

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

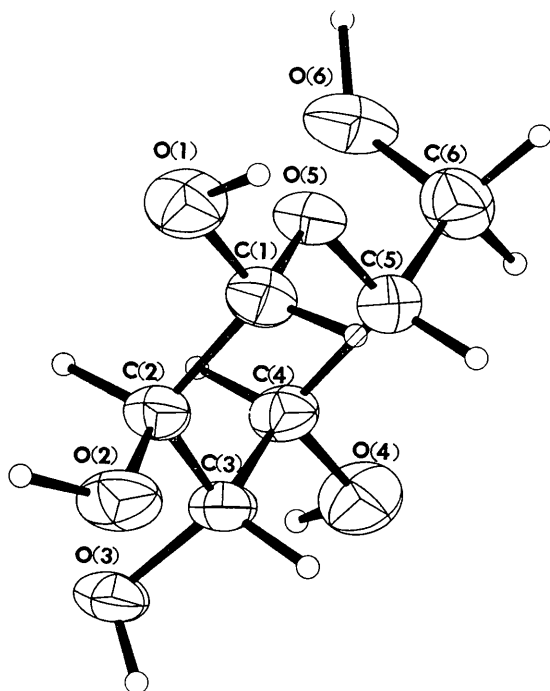


Fig. 1. The structure of one asymmetric unit of β -D-glucose viewed down the c axis. The diagram is produced by ORTEP (Johnson, 1965).

Table 1. Crystallographic data

Space group	β -D-Glucose $P2_12_12_1$	Cellobiose $P2_1$
a	$9.205 \pm 0.004 \text{ \AA}$	$10.972 \pm 0.004 \text{ \AA}$
b	12.640 ± 0.005	13.048 ± 0.005
c	6.654 ± 0.003	5.091 ± 0.003
β		$90.83 \pm 0.05^\circ$
D_x	1.545 g.cm^{-3}	1.560 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 0.073 and 0.067 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)	-0.0611 (3)	0.2279 (2)	0.5825 (4)	0.0147 (3)	0.0055 (2)	0.0203 (6)	0.0001 (2)	0.0017 (4)	-0.0037 (3)
O(2)	-0.1119 (3)	0.0060 (2)	0.5587 (4)	0.0155 (4)	0.0042 (1)	0.0235 (6)	0.0002 (2)	0.0051 (4)	0.0031 (3)
O(3)	-0.1147 (3)	-0.0647 (2)	0.1445 (4)	0.0120 (3)	0.0028 (1)	0.0314 (7)	-0.0007 (2)	-0.0037 (4)	-0.0010 (3)
O(4)	0.1297 (3)	0.0173 (2)	-0.0825 (4)	0.0146 (4)	0.0060 (2)	0.0264 (7)	0.0009 (2)	0.0060 (4)	-0.0045 (3)
O(5)	0.0636 (3)	0.2220 (1)	0.2893 (3)	0.0113 (3)	0.0032 (1)	0.0165 (5)	-0.0005 (2)	0.0013 (3)	-0.0000 (2)
O(6)	0.0992 (3)	0.2936 (2)	-0.1079 (4)	0.0188 (4)	0.0040 (1)	0.0192 (6)	-0.0013 (2)	-0.0029 (4)	0.0010 (2)
C(1)	0.0198 (4)	0.1614 (2)	0.4610 (5)	0.0109 (4)	0.0040 (2)	0.0166 (7)	-0.0006 (2)	-0.0001 (5)	0.0008 (3)
C(2)	-0.0786 (4)	0.0717 (2)	0.3902 (5)	0.0098 (4)	0.0034 (2)	0.0184 (7)	-0.0002 (2)	0.0000 (5)	0.0010 (3)
C(3)	-0.0081 (4)	0.0059 (2)	0.2259 (5)	0.0097 (4)	0.0028 (1)	0.0217 (8)	0.0001 (2)	-0.0020 (4)	-0.0003 (3)
C(4)	0.0486 (4)	0.0764 (2)	0.0600 (5)	0.0100 (4)	0.0039 (2)	0.0171 (7)	0.0007 (2)	0.0013 (5)	-0.0015 (3)
C(5)	0.1479 (3)	0.1614 (2)	0.1486 (5)	0.0088 (4)	0.0039 (2)	0.0205 (8)	0.0001 (2)	0.0007 (5)	0.0001 (3)
C(6)	0.2099 (4)	0.2385 (3)	-0.0027 (6)	0.0117 (4)	0.0055 (2)	0.0238 (9)	-0.0011 (3)	0.0041 (6)	0.0010 (4)
H(O1)	0.010	0.252	0.676						
H(O2)	-0.212	0.020	0.622						
H(O3)	-0.085	-0.128	0.188						
H(O4)	0.067	-0.002	-0.196						
H(O6)	0.085	0.370	-0.120						
H(C1)	0.116	0.137	0.540						
H(C2)	-0.175	0.104	0.337						
H(C3)	0.081	-0.035	0.296						
H(C4)	-0.041	0.107	-0.008						
H(C5)	0.238	0.125	0.218						
H(C6-1)	0.289	0.292	0.071						
H(C6-2)	0.271	0.196	-0.109						

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 10 σ , 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.

