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Crystal structure of (*E*)-2-{[(6-methoxy-1,3-benzothiazol-2-yl)imino]methyl}phenol

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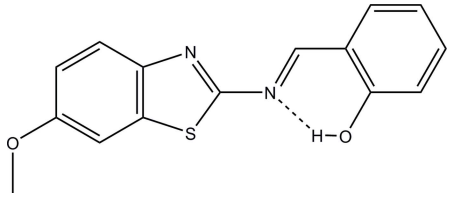
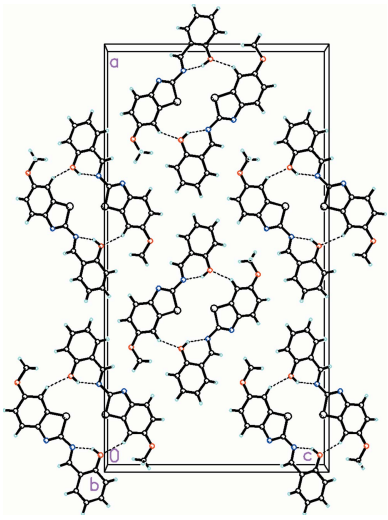
The title compound, $C_{15}H_{12}N_2O_2S$, crystallizes in the orthorhombic space group $Pna2_1$, with two molecules in the asymmetric unit ($Z' = 2$). Each molecule consists of a 2-hydroxy Schiff base moiety linked through a spacer to a 2-aminobenzothiazole moiety. Each molecule contains an intramolecular hydrogen bond between the –OH group and imine N atom, forming a six-membered ring. The two independent molecules are linked by a pair of C—H···O hydrogen bonds, forming dimers with an $R_2^2(20)$ ring motif. These dimers are further lined into sheets in the *ab* plane by weak intermolecular C—H···N interactions. The structure was refined as an inversion twin

1. Chemical context

A wide range of biological activities have been attributed to aminothiazoles and compounds having similar structures (Tahiliani *et al.*, 2003) and they have many applications in both human and veterinary medicine (Smith *et al.*, 1999; Sarhan *et al.*, 2010). Certain 2-aminobenzothiazole derivatives act on the central nervous system (Funderburk *et al.*, 1953), possess antimicrobial (Murhekar & Khadsan, 2010; Ravi *et al.*, 2014), antifungal (Catalano *et al.*, 2013) and antibacterial properties (Asiri *et al.*, 2013), serve as selective receptors for anion sensing (Hijji & Wairia, 2005), are active in corrosion inhibition (Quraishi *et al.*, 1997; Rawat & Quraishi, 2003) and act as plant-growth regulators (Mahajan *et al.*, 2013). In addition, some metal complexes of Schiff bases of 2-aminobenzothiazole derivatives have potent antibacterial properties (Sharma *et al.*, 2002; Song *et al.*, 2010). Among antitumor agents discovered in recent years, the identification of various 2-(4-aminophenyl)benzothiazoles as potent and selective antitumor drugs against breast, ovarian, colon and renal cell lines has stimulated remarkable interest (Usman *et al.*, 2003; Shi *et al.*, 1996; Havrylyuk *et al.* 2010) in this class of compound from both a synthetic, and particularly, a structural point of view. Aminothiazole Schiff bases have been prepared as intermediate ligands and for complexation with various metals (Liang *et al.*,1999; Liu *et al.*, 2009).



In this context, the synthesis and structural characterization of new 2-aminobenzothiazole Schiff base derivatives is of interest (El'tsov & Mokrushin, 2002).



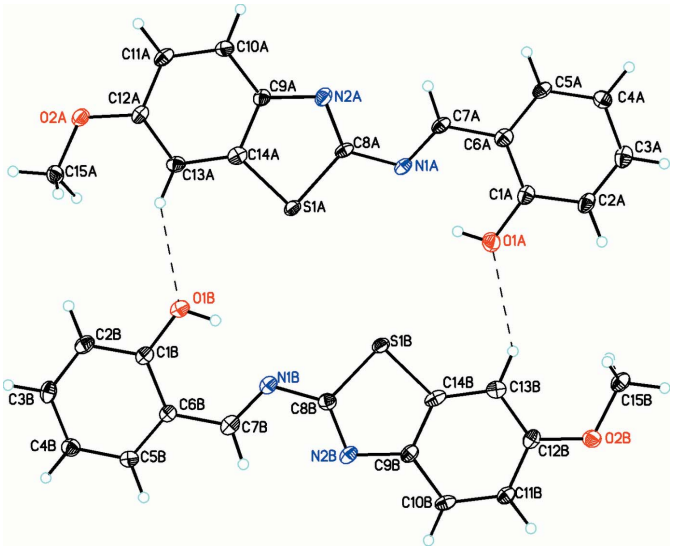


Figure 1
Molecular diagram for molecules *A* and *B* of the title compound, showing the atom labeling. Displacement parameters are drawn at the 30% probability level. The diagram shows the two molecules (*A* and *B*) linked into dimers by $R_2^2(20)$ C—H···O hydrogen bonds (dashed lines; see Table 1 for details).

