organic compounds

(R)-[(R)-3-Benzyl-2-oxooxazolidin-4-yl]-[4-(methylsulfonyl)phenyl]methyl acetate

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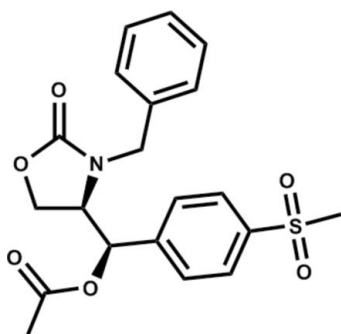Correspondence e-mail: chjin641@163.com

The structure of the title compound, $C_{20}H_{21}NO_6S$, is of interest with respect to its antibacterial properties. The oxazolidine ring makes dihedral angles of 79.63 (14) and 56.16 (12)° with the phenyl and benzene rings, respectively, while the phenyl and benzene rings make a dihedral angle of 64.37 (13)°. In the crystal, non-classical C—H⋯O hydrogen bonds link adjacent molecules along the c axis.

Related literature

For the original synthesis of the title compound, see: Li *et al.* (2011). For inversion of the configuration of the sulfonyloxy moiety, see: Shi *et al.* (2010). For background to the antibacterial properties of thiamphenicol-like compounds, see: Nagabhushan (1980, 1981); Jommi *et al.* (1985).

Experimental

Crystal data

$C_{20}H_{21}NO_6S$	V = 952.0 (7) Å^3
M_r = 403.44	Z = 2
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
a = 5.837 (3) Å	μ = 0.21 mm^{-1}
b = 21.021 (10) Å	T = 296 K
c = 7.884 (4) Å	$0.30 \times 0.25 \times 0.16$ mm
β = 100.256 (7)°	

Data collection

Bruker SMART CCD area-detector diffractometer	6495 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	3658 independent reflections
T_{min} = 0.940, T_{max} = 0.968	3254 reflections with $I > 2\sigma(I)$
	R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$wR(F^2)$ = 0.091	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
S = 1.02	Absolute structure: Flack (1983), 1356 Friedel pairs
3658 reflections	Absolute structure parameter: −0.06 (6)
255 parameters	
1 restraint	
H-atom parameters constrained	

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
C7—H7A⋯O4i	0.97	2.52	3.373 (3)	147
C10—H10⋯O6i	0.98	2.54	3.384 (3)	144
C13—H13C⋯O1ii	0.96	2.55	3.305 (3)	135

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5390).

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supporting information

(*R*)-[(*R*)-3-Benzyl-2-oxooxazolidin-4-yl][4-(methylsulfonyl)phenyl]methyl acetate

Feng Li, Ming-Zhong Zhao, Chun-Hua Jin and Jian-Wei Zou

S1. Comment

During the study on the synthesis of florfenicol, a class of antibiotics with pronounced broad-spectrum antibacterial activity, (Nagabhushan, 1980 & Jommi *et al.*, 1985). the title compound was produced and is a key intermediate in the synthetic route to florfenicol (Li *et al.*, 2011). The title compound was synthesized through the nucleophilic substitution reaction of (*S*)-((*R*)-3-benzyl-2-oxooxazolidin-4-yl)(4-(methylsulfonyl) phenyl)methylmethane sulfonate. Here we report the crystal structure of the title compound.

Fig. 1 shows the molecular structure of the title compound. The enantiomer was selected on the basis of the configuration of the starting material. All chiral carbon atoms (C10 and C11) are *R*-configuration. Only one molecule is included in the asymmetrical unit of this compound (Fig. 1). All the bond lengths and relevant angles are in the typical ranges. Although there is no –NH or –OH group available in the structure to form strong hydrogen bonds, the C atoms are involved in the formation of non-classical inter-molecular C—H···O hydrogen bonds (Fig 2).

