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3-Amino-N-benzyl-6-(4-fluorophenyl)-thieno[2,3-*b*]pyridine-2-carboxamide

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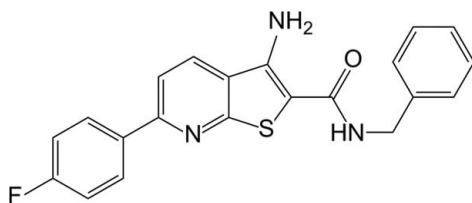
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.044; wR factor = 0.104; data-to-parameter ratio = 14.3.

In the title compound, $\text{C}_{21}\text{H}_{16}\text{FN}_3\text{OS}$, the thieno[2,3-*b*]pyridine system forms dihedral angles of 10.57 (12) and 83.87 (5)° with the fluorophenyl ring at the 6-position and the phenyl ring of the benzyl group, respectively. In the crystal, molecules are linked by weak $\text{N}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds and $\pi-\pi$ stacking interactions involving fluorophenyl rings of adjacent molecules, with a centroid-centroid distance of 3.648 (10) Å. In addition, intramolecular $\text{N}-\text{H}\cdots\text{S}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds contribute to the stability of the molecular conformation.

Related literature

For the biological activity of thieno[2,3-*b*]pyridine derivatives, see: Litvinov *et al.* (2005).



Experimental

Crystal data

 $\text{C}_{21}\text{H}_{16}\text{FN}_3\text{OS}$
 $M_r = 377.43$

 Monoclinic, $P2_1/c$
 $a = 18.9008$ (7) Å

 $b = 9.9828$ (4) Å
 $c = 9.5924$ (4) Å
 $\beta = 102.224$ (4)°
 $V = 1768.89$ (11) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 0.21$ mm⁻¹
 $T = 293$ K
 $0.40 \times 0.30 \times 0.10$ mm

Data collection

 Oxford Diffraction Xcalibur Eos diffractometer
 Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2006)
 $T_{\min} = 0.991$, $T_{\max} = 1.000$

 7919 measured reflections
 3609 independent reflections
 2665 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.104$
 $S = 1.03$
 3609 reflections
 252 parameters

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3}\cdots\text{S1}$	0.86	2.68	3.0897 (16)	111
$\text{N3}-\text{H3}\cdots\text{N2}^{\text{i}}$	0.86	2.51	3.253 (2)	146
$\text{N2}-\text{H2B}\cdots\text{O1}$	0.90 (2)	2.15 (2)	2.741 (2)	122.7 (17)
$\text{N2}-\text{H2B}\cdots\text{O1}^{\text{ii}}$	0.90 (2)	2.20 (2)	3.015 (2)	150.0 (17)

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *OLEX2*.

We thank the Analytical and Testing Center of Sichuan University for the X-ray measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2191).

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supplementary materials

Acta Cryst. (2012). E68, o1823 [doi:10.1107/S160053681202212X]

3-Amino-*N*-benzyl-6-(4-fluorophenyl)thieno[2,3-*b*]pyridine-2-carboxamide

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Comment

Thieno[2,3-*b*]pyridine derivatives are of great importance owing to their wide biological properties (Litvinov *et al.*, 2005). The title compound is one of the key intermediates in our synthetic investigations of anticancer drugs. Herein we report its crystal structure.

As shown in Fig. 1, the thieno[2,3-*b*]pyridine ring forms dihedral angles of 10.57(0.12)° and 83.87(0.05)° with the monofluoro-benzene at 6-position and the phenyl rings at 2-position, respectively. In the crystal packing, stacking interactions involving phenyl rings containing fluorine atom of adjacent molecules are helpful for the stabilization of the crystal as well as intermolecular N—H···N hydrogen bonds. In addition, intramolecular N—H···O and N—H···S hydrogen bonds help to stabilize the molecular conformation (Table 1 and Fig. 2).

