Structural Characterization and Hirshfeld surface analysis of 4-(pentafluoro thio)-2-iodobenzonitrile

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Abstract

Herein, we report the crystal structure and Hirshfeld surface analysis of the title compound ($C_7F_5H_3N_1S_1$), a pentafluoro thio (SF_5) containing arene which was synthesized from 4-(pentafluorothio)benzonitrile and lithium tetramethylpiperidide following a variation to the standard approach. Our synthesis of the title compound features simple and mild conditions that allow direct access to trisubstituted SF_5 intermediates that have not been demonstrated using previous methods. The title compound was recrystallized by slow evaporation of a saturated solution in dicloromethane. The molecule displays a planar geometry for which the benzene ring is in the same plane of its 3 substituents. However, the pentafluorothio group is present in a staggered fashion relative to the ring and the two hydrogens ortho to the substituent. S—F bond lengths of the pentafluorothio group are unequal: the S1—F2$_{(eq)}$ bond facing the iodo moiety's side of the molecule have a longer distance (1.573 (2) Å) and wider angle as compared to the S1—F1$_{(eq)}$ bond (1.561 (4) Å) facing the side of the molecules with the two hydrogens. As expected, the longest sulfur-fluorine bond distance corresponded to the S1—F3$_{(ax)}$ bond, with a bond distance of 1.582 (5) Å. In-plane intermolecular interactions are observed between C—H···F and N···I propagating along the [001] direction, and out-of-plane ones are observed between F···C. According to the Hirshfeld plots, the principal intermolecular contacts on the title compound and their % contributions arise from F···H at 29.4%, F···I at 15.8%, F···N at 11.4%, F···F at 6.0%, N···I at 5.6%, and F···C at 4.5%.

0.0.1. Chemical context

Organic compounds containing the trifluoromethyl (CF_3) or pentafluorothio (SF_5) groups have an important role in organofluorine chemistry due to their special properties including low surface energy, hydrophobicity, high chemical resistance, high thermal stability, and high electronegativity (Kirsch *et al.*, 1999; Kirsch *et al.*, 2014; Iida *et al.*, 2015; Beier *et al.*, 2011). SF_5, coined as the 'super-trifluoromethyl' group, is often prefered to CF_3 as it is more electronegative, lipophilic, chemically stable and possesses a higher steric effect (Bowden *et al.*, 2000). Current interest in the field of drug discovery of fluorinated substituents resides in the possibility of improving both the metabolic stability and bioavailability of receptor binders upon the incorporation of susbtituents with one or more fluorine atoms (Altomonte *et al.*, 2014; Savoie *et al.* 2014; Sowaileh *et al.*, 2017). In fact, there are several blockbuster drugs displaying such group demonstrating the prominent role of the trifluoromethyl group in the area of drug discovery (O'Hagan, 2010; Muller *et al.*, 2007; Purser *et al.*, 2008). New molecules incorporating the SF_5 group are thus potential alternatives to already existing biologically active molecules containing the CF_3 substitution. Additionally, the SF_5's chemical robustness is explored in other areas such as polymer chemsitry (Zhou *et al.*, 2016). Despite its popularity, the crystallographic characterization of the title compound, an important precursor in organofluorine chemsitry, has not been reported, which is an important milestone in the synthesis of next generation materials containing this motif. Herein, we include a variation to the synthetic approach and details of its simple crystallization through slow evaporation methods, yielding X-ray diffraction quality single crystals.

The title compound illustrated in **Scheme 1** was obtained as part of our studies toward the synthesis of functionalized arenes containing the SF$_5$ moiety. Its synthesis involved a one-pot reaction in which the interaction of the cyano group in 4-(pentafluorothio)benzonitrile to the Lewis acidic lithium cation in lithium tetramethylpiperidide (LiTMP) allowed the deprotonation from the nearest ortho-position H on the arene. The SF$_5$-containing organolithium species was then quenched with iodine to yield the title compound. This reaction pathway was recently proposed by Iida *et al.* for the synthesis of SF$_5$-substituted zinc phthalocyanines (Iida *et al.*, 2015). We modified the synthesis by adding tetramethyl ethylenediamine (TMEDA), an amine additive that serves to break up the lithiated base aggregates, allowing for accelerated reactivity due to increased basicity. This variation improved the total yield of the title compound by 8%.

