Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Potassium *N*-bromo-2-chlorobenzenesulfonamidate sesquihydrate

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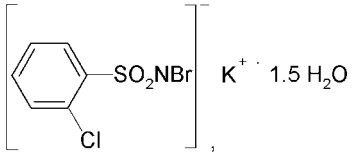
Received 29 May 2011; accepted 7 June 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.026; wR factor = 0.067; data-to-parameter ratio = 13.5.

In the structure of the title compound, $K^+\cdot C_6H_4BrClNO_2S^-\cdot 1.5H_2O$, the K^+ ion is heptacoordinated by three O atoms from water molecules and by four sulfonyl O atoms of *N*-bromo-2-chlorobenzenesulfonamidate anions. The S—N distance of 1.582 (4) Å is consistent with an S═N double bond. The crystal structure is stabilized by intermolecular O—H···Br and O—H···N hydrogen bonds. The asymmetric unit consits of one potassium cation, one *N*-bromo-2-chlorobenzenesulfonamidate anion and one water molecule in general positions and one water molecule located on a twofold rotation axis.

Related literature

For preparation of *N*-haloarylsulfonamides, see: Usha & Gowda (2006). For our study of the effect of substituents on the structures of *N*-haloarylsulfonamides, see: Gowda *et al.* (2010, 2011*a*,*b*). For related structures, see: George *et al.* (2000); Olmstead & Power (1986).



Experimental

Crystal data

$K^+\cdot C_6H_4BrClNO_2S^-\cdot 1.5H_2O$
M_r = 335.65
Orthorhombic, *Fdd*2
a = 12.343 (2) Å
b = 52.066 (6) Å
c = 6.942 (1) Å
V = 4461.3 (11) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 4.47 mm^{-1}
T = 293 K
0.44 × 0.40 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.244, T_{max} = 0.468
4075 measured reflections
1909 independent reflections
1841 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.06
1909 reflections
141 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 671 Friedel pairs
Flack parameter: 0.019 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···N1^{i}	0.80 (2)	2.16 (2)	2.937 (4)	164 (5)
O3—H32···Br1^{ii}	0.80 (2)	2.83 (3)	3.574 (3)	156 (4)
O4—H41···N1^{iii}	0.82 (2)	2.13 (3)	2.905 (4)	157 (5)

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

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*.

BTG thanks the University Grants Commission, Government of India, New Delhi, for a UGC-BSR one-time grant to Faculty/Professors.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2232).

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supporting information

Acta Cryst. (2011). E**67**, m926 [doi:10.1107/S1600536811022136]

Potassium *N*-bromo-2-chlorobenzenesulfonamidate sesquihydrate

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S1. Comment

To explore the effect of replacing sodium by potassium on the solid state structures of *N*-haloarylsulfonamidates (Gowda *et al.*, 2011*a,b*), the structure of potassium *N*-bromo-2-chloro-benzenesulfonamidate sesquihydrate (I) has been determined (Fig. 1). The structure of I resembles those of sodium *N*-bromo-2-chloro-benzenesulfonamidate sesquihydrate (II) (Gowda *et al.*, 2011*b*), sodium *N*-chloro-2-chloro- benzenesulfonamidate sesquihydrate (III)(Gowda *et al.*, 2010), potassium *N*-chloro-4-chloro-benzenesulfonamidate monohydrate (IV)(Gowda *et al.*, 2011*a*), and other sodium *N*-chloro-arylsulfonamidates (George *et al.*, 2000; Olmstead & Power, 1986).

In the structure of the title compound the K^+ ion is hepta coordinated by three O atoms from water molecules and by four sulfonyl O atoms of *N*-bromo-2-chloro-benzenesulfonamide anions. The replacement of Na^+ by K^+ changes the coordination from hexa to hepta coordination (Gowda *et al.*, 2011*b*).

The S—N distance of 1.582 (4)Å is consistent with an S—N double bond and is in agreement with the observed values of 1.579 (6) Å in (II), 1.588 (2) Å in (III) and 1.588 (2) Å in (IV)

In the crystal structure two-dimensional polymeric layer are found that are located parallel to the *ac* plane (Fig. 2). The molecular packing is stabilized by O3—H31···N1, O3—H32···Br1 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 (176 °). It was characterized by recording its infrared and NMR spectra. Yellow prisms of the title compound used in X-ray diffraction studies were obtained from its aqueous solution at room temperature.