S2. Experimental

The literature procedure according to Li *et al.* (2011) was followed. A solution of 1,8-diazabicyclo[5.4.0]undec-7-ene (700 mg, 4.56 mmol) and glacial acetic acid (550 mg, 9.11 mmol) in anhydrous toluene (5 mL) was stirred for 1.5 h at room temperature. (*S*)-((*R*)-3-benzyl-2-oxooxazolidin-4-yl)(4-(methylsulfonyl)phenyl)methylmethanesulfonate was added and the reaction mixture was heated to 363 K for 8 h. The resulting mixture was cooled to r.t., diluted with CH_2Cl_2 (40 mL) and washed with 2M aq. HCl (30 mL), 10% aq. K_2CO_3 (30 mL), and brine (30 mL) successively. The organic phase was dried over Na_2SO_4, concentrated in vacuo. The residue was purified by flash chromatography to afford the title compound 850 mg (92%) as a white solid. Suitable crystals for X-ray experiments were obtained by slow evaporation from an AcOEt/CHCl$_3$ solution at room temperature.

S2.1. Refinement

Hydrogen atoms bonded to the carbon atoms were placed in calculated positions and refined as riding mode, with C—H = 0.93Å (methane) or 0.96Å (methyl) and $U_{iso}(H) = 1.2U_{eq}(C_{methane})$ or $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$.
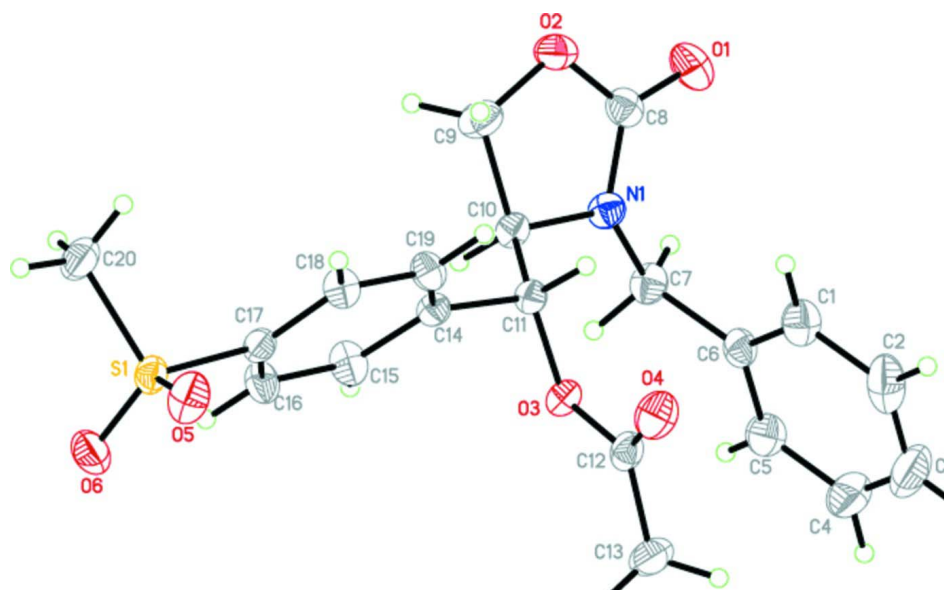
Figure 1

