

Arnaud Bonnet,^a William Jones^a
 and W. D. Samuel Motherwell^{b*}
^aThe Pfizer Institute for Pharmaceutical Materials Science, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England, and ^bThe Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England

 Correspondence e-mail:
 motherwell@ccdc.cam.ac.uk

Key indicators

 Single-crystal X-ray study
 $T = 180$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.036
 wR factor = 0.102
 Data-to-parameter ratio = 12.5

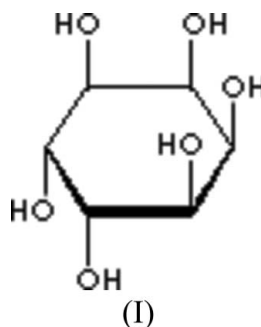
 For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

allo-Inositol

In the crystal structure of the title compound, $\text{C}_6\text{H}_{12}\text{O}_6$, molecules adopt a chair conformation. The H atoms were located and their positions refined satisfactorily. The molecules form one intramolecular and 12 intermolecular hydrogen bonds; all hydroxyl groups act as hydrogen-bond donors and acceptors.

Comment

Inositols are isomers of pyranose sugars ($\text{C}_6\text{H}_{12}\text{O}_6$), and are present in nature and in biological systems (Podeschwa *et al.*, 2003). We have reported elsewhere on the hydrogen bonds in crystal structures of some cyclohexanol derivatives (Bonnet *et al.*, 2005), and a study of the Cambridge Structural Database (Version 5.27; Allen, 2002) reveals that the crystal structures of only five of the nine isomeric inositols have been reported. Here we report the crystal structure of *allo*-inositol (Fig. 1). Fig. 2 provides a view along the a axis, showing each molecule linked to eight neighbouring molecules by hydrogen bonds.


Experimental

allo-Inositol (97%) was obtained from Sigma–Aldrich UK as a crystalline powder, and its purity was confirmed by solution NMR and elemental analysis. Suitable single crystals were obtained by vapour diffusion of acetone into an aqueous solution of the inositol, after a week at room temperature. Elemental analysis gave C 40.10, H 6.66, O 53.24%; expected: C 40.00, H 6.71, O 53.28%. The onset melting temperature was determined using differential scanning calorimetry, and gave a value of 454 K with reproducibility [literature: 583 K, with decomposition (Tschamber *et al.*, 1992)].

Crystal data

$\text{C}_6\text{H}_{12}\text{O}_6$	$Z = 4$
$M_r = 180.16$	$D_x = 1.678$ Mg m ⁻³
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 4.9520$ (2) Å	$\mu = 0.15$ mm ⁻¹
$b = 11.3145$ (6) Å	$T = 180$ (2) K
$c = 12.7326$ (6) Å	Block, colourless
$\beta = 91.142$ (3)°	$0.23 \times 0.18 \times 0.18$ mm
$V = 713.26$ (6) Å ³	

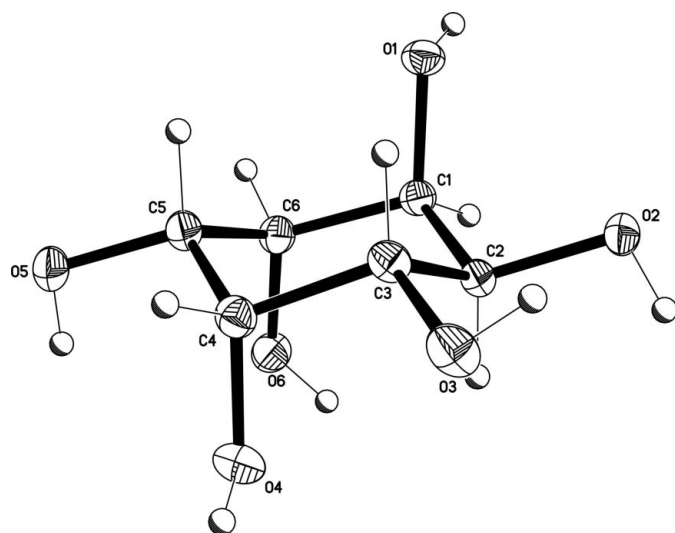


Figure 1
The molecular structure of *allo*-inositol. Displacement ellipsoids are drawn at the 50% probability level.

