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# 2,3,4-Trihydroxybenzoic acid 0.25-hydrate

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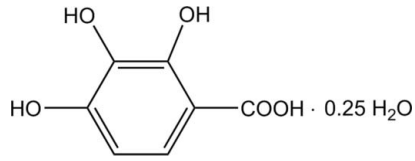
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.036; $wR$ factor = 0.090; data-to-parameter ratio = 11.5.

The asymmetric unit of the title compound, $C_7H_6O_5\cdot 0.25H_2O$, contains two molecules of 2,3,4-trihydroxybenzoic acid, with similar conformations, and one water molecule which lies on a twofold rotation axis. Both acid molecules are essentially planar [maximum r.m.s deviations = 0.0324 (2) and 0.0542 (3) Å for the two acid molecules]. The molecular conformations are stabilized by intramolecular O(phenol)—H···O(carboxyl/phenol) interactions. A cyclic intermolecular association is formed between the two acid and one water molecule [graph set $R_3^3(12)$] involving O—H···O hydrogen bonds. The two acid molecules are further linked through a cyclic $R_2^2(8)$ carboxylic acid hydrogen-bonding association, which together with intermolecular O—H···O hydrogen-bonding interactions involving the phenol groups and the water molecule, and weak $\pi$–$\pi$ interactions [minimum ring centroid separation = 3.731 (3) Å], give a three-dimensional network.

## Related literature

For the natural distribution of 2,3,4-trihydroxybenzoic acid, see: Zhai *et al.* (2010); Xu & Chang (2010). For its antioxidant and antibacterial activities, see: Kodama *et al.* (2007); Friedman *et al.* (2003). For the inhibition of xanthine oxidase, see: Chang *et al.* (1995). For the crystal structure of the dihydrate pseudopolymorph, see: Prior & Sharp (2010). For $\pi$–$\pi$ interactions in gallic acid pyridine monosolvate and in natural flavonoids, see: Dong *et al.* (2011); Jiang *et al.* (2009, 2002). For graph-set analysis, see: Etter *et al.* (1990); Bernstein *et al.* (1995).




## Experimental

### Crystal data

$C_7H_6O_5\cdot 0.25H_2O$
$M_r$ = 174.62
Orthorhombic, $P2_12_12$
$a$ = 11.8364 (12) Å
$b$ = 32.598 (3) Å
$c$ = 3.7306 (4) Å
$V$ = 1439.4 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.14 mm$^{-1}$
$T$ = 291 K
0.42 × 0.28 × 0.20 mm

### Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.874, $T_{max}$ = 1.000
7863 measured reflections
2552 independent reflections
2010 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.060

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
$S$ = 0.97
2552 reflections
222 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$WA$···O2 | 0.82 | 2.19 | 2.963 (2) | 156 |
| O1—H1$A$···O4 | 0.82 | 1.88 | 2.587 (3) | 143 |
| O2—H2$A$···O2$'^{i}$ | 0.82 | 2.05 | 2.839 (4) | 161 |
| O3—H3$A$···O3$'^{ii}$ | 0.82 | 2.06 | 2.828 (3) | 155 |
| O5—H5$B$···O4$'^{iii}$ | 0.82 | 1.88 | 2.679 (4) | 165 |
| O1′—H1′$A$···O4′ | 0.82 | 1.87 | 2.588 (3) | 145 |
| O2′—H2′$A$···O1 | 0.82 | 1.95 | 2.729 (4) | 159 |
| O3′—H3′$A$···O1$W$ | 0.82 | 2.06 | 2.841 (3) | 158 |
| O5′—H5′$B$···O4$^{iv}$ | 0.82 | 1.85 | 2.659 (4) | 171 |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Siemens, 1998); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2181).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o825–o826 [doi:10.1107/S160053681200709X]

