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(2*Z*)-2-(5-Fluoro-1-methyl-2-oxoindolin-3-ylidene)-*N*-(3-fluorophenyl)hydrazine-1-carbothioamide

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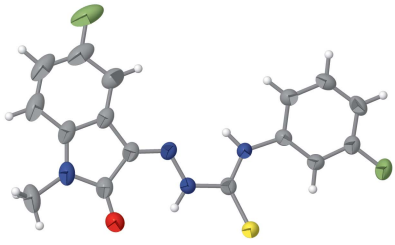
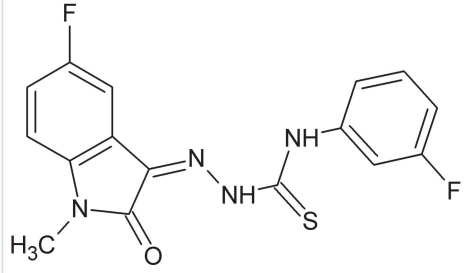
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{12}F_2N_4OS$, the whole molecule is essentially planar (r.m.s deviation = 0.003 Å), with only the H atoms of the methyl group lying out of the molecular plane. A planar indole fused-ring system (r.m.s deviation = 0.004 Å) is linked through a hydrazine–carbothioamide bridge to a fluorobenzene ring, with the indole ring system and inclined to the fluorobenzene ring by 4.26 (14)°. The planarity of the molecule is strengthened by three intramolecular N—H···N, N—H···O and C—H···S hydrogen bonds that generate *S*(5), *S*(6) and *S*(6) ring motifs, respectively. In the crystal, π–π stacking interactions combine with C—H···F hydrogen bonds to link the molecules into layers parallel to the $(10\bar{1})$ plane.

3D view



Chemical scheme



Structure description

The indole heterocyclic ring system is a significant component of many pharmaceutical agents, including compounds with antiviral, anti-inflammatory and antineoplastic properties (Ma *et al.*, 2015). Halogenated and *N*-alkylated isatin derivatives demonstrate antitumour activity (Karalı *et al.*, 2007; Podichetty *et al.*, 2009). Thiosemicarbazone compounds that incorporate isatin units also have various types of biological effects, including antiviral, antibacterial and antitumour activity (Thanh *et al.*, 2016). Isatin 3-thiosemicarbazones, which show anti-HIV effects, are also used in the treatment of smallpox and vaccinia viruses, and of other groups of viruses, including adenovirus and herpesvirus (Bal *et al.*, 2005; Hall *et al.*, 2009; Thanh *et al.*, 2016). Finally, isatin

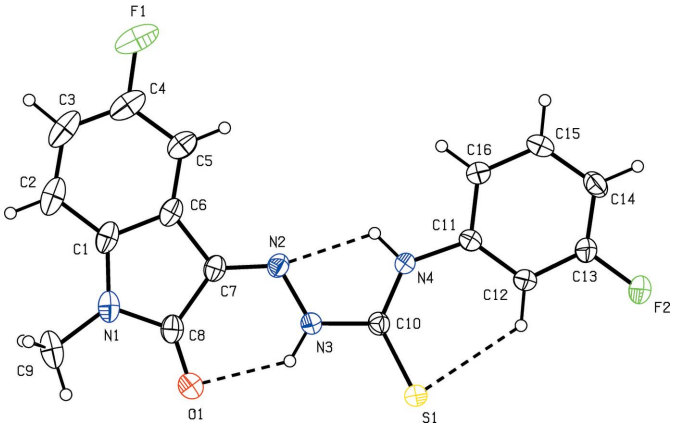


Figure 1
The structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

[N^4-(phenyl substituted)thiosemicarbazone] derivatives have been shown to be significantly more selective and effective against multidrug resistance when compared to the activity of N^4-alkyl and N^4-cycloalkylthiosemicarbazones (Hall *et al.*, 2009, 2011).

As shown in Fig. 1, the molecule of the title compound is essentially planar (r.m.s deviation = 0.003 Å), with only the H atoms of the C9 methyl group protruding from the molecular plane. The almost planar indole fused-ring (N1/C1–C8) (r.m.s deviation deviation = 0.004 Å) makes a dihedral angle of 4.26 (14)° with the C11–C16 benzene ring. The N2—N3—C10═S1 and N2—N3—C10—N4 torsion angles are 172.6 (2) and −6.1 (4)°, respectively, again in keeping with the planarity of the molecule. Three intramolecular N—H···N, N—H···O and C—H···S hydrogen bonds (Table 1) generate $S(5)$, $S(6)$ and $S(6)$ ring motifs, respectively, and also contribute significantly to the molecular planarity.

