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N-(1,3-Benzothiazol-2-yl)acetamide

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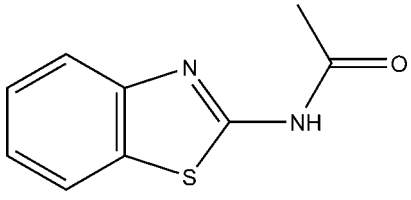
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.109; data-to-parameter ratio = 25.0.

The title compound, $C_9H_8N_2OS$, crystallizes with two molecules (*A* and *B*) in the asymmetric unit. The dihedral angles between the mean planes of the 1,3-benzothiazol-2-yl ring system and the acetamide group are 2.7 (4) (molecule *A*) and 7.2 (2) Å (molecule *B*). In the crystal, pairs of N—H···N hydrogen bonds link the *A* and *B* molecules into dimers, generating $R_2^2(8)$ loops. The dimers stack along [100].

Related literature

For the related crystal structure of the acetamide derivatives, see: Jasinski *et al.* (2013); Fun *et al.* (2011*a*,*b*, 2012).



Experimental

Crystal data

$C_9H_8N_2OS$
M_r = 192.24
Monoclinic, $P2_1/c$
a = 11.1852 (4) Å
b = 7.4037 (4) Å
c = 20.9189 (8) Å
β = 94.408 (3)°
V = 1727.21 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 173 K
0.45 × 0.24 × 0.15 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.770, T_{max} = 1.000
20845 measured reflections
5918 independent reflections
4622 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.08
5918 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2*A*—H2*A*···N1*B*	0.86	2.11	2.9700 (16)	176
N2*B*—H2*B*···N1*A*	0.86	2.14	2.9749 (16)	165

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7144).

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supporting information

Acta Cryst. (2013). E**69**, o1622 [doi:10.1107/S160053681302730X]

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S1. Comment

In continuation of our work on the synthesis of acetamide derivatives (Jasinski *et al.* 2013), we report herein the crystal structure of the title compound, $C_9H_8N_2OS$, (I). Some of the related crystal structures of similar acetamide derivatives include, N-(3-chloro-4-fluorophenyl)acetamide, N-(4-bromophenyl)-2-(naphthalen-1- yl)acetamide and N-(3,5-dichlorophenyl)-2-(naphthalen-1-yl)acetamide (Fun *et al.* 2011*a*,*b*, 2012).

The title compound, (I) crystallizes with two independent molecules (A & B) in the asymmetric unit (Fig.1). The dihedral angle between the mean planes of the 1,3-benzothiazol-2-yl ring and the acetamide group is 2.7 (4)° (A) and 7.2 (2)Å (B),(Fig. 2). In the crystal, N—H···N hydrogen bonds forming $R_2^2(8)$ graph set motifs which link the molecules into dimers, which stack along [100].

S2. Experimental

2-Aminobenzothiazole (1 mmol) were dissolved in a 30 ml acetic acid and it was refluxed for 3 hrs (Fig.3). The reaction mixture was cooled and poured into ice cold water. The precipitate obtained was obtained by filtration and recrystallized in ethanol. Colorless blocks were grown from methanol solution by the slow evaporation method and was used as such for X-ray studies (M.P.: 453-455 K).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.93Å (CH), 0.96Å (CH_3) or 0.86Å (NH). Isotropic displacement parameters for these atoms were set to 1.2 (CH, NH) or 1.5 (CH_3) times U_{eq} of the parent atom. Idealised methyl were refined as rotating groups.

