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Crystal structure and Hirshfeld surface analysis of 2-amino-5-bromo-1,3,4-triazol-3-ium chloride monohydrate

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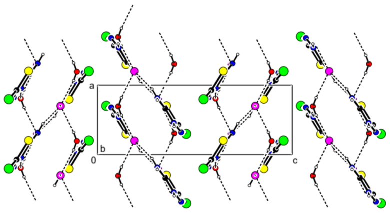
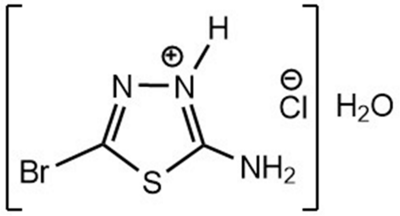
In the title salt, $C_2H_3BrN_3S^+\cdot Cl^-\cdot H_2O$, the cation $C_2H_3BrN_3S^+$ cation, the Cl^- anion and the water molecule are linked by N—H···Cl, N—H···O and O—H···Cl hydrogen bonds, forming molecular layers parallel to the (002) plane. The crystal packing is further reinforced by van der Waals interactions between these layers but C—H···π and π–π interactions are not observed. Hirshfeld surface analysis and two-dimensional fingerprint plots were used to study the intermolecular interactions.



1. Chemical context

Thiadiazole is a five-membered ring system containing a chalcogen-bond-donor sulfur atom (Gurbanov *et al.*, 2023), a hydrogen-bonding domain, and a two-electron donor nitrogen system that exhibits a strong coordination ability (Khojabaeva *et al.*, 2025; Mahmudov *et al.*, 2021). The 1,3,4-thiadiazole moiety is present as a core structural component in an array of drug categories such as anti-inflammatory, antimicrobial, analgesic, anticancer, anti-epileptic, antineoplastic, antiviral, and antitubercular agents (Jain *et al.*, 2013; Torambetov *et al.*, 2026). Transition-metal complexes of thiadiazole ligands have also attracted much attention due to their high synthetic potential for synthesis, crystal engineering and catalysis (Mamedov *et al.*, 2006; Nuralieva *et al.*, 2025, 2026). Functionalization of the thiadiazol moiety with a non-covalent bond-donor or acceptor sites can be used a synthetic tool to improve their functional properties (Huseynov *et al.*, 2021; Naghiyev *et al.*, 2023).



In a continuation of our work in this area, we functionalized a thiadiazol, 5-bromo-1,3,4-thiadiazol-2-amine, which exhibits various sorts of intermolecular non-covalent interactions.

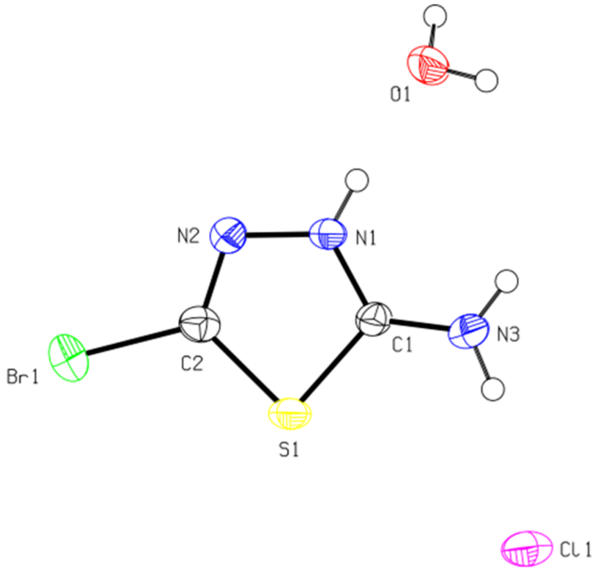


Figure 1
View of the asymmetric unit the title salt, showing the atom labeling and the 50% probability ellipsoids for non-hydrogen atoms.

