metal-organic compounds

Potassium N-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate

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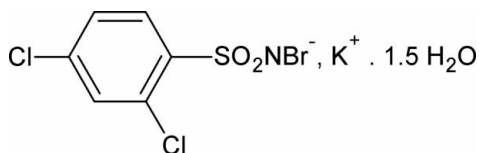Correspondence e-mail: gowdabt@yahoo.com

The asymmetric unit of the title salt, $K^+ \cdot C_6H_3BrCl_2NO_2S^- \cdot 1.5H_2O$, contains one K^+ cation, one N-bromo-2,4-dichlorobenzenesulfonamidate anion, one water molecule in general position and one water molecule located on a twofold rotation axis. The K^+ cation is hepta-coordinated by three water O atoms and four sulfonyl O atoms from three symmetry-related N-bromo-2,4-dichlorobenzenesulfonamide anions. The S=N distance of 1.575 (3) Å is consistent with that of a double bond. In the crystal, the anions are linked by O—H···Br and O—H···N hydrogen bonds into layers parallel to the *ac* plane.

Related literature

For preparation of N-haloarylsulfonamides, see: Gowda & Mahadevappa (1983). For studies of the effect of substituents on the structures of N-haloarylsulfonamides, see: George *et al.* (2000); Gowda *et al.* (2007, 2011*a*,*b*); Olmstead & Power (1986).

Experimental

Crystal data

$K^+ \cdot C_6H_3BrCl_2NO_2S^- \cdot 1.5H_2O$	$b = 6.7638$ (4) Å
$M_r = 740.18$	$c = 29.703$ (2) Å
Monoclinic, $C2/c$	$\beta = 98.352$ (5)°
$a = 12.5263$ (7) Å	$V = 2489.9$ (3) Å³

$Z = 4$	$T = 293$ K
Mo $K\alpha$ radiation	$0.32 \times 0.32 \times 0.28$ mm
$\mu = 4.22$ mm^{-1}	

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector	Diffraction, 2009)
	$T_{min} = 0.345$, $T_{max} = 0.384$
	4960 measured reflections
Absorption correction: multi-scan (*CrysAlis RED*; Oxford	2535 independent reflections
	2204 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.014$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.093$	
$S = 1.09$	
2535 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
150 parameters	$\Delta\rho_{min} = -0.65$ e Å^{-3}
3 restraints	

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···Br1[i]	0.80 (2)	2.78 (2)	3.550 (3)	160 (4)
O3—H32···N1	0.81 (2)	2.15 (3)	2.917 (4)	158 (5)
O4—H41···N1[ii]	0.82 (2)	2.16 (2)	2.957 (3)	165 (5)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2295).

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supporting information

Potassium *N*-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate

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S1. Comment

The present work was undertaken in order to explore the effect of replacing sodium ion by potassium ion on the solid state structures of metal salts of *N*-haloarylsulfonamidates (Gowda *et al.*, 2007, 2011*a*,*b*). As part of this work, the structure of potassium *N*-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate (I) has been determined (Fig. 1). The structure of (I) resembles those of potassium *N*-bromo-2-chlorobenzenesulfonamidate sesquihydrate (II) (Gowda *et al.*, 2011*a*), potassium *N*-bromo-4-chlorobenzenesulfonamidate sesquihydrate (III) (Gowda *et al.*, 2011*b*), sodium *N*-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate (IV) (Gowda *et al.*, 2007) and other sodium *N*-chloro-aryl-sulfonamidates (George *et al.*, 2000; Olmstead & Power, 1986).

In the title compound, K$^+$ ion is hepta coordinated by three O atoms from water molecules and four sulfonyl O atoms of three different *N*-bromo-2,4-dichlorobenzenesulfonamide anions. The replacement of Na$^+$ by K$^+$ changes co-ordination from hexa to hepta in the structure (Gowda *et al.*, 2007) and other parameters.

The S—N distance of 1.575 (3) Å is consistent with a S—N double bond and is in agreement with the observed values of 1.582 (4) Å in (II), 1.584 (6) Å in (III) and 1.590 (6) Å in (IV).

The asymmetric unit of (I) consists of one potassium cation, one *N*-bromo-2,4-dichlorobenzenesulfonamidate anion and one water molecule in general position and and one water molecule located on a twofold rotation axis.

