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Sodium *N*-bromo-2-chlorobenzene-sulfonamidate sesquihydrateB. Thimme Gowda,^{a*} Sabine Foro^b and K. Shakuntala^a^aDepartment of Chemistry, Mangalore University, Mangalagangothri 574 199, Mangalore, India, and ^bInstitute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany

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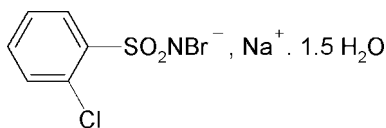
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.049; wR factor = 0.128; data-to-parameter ratio = 15.2.

In the title compound, $\text{Na}^+\cdot\text{C}_6\text{H}_4\text{BrClNO}_2\text{S}^-\cdot 1.5\text{H}_2\text{O}$, one water molecule has crystallographically imposed twofold symmetry. The Na^+ cation shows a pseudo-octahedral coordination provided by three O atoms of water molecules and three sulfonyl O atoms of different *N*-bromo-2-chlorobenzene-sulfonamidate anions. The S–N distance of 1.579 (6) Å is consistent with an S=N double-bond character. The crystal structure is stabilized by O–H...Br, O–H...N and O–H...O hydrogen bonds.

Related literature

For background to the chemistry of *N*-haloarylsulfonamides, see: Gowda & Shetty (2004); Usha & Gowda (2006). For our study of the effect of substituents on the structures of *N*-haloarylsulfonamides, see: Gowda, Kožíšek *et al.* (2007); Gowda, Usha *et al.* (2007). For related structures, see: George *et al.* (2000); Olmstead & Power (1986). For an isostructural compound, see: Gowda *et al.* (2010).



Experimental

Crystal data

$\text{Na}^+\cdot\text{C}_6\text{H}_4\text{BrClNO}_2\text{S}^-\cdot 1.5\text{H}_2\text{O}$
 $M_r = 319.53$
 Monoclinic, $C2/c$
 $a = 11.200$ (2) Å
 $b = 6.728$ (1) Å

$c = 28.304$ (3) Å
 $\beta = 100.94$ (1)°
 $V = 2094.0$ (5) Å³
 $Z = 8$
 Mo $K\alpha$ radiation

$\mu = 4.41$ mm⁻¹
 $T = 293$ K

0.34 × 0.30 × 0.14 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD area detector
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
 $T_{\text{min}} = 0.316$, $T_{\text{max}} = 0.578$

7442 measured reflections
 2147 independent reflections
 1955 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.128$
 $S = 1.25$
 2147 reflections
 141 parameters
 4 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 2.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3–H31 ⁱ ···Br ¹	0.82 (2)	2.70 (2)	3.518 (5)	171 (8)
O3–H32 ⁱ ···N1	0.81 (2)	2.21 (5)	2.934 (7)	149 (8)
O3–H32 ⁱ ···O2	0.81 (2)	2.51 (5)	3.232 (7)	148 (8)
O4–H41 ⁱ ···N1 ⁱⁱ	0.82 (2)	2.20 (3)	3.002 (7)	168 (8)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2602).

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supporting information

Acta Cryst. (2011). E67, m870 [doi:10.1107/S160053681102071X]

Sodium *N*-bromo-2-chlorobenzenesulfonamidate sesquihydrate

B. Thimme Gowda, Sabine Foro and K. Shakuntala

S1. Comment

The chemistry of *N*-halo arylsulfonamides are of interest in synthetic, mechanistic, analytical and biological chemistry (Gowda & Shetty, 2004; Usha & Gowda, 2006). In the present work, as a part of exploring the substituent effects on the crystal structures of *N*-haloarylsulfonamidates, the structure of sodium *N*-bromo-2-chlorobenzenesulfonamidate (I) has been determined (Fig. 1). The structure of (I) resembles those of sodium *N*-bromo-benzenesulfonamidate (II) (Gowda, Usha et al., 2007), sodium *i*-*N*-bromo-4-chlorobenzenesulfonamidate (III) (Gowda, Kožíšek et al., 2007) and other sodium *N*-chloro-arylsulfonamidates (George et al., 2000; Olmstead & Power, 1986), and is isostructural with the previously reported *N*-chloro-2-chloro-benzenesulfonamidate (Gowda et al., 2010) (IV).

In the title compound, one water molecule (O4) has crystallographically imposed twofold axis. The sodium ion shows octahedral coordination by three O atoms of water molecules and by three sulfonyl O atoms of three different *N*-bromo-2-chloro-benzenesulfonamide anions.

