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Rubidium bis(2-methyllactato)borate monohydrate

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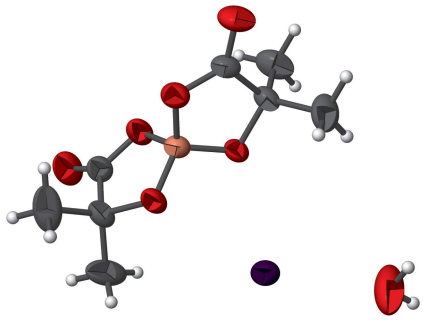
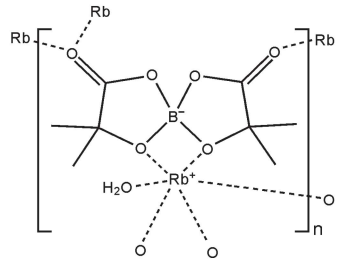
The asymmetric unit of the inorganic–organic hybrid salt, poly[aqua[μ_4-bis(2-methyllactato)borato]rubidium], $[Rb(C_8H_{12}BO_6)(H_2O)]_n$, comprises a rubidium cation, a bis(2-methyllactato)borate anion, and a water molecule of crystallization. The rubidium cation is pseudo-octahedrally coordinated by five O atoms from four bis(2-methyllactato)borate ligands and by a water molecule. The presence of four coordinating O atoms within the anion lead to the formation of a polymeric three-dimensional framework structure that is consolidated by additional O—H···O hydrogen-bonding interactions.

3D view



Chemical scheme



Structure description

Alkaline cations such as lithium and potassium are used in the development of batteries. Allen *et al.* (2012) have reported the crystal structure of lithium bis(2-methyllactato)borate monohydrate. In our current study we have replaced the lithium cation by a rubidium cation and report here single-crystal growth and structural analysis of rubidium bis(2-methyllactato)borate monohydrate. Whereas the lithium salt crystallizes in the space group *Pbca* with $Z = 8$, the rubidium salt crystallizes in space group $P2_1/n$ with $Z = 4$.

The asymmetric unit of the title compound comprises a rubidium cation, a bis(2-methyllactato)borate anion, and a water molecule of crystallization (Fig. 1). The structural features of the anion are very similar to that of the lithium salt (Allen *et al.*, 2012), in particular with respect to B—O bond lengths (Table 1). The five-membered ring O1/C2/C1/O2/B1 adopts a half-chair conformation with a twist on the O1—C2 bond [puckering parameters $Q_2 = 0.077$ (3) Å, $\varphi_2 = 198$ (2)°] whereas the O4/C5/C6/O5/B1 ring adopts a slightly distorted half-chair conformation with a twist on the O5—B1 bond [puckering parameters $Q_2 = 0.141$ (3) Å, $\varphi_2 = 303$ (1)°]. The dihedral angle between the least-squares

Table 1
Selected bond lengths (Å).

Rb1—O7	2.833 (3)	Rb1—O3^{iii}	3.115 (2)
Rb1—O6^{i}	2.8852 (19)	O1—B1	1.432 (3)
Rb1—O6^{ii}	2.932 (2)	O2—B1	1.507 (3)
Rb1—O5	2.9766 (17)	O4—B1	1.506 (3)
Rb1—O1	3.0316 (18)	O5—B1	1.438 (3)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H2···O5^{iii}	0.84 (2)	2.22 (2)	3.049 (3)	169 (5)
O7—H1···O3^{iv}	0.86 (4)	2.14 (4)	2.826 (4)	137 (4)

Symmetry codes: (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, y+1, z$.

planes of the two five-membered rings is 89.30 (14)°. The rubidium cation is sixfold coordinated by one water molecule (O7) and five O atoms (O1, O6^{i}, O6^{ii}, O3^{iii} and O5; symmetry codes as in Table 1) from four bis(2-methyllactato)borate ligands, one of which coordinates in a bidentate mode (Table 1). The presence of four coordinating oxygen atoms per anion leads to the formation of a three-dimensional framework structure. Additional hydrogen bonds between the water molecules and one of the O atoms of the BO_4 tetrahedron (O5) and one of the carbonyl O atoms (O3) stabilizes the structural set-up (Fig. 2, Table 2).

Synthesis and crystallization

The title compound was synthesized by reacting 2-methyllactic acid, boric acid and rubidium carbonate (molar ratio 4:2:1) in double distilled water. Slow evaporation of the solvent yielded good quality crystals within a period of 50 days.

