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(2*Z*)-2-(4-Chlorobenzylidene)-4-[2-(2-oxooxazolidin-3-yl)ethyl]-3,4-dihydro-2*H*-1,4-benzothiazin-3-one

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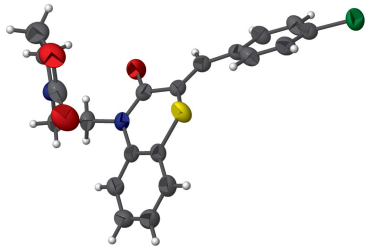
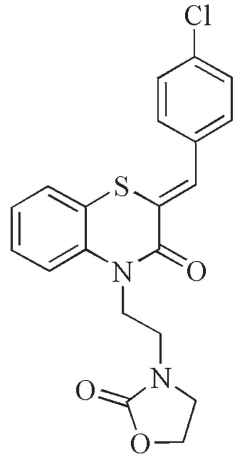
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{20}H_{17}ClN_2O_3S$, the oxazolidine ring is oriented towards the benzothiazine moiety so that the centroid of the former is *ca* 5.05 Å from the sulfur atom of the latter. In the crystal, the molecules are arranged in layers parallel to (101) and held together by the aid of C—H···O interactions, resulting in a three-dimensional network structure.

3D view



Chemical scheme



Structure description

A number of pharmacological tests have revealed 1,4-benzothiazine derivatives to possess a wide spectrum of biological activities, even when they are part of a complex molecule (Schiaffella *et al.*, 2006; Gupta *et al.*, 2009). As a result of the presence of a fold along the nitrogen–sulfur axis, the biological activities of some 1,4-benzothiazines are similar to that of phenothiazines, featuring the same structural specificity (Bansode *et al.*, 2009; Dixit *et al.*, 2009; Thomas *et al.*, 2003). Generally, 1,4-benzothiazine derivatives have found widespread applications as analgesic (Warren & Knaus, 1987), antibacterial (Armenise *et al.*, 2012; Sabatini *et al.*, 2008), anticancer (Jacquot *et al.*, 2001), anticonvulsant (Kalluraya *et al.*, 2005) or anthelmintic (Munirajasekar *et al.*, 2011) agents. In a continuation of our research activities devoted to the development of N-substituted 1,4-benzothiazine derivatives and the evaluation of their potential pharmacological activities (Sebbar *et al.*, 2016; Ellouz *et al.*, 2015), we have synthesized a new heterocyclic system containing 1,4-benzothiazine and oxazolidinone moieties.

In the title molecule (Fig. 1), the dihedral angle between the two benzene rings (C1–C6 and C10–C15) is 51.62 (5)°. A puckering analysis of the oxazolidine ring revealed a

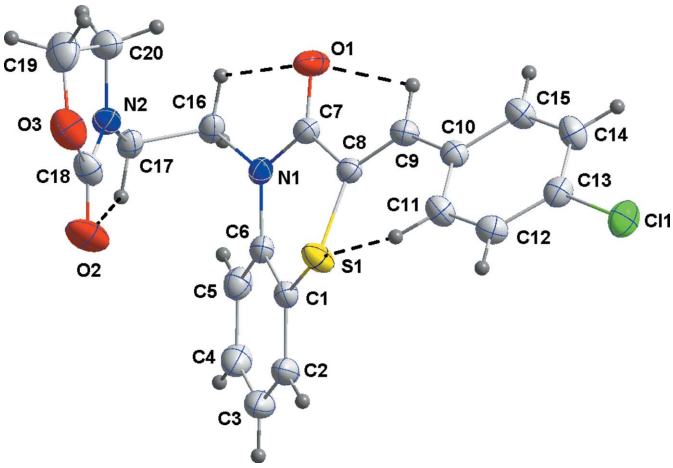


Figure 1
The molecular structure of the title compound drawn with displacement ellipsoids at the 50% probability level. Intramolecular C—H···O hydrogen bonds are shown by dashed lines.

