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Crystal structure and Hirshfeld surface analysis of 3-(2-chloro-6-fluorophenyl)-1,5-bis(thiophen-2-yl)-pentane-1,5-dione

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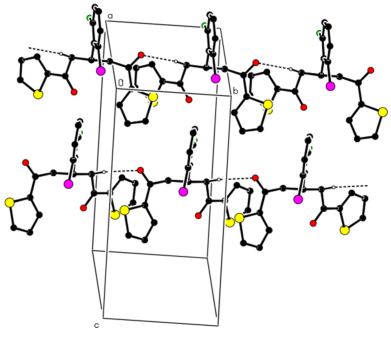
In the title compound, $C_{19}H_{14}ClFO_2S_2$, the molecular conformation is stabilized by intramolecular C—H···F, C—H···Cl and C—H···O hydrogen bonds. In the crystal, the molecules are linked into [010] chains by C—H···O hydrogen bonds, creating a $C(6)$ motif and weak C—H···F and C—H···Cl interactions link these chains into sheets parallel to the (100) plane. The entire $-C_6H_3FCl$ group is disordered over two positions in a 0.931 (4):0.069 (4) ratio. A Hirshfeld surface analysis indicates that the most important contributions to the crystal packing are from H···H (26.7%), C···H/H···C (17.2%), S···H/H···S (15.0%) and O···H/H···O (12.0%) interactions.

1. Chemical context

Substituted thiophenes are important intermediates in organic synthesis, and are widely used in medicine, industrial chemistry, and materials science (Peng *et al.*, 2024). Thiophenes with anti-inflammatory, antibacterial, anti-cancer and other biological activities are widely used in the pharmaceutical industry, and a number of thiophene-containing drugs have been approved by the Food and Drug Administration (FDA), such as Cefoxitin, Raloxifene and Suprofen (Schweizer *et al.*, 2011). In addition, thiophenes exhibit adequate electrical conductivity because of the presence of sulfur atoms. In particular, polythiophenes have found applications in organic light-emitting diodes, organic semiconductors, field effect transistors, *etc.* (Turkoglu *et al.*, 2019; Zhang *et al.*, 2015). Functional properties of thiophenes are strongly dependent on the intermolecular interactions, such as hydrogen and chalcogen bonds (Gurbanov *et al.*, 2020, 2022; Mahmudov *et al.*, 2021, 2023). The cooperation of –Cl, –F and C═O groups with the thiophen-2-yl synthon in thiophenes can improve the functional properties of the corresponding organic materials (Gurbanov *et al.*, 2023; Mahmoudi *et al.*, 2017, 2018; Velásquez *et al.*, 2019). Thus, in the current work we have synthesized a new thiophene derivative, 3-(2-chloro-6-fluorophenyl)-1,5-di(thiophen-2-yl)pentane-1,5-dione, which provides multiple intermolecular interactions.



2. Structural commentary

Intramolecular C2—H2*A*···F1, C1—H1···Cl1 and C13—H13···O1 interactions (Fig. 1, Table 1) maintain the molecular conformation of the major disorder component of the title compound, resulting in $C(6)$, $C(5)$ and $C(9)$ motifs

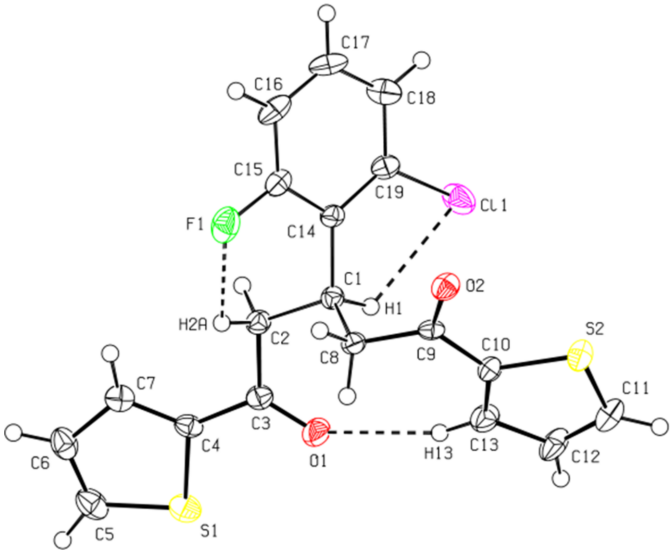


Figure 1
The title molecule with the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level. Only the major disorder component is displayed. Intramolecular C—H···Cl, C—H···F, and C—H···O hydrogen bonds are shown as dashed lines.

(Bernstein *et al.*, 1995), respectively. The major and minor occupancy benzene rings (C14–C19 and C14*A*–C19*A*) of the disordered 2-chloro-6-fluorophenyl group form an angle of 3.3 (5)° with one another. The angles between the planes of the two thiophen-2-yl rings (S1/C4–C7 and S2/C10–C13) and the major occupancy ring (C14–C19) of the disordered 2-chloro-6-fluorophenyl group are 40.9 (1) and 51.6 (1)°, respectively. The dihedral angle between the two thiophen-2-yl rings is 19.3 (1)°. The torsion angles C3—C2—C1—C14, C3—C2—C1—C8, C2—C1—C8—C9, C14—C1—C8—C9, C1—C8—C9—C10 and C8—C9—C10—C13 are 165.2 (2), −70.4 (2), 169.8 (2), −65.8 (3), −81.2 (2), and 0.4 (4)°, respectively. The sum of the angles about C1 is 333.6 (2)° for the major disorder component. All geometric parameters are normal and consistent with those of related compounds listed in the section *Database survey*.

