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Crystal structure and Hirshfeld surface analysis of 2-(4-chlorophenyl)-4-(dimethoxymethyl)-5-phenyl-1,3-thiazole

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Keywords: crystal structure; thiazole ring; chlorophenyl ring; C—H···π interactions; Hirshfeld surface analysis.

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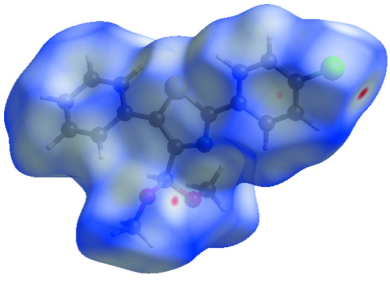
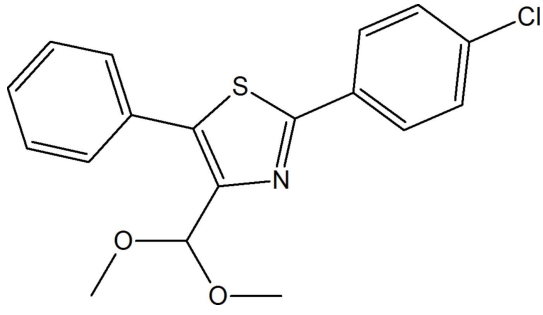
In the title compound, $C_{18}H_{16}ClNO_2S$, the thiazole ring subtends dihedral angles of 13.12 (14) and 43.79 (14) ° with the attached chlorophenyl and phenyl rings, respectively. In the crystal, C—H···π interactions link the molecules, forming a three-dimensional network. The roles of the various intermolecular interactions were clarified by Hirshfeld surface analysis, which reveals that the most important contributions to the crystal packing are from H···H (39.2%), H···C/C···H (25.2%), Cl···H/H···Cl (11.4%) and O···H/H···O (8.0%) contacts.

1. Chemical context

Thiazole and its derivatives have attracted much synthetic interest due to their antimicrobial, antiviral, anti-diabetic, diuretic, anticonvulsant, antioxidant, anti-HIV, analgesic, anti-inflammatory, neuroprotective and antitumor activities (Dondoni 2010; Grover & Jachak 2015). In fact, the thiazole moiety is a prominent structural feature in a variety of natural products, such as vitamin B and penicillin (Yariv *et al.*, 2015). On the other hand, the thiazole synthon is also useful in coordination chemistry and catalytic transformations due to its coordination ability and non-covalent bond donor or acceptor character (Gurbanov *et al.*, 2020). As part of our studies in this area, we now report the synthesis and structure of the title compound and quantify its intermolecular non-covalent interactions by Hirshfeld surface analysis.





2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The central 1,3-thiazolidine ring (S1/N1C1–C3) makes dihedral angles of 13.12 (14) and 43.79 (14)°, respectively, with

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

*Cg*1 and *Cg*3 are the centroids of the C1–C3/S1/N1 and C13–C18 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···S1	0.95	2.74	3.143 (3)	106
C6—H6···*Cg*3^{i}	0.95	2.81	3.620 (3)	144
C12—H12*C*···*Cg*3^{ii}	0.98	2.81	3.406 (3)	120
C15—H15···*Cg*1^{iii}	0.95	2.95	3.481 (3)	117

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

the chlorophenyl ring (C4–C9) and the phenyl ring (C13–C18). The dimethoxymethane moiety features one *anti* conformation [C2—C10—O2—C12 = 172.5 (2)°] and one *gauche* conformation [C2—C10—O1—C11 = −78.1 (3)°] for its pendant bonds. The molecular conformation may be consolidated by a weak intramolecular C5—H5···S1 contact [H5···S1 = 2.74 Å; C5—H5···S1 = 106°].

