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

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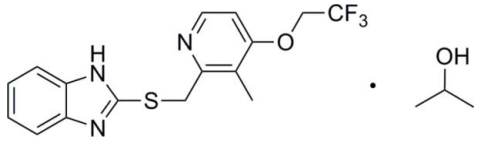
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.116; data-to-parameter ratio = 13.4.

In the crystal structure of the title compound, $C_{16}H_{14}F_3N_3OS\cdot C_3H_8O$, the molecules are linked into chains along [010] *via* N—H···O and O—H···N hydrogen bonds. The triclinic form was reported by Ren *et al.* [(2011). *Acta Cryst.* E**67**, o270] and the first monoclinic form by Chen *et al.* [(2012). *Acta Cryst.* E**68**, o2015–o2016]. The fused five-and six-membered rings make a dihedral angle of 1.22 (2)°, while the benzene and pyridine rings make a dihedral angle of 10.15 (2)°.

Related literature

For the use of the title compound as an intermediate 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 *et al.* (2010). For the triclinic polymorph of the title propan-2-ol solvo-polymorph, see: Ren *et al.* (2011) and for the monoclinic monohydrate, see: Chen *et al.* (2012).



Experimental

Crystal data

$C_{16}H_{14}F_3N_3OS\cdot C_3H_8O$
M_r = 413.46
Monoclinic, $P2_1/c$
a = 17.4583 (2) Å
b = 7.4162 (1) Å
c = 16.9622 (2) Å
β = 116.255 (2)°
V = 1969.60 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 296 K
0.31 × 0.23 × 0.15 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.592, T_{max} = 0.765
13351 measured reflections
3410 independent reflections
3266 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.116
S = 1.06
3410 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···N1^{i}	0.82	2.01	2.8142 (18)	167
N2—H2A···O2^{ii}	0.86	1.98	2.8027 (18)	161

Symmetry codes: (i) $x, y, z-1$; (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: BG2460).

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supplementary materials

Acta Cryst. (2012). E**68**, o2017 [doi:10.1107/S1600536812022143]

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

Jin-Ju Ma, Ming-Hui Qi, Ming-Huang Hong, Jie Lu and Guo-Bin Ren

Comment

Lansoprazole (Del Rio *et al.*, 2007; Reddy *et al.*, 2008) and many of its analogues are characterized by an anti-ulcer effect (Iwahi *et al.*,1991) The title compound, (I), is the critical reaction intermediate of lansoprazole Recently, the compound was successfully crystallized from 2-propanol, and the crystal structure is now firstly reported.

The crystral structure (Fig 1) contains one independent molecule and one 2-propanol solvato which are involved in the formation of hydrogen-bonded chains running along [010] *via* N—H···O and O—H···N hydrogen bonds (Table 1 and Fig. 2). The 2-propanol molecules acts as a hydrogen-bond bridge, providing further stability to the crystal lattice.

Experimental

The raw material was kindly provided by Shanghai Enran Sci-Tech Investment Management Co., Ltd. The compound was dissolved in 2-propanol and suitable crystals of X-ray were obtained by slow evaporation at room temperature over a period of one week.

Refinement

All C-H atoms were constrained to an ideal geometry with C—H distances of 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH; 0.97 Å and U_{iso}(H) = 1.2U_{eq} (C) for CH_2; 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3; 0.82 Å and U_{iso}(H) = 1.5U_{eq}(C)for OH atoms; and 0.86 Å and U_{iso}(H) = 1.5U_{eq}(C) for NH 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).

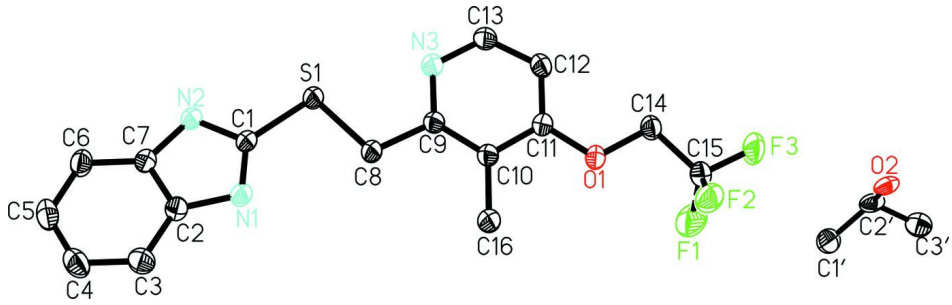

Figure 1

The content of asymmetric unit (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines denote hydrogen bonds. H atoms have been omitted for clarity.