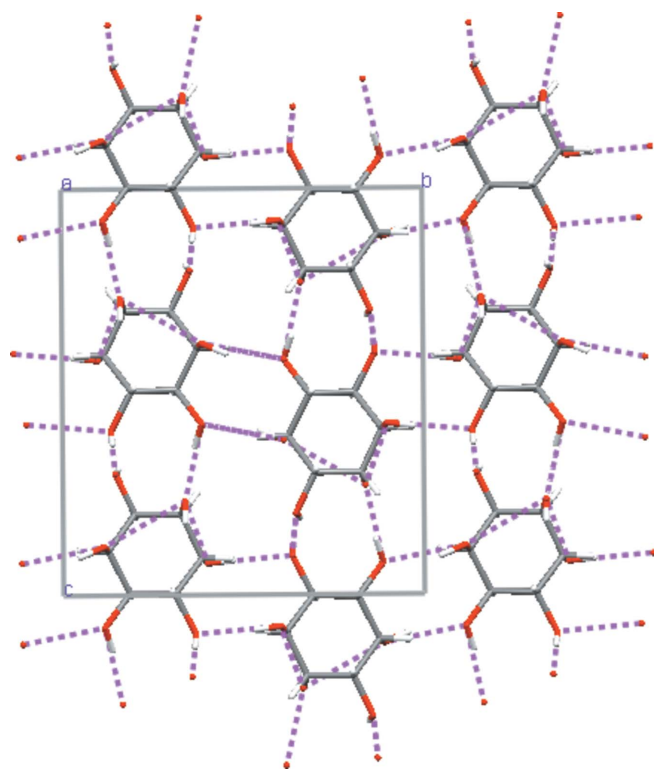


Figure 2
Packing diagram for *allo*-inositol, viewed along the *a* axis. The dashed lines show O...O contacts for hydrogen bonds.

Data collection

Nonius KappaCCD diffractometer	5743 measured reflections
thin-slice ω and φ scans	1627 independent reflections
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	1387 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.896$, $T_{\max} = 0.975$	$R_{\text{int}} = 0.038$
	$\theta_{\text{max}} = 27.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.102$
 $S = 1.06$
 1627 reflections
 130 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.2778P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.004$
 $\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.46 \text{ e } \text{Å}^{-3}$

Table 1

Hydrogen-bond geometry (Å , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2 ⁱ	0.82 (2)	1.95 (2)	2.7695 (14)	174 (2)
O2—H2 \cdots O5 ⁱⁱ	0.82 (2)	1.91 (2)	2.7289 (14)	179 (2)
O3—H3 \cdots O6 ⁱⁱⁱ	0.85 (2)	1.90 (2)	2.7423 (13)	171 (2)
O4—H4 \cdots O3 ^{iv}	0.84 (2)	1.93 (2)	2.7461 (14)	164 (2)
O5—H5 \cdots O2 ^v	0.86 (2)	2.12 (2)	2.9014 (14)	152 (2)
O6—H6 \cdots O1 ^{vi}	0.82 (2)	2.05 (2)	2.8248 (13)	158 (2)

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

The O-bound H atoms were all located in a difference map and refined with a common isotropic displacement parameter [$0.041(2) \text{ Å}^2$]; O—H distances were restrained to a target value of $0.83(1) \text{ Å}$. The C-bound H atoms were placed in calculated positions, with C—H = 1.00 Å , and refined as riding with a common isotropic displacement parameter [$0.016(2) \text{ Å}^2$].

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Version 1.4; Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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supporting information

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***allo*-Inositol**

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hexahydroxycyclohexane*Crystal data*

$C_6H_{12}O_6$

$M_r = 180.16$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 4.9520$ (2) Å

$b = 11.3145$ (6) Å

$c = 12.7326$ (6) Å

$\beta = 91.142$ (3)°

$V = 713.26$ (6) Å³

$Z = 4$

$F(000) = 384$

$D_x = 1.678$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 8271 reflections

$\theta = 1.0$ – 27.5 °

$\mu = 0.15$ mm⁻¹

$T = 180$ K

Block, colourless

$0.23 \times 0.18 \times 0.18$ mm

Data collection

Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed tube
thin-slice ω and φ scans