Experimental

To a solution of 6-(4-fluorophenyl)-2-thioxo-1,2-dihydropyridine-3-carbonitrile (2.30 g, 10 mmol) in DMF (15.00 ml) was added dropwise a solution of 10% sodium hydroxide (8.00 ml). After stirring at room temperature for 0.5 h and then the temperature was raised to 85 °C and then 10% sodium hydroxide (8.00 ml) and *N*-benzyl-2-chloroacetamide (2.20 g, 12.0 mmol) were added. The reaction mixture was stirred under reflux until complete conversion of the starting materials (6 h, monitored by TLC). The mixture was then cooled to room temperature and crystallized to give 3.17 g of a yellow solid (84% yield). The product was recrystallized from ethanol to afford the title compound as an off-yellow solid (yield: 60%). Crystals suitable for X-ray analysis were obtained by slow evaporation using dichloromethane:methanol (2:1 v/v) as eluent.

Refinement

H atoms of the amino group were located in a difference map and refined freely. The remaining H atoms were positioned geometrically (C—H = 0.93–0.97 Å, N—H = 0.82–0.90 Å) and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2006); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

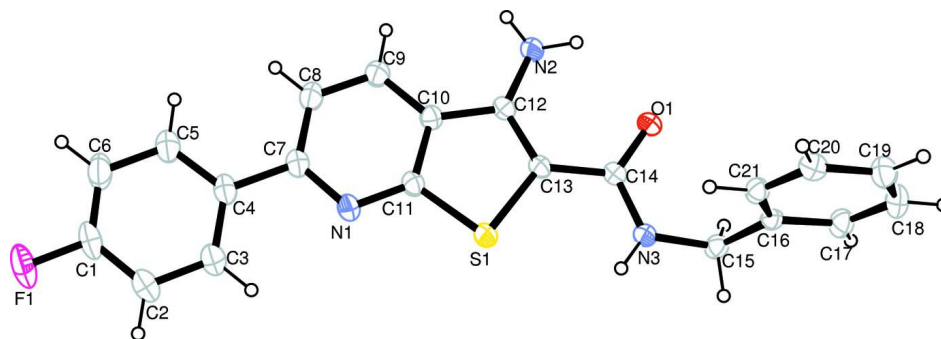


Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

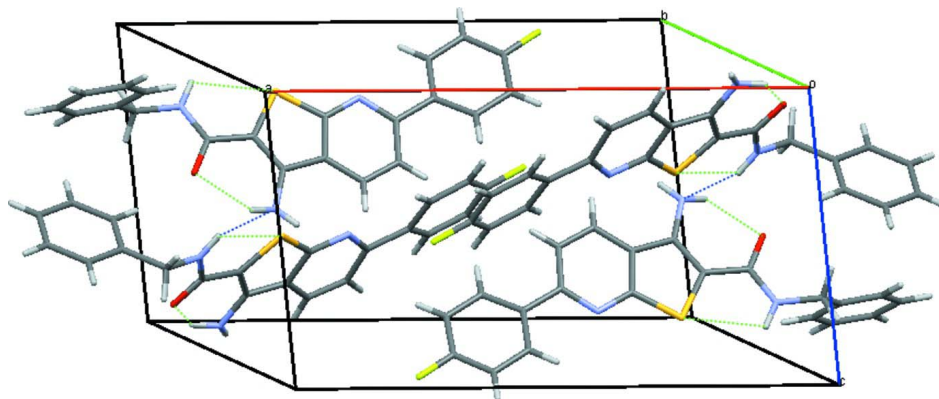


Figure 2

A packing diagram of the title compound, showing intermolecular hydrogen bonds of N—H...N as blue dashed lines, and intramolecular hydrogen bonds of N—H...O and N—H...S as green dashed lines

3-Amino-*N*-benzyl-6-(4-fluorophenyl)thieno[2,3-*b*]pyridine-2- carboxamide

Crystal data

$C_{21}H_{16}FN_3OS$

$M_r = 377.43$

Monoclinic, $P2_1/c$

$a = 18.9008 (7) \text{ \AA}$

$b = 9.9828 (4) \text{ \AA}$

$c = 9.5924 (4) \text{ \AA}$

$\beta = 102.224 (4)^\circ$

$V = 1768.89 (11) \text{ \AA}^3$

$Z = 4$

$F(000) = 784$

$D_x = 1.417 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.7107 \text{ \AA}$