2. Structural commentary

In the $(C_2H_3BrN_3S)^+$ cation of the title salt, (Fig. 1), the five-membered ring is quite planar (r.m.s. deviation = 0.004 Å). The N1—N2—C2—Br1 and C1—S1—C2—Br1 torsion angles are −179.2 (3) and 178.6 (3)°, respectively. The Br—C [Br1—C2 = 1.855 (5) Å], S—C [S1—C1 = 1.733 (5) and S1—C2 = 1.740 (5) Å], N═C [N1—C1 = 1.323 (6) and N2—C2 =1.277 (7) Å] and N—N [N1—N2 = 1.364 (6) Å] bond lengths, and the C—S—C [C1—S1—C2) 86.9 (2)°] and C═N—N [C1═N1—N2 = 117.5 (4) and C2═N2—N1 = 108.9 (4)°] angles are within normal values and are also compatible with those of the structures in the database survey section.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1*A*⋯Cl1^{i}	0.85	2.32	3.144 (4)	163
O1—H1*B*⋯Cl1^{ii}	0.85	2.37	3.196 (4)	163
N3—H3*A*⋯Cl1^{i}	0.86	2.38	3.221 (5)	168
N3—H3*B*⋯Cl1	0.86	2.29	3.127 (5)	163
N1—H1⋯O1	0.83 (3)	1.86 (3)	2.685 (6)	176 (7)

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

3. Supramolecular features and Hirshfeld surface analysis

In the title salt, the $(C_2H_3BrN_3S)^+$ cation, the Cl^- anion, and the water molecule are linked by N—H⋯Cl, N—H⋯O, and O—H⋯Cl hydrogen bonds, forming molecular layers parallel to the (002) plane (Table 1, Figs. 2, 3 and 4). van der Waals

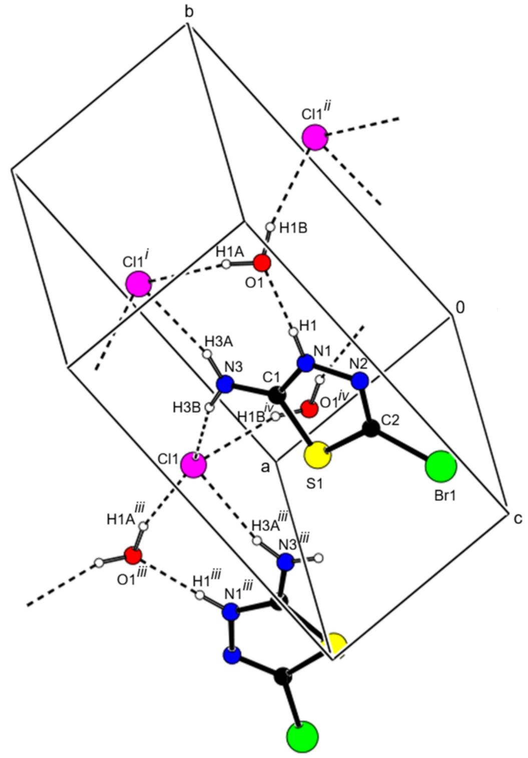


Figure 2
A partial packing diagram showing the O—H⋯Cl, N—H⋯Cl and N—H⋯O hydrogen bonds (dashed lines). Symmetry codes: (i) $2-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $-1+x, y, z$; (iii) $2-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (iv) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$.

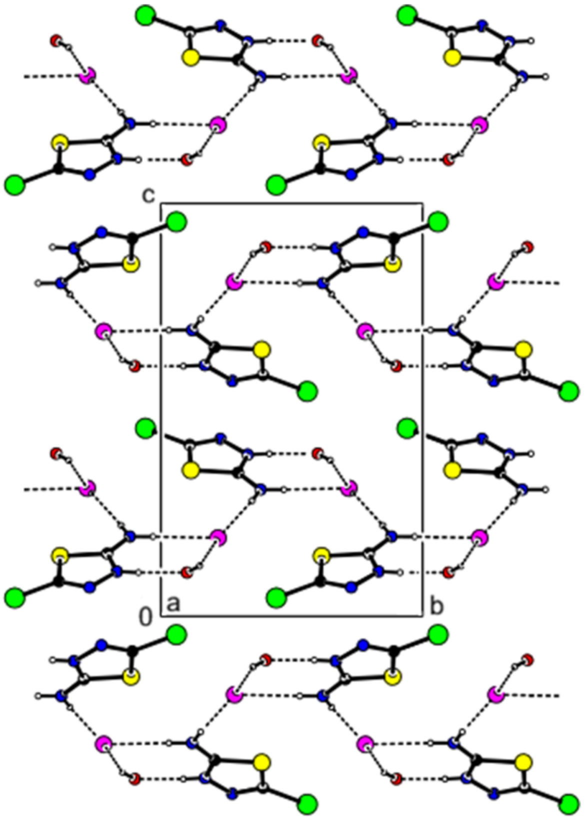


Figure 3
Crystal packing of the title salt viewed along the *a*-axis direction. Intermolecular hydrogen bonds are shown as dashed lines.

