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Crystal structure of 4-bromo-3-[(5-bromothiophen-2-yl)methylidene]-2-(dicyanomethylidene)-5,6-difluoro-2,3-dihydroinden-1-one

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Keywords: crystal structure; dicyanomethylene indenone; bromothiophene; pi-conjugated system; halogen bond (Br···O); C—H···N hydrogen bond.

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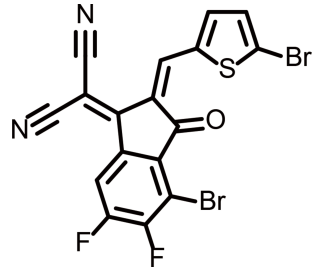
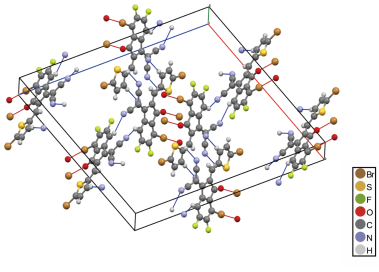
In the molecular structure of the title compound, $C_{17}H_4Br_2F_2N_2OS$, the indenone moiety is close to planar [the dihedral angle between the phenyl and the five-membered ring plane is 4.2 (4)°], and the thiophene ring is only slightly inclined to this fragment. In the extended structure, a short Br···O contact considered as a halogen bond and a weak C—H···N interaction contribute to the crystal packing.

1. Chemical context

Polyhalogenation is a convenient strategy for tuning the properties of π-conjugated organic building blocks, because halogen substituents can be introduced without altering the underlying conjugated framework while still allowing systematic modulation of the electronic structure and crystal packing (Baker *et al.*, 2012; Facchetti, 2011). In particular, combinations of heavier and lighter halogens (*e.g.* Br and F) can influence the molecular electrostatic potential and polarizability, and may facilitate directional intermolecular contacts, including halogen bonding, which contribute to the definition of packing motifs (Metrangolo & Resnati, 2001; Cavallo *et al.*, 2016; Desiraju *et al.*, 2013). Such effects are especially relevant for donor···acceptor-type conjugated molecules, in which optical and charge-transport properties can be sensitive to subtle changes in the intermolecular arrangement (Coropceanu *et al.*, 2007; Sirringhaus, 2014).



The title compound, $C_{17}H_4Br_2F_2N_2OS$, comprises an electron-withdrawing dicyanomethylene fragment and a carbonyl group within a conjugated indanone-based framework, together with a multi-halogenated substitution pattern that is frequently employed in the design of electron-deficient chromophores (Lin & Zhan, 2016). Although no device performance data are reported here, determination of the crystal structure is useful for assessing the conformational prefer-



ences of the conjugated skeleton and for identifying the intermolecular contacts promoted by the Br/F substitution.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The molecule consists of a dicyanomethylene-substituted 2,3-dihydro-1*H*-inden-1-one (indenone) unit that is connected to a 5-bromothiophene ring through an exocyclic C═C linkage involving atoms C1, C10 and C12. In the resulting π-conjugated molecule, the indenone carbonyl group and the dicyanomethylene fragment form an electron-deficient core, while the thienyl substituent further extends the conjugation. In line with the materials-guided use of multihalogenation, the presence of two bromine and two fluorine atoms may provide electronic tuning as well as potential sites for structure-directing intermolecular contacts in the solid state.

The indenone ring system is close to planar. The phenyl ring (C3–C8; r.m.s. deviation = 0.011 Å) and the five-membered ring (C1/C2/C3/C8/C9; r.m.s. deviation = 0.008 Å) form a dihedral angle of 4.2 (4)°. The thiophene ring P (S11/C12–C15; r.m.s. deviation = 0.005 Å) is slightly twisted with respect to the indenone core, making dihedral angles of 7.5 (3)° with the phenyl ring and 5.4 (3)° with the five-membered ring. The near-coplanar arrangement across the linking fragments is supported by the torsion angles C9—C1—C10—C12 [–176.6 (7)°] and C1—C10—C12—S1 [3.7 (13)°]. In the dicyanomethylene substituent, torsion angles C1—C9—C21—C22 [173.2 (7)°] and C1—C9—C21—C24 [–6.3 (11)°] indicate an overall nearly planar conjugated skeleton with a small asymmetry in the orientations of the two cyano groups. The molecular conformation is stabilized by two weak C—H···N intramolecular hydrogen bonds (entries 1 and 2 in Table 1).