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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 (3)
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 ($\times 10$).

2	50	59	53	0	2	557	557	0	557	0	54	55	0	55	1	94	93	7	93	0	44	50	50	0	0
4	876	908	908	0	4	184	180	0	176	0	1	29	32	0	32	4	84	80	66	45	1	31	34	33	4
6	10*	7	7	0	5	57	51	0	51	3	60	60	54	11	6	69	71	11	38	3	26	27	11	22	
8	58	62	62	0	6	100	120	0	120	4	26	28	25	12	7	21	23	17	15	4	55	57	39	41	
10	67	70	70	0	7	185	174	0	174	5	30	36	37	12	8	39	34	19	29	5	44	48	8	47	
12	162	169	164	0	8	11*	0	0	0	6	19	15	3	15	9	29	27	0	27	7	20	16	14	19	
14	213	226	222	0	9	111	112	0	112	0	872	845	845	0	10	40	47	45	14	8	53	51	46	24	
1	36	42	0	42	11	30	33	0	33	1	616	645	645	0	2	44	45	21	43	2	44	43	46	24	
2	270	293	293	0	12	59	60	0	60	2	95	78	78	0	3	60	60	43	41	0	21	20	0	20	
3	100	135	0	135	13	12*	0	0	0	3	21	28	28	0	4	38	37	23	30	1	59	57	34	45	
4	177	196	196	0	14	204	204	0	204	4	238	261	261	0	5	26	23	23	11	2	10*	14	60	34	
5	34	31	0	31	0	0	0	0	0	5	83	85	85	0	6	0	0	0	0	3	29	29	10	24	
6	27	29	29	0	0	459	478	0	478	6	24	21	21	0	7	240	251	164	281	4	27	22	19	11	
7	27	25	0	25	1	188	196	0	196	7	158	153	153	0	8	172	167	0	167	4	27	22	19	11	
8	129	126	126	0	2	318	320	249	201	8	30	26	26	0	9	36	27	0	27	0	431	430	430	0	
9	11*	11	0	11	3	195	198	336	24	9	37	37	37	0	4	23	25	0	25	1	37	36	36	0	
10	12*	7	7	0	4	276	267	247	102	10	73	73	73	0	5	70	62	0	62	4	295	290	290	0	
11	186	168	0	168	5	352	362	362	16	11	27	27	27	0	6	117	114	0	114	3	31	34	44	0	
12	35	35	35	0	6	176	168	132	107	12	20	64	64	0	7	106	100	77	104	4	130	127	127	0	
13	37	34	0	34	7	3*	3*	3*	0	11	53	53	53	0	8	147	147	0	147	5	5*	5*	63	0	
14	46	50	50	0	8	105	105	92	91	14	127	125	125	0	9	55	49	0	49	6	99	94	94	0	
0	430	416	416	0	9	136	133	132	102	15	11*	1	1	0	10	136	133	132	102	7	136	136	136	0	
1	261	280	0	280	11	87	87	36	78	0	844	900	0	900	11	12*	1	0	1	8	84	81	81	0	
2	169	171	0	171	13	36	35	32	13	3	503	512	417	298	14	18	13	0	13	11	52	49	49	0	
3	164	171	0	171	13	36	35	32	13	3	503	512	417	298	14	18	13	0	13	11	52	49	49	0	
4	104	92	92	0	14	102	104	82	82	4	475	468	23	459	0	153	151	151	150	12	25	27	27	0	
5	165	158	0	158	14	66	66	26	14	5	361	362	335	70	5	187	184	0	184	13	54	54	60	0	
6	21	16	16	0	0	416	437	437	0	6	212	197	135	144	1	235	242	98	221	1	150	1	1	0	
7	132	136	0	136	1	165	169	169	8	7	37	35	29	26	2	216	217	145	162	0	142	150	0	150	
8	12	14	0	14	2	154	156	152	214	8	154	156	152	214	8	154	156	152	214	8	154	156	152	214	
9	16	24	0	24	3	132	161	196	140	9	183	186	194	104	4	465	459	368	249	2	30	31	31	51	
10	25	22	22	0	4	410	409	376	360	10	125	126	24	124	5	157	152	100	116	3	174	174	127	124	
