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α-D,L-Sorbose

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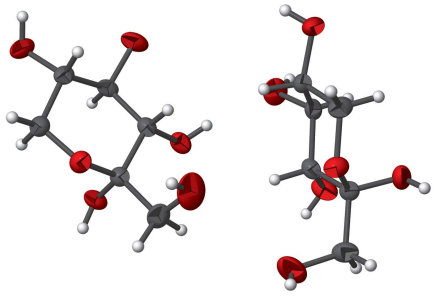
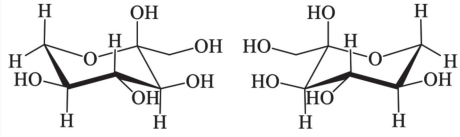
The racemic title compound, $C_6H_{12}O_6$, consisting of C-4 epimers of psicose, was crystallized from an aqueous solution of an equimolar mixture of D- and L-sorboses. It was confirmed that D-sorbose (or L-sorbose) formed α-pyranose with a $^4C_1$ (or $^1C_4$) conformation where the anomer position was designated as carbon-1. The asymmetric unit comprises two crystallographically independent molecules. In the crystal, molecules are linked by O—H···O hydrogen bonds, forming a three-dimensional framework. The unit-cell volume of the title racemic α-D,L-sorbose is 1450.86 (6) Å^3 (Z = 8), which is about 41 Å^3 smaller than that of twice the amount of chiral α-L-sorbose [V = 745.942 Å^3 (Z = 4)].

3D view



Chemical scheme



Structure description

D- and L-sorboses are classified as rare sugars. L-Sorbose is the first L-form hexose found in nature (Nordenson *et al.*, 1979). In this study, we aimed to create a racemic single crystal including both D- and L-sorbose in a 1:1 ratio. There are two independent sorbose molecules, *A* and *B*, in the asymmetric unit (Fig. 1). Therefore, there are a total of eight sorbose molecules (four L- and four D-forms) in the unit cell.

In the crystal, the D- and L-sorbose molecules are linked weakly, as well as the strong homo-chiral D–D (and L–L) links, *via* O—H···O hydrogen bonds (Table 1), forming a three-dimensional network (Fig. 2). The crystal structure of the title compound with two independent molecules in the asymmetric unit in space group $P2_1/a$ (Z = 8) is significantly different from the structures previously reported by us, *viz*. racemic β-D,L-allose ($P2_1/c$, Z = 4; Ishii, Senoo *et al.*, 2015*a*), β-D,L-psicose ($Pna2_1$, Z = 4; Ishii, Sakane *et al.*, 2015) and β-D,L-fructose ($P\overline{1}$, Z = 2; Ishii, Senoo *et al.*, 2015*b*), where each asymmetric unit consists of one molecule.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O4^{i}	0.82	2.37	3.174 (3)	167
O2—H2A···O5^{ii}	0.82	1.96	2.757 (2)	164
O3—H3A···O10	0.82	1.99	2.807 (2)	172
O4—H4A···O6^{iii}	0.82	2.11	2.917 (2)	170
O5—H5A···O2^{iv}	0.82	2.30	2.875 (2)	128
O5—H5A···O3^{iv}	0.82	2.10	2.8683 (18)	156
O7—H7A···O9^{i}	0.82	2.14	2.915 (2)	159
O7—H7A···O10^{i}	0.82	2.52	3.047 (3)	123
O8—H8A···O11^{v}	0.82	2.00	2.814 (2)	169
O9—H9A···O4^{vi}	0.82	1.93	2.747 (2)	172
O10—H10A···O12^{iii}	0.82	2.25	3.051 (2)	165
O11—H11A···O8^{iv}	0.82	2.41	2.976 (2)	127
O11—H11A···O9^{iv}	0.82	2.28	3.060 (2)	158

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

Synthesis and crystallization

L-Sorbose was purchased from Wako Pure Chemical Industries. D-Sorbose was prepared by microbial oxidation of galactitol to D-tagatose followed by enzymatic epimerization using D-tagatose 3-epimerase (Khan *et al.*, 1992; Itoh *et al.*, 1995). L-Sorbose and D-sorbose were each dissolved in hot water to give a 30 wt% solution and the solutions were mixed in equal volume. Single crystals were obtained from the mixed solution by keeping it at 20°C.