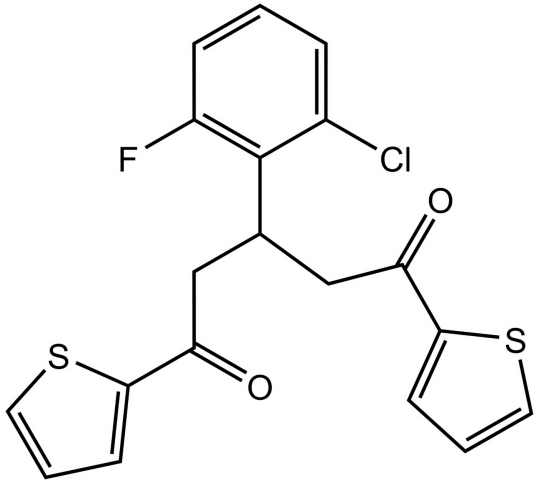


Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Cl1	1.00	2.57	3.128 (3)	115
C1—H1···F1*A*	1.00	2.21	2.86 (5)	122
C2—H2*A*···Cl1*A*	0.99	2.31	2.91 (3)	118
C2—H2*A*···F1	0.99	2.32	2.898 (5)	116
C2—H2*B*···O2^{i}	0.99	2.48	3.417 (3)	157
C5—H5···Cl1*A*^{ii}	0.95	2.49	3.12 (3)	123
C8—H8*A*···Cl1*A*	0.99	2.35	3.01 (3)	123
C13—H13···O1	0.95	2.45	3.367 (3)	163
C16—H16···F1*A*^{iii}	0.95	2.50	3.35 (3)	149

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

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, C—H···O hydrogen bonds (Table 1) link the molecules into chains extending along the [010] direction (Fig. 2) and weak C—H···F and C—H···Cl interactions (Table 1) further link these chains into sheets parallel to the (100) plane (Figs. 1 and 2 in the supporting information). van der Waals interactions between the sheets also contribute to the cohesion of the molecular packing. No π–π or C—H···π interactions are found.

We carried out a Hirshfeld surface analysis to further investigate the intermolecular interactions using *Crystal Explorer 17.5* (Spackman *et al.*, 2021). The Hirshfeld surface mapped over $d_{\rm norm}$ is illustrated in Fig. 3. The red spots on the Hirshfeld surface plot indicate the intermolecular C2—H2*B*···O2, C5—H5···Cl1*A* and C16—H16···F1A contacts shown in Table 1. The overall two-dimensional fingerprint plot is shown in Fig. 4*a*. The Hirshfeld surface analysis reveals that H···H (26.7%) and C···H/H···C (17.2%) contacts are the main contributors to the crystal

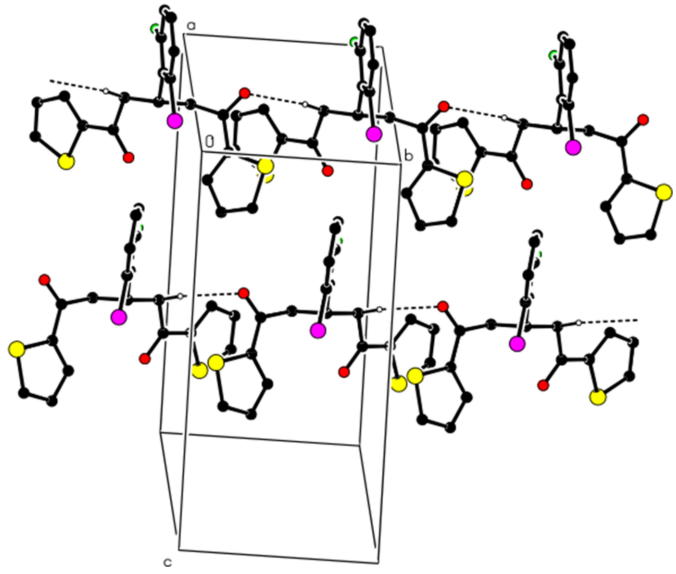


Figure 2
A partial packing diagram showing the unit cell. Dashed lines indicate C—H···O hydrogen bonds. Only H atoms involved in the hydrogen bonds and the major disorder component are shown for clarity.

Table 2
Summary of short interatomic contacts (Å).

