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Crystal structure of 1-(4-formylbenzylidene)thiosemicarbazone

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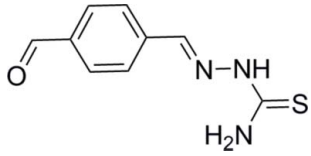
The asymmetric unit of the title compound, $C_9H_9N_3OS$, contains two approximately planar molecules (r.m.s. deviations for 14 non-H atoms = 0.094 and 0.045 Å), with different conformations. In one of them, the C=O group is *syn* to the S atom and in the other it is *anti*. Each molecule features an intramolecular N—H···N hydrogen bond, which generates an *S*(5) ring. In the crystal, molecules are linked by N—H···O and N—H···S hydrogen bonds, generating discrete networks; the *syn* molecules form [010] chains and the *anti* molecules form (100) sheets.

Keywords: crystal structure; thiosemicarbazone; hydrogen bonds.

CCDC reference: 1016158

1. Related literature

For further synthetic details, see: Jagst *et al.* (2005). For structure–biological activity relationships in thiosemicarbazones, see: Lukmantara *et al.* (2013). For their biological properties, see: Serda *et al.* (2012).



2. Experimental

2.1. Crystal data

$C_9H_9N_3OS$
M_r = 207.25
Monoclinic, $P2_1/c$
a = 12.3888 (9) Å
b = 11.7972 (8) Å
c = 14.9428 (11) Å
β = 110.286 (1)°
V = 2048.5 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 293 K
0.51 × 0.44 × 0.33 mm

2.2. Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.693, T_{max} = 0.746
19018 measured reflections
4920 independent reflections
3344 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.119
S = 1.03
4920 reflections
277 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1NA···N3A	0.84 (3)	2.32 (2)	2.630 (2)	102.0 (19)
N1A—H1NA···O1A^{i}	0.84 (3)	2.41 (3)	3.190 (3)	154 (2)
N1A—H2NA···S1A^{ii}	0.87 (3)	2.52 (3)	3.391 (2)	172 (2)
N2A—H3NA···S1B^{iii}	0.84 (2)	2.50 (2)	3.3270 (19)	166.1 (19)
N1B—H1NB···N3B	0.91 (3)	2.21 (3)	2.619 (3)	106 (3)
N1B—H2NB···O1B^{iv}	0.88 (3)	2.01 (3)	2.857 (3)	161 (3)
N2B—H3NB···S1A^{v}	0.84 (2)	2.58 (2)	3.409 (2)	171 (2)

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

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7254).

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supporting information

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Crystal structure of 1-(4-formylbenzylidene)thiosemicarbazone

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S1. Chemical context

The study of the thiosemicarbazones is interesting because they are compounds which show diverse biological properties (Serda *et al.*, 2012) and pharmacological activities (Lukmantara *et al.*, 2013). Also the thiosemicarbazones are of interest from a supramolecular point of view since they can be functionalized to give different supramolecular arrays by hydrogen bonds.

S2. Structural commentary

We report here the synthesis and structural characterization of (4-formylbenzylidine)-thiosemicarbazone (Fig.1). The two molecules in the asymmetric unit are structurally different due to the different orientation of the carbonyl group respect to the thiosemicarbazone chain. The thiosemicarbazone moiety in both molecules shows an E conformation with the sulfur atom trans to the iminic nitrogen N3 atom. The molecules labeled as B are linked into lineal chains by N—H···O hydrogen bonds with a d(N···O) of 2.857 (3) Å but the molecules labeled as A use the same kind of hydrogen bond with a longer d(N···O) of 3.190 (3) Å to form helical chains (Fig. 2). The two types of chains are packed by N—H···S hydrogen bonds with d(N—S) in the range 3.32-3.41 Å and (NHS) angles close to linearity (between 166 and 172°).