In the crystal structure the anions are linked by intermolecular O—H⋯Br and O—H⋯N hydrogen bonding into layers, that are parallel to the *ac* plane (Fig. 2 and Table 1).
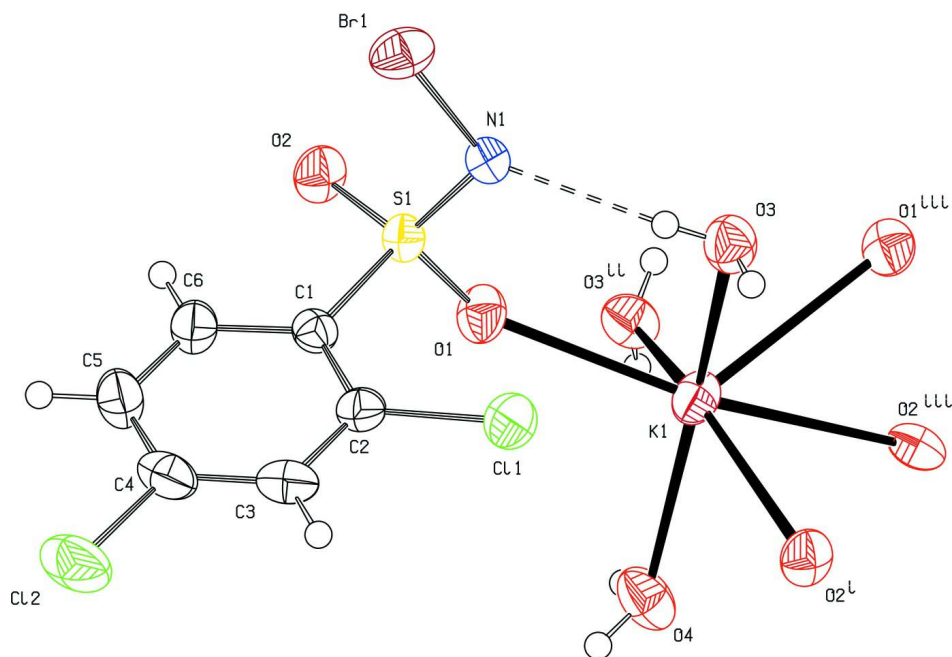
S2. Experimental

The title compound was prepared by a method similar to the one described by Gowda & Mahadevappa (Gowda & Mahadevappa, 1983). 2 g of 2,4-dichlorobenzenesulfonamide was dissolved with stirring in 40 ml of 5*M* KOH at room temperature. The resultant solution was cooled in ice and 4 ml of liquid bromine was added drop wise with constant stirring. The resultant potassium salt of *N*-bromo-2,4-dichlorobenzenesulfonamide was filtered under suction, washed quickly with a minimum quantity of ice cold water. The purity of the compound was checked by determining its melting point (203–205° C) and estimating, iodometrically, the amount of active bromine present in it. It was further characterized from its infrared spectrum.

Prism like yellow single crystals of the title compound used in the X-ray diffraction studies were obtained from its aqueous solution at room temperature.

S3. Refinement

H atoms bonded to C were positioned with idealized geometry using a riding model with the aromatic C—H = 0.93 Å. The H atoms bound to O atoms were located in difference map and later restrained to O—H = 0.82 (2) Å. All H atoms were refined with isotropic displacement parameters set at 1.2 U_{eq} of the parent atom.

Figure 1

Molecular structure of the title compound, showing the atom labelling scheme for the asymmetric unit and extended to show the coordination geometry for the K^+. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii.

Figure 2

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

Potassium *N*-bromo-2,4-dichlorobenzenesulfonamidate sesquihydrate

Crystal data

K⁺·C₆H₃BrCl₂NO₂S⁻·1.5H₂O	$F(000) = 1448$
$M_r = 740.18$	$D_x = 1.975$ Mg m⁻³
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 2489 reflections
$a = 12.5263$ (7) Å	$\theta = 3.0–27.7°$
$b = 6.7638$ (4) Å	$\mu = 4.22$ mm⁻¹
$c = 29.703$ (2) Å	$T = 293$ K
$\beta = 98.352$ (5)°	Prism, yellow
$V = 2489.9$ (3) Å³	$0.32 \times 0.32 \times 0.28$ mm
$Z = 4$	

K⁺·C₆H₃BrCl₂NO₂S⁻·1.5H₂O, $M_r = 740.18$, Monoclinic, $C2/c$. Hall symbol: -C 2yc. $a = 12.5263$ (7) Å, $b = 6.7638$ (4) Å, $c = 29.703$ (2) Å, $\beta = 98.352$ (5)°, $V = 2489.9$ (3) Å³, $Z = 4$. $F(000) = 1448$, $D_x = 1.975$ Mg m⁻³, Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å, cell parameters from 2489 reflections, $\theta = 3.0–27.7°$, $\mu = 4.22$ mm⁻¹, $T = 293$ K. Prism, yellow, $0.32 \times 0.32 \times 0.28$ mm.