3. Supramolecular features and Hirshfeld surface analysis

The extended structure features C—H···π interactions, forming a three-dimensional network (Table 1, Fig. 2) in which the thiazole ring accepts once such bond and the phenyl ring two, but no significant π–π stacking contacts are observed [shortest centroid–centroid separation = 4.1887 (16) Å]. A Hirshfeld surface analysis was performed, and two-dimensional fingerprint plots were created with *Crystal Explorer17.5* (Turner *et al.*, 2017) to quantify the intermolecular interactions present in the extended structure. Fig. 3 depicts the Hirshfeld surface projected on d_{norm} and the related colours reflecting various interactions. The C—H···Cl interaction is represented by the red spot on the surface. Fig. 4 depicts the two-dimensional fingerprint plots. The weak van der Waals H···H connections provide the most (39.2%, Fig. 4*b*) to the Hirshfeld surface. The other principal contributions to the overall surface are from C···H/H···C (25.2%, Fig. 4*c*), Cl···H/H···Cl (11.4%, Fig. 4*d*) and O···H/H···O (8.0%, Fig. 4*e*) interactions. The contributions of the remaining less important interactions are given in Table 2.

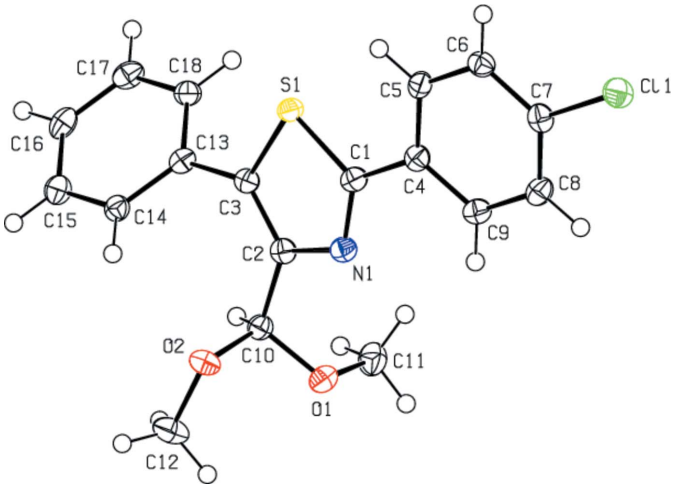


Figure 1
The title molecule with displacement ellipsoids drawn at the 50% probability level.

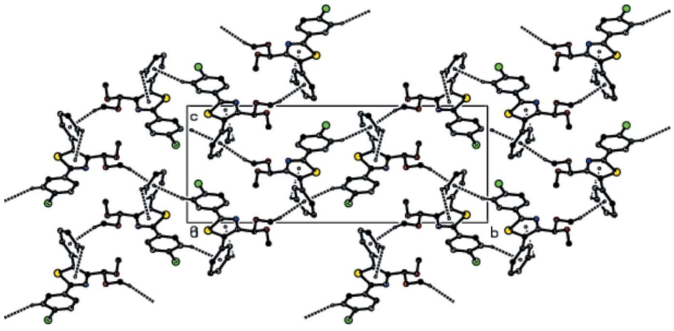


Figure 2
The packing viewed along the *a*-axis direction with the C—H···π interactions indicated by dashed lines.

Table 2
Percentage contributions of interatomic contacts to the Hirshfeld surface for the title compound.

Contact	Percentage contribution
H···H	39.2
H···C/C···H	25.2
Cl···H/H···Cl	11.4
O···H/H···O	8.0
S···H/H···S	5.1
N···H/H···N	3.9
C···C	2.4
Cl···C/C···Cl	1.7
S···C/C···S	1.5
Cl···Cl	0.6
S···S	0.2
O···C/C···O	0.1

4. Database survey

The most closely related four structures containing the 1,3-thiazole moiety are as follows: methyl(2-(cyclopentylidenehydrazono)-4-oxo-3-phenyl-1,3-thiazolidin-5-ylidene)-

