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4,4-Dimethyl-3,4-dihydropyrido-[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazin-2-amine ethanol monosolvate[1]

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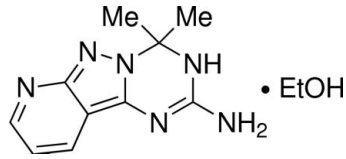
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; disorder in solvent or counterion; R factor = 0.050; wR factor = 0.133; data-to-parameter ratio = 15.0.

In the title compound, $C_{10}H_{12}N_6{\cdot}C_2H_5OH$, the planarity of the heterocyclic system is slightly distorted at the triazine ring (r.m.s. deviation = 0.1191 Å), which adopts a conformation best described as intermediate between a flattened twisted boat and a half-boat with the tertiary Csp^3 atom at the bow. In the crystal, molecules form centrosymmetric dimers connected by N···H—O and O···H—N hydrogen bonds between the amino group H atom, the ethanol solvent molecule and the triazine N atom, making an $R_4^4(12)$ graph-set motif. The other H atom of the amino group and the H atom on the endocyclic N atom form N···H—N hydrogen bonds with the N atoms of the pyrazole and pyridine rings, respectively, linking the molecules into $C(7)C(7)$ chains with the $R_2^2(8)$ binary graph-set motif running along [010].

Related literature

For a review on the synthesis and biological activity of pyrazolo[1,5-*a*]triazines, see: Dolzhenko *et al.* (2008). For the synthesis, crystal structure studies and biological activity of related fused *gem*-dimethyl-substituted amino-1,3,5-triazines, see: Dolzhenko *et al.* (2007*a*,*b*, 2009), Toyoda *et al.* (1997). For graph-set analysis of hydrogen bonding, see: Bernstein *et al.* (1995). For a related structure, see: Sachdeva *et al.* (2010).



Experimental

Crystal data

$C_{10}H_{12}N_6{\cdot}C_2H_6O$
M_r = 262.32
Monoclinic, $C2/c$
a = 12.1250 (19) Å
b = 13.913 (2) Å
c = 16.598 (3) Å
β = 101.683 (4)°
V = 2742.0 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.60 × 0.38 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.950, T_{max} = 0.991
9471 measured reflections
3129 independent reflections
2657 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.133
S = 1.06
3129 reflections
209 parameters
38 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···N1^{i}	0.86 (2)	2.16 (2)	3.0077 (18)	169.5 (18)
N6—H6B···N2^{i}	0.90 (2)	2.08 (2)	2.9754 (18)	171.5 (18)
N6—H6A···O1S^{ii}	0.85 (2)	2.03 (2)	2.8540 (18)	163.2 (18)
O1S—H1S···N4	0.87 (2)	1.93 (2)	2.7943 (17)	170 (2)

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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: HG2760).

[1] Fused heterocyclic systems with *s*-triazine ring. Part 16. for part 15, see Sachdeva *et al.* (2010).
§ Thomson Reuters ResearcherID: B-1130-2008.

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supporting information

Acta Cryst. (2011). E**67**, o83–o84 [https://doi.org/10.1107/S160053681005097X]

4,4-Dimethyl-3,4-dihydropyrido[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazin-2-amine ethanol monosolvate

Anton V. Dolzhenko, Geok Kheng Tan, Anna V. Dolzhenko, Lip Lin Koh and Wai Keung Chui

S1. Comment

The pyrazolo[1,5-*a*]triazine heterocyclic system has been recognized as a template for the construction of new potential therapeutic agents (Dolzhenko *et al.*, 2008). However data on pyrido[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazines are limited and no details on their structure are available. Herein, we report molecular and crystal structure of 4,4-dimethyl-3,4-dihydropyrido[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazin-2-amine, which crystallizes with a ethanol molecule to give the title compound, $C_{10}H_{12}N_6.C_2H_5OH$ (Fig. 1 & 2). This molecule has a close structural resemblance with some known dihydrofolate reductase inhibitors such as antimalarial drug cycloguanil and its fused analogue (Toyoda *et al.*, 1997) (Fig. 3). Due to annular tautomerism, four tautomeric forms are theoretically possible for the compound (Fig. 4). Similarly to the previously reported (Dolzhenko *et al.*, 2007*b*) related fused *gem*-dimethyl substituted amino-1,3,5-triazine, the compound exists in the crystal as a tautomer with the labile hydrogen atom located at the triazine nitrogen atom adjacent to the sp^3 hybridized carbon atom.