2. Structural commentary

The title compound, $C_{15}H_{12}N_2O_2S$, crystallizes in the orthorhombic space group, $Pna2_1$, with two molecules (*A* and *B*) in the asymmetric unit (Z' = 2). Each molecule consists of a 2-hydroxy Schiff base moiety linked through a spacer to a 2-aminobenzothiazole moiety. This spacer is both planar [r.m.s. deviations of fitted atoms of 0.004 (3) and 0.007 (3) Å, respectively for molecules *A* and *B*] and very close to coplanar with both the Schiff base and 2-aminobenzothiazole end moieties [making dihedral angles of 2.6 (9) and 4.0 (3)°, respectively, in molecule *A* and 3.3 (8) and 3.9 (7)° in molecule *B*]. The molecules themselves are very close to planar, as is shown by the dihedral angles of 4.0 (3) and 6.3 (2) between the two end groups for molecules *A* and *B*, respectively. Each molecule contains an intramolecular hydrogen bond between the OH group and imine N atom, forming a six-membered ring.

3. Supramolecular features

In addition to the intramolecular hydrogen bond mentioned above, the molecules are linked by a pair of C—H···O hydrogen bonds (Table 1), forming dimers with an $R_2^2(20)$ ring motif, as shown in Fig. 1. These dimers are further linked into sheets in the *ab* plane by weak intermolecular C—H···N interactions involving C15 and N2*B*, as shown in Fig. 2.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.35, last update November 2014; Groom & Allen, 2014) for related Schiff base derivatives of 2-aminobenzothiazole gave 23 hits of which the closest example to the title compound was (*E*)-2-[(6-ethoxybenzothiazol-2-yl)iminomethyl]-6-methoxyphenol (Kong, 2009).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···N1*A*	0.84	1.93	2.647 (9)	143
C13*A*—H13*A*···O1*B*	0.95	2.48	3.289 (9)	144
C15*A*—H15*A*···N2*B*^{i}	0.98	2.57	3.525 (10)	166
O1*B*—H1*B*···N1*B*	0.84	1.89	2.636 (9)	147
C13*B*—H13*B*···O1*A*	0.95	2.53	3.356 (10)	145

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{3}{2}, z-\frac{1}{2}$.

5. Synthesis and crystallization

A mixture of 0.505 g (4.10 mmol) salicylaldehyde and 0.746 g (4.10 mmol) 2-amino-6-methoxybenzothiozole was dissolved in 2 ml of acetonitrile in a vial. The mixture was reacted in a Biotage initiator eight mono mode microwave at 423 K for 2 min and then allowed to cool for 15 min. The resulting product was recrystallized from acetonitrile, filtered and then

