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Crystal structure of 4-amino-5-chloro-2,6-dimethylpyrimidinium thiophene-2,5-dicarboxylate

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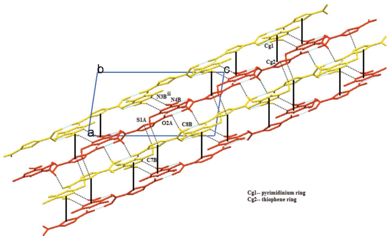
In the title salt, $C_6H_9ClN_3^+\cdot C_6H_3O_4S^-$, the cations and anions are linked *via* O—H$\cdots$O and N—H$\cdots$O hydrogen bonds, forming $R_6^6(37)$ ring motifs that are interconnected with each other, producing sheets. Separate parallel inversion-related sheets are linked through N—H$\cdots$N and π–π stacking interactions [centroid–centroid distance = 3.5414 (13) Å], forming double layers parallel to (101). Weak C—H$\cdots$O and C—H$\cdots$S hydrogen bonds, as well as C—H$\cdots\pi$ interactions, connect the double layers into a three-dimensional network.



1. Chemical context

In crystal engineering, non-covalent interactions, such as hydrogen bonding, play a key role in molecular recognition processes (Desiraju, 1989). Pyrimidine derivatives have gained considerable importance because of their remarkable biological properties, for example as anti-fungal, antiviral, anticancer and anti-allergenic agents (Ding *et al.*, 2004). Thiophenecarboxylic acid and its derivatives have attracted attention because of their wide range of pharmacological properties and numerous applications, such as the preparation of DNA hybridization indicators, single-molecule magnets, photoluminescence materials and the treatment of osteoporosis as inhibitors of bone resorption in the tissue culture (Bharti *et al.*, 2003; Taş *et al.*, 2014; Boulsourani *et al.*, 2011). The present study investigates the hydrogen-bonding patterns in 4-amino-5-chloro-2,6-dimethylpyrimidinium thiophene-2,5-dicarboxylate (I).

2. Structural commentary

The asymmetric unit of $C_6H_9ClN_3^+\cdot C_6H_3O_4S^-$, (I), contains one 4-amino-5-chloro-2,6-dimethylpyrimidinium cation and one thiophene-2,5-dicarboxylate anion (Fig. 1). Protonation of the pyrimidine occurs at atom N1, leading to a C2*B*—N1*B*—

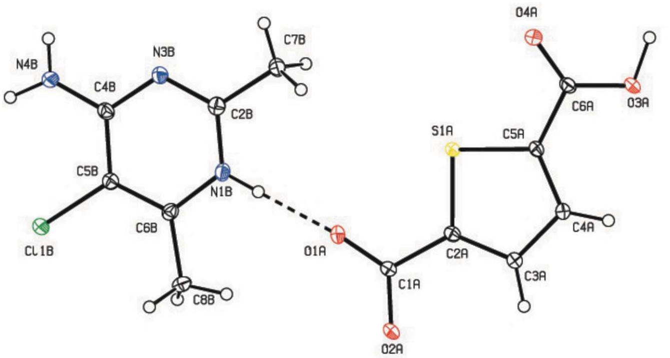


Figure 1
The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

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

Cg is the centroid of the S1*A*/C2*A*–C5*A* ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*A*—H3*A*···O2*A*^{i}	1.04 (4)	1.44 (4)	2.475 (2)	176 (4)
N1*B*—H1*B*···O1*A*	0.85 (3)	1.87 (3)	2.719 (3)	178 (3)
N4*B*—H4*B*1···N3*B*^{ii}	0.86 (3)	2.40 (3)	3.218 (3)	158 (3)
N4*B*—H4*B*2···O4*A*^{iii}	0.94 (3)	1.86 (3)	2.784 (3)	170 (3)
C7*B*—H7*BB*···S1*A*^{iv}	0.98	2.86	3.807 (2)	164
C8*B*—H8*BB*···O3*A*^{v}	0.98	2.53	3.281 (3)	134
C8*B*—H8*BC*···O2*A*^{vi}	0.98	2.47	3.301 (3)	143
C7*B*—H7*BB*···*Cg*^{iv}	0.98	2.69	3.556 (3)	148

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

C6*B* angle of 122.5 (2)° which an increase of *ca* 3.8° compared to the C2*B*—N3*B*—C4*B* angle 118.7 (2)° involving the unprotonated N3 atom.