The *ORTEP* view of the title compound with 30% probability level ellipsoids.
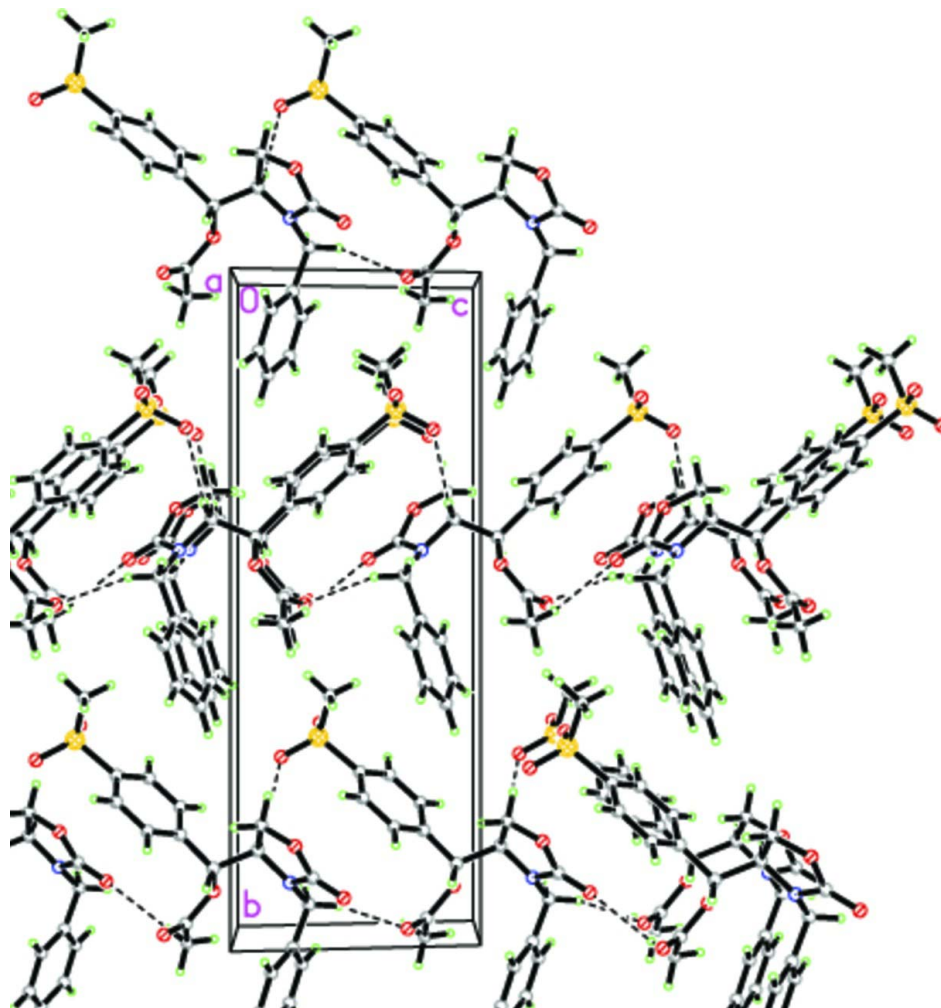
Figure 2
The molecular packing diagram of the title compound.

(*R*)-[(*R*)-3-Benzyl-2-oxooxazolidin-4-yl][4-(methylsulfonyl)phenyl]methyl acetate

Crystal data

$C_{20}H_{21}NO_6S$	$F(000) = 424$
$M_r = 403.44$	$D_x = 1.407$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 2349 reflections
$a = 5.837$ (3) Å	$\theta = 2.6$–25.3°
$b = 21.021$ (10) Å	$\mu = 0.21$ mm^{-1}
$c = 7.884$ (4) Å	$T = 296$ K
$\beta = 100.256$ (7)°	Block, colourless
$V = 952.0$ (7) Å^3	$0.30 \times 0.25 \times 0.16$ mm
$Z = 2$	

Data collection

Bruker SMART CCD area-detector diffractometer	Graphite monochromator
	phi and ω scans
Radiation source: fine-focus sealed tube	

Absorption correction: multi-scan
(*SADABS*; Bruker, 2000)
$T_{min} = 0.940$, $T_{max} = 0.968$
6495 measured reflections
3658 independent reflections
3254 reflections with $I > 2\sigma(I)$

$R_{int} = 0.022$
$\theta_{max} = 27.8°$, $\theta_{min} = 1.9°$
$h = -7 \rightarrow 7$
$k = -19 \rightarrow 27$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.091$
$S = 1.02$
3658 reflections
255 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Absolute structure: Flack (1983), 1356 Friedel pairs
Absolute structure parameter: −0.06 (6)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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.

