Crystal structure of MgK$_{0.5}$[B$_6$O$_{10}$](OH)$_{0.5}$$\cdot$0.5H$_2$O, poly[dimagnesium potassium bis(hexaborate) hydroxide monohydrate]

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The solvothermal reaction of H$_3$BO$_3$, KCF$_3$SO$_3$, Mg(CF$_3$SO$_3$)$_2$ and pyridine led to a new alkali- and alkaline-earth-metal borate, MgK$_{0.5}$[B$_6$O$_{10}$](OH)$_{0.5}$$\cdot$0.5H$_2$O. Its structure features an intricate three-dimensional framework built from [B$_6$O$_{13}$]$_2$$^{2-}$ clusters, thus resulting in a six-connected achiral net with high symmetry. Each [B$_6$O$_{13}$]$_2$$^{2-}$ building block is composed of three trigonal BO$_3$ and three tetrahedral BO$_4$ units, with these BO$_4$ units being further connected to neighboring BO$_3$ units, giving rise to an oxoboron cluster of the general formula [B$_6$O$_{10}$]$^{2-}$.

1. Chemical context

As inorganic materials, borates are an important class of nonlinear optical crystals, mainly because they can easily crystallize in non-centrosymmetric space groups and such structures often show a large second-harmonic generation response (Qiu et al., 2021a; Qui & Yang, 2021a). The combination of BO$_3$-trigonal and BO$_4$-tetrahedral units makes it possible to form a variety of isolated anionic clusters. Extended chains, layers and three-dimensional frameworks can be formed between clusters through the dehydration and condensation of the terminal hydroxyl groups of oxoboron clusters (Wang et al., 2017). In addition, negatively charged oxoboron clusters can also combine with a variety of counter-cations, making the structure of borates more complex and diverse. Here, single crystals of MgK$_{0.5}$[B$_6$O$_{10}$](OH)$_{0.5}$$\cdot$0.5H$_2$O with alkali- and alkaline-earth metals have been obtained under solvothermal conditions.
2. Structural commentary

The asymmetric unit of the title compound consists of 2 B, 10/3 O, 1/3 Mg, 1/6 K, 1/6 OH, and 1/6 H2O. The Mg, K, O4, O5 and O6 atoms are located on special positions with occupancy of 1/3 or 1/6, while the remaining B and O atoms are located at general positions with an occupancy of 1. Bond-valence-sum calculations show that Mg, K and B are consistent with the expected oxidation states (Brown & Altermatt, 1985; Brese & O’Keeffe, 1991). Three BO4 units are joined together through corner-sharing of the O4 atom and three BO4 units are connected with three neighboring BO3 units to form a [B6O13]8– oxoboron cluster (Fig. 1). To the best of our knowledge, this is the first example of a mixed alkali- and alkaline-earth-metal borate crystal with the [B6O13]8– cluster anion. In this cluster, the B—O4 bonds are unique because their bond distances [1.529 (2) Å] are longer than other B—O bonds [1.359 (2)–1.453 (2) Å] in the BO3 and BO4 units. Each [B6O13]8– unit is further connected to six other clusters by corner-sharing O atoms, resulting in a three-dimensional framework (Fig. 2).

