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2-{[3-Methyl-4-(2,2,2-trifluoroethoxy)-pyridin-2-yl]methylsulfanyl}-1*H*-benzimidazole monohydrate: a monoclinic polymorph

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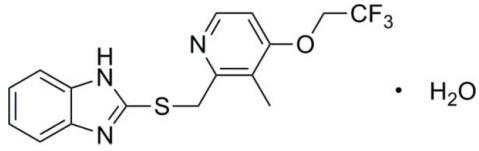
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.152; data-to-parameter ratio = 12.5.

The title compound, $C_{16}H_{14}F_3N_3OS\cdot H_2O$, which had been previously characterized in the space group $P\overline{1}$ [Ren *et al.* (2011). *Acta Cryst.* E**67**, o270], has now been crystallized from 1-propanol in the monoclinic form in the space group $P2_1/c$. While the triclinic form is a Z' = 2 crystal, the new monoclinic polymorph includes one main molecule and one water lattice molecule in the asymmetric unit. In the crystal, the water molecule is sandwiched between neighboring main molecules and behaves as both donor and acceptor in O—H···N and N—H···O hydrogen bonds with the imidazole N atoms. This pattern of chains parallel to [100] further interacts *via* O—H···N(pyridine) contacts.

Related literature

For the role of the title compound in the synthesis of the anti-ulcer drug lansoprazole {systematic name: (*RS*)-2-([3-methyl-4-(2,2,2-trifluoroethoxy)pyridin-2-yl]methylsulfinyl)-1*H*-benzo[*d*]imidazole}, see: Del Rio *et al.* (2007); Reddy *et al.* (2008); Iwahi *et al.* (1991). For related structures, see: Swamy & Ravikumar (2007); Hakim Al-arique *et al.* (2010). For the triclinic polymorph of the title hydrate, see: Ren *et al.* (2011) and for the structure of the propan-2-ol solvo-polymorph, see: Ma *et al.* (2012)



Experimental

Crystal data

$C_{16}H_{14}F_3N_3OS\cdot H_2O$
M_r = 371.39
Monoclinic, $P2_1/c$
a = 7.3886 (15) Å
b = 25.497 (5) Å
c = 8.8579 (18) Å
β = 93.64 (3)°
V = 1665.4 (6) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.17 mm^{-1}
T = 296 K
0.27 × 0.16 × 0.15 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.592, T_{max} = 0.737
7679 measured reflections
2827 independent reflections
2713 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.152
S = 1.15
2827 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1′—H1′B···N2^{i}	0.85	2.10	2.869 (3)	150
N1—H1A···O1′^{ii}	0.86	1.91	2.765 (3)	170
O1′—H1′A···N3	0.85	2.36	3.077 (4)	143

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2435).

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supplementary materials

Acta Cryst. (2012). E**68**, o2015–o2016 [doi:10.1107/S1600536812022131]

2-{[3-Methyl-4-(2,2,2-trifluoroethoxy)pyridin-2-yl]methylsulfanyl}-1*H*-benzimidazole monohydrate: a monoclinic polymorph

Yu-Feng Chen, Jin-Yao Chen, Ming-Huang Hong, Jie Lu and Guo-Bin Ren

Comment

The title compound is the critical reaction intermediate for the synthesis of lansoprazole (Del Rio *et al.*, 2007; Reddy *et al.*, 2008), and its analogs, used as drugs for their anti-ulcer effects (Iwahi *et al.*, 1991). Recently, the compound was successfully crystallized from 1-propanol, and the crystal structure is reported here. A first polymorph was X-ray characterized in space group $P\bar{1}$ (Ren *et al.*, 2011).

The asymmetric unit (Fig. 1) contains one independent molecule and one water molecule which are involved in the formation of hydrogen-bonded chains *via*, N—H···O and O—H···N hydrogen bonds. These chains further interact through O—H···N(pyridine) contacts (Fig. 2). The water molecule could thus be considered to be a hydrogen-bond bridge, which provides stability to the crystal lattice. The hydrogen bond characteristics and geometric parameters are given in Table 1. The geometry of the main molecule is close to that reported for analog systems (Hakim Al-arique *et al.*, 2010; Swamy & Ravikumar, 2007).