puckering amplitude with parameters $Q(2)$ = 0.206 (2) Å and $\varphi(2)$ = 131.9 (5)°. The ring has an envelope conformation with a twist on the C19—C20 bond and atom C20 as the flap. A similar analysis of the heterocyclic portion of the benzothiazene moiety gave Q = 0.426 (1) Å, θ = 73.1 (6)° and φ = 341.4 (2)°. The oxazolidine ring is oriented towards the benzothiazine unit such that the centroid of the oxazolidine ring is only 4.094 (2) Å from C7 and 5.053 (2) Å from S1 (Fig. 1). The overall conformation of the molecule is determined in part by intramolecular C—H···O and C—H···S hydrogen bonds (Fig. 1 and Table 1). In the crystal, the layered arrangement of the molecules is sustained by a three-dimensional network of C—H···O interactions (Table 1, Fig. 2).

Synthesis and crystallization

To a solution of (2*Z*)-2-(4-chlorobenzylidene)-3,4-dihydro-2*H*-1,4-benzothiazin-3-one (0.29 g, 1.00 mmol) in DMF (15 ml), was added tetra-*n*-butylammonium bromide (0.1 mmol), 2.2 eq of bis (2-chloroethyl)amine hydrochloride and 2.00 eq of potassium carbonate. The mixture was stirred at 353 K for 6 h. After removal of salts by filtration, the solution was evaporated under reduced pressure and the residue obtained was dissolved in dichloromethane. The remaining salts were extracted with distilled water, and the mixture obtained was chromatographed on a silica gel column (eluent: ethyl acetate/hexane: 4/1). The solid isolated was recrystallized from ethanol to afford colorless crystals in 64% yield.

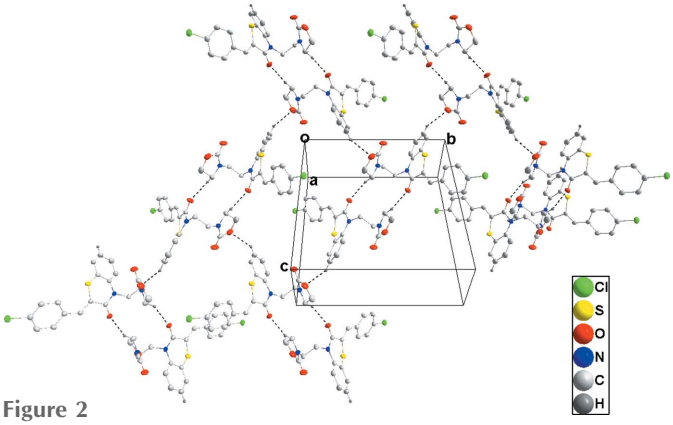


Figure 2
A portion of the crystal structure with C—H···O and C—H···S hydrogen bonds shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O3^{i}	0.93	2.60	3.380 (2)	142
C9—H9···O1	0.93	2.34	2.7344 (18)	105
C11—H11···S1	0.93	2.50	3.1463 (15)	127
C16—H16*B*···O1	0.97	2.23	2.6923 (19)	108
C17—H17*B*···O2	0.97	2.54	2.9049 (18)	102
C20—H20*A*···O1^{ii}	0.97	2.43	3.159 (2)	132

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{17}ClN_2O_3S$
M_r	400.86
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	6.2315 (3), 15.5466 (8), 18.9162 (10)
β (°)	98.845 (1)
V (Å^3)	1810.78 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.35
Crystal size (mm)	0.45 × 0.33 × 0.16
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.86, 0.95
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33990, 4719, 3743
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.678
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.123, 1.09
No. of reflections	4719
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.28

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170646 [https://doi.org/10.1107/S2414314617006460]

(2*Z*)-2-(4-Chlorobenzylidene)-4-[2-(2-oxooxazoliden-3-yl)ethyl]-3,4-dihydro-2*H*-1,4-benzothiazin-3-one

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Crystal data

$C_{20}H_{17}ClN_2O_3S$
M_r = 400.86
Monoclinic, $P2_1/n$
a = 6.2315 (3) Å
b = 15.5466 (8) Å
c = 18.9162 (10) Å
β = 98.845 (1)°
V = 1810.78 (16) Å^3
Z = 4
$F(000)$ = 832
D_x = 1.470 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9941 reflections
θ = 2.2–28.5°
μ = 0.35 mm^{-1}
T = 296 K
Block, colourless
0.45 × 0.33 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.86, T_{max} = 0.95
33990 measured reflections
4719 independent reflections
3743 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 28.8°, θ_{min} = 1.7°
h = −8→8
k = −21→21
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.123
S = 1.09
4719 reflections
244 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 0.1928P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, collected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 15 sec/frame.

