Table 4 (*cont.*)

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8	3	-2	128	131
8	3	-3	323	311
8	3	3	53	47
8	3	-4	192	177
8	3	4	34	19
8	3	-5	106	138
8	3	5	108	107
8	3	6	43	41
8	3	-6	76	75
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8	3	-7	82	84
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8	6	3	87	82
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8	6	-5	96	107
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8	6	-7	43	43
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8	7	-2	107	111
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8	8	1	143	173
8	8	-1	29	28
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8	9	-4	24	34
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8	10	3	47	68
8	10	-3	22	24
8	10	-4	36	54
8	11	0	60	61
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8	11	-1	62	67
8	11	-2	45	56
8	11	-3	22	9
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9	0	-2	66	88
9	0	-3	485	450
9	0	3	97	84
9	0	-4	43	46
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9	0	5	143	146
9	0	-5	111	123
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9	0	6	8	10
9	0	-7	42	49
9	0	-8	76	61
9	1	0	29	17
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9	6	-6	19	35
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10	0	-4	87	78
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10	0	-7	43	44
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10	4	-5	89	93
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10	8	-4	74	63
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10	9	2	45	66
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11	0	-3	115	102
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14	4	-3	53	61
14	5	-1	26	25
15	0	-1	67	62
15	0	-2	15	11
15	1	-1	30	17

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The Refinement of the Crystal Structures of β-D-Glucose and Cellobiose

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The structures of β-D-glucose and cellobiose have been refined anisotropically from new data obtained at room temperature with Cu Kα radiation on an automatic diffractometer. The earlier results are confirmed except for small changes in bond distances and bond angles. In both structures, the equatorial glycosidic C(1)–O(1) bonds are significantly short.

The crystal structure of β-D-glucose was determined by Ferrier (1963) and that of cellobiose by Jacobson, Wunderlich & Lipscomb (1961) and by Brown (1966). These structures have now been refined from new experimental data obtained on a Picker four-angle automatic diffractometer. The primary purpose of this refinement was to obtain bond distances with an accuracy comparable to those from other recent structure determinations of pyranose sugars (Berman, Chu & Jeffrey, 1967). The cell parameters, remeasured on the

diffractometer, are given in Table 1. The corresponding calculated densities are in good agreement with the observed values previously reported.
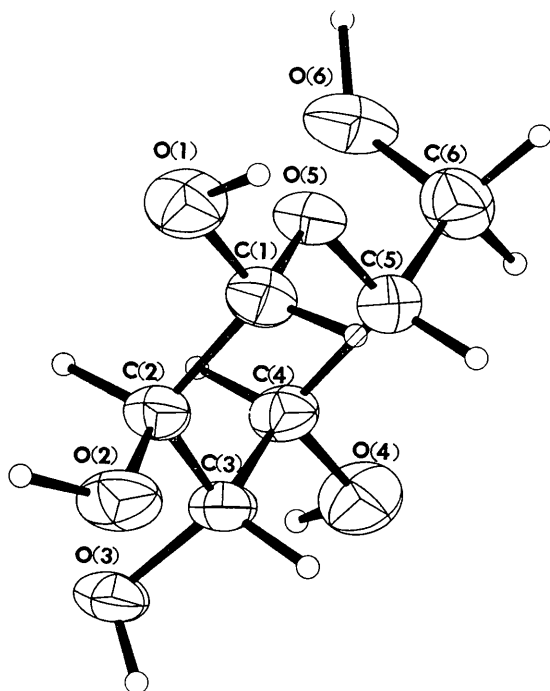

Fig. 1. The structure of one asymmetric unit of β-D-glucose viewed down the c axis. The diagram is produced by ORTEP (Johnson, 1965).

Table 1. *Crystallographic data*

Space group	β-D-Glucose $P2_12_12_1$	Cellobiose $P2_1$
a	$9{\cdot}205 \pm 0{\cdot}004$ Å	$10{\cdot}972 \pm 0{\cdot}004$ Å
b	$12{\cdot}640 \pm 0{\cdot}005$	$13{\cdot}048 \pm 0{\cdot}005$
c	$6{\cdot}654 \pm 0{\cdot}003$	$5{\cdot}091 \pm 0{\cdot}003$
β		$90{\cdot}83 \pm 0{\cdot}05°$
D_x	$1{\cdot}545$ g.cm^{-3}	$1{\cdot}560$ g.cm^{-3}

For β-D-glucose, 775 independent reflections with 2θ values below 130° were measured, of which 716 reflections had intensities significantly above the background. For cellobiose, 1239 of the 1257 independent reflections measured were significantly above background. In both cases, the intensity data were collected in two different quadrants of the reciprocal lattice and the arithmetic mean values were used.

