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4-(2-Fluorophenyl)-1-(2-oxoindolin-3-ylidene)thiosemicarbazide

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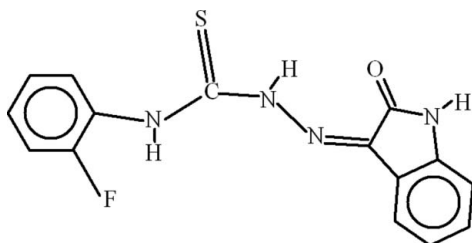
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.047; wR factor = 0.114; data-to-parameter ratio = 13.2.

The title compound, $\text{C}_{15}\text{H}_{11}\text{FN}_4\text{OS}$, is almost planar, the dihedral angle between the aromatic ring systems being 5.00 (13)°. The conformation is stabilized by intramolecular $\text{N}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, which generate $S(5)$ and $S(6)$ rings, respectively. $\text{N}-\text{H}\cdots\text{F}$ and $\text{C}-\text{H}\cdots\text{S}$ interactions also occur. In the crystal, inversion dimers linked by pairs of $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds occur, generating $R_2^2(8)$ loops.

Related literature

For related structures and medicinal background, see: Pervez *et al.* (2009, 2010). For graph-set theory, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{11}\text{FN}_4\text{OS}$
 $M_r = 314.34$
 Monoclinic, $P2_1/c$
 $a = 5.7646$ (3) Å

$b = 18.4939$ (12) Å
 $c = 13.6772$ (8) Å
 $\beta = 91.212$ (3)°
 $V = 1457.80$ (15) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹

$T = 296$ K
 $0.30 \times 0.14 \times 0.12$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.963$, $T_{\max} = 0.971$

11407 measured reflections
 2626 independent reflections
 1437 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.068$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.114$
 $S = 0.96$
 2626 reflections

199 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}^i$	0.86	2.07	2.912 (3)	164
$\text{N3}-\text{H3}\cdots\text{O1}$	0.86	2.08	2.762 (3)	135
$\text{N4}-\text{H4A}\cdots\text{F1}$	0.86	2.21	2.613 (2)	109
$\text{N4}-\text{H4A}\cdots\text{N2}$	0.86	2.13	2.585 (3)	113
$\text{C15}-\text{H15}\cdots\text{S1}$	0.93	2.56	3.216 (3)	128

Symmetry code: (i) $-x + 2, -y, -z$.

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5381).

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supporting information

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4-(2-Fluorophenyl)-1-(2-oxoindolin-3-ylidene)thiosemicarbazide

Humayun Pervez, Muhammad Yaqub, Muhammad Ramzan, Mohammad S. Iqbal and M. Nawaz Tahir

S1. Comment

As part of our ongoing studies of N⁴-arylsubstituted isatins-3-thiosemicarbazones with certain medicinal applications (Pervez *et al.*, 2009, 2010), we now report the synthesis and crystal structure of the title compound (I, Fig. 1).

The crystal structure of (II) i.e. 1-(5-nitro-2-oxoindolino-3-ylidene)-4-*o*-tolylthiosemicarbazide methanol monosolvate (Pervez *et al.*, 2009) has been published. The title compound (I) differs from (II) due to the absence of nitro function at position-5 of the isatin scaffold and presence of fluoro instead of methyl group at position-2 of the phenyl ring substituted at N⁴ of the thiosemicarbazone moiety. In (I), the 2-oxoindolin A (C1–C8/N1/O1), thiosemicarbazide B (N2/N3/C9/S1/N4) and the 2-fluorophenyl C (C10—C15/F1) are planar with maximum r. m. s. deviations of 0.0289, 0.0261 and 0.0056 Å, respectively. Due to intramolecular H-bondings (Table 1, Fig. 1), two S(5) and two S(6) (Bernstein *et al.*, 1995) ring motifs are formed. The molecules are dimerised due to intermolecular H-bonding of N—H···O type with R₂²(8) ring motifs.