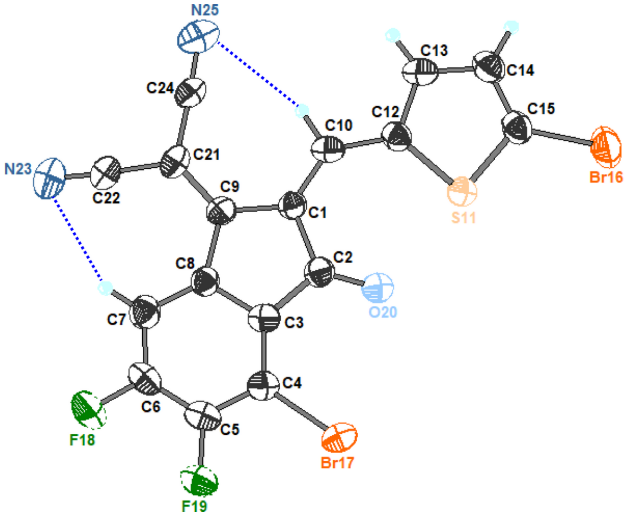


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius. C—H···N hydrogen bonds are shown as blue dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···N23	0.93	2.59	3.394 (12)	145
C10—H10···N25	0.93	2.61	3.489 (10)	159
C13—H13···N25^{i}	0.93	2.48	3.405 (11)	171

Symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{5}{2}, -z+1$.

3. Supramolecular features

In the extended structure, a short and highly directional intermolecular Br···O contact involving the carbonyl O atom is present. As shown in Fig. 2, this halogen bond (Cavallo *et al.*, 2016; Desiraju *et al.*, 2013) is nearly linear [Br17···O20^{i} = 3.141 (5) Å; C4—Br17···O20^{i} = 177.6 (2)°; symmetry code: (i) 1 − *x*, −*y*, 1 − *z*] and connects adjacent molecules into a centrosymmetric dimer.

In addition, a weak C—H···N interaction involving the phenyl ring and one of the cyanomethylene N atoms is present (entry 3 in Table 1) that may help to consolidate the crystal packing.

4. Database survey

A substructure search of the Cambridge Structural Database (CSD: version 2026.1; Groom *et al.*, 2016) was carried out for neutral molecules containing the same conjugated indenone/dicyanomethylene framework as the title compound. The search returned 51 hits. Representative closely related structures include CAPYUN (Popova *et al.*, 1983), IDOYUW (Palusiak *et al.*, 2006), RAZMEM and RAZLUB (Capobianco *et al.*, 2012), TETVAT (Shao *et al.*, 2023), PAWMUZ (Terenti *et al.*, 2022), SOFPOT and SOFPUZ (Masuda *et al.*, 2008) and XAKJAX (Francos *et al.*, 2016).

Structural variations are mainly associated with the substituents on the indenone ring and the exocyclic aryl(heteroaryl) methylidene fragment, including differences in halogen

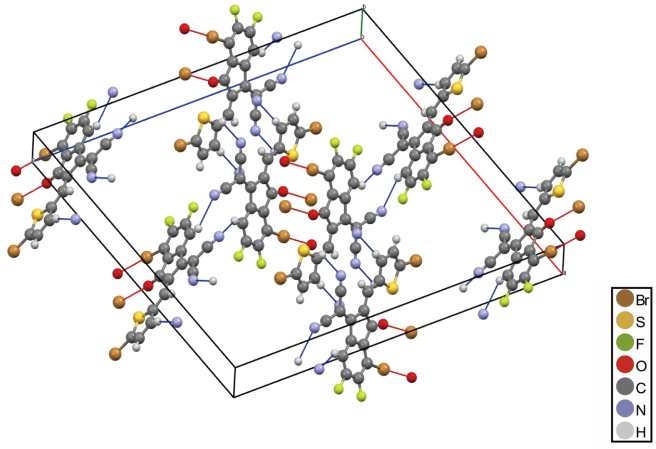


Figure 2
Crystal packing of the title compound viewed approximately along the *b* axis. Intermolecular Br···O contacts are shown as red lines, and intermolecular C—H···N interactions as blue lines.