The refinements were by the full-matrix least-squares IBM 7090 program (Busing, Martin & Levy, 1962; Shiono, 1966) starting with the positional and thermal parameters of the carbon and oxygen atoms in β-D-glucose given by Ferrier (1963) and those of cellobiose given by Brown (1966). Cruickshank's (1961) weighting scheme was used in the refinement, except that zero weights were assigned to unobserved reflections. The atomic scattering factors used were those of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955). After two cycles of anisotropic refinement, the R values were reduced to $0{\cdot}073$ and $0{\cdot}067$ for β-D-glucose and cellobiose, respectively. All the hydrogen atoms were clearly revealed in difference Fourier syntheses, at reasonable positions with respect to the car-

Table 2. *Fractional atomic coordinates and thermal parameters for β-D-glucose*

The estimated standard deviations are given in parentheses and refer to the last decimal positions of respective values. The expression for the temperature factor exponent consistent with the β-values is:
$$-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl).$$

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)	$-0{\cdot}0611$ (3)	$0{\cdot}2279$ (2)	$0{\cdot}5825$ (4)	$0{\cdot}0147$ (3)	$0{\cdot}0055$ (2)	$0{\cdot}0203$ (6)	$0{\cdot}0001$ (2)	$0{\cdot}0017$ (4)	$-0{\cdot}0037$ (3)
O(2)	$-0{\cdot}1119$ (3)	$0{\cdot}0060$ (2)	$0{\cdot}5587$ (4)	$0{\cdot}0155$ (4)	$0{\cdot}0042$ (1)	$0{\cdot}0235$ (6)	$0{\cdot}0002$ (2)	$0{\cdot}0051$ (4)	$0{\cdot}0031$ (3)
O(3)	$-0{\cdot}1147$ (3)	$-0{\cdot}0647$ (2)	$0{\cdot}1445$ (4)	$0{\cdot}0120$ (3)	$0{\cdot}0028$ (1)	$0{\cdot}0314$ (7)	$-0{\cdot}0007$ (2)	$-0{\cdot}0037$ (4)	$-0{\cdot}0010$ (3)
O(4)	$0{\cdot}1297$ (3)	$0{\cdot}0173$ (2)	$-0{\cdot}0825$ (4)	$0{\cdot}0146$ (4)	$0{\cdot}0060$ (2)	$0{\cdot}0264$ (7)	$0{\cdot}0009$ (2)	$0{\cdot}0060$ (4)	$-0{\cdot}0045$ (3)
O(5)	$0{\cdot}0636$ (3)	$0{\cdot}2220$ (1)	$0{\cdot}2893$ (3)	$0{\cdot}0113$ (3)	$0{\cdot}0032$ (1)	$0{\cdot}0165$ (5)	$-0{\cdot}0005$ (2)	$0{\cdot}0013$ (3)	$-0{\cdot}0000$ (2)
O(6)	$0{\cdot}0992$ (3)	$0{\cdot}2936$ (2)	$-0{\cdot}1079$ (4)	$0{\cdot}0188$ (4)	$0{\cdot}0040$ (1)	$0{\cdot}0192$ (6)	$-0{\cdot}0013$ (2)	$-0{\cdot}0029$ (4)	$0{\cdot}0010$ (3)
C(1)	$0{\cdot}0198$ (4)	$0{\cdot}1614$ (2)	$0{\cdot}4610$ (5)	$0{\cdot}0109$ (4)	$0{\cdot}0040$ (2)	$0{\cdot}0166$ (7)	$-0{\cdot}0006$ (2)	$-0{\cdot}0001$ (5)	$0{\cdot}0008$ (3)
C(2)	$-0{\cdot}0786$ (4)	$0{\cdot}0717$ (2)	$0{\cdot}3902$ (5)	$0{\cdot}0098$ (4)	$0{\cdot}0034$ (2)	$0{\cdot}0184$ (7)	$-0{\cdot}0002$ (2)	$0{\cdot}0000$ (5)	$0{\cdot}0010$ (3)
C(3)	$-0{\cdot}0081$ (4)	$0{\cdot}0059$ (2)	$0{\cdot}2259$ (5)	$0{\cdot}0097$ (4)	$0{\cdot}0028$ (1)	$0{\cdot}0217$ (8)	$0{\cdot}0001$ (2)	$-0{\cdot}0020$ (4)	$-0{\cdot}0003$ (3)
C(4)	$0{\cdot}0486$ (4)	$0{\cdot}0764$ (2)	$0{\cdot}0600$ (5)	$0{\cdot}0100$ (4)	$0{\cdot}0039$ (2)	$0{\cdot}0171$ (7)	$0{\cdot}0007$ (2)	$0{\cdot}0013$ (5)	$-0{\cdot}0015$ (3)
C(5)	$0{\cdot}1479$ (3)	$0{\cdot}1614$ (2)	$0{\cdot}1486$ (5)	$0{\cdot}0088$ (4)	$0{\cdot}0039$ (2)	$0{\cdot}0205$ (8)	$0{\cdot}0001$ (2)	$0{\cdot}0007$ (5)	$0{\cdot}0001$ (3)
C(6)	$0{\cdot}2099$ (4)	$0{\cdot}2385$ (3)	$-0{\cdot}0027$ (6)	$0{\cdot}0117$ (4)	$0{\cdot}0055$ (2)	$0{\cdot}0238$ (9)	$-0{\cdot}0011$ (3)	$0{\cdot}0041$ (6)	$0{\cdot}0010$ (4)
H(O1)	$0{\cdot}010$	$0{\cdot}252$	$0{\cdot}676$						
H(O2)	$-0{\cdot}212$	$0{\cdot}020$	$0{\cdot}622$						
H(O3)	$-0{\cdot}085$	$-0{\cdot}128$	$0{\cdot}188$						
H(O4)	$0{\cdot}067$	$-0{\cdot}002$	$-0{\cdot}196$						
H(O6)	$0{\cdot}085$	$0{\cdot}370$	$-0{\cdot}120$						
H(C1)	$0{\cdot}116$	$0{\cdot}137$	$0{\cdot}540$						
H(C2)	$-0{\cdot}175$	$0{\cdot}104$	$0{\cdot}337$						
H(C3)	$0{\cdot}081$	$-0{\cdot}035$	$0{\cdot}296$						
H(C4)	$-0{\cdot}041$	$0{\cdot}107$	$-0{\cdot}008$						
H(C5)	$0{\cdot}238$	$0{\cdot}125$	$0{\cdot}218$						
H(C6–1)	$0{\cdot}289$	$0{\cdot}292$	$0{\cdot}071$						
H(C6–2)	$0{\cdot}271$	$0{\cdot}196$	$-0{\cdot}109$						