S2. Experimental

To a hot solution of isatin (0.74 g, 5.0 mmol) in ethanol (10 ml) containing a few drops of glacial acetic acid was added 4-*o*-fluorophenylthiosemicarbazide (0.93 g, 5.0 mmol) dissolved in ethanol (10 ml) under stirring. The reaction mixture was then heated under reflux for 2 h. The yellow crystalline solid formed during refluxing was collected by suction filtration. Thorough washing with hot ethanol followed by ether furnished the target compound (I) in pure form (1.20 g, 76%), m.p. 505-507 K (d). The dark yellow needles of (I) were grown in ethyl acetate-petroleum ether (1:5) system by diffusion method at room temperature.

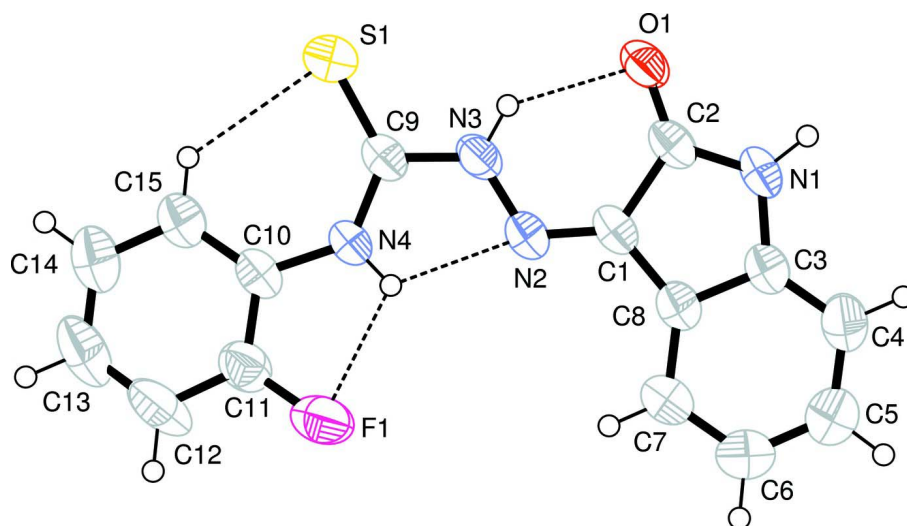


Figure 1

View of (I) with ellipsoids drawn at the 50% probability level. The dotted lines indicate the intramolecular H-bonds.

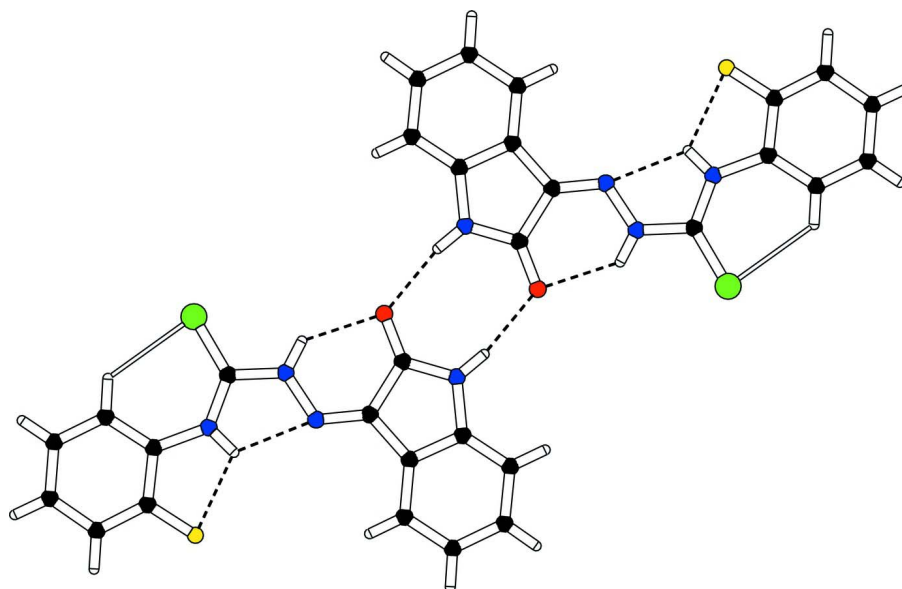


Figure 2

The partial packing of (I), which shows that molecules form inversion dimers.

