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N-[(3-Bromo-1-phenylsulfonyl-1*H*-indol-2-yl)methyl]-4-fluoroaniline

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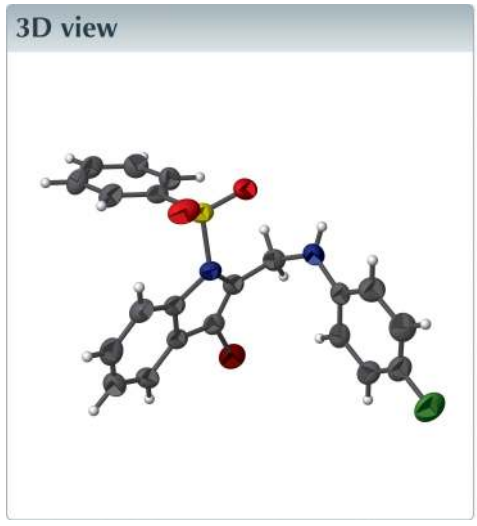
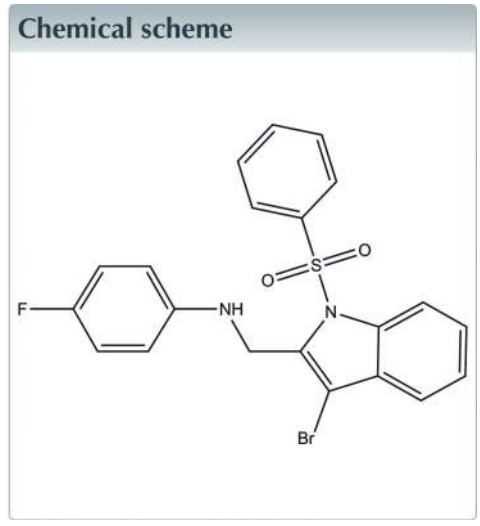
In the title compound, $C_{21}H_{16}BrFN_2O_2S$, the indole ring system makes dihedral angles of 87.23 (10) and 77.58 (9)° with the fluorobenzene and phenyl rings, respectively. The molecular structure is stabilized by a C—H···O and a C—H···Br intramolecular hydrogen bond, which generate *S*(6) and *S*(8) ring motifs, respectively. In the crystal, molecules are linked by C—H···π interactions, forming ribbons propagating along the *a*-axis direction. Within the ribbons, there are offset π–π interactions present involving inversion-related molecules [intercentroid distance = 3.650 (1) Å].





Structure description

Indole is an important heterocyclic system because it is built into proteins in the form of the amino acid tryptophan as well as being the basis of drugs such as indomethacin and providing the skeleton of indole alkaloids, the biologically active compounds from plants (Sharma *et al.*, 2010). As part of our investigations of indole derivatives, we have undertaken the synthesis and crystal structure analysis of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The molecular structure is stabilized by a C—H···O and a C—H···Br intramolecular hydrogen bond, which generate *S*(6) and *S*(8) ring motifs, respectively (Fig. 1 and Table 1). The indole ring system (N2/C8–C15) adopts a planar conformation with a maximum deviation of 0.0340 (1) Å for atom C11. Atom F1 deviates by 0.0107 (1) Å from the plane of the benzene ring (C1–C6) to which it is attached. The mean plane of the indole ring system makes dihedral angles of 87.23 (10) and 77.58 (9)° with the fluorobenzene and phenyl (C16–C21) rings, respectively. The fluorobenzene and phenyl rings are inclined to one another by 81.44 (11)°. The indole and fluorobenzene rings are connected through the

