Methyl 5-chloro-4-hydroxy-2,2-dioxo-1H-2λ⁶,1-benzothiazine-3-carboxylate: structure and Hirshfeld surface analysis

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The title compound, $C_{10}H_8ClNO_5S$, which has potential analgesic activity, crystallizes in space group $P2_1/n$. The benzothiazine ring system adopts an intermediate form between sofa and twist-boat conformations. The coplanarity of the ester substituent to the bicyclic fragment is stabilized by an O—H⋯O intramolecular hydrogen bond. In the crystal, hydrogen bonds of type N—H⋯O(SO₂) link the molecules into zigzag chains extending along the b-axis direction. Neighbouring chains are linked by both O—H⋯Cl and C—H⋯Cl interactions. A Hirshfeld surface analysis was used to compare different types of intermolecular interactions, giving contributions of O⋯H/H⋯O = 42.0%, C⋯H/H⋯C = 17.3%, Cl⋯H/H⋯Cl = 14.2%, H⋯H = 11.1%.

1. Chemical context

Alkyl 4-hydroxy-2,2-dioxo-1H-2λ⁶,1-benzothiazine-3-carboxylates are known to be highly active analgesics (Ukrainets et al., 2013). The influence of substituents at the cyclic nitrogen atom on the biological properties of these substances has been studied in detail (Ukrainets et al., 2013, 2017). Continuing our research in this direction, we have synthesized and studied a new compound of this class with a substituent on the benzene part of the molecule. The biological properties of benzothiazine derivatives are known to depend on their molecular structure (Ukrainets et al., 2019a,b). In addition, such molecules can form polymorphic modifications possessing different biological activity, as was shown in our previous studies (Ukrainets et al., 2016a, 2018). Therefore, the molecular and crystal structure study as well as a Hirshfeld surface analysis were performed for the title compound, **1**.

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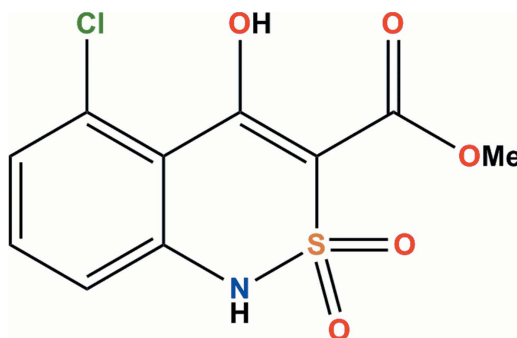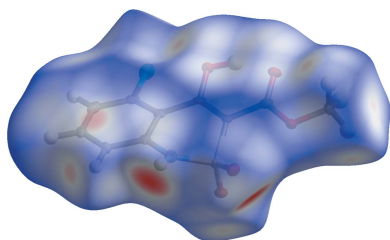
Table 1
Hydrogen-bond geometry (Å, °).

| D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$O\cdots$O2	0.84	1.76	2.509 (5)	148
N1—H1$N\cdots$O4[i]	0.88	2.07	2.841 (5)	145
O1—H1$O\cdots$Cl1[ii]	0.84	2.87	3.203 (4)	106
C10—H10$C\cdots$Cl1[iii]	0.98	2.84	3.399 (5)	117