4-(2-Fluorophenyl)-1-(2-oxoindolin-3-ylidene)thiosemicarbazide

Crystal data

$C_{15}H_{11}FN_4OS$

$M_r = 314.34$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 5.7646\ (3)\ \text{\AA}$

$b = 18.4939\ (12)\ \text{\AA}$

$c = 13.6772\ (8)\ \text{\AA}$

$\beta = 91.212\ (3)^\circ$

$V = 1457.80\ (15)\ \text{\AA}^3$

$Z = 4$

$F(000) = 648$

$D_x = 1.432\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2626 reflections

$\theta = 3.5\text{--}25.3^\circ$

$\mu = 0.24\ \text{mm}^{-1}$

$T = 296$ K $0.30 \times 0.14 \times 0.12$ mm
 Needle, dark yellow

Data collection

Bruker Kappa APEXII CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator Detector resolution: 7.80 pixels mm^{-1} ω scans Absorption correction: multi-scan (SADABS; Bruker, 2005) $T_{\min} = 0.963$, $T_{\max} = 0.971$	11407 measured reflections 2626 independent reflections 1437 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.068$ $\theta_{\max} = 25.3^\circ$, $\theta_{\min} = 3.5^\circ$ $h = -6 \rightarrow 6$ $k = -21 \rightarrow 22$ $l = -16 \rightarrow 16$
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Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.047$ $wR(F^2) = 0.114$ $S = 0.96$ 2626 reflections 199 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 $w = 1/[\sigma^2(F_o^2) + (0.0467P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$
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Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R - factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.09191 (15)	0.20047 (5)	0.00689 (6)	0.0742 (3)
F1	-0.0601 (3)	0.14317 (12)	0.37578 (11)	0.0911 (9)
O1	0.7157 (3)	0.04818 (11)	0.01234 (13)	0.0575 (8)
N1	0.9081 (4)	-0.02584 (13)	0.12316 (16)	0.0547 (9)
N2	0.4000 (4)	0.06836 (12)	0.18384 (15)	0.0489 (8)
N3	0.3340 (4)	0.10541 (12)	0.10344 (15)	0.0510 (8)
N4	0.0393 (3)	0.15113 (12)	0.19057 (14)	0.0499 (8)
C1	0.5848 (5)	0.02916 (15)	0.17922 (19)	0.0474 (10)
C2	0.7385 (5)	0.01971 (16)	0.0932 (2)	0.0494 (11)
C3	0.8851 (5)	-0.04562 (15)	0.2217 (2)	0.0513 (10)
C4	1.0273 (5)	-0.08819 (17)	0.2785 (2)	0.0696 (12)
C5	0.9689 (6)	-0.09758 (19)	0.3747 (3)	0.0803 (14)
C6	0.7757 (6)	-0.06518 (19)	0.4128 (2)	0.0774 (15)
C7	0.6305 (5)	-0.02238 (17)	0.3550 (2)	0.0658 (11)

