

2,8-Dimethyl-5,11-bis[3-(methylsulfanyl)propyl]-1*H*,7*H*-diimidazo[*c,h*][1,6]diazecine

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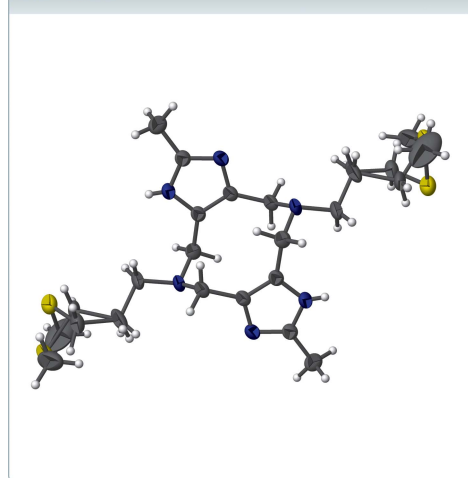
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Keywords: crystal structure; diazecine; twinning; disorder; *SQUEEZE* algorithm.

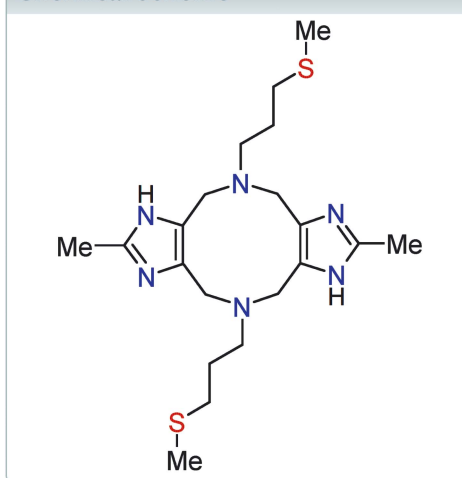
Structural data: full structural data are available from iucrdata.iucr.org

The refinement of the crystal structure of the title compound, C₂₀H₃₄N₆S₂, was challenging, as a consequence of three issues: crystals are twinned, disordered, and include large empty voids corresponding to *ca* 8% of the unit-cell volume. A satisfactory model was obtained using data collected at 153 K. The diazecine ring is centrosymmetric, and displays the expected boat–chair–boat conformation. The 3-(methylsulfanyl)propyl chain is disordered over two sites with equal occupancies, and different conformations, *i.e.* *trans-gauche-gauche* for the first chain [N_{diaz}–C_{meth}–C_{meth}–C_{meth} torsion angles: 169.9 (4), 66.8 (5), 62.4 (5)^o; diaz = diazecine and meth = methylene] and *trans-trans-gauche* for the second component [torsion angles: 169.9 (4), –177.6 (4), 64.4 (5)^o]. In the crystal, N–H···N hydrogen bonds between imidazole rings are evident; weak intermolecular C–H···S contacts are also noted. The crystal studied was modelled as a two-component twin.

3D view



Chemical scheme



Structure description

The chemistry of [1,6]diazecine derivatives bearing imidazole rings started in the 1990's, through a collaboration between groups from Mexico and The Netherlands (Mendoza-Díaz *et al.*, 1996), when a suitable methodology was established for their preparation, based on the Mannich reaction. Here, the one-pot reaction between propylamine, formaldehyde and 2-methylimidazole resulted in the double addition of formaldehyde on the imidazole, followed by condensation with propylamine, to afford the ten-membered ring characterizing the diazecines. Some other related structures were characterized by X-ray diffraction, upon modification of the group substituting the N sites in positions 1 and 6 in the ring (Mendoza-Díaz *et al.*, 2002, 2010). On the other hand, the coordination chemistry of Cu^{II} with these molecules was studied, which has been relevant towards