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector	4960 measured reflections
Radiation source: fine-focus sealed tube	2535 independent reflections
Graphite monochromator	2204 reflections with $I > 2\sigma(I)$
Rotation method data acquisition using ω scans.	$R_{int} = 0.014$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)	$\theta_{max} = 26.4°$, $\theta_{min} = 3.3°$
$T_{min} = 0.345$, $T_{max} = 0.384$	$h = -15 \rightarrow 13$
	$k = -8 \rightarrow 5$
	$l = -37 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.093$	$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 8.3581P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	
2535 reflections	$(\Delta/\sigma)_{max} = 0.001$
150 parameters	$\Delta\rho_{max} = 0.76$ e Å⁻³
3 restraints	$\Delta\rho_{min} = -0.65$ e Å⁻³
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. 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 (Å²)

	x	y	z	$U_{iso}*/U_{eq}$
C1	0.0780 (3)	0.4566 (5)	0.11591 (11)	0.0271 (7)
C2	0.1438 (3)	0.3775 (5)	0.08637 (12)	0.0317 (7)

C3	0.1538 (3)	0.4716 (6)	0.04598 (12)	0.0392 (9)
H3	0.1980	0.4192	0.0264	0.047*
C4	0.0974 (3)	0.6446 (6)	0.03496 (13)	0.0426 (9)
C5	0.0320 (3)	0.7248 (6)	0.06337 (14)	0.0447 (9)
H5	−0.0056	0.8413	0.0556	0.054*
C6	0.0228 (3)	0.6302 (5)	0.10361 (13)	0.0367 (8)
H6	−0.0214	0.6841	0.1230	0.044*
Br1	−0.11245 (3)	0.10625 (6)	0.130655 (14)	0.04440 (14)
Cl1	0.21550 (9)	0.15999 (15)	0.09788 (4)	0.0485 (3)
Cl2	0.10726 (10)	0.7571 (2)	−0.01671 (4)	0.0650 (4)
K1	0.34306 (6)	0.13766 (12)	0.23492 (3)	0.0366 (2)
N1	0.0277 (2)	0.1274 (4)	0.16389 (10)	0.0319 (6)
O1	0.1712 (2)	0.3416 (4)	0.19584 (8)	0.0386 (6)
O2	−0.0093 (2)	0.4804 (4)	0.18845 (8)	0.0383 (6)
O3	0.2037 (2)	−0.1486 (4)	0.19206 (10)	0.0426 (6)
H31	0.234 (3)	−0.195 (7)	0.1725 (12)	0.051*
H32	0.155 (3)	−0.088 (6)	0.1774 (14)	0.051*
O4	0.5000	0.4277 (6)	0.2500	0.0471 (10)
H41	0.490 (4)	0.502 (6)	0.2710 (11)	0.056*
S1	0.06429 (7)	0.34987 (12)	0.16983 (3)	0.02745 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0271 (16)	0.0256 (16)	0.0280 (16)	−0.0039 (13)	0.0014 (12)	−0.0003 (13)
C2	0.0261 (16)	0.0319 (18)	0.0371 (18)	−0.0031 (14)	0.0042 (14)	0.0000 (15)
C3	0.0350 (19)	0.048 (2)	0.0364 (19)	−0.0108 (17)	0.0109 (15)	−0.0008 (17)
C4	0.040 (2)	0.048 (2)	0.038 (2)	−0.0161 (18)	−0.0006 (16)	0.0113 (17)
C5	0.047 (2)	0.036 (2)	0.050 (2)	0.0043 (18)	0.0016 (18)	0.0116 (18)
C6	0.0359 (19)	0.0322 (18)	0.041 (2)	0.0040 (15)	0.0036 (15)	0.0029 (15)
Br1	0.0342 (2)	0.0494 (3)	0.0498 (2)	−0.00725 (17)	0.00672 (16)	−0.01193 (18)
Cl1	0.0484 (6)	0.0376 (5)	0.0645 (7)	0.0110 (4)	0.0250 (5)	0.0029 (5)
Cl2	0.0592 (7)	0.0857 (9)	0.0483 (6)	−0.0170 (6)	0.0024 (5)	0.0322 (6)
K1	0.0312 (4)	0.0354 (4)	0.0423 (4)	0.0051 (3)	0.0021 (3)	−0.0034 (3)
N1	0.0307 (15)	0.0279 (15)	0.0373 (16)	0.0006 (12)	0.0060 (12)	0.0047 (12)
O1	0.0373 (14)	0.0399 (14)	0.0353 (14)	0.0026 (11)	−0.0064 (11)	0.0010 (11)
O2	0.0444 (15)	0.0387 (14)	0.0339 (13)	0.0094 (12)	0.0130 (11)	−0.0046 (11)
O3	0.0475 (17)	0.0380 (15)	0.0434 (16)	0.0052 (12)	0.0099 (13)	0.0004 (12)
O4	0.073 (3)	0.031 (2)	0.041 (2)	0.000	0.022 (2)	0.000
S1	0.0302 (4)	0.0260 (4)	0.0260 (4)	0.0028 (3)	0.0033 (3)	0.0000 (3)