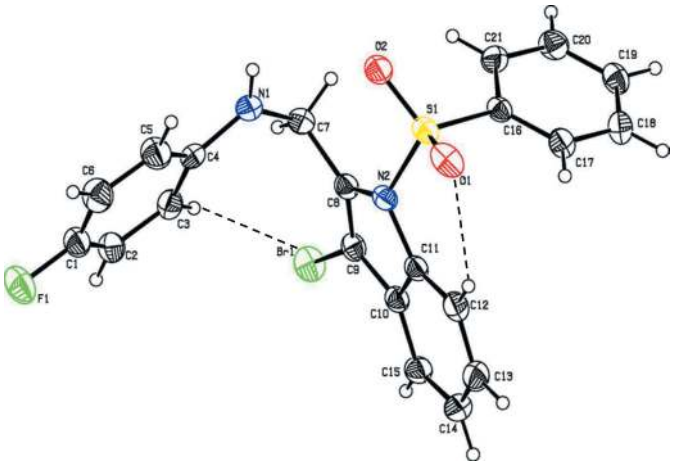


Figure 1
The molecular structure of the title compound, showing the atom labelling and with displacement ellipsoids drawn at 30% probability level. Hydrogen bonds are shown as dashed lines

atoms N1 and C7 with torsion angle C8—C7—N1—C4 = 66.9 (3)°. Atom S1 has a distorted tetrahedral configuration. The widening of angle O1—S1—O2 = 119.87 (10) ° and narrowing of angle N2—S1—C16 = 105.53 (8)° from the ideal tetrahedral value are attributed to the Thorpe–Ingold effect (Bassindale, 1984).

In the crystal, molecules are linked by C—H···π interactions, forming ribbons propagating along the *a*-axis direction (Table 1 and Fig. 2). Within the ribbons there are offset π–π interactions involving inversion-related molecules [*Cg*3···*Cg*3^{iii} = 3.650 (1) Å; *Cg*3 is the centroid of the C10-C15 ring; interplanar distance = 3.440 (1) Å; slippage 1.22 Å; symmetry code: (iii) $-x+2, -y+2, -z+1$].

Synthesis and crystallization

A solution of 1-phenylsulfonyl-2-bromomethyl-3-bromoindole (1.07 g, 2.5 mmol, 1.0 equiv) and 4-fluoroaniline (0.27 g, 2.5 mmol, 1.0 equiv) in dry DMF (10 ml) containing finely powdered K_2CO_3 (0.69 g, 5.0 mmol, 2.0 equiv) was stirred at room temperature for 12 h. The reaction mixture was then poured onto ice (200 g) and the solid formed was filtered immediately and washed with an excess of water. The crude product was dried over $CaCl_2$ and recrystallized from ethyl acetate–hexane (1: 9) to give a half-white coloured solid in 72% yield. Block-like colourless crystals were obtained by slow evaporation of a solution in CH_3OH.

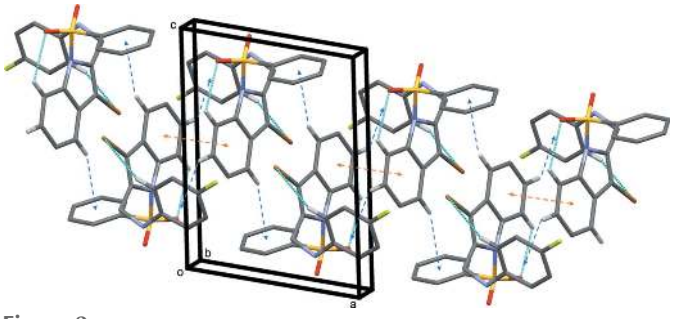


Figure 2
A partial view along the *b* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines, C—H···π interactions as blue dashed arrows and π–π interactions as orange dashed double arrows. H atoms not involved in these interactions have been excluded for clarity.

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

*Cg*2 and *Cg*4 are the centroids of rings C1-C6 and C16–C21, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Br1	0.93	2.92	3.765 (2)	151
C12—H12···O1	0.93	2.38	2.957 (3)	120
C13—H13···*Cg*2^{i}	0.93	2.90	3.8382 (3)	151
C15—H15···*Cg*4^{ii}	0.93	2.72	3.6522 (2)	154

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{16}BrFN_2O_2S$
M_r	459.33
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, *b*, *c* (Å)	8.1732 (5), 10.5828 (7), 12.1781 (8)
α, β, γ (°)	113.699 (1), 94.617 (1), 99.203 (1)
V (Å^3)	939.81 (11)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	2.33
Crystal size (mm)	0.24 × 0.19 × 0.12
Data collection	
Diffractometer	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.753, 0.856
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11107, 4427, 3778
R_{int}	0.018
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.032, 0.096, 1.05
No. of reflections	4427
No. of parameters	253
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *SHELXL2016* (Sheldrick, 2015).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170147 [https://doi.org/10.1107/S2414314617001470X]

