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Synthesis and crystal structure of (*E*)-4-(benzo[*d*]-thiazol-2-ylimino)-1-cyclohexyl-1,3,5-triazinane-2-thione

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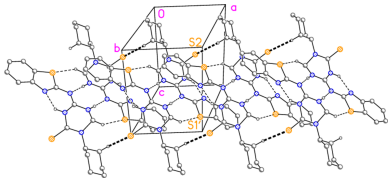
The title compound, $C_{16}H_{19}N_5S_2$, crystallizes in space group $P\overline{1}$ with $Z = 2$. The two heterocyclic systems are bridged by a nitrogen atom and further connected *via* an intramolecular hydrogen bond N—H···N, associated with an *E* configuration around the exocyclic C=N double bond at the thiazole ring. The associated $N_{thiazole}—C_{thiazole}=N$ angle of 129.58 (4)° is very wide. The triazinane ring displays a flattened boat conformation. The double bond lengths C=N and C=S at this ring are 1.3215 (5) and 1.6679 (4) Å, respectively. In the crystal, molecules are linked into inversion-symmetric dimers by a classical N—H···N hydrogen bond from the other NH group at the triazinane ring to the nitrogen atom that links the ring systems.

1. Chemical context

Triazines represent one of the key heterocyclic cores for drug discovery because of their molecular structural significance and broad-spectrum bioactivity (Mohamed-Ezzat *et al.*, 2024, 2025). Triazines, as nitrogen-enriched analogues of pyrimidine, have been developed in parallel with the synthesis of various antimetabolite pyrimidine derivatives (Elgemeie *et al.*, 2015). They have been widely exploited in designing antimetabolite agents because of their structural similarity to nucleic acid bases (Parker *et al.*, 2009; Brown, 2002; Jordheim *et al.*, 2013). Notably, there are various naturally occurring compounds that contain a triazine ring (Cascioferro *et al.*, 2017). Many triazines are potent compounds with inhibitory activity towards metalloproteinases (Cheng *et al.*, 2008), histone deacetylases (Bouchain & Delorme, 2003), tubulin (Lu *et al.*, 2012), urease and tyrosinase (Mojzych *et al.*, 2017).

Similarly to triazines, benzothiazoles are considered as privileged scaffolds widely explored for their pharmacological potential. Benzothiazoles are nitrogen- and sulfur-containing heterocycles contributing significantly to modern therapeutic chemistry because of their successful applications, such as their incorporation into various pharmaceutical agents for the treatment of several diseases (Mohamed-Ezzat & Elgemeie, 2024, 2025; Bulsara *et al.*, 2026; Elboshi *et al.*, 2026).

The triazine–benzothiazole combination thus represents a considerable potential for improving molecular diversity and biological efficacy in drug design. Although such materials have been studied (Bulsara *et al.*, 2026; Yurttas *et al.*, 2017), the number of investigations remains limited, and these have mainly explored their therapeutic applications, thus providing impetus for further development of these combined scaffolds.



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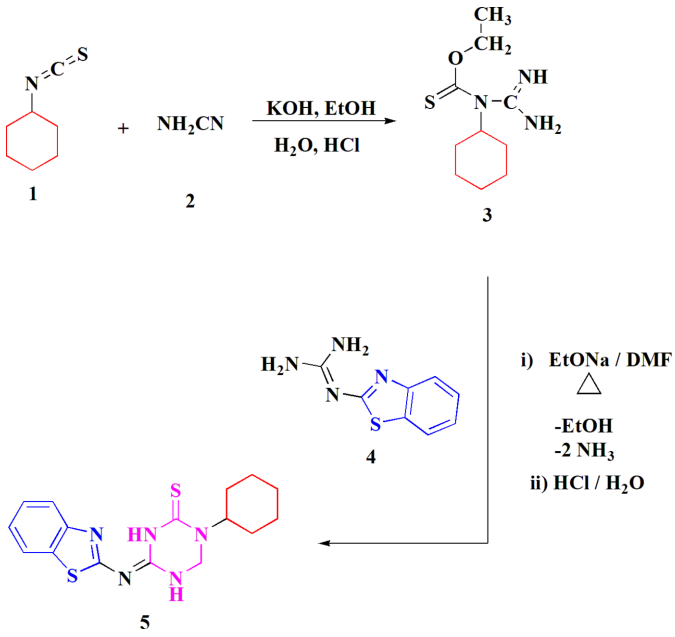
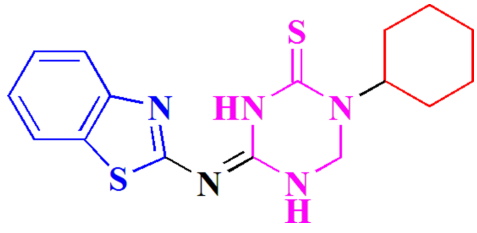


Figure 1
Synthesis scheme of compound **5**.

