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(2*Z*)-2-Benzylidene-4-octadecyl-3,4-dihydro-2*H*-1,4-benzothiazin-3-one

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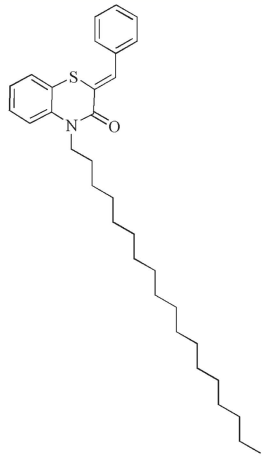
Structural data: full structural data are available from iucrdata.iucr.org

The octadecyl chain in the title compound, $C_{33}H_{47}NOS$, is in the 'fully extended' conformation. A puckering analysis of the thiazine ring was performed. The molecules form micellar blocks in the crystal by intercalation of the extended octadecyl chains and association of the dihydro benzothiazine units through C—H···O hydrogen bonds. These blocks are associated through intercalation of the pendant phenyl groups which reside on the outer edges of each block.

3D view

Chemical scheme



Structure description

1,4-Benzothiazine derivatives constitute an important class of heterocyclic compounds which, even when part of a complex molecule, possess a wide spectrum of biological activities (Sebbar *et al.*, 2016*a*; Gupta *et al.*, 2009). Several sulfur- and nitrogen-containing heterocycles have been well studied and various 1,4-benzothiazine derivatives have been synthesized by several methods (Dixit *et al.*, 2008, 2009). Benzothiazines have found widespread application as antibacterial (Armenise *et al.*, 2012; Sabatini *et al.*, 2008), analgesic (Warren *et al.*, 1987), anticancer (Jacquot *et al.*, 2001) and anticonvulsant (Kalluraya *et al.*, 2005) agents. As a continuation of our research work devoted to the development of N-substituted benzothiazine derivatives and evaluating their potential pharmacological activities, we have studied the condensation reaction of 1-bromooctadecane with (*E*)-2-(benzylidene)-3,4-dihydro-2*H*-1,4-benzothiazin-3-one under phase-transfer catalysis conditions using tetra-*n*-butylammonium bromide (TBAB) as catalyst and potassium carbonate as base (Sebbar *et al.*, 2016*b*, Sebbar *et al.*, 2014; Ellouz *et al.*, 2016). The crystal structure of the compound obtained is reported in this work (Fig. 1).

In the title compound, the octadecyl chain is in the 'fully extended' conformation. A Cremer–Pople puckering analysis of the six-membered heterocyclic ring gave the

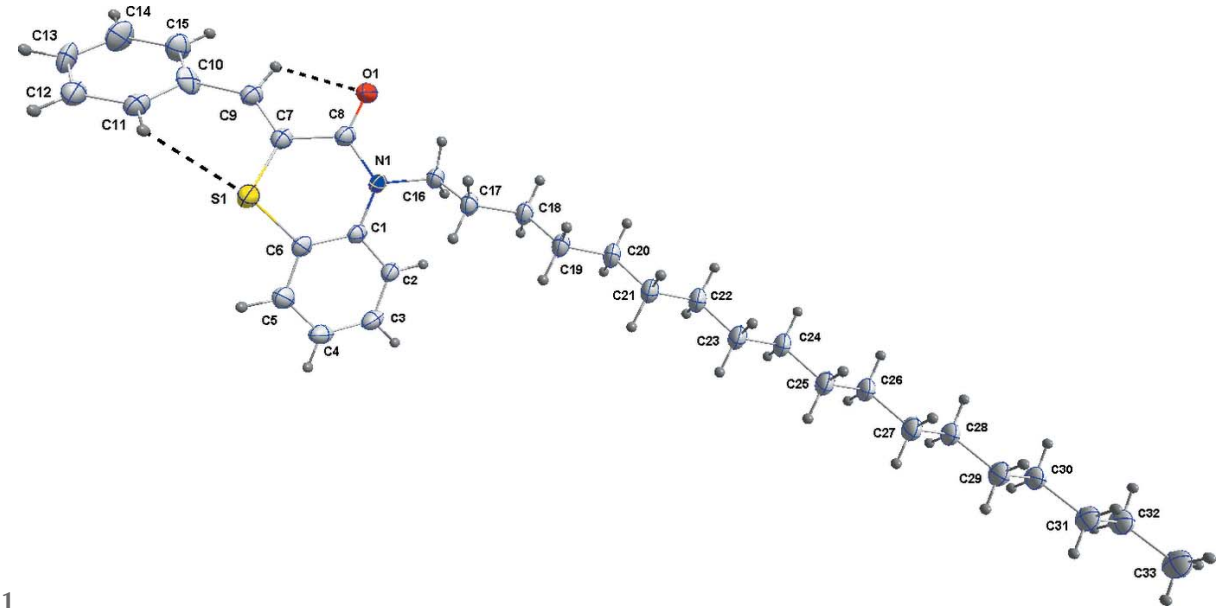


Figure 1
The title molecule with the labelling scheme and 50% probability displacement ellipsoids. Intramolecular hydrogen bonds are shown as dashed lines.

parameters Q = 0.443 (1) Å, θ = 109.7 (2)° and φ = 154.3 (2)°. The pendant phenyl ring is rotationally disordered over two sites having approximately equal occupancy about the C9—C10 bond by 41.1 (2)°. The dihedral angle between the C10–C15 and the C1–C6 rings is 58.4 (1)° while that for the other component (C10*A*–C15*A*) is 32.9 (1)°. Intramolecular C—H···O and C—H···S interactions occur (Table 1 and Fig. 1).