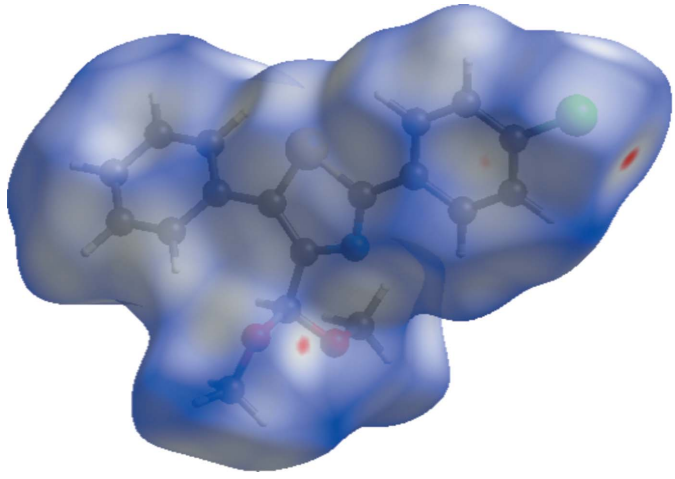


Figure 3
The three-dimensional Hirshfeld surface for the title compound, plotted over d_{norm} in the range −0.08 to +1.30 a.u.

acetate [Cambridge Structural Database (Groom *et al.*, 2016) refcode GUVVAW (I); Akkurt *et al.*, 2015], 2-(5-methyl-4-phenyl-1,3-thiazol-2-yl)-1-phenylethanol [EKEZUP (II); Rybakov *et al.*, 2003], 2-{(*E*)-2-[(2-chlorophenyl)methylidene]hydrazin-1-yl}-4-phenyl-1,3-thiazole [WOJKOX (III); Mague *et al.*, 2014] and 2-[4-(4-methoxyphenyl)-1,3-thiazol-2-yl]-2,3-dihydro-1*H*-isoindole-1,3-dione [IQUHOT (IV); Saravanan *et al.*, 2016].

In the crystal of (I), the thiazolidinyl ring (r.m.s. deviation = 0.024 Å) forms a dihedral angle of 65.13 (8)° with the attached phenyl ring. The molecular packing features C—H···O and C—H···π interactions, forming a three-dimensional network. In (II), molecules form extended chains through O—H···N hydrogen bonds and in (III), the two independent molecules are associated *via* complementary N—H···N hydrogen bonds into a dimer. These dimers are associated through weak C—H···Cl and C—H···S interactions into supramolecular chains propagating along the *a*-axis direction. In (IV), the molecules are linked *via* C—H···O interactions, which form *C*(7) chains propagating along [010]. In addition to this, weak π–π interactions are also observed.