3. Supramolecular features

The carboxylate group of the thiophene-2,5-dicarboxylate anion interacts with the protonated N1 atom of the pyrimidinium moiety with a single point heterosynthon *via* N—H···O hydrogen bonds (Table 1). In addition, the components are connected through O—H···O and N—H···O hydrogen bonds (Table 1) to form an $R_6^6(37)$ ring graph set motif. This motif includes anions connected by O—H.·O hydrogen bonds along [10$\overline{1}$] and involves the cations along [010] to form a 2D sheet (Fig. 2). Two separate 2D sheets (which are indicated in red and yellow in Fig. 3) are interconnected by a self-complementary base pair between the pyrimidinium moiety through N—H···N hydrogen bond interactions with an $R_2^2(8)$ ring graph set motif and π–π stacking interactions between the pyrimidinium ring and the thiophene ring with an observed interplanar distance of 3.4188 (10) Å, a centroid-to-centroid (*Cg*1–*Cg*2) distance of 3.5414 (13) Å (where *Cg*1 is the centroid of the ring N1*B*/C2*B*–C6*B* and *Cg*2 is the centroid of the ring S1*A*/C2*A*–C5*A*) and slip angle (the angle between the centroid vector and the normal to the plane) of 18.0°; these are typical aromatic stacking values (Hunter, 1994). Through these interactions, parallel inversion-related sheets are connected into double layers parallel to (101). In addition, weak C—H···O, C—H···S and C—H···π intermolecular interactions connect the double layers into a three-dimensional network (Fig. 3).

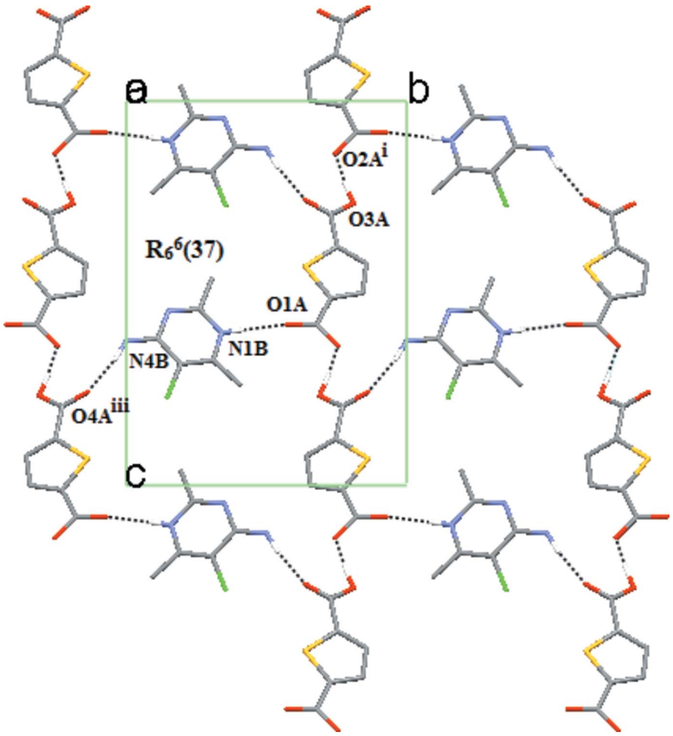


Figure 2
Packing diagram for (I), viewed along the *a* axis, showing a single sheet formed by O—H···O and N—H···O hydrogen bonds. Symmetry codes are given in Table 1. Dashed lines represent hydrogen bonds.