substitution. In comparison with these related compounds, the title molecule bears two Br atoms (on the indenone ring and the thiophene ring) together with two F atoms on the fused benzene ring. Such substitutions change the steric demand and the distribution of electron density around the carbonyl and nitrile groups, which can influence the balance of weak intermolecular contacts. Consistent with this, the crystal structure of the title compound is primarily stabilized by C—H···N interactions involving the nitrile N atoms and by a directional Br···O contact involving the carbonyl O atom; the latter interaction is enabled by the presence and orientation of the bromine substituent and is not necessarily present in all related structures lacking an appropriately positioned halogen donor.

5. Synthesis and crystallization

The synthesis scheme to obtain the title compound is given in Fig. 3. Starting material 1 (40 mg, 0.129 mmol) and 5-bromothiophene-2-carbaldehyde (31 mg, 0.162 mmol) were dissolved in 1,2-dichloroethane (12 ml). Trifluoroboric acid diethyl etherate ($BF_3{\cdot}Et_2O$, 0.10 ml) and acetic anhydride (Ac_2O, 0.10 ml) were added, and the reaction mixture was stirred at room temperature for 30 min. The mixture was then extracted with dichloromethane and the combined organic layers dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography using chloroform as eluent to afford the title compound as an orange–red solid (44 mg, 0.091 mmol, 71% based on starting material **1**. The product was characterized by ^{1}H NMR spectroscopy (details given in the electronic supplementary information). Single crystals suitable for X-ray diffraction were obtained by gas-liquid diffusion of *n*-hexane into a dichloromethane solution of the product over 2 d at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were placed in calculated positions and refined using a riding model [C—H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C)]. Six reflections, −20 4 18, 14 2 12, −5 3 21, −8 2 25, −9 1 28 and 12 4 11, were omitted as clear outliers. The maximum and minimum residual electron-density peaks are 1.70 and 0.97 Å, respectively, from atom Br17.

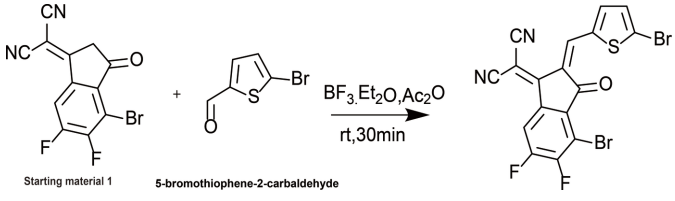


Figure 3
Synthesis scheme of the title compound.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_4Br_2F_2N_2OS$
M_r	482.08
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	22.9059 (8), 5.6693 (2), 25.9096 (9)
β (°)	108.971 (4)
V (Å^3)	3181.9 (2)
Z	8
Radiation type	Cu *K*α
μ (mm^{-1})	7.98
Crystal size (mm)	0.25 × 0.20 × 0.20
Data collection	
Diffractometer	XtaLAB Synergy R, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.116, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9183, 3095, 2432
R_{int}	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.636
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.042, 0.132, 1.15
No. of reflections	3095
No. of parameters	226
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.77, −1.15

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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supporting information

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Crystal structure of 4-bromo-3-[(5-bromothiophen-2-yl)methylidene]-2-(dicyanomethylidene)-5,6-difluoro-2,3-dihydroinden-1-one

Sunyu Cao, Xiaofeng Chen and Zhipeng Yu

Computing details

2-{4-Bromo-3-[(*E*)-(5-bromothiophen-2-yl)methylidene]-5,6-difluoro-1-oxoinden-2-ylidene}propanedinitrile

Crystal data

$C_{17}H_4Br_2F_2N_2OS$
M_r = 482.08
Monoclinic, *C*2/*c*
a = 22.9059 (8) Å
b = 5.6693 (2) Å
c = 25.9096 (9) Å
β = 108.971 (4)°
V = 3181.9 (2) Å^3
Z = 8
F(000) = 1856
D_x = 2.013 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 4587 reflections
θ = 3.6–76.1°
μ = 7.98 mm^{-1}
T = 293 K
Block, orange-red
0.25 × 0.20 × 0.20 mm