C8	0.6871 (4)	-0.01264 (15)	0.25825 (19)	0.0494 (10)
C9	0.1480 (5)	0.15218 (15)	0.10471 (18)	0.0486 (10)
C10	-0.1520 (4)	0.19126 (15)	0.22268 (19)	0.0479 (10)
C11	-0.2029 (5)	0.18597 (18)	0.3198 (2)	0.0626 (11)
C12	-0.3861 (6)	0.2210 (2)	0.3614 (3)	0.0864 (14)
C13	-0.5248 (6)	0.2633 (2)	0.3026 (3)	0.0849 (16)
C14	-0.4818 (5)	0.26920 (18)	0.2062 (3)	0.0743 (14)
C15	-0.2977 (5)	0.23337 (16)	0.1658 (2)	0.0623 (11)
H1	1.01726	-0.04097	0.08643	0.0657*
H3	0.40914	0.09984	0.05030	0.0611*
H4	1.15840	-0.10996	0.25313	0.0834*
H4A	0.09573	0.12107	0.23275	0.0598*
H5	1.06218	-0.12647	0.41499	0.0960*
H6	0.74193	-0.07212	0.47828	0.0929*
H7	0.49911	-0.00091	0.38065	0.0791*
H12	-0.41496	0.21619	0.42776	0.1037*
H13	-0.64912	0.28809	0.32902	0.1015*
H14	-0.57770	0.29779	0.16668	0.0892*
H15	-0.27161	0.23771	0.09919	0.0747*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0779 (6)	0.0878 (7)	0.0577 (5)	0.0167 (5)	0.0193 (4)	0.0148 (5)
F1	0.0833 (14)	0.1408 (19)	0.0495 (10)	0.0171 (13)	0.0103 (9)	-0.0024 (11)
O1	0.0453 (12)	0.0735 (15)	0.0543 (12)	0.0021 (10)	0.0167 (9)	-0.0014 (11)
N1	0.0398 (14)	0.0640 (17)	0.0610 (15)	0.0076 (12)	0.0148 (11)	-0.0042 (13)
N2	0.0410 (14)	0.0541 (15)	0.0519 (14)	0.0019 (12)	0.0100 (11)	-0.0051 (12)
N3	0.0481 (14)	0.0577 (16)	0.0477 (14)	0.0049 (12)	0.0153 (11)	-0.0039 (12)
N4	0.0460 (14)	0.0585 (16)	0.0455 (13)	0.0098 (12)	0.0118 (11)	-0.0016 (11)
C1	0.0397 (16)	0.0486 (18)	0.0544 (17)	-0.0033 (14)	0.0127 (13)	-0.0092 (14)
C2	0.0399 (17)	0.055 (2)	0.0537 (18)	-0.0072 (15)	0.0124 (13)	-0.0104 (15)
C3	0.0417 (17)	0.0550 (19)	0.0574 (18)	0.0009 (15)	0.0072 (14)	-0.0036 (16)
C4	0.054 (2)	0.076 (2)	0.079 (2)	0.0149 (18)	0.0073 (17)	0.0046 (19)
C5	0.075 (2)	0.089 (3)	0.077 (2)	0.017 (2)	0.0008 (19)	0.012 (2)
C6	0.086 (3)	0.090 (3)	0.0564 (19)	0.010 (2)	0.0068 (18)	0.0090 (19)
C7	0.065 (2)	0.077 (2)	0.0558 (19)	0.0075 (19)	0.0142 (16)	-0.0024 (17)
C8	0.0425 (17)	0.0527 (19)	0.0532 (17)	0.0001 (14)	0.0055 (13)	-0.0062 (15)
C9	0.0448 (17)	0.0512 (18)	0.0504 (16)	-0.0002 (15)	0.0124 (13)	-0.0052 (14)
C10	0.0404 (16)	0.0517 (19)	0.0518 (17)	-0.0038 (15)	0.0073 (13)	-0.0137 (14)
C11	0.0508 (19)	0.085 (2)	0.0519 (18)	0.0027 (18)	0.0005 (15)	-0.0134 (17)
C12	0.065 (2)	0.131 (3)	0.064 (2)	0.001 (2)	0.0214 (18)	-0.036 (2)
C13	0.049 (2)	0.106 (3)	0.100 (3)	0.008 (2)	0.010 (2)	-0.044 (2)
C14	0.053 (2)	0.075 (2)	0.095 (3)	0.0098 (18)	0.0041 (18)	-0.016 (2)
C15	0.0504 (18)	0.069 (2)	0.068 (2)	0.0058 (17)	0.0099 (15)	-0.0038 (17)

Geometric parameters (Å, °)