## 2,3,4-Trihydroxybenzoic acid 0.25-hydrate

**Jin-Hang Li, Fu-Yue Dong, Fang Cai, Xiao-Feng Yuan and Ren-Wang Jiang**

### Comment

2,3,4-Trihydroxybenzoic acid is a polyphenolic acid which has been isolated from *Pachysandra terminalis* (Zhai *et al.*, 2010) and the lentil (Xu & Chang, 2010). It has been found to show antioxidant (Kodama *et al.*, 2007) and antibacterial activities (Friedman *et al.*, 2003) and also to inhibit the xanthine oxidase enzyme (Chang *et al.*, 1995). This compound contains two of the most common functional groups in natural products: the carboxylic acid and the phenolic groups. The dihydrate pseudopolymorph of the acid with a space group *P*-1 has previously been reported (Prior & Sharp, 2010). In this study, we report the structure of the second pseudopolymorph, the partial hydrate $C_7H_6O_5$ . $0.25H_2O$.

The asymmetric unit of the title compound contains two molecules of 2,3,4-trihydroxybenzoic acid [(1) and (2)] with similar conformations, and one water molecule of solvation which lies on a crystallographic twofold rotation axis (Fig. 1). Both acid molecules are essentially planar [maximum r.m.s deviation 0.0324 (2) and 0.0542 (3) Å for the two acid molecules], with a dihedral angle of 49.4 (3)° between the planes. The molecular conformation of the acid molecules is stabilized by a number of intramolecular phenolic O—H···O interactions (Table 1).

The water molecule and the acid molecules are linked through O—H···O hydrogen bonds (Table 1) with both acting as donors and acceptors, giving a cyclic association [graph set $R^3_3(12)$ (Etter *et al.*, 1990; Bernstein *et al.*, 1995)]. The 2,3,4-trihydroxybenzoic acid molecules form head-to-head pairs through intermolecular hydrogen bonds [graph set $R^2_2(8)$. The molecular pairs are further extended into chains through hydrogen bond O2–H···O2$^{i}$ , while adjacent chains are connected *via* hydrogen bond O3–H···O3$^{ii}$ into a three-dimensional network (Fig. 2) [for symmetry codes (i) and (ii), see Table 1]. It is noteworthy that aromatic $\pi$–$\pi$ associations also play an important role in the molecular packing. Adjacent 2,3,4-trihydroxybenzoic acid molecules form stacks which extend down the *c*-axis giving weak $\pi$–$\pi$ interactions [minimum ring centroid separation, 3.731 (3) Å], which is larger than that in the dihydrate form of the acid (Prior & Sharp, 2010) and in gallic acid pyridine monosolvate (Dong *et al.*, 2011), but comparable with those in natural flavonoids (Jiang *et al.*, 2002, 2009).

### Experimental

2,3,4-Trihydroxybenzoic acid (purity >98%) was purchased from the Sigma-Aldrich Company. Sample of 34 mg (0.2 mmol) was dissolved in methanol (1.5 ml) in a tube (4 ml) and sealed by parafilm. Light brown crystals were formed after three days at room temperature.

### Refinement

The C-bound H atoms were positioned geometrically and were included in the refinement in the riding-model approximation, with C—H = 0.96 Å (methyl C) and $U_{iso}$(H) = 1.5$U_{eq}$(C); 0.97 Å (methylene C) and $U_{iso}$(H) = 1.2$U_{eq}$(C); 0.93 Å (aryl H) and $U_{iso}$(H)= 1.2$U_{eq}$(C); O—H = 0.82 Å and $U_{iso}$(H) = 1.5$U_{eq}$(O).