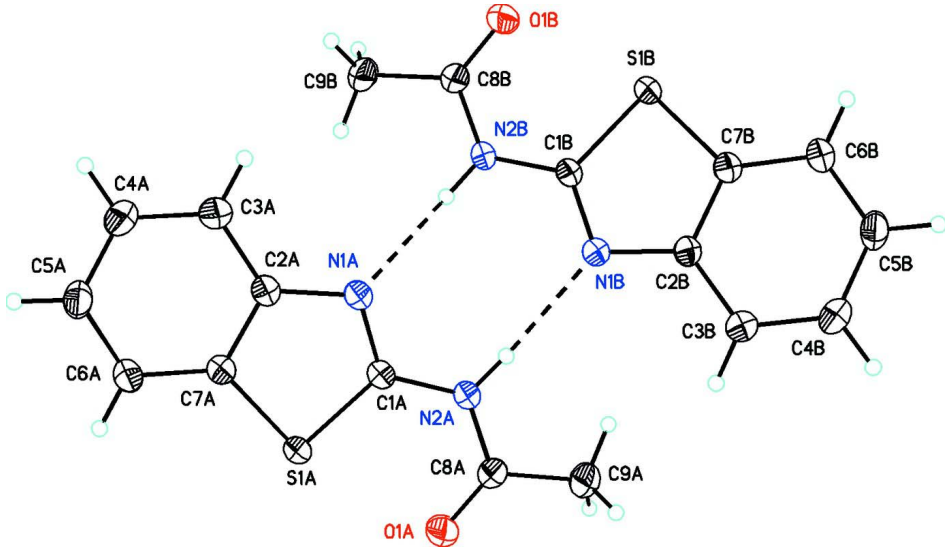

Figure 1

ORTEP drawing of (I) showing 50% probability displacement ellipsoids. Dashed lines indicate N—H···N intermolecular hydrogen bonds between A and B forming $R_2^2(8)$ graph set motifs.

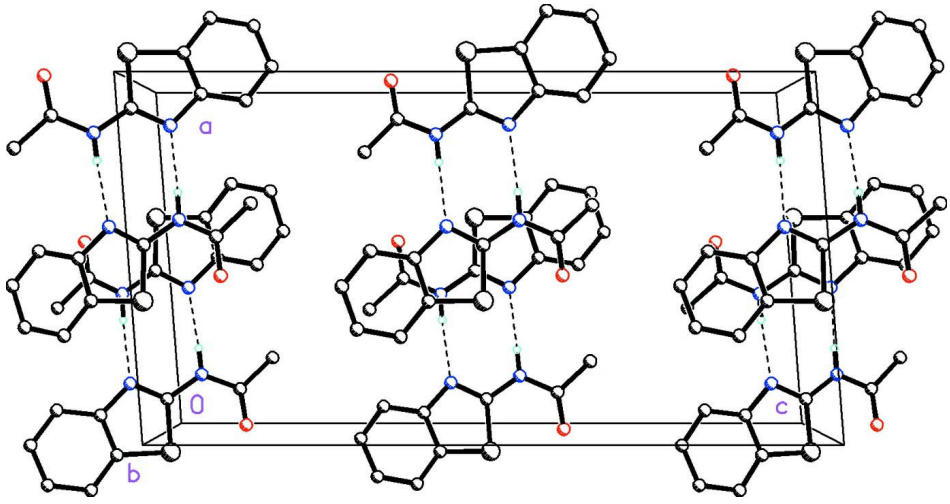

Figure 2

Molecular packing for (I) viewed along the *b* axis. Dashed lines indicate N—H···N intermolecular hydrogen bonds forming $R_2^2(8)$ graph set motifs which link the molecules into dimers along [100]. H atoms not involved in hydrogen bonding have been removed for clarity.

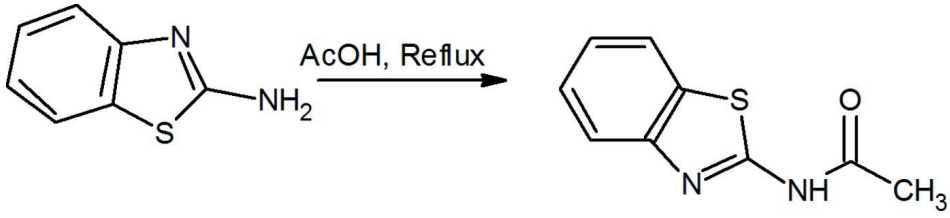

Figure 3

Synthesis scheme for (I).