All bond lengths and angles are within normal ranges and are in agreement with those reported for the related compounds 2-(5-fluoro-1-methyl-2-oxoindolin-3-ylidene)-*N*-[4-(methylsulfanyl)phenyl]hydrazine-1-carbothioamide (Atioğlu *et al.*, 2017), (3*E*)-3-[(4-butylphenyl)imino]-1,3-dihydro-2*H*-indol-2-one (Akkurt *et al.*, 2003), *N*′-[(2*Z*)-3-allyl-4-oxo-1,3-thiazolidin-2-ylidene]-5-fluoro-3-phenyl-1*H*-indole-2-carbohydrazide (Akkurt *et al.*, 2009), 2-(4-isobutylphenyl)-*N*′-[(3*Z*)-2-oxoindolin-3-ylidene]propanohydrazide (Mohamed *et al.*, 2012) and series of 5-fluoro-1*H*-indole-2,3-dione 3-thiosemicarbazone (Özbey *et al.*, 2006) and 5-trifluoromethoxy-1*H*-indole-2,3-dione 3-thiosemicarbazone derivatives (Kaynak *et al.*, 2013).

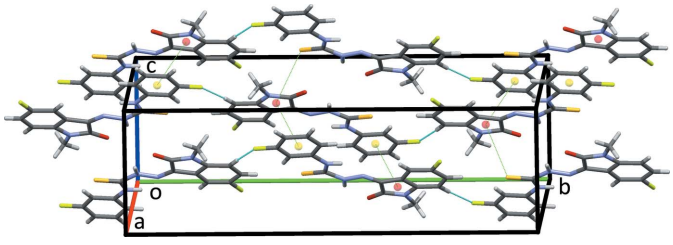


Figure 2
The layers of molecules of the title compound, viewed along the *a*-axis direction.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3N···O1	0.88 (3)	2.08 (3)	2.761 (3)	134 (2)
N4—H4N···N2	0.87 (3)	2.07 (3)	2.579 (3)	117 (3)
C2—H2···F2^{i}	0.93	2.44	3.370 (5)	176
C12—H12···S1	0.93	2.60	3.251 (3)	127

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{12}F_2N_4OS$
M_r	346.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	8.2648 (8), 25.571 (2), 7.6662 (6)
β (°)	108.248 (3)
V (Å^3)	1538.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.24
Crystal size (mm)	0.18 × 0.16 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.664, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33521, 3145, 2536
R_{int}	0.061
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.627
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.125, 1.20
No. of reflections	3145
No. of parameters	227
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.22

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

In the crystal structure of the title compound, C2—H···F2 hydrogen bonds link molecules into zigzag $C(14)$ chains along *b*. π–π stacking interactions between the oxopyrrole and benzene rings [$Cg1\cdots Cg3^{iii}$ = 3.818 (2) Å; symmetry code: (iii) $1-x, 1-y, 1-z$; $Cg1$ and $Cg3$ are the centroids of the N1/C1–C8 and C11–C16 rings, respectively] (Table 1) link these chains into layers parallel to the $(10\bar{1})$ plane (Fig. 2).

Synthesis and crystallization

Steps in the synthesis of the title compound (**5**) are shown in Fig. 3.

(i) *N*-(3-Fluorophenyl)thiosemicarbazide (2)