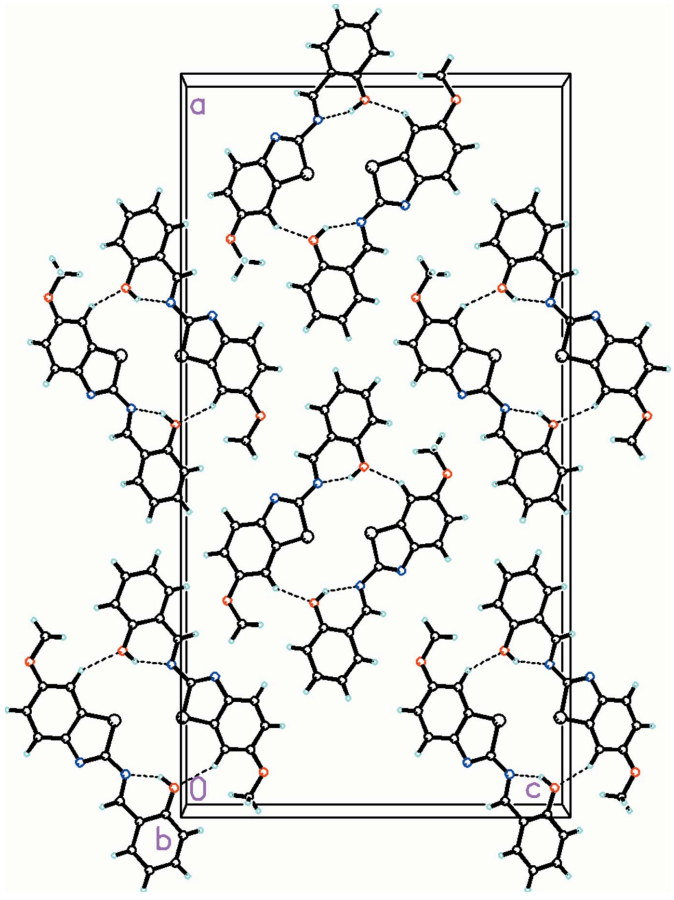


Figure 2
Packing diagram, viewed along the *b* axis, showing a sheet of $R_2^2(20)$ C—H···O-linked dimers in the *ac* plane.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{12}N_2O_2S$
M_r	284.33
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	120
a, b, c (Å)	35.623 (2), 3.8172 (2), 18.6525 (8)
V (Å^3)	2536.4 (2)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.30
Crystal size (mm)	0.38 × 0.09 × 0.06
Data collection	
Diffractometer	Agilent SuperNova (Dual, Cu at zero, Atlas)
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.573, 0.863
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6990, 3895, 3677
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.073, 0.189, 1.09
No. of reflections	3895
No. of parameters	364
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.01, −0.74
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.65 (5)

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SUPERFLIP* (Palatinus *et al.*, 2007), *SHELXL2013* (Sheldrick, 2015) and *SHELXTL* (Sheldrick, 2008).

vacuum dried to afford 0.971 g (86% yield) of a yellow crystalline solid (m.p. 399–403 K). A sample was dissolved in ethanol and allowed to crystallize by slow evaporation to give yellow needles used for X-ray structural determination.

^{1}H NMR (300 MHz, $CDCl_3$): δ 12.07 (*s*, 1H), 9.36 (*s*, 1H), 8.81 (*dd*, J = 9.0, 2.5 Hz, 1H), 8.39 (*d*, J = 7.5 Hz, 1H), 8.05 (*d*, J = 9.0 Hz. 1H), 7.55 (*m*, 2H), 7.09 (*d*, 7.5 Hz, 1H), 7.04 (*t*, J = 7.5 Hz, 1H), 3.83 (*s*, 3H)

^{13}C NMR (300 MHz, $CDCl_3$, p.p.m.): δ 55.07, 105.07, 115.46, 118.4, 121.2, 122.88, 125.26, 130.4, 132.44, 135.07, 145.59, 157.8 162.69, 165.36, 169.49

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were positioned geometrically and refined as riding: C–H = 0.93–0.99 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and = 1.2U_{eq}(C) for other H atoms. Phenol H atoms were located in a difference Fourier map and then refined as riding on their attached O atoms.

Acknowledgements

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Acta Cryst. (2015). E**71**, 385-387 [doi:10.1107/S2056989015005228]

Crystal structure of (*E*)-2-{[(6-methoxy-1,3-benzothiazol-2-yl)imino]methyl}-phenol

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Computing details

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

(*E*)-2-{[(6-Methoxy-1,3-benzothiazol-2-yl)imino]methyl}phenol

Crystal data

$C_{15}H_{12}N_2O_2S$
$M_r = 284.33$
Orthorhombic, $Pna2_1$
$a = 35.623$ (2) Å
$b = 3.8172$ (2) Å
$c = 18.6525$ (8) Å
$V = 2536.4$ (2) Å^3
$Z = 8$
$F(000) = 1184$
$D_x = 1.489$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 2917 reflections
$\theta = 4.7$–$76.1°$
$\mu = 2.30$ mm^{-1}
$T = 120$ K
Needle, yellow–orange
0.38 × 0.09 × 0.06 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
Radiation source: sealed X-ray tube
Detector resolution: 5.3250 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2012)
$T_{min} = 0.573$, $T_{max} = 0.863$
6990 measured reflections
3895 independent reflections
3677 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 76.2°$, $\theta_{min} = 3.4°$
$h = -41 \rightarrow 44$
$k = -2 \rightarrow 4$
$l = -20 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.189$
$S = 1.09$
3895 reflections
364 parameters
1 restraint
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0845P)^2 + 6.6687P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.01$ e Å^{-3}
$\Delta\rho_{min} = -0.74$ e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.65 (5)