4. Database survey

The crystal structures of aminopyrimidine derivatives (Schwalbe & Williams, 1982) and aminopyrimidine carboxylates (Hu *et al.*, 2002), have been reported. Several co-crystals/salts of aminopyrimidine derivatives have been reported from our laboratory including co-crystals/salts of aminopyrimidines with carboxylic acid (Muthiah *et al.*, 2006; Devi & Muthiah, 2007; Subashini *et al.*, 2008; Thanigaimani *et al.*, 2009; Ebenezer & Muthiah, 2010, 2012; Ebenezer *et al.*, 2011), aminopyrimidines–thiophenecarboxylic acid (Jegan Jennifer *et al.*, 2014), the crystal structure of 2-amino-4,6-dimethoxypyrimidiniumthiophene-2-carboxylate (Rajam *et al.*, 2015) and metal complexes with 4-amino-5-chloro-2,6-dimethylpyrimidine (Karthikeyan *et al.*, 2016)

5. Synthesis and crystallization

A hot DMF solution of 4-amino-5-chloro-2,6-dimethylpyrimidine (39 mg, Alfa Aesar) and thiophene-2,5-dicarboxylic acid (43 mg, Alfa Aesar) were mixed and warmed for

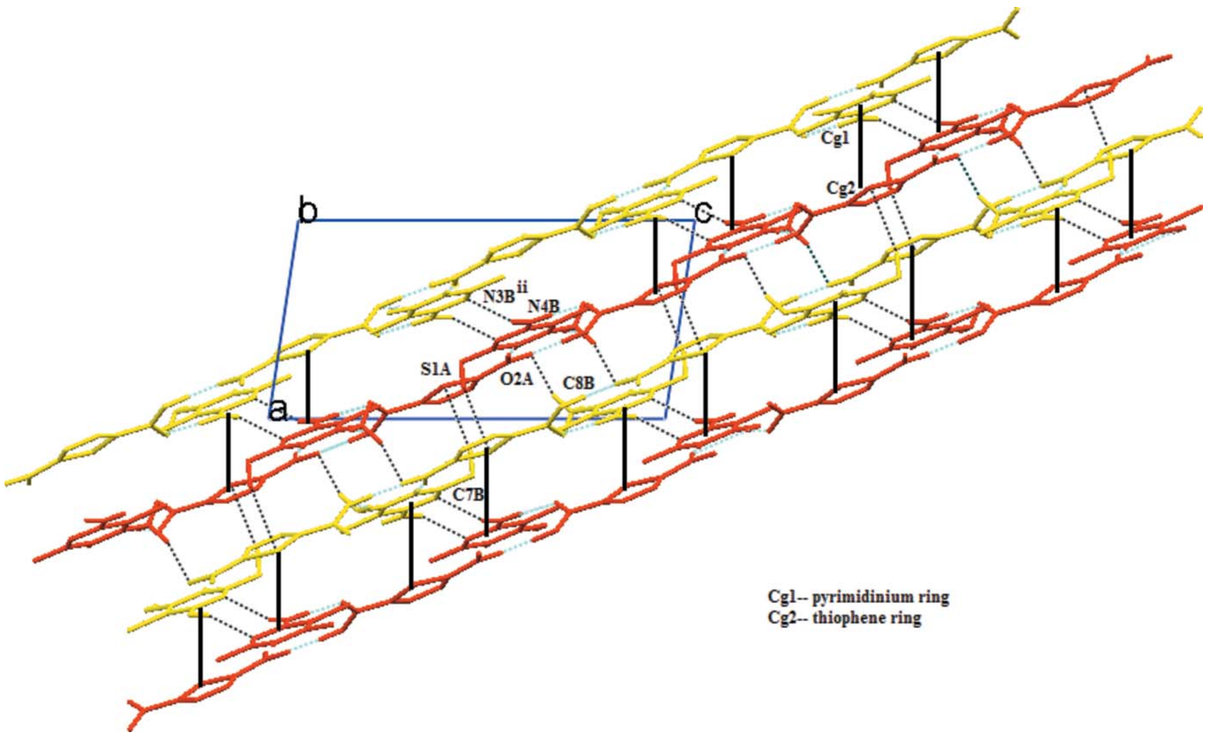


Figure 3
A view along the *b* axis, showing double layers (indicated in red and yellow) formed by hydrogen bonds and π–π stacking interactions. The weak C—H$\cdots$O and C—H$\cdots$S hydrogen bonds connect the double layers to form a three-dimensional network. Dotted lines represent N—H$\cdots$N, C—H$\cdots$O and C—H$\cdots$S interactions. Solid lines indicate the stacking interactions.