11	12*	1	0	1	5	194	190	110	101	11	87	88	64	76	6	140	138	0	138	4	256	257	257	61	
12	84	92	92	0	6	66	66	23	54	12	78	75	14	74	7	66	61	15	59	5	255	243	247	176	
13	98	90	0	90	7	95	92	91	14	13	38	33	23	24	8	113	117	21	115	6	121	113	113	101	
14	26	19	19	0	8	75	76	36	70	14	65	68	36	52	9	76	77	77	90	7	178	174	138	107	
1	100	98	0	98	9	107	105	95	45	0	54	60	60	0	11	83	79	58	58	8	150	146	146	41	
2	120	121	121	0	11	11*	7	5	16	1	119	127	118	64	12	39	39	37	12	10	74	76	15	76	
3	5	52	0	52	12	57	57	54	20	2	374	376	33	378	13	41	43	35	27	11	86	86	75	47	
4	10*	8	0	8	13	73	76	78	1	3	111	104	55	43	14	47	51	34	38	12	23	19	10	10	
5	165	158	0	158	14	66	66	26	14	5	169	165	32*	85	4	169	165	32*	85	11	39	36	11	33	
6	158	162	162	0	15	99	89	53	71	0	518	534	534	0	5	518	534	534	0	17	0	75	73	0	
7	166	161	0	161	0	415	421	0	421	6	22	21	10	19	1	40	40	36	17	0	75	73	73	0	
8	12	14	0	14	1	149	150	139	54	6	87	81	34	74	2	157	154	122	53	1	107	106	106	8*	
9	67	67	0	67	2	193	201	190	146	8	147	148	132	67	3	74	72	52	49	2	208	206	206	63	
10	247	246	246	0	3	61	67	70	35	9	85	85	7	84	4	309	309	364	59	3	312	304	236	193	
11	86	84	0	84	4	569	569	515	430	10	226	229	52	223	5	363	369	251	227	4	308	308	215	223	
12	27	24	24	0	5	22	21	61	20	11	13*	10	7	8	6	125	113	58	97	5	175	176	164	52	
13	65	67	0	67	6	169	163	61	157	12	99	95	20	93	7	162	161	27	98	6	155	148	148	101	
0	181	187	187	0	7	209	201	200	20	13	37	33	33	2	8	71	77	72	79	122	122	106	56		
1	15	22	0	22	8	265	266	105	244	0	110	111	8	111	10	125	127	73	164	9	86	88	82	62	
2	40	53	53	0	10	167	133	95	104	1	23	16	9	13	11	62	62	42	42	10	166	168	130	108	
3	30	27	0	27	11	76	81	95	60	2	165	164	119	112	12	66	65	65	23	11	86	86	75	47	
4	66	62	62	0	12	62	60	11	59	3	167	166	149	73	13	47	50	36	34	12	16	16	16	7	
5	90	92	0	92	13	30	31	26	19	4	198	197	64	178	0	198	197	64	178	13	30	30	11	33	
6	56	52	52	0	14	113	112	132	102	5	143	142	136	36	0	86	91	0	93	0	20	20	0	20	
7	176	176	0	176	0	115	132	132	0	6	130	140	57	128	1	80	87	74	46	0	20	20	0	20	
8	190	192	192	0	1	112	113	98	56	7	29	25	19	16	2	149	147	82	123	1	76	85	66	93	
9	161	157	0	157	2	72	75	49	57	8	64	67	46	46	3	71	67	0	67	2	27	20	20	4	
10	20	20	0	20	3	94	90	63	49	9	98	101	73	70	4	138	135	135	18	7	127	128	8	128	
11	51	52	0	52	4	195	198	106	87	10	125	127	118	10	5	53	53	53	2	4	110	106	106	160	
12	53	56	56	0	5	194	191	181	12	11	34	33	33	7	6	56	56	16	24	5	82	83	78	28	
1	57	54	0	54	7	200	204	127	164	12	21	24	44	23	7	54	58	51	27	6	124	13	9	10	
2	55	54	54	0	8	101	101	95	56	0	10*	11	13	0	9	70	71	54	46	8	88	86	85	10	
3	57	54	0	54	8	50	48	2	7	1	65	64	31	34	10	69	72	72	3	9	56	47	50		
4	87	84	84	0	10	30	36	34	16	1	45	46	31	34	11	62	66	66	66	10	124	9	7	9	
5	52	53	0	53	11	45	46	11																	