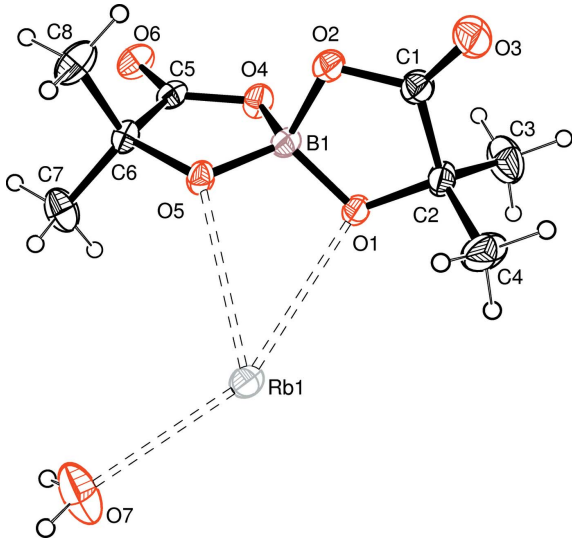


Figure 1
The asymmetric unit of the title compound showing the atom numbering with displacement ellipsoids drawn at the 25% probability level.

Table 3
Experimental details.

Crystal data	
Chemical formula	[Rb($C_8H_{12}BO_6$)(H_2O)]
M_r	318.47
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	8.3075 (3), 10.4488 (4), 15.5630 (6)
β (°)	92.202 (2)
V (Å^3)	1349.92 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.69
Crystal size (mm)	0.15 × 0.10 × 0.10
Data collection	
Diffractometer	Bruker Kappa APEX3 CMOS diffractometer
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.518, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	39188, 4927, 2964
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.760
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.105, 1.05
No. of reflections	4927
No. of parameters	160
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.54, −0.80

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* 2014/5 (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

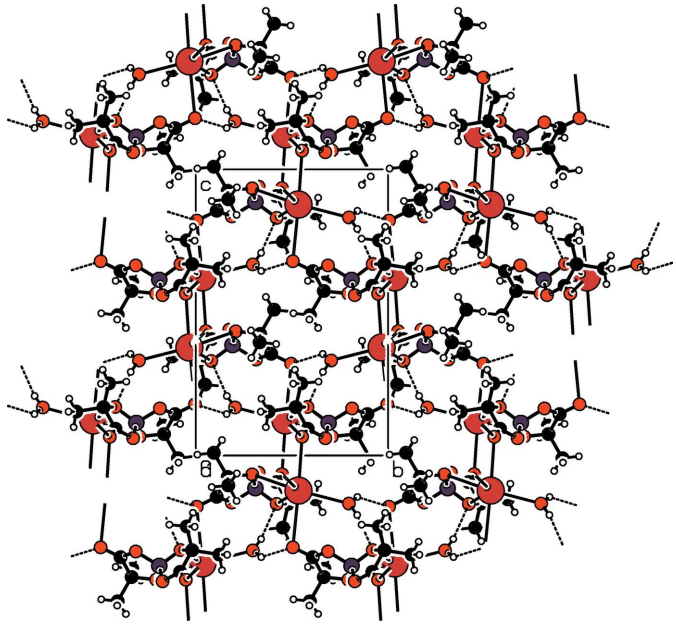


Figure 2
Packing diagram of the title compound viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Acknowledgements

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full crystallographic data

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Rubidium bis(2-methyllactato)borate monohydrate

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Poly[aqua[μ_4-bis(2-methyllactato)borato]rubidium]

Crystal data

$[Rb(C_8H_{12}BO_6)(H_2O)]$
M_r = 318.47
Monoclinic, $P2_1/n$
a = 8.3075 (3) Å
b = 10.4488 (4) Å
c = 15.5630 (6) Å
β = 92.202 (2)°
V = 1349.92 (9) Å^3
Z = 4
$F(000)$ = 640
D_x = 1.567 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9895 reflections
θ = 3.1–30.4°
μ = 3.69 mm^{-1}
T = 296 K
Block, colourless
0.15 × 0.10 × 0.10 mm

Data collection

Bruker Kappa APEX3 CMOS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.518, T_{max} = 0.746
39188 measured reflections
4927 independent reflections
2964 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 32.7°, θ_{min} = 3.4°
h = −10→12
k = −15→15
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.105
S = 1.05
4927 reflections
160 parameters
3 restraints
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.7957P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 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.

