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Crystal structure of (*E*)-*N*-cyclohexyl-2-(2-hydroxy-3-methylbenzylidene)hydrazine-1-carbothioamide

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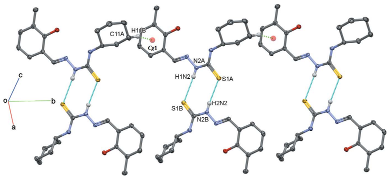
The asymmetric unit of the title compound, $C_{15}H_{21}N_3OS$, comprises of two crystallographically independent molecules (*A* and *B*). Each molecule consists of a cyclohexane ring and a 2-hydroxy-3-methylbenzylidene ring bridged by a hydrazinecarbothioamine unit. Both molecules exhibit an *E* configuration with respect to the azomethine C═N bond. There is an intramolecular O—H⋯N hydrogen bond in each molecule forming an *S*(6) ring motif. The cyclohexane ring in each molecule has a chair conformation. The benzene ring is inclined to the mean plane of the cyclohexane ring by 47.75 (9)° in molecule *A* and 66.99 (9)° in molecule *B*. The mean plane of the cyclohexane ring is inclined to the mean plane of the thiourea moiety [N—C(═S)—N] by 55.69 (9) and 58.50 (8)° in molecules *A* and *B*, respectively. In the crystal, the *A* and *B* molecules are linked by N—H⋯S hydrogen bonds, forming 'dimers'. The *A* molecules are further linked by a C—H⋯π interaction, hence linking the *A*–*B* units to form ribbons propagating along the *b*-axis direction. The conformation of a number of related cyclohexanehydrazinecarbothioamides are compared to that of the title compound.



1. Chemical context

Schiff bases are significant agents in both organic and inorganic chemistry, and are widely used in biological applications, particularly for anticancer screening (Ziessel, 2001; Salam *et al.*, 2012*a*; Arafath *et al.*, 2017*b*). They have attracted a great deal of attention because of the presence of hard and soft atoms together in one molecule. Thiosemicarbazone Schiff base compounds have soft sulfur and hard nitrogen as well hard oxygen atoms (Mohamed *et al.*, 2009). These Schiff base compounds are of special interest because of their diversity in coordinating to hard and soft metals using the hard and soft coordinating sites such as NSO (Arion *et al.*, 2001; Leovac & Češljević, 2002; Chandra & Sangeetika, 2004; Singh *et al.*, 2000; Gerbeleu *et al.*, 2008; Mohamed *et al.*, 2009). Many Schiff base compounds and their complexes with transition metals have wide biological and pharmaceutical applications (Padhyé & Kauffman, 1985; Salam *et al.*, 2012*b*). Thiosemicarbazones having ONS-coordinating sites are important for coordination chemistry because of their strong bonding ability with transition metals (Rayati *et al.*, 2007; Alomar *et al.*, 2009; Vieites *et al.*, 2009; Siddiki *et al.*, 2012).

2. Structural commentary

The asymmetric unit of the title compound consists of two crystallographic independent molecules (*A* and *B*), as

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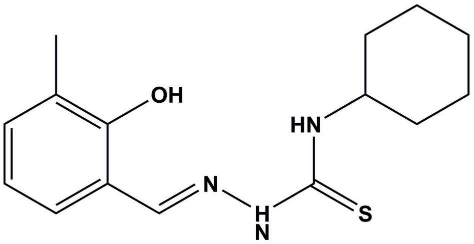
Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of benzene ring C1*A*–C6*A*.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1*A*—H1*O*1⋯N1*A*	0.80 (2)	1.98 (2)	2.6844 (19)	146 (2)
O1*B*—H1*O*2⋯N1*B*	0.84 (2)	1.91 (2)	2.664 (2)	148 (2)
N2*A*—H1*N*2⋯S1*B*^{i}	0.85 (2)	2.60 (2)	3.4414 (16)	170 (2)
N2*B*—H2*N*2⋯S1*A*^{i}	0.85 (2)	2.53 (2)	3.3568 (15)	164 (2)
C11*A*—H11*B*⋯*Cg*1^{ii}	0.99	2.93	3.801 (2)	148

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $x, y+1, z$.

illustrated in Fig. 1. In each molecule a cyclohexane ring and a 2-hydroxy-3-methylbenzylidene ring are interconnected by a hydrazinecarbothioamine bridge. Both molecules exhibit an *E* configuration with respect to the azomethine C7═N1 bond, and in each molecule there is an intramolecular O—H⋯N hydrogen bond forming an *S*(6) ring motif (Table 1and Fig. 1). The best AutoMolFit (*PLATON*; Spek, 2009) image of the two molecules, *viz*. inverted molecule *B* (red) on molecule *A* (black), which has an r.m.s. deviation of 0.654 Å, is shown in Fig. 2.



The cyclohexane ring (C9–C14) in each molecule has a chair conformation. The mean plane of the four central C atoms (C10/C11/C13/C14) is inclined to the mean plane of the thiourea moiety [N2—C8(═S1)—N3] by 54.83 (11) and 55.64 (10)° in molecules *A* and *B*, respectively, and by 50.33 (10) and 65.30 (10)° to the benzene rings (C1–C6) in molecules *A* and *B*, respectively. The benzene ring is inclined to the mean plane of the thiourea moiety by 10.95 (8)° in molecule *A* and 9.80 (8)° in molecule *B*.

