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ISSN 2414-3146

α-L-Glucose

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Received 21 August 2026
Accepted 26 August 2026

Edited by L. Van Meervelt, Katholieke Universiteit Leuven, Belgium

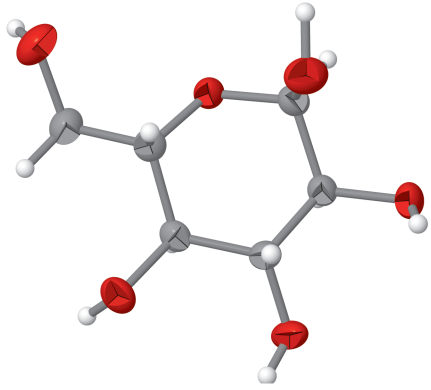
Keywords: crystal structure; hydrogen bonding; rare sugar; glucose; monosaccharide.

CCDC reference: 2577717

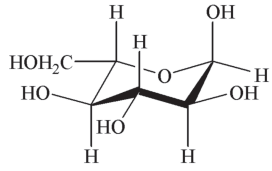
Structural data: full structural data are available from iucrdata.iucr.org

Commercially available L-glucose, $C_6H_{12}O_6$, was crystallized by slow evaporation from aqueous solution at room temperature affording colorless block-shaped single crystals suitable for single-crystal X-ray diffraction. The title compound crystallizes as α-L-glucose in the orthorhombic space group $P2_12_12_1$, with one molecule in the asymmetric unit and $Z = 4$. In the crystal, the molecules are linked by O—H···O hydrogen bonds, forming a three-dimensional hydrogen-bonded network. This study provides an experimentally determined structural dataset for the rare L enantiomer, which is not currently represented in the Cambridge Structural Database.

3D view



Chemical scheme



Structure description

Rare sugars are monosaccharides and derivatives that occur only in limited quantities in nature. The development of systematic bioproduction strategies has facilitated access to a wide range of rare hexoses (Izumori, 2002). L-Glucose is a rare sugar and the enantiomer of the naturally occurring D-glucose. The Cambridge Structural Database (CSD, version 6.00, update of August 2025; Groom *et al.*, 2016) contains several crystal structures of α-D-glucose, including the neutron-diffraction structures reported by Brown & Levy (1965, 1979; CSD refcodes GLUCSA and GLUCSA10, respectively). In contrast, no experimentally determined crystal structure of α-L-glucose was identified in our CSD search. Although the L enantiomer is expected to be related to the D enantiomer by inversion, its direct experimental determination provides an enantiomer-specific dataset comprising atomic coordinates, molecular conformation and hydrogen-bond geometry. The present structure therefore fills a gap in the crystallographic record and contributes to the systematic accumulation of structural data for rare sugars.

The title compound crystallizes in the orthorhombic space group $P2_12_12_1$. The asymmetric unit contains one molecule of α-L-glucose in the pyranose form (Fig. 1). The pyranose ring adopts a $^1C_4$ chair conformation, with the anomeric hydroxy group at C1

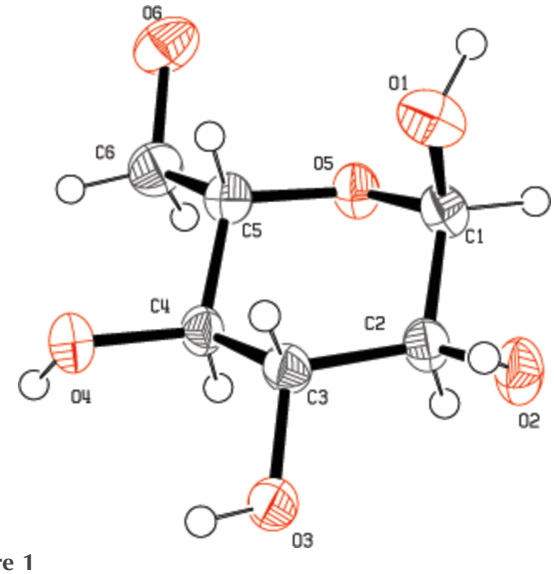


Figure 1
The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

occupying an axial position, while the hydroxy groups at C2, C3 and C4 and the hydroxymethyl group at C5 occupy equatorial positions. The Flack parameter of −0.29 (12) was not sufficiently precise to establish the absolute structure independently. The absolute configuration was therefore assigned on the basis of the known identity of the commercially available L-glucose used for crystallization. On this basis, the configurations of the stereogenic centres C1, C2, C3, C4 and C5 are *R*, *S*, *R*, *R* and *S*, respectively. The conformation of the hydroxymethyl group is characterized by an O5—C5—C6—O6 torsion angle of −70.7 (3)°. A least-squares