half an hour over a water bath. The mixture was cooled slowly and kept at room temperature. After a few days colourless plate-like crystals were obtained.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_9ClN_3^+\cdot C_6H_3O_4S^-$
M_r	329.76
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, *b*, *c* (Å)	7.9948 (3), 11.3928 (4), 15.7757 (6)
β (°)	98.520 (2)
V (Å^3)	1421.04 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.44
Crystal size (mm)	0.23 × 0.19 × 0.06
Data collection	
Diffractometer	Bruker AXS D8 Quest CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.424, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10749, 3911, 2862
R_{int}	0.053
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.185, 1.10
No. of reflections	3911
No. of parameters	208
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.59, −0.69

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SIR92* (Altomare *et al.*, 1993), *SHELXL2014* (Sheldrick, 2015), *SHELXLE* (Hübschle *et al.*, 2011), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The N—H and O—H H atoms were located in difference Fourier maps and refined isotropically. All other H atoms were placed in calculated positions and refined using a riding-model approximation with C—H = 0.95 Å (CH) or 0.98 Å (CH$_3$). Isotropic displacement parameters for these atoms were set to 1.2 (CH) or 1.5 (CH$_3$) times U_{eq} of the parent atom. Idealized Me H atoms were refined as rotating groups. There are larger than expected residual density peaks close to the Cl and S atoms but these are not chemically sensible and are assumed to be related to the quality of the crystal.

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supporting information

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Crystal structure of 4-amino-5-chloro-2,6-dimethylpyrimidinium thiophene-2,5-dicarboxylate

Ammaiyappan Rajam, Packianathan Thomas Muthiah, Ray J. Butcher and Matthias Zeller

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015) and *SHELXLE* (Hübschle *et al.*, 2011); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

4-Amino-5-chloro-2,6-dimethylpyrimidinium thiophene-2,5-dicarboxylate

Crystal data

$C_6H_9ClN_3^+\cdot C_6H_3O_4S^-$
M_r = 329.76
Monoclinic, $P2_1/n$
a = 7.9948 (3) Å
b = 11.3928 (4) Å
c = 15.7757 (6) Å
β = 98.520 (2)°
V = 1421.04 (9) Å^3
Z = 4
$F(000)$ = 680
D_x = 1.541 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6601 reflections
θ = 3.1–30.0°
μ = 0.44 mm^{-1}
T = 100 K
Plate, colourless
0.23 × 0.19 × 0.06 mm