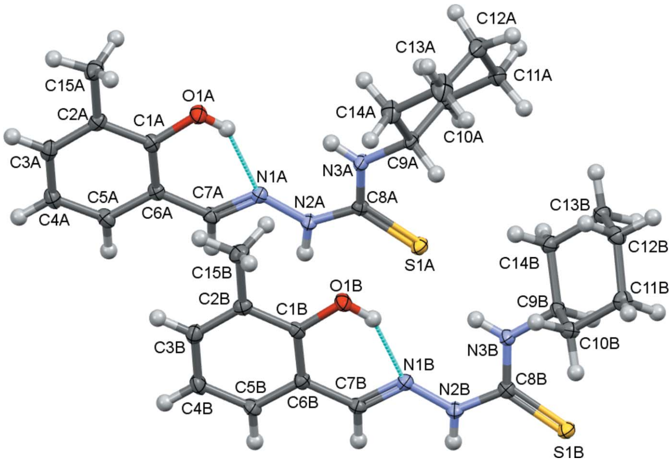


Figure 1
A view of the molecular structure of the two independent molecules (*A* and *B*) of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular O—H⋯N hydrogen bonds (Table 1) are shown as dashed cyan lines.

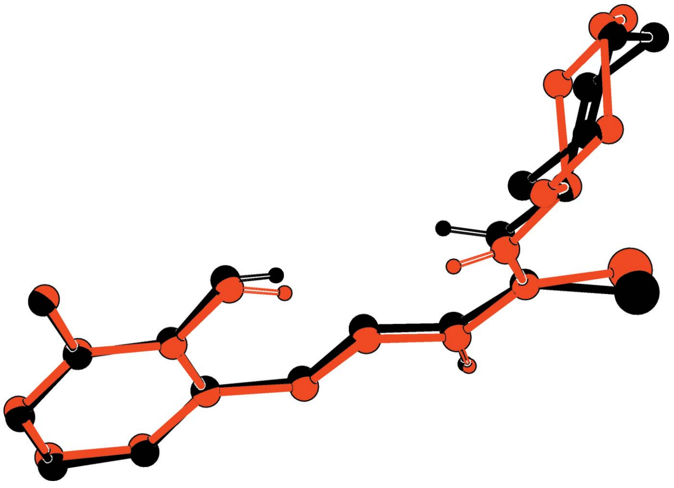


Figure 2
An AutoMolFit figure (*PLATON*; Spek, 2009) of inverted molecule *B* (red) on molecule *A* (black).

The unique molecular conformations of the two molecules can be characterized by five torsion angles, *i.e.* τ_1 (C1—C6—C7—N1), τ_2 (C7—N1—N2—C8), τ_3 (N1—N2—C8—N3), τ_4 (N2—C8—N3—C9) and τ_5 (C8—N3—C9—C10), as illustrated in Fig. 3. The torsion angle τ_1 between the benzylidine ring and the azomethine double bond for both molecules are approximately 0° [3.0 (2)° in molecule *A* and 1.9 (2)° in molecule *B*], signifying the coplanarity between benzylidine ring and the azomethine double bond (C7═N1). In molecule *B*, the azomethine double bond is close to planar with the hydrazine moiety [τ_2 = 177.23 (14)°], whereas τ_2 in molecule *A* is slightly twisted [τ_2 = 171.68 (14)°]. In both molecules, the torsion angle between the hydrazine moiety and the carbothio group are also slight twisted with τ_3 values in molecules *A* and *B* of 7.4 (2) and −10.2 (2)°, respectively. Similarly to τ_1, the carbothio group is almost coplanar with the thioamide group

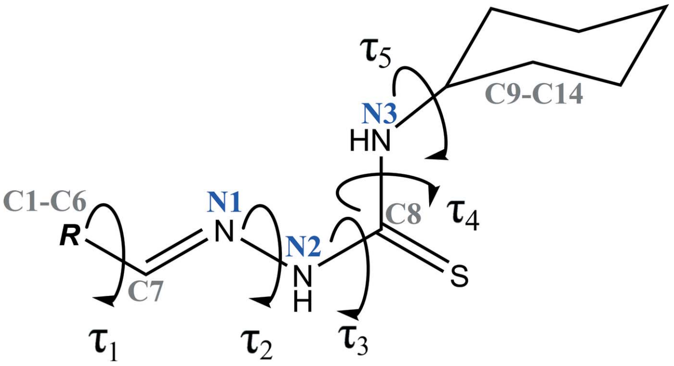


Figure 3
General chemical diagram showing torsion angles, τ_1, τ_2, τ_3, τ_4 and τ_5 in the title compound.

Table 2
Torsion angles τ_1, τ_2, τ_3, τ_4 and τ_5 (°).

Compound	*R*	τ_1	τ_2	τ_3	τ_4	τ_5
Title compound	2-hydroxy-3-methylbenzylidene	3.2, 1.9	171.7, 177.2	7.4, 10.2	178.1, 175.6	85.3, 81.6
ABUHEN (Basheer *et al.*, 2017)	pyren-1-ylmethylene	10.1	174.9	1.2	180.0	81.6
BEFZIY (Basheer *et al.*, 2016*a*)	2-hydroxy-1-naphthyl)methylene	0.9	179.3	6.8	176.6	83.4
BEVNAR (Koo *et al.*, 1981)	4-aminobenzylidene	14.3	175.0	7.4	178.5	94.5
LAQCIR (Jacob & Kurup, 2012)	5-bromo-2-hydroxy-3-methoxybenzylidene	10.1	176.8	4.1	179.5	86.2
LEPFIW (Seena *et al.*, 2006)	1-(2-hydroxyphenyl)ethylidene	3.9, 6.6	155.0, 153.5	14.0, 14.7	175.7, 171.8	91.9, 81.6
NALKOD (Basheer *et al.*, 2016*b*)	anthracen-9-ylmethylene	25.8, 36.2	171.6, 178.6	0.8, 1.4	172.9, 176.2	79.0, 79.2
OBOLOJ (Arafath, 2017*a*)	5-chloro-2-hydroxybenzylidene	4.7	176.0	5.5	176.7	83.7
XOYKAZ (Bhat *et al.*, 2015)	4-ethoxybenzylidene	0.5	169.3	11.6	176.2	85.8
YUXJOS (Arafath *et al.*, 2018)	3-*t*-butyl-2-hydroxyphenyl)methylidene	11.8	170.1	12.5	176.2	78.3

Note: The title compound and compounds LEPFIW and NALKOD crystallize with two independent molecules in the asymmetric unit.

for both molecules, as implied by torsion angle τ_4 [178.07 (14)° in molecule *A* and 175.59 (14)° in molecule *B*], which are approximately 180°. The thioamide group and the cyclohexane ring are almost perpendicular to each other with τ_5 torsion angles of 85.3 (2) and −81.6 (2)° in molecules *A* and *B*, respectively. This may arise from the steric repulsion between the cyclohexane ring and adjacent sulfur atom.