N-(1,3-Benzothiazol-2-yl)acetamide

Crystal data

$C_9H_8N_2OS$
$M_r = 192.24$
Monoclinic, $P2_1/c$
$a = 11.1852$ (4) Å
$b = 7.4037$ (4) Å
$c = 20.9189$ (8) Å
$\beta = 94.408$ (3)°
$V = 1727.21$ (13) Å^3
$Z = 8$
$F(000) = 800$
$D_x = 1.479$ Mg m^{-3}
Melting point: 453 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5326 reflections
$\theta = 3.3$–$32.7°$
$\mu = 0.33$ mm^{-1}
$T = 173$ K
Block, colorless
0.45 × 0.24 × 0.15 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Radiation source: Enhance (Mo) X-ray Source
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan *CrysAlis PRO* and *CrysAlis RED*, Agilent (2012).
$T_{min} = 0.770$, $T_{max} = 1.000$
20845 measured reflections
5918 independent reflections
4622 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 32.8°$, $\theta_{min} = 3.3°$
$h = -16 \rightarrow 16$
$k = -10 \rightarrow 9$
$l = -30 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.109$
$S = 1.08$
5918 reflections
237 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.4973P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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	0.38148 (3)	0.72688 (5)	0.50197 (2)	0.02464 (9)
O1A	0.45185 (9)	0.64286 (18)	0.62295 (5)	0.0349 (3)
N1A	0.58652 (10)	0.79642 (18)	0.45587 (5)	0.0242 (2)
N2A	0.60552 (10)	0.72112 (17)	0.56435 (5)	0.0232 (2)

H2A	0.6815	0.7393	0.5650	0.028*
C1A	0.53676 (11)	0.75086 (19)	0.50776 (6)	0.0208 (3)
C2A	0.49856 (11)	0.8192 (2)	0.40579 (6)	0.0228 (3)
C3A	0.51887 (13)	0.8704 (2)	0.34317 (7)	0.0301 (3)
H3A	0.5961	0.8949	0.3320	0.036*
C4A	0.42227 (14)	0.8841 (2)	0.29819 (7)	0.0315 (3)
H4A	0.4349	0.9165	0.2563	0.038*
C5A	0.30593 (13)	0.8500 (2)	0.31478 (7)	0.0303 (3)
H5A	0.2423	0.8596	0.2837	0.036*
C6A	0.28360 (13)	0.8024 (2)	0.37647 (7)	0.0284 (3)
H6A	0.2059	0.7813	0.3876	0.034*
C7A	0.38110 (12)	0.7869 (2)	0.42159 (6)	0.0225 (3)
C8A	0.55898 (12)	0.6640 (2)	0.61966 (6)	0.0241 (3)
C9A	0.64887 (14)	0.6310 (2)	0.67511 (7)	0.0312 (3)
H9AA	0.7267	0.6141	0.6597	0.047*
H9AB	0.6268	0.5247	0.6977	0.047*
H9AC	0.6508	0.7329	0.7035	0.047*
S1B	1.06929 (3)	0.76516 (5)	0.50481 (2)	0.02415 (9)
O1B	0.99661 (9)	0.63954 (18)	0.38920 (5)	0.0338 (3)
N1B	0.86730 (10)	0.77933 (17)	0.55907 (5)	0.0230 (2)
N2B	0.84393 (10)	0.70106 (17)	0.45051 (5)	0.0232 (2)
H2B	0.7673	0.7064	0.4517	0.028*
C1B	0.91433 (11)	0.74614 (19)	0.50500 (6)	0.0200 (2)
C2B	0.95787 (11)	0.8261 (2)	0.60567 (6)	0.0210 (3)
C3B	0.94173 (13)	0.8677 (2)	0.66959 (7)	0.0288 (3)
H3B	0.8654	0.8664	0.6844	0.035*
C4B	1.04033 (14)	0.9107 (2)	0.71058 (7)	0.0316 (3)
H4B	1.0302	0.9376	0.7533	0.038*
C5B	1.15469 (13)	0.9140 (2)	0.68865 (7)	0.0303 (3)
H5B	1.2198	0.9446	0.7169	0.036*
C6B	1.17329 (12)	0.8727 (2)	0.62580 (7)	0.0273 (3)
H6B	1.2499	0.8745	0.6114	0.033*
C7B	1.07368 (11)	0.8283 (2)	0.58475 (6)	0.0219 (3)
C8B	0.88922 (12)	0.6480 (2)	0.39429 (6)	0.0242 (3)
C9B	0.79789 (13)	0.5998 (2)	0.34107 (7)	0.0300 (3)
H9BA	0.7214	0.5827	0.3581	0.045*
H9BB	0.8214	0.4902	0.3210	0.045*
H9BC	0.7922	0.6954	0.3100	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.01604 (15)	0.0370 (2)	0.02094 (15)	−0.00082 (13)	0.00206 (11)	0.00004 (13)
O1A	0.0235 (5)	0.0539 (8)	0.0277 (5)	−0.0055 (5)	0.0038 (4)	0.0070 (5)
N1A	0.0172 (5)	0.0334 (7)	0.0218 (5)	−0.0006 (4)	0.0010 (4)	0.0034 (5)
N2A	0.0165 (5)	0.0327 (7)	0.0203 (5)	−0.0008 (4)	0.0007 (4)	0.0012 (5)
C1A	0.0166 (5)	0.0248 (7)	0.0211 (6)	0.0002 (5)	0.0012 (4)	−0.0005 (5)
C2A	0.0187 (6)	0.0268 (7)	0.0226 (6)	0.0007 (5)	0.0003 (5)	0.0013 (5)

