol-2-amine

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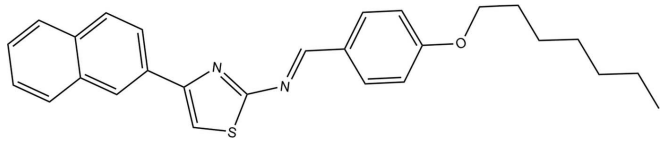
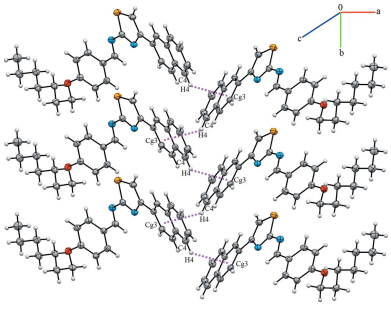
In the title compound, $C_{27}H_{28}N_2OS$, the naphthalene unit is planar to within 0.015 (2) Å and makes a dihedral angle of 14.24 (16)° with the thiazole ring. The anisole ring is inclined to the thiazole ring by a dihedral angle of 13.18 (23)°. The torsion angle between the heptyl chain and the anisole ring is 61.1 (4)°. These dihedral and torsion angles render the molecule non-planar. In the crystal, molecules are linked by C—H···π interactions, forming zigzag chains that propagate parallel to the *b* axis. The roles of the various intermolecular interactions in the crystal packing were clarified by Hirshfeld surface analysis; the most important contributions are from H···H (51.5%) and C···H/H···C (31.8%) contacts.

1. Chemical context

Schiff bases, *i.e.* compounds containing the azomethine group (–CH═N– or >C═N–), are important because of their physiological and pharmacological properties. They are typically synthesized by the condensation of primary amines and active carbonyl groups. The pharmacological activities of Schiff bases include anti-bacterial, anti-fungal, anti-cancer and anti-viral properties (Wang *et al.*, 2001; Yadav & Singh, 2001).



One of the most important scaffolds in drug design and heterocyclic chemistry is thiazole, which is widely found in various pharmacologically active substances and in some naturally occurring compounds (Ayati *et al.*, 2015). Various thiazole-bearing compounds have shown activities such as anti-bacterial, anti-fungal, anti-inflammatory, anti-hypertensive, anti-HIV, anti-tumor, anti-filarial, anti-convulsant, herbicidal, insecticidal, schistosomicidal and anthelmintic (Bharti *et al.*, 2010). The synthesis of thiazole derivatives by various methods and their biological evaluation have been described by several researchers and the thiazole nucleus has therefore attracted a lot of interest for the development of pharmacologically active compounds (Breslow, 1958). In our studies, a new Schiff base, 4-{[(*E*)-4-(heptyloxy)benzylidene]amino}-*N*-(naphthalen-2-yl)-1,3-thiazol-2-amine, was obtained in crystalline form from the reaction of 2-amino-4-(2-



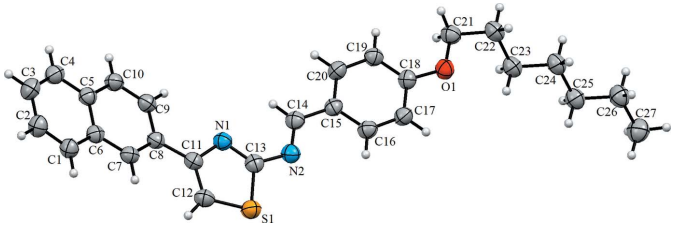


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 40% probability level.

naphthyl)thiazole with 4-*N*-(heptyloxy)benzaldehyde. We report here the synthesis and the crystal and molecular structures of the title compound, including a Hirshfeld surface analysis to assess the relative importance of the various intermolecular interactions on the crystal packing.

