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2,3:4,5-Di-*O*-isopropylidene-*β*-L-fructopyranose

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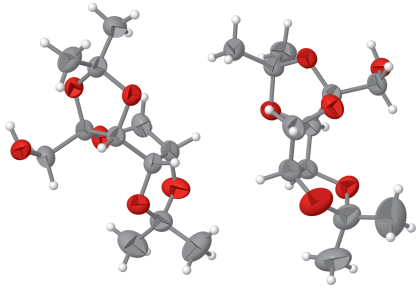
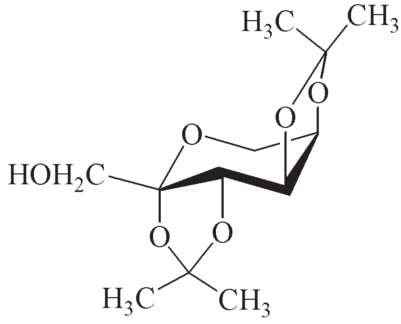
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{12}H_{20}O_6$, crystallizes in the tetragonal space group *P*4, with two crystallographically independent molecules in the asymmetric unit. Each independent molecule contains one hydroxy group that acts as both a hydrogen-bond donor and an acceptor. In the crystal, separate O—H···O hydrogen-bonding interactions connect four symmetry-related molecules into cyclic tetrameric assemblies around the crystallographic fourfold axes. The corresponding D-enantiomer has previously been determined at room temperature [CSD refcode FOYTAO; Lis & Weichsel (1987). *Acta Cryst.* C**43**, 1954–1956] and redetermined at 173 K [Yathirajan *et al.* (2004). *CSD Communication* (FOYTAO01). CCDC, Cambridge, England]. The close agreement in space group, asymmetric-unit contents and crystal packing indicates that the present L-enantiomer is isostructural with the previously reported D-enantiomer.

3D view



Chemical scheme



Structure description

The title compound, $C_{12}H_{20}O_6$, was prepared by acetonide protection of L-fructose. The molecular structure is shown in Fig. 1. The compound crystallizes in the tetragonal space group *P*4, with two crystallographically independent molecules, *A* (containing O1) and *B* (containing O7), in the asymmetric unit (Z' = 2). The two independent molecules have closely similar molecular conformations (r.m.s. deviation = 0.111 Å).

The crystal structure of the corresponding D-enantiomer, 2,3:4,5-di-*O*-isopropylidene-*β*-D-fructopyranose, was first reported at room temperature (CSD refcode FOYTAO; Lis & Weichsel, 1987) and was subsequently redetermined at 173 K (FOYTAO01; Yathirajan *et al.*, 2004). The structures were identified in the Cambridge Structural Database (CSD; Groom *et al.*, 2016). Both reported D-enantiomer structures crystallize in space group *P*4, with two crystallographically independent molecules in the asymmetric unit, as observed for the present L-enantiomer.

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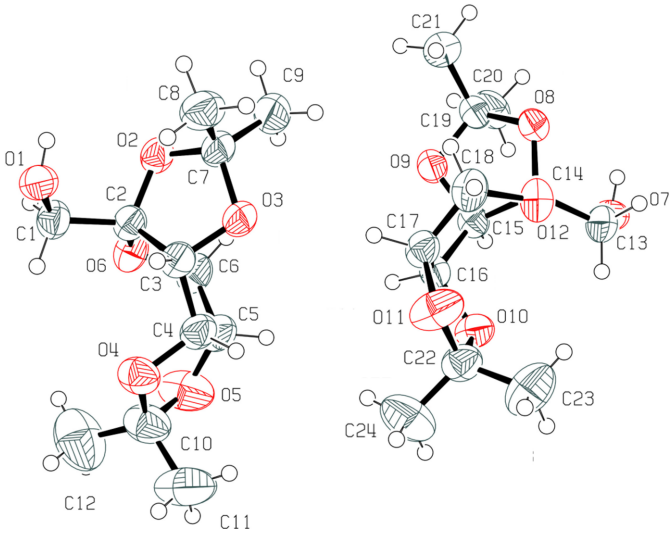

Figure 1
The two crystallographically independent molecules *A* (left) and *B* (right) in the asymmetric unit of 2,3:4,5-di-*O*-isopropylidene-*β*-L-fructopyranose, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as small spheres of arbitrary radii.

