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6-Hydroxymethyl-4-methoxy-2H-pyran-2-one (Opuntiol)

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.094; data-to-parameter ratio = 12.1.

The title compound, C7H8O4, isolated from Opuntia dillenii Haw (Cactaceae), is almost planar [maximum deviation of 0.027(2) Å] except for the H atoms of the methylene and methyl groups. The crystal packing is stabilized by $C-H \cdots O$ and $O-H \cdots O$ intermolecular hydrogen bonds, resulting in the formation of a three-dimensional network.

Related literature

For the use of the stem and fruit of Opuntia dillenii Haw (Cactaceae) in folk medicine, see: Chang et al. (2008). For phytochemical investigations of this plant, see: Qiu et al. (2002). For comparitive bond lengths, see: Allen et al. (1987).



Experimental

Crystal data

 $C_7H_8O_4$ $M_r = 156.13$ Monoclinic, $P2_1/c$ a = 4.0499 (5) Å b = 18.101 (2) Å c = 9.4743 (13) Å $\beta = 96.720 \ (7)^{\circ}$

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V = 689.76 (15) \text{ Å}^3
Z = 4
Mo K\alpha radiation
\mu = 0.13 \text{ mm}^{-1}
T = 296 \text{ K}
0.34 \times 0.25 \times 0.19 \; \text{mm}
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Data collection

Bruker Kappa APEXII CCD area-	1268 independent reflections
detector diffractometer	882 reflections with $I > 2\sigma(I)$
6516 measured reflections	$R_{\rm int} = 0.046$
6516 measured reflections	$R_{\rm int} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of
$wR(F^2) = 0.094$	independent and constrained
S = 1.02	refinement
1268 reflections	$\Delta \rho_{\rm max} = 0.16 \text{ e } \text{\AA}^{-3}$
105 parameters	$\Delta \rho_{\rm min} = -0.16 \text{ e } \text{\AA}^{-3}$
1 restraint	

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$\begin{array}{c} 04 - H1 \cdots 01^{i} \\ 04 - H1 \cdots 02^{i} \\ 07 - H7B \cdots 04^{ii} \\ 07 - H7C \cdots 02^{iii} \end{array}$	0.836 (14) 0.836 (14) 0.96 0.96	2.47 (2) 2.073 (13) 2.58 2.57	3.1840 (19) 2.8678 (18) 3.494 (2) 3.504 (2)	144.2 (17) 158.6 (18) 159 164

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare et al., 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2184).

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supplementary materials

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6-Hydroxymethyl-4-methoxy-2H-pyran-2-one (Opuntiol)

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Comment

Opuntia dillenii Haw (Cactaceae) usually grows in semi-desert regions in the tropics and subtropics. The stem and fruit of this plant are used in a folk medicine for reducing cholesterol levels, treatment of gastric ulcers, inflammation, diabetes and several other diseases (Chang *et al.*, 2008). The phytochemical investigations on this plant have led to the isolation of various oxygenated constituents namely *opuntiol*, opuntioside-I, *p*-hydroxybenzoic acid, ethyl 3,4-dihydroxybenzoate, 3,4-dihydroxybenzoic acid, *L*-(-)-malic acid, (*E*)-ferulic acid, 4-ethoxy-6-hydroxymethyl- α -pyrone, 1-heptanecanol, vanillic acid, isorhamnetin, isorhamnetin-3-*O*-rutinoside, rutin, quercetin, 3,3'-dimethyl quercetin, 3-*O*-methyl quercetin, 3-*O*-methyl quercetin, 7-*O*- β -*D*-glucopyranoside, kaempferol, kaempferol 7-*O*- β -*D*-glucopyranoside, kaempferide, β -sitosterol, and manghaslin (Qiu *et al.*, 2002). In the present study we first time report the crystal structure of opuntiol using single-crystal XRD.

In the title molecule, **I**, shown in Fig. 1, bond lengths and angles display normal values (Allen *et al.*, 1987). Except the H atoms of the methlene and methyl groups, the molecule of **I** is almost planar, with maximum deviations of 0.027 (2)Å for O4, 0.023 (2)Å for C7, 0.020 (1)Å for O2 and -0.019 (2)Å for C2. For the methoxy and hydroxy methyl groups at the C3 and C5 positions in **I**, the C2–C3–O3–C7 and C4–C3–O3–C7 torsion angles are 0.9 (2)° and -178.94 (15)°, the O1–C5–C6–O4 and C4–C5–C6–O4 torsion angles are 177.77 (14)° and -2.9 (3)°, respectively.

In the crystal structure of I, there are non-classical C–H \cdots O and classical O–H \cdots O intermolecular hydrogen bonds (Table 1), forming a three-dimensional network (Figs. 2 and 3).

Experimental

Plant Material: *Opuntia dillenii Haw* (whole plant) was collected from the areas of Mar Balochan, Sangla Hill, Distt. Nankana, Pakistan, in April 2008, and identified by Muhammad Ajaib (Taxonomist), Department of Botany, Government College University, Lahore.

Extraction and isolation: The shade-dried ground whole plant (7 kg) of *Opuntia dillenii Haw* was exhaustively extracted with methanol ($10L \times 4$) at room temperature. The extract was evaporated to yield the residue (1.1 kg), which was dissolved in distilled water (2.0 L) and partitioned with *n*-hexane ($2L \times 4$), chloroform ($2L \times 4$), ethyl acetate ($2L \times 4$) and *n*-butanol ($2L \times 4$) respectively. The chloroform soluble extract (157 g) was subjected to column chromatography using hexane with gradient of CHCl₃ and followed by methanol up to 100%. Fifteen fractions (Fr. 1-15) were collected. The Fr. 14 was loaded on flash silica gel and eluted with *Me*OH : CHCl₃ (2 : 98) to get purified crystals of *opuntiol* (84.7 mg).

Refinement

The H atom of the OH group was located in difference Fourier maps and were refined with a O–H distance restrained to 0.83 (1)Å, with displacement parameters fixed at 1.5 times U_{eq} of the parent O atom. The rest H atoms were placed geometrically, with C–H = 0.93-0.97 Å, and treated using a riding model, with $U_{iso}(H) = 1.2$ or $1.5U_{eq}$ (parent atom).

Figures



Fig. 1. Molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.



Fig. 2. The packing and hydrogen bonding of the title compound viewed down *a* axis. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.



Fig. 3. The packing and hydrogen bonding of the title compound viewed down b axis. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

6-Hydroxymethyl-4-methoxy-2H-pyran-2-one

Crystal data	
$C_7H_8O_4$	F(000) = 328
$M_r = 156.13$	$D_{\rm x} = 1.503 {\rm ~Mg~m^{-3}}$
Monoclinic, $P2_1/c$	Mo K α radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1306 reflections
a = 4.0499 (5) Å	$\theta = 2.3 - 23.4^{\circ}$
b = 18.101 (2) Å	$\mu = 0.13 \text{ mm}^{-1}$
c = 9.4743 (13) Å	T = 296 K
$\beta = 96.720 \ (7)^{\circ}$	Needle, colourless
$V = 689.76 (15) \text{ Å}^3$	$0.34 \times 0.25 \times 0.19 \text{ mm}$
Z = 4	

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

882 reflections with $I > 2\sigma(I)$

Radiation source: sealed tube	$R_{\rm int} = 0.046$
graphite	$\theta_{\text{max}} = 25.5^{\circ}, \ \theta_{\text{min}} = 2.4^{\circ}$
φ - and ω -scans	$h = -4 \rightarrow 4$
6516 measured reflections	$k = -21 \rightarrow 21$
1268 independent reflections	$l = -11 \rightarrow 11$

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
$wR(F^2) = 0.094$	$w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0406P)^{2} + 0.1053P]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
<i>S</i> = 1.01	$(\Delta/\sigma)_{max} < 0.001$
1268 reflections	$\Delta \rho_{max} = 0.16 \text{ e} \text{ Å}^{-3}$
105 parameters	$\Delta \rho_{\rm min} = -0.16 \text{ e } \text{\AA}^{-3}$
1 restraint	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), FC [*] =KFC[1+0.001XFC ² Λ^3 /SIN(2 Θ)] ^{-1/4}
Primary atom site location: structure-invariant direct	

methods Extinction coefficient: 0.0080 (19)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (A^2)

