organic compounds

6-Amino-8-(2-bromophenyl)-1,7,8,8a-tetrahydro-3*H*-isothiochromene-5,7,7-tricarbonitrile dimethylformamide solvate

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In the title compound, $C_{18}H_{13}BrN_4S \cdot C_3H_7NO$, the thiopyran ring and the adjacent six-numbered ring adopt distorted boat conformations. The molecules, lying about inversion centers, form hydrogen-bonded dimers involving one of the H atoms on the amino group with the N atom of a cyano group of an adjacent molecule, resulting in a 12-membered ring system [$R_2^2(12)$ ring motif]. The other H atom of the amino group forms an intermolecular hydrogen bond with the O atom of the dimethylformamide (DMF) molecule. Another lone pair of electrons on the same carbonyl O atom of DMF molecule forms a non-classical C—H···O intermolecular hydrogen bond, resulting in a chain of molecules.

Related literature

For the biological activity of related compounds, see: Karsten & Krisztina (2007); Wang *et al.* (1998, 2006); Zhang *et al.* (2008). For a related structure, see: (Mereiter *et al.* 2000). For graph-set notation, see: Bernstein *et al.* (1994).
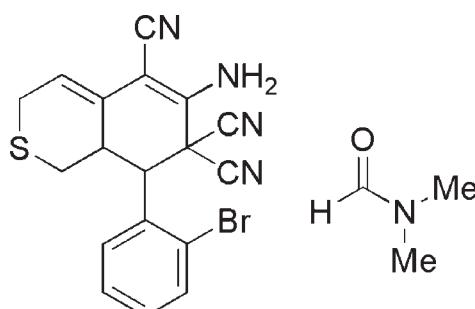
Experimental

Crystal data

$C_{18}H_{13}BrN_4S \cdot C_3H_7NO$	V = 2137.28 (11) Å^3
M_r = 470.39	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 14.7733 (4) Å	μ = 2.04 mm^{-1}
b = 9.1710 (3) Å	T = 296 K
c = 15.7897 (4) Å	0.44 × 0.36 × 0.05 mm
β = 92.478 (2)°	

Data collection

Bruker SMART CCD area-detector diffractometer	13894 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3841 independent reflections
	2723 reflections with $I > 2\sigma(I)$
T_{min} = 0.422, T_{max} = 0.900	R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.098	
S = 1.04	
3841 reflections	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
270 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O1[i]	0.89 (4)	1.96 (4)	2.856 (4)	178 (3)
N3—H3A···N4[ii]	0.79 (3)	2.54 (3)	3.294 (4)	162 (3)
C15—H15A···O1[iii]	0.93	2.54	3.438 (4)	162

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

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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supporting information

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6-Amino-8-(2-bromophenyl)-1,7,8,8a-tetrahydro-3*H*-isothiochromene-5,7,7-tricarbonitrile dimethylformamide solvate

Hai-Yan Zhang, Jian-Rong Wu and Xiang-Shan Wang

S1. Comment

Iso(thio)chromene derivatives are important and useful skeletons in organic synthesis. For example, it was reported that many isochromene derivatives displayed a wide range of biological activities, such as antiinflammatory activity (Wang *et al.* 2006), antitumor activity (Wang *et al.* 1998), antiviral activity (Karsten & Krisztina, 2007), and anti-apoptotic activity (Zhang, *et al.* 2008). We report here the crystal structure of the title compound, (I).

In the crystal structure of (I) (Fig. 1), the thiopyran ring adopts a distorted boat conformation: the atoms C5—C6, C8—C9 are coplanar, while the atoms C7 and S1 deviate from the plane by 0.332 (6) and -0.628 (6) Å, respectively. The adjacent six-numbered ring (C1—C6) also adopts a distorted boat conformation, with the atoms C1 and C6 deviating from the plane defined by atoms C2—C5 by 0.330 (5) and -0.404 (5) Å, respectively. The basal plane of the ring C1—C6 forms a dihedral angle of 16.5 (2) ° to the thiopyran ring and is nearly perpendicular to the benzene ring (C13—C18), forming a dihedral angle of 86.8 (1) °

