Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hydrogen-bonded sheets in 4-amino-8,8-dimethyl-2-(methylsulfanyl)-8,9-dihydropyrimidino[4,5-*b*]quinolin-6(7*H*)-one

Silvia Cruz,[a] Justo Cobo,[b] John N. Low[c] and Christopher Glidewell[d]*

[a]Departamento de Química, Universidad de Nariño, Ciudad Universitaria, Torobajo, AA 1175, Pasto, Colombia, [b]Departamento de Química Inorgánica y Orgánica, Universidad de Jaén, 23071 Jaén, Spain, [c]Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and [d]School of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland

Correspondence e-mail: cg@st-andrews.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.143
Data-to-parameter ratio = 17.6

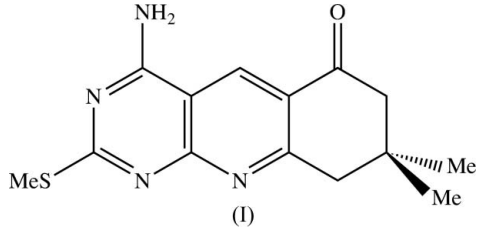
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 2 October 2006
Accepted 2 October 2006

The title molecule, $C_{14}H_{16}N_4OS$, shows strong bond fixation within the fused heterocyclic rings. In the crystal structure, molecules are linked into sheets by a combination of N—H···N and N—H···O hydrogen bonds.

Comment

We report here the structure of the title compound, (I) (Fig. 1), which was prepared by microwave irradiation of a two-component mixture of a 6-aminopyrimidine and the condensation product formed from dimedone and formaldehyde. By contrast a similar reaction between 6-aminopyrimidines, 5,5-dimethylcyclohexane-1,3-dione and a large excess of formaldehyde yielded spiranopyridopyrimidines (Quiroga *et al.*, 2006).



(I)

The bond distances within the fused heterocyclic system (Table 1) provide evidence for significant bond fixation of the naphthalene type. Thus, for example, the bonds N1—C2, N3—C4 and C9*A*—N10 are all significantly shorter than the bonds C2—N3, N10—C10*A* and C10*A*—N1, while C5—C5*A* is the shortest of the C—C bonds. The carbocyclic ring adopts a

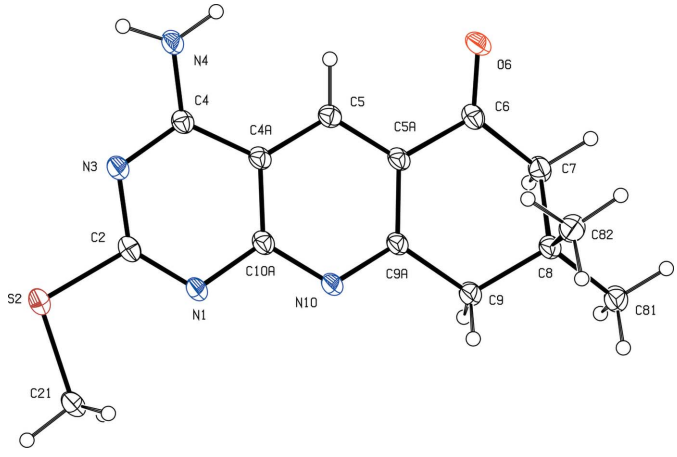


Figure 1
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

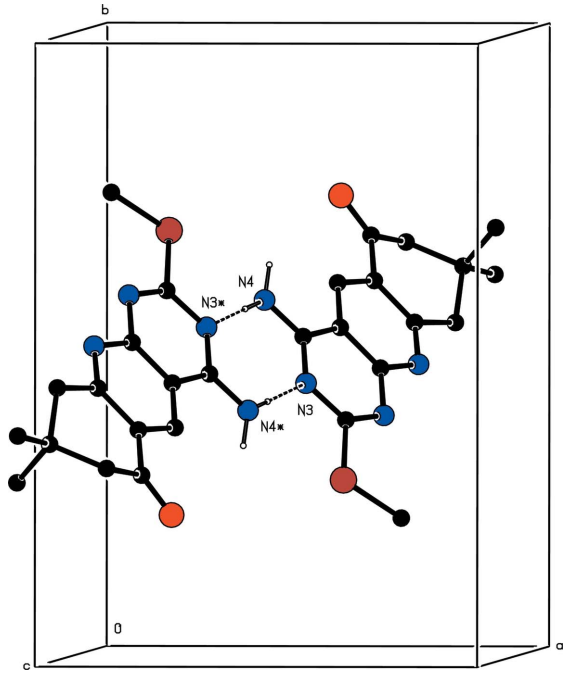


Figure 2
Part of the crystal structure of compound (I), showing the formation of the $R_2^2(8)$ substructure. Hydrogen bonds are shown as dashed lines and for the sake of clarity the H atoms bonded to C atoms have been omitted. The atoms marked with an asterisk (*) are at the symmetry position $(1-x, 1-y, 2-z)$.