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
01	0.6125 (3)	0.16542 (6)	0.30332 (12)	0.0376 (4)
O2	0.9490 (3)	0.11978 (7)	0.48000 (14)	0.0495 (5)
O3	0.3187 (3)	-0.03651 (6)	0.14748 (13)	0.0392 (4)
O4	0.0594 (4)	0.22405 (7)	0.00555 (16)	0.0558 (5)
C1	0.7497 (4)	0.10447 (9)	0.3778 (2)	0.0362 (6)
C2	0.6491 (4)	0.03392 (9)	0.32627 (18)	0.0336 (6)
C3	0.4283 (4)	0.02721 (9)	0.20778 (18)	0.0303 (5)
C4	0.2914 (4)	0.09149 (9)	0.13544 (18)	0.0334 (6)
C5	0.3878 (4)	0.15778 (9)	0.18521 (18)	0.0325 (6)
C6	0.2807 (5)	0.23160 (9)	0.1300 (2)	0.0413 (6)

supplementary materials

C7	0.4484 (5)	-0.10405 (10)	0.2121 (2)	0.0437 (7)
H1	-0.003 (6)	0.2662 (7)	-0.022 (2)	0.0840*
H2	0.73440	-0.00810	0.37370	0.0400*
H4	0.13750	0.08710	0.05500	0.0400*
H6A	0.17300	0.25800	0.20100	0.0500*
H6B	0.47320	0.25990	0.11000	0.0500*
H7A	0.68640	-0.10410	0.21640	0.0660*
H7B	0.35940	-0.14530	0.15650	0.0660*
H7C	0.38600	-0.10780	0.30650	0.0660*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0434 (7)	0.0266 (7)	0.0405 (8)	-0.0032 (5)	-0.0045 (6)	-0.0040 (6)
O2	0.0590 (9)	0.0408 (8)	0.0437 (8)	-0.0065 (7)	-0.0149 (7)	-0.0057 (7)
O3	0.0503 (8)	0.0224 (7)	0.0420 (8)	-0.0014 (6)	-0.0073 (6)	-0.0020(6)
O4	0.0688 (10)	0.0331 (8)	0.0596 (10)	0.0072 (7)	-0.0169 (8)	0.0056 (7)
C1	0.0385 (10)	0.0342 (11)	0.0347 (11)	-0.0020 (8)	-0.0002 (8)	0.0000 (9)
C2	0.0385 (10)	0.0256 (10)	0.0355 (11)	-0.0003 (8)	-0.0008 (8)	0.0019 (8)
C3	0.0333 (9)	0.0238 (9)	0.0335 (10)	-0.0023 (7)	0.0026 (8)	-0.0030 (8)
C4	0.0371 (10)	0.0312 (10)	0.0305 (10)	0.0010 (8)	-0.0021 (8)	0.0002 (8)
C5	0.0349 (10)	0.0274 (10)	0.0347 (10)	-0.0006 (8)	0.0022 (8)	0.0007 (8)
C6	0.0459 (11)	0.0267 (10)	0.0500 (12)	0.0014 (8)	0.0000 (9)	0.0015 (9)
C7	0.0548 (12)	0.0240 (10)	0.0501 (13)	0.0006 (8)	-0.0028 (10)	0.0008 (9)

Geometric parameters (Å, °)

O1—C1	1.390 (2)	C4—C5	1.331 (2)
O1—C5	1.364 (2)	C5—C6	1.481 (2)
O2—C1	1.218 (2)	С2—Н2	0.9300
O3—C3	1.340 (2)	C4—H4	0.9300
O3—C7	1.439 (2)	С6—Н6А	0.9700
O4—C6	1.402 (2)	С6—Н6В	0.9700
O4—H1	0.836 (14)	С7—Н7А	0.9600
C1—C2	1.410 (2)	С7—Н7В	0.9600
C2—C3	1.356 (2)	C7—H7C	0.9600
C3—C4	1.429 (2)		
O1···O4 ⁱ	3.1840 (19)	C2…H7C	2.7800
O2…O4 ⁱ	2.8678 (18)	С2…Н7А	2.7200
O2···C6 ⁱ	3.258 (2)	С7…Н2	2.5100
O3···C4 ⁱⁱ	3.415 (2)	C7…H7A ^{vii}	3.0900
O4…O2 ⁱⁱⁱ	2.8678 (18)	C7···H6A ^x	2.9900
O4…O1 ⁱⁱⁱ	3.1840 (19)	C7···H6B ^x	2.9800
O1…H1 ⁱ	2.47 (2)	H1…H6B ^{vii}	2.5900
O2…H2 ^{iv}	2.6900	H1…O1 ⁱⁱⁱ	2.47 (2)
$O2 \cdots H7C^{v}$	2.5700	H1…O2 ⁱⁱⁱ	2.073 (13)
O2…H1 ⁱ	2.073 (13)	H1…C1 ⁱⁱⁱ	2.676 (15)