3. Supramolecular features

In the title compound, the Mg and K atoms are six-coordinated, with Mg—O and distances in the range 2.332 (1)–2.374 (1) Å and K—O = 2.845 (1) Å. The three-dimensional structure is stabilized by a water cluster formed by O5—H5i 0.85 1.67 2.42 (3) 145 O6—H6Ai 0.85 2.58 3.276 (15) 140 O5—H5ii 0.85 1.78 2.484 (19) 139 O5—H5iii 0.85 2.30 3.06 (3) 150 K cations as templates has no effect on the crystallization of the oxoboron three-dimensional framework. However, after the introduction of Cl (Wu et al., 2011) or Br (Al-Ama et al., 2006), the new compounds crystallize in the trigonal space group R3̅m with a large second-harmonic generation response. The introduction of different anions can therefore play a key role in changing the crystalline structure to a non-centrosymmetric system.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.43, update June 2022; Groom et al., 2016) for the [B6O13]8– oxoboron cluster gave 23 hits. The terminal oxygen atoms of this type of [B6Ox] unit can be completely deprotonated [B6O13]8–, partially protonated [B6O11(OH)2]6– or completely protonated [B6O12(OH)6]2–. Among the above 23 compounds, most of them are inorganic–organic hybrid solids, which contain transition-metal complexes and the [B6O12(OH)6]2– cluster (refs: CAFYIV, CAFYOB, Altahan et al., 2021; CECWEM, Heller & Schellhaas, 1983; EMEHIP, Li et al., 2016; HIXNAF, Jamai et al., 2014; JOCCUC, JOCDAJ, Altahan et al., 2019a; JUZLIC, Altahan et al., 2020; MEBQUI, MEBRET, Altahan et al., 2017; POJVIW, POJVOC, Altahan

Table 1

| D—H···A   | D—H     | D···A   | D—H···A   |
|-----------|---------|---------|-----------|
| O5—H5···O5 | 0.85    | 1.67    | 2.42 (3)  | 145       |
| O6—H6A···O2i | 0.85   | 2.58    | 3.276 (15) | 140       |
| O5—H5···O6c | 0.85   | 1.78    | 2.484 (19) | 139       |
| O5—H5···O5a | 0.85   | 2.30    | 3.06 (3)   | 150       |

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

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![Figure 1](image1.png)

The asymmetric unit of the [B6O13]8– oxoboron cluster. Displacement ellipsoids are drawn at the 50% probability level.

![Figure 2](image2.png)

View of the three-dimensional supramolecular framework along the [100] direction. Color code: BO3 trigonal, yellow, orange and brown; BO4 tetrahedral, blue.

[45x55]3. Supramolecular features

In the title compound, the Mg and K atoms are six-coordinated, with Mg—O and distances in the range 2.332 (1)–2.374 (1) Å and K—O = 2.845 (1) Å. The three-dimensional structure is stabilized by a water cluster formed by O5—H5···O5, O5—H5···O6 and O6—H6A···O2 hydrogen bonds involving the water molecule, hydroxyl group and oxoboron cluster (Table 1). The channels of the compound are filled with ions/molecules (Mg2+, K+ , OH– and H2O). The title structure is similar to previously reported analogues NH4NaB6O10 (Wang et al., 2014), K0.5[B6O10]3H2O-1.5H2O (Qiu & Yang, 2021b), and NaRb0.5[B6O10]0.5H3O (Qiu et al., 2021b), so the simultaneous use of NH4 and Na or K or Na and Rb or Mg and

![Table 1](image3.png)

Hydrogen-bond geometry (Å, °).

| D—H···A   | D—H     | D···A   | D—H···A   |
|-----------|---------|---------|-----------|
| O5—H5···O5 | 0.85    | 1.67    | 2.42 (3)  | 145       |
| O6—H6A···O2i | 0.85   | 2.58    | 3.276 (15) | 140       |
| O5—H5···O6c | 0.85   | 1.78    | 2.484 (19) | 139       |
| O5—H5···O5a | 0.85   | 2.30    | 3.06 (3)   | 150       |

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

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![Figure 1](image1.png)

The asymmetric unit of the [B6O13]8– oxoboron cluster. Displacement ellipsoids are drawn at the 50% probability level.
et al., 2019b; TAFROI, Natarajan et al., 2003; VUVLOP, Jemai et al., 2015; BATCUY, Jemai et al., 2022; SAZVEY, Xin et al., 2022). It is worth noting that this oxoboron cluster contains too many active hydroxyl groups and therefore tends to form isolated structures. In the crystal of [Cd(1,2-dap)]/[B6O11(OH)2]4H2O (refcode: ZUXLIQ, He et al., 2020), partially protonated [B6O11(OH)2]64− was successfully extended to layered structures via B—O—B bonds, leading to a 3D framework, similar to that of the title compound.