The unit-cell parameters of the present L-enantiomer at 296 K are: $a = b = 21.5539\ (14)$, $c = 5.9556\ (2)$ Å and $V = 2766.8\ (4)$ Å^3. These values are close to those reported for FOYTAO at 295 K: $a = b = 21.510\ (10)$, $c = 5.940\ (3)$ Å and $V = 2748.3$ Å^3. The unit-cell parameters reported for the low-temperature redetermination FOYTAO01 are: $a = b = 21.4209\ (15)$, $c = 5.8879\ (6)$ Å and $V = 2701.7\ (4)$ Å^3. Its smaller unit-cell dimensions and volume are consistent with the lower measurement temperature of 173 K. The agreement in the space group, number of independent molecules and overall crystal-packing arrangement indicates that the present L-enantiomer is isostructural with both reported structures of the D-enantiomer.

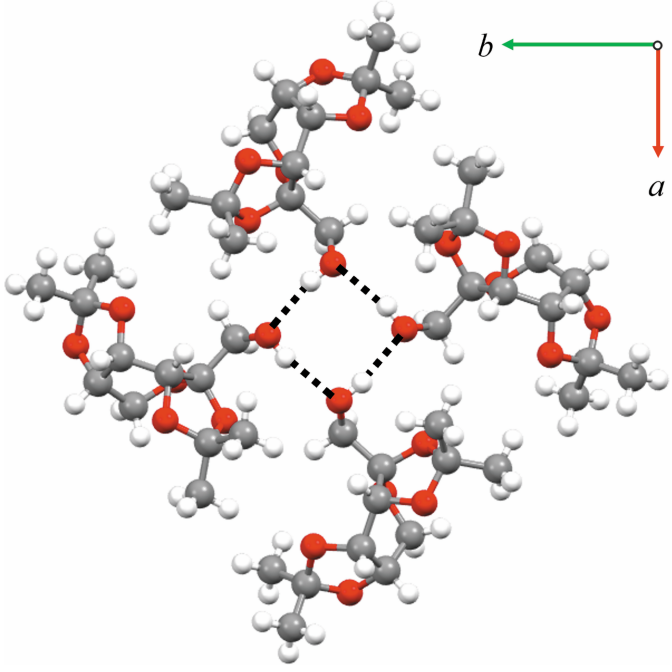

Figure 2
Cyclic tetrameric assembly formed by four symmetry-related molecules of type *A*, viewed along the *c* axis. O—H···O hydrogen bonds are shown as black dashed lines. Molecules of type *B* form a separate cyclic tetrameric assembly of the same kind.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.82	1.97	2.776 (2)	166
O7—H7···O7^{ii}	0.82	1.94	2.738 (2)	164

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{20}O_6$
M_r	260.28
Crystal system, space group	Tetragonal, *P*4
Temperature (K)	296
a, *c* (Å)	21.5539 (14), 5.9556 (2)
V (Å^3)	2766.8 (4)
Z	8
Radiation type	Cu *Kα*
μ (mm^{-1})	0.84
Crystal size (mm)	0.10 × 0.10 × 0.10
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min}, T_{max}	0.713, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31542, 4815, 4338
R_{int}	0.042
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.034, 0.085, 1.05
No. of reflections	4815
No. of parameters	343
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.10, −0.14
Absolute structure	Flack *x* determined using 1623 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.08 (6)

Computer programs: *RAPID-AUTO* (Rigaku, 2009), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* 1.3 (Dolomanov *et al.*, 2009).

In the crystal of the title compound, the hydroxy group of each independent molecule acts as both a hydrogen-bond donor and an acceptor. Molecules of type *A* are linked by O1—H1···O1 hydrogen bonds, with an O···O distance of 2.776 (2) Å and an O—H···O angle of 166°. Independently, molecules of type *B* are linked by O7—H7···O7 hydrogen bonds, with an O···O distance of 2.738 (2) Å and an O—H···O angle of 164°. Each hydrogen-bonding interaction connects four symmetry-related molecules around a crystallographic fourfold axis, producing two crystallographically independent cyclic tetrameric assemblies (Fig. 2, Table 1).

Synthesis and crystallization

A mixture of acetone, L-fructose and 2,2-dimethoxypropane was cooled to 10°C with stirring. A 70% aqueous solution of perchloric acid was added dropwise, and the reaction mixture was stirred for 18 h. The mixture was subsequently neutralized with 1 *M* aqueous sodium hydroxide solution and adjusted to pH 7.

The product was extracted with ethyl acetate and water. Separation and recovery of the organic phase were repeated three times. The combined organic layers were dried over anhydrous sodium sulfate and filtered. The filtrate was concentrated under reduced pressure to give a syrup.