Data collection

XtaLAB Synergy R, HyPix diffractometer
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2024)
T_{min} = 0.116, T_{max} = 1.000
9183 measured reflections
3095 independent reflections
2432 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 78.8°, θ_{min} = 3.6°
h = −27→28
k = −5→7
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.132
S = 1.15
3095 reflections
226 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.015P)^2 + 49.4493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −1.15 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}
Br17	0.54902 (3)	0.06639 (13)	0.57194 (3)	0.0452 (2)
Br16	0.25776 (5)	0.26446 (16)	0.29651 (3)	0.0663 (3)
S11	0.33207 (7)	0.4103 (3)	0.41385 (6)	0.0407 (4)
F18	0.62344 (18)	0.2168 (8)	0.68610 (17)	0.0589 (11)
F19	0.6063 (2)	0.5718 (9)	0.74651 (17)	0.0664 (13)
O20	0.4295 (2)	0.3420 (9)	0.5018 (2)	0.0554 (13)
C1	0.3949 (3)	0.6807 (11)	0.5405 (3)	0.0357 (13)
C3	0.4832 (3)	0.4643 (11)	0.5943 (3)	0.0370 (14)
C4	0.5329 (3)	0.3126 (11)	0.6139 (3)	0.0376 (14)
N25	0.3078 (3)	1.2489 (12)	0.5599 (3)	0.0602 (17)
C2	0.4346 (3)	0.4760 (11)	0.5400 (3)	0.0384 (14)
C9	0.4182 (3)	0.7844 (11)	0.5951 (3)	0.0358 (13)
C21	0.3949 (3)	0.9738 (11)	0.6149 (3)	0.0402 (15)
C12	0.3154 (3)	0.6618 (11)	0.4446 (3)	0.0362 (13)
C8	0.4730 (3)	0.6469 (11)	0.6271 (2)	0.0357 (13)
C10	0.3448 (3)	0.7501 (11)	0.4982 (3)	0.0376 (14)
H10	0.325749	0.883990	0.505978	0.045*
C24	0.3456 (3)	1.1198 (11)	0.5828 (3)	0.0399 (14)
C13	0.2659 (3)	0.7793 (12)	0.4081 (3)	0.0451 (16)
H13	0.249940	0.918681	0.416920	0.054*
C7	0.5150 (3)	0.6862 (13)	0.6790 (3)	0.0459 (16)
H7	0.509451	0.809712	0.700609	0.055*
C5	0.5740 (3)	0.3538 (13)	0.6655 (3)	0.0443 (16)
C15	0.2725 (3)	0.4711 (12)	0.3549 (3)	0.0429 (15)
C14	0.2420 (3)	0.6726 (13)	0.3572 (3)	0.0464 (16)
H14	0.209246	0.732103	0.328524	0.056*
C6	0.5642 (3)	0.5386 (13)	0.6972 (3)	0.0460 (16)
N23	0.4306 (4)	1.1109 (15)	0.7145 (3)	0.082 (2)
C22	0.4170 (3)	1.0470 (13)	0.6707 (3)	0.0498 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br17	0.0427 (4)	0.0407 (4)	0.0553 (4)	0.0068 (3)	0.0203 (3)	0.0006 (3)
Br16	0.0885 (7)	0.0584 (5)	0.0404 (4)	−0.0060 (5)	0.0049 (4)	−0.0067 (4)
S11	0.0414 (8)	0.0371 (8)	0.0388 (8)	0.0041 (7)	0.0064 (7)	−0.0021 (7)
F18	0.047 (2)	0.070 (3)	0.051 (2)	0.015 (2)	0.0043 (19)	0.004 (2)
F19	0.063 (3)	0.075 (3)	0.045 (2)	0.004 (2)	−0.006 (2)	−0.001 (2)
O20	0.054 (3)	0.054 (3)	0.048 (3)	0.017 (2)	0.001 (2)	−0.011 (2)
C1	0.035 (3)	0.032 (3)	0.039 (3)	0.002 (3)	0.011 (3)	0.000 (3)
C3	0.032 (3)	0.033 (3)	0.045 (3)	−0.002 (3)	0.011 (3)	0.003 (3)
C4	0.036 (3)	0.038 (3)	0.041 (3)	0.002 (3)	0.016 (3)	0.005 (3)
N25	0.064 (4)	0.047 (4)	0.076 (5)	0.011 (3)	0.031 (4)	0.003 (4)
C2	0.033 (3)	0.035 (3)	0.044 (4)	−0.003 (3)	0.008 (3)	−0.005 (3)
C9	0.038 (3)	0.030 (3)	0.040 (3)	−0.003 (3)	0.014 (3)	0.000 (3)