bon and oxygen atoms. Two further cycles of least-squares refinement, including all the hydrogen atoms, gave final R values of 0·043 for β-D-glucose and 0·037 for cellobiose. The positional parameters of the hydrogen atoms were not refined and the hydrogens were assigned the same thermal parameters as the carbon or oxygen atoms to which they are bonded. The final positional and thermal parameters are given in Tables 2 and 3. The observed and calculated structure factors are given in Tables 4 and 5.

The identification of the atoms and the illustration of the thermal ellipsoids (Johnson, 1965) are shown in Figs. 1 and 2. The bond lengths and bond angles, with their standard deviations, are given in Tables 6 and 7. The mean C–C bond length is 1·520 Å ($\sigma=0·0018$), for β-D-glucose and 1·522 Å ($\sigma=0·0016$) for cellobiose.

The mean C–O bond lengths, excluding the ring oxygen and anomeric carbon atoms, are 1·425 ($\sigma=0·0021$) and 1·420 Å ($\sigma=0·0017$) for β-D-glucose and cellobiose, respectively. In both structures, the equatorial glycosidic C(1)–O(1) bonds are shortened by 5 to 10σ, which is in agreement with the observations made on other β-pyranosides (Chu & Jeffrey, 1967; Berman, Chu & Jeffrey, 1967). Apart from changes in individual bond distances and angles (up to 0·06 Å and 3° in cellobiose, and 0·02 Å and 2° in β-D-glucose), the structures are unchanged from those previously reported.