Data collection

Bruker AXS D8 Quest CMOS diffractometer
Radiation source: I-mu-S microsource X-ray tube
Laterally graded multilayer (Goebel) mirror monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.424, T_{max} = 0.746
10749 measured reflections
3911 independent reflections
2862 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 30.0°, θ_{min} = 2.6°
$h = -11 \rightarrow 9$
$k = -15 \rightarrow 16$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.185
S = 1.10
3911 reflections
208 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1146P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.59$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}
S1A	0.83375 (7)	0.63795 (4)	0.43028 (4)	0.01808 (18)
O1A	0.6790 (2)	0.57301 (14)	0.58125 (10)	0.0252 (4)
O2A	0.6743 (2)	0.75418 (14)	0.63699 (10)	0.0218 (4)
O3A	1.0617 (2)	0.81066 (15)	0.26723 (10)	0.0227 (4)
H3A	1.110 (5)	0.780 (3)	0.214 (2)	0.060 (11)*
O4A	0.9244 (3)	0.63757 (15)	0.25678 (12)	0.0309 (4)
C1A	0.7104 (3)	0.6802 (2)	0.58237 (14)	0.0178 (4)
C2A	0.7953 (3)	0.7287 (2)	0.51203 (14)	0.0187 (4)
C3A	0.8446 (3)	0.84283 (19)	0.49963 (15)	0.0204 (5)
H3AA	0.8325	0.9054	0.5381	0.024*
C4A	0.9151 (3)	0.85594 (18)	0.42313 (15)	0.0199 (5)
H4AA	0.9568	0.9282	0.4046	0.024*
C5A	0.9166 (3)	0.75252 (19)	0.37866 (14)	0.0182 (4)
C6A	0.9689 (3)	0.7288 (2)	0.29484 (14)	0.0198 (5)
Cl1B	0.43554 (7)	0.14586 (5)	0.77201 (3)	0.02236 (18)
N1B	0.6246 (2)	0.34003 (17)	0.60286 (13)	0.0206 (4)
H1B	0.639 (4)	0.413 (3)	0.5956 (19)	0.031 (7)*
N3B	0.6059 (2)	0.14982 (16)	0.54703 (13)	0.0205 (4)
N4B	0.5127 (3)	−0.00013 (17)	0.62434 (14)	0.0242 (4)
H4B1	0.512 (4)	−0.043 (3)	0.5793 (19)	0.040 (9)*
H4B2	0.478 (4)	−0.039 (3)	0.671 (2)	0.045 (9)*
C2B	0.6450 (3)	0.2616 (2)	0.54118 (15)	0.0204 (5)
C4B	0.5460 (3)	0.1121 (2)	0.61845 (15)	0.0205 (5)
C5B	0.5201 (3)	0.1938 (2)	0.68398 (14)	0.0196 (4)
C6B	0.5592 (3)	0.3099 (2)	0.67489 (15)	0.0191 (4)
C7B	0.7142 (3)	0.3044 (2)	0.46395 (15)	0.0235 (5)
H7BA	0.6941	0.2453	0.4185	0.035*
H7BB	0.8360	0.3181	0.4787	0.035*
H7BC	0.6579	0.3778	0.4439	0.035*
C8B	0.5357 (3)	0.4046 (2)	0.73702 (15)	0.0250 (5)
H8BA	0.4198	0.4019	0.7502	0.037*
H8BB	0.5563	0.4810	0.7120	0.037*
H8BC	0.6156	0.3931	0.7898	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0222 (3)	0.0148 (3)	0.0193 (3)	−0.00038 (18)	0.0096 (2)	−0.00055 (19)
O1A	0.0324 (9)	0.0188 (8)	0.0273 (9)	−0.0044 (7)	0.0142 (7)	0.0021 (7)
O2A	0.0242 (8)	0.0230 (8)	0.0207 (8)	−0.0008 (6)	0.0118 (6)	−0.0003 (6)
O3A	0.0267 (8)	0.0229 (8)	0.0217 (8)	−0.0026 (7)	0.0140 (7)	−0.0021 (7)
O4A	0.0445 (11)	0.0221 (9)	0.0308 (10)	−0.0068 (7)	0.0212 (8)	−0.0064 (7)
C1A	0.0186 (9)	0.0192 (10)	0.0164 (10)	0.0001 (8)	0.0054 (8)	−0.0009 (8)
C2A	0.0169 (9)	0.0197 (10)	0.0207 (10)	0.0010 (8)	0.0064 (8)	−0.0006 (9)
C3A	0.0234 (11)	0.0193 (10)	0.0199 (11)	−0.0029 (8)	0.0078 (9)	−0.0015 (8)
C4A	0.0208 (10)	0.0183 (11)	0.0218 (11)	−0.0040 (8)	0.0076 (9)	−0.0013 (8)
C5A	0.0166 (9)	0.0184 (10)	0.0210 (11)	−0.0010 (8)	0.0081 (8)	−0.0002 (8)
C6A	0.0212 (10)	0.0203 (11)	0.0197 (11)	0.0030 (8)	0.0089 (8)	0.0015 (9)
Cl1B	0.0281 (3)	0.0207 (3)	0.0200 (3)	−0.0013 (2)	0.0090 (2)	−0.0002 (2)
N1B	0.0218 (9)	0.0168 (9)	0.0239 (10)	−0.0020 (7)	0.0055 (8)	0.0024 (8)
N3B	0.0225 (9)	0.0188 (10)	0.0212 (10)	0.0004 (7)	0.0059 (8)	0.0018 (7)
N4B	0.0349 (11)	0.0171 (10)	0.0227 (10)	0.0003 (8)	0.0116 (9)	0.0000 (8)
C2B	0.0165 (9)	0.0210 (11)	0.0235 (11)	0.0009 (8)	0.0021 (8)	0.0015 (9)
C4B	0.0183 (10)	0.0215 (11)	0.0228 (11)	0.0013 (8)	0.0071 (8)	0.0006 (9)
C5B	0.0201 (10)	0.0187 (10)	0.0207 (11)	0.0003 (8)	0.0050 (8)	0.0002 (9)
C6B	0.0176 (9)	0.0163 (10)	0.0233 (11)	0.0006 (8)	0.0026 (8)	−0.0003 (9)
C7B	0.0240 (10)	0.0208 (11)	0.0273 (12)	0.0000 (9)	0.0094 (9)	0.0024 (10)
C8B	0.0327 (12)	0.0177 (11)	0.0256 (12)	0.0009 (9)	0.0078 (10)	−0.0044 (9)