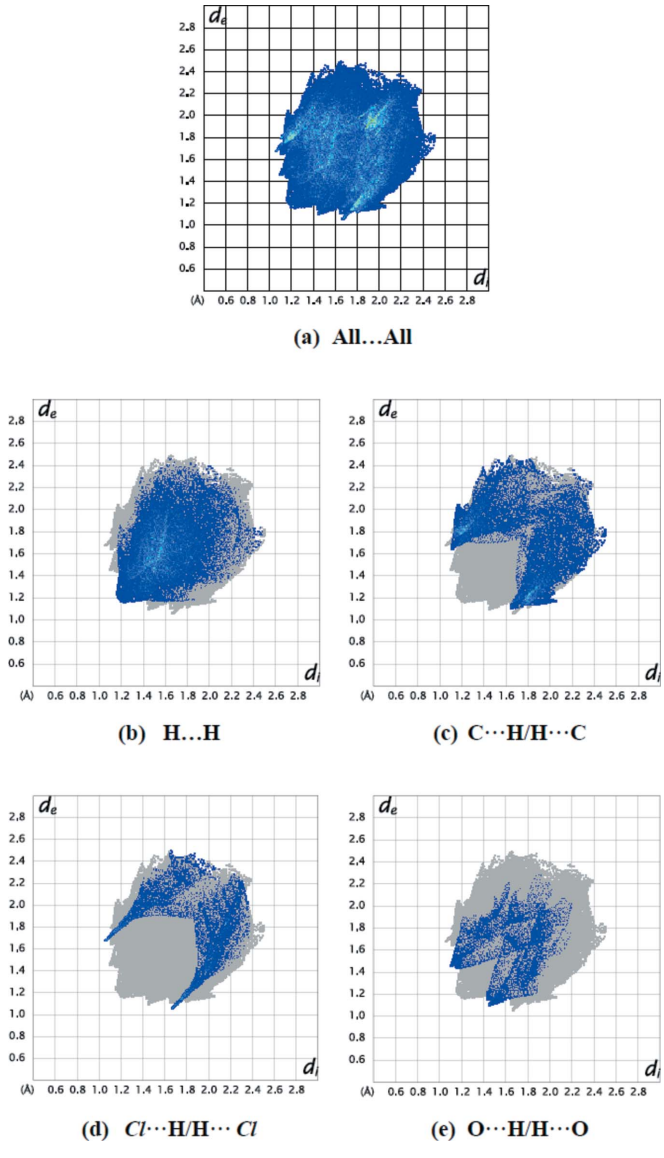


Figure 4
A view of the two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C, (*d*) Cl···H/H···Cl and (*e*) O···H/H···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{16}ClNO_2S$
M_r	345.83
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	6.6235 (1), 25.1848 (3), 9.8283 (1)
β (°)	96.504 (1)
V (Å^3)	1628.92 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.34
Crystal size (mm)	0.2 × 0.12 × 0.04
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.638, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31880, 3497, 3304
R_{int}	0.064
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.153, 1.12
No. of reflections	3497
No. of parameters	210
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −0.52

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2016/6* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

5. Synthesis and crystallization

A mixture of 1-chloro-3,3-diethoxy-1-phenylpropan-2-one (0.769 g, 2 mmol) and 4-chlorobenzothioamide (0.514 g, 3 mmol) was refluxed in methanol (15 ml) for 3 h. Then, the solvent was distilled off in a rotary evaporator under a vacuum. The residue was recrystallized from diethyl ether. Crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of a acetone solution. Colourless solid, yield 0.891 g (86%); m.p. 401–402 K. Analysis calculated for $C_{18}H_{16}ClNO_2S$: C 62.51, H 4.66, N 4.05; found: C 62.47, H 4.61, N 4.01%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.52 (6H, $2CH_3$), 4.62 (1H, CH), 7.22–8.90 (9H, Ar). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.6, 168.2, 154.4, 144.00, 142.4, 130.8, 129.6, 128.2, 127.4, 126.8, 126.00, 115.2 and 55.8. ESI–MS: *m*/*z*: 346.88 $[M + H]^+$.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms bonded to C atoms

were positioned geometrically (C—H = 0.93–1.00 Å) and constrained to ride on their parent atoms with U_{iso}(H) = 1.2–1.5U_{eq}(C)

Acknowledgements

The authors' contributions are as follows. Conceptualization, FIG, MA and AB; synthesis, FIG and KIK; X-ray analysis, EVS, EIT, MA and SÖY; writing (review and editing of the manuscript), FIG, MA, SÖY and AB.

References

Akkurt, M., Smolenski, V. A., Mohamed, S. K., Jasinski, J. P., Hassan, A. A. & Albayati, M. R. (2015). *Acta Cryst.* E**71**, o776–o777.
Dondoni, A. (2010). *Org. Biomol. Chem.* **8**, 3366–3385.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Grover, J. & Jachak, S. M. (2015). *RSC Adv.* **5**, 38892–38905.
Gurbanov, A. V., Kuznetsov, M. L., Demukhamedova, S. D., Alieva, I. N., Godjaev, N. M., Zubkov, F. I., Mahmudov, K. T. & Pombeiro, A. J. L. (2020). *CrystEngComm*, **22**, 628–633.
Mague, J. T., Mohamed, S. K., Akkurt, M., Hassan, A. A. & Albayati, M. R. (2014). *Acta Cryst.* E**70**, o907–o908.
Rigaku OD (2022). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Rybakov, V. B., Liakina, A. Y., Popova, I. S., Formanovsky, A. A. & Aslanov, L. A. (2003). *Acta Cryst.* E**59**, o1293–o1295.
Saravanan, K., Archana, K., Lakshmithendral, K., Kabilan, S. & Selvanayagam, S. (2016). *IUCrData*, **1**, x161053.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.
Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17*. University of Western Australia. http://hirshfeldsurface.net
Yariv, I., Lipovsky, A., Gedanken, A., Lubart, R. & Fixler, D. (2015). *Int. J. Nanomedicine*, **10**, 3593–3601.