Table 3. *Fractional atomic coordinates and thermal parameters for cellobiose*

Estimated standard deviations and temperature factor expression are as in Table 2.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)	0·1955 (2)	0·0000	0·3013 (4)	0·0039 (2)	0·0025 (1)	0·0210 (8)	0·0006 (1)	−0·0025 (3)	0·0003 (3)
O(2)	0·1551 (2)	−0·2025 (2)	0·4254 (5)	0·0048 (2)	0·0041 (1)	0·0306 (10)	−0·0017 (1)	−0·0043 (3)	0·0021 (3)
O(3)	0·3456 (2)	−0·3075 (2)	0·7189 (5)	0·0054 (2)	0·0024 (1)	0·0316 (10)	−0·0001 (1)	−0·0005 (3)	0·0013 (3)
O(4)	0·4967 (2)	−0·1753 (2)	1·0343 (5)	0·0038 (2)	0·0044 (2)	0·0250 (9)	0·0001 (1)	−0·0025 (3)	0·0038 (3)
O(5)	0·3692 (2)	0·0049 (2)	0·5507 (4)	0·0041 (2)	0·0028 (1)	0·0250 (9)	−0·0005 (1)	−0·0031 (3)	0·0016 (3)
O(6)	0·5418 (3)	0·1338 (3)	0·7271 (5)	0·0087 (3)	0·0027 (1)	0·0309 (10)	−0·0010 (2)	−0·0028 (4)	−0·0011 (3)
C(1)	0·2517 (3)	−0·0409 (3)	0·5259 (6)	0·0032 (2)	0·0028 (2)	0·0213 (11)	0·0004 (2)	−0·0018 (4)	0·0003 (4)
C(2)	0·2684 (3)	−0·1560 (3)	0·4883 (6)	0·0039 (2)	0·0032 (2)	0·0185 (11)	−0·0003 (2)	−0·0014 (4)	−0·0001 (4)
C(3)	0·3292 (3)	−0·1992 (3)	0·7346 (6)	0·0035 (2)	0·0027 (2)	0·0231 (12)	0·0004 (2)	0·0004 (4)	0·0002 (4)
C(4)	0·4506 (3)	−0·1438 (3)	0·7852 (6)	0·0035 (2)	0·0031 (2)	0·0186 (11)	0·0002 (2)	−0·0013 (4)	0·0010 (3)
C(5)	0·4330 (3)	−0·0273 (3)	0·7848 (6)	0·0040 (2)	0·0028 (2)	0·0217 (12)	0·0001 (2)	−0·0028 (4)	−0·0002 (4)
C(6)	0·5550 (3)	0·0277 (3)	0·7793 (7)	0·0051 (3)	0·0034 (2)	0·0354 (15)	−0·0007 (2)	−0·0050 (5)	0·0008 (5)
O(1')	−0·0138 (2)	0·3603 (3)	−0·0007 (6)	0·0054 (2)	0·0037 (1)	0·0394 (11)	0·0007 (1)	−0·0024 (4)	0·0032 (3)
O(2')	0·2471 (2)	0·3360 (3)	−0·0377 (6)	0·0045 (2)	0·0046 (2)	0·0592 (15)	0·0002 (2)	0·0002 (4)	0·0089 (4)
O(3')	0·3425 (3)	0·1943 (3)	0·3122 (8)	0·0050 (2)	0·0055 (2)	0·1012 (24)	−0·0025 (2)	−0·0145 (6)	0·0140 (6)
O(5')	−0·0263 (2)	0·2036 (2)	0·1873 (5)	0·0034 (2)	0·0028 (1)	0·0310 (9)	0·0006 (1)	0·0006 (3)	0·0014 (3)
O(6')	−0·1830 (2)	0·0271 (3)	0·2428 (6)	0·0035 (2)	0·0037 (2)	0·0640 (15)	−0·0001 (1)	−0·0023 (4)	−0·0031 (4)
C(1')	0·0449 (3)	0·2670 (3)	0·0176 (7)	0·0040 (2)	0·0035 (2)	0·0319 (12)	0·0005 (2)	0·0002 (4)	0·0030 (4)
C(2')	0·1711 (3)	0·2807 (3)	0·1365 (7)	0·0042 (2)	0·0033 (2)	0·0348 (14)	−0·0002 (2)	−0·0024 (4)	0·0025 (4)
C(3')	0·2311 (3)	0·1769 (3)	0·1783 (8)	0·0035 (2)	0·0033 (2)	0·0410 (15)	−0·0003 (2)	−0·0023 (4)	0·0038 (4)
C(4')	0·1481 (3)	0·1029 (3)	0·3256 (6)	0·0037 (2)	0·0026 (2)	0·0249 (12)	0·0003 (2)	−0·0016 (4)	0·0004 (3)
C(5')	0·0188 (3)	0·1006 (3)	0·2101 (6)	0·0041 (2)	0·0025 (2)	0·0270 (12)	0·0007 (2)	−0·0011 (4)	−0·0011 (4)
C(6')	−0·0702 (3)	−0·0438 (3)	0·3772 (7)	0·0038 (3)	0·0034 (2)	0·0393 (15)	−0·0002 (2)	−0·0003 (5)	−0·0003 (4)
H(O2)	0·112	−0·214	0·593						
H(O3)	0·382	−0·312	0·564						
H(O4)	0·585	−0·195	1·028						
H(O6)	0·545	0·170	0·886						
H(C1)	0·205	−0·025	0·690						
H(C2)	0·320	−0·170	0·320						
H(C3)	0·270	−0·180	0·865						
H(C4)	0·510	−0·170	0·640						
H(C5)	0·385	0·005	0·942						
H(C6–1)	0·610	−0·002	0·640						
H(C6–2)	0·590	0·000	0·970						
H(O1')	−0·040	0·370	−0·185						
H(O2')	0·216	0·393	−0·115						
H(O3')	0·375	0·140	0·420						
H(O6')	−0·230	0·084	0·200						
H(C1')	0·055	0·245	−0·192						
H(C2')	0·165	0·318	0·315						
H(C3')	0·255	0·140	0·000						
H(C4')	0·140	0·120	0·515						
H(C5')	0·030	0·065	0·025						
H(C6'–1)	−0·028	0·080	0·540						
H(C6'–2)	−0·025	−0·020	0·440						