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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.87886 (7)	−0.06538 (3)	0.34978 (2)	0.06434 (14)
S1	0.61719 (6)	0.22088 (3)	0.61074 (2)	0.05320 (13)
O1	0.0726 (2)	0.31674 (8)	0.51581 (6)	0.0664 (3)
O2	0.63844 (18)	0.47048 (12)	0.70186 (8)	0.0800 (4)
O3	0.6080 (2)	0.54626 (10)	0.59946 (8)	0.0758 (4)
N1	0.20199 (18)	0.31452 (7)	0.63432 (6)	0.0413 (3)
N2	0.30695 (17)	0.50294 (8)	0.63633 (7)	0.0459 (3)
C1	0.5149 (2)	0.23083 (9)	0.69107 (7)	0.0431 (3)
C2	0.6326 (3)	0.19328 (11)	0.75182 (8)	0.0564 (4)
H2	0.7598	0.1634	0.7483	0.068*
C3	0.5618 (3)	0.20006 (12)	0.81746 (9)	0.0660 (5)
H3	0.6426	0.1761	0.8581	0.079*
C4	0.3727 (3)	0.24218 (12)	0.82193 (9)	0.0639 (5)
H4	0.3245	0.2466	0.8659	0.077*
C5	0.2508 (3)	0.27862 (10)	0.76182 (9)	0.0545 (4)
H5	0.1204	0.3060	0.7658	0.065*
C6	0.3219 (2)	0.27462 (8)	0.69553 (7)	0.0411 (3)
C7	0.2053 (2)	0.28940 (9)	0.56473 (8)	0.0432 (3)
C8	0.3787 (2)	0.22887 (8)	0.54877 (7)	0.0394 (3)
C9	0.3506 (2)	0.19155 (9)	0.48386 (7)	0.0432 (3)
H9	0.2205	0.2054	0.4551	0.052*
C10	0.4893 (2)	0.13308 (9)	0.45089 (7)	0.0424 (3)
C11	0.7127 (2)	0.12295 (10)	0.47337 (8)	0.0490 (3)
H11	0.7826	0.1570	0.5103	0.059*
C12	0.8304 (2)	0.06316 (11)	0.44155 (8)	0.0498 (3)
H12	0.9787	0.0572	0.4570	0.060*
C13	0.7282 (2)	0.01232 (10)	0.38690 (8)	0.0475 (3)
C14	0.5106 (3)	0.02288 (11)	0.36082 (8)	0.0543 (4)
H14	0.4435	−0.0105	0.3229	0.065*
C15	0.3944 (2)	0.08405 (11)	0.39213 (8)	0.0500 (3)
H15	0.2489	0.0929	0.3737	0.060*

