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

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In the title compound, C_{18}H_{16}ClNO_{2}S, 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/Cl···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/N1/C1–C3) makes dihedral angles of 13.12 (14) and 43.79 (14)°, respectively, with...
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-dimen-
sional 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 dnorm and the related colours reflecting
various interactions. The C—H···π interaction is represented
by the red spot on the surface. Fig. 4 depicts the two-dimen-
sional fingerprint plots. The weak van der Waals H···H
connections provide the most (39.2%, Fig. 4b) to the Hirshfeld
surface. The other principal contributions to the overall
surface are from C···H···C (25.2%, Fig. 4c), Cl···H···Cl
(11.4%, Fig. 4d) and O···H···O (8.0%, Fig. 4e) interactions.
The contributions of the remaining less important interactions
are given in Table 2.

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

Table 1
Hydrogen-bond geometry (Å, °).
Cg1 and Cg3 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···Cg3 | 0.95 | 2.81  | 3.620 (3) | 144 |
| C12—H12C···Cg3 | 0.98 | 2.81  | 3.406 (3) | 120 |
| C15—H15···Cg1 | 0.95 | 2.95  | 3.481 (3) | 117 |

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

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                   |

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.

Figure 3
The three-dimensional Hirshfeld surface for the title compound, plotted
over dnorm 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-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-{[E]-2-[(2-chlorophenyl)methylidene]hydrazin-1-yl}-4-phenyl-1,3-thiazole [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/C1/C1/C1 O and
C—H/C1/C1/C1/C25 interactions, forming a three-dimensional network.

In (II), molecules form extended chains through O—H/C1/C1/C1 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 inter-
actions are also observed.

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 C18H16ClNO2S: C 62.51, H 4.66, N 4.05; found: C 62.47, H 4.61, N 4.01%. 1H NMR (300 MHz, CDCl3) δ 3.52 (6H, 2CH3), 4.62 (1H, CH), 7.22–8.90 (9H, Ar). 13CN M R (75 MHz, CDCl3) 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

| Crystal data | Chemical formula | C18H16ClNO2S |
|--------------|------------------|---------------|
| M (g/mol)    | 345.83           |               |
| Crystal system, space group | Monoclinic, P21/c |               |
| Temperature (K) | 100             |               |
| a, b, c (Å) | 6.6235 (1), 25.1848 (3), 9.8283 (1) |               |
| β (°)       | 96.504 (1)       |               |
| V (Å3)      | 1628.92 (4)      |               |
| Z           | 4                |               |
| µ (mm⁻¹)    | 3.34             |               |
| Crystal size (mm) | 0.2 × 0.12 × 0.04 |               |

Table 3
Experimental details.

Crystal data
Chemical formula
M
Crystal system, space group
Temperature (K)
a, b, c (Å)
β (°)
V (Å3)
Z
µ (mm⁻¹)
Crystal size (mm)

Data collection
Diffractometer
Absorption correction
Tmin, Tmax
No. of measured, independent and observed [I > 2σ(I)] reflections
Rint
(sin θ/λ)max (Å⁻¹)

Refinement
R[F² > 2σ(F²)], wR(F²), S
No. of reflections
No. of parameters
H-atom treatment
Δρmax, Δρmin (e Å⁻³)

H-atom parameters constrained

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

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 d₁ and
d₂ values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

were positioned geometrically \((C-H = 0.93–1.00 \text{ Å})\) 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.

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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

\[
\begin{align*}
C_{18}H_{16}ClNO_2S \\
M_r &= 345.83 \\
\text{Monoclinic, } P2_1/c \\
a &= 6.6235 (1) \text{ Å} \\
b &= 25.1848 (3) \text{ Å} \\
c &= 9.8283 (1) \text{ Å} \\
\beta &= 96.504 (1)^\circ \\
V &= 1628.92 (4) \text{ Å}^3 \\
Z &= 4
\end{align*}
\]

\[
\begin{align*}
F(000) &= 720 \\
D_d &= 1.410 \text{ Mg m}^{-3} \\
\text{Cu } K\alpha \text{ radiation, } \lambda = 1.54184 \text{ Å} \\
\text{Cell parameters from 20657 reflections} \\
\theta &= 3.5 \text{–} 79.0^\circ \\
\mu &= 3.34 \text{ mm}^{-1} \\
T &= 100 \text{ K} \\
\text{Block, colourless} \\
0.2 \times 0.12 \times 0.04 \text{ mm}
\end{align*}
\]