The classical (N—H···O and N—H···N) and non-classical (C—H···O) inter-molecular hydrogen bonds are present in the crystal structure of (I). The molecules of (I) lying about inversion centers form hydrogen bonded dimers involving one of the hydrogen atoms (H3A) on the amino group with the atom N4 of the cyano group of an adjacent molecule, resulting in a twelve membered ring system which may be described in terms of graph set notation (Bernstein *et al.* 1994) as $R_2^2(12)$ ring motif; details are given in Table 1 and Figure 2. The other hydrogen atom (H3B) of the amino group forms an intermolecular hydrogen bond with atom O1 of the DMF molecule. An other lone pair of electrons on the same carbonyl O1 atom of DMF molecule form a non-classical intermolecular (C15—H15A···O1) hydrogen bond, thus resulting in a chain of molecules.

The crystal structure of a closely related compound has been reported (Mereiter *et al.* 2000).

S2. Experimental

The title compound, (I), was prepared by the reaction of 2-bromobenzaldehyde (1 mmol, 0.185 g), malononitrile (1.2 mmol, 0.079 g) and 2-(tetrahydrothiopyran-4-ylidene)malononitrile (1 mmol, 0.164 g) in 1-butyl-3-methylimidazolium fluoroborate (20 ml) at 353 K. The single crystals suitable for X-ray diffraction were obtained by slow evaporation from a DMF solution.

S3. Refinement

The H atoms bonded to C atoms were included at geometrically calculated positions and in riding mode at C—H distances 0.93, 0.96, 0.97 and 0.98 Å for aryl, methyl, methine and methylene type H-atoms, respectively, with $U_{iso}(H) = 1.5U_{eq}$(methyl C-atoms) and $1.2U_{eq}$(non-methyl C-atoms). The H-atoms bonded to N3 were allowed to refine with isotropic displacement parameters.
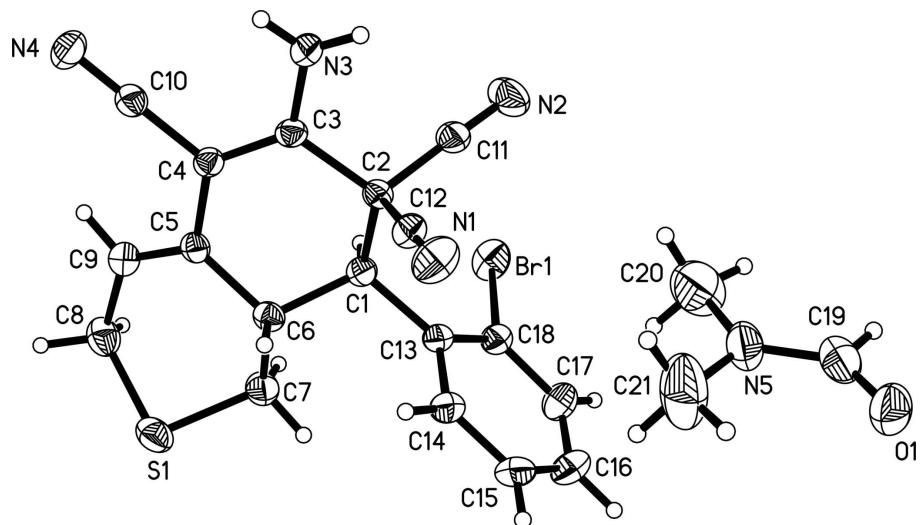
Figure 1