3. Supramolecular features

In the crystal, the *A* and *B* molecules are connected into 'dimers' with an $R_2^2(8)$ ring motif, *via* N2*A*—H1*N*2···S1*B*$^{\rm i}$ and N2*B*—H2*N*2···S1*A*$^{\rm i}$ hydrogen bonds (Fig. 4 and Table 1). The *A* molecules are further linked by a C—H···π interaction, so linking the *A*–*B* units to form ribbons propagating along the *b*-axis direction, as illustrated in Fig. 4.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.40, last update February 2019; Groom *et al.*, 2016) using (*E*)-2-benzylidene-*N*-cyclohexylhydrazine-1-carbothioamide as the reference moiety resulted in nine structures containing a cyclohexylhydrazinecarbothioamide moiety with different substituents (*R*). The different substituents (*R*) together with the torsion angles of the hydrazinecarbothioamide connecting bridge are compiled in Table 2 (*cf*. Fig. 3). In these structures, including the title compound, the hydrazinecarbothioamide connecting bridge is nearly planar as τ_2, τ_3 and τ_4 are in, respectively, anti-periplanar (153.5 to 179.3°), syn-periplanar (0.8 to 14.7°) and anti-periplanar (from 171.8 to 180.0°) conformations. The attached cyclohexane ring is always close to perpendicular to the thioamide group and with a syn/anti-clinal (τ_5 = 78.3 to 94.5°) conformation. Furthermore, torsion angle τ_1 for most of these structures exists in a syn-periplanar conformation, ranging from 0 to 25.8°, but there is one outlier (molecule *B* in NALKOD; Basheer *et al.*, 2016*b*) where torsion angle τ_1 is in a syn-clinal (36.2°) conformation. The cyclohexylhydrazinecarbothioamide moiety of this structure is substituted with an anthracen-9-ylmethylene ring system.

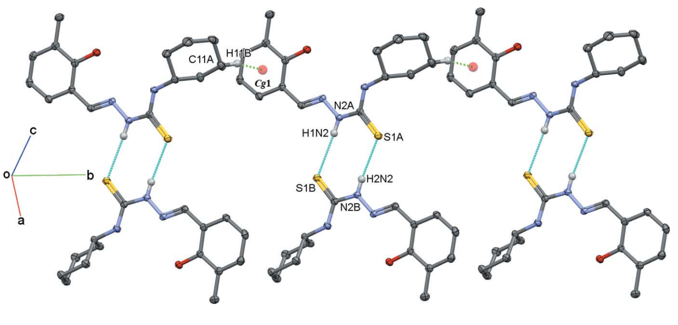


Figure 4
A partial view, normal to the *ac* plane, of the crystal packing of the title compound. The N—H···S hydrogen bonds are shown as cyan dotted lines, and the C—H···π interactions as green dotted lines (see Table 1 for details). For clarity, only the hydrogen atoms involved in these interactions have been included.

5. Synthesis and crystallization

The reaction scheme for the synthesis of the title Schiff base compound is given in Fig. 5.

2-Hydroxy-3-methylbenzaldehyde (0.68 g, 5.00 mmol) was dissolved in 20 ml of methanol. Glacial acetic acid (0.20 ml) was added and the mixture was refluxed for 30 min. A solution of *N*-cyclohexylhydrazine carbothioamide (0.87 g, 5 mmol) in 20 ml methanol was added dropwise with stirring to the aldehyde solution. The resulting colourless solution was refluxed for 4 h with stirring. A colourless precipitate was obtained on evaporation of the solvent. The crude product was washed with *n*-hexane (5 ml). The recovered product was dissolved in acetonitrile and purified by recrystallization. Colourless block-like crystals suitable for X-ray diffraction analysis were obtained on slow evaporation of the acetonitrile solvent (m.p. 513–514 K, yield 93%).

Spectroscopic and analytical data: ^{1}H NMR (500 MHz, DMSO-d_6, Me$_4$Si ppm): δ 11.27 (*s*, N—NH), δ 9.51 (*s*, OH), δ

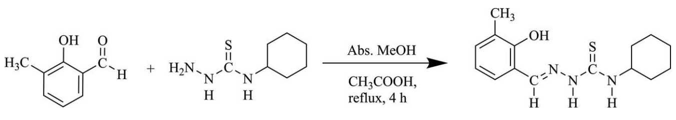


Figure 5
Reaction scheme for the synthesis of the title compound.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{21}N_3OS$
M_r	291.41
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	10.7799 (11), 10.9481 (11), 14.1895 (15)
α, β, γ (°)	74.526 (2), 68.246 (1), 80.207 (2)
V (Å^3)	1494.2 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.22
Crystal size (mm)	0.34 × 0.14 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
$T_{\min}$, $T_{\max}$	0.873, 0.935
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	50505, 8135, 5805
R_{int}	0.069
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.690
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.119, 1.04
No. of reflections	8135
No. of parameters	387
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.42, −0.36