C16	0.0506 (2)	0.38381 (9)	0.64572 (8)	0.0445 (3)
H16A	−0.0503	0.3627	0.6760	0.053*
H16B	−0.0327	0.4001	0.6001	0.053*
C17	0.1671 (2)	0.46259 (9)	0.68036 (8)	0.0440 (3)
H17A	0.0599	0.5041	0.6907	0.053*
H17B	0.2530	0.4458	0.7254	0.053*
C18	0.5244 (2)	0.50246 (11)	0.65165 (9)	0.0536 (4)
C19	0.4331 (4)	0.58882 (14)	0.55426 (12)	0.0787 (6)
H19A	0.4513	0.5845	0.5044	0.094*
H19B	0.4264	0.6491	0.5669	0.094*
C20	0.2305 (3)	0.54183 (12)	0.56775 (10)	0.0616 (4)
H20A	0.1113	0.5812	0.5703	0.074*
H20B	0.1858	0.4988	0.5313	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0707 (3)	0.0563 (2)	0.0708 (3)	0.00881 (19)	0.0257 (2)	−0.00626 (19)
S1	0.03737 (19)	0.0733 (3)	0.0475 (2)	0.00586 (16)	0.00185 (14)	−0.01277 (17)
O1	0.0699 (7)	0.0718 (8)	0.0531 (6)	0.0307 (6)	−0.0048 (5)	0.0007 (6)
O2	0.0369 (6)	0.1218 (13)	0.0767 (8)	0.0130 (7)	−0.0055 (6)	−0.0065 (8)
O3	0.0541 (7)	0.0942 (10)	0.0820 (9)	−0.0240 (7)	0.0199 (6)	−0.0076 (8)
N1	0.0388 (6)	0.0353 (5)	0.0492 (6)	0.0031 (4)	0.0052 (5)	−0.0034 (5)
N2	0.0322 (5)	0.0462 (6)	0.0571 (7)	0.0000 (5)	0.0004 (5)	0.0027 (5)
C1	0.0459 (7)	0.0392 (7)	0.0421 (7)	0.0007 (5)	0.0000 (5)	−0.0066 (5)
C2	0.0614 (9)	0.0510 (8)	0.0519 (8)	0.0117 (7)	−0.0072 (7)	−0.0078 (7)
C3	0.0911 (13)	0.0568 (9)	0.0454 (8)	0.0081 (9)	−0.0046 (8)	0.0007 (7)
C4	0.0907 (14)	0.0563 (10)	0.0462 (8)	0.0019 (9)	0.0153 (8)	−0.0001 (7)
C5	0.0650 (10)	0.0478 (8)	0.0535 (8)	0.0019 (7)	0.0178 (7)	−0.0023 (6)
C6	0.0450 (7)	0.0330 (6)	0.0448 (7)	−0.0014 (5)	0.0051 (5)	−0.0029 (5)
C7	0.0438 (7)	0.0385 (7)	0.0464 (7)	0.0021 (5)	0.0040 (6)	0.0016 (5)
C8	0.0387 (6)	0.0373 (6)	0.0416 (6)	−0.0008 (5)	0.0048 (5)	0.0024 (5)
C9	0.0413 (7)	0.0469 (7)	0.0405 (6)	0.0010 (6)	0.0037 (5)	0.0018 (5)
C10	0.0445 (7)	0.0455 (7)	0.0379 (6)	−0.0022 (6)	0.0088 (5)	0.0012 (5)
C11	0.0437 (7)	0.0597 (9)	0.0436 (7)	−0.0052 (6)	0.0062 (6)	−0.0088 (6)
C12	0.0436 (7)	0.0597 (9)	0.0467 (7)	0.0027 (6)	0.0088 (6)	0.0005 (6)
C13	0.0540 (8)	0.0463 (7)	0.0457 (7)	0.0006 (6)	0.0190 (6)	0.0016 (6)
C14	0.0525 (8)	0.0617 (9)	0.0496 (8)	−0.0085 (7)	0.0110 (6)	−0.0146 (7)
C15	0.0425 (7)	0.0634 (9)	0.0442 (7)	−0.0027 (6)	0.0064 (6)	−0.0070 (6)
C16	0.0328 (6)	0.0392 (7)	0.0613 (8)	0.0022 (5)	0.0069 (6)	−0.0066 (6)
C17	0.0357 (6)	0.0401 (7)	0.0562 (8)	0.0038 (5)	0.0076 (5)	−0.0063 (6)
C18	0.0347 (7)	0.0639 (9)	0.0618 (9)	−0.0036 (6)	0.0066 (6)	−0.0171 (7)
C19	0.0960 (15)	0.0654 (11)	0.0780 (13)	−0.0226 (11)	0.0243 (11)	0.0038 (10)
C20	0.0598 (9)	0.0572 (9)	0.0638 (10)	−0.0026 (8)	−0.0030 (8)	0.0099 (8)