S3. Synthesis and crystallization

A solution of thiosemicarbazide (342mg, 3.72 mmol) in 50 ml of water was slowly added at 50°C to a solution of terephthaldicarboxaldehyde (500 mg, 3.73 mmol) in 100 ml water. Then the mixture was stirred at 50°C for 30 mins. Once cooled to room temperature, the yellow solid was filtered off and vacuum dried. Yellow prisms were obtained by recrystallization from EtOH/H_2O (1:1) solution. Yield: 78%. M.pt: 212–214°C. IR data (KBr, cm^{-1}): 3452w, 3328m, 3152m *ν*(NH); 2974w, 2863w *ν*(C—H aldehyde); 1686s *ν*(C=O); 1533s, 1281m *ν*(C=N), 830m, 793m *ν*(C=S). ^{1}H NMR data (DMSO-d_6, ppm): 10.60 (s, 1H, N(2)—H); 10.01 (s, 1H, C(1)—H); 8.32 (s, 1H, N(2)—H); 8.15 (s, 1H, N(2)—H); 8.09 (s, 1H, C(8)—H); 8.02 (d, 2H, J = 8.2 Hz, C(3,7)-H); 7.91 (d, 2H, J = 8.2 Hz, C(4,6)-H).

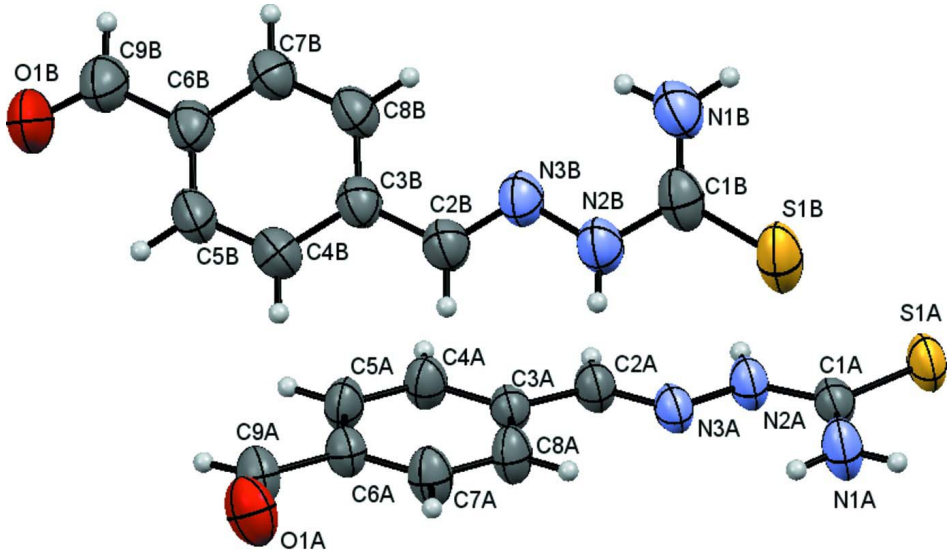

Figure 1

ORTEP view of the two molecules of the title compound. Displacement ellipsoids shown at the 50% probability level.