The syrup was allowed to stand at room temperature, resulting in the formation of crystals. A suitable crystal was selected for single-crystal X-ray diffraction analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank Professor Genta Sakane (Okayama University of Science) for constructive discussions and technical guidance, and Associate Professor Yoji Horii (Kagawa University) for technical guidance on single-crystal X-ray diffraction measurements. The authors also acknowledge support from the JST Support for Pioneering Research Initiated by the Next Generation (SPRING) program.

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full crystallographic data

IUCrData (2026). **11**, x261124 [https://doi.org/10.1107/S2414314626011247]

2,3:4,5-Di-*O*-isopropylidene-*β*-L-fructopyranose

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2,3:4,5-Di-*O*-isopropylidene-*β*-*L*-fructopyranose

Crystal data

$C_{12}H_{20}O_6$
M_r = 260.28
Tetragonal, $P4$
a = 21.5539 (14) Å
c = 5.9556 (2) Å
V = 2766.8 (4) Å^3
Z = 8
$F(000)$ = 1120
D_x = 1.250 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.5418 Å
Cell parameters from 28410 reflections
θ = 4.1–68.1°
μ = 0.84 mm^{-1}
T = 296 K
Block, clear light colourless
0.1 × 0.1 × 0.1 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min} = 0.713, T_{max} = 1.000
31542 measured reflections
4815 independent reflections
4338 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 68.1°, θ_{min} = 4.1°
h = −25→25
k = −25→25
l = −7→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.085
S = 1.05
4815 reflections
343 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 0.1529P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack x determined using 1623 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.08 (6)

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 H atoms attached to C1 were located in a difference-Fourier map and refined freely with isotropic displacement parameters. The remaining C-bound H atoms were placed in geometrically calculated positions and refined using a riding model, with C—H distances of 0.96–0.98 Å. Hydroxy H atoms were placed at calculated positions with O—H distances of 0.82 Å and refined as rotating groups.
The isotropic displacement parameters were set at U_{iso}(H) = 1.2U_{eq}(C) for methine and methylene H atoms and 1.5U_{eq}(C, O) for methyl and hydroxy H atoms. The absolute structure was determined using 1623 quotients of the form [(I+) - (I–)]/[(I+) + (I–)], giving a Flack parameter of 0.08 (6).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.40902 (7)	0.50423 (7)	0.0959 (4)	0.0585 (5)
H1	0.432457	0.534186	0.098235	0.088*
O2	0.35138 (7)	0.61784 (7)	0.1992 (3)	0.0504 (4)
O3	0.27266 (7)	0.61725 (7)	−0.0510 (3)	0.0549 (4)
O4	0.21488 (8)	0.47003 (8)	0.1486 (4)	0.0624 (5)
O5	0.15362 (10)	0.51805 (10)	0.4038 (5)	0.0920 (8)
O6	0.28592 (7)	0.56325 (8)	0.4383 (3)	0.0559 (4)
C1	0.36612 (12)	0.50913 (12)	0.2726 (5)	0.0549 (6)
H1A	0.3841 (13)	0.5149 (13)	0.424 (6)	0.075 (9)*
H1B	0.3434 (12)	0.4712 (12)	0.287 (5)	0.058 (7)*
C2	0.31924 (10)	0.56081 (10)	0.2366 (5)	0.0470 (5)
C3	0.27778 (11)	0.55522 (10)	0.0291 (4)	0.0484 (6)
H3	0.297236	0.528595	−0.084240	0.058*
C4	0.21237 (11)	0.53327 (10)	0.0800 (5)	0.0535 (6)
H4	0.185960	0.537717	−0.052962	0.064*
C5	0.18308 (11)	0.56620 (11)	0.2810 (5)	0.0597 (7)
H5	0.152024	0.596113	0.228776	0.072*
C6	0.23011 (11)	0.59846 (12)	0.4263 (5)	0.0582 (7)
H6A	0.238985	0.639176	0.364892	0.070*
H6B	0.213313	0.603936	0.576146	0.070*
C7	0.33040 (11)	0.64682 (11)	−0.0034 (5)	0.0562 (7)
C8	0.37644 (13)	0.63633 (15)	−0.1909 (5)	0.0719 (8)
H8A	0.415912	0.653440	−0.149266	0.108*
H8B	0.361862	0.656253	−0.325109	0.108*
H8C	0.380786	0.592616	−0.217617	0.108*
C9	0.31850 (13)	0.71473 (12)	0.0394 (7)	0.0834 (11)
H9A	0.289930	0.719124	0.162000	0.125*
H9B	0.301144	0.733340	−0.092940	0.125*
H9C	0.356844	0.734969	0.076231	0.125*
C10	0.16479 (14)	0.46018 (13)	0.2986 (7)	0.0756 (9)
C11	0.10731 (17)	0.44069 (19)	0.1687 (9)	0.1144 (15)
H11A	0.097753	0.471569	0.057846	0.172*
H11B	0.072988	0.436517	0.270360	0.172*
H11C	0.114875	0.401671	0.095992	0.172*
C12	0.1840 (2)	0.4143 (2)	0.4743 (9)	0.1260 (17)
H12A	0.191654	0.374784	0.405220	0.189*
H12B	0.151546	0.410152	0.583644	0.189*

