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4-[2-(1,3-Dioxoisoindolin-2-yl)-1,3-thiazol-4-yl]-benzonitrile

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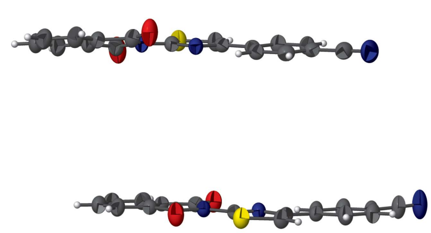
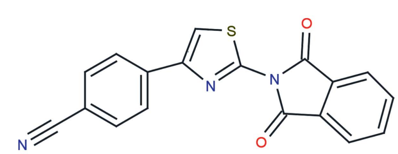
The title isoindole, $C_{18}H_8N_3O_2S$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit whose geometrical features are similar. The benzonitrile ring is oriented at an angle of 2.1 (1)° (molecule *A*) and 16.0 (1)° (molecule *B*), with respect to the isoindole ring system. In the crystal, *A* molecules are linked *via* C—H···N hydrogen bonds, forming *C*(15) chains propagating along along the *c* axis. *B* molecules are linked *via* C—H···O interactions, forming dimers with an $R_2^2(10)$ graph-set motif. C—H···O and C—H···N interactions, charcterized by $R_2^2(15)$ and $R_2^1(7)$ motifs, are observed between molecules *A* and *B*.

3D view



Chemical scheme



Structure description

In a continuation of our work on the crystal structure analysis of isoindole derivatives (Saravanan *et al.*, 2016), we have undertaken a single-crystal X-ray diffraction study of the title compound which has confirmed the molecular structure and atomic connectivity, as illustrated in Fig. 1. The asymmetric unit of contains two molecules (*A* and *B*) (Fig. 1); their corresponding bond lengths and bond angles are in good agreement. Fig. 2 shows a superposition of the two molecules using *Qmol* (Gans & Shalloway, 2001); the r.m.s. deviation is 0.2 Å.

The thiazole ring is planar with the maximum deviation of 0.001 (3) Å for atoms C9 and C9′ in molecules *A* and *B*. Keto atoms O2 and O3 deviate from the mean plane of the ring to which they are attached by 0.032 (2) and −0.044 (3) Å, respectively, in molecule *A*, −0.011 (3) and −0.122 (3) Å in molecule *B*. The nitrile group atoms (C18 and N1/C18′ and N1′) deviate by −0.036 (4) and −0.145 (2) Å, respectively, in molecule *A*, −0.015 (3)

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
C1—H1$\cdots$N1	0.93	2.48	2.818 (4)	102
C1′—H1′$\cdots$N1′	0.93	2.52	2.856 (4)	101
C2—H2$\cdots$N3′^{i}	0.93	2.61	3.376 (4)	141
C13—H13$\cdots$N3^{ii}	0.93	2.51	3.324 (5)	146
C5′—H5′$\cdots$O2^{iii}	0.93	2.55	3.444 (3)	161
C8′—H8′$\cdots$O2^{iii}	0.93	2.48	3.346 (3)	156
C12′—H12′$\cdots$O2′^{iv}	0.93	2.50	3.285 (4)	143
C2′—H2′$\cdots$O3^{v}	0.93	2.61	3.395 (3)	142

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

and −0.028 (3) Å in molecule *B*. The benzonitrile rings make dihedral angles of 4.2 (1) (molecule *A*) and 3.4 (1)° (molecule *B*) with thiazole rings. The benzonitrile ring in molecule *A* is oriented at an angle of 2.1 (1)° with respect to the isoindole ring system whereas it is oriented at an angle of 16.0 (1)° in molecule *B*.

The molecular structure is influenced by intramolecular C—H$\cdots$N hydrogen bonds (Table 1). In the crystal, C13—H13$\cdots$N3 hydrogen bonds link *A* molecules, forming $C(15)$ chains propagating along the *c* axis; see Fig. 3. C12′—H12′$\cdots$O2′ interactions form dimers of *B* molecules with graph-set motif $R_2^2(10)$. There are intermolecular interactions between molecules *A* and *B*: C2—H2$\cdots$N3′ and C2′—H2′$\cdots$O3 form an $R_2^2(15)$ ring, while C5′—H5′$\cdots$O2 and C8′—H8′$\cdots$O2 form an $R_1^2(7)$ ring; see Fig. 4.