The molecular structure of (I) showing 50% probability of displacement ellipsoids and the atom-numbering scheme.
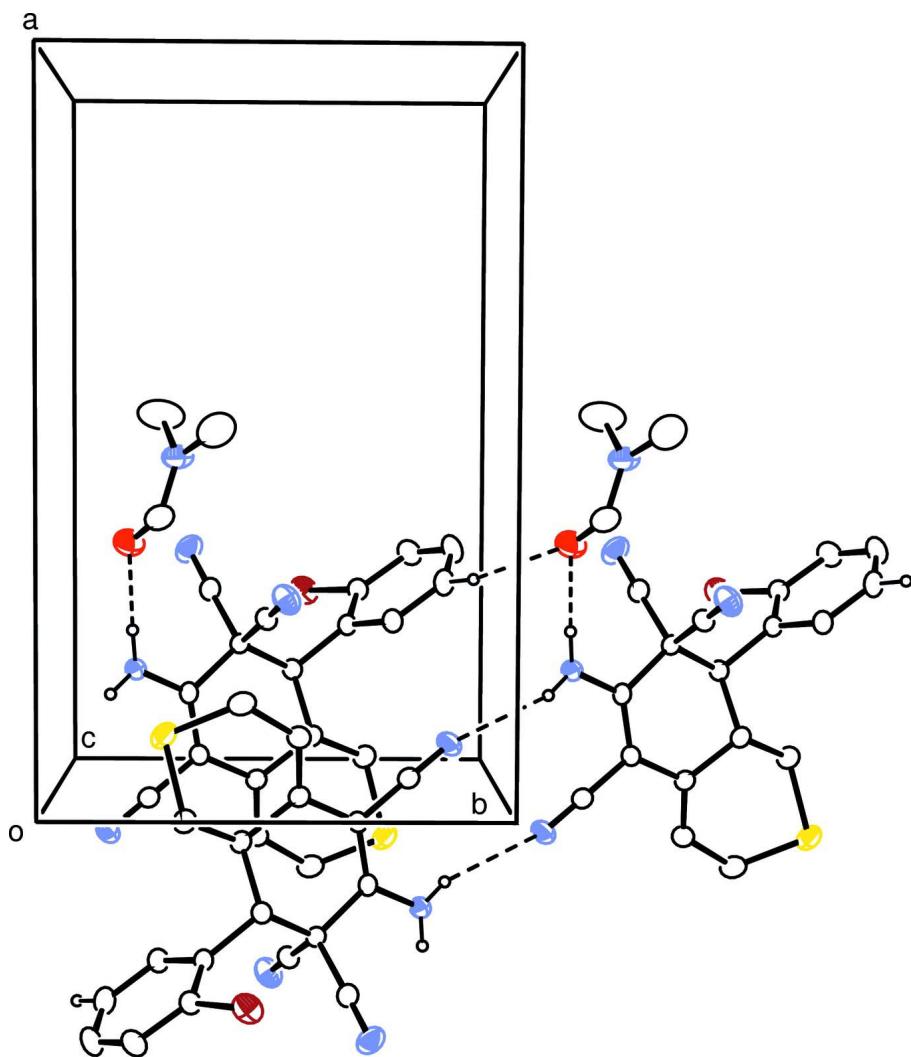
Figure 2

The molecular packing diagram showing the hydrogen bonds in the crystal of (I).

6-Amino-8-(2-bromophenyl)-1,7,8,8a-tetrahydro-3H-isothiochromene- 5,7,7-tricarbonitrile dimethylformamide solvate

Crystal data

$C_{18}H_{13}BrN_4S\cdot C_3H_7NO$	$F(000) = 960$
$M_r = 470.39$	$D_x = 1.462$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 530–532 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 14.7733$ (4) Å	Cell parameters from 4434 reflections
$b = 9.1710$ (3) Å	$\theta = 2.6$–22.6°
$c = 15.7897$ (4) Å	$\mu = 2.04$ mm^{-1}
$\beta = 92.478$ (2)°	$T = 296$ K
$V = 2137.28$ (11) Å^3	Plate, colourless
$Z = 4$	0.44 × 0.36 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer	13894 measured reflections
Radiation source: fine-focus sealed tube	3841 independent reflections
Graphite monochromator	2723 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.032$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.2°$, $\theta_{min} = 1.4°$
	$h = -14 \rightarrow 17$
$T_{min} = 0.422$, $T_{max} = 0.900$	$k = -9 \rightarrow 10$
	$l = -18 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.036$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.098$	
$S = 1.04$	H atoms treated by a mixture of independent and constrained refinement
3841 reflections	
270 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.4516P]$
0 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} = 0.001$
	$\Delta\rho_{max} = 0.32$ e Å⁻³
	$\Delta\rho_{min} = -0.23$ 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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Br1	0.26620 (2)	0.56202 (4)	0.85086 (2)	0.06278 (16)
S1	−0.08662 (5)	0.75087 (9)	0.66332 (5)	0.0568 (2)
C9	−0.08406 (19)	0.4522 (3)	0.65402 (18)	0.0437 (7)
H9A	−0.1163	0.3654	0.6481	0.052*
C1	0.15871 (17)	0.5338 (3)	0.66735 (17)	0.0353 (6)
H1A	0.1505	0.4901	0.7231	0.042*
C5	0.00049 (18)	0.4509 (3)	0.62871 (16)	0.0347 (6)
C6	0.06373 (18)	0.5807 (3)	0.63235 (17)	0.0361 (6)
H6A	0.0694	0.6179	0.5746	0.043*
C4	0.03938 (18)	0.3190 (3)	0.59218 (15)	0.0341 (6)
N3	0.1653 (2)	0.1753 (3)	0.54913 (17)	0.0465 (7)
C2	0.19932 (18)	0.4123 (3)	0.61042 (17)	0.0347 (6)
C10	−0.02003 (18)	0.2040 (3)	0.56411 (17)	0.0400 (7)
C3	0.12949 (18)	0.2955 (3)	0.58223 (16)	0.0351 (6)
C11	0.2753 (2)	0.3418 (3)	0.66002 (19)	0.0447 (7)