The heterocyclic system is nearly planar (with r.m.s. deviation of 0.1191 Å) with a distortion at the triazine ring. The triazine ring adopts the conformation best described as an intermediate between a flatten twist boat and a half-boat with atoms C-8 and N-4 at the bow and the stern. The angle between the geminal flagpole and bowsprit methyl groups is 112.40 (14)°. The N4—C7, N5—C7 and N6—C7 bond distances are similar suggesting guanidine-like electron delocalization in the N4—N6/C7 fragment of the molecule.

In the crystal, the molecules form centrosymmetric dimers connected by the N···HO and O···HN hydrogen bonds between the amino group N6—H6A, ethanol molecule and the triazine N4 atom making a $R_4^4(12)$ graph-set motif (Bernstein *et al.*, 1995). Another hydrogen atom of the amino group N6—H6B and the hydrogen atom at the endocyclic N5 atom act as hydrogen donors forming N···HN contacts with the pyrazole and pyridine N2 and N1 atoms, respectively. They arrange molecules into the running along a [010] axis $C(7)C(7)$ chains with the $R_2^2(8)$ binary graph-set motif.

S2. Experimental

4,4-Dimethyl-3,4-dihydropyrido[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazin-2-amine was prepared by the cyclocondensation of pyrazolo[3,4-*b*]pyridin-3-guanidine with acetone similarly to the previously described methods (Dolzhenko *et al.*, 2007*a*; Dolzhenko *et al.*, 2009). 1*H*-Pyrazolo[3,4-*b*]pyridin-3-guanidine (0.88 g, 5.0 mmol) and piperidine (0.30 ml, 3.0 mmol) were heated in acetone (30 ml) under reflux for 10 h. After cooling, the product was filtered and washed with acetone. Yield: 0.89 g (82%). The crystals suitable for crystallographic analysis were grown by recrystallization from ethanol. m.p. 559 K.

S3. Refinement

All C-bound H atoms were positioned geometrically and included in the refinement in riding-motion approximation [0.95 Å for CH of pyridine ring, 0.98 Å for methyl groups, and 0.99 Å for methylenic protons; U_{iso}(H) = 1.2U_{eq}(C_{py}), U_{iso}(H) = 1.5U_{eq}(C_{Me}) and U_{iso}(H)= 1.2U_{eq}($C_{methylenic}$)] while the N-bound H atoms were located in a difference map and refined freely. The ethyl group of ethanol molecule was disordered into two positions with occupancy ratio of 78:22.

