

Structural characterization and Hirshfeld surface analysis of 2-iodo-4-(pentafluoro- λ^6 -sulfanyl)-benzonitrile

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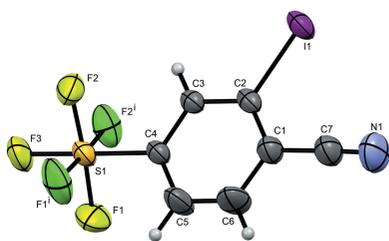
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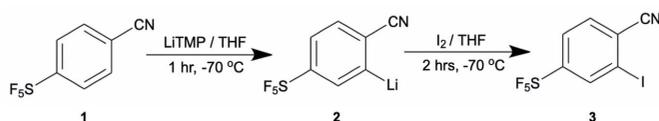
The title compound, C₇H₃F₅INS, a pentafluorosulfanyl (SF₅) containing arene, was synthesized from 4-(pentafluorosulfanyl)benzonitrile and lithium tetramethylpiperidide following a variation to the standard approach, which features simple and mild conditions that allow direct access to tri-substituted SF₅ intermediates that have not been demonstrated using previous methods. The molecule displays a planar geometry with the benzene ring in the same plane as its three substituents. It lies on a mirror plane perpendicular to [010] with the iodo, cyano, and the sulfur and axial fluorine atoms of the pentafluorosulfanyl substituent in the plane of the molecule. The equatorial F atoms have symmetry-related counterparts generated by the mirror plane. The pentafluorosulfanyl group exhibits a staggered fashion relative to the ring and the two hydrogen atoms *ortho* to the substituent. S—F bond lengths of the pentafluorosulfanyl group are unequal: the equatorial bond facing the iodo moiety has a longer distance [1.572 (3) Å] and wider angle compared to that facing the side of the molecules with two hydrogen atoms [1.561 (4) Å]. As expected, the axial S—F bond is the longest [1.582 (5) Å]. In the crystal, in-plane C—H···F and N···I interactions as well as out-of-plane F···C interactions are observed. According to the Hirshfeld analysis, the principal intermolecular contacts for the title compound are F···H (29.4%), F···I (15.8%), F···N (11.4%), F···F (6.0%), N···I (5.6%) and F···C (4.5%).

1. Chemical context

Organic compounds containing the trifluoromethyl (CF₃) or pentafluorothio (or pentafluoro- λ^6 -sulfanyl, SF₅) groups play an important role in organofluorine chemistry because of their special properties including low surface energy, hydrophobicity, high chemical resistance, high thermal stability and high electronegativity (Kirsch *et al.*, 1999, 2014; Iida *et al.*, 2015; Beier *et al.*, 2011). SF₅, coined as the ‘super-trifluoromethyl’ group, is often preferred to CF₃ as it is more electronegative, lipophilic and chemically stable, and possesses a higher steric effect (Bowden *et al.*, 2000). The current interest in the field of drug discovery of fluorinated substituents is based on the possibility of improving both the metabolic stability and bioavailability of receptor binders upon the incorporation of substituents with one or more fluorine atoms (Altomonte *et al.*, 2014; Savoie & Welch, 2015; Sowaileh *et al.*, 2017). In fact, several blockbuster drugs include such a group, demonstrating the prominent role of the trifluoromethyl group in the area of drug discovery (O’Hagan, 2010; Müller *et al.*, 2007; Purser *et al.*, 2008). New molecules incorporating the SF₅ group are thus potential alternatives to already existing biologically active molecules containing the CF₃ substitution.



Additionally, the chemical robustness of SF₅ has been explored in other areas such as polymer chemistry (Zhou *et al.*, 2016). Despite the popularity of the title compound, an important precursor in organofluorine chemistry, its crystallographic characterization, which is an important milestone in the synthesis of next-generation materials containing this motif, has not been reported. Herein, we describe a variation to the synthetic approach and give details of its simple crystallization through slow evaporation methods, yielding X-ray diffraction-quality single crystals.