There is no interaction between the N and Na atoms in the molecule. The S—N distance of N1—S1, 1.579 (6) Å is consistent with a S—N double bond and is in agreement with the observed values of 1.578 (4) Å in (II), 1.588 (2) Å in (IV), and N1—S1, 1.574 (5) Å and N2—S2 1.579 (4) Å in (III).

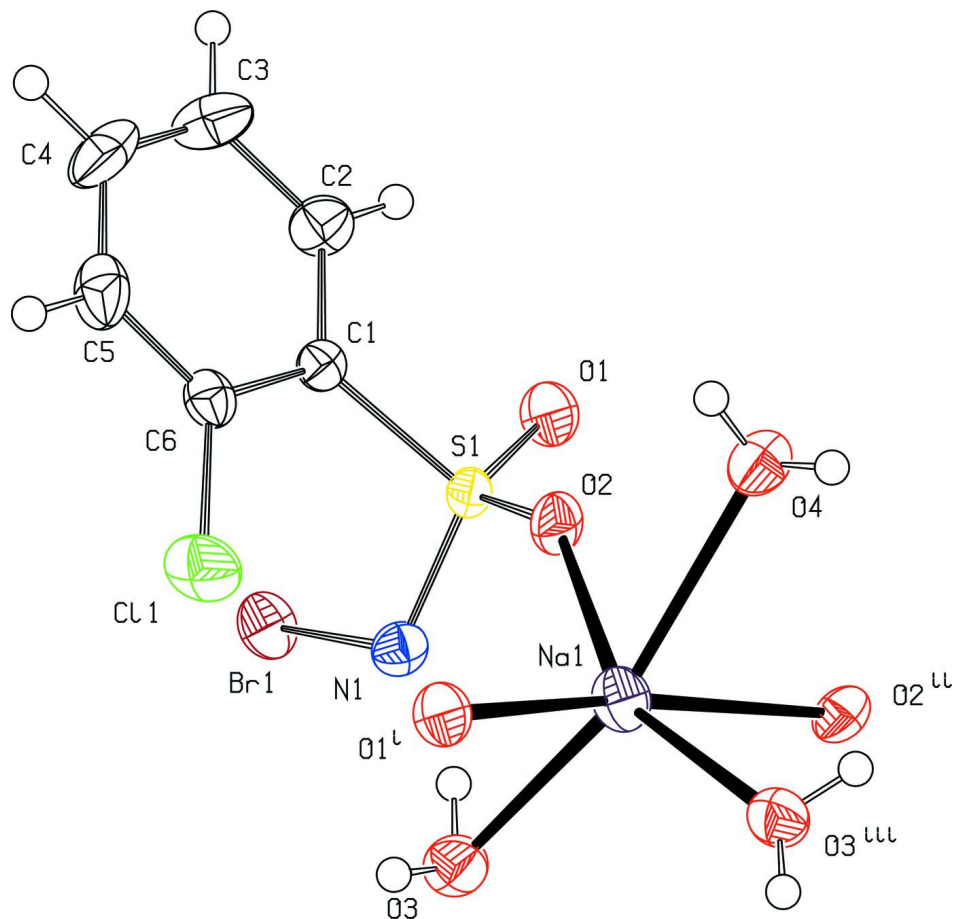
The crystal packing consists of a two-dimensional polymeric layers running parallel to the *ac* plane (Fig. 2). The molecular packing is stabilized by O3—H31⋯Br1, O3—H32⋯N1, O3—H32⋯O2 and O4—H41⋯N1 hydrogen bonds (Table 1).