1. Structural commentary

Figure 1 shows the molecular structure of the title compound, which crystallizes in the space group *Pnma.* Its asymmetric unit consists of a single molecule lying on a mirror plane perpendicular to [010] containing the iodo, cyano, and the sulfur and axial fluorine of the pentafluorosulfanyl substituent in the plane of the molecule. Fluorine atoms from the penta fluorosulfany group at equatorial positions lie above and below the plane in a staggered fashion relative to the two hydrogens ortho to the substituent; of those, two of the four florine atoms are symmetrically generated by the mirror plane. The S1—F$_{(eq)}$ bond distances differ from each other depending on the side of the molecule the bond is located at (**Table 1**). Bond S1—F2$_{(eq)}$ and its symmetry analogue F2 $^i_{(eq)}$ (i= x, -y+3/2, z) are on the same side of the iodine and exhibit a longer bond distance of 1.573 (2) Å in comparison to S1—F1$_{(eq)}$ and its symmetry analogue F1 $^i_{(eq)}$ (i= x, -y+3/2, z) which are further away from the iodine and have a shorter bond length distance of 1.561 (4) Å. The S1—F3$_{(ax)}$ bond length of 1.582 (5) Å is consistent with that of similar structures (1.588 (2) Å and 1.573 (3) Å from Du *et al.*, 2016).

2. Supramolecular features

The packing of the compound is consolidated through a series of intermolecular interactions which can be classified as in-plane and out-of-plane (**Table 2**). Each molecule acts as a C—H donor through the hydrogen atoms in the ortho and meta positions of each phenyl ring counter to the iodine atom. Propagating along the plane perpendicular to [010], there are two C—H⋯F hydrogen bonds between adjacent molecules creating an in plane network, one from C5—H5⋯F3 and the other between C6—H6⋯F3 with a contact distance of 2.57 Å and 2.56 Å, respectively (**Figure 2**). Both H5 and H6 atoms are highly acidic due to the electron withdrawing effects of the -SF$_5$ and -CN substituents. Additionally, significant in-plane intermolecular interactions attributed to halogen bonding between N1⋯I1 from neighboring molecules is observed, with a contact length of 3.408 (1) Å (Metrangolo *et al.*, 2005). Out-of-plane intermolecular interactions arise primarily from F⋯π ring interactions at one of the corners of the ring (**Figure** 3). The F⋯π intermolecular contact occur between F2⋯C3 with a distance of 3.123 (1) Å along [010].

3. (Hirshfeld Surface Analysis)

Figure 4 shows the Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) for the title compound and **Figure 5** shows the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007), both performed with *CrystalExplorer17* (Turner *et al.*, 2017). Red spots on the Hirshfeld surface mapped over d$_{norm}$ in the coulour range of -0.4869 to 1.4157 arbitrary units confirm the previously mentioned main intermolecular contacts with additional ones, which include F⋯F, F⋯I, F⋯N, N⋯H, C⋯H, I⋯H, C⋯N, F⋯F, and I⋯I interactions. In the case of the title compound, the attributed individual contacts and their reciprocals account for the following percenteges: F⋯H/H ⋯F at 29.4% (Fig.5(b)), F⋯I/I⋯F at 15.8% (Fig.5(c)), F⋯N/N⋯F at 11.4% (Fig.5(d)), H⋯N/N⋯H at 6.3% (Fig.5(e)), I⋯N/N⋯I at 5.6% (Fig.5(f)), C⋯F/F⋯C at 4.5% (Fig.5(g)), C⋯H/H ⋯ C at 4.5% (Fig. 5(h)), I⋯H/H⋯I at 3.3% (Fig.5(i)), C⋯N/N⋯C at 1.6% (Fig.5(j)), C⋯C at 9.5% (Fig.5(k)), F⋯F at 6.0% (Fig.5(l)), and I⋯I at 2.2% (Fig.5(m))(**Table 3**). Thus, the Hirshfeld

surface analysis points out that the most significant contributions arise mainly from F ⋯ H and F ⋯ I intermolecular contacts.