The title compound was obtained as part of our studies toward the synthesis of functionalized arenes containing the SF₅ moiety. Its synthesis involves a one-pot reaction in which the interaction of the cyano group in 4-(pentafluorosulfanyl)benzonitrile to the Lewis acidic lithium cation in lithium tetramethylpiperidide (LiTMP) allows deprotonation from the nearest *ortho*-H atom on the arene. The SF₅-containing organolithium species is then quenched with iodine to yield the title compound. This reaction pathway was proposed by Iida *et al.* (2015) for the synthesis of SF₅-substituted zinc phthalocyanines. We modified the synthesis by adding tetramethylethylenediamine (TMEDA), an amine additive that serves to break up the lithiated base aggregates, allowing for accelerated reactivity because of the increased basicity. This variation improves the total yield of the title compound by 8%.

2. Structural commentary

Fig. 1 shows the molecular structure of the title compound, which crystallizes in the space group *Pnma*. Its asymmetric unit comprises a single molecule lying on a mirror plane perpendicular to [010] with the iodo, cyano, and the sulfur and

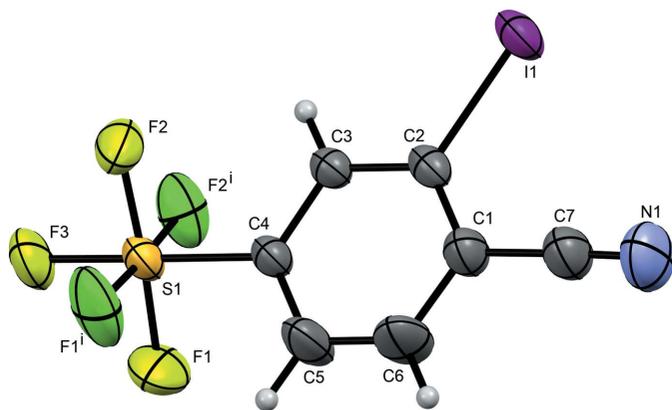


Figure 1
Molecular structure of the title compound, including atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Atoms generated by the mirror plane [symmetry code: (i) $x, -y + \frac{3}{2}, z$] are depicted in dark green.

Table 1
Selected bond lengths and angles.

S1—F1 _(eq) and S1—F1 ⁱ _(eq)	1.561 (4)
S1—F2 _(eq) and S1—F2 ⁱ _(eq)	1.572 (3)
S1—F3 _(ax)	1.582 (5)
C4—S1—F2 _(eq)	92.0 (2)
C4—S1—F1 _(eq)	92.2 (2)

Symmetry code: (i) $x, -y + \frac{3}{2}, z$.

axial fluorine atoms of the pentafluorosulfanyl substituent in the plane of the molecule. The fluorine atoms of the pentafluorosulfanyl group in the equatorial positions lie above and below the plane in a staggered fashion relative to the two hydrogen atoms *ortho* to the substituent; of those, two of the four fluorine atoms are generated symmetrically by the mirror plane. The S1—F_(eq) bond distances differ from each other depending on which side of the molecule the bond is located (Table 1). The S1—F2_(eq) bond and its symmetry equivalent S1—F2ⁱ_(eq) [symmetry code: (i) $x, -y + \frac{3}{2}, z$] are on the same side as the iodine atom and exhibit a longer bond distance of 1.572 (3) Å in comparison to S1—F1_(eq) and S1—F1ⁱ_(eq), 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 the longest and is consistent with those in similar structures [1.588 (2) and 1.573 (3) Å; Du *et al.*, 2016].