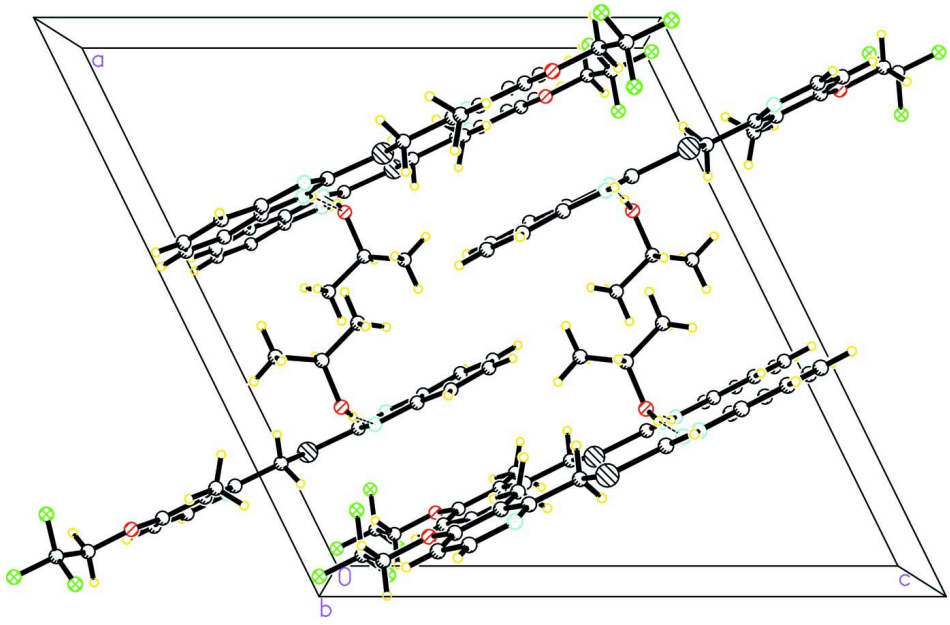

Figure 2

A packing diagram, projected along the [010] chains.

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

Crystal data

$C_{16}H_{14}F_3N_3OS·C_3H_8O$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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b = 7.4162 (1) Å
c = 16.9622 (2) Å
β = 116.255 (2)°
V = 1969.60 (5) Å^3
Z = 4

$F(000)$ = 864
D_x = 1.394 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 3266 reflections
θ = 6.1–67.0°
μ = 1.89 mm^{-1}
T = 296 K
Column, colorless
0.31 × 0.23 × 0.15 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.592, T_{max} = 0.765
13351 measured reflections
3410 independent reflections
3266 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 67.0°, θ_{min} = 6.1°
h = −19→20
k = −8→8
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.116
S = 1.06
3410 reflections
254 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
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.5861P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0024 (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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.22271 (3)	0.11157 (5)	1.05242 (3)	0.04524 (17)
O1	0.09818 (8)	0.61043 (16)	0.71885 (7)	0.0497 (3)
O2	0.32047 (8)	0.67645 (16)	0.17242 (10)	0.0573 (4)
H2B	0.3016	0.5801	0.1800	0.086*
N1	0.28104 (9)	0.32274 (18)	1.20227 (9)	0.0417 (3)
N2	0.29844 (8)	0.02492 (18)	1.22301 (8)	0.0419 (3)
H2A	0.2958	−0.0880	1.2105	0.050*
N3	0.14436 (10)	0.1600 (2)	0.87641 (9)	0.0476 (4)
F1	0.13495 (9)	0.8359 (2)	0.61276 (11)	0.0938 (5)
F2	0.01560 (8)	0.89596 (15)	0.61011 (8)	0.0681 (3)
F3	0.02040 (11)	0.76215 (19)	0.50116 (8)	0.0893 (5)
C1	0.26983 (10)	0.1637 (2)	1.16472 (10)	0.0375 (3)
C1′	0.47122 (13)	0.6930 (4)	0.26857 (17)	0.0747 (6)
H1′A	0.4639	0.6167	0.3104	0.112*
H1′B	0.4658	0.8169	0.2816	0.112*