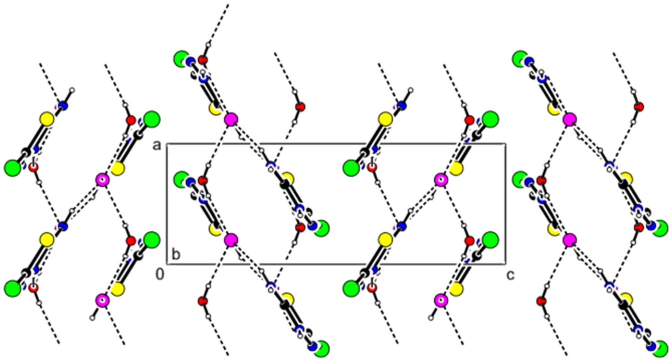


Figure 4
Crystal packing of the title salt viewed along the *b*-axis direction.

interactions between these layers consolidate the crystal packing. C—H$\cdots\pi$ and π–π interactions were not observed.

Hirshfeld surface analysis was performed to visualize and quantify the intermolecular interactions in the cation of the title salt using *CrystalExplorer* (Spackman *et al.*, 2021). The Hirshfeld surfaces were mapped over $d_{\rm norm}$ in the range −0.7220 (red) to +0,9614 (blue) a.u. (Fig. 5). The red regions are attributed to the N1—H1···O1 and N3—H3B···Cl1 interactions (Tables 1 and 2). The two-dimensional fingerprint plots indicate that the major contributions to the crystal packing are from Br···H/H···Br (21.4%), H···H (9.6%) and Cl···H/H···Cl (7.5%) interactions as shown in Fig. 6. Other, less notable contacts are from N···C/C···N (5.5%), N···N (5.3%), O···H/H···O (5.2%), N···H/H···N (5.1%), S···N/N···S (4.6%), Br···S/S···Br (4.3%), Br···O/O···Br (4.1%), C···H/H···C (4.1%), Cl···S/S···Cl (3.1%), Br···Cl/Cl···Br (2.2%), Cl···C/C···Cl (2.0%), Br···N/N···Br (1.8%), Cl···N/N···Cl (1.2%), S···O/O···S (0.8%), S···C/C···S (0.7%), Br···C/C···Br (0.3%), C···C (0.1%) and O···C/C···O (0.1%) interactions.

Table 2
Summary of short interatomic contacts (Å).

Contact	Distance	Symmetry operation
Br1···H1*B*	3.09	$x, -1+y, z$
Br1···O1	3.50	$-\frac{1}{2}+x, \frac{1}{2}-y, 1-z$
Br1···O1	3.56	$\frac{1}{2}+x, \frac{1}{2}-y, 1-z$
H1···O1	1.85	x, y, z
H3*B*···Cl1	2.29	x, y, z
H3*A*···Cl1	2.38	$2-x, \frac{1}{2}+y, \frac{1}{2}-z$
C1···Cl1	3.51	$-1+x, y, z$
Cl1···H1*B*	2.37	$1-x, -\frac{1}{2}+y, \frac{1}{2}-z$
Cl1···H1*A*	2.32	$2-x, -\frac{1}{2}+y, \frac{1}{2}-z$