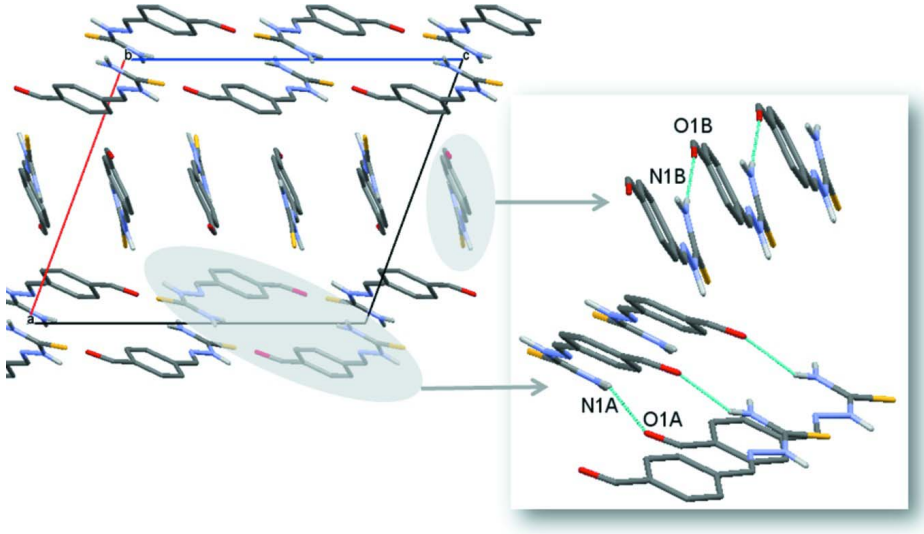

Figure 2

View of the crystal packing showing the two different chains.

1-(4-Formylbenzylidene)thiosemicarbazone

Crystal data

$C_9H_9N_3OS$
$M_r = 207.25$
Monoclinic, $P2_1/c$
$a = 12.3888$ (9) Å
$b = 11.7972$ (8) Å
$c = 14.9428$ (11) Å
$\beta = 110.286$ (1)°
$V = 2048.5$ (3) Å^3
$Z = 8$
$F(000) = 864$
$D_x = 1.344$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6097 reflections
$\theta = 2.3$–27.2°
$\mu = 0.29$ mm^{-1}
$T = 293$ K
Prism, yellow
0.51 × 0.44 × 0.33 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.693, T_{max} = 0.746
19018 measured reflections
4920 independent reflections
3344 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.1°, θ_{min} = 1.8°
h = −16→16
k = −15→15
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.119
S = 1.03
4920 reflections
277 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.8755P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N3A	0.89210 (14)	0.63007 (12)	−0.01356 (11)	0.0479 (4)
S1A	0.90693 (5)	0.91696 (4)	−0.13892 (4)	0.06120 (17)
O1A	0.89088 (17)	0.16790 (14)	0.29083 (12)	0.0778 (5)
N1A	0.97843 (19)	0.83357 (16)	0.03697 (14)	0.0646 (5)
C1A	0.92577 (17)	0.81529 (15)	−0.05446 (14)	0.0488 (4)
N2A	0.88481 (15)	0.71091 (13)	−0.08158 (13)	0.0519 (4)
C2A	0.84890 (17)	0.53375 (15)	−0.04474 (14)	0.0499 (4)
H2A	0.8172	0.5214	−0.1102	0.060*
C3A	0.84875 (16)	0.44243 (14)	0.02136 (13)	0.0446 (4)
C4A	0.80002 (18)	0.33905 (16)	−0.01569 (14)	0.0536 (5)
H4A	0.7659	0.3300	−0.0813	0.064*
C5A	0.80199 (18)	0.24931 (15)	0.04467 (14)	0.0549 (5)
H5A	0.7691	0.1803	0.0195	0.066*
C6A	0.85265 (17)	0.26217 (15)	0.14207 (14)	0.0487 (4)
C7A	0.9008 (2)	0.36573 (16)	0.17931 (14)	0.0576 (5)
H7A	0.9348	0.3746	0.2450	0.069*
C8A	0.89848 (19)	0.45524 (16)	0.11987 (14)	0.0550 (5)
H8A	0.9302	0.5245	0.1455	0.066*
C9A	0.8559 (2)	0.16499 (18)	0.20519 (17)	0.0615 (5)
H9A	0.8286	0.0959	0.1763	0.074*
H1NA	0.990 (2)	0.782 (2)	0.0779 (17)	0.069 (7)*
H2NA	1.007 (2)	0.900 (2)	0.0570 (17)	0.075 (7)*