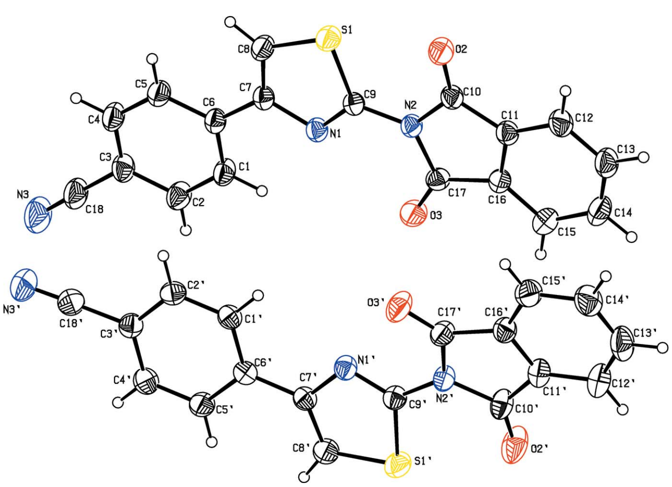


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

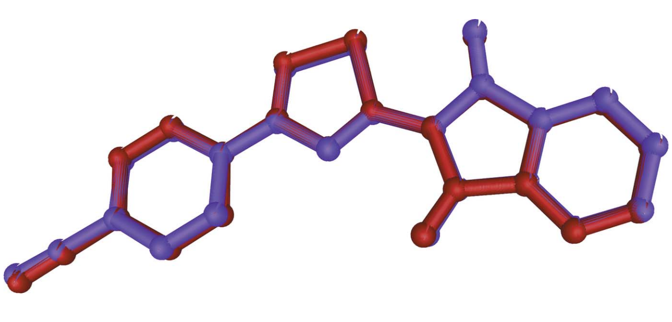


Figure 2
Superposition of molecule *A* (red) with molecule *B* (blue).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_9N_3O_2S$
M_r	331.34
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	7.915 (7), 12.1641 (10), 17.255 (14)
α, β, γ (°)	69.51 (2), 79.50 (2), 82.93 (3)
V (Å^3)	1527.0 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.22 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9065, 6901, 4330
R_{int}	0.078
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.652
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.183, 1.02
No. of reflections	6901
No. of parameters	433
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.36

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXS97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

Synthesis and crystallization

A mixture of 4-(2-aminothiazol-4-yl)benzonitrile (300 mg, 1.49 mmol), phthalic anhydride (441 mmol, 2.98 mmol) in

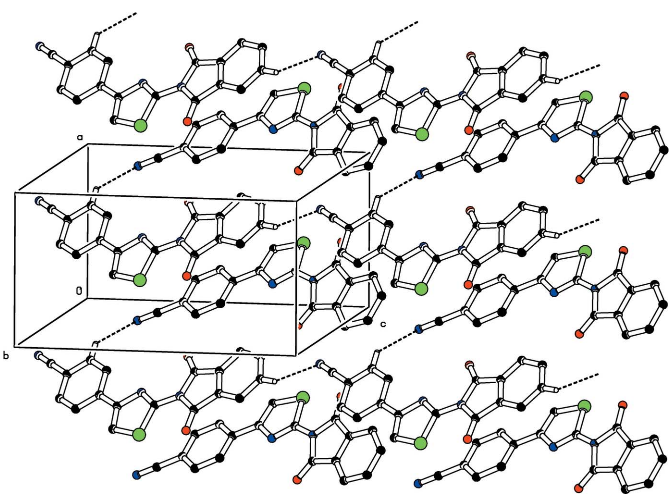


Figure 3
Crystal packing of the title compound, viewed approximately along the *b* axis. The C13—H13$\cdots$N3 and the C2—H2$\cdots$N3′ hydrogen bonds along the *c* and *a* axes, respectively, are shown with dashed lines.

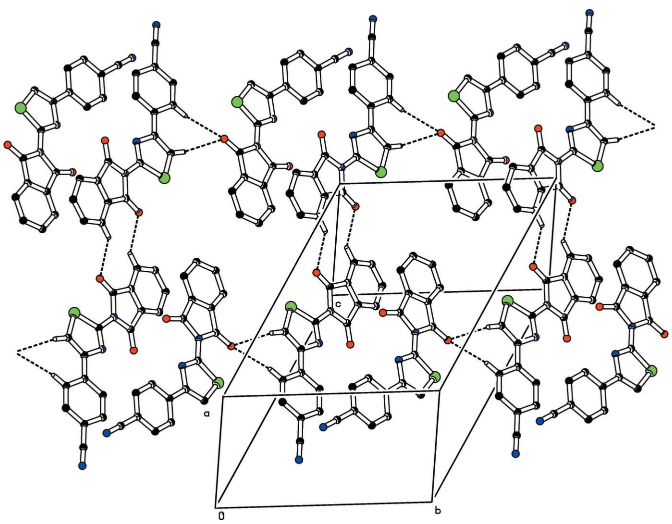


Figure 4
The C12′—H12′···O2 interactions along the *a* axis exhibit an $R_2^2(10)$ motif, while C5′—H5′···O2 and C8′—H8′···O2 hydrogen bonds form a ring with an $R_1^2(7)$ graph-set motif.

glacial acetic acid (5 ml) was refluxed for 3 h. After cooling, the resulting solid was collected by filtration, washed with petroleum ether and dried under vacuum, giving the compound as a lemon-yellow solid. The solid was further recrystallized in DMF to yield yellow crystals of the title compound.