4. Database survey

A search of the Cambridge Structural Database (Version 5.39, updated May 2017; Groom *et al.*, 2016) revealed no matching compounds with the title compound substructure and the three substituents. However, a search for SF_5-aryl compounds fragment revealed about 85 hits: 77 of these structures were reported in the last 10 years which shows the increasing interest in the SF_5 group. Most of these compounds are used as reagents in the synthesis and modification of pharmaceuticals, such as the antimalarial agent mefloquine (Wipf *et al.*, 2009). and the anti-obesity drug fenfluramine (Welch *et al.*, 2007).

5. Synthesis and crystallization

All solvents and reagents were purified prior to being used. 4-(Pentafluorothio)benzonitrile was commercially obtained and used without further purification. A solution of 2.5 M n-butyl lithium in hexanes was used. Column chromatography was carried out on a column packed with silica gel 70-230 mesh.

The synthesis of the title compound was performed through the regioselective ortho-lithiation of 4-(pentafluorothio) benzonitrile with lithium tetramethylpiperidide (LiTMP) in THF as solvent, favoring the formation of the ortho product (1,2,4-substituted arene) over the meta product (1,3,4-substituted arene). The ortho metalated product was subsequently quenched with I_2 to afford the iodinated trisubstituted arene. A dry 50 mL Schlenk tube was charged with 4 mL of dry THF and 300 μL of 2,2,6,6-tetramethyl piperidine (1.75 mmol, 2 eq.) and 262 μL of N,N,N,N- tetramethylethylendiamine (1.75 mmol) were added under inert atmosphere. The solution was cooled to 0°C and 700 μL of 2.5 M n-butyl lithium in hexane (1.75mmol, 2 eq.) were added slowly. The reaction mixture was stirred at 0 °C for 30 minutes and posteriorly cooled to -78 °C. A solution containing 200 mg of 4-(pentafluorothio)benzonitrile (0.872mmol, 1 eq.) in 4 mL THF was added dropwise: the solution progressed from a pale yellow to a dark brown upon formation of the metalated inter mediary. After stirring for 1 hour at -78 °C, a solution of 244 mg I_2 (0.960mmol, 1.2 eq.) in 4 mL THF was added dropwise and stirred for 2 hours. The mixture was then warmed to room temperature and stirred for 1 hour.

The reaction was quenched with water and THF was removed under reduced pressure, followed by extraction with di ethyl ether. The combined organic phase was washed with aqueous 0.1 M HCl, 0.1 M $Na_2S_2O_3$ and brine, then dried over $MgSO_4$. The crude product was purified by column chromatography (9:1, hexane: ethyl acetate) to yield 71 mg (46%) of pure arene product as a yellow solid (m.p. 94-96 °C). Block-like yellow crystals suitable for X-ray diffraction were obtained by slow evaporation of a saturated solution a CH_2Cl_2 solution of the 4-(pentafluorothio)-2-iodobenzonitrile at room temperature over a period of four days. NMR analyses were performed on a Bruker AV-500 spectrometer using chloroform-d as solvent ($CDCl_3$). The solvent signals at 7.26 and 77.00 ppm were used as internal standards for proton and carbon, respectively. ^1H NMR (500 MHz, Chloroform-d) d 8.31 (d, J = 2.1 Hz, 1H), 7.89 (dd, J = 8.6, 2.1 Hz, 1H), 7.75 (d, J = 8.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) d, 98.22, 117.83, 124.10, 126.16, 134.39, 136.82, 156.15.

6. Refinement

Data collection, crystal data and structure refinement parameters are summarized in **Table 4**. H atoms were included in geometrically calculated positions for the aryl carbon atoms and refined as riding atoms with C—H = 0.93 Å and U_{iso}(H) $1.2U_{eq}$(C).

F1 and F2 atoms from the SF_5 substituent have symmetry related counterparts at x, -y+3/2, z generated by a mirror plane perpendicular to [010].