Refinement. H atoms of the water molecule were discernable from difference Fourier maps and were refined with a distance constraint of d(O—H) = 0.85 (2) Å and U_{iso}(H) = 1.2U_{eq}(O).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Rb1	0.15594 (3)	1.03371 (3)	0.62254 (2)	0.04816 (10)
C1	0.3793 (3)	0.6083 (3)	0.64453 (16)	0.0424 (6)
C2	0.2674 (3)	0.6658 (3)	0.57496 (16)	0.0421 (6)
C3	0.2814 (5)	0.5932 (4)	0.4905 (2)	0.0764 (11)
H3A	0.241898	0.507568	0.497088	0.115*
H3B	0.218825	0.635964	0.445976	0.115*
H3C	0.392203	0.590459	0.475235	0.115*
C4	0.0954 (4)	0.6685 (4)	0.6045 (3)	0.0769 (11)
H4A	0.056836	0.582433	0.610491	0.115*
H4B	0.092286	0.711533	0.658929	0.115*
H4C	0.028243	0.713139	0.562860	0.115*
C5	0.7099 (3)	0.9182 (3)	0.59312 (15)	0.0379 (5)
C6	0.6303 (3)	0.9805 (3)	0.66890 (15)	0.0368 (5)
C7	0.6093 (4)	1.1224 (3)	0.6535 (2)	0.0615 (8)
H7A	0.713066	1.162725	0.653085	0.092*
H7B	0.553519	1.135858	0.599030	0.092*
H7C	0.547865	1.158700	0.698425	0.092*
C8	0.7251 (4)	0.9526 (4)	0.75202 (19)	0.0634 (9)
H8A	0.828318	0.993751	0.750896	0.095*
H8B	0.667126	0.984611	0.799709	0.095*
H8C	0.739760	0.861916	0.758072	0.095*
O1	0.32554 (19)	0.79284 (16)	0.56594 (11)	0.0390 (4)
O2	0.4970 (2)	0.68714 (18)	0.66442 (12)	0.0474 (5)
O3	0.3631 (3)	0.5045 (2)	0.67894 (15)	0.0624 (6)
O4	0.6196 (2)	0.82640 (19)	0.56029 (11)	0.0459 (4)
O5	0.47576 (18)	0.91984 (17)	0.66951 (10)	0.0372 (4)
O6	0.8396 (2)	0.9478 (2)	0.56534 (13)	0.0547 (5)
B1	0.4744 (3)	0.8096 (3)	0.61421 (17)	0.0365 (6)
O7	0.1465 (4)	1.2961 (3)	0.6680 (2)	0.0984 (10)
H1	0.221 (4)	1.340 (4)	0.645 (3)	0.118*
H2	0.108 (5)	1.339 (4)	0.708 (2)	0.118*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1	0.03750 (14)	0.05453 (19)	0.05188 (16)	0.00398 (12)	−0.00565 (10)	−0.00967 (13)
C1	0.0420 (13)	0.0423 (16)	0.0427 (13)	−0.0021 (12)	−0.0025 (10)	0.0019 (12)
C2	0.0403 (13)	0.0405 (15)	0.0449 (13)	−0.0107 (11)	−0.0069 (10)	0.0040 (11)
C3	0.121 (3)	0.055 (2)	0.0518 (18)	−0.008 (2)	−0.0172 (19)	−0.0080 (16)
C4	0.0384 (16)	0.075 (3)	0.117 (3)	−0.0077 (16)	0.0017 (17)	0.034 (2)
C5	0.0289 (11)	0.0460 (15)	0.0384 (12)	−0.0019 (10)	−0.0009 (9)	0.0065 (11)
C6	0.0341 (11)	0.0423 (15)	0.0337 (11)	−0.0091 (11)	−0.0021 (9)	0.0000 (10)
C7	0.078 (2)	0.0421 (17)	0.0656 (18)	−0.0124 (16)	0.0160 (16)	−0.0013 (15)
C8	0.0521 (17)	0.096 (3)	0.0408 (14)	−0.0111 (17)	−0.0098 (12)	0.0050 (16)
O1	0.0356 (9)	0.0355 (10)	0.0450 (9)	−0.0057 (7)	−0.0100 (7)	0.0052 (7)