N4	−0.06658 (17)	0.1117 (3)	0.53989 (18)	0.0582 (7)
C12	0.2385 (2)	0.4739 (3)	0.5331 (2)	0.0428 (7)
C13	0.22316 (18)	0.6621 (3)	0.68104 (17)	0.0379 (6)
C18	0.27173 (19)	0.6886 (3)	0.75675 (17)	0.0431 (7)
C7	0.02957 (19)	0.7038 (3)	0.6874 (2)	0.0506 (8)
H7A	0.0670	0.7893	0.6799	0.061*
H7B	0.0361	0.6749	0.7465	0.061*
N1	0.2686 (2)	0.5194 (3)	0.47443 (19)	0.0646 (8)
N2	0.3323 (2)	0.2913 (3)	0.69975 (19)	0.0716 (8)
C14	0.2323 (2)	0.7653 (3)	0.6164 (2)	0.0489 (8)
H14A	0.2002	0.7527	0.5650	0.059*
C8	−0.1330 (2)	0.5780 (3)	0.6909 (2)	0.0555 (8)
H8A	−0.1309	0.5687	0.7522	0.067*
H8B	−0.1961	0.5745	0.6713	0.067*
C15	0.2877 (2)	0.8846 (3)	0.6273 (2)	0.0628 (9)
H15A	0.2939	0.9498	0.5829	0.075*
C17	0.3260 (2)	0.8109 (4)	0.7679 (2)	0.0633 (9)
H17A	0.3570	0.8270	0.8196	0.076*
C16	0.3338 (3)	0.9082 (4)	0.7027 (3)	0.0738 (11)
H16A	0.3704	0.9901	0.7099	0.089*
O1	0.65268 (16)	0.8365 (3)	0.50459 (17)	0.0758 (7)
N5	0.53153 (19)	0.7245 (3)	0.55611 (19)	0.0675 (8)
C19	0.6160 (2)	0.7654 (4)	0.5584 (3)	0.0671 (10)
H19A	0.6517	0.7376	0.6056	0.081*
C20	0.4938 (3)	0.6366 (6)	0.6229 (3)	0.1171 (17)
H20A	0.5399	0.6179	0.6662	0.176*
H20B	0.4721	0.5458	0.5995	0.176*
H20C	0.4445	0.6882	0.6469	0.176*
C21	0.4730 (3)	0.7652 (6)	0.4850 (3)	0.1229 (18)
H21A	0.5064	0.8220	0.4460	0.184*
H21B	0.4233	0.8218	0.5044	0.184*
H21C	0.4501	0.6790	0.4571	0.184*
H3A	0.131 (2)	0.119 (3)	0.5268 (18)	0.042 (9)*
H3B	0.222 (3)	0.169 (4)	0.533 (2)	0.074 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0733 (3)	0.0739 (3)	0.0399 (2)	−0.01304 (18)	−0.01097 (16)	0.00090 (16)
S1	0.0557 (5)	0.0529 (5)	0.0613 (5)	0.0176 (4)	−0.0045 (4)	−0.0084 (4)
C9	0.0404 (18)	0.0459 (17)	0.0447 (17)	−0.0014 (14)	0.0006 (14)	−0.0004 (13)
C1	0.0387 (15)	0.0341 (15)	0.0329 (15)	−0.0012 (12)	−0.0014 (12)	0.0010 (12)
C5	0.0372 (16)	0.0374 (16)	0.0289 (14)	0.0018 (12)	−0.0060 (12)	0.0021 (11)
C6	0.0403 (16)	0.0359 (16)	0.0317 (15)	0.0042 (12)	−0.0025 (12)	−0.0003 (12)
C4	0.0368 (16)	0.0320 (14)	0.0333 (14)	−0.0021 (12)	−0.0014 (12)	0.0026 (12)
N3	0.0385 (16)	0.0382 (16)	0.0624 (18)	−0.0015 (13)	−0.0031 (14)	−0.0120 (13)
C2	0.0353 (15)	0.0323 (15)	0.0359 (15)	0.0021 (12)	−0.0037 (12)	0.0026 (12)
C10	0.0356 (16)	0.0396 (17)	0.0450 (17)	0.0027 (14)	0.0039 (13)	0.0003 (13)