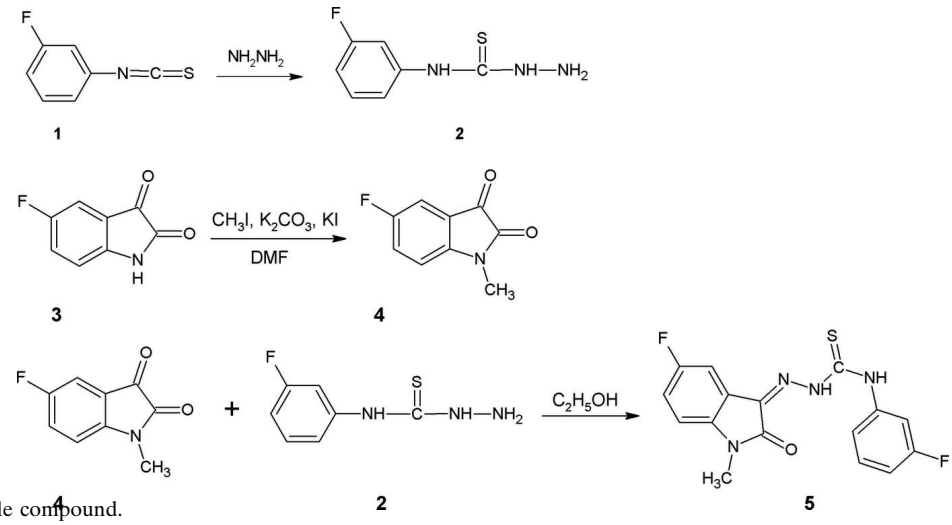


Figure 3
The synthesis of the title compound.

To a solution of hydrazine hydrate (5 mmol) in ethanol (10 ml), a suspension of 3-fluorophenyl isothiocyanate, **1** (5 mmol), in ethanol (10 ml) was added dropwise with vigorous stirring and cooling in an ice bath. The mixture was allowed to stand overnight. The crystals formed were recrystallized from ethanol solution.

(ii) 5-Fluoro-1-methyl-1*H*-indole-2,3-dione (4)

A suspension of 5-fluoro-1*H*-indole-2,3-dione, **3** (5 mmol), K_2CO_3 (7 mmol) and KI (1 mmol) in anhydrous DMF (5 ml) was stirred for 30 min at room temperature. After addition of iodomethane (15 mmol), the mixture was refluxed for 4 h. The product was poured onto ice–water and filtered.

(iii) (2*Z*)-2-(5-Fluoro-1-methyl-2-oxoindolin-1-ylidene)-*N*-(3-fluorophenyl)hydrazine-1-carbothioamide (5)

A solution of *N*-(3-fluorophenyl)thiosemicarbazide, **2** (2.5 mmol), in ethanol (10 ml) was added to a solution of 5-fluoro-1-methyl-1*H*-indole-2,3-dione, **4** (2.5 mmol), in ethanol (20 ml). The mixture was refluxed on a water bath for 8 h. The product formed after cooling was filtered off and washed with ethanol or recrystallized from ethanol. Orange crystals were obtained (82% yield; m.p. 510–516 K).

IR (KBr): ν 3288, 3226 (NH), 1695 (C═O), 1276 (C═S); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 3.20 (*s*, 3H, ind. N—CH_3), 7.09–7.16 (*m*, 2H, ind. C_7—H, fen. C_4—H), 7.28 (*dt*, J = 9.00, 2.70 Hz, 1H, ind. C_6—H), 7.43–7.51 (*m*, 2H, fen. $C_{5,6}$—H), 7.59–7.65 (*m*, 2H, ind. C_4—H, fen. C_2—H), 10.86 (*s*, 1H, N_4—H), 12.62 (*s*, 1H, N_2—H). Analysis calculated for $C_{16}H_{12}F_2N_4OS$: C 55.48, H 3.49, N 16.18%; found: C 55.26, H 3.41, N 16.18%.

Refinement

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

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full crystallographic data

IUCrData (2017). **2**, x170900 [https://doi.org/10.1107/S2414314617009002]

(2*Z*)-2-(5-Fluoro-1-methyl-2-oxoindolin-3-ylidene)-*N*-(3-fluorophenyl)-hydrazine-1-carbothioamide

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Crystal data

$C_{16}H_{12}F_2N_4OS$
M_r = 346.36
Monoclinic, $P2_1/c$
a = 8.2648 (8) Å
b = 25.571 (2) Å
c = 7.6662 (6) Å
β = 108.248 (3)°
V = 1538.7 (2) Å^3
Z = 4
$F(000)$ = 712
D_x = 1.495 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9857 reflections
θ = 3.1–26.4°
μ = 0.24 mm^{-1}
T = 296 K
Block, orange
0.18 × 0.16 × 0.15 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.664, T_{max} = 0.745
33521 measured reflections
3145 independent reflections
2536 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 26.5°, θ_{min} = 2.9°
h = −10→10
k = −31→32
l = −8→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.125
S = 1.20
3145 reflections
227 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.016P)^2 + 1.7256P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: Shelxl-2014/7 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0148 (18)