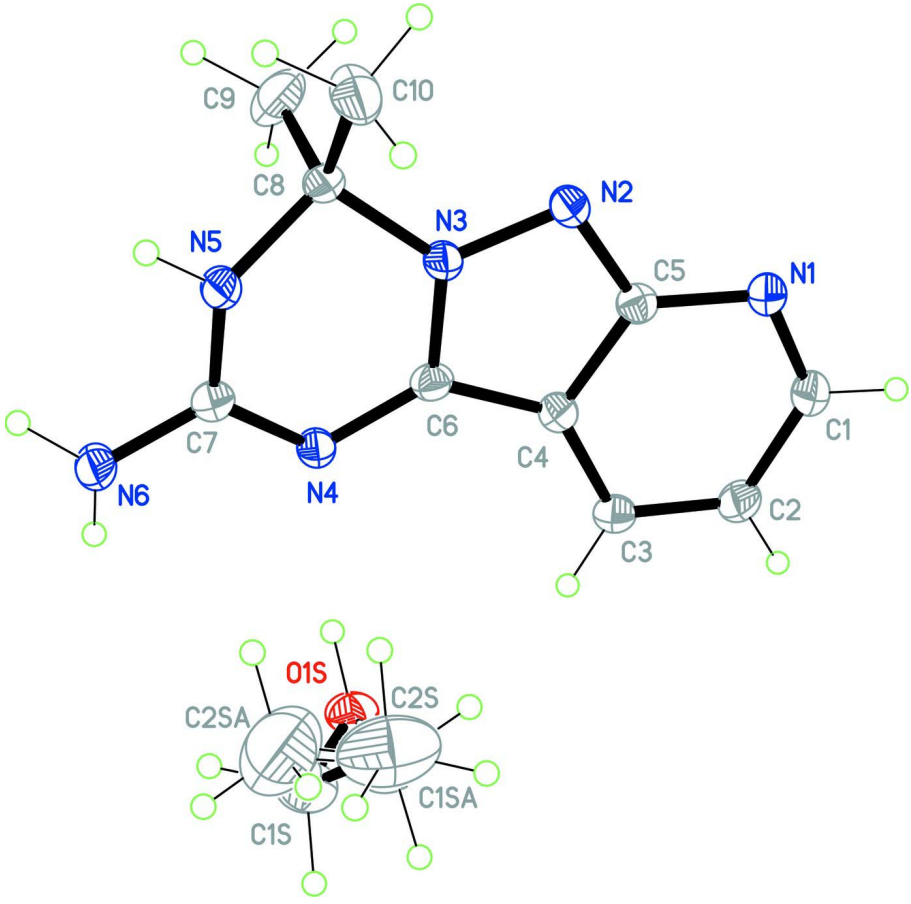


Figure 1

The molecular structure of 4,4-dimethyl-3,4-dihydropyrido[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazin-2-amine ethanol solvate showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

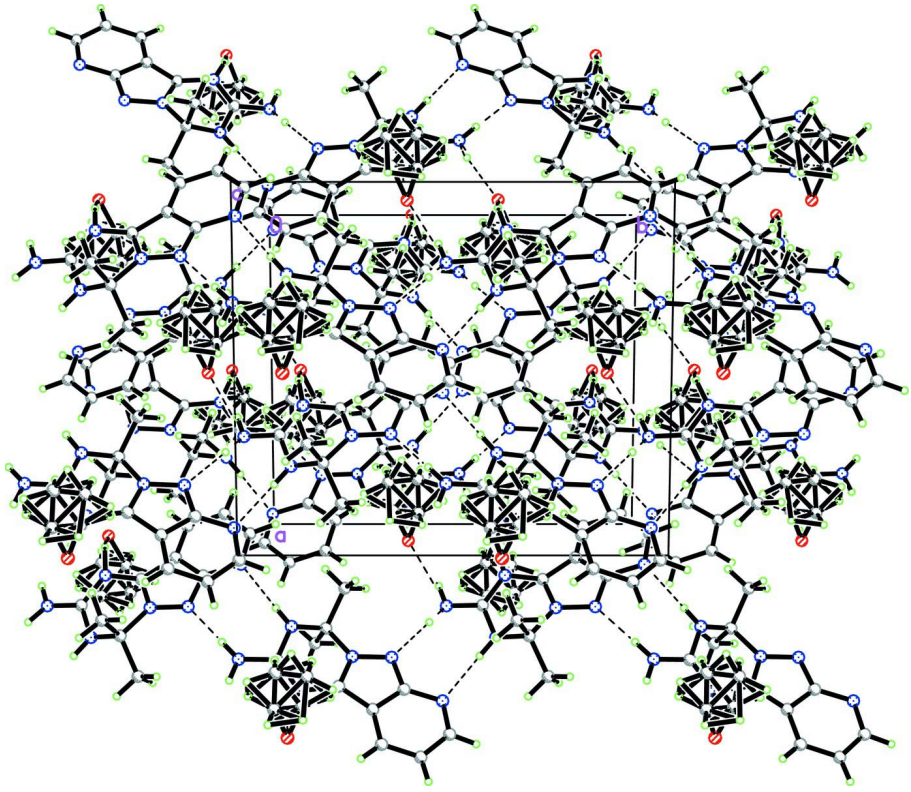
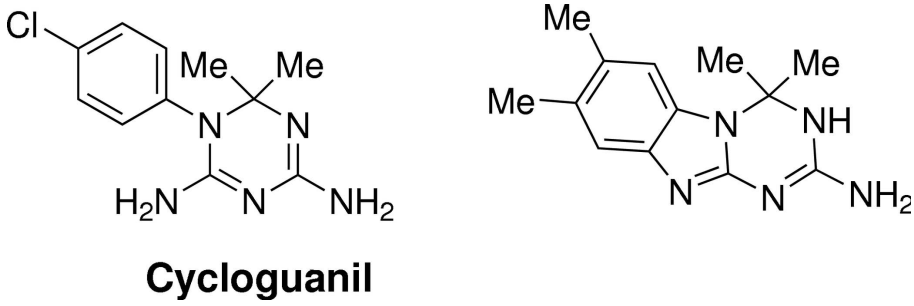