### Computing details

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Siemens, 1998); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

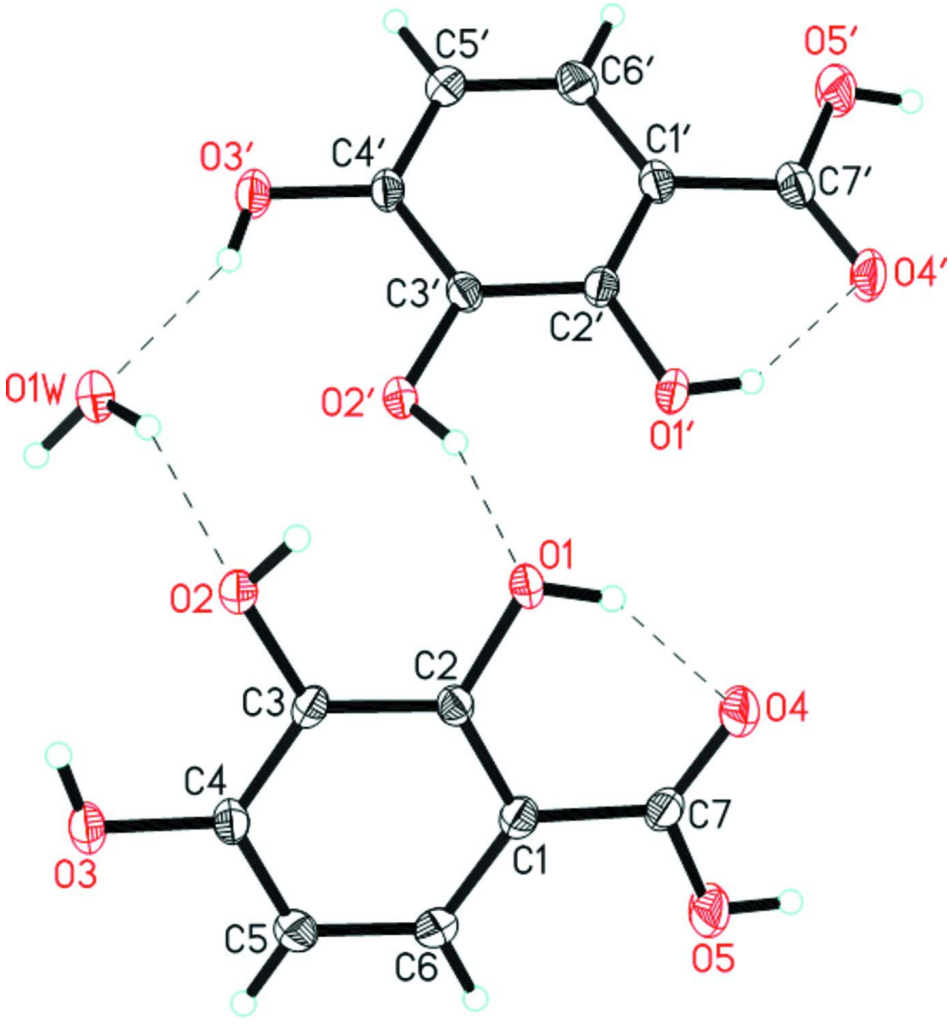


**Figure 1**

An ORTEP plot of the asymmetric unit of the title compound with atoms shown as 30% probability ellipsoids. The water molecule lies on a crystallographic twofold rotation axis and hydrogen bonds are shown as dashed lines.