2. Structural commentary

The asymmetric unit of the title compound contains one molecule (Fig. 1). The naphthalene unit makes a dihedral angle of 14.24 (16)° with the thiazole ring. The anisole ring is inclined to the thiazole ring by a dihedral angle of 13.18 (22)°. The heptyl chain attached to O1 is twisted out of this plane with the O1—C21—C22–C23 torsion angle being 61.1 (4)°. In the thiazole ring, the C11—N1 [1.373 (4) Å] and C13—N1 [1.298 (4) Å] distances indicate substantial electronic delocalization (Table 1).

3. Supramolecular features

In the crystal, the most important intermolecular contacts are C—H···π interactions, which link screw-related molecules *via* C4—H4···*Cg*3^{i} [symmetry code: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$), forming zigzag chains that extend parallel to the *b* axis (Fig. 2 and

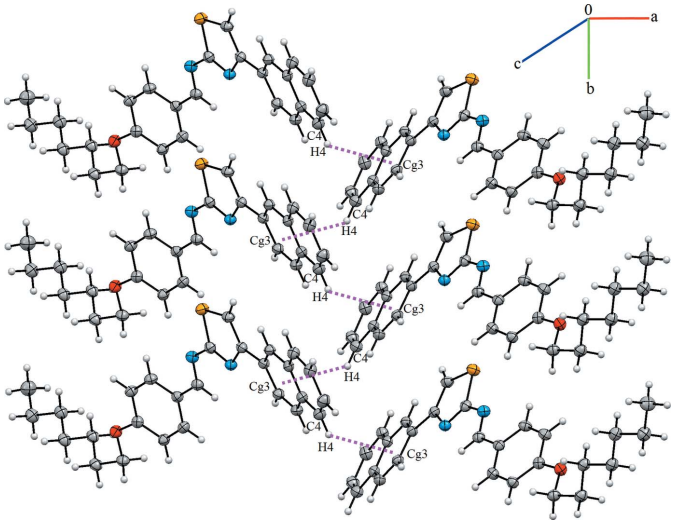


Figure 2
A view of the crystal packing of the title compound. The C—H···π(ring) interactions are indicated by dashed lines.

Table 1
Selected bond lengths (Å).

S1—C12	1.674 (4)	N1—C13	1.298 (4)
S1—C13	1.719 (4)	N1—C11	1.373 (4)
O1—C18	1.345 (4)	N2—C14	1.275 (4)
O1—C21	1.434 (4)	N2—C13	1.377 (4)

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

*Cg*3 is the centroid of the C5–C10 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···*Cg*3^{i}	0.93	2.85	3.522 (4)	130

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

Table 2). The distance of between the carbon atom C4 and the centroid (*Cg*3^{i}) of the adjacent C5-C10 ring is 3.522 (4) Å.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.39; Groom *et al.*, 2016) for the (*E*)-1-(4-(heptyloxy)phenyl)-*N*-(4-(naphthalen-2-yl)thiazol-2-yl)methanimine fragment revealed three hits. These structures are 4-(pyren-1-yl)-1,3-thiazol-2-amine (pyrene thiazole conjugate, PTC), $C_{19}H_{12}N_2S$ (SOPREW; Mahapatra *et al.*, 2014), 2-amino-4-(2-naphthyl)-1,3-thiazolium bromide, $C_{13}H_{11}N_2S^{+}\cdot Br^{-}$ (XUNKOG; Lynch *et al.*, 2002) 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 XUNKOG, the molecules are connected to each other *via* N—H···Br hydrogen bonds while in XAZJUE, they are linked by a weak C—H···O hydrogen bond. In SOPREW, the two pyrene thiazole conjugate molecules are connected into symmetrical homodimers by pairs of N—H···N hydrogen bonds.