$O4 - HTB^{vi}$ 2.5800 $H2 - HTA$ 2.2800 $O4 - H4$ 2.5400 $H2 - HTC$ 2.3300 $O4 - H6B^{vii}$ 2.7500 $H2 - O2^{vi}$ 2.6900 $C1 - C4^{viii}$ 3.65(2) $H4 - O3^{vi}$ 2.6700 $C2 - C3^{viii}$ 3.470 (2) $H6 - O4^{viii}$ 2.9900 $C2 - C3^{viii}$ 3.496 (2) $H6B - O4^{viii}$ 2.9900 $C2 - C2^{vii}$ 3.496 (2) $H6B - O4^{viii}$ 2.900 $C4 - C2^{vii}$ 3.496 (2) $H6B - O4^{viii}$ 2.900 $C4 - C2^{vii}$ 3.496 (2) $H6B - C7^{vii}$ 2.900 $C4 - C7^{vii}$ 3.365 (2) $H7A - C2$ 2.7200 $C4 - C7^{vii}$ 3.580 (3) $H7A - C2$ 2.7200 $C4 - C7^{vii}$ 3.451 (2) $H7A - C2$ 2.7800 $C5 - C1^{vii}$ 3.451 (3) $H7C - C2$ 2.7800 $C5 - C6^{vii}$ 3.451 (3) $H7C - H2$ 2.300 $C7 - C6^{x}$ 3.451 (3) $H7C - H2$ 2.300 $C1 - O1 - C5$ 12.164 (13) $C1 - C2 - H2$ 12.000 $C1 - O1 - C5$	O3…H4 ^{vi}	2.6700	H2…C7	2.5100
$04-H4$ $2,5400$ $H2-H7C$ $2,3300$ $04-H4B^{vii}$ $2,7500$ $H2-O2^{iv}$ $2,6900$ $C1-C4^{viii}$ $3,365 (2)$ $H4-O4$ $2,5400$ $C1-C5^{viii}$ $3,470 (2)$ $H4-O3^{vi}$ $2,6700$ $C2-C4^{viii}$ $3,473 (2)$ $H6B-O4^{viii}$ $2,9900$ $C2-C4^{viii}$ $3,473 (2)$ $H6B-O4^{viii}$ $2,500$ $C4-C2^{vii}$ $3,473 (2)$ $H6B-H1^{viii}$ $2,5900$ $C4-C2^{vii}$ $3,496 (2)$ $H6B-C7^{1x}$ $2,5700$ $C4-C1^{viii}$ $3,580 (3)$ $H7A-C2$ $2,7200$ $C4-C1^{viii}$ $3,580 (3)$ $H7A-C2$ $2,7200$ $C4-C7^{1ii}$ $3,470 (2)$ $H7A-C7^{viii}$ $3,9900$ $C5-C1^{vii}$ $3,451 (3)$ $H7C-H2$ $2,5800$ $C6-C2^{10i}$ $3,451 (3)$ $H7C-H2$ $2,5800$ $C6-C2^{10i}$ $3,451 (3)$ $H7C-H2$ $2,3300$ $C7-C6^{k}$ $3,451 (3)$ $H7C-H2$ $2,300$ $C7-C6^{k}$ $3,451 (3)$ $H7C-H2$ $2,5700$ $C1-H1^{1}$ $2,676 (15)$ $H7C-O2^{v}$ $2,5700$ $C1-H1^{1}$ $2,676 (15)$ $H7C-O2^{v}$ $2,5700$ $C1-C1-C2$ $11,264 (13)$ $C1-C2-H2$ $12,000$ $C6-O4+H11$ $1083 (14)$ $C3-C4-H4$ $12,100$ $O1-C1-O2$ $11,292 (15)$ $C3-C4-H4$ $10,001$ $O1-C1-C2$ $11,292 (15)$ $C3-C4-H4$ $10,001$ $O1-C1-C2$ $11,292 (15)$ $C3-C4-H4$ $10,001$ $O1-C2-C3$ $12,292 (15)$ <td>O4…H7B^{vi}</td> <td>2.5800</td> <td>Н2…Н7А</td> <td>2.2800</td>	O4…H7B ^{vi}	2.5800	Н2…Н7А	2.2800
$O4 - H6B^{vii}$ 2.7500 $H2 - O2^{iv}$ 2.6900 $C1 - C4^{viii}$ $3.365(2)$ $H4 - O4$ 2.5400 $C1 - C4^{viii}$ $3.470(2)$ $H4 - O3^{vii}$ 2.6700 $C2 - C3^{viii}$ $3.473(2)$ $H6B - O4^{viii}$ 2.7500 $C2 - C4^{viii}$ $3.473(2)$ $H6B - O4^{viii}$ 2.7500 $C3 - C2^{vii}$ $3.473(2)$ $H6B - H7c^{iv}$ 2.5900 $C4 - C2^{vii}$ $3.473(2)$ $H6B - H7c^{iv}$ 2.5900 $C4 - C1^{vii}$ $3.365(2)$ $H6B - H7c^{iv}$ 2.5900 $C4 - C1^{vii}$ $3.365(2)$ $H7A - C2$ 2.7200 $C4 - C1^{vii}$ $3.580(3)$ $H7A - C2$ 2.5000 $C4 - C1^{vii}$ $3.580(3)$ $H7A - C7^{viii}$ 2.5800 $C6 - C1^{vii}$ $3.451(3)$ $H7B - 04^{vi}$ 2.5800 $C6 - C2^{vii}$ $3.580(3)$ $H7C - H2$ 2.5000 $C7 - C4^{vii}$ $3.580(3)$ $H7C - H6B^{vii}$ 2.5700 $C1 - H1^{ii}$ $2.670(5)$ $H7C - C2^{vii}$ 2.5700 $C1 - 01 - C5$ $12.164(13)$ $C1 - C2 - H2$ 12.000 $C3 - 03 - C7$ $17.64(14)$ $C3 - C4 - H4$ 121.00 $O1 - C1 - O2$ $14.29(14)$ $C5 - C4 - H6A$ 110.00 $O2 - C1 - C2$ $12.570(15)$ $C5 - C6 - H6B$ 110.00 $O3 - C3 - C4$ $12.59(16)$ $O4 - C6 - H6B$ 110.00 $O3 - C3 - C4$ $12.570(15)$ $C5 - C6 - H6B$ 110.00 $O3 - C3 - C4$ $12.570(15)$ $C3 - C4 - H7A$ 199.00 </td <td>O4…H4</td> <td>2.5400</td> <td>H2…H7C</td> <td>2.3300</td>	O4…H4	2.5400	H2…H7C	2.3300
C1···C4 ^{viii} 3.365 (2)H4···O42.5400C1···C5 ^{viii} 3.470 (2)H4···O3 ^{vi} 2.6700C2···C3 ^{viii} 3.473 (2)H6A···C7 ^{ix} 2.9900C2···C4 ^{viii} 3.496 (2)H6B···O4 ^{viii} 2.7500C3···C2 ^{viii} 3.473 (2)H6B···I1 ^{viii} 2.5900C4···C1 ^{viii} 3.365 (2)H6B···T7 ^{ix} 2.9800C4···C1 ^{viii} 3.365 (2)H6B···T7 ^{ix} 2.5700C4···C1 ^{viii} 3.580 (3)H7A···C22.7200C4···C1 ^{viii} 3.415 (2)H7A···C7 ^{viii} 3.0900C5···C1 ^{viii} 3.470 (2)H7A···C12.2800C6···C2 ⁱⁱⁱ 3.258 (2)H7C···C22.7800C7···C6 ^x 3.451 (3)H7C···H22.300C7···C6 ^x 3.451 (3)H7C···H22.300C7···C4 ⁱⁱⁱ 3.580 (3)H7C···H22.300C1···H1 ¹ 2.676 (15)H7C··O2 ^x 2.5700C1···H1 ¹ 2.676 (15)H7C··O2 ^x 2.5700C1···H1 ¹ 2.676 (15)H7C··O2 ^x 2.5700C1···H1 ¹ 10.83 (14)C3··C2··H210.00C6···O4·III10.83 (14)C3··C2··H210.00C1···C1··C211.42 (14)C3··C4··H4121.00O1··C1··C212.52 (16)O4··C6··H6B110.00O2··C1··C212.52 (16)O4··C6··H6B10.00O1··C1··C212.52 (16)O4··C6··H6B10.00O2··C1··C212.52 (16)O4··C6··H6B10.00O1··C1··C213.85 (15)O3··C7··H7A109.0	O4…H6B ^{vii}	2.7500	H2···O2 ^{iv}	2.6900
C1-C5 ^{viii} 3.470 (2) $H4-03^{vi}$ 2.6700C2-C3 ^{viii} 3.473 (2) $H6AC7^{1k}$ 2.9900C2-C4 ^{viii} 3.496 (2) $H6BH1^{viii}$ 2.5500C4-C2 ^{vii} 3.473 (2) $H6BH1^{viii}$ 2.5900C4-C2 ^{vii} 3.496 (2) $H6BT1^{vii}$ 2.9800C4-C1 ^{viii} 3.365 (2) $H6BT1^{vii}$ 2.5700C4-C1 ^{viii} 3.365 (2) $H6BT1^{viii}$ 3.0900C5-C1 ^{viii} 3.415 (2) $H7AC2$ 2.7200C4-O3 ⁱⁱ 3.415 (2) $H7AC2^{viii}$ 3.0900C5-C1 ^{viii} 3.451 (3) $H7B-O4^{vii}$ 2.5800C6-C2 ⁱⁱⁱ 3.451 (3) $H7C-H2$ 2.300C7-C6 ^X 3.451 (3) $H7C-H2$ 2.300C7-C6 ^X 3.451 (3) $H7C-H2$ 2.5700C1-H1 ⁱ 2.676 (15) $H7C-M2$ 2.5700C1-H1 ⁱ 2.676 (15) $H7C-M2$ 2.5700C1-O1-C5121.64 (13)C1-C2-H2120.00C6-O4-H1108.3 (14)C3-C2-H2120.00C6-O4-H1108.3 (14)C3-C2-H2120.00C6-O4-H1108.3 (14)C3-C2-H2120.00C6-O4-H1108.3 (14)C3-C2-H2120.00C6-O2-C2125.270 (15)C5-C6-H6A110.00C1-C2-C3120.23 (15)C5-C6-H6A110.00C1-C2-C3120.23 (15)C5-C6-H6A100.01C1-C2-C4125.70 (15)C5-C6-H6B100.01C1-C2-C5125.70 (15)C5-C6-H6B100.01C1-C2-C6 <td< td=""><td>C1····C4^{viii}</td><td>3.365 (2)</td><td>H4···O4</td><td>2.5400</td></td<>	C1····C4 ^{viii}	3.365 (2)	H4···O4	2.5400