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Crystal data

$C_{21}H_{16}BrFN_2O_2S$
M_r = 459.33
Triclinic, $P\overline{1}$
a = 8.1732 (5) Å
b = 10.5828 (7) Å
c = 12.1781 (8) Å
α = 113.699 (1)°
β = 94.617 (1)°
γ = 99.203 (1)°
V = 939.81 (11) Å^3
Z = 2
$F(000)$ = 464
D_x = 1.623 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4427 reflections
θ = 2.2–28.3°
μ = 2.33 mm^{-1}
T = 293 K
Block, colourless
0.24 × 0.19 × 0.12 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.753, T_{max} = 0.856
11107 measured reflections
4427 independent reflections
3778 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 28.3°, θ_{min} = 2.2°
h = −10→10
k = −13→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.096
S = 1.05
4427 reflections
253 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.1305P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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}
C1	1.0439 (3)	0.3846 (2)	0.3063 (2)	0.0524 (5)
C2	0.8963 (3)	0.4075 (2)	0.3480 (2)	0.0510 (5)
H2	0.870710	0.391539	0.415005	0.061*
C3	0.7849 (3)	0.4548 (2)	0.2890 (2)	0.0466 (4)
H3	0.684493	0.471193	0.317208	0.056*
C4	0.8213 (3)	0.47778 (19)	0.18896 (17)	0.0433 (4)
C5	0.9754 (3)	0.4538 (3)	0.1506 (2)	0.0599 (6)
H5	1.003760	0.470852	0.084643	0.072*
C6	1.0853 (3)	0.4057 (3)	0.2082 (2)	0.0613 (6)
H6	1.185730	0.387984	0.180567	0.074*
C7	0.5735 (3)	0.5820 (2)	0.17222 (19)	0.0491 (5)
H7A	0.507416	0.521160	0.201672	0.059*
H7B	0.500965	0.587821	0.108060	0.059*
C8	0.6282 (2)	0.7267 (2)	0.27416 (17)	0.0395 (4)
C9	0.6028 (2)	0.7717 (2)	0.39091 (18)	0.0401 (4)
C10	0.6911 (2)	0.9145 (2)	0.46065 (17)	0.0396 (4)
C11	0.7743 (2)	0.9561 (2)	0.38144 (16)	0.0378 (4)
C12	0.8800 (3)	1.0883 (2)	0.4218 (2)	0.0476 (5)
H12	0.936670	1.115759	0.369150	0.057*
C13	0.8966 (3)	1.1766 (2)	0.5435 (2)	0.0562 (5)
H13	0.966282	1.265694	0.572957	0.067*
C14	0.8138 (3)	1.1379 (2)	0.6233 (2)	0.0559 (5)
H14	0.827849	1.201048	0.704601	0.067*
C15	0.7107 (3)	1.0068 (2)	0.58341 (18)	0.0488 (5)
H15	0.655233	0.980097	0.636937	0.059*
C16	0.5460 (2)	0.9385 (2)	0.13481 (16)	0.0372 (4)
C17	0.5621 (3)	1.0827 (2)	0.1861 (2)	0.0470 (4)
H17	0.667034	1.142071	0.220819	0.056*
C18	0.4198 (3)	1.1384 (2)	0.1854 (2)	0.0524 (5)
H18	0.428905	1.235653	0.220589	0.063*
C19	0.2653 (3)	1.0502 (2)	0.1329 (2)	0.0493 (5)
H19	0.170302	1.088132	0.132396	0.059*
C20	0.2503 (3)	0.9069 (3)	0.0815 (2)	0.0528 (5)
H20	0.145091	0.848001	0.046733	0.063*
C21	0.3913 (3)	0.8489 (2)	0.08082 (19)	0.0476 (4)
H21	0.381825	0.751566	0.044744	0.057*