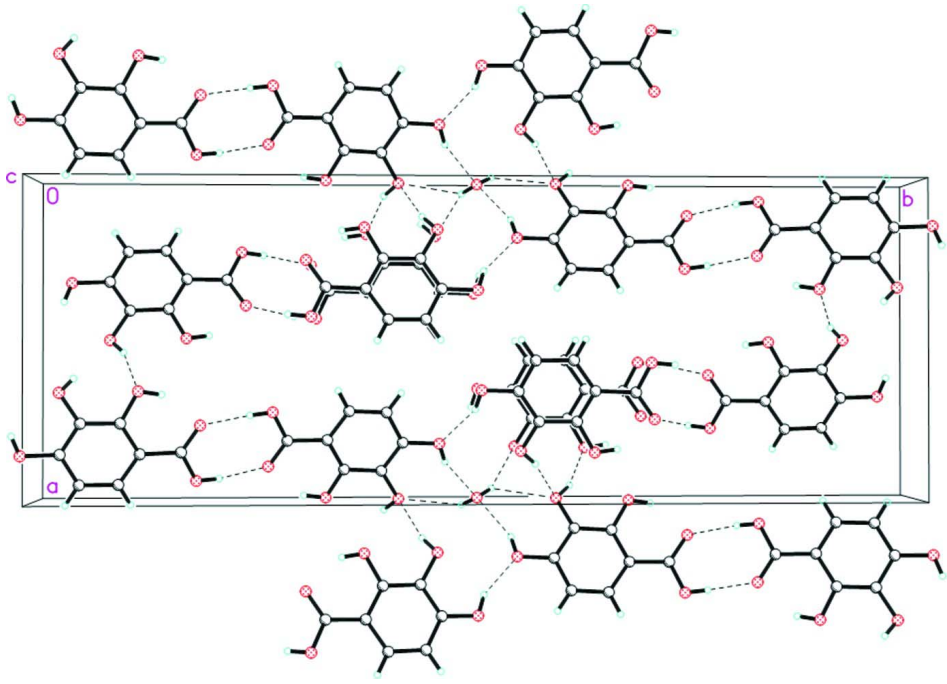


**Figure 2**

Packing diagram viewed down the *c*-axis showing hydrogen bonds as dashed lines.

### 2,3,4-Trihydroxybenzoic acid 0.25-hydrate

*Crystal data*

$C_7H_6O_5 \cdot 0.25H_2O$
$M_r = 174.62$
Orthorhombic, $P2_12_12$
Hall symbol: P 2ac 2ab
$a = 11.8364$ (12) Å
$b = 32.598$ (3) Å
$c = 3.7306$ (4) Å
$V = 1439.4$ (3) Å$^3$
$Z = 8$
$F(000) = 724$
$D_x = 1.612$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2552 reflections
$\theta = 2.1$–$50.0°$
$\mu = 0.14$ mm$^{-1}$
$T = 291$ K
Prism, light brown
0.42 × 0.28 × 0.20 mm

*Data collection*

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.874$, $T_{max} = 1.000$
7863 measured reflections
2552 independent reflections
2010 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -13 \rightarrow 14$
$k = -38 \rightarrow 34$
$l = -4 \rightarrow 4$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.090$
$S = 0.97$
2552 reflections
222 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