S1—C9	1.635 (3)	C5—C6	1.377 (5)
F1—C11	1.365 (4)	C6—C7	1.387 (4)
O1—C2	1.229 (3)	C7—C8	1.381 (4)
N1—C2	1.348 (4)	C10—C15	1.375 (4)
N1—C3	1.406 (4)	C10—C11	1.370 (4)
N2—N3	1.344 (3)	C11—C12	1.373 (5)
N2—C1	1.291 (4)	C12—C13	1.368 (5)
N3—C9	1.378 (4)	C13—C14	1.351 (6)
N4—C9	1.343 (3)	C14—C15	1.377 (4)
N4—C10	1.407 (3)	C4—H4	0.9300
N1—H1	0.8600	C5—H5	0.9300
N3—H3	0.8600	C6—H6	0.9300
N4—H4A	0.8600	C7—H7	0.9300
C1—C8	1.445 (4)	C12—H12	0.9300
C1—C2	1.498 (4)	C13—H13	0.9300
C3—C8	1.396 (4)	C14—H14	0.9300
C3—C4	1.367 (4)	C15—H15	0.9300
C4—C5	1.376 (5)		
S1…C15	3.216 (3)	C9…C2 ^{vi}	3.403 (4)
S1…C13 ⁱ	3.661 (4)	C9…C14 ⁱⁱⁱ	3.323 (4)
S1…C11 ⁱⁱ	3.696 (3)	C9…O1 ^{vi}	3.372 (3)
S1…C12 ⁱⁱ	3.665 (4)	C10…C1 ^{vi}	3.407 (4)
S1…H15	2.5600	C11…S1 ^{vii}	3.696 (3)
S1…H13 ⁱ	2.8900	C12…S1 ^{vii}	3.665 (4)
F1…N4	2.613 (2)	C13…S1 ^{viii}	3.661 (4)
F1…H4A	2.2100	C14…C9 ^{vi}	3.323 (4)
O1…N2	3.022 (3)	C15…N3 ^{vi}	3.280 (4)
O1…N3	2.762 (3)	C15…S1	3.216 (3)
O1…C9 ⁱⁱⁱ	3.372 (3)	C2…H3	2.4700
O1…N3 ^{iv}	3.262 (3)	C2…H3 ^{iv}	3.0600
O1…O1 ^{iv}	3.072 (3)	C2…H1 ^v	2.8800
O1…N1 ^v	2.912 (3)	C5…H14 ^{ix}	3.0200
O1…C2 ^{iv}	3.218 (3)	C6…H14 ^{ix}	2.9800
O1…H3	2.0800	C9…H15	2.8900
O1…H1 ^v	2.0700	C14…H4 ^x	2.9600
N1…O1 ^v	2.912 (3)	H1…O1 ^v	2.0700
N2…O1	3.022 (3)	H1…C2 ^v	2.8800
N2…N4	2.585 (3)	H3…O1	2.0800
N3…O1 ^{iv}	3.262 (3)	H3…C2	2.4700
N3…O1	2.762 (3)	H3…C2 ^{iv}	3.0600
N3…C15 ⁱⁱⁱ	3.280 (4)	H4…C14 ^{xi}	2.9600
N4…C2 ^{vi}	3.254 (4)	H4A…F1	2.2100
N4…F1	2.613 (2)	H4A…N2	2.1300
N4…N2	2.585 (3)	H13…S1 ^{viii}	2.8900
N2…H4A	2.1300	H14…C5 ^{xii}	3.0200