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2022); cell refinement: *CrysAlis PRO* (Rigaku OD, 2022); data reduction: *CrysAlis PRO* (Rigaku OD, 2022); program(s) used to solve structure: *SHELXT2016/6* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

2-(4-Chlorophenyl)-4-(dimethoxymethyl)-5-phenyl-1,3-thiazole

Crystal data

$C_{18}H_{16}ClNO_2S$
$M_r = 345.83$
Monoclinic, $P2_1/c$
$a = 6.6235$ (1) Å
$b = 25.1848$ (3) Å
$c = 9.8283$ (1) Å
$\beta = 96.504$ (1)°
$V = 1628.92$ (4) Å^3
$Z = 4$
$F(000) = 720$
$D_x = 1.410$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 20657 reflections
$\theta = 3.5$–79.0°
$\mu = 3.34$ mm^{-1}
$T = 100$ K
Block, colourless
0.2 × 0.12 × 0.04 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
$T_{min} = 0.638$, $T_{max} = 1.000$
31880 measured reflections
3497 independent reflections
3304 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 79.5°$, $\theta_{min} = 3.5°$
$h = -7 \rightarrow 8$
$k = -32 \rightarrow 32$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.153$
$S = 1.12$
3497 reflections
210 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

$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 4.0625P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.46338 (11)	0.46239 (3)	0.83382 (7)	0.0279 (2)
S1	0.51773 (10)	0.42961 (2)	0.43335 (7)	0.01922 (18)
O1	0.4944 (3)	0.23523 (8)	0.4398 (2)	0.0232 (4)
O2	0.2192 (3)	0.27028 (8)	0.5252 (2)	0.0234 (4)
N1	0.6210 (4)	0.33759 (9)	0.5297 (2)	0.0195 (5)
C1	0.6779 (4)	0.38728 (11)	0.5353 (3)	0.0197 (5)
C2	0.4449 (4)	0.33113 (11)	0.4441 (3)	0.0194 (5)
C3	0.3640 (4)	0.37626 (10)	0.3799 (3)	0.0184 (5)
C4	0.8675 (4)	0.40656 (11)	0.6128 (3)	0.0195 (5)
C5	0.9086 (4)	0.46059 (11)	0.6290 (3)	0.0204 (5)
H5	0.809694	0.485762	0.593256	0.025*
C6	1.0909 (4)	0.47816 (11)	0.6960 (3)	0.0210 (5)
H6	1.118224	0.515046	0.706735	0.025*
C7	1.2333 (4)	0.44064 (12)	0.7474 (3)	0.0213 (6)
C8	1.1971 (4)	0.38669 (12)	0.7341 (3)	0.0229 (6)
H8	1.296580	0.361728	0.770269	0.028*
C9	1.0129 (4)	0.36970 (11)	0.6669 (3)	0.0217 (6)
H9	0.985437	0.332781	0.657512	0.026*
C10	0.3501 (4)	0.27646 (11)	0.4245 (3)	0.0194 (5)
H10	0.270809	0.274179	0.331869	0.023*
C11	0.5988 (5)	0.22879 (13)	0.3220 (3)	0.0296 (7)
H11A	0.501099	0.230402	0.239378	0.044*
H11B	0.667819	0.194318	0.326277	0.044*
H11C	0.699242	0.257220	0.319221	0.044*
C12	0.0998 (5)	0.22282 (13)	0.5072 (3)	0.0315 (7)
H12A	0.051128	0.218272	0.410015	0.047*
H12B	−0.016708	0.225524	0.560094	0.047*
H12C	0.183243	0.192197	0.539363	0.047*
C13	0.1824 (4)	0.38355 (11)	0.2793 (3)	0.0188 (5)
C14	−0.0001 (4)	0.35859 (11)	0.2967 (3)	0.0201 (5)
H14	−0.009865	0.337216	0.375383	0.024*