H3NA	0.8488 (18)	0.6956 (18)	−0.1392 (16)	0.054 (6)*
S1B	0.70719 (7)	0.87078 (5)	0.20508 (5)	0.0836 (2)
O1B	0.36864 (17)	−0.02352 (14)	0.06781 (17)	0.1027 (7)
N1B	0.5055 (2)	0.77556 (19)	0.11523 (17)	0.0728 (6)
C1B	0.6141 (2)	0.76241 (17)	0.16872 (15)	0.0633 (6)
N2B	0.6506 (2)	0.65472 (15)	0.19199 (15)	0.0659 (5)
C2B	0.61285 (19)	0.46749 (17)	0.18659 (16)	0.0596 (5)
H2B	0.6866	0.4587	0.2310	0.072*
N3B	0.57577 (16)	0.56654 (14)	0.15795 (13)	0.0591 (4)
C3B	0.54146 (18)	0.36782 (16)	0.15082 (15)	0.0539 (5)
C4B	0.5824 (2)	0.26093 (18)	0.18761 (17)	0.0636 (6)
H4B	0.6538	0.2549	0.2358	0.076*
C5B	0.5189 (2)	0.16464 (18)	0.15366 (18)	0.0663 (6)
H5B	0.5477	0.0941	0.1784	0.080*
C6B	0.41212 (19)	0.17280 (17)	0.08275 (16)	0.0574 (5)
C7B	0.37016 (19)	0.27858 (17)	0.04567 (16)	0.0592 (5)
H6B	0.2983	0.2843	−0.0020	0.071*
C8B	0.43420 (19)	0.37484 (17)	0.07894 (16)	0.0583 (5)
H7B	0.4056	0.4451	0.0532	0.070*
C9B	0.3412 (2)	0.07213 (19)	0.0444 (2)	0.0723 (6)
H9B	0.2691	0.0838	−0.0017	0.087*
H1NB	0.463 (3)	0.712 (3)	0.093 (2)	0.107 (10)*
H2NB	0.478 (2)	0.844 (2)	0.1003 (19)	0.085 (8)*
H3NB	0.717 (2)	0.642 (2)	0.2304 (17)	0.065 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N3A	0.0572 (9)	0.0343 (7)	0.0505 (8)	0.0015 (7)	0.0167 (7)	0.0081 (6)
S1A	0.0797 (4)	0.0362 (2)	0.0594 (3)	−0.0022 (2)	0.0134 (3)	0.0123 (2)
O1A	0.1133 (14)	0.0633 (10)	0.0600 (10)	0.0069 (9)	0.0341 (9)	0.0169 (8)
N1A	0.0936 (15)	0.0363 (9)	0.0541 (10)	−0.0053 (9)	0.0130 (10)	0.0050 (8)
C1A	0.0554 (11)	0.0351 (9)	0.0545 (11)	0.0034 (8)	0.0174 (9)	0.0043 (8)
N2A	0.0682 (11)	0.0343 (7)	0.0479 (9)	−0.0020 (7)	0.0135 (8)	0.0067 (7)
C2A	0.0602 (11)	0.0375 (9)	0.0477 (10)	−0.0014 (8)	0.0131 (8)	0.0043 (8)
C3A	0.0498 (10)	0.0347 (8)	0.0480 (10)	0.0006 (7)	0.0151 (8)	0.0032 (7)
C4A	0.0647 (12)	0.0430 (9)	0.0447 (10)	−0.0084 (9)	0.0082 (9)	0.0010 (8)
C5A	0.0638 (12)	0.0367 (9)	0.0586 (12)	−0.0116 (8)	0.0141 (10)	−0.0017 (8)
C6A	0.0576 (11)	0.0383 (9)	0.0507 (10)	−0.0004 (8)	0.0193 (9)	0.0057 (8)
C7A	0.0817 (15)	0.0445 (10)	0.0439 (10)	−0.0040 (10)	0.0183 (10)	−0.0002 (8)
C8A	0.0774 (14)	0.0351 (9)	0.0498 (10)	−0.0068 (9)	0.0187 (10)	−0.0045 (8)
C9A	0.0775 (15)	0.0449 (10)	0.0641 (13)	−0.0005 (10)	0.0271 (11)	0.0082 (9)
S1B	0.1164 (6)	0.0470 (3)	0.0657 (4)	−0.0135 (3)	0.0042 (3)	0.0020 (3)
O1B	0.0916 (13)	0.0436 (9)	0.158 (2)	−0.0036 (9)	0.0239 (13)	−0.0026 (11)
N1B	0.0818 (15)	0.0507 (11)	0.0826 (14)	0.0090 (11)	0.0243 (12)	0.0030 (11)
C1B	0.0916 (17)	0.0453 (11)	0.0517 (11)	0.0007 (11)	0.0233 (11)	−0.0012 (9)
N2B	0.0739 (13)	0.0445 (9)	0.0669 (12)	−0.0017 (9)	0.0088 (10)	−0.0003 (8)
C2B	0.0632 (13)	0.0471 (11)	0.0647 (13)	0.0019 (10)	0.0172 (10)	0.0008 (9)