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

8.34 (*s*, HC═N), δ 8.05 (*d*, J = 8.35 Hz, CS═NH), δ 7.39–6.81 (multiplet, aromatic-H), δ 2.20 (*s*, Ph—CH_3), δ 1.87–1.14 (multiplet, cyclohexyl-H) ppm. ^{13}C NMR (DMSO-d_6, Me_4Si ppm): δ 175.79 (C═S), δ 154.29 (C═N), δ 143.76-119.17 (C-aromatic), δ 15.93 (CH_3), δ 52.87–24.90 (C-cyclohexyl) ppm. IR (KBr pellets, cm^{-1}): 3364 (NH), 3148 (OH), 2989(CH_3), 2931 and 2854 (CH, cyclohexyl), 1620 (C═N), 1540 (C═C, aromatic), 1268 (C═S), 1218 (CH, bend., aromatic), 1122 (C—O). 1075 (C—N). Elemental analysis calculated for $C_{15}H_{21}N_3OS$ (M_r = 291.41 g mol^{-1}); C, 61.77; H, 7.21; N, 14.42%; found: C, 61.81; H, 7.19; N, 14.42%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The O and N-bound H atoms were located in a difference-Fourier map and freely refined. The C-bound H atoms were positioned geometrically and refined using a riding model: C—H = 0.95–1.00 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

Funding information

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supporting information

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Crystal structure of (*E*)-*N*-cyclohexyl-2-(2-hydroxy-3-methylbenzylidene)hydrazine-1-carbothioamide

Md. Azharul Arafath, Huey Chong Kwong and Farook Adam

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

(*E*)-*N*-Cyclohexyl-2-(2-hydroxy-3-methylbenzylidene)hydrazine-1-\ carbothioamide

Crystal data

$C_{15}H_{21}N_3OS$
$M_r = 291.41$
Triclinic, $P\overline{1}$
$a = 10.7799$ (11) Å
$b = 10.9481$ (11) Å
$c = 14.1895$ (15) Å
$\alpha = 74.526$ (2)°
$\beta = 68.246$ (1)°
$\gamma = 80.207$ (2)°
$V = 1494.2$ (3) Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6929 reflections
$\theta = 2.2$–29.3°
$\mu = 0.22$ mm^{-1}
$T = 100$ K
Block, colourless
0.34 × 0.14 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
$T_{\min} = 0.873$, $T_{\max} = 0.935$
50505 measured reflections
8135 independent reflections
5805 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.069$
$\theta_{\max} = 29.4°$, $\theta_{\min} = 1.6°$
$h = -14 \rightarrow 14$
$k = -15 \rightarrow 15$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.119$
$S = 1.03$
8135 reflections
387 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
$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.3685P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.42$ e Å^{-3}
$\Delta\rho_{\min} = -0.36$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.69733 (4)	0.60902 (4)	0.10987 (3)	0.01869 (11)
O1A	0.20574 (12)	0.29193 (12)	0.27567 (9)	0.0204 (3)
H1O1	0.264 (2)	0.340 (2)	0.2474 (19)	0.047 (7)*
N1A	0.44459 (13)	0.36989 (12)	0.14267 (10)	0.0157 (3)
N2A	0.54998 (14)	0.44583 (13)	0.10122 (11)	0.0168 (3)
H1N2	0.617 (2)	0.4267 (19)	0.0507 (16)	0.032 (6)*
N3A	0.45512 (13)	0.54155 (13)	0.23929 (11)	0.0180 (3)
H1N3	0.387 (2)	0.5075 (19)	0.2500 (16)	0.031 (6)*
C1A	0.23068 (15)	0.20058 (15)	0.22090 (12)	0.0166 (3)
C2A	0.13421 (16)	0.11183 (15)	0.25585 (13)	0.0180 (3)
C3A	0.15680 (17)	0.01785 (16)	0.20070 (13)	0.0212 (4)
H3AA	0.0925	−0.0427	0.2231	0.025*
C4A	0.27061 (17)	0.00986 (16)	0.11389 (14)	0.0219 (4)
H4AA	0.2840	−0.0557	0.0779	0.026*
C5A	0.36387 (17)	0.09792 (16)	0.08048 (13)	0.0204 (3)
H5AA	0.4412	0.0933	0.0206	0.024*
C6A	0.34648 (16)	0.19418 (15)	0.13340 (12)	0.0163 (3)
C7A	0.45032 (16)	0.28267 (15)	0.09523 (13)	0.0173 (3)
H7AA	0.5243	0.2759	0.0337	0.021*
C8A	0.55885 (15)	0.52858 (15)	0.15423 (12)	0.0154 (3)
C9A	0.44553 (15)	0.62215 (16)	0.30920 (12)	0.0175 (3)
H9AA	0.5368	0.6226	0.3119	0.021*
C10A	0.39567 (17)	0.75839 (16)	0.27188 (14)	0.0223 (4)
H10A	0.3072	0.7594	0.2653	0.027*
H10B	0.4588	0.7950	0.2024	0.027*
C11A	0.38338 (17)	0.83900 (17)	0.34832 (14)	0.0249 (4)
H11A	0.4734	0.8448	0.3495	0.030*
H11B	0.3465	0.9261	0.3246	0.030*
C12A	0.29295 (17)	0.78223 (19)	0.45741 (15)	0.0300 (4)
H12A	0.2924	0.8328	0.5059	0.036*
H12B	0.2002	0.7864	0.4580	0.036*
C13A	0.3395 (2)	0.64536 (19)	0.49414 (14)	0.0334 (5)
H13A	0.2742	0.6092	0.5627	0.040*
H13B	0.4269	0.6425	0.5031	0.040*
C14A	0.35411 (18)	0.56458 (17)	0.41752 (13)	0.0253 (4)
H14A	0.3914	0.4777	0.4415	0.030*
H14B	0.2648	0.5581	0.4153	0.030*
C15A	0.01137 (16)	0.12174 (18)	0.34918 (14)	0.0246 (4)
H15A	−0.0495	0.0589	0.3588	0.037*