Refinement

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

Acknowledgements

The authors are sincerely grateful to Professor Genta Sakane (Okayama University of Science) for excellent discussions and useful technical advice.

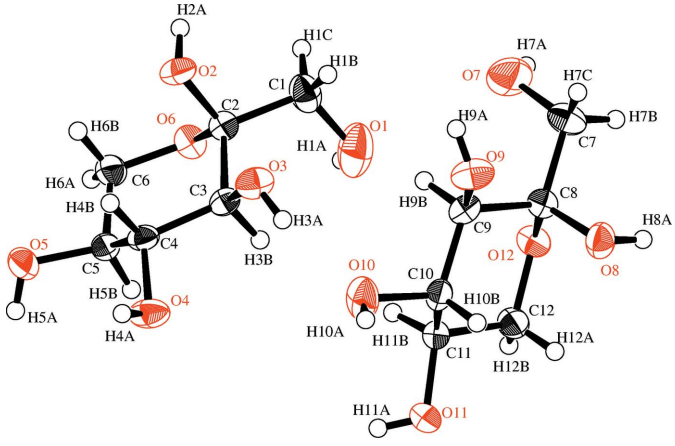


Figure 1
An *ORTEP* view of the title compound, molecule *A* (left) and molecule *B* (right), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_{12}O_6$
M_r	180.16
Crystal system, space group	Monoclinic, $P2_1/a$
Temperature (K)	296
a, b, c (Å)	12.8152 (3), 6.29489 (13), 18.9482 (4)
β (°)	108.3472 (12)
V (Å^3)	1450.86 (6)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.31
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}	0.728, 0.877
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	24139, 2658, 2161
R_{int}	0.051
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.120, 1.08
No. of reflections	2658
No. of parameters	228
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.57, −0.29

Computer programs: *RAPID-AUTO* (Rigaku, 2009), *SIR2011* (Burla *et al.*, 2012), *SHELXL2013* (Sheldrick, 2015) and *CrystalStructure* (Rigaku, 2014).

Funding information

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References

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Mallamo, M., Mazzone, A., Polidori, G. & Spagna, R. (2012). *J. Appl. Cryst.* **45**, 357–361.

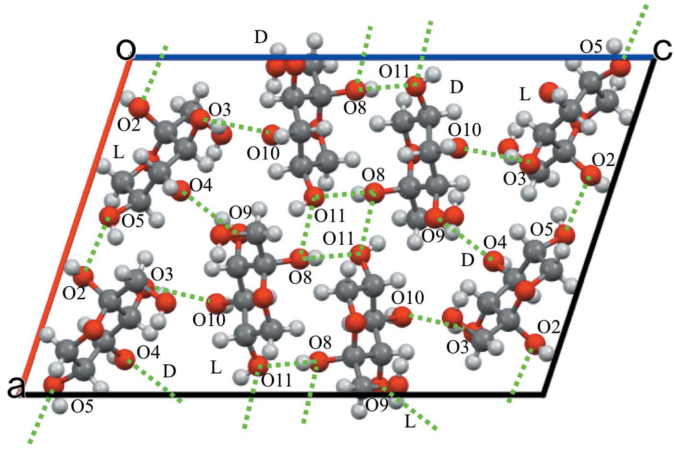

Figure 2
A packing diagram of the title compound viewed down the *b* axis, showing the hydrogen-bonding network (dotted lines). In this figure, D and L denote the D- and L-forms, respectively.

Ishii, T., Sakane, G., Yoshihara, A., Fukada, K. & Senoo, T. (2015). *Acta Cryst.* E**71**, o289–o290.
Ishii, T., Senoo, T., Kozakai, T., Fukada, K. & Sakane, G. (2015*a*). *Acta Cryst.* E**71**, o139.
Ishii, T., Senoo, T., Yoshihara, A., Fukada, K. & Sakane, G. (2015*b*). *Acta Cryst.* E**71**, o719–o720.
Itoh, H., Sato, T., Takeuchi, T., Khan, A. R. & Izumori, K. (1995). *J. Ferment. Bioeng.* **79**, 184–185.
Khan, A. R., Takahata, S., Okaya, H., Tsumura, T. & Izumori, K. (1992). *J. Ferment. Bioeng.* **74**, 149–152.
Nordenson, S., Takagi, S. & Jeffrey, G. A. (1979). *Acta Cryst.* B**35**, 1005–1007.
Rigaku (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2009). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2014). *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