N3B	0.0685 (11)	0.0429 (9)	0.0635 (10)	−0.0031 (8)	0.0199 (9)	−0.0036 (8)
C3B	0.0603 (12)	0.0434 (10)	0.0616 (12)	0.0037 (9)	0.0259 (10)	−0.0003 (9)
C4B	0.0605 (13)	0.0517 (11)	0.0738 (14)	0.0066 (10)	0.0172 (11)	0.0103 (10)
C5B	0.0705 (15)	0.0419 (10)	0.0884 (16)	0.0083 (10)	0.0299 (13)	0.0111 (10)
C6B	0.0607 (13)	0.0434 (10)	0.0742 (14)	0.0031 (9)	0.0312 (11)	−0.0022 (9)
C7B	0.0583 (12)	0.0483 (11)	0.0697 (13)	0.0068 (9)	0.0207 (10)	−0.0036 (10)
C8B	0.0650 (13)	0.0423 (10)	0.0672 (13)	0.0103 (9)	0.0225 (11)	0.0015 (9)
C9B	0.0709 (15)	0.0517 (12)	0.0965 (18)	−0.0014 (11)	0.0320 (13)	−0.0068 (12)

Geometric parameters (Å, º)

N3A—C2A	1.274 (2)	S1B—C1B	1.681 (2)
N3A—N2A	1.374 (2)	O1B—C9B	1.195 (3)
S1A—C1A	1.6976 (18)	N1B—C1B	1.314 (3)
O1A—C9A	1.201 (3)	N1B—H1NB	0.91 (3)
N1A—C1A	1.312 (3)	N1B—H2NB	0.88 (3)
N1A—H1NA	0.84 (3)	C1B—N2B	1.353 (3)
N1A—H2NA	0.87 (3)	N2B—N3B	1.369 (2)
C1A—N2A	1.340 (2)	N2B—H3NB	0.84 (2)
N2A—H3NA	0.84 (2)	C2B—N3B	1.274 (3)
C2A—C3A	1.462 (2)	C2B—C3B	1.457 (3)
C2A—H2A	0.9300	C2B—H2B	0.9300
C3A—C4A	1.388 (2)	C3B—C8B	1.392 (3)
C3A—C8A	1.393 (3)	C3B—C4B	1.399 (3)
C4A—C5A	1.386 (3)	C4B—C5B	1.375 (3)
C4A—H4A	0.9300	C4B—H4B	0.9300
C5A—C6A	1.379 (3)	C5B—C6B	1.382 (3)
C5A—H5A	0.9300	C5B—H5B	0.9300
C6A—C7A	1.388 (3)	C6B—C7B	1.391 (3)
C6A—C9A	1.476 (3)	C6B—C9B	1.470 (3)
C7A—C8A	1.374 (3)	C7B—C8B	1.376 (3)
C7A—H7A	0.9300	C7B—H6B	0.9300
C8A—H8A	0.9300	C8B—H7B	0.9300
C9A—H9A	0.9300	C9B—H9B	0.9300
C2A—N3A—N2A	115.92 (16)	C1B—N1B—H1NB	118 (2)
C1A—N1A—H1NA	122.5 (16)	C1B—N1B—H2NB	119.2 (18)
C1A—N1A—H2NA	120.1 (16)	H1NB—N1B—H2NB	122 (3)
H1NA—N1A—H2NA	117 (2)	N1B—C1B—N2B	116.6 (2)
N1A—C1A—N2A	117.74 (17)	N1B—C1B—S1B	123.36 (18)
N1A—C1A—S1A	123.28 (15)	N2B—C1B—S1B	120.0 (2)
N2A—C1A—S1A	118.98 (15)	C1B—N2B—N3B	119.7 (2)
C1A—N2A—N3A	119.56 (17)	C1B—N2B—H3NB	120.4 (17)
C1A—N2A—H3NA	121.2 (15)	N3B—N2B—H3NB	119.7 (16)
N3A—N2A—H3NA	119.0 (15)	N3B—C2B—C3B	121.0 (2)
N3A—C2A—C3A	120.60 (17)	N3B—C2B—H2B	119.5
N3A—C2A—H2A	119.7	C3B—C2B—H2B	119.5
C3A—C2A—H2A	119.7	C2B—N3B—N2B	116.96 (19)