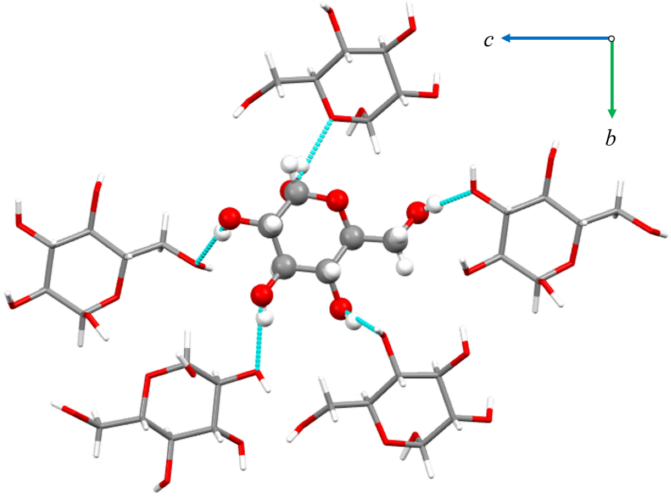


Figure 2
Crystal packing of the title compound viewed along the *a* axis (projection onto the *bc* plane), with the *b* and *c* unit-cell directions indicated. The central glucose molecule is shown using a ball-and-stick representation, whereas the surrounding molecules are shown using a capped-stick representation. The O1—H1···O5, O2—H2···O6, O3—H3···O2, O4—H4···O4 and O6—H6···O3 hydrogen bonds listed in Table 1 are shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5^{i}	0.95 (4)	1.91 (4)	2.836 (3)	163 (4)
O2—H2···O6^{ii}	0.90 (4)	1.87 (4)	2.760 (3)	166 (4)
O3—H3···O2^{iii}	0.83 (4)	1.89 (4)	2.698 (3)	165 (3)
O4—H4···O4^{iv}	0.85 (5)	1.93 (5)	2.7625 (17)	165 (5)
O6—H6···O3^{v}	0.84 (4)	1.86 (4)	2.704 (3)	175 (4)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (ii) $-x+\frac{3}{2}, -y+1, z+\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (v) $-x+\frac{1}{2}, -y+1, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_{12}O_6$
M_r	180.16
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, *b*, *c* (Å)	4.9536 (4), 10.3185 (7), 14.7798 (11)
V (Å^3)	755.45 (9)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	1.26
Crystal size (mm)	0.1 × 0.1 × 0.1
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min}, T_{max}	0.656, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8312, 1374, 1271
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.076, 1.06
No. of reflections	1374
No. of parameters	133
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.16
Absolute structure	Flack *x* determined using 457 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.29 (12)

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

fit of the 12 non-hydrogen atoms of the title molecule to those of the α-D-glucose structure reported by Brown & Levy (1965; CSD refcode GLUCSA) gave r.m.s. deviations of 0.910 Å and 0.013 Å without and with inversion, respectively. The very small r.m.s. deviation obtained after inversion indicates that there is no appreciable difference between the molecular conformations of the two enantiomers.

In the crystal, each hydroxy group acts as a donor in an O—H···O hydrogen bond (Table 1). Collectively, these interactions link the molecules into a three-dimensional hydrogen-bonded network, as shown in Fig. 2.

Synthesis and crystallization

Commercially available L-glucose (Sigma–Aldrich) was used as received without further purification. The sample was

dissolved in water, and the solution was allowed to evaporate slowly at room temperature. Colorless block-shaped single crystals suitable for single-crystal X-ray diffraction were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The Flack parameter was −0.29 (12), determined using 457 quotients (Parsons *et al.*, 2013), and did not permit a reliable determination of the absolute structure from the diffraction data alone. The absolute configuration was therefore assigned from the known identity of the commercially available L-glucose used for crystallization.