C2-C3 ^{viii} 3.473 (2) $H6A-·C7^{ik}$ 2.9900C2C4 ^{viii} 3.496 (2) $H6B-··O4^{viii}$ 2.5500C3C2 ^{viii} 3.473 (2) $H6B-··O1^{viii}$ 2.5900C4C2 ^{viii} 3.496 (2) $H6B-··C7^{ik}$ 2.9800C4C1 ^{viii} 3.365 (2) $H6B-··H7C^{ik}$ 2.5700C4C7 ⁱⁱⁱ 3.358 (3) $H7A-·C2$ 2.7200C4C3 ^{viii} 3.415 (2) $H7A-··C7^{viii}$ 3.9900C5C1 ^{viii} 3.470 (2) $H7A-··C7^{viii}$ 2.5800C6C7 ^{ik} 3.451 (3) $H7B-·O4^{vi}$ 2.5800C6C9 ⁱⁱⁱ 3.258 (2) $H7C-·C2$ 2.7800C7C6 ^k 3.451 (3) $H7C-·H2$ 2.3300C7C6 ^k 3.451 (3) $H7C-·H2$ 2.300C7C6 ^k 3.451 (3) $H7C-·H2$ 2.5700C1H1 ⁱ 2.676 (15) $H7C-·O2^{v}$ 2.5700C1H1 ⁱ 2.676 (15) $H7C-·O2^{v}$ 2.5700C1O1-C5121.64 (13)C1-C2-H2120.00C6-04-H1108.3 (14)C3-C4-H4121.00O1-C1-O2117.64 (14)C3-C4-H4121.00O1-C1-C2122.63 (15)C5-C6-H6B110.00C2-C3-C4120.23 (15)C5-C6-H6B110.00C2-C3-C4120.35 (15)H6A-·C6-H6B108.00O3-C3-C4120.35 (15)H6A-·C6-H6B108.00O3-C3-C4128.79 (16)H7A-·C7-H7B109.00C4-C5-C6128.79 (16)H7A-·C7-H7B109.00C4-C5-C6128.79 (16)H7A-·C7-H7C<	C1···C5 ^{viii}	3.470 (2)	H4…O3 ^{vi}	2.6700
$C2-C4^{4ii}$ $3.496 (2)$ $H6B-··O4^{4ii}$ 2.5900 $C3-C2^{vii}$ $3.473 (2)$ $H6B-··O1^{vii}$ 2.5900 $C4-C2^{vii}$ $3.496 (2)$ $H6B-··C7^{1k}$ 2.9800 $C4-C2^{vii}$ $3.365 (2)$ $H6B-··H7c^{1k}$ 2.5700 $C4-··C7^{1i}$ $3.365 (2)$ $H7A-··C2$ 2.7200 $C4-··C7^{1ii}$ $3.580 (3)$ $H7A-··C2$ 2.7200 $C4-··O3^{1i}$ $3.415 (2)$ $H7A-··C7^{1ii}$ 3.0900 $C5-··C1^{vii}$ $3.470 (2)$ $H7A-··C7^{1ii}$ 2.5800 $C6-··C7^{1k}$ $3.451 (3)$ $H7C-··C2$ 2.7800 $C6-··O2^{1ii}$ $3.258 (2)$ $H7C-··C2$ 2.7800 $C7-··C6^{x}$ $3.451 (3)$ $H7C-··H2$ 2.3300 $C7-··C6^{x}$ $3.451 (3)$ $H7C-··H2$ 2.5700 $C1-··H1^{1}$ $2.676 (15)$ $H7C-··H2$ 2.5700 $C101-C5$ $121.64 (13)$ $C1C2-H2$ 120.00 $C404-H1$ $1083 (14)$ $C3C2-H2$ 120.00 $C304-C7$ $17.64 (14)$ $C3C2-H2$ 120.00 $C102$ $114.29 (14)$ $C3C2-H2$ 120.00 $C102$ $114.29 (14)$ $C3C2-H2$ 10.00 $O1C1-C2$ $125.70 (15)$ $C5C6-H6B$ 110.00 $C2C3C4$ $120.33 (15)$ $HA-·C6-H6B$ 100.00 $C3C4C5$ $128.79 (16)$ $H7AC7-H7B$ 199.00 $C4C5-C6$ $128.79 (16)$ $H7AC7-H7B$ 199.00 $C4C5-C6$ $199.79 (15)$ $C1-C2-C3C4$ <t< td=""><td>C2···C3^{viii}</td><td>3.473 (2)</td><td>H6A····C7^{ix}</td><td>2.9900</td></t<>	C2···C3 ^{viii}	3.473 (2)	H6A····C7 ^{ix}	2.9900
C3C2 ^{vii} 3.473 (2)H6BH1 ^{viii} 2.5900 C4C2 ^{vii} 3.496 (2)H6BC7 ^{ix} 2.9800 C4C1 ^{viii} 3.365 (2)H6BH7C ^{ix} 2.5700 C4C7 ⁱⁱⁱ 3.580 (3)H7AC2 2.7200 C4C9 ⁱⁱⁱ 3.451 (2)H7AC7 ^{viiii} 3.9900 C5C1 ^{viii} 3.470 (2)H7AH2 2.2800 C6C7 ^{ix} 3.451 (3)H7BO4 ^{vii} 2.5800 C6C2 ⁱⁱⁱ 3.258 (2)H7CC2 2.7800 C7C6 ^x 3.451 (3)H7CH2 2.3300 C7C6 ^x 3.451 (3)H7CQ2 2.5700 C1H1 ⁱ 2.676 (15)H7CQ2 ^v 2.5700 C1O1C5121.64 (13)C1C2H2120.00C604H1108.3 (14)C3C2H2120.00C6-04H1108.3 (14)C3C4H4121.00O1C1-O2114.29 (14)C3C4H4121.00O1-C1-O2112.570 (15)C5C6H6A110.00O2-C1-C2128.25 (16)O4C6H6B110.00O3-C3-C4120.35 (15)H6A-C6-H6B100.00O3-C3-C4121.46 (15)O3C7H7A109.00O1-C5-C4128.79 (16)H7A-C7-H7B109.00O1-C5-C6128.79 (16)H7A-C7-H7C109.00O1-C5-C6129.79 (15)C1-C2-C3-O3178.79 (16)O1-C5-C6199.90 (15)C2-C3-C4-C5.9 (2)C7-O3-C3-C2-0.9 (2)C3C4-C5.9 (2)C7-O3-C3-C419.00 (15)C2-C3-C4	C2…C4 ^{viii}	3.496 (2)	H6B…O4 ^{viii}	2.7500
$C4-C2^{vii}$ $3.496 (2)$ $H6B-··C7^{ix}$ 2.9800 $C4-C1^{vii}$ $3.365 (2)$ $H6B-··H7C^{ix}$ 2.5700 $C4-C7^{ii}$ $3.580 (3)$ $H7A-·C2$ 2.7200 $C4-O3^{ii}$ $3.415 (2)$ $H7A-·C7^{viii}$ 3.0900 $C5-C1^{vii}$ $3.470 (2)$ $H7A-·H2$ 2.2800 $C6-C7^{ix}$ $3.470 (2)$ $H7A-·H2$ 2.2800 $C6-C7^{iix}$ $3.451 (3)$ $H7B-·04^{vi}$ 2.5800 $C6-C7^{iix}$ $3.451 (3)$ $H7C-·H2$ 2.3300 $C7-·C6^{x}$ $3.451 (3)$ $H7C-·H2$ 2.3300 $C7-·C4^{ii}$ $3.580 (3)$ $H7C-·H6B^{x}$ 2.5700 $C1-·H1^{i}$ $2.676 (15)$ $H7C-O2^{v}$ 2.5700 $C1-O1-C5$ $121.64 (13)$ $C1-C2-H2$ 120.00 $C3-O3-C7$ $11.764 (14)$ $C3-C2-H2$ 120.00 $C3-O3-C7$ $11.744 (15)$ $O4-C6-H6A$ 110.00 $O2-C1-C2$ $128.25 (16)$ $O4-C6-H6A$ 110.00 $O2-C1-C2$ $128.25 (15)$ $O4-C6-H6B$ 10.00 $O2-C1-C2$ $128.25 (15)$ $O4-C6-H6B$ 10.00 $C2-C3-C4$ $120.35 (15)$ $H6A-C6-H6B$ 108.00 $O3-C3-C4$ $120.35 (15)$ $H6A-C6-H6B$ 100.00 $C2-C5-C6$ $19.97 (14)$ $17A-C7-H7C$ 109.00 $C4-C5-C6$ $19.75 (14)$ $H7A-C7-H7C$ 109.00 $C4-C5-C6$ $10.97 (14)$ $H7A-C7-H7C$ 109.00 $C4-C5-C6$ $10.97 (14)$ $H7A-C7-H7C$ 109.00 $C2-O1-C1-C2$	C3···C2 ^{vii}	3.473 (2)	H6B…H1 ^{viii}	2.5900
$C4 - C1^{vii}$ $3.365 (2)$ $H6B - H7C^{ix}$ 2.5700 $C4 - C7^{ii}$ $3.580 (3)$ $H7A - C2$ 2.7200 $C4 - O3^{ii}$ $3.415 (2)$ $H7A - C7^{viii}$ 3.0900 $C5 - C1^{vii}$ $3.470 (2)$ $H7A - H2$ 2.2800 $C6 - C7^{ix}$ $3.451 (3)$ $H7B - O4^{vi}$ 2.5800 $C6 - O2^{iii}$ $3.258 (2)$ $H7C - C2$ 2.7800 $C7 - C6^{x}$ $3.451 (3)$ $H7C - H2$ 2.3300 $C7 - C4^{ii}$ $3.580 (3)$ $H7C - H6B^{x}$ 2.5700 $C1 - H1^{i}$ $2.676 (15)$ $H7C - O2^{v}$ 2.5700 $C1 - 01 - C5$ $121.64 (13)$ $C1 - C2 - H2$ 12000 $C3 - O3 - C7$ $117.64 (14)$ $C3 - C2 - H2$ 12000 $C3 - O3 - C7$ $117.64 (14)$ $C3 - C4 - H4$ 121.00 $O1 - C1 - O2$ $114.29 (14)$ $C5 - C4 - H6B$ 110.00 $O2 - C1 - C2$ $128.25 (16)$ $O4 - C6 - H6B$ 110.00 $C2 - C3 - C4$ $120.23 (15)$ $C5 - C6 - H6B$ 110.00 $C2 - C3 - C4$ $123.50 (14)$ $O3 - C7 - H7A$ 109.00 $C3 - C4 - C5$ $118.87 (15)$ $O3 - C7 - H7A$ 109.00 $C4 - C5 - C6$ $128.79 (16)$ $H7A - C7 - H7B$ 109.00 $C4 - C5 - C6$ $128.79 (16)$ $H7A - C7 - H7C$ 109.00 $C4 - C5 - C6$ $128.79 (16)$ $H7A - C7 - H7C$ 109.00 $C4 - C5 - C6$ $109.94 (14)$ $H7B - C7 - H7C$ 109.00 $C4 - C5 - C6$ $109.94 (14)$ $H7B - C7 - H7C$ <td< td=""><td>C4…C2^{vii}</td><td>3.496 (2)</td><td>H6B····C7^{ix}</td><td>2.9800</td></td<>	C4…C2 ^{vii}	3.496 (2)	H6B····C7 ^{ix}	2.9800