Geometric parameters (Å, º)

Cl1—C13	1.7426 (15)	C8—C9	1.3448 (19)
S1—C1	1.7427 (15)	C9—C10	1.459 (2)
S1—C8	1.7501 (13)	C9—H9	0.9300
O1—C7	1.2190 (17)	C10—C11	1.4004 (19)
O2—C18	1.203 (2)	C10—C15	1.4015 (19)
O3—C18	1.367 (2)	C11—C12	1.378 (2)
O3—C19	1.439 (3)	C11—H11	0.9300
N1—C7	1.3763 (18)	C12—C13	1.377 (2)
N1—C6	1.4207 (18)	C12—H12	0.9300
N1—C16	1.4696 (16)	C13—C14	1.380 (2)
N2—C18	1.3416 (17)	C14—C15	1.383 (2)
N2—C17	1.4386 (19)	C14—H14	0.9300
N2—C20	1.444 (2)	C15—H15	0.9300
C1—C2	1.393 (2)	C16—C17	1.5201 (19)
C1—C6	1.396 (2)	C16—H16A	0.9700
C2—C3	1.384 (2)	C16—H16B	0.9700
C2—H2	0.9300	C17—H17A	0.9700
C3—C4	1.362 (3)	C17—H17B	0.9700
C3—H3	0.9300	C19—C20	1.514 (3)
C4—C5	1.388 (3)	C19—H19A	0.9700
C4—H4	0.9300	C19—H19B	0.9700
C5—C6	1.394 (2)	C20—H20A	0.9700
C5—H5	0.9300	C20—H20B	0.9700
C7—C8	1.4980 (19)		
C1—S1—C8	101.01 (7)	C10—C11—H11	119.5
C18—O3—C19	108.68 (13)	C13—C12—C11	119.94 (14)
C7—N1—C6	124.90 (11)	C13—C12—H12	120.0
C7—N1—C16	116.93 (11)	C11—C12—H12	120.0
C6—N1—C16	118.01 (11)	C12—C13—C14	121.05 (14)
C18—N2—C17	123.65 (13)	C12—C13—Cl1	118.99 (12)
C18—N2—C20	112.28 (14)	C14—C13—Cl1	119.95 (12)
C17—N2—C20	123.86 (12)	C13—C14—C15	118.65 (14)
C2—C1—C6	120.25 (14)	C13—C14—H14	120.7
C2—C1—S1	117.74 (12)	C15—C14—H14	120.7
C6—C1—S1	122.01 (11)	C14—C15—C10	121.91 (14)
C3—C2—C1	120.54 (15)	C14—C15—H15	119.0
C3—C2—H2	119.7	C10—C15—H15	119.0
C1—C2—H2	119.7	N1—C16—C17	112.26 (11)
C4—C3—C2	119.37 (16)	N1—C16—H16A	109.2
C4—C3—H3	120.3	C17—C16—H16A	109.2
C2—C3—H3	120.3	N1—C16—H16B	109.2
C3—C4—C5	121.02 (16)	C17—C16—H16B	109.2
C3—C4—H4	119.5	H16A—C16—H16B	107.9
C5—C4—H4	119.5	N2—C17—C16	113.18 (12)
C4—C5—C6	120.60 (16)	N2—C17—H17A	108.9

C4—C5—H5	119.7	C16—C17—H17A	108.9
C6—C5—H5	119.7	N2—C17—H17B	108.9
C5—C6—C1	118.19 (14)	C16—C17—H17B	108.9
C5—C6—N1	120.89 (13)	H17A—C17—H17B	107.8
C1—C6—N1	120.92 (13)	O2—C18—N2	128.85 (17)
O1—C7—N1	121.25 (13)	O2—C18—O3	122.14 (14)
O1—C7—C8	119.49 (13)	N2—C18—O3	109.02 (14)
N1—C7—C8	119.24 (12)	O3—C19—C20	104.66 (15)
C9—C8—C7	117.29 (12)	O3—C19—H19A	110.8
C9—C8—S1	123.97 (11)	C20—C19—H19A	110.8
C7—C8—S1	118.30 (10)	O3—C19—H19B	110.8
C8—C9—C10	131.05 (13)	C20—C19—H19B	110.8
C8—C9—H9	114.5	H19A—C19—H19B	108.9
C10—C9—H9	114.5	N2—C20—C19	100.66 (14)
C11—C10—C15	117.29 (13)	N2—C20—H20A	111.6
C11—C10—C9	124.53 (12)	C19—C20—H20A	111.6
C15—C10—C9	118.18 (12)	N2—C20—H20B	111.6
C12—C11—C10	120.92 (13)	C19—C20—H20B	111.6
C12—C11—H11	119.5	H20A—C20—H20B	109.4