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	0.3755 (4)	0.68818 (11)	0.1055 (4)	0.0491 (8)
C2	0.3839 (6)	0.74228 (13)	0.1121 (6)	0.0656 (10)
H2	0.2990	0.7627	0.0334	0.079*
C3	0.5238 (6)	0.76481 (13)	0.2405 (6)	0.0737 (12)
H3	0.5339	0.8010	0.2482	0.088*
C4	0.6471 (5)	0.73406 (14)	0.3560 (6)	0.0671 (11)
C5	0.6409 (4)	0.68024 (12)	0.3531 (5)	0.0532 (8)
H5	0.7255	0.6602	0.4339	0.064*
C6	0.5028 (4)	0.65757 (10)	0.2241 (4)	0.0438 (7)
C7	0.4530 (4)	0.60370 (11)	0.1799 (4)	0.0397 (6)
C8	0.2885 (4)	0.60452 (11)	0.0230 (4)	0.0440 (7)
C9	0.0958 (5)	0.67445 (15)	−0.1501 (5)	0.0724 (11)
H9A	0.0309	0.6450	−0.2121	0.109*
H9B	0.1258	0.6961	−0.2376	0.109*
H9C	0.0289	0.6944	−0.0916	0.109*
C10	0.5401 (3)	0.47150 (10)	0.3010 (4)	0.0358 (6)
C11	0.8089 (3)	0.44869 (10)	0.5535 (4)	0.0363 (6)
C12	0.8077 (4)	0.39485 (11)	0.5441 (4)	0.0469 (7)
H12	0.7225	0.3771	0.4553	0.056*
C13	0.9371 (4)	0.36828 (11)	0.6708 (5)	0.0496 (8)
C14	1.0649 (4)	0.39157 (13)	0.8042 (4)	0.0493 (8)
H14	1.1501	0.3721	0.8868	0.059*
C15	1.0629 (4)	0.44527 (13)	0.8118 (4)	0.0521 (8)
H15	1.1480	0.4627	0.9019	0.063*
C16	0.9369 (4)	0.47364 (11)	0.6882 (4)	0.0449 (7)
H16	0.9378	0.5100	0.6954	0.054*
N1	0.2499 (3)	0.65613 (10)	−0.0125 (4)	0.0514 (7)
N2	0.5351 (3)	0.56333 (8)	0.2634 (3)	0.0383 (5)
N3	0.4656 (3)	0.51577 (9)	0.2078 (3)	0.0398 (6)
H3N	0.368 (4)	0.5131 (11)	0.119 (4)	0.041 (8)*
N4	0.6882 (3)	0.48115 (9)	0.4309 (3)	0.0410 (6)
H4N	0.710 (4)	0.5146 (12)	0.441 (4)	0.045 (8)*
O1	0.2066 (3)	0.56682 (8)	−0.0540 (3)	0.0530 (6)
S1	0.43668 (10)	0.41527 (3)	0.24325 (11)	0.0501 (3)
F1	0.7820 (3)	0.75761 (9)	0.4809 (4)	0.0957 (8)
F2	0.9353 (3)	0.31510 (7)	0.6611 (3)	0.0879 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.068 (2)	0.0349 (15)	0.0554 (19)	0.0101 (14)	0.0353 (17)	0.0061 (13)
C2	0.099 (3)	0.0398 (18)	0.076 (2)	0.0161 (19)	0.053 (2)	0.0130 (17)
C3	0.118 (4)	0.0343 (17)	0.093 (3)	−0.007 (2)	0.068 (3)	−0.0037 (19)
C4	0.092 (3)	0.048 (2)	0.080 (3)	−0.023 (2)	0.053 (2)	−0.0183 (19)
C5	0.062 (2)	0.0440 (17)	0.063 (2)	−0.0084 (15)	0.0328 (17)	−0.0069 (15)