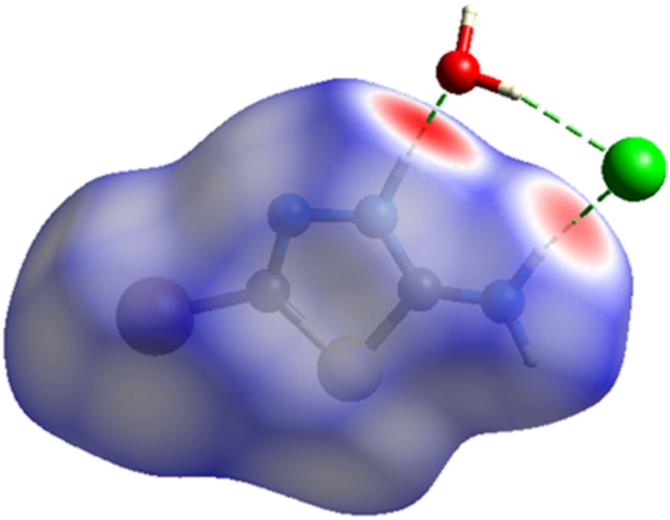
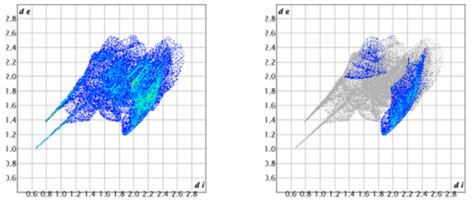
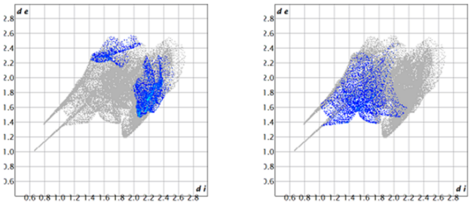


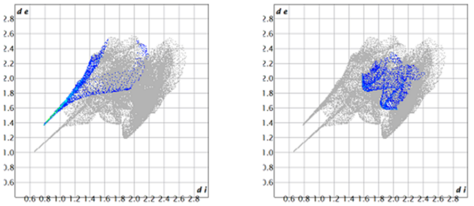
Figure 5
The Hirshfeld surface of the $(C_2H_3BrN_3S)^+$ cation of the title salt mapped over $d_{\rm norm}$ (color code. Br: green, C: gray; Cl: violet, H: white; O: red; N: blue; S: yellow).



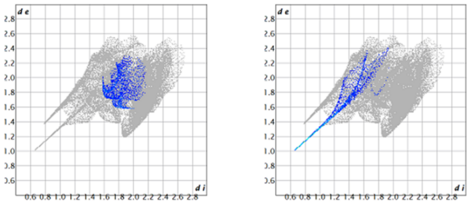
(a) All…All
(b) Br….H/H…Br



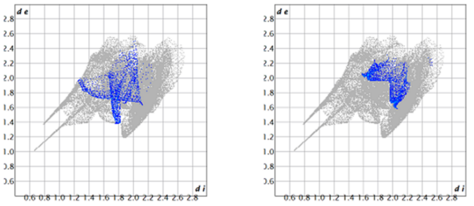
(c) S…H/H…S
(d) H…H



(e) Cl…H/H…Cl
(f) N…C/C…N



(g) N…N
(h) O…H/H…O



(i) N…H/H….N
(j) S…N/N…S

Figure 6
The two-dimensional fingerprint plots, showing (*a*) all interactions, and those delineated into (*b*) Br···H/H···Br, (*c*) S···H/H···S, (*d*) H···H, (*e*) Cl···H/H···Cl, (*f*) N···C/C···N, (*g*) N···N, (*h*) O···H/H···O, (i) N···H/H···N and (*j*) S···N/N···S interactions; d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.00, last update April 2025; Groom *et al.*, 2016) for the cation without the Br atom gave one hit and this is a copper complex. When the unprotonated molecule is searched for by removing Br, 240 results are obtained, and most of these are metal complexes. The three most similar compounds to the title salt containing the 2-amino-5-bromo-1,3,4-triazol-3-ium unit are CSD refcodes AYOVAM (Zhang *et al.*, 2011), VIKSOZ (Smith & Lynch, 2013) and BOMROM (Smith & Lynch, 2014).

In AYOVAM, the strongest N—H⋯N intermolecular hydrogen bond, between the amine group and one thiadiazole N atom, forms centrosymmetric dimers. The other amine H atom extends the supramolecular network, forming an N—H⋯N contact with the other thiadiazole N atom. In VIKSOZ, the amine-heteroatom N—H⋯N hydrogen bond between the heterodimers results in a one-dimensional chain structure stretching along the *c*-axis direction. In BOMROM, the heterodimers are extended into a chain along the *b*-axis direction through an amine N—H⋯N thiadiazole hydrogen bond. In the title compound, the crystal packing is achieved through intermolecular O—H⋯Cl and N—H⋯Cl hydrogen bonds.