Figure 2

Crystal packing in the cell (view along axis *c*).



Cycloguanil

Figure 3

Dihydrofolate reductase inhibitors with dihydro-1,3,5-triazine ring.

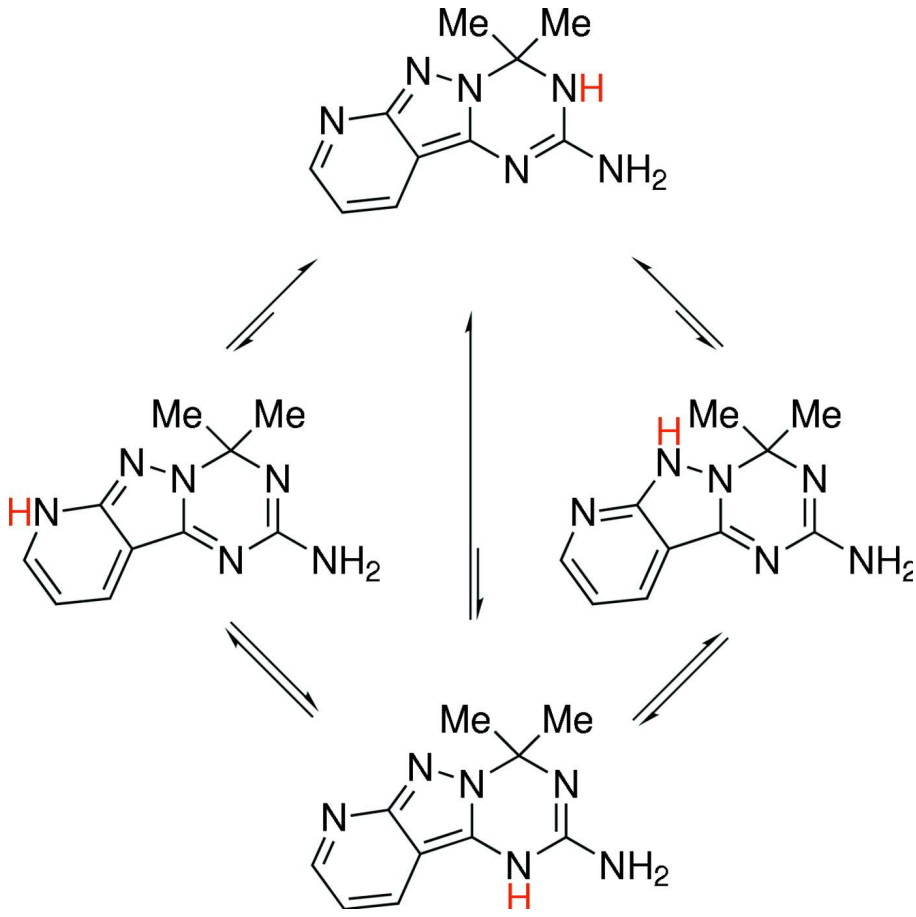


Figure 4

Annular tautomerism in 4,4-dimethyl-3,4-dihydropyrido[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazin-2-amine.