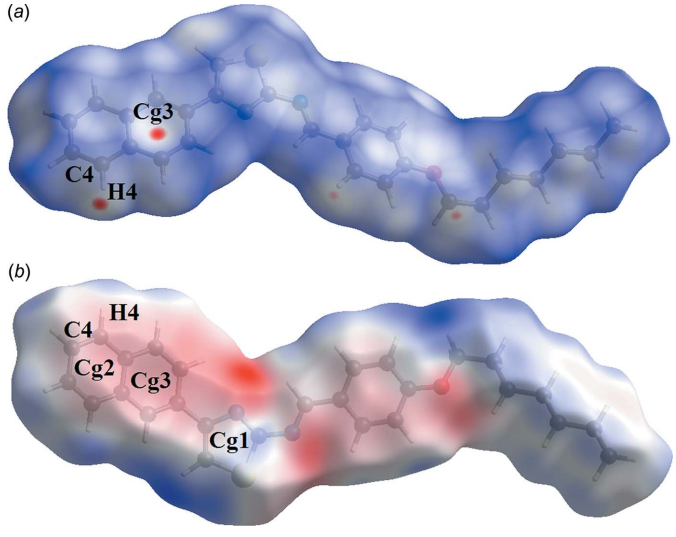


Figure 3
The Hirshfeld surfaces of the title compound mapped over (*a*) d_{norm}, and (*b*) electrostatic potential.

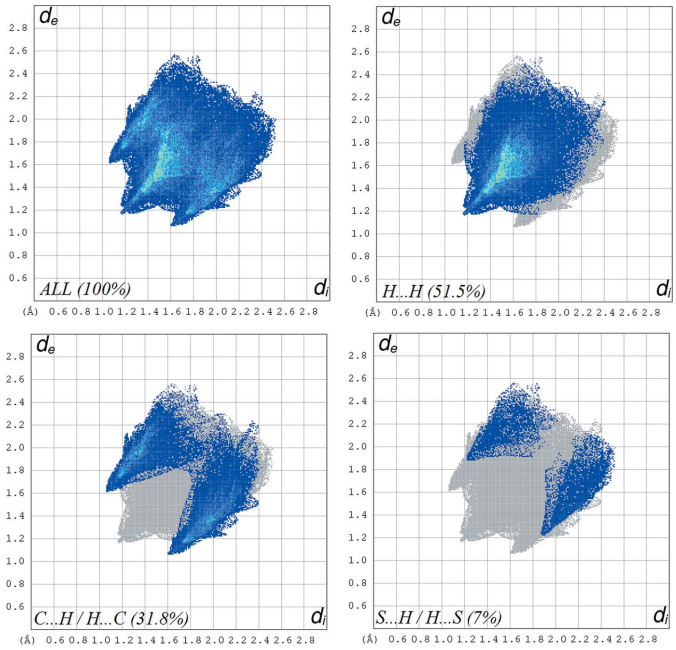


Figure 4
Two-dimensional fingerprint plots, showing the relative contribution of the atom-pair interactions to the Hirshfeld surface.

5. Hirshfeld surface analysis

To investigate the intermolecular interactions, Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and fingerprint plots were generated using *CrystalExplorer17.5* (Turner *et al.*, 2017). Hirshfeld surface analysis depicts intermolecular interactions by different colours, representing short or long contacts, which reflect the relative strength of the interaction. The generated Hirshfeld surface mapped over d_{norm} is shown in Fig. 3*a* where the red spots correspond to the C—H···π(ring) close contacts (Table 2). The three-dimensional Hirshfeld surface plotted over electrostatic potential shows donor (red) and acceptor (blue) regions (Fig. 3*b*). The crystal packing is dominated by H···H contacts, representing van der Waals interactions (51.5% contribution to the surface), followed by C···H/H···C and S···H/H···S interactions, which contribute 31.8% and 7%, respectively (Fig. 4).

6. Synthesis and crystallization

The title compound was prepared by adding 4-*N*-(heptyloxy)benzaldehyde (0.1947 g, 0.885 mmol) dropwise to a constantly stirring 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 was stirred for 3 h in a water bath at 278–283 K. The reaction was monitored with thin-layer chromatography (TLC) using a 3:7 ratio of ethyl acetate to *n*-hexane (R_f = 0.775). The precipitate was filtered, washed with 1-propanol, and dried. The resulting solid was further purified by recrystallization from ethanol and diethyl ether. Single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of an acetone solution (yield 81.7%, m.p. 387.5–389.5 K).