Cell parameters from 2427 reflections

$\theta = 3.0\text{--}29.2^\circ$

$\mu = 0.21 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, yellow

$0.40 \times 0.30 \times 0.10 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur Eos
diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: $16.0874 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2006)

$T_{\min} = 0.991$, $T_{\max} = 1.000$

7919 measured reflections

3609 independent reflections

2665 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 3.0^\circ$
 $h = -21 \rightarrow 23$

$k = -12 \rightarrow 11$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.104$
 $S = 1.03$
 3609 reflections
 252 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.2875P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.20491 (3)	0.22083 (5)	0.33501 (5)	0.04353 (16)
F1	0.68007 (7)	0.14850 (17)	0.54263 (17)	0.0879 (5)
O1	0.01663 (7)	0.12650 (13)	0.08498 (13)	0.0415 (3)
N1	0.34252 (8)	0.16214 (16)	0.32473 (17)	0.0430 (4)
N2	0.12841 (11)	0.01149 (18)	-0.01334 (18)	0.0431 (4)
N3	0.03925 (8)	0.26248 (15)	0.27578 (16)	0.0371 (4)
H3	0.0698	0.2893	0.3502	0.044*
C1	0.61019 (12)	0.1375 (3)	0.4718 (3)	0.0612 (6)
C2	0.55976 (13)	0.2160 (3)	0.5132 (3)	0.0649 (7)
H2	0.5730	0.2768	0.5876	0.078*
C3	0.48814 (12)	0.2039 (2)	0.4427 (3)	0.0588 (6)
H3A	0.4532	0.2570	0.4706	0.071*
C4	0.46761 (11)	0.1141 (2)	0.3312 (2)	0.0467 (5)
C5	0.52116 (12)	0.0370 (3)	0.2941 (3)	0.0629 (7)
H5	0.5088	-0.0248	0.2204	0.075*
C6	0.59308 (12)	0.0489 (3)	0.3640 (3)	0.0682 (7)
H6	0.6287	-0.0031	0.3369	0.082*
C7	0.38985 (11)	0.0995 (2)	0.2613 (2)	0.0441 (5)
C8	0.36703 (11)	0.0228 (2)	0.1384 (2)	0.0560 (6)
H8	0.4013	-0.0189	0.0964	0.067*
C9	0.29486 (11)	0.0081 (2)	0.0786 (2)	0.0514 (6)
H9	0.2799	-0.0429	-0.0035	0.062*
C10	0.24457 (10)	0.07078 (18)	0.14290 (19)	0.0363 (4)