In the crystal, the molecules form micellar blocks through intercalation of the octadecyl chains and association of the polar head groups along the *c*-axis direction through C3—H3···O1 hydrogen bonds (Table 2 and Fig. 2). These blocks are associated through intercalation of the pendant phenyl rings, which reside on the outer edges of each block (Fig. 2).

Synthesis and crystallization

To a solution of 2-(benzylidene)-3,4-dihydro-2*H*-1,4-benzothiazin-3-one (0.5 g, 2 mmol), potassium carbonate (0.55 g,

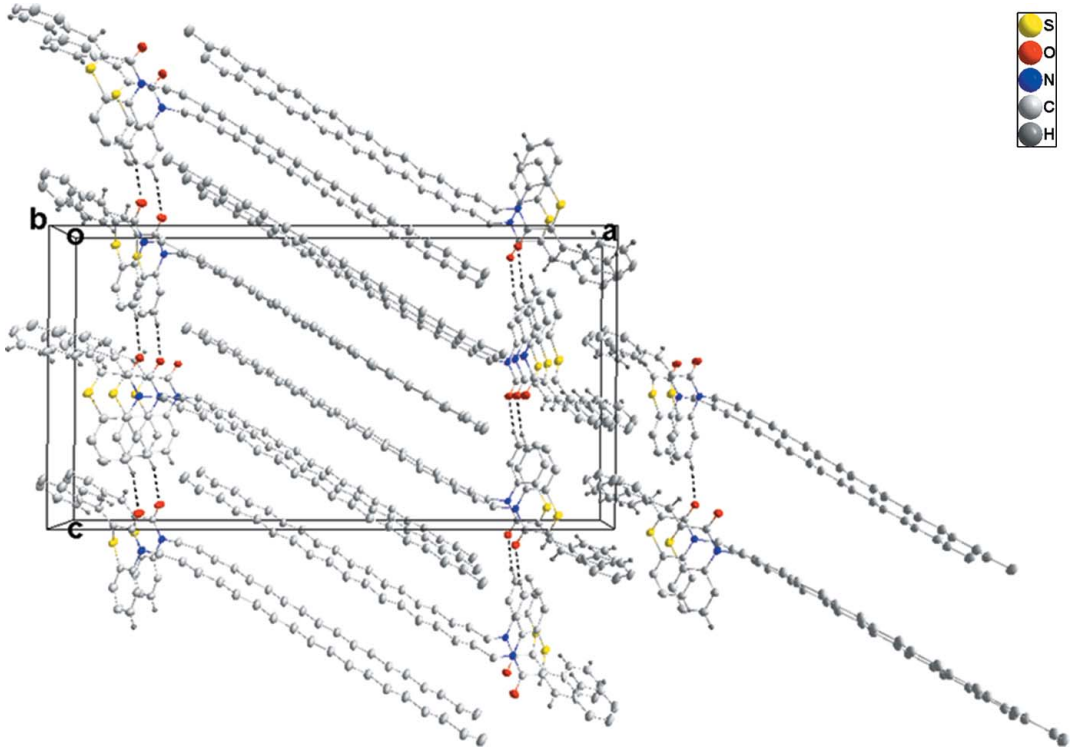


Figure 2
The packing of the title molecule, viewed along the *b*-axis direction, with C—H···O hydrogen bonds shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.95 (2)	2.40 (2)	3.298 (2)	158.0 (18)
C9—H9···O1	0.97 (2)	2.367 (19)	2.769 (2)	104.1 (13)
C11—H11···S1	0.95	2.58	3.225 (2)	126
C16—H16B···O1	0.97 (2)	2.17 (2)	2.679 (2)	111.3 (15)

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

4 mmol) and tetra-*n*-butyl ammonium bromide (0.064 g, 0.2 mmol) in DMF (15 ml) was added 1-bromooctadecane (1.33 g, 4 mmol). Stirring was continued at room temperature for 12 h. The mixture was filtered and the solvent removed. The residue was extracted with water. The organic compound was chromatographed on a column of silica gel with ethyl acetate–hexane (9/1) as eluent. The solid product was purified by recrystallization from ethanol solution to afford colourless crystals in 63% yield.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The pendant phenyl ring is rotationally disordered over two sites having approximately equal occupancy [ratio 0.503 (4):0.497 (4)]. The two components were refined as rigid hexagons with the attached hydrogen atoms in idealized positions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{33}H_{47}NOS$
M_r	505.77
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	33.8411 (7), 4.7106 (1), 18.0987 (4)
β (°)	90.470 (1)
V (Å^3)	2885.05 (11)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.17
Crystal size (mm)	0.24 × 0.11 × 0.03
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.81, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21375, 5792, 4927
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.120, 1.06
No. of reflections	5792
No. of parameters	524
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.46

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170695 [https://doi.org/10.1107/S2414314617006952]