5. Synthesis and crystallization
A mixture of H3BO3 (0.618 g, 10 mmol), KCF3SO3 (0.188 g, 1 mmol) and Mg(CF3SO3)2 (0.322 g, 1 mmol) was added to pyridine (3.0 mL). After stirring for 20 min, the resulting mixture was sealed in a 25 mL Teflon-lined stainless steel autoclave, heated at 488 K for 9 d, and then slowly cooled to room temperature and colorless block-shaped crystals MgK0.5[B6O10](OH)0.5−0.5H2O (refcode: U7786, Deng et al., 2020) were obtained (yield 56% based on H3BO3). Infrared (KBr pallet, cm−1): 3190 vs, 1631 vs, 1360w, 1268m, 1188m, 1134m, 1099m, 964s, 845m, 781m, 741m, 718m, 630w, 564w, 540w, 480w, 455w.

6. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were positioned geometrically (O—H = 0.85 Å) and refined as riding with Uiso(H) 1.2Ueq(O).

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Table 2
Experimental details.

| Crystal data | Chemical formula | Mg$_2$K[B$_6$O$_{10}$](OH)$_2$H$_2$O |
|--------------|------------------|----------------------------------|
| Chemical name|                  | M$_2$                            |
| System, space | Crystal system, | Cubic, Pn3                       |
| group        |                  |                                  |
| Temperature  | Temperature (K)  | (12.296) (2)                     |
|              |                  | 1859.32 (9)                      |
| Radiation    | Radiation type  | Mo Kα                            |
|              | µ (mm$^{-1}$)    | 0.47                             |
|              | Crystal size (mm)| 0.10 × 0.08 × 0.08                |
| Data collection |                  |                                  |
| Refinement   | R$_{int}$ (sin θ/λ)$_{max}$ (Å$^{-1}$) | 0.056, 0.714                       |
|              | R$_{w}$<2σ(F$_{w}$), S | 0.039, 0.116, 1.16               |
|              | No. of reflections | 952                            |
|              | No. of parameters | 72                              |
|              | H-atom treatment | H-atom parameters constrained   |
|              | Δρ$_{free}$, Δρ$_{calc}$ (e Å$^{-3}$) | 0.66, −0.64                     |

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Poly[dimagnesium potassium bis(hexaborate) hydroxide monohydrate]

Crystal data

MgK_{0.5}[B_{6}O_{10}](OH)_{0.5}·0.5H_{2}O
Mr = 572.46
Cubic, Pa3
a = 12.2966 (2) Å
V = 1859.32 (9) Å³
Z = 4
F(000) = 1128
Dₐ = 2.045 Mg m⁻³

Mo Kα radiation, λ = 0.71073 Å
Cell parameters from 5324 reflections
θ = 2.9–30.3°
µ = 0.47 mm⁻¹
T = 296 K
Block, colorless
0.10 × 0.08 × 0.08 mm

Data collection

Bruker APEX2 CCD
diffractometer
Radiation source: fine-focus sealed tube, Bruker
(Mo) X-ray Source
φ and ω scans
Absorption correction: multi-scan
(SADABS; Krause et al., 2015)
Tmin = 0.762, Tmax = 0.936
23808 measured reflections
952 independent reflections
828 reflections with I > 2σ(I)
Rint = 0.056
θmax = 30.5°, θmin = 3.3°
h = -16→17
k = -16→16
l = -16→17

Refinement

Refinement on F^2
Least-squares matrix: full
R[F^2 > 2σ(F^2)] = 0.039
wR(F^2) = 0.116
S = 1.16
952 reflections
72 parameters
0 restraints
Hydrogen site location: difference Fourier map
H-atom parameters constrained
w = 1/[σ^2(F^2) + (0.0658P)^2 + 0.9552P]
where P = (F^2 + 2F'^2)/3
(Δ/σ)max < 0.001
Δρmax = 0.66 e Å⁻³
Δρmin = -0.64 e Å⁻³
Supporting Information

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. The structure was solved by direct methods and refined by the full-matrix least-squares method on $\mathbf{F}^2$ using the SHELXL programs (Bruker, 2006; Sheldrick, 2015a). All non-hydrogen atoms in the complex were refined anisotropically.