Contact	Distance	Symmetry operation
H18*A*···H11	2.50	$-x, 1-y, 1-z$
F1*A*···H16	2.50	$x, \frac{3}{2}-y, \frac{1}{2}+z$
H5···O1	2.64	$1-x, \frac{1}{2}+y, \frac{3}{2}-z$
O2···H2*B*	2.48	$x, -1+y, z$
O2···H17*A*	2.44	$-x, -\frac{1}{2}+y, \frac{1}{2}-z$
H5···Cl1*A*	2.49	$1-x, 2-y, 1-z$
O2···H11	2.68	$x, \frac{1}{2}-y, \frac{1}{2}+z$
H6···H6	2.32	$1-x, 3-y, 1-z$

packing (Tables 1 and 2; Fig. 4*b*–*c*), followed by S···H/H···S (15.0%), O···H/H···O (12.0%), F···H/H···F (7.6%) and Cl···H/H···Cl (6.4%) contacts. The other minor contributions are less than 4.5%. The Hirshfeld surface analysis confirms the importance of H-atom contacts in the crystal (Hathwar *et al.*, 2015).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.00, update of April 2025; Groom *et al.*, 2016) found that the most closely related structures containing the 4-(2-chloro-6-fluorophenyl)-1,7-di(thiophen-2-yl)heptane-1,7-di-one unit are MIGVEE (Butcher *et al.*, 2007), WEPJOR (Yathirajan *et al.*, 2006) and XUJRAZ (Sharmoukh *et al.*, 2025).

The angles between the plane of the benzene ring and those of the two thiophene rings are 89.7 (5) and 63.7 (1)° for MIGVEE, 84.9 (2) and 68.8 (2) ° for WEPJOR, and 75.27 (5) and 83.8 (2)° for XUJRAZ. In MIGVEE, the molecules are linked by C—Br···π and C—Cl···π interactions and there are no classical hydrogen bonds. In WEPJOR, the molecules form layers parallel to (200) through C—H···O hydrogen bonds. C—H···π, C—Br···π, and C—O···π interactions formed between the layers strengthen the molecular packing. In the crystal of XUJRAZ, C—H···O hydrogen bonds form chains of molecules extending along the *c*-axis direction. These are linked by C—H···S hydrogen bonds and C—H···π interactions into corrugated layers parallel to the *bc* plane.

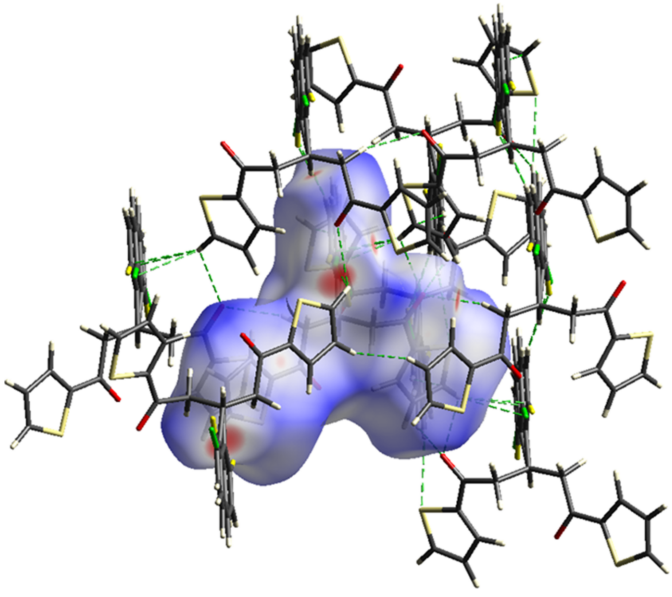


Figure 3
View of the three-dimensional Hirshfeld surface of the compound plotted over d_{norm}.

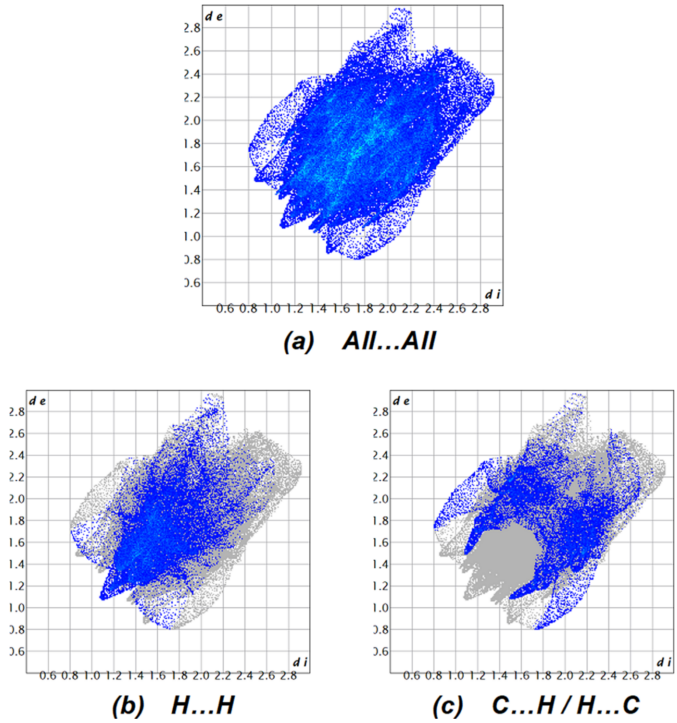


Figure 4
The two-dimensional fingerprint plots, showing (*a*) all interactions, and delineated into (*b*) H···H and (*c*) C···H/H···C interactions [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