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$
C1	0.2302 (4)	1.05248 (14)	1.2707 (4)	0.0558 (6)
H1	0.1259	1.0324	1.3295	0.067*
C2	0.1916 (6)	1.11380 (17)	1.2191 (5)	0.0781 (10)
H2	0.0605	1.1349	1.2422	0.094*
C3	0.3431 (7)	1.14521 (16)	1.1331 (5)	0.0833 (11)
H3	0.3155	1.1872	1.0981	0.100*
C4	0.5382 (6)	1.11300 (16)	1.0994 (4)	0.0701 (9)
H4	0.6428	1.1335	1.0417	0.084*
C5	0.5769 (4)	1.05031 (13)	1.1517 (3)	0.0506 (6)
H5	0.7077	1.0290	1.1290	0.061*
C6	0.4227 (4)	1.01946 (11)	1.2373 (3)	0.0395 (5)
C7	0.4569 (4)	0.95231 (11)	1.3036 (3)	0.0418 (5)
H7A	0.5095	0.9540	1.4274	0.050*
H7B	0.3070	0.9311	1.2832	0.050*
C8	0.8331 (4)	0.90008 (12)	1.3230 (3)	0.0418 (5)
C9	0.7678 (4)	0.82331 (14)	1.1163 (3)	0.0491 (6)
H9A	0.7290	0.7800	1.1428	0.059*

H9B	0.8324	0.8231	1.0112	0.059*
C10	0.5504 (3)	0.86602 (11)	1.0957 (3)	0.0347 (4)
H10	0.4169	0.8418	1.1206	0.042*
C11	0.4959 (3)	0.89357 (10)	0.9143 (2)	0.0325 (4)
H11	0.6286	0.9188	0.8923	0.039*
C12	0.2825 (4)	0.98383 (11)	0.7947 (3)	0.0401 (5)
C13	0.0631 (5)	1.02073 (14)	0.7899 (3)	0.0567 (7)
H13A	0.0890	1.0643	0.7625	0.085*
H13B	0.0163	1.0185	0.9005	0.085*
H13C	−0.0571	1.0031	0.7037	0.085*
C14	0.4399 (3)	0.84297 (10)	0.7772 (2)	0.0329 (4)
C15	0.2402 (4)	0.80602 (13)	0.7690 (3)	0.0453 (6)
H15	0.1481	0.8107	0.8531	0.054*
C16	0.1773 (4)	0.76262 (12)	0.6378 (3)	0.0435 (5)
H16	0.0425	0.7386	0.6324	0.052*
C17	0.3164 (3)	0.75514 (10)	0.5144 (2)	0.0343 (4)
C18	0.5208 (4)	0.78958 (12)	0.5248 (3)	0.0394 (5)
H18	0.6177	0.7831	0.4447	0.047*
C19	0.5795 (3)	0.83348 (11)	0.6545 (3)	0.0380 (5)
H19	0.7151	0.8572	0.6600	0.046*
C20	0.4084 (5)	0.63552 (13)	0.3899 (3)	0.0563 (6)
H20A	0.3814	0.6170	0.4959	0.084*
H20B	0.5685	0.6483	0.4022	0.084*
H20C	0.3739	0.6048	0.2988	0.084*
N1	0.6212 (3)	0.91344 (9)	1.2290 (2)	0.0373 (4)
O1	0.9319 (3)	0.92759 (11)	1.4488 (2)	0.0607 (5)
O2	0.9295 (3)	0.84974 (9)	1.2545 (2)	0.0530 (4)
O3	0.2955 (2)	0.93443 (7)	0.90796 (18)	0.0374 (3)
O4	0.4311 (3)	0.99426 (10)	0.7128 (2)	0.0566 (5)
O5	−0.0080 (3)	0.68428 (10)	0.3436 (2)	0.0585 (5)
O6	0.2809 (3)	0.73099 (10)	0.1869 (2)	0.0574 (5)
S1	0.22845 (9)	0.70219 (3)	0.34050 (6)	0.03925 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0543 (14)	0.0493 (16)	0.0618 (15)	0.0027 (12)	0.0052 (11)	−0.0131 (13)
C2	0.078 (2)	0.0510 (19)	0.098 (2)	0.0168 (16)	−0.0056 (18)	−0.0156 (19)
C3	0.121 (3)	0.0371 (17)	0.078 (2)	0.0108 (18)	−0.020 (2)	0.0006 (15)
C4	0.105 (2)	0.0517 (18)	0.0496 (15)	−0.0264 (18)	0.0039 (15)	0.0018 (13)
C5	0.0619 (14)	0.0468 (15)	0.0438 (12)	−0.0066 (12)	0.0115 (11)	0.0000 (11)
C6	0.0452 (11)	0.0367 (12)	0.0348 (10)	−0.0035 (9)	0.0024 (8)	−0.0088 (9)
C7	0.0467 (11)	0.0398 (13)	0.0421 (11)	0.0015 (10)	0.0171 (9)	−0.0043 (10)
C8	0.0404 (10)	0.0444 (14)	0.0412 (11)	−0.0061 (10)	0.0089 (9)	0.0045 (11)
C9	0.0546 (13)	0.0496 (15)	0.0416 (11)	0.0159 (11)	0.0044 (9)	−0.0041 (11)
C10	0.0395 (10)	0.0320 (11)	0.0328 (10)	0.0023 (9)	0.0073 (8)	0.0002 (8)
C11	0.0349 (9)	0.0303 (11)	0.0326 (10)	−0.0006 (8)	0.0066 (8)	0.0007 (8)
C12	0.0548 (12)	0.0301 (11)	0.0323 (10)	0.0006 (10)	−0.0011 (9)	−0.0026 (9)