4,4-Dimethyl-3,4-dihydropyrido[2′,3′:3,4]pyrazolo[1,5-*a*][1,3,5]triazin- 2-amine ethanol monosolvate

Crystal data

$C_{10}H_{12}N_6{\cdot}C_2H_6O$
M_r = 262.32
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 12.1250 (19) Å
b = 13.913 (2) Å
c = 16.598 (3) Å
β = 101.683 (4)°
V = 2742.0 (7) Å^3
Z = 8
F(000) = 1120
D_x = 1.271 Mg m^{-3}
Melting point: 559 K
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 782 reflections
θ = 2.7–27.3°
μ = 0.09 mm^{-1}
T = 100 K
Plate, yellow
0.60 × 0.38 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.950, T_{max} = 0.991
9471 measured reflections
3129 independent reflections
2657 reflections with $I > 2\sigma(I)$

R_{int} = 0.030
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −15→14
k = −18→17
l = −18→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.133
S = 1.06
3129 reflections
209 parameters
38 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
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 1.8445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1S	0.49619 (10)	0.11324 (8)	0.46397 (7)	0.0285 (3)	
H1S	0.5246 (18)	0.1117 (15)	0.5165 (14)	0.039 (6)*	
C1S	0.5838 (2)	0.0860 (2)	0.42339 (15)	0.0384 (7)	0.781 (6)
H1SA	0.5526	0.0769	0.3640	0.046*	0.781 (6)
H1SB	0.6169	0.0243	0.4461	0.046*	0.781 (6)
C2S	0.6736 (3)	0.1618 (3)	0.4346 (2)	0.0648 (11)	0.781 (6)
H2SA	0.7335	0.1420	0.4063	0.097*	0.781 (6)
H2SB	0.7051	0.1701	0.4934	0.097*	0.781 (6)
H2SC	0.6410	0.2226	0.4114	0.097*	0.781 (6)
C1SA	0.5898 (9)	0.1503 (9)	0.4290 (6)	0.044 (2)	0.219 (6)
H1SC	0.5651	0.1572	0.3687	0.053*	0.219 (6)
H1SD	0.6120	0.2146	0.4523	0.053*	0.219 (6)
C2SA	0.6822 (14)	0.0883 (12)	0.4464 (9)	0.077 (4)	0.219 (6)
H2SD	0.7437	0.1142	0.4227	0.116*	0.219 (6)
H2SE	0.6605	0.0250	0.4226	0.116*	0.219 (6)
H2SF	0.7072	0.0823	0.5062	0.116*	0.219 (6)
N1	0.56023 (10)	0.47488 (8)	0.67409 (7)	0.0203 (3)	
N2	0.67666 (10)	0.34962 (9)	0.74160 (7)	0.0205 (3)	
N3	0.68205 (10)	0.25362 (8)	0.72312 (7)	0.0187 (3)	
N4	0.59745 (10)	0.13025 (8)	0.63025 (7)	0.0208 (3)	
N5	0.77009 (11)	0.10579 (9)	0.72296 (8)	0.0220 (3)	