Table 1

Selected bond lenghts and distances

Atoms	Distance (Å) and angles (°)
S1-F1$_{(eq)}$ and S1-F1$^i_{(eq)}$	1.561 (4)
S1-F2$_{(eq)}$ and S1-F2$^i_{(eq)}$	1.573 (2)
S1-F3$_{(ax)}$	1.582 (5)
C4-S1-F2$_{(eq)}$	[92.02 (19)]
C4-S1-F1$_{(eq)}$	[92.16 (2)]

Symmetry codes: (i) x, -y+3/2, z

Table 2

Hydrogen-bond and short contacts geometry (Å, °)

D-H⋯A/D⋯A	D-H	H⋯A	D⋯A	D-H⋯A
C5-H5⋯F3	0.93	2.57	3.501 (1)	174
F2⋯C3	-	-	3.123 (1)	-
C6-H6⋯F3	0.93	2.56	3.476 (1)	169
N1⋯I1	-	-	3.408 (1)	-

Table 3

Percentage contributions of interatomic contacts to the Hirshfeld surface

Contact	% contribution	Contact	% contribution
F⋯H/ H⋯F	29.4	C⋯C	9.5
F⋯I / I⋯F	15.8	F⋯F	6.0
F⋯N / N⋯F	11.4	I⋯I	2.2
H⋯N/ N⋯H	6.3		
I⋯N/ N⋯I	5.6		
C⋯F/ F⋯C	4.5		
C⋯H/ H⋯C	4.5		
I⋯H/ H⋯I	3.3		
C⋯N/ N⋯C	1.6		

Table 4

Experimental details

Crystal data	
Chemical formula	$C_7H_3F_5INS$
M_r	355.06
Crystal system, space group	Orthorhombic, *Pnma*
Temperature (K)	300
a, b, c (Å)	8.0634 (1), 7.7088 (1), 16.4410 (3)
V (Å^3)	1021.96 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	26.99
Crystal size (mm)	0.26 × 0.17 × 0.12

Data collection

Diffractometer	SuperNova, Single source at offset/far, HyPix3000
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.39.46 (Rigaku Oxford Diffraction, 2018) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.287, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9403, 1020, 953
R_{int}	0.082
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.605

Refinement

$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.111, 1.03
No. of reflections	1020
No. of parameters	85
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.74, −1.77

Computer programs: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018), ShelXT (Sheldrick, 2015), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009).

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Figure 1

Molecular structure of the title compound, including atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Atoms symmetrically generated by the mirror plane (symmetry code: (i) x, -y+3/2, z) are depicted in dark green.

Figure 2

In plane contacts. A view along the a axis of crystal packing of the title compound, with short contact interactions shown as dashed lines.

Figure 3

Out of plane contacts. Partial view along the b axis of the title compound's crystal packing; F···π interactions are shown as dashed lines.

Figure 4

A view of the Hirshfeld surface of the title compound mapped over d_{norm} with the four main intermolecular contacts in the crystal lattice.

Figure 5

Full (a) and individual (b-m) two dimensional fingerprint plots showing the 12 intermolecular contacts present in the crystal lattice.

supporting information

Structural Characterization and Hirshfeld surface analysis of 4-(pentafluoro thio)-2-iodobenzonitrile

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Computing details

Data collection: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); data reduction: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); program(s) used to solve structure: ShelXT (Sheldrick, 2015); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

4-(pentafluorothio)-2-iodo-benzonitrile

Crystal data

$C_7H_3F_5INS$	$D_x = 2.308$ Mg m^{-3}
$M_r = 355.06$	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Orthorhombic, *Pnma*	Cell parameters from 6922 reflections
$a = 8.0634$ (1) Å	$\theta = 2.7–68.4°$
$b = 7.7088$ (1) Å	$\mu = 26.99$ mm^{-1}
$c = 16.4410$ (3) Å	$T = 300$ K
$V = 1021.96$ (3) Å^3	Irregular, clear light yellow
$Z = 4$	$0.26 \times 0.17 \times 0.12$ mm
$F(000) = 664$	

Data collection

SuperNova, Single source at offset/far, HyPix3000 diffractometer	9403 measured reflections
	1020 independent reflections
ω scans	953 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan *CrysAlis PRO* 1.171.39.46 (Rigaku Oxford Diffraction, 2018) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	$R_{int} = 0.082$
	$\theta_{max} = 68.8°$, $\theta_{min} = 5.4°$
	$h = -9 \rightarrow 9$
	$k = -9 \rightarrow 9$
	$l = -19 \rightarrow 19$
$T_{min} = 0.287$, $T_{max} = 1.000$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.111$	$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 1.8371P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	
1020 reflections	$(\Delta/\sigma)_{max} < 0.001$
85 parameters	$\Delta\rho_{max} = 0.74$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -1.77$ 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. ShelXL