C11	0.27268 (10)	0.14647 (18)	0.26477 (19)	0.0370 (4)
C12	0.16689 (10)	0.07362 (17)	0.10565 (19)	0.0335 (4)
C13	0.13826 (10)	0.15083 (17)	0.19911 (18)	0.0334 (4)
C14	0.06103 (10)	0.17874 (17)	0.18296 (18)	0.0322 (4)
C15	-0.03518 (10)	0.30762 (18)	0.2511 (2)	0.0383 (5)
H15A	-0.0510	0.3280	0.1504	0.046*
H15B	-0.0365	0.3905	0.3032	0.046*
C16	-0.08885 (10)	0.21225 (17)	0.29233 (18)	0.0337 (4)
C17	-0.16173 (11)	0.2454 (2)	0.2581 (2)	0.0465 (5)
H17	-0.1762	0.3236	0.2073	0.056*
C18	-0.21297 (12)	0.1646 (2)	0.2981 (3)	0.0582 (6)
H18	-0.2615	0.1892	0.2755	0.070*
C19	-0.19253 (12)	0.0472 (2)	0.3715 (2)	0.0540 (6)
H19	-0.2270	-0.0075	0.3988	0.065*
C20	-0.12068 (11)	0.0121 (2)	0.4037 (2)	0.0451 (5)
H20	-0.1066	-0.0674	0.4521	0.054*
C21	-0.06921 (10)	0.09380 (18)	0.36486 (19)	0.0382 (4)
H21	-0.0207	0.0689	0.3877	0.046*
H2A	0.1510 (12)	-0.042 (2)	-0.052 (2)	0.056 (7)*
H2B	0.0817 (12)	-0.005 (2)	-0.013 (2)	0.050 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0332 (3)	0.0534 (3)	0.0409 (3)	-0.0001 (2)	0.0009 (2)	-0.0129 (2)
F1	0.0331 (7)	0.1281 (13)	0.0949 (12)	-0.0129 (8)	-0.0034 (7)	0.0030 (10)
O1	0.0347 (7)	0.0465 (8)	0.0401 (8)	-0.0024 (6)	0.0006 (6)	-0.0115 (6)
N1	0.0315 (9)	0.0477 (10)	0.0467 (10)	-0.0001 (8)	0.0010 (8)	-0.0024 (8)
N2	0.0341 (10)	0.0547 (11)	0.0402 (10)	-0.0041 (9)	0.0074 (8)	-0.0145 (8)
N3	0.0326 (9)	0.0431 (9)	0.0338 (8)	-0.0009 (7)	0.0032 (7)	-0.0076 (7)
C1	0.0297 (12)	0.0809 (17)	0.0694 (16)	-0.0101 (12)	0.0023 (11)	0.0138 (14)
C2	0.0439 (14)	0.0742 (16)	0.0707 (17)	-0.0118 (13)	-0.0009 (12)	-0.0073 (13)
C3	0.0385 (13)	0.0658 (15)	0.0693 (16)	-0.0040 (12)	0.0050 (11)	-0.0043 (12)
C4	0.0320 (11)	0.0515 (12)	0.0553 (13)	-0.0018 (10)	0.0060 (10)	0.0072 (10)
C5	0.0375 (13)	0.0783 (17)	0.0714 (17)	0.0007 (12)	0.0083 (12)	-0.0095 (13)
C6	0.0351 (13)	0.0916 (19)	0.0772 (18)	0.0046 (13)	0.0108 (12)	-0.0017 (15)
C7	0.0341 (11)	0.0488 (12)	0.0481 (12)	0.0001 (10)	0.0057 (9)	0.0025 (9)
C8	0.0366 (12)	0.0725 (15)	0.0592 (14)	0.0053 (11)	0.0109 (11)	-0.0146 (12)
C9	0.0399 (12)	0.0651 (14)	0.0478 (13)	0.0023 (11)	0.0057 (10)	-0.0162 (10)
C10	0.0332 (10)	0.0390 (10)	0.0357 (10)	0.0003 (9)	0.0049 (8)	0.0007 (8)
C11	0.0320 (10)	0.0388 (10)	0.0379 (10)	-0.0003 (9)	0.0024 (8)	0.0020 (8)
C12	0.0337 (10)	0.0339 (9)	0.0317 (10)	-0.0023 (8)	0.0040 (8)	0.0024 (8)
C13	0.0319 (10)	0.0345 (10)	0.0318 (9)	-0.0022 (8)	0.0022 (8)	-0.0003 (8)
C14	0.0336 (10)	0.0316 (9)	0.0301 (9)	-0.0017 (8)	0.0040 (8)	0.0028 (7)
C15	0.0375 (11)	0.0389 (10)	0.0375 (11)	0.0074 (9)	0.0058 (9)	-0.0005 (8)
C16	0.0346 (10)	0.0358 (10)	0.0298 (9)	0.0027 (9)	0.0046 (8)	-0.0074 (7)
C17	0.0375 (12)	0.0476 (12)	0.0527 (13)	0.0085 (10)	0.0060 (10)	0.0030 (9)
C18	0.0320 (12)	0.0698 (15)	0.0725 (16)	0.0062 (12)	0.0104 (11)	-0.0006 (13)
C19	0.0427 (13)	0.0606 (14)	0.0607 (14)	-0.0075 (11)	0.0157 (11)	-0.0009 (11)
C20	0.0473 (13)	0.0445 (11)	0.0435 (12)	-0.0018 (10)	0.0094 (10)	0.0000 (9)