C3A	0.0244 (7)	0.0408 (9)	0.0253 (7)	0.0003 (6)	0.0038 (5)	0.0061 (6)
C4A	0.0329 (8)	0.0394 (9)	0.0222 (6)	0.0038 (6)	0.0014 (5)	0.0054 (6)
C5A	0.0278 (7)	0.0382 (9)	0.0239 (6)	0.0065 (6)	−0.0045 (5)	−0.0010 (6)
C6A	0.0201 (6)	0.0391 (9)	0.0256 (6)	0.0033 (6)	−0.0010 (5)	−0.0024 (6)
C7A	0.0192 (6)	0.0273 (7)	0.0210 (6)	0.0017 (5)	0.0015 (4)	−0.0012 (5)
C8A	0.0243 (6)	0.0273 (7)	0.0206 (6)	−0.0008 (5)	0.0015 (5)	−0.0001 (5)
C9A	0.0303 (7)	0.0387 (9)	0.0240 (7)	0.0007 (6)	−0.0016 (5)	0.0046 (6)
S1B	0.01533 (15)	0.0370 (2)	0.02013 (15)	−0.00067 (12)	0.00165 (11)	−0.00226 (13)
O1B	0.0229 (5)	0.0521 (8)	0.0269 (5)	−0.0017 (5)	0.0051 (4)	−0.0072 (5)
N1B	0.0174 (5)	0.0326 (7)	0.0190 (5)	0.0015 (4)	0.0010 (4)	−0.0006 (4)
N2B	0.0154 (5)	0.0346 (7)	0.0193 (5)	−0.0008 (4)	−0.0010 (4)	−0.0007 (5)
C1B	0.0154 (5)	0.0247 (7)	0.0199 (5)	0.0008 (4)	0.0002 (4)	0.0008 (5)
C2B	0.0181 (6)	0.0251 (7)	0.0194 (6)	0.0021 (5)	−0.0005 (4)	0.0006 (5)
C3B	0.0244 (7)	0.0398 (9)	0.0223 (6)	0.0002 (6)	0.0030 (5)	−0.0037 (6)
C4B	0.0332 (8)	0.0413 (9)	0.0200 (6)	−0.0007 (6)	−0.0002 (5)	−0.0040 (6)
C5B	0.0277 (7)	0.0366 (9)	0.0252 (7)	−0.0039 (6)	−0.0065 (5)	−0.0018 (6)
C6B	0.0194 (6)	0.0369 (9)	0.0249 (6)	−0.0025 (5)	−0.0020 (5)	−0.0010 (6)
C7B	0.0191 (6)	0.0255 (7)	0.0209 (6)	0.0006 (5)	0.0001 (4)	0.0006 (5)
C8B	0.0226 (6)	0.0297 (8)	0.0203 (6)	−0.0026 (5)	0.0010 (5)	−0.0004 (5)
C9B	0.0310 (7)	0.0377 (9)	0.0208 (6)	−0.0051 (6)	−0.0014 (5)	−0.0038 (6)