5. Synthesis and crystallization

2-Chloro-6-fluorobenzaldehyde (10 mmol) was added into a solution of 1-(thiophen-2-yl)ethan-1-one (20 mmol) in EtOH (60 mL). KOH pellets (25 mmol) were then added to the solution. The solution was stirred at room temperature for 8 h. The off-colourless solid was collected by filtration and washed with EtOH (3 × 10 mL). Recrystallization from $CHCl_3$–MeOH afforded a white crystalline solid of the title compound (yield, 52%). The synthesis is shown in Fig. 5. Analysis calculated for $C_{19}H_{14}ClFO_2S_2$: C, 58.09; H, 3.59. Found: C, 58.05; H, 3.55. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.83 (*dd*, *J* = 1.0, 3.8 Hz, 2H, ArH), 7.68 (*dd*, *J* = 1.0, 4.9 Hz, 2H, ArH), 7.55–7.52 (*m*, 2H, ArH), 7.24 (*d*, *J* = 8.0 Hz, 1H, ArH), 7.08 (*dd*, *J* = 3.9, 4.8 Hz, 2H, ArH), 4.60 (*p*, *J* = 7.2 Hz, 1H, CH), 3.51 (*dd*, *J* = 7.1, 16.9 Hz, 2H, CH_2), 3.39 (*dd*, *J* = 7.2, 16.9 Hz, 2H, CH_2); ^{13}C{H} NMR (125 MHz, $CDCl_3$): δ (ppm) 198.6, 160.0, 144.1, 136.6, 134.6, 134.4, 133.4, 128.7, 128.4, 124.2, 113.3, 45.0, 36.5.

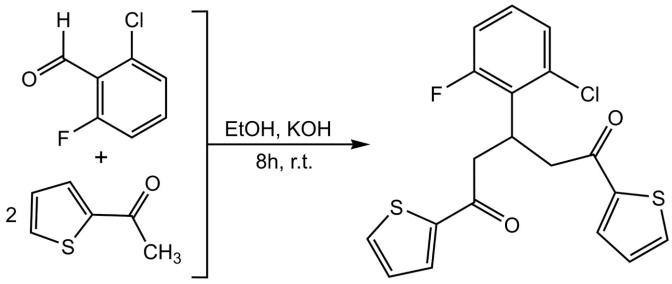


Figure 5
Synthesis of 3-(2-chloro-6-fluorophenyl)-1,5-di(thiophen-2-yl)pentane-1,5-dione.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All carbon-bound H atoms were positioned geometrically and refined as riding: C—H = 0.95–1.00 Å with U_{iso}(H) = 1.2U_{eq}(C). The –C_6H_3FCl group (C14–C19/Cl1/F1) atoms and the main group atom it is attached to (C1) were treated as disordered in a ratio of 0.931 (4):0.069 (4) over two positions. Refinement was performed by substituting the majority of the fluorine and chlorine atoms in the disorder with the minor portion's chlorine and fluorine atoms, respectively. The FLAT command was used to ensure that the atoms of the two disorder parts lie in the same plane. In the major and minor parts (C14–C19/Cl1/F1 and C14*A*–C19*A*/Cl1A/F1*A*) of the disorder group, the C—Cl and C—F bonds, as well as the corresponding C–C bond lengths (*e.g.* C14—C19 and C14A—C19*A*) of the benzene ring, and the C1—C14 and C1—C14*A* distances connecting the –C_6H_3FCl group to the main group, were forced to have the same value using the SADI command. Displacement parameters of similar corresponding atoms were forced to be the same using the EADP command. For the disordered main group atom (C1/C1*A*), the EXYZ and EADP commands were applied. One reflection (1 0 0), affected by the incident beam-stop was omitted in the final cycles of refinement.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{14}ClFO_2S_2$
M_r	392.87
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	16.4479 (14), 7.6867 (6), 15.4738 (12)
β (°)	113.697 (2)
V (Å^3)	1791.4 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.47
Crystal size (mm)	0.28 × 0.21 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.868, 0.936
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24966, 3678, 2523
R_{int}	0.069
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.101, 1.02
No. of reflections	3678
No. of parameters	251
No. of restraints	19
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.33

Computer programs: *APEX4* and *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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Funding information