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

|    | x          | y          | z          | $U_{11}$/$U_{eq}$ | Occ. (<1) |
|----|------------|------------|------------|-------------------|-----------|
| Mg | 0.33884 (5)| 0.33884 (5)| 0.33884 (5)| 0.0205 (3)        | 0.1667    |
| K  | 0.500000   | 0.500000   | 0.500000   | 0.0257 (3)        | 0.1667    |
| O1 | 0.52065 (8)| 0.28854 (8)| 0.29782 (8)| 0.0110 (3)        | 0.1667    |
| O2 | 0.22982 (9)| 0.18931 (8)| 0.38027 (8)| 0.0118 (3)        | 0.1667    |
| O3 | 0.36386 (8)| 0.68000 (8)| 0.55901 (8)| 0.0113 (3)        | 0.1667    |
| O4 | 0.18887 (7)| 0.18887 (7)| 0.18887 (7)| 0.0057 (3)        | 0.1667    |
| O5 | 0.4745 (13)| 0.1216 (14)| 0.5078 (12)| 0.066 (4)         | 0.1667    |
| H5 | 0.504419   | 0.061354   | 0.523614   | 0.099*            | 0.1667    |
| O6 | 0.544 (2)  | 0.0524 (17)| 0.5575 (10)| 0.080 (6)         | 0.1667    |
| H6A| 0.548070   | 0.065436   | 0.625259   | 0.121*            | 0.1667    |
| H6B| 0.587560   | 0.097246   | 0.528419   | 0.121*            | 0.1667    |
| B1 | 0.21526 (12)| 0.22026 (12)| 0.48534 (12)| 0.0084 (3)        | 0.1667    |
| B2 | 0.16682 (11)| 0.13303 (11)| 0.29771 (11)| 0.0067 (3)        | 0.1667    |

### Atomic displacement parameters ($\AA^2$)

|    | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|----|----------|----------|----------|----------|----------|----------|
| Mg | 0.0205 (3)| 0.0205 (3)| 0.0205 (3)| 0.0007 (2)| 0.0007 (2)| 0.0007 (2)|
| K  | 0.0257 (3)| 0.0257 (3)| 0.0257 (3)| 0.0071 (2)| 0.0071 (2)| 0.0071 (2)|
| O1 | 0.0060 (4)| 0.0113 (5)| 0.0156 (5)| 0.0015 (3)| −0.0031 (3)| −0.0047 (4)|
| O2 | 0.0141 (5)| 0.0157 (5)| 0.0055 (4)| −0.0039 (4)| 0.0005 (3)| −0.0023 (3)|
| O3 | 0.0138 (5)| 0.0134 (5)| 0.0066 (4)| 0.0060 (4)| −0.0017 (4)| −0.0027 (3)|
| O4 | 0.0057 (3)| 0.0057 (3)| 0.0057 (3)| 0.0007 (3)| 0.0007 (3)| 0.0007 (3)|
| O5 | 0.058 (8) | 0.074 (11)| 0.067 (9) | 0.005 (7) | 0.011 (7) | −0.018 (8)|
| O6 | 0.123 (19)| 0.101 (16)| 0.017 (5) | 0.029 (12)| −0.018 (7)| −0.002 (6)|
| B1 | 0.0094 (6)| 0.0091 (6)| 0.0065 (6)| 0.0007 (5)| −0.0008 (5)| −0.0009 (5)|
| B2 | 0.0067 (6)| 0.0067 (6)| 0.0067 (6)| 0.0003 (4)| 0.0006 (4)| 0.0005 (5)|