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{28}N_2OS$
M_r	428.57
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	22.927 (4), 5.9315 (6), 17.191 (2)
β (°)	97.734 (12)
V (Å^3)	2316.6 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.16
Crystal size (mm)	0.49 × 0.24 × 0.11
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.955, 0.982
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10986, 4068, 2000
R_{int}	0.063
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.067, 0.155, 0.92
No. of reflections	4068
No. of parameters	281
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.17

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

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

Funding information

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

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (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-{[(*E*)-4-(Heptyloxy)benzylidene]amino}-*N*-(naphthalen-2-yl)-1,3-thiazol-2-amine

Crystal data

$C_{27}H_{28}N_2OS$
$M_r = 428.57$
Monoclinic, $P2_1/c$
$a = 22.927$ (4) Å
$b = 5.9315$ (6) Å
$c = 17.191$ (2) Å
$\beta = 97.734$ (12)°
$V = 2316.6$ (5) Å^3
$Z = 4$
$F(000) = 912$
$D_x = 1.229$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9222 reflections
$\theta = 1.4$–27.7°
$\mu = 0.16$ mm^{-1}
$T = 296$ K
Stick, yellow
0.49 × 0.24 × 0.11 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.955$, $T_{max} = 0.982$
10986 measured reflections
4068 independent reflections
2000 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.4°$
$h = -24\rightarrow27$
$k = -7\rightarrow7$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.155$
$S = 0.92$
4068 reflections
281 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ 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}
S1	0.22633 (5)	0.01514 (16)	0.57256 (6)	0.1138 (4)
O1	0.34973 (11)	0.7781 (4)	0.18878 (14)	0.1090 (7)
N1	0.17508 (13)	0.3977 (5)	0.56495 (16)	0.0951 (8)
N2	0.23575 (14)	0.3219 (5)	0.46375 (17)	0.1016 (8)
C6	0.09218 (14)	0.4575 (5)	0.81098 (19)	0.0907 (9)
C7	0.12144 (15)	0.3353 (5)	0.7578 (2)	0.0922 (9)
H7	0.138236	0.197033	0.773380	0.111*
C18	0.31570 (16)	0.7233 (6)	0.24384 (19)	0.0942 (9)
C8	0.12605 (15)	0.4127 (5)	0.68404 (19)	0.0893 (9)
C13	0.20898 (16)	0.2713 (6)	0.52869 (19)	0.0957 (9)
C15	0.25439 (16)	0.5758 (6)	0.36278 (18)	0.0911 (9)
C9	0.09865 (16)	0.6188 (6)	0.6604 (2)	0.0983 (10)
H9	0.100324	0.671600	0.609769	0.118*
C16	0.29941 (17)	0.4482 (6)	0.33942 (19)	0.1012 (10)
H16	0.309049	0.310612	0.363781	0.121*
C5	0.06665 (15)	0.6676 (6)	0.7867 (2)	0.0957 (9)
C19	0.27062 (16)	0.8513 (6)	0.2650 (2)	0.0987 (10)
H19	0.260471	0.986613	0.239358	0.118*
C11	0.16110 (15)	0.2922 (5)	0.63110 (19)	0.0905 (9)
C17	0.32949 (17)	0.5193 (6)	0.28215 (19)	0.1011 (10)
H17	0.359909	0.431246	0.267905	0.121*
C20	0.24043 (16)	0.7789 (6)	0.3243 (2)	0.1000 (10)
H20	0.210185	0.867189	0.338883	0.120*
C10	0.07004 (16)	0.7411 (6)	0.7095 (2)	0.1021 (10)
H10	0.052252	0.876263	0.692155	0.123*
C1	0.08963 (16)	0.3841 (7)	0.8886 (2)	0.1035 (10)
H1	0.105644	0.245213	0.905032	0.124*
C14	0.22370 (16)	0.5061 (6)	0.42680 (19)	0.0977 (9)
H14	0.194260	0.598284	0.441516	0.117*
C12	0.18554 (17)	0.0833 (6)	0.6429 (2)	0.1043 (10)
H12	0.180195	−0.009921	0.684812	0.125*
C4	0.04009 (17)	0.7950 (7)	0.8408 (2)	0.1113 (11)
H4	0.023035	0.933143	0.825662	0.134*
C23	0.37841 (18)	0.7782 (7)	0.0293 (2)	0.1100 (11)
H23A	0.385642	0.645391	0.062131	0.132*
H23B	0.340038	0.760901	−0.001570	0.132*
C21	0.33361 (18)	0.9678 (6)	0.1388 (2)	0.1106 (11)
H21A	0.334233	1.104756	0.169733	0.133*
H21B	0.294231	0.947554	0.111073	0.133*