3. Supramolecular features

The packing of the title compound is consolidated through a series of intermolecular interactions, which can be classified as being in-plane and out-of-plane (Table 2). Each molecule acts as a C—H donor through the *meta*- and *para*-hydrogen atoms of the phenyl ring counter to the iodine atom. Two C—H...F

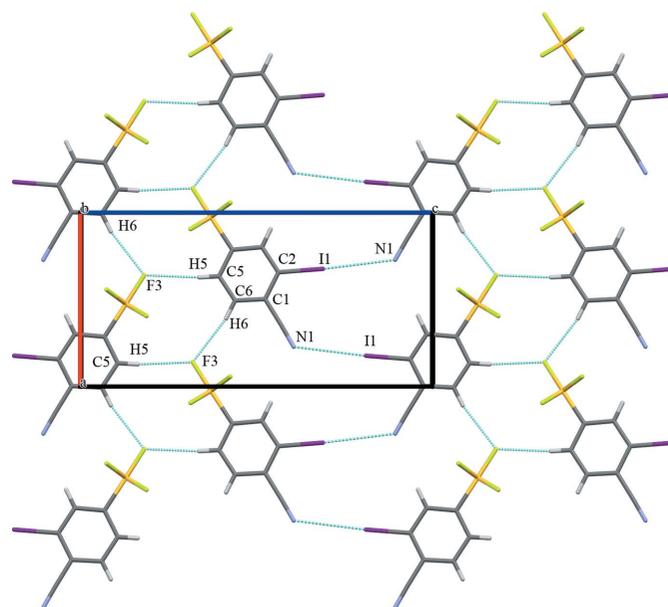


Figure 2
In plane contacts. A view along the *b* axis of crystal packing of the title compound, with short-contact interactions shown as dashed lines.

Table 2
 Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C5–H5···F3 ⁱ	0.93	2.57	3.501 (1)	174
C6–H6···F3 ⁱⁱ	0.93	2.56	3.476 (1)	169

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

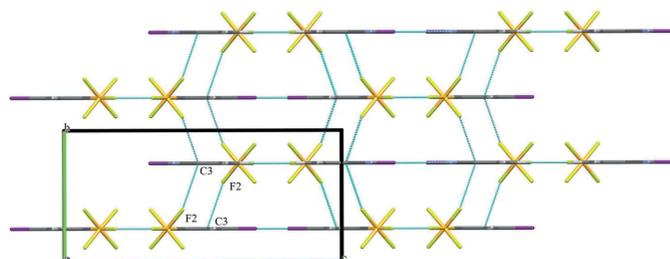
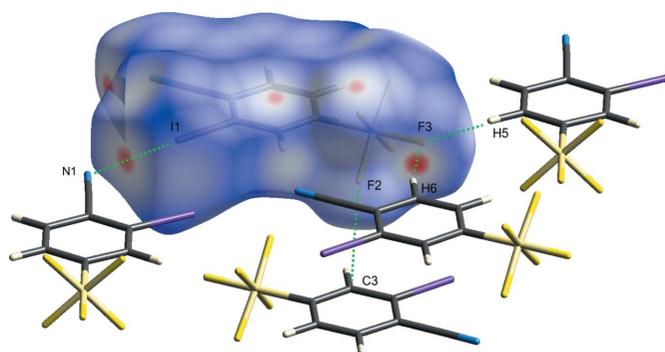
hydrogen bonds, C5–H5···F3 and C6–H6···F3 with H···F distances of 2.5 and 2.6 Å, respectively, create an in-plane network (Table 2 and Fig. 2). Both the H5 and H6 atoms are highly acidic because of the electron-withdrawing effects of the –SF₅ and –CN substituents. Additionally, significant in-plane halogen-bonding interactions [N1···I1($\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} - z$) = 3.408 (10) Å] are observed (Metrangolo *et al.*, 2005). Out-of-plane intermolecular interactions arise primarily from F··· π ring interactions at one of the ‘corners’ of the ring (Fig. 3) with an F2···C3($2 - x, -\frac{1}{2} + y, 1 - z$) distance of 3.124 (5) Å.