| | |
|---|---|
| Secondary atom site location: difference Fourier map | $w = 1/[\sigma^2(F_o^2) + (0.0443P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Hydrogen site location: inferred from neighbouring sites | $(\Delta/\sigma)_{max} < 0.001$ |
| H-atom parameters constrained | $\Delta\rho_{max} = 0.17$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.15$ 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**. 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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1W | 0.5000 | 0.0000 | −0.1102 (7) | 0.0395 (6) |
| H1WA | 0.5263 | 0.0173 | 0.0258 | 0.059* |
| O1 | 0.65345 (12) | 0.12870 (4) | 0.2193 (5) | 0.0334 (4) |
| H1A | 0.6637 | 0.1534 | 0.1900 | 0.040* |
| O2 | 0.65656 (13) | 0.04688 (4) | 0.3549 (4) | 0.0323 (4) |
| H2A | 0.6145 | 0.0640 | 0.4444 | 0.039* |
| O3 | 0.84576 (14) | 0.00203 (5) | 0.2010 (5) | 0.0445 (5) |
| H3A | 0.7859 | −0.0048 | 0.2940 | 0.053* |
| O4 | 0.75826 (14) | 0.19200 (4) | −0.0346 (6) | 0.0429 (5) |
| O5 | 0.93058 (15) | 0.18491 (4) | −0.2704 (6) | 0.0481 (5) |
| H5B | 0.9243 | 0.2098 | −0.2919 | 0.058* |
| C1 | 0.84467 (19) | 0.12653 (6) | −0.0250 (7) | 0.0273 (5) |
| C2 | 0.74982 (19) | 0.10787 (6) | 0.1337 (6) | 0.0245 (5) |
| C3 | 0.74932 (18) | 0.06626 (6) | 0.2074 (6) | 0.0254 (5) |
| C4 | 0.84311 (19) | 0.04271 (6) | 0.1272 (7) | 0.0295 (5) |
| C5 | 0.9374 (2) | 0.06046 (7) | −0.0324 (7) | 0.0330 (6) |
| H5A | 0.9998 | 0.0444 | −0.0891 | 0.040* |
| C6 | 0.9383 (2) | 0.10180 (7) | −0.1064 (7) | 0.0313 (6) |
| H6A | 1.0018 | 0.1135 | −0.2117 | 0.038* |
| C7 | 0.8406 (2) | 0.17017 (7) | −0.1079 (7) | 0.0310 (6) |
| O1′ | 0.49399 (13) | 0.17376 (4) | −0.2824 (5) | 0.0359 (4) |
| H1′A | 0.4856 | 0.1982 | −0.3270 | 0.043* |
| O2′ | 0.49999 (12) | 0.09083 (4) | −0.2151 (5) | 0.0308 (4) |
| H2′A | 0.5380 | 0.1075 | −0.1033 | 0.037* |
| O3′ | 0.32290 (14) | 0.04439 (4) | −0.4474 (5) | 0.0397 (5) |
| H3′A | 0.3817 | 0.0378 | −0.3464 | 0.048* |
| O4′ | 0.39072 (15) | 0.23703 (5) | −0.5434 (6) | 0.0446 (5) |
| O5′ | 0.22055 (15) | 0.23003 (5) | −0.7935 (6) | 0.0506 (5) |
| H5′B | 0.2294 | 0.2547 | −0.8259 | 0.061* |
| C1′ | 0.3088 (2) | 0.17066 (7) | −0.5659 (7) | 0.0293 (6) |
| C2′ | 0.40325 (19) | 0.15242 (6) | −0.4052 (6) | 0.0271 (6) |
| C3′ | 0.40863 (19) | 0.11019 (6) | −0.3646 (6) | 0.0267 (5) |