O2	0.0438 (10)	0.0402 (11)	0.0569 (11)	−0.0035 (8)	−0.0167 (8)	0.0063 (9)
O3	0.0730 (15)	0.0468 (12)	0.0664 (13)	−0.0106 (10)	−0.0102 (11)	0.0177 (10)
O4	0.0349 (9)	0.0563 (12)	0.0471 (9)	−0.0034 (8)	0.0086 (7)	−0.0139 (9)
O5	0.0292 (8)	0.0409 (10)	0.0418 (9)	−0.0081 (7)	0.0058 (7)	−0.0061 (7)
O6	0.0330 (9)	0.0748 (15)	0.0568 (11)	−0.0074 (9)	0.0094 (8)	0.0067 (10)
B1	0.0296 (12)	0.0405 (17)	0.0392 (14)	−0.0011 (11)	−0.0005 (10)	0.0008 (12)
O7	0.129 (3)	0.0592 (17)	0.111 (2)	−0.0272 (17)	0.0615 (19)	−0.0241 (16)

Geometric parameters (Å, º)

Rb1—O7	2.833 (3)	C4—H4B	0.9600
Rb1—O6^{i}	2.8852 (19)	C4—H4C	0.9600
Rb1—O6^{ii}	2.932 (2)	C5—O6	1.216 (3)
Rb1—O5	2.9766 (17)	C5—O4	1.309 (3)
Rb1—O1	3.0316 (18)	C5—C6	1.521 (4)
Rb1—O3^{iii}	3.115 (2)	C6—O5	1.432 (3)
Rb1—B1	3.539 (3)	C6—C7	1.511 (4)
Rb1—C5^{ii}	3.612 (2)	C6—C8	1.516 (4)
Rb1—C1^{iii}	3.730 (3)	C7—H7A	0.9600
Rb1—Rb1^{iv}	4.5823 (5)	C7—H7B	0.9600
Rb1—H1	3.27 (4)	C7—H7C	0.9600
C1—O3	1.219 (3)	C8—H8A	0.9600
C1—O2	1.307 (3)	C8—H8B	0.9600
C1—C2	1.523 (3)	C8—H8C	0.9600
C2—O1	1.421 (3)	O1—B1	1.432 (3)
C2—C4	1.518 (4)	O2—B1	1.507 (3)
C2—C3	1.526 (4)	O4—B1	1.506 (3)
C3—H3A	0.9600	O5—B1	1.438 (3)
C3—H3B	0.9600	O7—H1	0.857 (18)
C3—H3C	0.9600	O7—H2	0.844 (18)
C4—H4A	0.9600		
O7—Rb1—O6^{i}	110.16 (9)	O1—C2—C3	110.0 (2)
O7—Rb1—O6^{ii}	100.75 (8)	C4—C2—C3	112.0 (3)
O6^{i}—Rb1—O6^{ii}	76.06 (6)	C1—C2—C3	110.6 (3)
O7—Rb1—O5	111.01 (9)	C2—C3—H3A	109.5
O6^{i}—Rb1—O5	138.17 (6)	C2—C3—H3B	109.5
O6^{ii}—Rb1—O5	103.06 (5)	H3A—C3—H3B	109.5
O7—Rb1—O1	153.31 (8)	C2—C3—H3C	109.5
O6^{i}—Rb1—O1	94.58 (5)	H3A—C3—H3C	109.5
O6^{ii}—Rb1—O1	75.01 (5)	H3B—C3—H3C	109.5
O5—Rb1—O1	47.09 (4)	C2—C4—H4A	109.5
O7—Rb1—O3^{iii}	81.04 (8)	C2—C4—H4B	109.5
O6^{i}—Rb1—O3^{iii}	101.25 (6)	H4A—C4—H4B	109.5
O6^{ii}—Rb1—O3^{iii}	177.14 (6)	C2—C4—H4C	109.5
O5—Rb1—O3^{iii}	78.24 (5)	H4A—C4—H4C	109.5
O1—Rb1—O3^{iii}	104.41 (5)	H4B—C4—H4C	109.5
O7—Rb1—B1	132.64 (9)	O6—C5—O4	123.3 (2)