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α-D,L-Sorbose

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α-D,L-Sorbose

Crystal data

$C_6H_{12}O_6$
M_r = 180.16
Monoclinic, $P2_1/a$
a = 12.8152 (3) Å
b = 6.29489 (13) Å
c = 18.9482 (4) Å
β = 108.3472 (12)°
V = 1450.86 (6) Å^3
Z = 8
$F(000)$ = 768.00
D_x = 1.649 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 15393 reflections
θ = 3.6–68.3°
μ = 1.31 mm^{-1}
T = 296 K
Block, colorless
0.10 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
T_{min} = 0.728, T_{max} = 0.877
24139 measured reflections
2658 independent reflections
2161 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.051
θ_{max} = 68.3°, θ_{min} = 4.9°
h = −15→15
k = −7→7
l = −22→22

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 1.08
2658 reflections
228 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.7784P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: SHELXL2013 (Sheldrick, 2015)
Extinction coefficient: 0.0027 (4)

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).
H atoms were positioned geometrically (C—H = 0.98 or 0.97 Å, and O—H = 0.82 Å) and refined using as riding with U_{iso}(H) = 1.2U_{eq}(C or O), allowing for free rotation of the OH groups.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.22822 (19)	0.7791 (3)	0.22185 (11)	0.0629 (6)
O2	0.14999 (12)	0.4920 (2)	0.04746 (8)	0.0319 (4)
O3	0.18382 (11)	0.2570 (3)	0.17113 (8)	0.0338 (4)
O4	0.39585 (13)	0.0849 (3)	0.17903 (8)	0.0385 (4)
O5	0.47216 (12)	0.2681 (3)	0.05987 (8)	0.0404 (4)
O6	0.30811 (11)	0.6926 (2)	0.10091 (8)	0.0294 (4)
O7	0.02816 (17)	0.8374 (3)	0.28347 (10)	0.0547 (5)
O8	0.09763 (13)	0.5097 (3)	0.44959 (8)	0.0345 (4)
O9	0.02314 (12)	0.2877 (3)	0.31816 (9)	0.0368 (4)
O10	0.23099 (15)	0.1206 (3)	0.31891 (9)	0.0433 (4)
O11	0.41443 (12)	0.2925 (3)	0.43820 (8)	0.0386 (4)
O12	0.21295 (11)	0.7176 (2)	0.40376 (8)	0.0295 (4)
C1	0.16229 (19)	0.7191 (4)	0.15089 (13)	0.0380 (5)
C2	0.22188 (16)	0.5705 (3)	0.11388 (10)	0.0246 (4)
C3	0.27148 (15)	0.3795 (3)	0.16199 (11)	0.0239 (4)
C4	0.34130 (16)	0.2480 (3)	0.12745 (11)	0.0265 (5)
C5	0.42487 (16)	0.3835 (4)	0.10693 (11)	0.0274 (5)
C6	0.37037 (17)	0.5755 (4)	0.06332 (12)	0.0318 (5)
C7	0.02122 (18)	0.7524 (4)	0.35030 (13)	0.0365 (5)
C8	0.11366 (16)	0.5985 (3)	0.38604 (11)	0.0252 (4)
C9	0.12015 (16)	0.4150 (3)	0.33493 (11)	0.0256 (4)
C10	0.21984 (16)	0.2770 (3)	0.37048 (11)	0.0266 (4)
C11	0.32302 (16)	0.4106 (3)	0.39376 (11)	0.0268 (5)
C12	0.30878 (16)	0.5961 (4)	0.44065 (12)	0.0320 (5)
H3A	0.20162	0.20895	0.21349	0.0405*
H9B	0.12621	0.47356	0.28846	0.0307*
H11A	0.44627	0.23745	0.4115	0.0463*
H10B	0.21093	0.20623	0.4143	0.0319*
H8A	0.0954	0.60463	0.47871	0.0414*
H5B	0.48263	0.4284	0.15205	0.0329*
H2A	0.11709	0.59116	0.02195	0.0383*
H6A	0.42617	0.66733	0.05503	0.0381*
H6B	0.32208	0.53027	0.01517	0.0381*
H9A	−0.02006	0.32465	0.27811	0.0442*
H11B	0.33855	0.46362	0.34947	0.0321*
H5A	0.53459	0.2308	0.08379	0.0485*
H4B	0.29326	0.18044	0.08229	0.0318*
H4A	0.3784	−0.032	0.15987	0.0462*
H3B	0.31745	0.42981	0.21083	0.0287*
H10A	0.22195	0.00214	0.334	0.0519*
H12A	0.30313	0.54341	0.48742	0.0384*
H12B	0.37304	0.68699	0.45164	0.0384*
H7A	0.04068	0.96523	0.28858	0.0657*
H7C	−0.04858	0.67955	0.34064	0.0438*
H7B	0.02309	0.8675	0.38472	0.0438*