Experimental

The raw material was kindly provided by Shanghai Enran Sci-Tech Investment Management Co., Ltd. The compound was dissolved in 1-propanol and suitable crystals were obtained by slow evaporation at room temperature over a period of one week.

Refinement

Water H atoms were initially located in a difference map and then fixed in their as-found positions, while all other H atoms were constrained to an ideal geometry with C—H distances of 0.93 Å (aromatic CH), 0.96 Å (methyl CH_3), 0.97 Å (methylene CH_2) and N—H distance of 0.86 Å (imidazolic NH). Isotropic displacement parameters for H atoms were calculated as $U_{iso}(H) = xU_{eq}$(carrier atom) with x = 1.5 (H_2O and methyl group) or x = 1.2 (other H atoms).

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

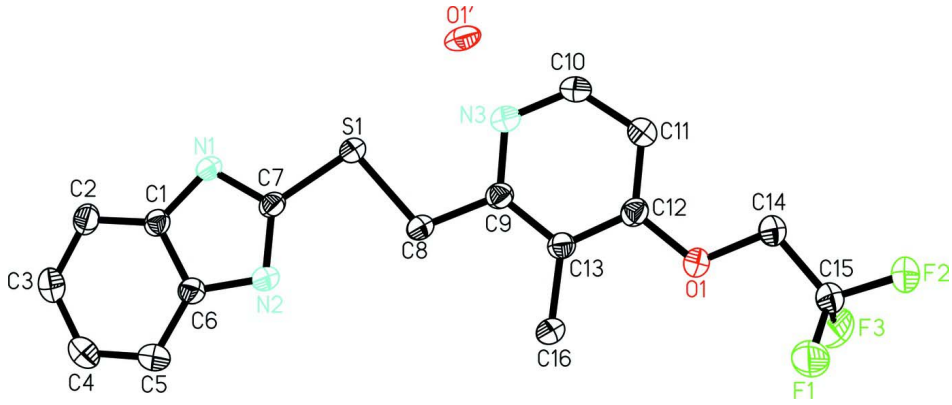

Figure 1

The content of the asymmetric unit of the title hydrate with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