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Crystal data

$C_{33}H_{47}NOS$
M_r = 505.77
Monoclinic, $P2_1/c$
a = 33.8411 (7) Å
b = 4.7106 (1) Å
c = 18.0987 (4) Å
β = 90.470 (1)°
V = 2885.05 (11) Å^3
Z = 4
$F(000)$ = 1104
D_x = 1.164 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9991 reflections
θ = 2.6–74.7°
μ = 1.17 mm^{-1}
T = 150 K
Plate, colourless
0.24 × 0.11 × 0.03 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.81, T_{max} = 0.97
21375 measured reflections
5792 independent reflections
4927 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 74.7°, θ_{min} = 2.6°
h = −42→42
k = −5→5
l = −21→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.120
S = 1.06
5792 reflections
524 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 1.3651P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. The pendant phenyl ring is rotationally disordered over two sites having approximately equal occupancies. The two components were refined as rigid hexagons with the attached hydrogen atoms in idealized positions.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.10593 (2)	0.77362 (9)	0.55251 (2)	0.03197 (13)	
O1	0.17114 (4)	0.2595 (3)	0.43940 (7)	0.0463 (4)	
N1	0.17320 (4)	0.3357 (3)	0.56293 (7)	0.0261 (3)	
C1	0.15506 (4)	0.4140 (3)	0.63057 (8)	0.0245 (3)	
C2	0.16804 (5)	0.2944 (4)	0.69743 (9)	0.0295 (3)	
H2	0.1873 (6)	0.151 (4)	0.6974 (10)	0.033 (5)*	
C3	0.15261 (5)	0.3838 (4)	0.76417 (9)	0.0348 (4)	
H3	0.1623 (6)	0.303 (5)	0.8089 (12)	0.047 (6)*	
C4	0.12362 (5)	0.5891 (4)	0.76594 (10)	0.0358 (4)	
H4	0.1125 (7)	0.651 (5)	0.8107 (13)	0.051 (6)*	
C5	0.10945 (5)	0.7024 (4)	0.70018 (10)	0.0339 (4)	
H5	0.0881 (6)	0.846 (5)	0.7002 (11)	0.040 (5)*	
C6	0.12506 (4)	0.6157 (3)	0.63291 (9)	0.0270 (3)	
C7	0.11658 (4)	0.5095 (4)	0.48802 (9)	0.0273 (3)	
C8	0.15556 (5)	0.3606 (4)	0.49388 (9)	0.0302 (4)	
C9	0.09375 (5)	0.4468 (4)	0.42866 (9)	0.0291 (3)	
H9	0.1057 (6)	0.313 (4)	0.3946 (10)	0.032 (5)*	
C10	0.05477 (6)	0.5456 (5)	0.40246 (18)	0.031 (2)	0.503 (4)
C11	0.03828 (7)	0.7998 (5)	0.42615 (15)	0.0306 (9)	0.503 (4)
H11	0.0532	0.9248	0.4566	0.037*	0.503 (4)
C12	−0.00007 (7)	0.8709 (5)	0.40525 (15)	0.0349 (9)	0.503 (4)
H12	−0.0113	1.0446	0.4214	0.042*	0.503 (4)
C13	−0.02194 (6)	0.6879 (6)	0.36066 (17)	0.036 (2)	0.503 (4)
H13	−0.0482	0.7366	0.3464	0.043*	0.503 (4)
C14	−0.00545 (9)	0.4338 (6)	0.3370 (2)	0.0456 (12)	0.503 (4)
H14	−0.0204	0.3088	0.3065	0.055*	0.503 (4)
C15	0.03290 (9)	0.3627 (5)	0.3579 (2)	0.0388 (10)	0.503 (4)
H15	0.0442	0.1890	0.3417	0.047*	0.503 (4)
C10A	0.05253 (6)	0.5378 (6)	0.41016 (14)	0.0224 (19)	0.497 (4)
C11A	0.02588 (7)	0.6580 (6)	0.45914 (11)	0.0300 (9)	0.497 (4)
H11A	0.0339	0.6986	0.5085	0.036*	0.497 (4)
C12A	−0.01246 (6)	0.7186 (6)	0.43597 (13)	0.0313 (9)	0.497 (4)
H12A	−0.0307	0.8006	0.4694	0.038*	0.497 (4)
C13A	−0.02416 (6)	0.6590 (7)	0.36382 (13)	0.034 (2)	0.497 (4)
H13A	−0.0504	0.7004	0.3480	0.040*	0.497 (4)
C14A	0.00249 (8)	0.5389 (7)	0.31484 (10)	0.0345 (10)	0.497 (4)
H14A	−0.0055	0.4982	0.2655	0.041*	0.497 (4)
C15A	0.04083 (7)	0.4783 (7)	0.33801 (13)	0.0297 (9)	0.497 (4)