H1C	0.13966	0.84507	0.1204	0.0456*
H1B	0.09662	0.64956	0.1545	0.0456*
H1A	0.27758	0.85718	0.2184	0.0755*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0933 (16)	0.0493 (13)	0.0544 (11)	−0.0043 (11)	0.0348 (11)	−0.0184 (10)
O2	0.0312 (8)	0.0310 (9)	0.0263 (7)	0.0003 (6)	−0.0014 (6)	0.0014 (6)
O3	0.0312 (8)	0.0350 (9)	0.0338 (8)	−0.0052 (7)	0.0082 (6)	0.0102 (7)
O4	0.0426 (9)	0.0250 (9)	0.0381 (9)	0.0065 (7)	−0.0013 (7)	0.0029 (7)
O5	0.0260 (8)	0.0569 (11)	0.0355 (9)	0.0092 (8)	0.0055 (6)	−0.0126 (8)
O6	0.0308 (8)	0.0237 (8)	0.0363 (8)	−0.0023 (6)	0.0143 (6)	0.0013 (6)
O7	0.0706 (12)	0.0396 (11)	0.0503 (11)	0.0128 (10)	0.0138 (9)	0.0158 (9)
O8	0.0441 (9)	0.0336 (9)	0.0306 (8)	0.0027 (7)	0.0186 (7)	0.0023 (7)
O9	0.0317 (8)	0.0305 (9)	0.0390 (9)	−0.0099 (7)	−0.0021 (6)	0.0024 (7)
O10	0.0629 (11)	0.0260 (9)	0.0445 (10)	0.0004 (8)	0.0221 (8)	−0.0111 (7)
O11	0.0311 (8)	0.0520 (11)	0.0333 (8)	0.0158 (7)	0.0112 (6)	0.0034 (7)
O12	0.0252 (7)	0.0241 (8)	0.0370 (8)	−0.0021 (6)	0.0066 (6)	−0.0042 (6)
C1	0.0465 (13)	0.0292 (13)	0.0444 (13)	0.0053 (10)	0.0231 (11)	0.0009 (10)
C2	0.0252 (10)	0.0223 (11)	0.0259 (10)	−0.0023 (8)	0.0076 (8)	−0.0008 (8)
C3	0.0252 (10)	0.0221 (11)	0.0220 (9)	−0.0038 (8)	0.0039 (8)	−0.0002 (8)
C4	0.0254 (10)	0.0252 (11)	0.0230 (10)	0.0015 (8)	−0.0007 (8)	−0.0019 (8)
C5	0.0224 (9)	0.0339 (13)	0.0231 (10)	0.0020 (9)	0.0030 (8)	−0.0054 (9)
C6	0.0283 (11)	0.0375 (13)	0.0315 (11)	0.0032 (9)	0.0123 (9)	0.0040 (10)
C7	0.0319 (11)	0.0285 (13)	0.0475 (14)	0.0044 (9)	0.0103 (10)	0.0052 (10)
C8	0.0247 (10)	0.0230 (11)	0.0283 (10)	−0.0012 (8)	0.0087 (8)	0.0019 (8)
C9	0.0288 (10)	0.0229 (11)	0.0230 (10)	−0.0054 (8)	0.0051 (8)	0.0016 (8)
C10	0.0352 (11)	0.0238 (11)	0.0224 (10)	0.0009 (9)	0.0115 (8)	−0.0006 (8)
C11	0.0266 (10)	0.0313 (12)	0.0231 (10)	0.0042 (9)	0.0089 (8)	0.0007 (8)
C12	0.0244 (10)	0.0361 (13)	0.0319 (11)	0.0000 (9)	0.0037 (8)	−0.0093 (9)