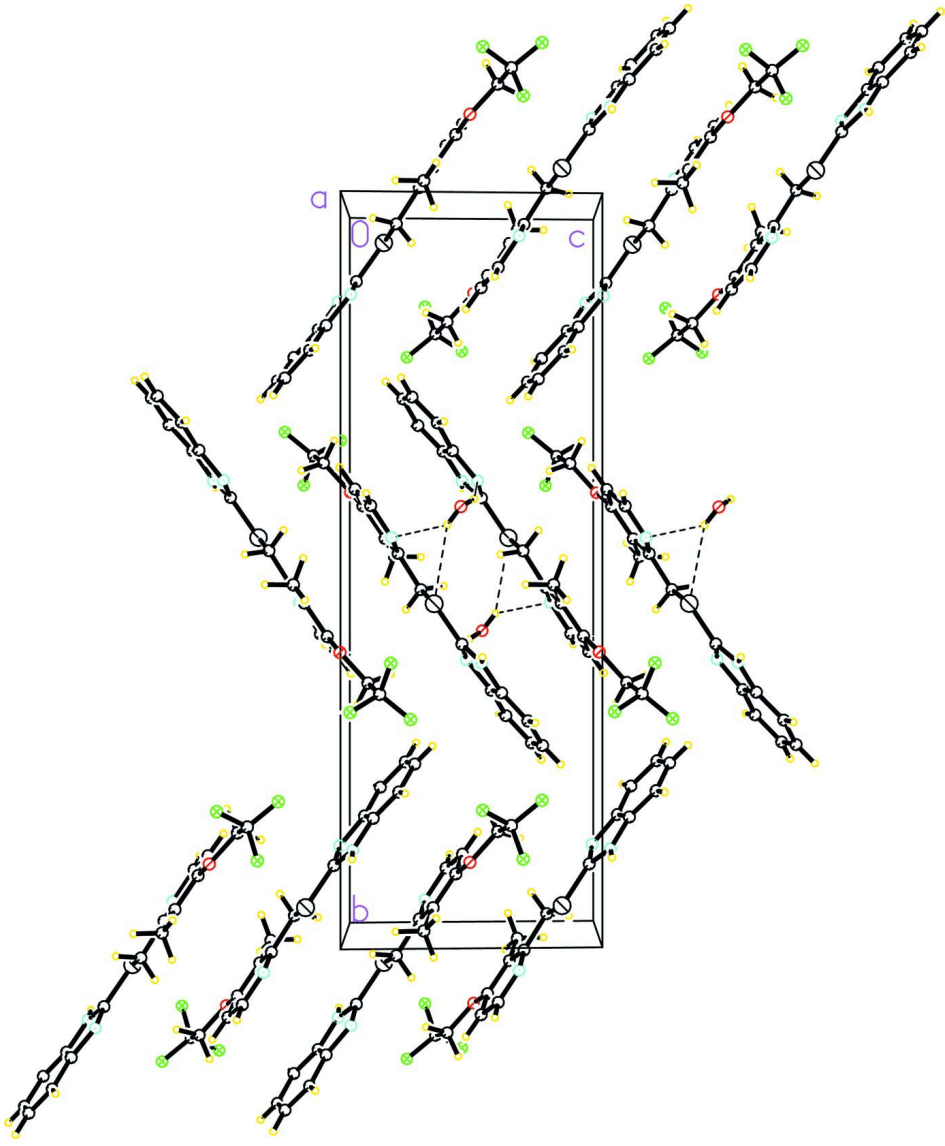

Figure 2

A packing diagram of the title compound. Supramolecular chains are running in the [100] direction, and dashed bonds indicate secondary hydrogen bonds connecting the chains in the crystal.

2-{[3-Methyl-4-(2,2,2-trifluoroethoxy)pyridin-2-yl]methylsulfanyl}- 1*H*-benzimidazole monohydrate

Crystal data

$C_{16}H_{14}F_3N_3OS·H_2O$
$M_r = 371.39$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3886$ (15) Å
$b = 25.497$ (5) Å
$c = 8.8579$ (18) Å
$\beta = 93.64$ (3)°
$V = 1665.4$ (6) Å^3
$Z = 4$

$F(000) = 768$
$D_x = 1.481$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 2713 reflections
$\theta = 3.5$–67.0°
$\mu = 2.17$ mm^{-1}
$T = 296$ K
Column, colorless
0.27 × 0.16 × 0.15 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.592, T_{max} = 0.737
7679 measured reflections
2827 independent reflections
2713 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 67.0°, θ_{min} = 3.5°
h = −8→8
k = −30→29
l = −9→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.152
S = 1.15
2827 reflections
227 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2 + 1.4537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0160 (11)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.30666 (8)	0.45480 (3)	0.64708 (8)	0.0437 (3)
O1	0.8564 (3)	0.60957 (8)	0.9928 (2)	0.0480 (5)
O1′	0.1360 (3)	0.58511 (9)	0.5422 (3)	0.0625 (6)
H1′B	0.2211	0.5963	0.4904	0.094*
H1′A	0.1850	0.5606	0.5956	0.094*
N1	0.2125 (3)	0.37523 (8)	0.4607 (3)	0.0403 (5)
H1A	0.0998	0.3838	0.4597	0.048*
N2	0.5109 (3)	0.37741 (9)	0.5223 (3)	0.0450 (6)
N3	0.3764 (3)	0.54450 (10)	0.8138 (3)	0.0485 (6)
F1	1.1369 (3)	0.62171 (9)	1.1942 (3)	0.0881 (8)
F2	1.0471 (3)	0.69647 (9)	1.2672 (3)	0.0814 (7)
F3	1.1303 (3)	0.68563 (10)	1.0413 (3)	0.0862 (7)
C1	0.2856 (3)	0.33433 (10)	0.3837 (3)	0.0394 (6)
C2	0.2097 (4)	0.29744 (11)	0.2827 (4)	0.0494 (7)
H2B	0.0858	0.2967	0.2566	0.059*
C3	0.3268 (5)	0.26218 (12)	0.2231 (4)	0.0567 (8)
H3B	0.2811	0.2374	0.1539	0.068*
C4	0.5115 (5)	0.26269 (13)	0.2636 (4)	0.0628 (9)
H4A	0.5861	0.2379	0.2221	0.075*
C5	0.5867 (4)	0.29905 (13)	0.3639 (4)	0.0593 (8)
H5A	0.7104	0.2991	0.3910	0.071*
C6	0.4717 (4)	0.33567 (11)	0.4233 (3)	0.0442 (6)
C7	0.3531 (3)	0.39957 (10)	0.5389 (3)	0.0389 (6)