C15	−0.1681 (5)	0.36470 (12)	0.2001 (3)	0.0239 (6)
H15	−0.291864	0.347268	0.212459	0.029*
C16	−0.1560 (5)	0.39635 (12)	0.0848 (3)	0.0248 (6)
H16	−0.270937	0.400469	0.018481	0.030*
C17	0.0259 (5)	0.42183 (12)	0.0677 (3)	0.0245 (6)
H17	0.034629	0.443579	−0.010394	0.029*
C18	0.1943 (4)	0.41573 (11)	0.1636 (3)	0.0213 (6)
H18	0.317831	0.433298	0.151148	0.026*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0244 (4)	0.0301 (4)	0.0270 (4)	−0.0046 (3)	−0.0063 (3)	0.0036 (3)
S1	0.0205 (3)	0.0162 (3)	0.0206 (3)	0.0005 (2)	0.0007 (2)	0.0009 (2)
O1	0.0250 (10)	0.0203 (10)	0.0236 (10)	0.0031 (8)	−0.0004 (8)	−0.0006 (7)
O2	0.0281 (11)	0.0210 (10)	0.0217 (10)	−0.0055 (8)	0.0051 (8)	0.0013 (8)
N1	0.0219 (12)	0.0199 (11)	0.0168 (10)	0.0006 (9)	0.0024 (9)	0.0009 (8)
C1	0.0238 (14)	0.0192 (13)	0.0169 (12)	0.0028 (10)	0.0056 (10)	0.0010 (10)
C2	0.0216 (14)	0.0203 (13)	0.0167 (12)	0.0004 (10)	0.0044 (10)	−0.0005 (10)
C3	0.0195 (13)	0.0181 (12)	0.0180 (12)	−0.0005 (10)	0.0030 (10)	−0.0006 (9)
C4	0.0210 (13)	0.0216 (13)	0.0165 (12)	0.0016 (10)	0.0044 (10)	−0.0005 (10)
C5	0.0183 (13)	0.0228 (13)	0.0204 (13)	0.0037 (10)	0.0029 (10)	0.0014 (10)
C6	0.0230 (14)	0.0200 (13)	0.0205 (13)	−0.0015 (10)	0.0047 (11)	−0.0005 (10)
C7	0.0204 (13)	0.0278 (14)	0.0161 (12)	−0.0009 (11)	0.0031 (10)	0.0002 (10)
C8	0.0239 (14)	0.0242 (14)	0.0204 (13)	0.0045 (11)	0.0009 (11)	0.0013 (10)
C9	0.0254 (14)	0.0191 (13)	0.0209 (13)	0.0009 (10)	0.0032 (11)	0.0002 (10)
C10	0.0193 (13)	0.0204 (13)	0.0180 (12)	0.0001 (10)	0.0000 (10)	0.0012 (10)
C11	0.0258 (15)	0.0309 (16)	0.0323 (16)	0.0035 (12)	0.0051 (12)	−0.0037 (12)
C12	0.0367 (18)	0.0257 (15)	0.0318 (16)	−0.0109 (13)	0.0028 (13)	0.0037 (12)
C13	0.0220 (14)	0.0183 (12)	0.0160 (12)	0.0025 (10)	0.0014 (10)	−0.0011 (9)
C14	0.0205 (13)	0.0211 (13)	0.0191 (12)	0.0024 (10)	0.0044 (10)	0.0007 (10)
C15	0.0231 (14)	0.0247 (14)	0.0241 (14)	0.0024 (11)	0.0035 (11)	−0.0017 (11)
C16	0.0243 (14)	0.0275 (14)	0.0212 (13)	0.0075 (11)	−0.0031 (11)	−0.0015 (11)
C17	0.0319 (16)	0.0240 (14)	0.0176 (13)	0.0051 (12)	0.0024 (11)	0.0022 (10)
C18	0.0238 (14)	0.0186 (12)	0.0224 (13)	0.0004 (10)	0.0057 (11)	0.0008 (10)