In this context, syntheses of new benzothiazole–triazine systems have been developed to provide promising materials for bioactive compound systems. We have now synthesized a novel 'triazine'–benzothiazole system, the title compound **5**, *via* a new synthetic pathway (Fig. 1) that utilizes the reaction of *O*-ethyl *N*-cyclohexylcarbamothioate **3** with 2-(benzo[*d*]thiazol-2-yl)guanidine **4** in refluxing dimethyl formamide containing sodium ethoxide. However, the triazine ring in **5** is formally saturated and it is thus more properly described as a triazinane. The crystal structure has been determined to confirm the structure of product **5** (as deduced from spectroscopic results) and is presented here.



2. Structural commentary

The molecular structure of the title compound **5** is shown in Fig. 2, with selected bond lengths and angles in Table 1. Standard numbering is used for the triazine ring and for the benzathiazole unit, the latter however with primes (′). A side view (Fig. 3) shows that a substantial proportion of the molecule is approximately planar. The two heterocyclic systems are connected via the nitrogen atom N7, whereby the atom sequence S1′—C2′—N7—C4—N3 has an extended conformation, and also by the intramolecular hydrogen bond N5—H05···N3′ (Table 2), which is associated with the *E* configuration around the exocyclic double bond C2′═N7. The

Table 1
Selected geometric parameters (Å, °).

N1—C6	1.3398 (5)	C6—S2	1.6679 (4)
N1—C2	1.4683 (6)	N7—C2′	1.3631 (5)
C2—N3	1.4440 (6)	S1′—C7*A*′	1.7343 (4)
N3—C4	1.3343 (5)	S1′—C2′	1.7631 (4)
C4—N7	1.3215 (5)	C2′—N3′	1.3127 (5)
C4—N5	1.3800 (5)	N3′—C3*A*′	1.3895 (5)
N5—C6	1.3958 (5)	C3*A*′—C7*A*′	1.4094 (6)
C6—N1—C2	115.40 (3)	N3′—C2′—N7	129.58 (4)
N3—C2—N1	108.40 (3)	N3′—C2′—S1′	115.10 (3)
C4—N3—C2	116.42 (4)	C2′—N3′—C3*A*′	110.82 (4)
N3—C4—N5	114.65 (4)	N3′—C3*A*′—C4′	125.32 (4)
C4—N5—C6	121.37 (3)	N3′—C3*A*′—C7*A*′	115.34 (4)
N1—C6—N5	114.73 (4)	C7′—C7*A*′—S1′	128.93 (4)
C4—N7—C2′	120.95 (4)	C3*A*′—C7*A*′—S1′	109.34 (3)
C7*A*′—S1′—C2′	89.39 (2)		
C6—N1—C2—N3	50.41 (5)	N3—C4—N7—C2′	176.98 (4)
N1—C2—N3—C4	−51.16 (5)	C6—N1—C11—C16	−150.72 (4)
C2—N3—C4—N5	13.28 (6)	C2—N1—C11—C16	35.19 (5)
N3—C4—N5—C6	29.74 (6)	C6—N1—C11—C12	84.33 (5)
C2—N1—C6—N5	−12.44 (5)	C2—N1—C11—C12	−89.75 (5)
C4—N5—C6—N1	−29.90 (6)	C4—N7—C2′—S1′	179.78 (3)

benzothiazine system is planar [root-mean-square (r.m.s.) deviation of nine atoms 0.018 Å]; its dimensions are much as expected, e.g. the large exocyclic angles at C3*A*′ and C7*A*′, but the wide angle N3′—C2′—N7 of 129.58 (4)° is perhaps surprising (but see *Database survey*). The triazinane ring displays a flattened boat conformation (cf. torsion angles in Table 1), with C2 and N5 lying 0.594 (1) and 0.307 (1) Å, respectively, to the same side of the plane of the other four atoms (r.m.s. deviation < 0.001 Å); the puckering parameters (Cremer & Pople, 1975) are Q = 0.5322 (5) Å, θ = 103.05 (5)°, φ = 240.13 (5)°. The bond lengths and angles suggest a good deal of delocalization in most of the ring, although C2 essentially shows sp^3 hybridization, with a N1—C2—N3 angle