C25	0.42596 (19)	0.5902 (7)	−0.0784 (2)	0.1155 (12)
H25A	0.432021	0.455243	−0.046493	0.139*
H25B	0.388034	0.576225	−0.110681	0.139*
C24	0.42408 (18)	0.7903 (7)	−0.0250 (2)	0.1128 (11)
H24A	0.462375	0.806563	0.006187	0.135*
H24B	0.417052	0.924663	−0.057046	0.135*
C2	0.06433 (18)	0.5126 (8)	0.9391 (2)	0.1156 (11)
H2	0.063744	0.463555	0.990321	0.139*
C22	0.37726 (19)	0.9836 (7)	0.0817 (2)	0.1149 (11)
H22A	0.416186	1.005154	0.110597	0.138*
H22B	0.368155	1.115365	0.048834	0.138*
C26	0.4728 (2)	0.6016 (8)	−0.1311 (2)	0.1277 (14)
H26A	0.510749	0.615254	−0.098731	0.153*
H26B	0.466844	0.736962	−0.162780	0.153*
C3	0.0389 (2)	0.7194 (8)	0.9150 (3)	0.1247 (13)
H3	0.021019	0.806070	0.950183	0.150*
C27	0.4750 (2)	0.4030 (8)	−0.1848 (3)	0.1497 (17)
H27A	0.438855	0.394620	−0.220161	0.225*
H27B	0.480019	0.267150	−0.154273	0.225*
H27C	0.507361	0.420161	−0.214350	0.225*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.1338 (8)	0.0960 (6)	0.1147 (7)	0.0124 (6)	0.0282 (6)	0.0065 (5)
O1	0.1105 (17)	0.1179 (17)	0.1008 (15)	0.0099 (14)	0.0219 (14)	0.0124 (14)
N1	0.101 (2)	0.0915 (16)	0.0922 (17)	0.0001 (15)	0.0123 (15)	0.0032 (15)
N2	0.117 (2)	0.0974 (19)	0.0913 (17)	−0.0022 (17)	0.0169 (16)	0.0002 (16)
C6	0.085 (2)	0.091 (2)	0.094 (2)	−0.0032 (17)	0.0068 (17)	−0.0021 (18)
C7	0.095 (2)	0.0804 (19)	0.099 (2)	−0.0006 (17)	0.0065 (19)	0.0057 (17)
C18	0.096 (2)	0.102 (2)	0.0839 (19)	0.000 (2)	0.0095 (18)	−0.0011 (19)
C8	0.088 (2)	0.0826 (19)	0.097 (2)	−0.0055 (16)	0.0109 (18)	0.0054 (17)
C13	0.096 (2)	0.101 (2)	0.089 (2)	−0.0075 (19)	0.0092 (19)	−0.0060 (19)
C15	0.096 (2)	0.091 (2)	0.0856 (19)	0.0002 (18)	0.0093 (17)	−0.0069 (17)
C9	0.098 (2)	0.093 (2)	0.103 (2)	−0.0053 (19)	0.012 (2)	0.0107 (19)
C16	0.121 (3)	0.090 (2)	0.092 (2)	0.009 (2)	0.013 (2)	0.0028 (18)
C5	0.087 (2)	0.091 (2)	0.109 (3)	−0.0041 (18)	0.0102 (19)	−0.0008 (19)
C19	0.104 (3)	0.094 (2)	0.098 (2)	0.007 (2)	0.014 (2)	0.0085 (18)
C11	0.093 (2)	0.085 (2)	0.092 (2)	−0.0088 (18)	0.0082 (18)	0.0037 (17)
C17	0.113 (3)	0.097 (2)	0.095 (2)	0.016 (2)	0.018 (2)	−0.001 (2)
C20	0.101 (2)	0.096 (2)	0.102 (2)	0.0135 (19)	0.014 (2)	−0.003 (2)
C10	0.100 (2)	0.085 (2)	0.120 (3)	0.0019 (18)	0.015 (2)	0.010 (2)
C1	0.103 (3)	0.110 (2)	0.098 (2)	0.005 (2)	0.014 (2)	0.005 (2)
C14	0.103 (2)	0.096 (2)	0.093 (2)	−0.002 (2)	0.0103 (19)	−0.005 (2)
C12	0.116 (3)	0.091 (2)	0.106 (2)	0.001 (2)	0.012 (2)	0.0129 (18)
C4	0.110 (3)	0.103 (2)	0.121 (3)	0.006 (2)	0.015 (2)	−0.005 (2)
C23	0.109 (3)	0.117 (3)	0.104 (2)	−0.009 (2)	0.014 (2)	0.011 (2)
C21	0.122 (3)	0.102 (2)	0.107 (2)	−0.001 (2)	0.015 (2)	0.008 (2)