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

2. Structural commentary

The dihydrothiazine ring in molecule **1** adopts a conformation that is intermediate between a sofa and twist-boat (Fig. 1) with puckering parameters $S = 0.53$, $\Theta = 35.1°$, $\Psi = 11.3°$ (Zefirov *et al.*, 1990). The S1 and C8 atoms deviate by 0.81 (1) and 0.22 (1) Å, respectively, from the mean-square plane of the remaining atoms in the ring. The Cremer–Pople ring puckering parameters for the dihydrothiazine ring are: $Q = 0.457$ (4) Å, $\Theta = 111.6$ (5)°, $\Psi = 192.1$ (6)°. The ester substituent is essentially coplanar to the C7—C8 endocyclic double bond [the C7—C8—C9—O2 torsion angle is 3.0 (7)°] as a result of the stabilizing influence of the O1—H1$O\cdots$O2 intramolecular hydrogen bond (Table 1). This hydrogen bond can be specified as $S(6)$ in terms of graph-set theory since the six atoms comprise a intramolecular hydrogen-bonded motif. The formation of the O—H$\cdots$O hydrogen bond causes some elongation of the C9—O2 and C7—C8 bonds as compared with typical values of 1.210 Å (Csp^2=O bond) and 1.326 Å (Csp^2—Csp^2 bond), respectively (Bürgi & Dunitz, 1994). The C7—O1 bond is shortened to 1.320 (6) Å (the typical length for a Csp^2—O bond is 1.362 Å) for the same reason. The methyl group is located in an *anti*-periplanar position to the C8—C9 bond [the C10—O3—C9—C8 torsion angle is −178.4 (4)°]. The noticeable steric repulsion between chlorine and the hydroxyl group [the Cl1$\cdots$O1 distance is 2.793 (4) Å as compared with the van der Waals radii sum (Zefirov, 1997) of 3.19 Å] results in twisting of the Cl1—C5—C6—C7 and C5—C6—C7—O1 torsion angles up to 14.7 (7) and 14.5 (7)°, respectively.
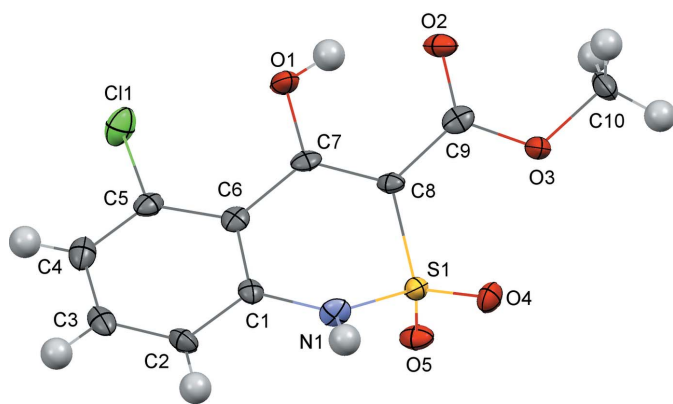
Figure 1
The molecular structure of compound **1**. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.
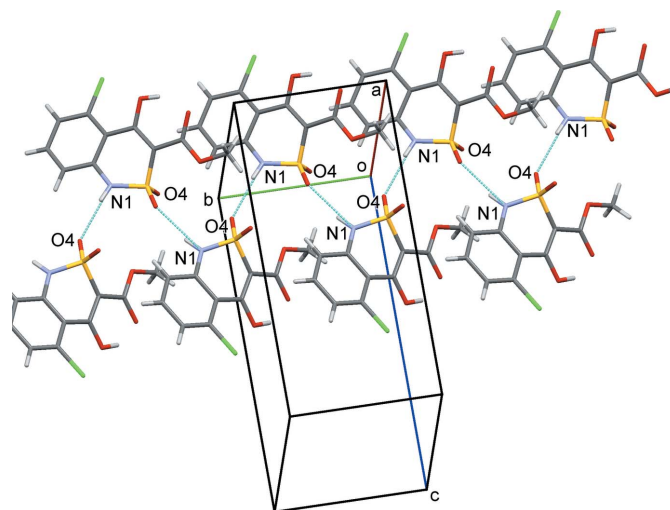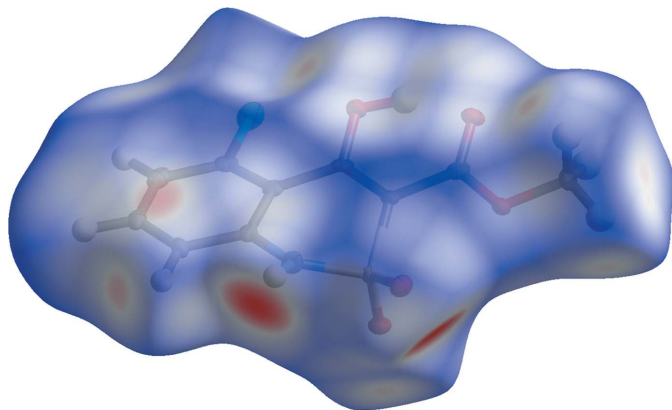

Figure 2
A chain of molecules of **1** bound by N—H$\cdots$O hydrogen bonds about the 2_1-screw axis parallel to the *b* axis.