S3. Refinement

The H atoms bound to O atoms were 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 atom).

The absolute structure was determined on the basis of 671 Friedel pairs pairs.

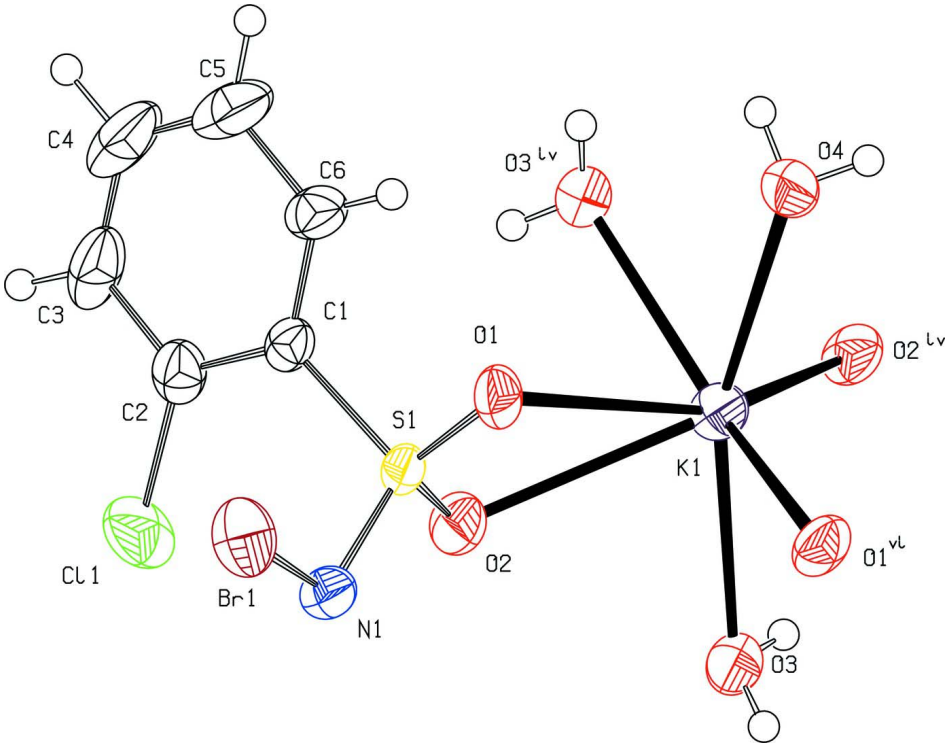

Figure 1

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

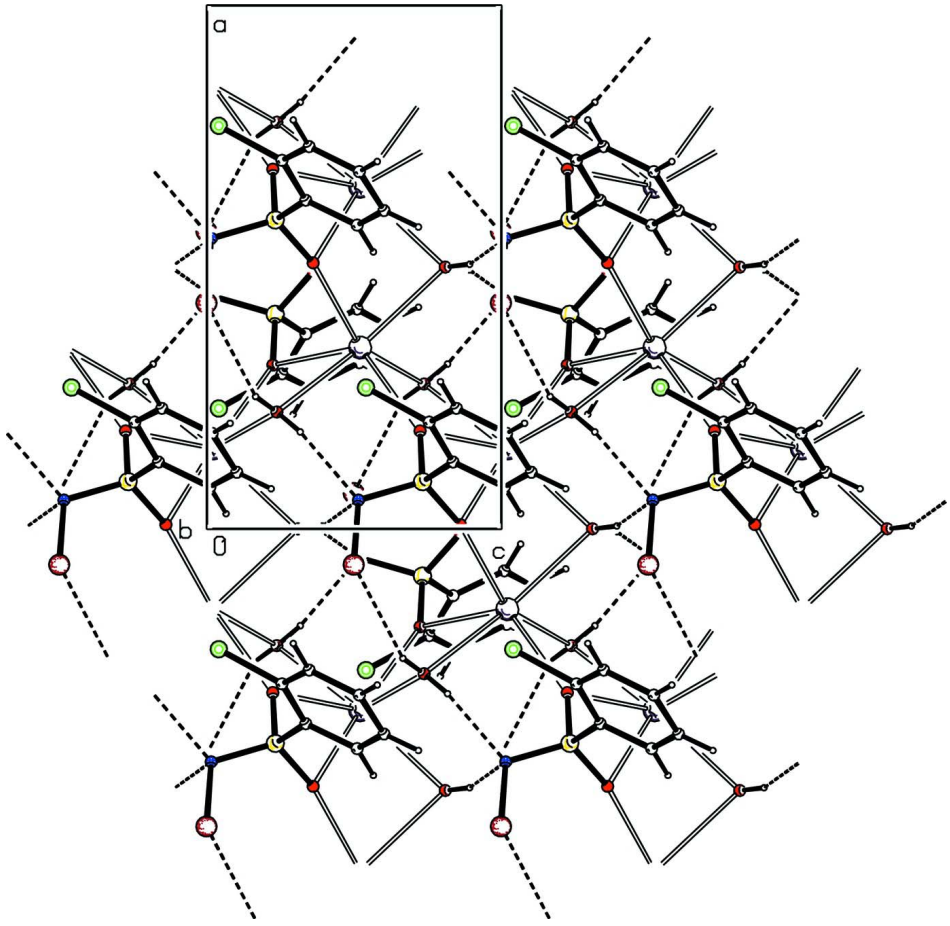

Figure 2

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

Potassium *N*-bromo-2-chlorobenzenesulfonamidate sesquihydrate

Crystal data

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M_r = 335.65
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
a = 12.343 (2) Å
b = 52.066 (6) Å
c = 6.942 (1) Å
V = 4461.3 (11) Å^3
Z = 16
F(000) = 2640
D_x = 1.999 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2515 reflections
θ = 2.9–27.9°
μ = 4.47 mm^{-1}
T = 293 K
Prism, yellow
0.44 × 0.40 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD 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} = 0.244, T_{max} = 0.468
4075 measured reflections
1909 independent reflections
1841 reflections with $I > 2\sigma(I)$

R_{int} = 0.026
θ_{max} = 26.4°, θ_{min} = 3.1°
h = −8→15
k = −56→64