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for (dpc149)

	x	y	z	U_{iso}*/U_{eq}
I1	0.67725 (6)	0.750000	0.31142 (3)	0.0540 (3)
S1	0.97572 (19)	0.750000	0.62917 (9)	0.0398 (4)
F3	1.1407 (6)	0.750000	0.6812 (3)	0.0641 (14)
F2	1.0576 (4)	0.6065 (5)	0.5743 (2)	0.0641 (9)
F1	0.9063 (5)	0.8925 (6)	0.68738 (19)	0.0819 (13)
C4	0.7869 (8)	0.750000	0.5682 (4)	0.0356 (13)
C3	0.8020 (7)	0.750000	0.4841 (4)	0.0335 (13)
H3	0.905856	0.750000	0.459508	0.040*
C2	0.6572 (8)	0.750000	0.4373 (4)	0.0352 (13)
C1	0.5034 (8)	0.750000	0.4752 (4)	0.0467 (16)
C7	0.3514 (9)	0.750000	0.4290 (5)	0.056 (2)
C5	0.6348 (10)	0.750000	0.6059 (5)	0.065 (3)
H5	0.628167	0.750000	0.662401	0.078*
N1	0.2295 (10)	0.750000	0.3943 (6)	0.080 (2)
C6	0.4948 (10)	0.750000	0.5606 (5)	0.072 (3)
H6	0.391926	0.750000	0.586180	0.087*

Atomic displacement parameters ($Å^2$) for (dpc149)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0575 (4)	0.0786 (4)	0.0259 (3)	0.000	−0.00566 (16)	0.000
S1	0.0409 (8)	0.0534 (9)	0.0250 (8)	0.000	−0.0044 (6)	0.000
F3	0.055 (3)	0.097 (4)	0.040 (3)	0.000	−0.020 (2)	0.000
F2	0.0622 (18)	0.0697 (19)	0.0605 (18)	0.0256 (16)	−0.0188 (15)	−0.0192 (17)
F1	0.081 (3)	0.110 (3)	0.055 (2)	0.022 (2)	−0.0146 (16)	−0.044 (2)
C4	0.038 (3)	0.045 (3)	0.024 (3)	0.000	−0.002 (3)	0.000
C3	0.037 (3)	0.038 (3)	0.026 (3)	0.000	0.000 (2)	0.000
C2	0.047 (4)	0.033 (3)	0.025 (3)	0.000	−0.003 (2)	0.000
C1	0.038 (3)	0.066 (4)	0.036 (4)	0.000	−0.003 (3)	0.000
C7	0.046 (4)	0.081 (6)	0.042 (5)	0.000	−0.004 (3)	0.000
C5	0.047 (4)	0.121 (8)	0.027 (4)	0.000	0.002 (3)	0.000
N1	0.049 (4)	0.121 (7)	0.071 (5)	0.000	−0.016 (4)	0.000
C6	0.036 (4)	0.139 (9)	0.042 (4)	0.000	0.014 (3)	0.000

Geometric parameters (Å, °) for (dpc149)

I1—C2	2.076 (6)	C3—H3	0.9300
S1—F3	1.582 (5)	C3—C2	1.399 (8)
S1—F2	1.572 (3)	C2—C1	1.388 (9)
S1—F2[i]	1.572 (3)	C1—C7	1.442 (10)
S1—F1[i]	1.561 (4)	C1—C6	1.406 (11)