C13	0.0597 (15)	0.0450 (15)	0.0611 (15)	0.0176 (12)	−0.0013 (12)	−0.0005 (13)
C14	0.0349 (10)	0.0312 (11)	0.0323 (9)	0.0023 (8)	0.0051 (7)	0.0027 (8)
C15	0.0449 (12)	0.0502 (15)	0.0455 (12)	−0.0083 (11)	0.0206 (9)	−0.0110 (11)
C16	0.0403 (11)	0.0418 (14)	0.0507 (12)	−0.0106 (10)	0.0142 (9)	−0.0058 (11)
C17	0.0405 (10)	0.0285 (11)	0.0326 (9)	0.0027 (8)	0.0028 (7)	0.0002 (8)
C18	0.0430 (11)	0.0425 (13)	0.0348 (10)	−0.0046 (10)	0.0131 (8)	−0.0015 (10)
C19	0.0380 (10)	0.0416 (13)	0.0356 (10)	−0.0076 (9)	0.0099 (8)	−0.0011 (9)
C20	0.0684 (15)	0.0354 (13)	0.0610 (15)	0.0102 (12)	0.0003 (12)	−0.0033 (12)
N1	0.0405 (9)	0.0381 (11)	0.0339 (9)	0.0046 (8)	0.0082 (7)	−0.0027 (8)
O1	0.0568 (9)	0.0691 (13)	0.0514 (10)	−0.0151 (9)	−0.0030 (7)	−0.0109 (10)
O2	0.0398 (8)	0.0539 (11)	0.0615 (10)	0.0085 (8)	−0.0013 (7)	−0.0069 (9)
O3	0.0427 (7)	0.0306 (8)	0.0391 (7)	0.0057 (6)	0.0080 (6)	0.0016 (6)
O4	0.0711 (11)	0.0478 (11)	0.0528 (10)	−0.0009 (9)	0.0166 (8)	0.0124 (9)
O5	0.0465 (9)	0.0559 (12)	0.0697 (11)	−0.0093 (8)	0.0005 (8)	−0.0189 (9)
O6	0.0903 (13)	0.0467 (11)	0.0347 (8)	−0.0012 (10)	0.0100 (7)	−0.0013 (8)
S1	0.0475 (3)	0.0299 (2)	0.0381 (3)	0.0003 (2)	0.0016 (2)	−0.0037 (2)

Geometric parameters (Å, º)