Geometric parameters (Å, º)

O1—C1	1.396 (3)	O1—H1A	0.820
O2—C2	1.395 (2)	O2—H2A	0.820
O3—C3	1.418 (3)	O3—H3A	0.820
O4—C4	1.438 (2)	O4—H4A	0.820
O5—C5	1.425 (3)	O5—H5A	0.820
O6—C2	1.429 (3)	O7—H7A	0.820
O6—C6	1.430 (3)	O8—H8A	0.820
O7—C7	1.403 (3)	O9—H9A	0.820
O8—C8	1.400 (3)	O10—H10A	0.820
O9—C9	1.428 (3)	O11—H11A	0.820
O10—C10	1.426 (3)	C1—H1C	0.970
O11—C11	1.419 (2)	C1—H1B	0.970
O12—C8	1.423 (2)	C3—H3B	0.980
O12—C12	1.429 (2)	C4—H4B	0.980

C1—C2	1.512 (3)	C5—H5B	0.980
C2—C3	1.522 (3)	C6—H6A	0.970
C3—C4	1.511 (3)	C6—H6B	0.970
C4—C5	1.513 (3)	C7—H7C	0.970
C5—C6	1.506 (3)	C7—H7B	0.970
C7—C8	1.515 (3)	C9—H9B	0.980
C8—C9	1.526 (3)	C10—H10B	0.980
C9—C10	1.516 (3)	C11—H11B	0.980
C10—C11	1.511 (3)	C12—H12A	0.970
C11—C12	1.513 (3)	C12—H12B	0.970

C2—O6—C6	113.05 (16)	C8—O8—H8A	109.471
C8—O12—C12	113.61 (15)	C9—O9—H9A	109.472
O1—C1—C2	111.89 (19)	C10—O10—H10A	109.479
O2—C2—O6	111.22 (16)	C11—O11—H11A	109.476
O2—C2—C1	110.54 (16)	O1—C1—H1C	109.244
O2—C2—C3	107.06 (16)	O1—C1—H1B	109.242
O6—C2—C1	106.13 (17)	C2—C1—H1C	109.230
O6—C2—C3	109.14 (15)	C2—C1—H1B	109.231
C1—C2—C3	112.80 (18)	H1C—C1—H1B	107.914
O3—C3—C2	107.78 (15)	O3—C3—H3B	108.924
O3—C3—C4	110.78 (16)	C2—C3—H3B	108.914
C2—C3—C4	111.47 (18)	C4—C3—H3B	108.910
O4—C4—C3	108.92 (17)	O4—C4—H4B	108.731
O4—C4—C5	110.20 (16)	C3—C4—H4B	108.728
C3—C4—C5	111.47 (17)	C5—C4—H4B	108.740
O5—C5—C4	110.39 (18)	O5—C5—H5B	109.860
O5—C5—C6	106.31 (18)	C4—C5—H5B	109.868
C4—C5—C6	110.49 (17)	C6—C5—H5B	109.864
O6—C6—C5	112.05 (19)	O6—C6—H6A	109.207
O7—C7—C8	112.6 (2)	O6—C6—H6B	109.204
O8—C8—O12	111.70 (15)	C5—C6—H6A	109.202
O8—C8—C7	109.51 (19)	C5—C6—H6B	109.203
O8—C8—C9	107.19 (16)	H6A—C6—H6B	107.889
O12—C8—C7	106.49 (16)	O7—C7—H7C	109.070
O12—C8—C9	108.98 (18)	O7—C7—H7B	109.069
C7—C8—C9	113.04 (16)	C8—C7—H7C	109.076
O9—C9—C8	110.39 (18)	C8—C7—H7B	109.068
O9—C9—C10	109.27 (16)	H7C—C7—H7B	107.828
C8—C9—C10	110.99 (15)	O9—C9—H9B	108.714
O10—C10—C9	110.08 (15)	C8—C9—H9B	108.713
O10—C10—C11	108.49 (19)	C10—C9—H9B	108.709
C9—C10—C11	110.40 (17)	O10—C10—H10B	109.288
O11—C11—C10	111.40 (17)	C9—C10—H10B	109.283
O11—C11—C12	106.60 (15)	C11—C10—H10B	109.285
C10—C11—C12	110.17 (18)	O11—C11—H11B	109.539
O12—C12—C11	111.71 (15)	C10—C11—H11B	109.544
C1—O1—H1A	109.482	C12—C11—H11B	109.542