N1	0.7090 (2)	0.51720 (19)	0.12096 (15)	0.0522 (4)
H1	0.721138	0.502532	0.047600	0.063*
N2	0.73770 (19)	0.83989 (17)	0.26447 (13)	0.0383 (3)
O1	0.87084 (18)	0.9732 (2)	0.15578 (15)	0.0572 (4)
O2	0.6999 (2)	0.73241 (18)	0.03837 (13)	0.0560 (4)
F1	1.1535 (2)	0.33908 (19)	0.36508 (16)	0.0767 (4)
S1	0.72622 (6)	0.86853 (6)	0.13829 (4)	0.04184 (12)
BR1	0.47945 (3)	0.66201 (3)	0.45649 (2)	0.05848 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0500 (12)	0.0487 (11)	0.0578 (12)	0.0118 (9)	−0.0011 (10)	0.0229 (10)
C2	0.0572 (12)	0.0466 (11)	0.0526 (11)	0.0107 (9)	0.0073 (10)	0.0245 (9)
C3	0.0459 (10)	0.0389 (10)	0.0538 (11)	0.0094 (8)	0.0074 (9)	0.0183 (9)
C4	0.0498 (11)	0.0313 (9)	0.0393 (9)	0.0072 (8)	−0.0008 (8)	0.0073 (7)
C5	0.0660 (14)	0.0713 (15)	0.0523 (12)	0.0263 (12)	0.0186 (11)	0.0300 (11)
C6	0.0515 (12)	0.0690 (15)	0.0673 (15)	0.0207 (11)	0.0156 (11)	0.0285 (12)
C7	0.0475 (11)	0.0483 (11)	0.0452 (10)	0.0112 (9)	−0.0048 (9)	0.0152 (9)
C8	0.0366 (9)	0.0442 (10)	0.0396 (9)	0.0127 (7)	0.0033 (7)	0.0184 (8)
C9	0.0362 (9)	0.0464 (10)	0.0452 (10)	0.0126 (8)	0.0098 (7)	0.0246 (8)
C10	0.0378 (9)	0.0467 (10)	0.0391 (9)	0.0161 (8)	0.0069 (7)	0.0203 (8)
C11	0.0354 (8)	0.0440 (10)	0.0375 (9)	0.0138 (7)	0.0038 (7)	0.0189 (8)
C12	0.0465 (11)	0.0475 (11)	0.0542 (11)	0.0104 (8)	0.0033 (9)	0.0277 (9)
C13	0.0564 (13)	0.0419 (11)	0.0628 (13)	0.0090 (9)	−0.0057 (11)	0.0178 (10)
C14	0.0652 (14)	0.0527 (12)	0.0440 (11)	0.0217 (11)	0.0033 (10)	0.0122 (10)
C15	0.0551 (12)	0.0562 (12)	0.0380 (9)	0.0203 (10)	0.0105 (9)	0.0191 (9)
C16	0.0364 (9)	0.0482 (10)	0.0335 (8)	0.0139 (7)	0.0097 (7)	0.0212 (8)
C17	0.0415 (10)	0.0477 (11)	0.0555 (11)	0.0071 (8)	0.0031 (9)	0.0274 (9)
C18	0.0535 (12)	0.0469 (11)	0.0648 (13)	0.0168 (9)	0.0096 (10)	0.0294 (10)
C19	0.0435 (10)	0.0625 (13)	0.0545 (12)	0.0224 (9)	0.0130 (9)	0.0322 (10)
C20	0.0374 (10)	0.0606 (13)	0.0563 (12)	0.0095 (9)	0.0012 (9)	0.0219 (10)
C21	0.0459 (11)	0.0453 (11)	0.0459 (10)	0.0112 (8)	0.0022 (8)	0.0139 (9)
N1	0.0645 (11)	0.0503 (10)	0.0374 (8)	0.0234 (8)	0.0025 (8)	0.0109 (7)
N2	0.0389 (8)	0.0460 (8)	0.0344 (7)	0.0131 (6)	0.0060 (6)	0.0199 (7)
O1	0.0391 (7)	0.0892 (11)	0.0636 (9)	0.0172 (7)	0.0186 (7)	0.0494 (9)
O2	0.0713 (10)	0.0687 (10)	0.0383 (7)	0.0377 (8)	0.0178 (7)	0.0227 (7)
F1	0.0660 (9)	0.0927 (11)	0.0872 (11)	0.0341 (8)	0.0043 (8)	0.0487 (9)
S1	0.0396 (2)	0.0592 (3)	0.0377 (2)	0.0207 (2)	0.01327 (18)	0.0264 (2)
BR1	0.05446 (15)	0.06742 (17)	0.06666 (17)	0.01190 (11)	0.02033 (11)	0.03985 (13)