O6^{i}—Rb1—B1	117.12 (6)	O6—C5—C6	125.7 (2)
O6^{ii}—Rb1—B1	88.23 (6)	O4—C5—C6	110.9 (2)
O5—Rb1—B1	23.52 (5)	O6—C5—Rb1^{ii}	47.56 (13)
O1—Rb1—B1	23.60 (5)	O4—C5—Rb1^{ii}	86.10 (13)
O3^{iii}—Rb1—B1	92.18 (6)	C6—C5—Rb1^{ii}	145.07 (17)
O7—Rb1—C5^{ii}	96.29 (8)	O5—C6—C7	109.7 (2)
O6^{i}—Rb1—C5^{ii}	93.82 (5)	O5—C6—C8	110.2 (2)
O6^{ii}—Rb1—C5^{ii}	17.83 (5)	C7—C6—C8	112.2 (2)
O5—Rb1—C5^{ii}	88.82 (5)	O5—C6—C5	103.41 (19)
O1—Rb1—C5^{ii}	71.47 (5)	C7—C6—C5	110.4 (2)
O3^{iii}—Rb1—C5^{ii}	164.71 (6)	C8—C6—C5	110.6 (2)
B1—Rb1—C5^{ii}	78.48 (6)	C6—C7—H7A	109.5
O7—Rb1—C1^{iii}	63.35 (8)	C6—C7—H7B	109.5
O6^{i}—Rb1—C1^{iii}	105.08 (6)	H7A—C7—H7B	109.5
O6^{ii}—Rb1—C1^{iii}	163.70 (6)	C6—C7—H7C	109.5
O5—Rb1—C1^{iii}	86.99 (5)	H7A—C7—H7C	109.5
O1—Rb1—C1^{iii}	120.69 (5)	H7B—C7—H7C	109.5
O3^{iii}—Rb1—C1^{iii}	17.75 (6)	C6—C8—H8A	109.5
B1—Rb1—C1^{iii}	105.10 (6)	C6—C8—H8B	109.5
C5^{ii}—Rb1—C1^{iii}	155.85 (6)	H8A—C8—H8B	109.5
O7—Rb1—Rb1^{iv}	109.65 (8)	C6—C8—H8C	109.5
O6^{i}—Rb1—Rb1^{iv}	38.39 (4)	H8A—C8—H8C	109.5
O6^{ii}—Rb1—Rb1^{iv}	37.67 (4)	H8B—C8—H8C	109.5
O5—Rb1—Rb1^{iv}	127.87 (3)	C2—O1—B1	110.61 (19)
O1—Rb1—Rb1^{iv}	83.38 (3)	C2—O1—Rb1	125.67 (15)
O3^{iii}—Rb1—Rb1^{iv}	139.63 (5)	B1—O1—Rb1	98.49 (15)
B1—Rb1—Rb1^{iv}	105.50 (4)	C1—O2—B1	109.58 (19)
C5^{ii}—Rb1—Rb1^{iv}	55.45 (4)	C1—O3—Rb1^{v}	111.07 (19)
C1^{iii}—Rb1—Rb1^{iv}	141.08 (4)	C5—O4—B1	109.10 (19)
O7—Rb1—H1	14.0 (5)	C6—O5—B1	109.72 (18)
O6^{i}—Rb1—H1	118.9 (8)	C6—O5—Rb1	127.82 (14)
O6^{ii}—Rb1—H1	92.0 (7)	B1—O5—Rb1	100.76 (13)
O5—Rb1—H1	103.0 (8)	C5—O6—Rb1^{vi}	141.11 (17)
O1—Rb1—H1	140.3 (6)	C5—O6—Rb1^{ii}	114.61 (16)
O3^{iii}—Rb1—H1	90.2 (7)	Rb1^{vi}—O6—Rb1^{ii}	103.94 (6)
B1—Rb1—H1	122.2 (7)	O1—B1—O5	113.5 (2)
C5^{ii}—Rb1—H1	84.8 (6)	O1—B1—O4	114.6 (2)
C1^{iii}—Rb1—H1	73.1 (6)	O5—B1—O4	104.6 (2)
Rb1^{iv}—Rb1—H1	109.0 (8)	O1—B1—O2	104.9 (2)
O3—C1—O2	123.4 (2)	O5—B1—O2	111.8 (2)
O3—C1—C2	126.1 (2)	O4—B1—O2	107.5 (2)
O2—C1—C2	110.5 (2)	O1—B1—Rb1	57.91 (12)
O3—C1—Rb1^{v}	51.18 (15)	O5—B1—Rb1	55.72 (12)
O2—C1—Rb1^{v}	89.28 (14)	O4—B1—Rb1	123.99 (16)
C2—C1—Rb1^{v}	134.79 (17)	O2—B1—Rb1	128.41 (16)
O1—C2—C4	109.9 (2)	Rb1—O7—H1	113 (3)
O1—C2—C1	103.79 (19)	Rb1—O7—H2	135 (3)
C4—C2—C1	110.3 (2)	H1—O7—H2	109 (3)