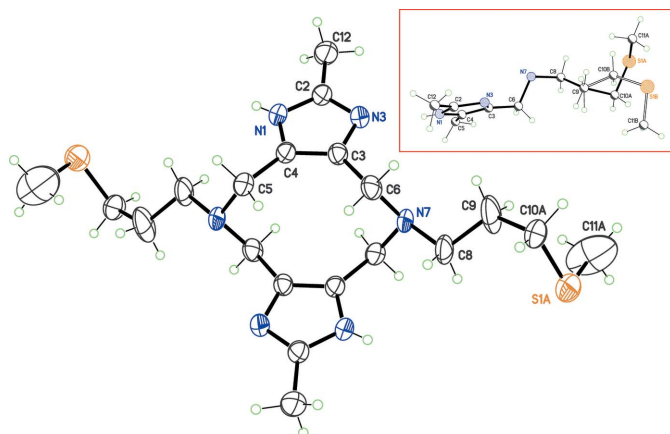


Figure 1
Molecular structure of the title compound, with 50% displacement ellipsoids for non-H atoms. Disordered sites *B* were omitted for clarity. The complete asymmetric unit is represented in the inset, including *A* and *B* disordered sites.

bioinorganic topics, including the modelling of the active site of catecholases (Mendoza-Díaz *et al.*, 2002; Mendoza-Quijano *et al.*, 2012; Zerón *et al.*, 2017).

Although the bioinorganic chemistry has grown steadily for this class of compound, it is clear that the chemical crystallography of the corresponding free ligands is rather poor, with very few structures deposited in the Cambridge Structural Database (Groom *et al.*, 2016). The reason probably stems in part from the fact that the refinement of these crystal structures is not always routine. In the case of the title compound, three issues made the refinement challenging: (i) crystals are

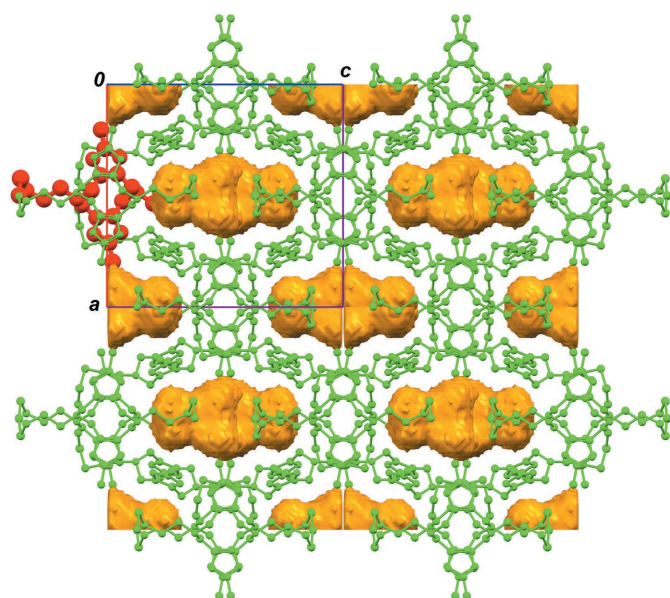


Figure 2
Part of the crystal structure of the title compound, viewed along the *b* axis. The minor part of the disorder and H atoms were omitted. The red molecule in the top-left unit cell includes the asymmetric unit. Void spaces in the crystal are delimited by gold surfaces calculated using the 'contact surface' tool in *Mercury*, with a probe radius of 1.2 Å and a grid spacing of 0.3 Å (Macrae *et al.*, 2008).

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1···N3 ⁱ	0.68 (3)	2.15 (3)	2.825 (2)	169 (3)
C6—H6 <i>B</i> ···S1A ⁱⁱ	0.99	2.93	3.837 (3)	153
C12—H12A···S1A ⁱⁱⁱ	0.98	3.01	3.926 (3)	156
C11 <i>B</i> —H11 <i>D</i> ···S1B ^{iv}	0.98	1.97	2.767 (6)	137

Symmetry codes: (i) $y - \frac{1}{4}, -x + \frac{3}{4}, z - \frac{1}{4}$; (ii) $-y + \frac{5}{4}, x - \frac{1}{4}, z - \frac{1}{4}$; (iii) $x - \frac{1}{2}, y, -z + \frac{1}{2}$; (iv) $-x + 1, -y + 1, -z + 1$.