C8	0.5380 (3)	0.47338 (11)	0.7022 (3)	0.0437 (6)
H8A	0.5965	0.4457	0.7622	0.052*
H8B	0.6051	0.4784	0.6127	0.052*
C9	0.5390 (3)	0.52327 (10)	0.7926 (3)	0.0394 (6)
C10	0.3747 (4)	0.58788 (13)	0.8963 (4)	0.0550 (8)
H10A	0.2631	0.6034	0.9101	0.066*
C11	0.5275 (4)	0.61143 (12)	0.9630 (4)	0.0504 (7)
H11A	0.5192	0.6411	1.0233	0.060*
C12	0.6938 (4)	0.58936 (10)	0.9371 (3)	0.0411 (6)
C13	0.7032 (3)	0.54422 (10)	0.8491 (3)	0.0391 (6)
C14	0.8503 (4)	0.65056 (11)	1.1002 (4)	0.0471 (7)
H14A	0.7841	0.6394	1.1857	0.056*
H14B	0.7905	0.6811	1.0549	0.056*
C15	1.0414 (4)	0.66317 (12)	1.1500 (4)	0.0550 (8)
C16	0.8805 (4)	0.51935 (12)	0.8153 (4)	0.0503 (7)
H16A	0.9786	0.5392	0.8632	0.075*
H16B	0.8918	0.5189	0.7079	0.075*
H16C	0.8845	0.4841	0.8532	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0305 (4)	0.0399 (4)	0.0604 (5)	−0.0018 (2)	0.0018 (3)	−0.0058 (3)
O1	0.0399 (10)	0.0434 (11)	0.0605 (13)	−0.0046 (8)	0.0004 (9)	−0.0123 (9)
O1′	0.0317 (10)	0.0713 (15)	0.0844 (16)	0.0044 (10)	0.0033 (10)	0.0137 (12)
N1	0.0268 (10)	0.0389 (12)	0.0549 (14)	−0.0020 (9)	−0.0001 (9)	0.0003 (10)
N2	0.0311 (11)	0.0432 (13)	0.0604 (15)	0.0009 (9)	0.0002 (10)	−0.0017 (11)
N3	0.0340 (12)	0.0533 (15)	0.0583 (15)	0.0010 (10)	0.0034 (11)	−0.0086 (11)
F1	0.0793 (15)	0.0701 (14)	0.1096 (18)	0.0313 (11)	−0.0360 (13)	−0.0204 (12)
F2	0.0623 (12)	0.0790 (14)	0.1000 (17)	0.0072 (10)	−0.0181 (11)	−0.0482 (13)
F3	0.0635 (13)	0.0855 (16)	0.1106 (18)	−0.0273 (12)	0.0131 (12)	−0.0078 (14)
C1	0.0371 (14)	0.0354 (13)	0.0455 (14)	−0.0030 (10)	0.0013 (11)	0.0058 (11)
C2	0.0482 (16)	0.0424 (15)	0.0570 (18)	−0.0087 (12)	−0.0022 (13)	0.0007 (13)
C3	0.069 (2)	0.0429 (16)	0.0582 (19)	−0.0049 (15)	0.0002 (15)	−0.0058 (14)
C4	0.067 (2)	0.0494 (18)	0.073 (2)	0.0103 (16)	0.0083 (17)	−0.0107 (16)
C5	0.0447 (17)	0.0555 (19)	0.078 (2)	0.0098 (14)	0.0025 (15)	−0.0061 (16)
C6	0.0374 (14)	0.0377 (14)	0.0577 (17)	0.0010 (11)	0.0036 (12)	0.0029 (12)
C7	0.0302 (12)	0.0360 (13)	0.0504 (15)	−0.0030 (10)	0.0008 (11)	0.0059 (11)
C8	0.0298 (13)	0.0415 (14)	0.0595 (17)	−0.0010 (11)	−0.0004 (11)	−0.0026 (12)
C9	0.0342 (13)	0.0369 (13)	0.0471 (15)	−0.0007 (10)	0.0034 (11)	0.0036 (11)
C10	0.0366 (15)	0.0595 (19)	0.069 (2)	0.0064 (13)	0.0065 (14)	−0.0149 (15)
C11	0.0450 (16)	0.0470 (16)	0.0594 (18)	0.0022 (13)	0.0052 (13)	−0.0100 (13)
C12	0.0380 (14)	0.0381 (14)	0.0468 (15)	−0.0045 (11)	0.0007 (11)	0.0026 (11)
C13	0.0347 (14)	0.0347 (14)	0.0481 (16)	−0.0005 (10)	0.0029 (11)	0.0046 (10)
C14	0.0461 (16)	0.0379 (14)	0.0569 (17)	−0.0021 (12)	0.0008 (13)	−0.0065 (12)
C15	0.0499 (17)	0.0446 (16)	0.069 (2)	0.0029 (13)	−0.0052 (15)	−0.0146 (14)
C16	0.0331 (14)	0.0481 (16)	0.069 (2)	−0.0004 (12)	−0.0021 (13)	−0.0076 (14)