Absorption correction: multi-scan
(SORTAV; Blessing, 1995)

$T_{\min} = 0.896$, $T_{\max} = 0.975$

5743 measured reflections

1627 independent reflections

1387 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 27.4$ °, $\theta_{\min} = 3.6$ °

$h = -6 \rightarrow 6$

$k = -14 \rightarrow 14$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.102$

$S = 1.06$

1627 reflections

130 parameters

6 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.2778P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.004$

$\Delta\rho_{\max} = 0.31$ e Å⁻³

$\Delta\rho_{\min} = -0.46$ e Å⁻³

Special details

Experimental. The –OH hydrogen atoms were all located and their positions were refined satisfactorily.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.58505 (18)	0.10025 (9)	0.42187 (7)	0.0175 (2)
H1	0.622 (4)	0.0302 (16)	0.4147 (15)	0.041 (2)*
C1	0.2986 (3)	0.11545 (11)	0.40831 (10)	0.0144 (3)
H1A	0.2090	0.0363	0.4105	0.0158 (15)*
O2	0.2568 (2)	0.13354 (8)	0.59619 (7)	0.0167 (2)
H2	0.112 (4)	0.1375 (18)	0.6268 (16)	0.041 (2)*
C2	0.1944 (2)	0.19153 (11)	0.49771 (9)	0.0137 (3)
H2A	-0.0064	0.1981	0.4898	0.0158 (15)*
O3	0.2171 (2)	0.38616 (8)	0.57924 (7)	0.0204 (3)
H3	0.306 (4)	0.3661 (18)	0.6344 (15)	0.041 (2)*
C3	0.3147 (3)	0.31563 (11)	0.49478 (9)	0.0148 (3)
H3A	0.5160	0.3103	0.5003	0.0158 (15)*
O4	-0.05263 (19)	0.38676 (9)	0.38074 (8)	0.0201 (2)
H4	-0.100 (4)	0.4524 (16)	0.4050 (16)	0.041 (2)*
C4	0.2332 (3)	0.37526 (12)	0.39100 (10)	0.0160 (3)
H4A	0.3170	0.4556	0.3885	0.0158 (15)*
O5	0.2820 (2)	0.35459 (9)	0.20083 (7)	0.0207 (2)
H5	0.113 (4)	0.3447 (17)	0.1893 (16)	0.041 (2)*
C5	0.3387 (3)	0.30110 (12)	0.30029 (10)	0.0165 (3)
H5A	0.5398	0.2990	0.3089	0.0158 (15)*
O6	-0.03399 (19)	0.16142 (9)	0.26888 (7)	0.0193 (2)
H6	-0.133 (4)	0.1621 (17)	0.3195 (15)	0.041 (2)*
C6	0.2426 (3)	0.17232 (12)	0.30083 (9)	0.0159 (3)
H6A	0.3520	0.1284	0.2484	0.0158 (15)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0142 (5)	0.0162 (5)	0.0222 (5)	0.0024 (4)	0.0009 (4)	0.0007 (4)
C1	0.0140 (6)	0.0132 (6)	0.0159 (6)	0.0000 (5)	0.0007 (5)	0.0002 (4)
O2	0.0184 (5)	0.0189 (5)	0.0128 (4)	0.0022 (4)	0.0018 (3)	0.0023 (3)
C2	0.0139 (6)	0.0142 (6)	0.0130 (6)	0.0005 (5)	-0.0006 (4)	0.0014 (4)
O3	0.0267 (5)	0.0172 (5)	0.0173 (5)	0.0065 (4)	-0.0020 (4)	-0.0041 (4)
C3	0.0164 (6)	0.0126 (6)	0.0154 (6)	0.0015 (5)	-0.0008 (5)	-0.0017 (4)
O4	0.0164 (5)	0.0182 (5)	0.0255 (5)	0.0033 (4)	-0.0027 (4)	-0.0015 (4)
C4	0.0155 (6)	0.0140 (6)	0.0185 (6)	-0.0011 (5)	-0.0009 (5)	0.0016 (5)
O5	0.0198 (5)	0.0247 (6)	0.0176 (5)	-0.0008 (4)	0.0006 (4)	0.0073 (4)
C5	0.0155 (6)	0.0181 (7)	0.0158 (6)	-0.0004 (5)	-0.0004 (5)	0.0037 (5)
O6	0.0167 (5)	0.0248 (5)	0.0162 (5)	-0.0019 (4)	-0.0008 (3)	0.0001 (4)
C6	0.0165 (6)	0.0179 (7)	0.0134 (6)	0.0004 (5)	0.0006 (5)	0.0001 (5)