Refinement

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

Acknowledgements

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References

Bruker (2002). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gans, J. D. & Shalloway, D. (2001). *J. Mol. Graph. Model.* **19**, 557–559.
Saravanan, K., Archana, K., Lakshmithendral, K., Kabilan, S. & Selvanayagam, S. (2016). IUCrData 1, x161053.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

full crystallographic data

IUCrData (2016). **1**, x161117 [https://doi.org/10.1107/S2414314616011172]

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Crystal data

$C_{18}H_9N_3O_2S$
$M_r = 331.34$
Triclinic, $P\overline{1}$
$a = 7.915$ (7) Å
$b = 12.1641$ (10) Å
$c = 17.255$ (14) Å
$\alpha = 69.51$ (2)°
$\beta = 79.50$ (2)°
$\gamma = 82.93$ (3)°
$V = 1527.0$ (19) Å^3
$Z = 4$
$F(000) = 680$
$D_x = 1.441$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5982 reflections
$\theta = 3.3$–26.7°
$\mu = 0.23$ mm^{-1}
$T = 296$ K
Block, yellow
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scans
9065 measured reflections
6901 independent reflections
4330 reflections with $I > 2\sigma(I)$
$R_{int} = 0.078$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.1°$
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 15$
$l = -10 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.183$
$S = 1.02$
6901 reflections
433 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0829P)^2 + 0.1516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.38921 (8)	0.78889 (6)	0.39010 (4)	0.0571 (2)

O2	0.4162 (2)	0.76188 (17)	0.54965 (12)	0.0647 (5)
O3	0.8033 (2)	0.48462 (17)	0.48373 (12)	0.0654 (5)
N1	0.6111 (2)	0.63277 (17)	0.35764 (12)	0.0464 (5)
N2	0.5965 (2)	0.63508 (17)	0.49470 (12)	0.0438 (4)
N3	0.7847 (4)	0.4946 (3)	−0.04423 (19)	0.1041 (11)
C1	0.7234 (3)	0.5651 (2)	0.21528 (16)	0.0545 (6)
H1	0.7776	0.5324	0.2625	0.065*
C2	0.7744 (4)	0.5259 (3)	0.14837 (16)	0.0612 (7)
H2	0.8623	0.4672	0.1505	0.073*
C3	0.6945 (4)	0.5743 (3)	0.07798 (16)	0.0581 (7)
C4	0.5645 (4)	0.6618 (3)	0.07480 (17)	0.0614 (7)
H4	0.5111	0.6944	0.0273	0.074*
C5	0.5139 (4)	0.7006 (2)	0.14184 (16)	0.0586 (7)
H5	0.4264	0.7597	0.1393	0.070*
C6	0.5924 (3)	0.6524 (2)	0.21352 (14)	0.0467 (5)
C7	0.5361 (3)	0.6902 (2)	0.28647 (14)	0.0448 (5)
C8	0.4156 (3)	0.7758 (2)	0.29379 (16)	0.0551 (6)
H8	0.3542	0.8220	0.2513	0.066*
C9	0.5460 (3)	0.6755 (2)	0.41544 (14)	0.0428 (5)
C10	0.5266 (3)	0.6826 (2)	0.55746 (15)	0.0477 (5)
C11	0.6149 (3)	0.6191 (2)	0.62956 (15)	0.0478 (6)
C12	0.5935 (4)	0.6341 (3)	0.70662 (16)	0.0595 (7)
H12	0.5112	0.6885	0.7202	0.071*
C13	0.6988 (4)	0.5651 (3)	0.76203 (17)	0.0662 (8)
H13	0.6893	0.5737	0.8142	0.079*
C14	0.8181 (4)	0.4836 (3)	0.74229 (18)	0.0670 (8)
H14	0.8873	0.4380	0.7816	0.080*
C15	0.8387 (3)	0.4669 (2)	0.66527 (17)	0.0600 (7)
H15	0.9191	0.4111	0.6523	0.072*
C16	0.7339 (3)	0.5375 (2)	0.60933 (15)	0.0457 (5)
C17	0.7246 (3)	0.5424 (2)	0.52334 (15)	0.0472 (5)
C18	0.7454 (4)	0.5311 (3)	0.00934 (18)	0.0742 (9)
S1′	0.37678 (10)	−0.06821 (7)	0.74956 (5)	0.0658 (2)
O2′	0.4044 (3)	−0.0300 (2)	0.89536 (15)	0.0899 (7)
O3′	−0.0673 (3)	0.1952 (2)	0.79880 (13)	0.0790 (6)
N1′	0.1656 (2)	0.10281 (18)	0.68470 (12)	0.0479 (5)
N2′	0.1870 (2)	0.08009 (18)	0.82460 (13)	0.0493 (5)
N3′	−0.0485 (4)	0.2563 (3)	0.24512 (17)	0.0912 (9)
C1′	0.0585 (3)	0.1964 (2)	0.52348 (16)	0.0480 (5)
H1′	0.0214	0.2343	0.5625	0.058*
C2′	0.0002 (3)	0.2396 (2)	0.44717 (16)	0.0517 (6)
H2′	−0.0755	0.3060	0.4349	0.062*
C3′	0.0556 (3)	0.1831 (2)	0.38873 (16)	0.0497 (6)
C4′	0.1694 (3)	0.0849 (2)	0.40719 (16)	0.0576 (6)
H4′	0.2076	0.0477	0.3678	0.069*
C5′	0.2258 (3)	0.0424 (2)	0.48295 (16)	0.0548 (6)
H5′	0.3016	−0.0240	0.4949	0.066*
C6′	0.1714 (3)	0.0974 (2)	0.54304 (15)	0.0449 (5)