H1′C	0.5269	0.6734	0.2717	0.112*
C2	0.32070 (10)	0.2857 (2)	1.29233 (11)	0.0415 (4)
C2′	0.40380 (12)	0.6487 (3)	0.17709 (15)	0.0594 (5)
H2′A	0.4095	0.5217	0.1646	0.071*
C3	0.34706 (13)	0.4014 (3)	1.36387 (13)	0.0556 (5)
H3B	0.3384	0.5251	1.3561	0.067*
C3′	0.41146 (15)	0.7633 (4)	0.10808 (17)	0.0729 (6)
H3′A	0.3673	0.7311	0.0513	0.109*
H3′B	0.4663	0.7440	0.1092	0.109*
H3′C	0.4057	0.8880	0.1196	0.109*
C4	0.38645 (14)	0.3274 (3)	1.44666 (13)	0.0631 (5)
H4A	0.4048	0.4029	1.4954	0.076*
C5	0.39947 (13)	0.1429 (3)	1.45925 (13)	0.0595 (5)
H5A	0.4272	0.0979	1.5162	0.071*
C6	0.37235 (11)	0.0253 (3)	1.38953 (11)	0.0519 (4)
H6A	0.3803	−0.0985	1.3980	0.062*
C7	0.33245 (10)	0.0997 (2)	1.30578 (11)	0.0408 (4)
C8	0.20875 (11)	0.3377 (2)	1.00826 (11)	0.0443 (4)
H8A	0.1736	0.4076	1.0281	0.053*
H8B	0.2638	0.3969	1.0285	0.053*
C9	0.16630 (10)	0.3261 (2)	0.90919 (10)	0.0385 (3)
C10	0.15158 (10)	0.4812 (2)	0.85880 (10)	0.0393 (4)
C11	0.11201 (10)	0.4568 (2)	0.76766 (10)	0.0405 (4)
C12	0.08915 (12)	0.2862 (2)	0.73202 (11)	0.0493 (4)
H12A	0.0628	0.2686	0.6715	0.059*
C13	0.10670 (13)	0.1429 (2)	0.78931 (12)	0.0536 (5)
H13A	0.0913	0.0278	0.7657	0.064*
C14	0.05724 (12)	0.5917 (2)	0.62635 (11)	0.0454 (4)
H14A	−0.0010	0.5500	0.6070	0.054*
H14B	0.0875	0.5051	0.6076	0.054*
C15	0.05779 (11)	0.7721 (3)	0.58855 (11)	0.0495 (4)
C16	0.17477 (13)	0.6669 (3)	0.89758 (12)	0.0548 (5)
H16A	0.1592	0.7539	0.8511	0.082*
H16B	0.2352	0.6730	0.9344	0.082*
H16C	0.1448	0.6924	0.9320	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0616 (3)	0.0325 (3)	0.0362 (2)	−0.00018 (16)	0.0168 (2)	0.00201 (14)
O1	0.0649 (8)	0.0411 (7)	0.0345 (6)	−0.0002 (5)	0.0143 (5)	0.0050 (5)
O2	0.0481 (7)	0.0306 (6)	0.0920 (10)	−0.0005 (5)	0.0299 (7)	0.0013 (6)
N1	0.0517 (8)	0.0324 (7)	0.0404 (7)	0.0030 (6)	0.0199 (6)	0.0036 (5)
N2	0.0523 (8)	0.0304 (7)	0.0395 (7)	0.0015 (6)	0.0172 (6)	0.0040 (5)
N3	0.0613 (9)	0.0367 (7)	0.0395 (8)	−0.0012 (6)	0.0174 (7)	0.0000 (6)
F1	0.0650 (8)	0.1046 (11)	0.1088 (12)	−0.0198 (7)	0.0357 (8)	0.0334 (9)
F2	0.0844 (8)	0.0471 (7)	0.0706 (8)	0.0098 (5)	0.0322 (7)	0.0056 (5)
F3	0.1476 (14)	0.0680 (8)	0.0367 (6)	−0.0046 (8)	0.0267 (7)	0.0095 (6)
C1	0.0419 (8)	0.0318 (8)	0.0383 (8)	0.0007 (6)	0.0172 (7)	0.0037 (6)
C1′	0.0519 (11)	0.0715 (15)	0.0859 (16)	0.0019 (10)	0.0171 (11)	0.0122 (12)