Geometric parameters (Å, °)

O1—C1	1.4357 (15)	C3—H3A	1.0000
O1—H1	0.819 (17)	O4—C4	1.4248 (15)
C1—C2	1.5253 (17)	O4—H4	0.839 (17)
C1—C6	1.5325 (17)	C4—C5	1.5281 (18)
C1—H1A	1.0000	C4—H4A	1.0000
O2—C2	1.4432 (15)	O5—C5	1.4265 (15)
O2—H2	0.823 (18)	O5—H5	0.855 (18)
C2—C3	1.5259 (18)	C5—C6	1.5329 (18)
C2—H2A	1.0000	C5—H5A	1.0000
O3—C3	1.4309 (15)	O6—C6	1.4263 (16)
O3—H3	0.853 (18)	O6—H6	0.817 (17)
C3—C4	1.5305 (17)	C6—H6A	1.0000
C1—O1—H1	108.9 (15)	C4—O4—H4	109.2 (15)
O1—C1—C2	109.03 (10)	O4—C4—C5	109.56 (10)
O1—C1—C6	108.58 (10)	O4—C4—C3	111.33 (10)
C2—C1—C6	111.81 (10)	C5—C4—C3	108.80 (10)
O1—C1—H1A	109.1	O4—C4—H4A	109.0
C2—C1—H1A	109.1	C5—C4—H4A	109.0
C6—C1—H1A	109.1	C3—C4—H4A	109.0
C2—O2—H2	102.3 (15)	C5—O5—H5	105.8 (14)
O2—C2—C1	108.79 (10)	O5—C5—C4	111.95 (10)
O2—C2—C3	111.26 (10)	O5—C5—C6	110.59 (10)
C1—C2—C3	111.28 (10)	C4—C5—C6	114.06 (10)
O2—C2—H2A	108.5	O5—C5—H5A	106.6
C1—C2—H2A	108.5	C4—C5—H5A	106.6
C3—C2—H2A	108.5	C6—C5—H5A	106.6
C3—O3—H3	107.1 (14)	C6—O6—H6	111.2 (15)
O3—C3—C2	110.92 (10)	O6—C6—C1	111.98 (10)
O3—C3—C4	108.41 (10)	O6—C6—C5	112.17 (10)
C2—C3—C4	109.30 (10)	C1—C6—C5	110.63 (10)
O3—C3—H3A	109.4	O6—C6—H6A	107.3
C2—C3—H3A	109.4	C1—C6—H6A	107.3
C4—C3—H3A	109.4	C5—C6—H6A	107.3
O1—C1—C2—O2	-59.22 (12)	O4—C4—C5—O5	61.06 (13)
C6—C1—C2—O2	-179.29 (10)	C3—C4—C5—O5	-177.02 (10)
O1—C1—C2—C3	63.71 (13)	O4—C4—C5—C6	-65.47 (13)
C6—C1—C2—C3	-56.37 (14)	C3—C4—C5—C6	56.45 (14)
O2—C2—C3—O3	-58.16 (13)	O1—C1—C6—O6	164.10 (10)
C1—C2—C3—O3	-179.65 (10)	C2—C1—C6—O6	-75.56 (13)
O2—C2—C3—C4	-177.64 (10)	O1—C1—C6—C5	-69.97 (12)
C1—C2—C3—C4	60.87 (13)	C2—C1—C6—C5	50.37 (14)
O3—C3—C4—O4	-59.66 (13)	O5—C5—C6—O6	-53.13 (13)
C2—C3—C4—O4	61.36 (13)	C4—C5—C6—O6	74.11 (13)
O3—C3—C4—C5	179.51 (10)	O5—C5—C6—C1	-178.95 (10)

C2—C3—C4—C5 -59.48 (13) C4—C5—C6—C1 -51.71 (14)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots O2 ⁱ	0.82 (2)	1.95 (2)	2.7695 (14)	174 (2)
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