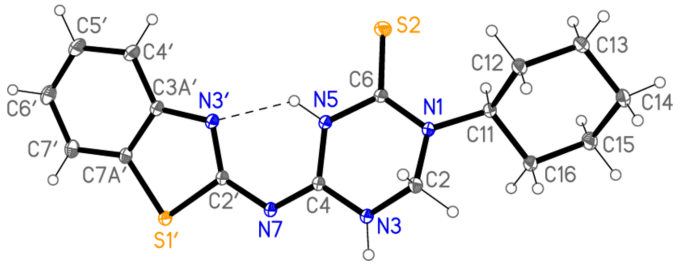


Figure 2
The molecule of the title compound **5** in the crystal. Ellipsoids represent 50% probability levels. The dashed line indicates the intramolecular hydrogen bond.

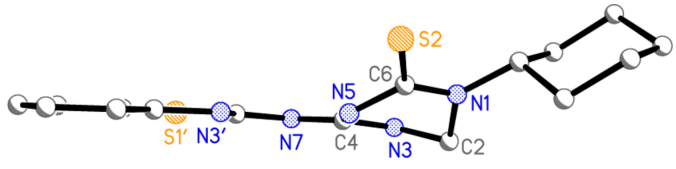


Figure 3
Side view of the molecule of **5** (H atoms omitted, radii arbitrary).

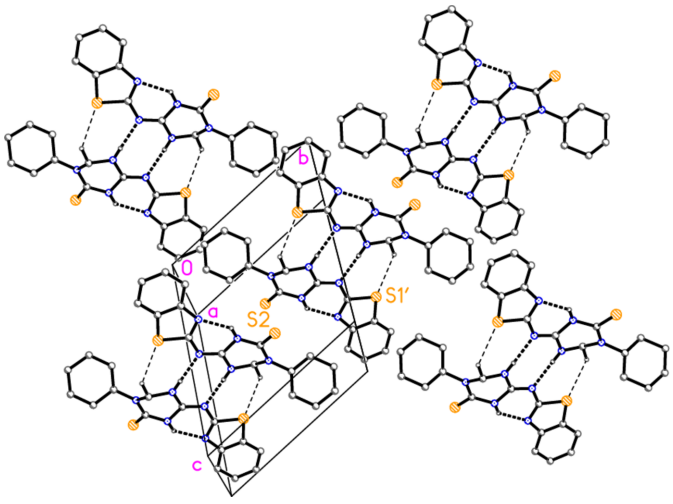


Figure 4
Packing of compound **5** viewed perpendicular to ($\bar{1}01$), showing the formation of dimers *via* classical (thick) and weak (thin) hydrogen bonds. Sulfur atom labels indicate the asymmetric unit. Hydrogen atoms not involved in these hydrogen bonds are omitted for clarity.

of 108.40 (3)°. The angle sums at C4 and C6 are both 360.0°, and the double bonds C4═N7 and C6═S2 are, at 1.3215 (5) and 1.6679 (4) Å, respectively, not significantly lengthened. In their extensive table of bond lengths, Allen *et al.* (1987) give a standard value of 1.681 (20) Å for the C═S bond length in thioureas, but no direct value for a system corresponding to C4═N7, although their general value for pyrimidines, 1.336 (14) Å, may be comparable.

3. Supramolecular features

Hydrogen bonds are listed in Table 2, which includes several borderline C—H···S contacts that we do not discuss further. In the crystal, molecules of **5** are linked to form inversion-symmetric dimers by the classical N3—H03···N7 hydrogen bond, supported by the weak C2—H2*A*···S1′ hydrogen bond (Fig. 4). The dimers are further linked *via* *x*-axis translation by the weak C16—H16*B*···S2 hydrogen bond (Fig. 5).