systematically twinned, a rather common feature for the tetragonal system. In the present case, a rotation axis about (110) is swapping unit cell vectors *a* and *b* in the Laue class $4/m$ (class I of twins by merohedry), to form an almost perfect twin; for the studied crystal, fractional contributions for the two-component twin were $k_1 = 0.486$ (2) and $k_2 = 0.514$ (2). (ii) A disorder is observed for the lateral 3-(methylsulfanyl)propyl chain, involving the S atom, which is the main scatterer in the crystal (see Fig. 1, inset). Indeed, this disorder could not be solved using room-temperature diffraction data. (iii) The packing efficiency of the molecules in the crystal is very poor, leaving *ca* 8% of the cell empty (Fig. 2). Apparently, each individual void of *ca* 100 Å³ is not filled with disordered solvent (ethanol or water), as evidenced by unsuccessful attempts to include the contribution of disordered solvents to structure factors using the *SQUEEZE* tool in *PLATON* (Spek, 2015); a non-significant density of 12 e⁻ per unit cell was recovered, corresponding to 1.5 e⁻/molecule.

Although these issues are decreased dramatically the scattering power of the crystals, data collected on a large sample at 153 K were suitable for refining the structure satisfactorily. The asymmetric unit contains half the formula, with the molecule lying on an inversion centre (Fig. 1). Atoms C10/S1/C11 belonging to the lateral chain are disordered over two sites, with occupancies equal to 0.5 for each part (sites *A* and *B*, Fig. 1, inset). The conformation of this chain is different for each disordered part: *trans-gauche-gauche* for part *A* [torsion angles starting from N7: 169.9 (4), 66.8 (5), 62.4 (5)°] and *trans-trans-gauche* for part *B* [torsion angles starting from N7: 169.9 (4), -177.6 (4), 64.4 (5)°]. The diazocine ten-membered ring adopts the skewed boat-chair-boat conformation, invariably found in other related derivatives (idealized symmetry: *C*_{2h}). In the imidazole ring, π -bonds are localized, with normal bond lengths C2=N3 [1.320 (3) Å] and C3=C4 [1.369 (3) Å]. As a consequence, the imidazolic H atom is localized on N1. This group serves as donor group for the formation of N1—H1···N3 hydrogen bonds with a symmetry-related imidazole ring. Other potentially stabilizing hydrogen bonds are weak intermolecular C—H···S contacts (Table 1).

Synthesis and crystallization

2-Methylimidazole (20 mmol, 1.64 g) was dissolved in water (100 ml). To this solution, with vigorous stirring, 3(methylthio)propylamine (20 mmol, 2.1 g) was added dropwise. This mixture formed an emulsion which was broken with the

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₀ H ₃₄ N ₆ S ₂
<i>M_r</i>	422.65
Crystal system, space group	Tetragonal, <i>I</i> 4 ₁ / <i>a</i>
Temperature (K)	153
<i>a</i> , <i>c</i> (Å)	16.8114 (6), 17.8288 (6)
<i>V</i> (Å ³)	5038.8 (4)
<i>Z</i>	8
Radiation type	Ag <i>K</i> α, λ = 0.56083 Å
μ (mm ⁻¹)	0.12
Crystal size (mm)	0.30 × 0.25 × 0.25
Data collection	
Diffractometer	Stoe Stadivari
Absorption correction	Multi-scan (<i>X-AREA</i> ; Stoe & Cie, 2018)
<i>T_{min}</i> , <i>T_{max}</i>	0.326, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	50278, 2943, 2296
<i>R_{int}</i>	0.098
(sin θ/λ) _{max} (Å ⁻¹)	0.653
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.048, 0.138, 0.97
No. of reflections	2943
No. of parameters	159
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.39, -0.19

Computer programs: *X-AREA*, *SHELXT2018* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *XP* in *SHELXTL-Plus* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *pubCIF* (Westrip, 2010).