O3—C1—C2—O1	172.0 (3)	C8—C6—O5—B1	−105.2 (3)
O2—C1—C2—O1	−7.0 (3)	C5—C6—O5—B1	13.0 (2)
Rb1^{v}—C1—C2—O1	103.7 (2)	C7—C6—O5—Rb1	8.8 (3)
O3—C1—C2—C4	54.3 (4)	C8—C6—O5—Rb1	132.8 (2)
O2—C1—C2—C4	−124.6 (3)	C5—C6—O5—Rb1	−108.92 (18)
Rb1^{v}—C1—C2—C4	−14.0 (4)	O4—C5—O6—Rb1^{vi}	−143.6 (2)
O3—C1—C2—C3	−70.1 (4)	C6—C5—O6—Rb1^{vi}	36.5 (4)
O2—C1—C2—C3	110.9 (3)	Rb1^{ii}—C5—O6—Rb1^{vi}	171.8 (4)
Rb1^{v}—C1—C2—C3	−138.4 (2)	O4—C5—O6—Rb1^{ii}	44.6 (3)
O6—C5—C6—O5	174.6 (2)	C6—C5—O6—Rb1^{ii}	−135.3 (2)
O4—C5—C6—O5	−5.3 (3)	C2—O1—B1—O5	−129.3 (2)
Rb1^{ii}—C5—C6—O5	109.6 (3)	Rb1—O1—B1—O5	4.0 (2)
O6—C5—C6—C7	57.3 (3)	C2—O1—B1—O4	110.6 (2)
O4—C5—C6—C7	−122.6 (3)	Rb1—O1—B1—O4	−116.0 (2)
Rb1^{ii}—C5—C6—C7	−7.7 (4)	C2—O1—B1—O2	−7.0 (3)
O6—C5—C6—C8	−67.4 (3)	Rb1—O1—B1—O2	126.33 (16)
O4—C5—C6—C8	112.7 (2)	C2—O1—B1—Rb1	−133.32 (19)
Rb1^{ii}—C5—C6—C8	−132.5 (2)	C6—O5—B1—O1	−141.1 (2)
C4—C2—O1—B1	126.4 (3)	Rb1—O5—B1—O1	−4.1 (2)
C1—C2—O1—B1	8.4 (3)	C6—O5—B1—O4	−15.5 (2)
C3—C2—O1—B1	−109.9 (3)	Rb1—O5—B1—O4	121.45 (15)
C4—C2—O1—Rb1	8.8 (3)	C6—O5—B1—O2	100.5 (2)
C1—C2—O1—Rb1	−109.23 (18)	Rb1—O5—B1—O2	−122.48 (16)
C3—C2—O1—Rb1	132.4 (2)	C6—O5—B1—Rb1	−136.98 (18)
O3—C1—O2—B1	−176.1 (3)	C5—O4—B1—O1	137.0 (2)
C2—C1—O2—B1	2.8 (3)	C5—O4—B1—O5	12.1 (3)
Rb1^{v}—C1—O2—B1	−135.54 (17)	C5—O4—B1—O2	−106.9 (2)
O2—C1—O3—Rb1^{v}	56.6 (3)	C5—O4—B1—Rb1	70.3 (2)
C2—C1—O3—Rb1^{v}	−122.2 (2)	C1—O2—B1—O1	2.4 (3)
O6—C5—O4—B1	175.9 (2)	C1—O2—B1—O5	125.8 (2)
C6—C5—O4—B1	−4.2 (3)	C1—O2—B1—O4	−120.0 (2)
Rb1^{ii}—C5—O4—B1	−152.81 (16)	C1—O2—B1—Rb1	63.0 (3)
C7—C6—O5—B1	130.8 (2)		

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iv) −*x*, −*y*+2, −*z*+1; (v) −*x*+1/2, *y*−1/2, −*z*+3/2; (vi) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H2···O5^{iii}	0.84 (2)	2.22 (2)	3.049 (3)	169 (5)
O7—H1···O3^{vii}	0.86 (4)	2.14 (4)	2.826 (4)	137 (4)

Symmetry codes: (iii) −*x*+1/2, *y*+1/2, −*z*+3/2; (vii) *x*, *y*+1, *z*.