C7′	0.2291 (3)	0.0505 (2)	0.62486 (15)	0.0461 (5)
C8′	0.3429 (3)	−0.0425 (2)	0.65024 (17)	0.0597 (7)
H8′	0.3960	−0.0870	0.6173	0.072*
C9′	0.2308 (3)	0.0485 (2)	0.75202 (15)	0.0473 (5)
C10′	0.2784 (3)	0.0368 (3)	0.89290 (17)	0.0601 (7)
C11′	0.1890 (3)	0.0870 (3)	0.95609 (16)	0.0561 (6)
C12′	0.2259 (4)	0.0738 (3)	1.03407 (19)	0.0738 (9)
H12′	0.3198	0.0260	1.0550	0.089*
C13′	0.1183 (5)	0.1343 (3)	1.07954 (19)	0.0792 (9)
H13′	0.1400	0.1267	1.1324	0.095*
C14′	−0.0192 (5)	0.2052 (3)	1.04946 (19)	0.0765 (9)
H14′	−0.0889	0.2452	1.0818	0.092*
C15′	−0.0558 (4)	0.2181 (3)	0.97160 (18)	0.0682 (8)
H15′	−0.1495	0.2662	0.9507	0.082*
C16′	0.0499 (3)	0.1579 (2)	0.92597 (15)	0.0528 (6)
C17′	0.0407 (3)	0.1526 (2)	0.84234 (16)	0.0541 (6)
C18′	−0.0037 (4)	0.2253 (2)	0.30838 (19)	0.0634 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0587 (4)	0.0613 (4)	0.0521 (4)	0.0151 (3)	−0.0127 (3)	−0.0241 (3)
O2	0.0701 (11)	0.0740 (13)	0.0571 (12)	0.0228 (10)	−0.0165 (9)	−0.0364 (10)
O3	0.0708 (12)	0.0683 (12)	0.0598 (12)	0.0211 (10)	−0.0134 (10)	−0.0317 (10)
N1	0.0489 (11)	0.0513 (11)	0.0420 (11)	0.0000 (9)	−0.0085 (9)	−0.0194 (9)
N2	0.0465 (10)	0.0470 (11)	0.0399 (10)	0.0023 (8)	−0.0081 (8)	−0.0179 (9)
N3	0.131 (3)	0.128 (3)	0.0669 (18)	0.038 (2)	−0.0350 (18)	−0.0558 (19)
C1	0.0574 (14)	0.0671 (16)	0.0398 (13)	0.0062 (12)	−0.0135 (11)	−0.0193 (12)
C2	0.0624 (16)	0.0743 (18)	0.0465 (15)	0.0122 (14)	−0.0104 (12)	−0.0242 (14)
C3	0.0672 (16)	0.0701 (17)	0.0401 (14)	−0.0036 (14)	−0.0082 (12)	−0.0225 (13)
C4	0.0690 (17)	0.0734 (19)	0.0437 (15)	0.0025 (14)	−0.0187 (13)	−0.0194 (13)
C5	0.0680 (16)	0.0619 (16)	0.0484 (15)	0.0081 (13)	−0.0182 (13)	−0.0210 (13)
C6	0.0498 (13)	0.0526 (14)	0.0380 (12)	−0.0076 (11)	−0.0083 (10)	−0.0131 (11)
C7	0.0473 (12)	0.0498 (13)	0.0391 (12)	−0.0062 (10)	−0.0064 (10)	−0.0160 (11)
C8	0.0599 (15)	0.0584 (15)	0.0458 (14)	0.0052 (12)	−0.0161 (12)	−0.0150 (12)
C9	0.0448 (12)	0.0451 (12)	0.0401 (12)	−0.0030 (10)	−0.0063 (10)	−0.0162 (10)
C10	0.0484 (12)	0.0521 (14)	0.0467 (14)	0.0027 (11)	−0.0087 (11)	−0.0229 (11)
C11	0.0526 (13)	0.0491 (13)	0.0426 (13)	−0.0079 (11)	−0.0065 (11)	−0.0153 (11)
C12	0.0742 (17)	0.0638 (16)	0.0431 (14)	−0.0063 (14)	−0.0049 (13)	−0.0225 (13)
C13	0.085 (2)	0.0716 (19)	0.0431 (15)	−0.0184 (16)	−0.0138 (14)	−0.0137 (14)
C14	0.0723 (18)	0.0733 (19)	0.0497 (16)	−0.0117 (15)	−0.0233 (14)	−0.0041 (14)
C15	0.0589 (15)	0.0610 (17)	0.0550 (16)	−0.0002 (13)	−0.0147 (13)	−0.0113 (13)
C16	0.0459 (12)	0.0478 (13)	0.0430 (13)	−0.0047 (10)	−0.0089 (10)	−0.0132 (11)
C17	0.0458 (12)	0.0448 (13)	0.0497 (14)	0.0022 (10)	−0.0080 (11)	−0.0157 (11)
C18	0.092 (2)	0.088 (2)	0.0480 (16)	0.0144 (18)	−0.0217 (15)	−0.0300 (16)
S1′	0.0709 (4)	0.0651 (5)	0.0625 (5)	0.0207 (4)	−0.0220 (4)	−0.0252 (4)
O2′	0.0619 (12)	0.137 (2)	0.0828 (16)	0.0369 (13)	−0.0346 (11)	−0.0536 (15)
O3′	0.0830 (13)	0.0973 (16)	0.0602 (13)	0.0427 (12)	−0.0321 (11)	−0.0362 (12)