Geometric parameters (Å, º)

C1—C6	1.384 (5)	K1—O3	2.788 (3)
C1—C2	1.395 (5)	K1—O1[iii]	2.895 (3)
C1—S1	1.787 (3)	K1—O2[iii]	3.045 (3)
C2—C3	1.380 (5)	K1—S1[iii]	3.4910 (12)
C2—Cl1	1.732 (4)	N1—S1	1.575 (3)

C3—C4	1.381 (6)	O1—S1	1.447 (3)
C3—H3	0.9300	O1—K1ii	2.895 (3)
C4—C5	1.370 (6)	O2—S1	1.443 (3)
C4—Cl2	1.734 (4)	O2—K1iv	2.683 (2)
C5—C6	1.375 (5)	O2—K1ii	3.045 (3)
C5—H5	0.9300	O3—K1iii	2.740 (3)
C6—H6	0.9300	O3—H31	0.802 (19)
Br1—N1	1.890 (3)	O3—H32	0.808 (19)
K1—O1	2.675 (3)	O4—K1v	2.767 (3)
K1—O2i	2.683 (2)	O4—H41	0.820 (19)
K1—O3ii	2.740 (3)	S1—K1ii	3.4910 (12)
K1—O4	2.767 (3)		
C6—C1—C2	118.5 (3)	O3—K1—K1v	130.38 (6)
C6—C1—S1	118.0 (3)	O1iii—K1—K1v	90.06 (6)
C2—C1—S1	123.4 (3)	O2iii—K1—K1v	43.27 (5)
C3—C2—C1	120.4 (3)	S1iii—K1—K1v	66.97 (2)
C3—C2—Cl1	117.0 (3)	O1—K1—K1iii	94.01 (7)
C1—C2—Cl1	122.6 (3)	O2i—K1—K1iii	103.41 (6)
C2—C3—C4	119.3 (4)	O3ii—K1—K1iii	93.78 (7)
C2—C3—H3	120.4	O4—K1—K1iii	157.36 (5)
C4—C3—H3	120.4	O3—K1—K1iii	38.92 (6)
C5—C4—C3	121.4 (4)	O1iii—K1—K1iii	38.01 (5)
C5—C4—Cl2	119.8 (3)	O2iii—K1—K1iii	84.35 (5)
C3—C4—Cl2	118.8 (3)	S1iii—K1—K1iii	61.08 (2)
C4—C5—C6	118.9 (4)	K1v—K1—K1iii	120.90 (2)
C4—C5—H5	120.5	O1—K1—K1ii	41.78 (6)
C6—C5—H5	120.5	O2i—K1—K1ii	149.20 (6)
C5—C6—C1	121.5 (4)	O3ii—K1—K1ii	39.74 (6)
C5—C6—H6	119.2	O4—K1—K1ii	78.55 (6)
C1—C6—H6	119.2	O3—K1—K1ii	108.70 (7)
O1—K1—O2i	123.54 (8)	O1iii—K1—K1ii	107.85 (6)
O1—K1—O3ii	79.66 (9)	O2iii—K1—K1ii	117.01 (6)
O2i—K1—O3ii	149.20 (9)	S1iii—K1—K1ii	113.48 (3)
O1—K1—O4	102.28 (8)	K1v—K1—K1ii	120.90 (2)
O2i—K1—O4	80.66 (7)	K1iii—K1—K1ii	104.55 (3)
O3ii—K1—O4	74.11 (7)	S1—N1—Br1	111.33 (16)
O1—K1—O3	75.45 (8)	S1—O1—K1	151.14 (16)
O2i—K1—O3	85.56 (9)	S1—O1—K1ii	101.80 (13)
O3ii—K1—O3	122.44 (5)	K1—O1—K1ii	100.21 (8)
O4—K1—O3	161.68 (7)	S1—O2—K1iv	165.01 (16)
O1—K1—O1iii	122.42 (5)	S1—O2—K1ii	95.45 (12)
O2i—K1—O1iii	102.09 (8)	K1iv—O2—K1ii	85.68 (7)
O3ii—K1—O1iii	76.13 (8)	K1iii—O3—K1	101.34 (10)
O4—K1—O1iii	119.42 (6)	K1iii—O3—H31	123 (4)
O3—K1—O1iii	75.21 (8)	K1—O3—H31	106 (4)
O1—K1—O2iii	157.55 (8)	K1iii—O3—H32	117 (4)
O2i—K1—O2iii	78.37 (9)	K1—O3—H32	106 (3)