5. Synthesis and crystallization

To a solution of 2-amino-1,3,4-thiadiazole (5 g, 48.45 mmol) in methanol (70 mL), sodium bicarbonate (8.14 g, 96.90 mmol) and bromine (2.5 mL, 48.45 mmol) were added. The reaction mixture was stirred at room temperature until the disappearance of the starting material (30–40 minutes). The methanol was removed under vacuum and the crude product was diluted with water (15 mL), filtered, dry *in vacuo* to give a brown solid, 5-bromo-1,3,4-thiadiazol-2-amine (94%). Colorless crystals suitable for X-ray analysis were obtained by slow evaporation of a mixture of 1 *M* HCl (pH = 0) and methanol (*v*/*v*, 1:2) solution. Analysis calculated for $C_2H_5BrClN_3OS$ (M = 234.50): C 10.24, H 2.15, N 17.95; found: C 10.20, H 2.10, N 17.92%. ^1H NMR (300 MHz, DMSO-d^6): δ 7.84 (3H). ^{13}C NMR (75 MHz, DMSO-d_6) δ 154.8 and 159.1.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The water H-atom positions were determined from the difference-Fourier map, with their thermal characteristics restricted to 1.5 times those of the oxygen atom. The hydrogen atom of the NH group was identified in the difference-Fourier map, refined freely with $1.2U_{eq}$(N), while the hydrogen atoms of the NH_2 groups were positioned geometrically and assigned thermal parameter values at 1.2 times that of the connected nitrogen atom.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_2H_3BrN_3S^+\cdot Cl^-\cdot H_2O$
M_r	234.51
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, b, c (Å)	5.3575 (1), 9.5328 (1), 15.0588 (2)
V (Å^3)	769.08 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	12.49
Crystal size (mm)	0.18 × 0.14 × 0.08
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2020)
T_{min}, T_{max}	0.341, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6293, 1495, 1485
R_{int}	0.056
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.097, 1.09
No. of reflections	1495
No. of parameters	90
No. of restraints	5
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.63, −0.48
Absolute structure	Flack x determined using 579 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).
Absolute structure parameter	0.03 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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The authors' contributions are as follows; conceptualization BT, MA and GMM; synthesis, KIH and BT; X-ray analysis JA and SK; founding KIH and BT; writing (review and editing of the manuscript) BT, and MA; supervision SK, MA and GMM.

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supporting information

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Crystal structure and Hirshfeld surface analysis of 2-amino-5-bromo-1,3,4-triazol-3-ium chloride monohydrate

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Computing details

2-Amino-5-bromo-1,3,4-triazol-3-ium chloride monohydrate

Crystal data

$C_2H_3BrN_3S^+\cdot Cl^-\cdot H_2O$
$M_r = 234.51$
Orthorhombic, $P2_12_12_1$
$a = 5.3575$ (1) Å
$b = 9.5328$ (1) Å
$c = 15.0588$ (2) Å
$V = 769.08$ (2) Å^3
$Z = 4$
$F(000) = 456$

$D_x = 2.025$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 6428 reflections
$\theta = 2.9$–$71.3°$
$\mu = 12.49$ mm^{-1}
$T = 293$ K
Block, colourles
0.18 × 0.14 × 0.08 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2020)