C8—S1—C1—C2	153.67 (12)	S1—C8—C9—C10	5.3 (2)
C8—S1—C1—C6	−26.30 (13)	C8—C9—C10—C11	−19.8 (2)
C6—C1—C2—C3	−1.0 (2)	C8—C9—C10—C15	160.93 (15)
S1—C1—C2—C3	178.98 (14)	C15—C10—C11—C12	−3.9 (2)
C1—C2—C3—C4	1.5 (3)	C9—C10—C11—C12	176.77 (14)
C2—C3—C4—C5	−0.3 (3)	C10—C11—C12—C13	−0.1 (2)
C3—C4—C5—C6	−1.5 (3)	C11—C12—C13—C14	3.1 (2)
C4—C5—C6—C1	1.9 (2)	C11—C12—C13—Cl1	−177.73 (12)
C4—C5—C6—N1	−177.67 (15)	C12—C13—C14—C15	−2.0 (2)
C2—C1—C6—C5	−0.7 (2)	Cl1—C13—C14—C15	178.92 (12)
S1—C1—C6—C5	179.28 (11)	C13—C14—C15—C10	−2.3 (2)
C2—C1—C6—N1	178.92 (13)	C11—C10—C15—C14	5.2 (2)
S1—C1—C6—N1	−1.12 (18)	C9—C10—C15—C14	−175.49 (15)
C7—N1—C6—C5	−154.04 (14)	C7—N1—C16—C17	−118.43 (14)
C16—N1—C6—C5	21.29 (19)	C6—N1—C16—C17	65.86 (16)
C7—N1—C6—C1	26.4 (2)	C18—N2—C17—C16	−110.69 (16)
C16—N1—C6—C1	−158.30 (12)	C20—N2—C17—C16	63.64 (18)
C6—N1—C7—O1	167.61 (14)	N1—C16—C17—N2	63.91 (16)
C16—N1—C7—O1	−7.8 (2)	C17—N2—C18—O2	−0.1 (3)
C6—N1—C7—C8	−13.8 (2)	C20—N2—C18—O2	−175.00 (18)
C16—N1—C7—C8	170.82 (12)	C17—N2—C18—O3	−179.91 (13)
O1—C7—C8—C9	−15.3 (2)	C20—N2—C18—O3	5.18 (19)
N1—C7—C8—C9	166.08 (13)	C19—O3—C18—O2	−170.22 (18)
O1—C7—C8—S1	157.32 (12)	C19—O3—C18—N2	9.62 (19)
N1—C7—C8—S1	−21.29 (17)	C18—O3—C19—C20	−19.5 (2)
C1—S1—C8—C9	−151.29 (12)	C18—N2—C20—C19	−16.49 (19)
C1—S1—C8—C7	36.61 (12)	C17—N2—C20—C19	168.61 (15)
C7—C8—C9—C10	177.49 (14)	O3—C19—C20—N2	20.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O3^{i}	0.93	2.60	3.380 (2)	142
C9—H9···O1	0.93	2.34	2.7344 (18)	105
C11—H11···S1	0.93	2.50	3.1463 (15)	127
C16—H16*B*···O1	0.97	2.23	2.6923 (19)	108
C17—H17*B*···O2	0.97	2.54	2.9049 (18)	102
C20—H20*A*···O1^{ii}	0.97	2.43	3.159 (2)	132

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