H5	0.8212 (17)	0.0662 (15)	0.7465 (12)	0.034 (5)*
N6	0.68817 (13)	−0.01616 (10)	0.63779 (9)	0.0302 (3)
H6A	0.6334 (17)	−0.0354 (14)	0.6007 (12)	0.028 (5)*
H6B	0.7326 (17)	−0.0588 (15)	0.6701 (12)	0.037 (5)*
C1	0.47528 (13)	0.49206 (10)	0.61227 (9)	0.0226 (3)
H1	0.4479	0.5562	0.6059	0.027*
C2	0.42132 (13)	0.42321 (11)	0.55453 (9)	0.0235 (3)
H2	0.3604	0.4420	0.5119	0.028*
C3	0.45708 (12)	0.32946 (11)	0.56021 (9)	0.0211 (3)
H3	0.4242	0.2824	0.5212	0.025*
C4	0.54476 (12)	0.30661 (10)	0.62667 (8)	0.0182 (3)
C5	0.59298 (12)	0.38088 (10)	0.68156 (8)	0.0180 (3)
C6	0.60627 (12)	0.22357 (10)	0.65668 (8)	0.0189 (3)
C7	0.68259 (13)	0.07377 (11)	0.66450 (9)	0.0220 (3)
C8	0.75702 (12)	0.18664 (10)	0.77658 (8)	0.0210 (3)
C9	0.70180 (17)	0.15481 (14)	0.84683 (10)	0.0384 (4)
H9A	0.6953	0.2100	0.8823	0.058*
H9B	0.7480	0.1049	0.8791	0.058*
H9C	0.6266	0.1291	0.8243	0.058*
C10	0.87144 (15)	0.23234 (12)	0.80702 (12)	0.0363 (4)
H10A	0.8983	0.2606	0.7604	0.055*
H10B	0.9249	0.1832	0.8332	0.055*
H10C	0.8651	0.2827	0.8471	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1S	0.0298 (6)	0.0327 (6)	0.0198 (6)	0.0020 (5)	−0.0023 (5)	−0.0027 (4)
C1S	0.0441 (15)	0.0418 (17)	0.0304 (12)	0.0038 (12)	0.0104 (10)	−0.0026 (11)
C2S	0.050 (2)	0.101 (3)	0.0473 (17)	−0.0189 (19)	0.0193 (14)	0.0019 (18)
C1SA	0.044 (5)	0.049 (6)	0.040 (4)	−0.019 (4)	0.008 (4)	0.007 (4)
C2SA	0.089 (8)	0.077 (8)	0.069 (7)	0.018 (6)	0.021 (6)	0.022 (6)
N1	0.0230 (6)	0.0168 (6)	0.0203 (6)	−0.0004 (5)	0.0025 (5)	0.0008 (5)
N2	0.0230 (6)	0.0159 (6)	0.0205 (6)	0.0006 (5)	−0.0001 (5)	−0.0021 (5)
N3	0.0195 (6)	0.0158 (6)	0.0184 (6)	0.0010 (4)	−0.0016 (5)	−0.0014 (4)
N4	0.0233 (6)	0.0164 (6)	0.0192 (6)	0.0016 (5)	−0.0042 (5)	−0.0017 (4)
N5	0.0227 (6)	0.0180 (6)	0.0217 (6)	0.0050 (5)	−0.0042 (5)	−0.0022 (5)
N6	0.0356 (8)	0.0196 (7)	0.0273 (7)	0.0063 (6)	−0.0128 (6)	−0.0040 (5)
C1	0.0255 (8)	0.0178 (7)	0.0235 (7)	0.0024 (6)	0.0027 (6)	0.0018 (6)
C2	0.0234 (7)	0.0232 (7)	0.0209 (7)	0.0015 (6)	−0.0028 (6)	0.0024 (6)
C3	0.0223 (7)	0.0213 (7)	0.0177 (7)	−0.0012 (5)	−0.0002 (5)	−0.0009 (5)
C4	0.0190 (7)	0.0170 (7)	0.0183 (7)	−0.0008 (5)	0.0029 (5)	−0.0004 (5)
C5	0.0173 (6)	0.0190 (7)	0.0177 (6)	−0.0011 (5)	0.0033 (5)	0.0001 (5)
C6	0.0185 (7)	0.0209 (7)	0.0158 (6)	−0.0005 (5)	0.0003 (5)	0.0001 (5)
C7	0.0254 (7)	0.0201 (7)	0.0182 (7)	0.0013 (6)	−0.0011 (6)	−0.0004 (5)
C8	0.0226 (7)	0.0194 (7)	0.0179 (7)	0.0046 (5)	−0.0031 (6)	−0.0015 (5)
C9	0.0475 (11)	0.0425 (10)	0.0257 (8)	0.0202 (8)	0.0088 (8)	0.0115 (7)
C10	0.0286 (9)	0.0244 (8)	0.0466 (10)	0.0042 (7)	−0.0146 (8)	−0.0081 (7)