C4A—C3A—C8A	119.25 (16)	C8B—C3B—C4B	118.45 (19)
C4A—C3A—C2A	118.70 (17)	C8B—C3B—C2B	122.07 (18)
C8A—C3A—C2A	122.03 (16)	C4B—C3B—C2B	119.5 (2)
C5A—C4A—C3A	120.31 (17)	C5B—C4B—C3B	121.1 (2)
C5A—C4A—H4A	119.8	C5B—C4B—H4B	119.5
C3A—C4A—H4A	119.8	C3B—C4B—H4B	119.5
C6A—C5A—C4A	120.11 (17)	C4B—C5B—C6B	119.92 (19)
C6A—C5A—H5A	119.9	C4B—C5B—H5B	120.0
C4A—C5A—H5A	119.9	C6B—C5B—H5B	120.0
C5A—C6A—C7A	119.67 (17)	C5B—C6B—C7B	119.61 (19)
C5A—C6A—C9A	119.37 (17)	C5B—C6B—C9B	121.8 (2)
C7A—C6A—C9A	120.96 (18)	C7B—C6B—C9B	118.6 (2)
C8A—C7A—C6A	120.50 (18)	C8B—C7B—C6B	120.5 (2)
C8A—C7A—H7A	119.8	C8B—C7B—H6B	119.7
C6A—C7A—H7A	119.8	C6B—C7B—H6B	119.7
C7A—C8A—C3A	120.15 (17)	C7B—C8B—C3B	120.43 (19)
C7A—C8A—H8A	119.9	C7B—C8B—H7B	119.8
C3A—C8A—H8A	119.9	C3B—C8B—H7B	119.8
O1A—C9A—C6A	125.3 (2)	O1B—C9B—C6B	125.3 (3)
O1A—C9A—H9A	117.3	O1B—C9B—H9B	117.4
C6A—C9A—H9A	117.3	C6B—C9B—H9B	117.4

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*NA*···N3*A*	0.84 (3)	2.32 (2)	2.630 (2)	102.0 (19)
N1*A*—H1*NA*···O1*A*^{i}	0.84 (3)	2.41 (3)	3.190 (3)	154 (2)
N1*A*—H2*NA*···S1*A*^{ii}	0.87 (3)	2.52 (3)	3.391 (2)	172 (2)
N2*A*—H3*NA*···S1*B*^{iii}	0.84 (2)	2.50 (2)	3.3270 (19)	166.1 (19)
N1*B*—H1*NB*···N3*B*	0.91 (3)	2.21 (3)	2.619 (3)	106 (3)
N1*B*—H2*NB*···O1*B*^{iv}	0.88 (3)	2.01 (3)	2.857 (3)	161 (3)
N2*B*—H3*NB*···S1*A*^{v}	0.84 (2)	2.58 (2)	3.409 (2)	171 (2)

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