C3	0.0416 (17)	0.0286 (15)	0.0343 (15)	0.0002 (12)	−0.0055 (12)	0.0018 (12)
C11	0.0474 (18)	0.0373 (17)	0.0487 (18)	0.0025 (14)	−0.0066 (14)	−0.0090 (14)
N4	0.0469 (16)	0.0502 (16)	0.077 (2)	−0.0109 (14)	0.0022 (14)	−0.0160 (14)
C12	0.0422 (17)	0.0393 (17)	0.0467 (19)	−0.0041 (13)	−0.0005 (15)	−0.0043 (14)
C13	0.0391 (16)	0.0300 (15)	0.0444 (16)	0.0005 (12)	−0.0024 (13)	−0.0013 (13)
C18	0.0443 (17)	0.0378 (16)	0.0468 (17)	−0.0017 (13)	−0.0022 (14)	−0.0030 (13)
C7	0.0465 (18)	0.0455 (17)	0.059 (2)	0.0053 (14)	−0.0028 (15)	−0.0130 (15)
N1	0.075 (2)	0.0656 (19)	0.0541 (18)	−0.0172 (15)	0.0148 (16)	−0.0007 (15)
N2	0.070 (2)	0.0647 (19)	0.077 (2)	0.0193 (16)	−0.0305 (16)	−0.0106 (16)
C14	0.0499 (19)	0.0363 (17)	0.0597 (19)	−0.0021 (14)	−0.0066 (15)	0.0070 (15)
C8	0.0440 (18)	0.066 (2)	0.057 (2)	0.0067 (15)	0.0035 (15)	−0.0056 (16)
C15	0.063 (2)	0.0366 (18)	0.089 (3)	0.0007 (17)	0.005 (2)	0.0175 (18)
C17	0.060 (2)	0.053 (2)	0.076 (2)	−0.0118 (17)	−0.0147 (18)	−0.0157 (19)
C16	0.071 (3)	0.040 (2)	0.109 (3)	−0.0164 (17)	−0.012 (2)	−0.004 (2)
O1	0.0585 (16)	0.0812 (18)	0.0890 (19)	−0.0077 (13)	0.0197 (14)	−0.0008 (15)
N5	0.0437 (17)	0.084 (2)	0.075 (2)	0.0016 (15)	0.0046 (15)	0.0082 (17)
C19	0.054 (2)	0.074 (3)	0.073 (3)	0.0110 (19)	−0.0049 (19)	−0.013 (2)
C20	0.099 (4)	0.121 (4)	0.135 (4)	0.020 (3)	0.041 (3)	0.047 (3)
C21	0.074 (3)	0.190 (5)	0.103 (4)	−0.014 (3)	−0.022 (3)	0.025 (4)

Geometric parameters (Å, º)