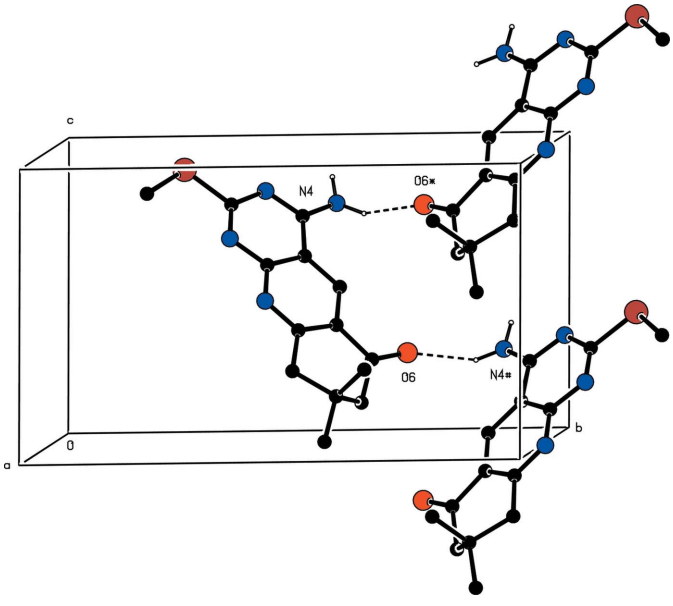


Figure 3
Part of the crystal structure of compound (I), showing the formation of the $C(8)$ substructure. The hydrogen bonds are shown as dashed lines and for the sake of clarity the H atoms bonded to C atoms have been omitted. The atoms marked with an asterisk (*) or a hash (#) are at the symmetry positions $(x, \frac{3}{2}-y, \frac{1}{2}+z)$ and $(x, \frac{3}{2}-y, -\frac{1}{2}+z)$, respectively.

conformation best described as intermediate between an envelope form, with the fold across the vector C7···C9, and a half-chair form. The ring-puckering parameters (Cremer & Pople, 1975) for the atom sequence C5*A*—C6—C7—C8—C9—C9*A* are $\theta = 129.2\ (2)^\circ$ and $\varphi = 342.4\ (4)^\circ$; the idealized values for the envelope and half-chair forms, respectively, are $\theta = 126.3$ and 129.8°, and $\varphi = (60k)$ and $(60k + 30)^\circ$, where k is zero or an integer. The two S—C distances are clearly different, and atom C21 lies almost in the plane of the adjacent pyrimidine ring.

The molecules are linked into sheets by two hydrogen bonds (Table 2), and the formation of the sheets is readily analysed in terms of two simple substructures, each formed by just one hydrogen bond. In the first substructure, amino atom N4 in the molecule at (x, y, z) acts as a hydrogen-bond donor, *via* H4*A*, to the pyrimidine ring atom N3 in the molecule at $(1-x, 1-y, 2-z)$, so generating by inversion an $R_2^2(8)$ (Bernstein *et al.*, 1995) ring centred at $(\frac{1}{2}, \frac{1}{2}, 1)$ (Fig. 2). In the second substructure, amino atom N4 at (x, y, z) acts as a hydrogen-bond donor, *via* H4*B*, to atom O6 in the molecule at $(x, \frac{3}{2}-y, \frac{1}{2}+z)$, so forming a simple $C(8)$ chain running parallel to the [001] direction and generated by the *c*-glide plane at $y = 0.75$ (Fig. 3). The combination of these two substructures generates a sheet parallel to (100) (Fig. 4), but there are no direction-specific interactions between adjacent sheets; in particular C—H···π hydrogen bonds and π–π stacking interactions are absent.