H15B	−0.0337	0.2073	0.3387	0.037*
H15C	0.0371	0.1055	0.4111	0.037*
S1B	1.20980 (4)	0.63000 (4)	0.11943 (3)	0.01957 (11)
O1B	0.72600 (12)	0.31105 (11)	0.27336 (9)	0.0204 (3)
H1O2	0.790 (2)	0.358 (2)	0.2455 (18)	0.042 (7)*
N1B	0.96393 (13)	0.38885 (13)	0.14385 (10)	0.0165 (3)
N2B	1.07086 (14)	0.46229 (13)	0.10739 (11)	0.0183 (3)
H2N2	1.141 (2)	0.4453 (19)	0.0585 (17)	0.035 (6)*
N3B	0.95163 (13)	0.58802 (14)	0.22201 (11)	0.0191 (3)
H2N3	0.8858 (19)	0.5517 (18)	0.2277 (14)	0.023 (5)*
C1B	0.74994 (15)	0.22243 (15)	0.21634 (12)	0.0160 (3)
C2B	0.64909 (16)	0.14034 (16)	0.24528 (13)	0.0182 (3)
C3B	0.67030 (16)	0.04933 (16)	0.18792 (13)	0.0212 (4)
H3BA	0.6019	−0.0055	0.2052	0.025*
C4B	0.78870 (17)	0.03605 (16)	0.10606 (14)	0.0221 (4)
H4BA	0.8018	−0.0285	0.0692	0.027*
C5B	0.88741 (16)	0.11750 (16)	0.07866 (13)	0.0198 (3)
H5BA	0.9683	0.1087	0.0224	0.024*
C6B	0.87008 (15)	0.21254 (15)	0.13242 (12)	0.0168 (3)
C7B	0.97581 (16)	0.29730 (15)	0.09955 (13)	0.0178 (3)
H7BA	1.0559	0.2846	0.0438	0.021*
C8B	1.06817 (16)	0.55741 (15)	0.15303 (12)	0.0165 (3)
C9B	0.93058 (15)	0.68143 (15)	0.28450 (12)	0.0171 (3)
H9BA	0.9867	0.7537	0.2406	0.021*
C10B	0.97252 (16)	0.62377 (16)	0.37971 (13)	0.0200 (3)
H10C	1.0684	0.5927	0.3570	0.024*
H10D	0.9197	0.5504	0.4230	0.024*
C11B	0.95005 (16)	0.72239 (16)	0.44436 (13)	0.0214 (4)
H11C	0.9730	0.6819	0.5077	0.026*
H11D	1.0100	0.7914	0.4034	0.026*
C12B	0.80487 (16)	0.77855 (17)	0.47574 (13)	0.0219 (4)
H12C	0.7460	0.7118	0.5248	0.026*
H12D	0.7953	0.8471	0.5120	0.026*
C13B	0.76067 (17)	0.83197 (17)	0.38142 (14)	0.0224 (4)
H13C	0.8111	0.9065	0.3372	0.027*
H13D	0.6642	0.8610	0.4051	0.027*
C14B	0.78417 (15)	0.73274 (16)	0.31723 (13)	0.0201 (4)
H14C	0.7268	0.6620	0.3590	0.024*
H14D	0.7592	0.7717	0.2546	0.024*
C15B	0.52399 (16)	0.15270 (17)	0.33654 (14)	0.0237 (4)
H15D	0.4569	0.1011	0.3383	0.036*
H15E	0.4886	0.2420	0.3299	0.036*
H15F	0.5447	0.1231	0.4010	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.01576 (19)	0.0224 (2)	0.0179 (2)	−0.00439 (16)	−0.00298 (16)	−0.00655 (17)