$C4-C7^{ii}$ $3.580 (3)$ $H7A-C2$ 2.7200 $C4-O3^{ii}$ $3.415 (2)$ $H7A-C7^{viii}$ 3.0900 $C5-C1^{vii}$ $3.470 (2)$ $H7A-H2$ 2.2800 $C6-C7^{ix}$ $3.451 (3)$ $H7B-O4^{vi}$ 2.5800 $C6-O2^{iii}$ $3.258 (2)$ $H7C-C2$ 2.7800 $C7-C6^{s}$ $3.451 (3)$ $H7C-H2$ 2.3300 $C7-C4^{ii}$ $3.580 (3)$ $H7C-H6B^{x}$ 2.5700 $C1-H1^{i}$ $2.676 (15)$ $H7C-O2^{v}$ 2.5700 $C1-O1-C5$ $121.64 (13)$ $C1-C2-H2$ 120.00 $C3-O3-C7$ $117.64 (14)$ $C3-C4-H4$ 121.00 $O1-C1-O2$ $114.29 (14)$ $C3-C4-H4$ 121.00 $O1-C1-O2$ $112.57 (15)$ $C5-C4-H4$ 110.00 $O2-C1-C2$ $128.25 (16)$ $O4-C6-H6B$ 110.00 $O2-C1-C2$ $128.25 (15)$ $C5-C6-H6B$ 110.00 $C2-C3-C4$ $120.35 (15)$ $C5-C6-H6B$ 100.00 $C3-C4-C5$ $18.87 (15)$ $O3-C7-H7B$ 109.00 $C3-C4-C5$ $128.79 (16)$ $H7A-C7-H7C$ 109.00 $C4-C5-C6$ $128.79 (16)$ $H7A-C7-H7C$ 109.00 $C4-C5-C6$ $129.79 (15)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-O2$ $179.27 (15)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-O2$ $179.27 (15)$ $C1-C2-C3-O3$ $178.94 (15)$ $C1-O1-C5-C6$ $109.90 (15)$ $C2-C3-C4-C5$ $09 (2)$ $C5-O1-C1-O2$ $03 (2)$ $C1-C2-C3-O3$ $178.94 (15)$	C4…C1 ^{vii}	3.365 (2)	H6B…H7C ^{ix}	2.5700
$C4-O3^{ii}$ $3.415 (2)$ $H7A-C7^{viii}$ 3.0900 $C5-C1^{vii}$ $3.470 (2)$ $H7A-H2$ 2.2800 $C6-C7^{ix}$ $3.451 (3)$ $H7B-O4^{ij}$ 2.5800 $C6-O2^{iii}$ $3.258 (2)$ $H7C-C2$ 2.7800 $C7-C6^x$ $3.451 (3)$ $H7C-H2$ 2.3300 $C7-C4^{ii}$ $3.580 (3)$ $H7C-H6B^x$ 2.5700 $C1-01-C5$ $21.64 (13)$ $C1-C2-H2$ 120.00 $C3-O3-C7$ $117.64 (14)$ $C3-C2-H2$ 120.00 $C3-O3-C7$ $117.64 (14)$ $C3-C4-H4$ 121.00 $O1-C1-O2$ $114.29 (14)$ $C5-C4-H4$ 121.00 $O1-C1-C2$ $117.44 (15)$ $04-C6-H6B$ 110.00 $O2-C1-C2$ $128.25 (16)$ $04-C6-H6B$ 110.00 $O2-C1-C2$ $128.25 (16)$ $04-C6-H6B$ 110.00 $O2-C2-C3-C4$ $120.35 (15)$ $16A-C6-H6B$ 100.00 $O2-C3-C4$ $123.51(15)$ $03-C7-H7A$ 109.00 $O3-C3-C4$ $13.95 (14)$ $O3-C7-H7B$ 109.00 $O1-C5-C6$ $109.75 (14)$ $H7A-C7-H7C$ 109.00 $O1-C5-C6$ $109.75 (14)$ $H7A-C7-H7C$ 109.00 $O1-C5-C6$ $109.94 (14)$ $H7B-C7-H7C$ 109.00 $O1-C5-C6$ $109.92 (15)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-O2$ $03 (2)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-C2$ $03 (2)$ $C1-C2-C3-O4$ $-1.1(3)$ $C1-C2-C3-C4$ $179.00 (15)$ $C2-C3-C4-C5$ $09 (2)$ $C1-O1-C5-C6$ <	C4···C7 ⁱⁱ	3.580 (3)	H7A…C2	2.7200
C5- $C1^{vii}$ 3.470 (2)H7A···H22.2800C6- $C7^{ix}$ 3.451 (3)H7B···O4 ^{vi} 2.5800C6- $O2^{iii}$ 3.258 (2)H7C···C22.7800C7-··C6^x3.451 (3)H7C···H22.3300C7-··C4^{ii}3.580 (3)H7C···H6B^x2.5700C1-··H1^12.676 (15)H7C···Q2^v2.5700C1-O1-C5121.64 (13)C1C2-H2120.00C3-O3C7117.64 (14)C3C2-H2120.00C6-O4-H1108.3 (14)C3C4-H4121.00O1-C1-O2114.29 (14)C5C4-H4121.00O1-C1-C217.44 (15)O4C6-H6A110.00O2-C1-C2128.25 (16)O4C6-H6B110.00C2C2-C3120.23 (15)C5C6-H6A110.00C3C4120.35 (15)H6AC6-H6B100.00C3C4-C5118.87 (15)O3C7-H7A109.00C3C4-C5118.87 (15)O3C7-H7B109.00C3C4-C5128.79 (16)H7AC7-H7B109.00C4C5-C6128.79 (16)H7AC7-H7B109.00C4C5-C6128.79 (16)H7A-C7-H7C109.00C5O1-C1-O2179.27 (15)C1C2-C3-O3178.79 (16)C5-O1-C1-C20.3 (2)C1C2-C3-O4-1.1 (3)C1-O1-C5-C6179.90 (15)C2-C3-C4-C50.9 (2)C3-O3-C3-C2-0.9 (2)C3-C4-C5-O1-0.2 (2)C7-O3-C3-C4178.94 (15)C3-C4-C5-O6-178.94 (15)C1-O1-C5-C6179.90 (15)C2-C3-C4-C50.9 (2) </td <td>C4…O3ⁱⁱ</td> <td>3.415 (2)</td> <td>H7A…C7^{viii}</td> <td>3.0900</td>	C4…O3 ⁱⁱ	3.415 (2)	H7A…C7 ^{viii}	3.0900
$C6-C7^{ix}$ $3.451 (3)$ $H7B-O4^{vi}$ 2.5800 $C6-C2^{iii}$ $3.258 (2)$ $H7C-C2$ 2.7800 $C7-C6^x$ $3.451 (3)$ $H7C-H2$ 2.3300 $C7-C4^{ii}$ $3.580 (3)$ $H7C-H6B^x$ 2.5700 $C1-H1^i$ $2.676 (15)$ $H7C-O2^v$ 2.5700 $C1-O1-C5$ $121.64 (13)$ $C1-C2-H2$ 120.00 $C3-O3-C7$ $117.64 (14)$ $C3-C2-H2$ 120.00 $C6-O4-H1$ $108.3 (14)$ $C3-C4-H4$ 121.00 $O1-C1-O2$ $117.44 (15)$ $O4-C6-H6A$ 110.00 $O2-C1-C2$ $128.25 (16)$ $O4-C6-H6B$ 110.00 $O2-C1-C2$ $128.25 (16)$ $O4-C6-H6B$ 110.00 $O2-C1-C2$ $128.25 (16)$ $O4-C6-H6B$ 110.00 $O3-C3-C2$ $120.23 (15)$ $C5-C6-H6A$ 110.00 $C3-C4-C5$ $118.87 (15)$ $O3-C7-H7A$ 109.00 $O3-C3-C4$ $121.36 (15)$ $O3-C7-H7B$ 109.00 $O1-C5-C4$ $121.46 (15)$ $O3-C7-H7B$ 109.00 $O1-C5-C4$ $121.46 (15)$ $O3-C7-H7B$ 109.00 $O1-C5-C4$ $129.70 (15)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-O2$ $179.94 (14)$ $H7A-C7-H7C$ 109.00 $O4-C6-C5$ $109.94 (14)$ $H7B-C7-H7C$ 109.00 $O4-C6-C5$ $109.94 (14)$ $H7B-C7-H7C$ 109.00 $C5-O1-C1-O2$ $179.94 (15)$ $C1-C2-C3-O4$ $-11.1(3)$ $C1-O1-C5-C6$ $109.90 (15)$ $C2-C3-C4-C5$ $09 (2)$ $C1-O1-C5-C6$ <td>C5…C1^{vii}</td> <td>3.470 (2)</td> <td>H7A…H2</td> <td>2.2800</td>	C5…C1 ^{vii}	3.470 (2)	H7A…H2	2.2800