N1′	0.0455 (10)	0.0549 (12)	0.0451 (12)	0.0023 (9)	−0.0078 (9)	−0.0202 (10)
N2′	0.0468 (10)	0.0600 (13)	0.0426 (11)	0.0038 (9)	−0.0120 (9)	−0.0189 (10)
N3′	0.123 (2)	0.087 (2)	0.0622 (18)	−0.0089 (18)	−0.0356 (17)	−0.0122 (15)
C1′	0.0465 (12)	0.0509 (14)	0.0486 (14)	−0.0012 (10)	−0.0024 (11)	−0.0221 (11)
C2′	0.0477 (13)	0.0487 (14)	0.0556 (15)	−0.0002 (11)	−0.0061 (11)	−0.0157 (12)
C3′	0.0507 (13)	0.0495 (14)	0.0462 (14)	−0.0088 (11)	−0.0057 (11)	−0.0117 (11)
C4′	0.0651 (16)	0.0614 (16)	0.0491 (15)	0.0014 (13)	−0.0037 (12)	−0.0261 (13)
C5′	0.0562 (14)	0.0554 (15)	0.0542 (15)	0.0106 (12)	−0.0086 (12)	−0.0248 (13)
C6′	0.0415 (11)	0.0464 (13)	0.0461 (13)	−0.0059 (10)	−0.0009 (10)	−0.0167 (11)
C7′	0.0439 (12)	0.0477 (13)	0.0482 (14)	−0.0031 (10)	−0.0047 (10)	−0.0190 (11)
C8′	0.0642 (16)	0.0601 (16)	0.0586 (17)	0.0122 (13)	−0.0121 (13)	−0.0285 (14)
C9′	0.0441 (12)	0.0508 (14)	0.0470 (14)	−0.0001 (10)	−0.0067 (11)	−0.0172 (11)
C10′	0.0473 (14)	0.0809 (19)	0.0542 (16)	0.0007 (13)	−0.0172 (12)	−0.0222 (14)
C11′	0.0558 (14)	0.0688 (17)	0.0454 (14)	−0.0097 (13)	−0.0113 (12)	−0.0175 (13)
C12′	0.0722 (18)	0.099 (2)	0.0525 (17)	−0.0070 (17)	−0.0211 (15)	−0.0222 (17)
C13′	0.099 (2)	0.099 (3)	0.0463 (17)	−0.027 (2)	−0.0124 (17)	−0.0247 (17)
C14′	0.099 (2)	0.080 (2)	0.0518 (18)	−0.0114 (19)	−0.0020 (17)	−0.0272 (16)
C15′	0.0832 (19)	0.0667 (18)	0.0537 (17)	0.0069 (15)	−0.0108 (15)	−0.0227 (14)
C16′	0.0605 (15)	0.0552 (15)	0.0418 (14)	−0.0055 (12)	−0.0070 (11)	−0.0152 (12)
C17′	0.0566 (14)	0.0568 (15)	0.0465 (14)	0.0061 (12)	−0.0104 (12)	−0.0163 (12)
C18′	0.0736 (18)	0.0568 (16)	0.0574 (18)	−0.0089 (14)	−0.0114 (15)	−0.0138 (14)