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer

\[
\begin{align*}
\text{Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source} \\
\text{Mirror monochromator} \\
\text{Detector resolution: 10.0000 pixels mm}^{-1} \\
\omega \text{ scans} \\
\text{Absorption correction: multi-scan} \\
\text{(CrysAlisPro; Rigaku OD, 2022)} \\
T_{\text{min}} &= 0.638, T_{\text{max}} = 1.000 \\
31880 \text{ measured reflections} \\
3497 \text{ independent reflections} \\
3304 \text{ reflections with } I > 2\sigma(I) \\
R_{\text{int}} &= 0.064 \\
\theta_{\text{max}} &= 79.5^\circ, \theta_{\text{min}} = 3.5^\circ \\
\h &= -7 \rightarrow 8 \\
\k &= -32 \rightarrow 32 \\
\l &= -12 \rightarrow 12
\end{align*}
\]

Refinement

Refinement on \(F^2\)

\[
\begin{align*}
\text{Least-squares matrix: full} \\
R(F^2 > 2\sigma(F^2)) &= 0.055 \\
wR(F^2) &= 0.153 \\
S &= 1.12 \\
3497 \text{ reflections} \\
210 \text{ parameters} \\
0 \text{ restraints}
\end{align*}
\]

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
\[ w = \frac{1}{\sigma^2(F_o^2) + (0.0621P)^2 + 4.0625P} \]
\[ \text{where } P = (F_o^2 + 2F_c^2)/3 \]
\[ (\Delta/\sigma)_{\text{max}} = 0.001 \]
\[ \Delta \rho_{\text{max}} = 0.67 \ \text{e Å}^{-3} \]
\[ \Delta \rho_{\text{min}} = -0.52 \ \text{e Å}^{-3} \]

**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 F² against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F², conventional R-factors R are based on F, with F set to zero for negative F². The threshold expression of F² > 2\sigma(F²) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F² 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) |
| S  | 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     | 0.560994     | 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  0.18481  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  0.43298  0.151148  0.026*  

**Atomic displacement parameters (Å²)**

|        | U₁₁  | U₂₂  | U₃₃  | U₁₂  | U₁₃  | U₂₃  |
|--------|------|------|------|------|------|------|
| C11    | 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, °)**

|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| C1—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) |        |        |        |
| Bond          | Length (Å) | Bond          | Length (Å) |
|--------------|------------|--------------|------------|
| 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     |              |            |

| Bond          | Length (Å) |
|--------------|------------|
| C3—S1—C1     | 89.91 (13) |
| C10—O1—C11   | 112.6 (2)  |
| C10—O2—C12   | 112.6 (2)  |
| C1—N1—C2     | 111.2 (2)  |
| N1—C1—S1     | 114.1 (2)  |
| N1—C1—C4     | 124.2 (3)  |
| C4—C1—S1     | 121.6 (2)  |
| N1—C2—C3     | 116.3 (2)  |
| N1—C2—C10    | 119.9 (2)  |
| C3—C2—C10    | 123.8 (3)  |
| C2—C3—S1     | 108.4 (2)  |
| C2—C3—C13    | 130.7 (3)  |
| C13—C3—S1    | 120.8 (2)  |
| C5—C4—C1     | 121.6 (3)  |
| C5—C4—C9     | 119.2 (3)  |
| C9—C4—C1     | 119.2 (2)  |
| C4—C5—H5     | 119.4      |
| C6—C5—C4     | 121.1 (3)  |
| C6—C5—H5     | 119.4      |
| C5—C6—H6     | 120.8      |
| C5—C6—C7     | 118.4 (3)  |
| C7—C6—H6     | 120.8      |
| C6—C7—C11    | 118.8 (2)  |
| C8—C7—C11    | 119.1 (2)  |
| C8—C7—C6     | 122.1 (3)  |
| C7—C8—H8     | 120.6      |
| C7—C8—C9     | 118.8 (3)  |
| C9—C8—H8     | 120.6      |
| C4—C9—H9     | 119.8      |
| C8—C9—C4     | 120.5 (3)  |
| C8—C9—H9     | 119.8      |
| O1—C10—C2    | 112.9 (2)  |
| O1—C10—H10   | 109.6      |
| O2—C10—O1    | 108.1 (2)  |

| Bond          | Angle (°)    |
|--------------|--------------|
| O2—C10—C2   | 107.0 (2)    |
| C2—C10—O1   | 109.6        |
| O1—C11—H11A | 109.5        |
| O1—C11—H11B | 109.5        |
| O1—C11—H11C | 109.5        |
| H11A—C11—H11B | 109.5 |
Hydrogen-bond geometry (Å, °)

Cg1 and Cg3 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···Cg3ii | 0.95 | 2.81 | 3.620 (3) | 144 |
| C12—H12C···Cg3i | 0.98 | 2.81 | 3.406 (3) | 120 |
| C15—H15···Cg1iii | 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 |
|---------|----------|--------------------|
| C11···H16 | 2.85 | 2 + x, y, 1 + z |
| H18···Cl1 | 3.00 | 2 - x, 1 - y, 1 - z |
| H11C···H15 | 2.50 | 1 + x, y, z |
| H6···C17 | 2.97 | 1 - x, 1 - y, 1 - z |
| O2···H11A | 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 |