S2. Experimental

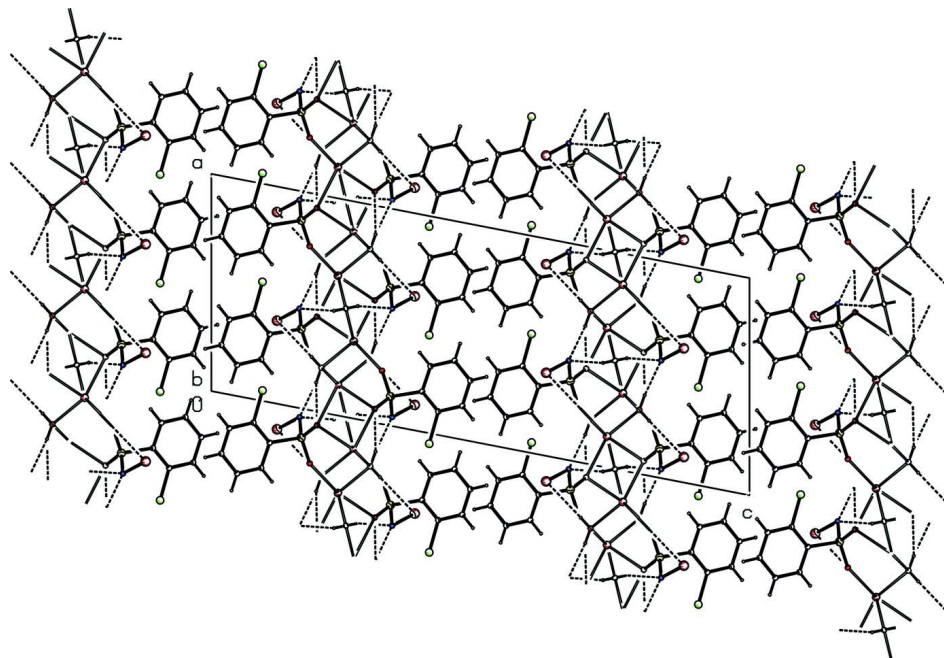
The title compound was prepared according to the literature method (Usha & Gowda, 2006). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. Prism like yellow single crystals of the title compound used in X-ray diffraction studies were obtained from slow evaporation of its aqueous solution at room temperature.

S3. Refinement

The H atoms bound to O3 were located in a difference Fourier map and later restrained to O—H = 0.82 (2) Å and H—H distance was restrained to 1.365 Å. The H atom bound to O4 was located in difference map and later restrained to O—H = 0.82 (2) Å. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å. All H atoms were refined with isotropic displacement parameters set to 1.2 times of the U_{eq} of the parent atoms. The residual electron-density features are located in the region of S1. The highest peak and the deepest hole are at 1.43 and 1.09 Å from S1, respectively.

**Figure 1**

The molecular structure of the title compound, showing the asymmetric unit extended to show the coordination geometry for the Na^+ ion. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii (symmetry codes: (i) $x + 1/2, y - 1/2, z$; (ii) $-x + 2, y, -z + 3/2$; (iii) $-x + 5/2, y - 1/2, -z + 3/2$).

**Figure 2**

Crystal packing of the title compound with hydrogen bonding shown as dashed lines.

Sodium *N*-bromo-2-chlorobenzenesulfonamidate sesquihydrate

Crystal data

$\text{Na}^+ \cdot \text{C}_6\text{H}_4\text{BrClNO}_2\text{S}^- \cdot 1.5\text{H}_2\text{O}$

$M_r = 319.53$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 11.200\ (2)\ \text{\AA}$

$b = 6.728\ (1)\ \text{\AA}$

$c = 28.304\ (3)\ \text{\AA}$

$\beta = 100.94\ (1)^\circ$

$V = 2094.0\ (5)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1256$

$D_x = 2.027\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 4107 reflections

$\theta = 2.9\text{--}27.8^\circ$

$\mu = 4.41\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, yellow

$0.34 \times 0.30 \times 0.14\ \text{mm}$

Data collection

Oxford Diffraction Xcalibur

diffractometer with Sapphire CCD area detector

Radiation source: fine-focus sealed tube

Graphite monochromator

rotation method data acquisition using ω scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.316$, $T_{\max} = 0.578$

7442 measured reflections

2147 independent reflections

1955 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -13 \rightarrow 13$

$k = -8 \rightarrow 7$

$l = -35 \rightarrow 35$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.128$