Geometric parameters (Å, º)

Cl1—C7	1.747 (3)	C8—C9	1.387 (4)
S1—C1	1.740 (3)	C9—H9	0.9500
S1—C3	1.731 (3)	C10—H10	1.0000
O1—C10	1.408 (3)	C11—H11A	0.9800
O1—C11	1.424 (4)	C11—H11B	0.9800
O2—C10	1.396 (3)	C11—H11C	0.9800
O2—C12	1.433 (4)	C12—H12A	0.9800
N1—C1	1.306 (4)	C12—H12B	0.9800
N1—C2	1.368 (4)	C12—H12C	0.9800
C1—C4	1.475 (4)	C13—C14	1.391 (4)

C2—C3	1.379 (4)	C13—C18	1.406 (4)
C2—C10	1.517 (4)	C14—H14	0.9500
C3—C13	1.480 (4)	C14—C15	1.387 (4)
C4—C5	1.393 (4)	C15—H15	0.9500
C4—C9	1.399 (4)	C15—C16	1.395 (4)
C5—H5	0.9500	C16—H16	0.9500
C5—C6	1.381 (4)	C16—C17	1.392 (4)
C6—H6	0.9500	C17—H17	0.9500
C6—C7	1.389 (4)	C17—C18	1.384 (4)
C7—C8	1.383 (4)	C18—H18	0.9500
C8—H8	0.9500		

C3—S1—C1	89.91 (13)	O2—C10—C2	107.0 (2)
C10—O1—C11	112.6 (2)	O2—C10—H10	109.6
C10—O2—C12	112.6 (2)	C2—C10—H10	109.6
C1—N1—C2	111.2 (2)	O1—C11—H11A	109.5
N1—C1—S1	114.1 (2)	O1—C11—H11B	109.5
N1—C1—C4	124.2 (3)	O1—C11—H11C	109.5
C4—C1—S1	121.6 (2)	H11A—C11—H11B	109.5
N1—C2—C3	116.3 (2)	H11A—C11—H11C	109.5
N1—C2—C10	119.9 (2)	H11B—C11—H11C	109.5
C3—C2—C10	123.8 (3)	O2—C12—H12A	109.5
C2—C3—S1	108.4 (2)	O2—C12—H12B	109.5
C2—C3—C13	130.7 (3)	O2—C12—H12C	109.5
C13—C3—S1	120.8 (2)	H12A—C12—H12B	109.5
C5—C4—C1	121.6 (3)	H12A—C12—H12C	109.5
C5—C4—C9	119.2 (3)	H12B—C12—H12C	109.5
C9—C4—C1	119.2 (2)	C14—C13—C3	120.9 (2)
C4—C5—H5	119.4	C14—C13—C18	119.3 (3)
C6—C5—C4	121.1 (3)	C18—C13—C3	119.8 (3)
C6—C5—H5	119.4	C13—C14—H14	119.8
C5—C6—H6	120.8	C15—C14—C13	120.4 (3)
C5—C6—C7	118.4 (3)	C15—C14—H14	119.8
C7—C6—H6	120.8	C14—C15—H15	119.9
C6—C7—Cl1	118.8 (2)	C14—C15—C16	120.3 (3)
C8—C7—Cl1	119.1 (2)	C16—C15—H15	119.9
C8—C7—C6	122.1 (3)	C15—C16—H16	120.3
C7—C8—H8	120.6	C17—C16—C15	119.4 (3)
C7—C8—C9	118.8 (3)	C17—C16—H16	120.3
C9—C8—H8	120.6	C16—C17—H17	119.7
C4—C9—H9	119.8	C18—C17—C16	120.6 (3)
C8—C9—C4	120.5 (3)	C18—C17—H17	119.7
C8—C9—H9	119.8	C13—C18—H18	120.0
O1—C10—C2	112.9 (2)	C17—C18—C13	120.0 (3)
O1—C10—H10	109.6	C17—C18—H18	120.0
O2—C10—O1	108.1 (2)		