3. Supramolecular features

In the crystal, molecules of **1** form zigzag chains in the [010] direction (Fig. 2) as a result of the formation of N1—H$\cdots$O4[i] hydrogen bonds about the 2_1 screw axis parallel to *b* [symmetry code: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; the N$\cdots$O distance is 2.841 (5) Å, the N—H$\cdots$O angle is 145.1° (Table 1)]. The crystal structure fragment formed by this hydrogen bond may be described as $C(4)$ in terms of graph-set theory. Neighbouring zigzag chains are connected by weaker O—H$\cdots$Cl[ii] interactions (Table 1) in the [001] direction [symmetry code: (ii) $\frac{3}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$]. As a result, the hydrogen-bonded layers parallel to the *bc* plane may be considered as secondary structural motifs. There are weak C—H$\cdots$Cl[iii] interactions [symmetry code: (iii) $x - \frac{1}{2}, -y - \frac{1}{2}, z - \frac{1}{2}$] between molecules of neighbouring layers. In addition, stacking interactions between inversion-related $(2 - x, 1 - y, 1 - z)$ benzene rings of molecules belonging to neighbouring layers are found. The distance between ring planes is 3.246 (2) Å. The stacking interactions are characterized by a centroid-to-centroid distance of 3.872 (2) Å, with a lateral shift of the benzene rings of 2.111 (2) Å.

4. Hirshfeld surface analysis

Hirshfeld surface analysis and 2D fingerprint plots are useful tools to investigate the different types of intra- and inter-molecular interactions in a crystal (Turner *et al.*, 2017). The Hirshfeld surface of the title compound was obtained using a standard (high) surface resolution, mapped over d_{norm}. The areas coloured red on the d_{norm} surfaces correspond to contacts that are shorter than the van der Waals radii sum of the closest atoms (Fig. 3). In this way, red spots on the Hirshfeld surface indicate atoms participating in hydrogen bonds or other short contacts. Such red spots are observed at the hydrogen atom of the NH group, one of the oxygen atoms

Figure 3
Hirshfeld surface of a molecule of **1** mapped over d_{norm}, with transparency to show the conformation.

of the SO_2 group, and the chlorine atom. Smaller red spots are also present at one of the hydrogen atoms of the methyl group.