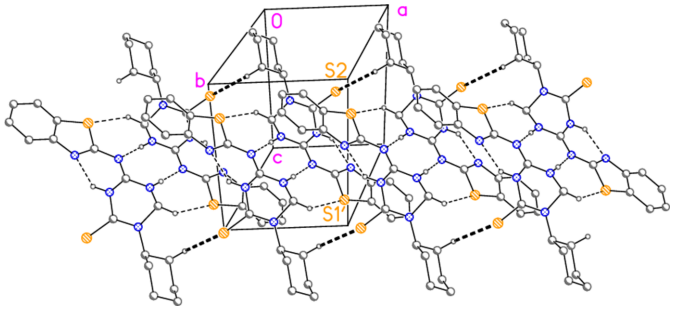


Figure 5
Packing of compound **5** viewed perpendicular to ($0\bar{1}1$), showing the linking of dimers parallel to the *x* axis *via* further C—H···S hydrogen bonds (thick dashed lines; hydrogen bonds within the dimers are shown as thin dashed lines). Sulfur atom labels indicate the asymmetric unit. Hydrogen atoms not involved in these hydrogen bonds are omitted for clarity.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H03···N7^{i}	0.865 (14)	2.039 (14)	2.8985 (5)	172.2 (13)
N5—H05···N3′	0.890 (11)	2.006 (11)	2.6968 (5)	133.5 (9)
C2—H2*A*···S1′^{i}	0.99	2.88	3.6836 (4)	138
C2—H2*B*···S2^{ii}	0.99	3.03	3.9585 (5)	157
C12—H12*B*···S2	0.99	3.01	3.5599 (5)	116
C16—H16*B*···S2^{iii}	0.99	2.83	3.7864 (5)	162
C4′—H4′···S2^{iv}	0.95	2.97	3.9042 (5)	168

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

4. Database survey

Searches were conducted using CSD Version 6.01, update Sept. 2026 (Groom *et al.*, 2016) and the ConQuest routine (Version 2026.2.0; Bruno *et al.*, 2002).

A search for structures of similar benzothiazyl derivatives to **5**, with a substituent —N(two-coordinate)—C(three-coordinate) at C2, gave 96 hits, with most showing the same very wide angles as N3′—C2′—N7 in **5**. However, a substantial subset showed values much closer to 120°. Closer inspection showed that the majority (74) of the structures, with a mean angle of 128.2 (18)°, has a *cis* configuration N—C—N—C (absolute torsion angles *ca.* 0°) about the exocyclic C═N bond, whereas the narrower angles, with a mean value of 120.9 (10)°, are associated with a *trans* configuration (absolute torsion angles *ca.* 180°).

A search for triazine/triazinane rings with no restriction on bond order or substituents, with coordination numbers 4 at C2 (based on the numbering of **5**) and 3 at all other atoms, showed that **5** may reasonably be described as a 'novel' compound. There were only 16 hits. All necessarily have formal double bonds from C2 and C4 to their substituents, but none has a C═N and a C═S double bond as in **5**. In 14 of the structures, there are two C═O groups [*e.g.* 3-(4-chlorophenyl)-1-methyl-1,3,5-triazinane-2,4-dione and its 3-(2-chlorophenyl) isomer (XOBLIN and XOBLOT; Panga *et al.*, 2022)]. The two exceptions are 2,4-bis(dinitromethylidene)-1,3,5-triazinane, an explosive compound with two C═C bonds (GOGHOC; Yan *et al.*, 2019) and *N*′-(4,4-dimethyl-2,6-disulfanylidene-1,3,5-triazinan-1-yl)-*N*,*N*-diethyldicarbonimidothioic diamide, with two C═S double bonds (TANXAK; Hussien *et al.*, 2017).

5. Synthesis and crystallization

A mixture of *O*-ethyl *N*-cyclohexylcarbamothioate **3** (2.29 g, 0.01 mol) and 2-(benzo[*d*]thiazol-2-yl)guanidine (1.92 g, 0.01 mol) **4** was reacted for 2 h under reflux in dry dimethylformamide (10 ml) containing sodium ethoxide (0.68 g, 0.01 mol). Following completion of the reaction, the reaction mixture was poured into ice-cold water and neutralized using hydrochloric acid. The precipitate thus formed was collected *via* filtration, washed thoroughly with water, dried, and then recrystallized from dimethyl sulfoxide, yielding compound **5** as colourless crystals in 42% yield (0.15 g), m.p. 509–510 K; ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm)1.20 (*m*, 3H, cyclohexyl),

1.44 (*m*, 2H, cyclohexyl), 1.58 (*d*, 1H, J = 10 Hz, cyclohexyl), 1.70 (*d*, 2H, *J* = 15 Hz, cyclohexyl), 1.77 (*d*, 2H, *J* = 10 Hz, cyclohexyl), 4.63 (*s*, 1H, NH), 4.74 (*s*, 2H, CH_2), 4.86 (*s*, 1H, NH), 7.17 (*t*, *J* = 7.5 Hz, 1H, benzothiazole-CH), 7.33 (*t*, *J* = 5 Hz, 1H, benzothiazole-CH), 7.58 (*d*, *J* = 8 Hz, 1H, benzothiazole-CH), 7.78 (*d*, *J* = 10 Hz, 1H, benzothiazole-CH); Analysis: calculated for $C_{16}H_{19}N_5S_2$: C 55.62, H 5.54, N 20.27, S 18.56. Found: C 55.59, H 5.50, N 20.21, S 18.53%.