C25	0.120 (3)	0.126 (3)	0.100 (2)	−0.006 (2)	0.015 (2)	0.009 (2)
C24	0.113 (3)	0.126 (3)	0.100 (2)	−0.011 (2)	0.017 (2)	0.015 (2)
C2	0.112 (3)	0.133 (3)	0.101 (2)	0.008 (3)	0.013 (2)	0.001 (3)
C22	0.121 (3)	0.114 (3)	0.112 (2)	−0.010 (2)	0.023 (2)	0.015 (2)
C26	0.137 (4)	0.142 (3)	0.107 (3)	−0.009 (3)	0.026 (3)	0.003 (3)
C3	0.128 (3)	0.128 (3)	0.122 (3)	0.013 (3)	0.030 (3)	−0.017 (3)
C27	0.173 (5)	0.157 (4)	0.121 (3)	0.002 (3)	0.029 (3)	−0.014 (3)

Geometric parameters (Å, º)

S1—C12	1.674 (4)	C10—H10	0.9300
S1—C13	1.719 (4)	C1—C2	1.343 (5)
O1—C18	1.345 (4)	C1—H1	0.9300
O1—C21	1.434 (4)	C14—H14	0.9300
N1—C13	1.298 (4)	C12—H12	0.9300
N1—C11	1.373 (4)	C4—C3	1.356 (5)
N2—C14	1.275 (4)	C4—H4	0.9300
N2—C13	1.377 (4)	C23—C24	1.495 (5)
C6—C7	1.406 (4)	C23—C22	1.517 (5)
C6—C1	1.413 (4)	C23—H23A	0.9700
C6—C5	1.416 (5)	C23—H23B	0.9700
C7—C8	1.366 (4)	C21—C22	1.497 (5)
C7—H7	0.9300	C21—H21A	0.9700
C18—C19	1.370 (5)	C21—H21B	0.9700
C18—C17	1.394 (5)	C25—C26	1.497 (5)
C8—C9	1.409 (5)	C25—C24	1.505 (5)
C8—C11	1.477 (4)	C25—H25A	0.9700
C15—C16	1.382 (5)	C25—H25B	0.9700
C15—C20	1.391 (5)	C24—H24A	0.9700
C15—C14	1.444 (5)	C24—H24B	0.9700
C9—C10	1.349 (4)	C2—C3	1.397 (6)
C9—H9	0.9300	C2—H2	0.9300
C16—C17	1.344 (5)	C22—H22A	0.9700
C16—H16	0.9300	C22—H22B	0.9700
C5—C4	1.400 (5)	C26—C27	1.502 (6)
C5—C10	1.409 (5)	C26—H26A	0.9700
C19—C20	1.376 (4)	C26—H26B	0.9700
C19—H19	0.9300	C3—H3	0.9300
C11—C12	1.364 (5)	C27—H27A	0.9600
C17—H17	0.9300	C27—H27B	0.9600
C20—H20	0.9300	C27—H27C	0.9600
C12—S1—C13	89.11 (18)	C11—C12—H12	124.1
C18—O1—C21	119.0 (3)	S1—C12—H12	124.1
C13—N1—C11	110.8 (3)	C3—C4—C5	120.8 (4)
C14—N2—C13	120.0 (3)	C3—C4—H4	119.6
C7—C6—C1	122.7 (3)	C5—C4—H4	119.6
C7—C6—C5	118.5 (3)	C24—C23—C22	113.7 (3)