Table 4. *Observed and calculated structure factors for β-D-glucose*

The running index is k; other columns are $|F_{obs}|$, $|F_{calc}|$, A, B ($\times 10$).

Table 4 (cont.)

Fig. 2. The structure of one asymmetric unit of cellobiose viewed down the c axis. Dotted line is intramolecular hydrogen bond. The diagram is produced by ORTEP (Johnson, 1965).

Table 5. *Observed and calculated structure factors for cellobiose*

Columns are as in Table 4.

Table 5 (cont.)

Table 5 (cont.)

Table 6. *Bond lengths (including hydrogen bonds) and bond angles in β-D-glucose*

Estimated standard deviations in parentheses refer to the last decimal positions of respective values.

i	j	D(ij)	i	j	k	∠(ijk)
C(1)	C(2)	1·525 (4) Å	C(2)	C(1)	O(1)	108·2 (3)°
C(2)	C(3)	1·520 (4)	C(2)	C(1)	O(5)	108·5 (2)
C(3)	C(4)	1·511 (4)	O(1)	C(1)	O(5)	107·0 (2)
C(4)	C(5)	1·529 (4)	C(1)	C(2)	C(3)	112·1 (3)
C(5)	C(6)	1·513 (5)	C(1)	C(2)	O(2)	108·5 (3)
			C(3)	C(2)	O(2)	109·7 (3)
C(1)	O(1)	1·383 (4)	C(2)	C(3)	C(4)	110·5 (3)
C(2)	O(2)	1·429 (4)	C(2)	C(3)	O(3)	108·7 (3)
C(3)	O(3)	1·432 (4)	C(4)	C(3)	O(3)	109·1 (3)
C(4)	O(4)	1·419 (4)	C(3)	C(4)	C(5)	109·8 (3)
C(1)	O(5)	1·433 (4)	C(3)	C(4)	O(4)	111·1 (3)
C(5)	O(5)	1·437 (4)	C(5)	C(4)	O(4)	108·2 (3)
C(6)	O(6)	1·419 (5)	C(4)	C(5)	C(6)	115·0 (3)
			C(4)	C(5)	O(5)	107·6 (2)
O(1)	O(6)a	2·666	C(6)	C(5)	O(5)	107·1 (3)
O(2)	O(3)b	2·686	C(5)	C(6)	O(6)	111·9 (3)
O(2)	O(6)c	2·708				
O(3)	O(5)c	2·772	C(1)	O(5)	C(5)	112·7 (2)