Geometric parameters (Å, º)

S1—C8	1.698 (3)	S1′—C8′	1.697 (3)
S1—C9	1.728 (3)	S1′—C9′	1.724 (3)
O2—C10	1.207 (3)	O2′—C10′	1.204 (3)
O3—C17	1.193 (3)	O3′—C17′	1.190 (3)
N1—C9	1.281 (3)	N1′—C9′	1.284 (3)
N1—C7	1.383 (3)	N1′—C7′	1.384 (3)
N2—C9	1.397 (3)	N2′—C10′	1.404 (3)
N2—C10	1.398 (3)	N2′—C9′	1.408 (3)
N2—C17	1.433 (3)	N2′—C17′	1.421 (3)
N3—C18	1.138 (4)	N3′—C18′	1.131 (4)
C1—C2	1.375 (4)	C1′—C2′	1.378 (4)
C1—C6	1.386 (3)	C1′—C6′	1.387 (3)
C1—H1	0.9300	C1′—H1′	0.9300
C2—C3	1.382 (4)	C2′—C3′	1.389 (3)
C2—H2	0.9300	C2′—H2′	0.9300
C3—C4	1.380 (4)	C3′—C4′	1.384 (4)
C3—C18	1.432 (4)	C3′—C18′	1.444 (4)
C4—C5	1.374 (4)	C4′—C5′	1.363 (4)
C4—H4	0.9300	C4′—H4′	0.9300
C5—C6	1.394 (3)	C5′—C6′	1.400 (3)
C5—H5	0.9300	C5′—H5′	0.9300
C6—C7	1.465 (3)	C6′—C7′	1.461 (4)
C7—C8	1.346 (3)	C7′—C8′	1.353 (3)
C8—H8	0.9300	C8′—H8′	0.9300

C10—C11	1.464 (3)	C10′—C11′	1.463 (4)
C11—C16	1.374 (3)	C11′—C16′	1.374 (4)
C11—C12	1.382 (3)	C11′—C12′	1.380 (4)
C12—C13	1.367 (4)	C12′—C13′	1.374 (5)
C12—H12	0.9300	C12′—H12′	0.9300
C13—C14	1.372 (4)	C13′—C14′	1.363 (5)
C13—H13	0.9300	C13′—H13′	0.9300
C14—C15	1.391 (4)	C14′—C15′	1.377 (4)
C14—H14	0.9300	C14′—H14′	0.9300
C15—C16	1.376 (4)	C15′—C16′	1.367 (4)
C15—H15	0.9300	C15′—H15′	0.9300
C16—C17	1.479 (3)	C16′—C17′	1.482 (4)
C8—S1—C9	87.83 (12)	C8′—S1′—C9′	88.02 (12)
C9—N1—C7	110.1 (2)	C9′—N1′—C7′	110.2 (2)
C9—N2—C10	123.2 (2)	C10′—N2′—C9′	123.8 (2)
C9—N2—C17	126.21 (19)	C10′—N2′—C17′	110.2 (2)
C10—N2—C17	110.61 (19)	C9′—N2′—C17′	125.9 (2)
C2—C1—C6	121.1 (2)	C2′—C1′—C6′	121.1 (2)
C2—C1—H1	119.4	C2′—C1′—H1′	119.4
C6—C1—H1	119.4	C6′—C1′—H1′	119.4
C1—C2—C3	119.7 (3)	C1′—C2′—C3′	119.5 (2)
C1—C2—H2	120.2	C1′—C2′—H2′	120.2
C3—C2—H2	120.2	C3′—C2′—H2′	120.2
C4—C3—C2	120.1 (2)	C4′—C3′—C2′	119.9 (2)
C4—C3—C18	120.5 (2)	C4′—C3′—C18′	119.0 (2)
C2—C3—C18	119.4 (3)	C2′—C3′—C18′	121.0 (2)
C5—C4—C3	120.0 (2)	C5′—C4′—C3′	120.2 (2)
C5—C4—H4	120.0	C5′—C4′—H4′	119.9
C3—C4—H4	120.0	C3′—C4′—H4′	119.9
C4—C5—C6	120.7 (3)	C4′—C5′—C6′	121.0 (2)
C4—C5—H5	119.6	C4′—C5′—H5′	119.5
C6—C5—H5	119.6	C6′—C5′—H5′	119.5
C1—C6—C5	118.4 (2)	C1′—C6′—C5′	118.2 (2)
C1—C6—C7	120.3 (2)	C1′—C6′—C7′	120.8 (2)
C5—C6—C7	121.3 (2)	C5′—C6′—C7′	121.0 (2)
C8—C7—N1	114.2 (2)	C8′—C7′—N1′	114.0 (2)
C8—C7—C6	127.5 (2)	C8′—C7′—C6′	126.3 (2)
N1—C7—C6	118.2 (2)	N1′—C7′—C6′	119.7 (2)
C7—C8—S1	111.79 (19)	C7′—C8′—S1′	111.73 (19)
C7—C8—H8	124.1	C7′—C8′—H8′	124.1
S1—C8—H8	124.1	S1′—C8′—H8′	124.1
N1—C9—N2	123.2 (2)	N1′—C9′—N2′	123.1 (2)
N1—C9—S1	116.02 (18)	N1′—C9′—S1′	116.08 (18)
N2—C9—S1	120.76 (16)	N2′—C9′—S1′	120.86 (18)
O2—C10—N2	124.1 (2)	O2′—C10′—N2′	123.7 (3)
O2—C10—C11	129.1 (2)	O2′—C10′—C11′	129.4 (3)
N2—C10—C11	106.7 (2)	N2′—C10′—C11′	106.8 (2)