C1—C6—C5	118.8 (3)	C24—C23—H23A	108.8
C8—C7—C6	122.3 (3)	C22—C23—H23A	108.8
C8—C7—H7	118.9	C24—C23—H23B	108.8
C6—C7—H7	118.9	C22—C23—H23B	108.8
O1—C18—C19	125.6 (3)	H23A—C23—H23B	107.7
O1—C18—C17	115.2 (3)	O1—C21—C22	107.5 (3)
C19—C18—C17	119.1 (3)	O1—C21—H21A	110.2
C7—C8—C9	118.2 (3)	C22—C21—H21A	110.2
C7—C8—C11	121.7 (3)	O1—C21—H21B	110.2
C9—C8—C11	120.0 (3)	C22—C21—H21B	110.2
N1—C13—N2	128.6 (3)	H21A—C21—H21B	108.5
N1—C13—S1	114.7 (2)	C26—C25—C24	114.6 (3)
N2—C13—S1	116.5 (3)	C26—C25—H25A	108.6
C16—C15—C20	118.0 (3)	C24—C25—H25A	108.6
C16—C15—C14	121.6 (3)	C26—C25—H25B	108.6
C20—C15—C14	120.4 (3)	C24—C25—H25B	108.6
C10—C9—C8	121.4 (3)	H25A—C25—H25B	107.6
C10—C9—H9	119.3	C23—C24—C25	115.0 (3)
C8—C9—H9	119.3	C23—C24—H24A	108.5
C17—C16—C15	121.2 (3)	C25—C24—H24A	108.5
C17—C16—H16	119.4	C23—C24—H24B	108.5
C15—C16—H16	119.4	C25—C24—H24B	108.5
C4—C5—C10	122.9 (3)	H24A—C24—H24B	107.5
C4—C5—C6	118.6 (3)	C1—C2—C3	120.4 (4)
C10—C5—C6	118.5 (3)	C1—C2—H2	119.8
C18—C19—C20	119.7 (3)	C3—C2—H2	119.8
C18—C19—H19	120.1	C21—C22—C23	113.9 (3)
C20—C19—H19	120.1	C21—C22—H22A	108.8
C12—C11—N1	113.6 (3)	C23—C22—H22A	108.8
C12—C11—C8	126.5 (3)	C21—C22—H22B	108.8
N1—C11—C8	119.8 (3)	C23—C22—H22B	108.8
C16—C17—C18	120.8 (3)	H22A—C22—H22B	107.7
C16—C17—H17	119.6	C25—C26—C27	115.0 (4)
C18—C17—H17	119.6	C25—C26—H26A	108.5
C19—C20—C15	121.1 (3)	C27—C26—H26A	108.5
C19—C20—H20	119.5	C25—C26—H26B	108.5
C15—C20—H20	119.5	C27—C26—H26B	108.5
C9—C10—C5	121.1 (3)	H26A—C26—H26B	107.5
C9—C10—H10	119.5	C4—C3—C2	120.6 (4)
C5—C10—H10	119.5	C4—C3—H3	119.7
C2—C1—C6	120.7 (4)	C2—C3—H3	119.7
C2—C1—H1	119.6	C26—C27—H27A	109.5
C6—C1—H1	119.6	C26—C27—H27B	109.5
N2—C14—C15	122.0 (3)	H27A—C27—H27B	109.5
N2—C14—H14	119.0	C26—C27—H27C	109.5
C15—C14—H14	119.0	H27A—C27—H27C	109.5
C11—C12—S1	111.8 (3)	H27B—C27—H27C	109.5