Geometric parameters (Å, º)

O1S—C1S	1.420 (3)	N5—C7	1.3596 (18)
O1S—C1SA	1.469 (9)	N5—C8	1.4628 (19)
O1S—H1S	0.87 (2)	N5—H5	0.86 (2)
C1S—C2S	1.500 (5)	N6—C7	1.334 (2)
C1S—H1SA	0.9900	N6—H6A	0.85 (2)
C1S—H1SB	0.9900	N6—H6B	0.90 (2)
C2S—H2SA	0.9800	C1—C2	1.418 (2)
C2S—H2SB	0.9800	C1—H1	0.9500
C2S—H2SC	0.9800	C2—C3	1.372 (2)
C1SA—C2SA	1.40 (2)	C2—H2	0.9500
C1SA—H1SC	0.9900	C3—C4	1.4047 (19)
C1SA—H1SD	0.9900	C3—H3	0.9500
C2SA—H2SD	0.9800	C4—C6	1.410 (2)
C2SA—H2SE	0.9800	C4—C5	1.4227 (19)
C2SA—H2SF	0.9800	C8—C10	1.517 (2)
N1—C1	1.3202 (19)	C8—C9	1.523 (2)
N1—C5	1.3651 (18)	C9—H9A	0.9800
N2—C5	1.3425 (18)	C9—H9B	0.9800
N2—N3	1.3749 (17)	C9—H9C	0.9800
N3—C6	1.3508 (17)	C10—H10A	0.9800
N3—C8	1.4682 (18)	C10—H10B	0.9800
N4—C7	1.3299 (19)	C10—H10C	0.9800
N4—C6	1.3678 (18)		

C1S—O1S—C1SA	36.3 (5)	N1—C1—C2	125.71 (14)
C1S—O1S—H1S	106.7 (14)	N1—C1—H1	117.1
C1SA—O1S—H1S	102.9 (14)	C2—C1—H1	117.1
O1S—C1S—C2S	110.4 (3)	C3—C2—C1	119.98 (13)
O1S—C1S—H1SA	109.6	C3—C2—H2	120.0
C2S—C1S—H1SA	109.6	C1—C2—H2	120.0
O1S—C1S—H1SB	109.6	C2—C3—C4	116.60 (13)
C2S—C1S—H1SB	109.6	C2—C3—H3	121.7
H1SA—C1S—H1SB	108.1	C4—C3—H3	121.7
C1S—C2S—H2SA	109.5	C3—C4—C6	136.46 (13)
C1S—C2S—H2SB	109.5	C3—C4—C5	119.08 (13)
H2SA—C2S—H2SB	109.5	C6—C4—C5	104.45 (12)
C1S—C2S—H2SC	109.5	N2—C5—N1	122.69 (12)
H2SA—C2S—H2SC	109.5	N2—C5—C4	113.00 (12)
H2SB—C2S—H2SC	109.5	N1—C5—C4	124.30 (13)
C2SA—C1SA—O1S	110.6 (11)	N3—C6—N4	123.49 (12)
C2SA—C1SA—H1SC	109.5	N3—C6—C4	104.98 (12)
O1S—C1SA—H1SC	109.5	N4—C6—C4	131.53 (13)
C2SA—C1SA—H1SD	109.5	N4—C7—N6	119.96 (13)
O1S—C1SA—H1SD	109.5	N4—C7—N5	122.51 (14)
H1SC—C1SA—H1SD	108.1	N6—C7—N5	117.38 (13)
C1SA—C2SA—H2SD	109.5	N5—C8—N3	104.50 (11)