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. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.87402 (5)	0.3471 (4)	0.32176 (9)	0.0241 (4)
O1A	0.97069 (15)	0.6508 (16)	0.4723 (3)	0.0337 (13)
H1A	0.9559	0.6313	0.4376	0.050*
O2A	0.78912 (15)	−0.1334 (15)	0.1150 (3)	0.0283 (12)
N1A	0.94790 (18)	0.3743 (16)	0.3497 (4)	0.0250 (13)
N2A	0.92781 (17)	0.1374 (18)	0.2372 (4)	0.0283 (13)
C1A	1.0055 (2)	0.5657 (19)	0.4512 (4)	0.0261 (15)
C2A	1.0359 (2)	0.648 (2)	0.4958 (4)	0.0306 (16)
H1	1.0314	0.7620	0.5402	0.037*
C3A	1.0718 (2)	0.568 (2)	0.4768 (4)	0.0318 (17)
H2	1.0919	0.6241	0.5082	0.038*
C4A	1.0793 (2)	0.403 (2)	0.4114 (5)	0.0274 (15)
H3	1.1045	0.3592	0.3970	0.033*
C5A	1.0495 (2)	0.303 (2)	0.3674 (4)	0.0274 (16)
H4	1.0542	0.1730	0.3249	0.033*
C6A	1.0126 (2)	0.394 (2)	0.3862 (4)	0.0274 (16)
C7A	0.9824 (2)	0.2951 (18)	0.3370 (4)	0.0238 (15)
H5	0.9884	0.1694	0.2946	0.029*
C8A	0.9213 (2)	0.2730 (17)	0.2996 (4)	0.0225 (14)
C9A	0.89431 (19)	0.0635 (19)	0.2017 (4)	0.0237 (14)
C10A	0.8905 (2)	−0.087 (2)	0.1348 (4)	0.0265 (15)
H10A	0.9120	−0.1510	0.1078	0.032*
C11A	0.8548 (2)	−0.1449 (19)	0.1075 (4)	0.0264 (16)
H11A	0.8521	−0.2508	0.0617	0.032*
C12A	0.8227 (2)	−0.0498 (17)	0.1462 (4)	0.0212 (14)
C13A	0.8255 (2)	0.1077 (19)	0.2129 (4)	0.0254 (15)
H13A	0.8037	0.1706	0.2392	0.031*
C14A	0.8617 (2)	0.1715 (18)	0.2403 (4)	0.0240 (14)
C15A	0.75623 (19)	−0.027 (2)	0.1521 (5)	0.0289 (16)
H15A	0.7340	−0.1033	0.1254	0.043*
H15B	0.7560	0.2289	0.1566	0.043*
H15C	0.7560	−0.1328	0.2000	0.043*
S1B	0.87656 (5)	0.8509 (4)	0.49182 (9)	0.0246 (4)
O1B	0.78077 (16)	0.5412 (16)	0.3390 (3)	0.0361 (14)
H1B	0.7960	0.6119	0.3701	0.054*
O2B	0.95964 (15)	1.3166 (15)	0.7026 (3)	0.0293 (12)
N1B	0.80272 (18)	0.8089 (15)	0.4624 (4)	0.0247 (13)
N2B	0.82255 (17)	1.0626 (16)	0.5746 (4)	0.0263 (13)