Symmetry code

	x	y	z
−	x	y	z
a	x	y	1 + z
b	−½ − x	−y	½ + z
c	−x	−½ + y	½ − z

Table 7. *Bond lengths (including hydrogen bonds) and bond angles in cellobiose*

Estimated standard deviations in parentheses refer to the last decimal positions of respective values.

i	j	D(ij)	i	j	k	∠(ijk)
C(1)	C(2)	1·525 (5) Å	C(2)	C(1)	O(1)	109·0 (3)*
C(2)	C(3)	1·520 (5)	C(2)	C(1)	O(5)	108·3 (3)
C(3)	C(4)	1·543 (5)	O(1)	C(1)	O(5)	107·4 (2)
C(4)	C(5)	1·532 (5)	C(1)	C(2)	C(3)	108·3 (3)
C(5)	C(6)	1·519 (5)	C(1)	C(2)	O(2)	110·0 (3)
			C(3)	C(2)	O(2)	113·6 (3)
C(1)	O(1)	1·397 (4)	C(2)	C(3)	C(4)	109·5 (3)
C(2)	O(2)	1·416 (4)	C(2)	C(3)	O(3)	112·0 (3)
C(3)	O(3)	1·427 (4)	C(4)	C(3)	O(3)	111·5 (3)
C(4)	O(4)	1·420 (4)	C(3)	C(4)	C(5)	111·0 (3)
C(1)	O(5)	1·425 (4)	C(3)	C(4)	O(4)	108·1 (2)
C(5)	O(5)	1·436 (4)	C(5)	C(4)	O(4)	109·4 (2)
C(6)	O(6)	1·416 (5)	C(4)	C(5)	C(6)	111·0 (3)
			C(4)	C(5)	O(5)	110·5 (3)
C(1')	C(2')	1·514 (5)	C(6)	C(5)	O(5)	105·4 (3)
C(2')	C(3')	1·519 (5)	C(5)	C(6)	O(6)	112·2 (3)
C(3')	C(4')	1·530 (5)				
C(4')	C(5')	1·527 (5)	C(2')	C(1')	O(1')	110·2 (3)
C(5')	C(6')	1·501 (5)	C(2')	C(1')	O(5')	109·3 (3)
			O(1')	C(1')	O(5')	107·0 (3)
C(1')	O(1')	1·381 (5)	C(1')	C(2')	C(3')	110·0 (3)
C(2')	O(2')	1·423 (5)	C(1')	C(2')	O(2')	110·6 (3)
C(3')	O(3')	1·410 (5)	C(3')	C(2')	O(2')	106·5 (3)
C(4')	O(1)	1·446 (4)	C(2')	C(3')	C(4')	111·8 (3)
C(1')	O(5')	1·435 (4)	C(2')	C(3')	O(3')	107·1 (3)
C(5')	O(5')	1·437 (4)	C(4')	C(3')	O(3)'	112·5 (3)
C(6')	O(6')	1·423 (5)	C(3')	C(4')	C(5')	112·3 (3)
			C(3')	C(4')	O(1)	109·0 (3)
O(2)	O(1')a	2·766	C(5')	C(4')	O(1)	106·4 (3)
O(2)	O(5')b	2·733	C(4')	C(5')	C(6')	113·6 (3)
O(3)	O(6)c	2·711	C(4')	C(5')	O(5')	109·2 (3)
O(3)	O(6')b	2·808	C(6')	C(5')	O(5')	106·4 (3)
O(4)	O(6)c	2·807	C(5')	C(6')	O(6')	111·8 (3)
O(4)	O(2')d	2·814				
O(5)	O(3')	2·767	C(1)	O(5)	C(5)	112·4 (2)
O(2')	O(6')e	2·789	C(1)	O(1)	C(4')	116·1 (2)
			C(1')	O(5')	C(5')	113·5 (3)

Symmetry code

	x	y	z
–	x	y	z
a	−x	−½+y	−z
b	−x	−½+y	1−z
c	1−x	−½+y	1−z
d	1−x	−½+y	−z
e	−x	½+y	−z

for providing the crystals of β-D-glucose and Dr R. Rosenstein of this laboratory for making the crystals of cellobiose.

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