O1A	0.0200 (6)	0.0223 (7)	0.0185 (6)	−0.0050 (5)	−0.0019 (5)	−0.0086 (5)
N1A	0.0150 (6)	0.0159 (7)	0.0166 (7)	−0.0018 (5)	−0.0052 (5)	−0.0041 (5)
N2A	0.0155 (6)	0.0188 (7)	0.0155 (7)	−0.0032 (5)	−0.0014 (6)	−0.0072 (6)
N3A	0.0142 (6)	0.0223 (8)	0.0187 (7)	−0.0050 (6)	−0.0020 (6)	−0.0095 (6)
C1A	0.0199 (8)	0.0162 (8)	0.0153 (8)	−0.0006 (6)	−0.0079 (6)	−0.0036 (6)
C2A	0.0177 (7)	0.0191 (8)	0.0173 (8)	−0.0022 (6)	−0.0080 (6)	−0.0012 (7)
C3A	0.0238 (8)	0.0177 (9)	0.0244 (9)	−0.0054 (7)	−0.0118 (7)	−0.0013 (7)
C4A	0.0291 (9)	0.0168 (9)	0.0238 (9)	−0.0012 (7)	−0.0122 (7)	−0.0070 (7)
C5A	0.0238 (8)	0.0177 (9)	0.0187 (9)	0.0002 (7)	−0.0056 (7)	−0.0061 (7)
C6A	0.0197 (8)	0.0146 (8)	0.0151 (8)	−0.0009 (6)	−0.0074 (6)	−0.0025 (6)
C7A	0.0180 (7)	0.0175 (8)	0.0146 (8)	−0.0015 (6)	−0.0032 (6)	−0.0043 (6)
C8A	0.0158 (7)	0.0158 (8)	0.0153 (8)	−0.0003 (6)	−0.0072 (6)	−0.0024 (6)
C9A	0.0162 (7)	0.0223 (9)	0.0159 (8)	−0.0045 (6)	−0.0036 (6)	−0.0081 (7)
C10A	0.0248 (8)	0.0215 (9)	0.0225 (9)	−0.0012 (7)	−0.0091 (7)	−0.0072 (7)
C11A	0.0223 (8)	0.0248 (10)	0.0327 (10)	0.0003 (7)	−0.0109 (8)	−0.0142 (8)
C12A	0.0206 (8)	0.0435 (12)	0.0320 (11)	−0.0055 (8)	−0.0022 (8)	−0.0262 (9)
C13A	0.0415 (11)	0.0405 (12)	0.0187 (10)	−0.0133 (9)	−0.0027 (8)	−0.0120 (8)
C14A	0.0295 (9)	0.0272 (10)	0.0180 (9)	−0.0086 (8)	−0.0031 (7)	−0.0066 (7)
C15A	0.0198 (8)	0.0282 (10)	0.0244 (9)	−0.0067 (7)	−0.0040 (7)	−0.0056 (8)
S1B	0.01561 (19)	0.0223 (2)	0.0206 (2)	−0.00340 (16)	−0.00332 (16)	−0.00756 (17)
O1B	0.0204 (6)	0.0208 (6)	0.0198 (6)	−0.0032 (5)	−0.0019 (5)	−0.0106 (5)
N1B	0.0154 (6)	0.0169 (7)	0.0173 (7)	−0.0020 (5)	−0.0052 (5)	−0.0042 (6)
N2B	0.0155 (7)	0.0203 (8)	0.0177 (7)	−0.0029 (6)	−0.0013 (6)	−0.0074 (6)
N3B	0.0148 (6)	0.0217 (8)	0.0227 (8)	−0.0024 (6)	−0.0035 (6)	−0.0117 (6)
C1B	0.0185 (7)	0.0145 (8)	0.0151 (8)	0.0014 (6)	−0.0067 (6)	−0.0039 (6)
C2B	0.0179 (7)	0.0185 (8)	0.0176 (8)	−0.0002 (6)	−0.0072 (6)	−0.0022 (7)
C3B	0.0217 (8)	0.0200 (9)	0.0244 (9)	−0.0034 (7)	−0.0103 (7)	−0.0047 (7)
C4B	0.0275 (9)	0.0198 (9)	0.0246 (9)	−0.0003 (7)	−0.0117 (7)	−0.0109 (7)
C5B	0.0208 (8)	0.0211 (9)	0.0176 (8)	0.0000 (7)	−0.0041 (7)	−0.0095 (7)
C6B	0.0179 (7)	0.0171 (8)	0.0163 (8)	−0.0011 (6)	−0.0066 (6)	−0.0042 (6)
C7B	0.0175 (7)	0.0186 (8)	0.0158 (8)	0.0003 (6)	−0.0042 (6)	−0.0049 (7)
C8B	0.0186 (7)	0.0160 (8)	0.0142 (8)	−0.0011 (6)	−0.0059 (6)	−0.0021 (6)
C9B	0.0178 (7)	0.0179 (8)	0.0167 (8)	−0.0032 (6)	−0.0035 (6)	−0.0079 (7)
C10B	0.0183 (8)	0.0215 (9)	0.0199 (9)	0.0017 (6)	−0.0066 (7)	−0.0063 (7)
C11B	0.0228 (8)	0.0252 (9)	0.0188 (9)	−0.0011 (7)	−0.0096 (7)	−0.0063 (7)
C12B	0.0225 (8)	0.0247 (9)	0.0196 (9)	−0.0005 (7)	−0.0062 (7)	−0.0092 (7)
C13B	0.0207 (8)	0.0245 (9)	0.0262 (10)	0.0035 (7)	−0.0107 (7)	−0.0121 (8)
C14B	0.0179 (8)	0.0236 (9)	0.0218 (9)	−0.0006 (7)	−0.0081 (7)	−0.0087 (7)
C15B	0.0199 (8)	0.0253 (9)	0.0231 (9)	−0.0036 (7)	−0.0036 (7)	−0.0048 (7)

Geometric parameters (Å, º)

S1A—C8A	1.6897 (15)	S1B—C8B	1.6914 (16)
O1A—C1A	1.3583 (19)	O1B—C1B	1.3569 (19)
O1A—H1O1	0.80 (2)	O1B—H1O2	0.83 (2)
N1A—C7A	1.289 (2)	N1B—C7B	1.284 (2)
N1A—N2A	1.3758 (18)	N1B—N2B	1.3762 (18)
N2A—C8A	1.357 (2)	N2B—C8B	1.357 (2)

N2A—H1N2	0.85 (2)	N2B—H2N2	0.85 (2)
N3A—C8A	1.328 (2)	N3B—C8B	1.330 (2)
N3A—C9A	1.461 (2)	N3B—C9B	1.463 (2)
N3A—H1N3	0.82 (2)	N3B—H2N3	0.840 (19)
C1A—C6A	1.404 (2)	C1B—C2B	1.401 (2)
C1A—C2A	1.406 (2)	C1B—C6B	1.409 (2)
C2A—C3A	1.390 (2)	C2B—C3B	1.387 (2)
C2A—C15A	1.499 (2)	C2B—C15B	1.500 (2)
C3A—C4A	1.390 (2)	C3B—C4B	1.388 (2)
C3A—H3AA	0.9500	C3B—H3BA	0.9500
C4A—C5A	1.378 (2)	C4B—C5B	1.382 (2)
C4A—H4AA	0.9500	C4B—H4BA	0.9500
C5A—C6A	1.400 (2)	C5B—C6B	1.397 (2)
C5A—H5AA	0.9500	C5B—H5BA	0.9500
C6A—C7A	1.458 (2)	C6B—C7B	1.453 (2)
C7A—H7AA	0.9500	C7B—H7BA	0.9500
C9A—C14A	1.517 (2)	C9B—C14B	1.522 (2)
C9A—C10A	1.520 (2)	C9B—C10B	1.526 (2)
C9A—H9AA	1.0000	C9B—H9BA	1.0000
C10A—C11A	1.529 (2)	C10B—C11B	1.530 (2)
C10A—H10A	0.9900	C10B—H10C	0.9900
C10A—H10B	0.9900	C10B—H10D	0.9900
C11A—C12A	1.519 (3)	C11B—C12B	1.526 (2)
C11A—H11A	0.9900	C11B—H11C	0.9900
C11A—H11B	0.9900	C11B—H11D	0.9900
C12A—C13A	1.513 (3)	C12B—C13B	1.523 (2)
C12A—H12A	0.9900	C12B—H12C	0.9900
C12A—H12B	0.9900	C12B—H12D	0.9900
C13A—C14A	1.526 (2)	C13B—C14B	1.529 (2)
C13A—H13A	0.9900	C13B—H13C	0.9900
C13A—H13B	0.9900	C13B—H13D	0.9900
C14A—H14A	0.9900	C14B—H14C	0.9900
C14A—H14B	0.9900	C14B—H14D	0.9900
C15A—H15A	0.9800	C15B—H15D	0.9800
C15A—H15B	0.9800	C15B—H15E	0.9800
C15A—H15C	0.9800	C15B—H15F	0.9800
C1A—O1A—H1O1	108.6 (17)	C1B—O1B—H1O2	107.4 (15)
C7A—N1A—N2A	116.82 (13)	C7B—N1B—N2B	116.97 (14)
C8A—N2A—N1A	119.82 (13)	C8B—N2B—N1B	120.46 (14)
C8A—N2A—H1N2	120.7 (13)	C8B—N2B—H2N2	119.4 (14)
N1A—N2A—H1N2	117.8 (14)	N1B—N2B—H2N2	120.0 (14)
C8A—N3A—C9A	125.71 (13)	C8B—N3B—C9B	124.99 (13)
C8A—N3A—H1N3	117.1 (14)	C8B—N3B—H2N3	116.0 (13)
C9A—N3A—H1N3	116.9 (14)	C9B—N3B—H2N3	118.9 (13)
O1A—C1A—C6A	122.24 (14)	O1B—C1B—C2B	116.63 (14)
O1A—C1A—C2A	116.68 (14)	O1B—C1B—C6B	122.02 (14)
C6A—C1A—C2A	121.08 (15)	C2B—C1B—C6B	121.35 (15)