H15A	0.0590	0.3962	0.3045	0.036*	0.497 (4)
C16	0.21002 (5)	0.1695 (4)	0.56682 (10)	0.0298 (4)	
H16A	0.2051 (6)	−0.004 (5)	0.5980 (11)	0.037 (5)*	
H16B	0.2162 (6)	0.114 (5)	0.5165 (12)	0.043 (6)*	
C17	0.24455 (5)	0.3396 (4)	0.59860 (10)	0.0304 (4)	
H17A	0.2350 (6)	0.459 (5)	0.6395 (11)	0.039 (5)*	
H17B	0.2534 (6)	0.473 (5)	0.5603 (12)	0.043 (6)*	
C18	0.27795 (5)	0.1485 (4)	0.62544 (11)	0.0333 (4)	
H18A	0.2663 (6)	0.011 (5)	0.6624 (12)	0.045 (6)*	
H18B	0.2885 (6)	0.046 (5)	0.5832 (12)	0.047 (6)*	
C19	0.31103 (5)	0.3118 (4)	0.66399 (10)	0.0331 (4)	
H19A	0.2991 (6)	0.421 (4)	0.7056 (11)	0.038 (5)*	
H19B	0.3222 (6)	0.448 (5)	0.6307 (11)	0.040 (5)*	
C20	0.34370 (5)	0.1221 (4)	0.69465 (11)	0.0363 (4)	
H20A	0.3316 (6)	−0.017 (5)	0.7293 (12)	0.046 (6)*	
H20B	0.3545 (7)	0.012 (5)	0.6542 (13)	0.052 (6)*	
C21	0.37560 (5)	0.2852 (4)	0.73656 (11)	0.0365 (4)	
H21A	0.3627 (6)	0.390 (5)	0.7799 (12)	0.045 (6)*	
H21B	0.3879 (6)	0.424 (5)	0.7029 (12)	0.045 (6)*	
C22	0.40833 (5)	0.0963 (5)	0.76801 (11)	0.0379 (4)	
H22A	0.3964 (7)	−0.048 (5)	0.8017 (13)	0.051 (6)*	
H22B	0.4214 (7)	−0.016 (5)	0.7276 (13)	0.052 (6)*	
C23	0.43998 (5)	0.2610 (5)	0.81015 (11)	0.0386 (4)	
H23A	0.4269 (6)	0.369 (5)	0.8512 (12)	0.046 (6)*	
H23B	0.4523 (7)	0.398 (5)	0.7763 (12)	0.048 (6)*	
C24	0.47278 (5)	0.0739 (5)	0.84179 (11)	0.0391 (4)	
H24A	0.4852 (7)	−0.046 (5)	0.8010 (13)	0.057 (7)*	
H24B	0.4609 (7)	−0.072 (5)	0.8751 (13)	0.053 (6)*	
C25	0.50452 (5)	0.2404 (5)	0.88337 (11)	0.0389 (4)	
H25A	0.4916 (6)	0.354 (5)	0.9245 (12)	0.047 (6)*	
H25B	0.5166 (7)	0.384 (5)	0.8489 (12)	0.050 (6)*	
C26	0.53738 (5)	0.0544 (5)	0.91556 (11)	0.0386 (4)	
H26A	0.5498 (7)	−0.069 (5)	0.8743 (13)	0.052 (6)*	
H26B	0.5253 (6)	−0.087 (5)	0.9512 (12)	0.046 (6)*	
C27	0.56926 (5)	0.2235 (5)	0.95610 (11)	0.0388 (4)	
H27A	0.5568 (7)	0.338 (5)	0.9957 (12)	0.049 (6)*	
H27B	0.5805 (6)	0.363 (5)	0.9208 (12)	0.046 (6)*	
C28	0.60229 (5)	0.0411 (4)	0.98870 (11)	0.0374 (4)	
H28A	0.5905 (6)	−0.100 (5)	1.0231 (11)	0.039 (5)*	
H28B	0.6146 (6)	−0.083 (5)	0.9474 (12)	0.044 (6)*	
C29	0.63446 (5)	0.2137 (4)	1.02729 (11)	0.0374 (4)	
H29A	0.6453 (7)	0.356 (5)	0.9902 (13)	0.053 (6)*	
H29B	0.6224 (6)	0.331 (5)	1.0664 (12)	0.045 (6)*	
C30	0.66771 (5)	0.0345 (4)	1.06014 (10)	0.0355 (4)	
H30A	0.6799 (6)	−0.094 (5)	1.0206 (12)	0.047 (6)*	
H30B	0.6561 (6)	−0.098 (5)	1.0982 (11)	0.042 (6)*	
C31	0.70000 (5)	0.2102 (4)	1.09748 (11)	0.0374 (4)	
H31A	0.6871 (7)	0.327 (5)	1.1351 (13)	0.052 (6)*	