C21	0.0339 (11)	0.0447 (11)	0.0349 (10)	0.0043 (9)	0.0045 (8)	-0.0008 (8)
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Geometric parameters (Å, °)

S1—C11	1.7353 (19)	C7—C8	1.394 (3)
S1—C13	1.7548 (18)	C8—H8	0.9300
F1—C1	1.356 (2)	C8—C9	1.371 (3)
O1—C14	1.235 (2)	C9—H9	0.9300
N1—C7	1.339 (2)	C9—C10	1.387 (3)
N1—C11	1.333 (2)	C10—C11	1.399 (2)
N2—C12	1.366 (2)	C10—C12	1.436 (3)
N2—H2A	0.82 (2)	C12—C13	1.377 (2)
N2—H2B	0.90 (2)	C13—C14	1.462 (2)
N3—H3	0.8600	C15—H15A	0.9700
N3—C14	1.348 (2)	C15—H15B	0.9700
N3—C15	1.448 (2)	C15—C16	1.504 (3)
C1—C2	1.357 (3)	C16—C17	1.387 (3)
C1—C6	1.347 (3)	C16—C21	1.382 (2)
C2—H2	0.9300	C17—H17	0.9300
C2—C3	1.384 (3)	C17—C18	1.376 (3)
C3—H3A	0.9300	C18—H18	0.9300
C3—C4	1.386 (3)	C18—C19	1.379 (3)
C4—C5	1.377 (3)	C19—H19	0.9300
C4—C7	1.488 (3)	C19—C20	1.373 (3)
C5—H5	0.9300	C20—H20	0.9300
C5—C6	1.388 (3)	C20—C21	1.380 (3)
C6—H6	0.9300	C21—H21	0.9300
C11—S1—C13	90.80 (9)	C11—C10—C12	112.62 (16)
C11—N1—C7	116.41 (17)	N1—C11—S1	121.82 (15)
C12—N2—H2A	116.1 (16)	N1—C11—C10	126.18 (18)
C12—N2—H2B	115.6 (13)	C10—C11—S1	112.00 (14)
H2A—N2—H2B	119 (2)	N2—C12—C10	122.31 (17)
C14—N3—H3	119.8	N2—C12—C13	125.82 (18)
C14—N3—C15	120.47 (15)	C13—C12—C10	111.78 (16)
C15—N3—H3	119.8	C12—C13—S1	112.79 (14)
F1—C1—C2	118.5 (2)	C12—C13—C14	123.99 (16)
C6—C1—F1	119.2 (2)	C14—C13—S1	123.12 (13)
C6—C1—C2	122.3 (2)	O1—C14—N3	120.75 (17)
C1—C2—H2	120.6	O1—C14—C13	120.16 (16)
C1—C2—C3	118.8 (2)	N3—C14—C13	119.09 (16)
C3—C2—H2	120.6	N3—C15—H15A	108.2
C2—C3—H3A	119.4	N3—C15—H15B	108.2
C2—C3—C4	121.2 (2)	N3—C15—C16	116.49 (15)
C4—C3—H3A	119.4	H15A—C15—H15B	107.3
C3—C4—C7	119.98 (19)	C16—C15—H15A	108.2
C5—C4—C3	117.4 (2)	C16—C15—H15B	108.2
C5—C4—C7	122.6 (2)	C17—C16—C15	118.56 (16)
C4—C5—H5	119.1	C21—C16—C15	123.34 (17)
C4—C5—C6	121.7 (2)	C21—C16—C17	118.10 (18)