C3A—C2A—C1A	117.85 (15)	C3B—C2B—C1B	117.95 (15)
C3A—C2A—C15A	122.40 (14)	C3B—C2B—C15B	122.57 (15)
C1A—C2A—C15A	119.74 (15)	C1B—C2B—C15B	119.48 (15)
C4A—C3A—C2A	122.00 (15)	C2B—C3B—C4B	121.87 (15)
C4A—C3A—H3AA	119.0	C2B—C3B—H3BA	119.1
C2A—C3A—H3AA	119.0	C4B—C3B—H3BA	119.1
C5A—C4A—C3A	119.37 (16)	C5B—C4B—C3B	119.48 (15)
C5A—C4A—H4AA	120.3	C5B—C4B—H4BA	120.3
C3A—C4A—H4AA	120.3	C3B—C4B—H4BA	120.3
C4A—C5A—C6A	121.01 (16)	C4B—C5B—C6B	120.98 (16)
C4A—C5A—H5AA	119.5	C4B—C5B—H5BA	119.5
C6A—C5A—H5AA	119.5	C6B—C5B—H5BA	119.5
C5A—C6A—C1A	118.68 (14)	C5B—C6B—C1B	118.35 (14)
C5A—C6A—C7A	118.22 (15)	C5B—C6B—C7B	118.96 (15)
C1A—C6A—C7A	123.09 (14)	C1B—C6B—C7B	122.70 (14)
N1A—C7A—C6A	121.83 (15)	N1B—C7B—C6B	121.80 (15)
N1A—C7A—H7AA	119.1	N1B—C7B—H7BA	119.1
C6A—C7A—H7AA	119.1	C6B—C7B—H7BA	119.1
N3A—C8A—N2A	116.73 (14)	N3B—C8B—N2B	116.78 (14)
N3A—C8A—S1A	123.76 (12)	N3B—C8B—S1B	124.07 (12)
N2A—C8A—S1A	119.51 (12)	N2B—C8B—S1B	119.15 (12)
N3A—C9A—C14A	108.61 (13)	N3B—C9B—C14B	109.69 (12)
N3A—C9A—C10A	112.01 (13)	N3B—C9B—C10B	111.20 (13)
C14A—C9A—C10A	111.06 (14)	C14B—C9B—C10B	110.58 (13)
N3A—C9A—H9AA	108.4	N3B—C9B—H9BA	108.4
C14A—C9A—H9AA	108.4	C14B—C9B—H9BA	108.4
C10A—C9A—H9AA	108.4	C10B—C9B—H9BA	108.4
C9A—C10A—C11A	110.55 (14)	C9B—C10B—C11B	110.68 (13)
C9A—C10A—H10A	109.5	C9B—C10B—H10C	109.5
C11A—C10A—H10A	109.5	C11B—C10B—H10C	109.5
C9A—C10A—H10B	109.5	C9B—C10B—H10D	109.5
C11A—C10A—H10B	109.5	C11B—C10B—H10D	109.5
H10A—C10A—H10B	108.1	H10C—C10B—H10D	108.1
C12A—C11A—C10A	111.31 (14)	C12B—C11B—C10B	111.23 (13)
C12A—C11A—H11A	109.4	C12B—C11B—H11C	109.4
C10A—C11A—H11A	109.4	C10B—C11B—H11C	109.4
C12A—C11A—H11B	109.4	C12B—C11B—H11D	109.4
C10A—C11A—H11B	109.4	C10B—C11B—H11D	109.4
H11A—C11A—H11B	108.0	H11C—C11B—H11D	108.0
C13A—C12A—C11A	111.40 (15)	C13B—C12B—C11B	111.49 (14)
C13A—C12A—H12A	109.3	C13B—C12B—H12C	109.3
C11A—C12A—H12A	109.3	C11B—C12B—H12C	109.3
C13A—C12A—H12B	109.3	C13B—C12B—H12D	109.3
C11A—C12A—H12B	109.3	C11B—C12B—H12D	109.3
H12A—C12A—H12B	108.0	H12C—C12B—H12D	108.0
C12A—C13A—C14A	111.91 (16)	C12B—C13B—C14B	111.59 (14)
C12A—C13A—H13A	109.2	C12B—C13B—H13C	109.3
C14A—C13A—H13A	109.2	C14B—C13B—H13C	109.3