addition of EtOH (*ca* 20 ml). Without pausing the agitation, formaldehyde (60 mmol, 37% aqueous solution) was added dropwise. This mixture was allowed to react at 333 K for approximately two days when the appearance of a white precipitate indicated the presence of the product. Analysis calculated (%) for C₂₀H₃₄N₆S₂: C, 56.37; H, 8.11; N, 19.88; S, 15.17. Found: C, 57.15; H, 8.25; N, 19.68, S, 15.30. ¹H-NMR (400 MHz, CD₃OD, p.p.m.) δ: 2.34 (*s*, 6H, **CH**₃-Im), 3.36 (*s*, 8H, Im-**CH**₂-N-*R*), 1.93 (*q*, 4H, -CH₂-**CH**₂-CH₂-S-CH₃), 2.12 (*s*, 6H, **CH**₃-S-), 2.92 (*t*, 4H, -CH₂-CH₂-**CH**₂-N-), 2.66 (*t*, 4H, -S-**CH**₂-CH₂-CH₂-N-). Crystalline samples were

obtained from the slow evaporation of ethanolic solutions of the compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal was modelled as a two-component twin, using the twin matrix (0 1 0, 1 0 0, 0 0 1) and one batch scale factor, which converged to 0.486 (2) (Sheldrick, 2015b). Occupancies for disordered sites *A* and *B* (atoms C10/S1/C11) were first refined, and since they converged towards a value very close to 1/2, they were fixed to 0.5 in the last cycles of refinement.

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full crystallographic data

IUCrData (2019). 4, x190441 [https://doi.org/10.1107/S2414314619004413]

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2,8-Dimethyl-5,11-bis[3-(methylsulfanyl)propyl]-1*H*,7*H*-diimidazo[*c,h*][1,6]diazecine

Crystal data

C₂₀H₃₄N₆S₂

$M_r = 422.65$

Tetragonal, $I4_1/a$

$a = 16.8114$ (6) Å

$c = 17.8288$ (6) Å

$V = 5038.8$ (4) Å³

$Z = 8$

$F(000) = 1824$

$D_x = 1.114$ Mg m⁻³

Ag $K\alpha$ radiation, $\lambda = 0.56083$ Å

Cell parameters from 29151 reflections

$\theta = 2.3$ – 25.6°

$\mu = 0.12$ mm⁻¹

$T = 153$ K

Prism, yellow

$0.30 \times 0.25 \times 0.25$ mm

Data collection

Stoe Stadivari

diffractometer

Radiation source: Sealed X-ray tube, Axo Astix-
f Microfocus source

Graded multilayer mirror monochromator

Detector resolution: 5.81 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(X-AREA; Stoe & Cie, 2018)

$T_{\min} = 0.326$, $T_{\max} = 1.000$

50278 measured reflections

2943 independent reflections

2296 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.098$

$\theta_{\max} = 21.5^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -21 \rightarrow 21$

$k = -21 \rightarrow 21$

$l = -23 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.138$

$S = 0.97$

2943 reflections

159 parameters

0 restraints

0 constraints

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0946P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.39$ e Å⁻³

$\Delta\rho_{\min} = -0.19$ e Å⁻³

Special details

Refinement. Refined as a 2-component twin, rotation axis (1 1 0). TWIN 0 1 0 1 0 0 0 0 -1 2 BASF 0.48572