6. Refinement

Details of data collection and structure refinement are summarized in Table 3. Hydrogen atoms of the NH groups were refined freely. Other hydrogens were introduced at calculated positions and refined using a riding model, with C—H 1.00 (methine), 0.99 (methylene) or 0.95 (aromatic) Å. The U_{iso}(H) values were fixed at 1.2 × U_{eq} of the parent carbon atoms. Nine reflections with $\Delta/\sigma > 8$ were omitted from the refinement.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{19}N_5S_2$
M_r	345.48
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	6.97438 (12), 10.81958 (19), 12.3192 (2)
α, β, γ (°)	114.1800 (18), 91.3132 (14), 103.0600 (14)
V (Å^3)	819.11 (3)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.33
Crystal size (mm)	0.2 × 0.1 × 0.1
Data collection	
Diffractometer	XtaLAB Synergy
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2025)
T_{min}, T_{max}	0.559, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	134638, 13416, 11462
R_{int}	0.030
θ values (°)	θ_{max} = 44.9, θ_{min} = 2.1
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.994
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.028, 0.089, 1.05
No. of reflections	13416
No. of parameters	216
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.62, −0.59

Computer programs: *CrysAlis PRO* (Rigaku OD, 2025), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *XP* (Bruker, 1998) and *publCIF* (Westrip, 2010).

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Synthesis and crystal structure of (*E*)-4-(benzo[*d*]thiazol-2-ylimino)-1-cyclohexyl-1,3,5-triazinane-2-thione

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Computing details

(*E*)-4-(Benzo[*d*]thiazol-2-ylimino)-1-cyclohexyl-1,3,5-triazinane-2-thione

Crystal data

$C_{16}H_{19}N_5S_2$
M_r = 345.48
Triclinic, $P\overline{1}$
a = 6.97438 (12) Å
b = 10.81958 (19) Å
c = 12.3192 (2) Å
α = 114.1800 (18)°
β = 91.3132 (14)°
γ = 103.0600 (14)°
V = 819.11 (3) Å^3
Z = 2
$F(000)$ = 364
D_x = 1.401 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 76587 reflections
θ = 3.0–45.1°
μ = 0.33 mm^{-1}
T = 100 K
Prism, colourless
0.2 × 0.1 × 0.1 mm