Geometric parameters (Å, º)

S1—C7	1.750 (3)	C3—H3B	0.9300
S1—C8	1.811 (3)	C4—C5	1.376 (5)
O1—C12	1.370 (3)	C4—H4A	0.9300
O1—C14	1.416 (3)	C5—C6	1.388 (4)
O1′—H1′B	0.8499	C5—H5A	0.9300
O1′—H1′A	0.8497	C8—C9	1.503 (4)
N1—C7	1.361 (3)	C8—H8A	0.9700
N1—C1	1.375 (4)	C8—H8B	0.9700
N1—H1A	0.8600	C9—C13	1.390 (4)
N2—C7	1.312 (3)	C10—C11	1.378 (4)
N2—C6	1.397 (4)	C10—H10A	0.9300
N3—C10	1.326 (4)	C11—C12	1.383 (4)
N3—C9	1.342 (4)	C11—H11A	0.9300
F1—C15	1.317 (4)	C12—C13	1.394 (4)
F2—C15	1.340 (4)	C13—C16	1.502 (4)
F3—C15	1.329 (4)	C14—C15	1.488 (4)
C1—C2	1.392 (4)	C14—H14A	0.9700
C1—C6	1.398 (4)	C14—H14B	0.9700
C2—C3	1.376 (5)	C16—H16A	0.9600
C2—H2B	0.9300	C16—H16B	0.9600
C3—C4	1.389 (5)	C16—H16C	0.9600
C7—S1—C8	98.25 (13)	H8A—C8—H8B	108.2
C12—O1—C14	117.0 (2)	N3—C9—C13	124.3 (3)
H1′B—O1′—H1′A	104.1	N3—C9—C8	116.2 (2)
C7—N1—C1	106.6 (2)	C13—C9—C8	119.5 (2)
C7—N1—H1A	126.7	N3—C10—C11	124.3 (3)
C1—N1—H1A	126.7	N3—C10—H10A	117.9
C7—N2—C6	104.4 (2)	C11—C10—H10A	117.9
C10—N3—C9	117.0 (3)	C10—C11—C12	117.6 (3)
N1—C1—C2	132.6 (3)	C10—C11—H11A	121.2
N1—C1—C6	105.6 (2)	C12—C11—H11A	121.2
C2—C1—C6	121.9 (3)	O1—C12—C11	123.7 (3)
C3—C2—C1	116.8 (3)	O1—C12—C13	116.0 (2)
C3—C2—H2B	121.6	C11—C12—C13	120.3 (3)
C1—C2—H2B	121.6	C9—C13—C12	116.4 (2)
C2—C3—C4	121.8 (3)	C9—C13—C16	121.2 (2)
C2—C3—H3B	119.1	C12—C13—C16	122.3 (2)
C4—C3—H3B	119.1	O1—C14—C15	106.8 (2)
C5—C4—C3	121.5 (3)	O1—C14—H14A	110.4
C5—C4—H4A	119.2	C15—C14—H14A	110.4
C3—C4—H4A	119.2	O1—C14—H14B	110.4
C4—C5—C6	117.8 (3)	C15—C14—H14B	110.4
C4—C5—H5A	121.1	H14A—C14—H14B	108.6
C6—C5—H5A	121.1	F1—C15—F3	106.3 (3)
C5—C6—N2	130.0 (3)	F1—C15—F2	106.8 (3)
C5—C6—C1	120.3 (3)	F3—C15—F2	107.2 (3)
N2—C6—C1	109.7 (2)	F1—C15—C14	113.3 (3)