C1—C2	1.359 (5)	C11—C14	1.511 (3)
C1—C6	1.385 (3)	C11—H11	0.9800
C1—H1	0.9300	C12—O4	1.191 (3)
C2—C3	1.375 (5)	C12—O3	1.363 (3)
C2—H2	0.9300	C12—C13	1.492 (3)
C3—C4	1.391 (5)	C13—H13A	0.9600
C3—H3	0.9300	C13—H13B	0.9600
C4—C5	1.387 (4)	C13—H13C	0.9600
C4—H4	0.9300	C14—C19	1.385 (3)
C5—C6	1.379 (3)	C14—C15	1.393 (3)
C5—H5	0.9300	C15—C16	1.379 (3)
C6—C7	1.506 (3)	C15—H15	0.9300
C7—N1	1.461 (3)	C16—C17	1.383 (3)
C7—H7A	0.9700	C16—H16	0.9300
C7—H7B	0.9700	C17—C18	1.385 (3)
C8—O1	1.203 (3)	C17—S1	1.769 (2)
C8—N1	1.354 (3)	C18—C19	1.374 (3)
C8—O2	1.355 (3)	C18—H18	0.9300
C9—O2	1.421 (3)	C19—H19	0.9300
C9—C10	1.539 (3)	C20—S1	1.753 (3)
C9—H9A	0.9700	C20—H20A	0.9600
C9—H9B	0.9700	C20—H20B	0.9600
C10—N1	1.454 (3)	C20—H20C	0.9600
C10—C11	1.523 (3)	O5—S1	1.4353 (18)
C10—H10	0.9800	O6—S1	1.4346 (19)
C11—O3	1.445 (2)		
C2—C1—C6	121.0 (3)	O4—C12—O3	122.3 (2)
C2—C1—H1	119.5	O4—C12—C13	126.5 (2)

C6—C1—H1	119.5	O3—C12—C13	111.1 (2)
C1—C2—C3	121.1 (3)	C12—C13—H13A	109.5
C1—C2—H2	119.5	C12—C13—H13B	109.5
C3—C2—H2	119.5	H13A—C13—H13B	109.5
C2—C3—C4	118.7 (3)	C12—C13—H13C	109.5
C2—C3—H3	120.6	H13A—C13—H13C	109.5
C4—C3—H3	120.6	H13B—C13—H13C	109.5
C5—C4—C3	120.1 (3)	C19—C14—C15	118.6 (2)
C5—C4—H4	120.0	C19—C14—C11	121.46 (18)
C3—C4—H4	120.0	C15—C14—C11	119.88 (17)
C6—C5—C4	120.4 (3)	C16—C15—C14	120.81 (19)
C6—C5—H5	119.8	C16—C15—H15	119.6
C4—C5—H5	119.8	C14—C15—H15	119.6
C5—C6—C1	118.7 (2)	C15—C16—C17	119.47 (19)
C5—C6—C7	123.6 (2)	C15—C16—H16	120.3
C1—C6—C7	117.7 (2)	C17—C16—H16	120.3
N1—C7—C6	116.12 (18)	C16—C17—C18	120.39 (19)
N1—C7—H7A	108.3	C16—C17—S1	119.40 (16)
C6—C7—H7A	108.3	C18—C17—S1	120.20 (15)
N1—C7—H7B	108.3	C19—C18—C17	119.54 (18)
C6—C7—H7B	108.3	C19—C18—H18	120.2
H7A—C7—H7B	107.4	C17—C18—H18	120.2
O1—C8—N1	127.5 (2)	C18—C19—C14	121.09 (19)
O1—C8—O2	122.1 (2)	C18—C19—H19	119.5
N1—C8—O2	110.35 (19)	C14—C19—H19	119.5
O2—C9—C10	106.0 (2)	S1—C20—H20A	109.5
O2—C9—H9A	110.5	S1—C20—H20B	109.5
C10—C9—H9A	110.5	H20A—C20—H20B	109.5
O2—C9—H9B	110.5	S1—C20—H20C	109.5
C10—C9—H9B	110.5	H20A—C20—H20C	109.5
H9A—C9—H9B	108.7	H20B—C20—H20C	109.5
N1—C10—C11	113.76 (18)	C8—N1—C10	111.57 (18)
N1—C10—C9	101.58 (17)	C8—N1—C7	119.80 (18)
C11—C10—C9	110.60 (17)	C10—N1—C7	123.54 (17)
N1—C10—H10	110.2	C8—O2—C9	110.15 (17)
C11—C10—H10	110.2	C12—O3—C11	115.21 (16)
C9—C10—H10	110.2	O6—S1—O5	118.39 (12)
O3—C11—C14	108.86 (15)	O6—S1—C20	108.39 (13)
O3—C11—C10	106.93 (14)	O5—S1—C20	109.06 (13)
C14—C11—C10	112.74 (18)	O6—S1—C17	108.20 (11)
O3—C11—H11	109.4	O5—S1—C17	107.41 (11)
C14—C11—H11	109.4	C20—S1—C17	104.53 (11)
C10—C11—H11	109.4		
C6—C1—C2—C3	−0.5 (5)	C17—C18—C19—C14	1.3 (3)
C1—C2—C3—C4	0.0 (5)	C15—C14—C19—C18	1.4 (3)
C2—C3—C4—C5	0.2 (4)	C11—C14—C19—C18	−176.6 (2)
C3—C4—C5—C6	0.0 (4)	O1—C8—N1—C10	−174.6 (2)