4. Hirshfeld surface analysis

The Hirshfeld surface (Spackman & Jayatilaka, 2009) for the title compound mapped over d_{norm} is shown in Fig. 4 while Fig. 5 shows the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007), both generated with *Crystal-Explorer17* (Turner *et al.*, 2017). Red spots on the Hirshfeld surface mapped over d_{norm} in the colour range –0.4869 to 1.4157 arbitrary units confirm the previously mentioned main intermolecular contacts. The fingerprint plots are given for all contacts and those delineated into F···H/H···F (29.4%; Fig. 5b), F···I/I···F (15.8%; Fig. 5c), F···N/N···F (11.4%; Fig. 5d), H···N/N···H (6.3%; Fig. 5e), I···N/N···I (5.6%; Fig. 5f), C···F/F···C (4.5%; Fig. 5g), C···H/H···C (4.5%; Fig. 5h), I···H/H···I (3.3%; Fig. 5i), C···N/N···C (1.6%; Fig. 5j), C···C (9.5%; Fig. 5k), F···F (6.0%; Fig. 5l) and I···I (2.2%; Fig. 5m) interactions. Thus, the Hirshfeld surface analysis indicates that the most significant contributions arise from F···H and F···I contacts.

5. 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

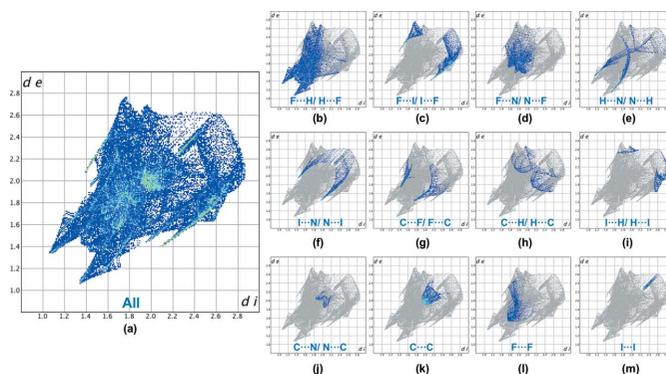

Figure 3
 Out-of-plane contacts. Partial packing diagram for the title compound viewed along the *a* axis. F··· π interactions are shown as dashed lines.

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.

three substituents. However, a search for SF₅ 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 SF₅ 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).

6. Synthesis and crystallization

All solvents and reagents were purified prior to being used. 4-(Pentafluorosulfanyl)benzotrile was obtained commercially 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-(pentafluorosulfanyl)benzotrile with lithium tetramethylpiperidide (LiTMP) in THF as solvent, favouring 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 I₂ to afford the iodinated trisubstituted arene. A dry 50 mL Schlenk tube was charged with 4 mL of dry THF and 300 μ L of 2,2,6,6-tetramethyl piperidine (1.75 mmol, 2 eq.) and 262 μ L of *N,N,N,N*-tetramethylethylenediamine (1.75 mmol) were added under an inert atmosphere. The


Figure 5
 Full (a) and individual (b)–(m) two-dimensional fingerprint plots showing the 12 intermolecular contacts present in the crystal structure.

solution was cooled to 273 K and 700 μL of 2.5 M *n*-butyl lithium in hexane (1.75 mmol, 2 eq.) were added slowly. The reaction mixture was stirred at 273 K for 30 minutes and then cooled to 195 K. A solution containing 200 mg of 4-(pentafluorosulfanyl)benzotrile (0.872 mmol, 1 eq.) in 4 mL THF was added dropwise: the solution changed from pale yellow to dark brown upon formation of the metalated intermediary. After stirring for 1 h at 195 K, a solution of 244 mg I_2 (0.960 mmol, 1.2 eq.) in 4 mL THF was added dropwise and stirred for 2 h. The mixture was then warmed to room temperature and stirred for 1 h.

The reaction was quenched with water and THF was removed under reduced pressure, followed by extraction with diethyl ether. The combined organic phase was washed with aqueous 0.1 M HCl, 0.1 M $\text{Na}_2\text{S}_2\text{O}_3$ 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 the pure arene product as a yellow solid (m.p. 367–369 K). Block-like yellow crystals suitable for X-ray diffraction were obtained by slow evaporation of a saturated CH_2Cl_2 solution of the 2-iodo-4-(pentafluoro- λ^6 -sulfanyl)benzotrile 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*) δ 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) δ , 98.22, 117.83, 124.10, 126.16, 134.39, 136.82, 156.15.