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supporting information

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Computing details

3-(2-Chloro-6-fluorophenyl)-1,5-bis(thiophen-2-yl)pentane-1,5-dione

Crystal data

$C_{19}H_{14}ClFO_2S_2$
$M_r = 392.87$
Monoclinic, $P2_1/c$
$a = 16.4479$ (14) Å
$b = 7.6867$ (6) Å
$c = 15.4738$ (12) Å
$\beta = 113.697$ (2)°
$V = 1791.4$ (3) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.457$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3391 reflections
$\theta = 2.7$–22.6°
$\mu = 0.47$ mm^{-1}
$T = 150$ K
Plate, colourless
0.28 × 0.21 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.868$, $T_{max} = 0.936$
24966 measured reflections
3678 independent reflections
2523 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.6°$
$h = -12\rightarrow20$
$k = -9\rightarrow9$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.101$
$S = 1.02$
3678 reflections
251 parameters
19 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
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.8461P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.48547 (5)	1.11343 (9)	0.68846 (5)	0.0347 (2)	
S2	0.17955 (5)	0.15490 (9)	0.57749 (4)	0.02808 (18)	
O1	0.35484 (12)	0.8198 (2)	0.63059 (11)	0.0325 (5)	
O2	0.20623 (11)	0.2763 (2)	0.40727 (11)	0.0257 (4)	
C1	0.23408 (15)	0.7006 (3)	0.45142 (15)	0.0185 (5)	0.931 (4)
H1	0.208985	0.704636	0.500503	0.022*	0.931 (4)
C1A	0.23408 (15)	0.7006 (3)	0.45142 (15)	0.0185 (5)	0.069 (4)
H1A	0.216615	0.704850	0.506277	0.022*	0.069 (4)
C2	0.29032 (16)	0.8652 (3)	0.46245 (16)	0.0211 (5)	
H2A	0.324906	0.852587	0.423181	0.025*	
H2B	0.249983	0.965811	0.437873	0.025*	
C3	0.35410 (16)	0.9041 (3)	0.56334 (16)	0.0222 (6)	
C4	0.41533 (16)	1.0496 (3)	0.57579 (16)	0.0216 (6)	
C5	0.53198 (18)	1.2697 (3)	0.6448 (2)	0.0334 (7)	
H5	0.577736	1.345670	0.683339	0.040*	
C6	0.49693 (17)	1.2742 (3)	0.54950 (19)	0.0296 (6)	
H6	0.515453	1.352724	0.513567	0.036*	
C7	0.42941 (17)	1.1482 (3)	0.50947 (18)	0.0256 (6)	
H7	0.397187	1.133687	0.443422	0.031*	
C8	0.29140 (16)	0.5332 (3)	0.46852 (16)	0.0195 (5)	
H8A	0.310864	0.518754	0.416146	0.023*	
H8B	0.345162	0.546509	0.527707	0.023*	
C9	0.24180 (15)	0.3726 (3)	0.47531 (16)	0.0192 (5)	
C10	0.23621 (16)	0.3363 (3)	0.56578 (16)	0.0206 (5)	
C11	0.20209 (19)	0.2051 (3)	0.69187 (18)	0.0319 (7)	
H11	0.183088	0.136201	0.731254	0.038*	
C12	0.24999 (19)	0.3535 (4)	0.72113 (17)	0.0328 (7)	
H12	0.267969	0.400652	0.782783	0.039*	
C13	0.26995 (18)	0.4295 (3)	0.64853 (17)	0.0300 (6)	
H13	0.303128	0.533825	0.656235	0.036*	
F1	0.2498 (2)	0.7339 (4)	0.2741 (3)	0.0361 (9)	0.931 (4)
Cl1	0.04217 (6)	0.63824 (16)	0.44021 (6)	0.0390 (3)	0.931 (4)
C14	0.15660 (18)	0.6954 (3)	0.35533 (18)	0.0185 (7)	0.931 (4)
C15	0.1675 (2)	0.7152 (5)	0.2710 (2)	0.0244 (8)	0.931 (4)
C16	0.1007 (2)	0.7139 (5)	0.1826 (2)	0.0326 (8)	0.931 (4)
H16	0.112992	0.728642	0.128086	0.039*	0.931 (4)
C17	0.0151 (2)	0.6907 (5)	0.1749 (2)	0.0361 (8)	0.931 (4)
H17	−0.032523	0.690595	0.114242	0.043*	0.931 (4)
C18	−0.0023 (2)	0.6679 (4)	0.2535 (3)	0.0328 (8)	0.931 (4)