l = −8→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.06
1909 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
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 7.9401P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 671 Friedel pairs
Absolute structure parameter: 0.019 (9)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.1277 (3)	0.07221 (6)	0.8359 (5)	0.0279 (7)
C2	0.2039 (3)	0.08804 (7)	0.7551 (6)	0.0366 (8)
C3	0.2302 (4)	0.11022 (8)	0.8473 (8)	0.0527 (12)
H3	0.2811	0.1213	0.7935	0.063*
C4	0.1824 (4)	0.11628 (8)	1.0178 (9)	0.0620 (14)
H4	0.2017	0.1315	1.0788	0.074*
C5	0.1081 (4)	0.10099 (9)	1.1015 (8)	0.0568 (13)
H5	0.0766	0.1055	1.2184	0.068*
C6	0.0802 (3)	0.07872 (7)	1.0103 (7)	0.0383 (8)
H6	0.0291	0.0678	1.0655	0.046*
Br1	−0.06844 (3)	0.067404 (8)	0.49856 (7)	0.04826 (13)
Cl1	0.26996 (9)	0.08136 (2)	0.54056 (16)	0.0559 (3)
K1	0.34639 (6)	0.007514 (14)	0.52051 (13)	0.03396 (18)
N1	0.0549 (2)	0.04684 (5)	0.5150 (5)	0.0326 (6)
O1	0.0081 (2)	0.03366 (5)	0.8608 (4)	0.0389 (6)
O2	0.1870 (2)	0.02816 (5)	0.7239 (5)	0.0386 (6)
O3	0.2768 (2)	−0.03195 (5)	0.7376 (5)	0.0412 (6)
H31	0.315 (3)	−0.0386 (9)	0.817 (6)	0.049*