Data collection

XtaLAB Synergy diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2025)
T_{min} = 0.559, T_{max} = 1.000
134638 measured reflections
13416 independent reflections
11462 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 44.9°, θ_{min} = 2.1°
h = −13→13
k = −21→21
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.089
S = 1.05
13416 reflections
216 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.0934P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.40469 (5)	0.57040 (4)	0.34132 (3)	0.01203 (5)
C2	0.29528 (6)	0.66914 (4)	0.41522 (4)	0.01326 (6)
H2A	0.170930	0.657958	0.367754	0.016*
H2B	0.260448	0.650407	0.485473	0.016*
N3	0.41976 (5)	0.80986 (4)	0.45469 (4)	0.01316 (5)
H03	0.370 (2)	0.8756 (15)	0.4529 (12)	0.047 (4)*
C4	0.60318 (6)	0.83452 (4)	0.50621 (4)	0.01122 (5)
N5	0.66216 (5)	0.71576 (4)	0.49148 (3)	0.01237 (5)
H05	0.7848 (16)	0.7305 (11)	0.5245 (9)	0.023 (2)*
C6	0.58871 (6)	0.58932 (4)	0.39008 (4)	0.01198 (6)
S2	0.73359 (2)	0.47973 (2)	0.33910 (2)	0.01797 (3)
N7	0.71508 (5)	0.96423 (4)	0.56399 (3)	0.01237 (5)
C11	0.31303 (6)	0.44990 (4)	0.22608 (4)	0.01190 (6)
H11	0.421766	0.428285	0.175542	0.014*
C12	0.21738 (7)	0.31865 (4)	0.24372 (4)	0.01497 (6)
H12A	0.106864	0.335503	0.292250	0.018*
H12B	0.316607	0.297302	0.287489	0.018*
C13	0.13876 (8)	0.19412 (5)	0.12180 (5)	0.01832 (8)
H13A	0.251521	0.171996	0.076744	0.022*
H13B	0.071544	0.110918	0.134304	0.022*
C14	−0.00719 (8)	0.22541 (5)	0.04805 (5)	0.01931 (8)
H14A	−0.047016	0.145971	−0.032418	0.023*
H14B	−0.127927	0.235678	0.088001	0.023*
C15	0.08641 (8)	0.35983 (5)	0.03479 (4)	0.01804 (7)
H15A	−0.013537	0.381174	−0.008498	0.022*
H15B	0.197709	0.345486	−0.013470	0.022*
C16	0.16323 (7)	0.48397 (4)	0.15712 (4)	0.01450 (6)
H16A	0.227436	0.568638	0.145888	0.017*
H16B	0.050948	0.503456	0.203459	0.017*
S1′	1.02952 (2)	1.16919 (2)	0.69377 (2)	0.01327 (2)
C2′	0.89915 (6)	0.99074 (4)	0.62152 (4)	0.01145 (5)
N3′	0.99177 (6)	0.90340 (4)	0.63392 (4)	0.01324 (5)
C3A′	1.17474 (6)	0.97534 (4)	0.70407 (4)	0.01259 (6)
C4′	1.30722 (7)	0.91391 (5)	0.73829 (5)	0.01677 (7)
H4′	1.276116	0.815309	0.713071	0.020*
C5′	1.48491 (7)	0.99956 (6)	0.80973 (5)	0.01940 (8)
H5′	1.574984	0.958792	0.833936	0.023*
C6′	1.53349 (7)	1.14506 (6)	0.84669 (5)	0.01934 (8)
H6′	1.656516	1.201398	0.894684	0.023*
C7′	1.40353 (7)	1.20771 (5)	0.81383 (4)	0.01657 (7)
H7′	1.436250	1.306223	0.838357	0.020*
C7A′	1.22374 (6)	1.12205 (4)	0.74386 (4)	0.01258 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.01022 (11)	0.00954 (11)	0.01345 (12)	0.00232 (9)	−0.00271 (9)	0.00241 (9)
C2	0.01028 (12)	0.01091 (13)	0.01525 (15)	0.00200 (10)	−0.00118 (11)	0.00284 (11)
N3	0.01047 (11)	0.00942 (11)	0.01636 (13)	0.00216 (9)	−0.00363 (10)	0.00284 (10)
C4	0.01044 (12)	0.00970 (12)	0.01170 (13)	0.00209 (10)	−0.00193 (10)	0.00321 (10)
N5	0.01138 (11)	0.00958 (11)	0.01435 (13)	0.00184 (9)	−0.00377 (9)	0.00408 (10)
C6	0.01051 (12)	0.00951 (12)	0.01480 (14)	0.00176 (10)	−0.00203 (10)	0.00469 (11)
S2	0.01294 (4)	0.01257 (4)	0.02556 (6)	0.00442 (3)	−0.00118 (4)	0.00494 (4)
N7	0.01059 (11)	0.00960 (11)	0.01399 (12)	0.00166 (9)	−0.00336 (9)	0.00290 (9)
C11	0.01230 (13)	0.00914 (12)	0.01231 (13)	0.00174 (10)	−0.00215 (10)	0.00340 (10)
C12	0.01691 (16)	0.01051 (13)	0.01603 (15)	0.00092 (11)	−0.00368 (12)	0.00588 (12)
C13	0.02185 (19)	0.00968 (13)	0.01983 (18)	0.00241 (13)	−0.00615 (14)	0.00409 (13)
C14	0.02080 (19)	0.01146 (14)	0.01967 (18)	0.00089 (13)	−0.00858 (15)	0.00307 (13)
C15	0.02236 (19)	0.01440 (15)	0.01444 (16)	0.00298 (14)	−0.00569 (14)	0.00460 (13)
C16	0.01568 (15)	0.01070 (13)	0.01548 (15)	0.00200 (11)	−0.00446 (12)	0.00502 (12)
S1′	0.01121 (4)	0.00949 (4)	0.01605 (4)	0.00150 (3)	−0.00309 (3)	0.00332 (3)
C2′	0.01045 (12)	0.01008 (12)	0.01183 (13)	0.00165 (10)	−0.00190 (10)	0.00342 (10)
N3′	0.01184 (12)	0.01099 (11)	0.01508 (13)	0.00188 (9)	−0.00368 (10)	0.00461 (10)
C3A′	0.01077 (13)	0.01270 (13)	0.01303 (14)	0.00247 (10)	−0.00186 (10)	0.00468 (11)
C4′	0.01419 (15)	0.01648 (16)	0.01959 (18)	0.00463 (12)	−0.00305 (13)	0.00756 (14)
C5′	0.01348 (15)	0.02231 (19)	0.0222 (2)	0.00522 (14)	−0.00384 (14)	0.00922 (16)
C6′	0.01149 (14)	0.02159 (19)	0.02114 (19)	0.00159 (13)	−0.00471 (13)	0.00713 (16)
C7′	0.01120 (14)	0.01547 (15)	0.01846 (17)	0.00011 (12)	−0.00319 (12)	0.00474 (13)
C7A′	0.00993 (12)	0.01246 (13)	0.01306 (14)	0.00160 (10)	−0.00143 (10)	0.00402 (11)