N2—C7—N1	113.7 (2)	F3—C15—C14	112.4 (3)
N2—C7—S1	127.9 (2)	F2—C15—C14	110.5 (3)
N1—C7—S1	118.38 (19)	C13—C16—H16A	109.5
C9—C8—S1	109.75 (18)	C13—C16—H16B	109.5
C9—C8—H8A	109.7	H16A—C16—H16B	109.5
S1—C8—H8A	109.7	C13—C16—H16C	109.5
C9—C8—H8B	109.7	H16A—C16—H16C	109.5
S1—C8—H8B	109.7	H16B—C16—H16C	109.5
C7—N1—C1—C2	−177.4 (3)	C10—N3—C9—C13	−1.1 (4)
C7—N1—C1—C6	1.2 (3)	C10—N3—C9—C8	178.5 (3)
N1—C1—C2—C3	178.3 (3)	S1—C8—C9—N3	−0.8 (3)
C6—C1—C2—C3	0.0 (4)	S1—C8—C9—C13	178.8 (2)
C1—C2—C3—C4	1.1 (5)	C9—N3—C10—C11	−1.3 (5)
C2—C3—C4—C5	−0.9 (6)	N3—C10—C11—C12	2.6 (5)
C3—C4—C5—C6	−0.3 (5)	C14—O1—C12—C11	9.6 (4)
C4—C5—C6—N2	−177.8 (3)	C14—O1—C12—C13	−170.9 (2)
C4—C5—C6—C1	1.3 (5)	C10—C11—C12—O1	178.1 (3)
C7—N2—C6—C5	179.0 (3)	C10—C11—C12—C13	−1.4 (4)
C7—N2—C6—C1	−0.3 (3)	N3—C9—C13—C12	2.1 (4)
N1—C1—C6—C5	−179.9 (3)	C8—C9—C13—C12	−177.5 (2)
C2—C1—C6—C5	−1.2 (4)	N3—C9—C13—C16	−177.5 (3)
N1—C1—C6—N2	−0.6 (3)	C8—C9—C13—C16	3.0 (4)
C2—C1—C6—N2	178.1 (3)	O1—C12—C13—C9	179.7 (2)
C6—N2—C7—N1	1.1 (3)	C11—C12—C13—C9	−0.7 (4)
C6—N2—C7—S1	−179.2 (2)	O1—C12—C13—C16	−0.7 (4)
C1—N1—C7—N2	−1.5 (3)	C11—C12—C13—C16	178.8 (3)
C1—N1—C7—S1	178.72 (18)	C12—O1—C14—C15	176.4 (2)
C8—S1—C7—N2	6.6 (3)	O1—C14—C15—F1	−51.6 (4)
C8—S1—C7—N1	−173.7 (2)	O1—C14—C15—F3	69.0 (3)
C7—S1—C8—C9	176.9 (2)	O1—C14—C15—F2	−171.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1′—H1′*B*···N2^{i}	0.85	2.10	2.869 (3)	150
N1—H1*A*···O1′^{ii}	0.86	1.91	2.765 (3)	170
O1′—H1′*A*···N3	0.85	2.36	3.077 (4)	143
O1′—H1′*A*···S1	0.85	2.87	3.653 (2)	154

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