H32	0.247 (4)	−0.0416 (8)	0.666 (6)	0.049*
O4	0.5000	0.0000	0.8095 (6)	0.0466 (10)
H41	0.505 (4)	0.0112 (7)	0.892 (6)	0.056*
S1	0.09016 (6)	0.043209 (13)	0.73226 (12)	0.02646 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0302 (16)	0.0232 (15)	0.0302 (17)	0.0029 (13)	−0.0063 (14)	0.0003 (13)
C2	0.0397 (18)	0.0328 (16)	0.037 (2)	−0.0047 (13)	−0.0093 (19)	0.0048 (18)
C3	0.060 (3)	0.030 (2)	0.068 (3)	−0.0135 (19)	−0.023 (2)	0.004 (2)
C4	0.078 (3)	0.032 (2)	0.075 (4)	0.001 (2)	−0.028 (3)	−0.019 (2)
C5	0.073 (3)	0.044 (2)	0.053 (3)	0.019 (2)	−0.013 (2)	−0.022 (2)
C6	0.048 (2)	0.0327 (17)	0.035 (2)	0.0119 (15)	−0.0027 (19)	−0.0056 (18)
Br1	0.0399 (2)	0.0498 (2)	0.0551 (3)	0.00658 (16)	−0.0060 (2)	0.0135 (2)
Cl1	0.0568 (6)	0.0659 (7)	0.0449 (6)	−0.0265 (5)	0.0108 (5)	0.0044 (5)
K1	0.0342 (4)	0.0329 (4)	0.0348 (4)	0.0038 (3)	0.0060 (3)	0.0016 (3)
N1	0.0353 (14)	0.0298 (13)	0.0328 (16)	0.0011 (11)	0.0023 (14)	−0.0036 (14)
O1	0.0466 (15)	0.0280 (12)	0.0421 (16)	−0.0063 (11)	0.0119 (12)	0.0061 (11)
O2	0.0422 (13)	0.0306 (11)	0.0429 (16)	0.0119 (10)	0.0037 (12)	0.0029 (12)
O3	0.0528 (16)	0.0311 (13)	0.0396 (16)	−0.0014 (11)	−0.0041 (15)	−0.0001 (13)
O4	0.070 (3)	0.038 (2)	0.031 (2)	−0.0152 (19)	0.000	0.000
S1	0.0315 (4)	0.0186 (3)	0.0293 (4)	0.0007 (3)	0.0042 (3)	0.0006 (3)

Geometric parameters (Å, º)

C1—C2	1.371 (5)	K1—O3^{ii}	2.790 (3)
C1—C6	1.387 (6)	K1—O2^{ii}	2.803 (3)
C1—S1	1.736 (3)	K1—O1^{ii}	3.008 (3)
C2—C3	1.360 (6)	K1—S1^{ii}	3.4047 (11)
C2—Cl1	1.733 (5)	K1—H32	3.01 (4)
C3—C4	1.360 (8)	N1—S1	1.582 (4)
C3—H3	0.9300	O1—S1	1.438 (3)
C4—C5	1.346 (8)	O1—K1^{iii}	2.659 (3)
C4—H4	0.9300	O1—K1^{iv}	3.008 (3)
C5—C6	1.365 (6)	O2—S1	1.431 (3)
C5—H5	0.9300	O2—K1^{iv}	2.803 (3)
C6—H6	0.9300	O3—K1^{iv}	2.790 (3)
Br1—N1	1.864 (3)	O3—H31	0.804 (19)
K1—O2	2.649 (3)	O3—H32	0.796 (19)
K1—O1^{i}	2.659 (3)	O4—K1^{v}	2.788 (3)
K1—O3	2.689 (3)	O4—H41	0.819 (19)
K1—O4	2.788 (3)	S1—K1^{iv}	3.4047 (11)
C2—C1—C6	120.0 (3)	O1^{i}—K1—S1^{ii}	88.82 (6)
C2—C1—S1	122.4 (3)	O3—K1—S1^{ii}	79.06 (7)
C6—C1—S1	117.5 (3)	O4—K1—S1^{ii}	99.07 (5)
C3—C2—C1	118.8 (4)	O3^{ii}—K1—S1^{ii}	93.74 (7)