H31B	0.7112 (7)	0.341 (5)	1.0589 (13)	0.057 (7)*
C32	0.73361 (5)	0.0345 (4)	1.13048 (11)	0.0392 (4)
H32A	0.7216 (7)	−0.103 (5)	1.1672 (13)	0.053 (6)*
H32B	0.7455 (7)	−0.088 (5)	1.0913 (13)	0.054 (6)*
C33	0.76560 (6)	0.2158 (5)	1.16623 (14)	0.0476 (5)
H33A	0.7546 (8)	0.322 (6)	1.2070 (15)	0.067 (8)*
H33B	0.7871 (8)	0.105 (6)	1.1857 (14)	0.065 (7)*
H33C	0.7764 (8)	0.352 (6)	1.1291 (16)	0.076 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0329 (2)	0.0295 (2)	0.0333 (2)	0.00240 (16)	−0.01019 (16)	0.00035 (16)
O1	0.0316 (6)	0.0827 (11)	0.0247 (6)	0.0151 (7)	−0.0012 (5)	−0.0048 (6)
N1	0.0202 (6)	0.0350 (7)	0.0230 (6)	−0.0002 (5)	−0.0045 (5)	−0.0004 (5)
C1	0.0185 (6)	0.0308 (8)	0.0240 (7)	−0.0039 (6)	−0.0033 (6)	−0.0003 (6)
C2	0.0244 (7)	0.0367 (9)	0.0272 (8)	0.0018 (7)	−0.0040 (6)	0.0034 (7)
C3	0.0333 (8)	0.0463 (10)	0.0248 (8)	−0.0042 (8)	−0.0043 (7)	0.0030 (7)
C4	0.0350 (9)	0.0454 (10)	0.0270 (8)	−0.0031 (8)	0.0017 (7)	−0.0054 (7)
C5	0.0293 (8)	0.0375 (9)	0.0349 (9)	0.0003 (7)	−0.0012 (7)	−0.0046 (7)
C6	0.0226 (7)	0.0293 (8)	0.0290 (8)	−0.0039 (6)	−0.0047 (6)	−0.0008 (6)
C7	0.0232 (7)	0.0326 (8)	0.0260 (8)	−0.0018 (6)	−0.0018 (6)	0.0052 (6)
C8	0.0230 (7)	0.0426 (9)	0.0250 (8)	−0.0015 (7)	−0.0035 (6)	0.0017 (7)
C9	0.0249 (7)	0.0373 (9)	0.0251 (8)	−0.0019 (7)	−0.0027 (6)	0.0035 (7)
C10	0.016 (3)	0.035 (5)	0.043 (4)	−0.004 (3)	0.007 (3)	0.003 (3)
C11	0.0276 (16)	0.036 (2)	0.0277 (17)	−0.0018 (14)	−0.0063 (14)	0.0041 (15)
C12	0.0316 (17)	0.041 (2)	0.0325 (18)	0.0055 (16)	−0.0018 (14)	0.0077 (16)
C13	0.024 (3)	0.037 (3)	0.047 (5)	0.004 (3)	−0.012 (3)	0.016 (3)
C14	0.033 (2)	0.052 (3)	0.052 (3)	−0.008 (2)	−0.021 (2)	0.005 (2)
C15	0.033 (2)	0.040 (2)	0.043 (2)	−0.0020 (18)	−0.0105 (17)	−0.0011 (19)
C10A	0.030 (3)	0.028 (4)	0.009 (2)	−0.004 (3)	−0.012 (2)	0.009 (2)
C11A	0.0283 (16)	0.0331 (19)	0.0285 (18)	−0.0023 (14)	−0.0025 (14)	0.0014 (15)
C12A	0.0259 (16)	0.0324 (19)	0.0357 (19)	−0.0026 (14)	−0.0003 (14)	0.0028 (15)
C13A	0.028 (4)	0.039 (4)	0.035 (4)	−0.009 (3)	−0.006 (3)	0.007 (3)
C14A	0.034 (2)	0.041 (2)	0.029 (2)	−0.0054 (17)	−0.0120 (16)	0.0041 (16)
C15A	0.0301 (18)	0.036 (2)	0.0224 (19)	0.0003 (16)	−0.0055 (14)	0.0004 (15)
C16	0.0222 (7)	0.0362 (9)	0.0308 (9)	0.0022 (7)	−0.0042 (6)	−0.0034 (7)
C17	0.0195 (7)	0.0363 (9)	0.0352 (9)	0.0005 (7)	−0.0031 (6)	0.0007 (7)
C18	0.0218 (7)	0.0388 (9)	0.0393 (10)	0.0013 (7)	−0.0058 (7)	−0.0014 (8)
C19	0.0209 (7)	0.0401 (10)	0.0383 (9)	0.0013 (7)	−0.0051 (7)	−0.0007 (8)
C20	0.0219 (7)	0.0456 (11)	0.0413 (10)	0.0032 (7)	−0.0058 (7)	−0.0013 (9)
C21	0.0223 (8)	0.0477 (11)	0.0395 (10)	0.0005 (7)	−0.0054 (7)	−0.0001 (8)
C22	0.0223 (8)	0.0505 (11)	0.0408 (10)	0.0019 (8)	−0.0048 (7)	−0.0015 (9)
C23	0.0235 (8)	0.0538 (12)	0.0385 (10)	0.0007 (8)	−0.0063 (7)	0.0008 (9)
C24	0.0223 (8)	0.0557 (12)	0.0392 (10)	0.0023 (8)	−0.0053 (7)	−0.0025 (9)
C25	0.0238 (8)	0.0555 (12)	0.0373 (10)	−0.0001 (8)	−0.0067 (7)	0.0012 (9)
C26	0.0233 (8)	0.0538 (12)	0.0385 (10)	0.0024 (8)	−0.0048 (7)	−0.0028 (9)
C27	0.0261 (8)	0.0523 (12)	0.0378 (10)	0.0012 (8)	−0.0067 (7)	0.0016 (9)