All of the hydrogen bonds and short contacts of the title compound are evident in the two-dimensional fingerprint plot presented in Fig. 4a. The pair of very sharp spikes indicates the presence of strong hydrogen bonds in the crystal of **1**. The
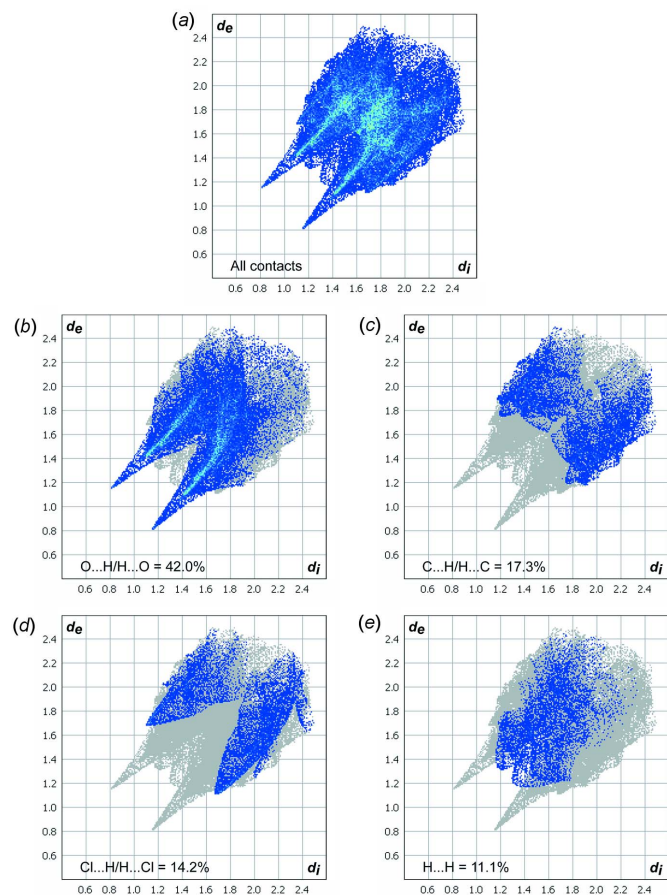
main contribution (42.0%) to these spikes is provided by O···H/H···O interactions (Fig. 4b). The contributions of C···H/H···C (17.3%) and Cl···H/H···Cl (14.2%) (Fig. 4c,d) interactions are similar, but the presence of sharp spikes in the fingerprint plot delineated Cl···H/H···Cl interactions suggests that these contacts are stronger. Surprisingly, the contribution of H···H interactions (11.1%) (Fig. 4e) is very small, which is unusual for molecular crystals.
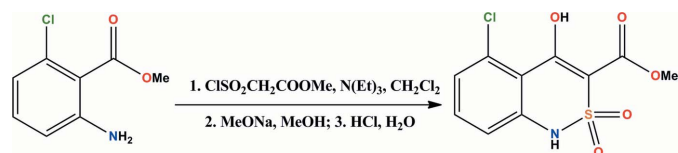
5. Database survey

A search of the Cambridge Structural Database (Version 5.41, update of November 2019; Groom *et al.*, 2016) for the benzothiazine fragment revealed only ten hits [refcodes AKIJIP, AKIJIP01 (Ukrainets *et al.*, 2016a), CABBEP (Lei *et al.*, 2016), IJUJAA (Ukrainets *et al.*, 2015b), LANNUM (Ukrainets *et al.*, 2016b), LOGHEW (Ukrainets *et al.*, 2014), MINJAW (Shishkina *et al.*, 2013), NODGUK (Ukrainets *et al.*, 2013), UWUCIA (Ukrainets *et al.*, 2015a) and XEKPUB (Ukrainets *et al.*, 2017)]. In all these structures, the conformation of the benzothiazine rings as well as the redistribution of the electron density as a result of the formation of the O—H···O intramolecular hydrogen bond are similar.

The title compound may be considered as a structural analogue of methyl 4-hydroxy-2,2-dioxo-1-methyl-1*H*-2,1-benzothiazine-3-carboxylate (Ukrainets *et al.*, 2013), which is substituted by chlorine on the benzene ring of the molecule and dealkylated at the cyclic nitrogen atom.

6. Synthesis and crystallization

Methyl (chlorosulfonyl)acetate (1.90 g, 0.011 mol) was added dropwise under stirring to a solution of methyl 6-chloro-anthranilate (1.85 g, 0.010 mol) and triethylamine (1.54 mL, 0.011 mol) in CH_2Cl_2 (20 mL) and the mixture was cooled (268 to 273 K) (Fig. 5). After 10 h, water (50 mL) was added to the reaction mixture, which was acidified up to pH = 4 with 1 *N* HCl and mixed thoroughly. The organic layer was separated, dried over anhydrous $CaCl_2$, and distilled (at reduced pressure at the end). A solution of sodium methylate in anhydrous methanol [from metallic sodium (0.69 g, 0.030 mol) and absolute methanol (20 mL)] was added, the mixture was boiled and stored for 15 h at room temperature. The reaction mixture was diluted with cold water and acidified with 1 *N* HCl to pH = 4. The solid methyl 5-chloro-4-hydroxy-2,2-dioxo-1*H*-2λ^6,1-benzothiazine-3-carboxylate was filtered, washed with water, and dried in air. Yield 2.43g (84%); colourless crystals; m.p. 464–466 K.