S1—F1	1.561 (4)	C7—N1	1.136 (10)
S1—C4	1.823 (7)	C5—H5	0.9300
C4—C3	1.388 (9)	C5—C6	1.353 (11)
C4—C5	1.374 (10)	C6—H6	0.9300
F3—S1—C4	179.4 (3)	C5—C4—C3	121.8 (6)
F2ⁱ—S1—F3	87.52 (18)	C4—C3—H3	120.8
F2—S1—F3	87.52 (18)	C4—C3—C2	118.4 (6)
F2ⁱ—S1—F2	89.4 (3)	C2—C3—H3	120.8
F2—S1—C4	92.04 (19)	C3—C2—I1	118.9 (5)
F2ⁱ—S1—C4	92.04 (19)	C1—C2—I1	121.2 (5)
F1ⁱ—S1—F3	88.3 (2)	C1—C2—C3	119.9 (6)
F1—S1—F3	88.3 (2)	C2—C1—C7	121.6 (6)
F1—S1—F2ⁱ	90.4 (2)	C2—C1—C6	119.5 (6)
F1—S1—F2	175.8 (2)	C6—C1—C7	118.9 (7)
F1ⁱ—S1—F2	90.4 (2)	N1—C7—C1	178.4 (9)
F1ⁱ—S1—F2ⁱ	175.8 (2)	C4—C5—H5	120.1
F1ⁱ—S1—F1	89.5 (4)	C6—C5—C4	119.8 (7)
F1ⁱ—S1—C4	92.2 (2)	C6—C5—H5	120.1
F1—S1—C4	92.2 (2)	C1—C6—H6	119.7
C3—C4—S1	118.3 (5)	C5—C6—C1	120.6 (7)
C5—C4—S1	119.8 (5)	C5—C6—H6	119.7
I1—C2—C1—C7	0.000 (2)	F1ⁱ—S1—C4—C5	44.79 (18)
I1—C2—C1—C6	180.000 (2)	C4—C3—C2—I1	180.000 (1)
S1—C4—C3—C2	180.000 (2)	C4—C3—C2—C1	0.000 (2)
S1—C4—C5—C6	180.000 (2)	C4—C5—C6—C1	0.000 (3)
F2—S1—C4—C3	−44.74 (15)	C3—C4—C5—C6	0.000 (3)
F2ⁱ—S1—C4—C3	44.74 (15)	C3—C2—C1—C7	180.000 (2)
F2ⁱ—S1—C4—C5	−135.26 (15)	C3—C2—C1—C6	0.000 (2)
F2—S1—C4—C5	135.26 (15)	C2—C1—C6—C5	0.000 (3)
F1ⁱ—S1—C4—C3	−135.21 (18)	C7—C1—C6—C5	180.000 (2)
F1—S1—C4—C3	135.21 (18)	C5—C4—C3—C2	0.000 (2)
F1—S1—C4—C5	−44.79 (18)		

Symmetry code: (i) *x*, −*y*+3/2, *z*.

Non-covalent intermolecular interaction lenghts (in Armstrongs)

N(1) — I(1)	F(2) — C(3)	F(3) — H(5)	F(3) — H(6)
3.408	3.123	2.573	2.558

Selected bond lenghts and distances

Atoms	Distance (Å) and angles (°)
S1-F1$_{(eq)}$ and S1-F1ⁱ$_{(eq)}$	1.561 (4)
S1-F2$_{(eq)}$ and S1-F2ⁱ$_{(eq)}$	1.573 (2)
S1-F3$_{(ax)}$	1.582 (5)
C4-S1-F2$_{(eq)}$	[92.02 (19)]
C4-S1-F1$_{(eq)}$	[92.16 (2)]

Symmetry codes: (i) x, -y+3/2, z

Hydrogen-bond and short contacts geometry (Å, °)

D-H···A/D···A	D-H	H···A	D···A	D-H···A
C5-H5···F3	0.93	2.57	3.501 (1)	174
F2···C3	-	-	3.123 (1)	-
C6-H6···F3	0.93	2.56	3.476 (1)	169
N1···I1	-	-	3.408 (1)	-

Percentage contributions of interatomic contacts to the Hirshfeld surface

Contact	% contribution	Contact	% contribution
F···H/ H···F	29.4	C···C	9.5
F···I / I···F	15.8	F···F	6.0
F···N / N···F	11.4	I···I	2.2
H···N/ N···H	6.3		
I···N/ N···I	5.6		
C···F/ F···C	4.5		
C···H/ H···C	4.5		
I···H/ H···I	3.3		
C···N/ N···C	1.6		