Geometric parameters (Å, º)

N1—C6	1.3398 (5)	C14—C15	1.5293 (7)
N1—C2	1.4683 (6)	C14—H14A	0.9900
N1—C11	1.4797 (5)	C14—H14B	0.9900
C2—N3	1.4440 (6)	C15—C16	1.5304 (6)
C2—H2A	0.9900	C15—H15A	0.9900
C2—H2B	0.9900	C15—H15B	0.9900
N3—C4	1.3343 (5)	C16—H16A	0.9900
N3—H03	0.865 (14)	C16—H16B	0.9900
C4—N7	1.3215 (5)	S1′—C7A′	1.7343 (4)
C4—N5	1.3800 (5)	S1′—C2′	1.7631 (4)
N5—C6	1.3958 (5)	C2′—N3′	1.3127 (5)
N5—H05	0.890 (11)	N3′—C3A′	1.3895 (5)
C6—S2	1.6679 (4)	C3A′—C4′	1.4008 (6)
N7—C2′	1.3631 (5)	C3A′—C7A′	1.4094 (6)
C11—C16	1.5294 (6)	C4′—C5′	1.3900 (7)
C11—C12	1.5298 (6)	C4′—H4′	0.9500
C11—H11	1.0000	C5′—C6′	1.4018 (8)
C12—C13	1.5305 (7)	C5′—H5′	0.9500
C12—H12A	0.9900	C6′—C7′	1.3895 (7)

C12—H12B	0.9900	C6′—H6′	0.9500
C13—C14	1.5302 (7)	C7′—C7A′	1.3946 (6)
C13—H13A	0.9900	C7′—H7′	0.9500
C13—H13B	0.9900		

C6—N1—C2	115.40 (3)	C15—C14—H14A	109.5
C6—N1—C11	121.71 (4)	C13—C14—H14A	109.5
C2—N1—C11	122.65 (3)	C15—C14—H14B	109.5
N3—C2—N1	108.40 (3)	C13—C14—H14B	109.5
N3—C2—H2A	110.0	H14A—C14—H14B	108.0
N1—C2—H2A	110.0	C14—C15—C16	111.41 (4)
N3—C2—H2B	110.0	C14—C15—H15A	109.3
N1—C2—H2B	110.0	C16—C15—H15A	109.3
H2A—C2—H2B	108.4	C14—C15—H15B	109.3
C4—N3—C2	116.42 (4)	C16—C15—H15B	109.3
C4—N3—H03	122.9 (9)	H15A—C15—H15B	108.0
C2—N3—H03	120.2 (9)	C11—C16—C15	109.63 (4)
N7—C4—N3	120.58 (4)	C11—C16—H16A	109.7
N7—C4—N5	124.76 (4)	C15—C16—H16A	109.7
N3—C4—N5	114.65 (4)	C11—C16—H16B	109.7
C4—N5—C6	121.37 (3)	C15—C16—H16B	109.7
C4—N5—H05	115.7 (7)	H16A—C16—H16B	108.2
C6—N5—H05	115.9 (7)	C7A′—S1′—C2′	89.39 (2)
N1—C6—N5	114.73 (4)	N3′—C2′—N7	129.58 (4)
N1—C6—S2	126.30 (3)	N3′—C2′—S1′	115.10 (3)
N5—C6—S2	118.95 (3)	N7—C2′—S1′	115.29 (3)
C4—N7—C2′	120.95 (4)	C2′—N3′—C3A′	110.82 (4)
N1—C11—C16	112.15 (3)	N3′—C3A′—C4′	125.32 (4)
N1—C11—C12	111.77 (3)	N3′—C3A′—C7A′	115.34 (4)
C16—C11—C12	110.67 (3)	C4′—C3A′—C7A′	119.33 (4)
N1—C11—H11	107.3	C5′—C4′—C3A′	118.93 (5)
C16—C11—H11	107.3	C5′—C4′—H4′	120.5
C12—C11—H11	107.3	C3A′—C4′—H4′	120.5
C11—C12—C13	109.97 (4)	C4′—C5′—C6′	121.14 (4)
C11—C12—H12A	109.7	C4′—C5′—H5′	119.4
C13—C12—H12A	109.7	C6′—C5′—H5′	119.4
C11—C12—H12B	109.7	C7′—C6′—C5′	120.67 (4)
C13—C12—H12B	109.7	C7′—C6′—H6′	119.7
H12A—C12—H12B	108.2	C5′—C6′—H6′	119.7
C14—C13—C12	111.52 (4)	C6′—C7′—C7A′	118.19 (4)
C14—C13—H13A	109.3	C6′—C7′—H7′	120.9
C12—C13—H13A	109.3	C7A′—C7′—H7′	120.9
C14—C13—H13B	109.3	C7′—C7A′—C3A′	121.72 (4)
C12—C13—H13B	109.3	C7′—C7A′—S1′	128.93 (4)
H13A—C13—H13B	108.0	C3A′—C7A′—S1′	109.34 (3)
C15—C14—C13	110.90 (4)		