### Geometric parameters ($\AA$, °)

|    | Mg—O2' | O2—B1    | O2—B2     | Mg—O2' | O2—B2     | O2—B2     |
|----|--------|----------|-----------|--------|-----------|-----------|
| Mg | 2.3319 (12)| 1.3587 (16)| 1.4525 (16)| 2.3319 (12)| 1.3570 (18)| 1.4519 (16)|
| Mg | 2.3319 (12)| 1.5285 (15)| 1.5285 (15)| 2.7714 (15)| 1.5285 (15)|

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| Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|--------------|--------------|--------------|
| Mg—B1i       | 2.7715 (15)  | O5—O6ix      | 0.96 (2)     |
| Mg—B1ii      | 2.7715 (15)  | O5—O6x       | 1.27 (3)     |
| Mg—K         | 3.4324 (11)  | O5—O6        | 1.35 (3)     |
| K—O3         | 2.8450 (10)  | O5—H5        | 0.8500       |
| K—O3ii       | 2.8450 (10)  | O5—H6B       | 1.4451       |
| K—O3i        | 2.8450 (10)  | O6—O6ix      | 0.70 (3)     |
| K—O3iv       | 2.8450 (10)  | O6—O6i       | 1.20 (3)     |
| K—O3v        | 2.8450 (10)  | O6—H5        | 0.6476       |
| O1—B1i       | 1.3821 (18)  | O6—H6A       | 0.8500       |
| O1—B2ii      | 1.4531 (16)  | O6—H6B       | 0.8500       |
| O2—Mg—O2     | 81.06 (5)    | B1ii—O1—B2vi | 123.77 (11) |
| O2—Mg—O2i    | 81.06 (5)    | B1ii—O1—Mg   | 91.19 (8)    |
| O2ii—Mg—O1i  | 112.48 (4)   | B1ii—O1—O2   | 144.28 (8)   |
| O2—Mg—O1i    | 112.48 (4)   | B1ii—O1—O2   | 136.70 (11)  |
| O2—Mg—O1i    | 112.48 (4)   | B1ii—O1—B2   | 93.59 (8)    |
| O2—Mg—O1     | 112.48 (4)   | B2—O2—O2ii   | 121.98 (8)   |
| O2—Mg—O1i    | 112.48 (4)   | B2—O2—O2ii   | 122.23 (11)  |
| O2—Mg—O1     | 112.48 (4)   | B2—O2—O2ii   | 125.09 (8)   |
| O2—Mg—O1     | 112.48 (4)   | B2—O2—O2ii   | 110.32 (7)   |
| O2—Mg—O1     | 112.48 (4)   | B2—O2—O2ii   | 117.97 (4)   |
| O2—O2—O2ii   | 81.06 (5)    | B2—O2—O2ii   | 117.97 (4)   |
| O2—Mg—O1     | 112.48 (4)   | O6—O5—O6ix   | 59 (2)       |
| O2—Mg—O1     | 112.48 (4)   | O6—O5—O6x    | 89.1 (19)    |
| O2—Mg—O1     | 112.48 (4)   | O6—O5—H5     | 47.9         |
| O2—Mg—B1     | 93.22 (5)    | O6—O5—H5     | 22.1         |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 94.6         |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 104.1        |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 35.2         |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 50.4         |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 71 (3)       |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 77 (3)       |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 101 (2)      |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 114 (2)      |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 136.9 (16)   |
| O2—Mg—B1i    | 93.22 (5)    | O6—O5—H5     | 45.7 (12)    |