C1...C10 ⁱⁱⁱ	3.407 (4)	H14...C6 ^{xii}	2.9800
C2...N4 ⁱⁱⁱ	3.254 (4)	H15...S1	2.5600
C2...C9 ⁱⁱⁱ	3.403 (4)	H15...C9	2.8900
C2...O1 ^{iv}	3.218 (3)		
C2—N1—C3	111.8 (2)	S1—C9—N4	129.5 (2)
N3—N2—C1	117.8 (2)	C11—C10—C15	116.6 (2)
N2—N3—C9	121.1 (2)	N4—C10—C15	126.6 (2)
C9—N4—C10	130.4 (2)	N4—C10—C11	116.8 (2)
C3—N1—H1	124.00	C10—C11—C12	123.4 (3)
C2—N1—H1	124.00	F1—C11—C10	116.5 (2)
N2—N3—H3	119.00	F1—C11—C12	120.1 (3)
C9—N3—H3	119.00	C11—C12—C13	118.1 (4)
C10—N4—H4A	115.00	C12—C13—C14	120.2 (3)
C9—N4—H4A	115.00	C13—C14—C15	120.8 (3)
N2—C1—C2	127.3 (2)	C10—C15—C14	120.8 (3)
C2—C1—C8	106.6 (2)	C3—C4—H4	121.00
N2—C1—C8	126.0 (2)	C5—C4—H4	121.00
N1—C2—C1	105.8 (2)	C4—C5—H5	119.00
O1—C2—N1	127.2 (3)	C6—C5—H5	119.00
O1—C2—C1	127.1 (3)	C5—C6—H6	119.00
N1—C3—C4	128.9 (3)	C7—C6—H6	119.00
N1—C3—C8	108.9 (2)	C6—C7—H7	121.00
C4—C3—C8	122.2 (3)	C8—C7—H7	121.00
C3—C4—C5	117.4 (3)	C11—C12—H12	121.00
C4—C5—C6	121.6 (3)	C13—C12—H12	121.00
C5—C6—C7	121.1 (3)	C12—C13—H13	120.00
C6—C7—C8	117.9 (3)	C14—C13—H13	120.00
C1—C8—C3	106.9 (2)	C13—C14—H14	120.00
C3—C8—C7	119.8 (2)	C15—C14—H14	120.00
C1—C8—C7	133.3 (2)	C10—C15—H15	120.00
S1—C9—N3	118.23 (19)	C14—C15—H15	120.00
N3—C9—N4	112.3 (2)		
C3—N1—C2—O1	177.5 (3)	C8—C3—C4—C5	-0.2 (5)
C3—N1—C2—C1	-1.8 (3)	N1—C3—C8—C1	-0.2 (3)
C2—N1—C3—C4	-177.2 (3)	N1—C3—C8—C7	-178.3 (3)
C2—N1—C3—C8	1.3 (3)	C4—C3—C8—C1	178.5 (3)
C1—N2—N3—C9	-175.5 (3)	C4—C3—C8—C7	0.3 (4)
N3—N2—C1—C2	0.0 (4)	C3—C4—C5—C6	-0.4 (5)
N3—N2—C1—C8	178.0 (2)	C4—C5—C6—C7	0.8 (5)
N2—N3—C9—S1	174.9 (2)	C5—C6—C7—C8	-0.7 (5)
N2—N3—C9—N4	-4.4 (4)	C6—C7—C8—C1	-177.4 (3)
C10—N4—C9—S1	-0.8 (4)	C6—C7—C8—C3	0.1 (4)
C10—N4—C9—N3	178.3 (2)	N4—C10—C11—F1	1.1 (4)
C9—N4—C10—C11	-170.6 (3)	N4—C10—C11—C12	-179.0 (3)
C9—N4—C10—C15	11.8 (4)	C15—C10—C11—F1	179.0 (3)
N2—C1—C2—O1	0.6 (5)	C15—C10—C11—C12	-1.1 (5)

N2—C1—C2—N1	180.0 (3)	N4—C10—C15—C14	179.0 (3)
C8—C1—C2—O1	-177.7 (3)	C11—C10—C15—C14	1.3 (4)
C8—C1—C2—N1	1.7 (3)	F1—C11—C12—C13	-180.0 (3)
N2—C1—C8—C3	-179.2 (3)	C10—C11—C12—C13	0.1 (5)
N2—C1—C8—C7	-1.5 (5)	C11—C12—C13—C14	0.7 (5)
C2—C1—C8—C3	-0.9 (3)	C12—C13—C14—C15	-0.5 (5)
C2—C1—C8—C7	176.9 (3)	C13—C14—C15—C10	-0.6 (5)
N1—C3—C4—C5	178.1 (3)		

Symmetry codes: (i) $x+1, -y+1/2, z-1/2$; (ii) $x, -y+1/2, z-1/2$; (iii) $x+1, y, z$; (iv) $-x+1, -y, -z$; (v) $-x+2, -y, -z$; (vi) $x-1, y, z$; (vii) $x, -y+1/2, z+1/2$; (viii) $x-1, -y+1/2, z+1/2$; (ix) $-x, y-1/2, -z+1/2$; (x) $-x+1, y+1/2, -z+1/2$; (xi) $-x+1, y-1/2, -z+1/2$; (xii) $-x, y+1/2, -z+1/2$.

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1...O1 ^v	0.86	2.07	2.912 (3)	164
N3—H3...O1	0.86	2.08	2.762 (3)	135
N4—H4A...F1	0.86	2.21	2.613 (2)	109
N4—H4A...N2	0.86	2.13	2.585 (3)	113
C15—H15...S1	0.93	2.56	3.216 (3)	128

Symmetry code: (v) $-x+2, -y, -z$.