Geometric parameters (Å, º)

S1A—C2A	1.716 (2)	N1B—H1B	0.85 (3)
S1A—C5A	1.722 (2)	N3B—C2B	1.318 (3)
O1A—C1A	1.247 (3)	N3B—C4B	1.358 (3)
O2A—C1A	1.269 (3)	N4B—C4B	1.312 (3)
O3A—C6A	1.306 (3)	N4B—H4B1	0.86 (3)
O3A—H3A	1.04 (4)	N4B—H4B2	0.94 (3)
O4A—C6A	1.226 (3)	C2B—C7B	1.492 (3)
C1A—C2A	1.490 (3)	C4B—C5B	1.429 (3)
C2A—C3A	1.381 (3)	C5B—C6B	1.372 (3)
C3A—C4A	1.414 (3)	C6B—C8B	1.488 (3)
C3A—H3AA	0.9500	C7B—H7BA	0.9800
C4A—C5A	1.372 (3)	C7B—H7BB	0.9800
C4A—H4AA	0.9500	C7B—H7BC	0.9800
C5A—C6A	1.470 (3)	C8B—H8BA	0.9800
Cl1B—C5B	1.721 (2)	C8B—H8BB	0.9800
N1B—C2B	1.348 (3)	C8B—H8BC	0.9800
N1B—C6B	1.363 (3)		
C2A—S1A—C5A	91.32 (10)	H4B1—N4B—H4B2	115 (3)
C6A—O3A—H3A	109 (2)	N3B—C2B—N1B	122.3 (2)
O1A—C1A—O2A	126.5 (2)	N3B—C2B—C7B	119.5 (2)

O1A—C1A—C2A	117.76 (19)	N1B—C2B—C7B	118.2 (2)
O2A—C1A—C2A	115.72 (19)	N4B—C4B—N3B	117.9 (2)
C3A—C2A—C1A	128.7 (2)	N4B—C4B—C5B	122.1 (2)
C3A—C2A—S1A	111.97 (17)	N3B—C4B—C5B	120.0 (2)
C1A—C2A—S1A	119.24 (16)	C6B—C5B—C4B	119.5 (2)
C2A—C3A—C4A	112.3 (2)	C6B—C5B—Cl1B	120.89 (18)
C2A—C3A—H3AA	123.9	C4B—C5B—Cl1B	119.55 (17)
C4A—C3A—H3AA	123.9	N1B—C6B—C5B	116.8 (2)
C5A—C4A—C3A	112.36 (19)	N1B—C6B—C8B	117.9 (2)
C5A—C4A—H4AA	123.8	C5B—C6B—C8B	125.2 (2)
C3A—C4A—H4AA	123.8	C2B—C7B—H7BA	109.5
C4A—C5A—C6A	130.0 (2)	C2B—C7B—H7BB	109.5
C4A—C5A—S1A	112.08 (16)	H7BA—C7B—H7BB	109.5
C6A—C5A—S1A	117.83 (16)	C2B—C7B—H7BC	109.5
O4A—C6A—O3A	125.4 (2)	H7BA—C7B—H7BC	109.5
O4A—C6A—C5A	119.7 (2)	H7BB—C7B—H7BC	109.5
O3A—C6A—C5A	114.8 (2)	C6B—C8B—H8BA	109.5
C2B—N1B—C6B	122.5 (2)	C6B—C8B—H8BB	109.5
C2B—N1B—H1B	121 (2)	H8BA—C8B—H8BB	109.5
C6B—N1B—H1B	116 (2)	C6B—C8B—H8BC	109.5
C2B—N3B—C4B	118.7 (2)	H8BA—C8B—H8BC	109.5
C4B—N4B—H4B1	118 (2)	H8BB—C8B—H8BC	109.5
C4B—N4B—H4B2	127 (2)		