$S = 1.25$

2147 reflections

141 parameters

4 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: inferred from neighbouring sites
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0182P)^2 + 43.7119P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 2.27 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.19 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. CrysAlis RED (Oxford Diffraction, 2009) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8143 (5)	-0.3307 (9)	0.6083 (2)	0.0205 (12)
C2	0.6903 (6)	-0.3509 (11)	0.5927 (2)	0.0311 (14)
H2	0.6375	-0.3101	0.6125	0.037*
C3	0.6437 (7)	-0.4309 (13)	0.5480 (3)	0.0433 (19)
H3	0.5600	-0.4409	0.5377	0.052*
C4	0.7209 (8)	-0.4957 (12)	0.5187 (3)	0.044 (2)
H4	0.6892	-0.5508	0.4888	0.053*
C5	0.8449 (8)	-0.4791 (11)	0.5336 (3)	0.0374 (17)
H5	0.8971	-0.5243	0.5140	0.045*
C6	0.8919 (6)	-0.3942 (9)	0.5782 (2)	0.0249 (13)
Br1	0.88260 (6)	0.14784 (10)	0.62206 (2)	0.0312 (2)
N1	0.9583 (5)	-0.0535 (8)	0.66407 (18)	0.0247 (11)
Na1	1.1437 (2)	-0.5132 (4)	0.73529 (9)	0.0303 (6)
O1	0.7549 (4)	-0.1730 (8)	0.68272 (16)	0.0324 (11)
O2	0.9370 (4)	-0.3782 (7)	0.69654 (15)	0.0286 (10)
O3	1.2055 (4)	-0.1890 (8)	0.70471 (17)	0.0335 (11)
H31	1.246 (5)	-0.241 (12)	0.687 (2)	0.040*
H32	1.1325 (19)	-0.199 (12)	0.695 (2)	0.040*
O4	1.0000	-0.7830 (10)	0.7500	0.0336 (16)
H41	0.979 (7)	-0.861 (9)	0.728 (2)	0.040*
S1	0.86584 (13)	-0.2281 (2)	0.66713 (5)	0.0198 (3)
Cl1	1.04842 (16)	-0.3824 (3)	0.59503 (7)	0.0414 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.023 (3)	0.017 (3)	0.021 (3)	0.001 (2)	0.003 (2)	0.002 (2)
C2	0.026 (3)	0.033 (4)	0.033 (3)	0.004 (3)	0.003 (3)	0.000 (3)

C3	0.030 (4)	0.050 (5)	0.045 (4)	-0.004 (4)	-0.007 (3)	-0.009 (4)
C4	0.056 (5)	0.043 (5)	0.027 (4)	-0.005 (4)	-0.009 (3)	-0.010 (3)
C5	0.055 (5)	0.032 (4)	0.028 (4)	-0.001 (3)	0.017 (3)	-0.005 (3)
C6	0.030 (3)	0.020 (3)	0.026 (3)	0.000 (3)	0.009 (3)	0.002 (2)
Br1	0.0358 (4)	0.0245 (3)	0.0342 (4)	0.0033 (3)	0.0092 (3)	0.0072 (3)
N1	0.022 (3)	0.025 (3)	0.025 (3)	0.003 (2)	0.001 (2)	0.002 (2)
Na1	0.0299 (14)	0.0312 (14)	0.0320 (14)	0.0047 (11)	0.0114 (11)	-0.0007 (11)
O1	0.030 (2)	0.040 (3)	0.030 (2)	0.001 (2)	0.0131 (19)	-0.006 (2)
O2	0.033 (2)	0.028 (2)	0.023 (2)	0.002 (2)	0.0021 (18)	0.0075 (19)
O3	0.027 (2)	0.039 (3)	0.034 (3)	0.002 (2)	0.006 (2)	-0.003 (2)
O4	0.044 (4)	0.024 (4)	0.030 (4)	0.000	0.000 (3)	0.000
S1	0.0209 (7)	0.0215 (7)	0.0170 (7)	0.0005 (6)	0.0038 (5)	0.0002 (6)
Cl1	0.0280 (8)	0.0478 (11)	0.0522 (11)	0.0018 (8)	0.0174 (8)	-0.0107 (9)

Geometric parameters (Å, °)