Geometric parameters (Å, º)

C1—C6	1.360 (4)	C12—C13	1.379 (3)
C1—F1	1.363 (3)	C12—H12	0.9300
C1—C2	1.366 (3)	C13—C14	1.381 (4)
C2—C3	1.387 (3)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.375 (3)
C3—C4	1.380 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.403 (3)	C16—C17	1.376 (3)
C4—N1	1.407 (3)	C16—C21	1.383 (3)
C5—C6	1.374 (3)	C16—S1	1.7562 (18)
C5—H5	0.9300	C17—C18	1.386 (3)
C6—H6	0.9300	C17—H17	0.9300
C7—N1	1.449 (3)	C18—C19	1.374 (3)
C7—C8	1.500 (3)	C18—H18	0.9300

C7—H7A	0.9700	C19—C20	1.368 (3)
C7—H7B	0.9700	C19—H19	0.9300
C8—C9	1.351 (3)	C20—C21	1.389 (3)
C8—N2	1.427 (3)	C20—H20	0.9300
C9—C10	1.431 (3)	C21—H21	0.9300
C9—BR1	1.8712 (19)	N1—H1	0.8600
C10—C11	1.392 (3)	N2—S1	1.6799 (15)
C10—C15	1.397 (3)	O1—S1	1.4215 (17)
C11—C12	1.392 (3)	O2—S1	1.4324 (17)
C11—N2	1.427 (2)		

C6—C1—F1	118.9 (2)	C14—C13—C12	122.5 (2)
C6—C1—C2	122.2 (2)	C14—C13—H13	118.7
F1—C1—C2	118.9 (2)	C12—C13—H13	118.7
C1—C2—C3	119.1 (2)	C15—C14—C13	120.5 (2)
C1—C2—H2	120.4	C15—C14—H14	119.8
C3—C2—H2	120.4	C13—C14—H14	119.8
C4—C3—C2	120.8 (2)	C14—C15—C10	118.5 (2)
C4—C3—H3	119.6	C14—C15—H15	120.7
C2—C3—H3	119.6	C10—C15—H15	120.7
C3—C4—C5	117.71 (19)	C17—C16—C21	121.15 (18)
C3—C4—N1	123.4 (2)	C17—C16—S1	118.91 (15)
C5—C4—N1	118.8 (2)	C21—C16—S1	119.94 (15)
C6—C5—C4	121.6 (2)	C16—C17—C18	119.11 (19)
C6—C5—H5	119.2	C16—C17—H17	120.4
C4—C5—H5	119.2	C18—C17—H17	120.4
C1—C6—C5	118.5 (2)	C19—C18—C17	120.2 (2)
C1—C6—H6	120.7	C19—C18—H18	119.9
C5—C6—H6	120.7	C17—C18—H18	119.9
N1—C7—C8	114.88 (17)	C20—C19—C18	120.40 (19)
N1—C7—H7A	108.5	C20—C19—H19	119.8
C8—C7—H7A	108.5	C18—C19—H19	119.8
N1—C7—H7B	108.5	C19—C20—C21	120.4 (2)
C8—C7—H7B	108.5	C19—C20—H20	119.8
H7A—C7—H7B	107.5	C21—C20—H20	119.8
C9—C8—N2	107.46 (17)	C16—C21—C20	118.8 (2)
C9—C8—C7	128.96 (19)	C16—C21—H21	120.6
N2—C8—C7	123.22 (18)	C20—C21—H21	120.6
C8—C9—C10	110.49 (17)	C4—N1—C7	121.22 (18)
C8—C9—BR1	125.55 (16)	C4—N1—H1	119.4
C10—C9—BR1	123.88 (14)	C7—N1—H1	119.4
C11—C10—C15	120.12 (19)	C11—N2—C8	107.49 (15)
C11—C10—C9	106.54 (16)	C11—N2—S1	120.22 (13)
C15—C10—C9	133.28 (19)	C8—N2—S1	122.79 (13)
C12—C11—C10	121.47 (18)	O1—S1—O2	119.87 (10)
C12—C11—N2	130.41 (18)	O1—S1—N2	106.12 (9)
C10—C11—N2	108.01 (16)	O2—S1—N2	106.04 (9)
C13—C12—C11	116.9 (2)	O1—S1—C16	109.28 (10)