Figure 4
Two-dimensional Hirshfeld fingerprint plot of (*a*) all contacts for compound **1** and those delineated into (*b*) O···H/ H···O (42.0%), (*c*) C···H/H···C (17.3%), (*d*) Cl···H/H···Cl (14.2%), (*e*) H···H (11.1%) contacts.

Figure 5
The synthesis of compound **1**.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All of the hydrogen atoms were located in difference-Fourier maps. They were included in calculated positions and treated as riding with C—H = 0.96 Å, O—H = 0.84 Å, $U_{iso}(H) = 1.5U_{eq}(C,O)$ for methyl and hydroxyl groups and with C—H = 0.93 Å, N—H = 0.88 Å, $U_{iso}(H) = 1.2U_{eq}(C,N)$ for all other hydrogen atoms.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_8ClNO_5S$
M_r	289.68
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	120
a, b, c (Å)	11.153 (3), 6.8926 (15), 14.600 (3)
β (°)	97.528 (5)
V (Å^3)	1112.6 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.54
Crystal size (mm)	$0.30 \times 0.10 \times 0.05$
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur, Sapphire3
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.428, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9166, 1957, 1343
R_{int}	0.111
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.145, 1.05
No. of reflections	1957
No. of parameters	165
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.38, −0.46

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *Mercury* (Macrae, 2020).

Methyl 5-chloro-4-hydroxy-2,2-dioxo-1*H*-2λ⁶,1-benzothiazine-3-carboxylate: structure and Hirshfeld surface analysis

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae, 2020).

Methyl 5-chloro-4-hydroxy-2,2-dioxo-1*H*-2λ⁶,1-benzothiazine-3-carboxylate

Crystal data

$C_{10}H_8ClNO_5S$	$F(000) = 592$
$M_r = 289.68$	$D_x = 1.729$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 11.153$ (3) Å	Cell parameters from 2736 reflections
$b = 6.8926$ (15) Å	$\theta = 3.3–34.2°$
$c = 14.600$ (3) Å	$\mu = 0.54$ mm^{-1}
$\beta = 97.528$ (5)°	$T = 120$ K
$V = 1112.6$ (4) Å^3	Plate, colourless
$Z = 4$	$0.30 \times 0.10 \times 0.05$ mm