| O2—B1—Mg—B1i| 112.48 (4)   | O5—O6—O6ix   | 134.5 (17)   |
| O2—B1—Mg—B1i| 112.48 (4)   | O5—O6—O6x    | 104.1        |
| O2—B1—Mg—B1i| 112.48 (4)   | O5—O6—O6x    | 33.1         |
| O2—B1—Mg—B1i| 112.48 (4)   | O5—O6—O6x    | 103.9        |
| O2—B1—Mg—B1i| 112.48 (4)   | O5—O6—O6x    | 117.5        |
| O2—B1—Mg—B1i| 112.48 (4)   | O5—O6—O6x    | 29.6         |
| Bond | Angle (°) | Bond | Angle (°) |
|------|----------|------|----------|
| O2—Mg—K | 131.38 (3) | O5xi—O6—H6A | 44.8 |
| O2ii—Mg—K | 131.38 (3) | O6xi—O6—H6A | 101.0 |
| O2—Mg—K | 131.38 (3) | O6xi—O6—H6A | 103.2 |
| O1i—Mg—K | 74.30 (3) | O5ii—O6—H6A | 111.4 |
| O1ii—Mg—K | 74.30 (3) | O5—O6—H6A | 111.4 |
| O1—Mg—K | 74.30 (3) | H5—O6—H6A | 130.2 |
| B1—Mg—K | 104.19 (4) | O5ui—O6—H6B | 149.2 |
| B1i—Mg—K | 104.19 (4) | O6xii—O6—H6B | 122.2 |
| B1ii—Mg—K | 104.19 (4) | O6xi—O6—H6B | 122.0 |
| B1—Mg—K | 104.19 (4) | O6—O6—H6B | 78.5 |
| O3—K—O3ii | 65.411 (16) | O5—O6—H6B | 76.7 |
| O3—K—O3i | 114.589 (16) | O5—O6—H6B | 95.3 |
| O3—K—O3i | 180.0 | O5—O6—H6B | 104.5 |
| O3—K—O3iv | 65.410 (16) | O5—O6—H6B | 58.1 (15) |
| O3—K—O3iv | 114.590 (15) | O5—O6—H6B | 74 (3) |
| O3—K—O3ii | 65.410 (15) | O5—O6—H6B | 28.4 (18) |
| O3—K—O3ii | 114.590 (15) | O5—O6—H6B | 74 (3) |
| O3—K—O3ii | 180.0 | O5—O6—H6B | 114 (3) |
| O3—K—O3iv | 65.410 (16) | H6A—O6—H5xi | 87.3 |
| O3—K—O3iv | 65.410 (16) | H6A—O6—H5xi | 97.8 |
| O3—K—Mgvi | 76.32 (2) | H6B—O6—H5xi | 148.0 |
| O3vi—K—Mgvi | 103.68 (2) | O3—B1—O2 | 123.87 (12) |
| O3vi—K—Mgvi | 76.32 (2) | O3—B1—O1i | 122.17 (12) |
| O3vi—K—Mgvi | 103.68 (2) | O2—B1—O1i | 113.96 (12) |
| O3vi—K—Mgvi | 103.68 (2) | O3—B1—Mg | 166.22 (10) |
| O3i—K—Mgvi | 76.32 (2) | O2—B1—Mg | 57.12 (7) |
| O3i—K—Mgvi | 103.68 (2) | O1i—B1—Mg | 58.91 (7) |
| O3i—K—Mgvi | 76.32 (2) | O3—B2—O2 | 112.28 (11) |
| O3i—K—Mgvi | 103.68 (2) | O3—B2—O1iv | 109.48 (11) |
| O3i—K—Mgvi | 76.32 (2) | O2—B2—O1iv | 110.35 (11) |
| O3i—K—Mgvi | 76.32 (2) | O3—B2—O4 | 109.12 (10) |
| O3i—K—Mgvi | 103.68 (2) | O2—B2—O4 | 107.66 (11) |
| Mgvi—K—Mgvi | 180.000 (17) | O1iv—B2—O4 | 107.83 (10) |
| O6xvi—O5—O6—O5xi | −36 (3) | B1—O2—B2—O3xiv | 21.1 (2) |
| O6xiv—O5—O6—O5xi | −94.9 (17) | Mg—O2—B2—O3xiv | −119.29 (10) |
| O6—O5—O6—O6xi | −59 (2) | B1—O2—B2—O1xv | −101.35 (17) |
| O6—O5—O6—O6xi | 52 (3) | Mg—O2—B2—O1xv | 118.27 (10) |
| O6—O5—O6—O6xi | −7 (5) | B1—O2—B2—O4 | 141.21 (14) |
| O6—O5—O6—O5xi | 117 (3) | Mg—O2—B2—O4 | 0.84 (12) |
| O6—O5—O6—O5xi | 58 (4) | B2—O4—B2—O3xiv | 45.6 (2) |
| B2—O2—B1—O3iii | 1.63 (2) | B2—O4—B2—O3xiv | −162.41 (10) |
| Mg—O2—B1—O3iii | 163.52 (12) | B2—O4—B2—O2 | −76.54 (15) |
| B2—O2—B1—O1i | −163.39 (13) | B2—O4—B2—O2 | 75.49 (15) |
Mg—O2—B1—O1i −16.21 (12) B2i—O4—B2—O1iv 164.40 (10) B2—O2—B1—Mg −147.18 (17) B2ii—O4—B2—O1xv −43.6 (2)