Experimental

A mixture of 4,6-diamino-2-methylsulfanylpyrimidine (1.0 mmol), 2,2-methylenebis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one) (1.0 mmol) and triethylamine (0.5 mmol) was placed in an open Pyrex-glass vessel and irradiated in a domestic microwave oven for 80 s at 600 W. The resulting solid product was collected by filtration, washed with cold ethanol, dried and then recrystallized from ethanol to provide crystals of compound (I) suitable for single-crystal X-ray diffraction; yield 60%, m.p. 580 K.

Crystal data

$C_{14}H_{16}N_4OS$
$M_r = 288.37$
Monoclinic, $P2_1/c$
$a = 10.7138\ (11)$ Å
$b = 15.1368\ (15)$ Å
$c = 8.9112\ (6)$ Å
$\beta = 101.208\ (6)^\circ$
$V = 1417.6\ (2)$ Å^3
$Z = 4$
$D_x = 1.351$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.23$ mm^{-1}
$T = 120\ (2)$ K
Block, colourless
0.40 × 0.24 × 0.18 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.926$, $T_{max} = 0.960$
20540 measured reflections
3245 independent reflections
2115 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.143$
$S = 1.02$
3245 reflections
184 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.6375P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

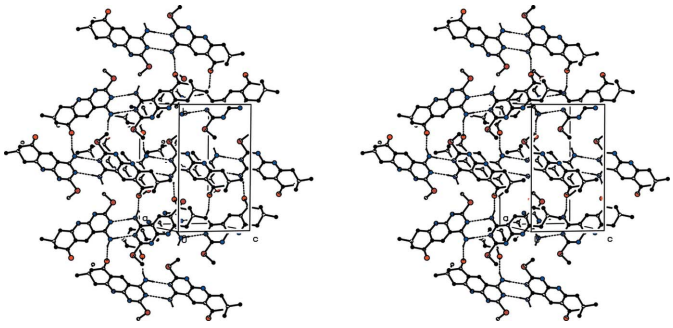


Figure 4
A stereoscopic view of part of the crystal structure of compound (I), showing the formation of a sheet parallel to (100). The hydrogen bonds are shown as dashed lines and for the sake of clarity the H atoms bonded to C atoms have been omitted.

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.314 (3)	C9*A*—N10	1.328 (3)
C2—N3	1.364 (3)	N10—C10*A*	1.356 (3)
N3—C4	1.338 (3)	C10*A*—N1	1.371 (3)
C4—C4*A*	1.445 (3)	C4*A*—C10*A*	1.408 (3)
C4*A*—C5	1.401 (3)	C2—S2	1.753 (2)
C5—C5*A*	1.384 (3)	S2—C21	1.794 (3)
C5*A*—C9*A*	1.413 (3)	C4—N4	1.332 (3)
C2—S2—C21	101.78 (12)		
N1—C2—S2—C21	2.1 (2)	N3—C2—S2—C21	−177.21 (17)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···N3^{i}	0.90	2.17	3.067 (3)	173
N4—H4*B*···O6^{ii}	0.90	2.15	2.946 (3)	147

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

All H atoms were located in difference maps and then treated as riding atoms with distances C—H = 0.95 Å (aromatic), 0.98 Å (CH_3) or 0.99 Å (CH_2) and N—H = 0.90 Å, and with $U_{iso}(H) = kU_{eq}(C,N)$, where k = 1.5 for methyl H atoms and 1.2 for all other H atoms.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. JC and JT thank the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. SC thanks COLCIENCIAS and UDENAR (Universidad de Nariño, Colombia) for financial support.

References

Bernstein, J., Davis, R., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Hooft, R. W. W. (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
McArdle, P. (2003). *OSCAIL for Windows*. Version 10. Crystallography Centre, Chemistry Department, NUI Galway, Ireland.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Quiroga, J., Cruz, S., Insuasty, B., Abonía, R., Nogueras, M. & Cobo, J. (2006). *Tetrahedron Lett.* **47**, 27–30.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

Acta Cryst. (2006). E**62**, o4933–o4935 [https://doi.org/10.1107/S1600536806040633]

Hydrogen-bonded sheets in 4-amino-8,8-dimethyl-2-(methylsulfanyl)-8,9-dihydropyrimidino[4,5-*b*]quinolin-6(7*H*)-one

Silvia Cruz, Justo Cobo, John N. Low and Christopher Glidewell

4-Amino-8,8-dimethyl-2- (methanesulfanyl)-8,9-dihydropyrimidino[4,5-*b*]quinolin-6(7*H*)-one