C3—C2—Cl1	117.5 (3)	O2^{ii}—K1—S1^{ii}	24.26 (5)
C1—C2—Cl1	123.6 (3)	O1^{ii}—K1—S1^{ii}	24.95 (5)
C2—C3—C4	120.2 (4)	O2—K1—H32	82.2 (9)
C2—C3—H3	119.9	O1^{i}—K1—H32	151.7 (9)
C4—C3—H3	119.9	O3—K1—H32	14.7 (6)
C5—C4—C3	122.3 (4)	O4—K1—H32	85.2 (7)
C5—C4—H4	118.9	O3^{ii}—K1—H32	113.7 (7)
C3—C4—H4	118.9	O2^{ii}—K1—H32	67.9 (6)
C4—C5—C6	118.3 (5)	O1^{ii}—K1—H32	76.2 (9)
C4—C5—H5	120.9	S1^{ii}—K1—H32	68.4 (8)
C6—C5—H5	120.9	S1—N1—Br1	110.60 (17)
C5—C6—C1	120.4 (4)	S1—O1—K1^{iii}	164.64 (17)
C5—C6—H6	119.8	S1—O1—K1^{iv}	93.13 (13)
C1—C6—H6	119.8	K1^{iii}—O1—K1^{iv}	85.96 (7)
O2—K1—O1^{i}	124.89 (9)	S1—O2—K1	149.8 (2)
O2—K1—O3	76.94 (8)	S1—O2—K1^{iv}	102.12 (15)
O1^{i}—K1—O3	149.87 (9)	K1—O2—K1^{iv}	103.41 (8)
O2—K1—O4	100.27 (10)	K1—O3—K1^{iv}	102.72 (8)
O1^{i}—K1—O4	82.02 (8)	K1—O3—H31	122 (4)
O3—K1—O4	72.95 (7)	K1^{iv}—O3—H31	92 (4)
O2—K1—O3^{ii}	77.62 (10)	K1—O3—H32	106 (4)
O1^{i}—K1—O3^{ii}	83.23 (9)	K1^{iv}—O3—H32	118 (4)
O3—K1—O3^{ii}	124.66 (5)	H31—O3—H32	116 (5)
O4—K1—O3^{ii}	160.21 (6)	K1—O4—K1^{v}	87.96 (13)
O2—K1—O2^{ii}	123.44 (5)	K1—O4—H41	117 (4)
O1^{i}—K1—O2^{ii}	98.26 (9)	K1^{v}—O4—H41	123 (4)
O3—K1—O2^{ii}	81.86 (9)	O2—S1—O1	115.10 (17)
O4—K1—O2^{ii}	122.39 (7)	O2—S1—N1	104.89 (17)
O3^{ii}—K1—O2^{ii}	72.84 (8)	O1—S1—N1	116.06 (16)
O2—K1—O1^{ii}	158.24 (8)	O2—S1—C1	105.67 (17)
O1^{i}—K1—O1^{ii}	76.30 (9)	O1—S1—C1	103.37 (17)
O3—K1—O1^{ii}	81.53 (9)	N1—S1—C1	111.42 (15)
O4—K1—O1^{ii}	76.07 (7)	O2—S1—K1^{iv}	53.61 (12)
O3^{ii}—K1—O1^{ii}	113.00 (8)	O1—S1—K1^{iv}	61.92 (11)
O2^{ii}—K1—O1^{ii}	49.09 (7)	N1—S1—K1^{iv}	135.78 (10)
O2—K1—S1^{ii}	143.01 (7)	C1—S1—K1^{iv}	111.69 (11)