Acknowledgements

The authors thank Professor Genta Sakane (Okayama University of Science) for constructive discussions and technical guidance, and Kei Takeshita (FUSHIMI Pharmaceutical Co., Ltd.) for helpful advice. 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**, x260887 [https://doi.org/10.1107/S2414314626008874]

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α-*L*-Glucose

Crystal data

$C_6H_{12}O_6$
M_r = 180.16
Orthorhombic, $P2_12_12_1$
a = 4.9536 (4) Å
b = 10.3185 (7) Å
c = 14.7798 (11) Å
V = 755.45 (9) Å^3
Z = 4
F(000) = 384
D_x = 1.584 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 7806 reflections
θ = 3.0–68.4°
μ = 1.26 mm^{-1}
T = 296 K
Block, clear light colourless
0.1 × 0.1 × 0.1 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} = 0.656, T_{max} = 1.000
8312 measured reflections
1374 independent reflections
1271 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 68.1°, θ_{min} = 5.2°
h = −5→5
k = −12→12
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.076
S = 1.06
1374 reflections
133 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 0.2146P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack x determined using 457 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.29 (12)

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. All non-hydrogen atoms were refined anisotropically. The hydroxy H atoms H1, H2, H3, H4 and H6 and the C-bound H atom H1A were located in difference-Fourier maps and refined freely. The remaining C-bound H atoms were placed in calculated positions and refined using constrained models.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8530 (4)	0.3471 (2)	0.60082 (14)	0.0418 (6)
H1	0.918 (10)	0.273 (4)	0.570 (3)	0.087 (14)*
O2	0.5651 (5)	0.38741 (19)	0.75979 (12)	0.0377 (5)
H2	0.703 (9)	0.441 (4)	0.774 (3)	0.082 (15)*
O3	0.3351 (5)	0.6328 (2)	0.71548 (13)	0.0412 (6)
H3	0.371 (8)	0.711 (4)	0.713 (2)	0.063 (12)*
O4	0.4329 (5)	0.71765 (18)	0.53468 (13)	0.0344 (5)
H4	0.289 (9)	0.752 (5)	0.514 (3)	0.085 (16)*
O5	0.4615 (4)	0.36546 (16)	0.51522 (11)	0.0302 (5)
O6	0.5544 (5)	0.4462 (2)	0.33123 (14)	0.0454 (6)
H6	0.437 (8)	0.417 (4)	0.295 (2)	0.058 (12)*
C1	0.5752 (6)	0.3328 (3)	0.60101 (17)	0.0295 (6)
H1A	0.526 (4)	0.233 (2)	0.6127 (14)	0.003 (5)*
C2	0.4535 (6)	0.4187 (2)	0.67401 (16)	0.0287 (6)
H2A	0.259784	0.399836	0.676647	0.034*
C3	0.4844 (6)	0.5609 (2)	0.65125 (16)	0.0282 (7)
H3A	0.675258	0.585394	0.654612	0.034*
C4	0.3795 (6)	0.5855 (2)	0.55691 (17)	0.0266 (6)
H4A	0.183949	0.571024	0.556111	0.032*
C5	0.5113 (6)	0.4965 (2)	0.48833 (16)	0.0282 (6)
H5	0.706301	0.512517	0.487074	0.034*
C6	0.3971 (7)	0.5145 (3)	0.39572 (18)	0.0376 (7)
H6A	0.212706	0.482996	0.394260	0.045*
H6B	0.395072	0.606009	0.380678	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0390 (14)	0.0445 (13)	0.0418 (12)	0.0081 (11)	−0.0048 (10)	−0.0091 (10)
O2	0.0585 (15)	0.0289 (11)	0.0258 (9)	0.0000 (11)	−0.0055 (10)	0.0038 (8)
O3	0.0674 (17)	0.0233 (11)	0.0329 (10)	0.0009 (10)	0.0165 (10)	−0.0026 (8)
O4	0.0400 (13)	0.0247 (10)	0.0385 (11)	−0.0014 (10)	−0.0010 (10)	0.0050 (8)
O5	0.0402 (12)	0.0248 (10)	0.0257 (9)	−0.0023 (9)	−0.0051 (8)	−0.0018 (7)
O6	0.0519 (15)	0.0552 (14)	0.0291 (11)	−0.0086 (13)	0.0052 (11)	−0.0083 (10)
C1	0.0334 (17)	0.0258 (14)	0.0292 (13)	0.0034 (13)	−0.0048 (12)	−0.0006 (11)
C2	0.0356 (17)	0.0241 (14)	0.0264 (13)	0.0001 (13)	−0.0021 (12)	0.0009 (10)
C3	0.0358 (18)	0.0232 (13)	0.0257 (13)	0.0009 (12)	0.0012 (11)	−0.0028 (10)
C4	0.0273 (16)	0.0217 (13)	0.0306 (14)	−0.0023 (11)	0.0008 (11)	0.0028 (10)
C5	0.0288 (17)	0.0274 (14)	0.0285 (13)	−0.0025 (11)	−0.0024 (11)	−0.0008 (10)
C6	0.0444 (19)	0.0399 (17)	0.0284 (14)	0.0009 (15)	−0.0005 (13)	−0.0009 (12)