| | | | | |
|---|---|---|---|---|
| C4′ | 0.31874 (19) | 0.08593 (6) | −0.4795 (7) | 0.0281 (6) |
| C5′ | 0.22322 (19) | 0.10389 (7) | −0.6322 (7) | 0.0328 (6) |
| H5′A | 0.1630 | 0.0876 | −0.7056 | 0.039* |
| C6′ | 0.2185 (2) | 0.14569 (7) | −0.6737 (7) | 0.0336 (6) |
| H6′A | 0.1546 | 0.1576 | −0.7746 | 0.040* |
| C7′ | 0.3098 (2) | 0.21492 (7) | −0.6310 (7) | 0.0349 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1W | 0.0469 (15) | 0.0229 (11) | 0.0486 (16) | −0.0056 (10) | 0.000 | 0.000 |
| O1 | 0.0299 (9) | 0.0177 (7) | 0.0527 (11) | 0.0023 (6) | 0.0057 (9) | 0.0020 (8) |
| O2 | 0.0280 (9) | 0.0212 (8) | 0.0475 (11) | 0.0003 (6) | 0.0064 (8) | 0.0020 (8) |
| O3 | 0.0386 (10) | 0.0215 (8) | 0.0734 (13) | 0.0038 (7) | 0.0121 (10) | 0.0077 (10) |
| O4 | 0.0398 (11) | 0.0244 (8) | 0.0644 (13) | −0.0006 (8) | 0.0084 (10) | 0.0075 (9) |
| O5 | 0.0463 (11) | 0.0268 (9) | 0.0713 (14) | −0.0031 (8) | 0.0157 (11) | 0.0094 (10) |
| C1 | 0.0298 (13) | 0.0244 (11) | 0.0278 (13) | −0.0029 (10) | −0.0040 (11) | 0.0009 (11) |
| C2 | 0.0265 (12) | 0.0208 (11) | 0.0261 (13) | 0.0014 (9) | −0.0058 (11) | −0.0024 (10) |
| C3 | 0.0285 (13) | 0.0211 (11) | 0.0268 (12) | −0.0056 (9) | −0.0017 (11) | 0.0004 (10) |
| C4 | 0.0334 (14) | 0.0193 (11) | 0.0359 (14) | 0.0014 (10) | −0.0033 (12) | 0.0009 (11) |
| C5 | 0.0278 (14) | 0.0303 (13) | 0.0409 (15) | 0.0041 (10) | 0.0006 (12) | −0.0034 (12) |
| C6 | 0.0257 (13) | 0.0324 (13) | 0.0360 (15) | −0.0042 (10) | −0.0001 (12) | 0.0006 (11) |
| C7 | 0.0315 (14) | 0.0255 (12) | 0.0361 (14) | −0.0068 (11) | −0.0040 (12) | 0.0019 (11) |
| O1′ | 0.0346 (9) | 0.0185 (7) | 0.0546 (11) | −0.0032 (6) | −0.0058 (10) | 0.0011 (8) |
| O2′ | 0.0294 (9) | 0.0191 (7) | 0.0440 (10) | 0.0016 (6) | −0.0038 (9) | 0.0011 (7) |
| O3′ | 0.0408 (11) | 0.0207 (8) | 0.0575 (12) | −0.0029 (7) | −0.0115 (9) | −0.0004 (9) |
| O4′ | 0.0476 (12) | 0.0208 (8) | 0.0655 (14) | 0.0004 (8) | −0.0142 (10) | 0.0057 (9) |
| O5′ | 0.0482 (11) | 0.0279 (9) | 0.0758 (14) | 0.0047 (8) | −0.0172 (12) | 0.0138 (10) |
| C1′ | 0.0340 (14) | 0.0227 (12) | 0.0312 (13) | 0.0031 (10) | 0.0040 (11) | −0.0003 (11) |
| C2′ | 0.0295 (13) | 0.0221 (12) | 0.0297 (14) | −0.0024 (10) | 0.0035 (12) | −0.0021 (10) |
| C3′ | 0.0280 (13) | 0.0231 (11) | 0.0290 (13) | 0.0037 (10) | 0.0045 (11) | 0.0009 (10) |
| C4′ | 0.0334 (14) | 0.0199 (11) | 0.0311 (14) | 0.0005 (10) | 0.0052 (11) | −0.0007 (11) |
| C5′ | 0.0297 (14) | 0.0299 (12) | 0.0388 (15) | −0.0033 (10) | −0.0005 (12) | −0.0019 (12) |
| C6′ | 0.0342 (14) | 0.0326 (12) | 0.0339 (15) | 0.0051 (10) | −0.0039 (12) | 0.0022 (12) |
| C7′ | 0.0399 (16) | 0.0271 (13) | 0.0376 (15) | 0.0071 (11) | 0.0020 (12) | 0.0021 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1W—H1WA | 0.8200 | O1′—C2′ | 1.359 (3) |
| O1—C2 | 1.365 (3) | O1′—H1′A | 0.8200 |
| O1—H1A | 0.8200 | O2′—C3′ | 1.371 (3) |
| O2—C3 | 1.381 (3) | O2′—H2′A | 0.8200 |
| O2—H2A | 0.8200 | O3′—C4′ | 1.360 (2) |
| O3—C4 | 1.355 (2) | O3′—H3′A | 0.8200 |
| O3—H3A | 0.8200 | O4′—C7′ | 1.243 (3) |
| O4—C7 | 1.237 (3) | O5′—C7′ | 1.314 (3) |
| O5—C7 | 1.317 (3) | O5′—H5′B | 0.8200 |
| O5—H5B | 0.8200 | C1′—C2′ | 1.401 (3) |
| C1—C6 | 1.404 (3) | C1′—C6′ | 1.403 (3) |
| C1—C2 | 1.407 (3) | C1′—C7′ | 1.463 (3) |