$C6-c02^{iii}$ $3.258 (2)$ $H7C-C2$ 2.7800 $C7-C6^x$ $3.451 (3)$ $H7C-H2$ 2.3300 $C7-C4^{ii}$ $3.580 (3)$ $H7C-H6B^x$ 2.5700 $C1-H1^{i}$ $2.676 (15)$ $H7C-O2^v$ 2.5700 $C1-O1-C5$ $121.64 (13)$ $C1-C2-H2$ 120.00 $C3-O3-C7$ $117.64 (14)$ $C3-C2-H2$ 120.00 $C6-O4-H1$ $108.3 (14)$ $C3-C4-H4$ 121.00 $O1-C1-O2$ $114.29 (14)$ $C5-C4-H4$ 121.00 $O1-C1-C2$ $122.52 (16)$ $O4-C6-H6A$ 110.00 $O2-C1-C2$ $122.52 (16)$ $O4-C6-H6B$ 110.00 $O3-C3-C2$ $120.23 (15)$ $C5-C6-H6B$ 110.00 $C2-C3-C4$ $120.35 (15)$ $H6A-C6-H6B$ 100.00 $C2-C3-C4$ $120.35 (15)$ $H6A-C6-H6B$ 100.00 $C3-C4-C5$ $118.87 (15)$ $O3-C7-H7A$ 109.00 $C4-C5-C6$ $128.79 (16)$ $H7A-C7-H7B$ 109.00 $C4-C5-C6$ $129.79 (16)$ $H7A-C7-H7B$ 109.00 $O4-C6-C5$ $109.94 (14)$ $H7B-C7-H7C$ 109.00 $C5-O1-C1-C2$ $03.(2)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-C2$ $03.(2)$ $C1-C2-C3-O4$ $-11.1(3)$ $C1-O1-C5-C6$ $179.00 (15)$ $C2-C3-C4-C5$ $0.9 (2)$ $C7-O3-C3-C2$ $-0.9 (2)$ $C3-C4-C5-O1$ $-0.2 (2)$ $C7-O3-C3-C4$ $178.94 (15)$ $C3-C4-C5-O6$ $-179.49 (17)$ $O1-C5-C6$ $179.90 (15)$ $C2-C5-C6-O4$ $-179.49 (17)$	C6····C7 ^{ix}	3.451 (3)	H7B…O4 ^{vi}	2.5800
$C7-C6^x$ $3.451(3)$ $H7C-H2$ 2.3300 $C7-C4^{ii}$ $3.580(3)$ $H7C-H6B^x$ 2.5700 $C1-H1^i$ $2.676(15)$ $H7C-O2^v$ 2.5700 $C1-O1-C5$ $121.64(13)$ $C1-C2-H2$ 120.00 $C3-O3-C7$ $117.64(14)$ $C3-C2-H2$ 120.00 $C6-04-H1$ $108.3(14)$ $C3-C4-H4$ 121.00 $O1-C1-O2$ $114.29(14)$ $C5-C4-H4$ 121.00 $O1-C1-C2$ $117.44(15)$ $04-C6-H6A$ 110.00 $O2-C1-C2$ $128.25(16)$ $04-C6-H6B$ 110.00 $O2-C1-C2$ $128.25(16)$ $04-C6-H6B$ 110.00 $O3-C3-C2$ $125.70(15)$ $C5-C6-H6B$ 110.00 $O3-C3-C4$ $120.55(15)$ $H6A-C6-H6B$ 108.00 $O3-C3-C4$ $120.55(15)$ $H6A-C6-H6B$ 109.00 $O1-C5-C4$ $121.46(15)$ $O3-C7-H7A$ 109.00 $O1-C5-C4$ $121.46(15)$ $O3-C7-H7C$ 109.00 $O1-C5-C6$ $128.79(16)$ $H7A-C7-H7B$ 109.00 $O1-C5-C6$ $129.94(14)$ $H7B-C7-H7C$ 109.00 $O4-C6-C5$ $109.94(14)$ $H7B-C7-H7C$ 109.00 $C5-O1-C1-O2$ $179.27(15)$ $C1-C2-C3-O3$ $178.79(16)$ $C5-O1-C1-D2$ $179.27(15)$ $C1-C2-C3-O3$ $178.79(16)$ $C5-O1-C1-C2$ $03(2)$ $C1-C2-C3-O4$ $-11(3)$ $C1-O1-C5-C4$ $-0.4(2)$ $O3-C3-C4-C5$ $0.9(2)$ $C7-O3-C3-C4$ $179.00(15)$ $C2-C3-C4-C5$ $0.9(2)$ $C7-O3-C3-C4$ $178.94(15)$ <	C6…O2 ⁱⁱⁱ	3.258 (2)	H7C…C2	2.7800
$C_7 - C_4^{ii}$ $3.580 (3)$ $H_7 C - H6B^x$ 2.5700 $C_1 - H_1^i$ $2.676 (15)$ $H_7 C - O2^v$ 2.5700 $C_1 - O_1 - C_5$ $121.64 (13)$ $C_1 - C_2 - H2$ 120.00 $C_3 - O_3 - C_7$ $117.64 (14)$ $C_3 - C_2 - H2$ 120.00 $C_6 - O_4 - H1$ $108.3 (14)$ $C_3 - C_4 - H4$ 121.00 $O_1 - C_1 - O_2$ $114.29 (14)$ $C_5 - C_4 - H4$ 121.00 $O_1 - C_1 - C_2$ $117.44 (15)$ $O_4 - C_6 - H6A$ 110.00 $O_2 - C_1 - C_2$ $128.25 (16)$ $O_4 - C_6 - H6B$ 110.00 $O_2 - C_1 - C_2$ $125.70 (15)$ $C_5 - C_6 - H6B$ 110.00 $C_2 - C_3 - C_4$ $120.23 (15)$ $C_5 - C_6 - H6B$ 110.00 $C_2 - C_3 - C_4$ $120.35 (15)$ $H6A - C_6 - H6B$ 108.00 $O_3 - C_3 - C_4$ $120.35 (15)$ $H6A - C_6 - H6B$ 109.00 $O_3 - C_3 - C_4$ $113.95 (14)$ $O_3 - C_7 - H7A$ 109.00 $O_3 - C_5 - C_6$ $118.87 (15)$ $O_3 - C_7 - H7B$ 109.00 $O_1 - C_5 - C_6$ $128.79 (16)$ $H7A - C_7 - H7C$ 109.00 $O_4 - C_6 - C_5$ $109.94 (14)$ $H7B - C_7 - H7C$ 109.00 $O_4 - C_6 - C_5$ $109.94 (14)$ $H7B - C_7 - H7C$ 109.00 $O_4 - C_6 - C_5$ $109.94 (14)$ $H7B - C_7 - H7C$ 109.00 $O_4 - C_6 - C_5$ $109.94 (14)$ $H7B - C_7 - H7C$ 109.00 $O_4 - C_6 - C_5$ $109.94 (14)$ $H7B - C_7 - H7C$ 109.00 $C_5 - O_1 - C_1 - C_2$ $03 (2)$ <td< td=""><td>C7…C6^x</td><td>3.451 (3)</td><td>H7C…H2</td><td>2.3300</td></td<>	C7…C6 ^x	3.451 (3)	H7C…H2	2.3300
$C1 \cdots H1^i$ $2.676 (15)$ $H7C \cdots O2^v$ 2.5700 $C1 - O1 - C5$ $121.64 (13)$ $C1 - C2 - H2$ 120.00 $C3 - O3 - C7$ $117.64 (14)$ $C3 - C2 - H2$ 120.00 $C6 - 04 - H1$ $108.3 (14)$ $C3 - C4 - H4$ 121.00 $O1 - C1 - O2$ $114.29 (14)$ $C5 - C4 - H4$ 121.00 $O1 - C1 - C2$ $117.44 (15)$ $O4 - C6 - H6A$ 110.00 $O2 - C1 - C2$ $128.25 (16)$ $O4 - C6 - H6B$ 110.00 $O3 - C3 - C2$ $125.70 (15)$ $C5 - C6 - H6A$ 110.00 $C2 - C3 - C4$ $120.35 (15)$ $H6A - C6 - H6B$ 108.00 $O3 - C3 - C2$ $125.70 (15)$ $C5 - C6 - H6B$ 109.00 $C3 - C4 - C5$ $118.87 (15)$ $O3 - C7 - H7A$ 109.00 $C3 - C4 - C5$ $118.87 (15)$ $O3 - C7 - H7B$ 109.00 $C4 - C5 - C6$ $128.79 (16)$ $H7A - C7 - H7C$ 109.00 $C4 - C5 - C6$ $109.75 (14)$ $H7A - C7 - H7C$ 109.00 $O1 - C5 - C6$ $109.75 (14)$ $H7A - C7 - H7C$ 109.00 $O1 - C5 - C6$ $109.75 (14)$ $H7A - C7 - H7C$ 109.00 $C5 - O1 - C1 - O2$ $179.27 (15)$ $C1 - C2 - C3 - O3$ $178.79 (16)$ $C5 - O1 - C1 - C2$ $03.(2)$ $C1 - C2 - C3 - C4$ $-11.1 (3)$ $C1 - O1 - C5 - C6$ $179.00 (15)$ $C2 - C3 - C4 - C5$ $0.9 (2)$ $C7 - O3 - C3 - C2$ $-0.9 (2)$ $C3 - C4 - C5 - O1$ $-0.2 (2)$ $C7 - O3 - C3 - C4$ $178.94 (15)$ $C3 - C4 - C5 - O4$ $-179.49 (17)$	C7···C4 ⁱⁱ	3.580 (3)	H7C····H6B ^x	2.5700
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1…H1 ⁱ	2.676 (15)	H7C····O2 ^v	2.5700
C3-O3-C7117.64 (14)C3-C2-H2120.00C6-O4-H1108.3 (14)C3-C4-H4121.00O1-C1-O2114.29 (14)C5-C4-H4121.00O1-C1-C2117.44 (15)O4-C6-H6A110.00O2-C1-C2128.25 (16)O4-C6-H6B110.00C3-C3-C2120.23 (15)C5-C6-H6A110.00C2-C3-C4120.35 (15)H6A-C6-H6B108.00O3-C3-C2125.70 (15)C5-C6-H6B108.00C3-C4-C5118.87 (15)O3-C7-H7A109.00C3-C4-C5128.79 (16)H7A-C7-H7B109.00C4-C5-C6128.79 (16)H7A-C7-H7C109.00O1-C5-C6109.75 (14)H7A-C7-H7C109.00O4-C6-C5109.94 (14)H7B-C7-H7C109.00C5-O1-C1-O2179.27 (15)C1-C2-C3-O3178.79 (16)C5-O1-C1-C20.3 (2)C1-C2-C3-C4-1.1 (3)C1-O1-C5-C6179.00 (15)C2-C3-C4-C50.9 (2)C7-O3-C3-C2-0.9 (2)C3-C4-C5-O1-0.2 (2)C7-O3-C3-C4178.94 (15)C3-C4-C5-C6-179.49 (17)O1-C1-C2-C30.4 (2)01-C5-C6-O4177.77 (14)O2-C1-C2-C30.4 (2)01-C5-C6-O4-2.9 (3)	C1—O1—C5	121.64 (13)	C1—C2—H2	120.00