C13—C12—H12	121.6	O2—S1—C16	109.01 (9)
C11—C12—H12	121.6	N2—S1—C16	105.53 (8)
C6—C1—C2—C3	−0.5 (3)	C21—C16—C17—C18	1.2 (3)
F1—C1—C2—C3	179.51 (19)	S1—C16—C17—C18	−178.91 (17)
C1—C2—C3—C4	0.4 (3)	C16—C17—C18—C19	−0.7 (3)
C2—C3—C4—C5	−1.0 (3)	C17—C18—C19—C20	0.3 (3)
C2—C3—C4—N1	175.91 (18)	C18—C19—C20—C21	−0.5 (4)
C3—C4—C5—C6	1.6 (3)	C17—C16—C21—C20	−1.4 (3)
N1—C4—C5—C6	−175.4 (2)	S1—C16—C21—C20	178.72 (17)
F1—C1—C6—C5	−178.9 (2)	C19—C20—C21—C16	1.1 (3)
C2—C1—C6—C5	1.0 (4)	C3—C4—N1—C7	21.2 (3)
C4—C5—C6—C1	−1.6 (4)	C5—C4—N1—C7	−162.0 (2)
N1—C7—C8—C9	−118.5 (2)	C8—C7—N1—C4	66.9 (3)
N1—C7—C8—N2	53.7 (3)	C12—C11—N2—C8	176.79 (19)
N2—C8—C9—C10	0.9 (2)	C10—C11—N2—C8	0.68 (19)
C7—C8—C9—C10	174.02 (18)	C12—C11—N2—S1	−36.0 (3)
N2—C8—C9—BR1	−176.08 (12)	C10—C11—N2—S1	147.90 (13)
C7—C8—C9—BR1	−3.0 (3)	C9—C8—N2—C11	−0.97 (19)
C8—C9—C10—C11	−0.5 (2)	C7—C8—N2—C11	−174.58 (16)
BR1—C9—C10—C11	176.56 (13)	C9—C8—N2—S1	−147.16 (14)
C8—C9—C10—C15	−177.6 (2)	C7—C8—N2—S1	39.2 (2)
BR1—C9—C10—C15	−0.6 (3)	C11—N2—S1—O1	47.52 (16)
C15—C10—C11—C12	0.9 (3)	C8—N2—S1—O1	−170.39 (15)
C9—C10—C11—C12	−176.67 (17)	C11—N2—S1—O2	176.02 (14)
C15—C10—C11—N2	177.44 (16)	C8—N2—S1—O2	−41.89 (17)
C9—C10—C11—N2	−0.15 (19)	C11—N2—S1—C16	−68.41 (15)
C10—C11—C12—C13	−0.8 (3)	C8—N2—S1—C16	73.69 (16)
N2—C11—C12—C13	−176.45 (18)	C17—C16—S1—O1	−20.95 (18)
C11—C12—C13—C14	0.1 (3)	C21—C16—S1—O1	158.89 (16)
C12—C13—C14—C15	0.5 (3)	C17—C16—S1—O2	−153.69 (16)
C13—C14—C15—C10	−0.4 (3)	C21—C16—S1—O2	26.15 (18)
C11—C10—C15—C14	−0.3 (3)	C17—C16—S1—N2	92.79 (16)
C9—C10—C15—C14	176.5 (2)	C21—C16—S1—N2	−87.37 (17)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg4 are the centroids of rings C1-C6 and C16–C21, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Br1	0.93	2.92	3.765 (2)	151
C12—H12···O1	0.93	2.38	2.957 (3)	120
C13—H13···*Cg*2^{i}	0.93	2.90	3.8382 (3)	151
C15—H15···*Cg*4^{ii}	0.93	2.72	3.6522 (2)	154

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