C1—C2	1.382 (9)	Na1—O3 ⁱⁱⁱ	2.459 (5)
C1—C6	1.393 (8)	Na1—O3	2.493 (6)
C1—S1	1.793 (6)	Na1—O4	2.512 (6)
C2—C3	1.383 (10)	Na1—O2	2.534 (5)
C2—H2	0.9300	Na1—S1 ⁱⁱ	3.381 (3)
C3—C4	1.378 (12)	Na1—H32	2.40 (9)
C3—H3	0.9300	O1—S1	1.444 (5)
C4—C5	1.378 (11)	O1—Na1 ^{iv}	2.371 (5)
C4—H4	0.9300	O2—S1	1.448 (5)
C5—C6	1.396 (9)	O2—Na1 ⁱⁱ	2.455 (5)
C5—H5	0.9300	O3—Na1 ^v	2.459 (5)
C6—Cl1	1.729 (7)	O3—H31	0.82 (2)
Br1—N1	1.893 (5)	O3—H32	0.81 (2)
N1—S1	1.579 (6)	O4—Na1 ⁱⁱ	2.512 (6)
Na1—O1 ⁱ	2.371 (5)	O4—H41	0.82 (2)
Na1—O2 ⁱⁱ	2.455 (5)	S1—Na1 ⁱⁱ	3.381 (3)
C2—C1—C6	118.6 (6)	O2 ⁱⁱ —Na1—S1 ⁱⁱ	22.28 (11)
C2—C1—S1	117.5 (5)	O3 ⁱⁱⁱ —Na1—S1 ⁱⁱ	80.37 (14)
C6—C1—S1	123.9 (5)	O3—Na1—S1 ⁱⁱ	80.85 (13)
C1—C2—C3	120.9 (6)	O4—Na1—S1 ⁱⁱ	98.86 (11)
C1—C2—H2	119.6	O2—Na1—S1 ⁱⁱ	88.99 (13)
C3—C2—H2	119.6	O1 ⁱ —Na1—H32	94.9 (14)
C4—C3—C2	120.2 (7)	O2 ⁱⁱ —Na1—H32	93.2 (15)
C4—C3—H3	119.9	O3 ⁱⁱⁱ —Na1—H32	136.1 (7)
C2—C3—H3	119.9	O3—Na1—H32	19.0 (5)
C5—C4—C3	120.1 (7)	O4—Na1—H32	137.7 (5)
C5—C4—H4	120.0	O2—Na1—H32	61.1 (5)
C3—C4—H4	120.0	S1 ⁱⁱ —Na1—H32	83.3 (15)
C4—C5—C6	119.7 (7)	S1—O1—Na1 ^{iv}	153.3 (3)
C4—C5—H5	120.2	S1—O2—Na1 ⁱⁱ	117.7 (3)
C6—C5—H5	120.2	S1—O2—Na1	149.0 (3)