C1B	0.7453 (2)	0.5753 (18)	0.3644 (4)	0.0248 (15)
C2B	0.7160 (2)	0.4583 (19)	0.3210 (5)	0.0291 (15)
H6	0.7209	0.3632	0.2749	0.035*
C3B	0.6790 (2)	0.484 (2)	0.3472 (4)	0.0299 (17)
H7	0.6587	0.4020	0.3187	0.036*
C4B	0.6717 (2)	0.628 (2)	0.4136 (4)	0.0287 (16)
H8	0.6466	0.6431	0.4301	0.034*
C5B	0.7005 (2)	0.7494 (18)	0.4564 (4)	0.0243 (15)
H9	0.6950	0.8494	0.5019	0.029*
C6B	0.7381 (2)	0.7258 (16)	0.4329 (4)	0.0204 (14)
C7B	0.7681 (2)	0.8352 (17)	0.4793 (4)	0.0245 (15)
H10	0.7618	0.9319	0.5247	0.029*
C8B	0.8289 (2)	0.9165 (19)	0.5123 (4)	0.0252 (15)
C9B	0.8560 (2)	1.1290 (19)	0.6098 (4)	0.0253 (15)
C10B	0.8589 (2)	1.2798 (19)	0.6777 (4)	0.0262 (16)
H10B	0.8370	1.3415	0.7040	0.031*
C11B	0.8943 (2)	1.3379 (19)	0.7062 (5)	0.0261 (15)
H11B	0.8967	1.4428	0.7522	0.031*
C12B	0.9269 (2)	1.2432 (18)	0.6678 (5)	0.0252 (16)
C13B	0.9242 (2)	1.0870 (17)	0.6009 (4)	0.0246 (14)
H13B	0.9460	1.0207	0.5748	0.029*
C14B	0.8884 (2)	1.0313 (17)	0.5736 (4)	0.0234 (14)
C15B	0.9936 (2)	1.235 (2)	0.6643 (5)	0.0288 (16)
H15D	1.0149	1.3469	0.6882	0.043*
H15E	0.9916	1.3226	0.6150	0.043*
H15F	0.9972	0.9808	0.6635	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0280 (8)	0.0261 (8)	0.0182 (9)	−0.0016 (6)	−0.0003 (7)	−0.0049 (7)
O1A	0.029 (3)	0.044 (3)	0.028 (3)	−0.005 (2)	0.000 (2)	0.001 (3)
O2A	0.031 (3)	0.031 (3)	0.023 (3)	−0.003 (2)	−0.002 (2)	−0.004 (2)
N1A	0.032 (3)	0.021 (3)	0.022 (3)	−0.002 (2)	−0.002 (3)	−0.006 (2)
N2A	0.032 (3)	0.033 (3)	0.020 (3)	−0.007 (2)	−0.003 (3)	0.001 (3)
C1A	0.033 (4)	0.025 (3)	0.020 (4)	−0.006 (3)	−0.003 (3)	0.006 (3)
C2A	0.040 (4)	0.034 (4)	0.018 (4)	−0.015 (3)	−0.002 (3)	0.002 (3)
C3A	0.039 (4)	0.033 (4)	0.024 (4)	−0.007 (3)	−0.008 (3)	0.009 (3)
C4A	0.027 (3)	0.026 (3)	0.030 (4)	0.004 (3)	0.001 (3)	0.002 (3)
C5A	0.038 (4)	0.030 (4)	0.014 (4)	−0.001 (3)	−0.001 (3)	0.000 (3)
C6A	0.034 (4)	0.025 (3)	0.023 (4)	−0.002 (3)	0.000 (3)	0.004 (3)
C7A	0.037 (4)	0.022 (3)	0.012 (3)	−0.003 (3)	0.000 (3)	0.003 (3)
C8A	0.034 (4)	0.017 (3)	0.017 (4)	0.000 (2)	0.002 (3)	−0.004 (2)
C9A	0.028 (3)	0.027 (3)	0.016 (3)	−0.004 (3)	0.001 (3)	0.007 (3)
C10A	0.030 (3)	0.028 (4)	0.022 (4)	0.003 (3)	0.003 (3)	−0.002 (3)
C11A	0.041 (4)	0.021 (3)	0.016 (4)	−0.008 (3)	0.000 (3)	0.003 (3)
C12A	0.032 (3)	0.014 (3)	0.018 (3)	−0.004 (2)	−0.003 (3)	0.004 (3)
C13A	0.030 (3)	0.027 (4)	0.019 (3)	0.002 (3)	0.004 (3)	0.004 (3)

C14A	0.033 (3)	0.016 (3)	0.023 (4)	−0.005 (3)	0.003 (3)	0.005 (3)
C15A	0.025 (3)	0.029 (3)	0.033 (4)	−0.003 (3)	−0.002 (3)	−0.005 (3)
S1B	0.0291 (9)	0.0271 (8)	0.0177 (9)	0.0008 (6)	−0.0003 (6)	−0.0047 (7)
O1B	0.033 (3)	0.046 (3)	0.029 (3)	−0.001 (2)	0.002 (2)	−0.013 (3)
O2B	0.029 (3)	0.036 (3)	0.022 (3)	0.004 (2)	−0.001 (2)	−0.001 (2)
N1B	0.032 (3)	0.020 (3)	0.022 (3)	0.002 (2)	−0.004 (3)	0.002 (2)
N2B	0.034 (3)	0.020 (3)	0.024 (3)	−0.002 (2)	−0.004 (3)	−0.003 (3)
C1B	0.033 (4)	0.018 (3)	0.023 (4)	0.001 (3)	−0.003 (3)	0.002 (3)
C2B	0.040 (4)	0.029 (3)	0.018 (4)	0.000 (3)	0.000 (3)	0.003 (3)
C3B	0.036 (4)	0.028 (4)	0.026 (4)	−0.002 (3)	−0.010 (3)	0.009 (3)
C4B	0.030 (4)	0.030 (4)	0.026 (4)	0.000 (3)	0.003 (3)	0.002 (3)
C5B	0.031 (4)	0.020 (3)	0.022 (4)	0.001 (3)	0.003 (3)	0.003 (3)
C6B	0.029 (3)	0.012 (3)	0.021 (4)	0.001 (2)	−0.002 (3)	0.004 (3)
C7B	0.040 (4)	0.014 (3)	0.019 (4)	−0.003 (2)	−0.003 (3)	0.009 (3)
C8B	0.028 (4)	0.022 (3)	0.025 (4)	0.002 (3)	0.001 (3)	0.000 (3)
C9B	0.033 (3)	0.019 (3)	0.024 (4)	−0.004 (2)	−0.001 (3)	−0.001 (3)
C10B	0.040 (4)	0.017 (3)	0.021 (4)	0.001 (3)	0.005 (3)	−0.002 (3)
C11B	0.033 (4)	0.021 (3)	0.024 (4)	−0.002 (3)	0.000 (3)	−0.002 (3)
C12B	0.033 (4)	0.014 (3)	0.028 (4)	−0.004 (2)	−0.003 (3)	0.002 (3)
C13B	0.033 (3)	0.018 (3)	0.023 (4)	0.002 (3)	0.003 (3)	0.006 (3)
C14B	0.045 (4)	0.014 (3)	0.011 (3)	0.000 (3)	0.003 (3)	0.006 (2)
C15B	0.040 (4)	0.025 (3)	0.021 (4)	−0.002 (3)	−0.004 (3)	0.001 (3)