C12A—C13A—H13B	109.2	C12B—C13B—H13D	109.3
C14A—C13A—H13B	109.2	C14B—C13B—H13D	109.3
H13A—C13A—H13B	107.9	H13C—C13B—H13D	108.0
C9A—C14A—C13A	111.02 (14)	C9B—C14B—C13B	110.42 (13)
C9A—C14A—H14A	109.4	C9B—C14B—H14C	109.6
C13A—C14A—H14A	109.4	C13B—C14B—H14C	109.6
C9A—C14A—H14B	109.4	C9B—C14B—H14D	109.6
C13A—C14A—H14B	109.4	C13B—C14B—H14D	109.6
H14A—C14A—H14B	108.0	H14C—C14B—H14D	108.1
C2A—C15A—H15A	109.5	C2B—C15B—H15D	109.5
C2A—C15A—H15B	109.5	C2B—C15B—H15E	109.5
H15A—C15A—H15B	109.5	H15D—C15B—H15E	109.5
C2A—C15A—H15C	109.5	C2B—C15B—H15F	109.5
H15A—C15A—H15C	109.5	H15D—C15B—H15F	109.5
H15B—C15A—H15C	109.5	H15E—C15B—H15F	109.5

C7A—N1A—N2A—C8A	−171.68 (14)	C7B—N1B—N2B—C8B	−177.23 (14)
O1A—C1A—C2A—C3A	179.53 (14)	O1B—C1B—C2B—C3B	179.53 (14)
C6A—C1A—C2A—C3A	−0.3 (2)	C6B—C1B—C2B—C3B	−0.7 (2)
O1A—C1A—C2A—C15A	0.2 (2)	O1B—C1B—C2B—C15B	−1.0 (2)
C6A—C1A—C2A—C15A	−179.68 (15)	C6B—C1B—C2B—C15B	178.77 (15)
C1A—C2A—C3A—C4A	0.3 (2)	C1B—C2B—C3B—C4B	1.9 (2)
C15A—C2A—C3A—C4A	179.61 (16)	C15B—C2B—C3B—C4B	−177.57 (16)
C2A—C3A—C4A—C5A	−0.5 (3)	C2B—C3B—C4B—C5B	−1.7 (3)
C3A—C4A—C5A—C6A	0.8 (3)	C3B—C4B—C5B—C6B	0.3 (3)
C4A—C5A—C6A—C1A	−0.9 (2)	C4B—C5B—C6B—C1B	0.8 (2)
C4A—C5A—C6A—C7A	178.73 (15)	C4B—C5B—C6B—C7B	−178.94 (15)
O1A—C1A—C6A—C5A	−179.23 (14)	O1B—C1B—C6B—C5B	179.16 (14)
C2A—C1A—C6A—C5A	0.6 (2)	C2B—C1B—C6B—C5B	−0.6 (2)
O1A—C1A—C6A—C7A	1.2 (2)	O1B—C1B—C6B—C7B	−1.1 (2)
C2A—C1A—C6A—C7A	−178.96 (14)	C2B—C1B—C6B—C7B	179.12 (15)
N2A—N1A—C7A—C6A	178.28 (13)	N2B—N1B—C7B—C6B	179.20 (14)
C5A—C6A—C7A—N1A	−176.61 (15)	C5B—C6B—C7B—N1B	177.83 (15)
C1A—C6A—C7A—N1A	3.0 (2)	C1B—C6B—C7B—N1B	−1.9 (2)
C9A—N3A—C8A—N2A	178.07 (14)	C9B—N3B—C8B—N2B	175.59 (14)
C9A—N3A—C8A—S1A	−2.3 (2)	C9B—N3B—C8B—S1B	−4.8 (2)
N1A—N2A—C8A—N3A	−7.4 (2)	N1B—N2B—C8B—N3B	−10.2 (2)
N1A—N2A—C8A—S1A	172.92 (11)	N1B—N2B—C8B—S1B	170.21 (11)
C8A—N3A—C9A—C14A	−151.70 (16)	C8B—N3B—C9B—C14B	155.77 (15)
C8A—N3A—C9A—C10A	85.26 (19)	C8B—N3B—C9B—C10B	−81.60 (19)
N3A—C9A—C10A—C11A	178.51 (13)	N3B—C9B—C10B—C11B	179.99 (13)
C14A—C9A—C10A—C11A	56.87 (18)	C14B—C9B—C10B—C11B	−57.90 (17)
C9A—C10A—C11A—C12A	−56.18 (19)	C9B—C10B—C11B—C12B	55.88 (18)
C10A—C11A—C12A—C13A	54.83 (19)	C10B—C11B—C12B—C13B	−54.08 (19)
C11A—C12A—C13A—C14A	−54.1 (2)	C11B—C12B—C13B—C14B	54.32 (19)
N3A—C9A—C14A—C13A	−179.67 (15)	N3B—C9B—C14B—C13B	−179.21 (14)
C10A—C9A—C14A—C13A	−56.06 (19)	C10B—C9B—C14B—C13B	57.79 (18)
C12A—C13A—C14A—C9A	54.7 (2)	C12B—C13B—C14B—C9B	−56.10 (19)

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of benzene ring C1*A*–C6*A*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*O*1···N1*A*	0.80 (2)	1.98 (2)	2.6844 (19)	146 (2)
O1*B*—H1*O*2···N1*B*	0.84 (2)	1.91 (2)	2.664 (2)	148 (2)
N2*A*—H1*N*2···S1*B*^{i}	0.85 (2)	2.60 (2)	3.4414 (16)	170 (2)
N2*B*—H2*N*2···S1*A*^{i}	0.85 (2)	2.53 (2)	3.3568 (15)	164 (2)
C11*A*—H11*B*···*Cg*1^{ii}	0.99	2.93	3.801 (2)	148

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) *x*, *y*+1, *z*.