H18	−0.061441	0.650549	0.247814	0.039*	0.931 (4)
C19	0.06845 (18)	0.6705 (4)	0.3424 (2)	0.0230 (7)	0.931 (4)
F1A	0.068 (3)	0.647 (5)	0.466 (2)	0.0361 (9)	0.069 (4)
Cl1A	0.2623 (17)	0.701 (4)	0.2830 (19)	0.0390 (3)	0.069 (4)
C14A	0.1464 (16)	0.672 (3)	0.366 (2)	0.0185 (7)	0.069 (4)
C15A	0.155 (2)	0.687 (8)	0.281 (3)	0.0244 (8)	0.069 (4)
C16A	0.078 (3)	0.687 (7)	0.200 (3)	0.0326 (8)	0.069 (4)
H16A	0.080506	0.698995	0.140011	0.039*	0.069 (4)
C17A	−0.002 (3)	0.669 (8)	0.206 (3)	0.0361 (8)	0.069 (4)
H17A	−0.054819	0.663755	0.150898	0.043*	0.069 (4)
C18A	−0.005 (3)	0.657 (6)	0.293 (3)	0.0328 (8)	0.069 (4)
H18A	−0.061667	0.648735	0.294035	0.039*	0.069 (4)
C19A	0.068 (2)	0.658 (6)	0.380 (2)	0.0230 (7)	0.069 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0333 (4)	0.0364 (4)	0.0268 (4)	−0.0097 (3)	0.0041 (3)	−0.0050 (3)
S2	0.0367 (4)	0.0245 (4)	0.0261 (3)	−0.0031 (3)	0.0158 (3)	0.0013 (3)
O1	0.0392 (12)	0.0314 (11)	0.0211 (9)	−0.0098 (9)	0.0061 (9)	0.0016 (8)
O2	0.0330 (11)	0.0240 (10)	0.0188 (9)	−0.0017 (8)	0.0091 (8)	−0.0026 (8)
C1	0.0195 (13)	0.0200 (13)	0.0167 (12)	0.0002 (11)	0.0080 (11)	0.0002 (10)
C1A	0.0195 (13)	0.0200 (13)	0.0167 (12)	0.0002 (11)	0.0080 (11)	0.0002 (10)
C2	0.0231 (14)	0.0188 (13)	0.0197 (12)	0.0000 (11)	0.0069 (11)	0.0005 (10)
C3	0.0216 (14)	0.0219 (13)	0.0227 (13)	0.0035 (11)	0.0085 (11)	0.0009 (11)
C4	0.0183 (13)	0.0193 (13)	0.0234 (13)	0.0021 (11)	0.0044 (11)	−0.0029 (11)
C5	0.0271 (16)	0.0265 (15)	0.0428 (17)	−0.0046 (13)	0.0102 (14)	−0.0078 (13)
C6	0.0267 (15)	0.0207 (14)	0.0433 (17)	−0.0006 (12)	0.0160 (14)	−0.0002 (12)
C7	0.0256 (15)	0.0238 (14)	0.0260 (13)	0.0024 (12)	0.0090 (12)	−0.0021 (11)
C8	0.0186 (13)	0.0226 (13)	0.0165 (12)	0.0017 (11)	0.0063 (11)	0.0018 (10)
C9	0.0158 (13)	0.0193 (13)	0.0187 (13)	0.0051 (11)	0.0030 (11)	0.0017 (10)
C10	0.0233 (14)	0.0171 (13)	0.0214 (13)	0.0019 (11)	0.0090 (11)	0.0025 (10)
C11	0.0451 (18)	0.0285 (16)	0.0260 (14)	0.0054 (14)	0.0184 (14)	0.0080 (12)
C12	0.0513 (19)	0.0312 (16)	0.0178 (13)	−0.0009 (14)	0.0157 (13)	0.0027 (11)
C13	0.0378 (17)	0.0260 (15)	0.0212 (13)	−0.0053 (13)	0.0066 (13)	−0.0003 (11)
F1	0.0400 (19)	0.0373 (17)	0.0408 (15)	0.0063 (11)	0.0263 (13)	0.0092 (11)
Cl1	0.0258 (6)	0.0652 (6)	0.0289 (5)	−0.0084 (5)	0.0141 (4)	−0.0055 (5)
C14	0.0194 (14)	0.0133 (13)	0.0198 (14)	0.0019 (11)	0.0049 (12)	0.0009 (10)
C15	0.0316 (17)	0.021 (2)	0.0197 (15)	0.0010 (14)	0.0093 (13)	0.0025 (12)
C16	0.047 (2)	0.0335 (19)	0.0164 (16)	0.0068 (16)	0.0118 (14)	0.0048 (13)
C17	0.035 (2)	0.045 (2)	0.0165 (17)	0.0075 (16)	−0.0020 (15)	0.0014 (15)
C18	0.0251 (16)	0.0401 (18)	0.0277 (19)	0.0020 (14)	0.0048 (17)	−0.0037 (18)
C19	0.0254 (16)	0.0236 (15)	0.0182 (16)	0.0024 (12)	0.0068 (14)	−0.0012 (13)
F1A	0.0400 (19)	0.0373 (17)	0.0408 (15)	0.0063 (11)	0.0263 (13)	0.0092 (11)
Cl1A	0.0258 (6)	0.0652 (6)	0.0289 (5)	−0.0084 (5)	0.0141 (4)	−0.0055 (5)
C14A	0.0194 (14)	0.0133 (13)	0.0198 (14)	0.0019 (11)	0.0049 (12)	0.0009 (10)
C15A	0.0316 (17)	0.021 (2)	0.0197 (15)	0.0010 (14)	0.0093 (13)	0.0025 (12)
C16A	0.047 (2)	0.0335 (19)	0.0164 (16)	0.0068 (16)	0.0118 (14)	0.0048 (13)

C17A	0.035 (2)	0.045 (2)	0.0165 (17)	0.0075 (16)	−0.0020 (15)	0.0014 (15)
C18A	0.0251 (16)	0.0401 (18)	0.0277 (19)	0.0020 (14)	0.0048 (17)	−0.0037 (18)
C19A	0.0254 (16)	0.0236 (15)	0.0182 (16)	0.0024 (12)	0.0068 (14)	−0.0012 (13)

Geometric parameters (Å, º)