Geometric parameters (Å, º)

O1—H1	0.95 (4)	C1—H1A	1.07 (2)
O1—C1	1.384 (4)	C1—C2	1.521 (4)

O2—H2	0.90 (4)	C2—H2A	0.9800
O2—C2	1.420 (3)	C2—C3	1.513 (4)
O3—H3	0.83 (4)	C3—H3A	0.9800
O3—C3	1.413 (3)	C3—C4	1.509 (3)
O4—H4	0.85 (5)	C4—H4A	0.9800
O4—C4	1.428 (3)	C4—C5	1.516 (3)
O5—C1	1.428 (3)	C5—H5	0.9800
O5—C5	1.430 (3)	C5—C6	1.493 (3)
O6—H6	0.84 (4)	C6—H6A	0.9700
O6—C6	1.419 (4)	C6—H6B	0.9700

C1—O1—H1	105 (3)	C2—C3—H3A	109.6
C2—O2—H2	111 (3)	C4—C3—C2	109.5 (2)
C3—O3—H3	111 (3)	C4—C3—H3A	109.6
C4—O4—H4	109 (3)	O4—C4—C3	108.0 (2)
C1—O5—C5	113.68 (19)	O4—C4—H4A	109.0
C6—O6—H6	103 (3)	O4—C4—C5	110.2 (2)
O1—C1—O5	111.4 (2)	C3—C4—H4A	109.0
O1—C1—H1A	109.2 (12)	C3—C4—C5	111.6 (2)
O1—C1—C2	109.5 (2)	C5—C4—H4A	109.0
O5—C1—H1A	106.2 (11)	O5—C5—C4	108.2 (2)
O5—C1—C2	109.7 (2)	O5—C5—H5	109.6
C2—C1—H1A	110.8 (12)	O5—C5—C6	107.9 (2)
O2—C2—C1	110.3 (2)	C4—C5—H5	109.6
O2—C2—H2A	107.5	C6—C5—C4	112.0 (2)
O2—C2—C3	112.3 (2)	C6—C5—H5	109.6
C1—C2—H2A	107.5	O6—C6—C5	110.2 (3)
C3—C2—C1	111.6 (2)	O6—C6—H6A	109.6
C3—C2—H2A	107.5	O6—C6—H6B	109.6
O3—C3—C2	107.9 (2)	C5—C6—H6A	109.6
O3—C3—H3A	109.6	C5—C6—H6B	109.6
O3—C3—C4	110.6 (2)	H6A—C6—H6B	108.1

O1—C1—C2—O2	−57.4 (3)	C1—O5—C5—C4	−62.1 (3)
O1—C1—C2—C3	68.1 (3)	C1—O5—C5—C6	176.5 (2)
O2—C2—C3—O3	−63.5 (3)	C1—C2—C3—O3	172.1 (2)
O2—C2—C3—C4	176.1 (2)	C1—C2—C3—C4	51.7 (3)
O3—C3—C4—O4	66.2 (3)	C2—C3—C4—O4	−175.0 (2)
O3—C3—C4—C5	−172.5 (2)	C2—C3—C4—C5	−53.8 (3)
O4—C4—C5—O5	177.8 (2)	C3—C4—C5—O5	57.8 (3)
O4—C4—C5—C6	−63.4 (3)	C3—C4—C5—C6	176.6 (2)
O5—C1—C2—O2	−179.9 (2)	C4—C5—C6—O6	170.3 (2)
O5—C1—C2—C3	−54.4 (3)	C5—O5—C1—O1	−60.5 (3)
O5—C5—C6—O6	−70.7 (3)	C5—O5—C1—C2	60.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5^{i}	0.95 (4)	1.91 (4)	2.836 (3)	163 (4)
O2—H2···O6^{ii}	0.90 (4)	1.87 (4)	2.760 (3)	166 (4)
O3—H3···O2^{iii}	0.83 (4)	1.89 (4)	2.698 (3)	165 (3)
O4—H4···O4^{iv}	0.85 (5)	1.93 (5)	2.7625 (17)	165 (5)
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