All C-bound H atoms were placed in calculated positions and refined as riding to their carrier C atoms with isotropic displacement parameters. The atomic coordinates for the N-bound H atom were refined; $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{N})$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C10A	0.5232 (4)	0.5267 (4)	0.3420 (3)	0.0508 (13)	0.5
H10A	0.559442	0.480455	0.338174	0.061*	0.5
H10B	0.482368	0.515233	0.380508	0.061*	0.5
S1A	0.57758 (8)	0.61513 (10)	0.36542 (7)	0.0531 (4)	0.5
C11A	0.5021 (6)	0.6863 (5)	0.3722 (7)	0.126 (4)	0.5
H11A	0.525322	0.737967	0.385065	0.189*	0.5
H11B	0.474258	0.690329	0.324065	0.189*	0.5
H11C	0.464325	0.670403	0.411337	0.189*	0.5
C10B	0.5452 (3)	0.5766 (5)	0.3314 (3)	0.0541 (14)	0.5
H10C	0.557718	0.633326	0.322144	0.065*	0.5
H10D	0.595553	0.546074	0.329966	0.065*	0.5
S1B	0.49849 (9)	0.56555 (13)	0.42257 (7)	0.0728 (5)	0.5
C11B	0.4927 (5)	0.4626 (7)	0.4248 (4)	0.099 (3)	0.5
H11D	0.467977	0.445643	0.471933	0.149*	0.5
H11E	0.460470	0.443912	0.382466	0.149*	0.5
H11F	0.546275	0.439992	0.421161	0.149*	0.5
N1	0.33547 (11)	0.45749 (11)	-0.05949 (9)	0.0340 (4)	
H1	0.3217 (17)	0.4482 (17)	-0.0945 (15)	0.041*	
C2	0.28871 (13)	0.49400 (12)	-0.00916 (11)	0.0337 (4)	
N3	0.32672 (11)	0.50618 (11)	0.05457 (9)	0.0342 (4)	
C3	0.40212 (12)	0.47426 (12)	0.04372 (11)	0.0308 (4)	
C4	0.40840 (12)	0.44355 (12)	-0.02712 (11)	0.0316 (4)	
C5	0.47564 (13)	0.40230 (13)	-0.06585 (12)	0.0369 (5)	
H5A	0.516715	0.390068	-0.027772	0.044*	
H5B	0.455497	0.350876	-0.085133	0.044*	
C6	0.46077 (13)	0.47487 (14)	0.10598 (10)	0.0361 (5)	
H6A	0.437275	0.447824	0.150050	0.043*	
H6B	0.508375	0.444327	0.090521	0.043*	
N7	0.48549 (11)	0.55613 (12)	0.12799 (8)	0.0373 (4)	
C8	0.53467 (15)	0.5544 (2)	0.19642 (12)	0.0559 (8)	
H8A	0.564999	0.604701	0.200290	0.067*	
H8B	0.573358	0.510160	0.192816	0.067*	
C9	0.48435 (19)	0.5437 (2)	0.26668 (12)	0.0732 (10)	
H9A	0.452184	0.592605	0.272717	0.088*	0.5
H9B	0.446619	0.499762	0.256607	0.088*	0.5
H9C	0.470416	0.487153	0.274937	0.088*	0.5
H9D	0.435047	0.575808	0.264417	0.088*	0.5
C12	0.20352 (15)	0.51376 (16)	-0.02429 (14)	0.0481 (6)	
H12A	0.184832	0.552542	0.012768	0.072*	
H12B	0.171306	0.465312	-0.020832	0.072*	
H12C	0.198561	0.536381	-0.074737	0.072*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C10A	0.052 (3)	0.072 (4)	0.028 (2)	-0.006 (3)	-0.007 (2)	-0.006 (2)
S1A	0.0488 (7)	0.0725 (9)	0.0379 (6)	0.0006 (7)	-0.0083 (5)	-0.0032 (6)
C11A	0.088 (6)	0.083 (6)	0.206 (10)	0.033 (5)	-0.044 (7)	-0.028 (7)
C10B	0.042 (3)	0.089 (5)	0.031 (2)	-0.013 (3)	-0.009 (2)	-0.020 (3)
S1B	0.0529 (8)	0.1376 (17)	0.0279 (5)	0.0111 (9)	0.0017 (5)	-0.0087 (7)
C11B	0.060 (4)	0.187 (10)	0.051 (3)	0.018 (5)	0.011 (3)	0.024 (4)
N1	0.0360 (9)	0.0387 (10)	0.0274 (8)	-0.0039 (8)	-0.0013 (7)	-0.0085 (7)
C2	0.0360 (11)	0.0316 (10)	0.0334 (10)	-0.0034 (8)	0.0016 (8)	-0.0043 (8)
N3	0.0362 (9)	0.0382 (9)	0.0282 (8)	-0.0026 (7)	0.0042 (7)	-0.0056 (7)
C3	0.0361 (11)	0.0300 (10)	0.0262 (8)	-0.0025 (8)	0.0028 (8)	-0.0002 (7)
C4	0.0349 (10)	0.0305 (10)	0.0295 (9)	-0.0045 (8)	0.0016 (7)	-0.0035 (8)
C5	0.0379 (12)	0.0345 (11)	0.0384 (10)	-0.0016 (9)	0.0009 (8)	-0.0108 (9)
C6	0.0398 (12)	0.0459 (12)	0.0227 (8)	-0.0001 (9)	0.0014 (8)	0.0035 (8)
N7	0.0384 (10)	0.0520 (12)	0.0216 (7)	-0.0023 (8)	-0.0016 (7)	-0.0124 (7)
C8	0.0432 (13)	0.099 (2)	0.0256 (10)	0.0152 (13)	-0.0079 (9)	-0.0217 (12)
C9	0.0659 (18)	0.131 (3)	0.0225 (10)	0.0355 (19)	-0.0047 (11)	-0.0117 (13)
C12	0.0383 (13)	0.0531 (14)	0.0529 (13)	0.0028 (11)	-0.0022 (10)	-0.0120 (11)