H12C	0.221174	0.428538	0.546742	0.189*
O7	0.03136 (7)	0.91583 (7)	−0.1048 (4)	0.0567 (5)
H7	0.053714	0.946614	−0.102355	0.085*
O8	0.15807 (7)	0.89231 (7)	−0.1922 (3)	0.0479 (4)
O9	0.17575 (7)	0.81666 (6)	0.0631 (3)	0.0487 (4)
O10	0.05030 (7)	0.72325 (7)	−0.1521 (3)	0.0553 (5)
O11	0.11500 (8)	0.67555 (9)	−0.3981 (4)	0.0794 (7)
O12	0.12620 (8)	0.81417 (8)	−0.4345 (3)	0.0532 (4)
C13	0.04996 (10)	0.87641 (11)	−0.2817 (5)	0.0535 (6)
H13A	0.052680	0.900266	−0.419495	0.064*
H13B	0.018856	0.844425	−0.303102	0.064*
C14	0.11241 (10)	0.84602 (10)	−0.2350 (4)	0.0440 (5)
C15	0.11551 (10)	0.80518 (10)	−0.0257 (4)	0.0426 (5)
H15	0.083521	0.817439	0.082449	0.051*
C16	0.11134 (10)	0.73627 (10)	−0.0755 (5)	0.0469 (5)
H16	0.120573	0.712117	0.059899	0.056*
C17	0.15305 (10)	0.71584 (10)	−0.2687 (5)	0.0509 (6)
H17	0.188941	0.693064	−0.210220	0.061*
C18	0.17449 (11)	0.76945 (11)	−0.4106 (5)	0.0544 (6)
H18A	0.210346	0.788742	−0.341223	0.065*
H18B	0.186747	0.754435	−0.557608	0.065*
C19	0.18940 (11)	0.88016 (10)	0.0158 (5)	0.0505 (6)
C20	0.16511 (14)	0.92255 (11)	0.1983 (5)	0.0657 (7)
H20A	0.121652	0.914952	0.220428	0.099*
H20B	0.171210	0.964985	0.154611	0.099*
H20C	0.187057	0.914596	0.335560	0.099*
C21	0.25853 (12)	0.88619 (13)	−0.0166 (7)	0.0761 (9)
H21A	0.279550	0.871490	0.115211	0.114*
H21B	0.268931	0.928947	−0.041539	0.114*
H21C	0.271117	0.861982	−0.143967	0.114*
C22	0.05386 (11)	0.67444 (12)	−0.3135 (5)	0.0594 (7)
C23	0.01034 (16)	0.68932 (19)	−0.5024 (7)	0.0958 (12)
H23A	−0.031670	0.687308	−0.449319	0.144*
H23B	0.016001	0.659852	−0.621512	0.144*
H23C	0.018817	0.730331	−0.557299	0.144*
C24	0.0415 (2)	0.61259 (14)	−0.2036 (8)	0.1050 (13)
H24A	0.070346	0.606422	−0.082786	0.157*
H24B	0.046385	0.580063	−0.312281	0.157*
H24C	−0.000060	0.611932	−0.145751	0.157*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0440 (8)	0.0432 (8)	0.0883 (14)	0.0012 (7)	0.0050 (9)	−0.0127 (9)
O2	0.0486 (8)	0.0469 (8)	0.0558 (11)	0.0018 (6)	−0.0156 (8)	−0.0080 (8)
O3	0.0485 (9)	0.0519 (9)	0.0641 (12)	−0.0020 (7)	−0.0187 (8)	−0.0010 (9)
O4	0.0646 (11)	0.0494 (9)	0.0733 (13)	−0.0023 (8)	0.0091 (9)	−0.0113 (9)
O5	0.0887 (14)	0.0776 (13)	0.110 (2)	−0.0151 (11)	0.0468 (14)	−0.0262 (14)