C21	0.046 (4)	0.033 (3)	0.045 (4)	−0.004 (3)	0.020 (3)	−0.007 (3)
C12	0.032 (3)	0.037 (3)	0.037 (3)	−0.003 (3)	0.007 (2)	0.000 (3)
C8	0.038 (3)	0.036 (3)	0.034 (3)	0.000 (3)	0.014 (3)	0.000 (3)
C10	0.034 (3)	0.032 (3)	0.046 (4)	0.003 (3)	0.011 (3)	0.006 (3)
C24	0.047 (4)	0.031 (3)	0.046 (4)	0.002 (3)	0.022 (3)	−0.002 (3)
C13	0.042 (4)	0.038 (4)	0.053 (4)	0.009 (3)	0.012 (3)	0.008 (3)
C7	0.054 (4)	0.045 (4)	0.041 (4)	0.000 (3)	0.019 (3)	0.001 (3)
C5	0.036 (3)	0.046 (4)	0.047 (4)	0.002 (3)	0.009 (3)	0.010 (3)
C15	0.045 (4)	0.040 (4)	0.038 (3)	−0.007 (3)	0.006 (3)	−0.001 (3)
C14	0.049 (4)	0.047 (4)	0.039 (3)	0.002 (3)	0.008 (3)	0.007 (3)
C6	0.040 (3)	0.052 (4)	0.038 (3)	−0.004 (3)	0.002 (3)	0.006 (3)
N23	0.096 (6)	0.090 (6)	0.057 (4)	0.026 (5)	0.018 (4)	−0.022 (4)
C22	0.058 (4)	0.045 (4)	0.047 (4)	0.008 (4)	0.017 (3)	−0.008 (3)

Geometric parameters (Å, º)

Br17—C4	1.877 (7)	C9—C8	1.480 (9)
Br16—C15	1.855 (7)	C21—C24	1.428 (9)
S11—C12	1.735 (7)	C21—C22	1.428 (9)
S11—C15	1.720 (7)	C12—C10	1.422 (9)
F18—C5	1.333 (8)	C12—C13	1.389 (9)
F19—C6	1.341 (7)	C8—C7	1.395 (9)
O20—C2	1.223 (8)	C10—H10	0.9300
C1—C2	1.477 (9)	C13—H13	0.9300
C1—C9	1.464 (8)	C13—C14	1.391 (9)
C1—C10	1.362 (8)	C7—H7	0.9300
C3—C4	1.385 (9)	C7—C6	1.359 (10)
C3—C2	1.485 (9)	C5—C6	1.394 (10)
C3—C8	1.405 (9)	C15—C14	1.352 (10)
C4—C5	1.382 (9)	C14—H14	0.9300
N25—C24	1.142 (9)	N23—C22	1.136 (9)
C9—C21	1.372 (9)		

C15—S11—C12	90.8 (3)	C7—C8—C9	130.5 (6)
C9—C1—C2	106.9 (5)	C1—C10—C12	133.8 (6)
C10—C1—C2	125.5 (6)	C1—C10—H10	113.1
C10—C1—C9	127.6 (6)	C12—C10—H10	113.1
C4—C3—C2	130.4 (6)	N25—C24—C21	175.0 (8)
C4—C3—C8	121.1 (6)	C12—C13—H13	122.6
C8—C3—C2	108.5 (5)	C12—C13—C14	114.9 (6)
C3—C4—Br17	122.9 (5)	C14—C13—H13	122.6
C5—C4—Br17	119.1 (5)	C8—C7—H7	121.0
C5—C4—C3	117.9 (6)	C6—C7—C8	118.0 (7)
O20—C2—C1	126.7 (6)	C6—C7—H7	121.0
O20—C2—C3	125.7 (6)	F18—C5—C4	120.7 (6)
C1—C2—C3	107.5 (5)	F18—C5—C6	118.7 (6)
C1—C9—C8	107.8 (5)	C4—C5—C6	120.5 (6)
C21—C9—C1	127.7 (6)	S11—C15—Br16	118.7 (4)