C28	0.0245 (8)	0.0507 (11)	0.0369 (10)	0.0025 (8)	−0.0057 (7)	−0.0034 (8)
C29	0.0274 (8)	0.0457 (11)	0.0388 (10)	0.0019 (8)	−0.0086 (7)	0.0006 (8)
C30	0.0261 (8)	0.0436 (10)	0.0367 (9)	0.0040 (7)	−0.0061 (7)	−0.0018 (8)
C31	0.0306 (8)	0.0414 (10)	0.0402 (10)	0.0044 (8)	−0.0111 (8)	0.0006 (8)
C32	0.0309 (8)	0.0441 (11)	0.0424 (10)	0.0060 (8)	−0.0091 (8)	−0.0007 (9)
C33	0.0365 (10)	0.0537 (13)	0.0524 (13)	0.0048 (9)	−0.0201 (9)	−0.0014 (10)

Geometric parameters (Å, º)

S1—C7	1.7456 (17)	C18—C19	1.523 (2)
S1—C6	1.7536 (16)	C18—H18A	1.01 (2)
O1—C8	1.219 (2)	C18—H18B	0.98 (2)
N1—C8	1.386 (2)	C19—C20	1.523 (2)
N1—C1	1.423 (2)	C19—H19A	1.00 (2)
N1—C16	1.473 (2)	C19—H19B	0.96 (2)
C1—C6	1.391 (2)	C20—C21	1.522 (2)
C1—C2	1.402 (2)	C20—H20A	1.00 (2)
C2—C3	1.385 (2)	C20—H20B	0.97 (2)
C2—H2	0.94 (2)	C21—C22	1.527 (2)
C3—C4	1.378 (3)	C21—H21A	1.03 (2)
C3—H3	0.95 (2)	C21—H21B	0.99 (2)
C4—C5	1.386 (3)	C22—C23	1.522 (3)
C4—H4	0.94 (2)	C22—H22A	1.00 (2)
C5—C6	1.392 (2)	C22—H22B	1.01 (2)
C5—H5	0.99 (2)	C23—C24	1.525 (3)
C7—C9	1.351 (2)	C23—H23A	1.01 (2)
C7—C8	1.497 (2)	C23—H23B	0.99 (2)
C9—C10	1.474 (2)	C24—C25	1.524 (3)
C9—C10A	1.495 (2)	C24—H24A	1.02 (2)
C9—H9	0.97 (2)	C24—H24B	1.00 (2)
C10—C11	1.3900	C25—C26	1.527 (3)
C10—C15	1.3900	C25—H25A	1.02 (2)
C11—C12	1.3900	C25—H25B	1.01 (2)
C11—H11	0.9500	C26—C27	1.524 (3)
C12—C13	1.3900	C26—H26A	1.04 (2)
C12—H12	0.9500	C26—H26B	1.02 (2)
C13—C14	1.3900	C27—C28	1.525 (2)
C13—H13	0.9500	C27—H27A	0.99 (2)
C14—C15	1.3900	C27—H27B	0.99 (2)
C14—H14	0.9500	C28—C29	1.524 (3)
C15—H15	0.9500	C28—H28A	1.00 (2)
C10A—C11A	1.3900	C28—H28B	1.04 (2)
C10A—C15A	1.3900	C29—C30	1.524 (2)
C11A—C12A	1.3900	C29—H29A	1.02 (2)
C11A—H11A	0.9500	C29—H29B	0.99 (2)
C12A—C13A	1.3900	C30—C31	1.524 (2)
C12A—H12A	0.9500	C30—H30A	1.03 (2)
C13A—C14A	1.3900	C30—H30B	1.01 (2)

C13A—H13A	0.9500	C31—C32	1.525 (2)
C14A—C15A	1.3900	C31—H31A	0.98 (2)
C14A—H14A	0.9500	C31—H31B	1.01 (3)
C15A—H15A	0.9500	C32—C33	1.519 (3)
C16—C17	1.526 (2)	C32—H32A	1.02 (2)
C16—H16A	1.01 (2)	C32—H32B	1.00 (2)
C16—H16B	0.97 (2)	C33—H33A	0.97 (3)
C17—C18	1.521 (2)	C33—H33B	0.96 (3)
C17—H17A	0.99 (2)	C33—H33C	1.00 (3)
C17—H17B	0.98 (2)		