O6	0.0527 (9)	0.0655 (10)	0.0494 (11)	0.0125 (8)	−0.0041 (8)	−0.0095 (9)
C1	0.0501 (13)	0.0508 (14)	0.0639 (19)	0.0094 (11)	−0.0042 (13)	−0.0030 (13)
C2	0.0460 (12)	0.0439 (11)	0.0511 (15)	0.0050 (9)	−0.0039 (11)	−0.0099 (11)
C3	0.0480 (12)	0.0445 (12)	0.0526 (16)	0.0037 (9)	−0.0060 (11)	−0.0132 (11)
C4	0.0475 (12)	0.0510 (13)	0.0621 (16)	−0.0005 (10)	−0.0094 (12)	−0.0105 (12)
C5	0.0466 (12)	0.0561 (14)	0.076 (2)	0.0067 (10)	0.0006 (13)	−0.0143 (14)
C6	0.0528 (13)	0.0603 (14)	0.0615 (17)	0.0138 (11)	−0.0010 (13)	−0.0193 (13)
C7	0.0494 (13)	0.0516 (13)	0.0676 (19)	−0.0022 (10)	−0.0202 (13)	−0.0004 (12)
C8	0.0613 (16)	0.087 (2)	0.067 (2)	−0.0149 (14)	−0.0109 (15)	0.0084 (16)
C9	0.0724 (18)	0.0483 (14)	0.130 (3)	−0.0013 (12)	−0.036 (2)	−0.0008 (18)
C10	0.0751 (18)	0.0645 (17)	0.087 (2)	−0.0077 (14)	0.0223 (17)	−0.0086 (17)
C11	0.089 (2)	0.106 (3)	0.148 (4)	−0.039 (2)	0.014 (3)	−0.022 (3)
C12	0.153 (4)	0.117 (3)	0.108 (4)	0.021 (3)	0.042 (3)	0.034 (3)
O7	0.0417 (8)	0.0393 (8)	0.0891 (14)	0.0014 (6)	0.0105 (9)	−0.0046 (9)
O8	0.0481 (8)	0.0449 (8)	0.0509 (11)	0.0005 (6)	0.0003 (7)	0.0101 (7)
O9	0.0538 (9)	0.0412 (8)	0.0509 (10)	−0.0006 (6)	−0.0087 (8)	0.0055 (8)
O10	0.0466 (8)	0.0530 (9)	0.0664 (13)	−0.0019 (7)	0.0024 (8)	−0.0114 (9)
O11	0.0554 (10)	0.0810 (13)	0.1018 (18)	−0.0014 (9)	0.0055 (11)	−0.0474 (13)
O12	0.0612 (10)	0.0569 (9)	0.0416 (10)	0.0164 (8)	0.0011 (8)	0.0001 (8)
C13	0.0476 (12)	0.0489 (12)	0.0641 (18)	0.0096 (10)	−0.0036 (12)	0.0030 (12)
C14	0.0445 (11)	0.0418 (11)	0.0457 (14)	0.0055 (9)	0.0017 (10)	0.0010 (10)
C15	0.0438 (11)	0.0407 (11)	0.0434 (14)	0.0030 (9)	0.0033 (10)	−0.0017 (10)
C16	0.0495 (12)	0.0396 (11)	0.0517 (15)	0.0019 (9)	−0.0038 (11)	0.0034 (11)
C17	0.0457 (11)	0.0448 (11)	0.0622 (16)	0.0091 (9)	−0.0038 (12)	−0.0085 (12)
C18	0.0531 (13)	0.0604 (14)	0.0498 (16)	0.0163 (11)	0.0059 (12)	−0.0064 (13)
C19	0.0543 (13)	0.0429 (11)	0.0544 (16)	−0.0024 (10)	−0.0054 (11)	0.0091 (11)
C20	0.0903 (19)	0.0469 (13)	0.0600 (19)	−0.0064 (13)	−0.0077 (16)	−0.0030 (13)
C21	0.0558 (15)	0.0677 (17)	0.105 (3)	−0.0085 (13)	−0.0138 (16)	0.0162 (17)
C22	0.0537 (13)	0.0571 (14)	0.0675 (18)	−0.0004 (11)	−0.0026 (13)	−0.0128 (13)
C23	0.080 (2)	0.127 (3)	0.081 (3)	0.009 (2)	−0.0206 (19)	−0.024 (2)
C24	0.141 (3)	0.0592 (18)	0.115 (3)	−0.0181 (19)	0.004 (3)	−0.011 (2)