| | | | |
|---|---|---|---|
| C1—C7 | 1.457 (3) | C2′—C3′ | 1.386 (3) |
| C2—C3 | 1.384 (3) | C3′—C4′ | 1.393 (3) |
| C3—C4 | 1.382 (3) | C4′—C5′ | 1.395 (3) |
| C4—C5 | 1.391 (3) | C5′—C6′ | 1.373 (3) |
| C5—C6 | 1.376 (3) | C5′—H5′A | 0.9300 |
| C5—H5A | 0.9300 | C6′—H6′A | 0.9300 |
| C6—H6A | 0.9300 | | |

| | | | |
|---|---|---|---|
| C2—O1—H1A | 109.5 | C2′—O1′—H1′A | 109.5 |
| C3—O2—H2A | 109.5 | C3′—O2′—H2′A | 109.5 |
| C4—O3—H3A | 109.5 | C4′—O3′—H3′A | 109.5 |
| C7—O5—H5B | 109.5 | C7′—O5′—H5′B | 109.5 |
| C6—C1—C2 | 118.2 (2) | C2′—C1′—C6′ | 119.0 (2) |
| C6—C1—C7 | 122.8 (2) | C2′—C1′—C7′ | 118.9 (2) |
| C2—C1—C7 | 119.0 (2) | C6′—C1′—C7′ | 122.1 (2) |
| O1—C2—C3 | 115.9 (2) | O1′—C2′—C3′ | 115.8 (2) |
| O1—C2—C1 | 123.35 (18) | O1′—C2′—C1′ | 123.89 (18) |
| C3—C2—C1 | 120.7 (2) | C3′—C2′—C1′ | 120.3 (2) |
| O2—C3—C4 | 118.08 (17) | O2′—C3′—C2′ | 122.5 (2) |
| O2—C3—C2 | 122.06 (19) | O2′—C3′—C4′ | 117.79 (18) |
| C4—C3—C2 | 119.9 (2) | C2′—C3′—C4′ | 119.7 (2) |
| O3—C4—C3 | 121.2 (2) | O3′—C4′—C3′ | 120.7 (2) |
| O3—C4—C5 | 118.4 (2) | O3′—C4′—C5′ | 118.9 (2) |
| C3—C4—C5 | 120.4 (2) | C3′—C4′—C5′ | 120.4 (2) |
| C6—C5—C4 | 119.9 (2) | C6′—C5′—C4′ | 119.7 (2) |
| C6—C5—H5A | 120.0 | C6′—C5′—H5′A | 120.1 |
| C4—C5—H5A | 120.0 | C4′—C5′—H5′A | 120.1 |
| C5—C6—C1 | 120.9 (2) | C5′—C6′—C1′ | 120.8 (2) |
| C5—C6—H6A | 119.6 | C5′—C6′—H6′A | 119.6 |
| C1—C6—H6A | 119.6 | C1′—C6′—H6′A | 119.6 |
| O4—C7—O5 | 122.0 (2) | O4′—C7′—O5′ | 121.6 (2) |
| O4—C7—C1 | 122.7 (2) | O4′—C7′—C1′ | 122.3 (2) |
| O5—C7—C1 | 115.3 (2) | O5′—C7′—C1′ | 116.1 (2) |