Data collection

Rigaku Oxford Diffraction Xcalibur, Sapphire3 diffractometer	9166 measured reflections
Radiation source: Enhance (Mo) X-ray Source	1957 independent reflections
Detector resolution: 16.1827 pixels mm^{-1}	1343 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.111$
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)	$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
	$h = -13 \rightarrow 13$
	$k = -8 \rightarrow 8$
$T_{min} = 0.428$, $T_{max} = 1.000$	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.063$	$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.6529P]$
$wR(F^2) = 0.145$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
1957 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
165 parameters	$\Delta\rho_{min} = -0.46$ e Å^{-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 ($Å^2$)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Cl1	0.84549 (13)	0.2458 (2)	0.73322 (9)	0.0298 (4)
S1	0.76398 (12)	0.09884 (18)	0.35643 (9)	0.0158 (3)
O1	0.6753 (3)	0.0566 (5)	0.6066 (2)	0.0218 (9)
H1O	0.638729	−0.048715	0.594436	0.033*
O2	0.5710 (3)	−0.2111 (5)	0.5105 (2)	0.0232 (9)
O3	0.6006 (3)	−0.2377 (5)	0.3617 (2)	0.0212 (9)
O4	0.6887 (3)	0.0811 (5)	0.2691 (2)	0.0209 (8)
O5	0.8815 (3)	0.0129 (5)	0.3625 (2)	0.0213 (9)
N1	0.7714 (4)	0.3285 (6)	0.3778 (3)	0.0200 (10)
H1N	0.750045	0.409629	0.331963	0.024*
C1	0.8100 (4)	0.4052 (7)	0.4653 (3)	0.0150 (11)
C2	0.8599 (4)	0.5923 (7)	0.4729 (4)	0.0187 (12)
H2	0.867292	0.666061	0.418938	0.022*
C3	0.8974 (4)	0.6672 (8)	0.5574 (4)	0.0215 (12)
H3	0.928646	0.795566	0.562115	0.026*
C4	0.8914 (5)	0.5596 (8)	0.6383 (4)	0.0225 (13)
H4	0.921192	0.611991	0.697051	0.027*
C5	0.8413 (4)	0.3765 (8)	0.6308 (3)	0.0182 (12)
C6	0.7937 (4)	0.2947 (7)	0.5441 (3)	0.0156 (11)
C7	0.7202 (4)	0.1186 (7)	0.5325 (3)	0.0163 (11)
C8	0.6938 (4)	0.0228 (7)	0.4494 (3)	0.0152 (11)
C9	0.6170 (4)	−0.1515 (7)	0.4434 (3)	0.0180 (12)
C10	0.5228 (5)	−0.4067 (7)	0.3536 (4)	0.0247 (13)
H10C	0.528740	−0.471978	0.294700	0.037*
H10B	0.438987	−0.366365	0.355781	0.037*
H10A	0.548102	−0.495994	0.404669	0.037*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0396 (9)	0.0322 (8)	0.0162 (7)	0.0041 (7)	−0.0016 (6)	0.0010 (6)
S1	0.0175 (7)	0.0156 (7)	0.0151 (7)	−0.0009 (6)	0.0050 (5)	−0.0007 (6)
O1	0.030 (2)	0.020 (2)	0.0181 (19)	−0.0045 (17)	0.0113 (17)	0.0001 (16)
O2	0.022 (2)	0.023 (2)	0.028 (2)	−0.0011 (17)	0.0127 (17)	0.0031 (17)
O3	0.023 (2)	0.021 (2)	0.022 (2)	−0.0081 (17)	0.0110 (16)	−0.0049 (16)
O4	0.023 (2)	0.025 (2)	0.0143 (18)	0.0003 (17)	−0.0004 (15)	−0.0031 (16)
O5	0.020 (2)	0.019 (2)	0.028 (2)	0.0041 (16)	0.0107 (16)	0.0025 (16)
N1	0.029 (3)	0.014 (2)	0.017 (2)	0.003 (2)	0.004 (2)	0.0069 (18)
C1	0.009 (2)	0.017 (3)	0.019 (3)	0.002 (2)	0.001 (2)	−0.002 (2)

C2	0.017 (3)	0.013 (3)	0.027 (3)	−0.002 (2)	0.005 (2)	0.001 (2)
C3	0.011 (3)	0.018 (3)	0.036 (3)	0.002 (2)	0.005 (2)	−0.008 (2)
C4	0.015 (3)	0.028 (3)	0.024 (3)	0.005 (2)	−0.001 (2)	−0.008 (2)
C5	0.011 (3)	0.027 (3)	0.017 (3)	0.003 (2)	0.003 (2)	0.000 (2)
C6	0.010 (3)	0.018 (3)	0.019 (3)	0.006 (2)	0.002 (2)	0.000 (2)
C7	0.010 (3)	0.022 (3)	0.018 (3)	0.005 (2)	0.006 (2)	0.002 (2)
C8	0.013 (3)	0.014 (3)	0.019 (3)	0.002 (2)	0.007 (2)	0.001 (2)
C9	0.014 (3)	0.020 (3)	0.020 (3)	0.010 (2)	0.003 (2)	0.003 (2)
C10	0.020 (3)	0.021 (3)	0.034 (3)	−0.008 (3)	0.007 (2)	−0.009 (3)

Geometric parameters (Å, º)