C16—C11—C12	122.1 (2)	C16′—C11′—C12′	120.7 (3)
C16—C11—C10	108.7 (2)	C16′—C11′—C10′	108.8 (2)
C12—C11—C10	129.2 (2)	C12′—C11′—C10′	130.4 (3)
C13—C12—C11	117.0 (3)	C13′—C12′—C11′	117.2 (3)
C13—C12—H12	121.5	C13′—C12′—H12′	121.4
C11—C12—H12	121.5	C11′—C12′—H12′	121.4
C12—C13—C14	121.3 (3)	C14′—C13′—C12′	122.0 (3)
C12—C13—H13	119.3	C14′—C13′—H13′	119.0
C14—C13—H13	119.3	C12′—C13′—H13′	119.0
C13—C14—C15	122.0 (3)	C13′—C14′—C15′	120.6 (3)
C13—C14—H14	119.0	C13′—C14′—H14′	119.7
C15—C14—H14	119.0	C15′—C14′—H14′	119.7
C16—C15—C14	116.5 (3)	C16′—C15′—C14′	117.9 (3)
C16—C15—H15	121.8	C16′—C15′—H15′	121.1
C14—C15—H15	121.8	C14′—C15′—H15′	121.1
C11—C16—C15	121.2 (2)	C15′—C16′—C11′	121.5 (3)
C11—C16—C17	109.0 (2)	C15′—C16′—C17′	129.9 (3)
C15—C16—C17	129.8 (2)	C11′—C16′—C17′	108.5 (2)
O3—C17—N2	125.4 (2)	O3′—C17′—N2′	125.6 (2)
O3—C17—C16	129.7 (2)	O3′—C17′—C16′	128.8 (2)
N2—C17—C16	104.86 (19)	N2′—C17′—C16′	105.6 (2)
N3—C18—C3	178.6 (4)	N3′—C18′—C3′	178.5 (3)

C6—C1—C2—C3	0.1 (4)	C6′—C1′—C2′—C3′	0.0 (4)
C1—C2—C3—C4	0.3 (4)	C1′—C2′—C3′—C4′	−0.6 (4)
C1—C2—C3—C18	−178.5 (3)	C1′—C2′—C3′—C18′	179.5 (2)
C2—C3—C4—C5	−0.3 (4)	C2′—C3′—C4′—C5′	0.8 (4)
C18—C3—C4—C5	178.5 (3)	C18′—C3′—C4′—C5′	−179.3 (2)
C3—C4—C5—C6	−0.1 (4)	C3′—C4′—C5′—C6′	−0.5 (4)
C2—C1—C6—C5	−0.5 (4)	C2′—C1′—C6′—C5′	0.3 (4)
C2—C1—C6—C7	178.0 (2)	C2′—C1′—C6′—C7′	−178.4 (2)
C4—C5—C6—C1	0.5 (4)	C4′—C5′—C6′—C1′	−0.1 (4)
C4—C5—C6—C7	−178.0 (2)	C4′—C5′—C6′—C7′	178.7 (2)
C9—N1—C7—C8	0.2 (3)	C9′—N1′—C7′—C8′	−0.5 (3)
C9—N1—C7—C6	−179.2 (2)	C9′—N1′—C7′—C6′	179.6 (2)
C1—C6—C7—C8	177.7 (2)	C1′—C6′—C7′—C8′	−177.6 (2)
C5—C6—C7—C8	−3.9 (4)	C5′—C6′—C7′—C8′	3.7 (4)
C1—C6—C7—N1	−3.1 (3)	C1′—C6′—C7′—N1′	2.3 (3)
C5—C6—C7—N1	175.4 (2)	C5′—C6′—C7′—N1′	−176.4 (2)
N1—C7—C8—S1	−0.1 (3)	N1′—C7′—C8′—S1′	−0.4 (3)
C6—C7—C8—S1	179.19 (19)	C6′—C7′—C8′—S1′	179.53 (19)
C9—S1—C8—C7	0.0 (2)	C9′—S1′—C8′—C7′	0.9 (2)
C7—N1—C9—N2	−180.0 (2)	C7′—N1′—C9′—N2′	−178.4 (2)
C7—N1—C9—S1	−0.2 (3)	C7′—N1′—C9′—S1′	1.2 (3)
C10—N2—C9—N1	179.4 (2)	C10′—N2′—C9′—N1′	−167.8 (2)
C17—N2—C9—N1	−0.1 (4)	C17′—N2′—C9′—N1′	16.6 (4)
C10—N2—C9—S1	−0.4 (3)	C10′—N2′—C9′—S1′	12.6 (3)
C17—N2—C9—S1	−179.84 (17)	C17′—N2′—C9′—S1′	−162.98 (19)