C6	0.0556 (18)	0.0321 (14)	0.0517 (17)	0.0035 (13)	0.0284 (15)	0.0015 (13)
C7	0.0459 (16)	0.0342 (14)	0.0434 (16)	0.0050 (12)	0.0205 (13)	0.0022 (12)
C8	0.0466 (17)	0.0416 (16)	0.0480 (17)	0.0089 (13)	0.0210 (14)	0.0060 (13)
C9	0.071 (3)	0.072 (2)	0.071 (2)	0.031 (2)	0.018 (2)	0.025 (2)
C10	0.0374 (15)	0.0358 (14)	0.0336 (14)	0.0046 (11)	0.0102 (11)	−0.0001 (11)
C11	0.0315 (13)	0.0381 (14)	0.0372 (14)	−0.0007 (11)	0.0079 (11)	−0.0003 (11)
C12	0.0385 (15)	0.0377 (15)	0.0534 (18)	0.0001 (12)	−0.0016 (13)	−0.0046 (13)
C13	0.0412 (17)	0.0354 (15)	0.064 (2)	0.0051 (12)	0.0043 (15)	0.0013 (14)
C14	0.0352 (15)	0.0566 (19)	0.0483 (18)	0.0069 (13)	0.0020 (13)	0.0066 (14)
C15	0.0394 (16)	0.0569 (19)	0.0484 (18)	−0.0045 (14)	−0.0030 (14)	−0.0038 (15)
C16	0.0432 (16)	0.0377 (15)	0.0477 (17)	−0.0046 (12)	0.0053 (13)	−0.0008 (12)
N1	0.0571 (16)	0.0451 (14)	0.0540 (16)	0.0174 (12)	0.0206 (13)	0.0116 (12)
N2	0.0425 (13)	0.0308 (11)	0.0417 (13)	0.0027 (10)	0.0135 (10)	−0.0007 (10)
N3	0.0398 (14)	0.0325 (12)	0.0396 (13)	0.0026 (10)	0.0018 (11)	−0.0008 (10)
N4	0.0407 (13)	0.0278 (12)	0.0450 (14)	−0.0004 (10)	−0.0003 (10)	0.0004 (10)
O1	0.0468 (12)	0.0502 (13)	0.0551 (13)	0.0028 (10)	0.0061 (10)	0.0019 (10)
S1	0.0461 (4)	0.0347 (4)	0.0553 (5)	−0.0032 (3)	−0.0047 (3)	0.0001 (3)
F1	0.114 (2)	0.0690 (15)	0.116 (2)	−0.0432 (14)	0.0545 (17)	−0.0386 (14)
F2	0.0730 (14)	0.0385 (11)	0.1170 (19)	0.0134 (10)	−0.0208 (13)	−0.0008 (11)

Geometric parameters (Å, º)

C1—C2	1.385 (4)	C9—H9C	0.9600
C1—C6	1.395 (4)	C10—N4	1.337 (3)
C1—N1	1.407 (4)	C10—N3	1.377 (3)
C2—C3	1.387 (6)	C10—S1	1.660 (3)
C2—H2	0.9300	C11—C12	1.378 (4)
C3—C4	1.370 (6)	C11—C16	1.381 (4)
C3—H3	0.9300	C11—N4	1.407 (3)
C4—F1	1.361 (4)	C12—C13	1.378 (4)
C4—C5	1.377 (4)	C12—H12	0.9300
C5—C6	1.382 (4)	C13—C14	1.357 (4)
C5—H5	0.9300	C13—F2	1.362 (3)
C6—C7	1.447 (4)	C14—C15	1.375 (4)
C7—N2	1.290 (3)	C14—H14	0.9300
C7—C8	1.507 (4)	C15—C16	1.375 (4)
C8—O1	1.219 (4)	C15—H15	0.9300
C8—N1	1.365 (4)	C16—H16	0.9300
C9—N1	1.454 (4)	N2—N3	1.356 (3)
C9—H9A	0.9600	N3—H3N	0.88 (3)
C9—H9B	0.9600	N4—H4N	0.87 (3)
C2—C1—C6	121.2 (3)	N4—C10—S1	129.3 (2)
C2—C1—N1	128.6 (3)	N3—C10—S1	117.7 (2)
C6—C1—N1	110.3 (2)	C12—C11—C16	119.5 (3)
C1—C2—C3	117.5 (4)	C12—C11—N4	124.2 (2)
C1—C2—H2	121.2	C16—C11—N4	116.3 (2)
C3—C2—H2	121.2	C13—C12—C11	117.6 (3)