Crystal data

$C_{14}H_{16}N_4OS$
$M_r = 288.37$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.7138$ (11) Å
$b = 15.1368$ (15) Å
$c = 8.9112$ (6) Å
$\beta = 101.208$ (6)°
$V = 1417.6$ (2) Å^3
$Z = 4$
$F(000) = 608$
$D_x = 1.351$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3245 reflections
$\theta = 2.4$–27.5°
$\mu = 0.23$ mm^{-1}
$T = 120$ K
Block, colourless
0.40 × 0.24 × 0.18 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.926$, $T_{max} = 0.960$
20540 measured reflections
3245 independent reflections
2115 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -13 \rightarrow 13$
$k = -19 \rightarrow 19$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.143$
$S = 1.02$
3245 reflections
184 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
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.6375P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Experimental. MS (70 eV) *m*/*z* (%) 290 (100, M^+), 289 (62), 275 (34), 259 (5), 245 (9), 220 (17)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.74462 (19)	0.39484 (12)	0.7310 (2)	0.0288 (5)
C2	0.6764 (2)	0.39091 (15)	0.8384 (3)	0.0290 (5)
S2	0.69070 (6)	0.29872 (4)	0.95954 (7)	0.0350 (2)
C21	0.8107 (3)	0.23543 (17)	0.8931 (3)	0.0355 (6)
N3	0.59209 (19)	0.45107 (12)	0.8743 (2)	0.0283 (5)
C4	0.5710 (2)	0.52293 (15)	0.7856 (2)	0.0250 (5)
N4	0.48914 (19)	0.58258 (13)	0.8191 (2)	0.0301 (5)
C4A	0.6340 (2)	0.53342 (14)	0.6572 (2)	0.0250 (5)
C5	0.6103 (2)	0.60132 (15)	0.5486 (2)	0.0260 (5)
C5A	0.6734 (2)	0.60094 (14)	0.4270 (2)	0.0247 (5)
C6	0.6463 (2)	0.66958 (15)	0.3058 (2)	0.0274 (5)
O6	0.58072 (17)	0.73385 (11)	0.32040 (18)	0.0338 (4)
C7	0.7028 (2)	0.65422 (16)	0.1666 (3)	0.0311 (6)
C8	0.8376 (2)	0.61671 (15)	0.2029 (2)	0.0274 (5)
C81	0.8854 (3)	0.59856 (16)	0.0546 (3)	0.0334 (6)
C82	0.9273 (3)	0.68183 (16)	0.3016 (3)	0.0358 (6)
C9	0.8344 (2)	0.52914 (15)	0.2897 (3)	0.0312 (6)
C9A	0.7636 (2)	0.53374 (14)	0.4198 (2)	0.0252 (5)
N10	0.78922 (18)	0.46986 (12)	0.5234 (2)	0.0279 (5)
C10A	0.7220 (2)	0.46742 (15)	0.6375 (2)	0.0263 (5)
H21A	0.7841	0.2243	0.7832	0.053*
H21B	0.8226	0.1790	0.9479	0.053*
H21C	0.8910	0.2684	0.9119	0.053*
H4A	0.4592	0.5712	0.9047	0.036*
H4B	0.4941	0.6379	0.7837	0.036*
H5	0.5517	0.6471	0.5583	0.031*
H7A	0.7041	0.7109	0.1115	0.037*
H7B	0.6476	0.6128	0.0975	0.037*
H81A	0.8307	0.5543	−0.0060	0.050*
H81B	0.9729	0.5764	0.0793	0.050*
H81C	0.8831	0.6534	−0.0044	0.050*
H82A	0.9243	0.7388	0.2489	0.054*
H82B	1.0144	0.6587	0.3190	0.054*
H82C	0.9008	0.6897	0.4000	0.054*
H9A	0.7943	0.4834	0.2165	0.037*
H9B	0.9230	0.5103	0.3305	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0383 (12)	0.0191 (10)	0.0309 (11)	0.0019 (9)	0.0112 (9)	0.0049 (8)
C2	0.0341 (14)	0.0219 (12)	0.0303 (12)	−0.0026 (10)	0.0048 (10)	0.0034 (9)
S2	0.0459 (4)	0.0266 (3)	0.0350 (4)	0.0031 (3)	0.0143 (3)	0.0098 (3)
C21	0.0468 (16)	0.0229 (12)	0.0380 (14)	0.0050 (12)	0.0111 (12)	0.0083 (10)
N3	0.0351 (11)	0.0213 (10)	0.0298 (11)	0.0004 (9)	0.0094 (8)	0.0029 (8)