C8—S1—C9—N1	0.1 (2)	C8′—S1′—C9′—N1′	−1.2 (2)
C8—S1—C9—N2	179.9 (2)	C8′—S1′—C9′—N2′	178.4 (2)
C9—N2—C10—O2	0.4 (4)	C9′—N2′—C10′—O2′	1.1 (4)
C17—N2—C10—O2	179.9 (2)	C17′—N2′—C10′—O2′	177.3 (3)
C9—N2—C10—C11	−178.65 (19)	C9′—N2′—C10′—C11′	−178.0 (2)
C17—N2—C10—C11	0.8 (3)	C17′—N2′—C10′—C11′	−1.8 (3)
O2—C10—C11—C16	−178.6 (3)	O2′—C10′—C11′—C16′	−179.3 (3)
N2—C10—C11—C16	0.4 (3)	N2′—C10′—C11′—C16′	−0.3 (3)
O2—C10—C11—C12	0.2 (5)	O2′—C10′—C11′—C12′	1.7 (5)
N2—C10—C11—C12	179.2 (2)	N2′—C10′—C11′—C12′	−179.3 (3)
C16—C11—C12—C13	1.2 (4)	C16′—C11′—C12′—C13′	0.0 (4)
C10—C11—C12—C13	−177.5 (2)	C10′—C11′—C12′—C13′	179.0 (3)
C11—C12—C13—C14	−1.1 (4)	C11′—C12′—C13′—C14′	−0.3 (5)
C12—C13—C14—C15	0.2 (4)	C12′—C13′—C14′—C15′	0.4 (5)
C13—C14—C15—C16	0.5 (4)	C13′—C14′—C15′—C16′	−0.1 (5)
C12—C11—C16—C15	−0.4 (4)	C14′—C15′—C16′—C11′	−0.2 (4)
C10—C11—C16—C15	178.5 (2)	C14′—C15′—C16′—C17′	178.5 (3)
C12—C11—C16—C17	179.6 (2)	C12′—C11′—C16′—C15′	0.3 (4)
C10—C11—C16—C17	−1.5 (3)	C10′—C11′—C16′—C15′	−178.9 (2)
C14—C15—C16—C11	−0.5 (4)	C12′—C11′—C16′—C17′	−178.7 (3)
C14—C15—C16—C17	179.5 (2)	C10′—C11′—C16′—C17′	2.1 (3)
C9—N2—C17—O3	−2.0 (4)	C10′—N2′—C17′—O3′	−174.7 (3)
C10—N2—C17—O3	178.5 (2)	C9′—N2′—C17′—O3′	1.4 (4)
C9—N2—C17—C16	177.8 (2)	C10′—N2′—C17′—C16′	3.0 (3)
C10—N2—C17—C16	−1.7 (2)	C9′—N2′—C17′—C16′	179.1 (2)
C11—C16—C17—O3	−178.3 (3)	C15′—C16′—C17′—O3′	−4.4 (5)
C15—C16—C17—O3	1.8 (4)	C11′—C16′—C17′—O3′	174.5 (3)
C11—C16—C17—N2	1.9 (3)	C15′—C16′—C17′—N2′	178.0 (3)
C15—C16—C17—N2	−178.0 (2)	C11′—C16′—C17′—N2′	−3.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1	0.93	2.48	2.818 (4)	102
C1′—H1′···N1′	0.93	2.52	2.856 (4)	101
C2—H2···N3′^{i}	0.93	2.61	3.376 (4)	141
C13—H13···N3^{ii}	0.93	2.51	3.324 (5)	146
C5′—H5′···O2^{iii}	0.93	2.55	3.444 (3)	161
C8′—H8′···O2^{iii}	0.93	2.48	3.346 (3)	156
C12′—H12′···O2′^{iv}	0.93	2.50	3.285 (4)	143
C2′—H2′···O3^{v}	0.93	2.61	3.395 (3)	142

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