Geometric parameters (Å, º)

S1A—C1A	1.7407 (13)	S1B—C1B	1.7392 (13)
S1A—C7A	1.7390 (14)	S1B—C7B	1.7333 (13)
O1A—C8A	1.2156 (17)	O1B—C8B	1.2157 (16)
N1A—C1A	1.3018 (17)	N1B—C1B	1.3068 (16)
N1A—C2A	1.3913 (17)	N1B—C2B	1.3945 (17)
N2A—H2A	0.8600	N2B—H2B	0.8600
N2A—C1A	1.3791 (17)	N2B—C1B	1.3757 (16)
N2A—C8A	1.3715 (17)	N2B—C8B	1.3733 (17)
C2A—C3A	1.3989 (19)	C2B—C3B	1.3974 (18)
C2A—C7A	1.3997 (18)	C2B—C7B	1.3988 (18)
C3A—H3A	0.9300	C3B—H3B	0.9300
C3A—C4A	1.381 (2)	C3B—C4B	1.381 (2)
C4A—H4A	0.9300	C4B—H4B	0.9300
C4A—C5A	1.395 (2)	C4B—C5B	1.392 (2)
C5A—H5A	0.9300	C5B—H5B	0.9300
C5A—C6A	1.379 (2)	C5B—C6B	1.381 (2)
C6A—H6A	0.9300	C6B—H6B	0.9300
C6A—C7A	1.3910 (19)	C6B—C7B	1.3928 (18)
C8A—C9A	1.4957 (19)	C8B—C9B	1.4952 (19)
C9A—H9AA	0.9600	C9B—H9BA	0.9600
C9A—H9AB	0.9600	C9B—H9BB	0.9600
C9A—H9AC	0.9600	C9B—H9BC	0.9600
C7A—S1A—C1A	88.25 (6)	C7B—S1B—C1B	88.51 (6)
C1A—N1A—C2A	109.66 (11)	C1B—N1B—C2B	109.42 (11)

C1A—N2A—H2A	118.3	C1B—N2B—H2B	118.2
C8A—N2A—H2A	118.3	C8B—N2B—H2B	118.2
C8A—N2A—C1A	123.41 (12)	C8B—N2B—C1B	123.62 (11)
N1A—C1A—S1A	117.17 (10)	N1B—C1B—S1B	117.01 (10)
N1A—C1A—N2A	120.74 (12)	N1B—C1B—N2B	121.32 (12)
N2A—C1A—S1A	122.08 (10)	N2B—C1B—S1B	121.66 (10)
N1A—C2A—C3A	125.57 (12)	N1B—C2B—C3B	125.69 (12)
N1A—C2A—C7A	115.07 (12)	N1B—C2B—C7B	115.13 (11)
C3A—C2A—C7A	119.36 (12)	C3B—C2B—C7B	119.18 (12)
C2A—C3A—H3A	120.6	C2B—C3B—H3B	120.4
C4A—C3A—C2A	118.89 (13)	C4B—C3B—C2B	119.29 (13)
C4A—C3A—H3A	120.6	C4B—C3B—H3B	120.4
C3A—C4A—H4A	119.6	C3B—C4B—H4B	119.7
C3A—C4A—C5A	120.87 (13)	C3B—C4B—C5B	120.63 (13)
C5A—C4A—H4A	119.6	C5B—C4B—H4B	119.7
C4A—C5A—H5A	119.4	C4B—C5B—H5B	119.4
C6A—C5A—C4A	121.23 (13)	C6B—C5B—C4B	121.29 (13)
C6A—C5A—H5A	119.4	C6B—C5B—H5B	119.4
C5A—C6A—H6A	121.1	C5B—C6B—H6B	121.1
C5A—C6A—C7A	117.84 (13)	C5B—C6B—C7B	117.86 (13)
C7A—C6A—H6A	121.1	C7B—C6B—H6B	121.1
C2A—C7A—S1A	109.84 (10)	C2B—C7B—S1B	109.90 (10)
C6A—C7A—S1A	128.36 (11)	C6B—C7B—S1B	128.35 (10)
C6A—C7A—C2A	121.80 (12)	C6B—C7B—C2B	121.74 (12)
O1A—C8A—N2A	121.82 (13)	O1B—C8B—N2B	121.45 (12)
O1A—C8A—C9A	122.81 (13)	O1B—C8B—C9B	123.07 (13)
N2A—C8A—C9A	115.37 (12)	N2B—C8B—C9B	115.48 (12)
C8A—C9A—H9AA	109.5	C8B—C9B—H9BA	109.5
C8A—C9A—H9AB	109.5	C8B—C9B—H9BB	109.5
C8A—C9A—H9AC	109.5	C8B—C9B—H9BC	109.5
H9AA—C9A—H9AB	109.5	H9BA—C9B—H9BB	109.5
H9AA—C9A—H9AC	109.5	H9BA—C9B—H9BC	109.5
H9AB—C9A—H9AC	109.5	H9BB—C9B—H9BC	109.5