Geometric parameters (\AA , $^\circ$)

C10A—C9	1.520 (5)	N3—C3	1.390 (3)
C10A—S1A	1.795 (7)	C3—C4	1.369 (3)
C10A—H10A	0.9900	C3—C6	1.485 (3)
C10A—H10B	0.9900	C4—C5	1.495 (3)
S1A—C11A	1.748 (8)	C5—N7 ⁱ	1.464 (3)
C11A—H11A	0.9800	C5—H5A	0.9900
C11A—H11B	0.9800	C5—H5B	0.9900
C11A—H11C	0.9800	C6—N7	1.481 (3)
C10B—C9	1.639 (6)	C6—H6A	0.9900
C10B—S1B	1.815 (6)	C6—H6B	0.9900
C10B—H10C	0.9900	N7—C8	1.474 (3)
C10B—H10D	0.9900	C8—C9	1.522 (4)
S1B—C11B	1.734 (11)	C8—H8A	0.9900
C11B—H11D	0.9800	C8—H8B	0.9900
C11B—H11E	0.9800	C9—H9A	0.9900
C11B—H11F	0.9800	C9—H9B	0.9900
N1—C2	1.341 (3)	C9—H9C	0.9900
N1—C4	1.375 (3)	C9—H9D	0.9900
N1—H1	0.68 (3)	C12—H12A	0.9800
C2—N3	1.320 (3)	C12—H12B	0.9800
C2—C12	1.495 (3)	C12—H12C	0.9800
C9—C10A—S1A	105.6 (4)	N7 ⁱ —C5—C4	117.74 (18)
C9—C10A—H10A	110.6	N7 ⁱ —C5—H5A	107.9
S1A—C10A—H10A	110.6	C4—C5—H5A	107.9