C6-O4-H1108.3 (14)C3-C4-H4121.00O1-C1-O2114.29 (14)C5-C4-H4121.00O1-C1-C2117.44 (15)O4-C6-H6A110.00O2-C1-C2128.25 (16)O4-C6-H6B110.00C1-C2-C3120.23 (15)C5-C6-H6A110.00O3-C3-C2125.70 (15)C5-C6-H6B108.00O3-C3-C4120.35 (15)H6A-C6-H6B108.00O3-C3-C4113.95 (14)O3-C7-H7A109.00C3-C4-C5118.87 (15)O3-C7-H7B109.00O1-C5-C4121.46 (15)O3-C7-H7B109.00O1-C5-C6109.75 (14)H7A-C7-H7C109.00O4-C6-C5109.94 (14)H7B-C7-H7C109.00O4-C6-C5109.94 (14)H7B-C7-H7C109.00C5-O1-C1-O2179.27 (15)C1-C2-C3-O3178.79 (16)C5-O1-C1-C20.3 (2)C1-C2-C3-C4-1.1 (3)C1-O1-C5-C6179.00 (15)C2-C3-C4-C50.9 (2)C7-O3-C3-C2-0.9 (2)C3-C4-C5-O1-0.2 (2)C7-O3-C3-C4178.94 (15)C3-C4-C5-C6-179.49 (17)O1-C1-C2-C30.4 (2)O1-C5-C6-O4177.77 (14)O2-C1-C2-C30.4 (2)O1-C5-C6-O4-2.9 (3)	C3—O3—C7	117.64 (14)	С3—С2—Н2	120.00
01C102 $114.29 (14)$ $C5C4H4$ 121.00 $01C1C2$ $117.44 (15)$ $04C6H6A$ 110.00 $02C1C2$ $128.25 (16)$ $04C6H6B$ 110.00 $C1C2C3$ $120.23 (15)$ $C5C6H6A$ 110.00 $03C3C2$ $125.70 (15)$ $C5C6H6B$ 108.00 $03C3C4$ $120.35 (15)$ $H6AC6H6B$ 108.00 $03C3C4$ $113.95 (14)$ $03C7H7A$ 109.00 $C3C4C5$ $118.87 (15)$ $03C7H7B$ 109.00 $01C5C4$ $121.46 (15)$ $03C7H7B$ 109.00 $01C5C6$ $128.79 (16)$ $H7AC7H7B$ 109.00 $01C5C6$ $109.75 (14)$ $H7AC7H7C$ 109.00 $04C6C5$ $109.94 (14)$ $H7BC7H7C$ 109.00 $04C6C5$ $109.94 (14)$ $H7BC7H7C$ 109.00 $C501C102$ $179.27 (15)$ $C1C2C3O3$ $178.79 (16)$ $C501C1C2$ $03 (2)$ $C1C2C3C4$ $-1.1 (3)$ $C101C5C6$ $179.00 (15)$ $C2C3C4C5$ $0.9 (2)$ $C703C3C2$ $-0.9 (2)$ $C3C4C5O1$ $-0.2 (2)$ $C703C3C4$ $178.94 (15)$ $C3C4C5C6$ $-179.49 (17)$ $01C1C2C3$ $0.4 (2)$ $01C5C6O4$ $177.77 (14)$ $02C1C2C3$ $-178.35 (18)$ $C4C5C6O4$ $-2.9 (3)$	C6—O4—H1	108.3 (14)	C3—C4—H4	121.00
01C1C2 $117.44 (15)$ $04C6H6A$ 110.00 $02C1C2$ $128.25 (16)$ $04C6H6B$ 110.00 $03C2C3$ $120.23 (15)$ $C5C6H6A$ 110.00 $03C3C2$ $125.70 (15)$ $C5C6H6B$ 110.00 $C2C3C4$ $120.35 (15)$ $H6AC6H6B$ 108.00 $03C3C4$ $113.95 (14)$ $03C7H7A$ 109.00 $C3C4C5$ $118.87 (15)$ $03C7H7B$ 109.00 $C4C5C6$ $128.79 (16)$ $H7AC7H7B$ 109.00 $01C5C6$ $109.75 (14)$ $H7AC7H7B$ 109.00 $04C6C5$ $109.94 (14)$ $H7BC7H7C$ 109.00 $04C6C5$ $109.94 (14)$ $H7BC7H7C$ 109.00 $C501C102$ $179.27 (15)$ $C1C2C3O3$ $178.79 (16)$ $C501C1C2$ $0.3 (2)$ $C1C2C3C4$ $-1.1 (3)$ $C101C5C6$ $179.00 (15)$ $C2C3C4C5$ $0.9 (2)$ $C703C3C2$ $-0.9 (2)$ $C3C4C5O1$ $-0.2 (2)$ $C703C3C4$ $178.94 (15)$ $C3C4C5C6$ $-179.49 (17)$ $01C1C2C3$ $0.4 (2)$ $01C5C6O4$ $-7.9 (3)$	O1—C1—O2	114.29 (14)	C5—C4—H4	121.00
02C1C2 $128.25 (16)$ $04C6H6B$ 110.00 $C1C2C3$ $120.23 (15)$ $C5C6H6A$ 110.00 $03C3C2$ $125.70 (15)$ $C5C6H6B$ 110.00 $C2C3C4$ $120.35 (15)$ $H6AC6H6B$ 108.00 $03C3C4$ $113.95 (14)$ $03C7H7A$ 109.00 $C3C4C5$ $118.87 (15)$ $03C7H7B$ 109.00 $O1C5C4$ $121.46 (15)$ $O3C7H7B$ 109.00 $O1C5C6$ $128.79 (16)$ $H7AC7H7B$ 109.00 $O1C5C6$ $109.75 (14)$ $H7AC7H7C$ 109.00 $O4C6C5$ $109.94 (14)$ $H7BC7H7C$ 109.00 $C5O1C1O2$ $179.27 (15)$ $C1C2C3O3$ $178.79 (16)$ $C5O1C1C2$ $0.3 (2)$ $C1C2C3C4$ $-1.1 (3)$ $C1O1C5C4$ $-0.4 (2)$ $O3C3C4C5$ $0.9 (2)$ $C7O3C3-C2$ $-0.9 (2)$ $C3C4C5O1$ $-0.2 (2)$ $C7O3C3C4$ $178.94 (15)$ $C3C4C5C6$ $-179.49 (17)$ $O1C1C2C3$ $0.4 (2)$ $O1C5C6O4$ $177.77 (14)$ $O2C1C2C3$ $-178.35 (18)$ $C4C5C6O4$ $-2.9 (3)$	O1—C1—C2	117.44 (15)	O4—C6—H6A	110.00
C1C2C3120.23 (15)C5C6H6A110.00 $O3C3C2$ 125.70 (15)C5C6H6B110.00 $C2C3C4$ 120.35 (15)H6AC6H6B108.00 $O3C3C4$ 113.95 (14) $O3C7H7A$ 109.00 $C3C4C5$ 118.87 (15) $O3C7H7B$ 109.00 $O1C5C4$ 121.46 (15) $O3C7H7B$ 109.00 $C4C5C6$ 128.79 (16)H7AC7H7B109.00 $O1C5C6$ 109.75 (14)H7AC7H7C109.00 $O4C6C5$ 109.94 (14)H7BC7H7C109.00 $C5O1C1O2$ 179.27 (15)C1C2C3O3178.79 (16) $C5O1C1C2$ 0.3 (2)C1C2C3C4-1.1 (3) $C1O1C5C6$ 179.00 (15)C2C3C4C50.9 (2) $C7O3C3C2$ -0.9 (2)C3C4C5O1-0.2 (2) $C7O3C3C4$ 178.94 (15)C3C4C5C6-179.49 (17) $O1C1C2C3$ 0.4 (2) $O1C5C6-O4$ 177.77 (14) $O2C1C2C3$ -178.35 (18)C4C5C6O4-2.9 (3)	O2—C1—C2	128.25 (16)	O4—C6—H6B	110.00
03-C3-C2 $125.70 (15)$ $C5-C6-H6B$ 110.00 $C2-C3-C4$ $120.35 (15)$ $H6A-C6-H6B$ 108.00 $03-C3-C4$ $113.95 (14)$ $03-C7-H7A$ 109.00 $C3-C4-C5$ $118.87 (15)$ $03-C7-H7B$ 109.00 $01-C5-C4$ $121.46 (15)$ $03-C7-H7C$ 109.00 $C4-C5-C6$ $128.79 (16)$ $H7A-C7-H7B$ 109.00 $01-C5-C6$ $109.75 (14)$ $H7A-C7-H7C$ 109.00 $04-C6-C5$ $109.94 (14)$ $H7B-C7-H7C$ 109.00 $C5-O1-C1-O2$ $179.27 (15)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-C2$ $0.3 (2)$ $C1-C2-C3-C4$ $-1.1 (3)$ $C1-O1-C5-C6$ $179.00 (15)$ $C2-C3-C4-C5$ $0.9 (2)$ $C7-O3-C3-C2$ $-0.9 (2)$ $C3-C4-C5-O1$ $-0.2 (2)$ $C7-O3-C3-C4$ $178.94 (15)$ $C3-C4-C5-C6$ $-179.49 (17)$ $01-C1-C2-C3$ $0.4 (2)$ $01-C5-C6-O4$ $177.77 (14)$ $02-C1-C2-C3$ $-178.35 (18)$ $C4-C5-C6-O4$ $-2.9 (3)$	C1—C2—C3	120.23 (15)	С5—С6—Н6А	110.00
C2C3C4120.35 (15)H6AC6H6B108.00O3C3C4113.95 (14)O3C7H7A109.00C3C4C5118.87 (15)O3C7H7B109.00O1C5C4121.46 (15)O3C7H7B109.00C4C5C6128.79 (16)H7AC7H7B109.00O1C5C6109.75 (14)H7AC7H7C109.00O4C6C5109.94 (14)H7BC7H7C109.00C5O1C1O2179.27 (15)C1C2C3O3178.79 (16)C5O1C1C20.3 (2)C1C2C3C4-1.1 (3)C1O1C5C4-0.4 (2)O3C3C4C5-178.94 (15)C1O1C5C6179.00 (15)C2C3C4C50.9 (2)C7O3C3C2-0.9 (2)C3C4C5O1-0.2 (2)C7O3C3C4178.94 (15)C3C4C5C6-179.49 (17)O1C1C2C30.4 (2)O1C5C6O4177.77 (14)O2C1C2C3-178.35 (18)C4C5C6O4-2.9 (3)	O3—C3—C2	125.70 (15)	С5—С6—Н6В	110.00