C7—S1—C6	100.11 (8)	C18—C19—H19A	107.8 (12)
C8—N1—C1	124.64 (13)	C20—C19—H19B	109.4 (12)
C8—N1—C16	116.50 (13)	C18—C19—H19B	110.0 (12)
C1—N1—C16	117.88 (13)	H19A—C19—H19B	107.0 (17)
C6—C1—C2	118.13 (15)	C21—C20—C19	113.28 (16)
C6—C1—N1	121.57 (14)	C21—C20—H20A	108.1 (12)
C2—C1—N1	120.28 (14)	C19—C20—H20A	108.3 (12)
C3—C2—C1	120.85 (16)	C21—C20—H20B	112.1 (13)
C3—C2—H2	119.1 (11)	C19—C20—H20B	108.3 (13)
C1—C2—H2	120.0 (11)	H20A—C20—H20B	106.3 (18)
C4—C3—C2	120.47 (16)	C20—C21—C22	113.64 (16)
C4—C3—H3	120.2 (13)	C20—C21—H21A	108.6 (12)
C2—C3—H3	119.3 (13)	C22—C21—H21A	107.9 (12)
C3—C4—C5	119.42 (17)	C20—C21—H21B	109.1 (12)
C3—C4—H4	121.7 (14)	C22—C21—H21B	107.9 (13)
C5—C4—H4	118.8 (14)	H21A—C21—H21B	109.7 (18)
C4—C5—C6	120.45 (17)	C23—C22—C21	113.26 (17)
C4—C5—H5	120.6 (12)	C23—C22—H22A	109.1 (13)
C6—C5—H5	118.9 (12)	C21—C22—H22A	109.2 (13)
C1—C6—C5	120.61 (15)	C23—C22—H22B	108.7 (13)
C1—C6—S1	121.94 (12)	C21—C22—H22B	110.8 (13)
C5—C6—S1	117.44 (13)	H22A—C22—H22B	105.5 (19)
C9—C7—C8	116.86 (15)	C22—C23—C24	113.61 (17)
C9—C7—S1	124.60 (13)	C22—C23—H23A	108.4 (12)
C8—C7—S1	118.24 (11)	C24—C23—H23A	109.8 (12)
O1—C8—N1	120.71 (15)	C22—C23—H23B	108.8 (13)
O1—C8—C7	120.83 (14)	C24—C23—H23B	107.6 (13)
N1—C8—C7	118.45 (14)	H23A—C23—H23B	108.4 (19)
C7—C9—C10	133.75 (18)	C25—C24—C23	113.32 (17)
C7—C9—C10A	129.94 (18)	C25—C24—H24A	110.4 (14)
C7—C9—H9	114.1 (11)	C23—C24—H24A	110.5 (13)
C10—C9—H9	112.1 (11)	C25—C24—H24B	109.9 (13)
C10A—C9—H9	115.8 (11)	C23—C24—H24B	109.2 (13)
C11—C10—C15	120.0	H24A—C24—H24B	103.0 (19)
C11—C10—C9	122.23 (17)	C24—C25—C26	113.65 (17)
C15—C10—C9	117.51 (17)	C24—C25—H25A	109.0 (12)
C12—C11—C10	120.0	C26—C25—H25A	109.8 (12)

C12—C11—H11	120.0	C24—C25—H25B	109.1 (13)
C10—C11—H11	120.0	C26—C25—H25B	109.0 (13)
C13—C12—C11	120.0	H25A—C25—H25B	106.0 (18)
C13—C12—H12	120.0	C27—C26—C25	113.19 (17)
C11—C12—H12	120.0	C27—C26—H26A	110.5 (13)
C12—C13—C14	120.0	C25—C26—H26A	110.1 (13)
C12—C13—H13	120.0	C27—C26—H26B	108.9 (12)
C14—C13—H13	120.0	C25—C26—H26B	108.9 (12)
C13—C14—C15	120.0	H26A—C26—H26B	104.9 (18)
C13—C14—H14	120.0	C26—C27—C28	113.91 (17)
C15—C14—H14	120.0	C26—C27—H27A	109.1 (13)
C14—C15—C10	120.0	C28—C27—H27A	109.9 (13)
C14—C15—H15	120.0	C26—C27—H27B	108.0 (13)
C10—C15—H15	120.0	C28—C27—H27B	109.8 (13)
C11A—C10A—C15A	120.0	H27A—C27—H27B	105.9 (19)
C11A—C10A—C9	125.66 (17)	C29—C28—C27	113.29 (17)
C15A—C10A—C9	114.25 (17)	C29—C28—H28A	111.0 (12)
C10A—C11A—C12A	120.0	C27—C28—H28A	108.8 (12)
C10A—C11A—H11A	120.0	C29—C28—H28B	109.9 (12)
C12A—C11A—H11A	120.0	C27—C28—H28B	109.6 (12)
C13A—C12A—C11A	120.0	H28A—C28—H28B	103.8 (17)
C13A—C12A—H12A	120.0	C30—C29—C28	113.95 (16)
C11A—C12A—H12A	120.0	C30—C29—H29A	110.6 (13)
C12A—C13A—C14A	120.0	C28—C29—H29A	108.0 (13)
C12A—C13A—H13A	120.0	C30—C29—H29B	109.7 (13)
C14A—C13A—H13A	120.0	C28—C29—H29B	109.2 (13)
C15A—C14A—C13A	120.0	H29A—C29—H29B	105.0 (18)
C15A—C14A—H14A	120.0	C29—C30—C31	113.38 (16)
C13A—C14A—H14A	120.0	C29—C30—H30A	110.7 (12)
C14A—C15A—C10A	120.0	C31—C30—H30A	109.8 (12)
C14A—C15A—H15A	120.0	C29—C30—H30B	108.5 (12)
C10A—C15A—H15A	120.0	C31—C30—H30B	108.3 (12)
N1—C16—C17	112.56 (14)	H30A—C30—H30B	105.8 (18)
N1—C16—H16A	108.3 (11)	C30—C31—C32	114.12 (16)
C17—C16—H16A	110.1 (11)	C30—C31—H31A	106.9 (14)
N1—C16—H16B	106.6 (12)	C32—C31—H31A	111.5 (13)
C17—C16—H16B	108.8 (13)	C30—C31—H31B	107.2 (14)
H16A—C16—H16B	110.3 (17)	C32—C31—H31B	108.7 (14)
C18—C17—C16	111.98 (15)	H31A—C31—H31B	108 (2)
C18—C17—H17A	110.1 (12)	C33—C32—C31	112.85 (17)
C16—C17—H17A	109.3 (12)	C33—C32—H32A	111.6 (13)
C18—C17—H17B	111.8 (12)	C31—C32—H32A	107.6 (13)
C16—C17—H17B	107.8 (12)	C33—C32—H32B	109.6 (13)
H17A—C17—H17B	105.5 (17)	C31—C32—H32B	109.8 (13)
C17—C18—C19	112.89 (15)	H32A—C32—H32B	105.1 (19)
C17—C18—H18A	107.3 (12)	C32—C33—H33A	109.8 (16)
C19—C18—H18A	107.9 (12)	C32—C33—H33B	112.7 (16)
C17—C18—H18B	108.6 (13)	H33A—C33—H33B	107 (2)