| | | | |
|---|---|---|---|
| C6—C1—C2—O1 | −178.9 (2) | C6′—C1′—C2′—O1′ | −178.2 (2) |
| C7—C1—C2—O1 | −0.8 (3) | C7′—C1′—C2′—O1′ | 4.6 (4) |
| C6—C1—C2—C3 | 0.1 (3) | C6′—C1′—C2′—C3′ | 2.1 (4) |
| C7—C1—C2—C3 | 178.2 (2) | C7′—C1′—C2′—C3′ | −175.1 (2) |
| O1—C2—C3—O2 | 0.7 (3) | O1′—C2′—C3′—O2′ | −0.9 (3) |
| C1—C2—C3—O2 | −178.4 (2) | C1′—C2′—C3′—O2′ | 178.8 (2) |
| O1—C2—C3—C4 | 179.6 (2) | O1′—C2′—C3′—C4′ | 179.3 (2) |
| C1—C2—C3—C4 | 0.5 (3) | C1′—C2′—C3′—C4′ | −1.0 (4) |
| O2—C3—C4—O3 | −2.0 (3) | O2′—C3′—C4′—O3′ | −0.8 (3) |
| C2—C3—C4—O3 | 179.0 (2) | C2′—C3′—C4′—O3′ | 179.0 (2) |
| O2—C3—C4—C5 | 177.9 (2) | O2′—C3′—C4′—C5′ | 179.7 (2) |
| C2—C3—C4—C5 | −1.0 (4) | C2′—C3′—C4′—C5′ | −0.5 (4) |
| O3—C4—C5—C6 | −179.1 (2) | O3′—C4′—C5′—C6′ | −178.6 (2) |
| C3—C4—C5—C6 | 1.0 (4) | C3′—C4′—C5′—C6′ | 0.9 (4) |
| C4—C5—C6—C1 | −0.4 (4) | C4′—C5′—C6′—C1′ | 0.3 (4) |

| | | | |
|---|---|---|---|
| C2—C1—C6—C5 | −0.1 (4) | C2′—C1′—C6′—C5′ | −1.8 (4) |
| C7—C1—C6—C5 | −178.2 (2) | C7′—C1′—C6′—C5′ | 175.3 (2) |
| C6—C1—C7—O4 | −179.6 (2) | C2′—C1′—C7′—O4′ | −1.2 (4) |
| C2—C1—C7—O4 | 2.3 (4) | C6′—C1′—C7′—O4′ | −178.3 (2) |
| C6—C1—C7—O5 | 1.0 (3) | C2′—C1′—C7′—O5′ | 177.7 (2) |
| C2—C1—C7—O5 | −177.1 (2) | C6′—C1′—C7′—O5′ | 0.6 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*WA*···O2 | 0.82 | 2.19 | 2.963 (2) | 156 |
| O1*W*—H1*WA*···O2′ | 0.82 | 2.58 | 2.987 (3) | 112 |
| O1—H1*A*···O4 | 0.82 | 1.88 | 2.587 (3) | 143 |
| O2—H2*A*···O2′$^{i}$ | 0.82 | 2.05 | 2.839 (4) | 161 |
| O2—H2*A*···O1 | 0.82 | 2.32 | 2.715 (2) | 111 |
| O3—H3*A*···O3′$^{ii}$ | 0.82 | 2.06 | 2.828 (3) | 155 |
| O3—H3*A*···O2 | 0.82 | 2.29 | 2.735 (3) | 115 |
| O5—H5*B*···O4′$^{iii}$ | 0.82 | 1.88 | 2.679 (4) | 165 |
| O1′—H1′*A*···O4′ | 0.82 | 1.87 | 2.588 (3) | 145 |
| O2′—H2′*A*···O1 | 0.82 | 1.95 | 2.729 (4) | 159 |
| O2′—H2′*A*···O1′ | 0.82 | 2.32 | 2.716 (2) | 110 |
| O3′—H3′*A*···O1*W* | 0.82 | 2.06 | 2.841 (3) | 158 |
| O3′—H3′*A*···O2′ | 0.82 | 2.28 | 2.727 (4) | 115 |
| O5′—H5′*B*···O4$^{iv}$ | 0.82 | 1.85 | 2.659 (4) | 171 |

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