Cl1—C7—C8—C9	179.2 (2)	C3—C2—C10—O1	150.2 (3)

S1—C1—C4—C5	12.2 (4)	C3—C2—C10—O2	−90.9 (3)
S1—C1—C4—C9	−165.3 (2)	C3—C13—C14—C15	−178.5 (3)
S1—C3—C13—C14	−137.1 (2)	C3—C13—C18—C17	178.7 (2)
S1—C3—C13—C18	43.4 (3)	C4—C5—C6—C7	0.0 (4)
N1—C1—C4—C5	−172.0 (3)	C5—C4—C9—C8	−0.9 (4)
N1—C1—C4—C9	10.5 (4)	C5—C6—C7—Cl1	−179.4 (2)
N1—C2—C3—S1	−0.9 (3)	C5—C6—C7—C8	−0.4 (4)
N1—C2—C3—C13	177.8 (3)	C6—C7—C8—C9	0.2 (4)
N1—C2—C10—O1	−29.8 (3)	C7—C8—C9—C4	0.5 (4)
N1—C2—C10—O2	89.1 (3)	C9—C4—C5—C6	0.7 (4)
C1—S1—C3—C2	0.5 (2)	C10—C2—C3—S1	179.0 (2)
C1—S1—C3—C13	−178.4 (2)	C10—C2—C3—C13	−2.2 (5)
C1—N1—C2—C3	1.0 (3)	C11—O1—C10—O2	163.7 (2)
C1—N1—C2—C10	−179.0 (2)	C11—O1—C10—C2	−78.1 (3)
C1—C4—C5—C6	−176.8 (2)	C12—O2—C10—O1	−65.6 (3)
C1—C4—C9—C8	176.6 (2)	C12—O2—C10—C2	172.5 (2)
C2—N1—C1—S1	−0.5 (3)	C13—C14—C15—C16	−0.5 (4)
C2—N1—C1—C4	−176.6 (2)	C14—C13—C18—C17	−0.7 (4)
C2—C3—C13—C14	44.2 (4)	C14—C15—C16—C17	−0.1 (4)
C2—C3—C13—C18	−135.2 (3)	C15—C16—C17—C18	0.4 (4)
C3—S1—C1—N1	0.0 (2)	C16—C17—C18—C13	0.1 (4)
C3—S1—C1—C4	176.2 (2)	C18—C13—C14—C15	1.0 (4)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*3 are the centroids of the C1–C3/S1/N1 and C13–C18 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···S1	0.95	2.74	3.143 (3)	106
C6—H6···*Cg*3^{i}	0.95	2.81	3.620 (3)	144
C12—H12*C*···*Cg*3^{ii}	0.98	2.81	3.406 (3)	120
C15—H15···*Cg*1^{iii}	0.95	2.95	3.481 (3)	117

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

Summary of short interatomic contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
Cl1···H16	2.85	2 + *x*, *y*, 1 + *z*
H18···Cl1	3.00	2 - *x*, 1 - *y*, 1 - *z*
H11*C*···H15	2.50	1 + *x*, *y*, *z*
H6···C17	2.97	1 - *x*, 1 - *y*, 1 - *z*
O2···H11*A*	2.65	*x*, 1/2 - *y*, 1/2 + *z*
C7···H17	2.85	1 + *x*, *y*, 1 + *z*
C11···H8	3.04	-1 + *x*, 1/2 - *y*, -1/2 + *z*