Geometric parameters (Å, º)

O1—H1	0.8200	O7—H7	0.8200
O1—C1	1.405 (3)	O7—C13	1.412 (3)
O2—C2	1.429 (3)	O8—C14	1.425 (3)
O2—C7	1.432 (3)	O8—C19	1.435 (3)
O3—C3	1.424 (3)	O9—C15	1.424 (3)
O3—C7	1.427 (3)	O9—C19	1.428 (3)
O4—C4	1.424 (3)	O10—C16	1.421 (3)
O4—C10	1.417 (4)	O10—C22	1.427 (3)
O5—C5	1.419 (3)	O11—C17	1.422 (3)
O5—C10	1.417 (3)	O11—C22	1.411 (3)
O6—C2	1.400 (3)	O12—C14	1.404 (3)
O6—C6	1.424 (3)	O12—C18	1.426 (3)
C1—H1A	0.99 (4)	C13—H13A	0.9700
C1—H1B	0.96 (3)	C13—H13B	0.9700

C1—C2	1.519 (3)	C13—C14	1.522 (3)
C2—C3	1.530 (3)	C14—C15	1.527 (3)
C3—H3	0.9800	C15—H15	0.9800
C3—C4	1.518 (3)	C15—C16	1.517 (3)
C4—H4	0.9800	C16—H16	0.9800
C4—C5	1.528 (4)	C16—C17	1.525 (4)
C5—H5	0.9800	C17—H17	0.9800
C5—C6	1.503 (4)	C17—C18	1.505 (4)
C6—H6A	0.9700	C18—H18A	0.9700
C6—H6B	0.9700	C18—H18B	0.9700
C7—C8	1.511 (4)	C19—C20	1.513 (4)
C7—C9	1.508 (4)	C19—C21	1.508 (3)
C8—H8A	0.9600	C20—H20A	0.9600
C8—H8B	0.9600	C20—H20B	0.9600
C8—H8C	0.9600	C20—H20C	0.9600
C9—H9A	0.9600	C21—H21A	0.9600
C9—H9B	0.9600	C21—H21B	0.9600
C9—H9C	0.9600	C21—H21C	0.9600
C10—C11	1.520 (5)	C22—C23	1.499 (4)
C10—C12	1.499 (5)	C22—C24	1.509 (4)
C11—H11A	0.9600	C23—H23A	0.9600
C11—H11B	0.9600	C23—H23B	0.9600
C11—H11C	0.9600	C23—H23C	0.9600
C12—H12A	0.9600	C24—H24A	0.9600
C12—H12B	0.9600	C24—H24B	0.9600
C12—H12C	0.9600	C24—H24C	0.9600

C1—O1—H1	109.5	C13—O7—H7	109.5
C2—O2—C7	110.72 (17)	C14—O8—C19	110.60 (17)
C3—O3—C7	106.58 (16)	C15—O9—C19	106.32 (16)
C10—O4—C4	107.17 (19)	C16—O10—C22	108.20 (17)
C10—O5—C5	109.9 (2)	C22—O11—C17	110.8 (2)
C2—O6—C6	114.2 (2)	C14—O12—C18	113.63 (18)
O1—C1—H1A	115.6 (17)	O7—C13—H13A	109.2
O1—C1—H1B	109.7 (17)	O7—C13—H13B	109.2
O1—C1—C2	112.8 (2)	O7—C13—C14	111.9 (2)
H1A—C1—H1B	103 (2)	H13A—C13—H13B	107.9
C2—C1—H1A	107.3 (17)	C14—C13—H13A	109.2
C2—C1—H1B	107.4 (15)	C14—C13—H13B	109.2
O2—C2—C1	109.29 (19)	O8—C14—C13	110.01 (17)
O2—C2—C3	103.0 (2)	O8—C14—C15	103.13 (18)
O6—C2—O2	110.52 (18)	O12—C14—O8	110.35 (18)
O6—C2—C1	104.3 (2)	O12—C14—C13	104.1 (2)
O6—C2—C3	113.35 (17)	O12—C14—C15	113.55 (16)
C1—C2—C3	116.4 (2)	C13—C14—C15	115.8 (2)
O3—C3—C2	103.99 (17)	O9—C15—C14	104.07 (17)
O3—C3—H3	110.6	O9—C15—H15	110.5
O3—C3—C4	106.71 (18)	O9—C15—C16	107.26 (17)