C1—C6—C7—C8	−176.9 (3)	C15—C16—C17—C18	−0.8 (5)
C5—C6—C7—C8	0.1 (5)	O1—C18—C17—C16	178.7 (3)
C21—O1—C18—C19	−9.9 (5)	C19—C18—C17—C16	−0.3 (5)
C21—O1—C18—C17	171.2 (3)	C18—C19—C20—C15	−0.8 (5)
C6—C7—C8—C9	−2.1 (5)	C16—C15—C20—C19	−0.3 (5)
C6—C7—C8—C11	174.8 (3)	C14—C15—C20—C19	177.8 (3)
C11—N1—C13—N2	−175.0 (3)	C8—C9—C10—C5	0.2 (5)
C11—N1—C13—S1	−0.1 (4)	C4—C5—C10—C9	176.6 (4)
C14—N2—C13—N1	−7.2 (6)	C6—C5—C10—C9	−2.3 (5)
C14—N2—C13—S1	178.0 (3)	C7—C6—C1—C2	175.9 (4)
C12—S1—C13—N1	0.2 (3)	C5—C6—C1—C2	−1.1 (5)
C12—S1—C13—N2	175.8 (3)	C13—N2—C14—C15	174.4 (3)
C7—C8—C9—C10	2.0 (5)	C16—C15—C14—N2	−1.4 (5)
C11—C8—C9—C10	−175.0 (3)	C20—C15—C14—N2	−179.4 (3)
C20—C15—C16—C17	1.0 (5)	N1—C11—C12—S1	0.2 (4)
C14—C15—C16—C17	−177.0 (3)	C8—C11—C12—S1	−175.5 (3)
C7—C6—C5—C4	−176.8 (3)	C13—S1—C12—C11	−0.2 (3)
C1—C6—C5—C4	0.3 (5)	C10—C5—C4—C3	−178.7 (4)
C7—C6—C5—C10	2.1 (5)	C6—C5—C4—C3	0.2 (5)
C1—C6—C5—C10	179.2 (3)	C18—O1—C21—C22	−177.7 (3)
O1—C18—C19—C20	−177.8 (3)	C22—C23—C24—C25	−179.3 (3)
C17—C18—C19—C20	1.1 (5)	C26—C25—C24—C23	−178.5 (3)
C13—N1—C11—C12	−0.1 (4)	C6—C1—C2—C3	1.4 (6)
C13—N1—C11—C8	176.0 (3)	O1—C21—C22—C23	61.1 (4)
C7—C8—C11—C12	9.5 (5)	C24—C23—C22—C21	−177.2 (3)
C9—C8—C11—C12	−173.7 (4)	C24—C25—C26—C27	−179.8 (4)
C7—C8—C11—N1	−166.1 (3)	C5—C4—C3—C2	0.1 (6)
C9—C8—C11—N1	10.8 (5)	C1—C2—C3—C4	−0.9 (6)

Hydrogen-bond geometry (Å, º)

*Cg*3 is the centroid of the C5–C10 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···*Cg*3^{i}	0.93	2.85	3.522 (4)	130

Symmetry code: (i) −*x*, *y*+1/2, −*z*+3/2.