S1—C5	1.703 (3)	C10—C13	1.375 (3)
S1—C4	1.731 (2)	C11—C12	1.357 (4)
S2—C11	1.700 (3)	C11—H11	0.9500
S2—C10	1.727 (2)	C12—C13	1.417 (3)
O1—C3	1.222 (3)	C12—H12	0.9500
O2—C9	1.226 (3)	C13—H13	0.9500
C1—C14	1.521 (3)	F1—C15	1.342 (5)
C1—C2	1.536 (3)	Cl1—C19	1.750 (3)
C1—C8	1.554 (3)	C14—C19	1.395 (4)
C1—H1	1.0000	C14—C15	1.395 (3)
C1A—C14A	1.529 (19)	C15—C16	1.368 (4)
C1A—C2	1.536 (3)	C16—C17	1.376 (5)
C1A—C8	1.554 (3)	C16—H16	0.9500
C1A—H1A	1.0000	C17—C18	1.368 (4)
C2—C3	1.520 (3)	C17—H17	0.9500
C2—H2A	0.9900	C18—C19	1.401 (4)
C2—H2B	0.9900	C18—H18	0.9500
C3—C4	1.465 (3)	F1A—C19A	1.341 (19)
C4—C7	1.369 (3)	Cl1A—C15A	1.75 (2)
C5—C6	1.350 (4)	C14A—C15A	1.390 (19)
C5—H5	0.9500	C14A—C19A	1.39 (2)
C6—C7	1.415 (4)	C15A—C16A	1.37 (2)
C6—H6	0.9500	C16A—C17A	1.36 (2)
C7—H7	0.9500	C16A—H16A	0.9500
C8—C9	1.507 (3)	C17A—C18A	1.36 (2)
C8—H8A	0.9900	C17A—H17A	0.9500
C8—H8B	0.9900	C18A—C19A	1.39 (2)
C9—C10	1.466 (3)	C18A—H18A	0.9500
C5—S1—C4	91.38 (13)	C13—C10—S2	110.85 (18)
C11—S2—C10	91.43 (12)	C9—C10—S2	119.83 (17)
C14—C1—C2	111.15 (19)	C12—C11—S2	113.1 (2)
C14—C1—C8	110.94 (19)	C12—C11—H11	123.4
C2—C1—C8	111.47 (19)	S2—C11—H11	123.4
C14—C1—H1	107.7	C11—C12—C13	111.8 (2)
C2—C1—H1	107.7	C11—C12—H12	124.1
C8—C1—H1	107.7	C13—C12—H12	124.1
C14A—C1A—C2	122.0 (10)	C10—C13—C12	112.8 (2)
C14A—C1A—C8	109.1 (9)	C10—C13—H13	123.6
C2—C1A—C8	111.47 (19)	C12—C13—H13	123.6
C14A—C1A—H1A	104.1	C19—C14—C15	113.4 (2)
C2—C1A—H1A	104.1	C19—C14—C1	123.9 (2)

C8—C1A—H1A	104.1	C15—C14—C1	122.7 (3)
C3—C2—C1	114.36 (19)	F1—C15—C16	115.5 (3)
C3—C2—C1A	114.36 (19)	F1—C15—C14	119.0 (3)
C3—C2—H2A	108.7	C16—C15—C14	125.5 (3)
C1—C2—H2A	108.7	C15—C16—C17	118.1 (3)
C3—C2—H2B	108.7	C15—C16—H16	121.0
C1—C2—H2B	108.7	C17—C16—H16	121.0
H2A—C2—H2B	107.6	C18—C17—C16	120.8 (3)
O1—C3—C4	121.5 (2)	C18—C17—H17	119.6
O1—C3—C2	122.5 (2)	C16—C17—H17	119.6
C4—C3—C2	116.1 (2)	C17—C18—C19	118.9 (3)
C7—C4—C3	129.7 (2)	C17—C18—H18	120.5
C7—C4—S1	110.67 (19)	C19—C18—H18	120.5
C3—C4—S1	119.58 (18)	C14—C19—C18	123.2 (3)
C6—C5—S1	112.9 (2)	C14—C19—Cl1	120.0 (2)
C6—C5—H5	123.6	C18—C19—Cl1	116.8 (2)
S1—C5—H5	123.6	C15A—C14A—C19A	127 (2)
C5—C6—C7	112.1 (2)	C15A—C14A—C1A	113 (3)
C5—C6—H6	124.0	C19A—C14A—C1A	119 (3)
C7—C6—H6	124.0	C16A—C15A—C14A	117 (3)
C4—C7—C6	113.0 (2)	C16A—C15A—Cl1A	125 (3)
C4—C7—H7	123.5	C14A—C15A—Cl1A	118 (3)
C6—C7—H7	123.5	C17A—C16A—C15A	120 (4)
C9—C8—C1	112.44 (19)	C17A—C16A—H16A	120.1
C9—C8—C1A	112.44 (19)	C15A—C16A—H16A	120.1
C9—C8—H8A	109.1	C18A—C17A—C16A	120 (5)
C1—C8—H8A	109.1	C18A—C17A—H17A	120.2
C9—C8—H8B	109.1	C16A—C17A—H17A	120.2
C1—C8—H8B	109.1	C17A—C18A—C19A	126 (5)
H8A—C8—H8B	107.8	C17A—C18A—H18A	116.8
O2—C9—C10	120.9 (2)	C19A—C18A—H18A	116.8
O2—C9—C8	121.3 (2)	F1A—C19A—C14A	122 (3)
C10—C9—C8	117.8 (2)	F1A—C19A—C18A	128 (4)
C13—C10—C9	129.3 (2)	C14A—C19A—C18A	110 (3)