C4—C5—C6—C1	−0.5 (3)	O2—C8—N1—C10	6.3 (2)
C4—C5—C6—C7	−177.8 (2)	O1—C8—N1—C7	−19.0 (3)
C2—C1—C6—C5	0.7 (4)	O2—C8—N1—C7	161.91 (19)
C2—C1—C6—C7	178.2 (3)	C11—C10—N1—C8	−122.93 (18)
C5—C6—C7—N1	−18.5 (3)	C9—C10—N1—C8	−4.1 (2)
C1—C6—C7—N1	164.21 (19)	C11—C10—N1—C7	82.5 (2)
O2—C9—C10—N1	0.6 (2)	C9—C10—N1—C7	−158.6 (2)
O2—C9—C10—C11	121.7 (2)	C6—C7—N1—C8	106.2 (2)
N1—C10—C11—O3	−64.6 (2)	C6—C7—N1—C10	−101.2 (2)
C9—C10—C11—O3	−178.14 (18)	O1—C8—O2—C9	175.1 (2)
N1—C10—C11—C14	175.82 (16)	N1—C8—O2—C9	−5.7 (3)
C9—C10—C11—C14	62.3 (2)	C10—C9—O2—C8	2.9 (3)
O3—C11—C14—C19	125.2 (2)	O4—C12—O3—C11	−3.3 (3)
C10—C11—C14—C19	−116.3 (2)	C13—C12—O3—C11	176.55 (18)
O3—C11—C14—C15	−52.7 (2)	C14—C11—O3—C12	−86.7 (2)
C10—C11—C14—C15	65.8 (2)	C10—C11—O3—C12	151.25 (17)
C19—C14—C15—C16	−2.5 (3)	C16—C17—S1—O6	139.88 (19)
C11—C14—C15—C16	175.5 (2)	C18—C17—S1—O6	−39.0 (2)
C14—C15—C16—C17	0.9 (4)	C16—C17—S1—O5	11.0 (2)
C15—C16—C17—C18	1.8 (3)	C18—C17—S1—O5	−167.86 (18)
C15—C16—C17—S1	−177.03 (19)	C16—C17—S1—C20	−104.8 (2)
C16—C17—C18—C19	−3.0 (3)	C18—C17—S1—C20	76.4 (2)
S1—C17—C18—C19	175.90 (18)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O4[i]	0.97	2.52	3.373 (3)	147
C10—H10···O6[i]	0.98	2.54	3.384 (3)	144
C13—H13C···O1[ii]	0.96	2.55	3.305 (3)	135

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