$T_{\min} = 0.341$, $T_{\max} = 1.000$
6293 measured reflections
1495 independent reflections
1485 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.056$
$\theta_{\max} = 71.4°$, $\theta_{\min} = 5.5°$
$h = -5 \rightarrow 6$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.097$
$S = 1.09$
1495 reflections
90 parameters
5 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.3887P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.63$ e Å^{-3}
$\Delta\rho_{\min} = -0.48$ e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0048 (8)
Absolute structure: Flack x determined using 579 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).
Absolute structure parameter: 0.03 (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	$U_{\rm iso}$*/$U_{\rm eq}$
Br1	0.29817 (13)	−0.05893 (6)	0.45541 (4)	0.0458 (3)
Cl1	1.2003 (2)	0.21834 (13)	0.18983 (8)	0.0381 (4)
S1	0.7039 (2)	0.11486 (12)	0.35421 (8)	0.0319 (3)
O1	0.3054 (8)	0.5998 (4)	0.3940 (3)	0.0435 (9)
H1A	0.431399	0.647416	0.377691	0.065*
H1B	0.180495	0.648222	0.377514	0.065*
N1	0.4579 (7)	0.3315 (4)	0.3915 (3)	0.0269 (8)
N2	0.3207 (8)	0.2273 (4)	0.4298 (3)	0.0288 (8)
N3	0.8144 (10)	0.3806 (5)	0.3069 (3)	0.0420 (11)
H3A	0.785060	0.469288	0.306957	0.050*
H3B	0.943662	0.348223	0.279993	0.050*
C1	0.6621 (8)	0.2948 (5)	0.3479 (3)	0.0254 (9)
C2	0.4283 (9)	0.1099 (5)	0.4153 (3)	0.0280 (10)
H1	0.406 (12)	0.414 (3)	0.394 (4)	0.036 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0516 (4)	0.0277 (4)	0.0581 (4)	−0.0044 (3)	0.0093 (3)	0.0041 (2)
Cl1	0.0264 (5)	0.0377 (7)	0.0501 (7)	0.0046 (5)	−0.0006 (5)	−0.0154 (5)
S1	0.0258 (5)	0.0263 (6)	0.0435 (6)	0.0058 (5)	0.0041 (5)	−0.0054 (5)
O1	0.0295 (17)	0.0276 (19)	0.073 (3)	0.0051 (16)	0.006 (2)	0.0073 (17)
N1	0.0231 (17)	0.022 (2)	0.036 (2)	0.0028 (16)	0.0047 (16)	−0.0036 (15)
N2	0.0259 (19)	0.026 (2)	0.0342 (19)	−0.0007 (17)	0.0043 (16)	−0.0015 (16)
N3	0.036 (2)	0.030 (2)	0.060 (3)	0.001 (2)	0.022 (2)	−0.006 (2)
C1	0.019 (2)	0.024 (2)	0.033 (2)	−0.0016 (17)	0.0011 (17)	−0.0043 (18)
C2	0.026 (2)	0.027 (2)	0.031 (2)	0.001 (2)	−0.0031 (18)	−0.0049 (18)

Geometric parameters (Å, º)

Br1—C2	1.855 (5)	N1—C1	1.323 (6)
S1—C1	1.733 (5)	N1—H1	0.83 (3)
S1—C2	1.740 (5)	N2—C2	1.277 (7)
O1—H1A	0.8500	N3—H3A	0.8600
O1—H1B	0.8501	N3—H3B	0.8600
N1—N2	1.364 (6)	N3—C1	1.309 (7)
C1—S1—C2	86.9 (2)	C1—N3—H3B	120.0
H1A—O1—H1B	104.5	N1—C1—S1	110.0 (4)

N2—N1—H1	119 (5)	N3—C1—S1	124.3 (4)
C1—N1—N2	117.5 (4)	N3—C1—N1	125.7 (5)
C1—N1—H1	123 (5)	S1—C2—Br1	121.0 (3)
C2—N2—N1	108.9 (4)	N2—C2—Br1	122.4 (4)
H3A—N3—H3B	120.0	N2—C2—S1	116.7 (4)
C1—N3—H3A	120.0		

N1—N2—C2—Br1	−179.2 (3)	C1—S1—C2—N2	−0.6 (4)
N1—N2—C2—S1	−0.1 (5)	C1—N1—N2—C2	1.0 (6)
N2—N1—C1—S1	−1.4 (5)	C2—S1—C1—N1	1.1 (4)
N2—N1—C1—N3	179.6 (5)	C2—S1—C1—N3	−180.0 (5)
C1—S1—C2—Br1	178.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1$^{\mathrm{i}}$	0.85	2.32	3.144 (4)	163
O1—H1*B*···Cl1$^{\mathrm{ii}}$	0.85	2.37	3.196 (4)	163
N3—H3*A*···Cl1$^{\mathrm{i}}$	0.86	2.38	3.221 (5)	168
N3—H3*B*···Cl1	0.86	2.29	3.127 (5)	163
N1—H1···O1	0.83 (3)	1.86 (3)	2.685 (6)	176 (7)

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