C2—C3—H3	110.6	C14—C15—H15	110.5
C4—C3—C2	113.9 (2)	C16—C15—C14	113.7 (2)
C4—C3—H3	110.6	C16—C15—H15	110.5
O4—C4—C3	108.69 (18)	O10—C16—C15	108.11 (17)
O4—C4—H4	110.3	O10—C16—H16	110.3
O4—C4—C5	103.6 (2)	O10—C16—C17	104.3 (2)
C3—C4—H4	110.3	C15—C16—H16	110.3
C3—C4—C5	113.30 (19)	C15—C16—C17	113.26 (19)
C5—C4—H4	110.3	C17—C16—H16	110.3
O5—C5—C4	104.4 (2)	O11—C17—C16	104.21 (19)
O5—C5—H5	109.8	O11—C17—H17	110.0
O5—C5—C6	110.1 (3)	O11—C17—C18	110.0 (2)
C4—C5—H5	109.8	C16—C17—H17	110.0
C6—C5—C4	112.8 (2)	C18—C17—C16	112.53 (18)
C6—C5—H5	109.8	C18—C17—H17	110.0
O6—C6—C5	110.6 (2)	O12—C18—C17	110.6 (2)
O6—C6—H6A	109.5	O12—C18—H18A	109.5
O6—C6—H6B	109.5	O12—C18—H18B	109.5
C5—C6—H6A	109.5	C17—C18—H18A	109.5
C5—C6—H6B	109.5	C17—C18—H18B	109.5
H6A—C6—H6B	108.1	H18A—C18—H18B	108.1
O2—C7—C8	110.5 (2)	O8—C19—C20	110.30 (19)
O2—C7—C9	109.6 (2)	O8—C19—C21	109.8 (2)
O3—C7—O2	104.4 (2)	O9—C19—O8	104.38 (18)
O3—C7—C8	111.0 (2)	O9—C19—C20	111.4 (2)
O3—C7—C9	108.60 (19)	O9—C19—C21	108.15 (19)
C9—C7—C8	112.4 (3)	C21—C19—C20	112.4 (2)
C7—C8—H8A	109.5	C19—C20—H20A	109.5
C7—C8—H8B	109.5	C19—C20—H20B	109.5
C7—C8—H8C	109.5	C19—C20—H20C	109.5
H8A—C8—H8B	109.5	H20A—C20—H20B	109.5
H8A—C8—H8C	109.5	H20A—C20—H20C	109.5
H8B—C8—H8C	109.5	H20B—C20—H20C	109.5
C7—C9—H9A	109.5	C19—C21—H21A	109.5
C7—C9—H9B	109.5	C19—C21—H21B	109.5
C7—C9—H9C	109.5	C19—C21—H21C	109.5
H9A—C9—H9B	109.5	H21A—C21—H21B	109.5
H9A—C9—H9C	109.5	H21A—C21—H21C	109.5
H9B—C9—H9C	109.5	H21B—C21—H21C	109.5
O4—C10—C11	110.0 (3)	O10—C22—C23	108.3 (2)
O4—C10—C12	109.2 (3)	O10—C22—C24	110.5 (3)
O5—C10—O4	106.0 (2)	O11—C22—O10	106.16 (18)
O5—C10—C11	109.3 (3)	O11—C22—C23	108.2 (3)
O5—C10—C12	108.6 (3)	O11—C22—C24	109.5 (3)
C12—C10—C11	113.5 (3)	C23—C22—C24	113.8 (3)
C10—C11—H11A	109.5	C22—C23—H23A	109.5
C10—C11—H11B	109.5	C22—C23—H23B	109.5
C10—C11—H11C	109.5	C22—C23—H23C	109.5

H11A—C11—H11B	109.5	H23A—C23—H23B	109.5
H11A—C11—H11C	109.5	H23A—C23—H23C	109.5
H11B—C11—H11C	109.5	H23B—C23—H23C	109.5
C10—C12—H12A	109.5	C22—C24—H24A	109.5
C10—C12—H12B	109.5	C22—C24—H24B	109.5
C10—C12—H12C	109.5	C22—C24—H24C	109.5
H12A—C12—H12B	109.5	H24A—C24—H24B	109.5
H12A—C12—H12C	109.5	H24A—C24—H24C	109.5
H12B—C12—H12C	109.5	H24B—C24—H24C	109.5