Br1—C18	1.890 (3)	C13—C18	1.389 (4)
S1—C8	1.788 (3)	C13—C14	1.402 (4)
S1—C7	1.795 (3)	C18—C17	1.385 (4)
C9—C5	1.328 (4)	C7—H7A	0.9700
C9—C8	1.494 (4)	C7—H7B	0.9700
C9—H9A	0.9300	C14—C15	1.372 (4)
C1—C13	1.523 (4)	C14—H14A	0.9300
C1—C6	1.546 (4)	C8—H8A	0.9700
C1—C2	1.568 (4)	C8—H8B	0.9700
C1—H1A	0.9800	C15—C16	1.363 (5)
C5—C4	1.468 (4)	C15—H15A	0.9300
C5—C6	1.512 (4)	C17—C16	1.371 (5)
C6—C7	1.525 (4)	C17—H17A	0.9300
C6—H6A	0.9800	C16—H16A	0.9300
C4—C3	1.364 (4)	O1—C19	1.216 (4)
C4—C10	1.431 (4)	N5—C19	1.302 (4)
N3—C3	1.339 (4)	N5—C21	1.436 (5)
N3—H3A	0.79 (3)	N5—C20	1.457 (5)
N3—H3B	0.89 (4)	C19—H19A	0.9300
C2—C12	1.485 (4)	C20—H20A	0.9600
C2—C11	1.488 (4)	C20—H20B	0.9600
C2—C3	1.539 (4)	C20—H20C	0.9600
C10—N4	1.145 (3)	C21—H21A	0.9600
C11—N2	1.128 (4)	C21—H21B	0.9600
C12—N1	1.126 (4)	C21—H21C	0.9600

C8—S1—C7	96.21 (14)	C6—C7—S1	113.2 (2)
C5—C9—C8	127.0 (3)	C6—C7—H7A	108.9
C5—C9—H9A	116.5	S1—C7—H7A	108.9
C8—C9—H9A	116.5	C6—C7—H7B	108.9
C13—C1—C6	112.8 (2)	S1—C7—H7B	108.9
C13—C1—C2	112.2 (2)	H7A—C7—H7B	107.7
C6—C1—C2	110.9 (2)	C15—C14—C13	121.5 (3)
C13—C1—H1A	106.8	C15—C14—H14A	119.2
C6—C1—H1A	106.8	C13—C14—H14A	119.2
C2—C1—H1A	106.8	C9—C8—S1	113.1 (2)
C9—C5—C4	121.0 (2)	C9—C8—H8A	109.0
C9—C5—C6	124.7 (2)	S1—C8—H8A	109.0
C4—C5—C6	114.3 (2)	C9—C8—H8B	109.0
C5—C6—C7	112.7 (2)	S1—C8—H8B	109.0
C5—C6—C1	110.2 (2)	H8A—C8—H8B	107.8
C7—C6—C1	108.6 (2)	C16—C15—C14	120.6 (3)
C5—C6—H6A	108.4	C16—C15—H15A	119.7
C7—C6—H6A	108.4	C14—C15—H15A	119.7
C1—C6—H6A	108.4	C16—C17—C18	119.9 (3)
C3—C4—C10	115.9 (2)	C16—C17—H17A	120.1
C3—C4—C5	125.2 (2)	C18—C17—H17A	120.1
C10—C4—C5	119.0 (2)	C15—C16—C17	119.8 (3)
C3—N3—H3A	117 (2)	C15—C16—H16A	120.1
C3—N3—H3B	124 (2)	C17—C16—H16A	120.1
H3A—N3—H3B	115 (3)	C19—N5—C21	119.4 (3)
C12—C2—C11	106.6 (2)	C19—N5—C20	122.4 (4)
C12—C2—C3	107.9 (2)	C21—N5—C20	118.2 (3)
C11—C2—C3	109.3 (2)	O1—C19—N5	126.2 (4)
C12—C2—C1	111.9 (2)	O1—C19—H19A	116.9
C11—C2—C1	107.8 (2)	N5—C19—H19A	116.9
C3—C2—C1	113.1 (2)	N5—C20—H20A	109.5
N4—C10—C4	178.4 (3)	N5—C20—H20B	109.5
N3—C3—C4	125.4 (3)	H20A—C20—H20B	109.5
N3—C3—C2	114.5 (2)	N5—C20—H20C	109.5
C4—C3—C2	120.1 (2)	H20A—C20—H20C	109.5
N2—C11—C2	177.7 (3)	H20B—C20—H20C	109.5
N1—C12—C2	179.4 (3)	N5—C21—H21A	109.5
C18—C13—C14	116.4 (2)	N5—C21—H21B	109.5
C18—C13—C1	123.6 (2)	H21A—C21—H21B	109.5
C14—C13—C1	119.9 (2)	N5—C21—H21C	109.5
C17—C18—C13	121.7 (3)	H21A—C21—H21C	109.5
C17—C18—Br1	116.2 (2)	H21B—C21—H21C	109.5
C13—C18—Br1	122.1 (2)		
C8—C9—C5—C4	−179.0 (3)	C11—C2—C3—C4	133.3 (3)
C8—C9—C5—C6	−0.4 (5)	C1—C2—C3—C4	13.2 (3)
C9—C5—C6—C7	13.9 (4)	C12—C2—C11—N2	121 (9)
C4—C5—C6—C7	−167.4 (2)	C3—C2—C11—N2	−123 (9)