C19—C18—H18B	109.7 (13)	C32—C33—H33C	109.8 (16)
H18A—C18—H18B	110.3 (18)	H33A—C33—H33C	109 (2)
C20—C19—C18	113.54 (16)	H33B—C33—H33C	108 (2)
C20—C19—H19A	108.8 (12)		

C8—N1—C1—C6	−24.7 (2)	C10—C11—C12—C13	0.0
C16—N1—C1—C6	167.07 (14)	C11—C12—C13—C14	0.0
C8—N1—C1—C2	157.30 (16)	C12—C13—C14—C15	0.0
C16—N1—C1—C2	−10.9 (2)	C13—C14—C15—C10	0.0
C6—C1—C2—C3	−2.8 (2)	C11—C10—C15—C14	0.0
N1—C1—C2—C3	175.29 (15)	C9—C10—C15—C14	174.3 (3)
C1—C2—C3—C4	1.2 (3)	C7—C9—C10A—C11A	−15.3 (3)
C2—C3—C4—C5	1.1 (3)	C7—C9—C10A—C15A	168.19 (19)
C3—C4—C5—C6	−1.7 (3)	C15A—C10A—C11A—C12A	0.0
C2—C1—C6—C5	2.2 (2)	C9—C10A—C11A—C12A	−176.3 (3)
N1—C1—C6—C5	−175.88 (15)	C10A—C11A—C12A—C13A	0.0
C2—C1—C6—S1	−178.72 (12)	C11A—C12A—C13A—C14A	0.0
N1—C1—C6—S1	3.2 (2)	C12A—C13A—C14A—C15A	0.0
C4—C5—C6—C1	0.1 (3)	C13A—C14A—C15A—C10A	0.0
C4—C5—C6—S1	−179.09 (14)	C11A—C10A—C15A—C14A	0.0
C7—S1—C6—C1	25.40 (15)	C9—C10A—C15A—C14A	176.7 (2)
C7—S1—C6—C5	−155.46 (13)	C8—N1—C16—C17	122.78 (16)
C6—S1—C7—C9	146.07 (15)	C1—N1—C16—C17	−68.02 (19)
C6—S1—C7—C8	−40.46 (14)	N1—C16—C17—C18	161.52 (15)
C1—N1—C8—O1	−171.61 (16)	C16—C17—C18—C19	−174.54 (15)
C16—N1—C8—O1	−3.2 (2)	C17—C18—C19—C20	177.06 (16)
C1—N1—C8—C7	7.2 (2)	C18—C19—C20—C21	−177.02 (16)
C16—N1—C8—C7	175.62 (14)	C19—C20—C21—C22	179.56 (16)
C9—C7—C8—O1	21.7 (3)	C20—C21—C22—C23	−179.70 (16)
S1—C7—C8—O1	−152.32 (15)	C21—C22—C23—C24	179.97 (16)
C9—C7—C8—N1	−157.19 (16)	C22—C23—C24—C25	179.53 (16)
S1—C7—C8—N1	28.8 (2)	C23—C24—C25—C26	179.72 (16)
C8—C7—C9—C10	−179.2 (2)	C24—C25—C26—C27	179.20 (16)
S1—C7—C9—C10	−5.6 (3)	C25—C26—C27—C28	179.93 (16)
C8—C7—C9—C10A	174.2 (2)	C26—C27—C28—C29	178.50 (16)
S1—C7—C9—C10A	−12.3 (3)	C27—C28—C29—C30	−179.97 (16)
C7—C9—C10—C11	20.0 (4)	C28—C29—C30—C31	179.07 (16)
C7—C9—C10—C15	−154.1 (2)	C29—C30—C31—C32	−179.82 (17)
C15—C10—C11—C12	0.0	C30—C31—C32—C33	179.12 (18)
C9—C10—C11—C12	−174.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.95 (2)	2.40 (2)	3.298 (2)	158.0 (18)
C9—H9···O1	0.97 (2)	2.367 (19)	2.769 (2)	104.1 (13)

C11—H11···S1	0.95	2.58	3.225 (2)	126
C16—H16*B*···O1	0.97 (2)	2.17 (2)	2.679 (2)	111.3 (15)

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