O1—C1—C2—O2	−55.0 (3)	O7—C13—C14—O8	−56.0 (3)
O1—C1—C2—O6	−173.2 (2)	O7—C13—C14—O12	−174.25 (19)
O1—C1—C2—C3	61.1 (3)	O7—C13—C14—C15	60.4 (3)
O2—C2—C3—O3	−21.9 (2)	O8—C14—C15—O9	−22.4 (2)
O2—C2—C3—C4	−137.70 (19)	O8—C14—C15—C16	−138.74 (18)
O3—C3—C4—O4	176.7 (2)	O9—C15—C16—O10	176.66 (19)
O3—C3—C4—C5	−68.7 (3)	O9—C15—C16—C17	−68.3 (3)
O4—C4—C5—O5	−19.1 (3)	O10—C16—C17—O11	−18.7 (2)
O4—C4—C5—C6	100.3 (2)	O10—C16—C17—C18	100.4 (2)
O5—C5—C6—O6	79.6 (3)	O11—C17—C18—O12	78.1 (2)
O6—C2—C3—O3	97.5 (2)	O12—C14—C15—O9	97.1 (2)
O6—C2—C3—C4	−18.3 (3)	O12—C14—C15—C16	−19.3 (3)
C1—C2—C3—O3	−141.5 (2)	C13—C14—C15—O9	−142.6 (2)
C1—C2—C3—C4	102.8 (2)	C13—C14—C15—C16	101.0 (2)
C2—O2—C7—O3	17.5 (2)	C14—O8—C19—O9	17.3 (2)
C2—O2—C7—C8	−101.9 (2)	C14—O8—C19—C20	−102.5 (2)
C2—O2—C7—C9	133.6 (2)	C14—O8—C19—C21	133.0 (2)
C2—O6—C6—C5	68.7 (3)	C14—O12—C18—C17	69.1 (3)
C2—C3—C4—O4	−69.1 (3)	C14—C15—C16—O10	−68.8 (2)
C2—C3—C4—C5	45.5 (3)	C14—C15—C16—C17	46.2 (3)
C3—O3—C7—O2	−32.0 (2)	C15—O9—C19—O8	−32.0 (2)
C3—O3—C7—C8	87.0 (3)	C15—O9—C19—C20	87.0 (2)
C3—O3—C7—C9	−148.8 (3)	C15—O9—C19—C21	−148.9 (2)
C3—C4—C5—O5	−136.8 (2)	C15—C16—C17—O11	−136.0 (2)
C3—C4—C5—C6	−17.3 (3)	C15—C16—C17—C18	−16.9 (3)
C4—O4—C10—O5	−28.9 (3)	C16—O10—C22—O11	−22.9 (3)
C4—O4—C10—C11	89.2 (3)	C16—O10—C22—C23	−138.9 (2)
C4—O4—C10—C12	−145.7 (3)	C16—O10—C22—C24	95.8 (3)
C4—C5—C6—O6	−36.5 (3)	C16—C17—C18—O12	−37.6 (3)
C5—O5—C10—O4	16.0 (3)	C17—O11—C22—O10	10.2 (3)
C5—O5—C10—C11	−102.5 (3)	C17—O11—C22—C23	126.3 (3)
C5—O5—C10—C12	133.2 (3)	C17—O11—C22—C24	−109.0 (3)
C6—O6—C2—O2	76.4 (2)	C18—O12—C14—O8	77.3 (2)
C6—O6—C2—C1	−166.2 (2)	C18—O12—C14—C13	−164.68 (19)
C6—O6—C2—C3	−38.6 (3)	C18—O12—C14—C15	−37.9 (3)
C7—O2—C2—O6	−118.7 (2)	C19—O8—C14—O12	−118.53 (19)
C7—O2—C2—C1	127.1 (2)	C19—O8—C14—C13	127.2 (2)
C7—O2—C2—C3	2.7 (2)	C19—O8—C14—C15	3.1 (2)

C7—O3—C3—C2	33.7 (2)	C19—O9—C15—C14	33.9 (2)
C7—O3—C3—C4	154.4 (2)	C19—O9—C15—C16	154.7 (2)
C10—O4—C4—C3	150.2 (2)	C22—O10—C16—C15	146.5 (2)
C10—O4—C4—C5	29.5 (3)	C22—O10—C16—C17	25.7 (2)
C10—O5—C5—C4	2.1 (3)	C22—O11—C17—C16	5.3 (3)
C10—O5—C5—C6	−119.2 (3)	C22—O11—C17—C18	−115.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.82	1.97	2.776 (2)	166
O7—H7···O7^{ii}	0.82	1.94	2.738 (2)	164

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