O3ⁱⁱ—K1—O2ⁱⁱⁱ	78.12 (8)	H31—O3—H32	102 (5)
O4—K1—O2ⁱⁱⁱ	74.58 (7)	K1—O4—K1ᵛ	89.71 (12)
O3—K1—O2ⁱⁱⁱ	114.43 (8)	K1—O4—H41	112 (3)
O1ⁱⁱⁱ—K1—O2ⁱⁱⁱ	48.19 (7)	K1ᵛ—O4—H41	119 (3)
O1—K1—S1ⁱⁱⁱ	142.27 (7)	O2—S1—O1	114.34 (16)
O2ⁱ—K1—S1ⁱⁱⁱ	91.31 (6)	O2—S1—N1	115.83 (16)
O3ⁱⁱ—K1—S1ⁱⁱⁱ	74.74 (7)	O1—S1—N1	104.73 (16)
O4—K1—S1ⁱⁱⁱ	96.86 (5)	O2—S1—C1	104.25 (15)
O3—K1—S1ⁱⁱⁱ	95.47 (7)	O1—S1—C1	107.00 (16)
O1ⁱⁱⁱ—K1—S1ⁱⁱⁱ	23.94 (5)	N1—S1—C1	110.46 (16)
O2ⁱⁱⁱ—K1—S1ⁱⁱⁱ	24.30 (5)	O2—S1—K1ⁱⁱ	60.25 (11)
O1—K1—K1ᵛ	145.05 (6)	O1—S1—K1ⁱⁱ	54.26 (11)
O2ⁱ—K1—K1ᵛ	51.05 (6)	N1—S1—K1ⁱⁱ	132.87 (12)
O3ⁱⁱ—K1—K1ᵛ	98.18 (7)	C1—S1—K1ⁱⁱ	115.93 (11)
O4—K1—K1ᵛ	45.15 (6)		
C6—C1—C2—C3	0.3 (5)	S1ⁱⁱⁱ—K1—O3—K1ⁱⁱⁱ	26.89 (8)
S1—C1—C2—C3	−177.6 (3)	K1ᵛ—K1—O3—K1ⁱⁱⁱ	91.14 (10)
C6—C1—C2—Cl1	−179.3 (3)	K1ⁱⁱ—K1—O3—K1ⁱⁱⁱ	−90.17 (8)
S1—C1—C2—Cl1	2.9 (4)	O1—K1—O4—K1ᵛ	−165.19 (7)
C1—C2—C3—C4	−0.3 (5)	O2ⁱ—K1—O4—K1ᵛ	−42.70 (6)
Cl1—C2—C3—C4	179.3 (3)	O3ⁱⁱ—K1—O4—K1ᵛ	119.46 (7)
C2—C3—C4—C5	0.1 (6)	O3—K1—O4—K1ᵛ	−84.4 (3)
C2—C3—C4—Cl2	−178.0 (3)	O1ⁱⁱⁱ—K1—O4—K1ᵛ	55.99 (7)
C3—C4—C5—C6	0.0 (6)	O2ⁱⁱⁱ—K1—O4—K1ᵛ	37.71 (5)
Cl2—C4—C5—C6	178.1 (3)	S1ⁱⁱⁱ—K1—O4—K1ᵛ	47.51 (2)
C4—C5—C6—C1	−0.1 (6)	K1ⁱⁱⁱ—K1—O4—K1ᵛ	59.77 (14)
C2—C1—C6—C5	−0.1 (5)	K1ⁱⁱ—K1—O4—K1ᵛ	160.16 (4)
S1—C1—C6—C5	177.9 (3)	K1ⁱᵛ—O2—S1—O1	−89.2 (6)
O2ⁱ—K1—O1—S1	77.2 (4)	K1ⁱⁱ—O2—S1—O1	4.50 (17)
O3ⁱⁱ—K1—O1—S1	−124.9 (3)	K1ⁱᵛ—O2—S1—N1	32.8 (7)
O4—K1—O1—S1	164.0 (3)	K1ⁱⁱ—O2—S1—N1	126.44 (14)