N1A—C2A—C3A—C4A	178.73 (15)	N1B—C2B—C3B—C4B	179.62 (15)
N1A—C2A—C7A—S1A	0.23 (17)	N1B—C2B—C7B—S1B	−1.33 (16)
N1A—C2A—C7A—C6A	−179.33 (14)	N1B—C2B—C7B—C6B	179.88 (14)
C1A—S1A—C7A—C2A	0.29 (11)	C1B—S1B—C7B—C2B	1.31 (11)
C1A—S1A—C7A—C6A	179.81 (15)	C1B—S1B—C7B—C6B	180.00 (15)
C1A—N1A—C2A—C3A	179.14 (15)	C1B—N1B—C2B—C3B	−178.89 (15)
C1A—N1A—C2A—C7A	−0.81 (19)	C1B—N1B—C2B—C7B	0.50 (18)
C1A—N2A—C8A—O1A	−3.1 (2)	C1B—N2B—C8B—O1B	−0.8 (2)
C1A—N2A—C8A—C9A	177.18 (14)	C1B—N2B—C8B—C9B	178.36 (13)
C2A—N1A—C1A—S1A	1.07 (16)	C2B—N1B—C1B—S1B	0.60 (16)
C2A—N1A—C1A—N2A	−179.72 (13)	C2B—N1B—C1B—N2B	−178.39 (13)
C2A—C3A—C4A—C5A	0.9 (3)	C2B—C3B—C4B—C5B	0.4 (3)
C3A—C2A—C7A—S1A	−179.73 (12)	C3B—C2B—C7B—S1B	178.10 (12)
C3A—C2A—C7A—C6A	0.7 (2)	C3B—C2B—C7B—C6B	−0.7 (2)

C3A—C4A—C5A—C6A	0.3 (3)	C3B—C4B—C5B—C6B	−0.7 (3)
C4A—C5A—C6A—C7A	−0.9 (3)	C4B—C5B—C6B—C7B	0.3 (2)
C5A—C6A—C7A—S1A	−179.09 (13)	C5B—C6B—C7B—S1B	−178.14 (13)
C5A—C6A—C7A—C2A	0.4 (2)	C5B—C6B—C7B—C2B	0.4 (2)
C7A—S1A—C1A—N1A	−0.82 (12)	C7B—S1B—C1B—N1B	−1.16 (12)
C7A—S1A—C1A—N2A	179.98 (13)	C7B—S1B—C1B—N2B	177.82 (12)
C7A—C2A—C3A—C4A	−1.3 (2)	C7B—C2B—C3B—C4B	0.2 (2)
C8A—N2A—C1A—S1A	2.6 (2)	C8B—N2B—C1B—S1B	7.6 (2)
C8A—N2A—C1A—N1A	−176.56 (14)	C8B—N2B—C1B—N1B	−173.46 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H2*A*···N1*B*	0.86	2.11	2.9700 (16)	176
N2*B*—H2*B*···N1*A*	0.86	2.14	2.9749 (16)	165