Geometric parameters (Å, º)

S1A—C14A	1.718 (8)	S1B—C14B	1.726 (8)
S1A—C8A	1.759 (8)	S1B—C8B	1.758 (8)
O1A—C1A	1.341 (10)	O1B—C1B	1.356 (9)
O1A—H1A	0.8399	O1B—H1B	0.8400
O2A—C12A	1.369 (9)	O2B—C12B	1.364 (9)
O2A—C15A	1.421 (9)	O2B—C15B	1.438 (10)
N1A—C7A	1.288 (10)	N1B—C7B	1.278 (10)
N1A—C8A	1.385 (10)	N1B—C8B	1.380 (10)
N2A—C8A	1.295 (10)	N2B—C8B	1.309 (10)
N2A—C9A	1.393 (9)	N2B—C9B	1.383 (9)
C1A—C6A	1.402 (11)	C1B—C2B	1.395 (11)
C1A—C2A	1.402 (11)	C1B—C6B	1.424 (10)
C2A—C3A	1.362 (12)	C2B—C3B	1.409 (11)
C2A—H1	0.9500	C2B—H6	0.9500
C3A—C4A	1.398 (12)	C3B—C4B	1.378 (12)
C3A—H2	0.9500	C3B—H7	0.9500
C4A—C5A	1.395 (11)	C4B—C5B	1.381 (11)
C4A—H3	0.9500	C4B—H8	0.9500
C5A—C6A	1.405 (12)	C5B—C6B	1.412 (10)
C5A—H4	0.9500	C5B—H9	0.9500
C6A—C7A	1.463 (11)	C6B—C7B	1.435 (10)
C7A—H5	0.9500	C7B—H10	0.9500
C9A—C10A	1.382 (11)	C9B—C14B	1.388 (11)