C9—C5—C6—C1	135.4 (3)	C1—C2—C11—N2	1 (9)
C4—C5—C6—C1	−46.0 (3)	C11—C2—C12—N1	40 (33)
C13—C1—C6—C5	−174.2 (2)	C3—C2—C12—N1	−77 (33)
C2—C1—C6—C5	58.9 (3)	C1—C2—C12—N1	158 (100)
C13—C1—C6—C7	−50.4 (3)	C6—C1—C13—C18	127.9 (3)
C2—C1—C6—C7	−177.3 (2)	C2—C1—C13—C18	−106.0 (3)
C9—C5—C4—C3	−164.3 (3)	C6—C1—C13—C14	−48.9 (3)
C6—C5—C4—C3	17.0 (4)	C2—C1—C13—C14	77.3 (3)
C9—C5—C4—C10	15.7 (4)	C14—C13—C18—C17	0.3 (4)
C6—C5—C4—C10	−163.0 (2)	C1—C13—C18—C17	−176.5 (3)
C13—C1—C2—C12	−47.4 (3)	C14—C13—C18—Br1	179.3 (2)
C6—C1—C2—C12	79.8 (3)	C1—C13—C18—Br1	2.4 (4)
C13—C1—C2—C11	69.6 (3)	C5—C6—C7—S1	−49.2 (3)
C6—C1—C2—C11	−163.2 (2)	C1—C6—C7—S1	−171.53 (19)
C13—C1—C2—C3	−169.4 (2)	C8—S1—C7—C6	62.6 (2)
C6—C1—C2—C3	−42.2 (3)	C18—C13—C14—C15	1.1 (4)
C3—C4—C10—N4	−48 (11)	C1—C13—C14—C15	178.1 (3)
C5—C4—C10—N4	131 (11)	C5—C9—C8—S1	22.8 (4)
C10—C4—C3—N3	−0.2 (4)	C7—S1—C8—C9	−47.3 (3)
C5—C4—C3—N3	179.8 (3)	C13—C14—C15—C16	−1.8 (5)
C10—C4—C3—C2	−179.9 (2)	C13—C18—C17—C16	−1.1 (5)
C5—C4—C3—C2	0.1 (4)	Br1—C18—C17—C16	179.9 (3)
C12—C2—C3—N3	69.1 (3)	C14—C15—C16—C17	1.0 (5)
C11—C2—C3—N3	−46.5 (3)	C18—C17—C16—C15	0.4 (5)
C1—C2—C3—N3	−166.6 (2)	C21—N5—C19—O1	−0.4 (6)
C12—C2—C3—C4	−111.2 (3)	C20—N5—C19—O1	178.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O1[i]	0.89 (4)	1.96 (4)	2.856 (4)	178 (3)
N3—H3A···N4[ii]	0.79 (3)	2.54 (3)	3.294 (4)	162 (3)
C15—H15A···O1[iii]	0.93	2.54	3.438 (4)	162

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