C9—C10A—H10B	110.6	N7 ⁱ —C5—H5B	107.9
S1A—C10A—H10B	110.6	C4—C5—H5B	107.9
H10A—C10A—H10B	108.8	H5A—C5—H5B	107.2
C11A—S1A—C10A	102.3 (4)	N7—C6—C3	113.01 (18)
S1A—C11A—H11A	109.5	N7—C6—H6A	109.0
S1A—C11A—H11B	109.5	C3—C6—H6A	109.0
H11A—C11A—H11B	109.5	N7—C6—H6B	109.0
S1A—C11A—H11C	109.5	C3—C6—H6B	109.0
H11A—C11A—H11C	109.5	H6A—C6—H6B	107.8
H11B—C11A—H11C	109.5	C5 ⁱ —N7—C8	112.67 (19)
C9—C10B—S1B	109.0 (4)	C5 ⁱ —N7—C6	111.42 (14)
C9—C10B—H10C	109.9	C8—N7—C6	111.0 (2)
S1B—C10B—H10C	109.9	N7—C8—C9	111.8 (2)
C9—C10B—H10D	109.9	N7—C8—H8A	109.3
S1B—C10B—H10D	109.9	C9—C8—H8A	109.3
H10C—C10B—H10D	108.3	N7—C8—H8B	109.3
C11B—S1B—C10B	98.5 (3)	C9—C8—H8B	109.3
S1B—C11B—H11D	109.5	H8A—C8—H8B	107.9
S1B—C11B—H11E	109.5	C10A—C9—C8	120.7 (3)
H11D—C11B—H11E	109.5	C8—C9—C10B	101.1 (3)
S1B—C11B—H11F	109.5	C10A—C9—H9A	107.2
H11D—C11B—H11F	109.5	C8—C9—H9A	107.2
H11E—C11B—H11F	109.5	C10A—C9—H9B	107.2
C2—N1—C4	108.65 (16)	C8—C9—H9B	107.2
C2—N1—H1	121 (2)	H9A—C9—H9B	106.8
C4—N1—H1	130 (2)	C8—C9—H9C	111.6
N3—C2—N1	111.29 (19)	C10B—C9—H9C	111.6
N3—C2—C12	125.80 (19)	C8—C9—H9D	111.6
N1—C2—C12	122.85 (19)	C10B—C9—H9D	111.6
C2—N3—C3	105.19 (17)	H9C—C9—H9D	109.4
C4—C3—N3	110.15 (18)	C2—C12—H12A	109.5
C4—C3—C6	129.9 (2)	C2—C12—H12B	109.5
N3—C3—C6	119.93 (17)	H12A—C12—H12B	109.5
C3—C4—N1	104.72 (18)	C2—C12—H12C	109.5
C3—C4—C5	131.3 (2)	H12A—C12—H12C	109.5
N1—C4—C5	124.00 (17)	H12B—C12—H12C	109.5
C9—C10A—S1A—C11A	62.4 (5)	C2—N1—C4—C5	178.75 (19)
C9—C10B—S1B—C11B	64.4 (5)	C3—C4—C5—N7 ⁱ	-111.7 (3)
C4—N1—C2—N3	0.9 (3)	N1—C4—C5—N7 ⁱ	69.1 (3)
C4—N1—C2—C12	-176.4 (2)	C4—C3—C6—N7	117.0 (2)
N1—C2—N3—C3	-0.8 (2)	N3—C3—C6—N7	-65.4 (2)
C12—C2—N3—C3	176.4 (2)	C3—C6—N7—C5 ⁱ	-61.5 (2)
C2—N3—C3—C4	0.4 (2)	C3—C6—N7—C8	172.04 (17)
C2—N3—C3—C6	-177.72 (19)	C5 ⁱ —N7—C8—C9	156.2 (3)
N3—C3—C4—N1	0.2 (2)	C6—N7—C8—C9	-78.0 (3)
C6—C3—C4—N1	178.0 (2)	S1A—C10A—C9—C8	66.8 (5)
N3—C3—C4—C5	-179.1 (2)	N7—C8—C9—C10A	169.9 (4)

C6—C3—C4—C5	-1.3 (4)	N7—C8—C9—C10B	-159.8 (3)
C2—N1—C4—C3	-0.6 (2)	S1B—C10B—C9—C8	-177.6 (4)

Symmetry code: (i) $-x+1, -y+1, -z$.

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1...N3 ⁱⁱ	0.68 (3)	2.15 (3)	2.825 (2)	169 (3)
C6—H6B...S1A ⁱⁱⁱ	0.99	2.93	3.837 (3)	153
C12—H12A...S1A ^{iv}	0.98	3.01	3.926 (3)	156
C11B—H11D...S1B ^v	0.98	1.97	2.767 (6)	137

Symmetry codes: (ii) $y-1/4, -x+3/4, z-1/4$; (iii) $-y+5/4, x-1/4, z-1/4$; (iv) $x-1/2, y, -z+1/2$; (v) $-x+1, -y+1, -z+1$.