C9A—C14A	1.428 (10)	C9B—C10B	1.396 (11)
C10A—C11A	1.385 (11)	C10B—C11B	1.388 (12)
C10A—H10A	0.9500	C10B—H10B	0.9500
C11A—C12A	1.401 (11)	C11B—C12B	1.410 (11)
C11A—H11A	0.9500	C11B—H11B	0.9500
C12A—C13A	1.385 (11)	C12B—C13B	1.387 (11)
C13A—C14A	1.407 (10)	C13B—C14B	1.391 (11)
C13A—H13A	0.9500	C13B—H13B	0.9500
C15A—H15A	0.9800	C15B—H15D	0.9800
C15A—H15B	0.9800	C15B—H15E	0.9800
C15A—H15C	0.9800	C15B—H15F	0.9800
C14A—S1A—C8A	88.5 (4)	C14B—S1B—C8B	89.2 (4)
C1A—O1A—H1A	109.5	C1B—O1B—H1B	109.3
C12A—O2A—C15A	116.6 (6)	C12B—O2B—C15B	116.0 (6)
C7A—N1A—C8A	117.5 (6)	C7B—N1B—C8B	117.6 (7)
C8A—N2A—C9A	110.8 (6)	C8B—N2B—C9B	110.5 (6)
O1A—C1A—C6A	122.3 (7)	O1B—C1B—C2B	117.6 (7)
O1A—C1A—C2A	119.1 (7)	O1B—C1B—C6B	121.3 (6)
C6A—C1A—C2A	118.6 (7)	C2B—C1B—C6B	121.1 (7)
C3A—C2A—C1A	121.4 (8)	C1B—C2B—C3B	118.4 (8)
C3A—C2A—H1	119.3	C1B—C2B—H6	120.8
C1A—C2A—H1	119.3	C3B—C2B—H6	120.8
C2A—C3A—C4A	120.5 (7)	C4B—C3B—C2B	121.0 (7)
C2A—C3A—H2	119.8	C4B—C3B—H7	119.5
C4A—C3A—H2	119.8	C2B—C3B—H7	119.5
C5A—C4A—C3A	119.4 (7)	C3B—C4B—C5B	120.9 (7)
C5A—C4A—H3	120.3	C3B—C4B—H8	119.5
C3A—C4A—H3	120.3	C5B—C4B—H8	119.5
C4A—C5A—C6A	119.9 (7)	C4B—C5B—C6B	120.2 (7)
C4A—C5A—H4	120.1	C4B—C5B—H9	119.9
C6A—C5A—H4	120.1	C6B—C5B—H9	119.9
C1A—C6A—C5A	120.0 (7)	C5B—C6B—C1B	118.3 (7)
C1A—C6A—C7A	122.1 (7)	C5B—C6B—C7B	120.0 (7)
C5A—C6A—C7A	117.9 (7)	C1B—C6B—C7B	121.6 (7)
N1A—C7A—C6A	121.7 (7)	N1B—C7B—C6B	123.1 (7)
N1A—C7A—H5	119.2	N1B—C7B—H10	118.4
C6A—C7A—H5	119.2	C6B—C7B—H10	118.4
N2A—C8A—N1A	126.7 (7)	N2B—C8B—N1B	127.5 (7)
N2A—C8A—S1A	116.5 (6)	N2B—C8B—S1B	114.9 (6)
N1A—C8A—S1A	116.8 (5)	N1B—C8B—S1B	117.6 (6)
C10A—C9A—N2A	126.7 (7)	N2B—C9B—C14B	115.8 (7)
C10A—C9A—C14A	119.7 (7)	N2B—C9B—C10B	124.8 (7)
N2A—C9A—C14A	113.6 (7)	C14B—C9B—C10B	119.3 (7)
C9A—C10A—C11A	119.2 (7)	C11B—C10B—C9B	118.8 (8)
C9A—C10A—H10A	120.4	C11B—C10B—H10B	120.6
C11A—C10A—H10A	120.4	C9B—C10B—H10B	120.6
C10A—C11A—C12A	121.2 (8)	C10B—C11B—C12B	120.8 (8)

C10A—C11A—H11A	119.4	C10B—C11B—H11B	119.6
C12A—C11A—H11A	119.4	C12B—C11B—H11B	119.6
O2A—C12A—C13A	123.1 (7)	O2B—C12B—C13B	125.1 (7)
O2A—C12A—C11A	115.8 (7)	O2B—C12B—C11B	114.2 (7)
C13A—C12A—C11A	121.1 (7)	C13B—C12B—C11B	120.7 (7)
C12A—C13A—C14A	117.8 (7)	C12B—C13B—C14B	117.3 (7)
C12A—C13A—H13A	121.1	C12B—C13B—H13B	121.4
C14A—C13A—H13A	121.1	C14B—C13B—H13B	121.4
C13A—C14A—C9A	120.8 (7)	C9B—C14B—C13B	123.0 (7)
C13A—C14A—S1A	128.5 (6)	C9B—C14B—S1B	109.6 (6)
C9A—C14A—S1A	110.5 (6)	C13B—C14B—S1B	127.4 (6)
O2A—C15A—H15A	109.5	O2B—C15B—H15D	109.5
O2A—C15A—H15B	109.5	O2B—C15B—H15E	109.5
H15A—C15A—H15B	109.5	H15D—C15B—H15E	109.5
O2A—C15A—H15C	109.5	O2B—C15B—H15F	109.5
H15A—C15A—H15C	109.5	H15D—C15B—H15F	109.5
H15B—C15A—H15C	109.5	H15E—C15B—H15F	109.5