C21—C9—C8	124.4 (6)	C14—C15—Br16	127.6 (5)
C9—C21—C24	124.4 (6)	C14—C15—S11	113.7 (5)
C9—C21—C22	123.5 (6)	C13—C14—H14	124.5
C22—C21—C24	112.0 (6)	C15—C14—C13	111.1 (6)
C10—C12—S11	129.2 (5)	C15—C14—H14	124.5
C13—C12—S11	109.5 (5)	F19—C6—C7	120.2 (7)
C13—C12—C10	121.3 (6)	F19—C6—C5	117.6 (6)
C3—C8—C9	109.1 (5)	C7—C6—C5	122.2 (6)
C7—C8—C3	120.1 (6)	N23—C22—C21	175.2 (8)

Br17—C4—C5—F18	−2.0 (9)	C2—C3—C8—C7	−175.3 (6)
Br17—C4—C5—C6	178.5 (5)	C9—C1—C2—O20	179.2 (7)
Br16—C15—C14—C13	179.4 (5)	C9—C1—C2—C3	−2.0 (7)
S11—C12—C10—C1	3.7 (11)	C9—C1—C10—C12	−176.6 (7)
S11—C12—C13—C14	0.0 (8)	C9—C8—C7—C6	−175.4 (6)
S11—C15—C14—C13	−1.4 (8)	C21—C9—C8—C3	179.2 (6)
F18—C5—C6—F19	1.7 (10)	C21—C9—C8—C7	−7.0 (11)
F18—C5—C6—C7	179.8 (6)	C12—S11—C15—Br16	−179.5 (4)
C1—C9—C21—C24	−6.3 (11)	C12—S11—C15—C14	1.2 (6)
C1—C9—C21—C22	173.2 (7)	C12—C13—C14—C15	0.9 (9)
C1—C9—C8—C3	−0.6 (7)	C8—C3—C4—Br17	−179.8 (5)
C1—C9—C8—C7	173.2 (7)	C8—C3—C4—C5	−3.3 (9)
C3—C4—C5—F18	−178.6 (6)	C8—C3—C2—O20	−179.5 (7)
C3—C4—C5—C6	1.9 (10)	C8—C3—C2—C1	1.7 (7)
C3—C8—C7—C6	−2.2 (10)	C8—C9—C21—C24	174.0 (6)
C4—C3—C2—O20	1.9 (12)	C8—C9—C21—C22	−6.5 (10)
C4—C3—C2—C1	−176.9 (6)	C8—C7—C6—F19	178.8 (6)
C4—C3—C8—C9	178.1 (6)	C8—C7—C6—C5	0.8 (11)
C4—C3—C8—C7	3.5 (9)	C10—C1—C2—O20	1.6 (11)
C4—C5—C6—F19	−178.8 (6)	C10—C1—C2—C3	−179.7 (6)
C4—C5—C6—C7	−0.7 (11)	C10—C1—C9—C21	−0.6 (11)
C2—C1—C9—C21	−178.1 (6)	C10—C1—C9—C8	179.2 (6)
C2—C1—C9—C8	1.6 (7)	C10—C12—C13—C14	179.8 (6)
C2—C1—C10—C12	0.5 (12)	C13—C12—C10—C1	−176.0 (7)
C2—C3—C4—Br17	−1.3 (10)	C15—S11—C12—C10	179.6 (6)
C2—C3—C4—C5	175.2 (6)	C15—S11—C12—C13	−0.7 (5)
C2—C3—C8—C9	−0.7 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···N23	0.93	2.59	3.394 (12)	145
C10—H10···N25	0.93	2.61	3.489 (10)	159
C13—H13···N25^{i}	0.93	2.48	3.405 (11)	171

Symmetry code: (i) −*x*+1/2, −*y*+5/2, −*z*+1.