Symmetry codes: (i) y, z, x; (ii) z, x, y; (iii) −y+1, −z+1, −x+1; (iv) −z+1, −x+1, −y+1; (v) −x+1, −y+1, −z+1; (vi) y+1/2, z, −x+1/2; (vii) −x+1/2, y+1/2, z; (viii) −y+1/2, −z+1, x+1/2; (ix) −y+1/2, z−1/2, x; (x) −z+1, x−1/2, −y+1/2; (xi) −x+1/2, y+1/2, z+1/2; (xii) y+1/2, −x+1, y+1/2; (xiii) −x+1/2, −x+1/2, −y+1; (xiv) z−1/2, −x+1/2, −y+1; (xv) −z+1/2, x−1/2, y.

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A   | D—H···A |
|---------|------|-------|---------|---------|
| O5—H5···O5xii | 0.85 | 1.67  | 2.42 (3) | 145 |
| O6—H6···O2xii | 0.85 | 2.58  | 3.276 (15) | 140 |
| O6—H5···O6x | 0.65 | 0.74  | 1.20 (3) | 119 |
| O6—H5···O6xvi | 0.65 | 1.23  | 1.84 (2) | 158 |
| O6—H5···O5vii | 0.65 | 1.82  | 2.19 (3) | 118 |
| O6—H5···O5viii | 0.65 | 1.79  | 2.34 (3) | 143 |
| O6—H5···O5ix | 0.65 | 2.09  | 2.484 (19) | 121 |
| O6—H5···O5x | 0.65 | 0.85  | 1.35 (3) | 128 |
| O5—H5···O6xvi | 0.85 | 1.78  | 2.484 (19) | 139 |
| O5—H5···O6xvii | 0.85 | 1.49  | 2.34 (3) | 179 |
| O5—H5···O6xvii | 0.85 | 1.82  | 2.30 (2) | 114 |
| O5—H5···O5xii | 0.85 | 1.67  | 2.42 (3) | 145 |
| O5—H5···O5xvi | 0.85 | 1.28  | 1.88 (3) | 122 |
| O5—H5···O5xvi | 0.85 | 2.30  | 3.06 (3) | 150 |

Symmetry codes: (ix) −y+1/2, z−1/2, x; (x) −z+1, x−1/2, −y+1/2; (xi) z, −x+1/2, y+1/2; (xii) y+1/2, −z+1/2, −x+1; (xvi) −x+1, −y, −z+1.