C2—O2—H2A	109.473	O12—C12—H12A	109.276
C3—O3—H3A	109.469	O12—C12—H12B	109.277
C4—O4—H4A	109.472	C11—C12—H12A	109.279
C5—O5—H5A	109.470	C11—C12—H12B	109.283
C7—O7—H7A	109.468	H12A—C12—H12B	107.938
C2—O6—C6—C5	−60.30 (17)	C3—C4—C5—O5	−166.84 (13)
C6—O6—C2—O2	−57.58 (18)	C3—C4—C5—C6	−49.53 (19)
C6—O6—C2—C1	−177.85 (12)	O5—C5—C6—O6	173.00 (14)
C6—O6—C2—C3	60.32 (17)	C4—C5—C6—O6	53.2 (2)
C8—O12—C12—C11	59.7 (2)	O7—C7—C8—O8	−176.16 (15)
C12—O12—C8—O8	58.4 (2)	O7—C7—C8—O12	62.9 (2)
C12—O12—C8—C7	177.90 (15)	O7—C7—C8—C9	−56.7 (2)
C12—O12—C8—C9	−59.9 (2)	O8—C8—C9—O9	56.92 (18)
O1—C1—C2—O2	172.38 (18)	O8—C8—C9—C10	−64.39 (19)
O1—C1—C2—O6	−66.9 (2)	O12—C8—C9—O9	177.97 (13)
O1—C1—C2—C3	52.6 (2)	O12—C8—C9—C10	56.6 (2)
O2—C2—C3—O3	−57.0 (2)	C7—C8—C9—O9	−63.8 (2)
O2—C2—C3—C4	64.77 (19)	C7—C8—C9—C10	174.84 (17)
O6—C2—C3—O3	−177.49 (14)	O9—C9—C10—O10	64.2 (2)
O6—C2—C3—C4	−55.71 (18)	O9—C9—C10—C11	−176.02 (15)
C1—C2—C3—O3	64.81 (19)	C8—C9—C10—O10	−173.79 (16)
C1—C2—C3—C4	−173.42 (14)	C8—C9—C10—C11	−54.0 (2)
O3—C3—C4—O4	−66.54 (17)	O10—C10—C11—O11	−69.2 (2)
O3—C3—C4—C5	171.66 (12)	O10—C10—C11—C12	172.67 (13)
C2—C3—C4—O4	173.44 (13)	C9—C10—C11—O11	170.05 (16)
C2—C3—C4—C5	51.64 (18)	C9—C10—C11—C12	52.0 (2)
O4—C4—C5—O5	72.10 (18)	O11—C11—C12—O12	−175.14 (16)
O4—C4—C5—C6	−170.59 (14)	C10—C11—C12—O12	−54.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O4^{i}	0.82	2.37	3.174 (3)	167
O2—H2*A*···O5^{ii}	0.82	1.96	2.757 (2)	164
O3—H3*A*···O10	0.82	1.99	2.807 (2)	172
O4—H4*A*···O6^{iii}	0.82	2.11	2.917 (2)	170
O5—H5*A*···O2^{iv}	0.82	2.30	2.875 (2)	128
O5—H5*A*···O3^{iv}	0.82	2.10	2.8683 (18)	156
O7—H7*A*···O9^{i}	0.82	2.14	2.915 (2)	159
O7—H7*A*···O10^{i}	0.82	2.52	3.047 (3)	123
O8—H8*A*···O11^{v}	0.82	2.00	2.814 (2)	169
O9—H9*A*···O4^{vi}	0.82	1.93	2.747 (2)	172
O10—H10*A*···O12^{iii}	0.82	2.25	3.051 (2)	165
O11—H11*A*···O8^{iv}	0.82	2.41	2.976 (2)	127
O11—H11*A*···O9^{iv}	0.82	2.28	3.060 (2)	158

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