C4	0.0286 (12)	0.0194 (12)	0.0266 (11)	−0.0033 (10)	0.0047 (9)	−0.0015 (9)
N4	0.0429 (12)	0.0191 (10)	0.0309 (11)	−0.0006 (9)	0.0137 (9)	0.0007 (8)
C4A	0.0317 (13)	0.0169 (11)	0.0267 (12)	−0.0025 (10)	0.0064 (9)	−0.0022 (9)
C5	0.0308 (13)	0.0197 (12)	0.0279 (12)	−0.0015 (10)	0.0068 (10)	−0.0022 (9)
C5A	0.0306 (13)	0.0156 (11)	0.0280 (12)	−0.0026 (9)	0.0058 (10)	−0.0012 (9)
C6	0.0338 (13)	0.0219 (12)	0.0258 (12)	−0.0026 (11)	0.0042 (10)	0.0007 (9)
O6	0.0452 (11)	0.0210 (9)	0.0362 (9)	0.0063 (8)	0.0104 (8)	0.0039 (7)
C7	0.0376 (14)	0.0277 (13)	0.0284 (12)	0.0010 (11)	0.0078 (10)	0.0048 (10)
C8	0.0372 (14)	0.0200 (12)	0.0265 (12)	−0.0008 (10)	0.0102 (10)	−0.0008 (9)
C81	0.0450 (16)	0.0258 (14)	0.0321 (13)	−0.0013 (11)	0.0138 (11)	0.0000 (10)
C82	0.0400 (15)	0.0307 (14)	0.0391 (14)	−0.0059 (12)	0.0137 (11)	−0.0054 (11)
C9	0.0448 (15)	0.0218 (12)	0.0300 (13)	0.0031 (11)	0.0152 (11)	0.0018 (10)
C9A	0.0329 (13)	0.0171 (11)	0.0264 (12)	−0.0009 (10)	0.0081 (10)	0.0001 (9)
N10	0.0381 (12)	0.0182 (10)	0.0294 (10)	0.0025 (9)	0.0117 (9)	0.0028 (8)
C10A	0.0336 (13)	0.0198 (12)	0.0257 (11)	−0.0018 (10)	0.0062 (9)	0.0001 (9)

Geometric parameters (Å, º)

N1—C2	1.314 (3)	C5—H5	0.95
C2—N3	1.364 (3)	C5A—C6	1.486 (3)
N3—C4	1.338 (3)	C6—O6	1.221 (3)
C4—C4A	1.445 (3)	C6—C7	1.501 (3)
C4A—C5	1.401 (3)	C7—C8	1.526 (3)
C5—C5A	1.384 (3)	C7—H7A	0.99
C5A—C9A	1.413 (3)	C7—H7B	0.99
C9A—N10	1.328 (3)	C8—C82	1.530 (3)
N10—C10A	1.356 (3)	C8—C81	1.532 (3)
C10A—N1	1.371 (3)	C8—C9	1.538 (3)
C4A—C10A	1.408 (3)	C81—H81A	0.98
C2—S2	1.753 (2)	C81—H81B	0.98
S2—C21	1.794 (3)	C81—H81C	0.98
C21—H21A	0.98	C82—H82A	0.98
C21—H21B	0.98	C82—H82B	0.98
C21—H21C	0.98	C82—H82C	0.98
C4—N4	1.332 (3)	C9—C9A	1.506 (3)
N4—H4A	0.90	C9—H9A	0.99
N4—H4B	0.90	C9—H9B	0.99
C2—N1—C10A	114.9 (2)	C8—C7—H7B	108.8
N1—C2—N3	128.9 (2)	H7A—C7—H7B	107.7
N1—C2—S2	119.38 (18)	C7—C8—C82	110.2 (2)
N3—C2—S2	111.68 (17)	C7—C8—C81	110.20 (19)
C2—S2—C21	101.78 (12)	C82—C8—C81	109.5 (2)
S2—C21—H21A	109.5	C7—C8—C9	108.33 (19)
S2—C21—H21B	109.5	C82—C8—C9	109.8 (2)
H21A—C21—H21B	109.5	C81—C8—C9	108.84 (18)
S2—C21—H21C	109.5	C8—C81—H81A	109.5
H21A—C21—H21C	109.5	C8—C81—H81B	109.5