O3—K1—O1—S1	2.7 (3)	K1ⁱᵛ—O2—S1—C1	154.3 (6)
O1ⁱⁱⁱ—K1—O1—S1	−58.8 (3)	K1ⁱⁱ—O2—S1—C1	−111.99 (12)
O2ⁱⁱⁱ—K1—O1—S1	−116.7 (3)	K1ⁱᵛ—O2—S1—K1ⁱⁱ	−93.7 (6)
S1ⁱⁱⁱ—K1—O1—S1	−77.2 (4)	K1—O1—S1—O2	134.2 (3)
K1ᵛ—K1—O1—S1	145.6 (3)	K1ⁱⁱ—O1—S1—O2	−4.81 (18)
K1ⁱⁱⁱ—K1—O1—S1	−31.8 (3)	K1—O1—S1—N1	6.3 (4)
K1ⁱⁱ—K1—O1—S1	−139.2 (4)	K1ⁱⁱ—O1—S1—N1	−132.65 (13)
O2ⁱ—K1—O1—K1ⁱⁱ	−143.58 (9)	K1—O1—S1—C1	−111.0 (3)
O3ⁱⁱ—K1—O1—K1ⁱⁱ	14.32 (8)	K1ⁱⁱ—O1—S1—C1	110.07 (14)
O4—K1—O1—K1ⁱⁱ	−56.74 (8)	K1—O1—S1—K1ⁱⁱ	139.0 (4)
O3—K1—O1—K1ⁱⁱ	141.96 (10)	Br1—N1—S1—O2	52.7 (2)
O1ⁱⁱⁱ—K1—O1—K1ⁱⁱ	80.46 (13)	Br1—N1—S1—O1	179.61 (16)
O2ⁱⁱⁱ—K1—O1—K1ⁱⁱ	22.6 (2)	Br1—N1—S1—C1	−65.5 (2)
S1ⁱⁱⁱ—K1—O1—K1ⁱⁱ	62.01 (13)	Br1—N1—S1—K1ⁱⁱ	125.06 (12)
K1ᵛ—K1—O1—K1ⁱⁱ	−75.18 (13)	C6—C1—S1—O2	1.3 (3)
K1ⁱⁱⁱ—K1—O1—K1ⁱⁱ	107.44 (7)	C2—C1—S1—O2	179.2 (3)

O1—K1—O3—K1^{iii}	−115.86 (10)	C6—C1—S1—O1	−120.2 (3)
O2^i—K1—O3—K1^{iii}	117.79 (9)	C2—C1—S1—O1	57.7 (3)
O3^{ii}—K1—O3—K1^{iii}	−48.49 (13)	C6—C1—S1—N1	126.4 (3)
O4—K1—O3—K1^{iii}	159.0 (2)	C2—C1—S1—N1	−55.8 (3)
O1^{iii}—K1—O3—K1^{iii}	14.03 (8)	C6—C1—S1—K1^{ii}	−62.2 (3)
O2^{iii}—K1—O3—K1^{iii}	42.71 (11)	C2—C1—S1—K1^{ii}	115.6 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···Br1^i	0.80 (2)	2.78 (2)	3.550 (3)	160 (4)
O3—H32···N1	0.81 (2)	2.15 (3)	2.917 (4)	158 (5)
O4—H41···N1^{ii}	0.82 (2)	2.16 (2)	2.957 (3)	165 (5)

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