C1SA—C2SA—H2SE	109.5	N5—C8—C10	108.70 (13)
H2SD—C2SA—H2SE	109.5	N3—C8—C10	110.36 (13)
C1SA—C2SA—H2SF	109.5	N5—C8—C9	111.15 (13)
H2SD—C2SA—H2SF	109.5	N3—C8—C9	109.45 (12)
H2SE—C2SA—H2SF	109.5	C10—C8—C9	112.40 (14)
C1—N1—C5	114.26 (12)	C8—C9—H9A	109.5
C5—N2—N3	102.25 (11)	C8—C9—H9B	109.5
C6—N3—N2	115.31 (11)	H9A—C9—H9B	109.5
C6—N3—C8	122.17 (12)	C8—C9—H9C	109.5
N2—N3—C8	122.23 (11)	H9A—C9—H9C	109.5
C7—N4—C6	114.85 (12)	H9B—C9—H9C	109.5
C7—N5—C8	121.41 (12)	C8—C10—H10A	109.5
C7—N5—H5	120.0 (13)	C8—C10—H10B	109.5
C8—N5—H5	111.9 (13)	H10A—C10—H10B	109.5
C7—N6—H6A	116.8 (13)	C8—C10—H10C	109.5
C7—N6—H6B	118.9 (13)	H10A—C10—H10C	109.5
H6A—N6—H6B	120.5 (18)	H10B—C10—H10C	109.5
C1SA—O1S—C1S—C2S	21.3 (7)	C8—N3—C6—C4	174.81 (13)
C1S—O1S—C1SA—C2SA	−39.4 (9)	C7—N4—C6—N3	−12.5 (2)
C5—N2—N3—C6	−1.02 (16)	C7—N4—C6—C4	168.49 (15)
C5—N2—N3—C8	−175.06 (13)	C3—C4—C6—N3	178.26 (17)
C5—N1—C1—C2	−2.2 (2)	C5—C4—C6—N3	−0.17 (15)
N1—C1—C2—C3	−0.2 (2)	C3—C4—C6—N4	−2.6 (3)
C1—C2—C3—C4	2.3 (2)	C5—C4—C6—N4	178.95 (15)
C2—C3—C4—C6	179.72 (16)	C6—N4—C7—N6	−173.68 (14)
C2—C3—C4—C5	−2.0 (2)	C6—N4—C7—N5	1.7 (2)
N3—N2—C5—N1	−177.97 (13)	C8—N5—C7—N4	26.4 (2)
N3—N2—C5—C4	0.87 (16)	C8—N5—C7—N6	−158.08 (14)
C1—N1—C5—N2	−178.85 (14)	C7—N5—C8—N3	−37.89 (18)
C1—N1—C5—C4	2.4 (2)	C7—N5—C8—C10	−155.73 (14)
C3—C4—C5—N2	−179.23 (13)	C7—N5—C8—C9	80.06 (17)
C6—C4—C5—N2	−0.46 (17)	C6—N3—C8—N5	27.26 (18)
C3—C4—C5—N1	−0.4 (2)	N2—N3—C8—N5	−159.11 (12)
C6—C4—C5—N1	178.35 (13)	C6—N3—C8—C10	143.94 (14)
N2—N3—C6—N4	−178.45 (13)	N2—N3—C8—C10	−42.42 (19)
C8—N3—C6—N4	−4.4 (2)	C6—N3—C8—C9	−91.86 (17)
N2—N3—C6—C4	0.77 (17)	N2—N3—C8—C9	81.78 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···N1^{i}	0.86 (2)	2.16 (2)	3.0077 (18)	169.5 (18)
N6—H6*B*···N2^{i}	0.90 (2)	2.08 (2)	2.9754 (18)	171.5 (18)
N6—H6*A*···O1*S*^{ii}	0.85 (2)	2.03 (2)	2.8540 (18)	163.2 (18)
O1*S*—H1*S*···N4	0.87 (2)	1.93 (2)	2.7943 (17)	170 (2)

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1, −*y*, −*z*+1.