H21B—C21—H21C	109.5	H81A—C81—H81B	109.5
C4—N3—C2	116.59 (19)	C8—C81—H81C	109.5
N4—C4—N3	117.5 (2)	H81A—C81—H81C	109.5
N4—C4—C4A	122.1 (2)	H81B—C81—H81C	109.5
N3—C4—C4A	120.4 (2)	C8—C82—H82A	109.5
C4—N4—H4A	114.8	C8—C82—H82B	109.5
C4—N4—H4B	117.8	H82A—C82—H82B	109.5
H4A—N4—H4B	122.0	C8—C82—H82C	109.5
C5—C4A—C10A	118.0 (2)	H82A—C82—H82C	109.5
C5—C4A—C4	125.3 (2)	H82B—C82—H82C	109.5
C10A—C4A—C4	116.6 (2)	C9A—C9—C8	114.27 (19)
C5A—C5—C4A	119.2 (2)	C9A—C9—H9A	108.7
C5A—C5—H5	120.4	C8—C9—H9A	108.7
C4A—C5—H5	120.4	C9A—C9—H9B	108.7
C5—C5A—C9A	118.7 (2)	C8—C9—H9B	108.7
C5—C5A—C6	120.7 (2)	H9A—C9—H9B	107.6
C9A—C5A—C6	120.6 (2)	N10—C9A—C5A	122.9 (2)
O6—C6—C5A	121.0 (2)	N10—C9A—C9	115.76 (19)
O6—C6—C7	123.0 (2)	C5A—C9A—C9	121.32 (19)
C5A—C6—C7	116.0 (2)	C9A—N10—C10A	118.2 (2)
C6—C7—C8	113.59 (19)	N10—C10A—N1	114.8 (2)
C6—C7—H7A	108.8	N10—C10A—C4A	122.7 (2)
C8—C7—H7A	108.8	N1—C10A—C4A	122.4 (2)
C6—C7—H7B	108.8		

C10A—N1—C2—N3	−3.9 (4)	C6—C7—C8—C82	−62.0 (3)
C10A—N1—C2—S2	176.91 (17)	C6—C7—C8—C81	177.1 (2)
N1—C2—S2—C21	2.1 (2)	C6—C7—C8—C9	58.1 (3)
N3—C2—S2—C21	−177.21 (17)	C7—C8—C9—C9A	−47.8 (3)
N1—C2—N3—C4	2.8 (4)	C82—C8—C9—C9A	72.6 (3)
S2—C2—N3—C4	−177.99 (16)	C81—C8—C9—C9A	−167.7 (2)
C2—N3—C4—N4	−179.9 (2)	C5—C5A—C9A—N10	1.1 (3)
C2—N3—C4—C4A	1.2 (3)	C6—C5A—C9A—N10	−178.5 (2)
N4—C4—C4A—C5	−5.2 (4)	C5—C5A—C9A—C9	179.4 (2)
N3—C4—C4A—C5	173.6 (2)	C6—C5A—C9A—C9	−0.3 (3)
N4—C4—C4A—C10A	177.7 (2)	C8—C9—C9A—N10	−161.0 (2)
N3—C4—C4A—C10A	−3.5 (3)	C8—C9—C9A—C5A	20.6 (3)
C10A—C4A—C5—C5A	0.2 (3)	C5A—C9A—N10—C10A	2.6 (3)
C4—C4A—C5—C5A	−176.9 (2)	C9—C9A—N10—C10A	−175.7 (2)
C4A—C5—C5A—C9A	−2.5 (3)	C9A—N10—C10A—N1	173.8 (2)
C4A—C5—C5A—C6	177.2 (2)	C9A—N10—C10A—C4A	−5.2 (3)
C5—C5A—C6—O6	9.5 (3)	C2—N1—C10A—N10	−177.8 (2)
C9A—C5A—C6—O6	−170.8 (2)	C2—N1—C10A—C4A	1.1 (3)
C5—C5A—C6—C7	−169.9 (2)	C5—C4A—C10A—N10	3.8 (3)
C9A—C5A—C6—C7	9.7 (3)	C4—C4A—C10A—N10	−178.9 (2)
O6—C6—C7—C8	140.8 (2)	C5—C4A—C10A—N1	−175.0 (2)
C5A—C6—C7—C8	−39.8 (3)	C4—C4A—C10A—N1	2.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···N3^{i}	0.90	2.17	3.067 (3)	173
N4—H4*B*···O6^{ii}	0.90	2.15	2.946 (3)	147

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