7. Refinement

Data collection, crystal data and structure refinement parameters are summarized in Table 3. H atoms were included in geometrically calculated positions and refined as riding atoms with $\text{C}-\text{H} = 0.93$ Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Funding information

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Table 3
Experimental details.

Crystal data	
Chemical formula	$\text{C}_7\text{H}_3\text{F}_5\text{INS}$
M_r	355.06
Crystal system, space group	Orthorhombic, <i>Pnma</i>
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 (<i>CrysAlis PRO</i> ; Rigaku OD, 2018)
$T_{\text{min}}, T_{\text{max}}$	0.287, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9403, 1020, 953
R_{int}	0.082
$(\sin \theta/\lambda)_{\text{max}}$ (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
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.74, -1.78

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

Acta Cryst. (2020). E76, 231-234 [https://doi.org/10.1107/S2056989020000365]

Structural characterization and Hirshfeld surface analysis of 2-iodo-4-(pentafluoro- λ^6 -sulfanyl)benzotrile

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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: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

2-Iodo-4-(pentafluoro- λ^6 -sulfanyl)benzotrile

Crystal data

$C_7H_3F_5INS$

$M_r = 355.06$

Orthorhombic, *Pnma*

$a = 8.0634$ (1) Å

$b = 7.7088$ (1) Å

$c = 16.4410$ (3) Å

$V = 1021.96$ (3) Å³

$Z = 4$

$F(000) = 664$

$D_x = 2.308$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 6922 reflections

$\theta = 2.7$ – 68.4°

$\mu = 26.99$ mm⁻¹

$T = 300$ K

Irregular, clear light yellow

$0.26 \times 0.17 \times 0.12$ mm

Data collection

SuperNova, Single source at offset/far,

HyPix3000

diffractometer

ω scans

Absorption correction: multi-scan

(*CrysAlisPro*; Rigaku OD, 2018)

$T_{\min} = 0.287$, $T_{\max} = 1.000$

9403 measured reflections

1020 independent reflections

953 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.082$

$\theta_{\max} = 68.8^\circ$, $\theta_{\min} = 5.4^\circ$

$h = -9 \rightarrow 9$

$k = -9 \rightarrow 9$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.111$

$S = 1.03$

1020 reflections

85 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 1.8371P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.74$ e Å⁻³

$\Delta\rho_{\min} = -1.77$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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 (\AA , $^\circ$)

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)
F2 ⁱ —S1—F3	87.52 (18)	C4—C3—H3	120.8
F2—S1—F3	87.52 (18)	C4—C3—C2	118.4 (6)
F2 ⁱ —S1—F2	89.4 (3)	C2—C3—H3	120.8
F2—S1—C4	92.04 (19)	C3—C2—I1	118.9 (5)
F2 ⁱ —S1—C4	92.04 (19)	C1—C2—I1	121.2 (5)
F1 ⁱ —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—F2 ⁱ	90.4 (2)	C2—C1—C6	119.5 (6)
F1—S1—F2	175.8 (2)	C6—C1—C7	118.9 (7)
F1 ⁱ —S1—F2	90.4 (2)	N1—C7—C1	178.4 (9)
F1 ⁱ —S1—F2 ⁱ	175.8 (2)	C4—C5—H5	120.1
F1 ⁱ —S1—F1	89.5 (4)	C6—C5—C4	119.8 (7)
F1 ⁱ —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)	F1 ⁱ —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)
F2 ⁱ —S1—C4—C3	44.74 (15)	C3—C2—C1—C7	180.000 (2)
F2 ⁱ —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)
F1 ⁱ —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) $x, -y+3/2, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5 \cdots F3 ⁱⁱ	0.93	2.57	3.501 (1)	174
C6—H6 \cdots F3 ⁱⁱⁱ	0.93	2.56	3.476 (1)	169

Symmetry codes: (ii) $x-1/2, -y+3/2, -z+3/2$; (iii) $x-1, -y+3/2, z$.

Non-covalent intermolecular interactions (Å)

N1—I1	3.408	F2—C3'	3.408
F3—H5	3.123	F3—H6	2.573, 2.558

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

<i>D—H...A/D...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
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		