C1—C6—C5	120.5 (6)	Na1 ⁱⁱ —O2—Na1	88.25 (17)
C1—C6—Cl1	122.4 (5)	Na1 ^v —O3—Na1	112.4 (2)
C5—C6—Cl1	117.1 (5)	Na1 ^v —O3—H31	104 (5)
S1—N1—Br1	110.3 (3)	Na1—O3—H31	94 (6)
O1 ⁱ —Na1—O2 ⁱⁱ	167.5 (2)	Na1 ^v —O3—H32	142 (5)
O1 ⁱ —Na1—O3 ⁱⁱⁱ	80.89 (18)	Na1—O3—H32	74 (6)
O2 ⁱⁱ —Na1—O3 ⁱⁱⁱ	86.70 (18)	H31—O3—H32	112 (4)
O1 ⁱ —Na1—O3	88.03 (19)	Na1—O4—Na1 ⁱⁱ	87.5 (3)
O2 ⁱⁱ —Na1—O3	96.71 (18)	Na1—O4—H41	116 (6)
O3 ⁱⁱⁱ —Na1—O3	117.45 (15)	Na1 ⁱⁱ —O4—H41	119 (6)
O1 ⁱ —Na1—O4	101.87 (19)	O1—S1—O2	114.5 (3)
O2 ⁱⁱ —Na1—O4	78.11 (16)	O1—S1—N1	115.9 (3)
O3 ⁱⁱⁱ —Na1—O4	85.18 (16)	O2—S1—N1	104.8 (3)
O3—Na1—O4	156.70 (19)	O1—S1—C1	103.8 (3)
O1 ⁱ —Na1—O2	115.86 (19)	O2—S1—C1	108.1 (3)
O2 ⁱⁱ —Na1—O2	76.42 (19)	N1—S1—C1	109.5 (3)
O3 ⁱⁱⁱ —Na1—O2	157.31 (19)	O1—S1—Na1 ⁱⁱ	74.5 (2)
O3—Na1—O2	80.02 (17)	N1—S1—Na1 ⁱⁱ	126.1 (2)
O4—Na1—O2	76.68 (15)	C1—S1—Na1 ⁱⁱ	119.0 (2)
O1 ⁱ —Na1—S1 ⁱⁱ	150.64 (16)		
C6—C1—C2—C3	-0.5 (10)	O1 ⁱ —Na1—O4—Na1 ⁱⁱ	-152.81 (18)
S1—C1—C2—C3	-179.3 (6)	O2 ⁱⁱ —Na1—O4—Na1 ⁱⁱ	39.93 (12)
C1—C2—C3—C4	1.4 (12)	O3 ⁱⁱⁱ —Na1—O4—Na1 ⁱⁱ	127.57 (16)
C2—C3—C4—C5	-0.7 (13)	O3—Na1—O4—Na1 ⁱⁱ	-39.3 (4)
C3—C4—C5—C6	-0.8 (12)	O2—Na1—O4—Na1 ⁱⁱ	-38.72 (11)
C2—C1—C6—C5	-1.0 (10)	S1 ⁱⁱ —Na1—O4—Na1 ⁱⁱ	48.11 (6)
S1—C1—C6—C5	177.7 (5)	Na1 ^{iv} —O1—S1—O2	73.2 (8)
C2—C1—C6—Cl1	-178.1 (5)	Na1 ^{iv} —O1—S1—N1	-49.0 (8)
S1—C1—C6—Cl1	0.6 (8)	Na1 ^{iv} —O1—S1—C1	-169.1 (7)
C4—C5—C6—C1	1.6 (11)	Na1 ^{iv} —O1—S1—Na1 ⁱⁱ	74.1 (7)
C4—C5—C6—Cl1	178.9 (6)	Na1 ⁱⁱ —O2—S1—O1	1.2 (4)
O1 ⁱ —Na1—O2—S1	-74.9 (6)	Na1—O2—S1—O1	-142.6 (5)
O2 ⁱⁱ —Na1—O2—S1	107.4 (5)	Na1 ⁱⁱ —O2—S1—N1	129.4 (3)
O3 ⁱⁱⁱ —Na1—O2—S1	150.4 (5)	Na1—O2—S1—N1	-14.4 (6)
O3—Na1—O2—S1	8.0 (6)	Na1 ⁱⁱ —O2—S1—C1	-113.9 (3)
O4—Na1—O2—S1	-171.8 (6)	Na1—O2—S1—C1	102.3 (6)
S1 ⁱⁱ —Na1—O2—S1	88.9 (6)	Na1—O2—S1—Na1 ⁱⁱ	-143.8 (7)
O1 ⁱ —Na1—O2—Na1 ⁱⁱ	136.66 (17)	Br1—N1—S1—O1	-57.6 (4)
O2 ⁱⁱ —Na1—O2—Na1 ⁱⁱ	-41.0 (2)	Br1—N1—S1—O2	175.1 (3)
O3 ⁱⁱⁱ —Na1—O2—Na1 ⁱⁱ	2.0 (6)	Br1—N1—S1—C1	59.4 (4)
O3—Na1—O2—Na1 ⁱⁱ	-140.47 (18)	Br1—N1—S1—Na1 ⁱⁱ	-146.92 (16)
O4—Na1—O2—Na1 ⁱⁱ	39.77 (14)	C2—C1—S1—O1	-5.0 (6)
S1 ⁱⁱ —Na1—O2—Na1 ⁱⁱ	-59.58 (15)	C6—C1—S1—O1	176.3 (5)
O1 ⁱ —Na1—O3—Na1 ^v	-108.3 (2)	C2—C1—S1—O2	117.0 (5)
O2 ⁱⁱ —Na1—O3—Na1 ^v	60.1 (2)	C6—C1—S1—O2	-61.7 (6)
O3 ⁱⁱⁱ —Na1—O3—Na1 ^v	-29.7 (2)	C2—C1—S1—N1	-129.4 (5)
O4—Na1—O3—Na1 ^v	135.6 (4)	C6—C1—S1—N1	51.9 (6)

O2—Na1—O3—Na1 ^v	135.0 (2)	C2—C1—S1—Na1 ⁱⁱ	74.7 (5)
S1 ⁱⁱ —Na1—O3—Na1 ^v	44.40 (17)	C6—C1—S1—Na1 ⁱⁱ	-103.9 (5)

Symmetry codes: (i) $x+1/2, y-1/2, z$; (ii) $-x+2, y, -z+3/2$; (iii) $-x+5/2, y-1/2, -z+3/2$; (iv) $x-1/2, y+1/2, z$; (v) $-x+5/2, y+1/2, -z+3/2$.

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O3—H31...Br1 ⁱ	0.82 (2)	2.70 (2)	3.518 (5)	171 (8)
O3—H32...N1	0.81 (2)	2.21 (5)	2.934 (7)	149 (8)
O3—H32...O2	0.81 (2)	2.51 (5)	3.232 (7)	148 (8)
O4—H41...N1 ^{vi}	0.82 (2)	2.20 (3)	3.002 (7)	168 (8)

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