O1A—C1A—C2A—C3A	−179.2 (2)	C4B—N3B—C2B—N1B	−1.3 (3)
O2A—C1A—C2A—C3A	2.2 (3)	C4B—N3B—C2B—C7B	178.83 (19)
O1A—C1A—C2A—S1A	3.9 (3)	C6B—N1B—C2B—N3B	−1.3 (3)
O2A—C1A—C2A—S1A	−174.75 (16)	C6B—N1B—C2B—C7B	178.6 (2)
C5A—S1A—C2A—C3A	0.03 (18)	C2B—N3B—C4B—N4B	−177.9 (2)
C5A—S1A—C2A—C1A	177.43 (18)	C2B—N3B—C4B—C5B	2.5 (3)
C1A—C2A—C3A—C4A	−177.4 (2)	N4B—C4B—C5B—C6B	179.2 (2)
S1A—C2A—C3A—C4A	−0.4 (3)	N3B—C4B—C5B—C6B	−1.2 (3)
C2A—C3A—C4A—C5A	0.6 (3)	N4B—C4B—C5B—Cl1B	−2.4 (3)
C3A—C4A—C5A—C6A	176.1 (2)	N3B—C4B—C5B—Cl1B	177.20 (17)
C3A—C4A—C5A—S1A	−0.6 (3)	C2B—N1B—C6B—C5B	2.4 (3)
C2A—S1A—C5A—C4A	0.31 (18)	C2B—N1B—C6B—C8B	−177.5 (2)
C2A—S1A—C5A—C6A	−176.79 (17)	C4B—C5B—C6B—N1B	−1.2 (3)
C4A—C5A—C6A—O4A	−162.8 (2)	Cl1B—C5B—C6B—N1B	−179.59 (16)
S1A—C5A—C6A—O4A	13.7 (3)	C4B—C5B—C6B—C8B	178.8 (2)
C4A—C5A—C6A—O3A	17.1 (3)	Cl1B—C5B—C6B—C8B	0.4 (3)
S1A—C5A—C6A—O3A	−166.44 (16)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the S1*A*/C2*A*–C5*A* ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*A*—H3*A*···O2*A*^{i}	1.04 (4)	1.44 (4)	2.475 (2)	176 (4)
N1*B*—H1*B*···O1*A*	0.85 (3)	1.87 (3)	2.719 (3)	178 (3)

N4*B*—H4*B*1···N3*B*^{ii}	0.86 (3)	2.40 (3)	3.218 (3)	158 (3)
N4*B*—H4*B*2···O4*A*^{iii}	0.94 (3)	1.86 (3)	2.784 (3)	170 (3)
C7*B*—H7*BB*···S1*A*^{iv}	0.98	2.86	3.807 (2)	164
C8*B*—H8*BB*···O3*A*^{v}	0.98	2.53	3.281 (3)	134
C8*B*—H8*BC*···O2*A*^{vi}	0.98	2.47	3.301 (3)	143
C7*B*—H7*BB*···*Cg*^{iv}	0.98	2.69	3.556 (3)	148

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