O1A—C1A—C2A—C3A	−179.9 (7)	O1B—C1B—C2B—C3B	178.6 (6)
C6A—C1A—C2A—C3A	0.7 (11)	C6B—C1B—C2B—C3B	−1.5 (11)
C1A—C2A—C3A—C4A	0.6 (12)	C1B—C2B—C3B—C4B	1.1 (11)
C2A—C3A—C4A—C5A	−3.6 (12)	C2B—C3B—C4B—C5B	−0.1 (12)
C3A—C4A—C5A—C6A	5.3 (12)	C3B—C4B—C5B—C6B	−0.6 (11)
O1A—C1A—C6A—C5A	−178.4 (7)	C4B—C5B—C6B—C1B	0.2 (10)
C2A—C1A—C6A—C5A	1.0 (11)	C4B—C5B—C6B—C7B	−176.6 (6)
O1A—C1A—C6A—C7A	−0.1 (11)	O1B—C1B—C6B—C5B	−179.3 (6)
C2A—C1A—C6A—C7A	179.3 (7)	C2B—C1B—C6B—C5B	0.9 (10)
C4A—C5A—C6A—C1A	−4.0 (11)	O1B—C1B—C6B—C7B	−2.5 (10)
C4A—C5A—C6A—C7A	177.6 (7)	C2B—C1B—C6B—C7B	177.6 (6)
C8A—N1A—C7A—C6A	179.3 (6)	C8B—N1B—C7B—C6B	−178.6 (6)
C1A—C6A—C7A—N1A	2.9 (11)	C5B—C6B—C7B—N1B	177.4 (6)
C5A—C6A—C7A—N1A	−178.8 (7)	C1B—C6B—C7B—N1B	0.7 (10)
C9A—N2A—C8A—N1A	179.1 (7)	C9B—N2B—C8B—N1B	179.2 (7)
C9A—N2A—C8A—S1A	−2.8 (8)	C9B—N2B—C8B—S1B	−0.3 (8)
C7A—N1A—C8A—N2A	−7.7 (11)	C7B—N1B—C8B—N2B	−4.1 (11)
C7A—N1A—C8A—S1A	174.3 (5)	C7B—N1B—C8B—S1B	175.5 (5)
C14A—S1A—C8A—N2A	1.2 (6)	C14B—S1B—C8B—N2B	0.4 (6)
C14A—S1A—C8A—N1A	179.5 (6)	C14B—S1B—C8B—N1B	−179.2 (6)
C8A—N2A—C9A—C10A	−178.8 (7)	C8B—N2B—C9B—C14B	0.0 (9)
C8A—N2A—C9A—C14A	3.3 (9)	C8B—N2B—C9B—C10B	−179.3 (7)
N2A—C9A—C10A—C11A	179.6 (7)	N2B—C9B—C10B—C11B	−178.8 (7)
C14A—C9A—C10A—C11A	−2.7 (11)	C14B—C9B—C10B—C11B	2.0 (11)
C9A—C10A—C11A—C12A	0.6 (11)	C9B—C10B—C11B—C12B	−0.7 (11)
C15A—O2A—C12A—C13A	4.5 (10)	C15B—O2B—C12B—C13B	2.6 (10)
C15A—O2A—C12A—C11A	−177.6 (6)	C15B—O2B—C12B—C11B	−178.0 (6)
C10A—C11A—C12A—O2A	−177.3 (6)	C10B—C11B—C12B—O2B	179.9 (7)
C10A—C11A—C12A—C13A	0.5 (11)	C10B—C11B—C12B—C13B	−0.6 (11)
O2A—C12A—C13A—C14A	178.2 (6)	O2B—C12B—C13B—C14B	179.9 (6)

C11A—C12A—C13A—C14A	0.5 (10)	C11B—C12B—C13B—C14B	0.5 (10)
C12A—C13A—C14A—C9A	−2.6 (10)	N2B—C9B—C14B—C13B	178.5 (6)
C12A—C13A—C14A—S1A	−177.6 (6)	C10B—C9B—C14B—C13B	−2.2 (11)
C10A—C9A—C14A—C13A	3.8 (10)	N2B—C9B—C14B—S1B	0.3 (8)
N2A—C9A—C14A—C13A	−178.3 (6)	C10B—C9B—C14B—S1B	179.6 (6)
C10A—C9A—C14A—S1A	179.6 (6)	C12B—C13B—C14B—C9B	0.9 (10)
N2A—C9A—C14A—S1A	−2.4 (8)	C12B—C13B—C14B—S1B	178.8 (5)
C8A—S1A—C14A—C13A	176.1 (7)	C8B—S1B—C14B—C9B	−0.4 (5)
C8A—S1A—C14A—C9A	0.7 (5)	C8B—S1B—C14B—C13B	−178.5 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···N1*A*	0.84	1.93	2.647 (9)	143
C13*A*—H13*A*···O1*B*	0.95	2.48	3.289 (9)	144
C15*A*—H15*A*···N2*B*^{i}	0.98	2.57	3.525 (10)	166
O1*B*—H1*B*···N1*B*	0.84	1.89	2.636 (9)	147
C13*B*—H13*B*···O1*A*	0.95	2.53	3.356 (10)	145

Symmetry code: (i) −*x*+3/2, *y*−3/2, *z*−1/2.