C4—C3—C2	120.4 (3)	C13—C12—H12	121.2
C4—C3—H3	119.8	C11—C12—H12	121.2
C2—C3—H3	119.8	C14—C13—F2	118.2 (3)
F1—C4—C3	118.7 (3)	C14—C13—C12	124.4 (3)
F1—C4—C5	118.1 (4)	F2—C13—C12	117.5 (3)
C3—C4—C5	123.2 (4)	C13—C14—C15	117.0 (3)
C4—C5—C6	116.7 (3)	C13—C14—H14	121.5
C4—C5—H5	121.7	C15—C14—H14	121.5
C6—C5—H5	121.7	C14—C15—C16	121.0 (3)
C5—C6—C1	121.1 (3)	C14—C15—H15	119.5
C5—C6—C7	132.6 (3)	C16—C15—H15	119.5
C1—C6—C7	106.3 (3)	C15—C16—C11	120.6 (3)
N2—C7—C6	125.4 (3)	C15—C16—H16	119.7
N2—C7—C8	127.6 (3)	C11—C16—H16	119.7
C6—C7—C8	107.0 (2)	C8—N1—C1	110.8 (3)
O1—C8—N1	127.5 (3)	C8—N1—C9	123.6 (3)
O1—C8—C7	126.9 (3)	C1—N1—C9	125.5 (3)
N1—C8—C7	105.6 (3)	C7—N2—N3	117.2 (2)
N1—C9—H9A	109.5	N2—N3—C10	119.9 (2)
N1—C9—H9B	109.5	N2—N3—H3N	120.5 (19)
H9A—C9—H9B	109.5	C10—N3—H3N	119.4 (19)
N1—C9—H9C	109.5	C10—N4—C11	132.9 (2)
H9A—C9—H9C	109.5	C10—N4—H4N	111 (2)
H9B—C9—H9C	109.5	C11—N4—H4N	116 (2)
N4—C10—N3	113.0 (2)		

C6—C1—C2—C3	0.2 (5)	C11—C12—C13—F2	180.0 (3)
N1—C1—C2—C3	−179.0 (3)	F2—C13—C14—C15	−179.5 (3)
C1—C2—C3—C4	−0.4 (5)	C12—C13—C14—C15	0.3 (5)
C2—C3—C4—F1	−179.7 (3)	C13—C14—C15—C16	−0.4 (5)
C2—C3—C4—C5	−0.1 (6)	C14—C15—C16—C11	0.2 (5)
F1—C4—C5—C6	−179.7 (3)	C12—C11—C16—C15	0.3 (5)
C3—C4—C5—C6	0.8 (5)	N4—C11—C16—C15	−178.5 (3)
C4—C5—C6—C1	−0.9 (5)	O1—C8—N1—C1	180.0 (3)
C4—C5—C6—C7	179.9 (3)	C7—C8—N1—C1	0.8 (3)
C2—C1—C6—C5	0.4 (5)	O1—C8—N1—C9	1.9 (5)
N1—C1—C6—C5	179.8 (3)	C7—C8—N1—C9	−177.3 (3)
C2—C1—C6—C7	179.8 (3)	C2—C1—N1—C8	179.3 (3)
N1—C1—C6—C7	−0.8 (3)	C6—C1—N1—C8	0.0 (4)
C5—C6—C7—N2	1.5 (5)	C2—C1—N1—C9	−2.7 (5)
C1—C6—C7—N2	−177.7 (3)	C6—C1—N1—C9	178.0 (3)
C5—C6—C7—C8	−179.5 (3)	C6—C7—N2—N3	177.4 (3)
C1—C6—C7—C8	1.2 (3)	C8—C7—N2—N3	−1.4 (4)
N2—C7—C8—O1	−1.5 (5)	C7—N2—N3—C10	−174.9 (3)
C6—C7—C8—O1	179.6 (3)	N4—C10—N3—N2	−6.1 (4)
N2—C7—C8—N1	177.7 (3)	S1—C10—N3—N2	172.6 (2)
C6—C7—C8—N1	−1.2 (3)	N3—C10—N4—C11	−177.7 (3)
C16—C11—C12—C13	−0.5 (5)	S1—C10—N4—C11	3.7 (5)

N4—C11—C12—C13	178.3 (3)	C12—C11—N4—C10	10.3 (5)
C11—C12—C13—C14	0.2 (5)	C16—C11—N4—C10	−170.9 (3)

Hydrogen-bond geometry (Å, º)

Cg1 is a centroid of the N1/C1/C6–C8 cyclopentene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···O1	0.88 (3)	2.08 (3)	2.761 (3)	134 (2)
N4—H4*N*···N2	0.87 (3)	2.07 (3)	2.579 (3)	117 (3)
C2—H2···F2^{i}	0.93	2.44	3.370 (5)	176
C9—H9*A*···O1	0.96	2.54	2.921 (4)	104
C12—H12···S1	0.93	2.60	3.251 (3)	127
C10—S1···*Cg*1^{ii}	1.66 (1)	3.78 (1)	4.467 (3)	103 (1)

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