O3-C3-C4 $113.95(14)$ $O3-C7-H7A$ 109.00 $C3-C4-C5$ $118.87(15)$ $O3-C7-H7B$ 109.00 $O1-C5-C4$ $121.46(15)$ $O3-C7-H7C$ 109.00 $C4-C5-C6$ $128.79(16)$ $H7A-C7-H7B$ 109.00 $O1-C5-C6$ $109.75(14)$ $H7A-C7-H7B$ 109.00 $O4-C6-C5$ $109.94(14)$ $H7B-C7-H7C$ 109.00 $C5-O1-C1-O2$ $179.27(15)$ $C1-C2-C3-O3$ $178.79(16)$ $C5-O1-C1-C2$ $0.3(2)$ $C1-C2-C3-C4$ $-1.1(3)$ $C1-O1-C5-C4$ $-0.4(2)$ $O3-C3-C4-C5$ $0.9(2)$ $C7-O3-C3-C2$ $-0.9(2)$ $C3-C4-C5-O1$ $-0.2(2)$ $C7-O3-C3-C4$ $178.94(15)$ $C3-C4-C5-C6$ $-179.49(17)$ $O1-C1-C2-C3$ $0.4(2)$ $O1-C5-C6-O4$ $177.77(14)$ $O2-C1-C2-C3$ $-178.35(18)$ $C4-C5-C6-O4$ $-2.9(3)$	C2—C3—C4	120.35 (15)	H6A—C6—H6B	108.00
C3-C4-C5 $118.87 (15)$ O3-C7-H7B 109.00 O1-C5-C4 $121.46 (15)$ O3-C7-H7C 109.00 C4-C5-C6 $128.79 (16)$ $H7A-C7-H7B$ 109.00 O1-C5-C6 $109.75 (14)$ $H7A-C7-H7C$ 109.00 O4-C6-C5 $109.94 (14)$ $H7B-C7-H7C$ 109.00 C5-O1-C1-O2 $179.27 (15)$ $C1-C2-C3-O3$ $178.79 (16)$ C5-O1-C1-C2 $0.3 (2)$ $C1-C2-C3-C4$ $-1.1 (3)$ C1-O1-C5-C4 $-0.4 (2)$ $O3-C3-C4-C5$ $0.9 (2)$ C7-O3-C3-C2 $-0.9 (2)$ $C3-C4-C5-O1$ $-0.2 (2)$ C7-O3-C3-C4 $178.94 (15)$ $C3-C4-C5-C6$ $-179.49 (17)$ O1-C1-C2-C3 $0.4 (2)$ $01-C5-C6-O4$ $177.77 (14)$ O2-C1-C2-C3 $-178.35 (18)$ $C4-C5-C6-O4$ $-2.9 (3)$	O3—C3—C4	113.95 (14)	O3—C7—H7A	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—C4—C5	118.87 (15)	O3—C7—H7B	109.00
C4—C5—C6128.79 (16)H7A—C7—H7B109.00O1—C5—C6109.75 (14)H7A—C7—H7C109.00O4—C6—C5109.94 (14)H7B—C7—H7C109.00C5—O1—C1—O2179.27 (15)C1—C2—C3—O3178.79 (16)C5—O1—C1—C20.3 (2)C1—C2—C3—C4 -1.1 (3)C1—O1—C5—C4 -0.4 (2)O3—C3—C4—C5 -178.94 (15)C1—O1—C5—C6179.00 (15)C2—C3—C4—C5 0.9 (2)C7—O3—C3—C2 -0.9 (2)C3—C4—C5—O1 -0.2 (2)C7—O3—C3—C4178.94 (15)C3—C4—C5—C6 -179.49 (17)O1—C1—C2—C3 0.4 (2)O1—C5—C6—O4177.77 (14)O2—C1—C2—C3 -178.35 (18)C4—C5—C6—O4 -2.9 (3)	O1—C5—C4	121.46 (15)	O3—C7—H7C	109.00
O1-C5-C6 $109.75 (14)$ $H7A-C7-H7C$ 109.00 $O4-C6-C5$ $109.94 (14)$ $H7B-C7-H7C$ 109.00 $C5-O1-C1-O2$ $179.27 (15)$ $C1-C2-C3-O3$ $178.79 (16)$ $C5-O1-C1-C2$ $0.3 (2)$ $C1-C2-C3-C4$ $-1.1 (3)$ $C1-O1-C5-C4$ $-0.4 (2)$ $O3-C3-C4-C5$ $-178.94 (15)$ $C1-O1-C5-C6$ $179.00 (15)$ $C2-C3-C4-C5$ $0.9 (2)$ $C7-O3-C3-C2$ $-0.9 (2)$ $C3-C4-C5-O1$ $-0.2 (2)$ $C7-O3-C3-C4$ $178.94 (15)$ $C3-C4-C5-C6$ $-179.49 (17)$ $O1-C1-C2-C3$ $0.4 (2)$ $O1-C5-C6-O4$ $177.77 (14)$ $O2-C1-C2-C3$ $-178.35 (18)$ $C4-C5-C6-O4$ $-2.9 (3)$	C4—C5—C6	128.79 (16)	H7A—C7—H7B	109.00
O4-C6-C5 $109.94(14)$ $H7B-C7-H7C$ 109.00 $C5-O1-C1-O2$ $179.27(15)$ $C1-C2-C3-O3$ $178.79(16)$ $C5-O1-C1-C2$ $0.3(2)$ $C1-C2-C3-C4$ $-1.1(3)$ $C1-O1-C5-C4$ $-0.4(2)$ $O3-C3-C4-C5$ $-178.94(15)$ $C1-O1-C5-C6$ $179.00(15)$ $C2-C3-C4-C5$ $0.9(2)$ $C7-O3-C3-C2$ $-0.9(2)$ $C3-C4-C5-O1$ $-0.2(2)$ $C7-O3-C3-C4$ $178.94(15)$ $C3-C4-C5-C6$ $-179.49(17)$ $O1-C1-C2-C3$ $0.4(2)$ $O1-C5-C6-O4$ $177.77(14)$ $O2-C1-C2-C3$ $-178.35(18)$ $C4-C5-C6-O4$ $-2.9(3)$	O1—C5—C6	109.75 (14)	H7A—C7—H7C	109.00
C501C102179.27 (15)C1C2C303178.79 (16)C501C1C2 $0.3 (2)$ $C1C2C3C4$ $-1.1 (3)$ C101C5C4 $-0.4 (2)$ $03C3C4C5$ $-178.94 (15)$ C101C5C6179.00 (15) $C2C3C4C5$ $0.9 (2)$ C703C3C2 $-0.9 (2)$ $C3C4C501$ $-0.2 (2)$ C703C3C4178.94 (15) $C3C4C5C6$ $-179.49 (17)$ 01C1C2C3 $0.4 (2)$ $01C5C604$ $177.77 (14)$ 02C1C2C3 $-178.35 (18)$ $C4C5C604$ $-2.9 (3)$	O4—C6—C5	109.94 (14)	Н7В—С7—Н7С	109.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5—O1—C1—O2	179.27 (15)	C1—C2—C3—O3	178.79 (16)
C1-O1-C5-C4 -0.4 (2) $O3-C3-C4-C5$ -178.94 (15) $C1-O1-C5-C6$ 179.00 (15) $C2-C3-C4-C5$ 0.9 (2) $C7-O3-C3-C2$ -0.9 (2) $C3-C4-C5-O1$ -0.2 (2) $C7-O3-C3-C4$ 178.94 (15) $C3-C4-C5-C6$ -179.49 (17) $O1-C1-C2-C3$ 0.4 (2) $O1-C5-C6-O4$ 177.77 (14) $O2-C1-C2-C3$ -178.35 (18) $C4-C5-C6-O4$ -2.9 (3)	C5—O1—C1—C2	0.3 (2)	C1—C2—C3—C4	-1.1 (3)
C1—O1—C5—C6 179.00 (15) C2—C3—C4—C5 0.9 (2) C7—O3—C3—C2 -0.9 (2) C3—C4—C5—O1 -0.2 (2) C7—O3—C3—C4 178.94 (15) C3—C4—C5—C6 -179.49 (17) O1—C1—C2—C3 0.4 (2) O1—C5—C6—O4 177.77 (14) O2—C1—C2—C3 -178.35 (18) C4—C5—C6—O4 -2.9 (3)	C1—O1—C5—C4	-0.4 (2)	O3—C3—C4—C5	-178.94 (15)
C7-O3-C3-C2 -0.9 (2) C3-C4-C5-O1 -0.2 (2) C7-O3-C3-C4 178.94 (15) C3-C4-C5-C6 -179.49 (17) O1-C1-C2-C3 0.4 (2) O1-C5-C6-O4 177.77 (14) O2-C1-C2-C3 -178.35 (18) C4-C5-C6-O4 -2.9 (3)	C1—O1—C5—C6	179.00 (15)	C2—C3—C4—C5	0.9 (2)
C7-O3-C3-C4 178.94 (15) C3-C4-C5-C6 -179.49 (17) O1-C1-C2-C3 0.4 (2) O1-C5-C6-O4 177.77 (14) O2-C1-C2-C3 -178.35 (18) C4-C5-C6-O4 -2.9 (3)	C7—O3—C3—C2	-0.9 (2)	C3—C4—C5—O1	-0.2 (2)
O1-C1-C2-C3 0.4 (2) O1-C5-C6-O4 177.77 (14) O2-C1-C2-C3 -178.35 (18) C4-C5-C6-O4 -2.9 (3)	C7—O3—C3—C4	178.94 (15)	C3—C4—C5—C6	-179.49 (17)
02-C1-C2-C3 -178.35 (18) C4-C5-C6-O4 -2.9 (3)	01-C1-C2-C3	0.4 (2)	01—C5—C6—O4	177.77 (14)
	02-C1-C2-C3	-178.35 (18)	C4—C5—C6—O4	-2.9 (3)

Symmetry codes: (i) *x*+1, -*y*+1/2, *z*+1/2; (ii) -*x*+1, -*y*, -*z*; (iii) *x*-1, -*y*+1/2, *z*-1/2; (iv) -*x*+2, -*y*, -*z*+1; (v) -*x*+1, -*y*, -*z*+1; (vi) -*x*, -*y*, -*z*; (vii) *x*-1, *y*, *z*; (viii) *x*+1, *y*, *z*; (ix) -*x*+1, *y*+1/2, -*z*+1/2; (x) -*x*+1, *y*-1/2, -*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A	
O4—H1···O1 ⁱⁱⁱ	0.836 (14)	2.47 (2)	3.1840 (19)	144.2 (17)	
O4—H1···O2 ⁱⁱⁱ	0.836 (14)	2.073 (13)	2.8678 (18)	158.6 (18)	
C7—H7B····O4 ^{vi}	0.96	2.58	3.494 (2)	159	
C7— $H7C$ ···O2 ^v	0.96	2.57	3.504 (2)	164	
Symmetry codes: (iii) $x-1$, $-y+1/2$, $z-1/2$; (vi) $-x$, $-y$, $-z$; (v) $-x+1$, $-y$, $-z+1$.					



Fig. 1







Fig. 3