C6—N1—C2—N3	50.41 (5)	N1—C11—C16—C15	175.46 (4)

C11—N1—C2—N3	−135.15 (4)	C12—C11—C16—C15	−58.99 (5)
N1—C2—N3—C4	−51.16 (5)	C14—C15—C16—C11	57.29 (5)
C2—N3—C4—N7	−167.85 (4)	C4—N7—C2′—N3′	−2.30 (7)
C2—N3—C4—N5	13.28 (6)	C4—N7—C2′—S1′	179.78 (3)
N7—C4—N5—C6	−149.08 (4)	C7A′—S1′—C2′—N3′	0.23 (4)
N3—C4—N5—C6	29.74 (6)	C7A′—S1′—C2′—N7	178.46 (4)
C2—N1—C6—N5	−12.44 (5)	N7—C2′—N3′—C3A′	−177.35 (4)
C11—N1—C6—N5	173.07 (4)	S1′—C2′—N3′—C3A′	0.58 (5)
C2—N1—C6—S2	169.16 (3)	C2′—N3′—C3A′—C4′	177.48 (4)
C11—N1—C6—S2	−5.33 (6)	C2′—N3′—C3A′—C7A′	−1.37 (6)
C4—N5—C6—N1	−29.90 (6)	N3′—C3A′—C4′—C5′	−179.49 (5)
C4—N5—C6—S2	148.62 (4)	C7A′—C3A′—C4′—C5′	−0.69 (7)
N3—C4—N7—C2′	176.98 (4)	C3A′—C4′—C5′—C6′	−0.58 (8)
N5—C4—N7—C2′	−4.27 (7)	C4′—C5′—C6′—C7′	0.77 (9)
C6—N1—C11—C16	−150.72 (4)	C5′—C6′—C7′—C7A′	0.33 (8)
C2—N1—C11—C16	35.19 (5)	C6′—C7′—C7A′—C3A′	−1.63 (7)
C6—N1—C11—C12	84.33 (5)	C6′—C7′—C7A′—S1′	177.43 (4)
C2—N1—C11—C12	−89.75 (5)	N3′—C3A′—C7A′—C7′	−179.26 (4)
N1—C11—C12—C13	−175.66 (4)	C4′—C3A′—C7A′—C7′	1.83 (7)
C16—C11—C12—C13	58.58 (5)	N3′—C3A′—C7A′—S1′	1.52 (5)
C11—C12—C13—C14	−56.31 (6)	C4′—C3A′—C7A′—S1′	−177.40 (4)
C12—C13—C14—C15	54.74 (6)	C2′—S1′—C7A′—C7′	179.90 (5)
C13—C14—C15—C16	−55.29 (6)	C2′—S1′—C7A′—C3A′	−0.95 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H03···N7^{i}	0.865 (14)	2.039 (14)	2.8985 (5)	172.2 (13)
N5—H05···N3′	0.890 (11)	2.006 (11)	2.6968 (5)	133.5 (9)
C2—H2*A*···S1′^{i}	0.99	2.88	3.6836 (4)	138
C2—H2*B*···S2^{ii}	0.99	3.03	3.9585 (5)	157
C12—H12*B*···S2	0.99	3.01	3.5599 (5)	116
C16—H16*B*···S2^{iii}	0.99	2.83	3.7864 (5)	162
C4′—H4′···S2^{iv}	0.95	2.97	3.9042 (5)	168

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