C6—C5—H5	119.1	C16—C17—H17	119.5
C1—C6—C5	118.6 (2)	C18—C17—C16	121.10 (19)
C1—C6—H6	120.7	C18—C17—H17	119.5
C5—C6—H6	120.7	C17—C18—H18	119.9
N1—C7—C4	116.12 (18)	C17—C18—C19	120.2 (2)
N1—C7—C8	121.59 (18)	C19—C18—H18	119.9
C8—C7—C4	122.28 (19)	C18—C19—H19	120.4
C7—C8—H8	119.5	C20—C19—C18	119.2 (2)
C9—C8—C7	121.0 (2)	C20—C19—H19	120.4
C9—C8—H8	119.5	C19—C20—H20	119.7
C8—C9—H9	120.6	C19—C20—C21	120.6 (2)
C8—C9—C10	118.70 (19)	C21—C20—H20	119.7
C10—C9—H9	120.6	C16—C21—H21	119.6
C9—C10—C11	116.14 (18)	C20—C21—C16	120.79 (18)
C9—C10—C12	131.23 (18)	C20—C21—H21	119.6
S1—C13—C14—O1	179.94 (13)	C9—C10—C11—N1	-0.9 (3)
S1—C13—C14—N3	0.3 (2)	C9—C10—C12—N2	-2.3 (3)
F1—C1—C2—C3	-179.1 (2)	C9—C10—C12—C13	-179.1 (2)
F1—C1—C6—C5	178.8 (2)	C10—C12—C13—S1	-0.40 (19)
N1—C7—C8—C9	-0.5 (3)	C10—C12—C13—C14	176.11 (16)
N2—C12—C13—S1	-177.12 (15)	C11—S1—C13—C12	0.46 (14)
N2—C12—C13—C14	-0.6 (3)	C11—S1—C13—C14	-176.09 (15)
N3—C15—C16—C17	-173.84 (16)	C11—N1—C7—C4	-178.27 (17)
N3—C15—C16—C21	7.2 (2)	C11—N1—C7—C8	0.5 (3)
C1—C2—C3—C4	-0.3 (4)	C11—C10—C12—N2	176.96 (16)
C2—C1—C6—C5	-0.6 (4)	C11—C10—C12—C13	0.1 (2)
C2—C3—C4—C5	0.4 (3)	C12—C10—C11—S1	0.2 (2)
C2—C3—C4—C7	177.6 (2)	C12—C10—C11—N1	179.78 (17)
C3—C4—C5—C6	-0.7 (4)	C12—C13—C14—O1	3.8 (3)
C3—C4—C7—N1	-9.0 (3)	C12—C13—C14—N3	-175.88 (16)
C3—C4—C7—C8	172.3 (2)	C13—S1—C11—N1	-179.96 (16)
C4—C5—C6—C1	0.8 (4)	C13—S1—C11—C10	-0.39 (14)
C4—C7—C8—C9	178.2 (2)	C14—N3—C15—C16	80.5 (2)
C5—C4—C7—N1	167.95 (19)	C15—N3—C14—O1	-8.7 (3)
C5—C4—C7—C8	-10.8 (3)	C15—N3—C14—C13	170.97 (15)
C6—C1—C2—C3	0.4 (4)	C15—C16—C17—C18	-177.43 (18)
C7—N1—C11—S1	179.73 (14)	C15—C16—C21—C20	178.02 (17)
C7—N1—C11—C10	0.2 (3)	C16—C17—C18—C19	-1.0 (3)
C7—C4—C5—C6	-177.7 (2)	C17—C16—C21—C20	-0.9 (3)
C7—C8—C9—C10	-0.2 (3)	C17—C18—C19—C20	-0.2 (3)
C8—C9—C10—C11	0.8 (3)	C18—C19—C20—C21	0.8 (3)
C8—C9—C10—C12	180.0 (2)	C19—C20—C21—C16	-0.3 (3)
C9—C10—C11—S1	179.59 (15)	C21—C16—C17—C18	1.5 (3)

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>
N3—H3...S1	0.86	2.68	3.0897 (16)	111

N3—H3···N2 ⁱ	0.86	2.51	3.253 (2)	146
N2—H2B···O1	0.90 (2)	2.15 (2)	2.741 (2)	122.7 (17)
N2—H2B···O1 ⁱⁱ	0.90 (2)	2.20 (2)	3.015 (2)	150.0 (17)

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