C2	0.0444 (8)	0.0411 (9)	0.0408 (9)	0.0024 (7)	0.0203 (7)	0.0022 (7)
C2′	0.0493 (10)	0.0350 (9)	0.0896 (15)	0.0018 (8)	0.0268 (10)	−0.0054 (9)
C3	0.0682 (12)	0.0485 (11)	0.0517 (11)	−0.0001 (9)	0.0280 (9)	−0.0078 (8)
C3′	0.0667 (13)	0.0789 (16)	0.0785 (15)	−0.0071 (11)	0.0369 (12)	−0.0080 (12)
C4	0.0703 (12)	0.0766 (14)	0.0434 (10)	−0.0044 (11)	0.0260 (9)	−0.0130 (9)
C5	0.0584 (11)	0.0791 (14)	0.0382 (9)	0.0024 (10)	0.0188 (8)	0.0082 (9)
C6	0.0554 (10)	0.0533 (11)	0.0442 (10)	0.0035 (8)	0.0195 (8)	0.0122 (8)
C7	0.0419 (8)	0.0412 (9)	0.0401 (8)	0.0006 (6)	0.0190 (7)	0.0044 (6)
C8	0.0566 (10)	0.0334 (8)	0.0365 (9)	0.0009 (7)	0.0147 (7)	0.0028 (7)
C9	0.0404 (8)	0.0363 (8)	0.0365 (8)	0.0010 (6)	0.0149 (6)	0.0004 (6)
C10	0.0406 (8)	0.0374 (8)	0.0367 (8)	0.0014 (6)	0.0143 (6)	0.0014 (6)
C11	0.0425 (8)	0.0388 (8)	0.0375 (8)	0.0016 (7)	0.0152 (6)	0.0044 (7)
C12	0.0595 (10)	0.0467 (10)	0.0337 (8)	−0.0012 (8)	0.0134 (7)	−0.0017 (7)
C13	0.0726 (12)	0.0376 (9)	0.0421 (9)	−0.0051 (8)	0.0176 (9)	−0.0053 (7)
C14	0.0536 (9)	0.0453 (10)	0.0341 (8)	0.0029 (7)	0.0165 (7)	0.0017 (7)
C15	0.0548 (10)	0.0539 (11)	0.0365 (8)	−0.0026 (8)	0.0170 (7)	0.0045 (7)
C16	0.0733 (12)	0.0383 (9)	0.0422 (9)	−0.0022 (8)	0.0159 (9)	0.0010 (7)

Geometric parameters (Å, º)

S1—C1	1.7517 (16)	C3′—H3′A	0.9600
S1—C8	1.8088 (17)	C3′—H3′B	0.9600
O1—C11	1.366 (2)	C3′—H3′C	0.9600
O1—C14	1.414 (2)	C4—C5	1.388 (3)
O2—C2′	1.436 (2)	C4—H4A	0.9300
O2—H2B	0.8200	C5—C6	1.374 (3)
N1—C1	1.313 (2)	C5—H5A	0.9300
N1—C2	1.397 (2)	C6—C7	1.390 (2)
N2—C1	1.360 (2)	C6—H6A	0.9300
N2—C7	1.376 (2)	C8—C9	1.510 (2)
N2—H2A	0.8600	C8—H8A	0.9700
N3—C13	1.331 (2)	C8—H8B	0.9700
N3—C9	1.337 (2)	C9—C10	1.387 (2)
F1—C15	1.311 (2)	C10—C11	1.398 (2)
F2—C15	1.326 (2)	C10—C16	1.502 (2)
F3—C15	1.331 (2)	C11—C12	1.383 (3)
C1′—C2′	1.512 (3)	C12—C13	1.380 (3)
C1′—H1′A	0.9600	C12—H12A	0.9300
C1′—H1′B	0.9600	C13—H13A	0.9300
C1′—H1′C	0.9600	C14—C15	1.486 (3)
C2—C3	1.388 (3)	C14—H14A	0.9700
C2—C7	1.398 (2)	C14—H14B	0.9700
C2′—C3′	1.499 (3)	C16—H16A	0.9600
C2′—H2′A	0.9800	C16—H16B	0.9600
C3—C4	1.375 (3)	C16—H16C	0.9600
C3—H3B	0.9300		
C1—S1—C8	99.09 (8)	C7—C6—H6A	121.5
C11—O1—C14	117.24 (13)	N2—C7—C6	132.68 (16)
C2′—O2—H2B	109.5	N2—C7—C2	105.36 (14)