C6—C1—C2—C3	−1.1 (5)	O1^{i}—K1—O4—K1^{v}	−41.28 (6)
S1—C1—C2—C3	−178.8 (3)	O3—K1—O4—K1^{v}	121.76 (7)
C6—C1—C2—Cl1	178.7 (3)	O3^{ii}—K1—O4—K1^{v}	−83.5 (3)
S1—C1—C2—Cl1	0.9 (5)	O2^{ii}—K1—O4—K1^{v}	53.47 (8)
C1—C2—C3—C4	0.8 (6)	O1^{ii}—K1—O4—K1^{v}	36.50 (6)
Cl1—C2—C3—C4	−178.9 (3)	S1^{ii}—K1—O4—K1^{v}	46.24 (2)
C2—C3—C4—C5	−0.2 (7)	K1—O2—S1—O1	139.5 (3)
C3—C4—C5—C6	−0.2 (7)	K1^{iv}—O2—S1—O1	−7.7 (2)
C4—C5—C6—C1	0.0 (6)	K1—O2—S1—N1	10.7 (4)
C2—C1—C6—C5	0.7 (6)	K1^{iv}—O2—S1—N1	−136.49 (13)
S1—C1—C6—C5	178.5 (3)	K1—O2—S1—C1	−107.1 (3)

O1^{i}—K1—O2—S1	71.6 (4)	K1^{iv}—O2—S1—C1	105.67 (15)
O3—K1—O2—S1	−131.4 (3)	K1—O2—S1—K1^{iv}	147.2 (4)
O4—K1—O2—S1	159.0 (3)	K1^{iii}—O1—S1—O2	−79.1 (7)
O3^{ii}—K1—O2—S1	−1.0 (3)	K1^{iv}—O1—S1—O2	7.01 (19)
O2^{ii}—K1—O2—S1	−60.5 (3)	K1^{iii}—O1—S1—N1	43.9 (7)
O1^{ii}—K1—O2—S1	−122.9 (3)	K1^{iv}—O1—S1—N1	130.04 (12)
S1^{ii}—K1—O2—S1	−80.6 (3)	K1^{iii}—O1—S1—C1	166.2 (6)
O1^{i}—K1—O2—K1^{iv}	−141.38 (9)	K1^{iv}—O1—S1—C1	−107.68 (12)
O3—K1—O2—K1^{iv}	15.65 (9)	K1^{iii}—O1—S1—K1^{iv}	−86.2 (6)
O4—K1—O2—K1^{iv}	−53.99 (9)	Br1—N1—S1—O2	−177.66 (15)
O3^{ii}—K1—O2—K1^{iv}	146.08 (11)	Br1—N1—S1—O1	54.1 (2)
O2^{ii}—K1—O2—K1^{iv}	86.54 (16)	Br1—N1—S1—C1	−63.8 (2)
O1^{ii}—K1—O2—K1^{iv}	24.1 (3)	Br1—N1—S1—K1^{iv}	129.71 (11)
S1^{ii}—K1—O2—K1^{iv}	66.47 (16)	C2—C1—S1—O2	60.1 (3)
O2—K1—O3—K1^{iv}	−15.68 (9)	C6—C1—S1—O2	−117.8 (3)
O1^{i}—K1—O3—K1^{iv}	124.69 (15)	C2—C1—S1—O1	−178.6 (3)
O4—K1—O3—K1^{iv}	89.55 (10)	C6—C1—S1—O1	3.6 (3)
O3^{ii}—K1—O3—K1^{iv}	−80.34 (16)	C2—C1—S1—N1	−53.3 (3)
O2^{ii}—K1—O3—K1^{iv}	−142.87 (10)	C6—C1—S1—N1	128.9 (3)
O1^{ii}—K1—O3—K1^{iv}	167.49 (10)	C2—C1—S1—K1^{iv}	116.6 (3)
S1^{ii}—K1—O3—K1^{iv}	−167.32 (9)	C6—C1—S1—K1^{iv}	−61.2 (3)
O2—K1—O4—K1^{v}	−165.44 (7)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H31···N1^{iv}	0.80 (2)	2.16 (2)	2.937 (4)	164 (5)
O3—H32···Br1^{vi}	0.80 (2)	2.83 (3)	3.574 (3)	156 (4)
O4—H41···N1^{vii}	0.82 (2)	2.13 (3)	2.905 (4)	157 (5)

Symmetry codes: (iv) −x+1/2, −y, z+1/2; (vi) −x, −y, z; (vii) x+1/2, y, z+1/2.