Cl1—C5	1.741 (5)	C1—C2	1.403 (7)
S1—O5	1.431 (4)	C1—C6	1.412 (7)
S1—O4	1.437 (3)	C2—C3	1.352 (7)
S1—N1	1.614 (4)	C3—C4	1.404 (7)
S1—C8	1.734 (5)	C4—C5	1.379 (7)
O1—C7	1.320 (6)	C5—C6	1.423 (7)
O2—C9	1.234 (6)	C6—C7	1.462 (7)
O3—C9	1.323 (6)	C7—C8	1.379 (7)
O3—C10	1.448 (6)	C8—C9	1.471 (7)
N1—C1	1.397 (6)		
O5—S1—O4	116.3 (2)	C4—C5—Cl1	116.2 (4)
O5—S1—N1	111.8 (2)	C6—C5—Cl1	121.6 (4)
O4—S1—N1	105.3 (2)	C1—C6—C5	116.0 (5)
O5—S1—C8	109.3 (2)	C1—C6—C7	118.9 (4)
O4—S1—C8	113.4 (2)	C5—C6—C7	124.8 (4)
N1—S1—C8	99.3 (2)	O1—C7—C8	120.3 (5)
C9—O3—C10	116.5 (4)	O1—C7—C6	116.2 (4)
C1—N1—S1	123.3 (3)	C8—C7—C6	123.5 (4)
N1—C1—C2	119.5 (4)	C7—C8—C9	119.9 (4)
N1—C1—C6	119.0 (4)	C7—C8—S1	118.5 (4)
C2—C1—C6	121.5 (5)	C9—C8—S1	121.3 (4)
C3—C2—C1	119.7 (5)	O2—C9—O3	122.9 (5)
C2—C3—C4	121.5 (5)	O2—C9—C8	121.6 (5)
C5—C4—C3	118.8 (5)	O3—C9—C8	115.5 (4)
C4—C5—C6	122.2 (5)		
O5—S1—N1—C1	−69.3 (4)	C5—C6—C7—O1	14.5 (7)
O4—S1—N1—C1	163.5 (4)	C1—C6—C7—C8	19.0 (7)
C8—S1—N1—C1	45.9 (4)	C5—C6—C7—C8	−167.7 (5)
S1—N1—C1—C2	154.5 (4)	O1—C7—C8—C9	−1.2 (7)
S1—N1—C1—C6	−27.8 (6)	C6—C7—C8—C9	−178.8 (4)
N1—C1—C2—C3	−180.0 (4)	O1—C7—C8—S1	−175.2 (3)
C6—C1—C2—C3	2.3 (7)	C6—C7—C8—S1	7.2 (7)
C1—C2—C3—C4	2.1 (7)	O5—S1—C8—C7	82.9 (4)
C2—C3—C4—C5	−2.7 (7)	O4—S1—C8—C7	−145.5 (4)

C3—C4—C5—C6	−1.2 (7)	N1—S1—C8—C7	−34.2 (4)
C3—C4—C5—Cl1	176.1 (4)	O5—S1—C8—C9	−91.1 (4)
N1—C1—C6—C5	176.5 (4)	O4—S1—C8—C9	40.5 (5)
C2—C1—C6—C5	−5.8 (7)	N1—S1—C8—C9	151.8 (4)
N1—C1—C6—C7	−9.7 (7)	C10—O3—C9—O2	1.1 (7)
C2—C1—C6—C7	168.0 (4)	C10—O3—C9—C8	−178.4 (4)
C4—C5—C6—C1	5.2 (7)	C7—C8—C9—O2	3.0 (7)
Cl1—C5—C6—C1	−171.9 (4)	S1—C8—C9—O2	176.9 (4)
C4—C5—C6—C7	−168.2 (5)	C7—C8—C9—O3	−177.5 (4)
Cl1—C5—C6—C7	14.7 (7)	S1—C8—C9—O3	−3.6 (6)
C1—C6—C7—O1	−158.7 (4)		

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1*O*⋯O2	0.84	1.76	2.509 (5)	148
N1—H1*N*⋯O4[i]	0.88	2.07	2.841 (5)	145
O1—H1*O*⋯Cl1[ii]	0.84	2.87	3.203 (4)	106
C10—H10*C*⋯Cl1[iii]	0.98	2.84	3.399 (5)	117

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