C14—C1—C2—C3	165.2 (2)	C11—C12—C13—C10	0.2 (4)
C8—C1—C2—C3	−70.4 (2)	C2—C1—C14—C19	−127.6 (3)
C14A—C1A—C2—C3	158.3 (16)	C8—C1—C14—C19	107.8 (3)
C8—C1A—C2—C3	−70.4 (2)	C2—C1—C14—C15	52.4 (3)
C1—C2—C3—O1	−6.0 (3)	C8—C1—C14—C15	−72.2 (3)
C1A—C2—C3—O1	−6.0 (3)	C19—C14—C15—F1	−177.7 (3)
C1—C2—C3—C4	174.0 (2)	C1—C14—C15—F1	2.2 (5)
C1A—C2—C3—C4	174.0 (2)	C19—C14—C15—C16	0.9 (5)
O1—C3—C4—C7	173.8 (3)	C1—C14—C15—C16	−179.2 (3)
C2—C3—C4—C7	−6.1 (4)	F1—C15—C16—C17	178.4 (3)
O1—C3—C4—S1	−4.3 (3)	C14—C15—C16—C17	−0.2 (6)
C2—C3—C4—S1	175.73 (17)	C15—C16—C17—C18	−0.6 (5)
C5—S1—C4—C7	−0.1 (2)	C16—C17—C18—C19	0.8 (5)

C5—S1—C4—C3	178.4 (2)	C15—C14—C19—C18	−0.7 (4)
C4—S1—C5—C6	−0.3 (2)	C1—C14—C19—C18	179.3 (3)
S1—C5—C6—C7	0.5 (3)	C15—C14—C19—Cl1	178.5 (2)
C3—C4—C7—C6	−177.9 (2)	C1—C14—C19—Cl1	−1.4 (4)
S1—C4—C7—C6	0.4 (3)	C17—C18—C19—C14	0.0 (5)
C5—C6—C7—C4	−0.6 (3)	C17—C18—C19—Cl1	−179.3 (2)
C14—C1—C8—C9	−65.8 (3)	C2—C1A—C14A—C15A	55 (3)
C2—C1—C8—C9	169.78 (19)	C8—C1A—C14A—C15A	−78 (3)
C14A—C1A—C8—C9	−52.7 (15)	C2—C1A—C14A—C19A	−118 (2)
C2—C1A—C8—C9	169.78 (19)	C8—C1A—C14A—C19A	110 (2)
C1—C8—C9—O2	97.9 (3)	C19A—C14A—C15A—C16A	0 (7)
C1A—C8—C9—O2	97.9 (3)	C1A—C14A—C15A—C16A	−172 (4)
C1—C8—C9—C10	−81.2 (2)	C19A—C14A—C15A—Cl1A	−179 (3)
C1A—C8—C9—C10	−81.2 (2)	C1A—C14A—C15A—Cl1A	9 (5)
O2—C9—C10—C13	−178.8 (3)	C14A—C15A—C16A—C17A	−2 (8)
C8—C9—C10—C13	0.4 (4)	Cl1A—C15A—C16A—C17A	178 (4)
O2—C9—C10—S2	0.5 (3)	C15A—C16A—C17A—C18A	2 (8)
C8—C9—C10—S2	179.57 (17)	C16A—C17A—C18A—C19A	−2 (9)
C11—S2—C10—C13	−0.3 (2)	C15A—C14A—C19A—F1A	−179 (4)
C11—S2—C10—C9	−179.7 (2)	C1A—C14A—C19A—F1A	−8 (5)
C10—S2—C11—C12	0.4 (2)	C15A—C14A—C19A—C18A	0 (6)
S2—C11—C12—C13	−0.4 (3)	C1A—C14A—C19A—C18A	172 (3)
C9—C10—C13—C12	179.4 (2)	C17A—C18A—C19A—F1A	180 (5)
S2—C10—C13—C12	0.1 (3)	C17A—C18A—C19A—C14A	0 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Cl1	1.00	2.57	3.128 (3)	115
C1—H1···F1*A*	1.00	2.21	2.86 (5)	122
C2—H2*A*···Cl1*A*	0.99	2.31	2.91 (3)	118
C2—H2*A*···F1	0.99	2.32	2.898 (5)	116
C2—H2*B*···O2^{i}	0.99	2.48	3.417 (3)	157
C5—H5···Cl1*A*^{ii}	0.95	2.49	3.12 (3)	123
C8—H8*A*···Cl1*A*	0.99	2.35	3.01 (3)	123
C13—H13···O1	0.95	2.45	3.367 (3)	163
C16—H16···F1*A*^{iii}	0.95	2.50	3.35 (3)	149

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