C1—N1—C2	104.42 (13)	C6—C7—C2	121.96 (17)
C1—N2—C7	106.91 (13)	C9—C8—S1	108.55 (11)
C1—N2—H2A	126.5	C9—C8—H8A	110.0
C7—N2—H2A	126.5	S1—C8—H8A	110.0
C13—N3—C9	117.35 (15)	C9—C8—H8B	110.0
N1—C1—N2	113.52 (14)	S1—C8—H8B	110.0
N1—C1—S1	128.56 (12)	H8A—C8—H8B	108.4
N2—C1—S1	117.92 (12)	N3—C9—C10	124.55 (15)
C2′—C1′—H1′A	109.5	N3—C9—C8	115.14 (14)
C2′—C1′—H1′B	109.5	C10—C9—C8	120.30 (14)
H1′A—C1′—H1′B	109.5	C9—C10—C11	116.09 (15)
C2′—C1′—H1′C	109.5	C9—C10—C16	123.33 (14)
H1′A—C1′—H1′C	109.5	C11—C10—C16	120.58 (14)
H1′B—C1′—H1′C	109.5	O1—C11—C12	123.98 (14)
C3—C2—N1	130.27 (16)	O1—C11—C10	115.48 (14)
C3—C2—C7	119.94 (16)	C12—C11—C10	120.53 (15)
N1—C2—C7	109.79 (15)	C13—C12—C11	117.74 (16)
O2—C2′—C3′	108.28 (17)	C13—C12—H12A	121.1
O2—C2′—C1′	109.59 (18)	C11—C12—H12A	121.1
C3′—C2′—C1′	112.37 (18)	N3—C13—C12	123.72 (17)
O2—C2′—H2′A	108.8	N3—C13—H13A	118.1
C3′—C2′—H2′A	108.8	C12—C13—H13A	118.1
C1′—C2′—H2′A	108.8	O1—C14—C15	107.09 (14)
C4—C3—C2	117.96 (19)	O1—C14—H14A	110.3
C4—C3—H3B	121.0	C15—C14—H14A	110.3
C2—C3—H3B	121.0	O1—C14—H14B	110.3
C2′—C3′—H3′A	109.5	C15—C14—H14B	110.3
C2′—C3′—H3′B	109.5	H14A—C14—H14B	108.6
H3′A—C3′—H3′B	109.5	F1—C15—F2	106.44 (17)
C2′—C3′—H3′C	109.5	F1—C15—F3	107.37 (16)
H3′A—C3′—H3′C	109.5	F2—C15—F3	106.68 (16)
H3′B—C3′—H3′C	109.5	F1—C15—C14	113.07 (16)
C3—C4—C5	121.61 (19)	F2—C15—C14	113.23 (14)
C3—C4—H4A	119.2	F3—C15—C14	109.68 (15)
C5—C4—H4A	119.2	C10—C16—H16A	109.5
C6—C5—C4	121.53 (18)	C10—C16—H16B	109.5
C6—C5—H5A	119.2	H16A—C16—H16B	109.5
C4—C5—H5A	119.2	C10—C16—H16C	109.5
C5—C6—C7	116.97 (19)	H16A—C16—H16C	109.5
C5—C6—H6A	121.5	H16B—C16—H16C	109.5

C2—N1—C1—N2	0.47 (18)	C13—N3—C9—C10	0.8 (3)
C2—N1—C1—S1	179.51 (12)	C13—N3—C9—C8	179.99 (15)
C7—N2—C1—N1	−0.99 (18)	S1—C8—C9—N3	3.65 (19)
C7—N2—C1—S1	179.85 (11)	S1—C8—C9—C10	−177.14 (12)
C8—S1—C1—N1	6.99 (17)	N3—C9—C10—C11	−0.9 (2)
C8—S1—C1—N2	−174.00 (12)	C8—C9—C10—C11	179.94 (14)
C1—N1—C2—C3	−179.33 (18)	N3—C9—C10—C16	178.21 (17)
C1—N1—C2—C7	0.23 (18)	C8—C9—C10—C16	−0.9 (2)

N1—C2—C3—C4	−178.76 (18)	C14—O1—C11—C12	0.6 (2)
C7—C2—C3—C4	1.7 (3)	C14—O1—C11—C10	−179.17 (14)
C2—C3—C4—C5	−0.3 (3)	C9—C10—C11—O1	−179.78 (13)
C3—C4—C5—C6	−1.1 (3)	C16—C10—C11—O1	1.1 (2)
C4—C5—C6—C7	1.0 (3)	C9—C10—C11—C12	0.5 (2)
C1—N2—C7—C6	−178.20 (18)	C16—C10—C11—C12	−178.69 (17)
C1—N2—C7—C2	1.05 (17)	O1—C11—C12—C13	−179.70 (17)
C5—C6—C7—N2	179.62 (17)	C10—C11—C12—C13	0.0 (3)
C5—C6—C7—C2	0.5 (3)	C9—N3—C13—C12	−0.2 (3)
C3—C2—C7—N2	178.81 (15)	C11—C12—C13—N3	−0.2 (3)
N1—C2—C7—N2	−0.81 (18)	C11—O1—C14—C15	−174.15 (14)
C3—C2—C7—C6	−1.8 (3)	O1—C14—C15—F1	59.7 (2)
N1—C2—C7—C6	178.54 (15)	O1—C14—C15—F2	−61.42 (19)
C1—S1—C8—C9	−178.94 (12)	O1—C14—C15—F3	179.55 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···N1^{i}	0.82	2.01	2.8142 (18)	167
N2—H2*A*···O2^{ii}	0.86	1.98	2.8027 (18)	161

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