Table 4 (cont.)

0	21	22	22	0	1	85	90	62	46	1	105	114	80-	82-	9	24	28	27	7-	7	15	15	15	6
1	11*	17	11	18	3	69	75	19	70	2	131	148	2	136-	10	20	29	27-	9	4	34	40	40	7-
2	27	26	1	26	4	44	47	30	27	4	87	81	72	36	0	11*	0	0	0	0	15	13	13-	0
3	11*	3	3-	2-	5	53	58	10	57	5	20	25	24	6	1	111	114	98-	59-	1	54	57	9	57-
4	26	56	47	29-	6	12*	20	12-	16*	6	38	42	62	6	2	190	190	16-	109-	2	40	41	32	26
5	16	19	16-	9	7	26	26	4	26-	7	31	28	3	28-	1	48	48	47	8-	3	20	15	1	15
6	42	40	8	19	8	47	48	-	48	8	28	31	8-	30	4	83	87	87-	3-	4	46	41	6-	40
7	33	33	6	32-	10	35	35	34-	9	10	16	31	29-	11-	6	29	29	27-	12-	6	28	24	24	3
8	44	40	0	40-	0	132	125	0	125	0	101	106	106*	0	7	34	29	27	10	4	5	5	4	1
9	36	35	23	4-	0	107	107	8	108-	1	167	169	145-	87-	9	31	24	8	23	1	26	26	25	11-
10	34	33	33-	2-	1	107	107	8	108-	2	78	79	63	47-	8	22	20	20	4	0	2	17	16	1
11	24	19	19-	0	2	88	92	45	80	2	78	79	63	47-	8	22	20	20	4	0	2	17	16	1
12	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
73	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
74	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75	10*	0	0	5	1	10*	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76	10*	0	0	5																				

Table 5. Observed and calculated structure factors for cellobiose
Columns are as in Table 4.

2	281	285	284	31-	10	235	232	232	42	12	84	83	57-	60	3	106	110	100	93-	3	90	94	94-	8	2	228	241	44-	236-	
4	453	454	444	410	11	44	70	25	67	13	71	68	7	68-	4	101	100	65-	75-	4	231	225	149-	169	6					
6	717	721	714	73	17	79	75	60	54	14	41	35	36	16-	6	147	154	114	153	6	174	183	114	143	7					
8	143	127	127	127-	13	57	57	20-	63																					
10	159	157	155	76						0	261	263	263	0	7	43	78	72	70	7	32	35	35-	7-						
12	204	211	74	198	0	57	47	47-	0	1	262	262	59-	255-	8	48	47	46-	11-	8	136	138	16	137-						
14	87	60	4-	60-	1	104	104	174	41-	2	90	87	40	54-	9	51	54	52	16-	9	67	63	61-	14-						
0	h	h	h	0	1	101	101	28	57-	4	30	17	3-	17-	11	16	9	8	4	11	52	53	29	45-						
1	110	308	308	351	4	141	160	156-	84	5	225	215	167-	138-																
2	158	140	110-	96	5	166	167	142-	68-	6	215	202	43	197	0	4+	3	3	0	13	67	68	36	57-						
3	130	124	121	27-	6	166	168	125-	112-	7	128	114	33	109-	1	10	207	130-	162-	14	26	28	27-	8						
4	156	197	48	191	7	168	163	159	36	8	43	39	17	15-	2	40	91	35	84-	4	11	52	53	29	45-					
5	254	264	161	169	8	131	117	99	105-	9	49	44	38	22-	3	110	107	75	76-	0	53	40	60	0						
6	199	361	361-	89	9	28	29	29	2	10	163	156	126-	90	4	58	60	30	52-	1	53	63	27	57-						
7	249	235	218	84	10	43	44	41-	106	11	30	31	22-	22	5	70	75	61	43-	2	174	159	5-	159						
8	23	27	26	6	11	40	37	47	73	12	71	66	57-	34	6	134	129	93	99	3	79	74	59-	44						
9	118	111	76	40	12	77	70	70-	8	13	29	27	26	4	7	96	100	86-	51-	4	119	116	114-	21-						
10	103	97	91	91-						14	20	19	16-	10-	8	68	66	55	57-	5	31	39	1-	39-						
11	146	134	42	104	0	15	15	15	0																					
12	100	97	41-	84	1	44	51	10	50	0	76	71	71	0	10	21	22	15	16-	7	25	24	0	24-						
13	54	58	58	11	2	117	118	107-	61-	1	258	257	40-	184-																
14	23	22	5	21	3	81	80	31-	53-	2	123	126	76-	101-	0	95	90	90	0	9	62	63	52-	36						
15	46	43	5	43	4	166	169	166-	32-	3	521	524	286	459-	1	160	170	119	121	10	56	57	53-	20						
0	h	h	h	0	6	68	65	62	17-	5	79	82	64-	51-	3	100	100	19-	98	12	65	68	38-	56						
1	279	266	250-	137-	7	126	126	114	52	6	91	81	37-	72	4	17	17	1-	17-	13	24	21	14-	16-						
2	126	120	116	116	5	170	170	40-	166-	4	134	126	41-	120-	6	115	116	87-	11	82	85	83	15-							
3	191	166	39-	182-	9	35	35	22-	26-	8	85	80	30	71-	6	107	103	31	97-	0	67	59	59-	0						
4	232	241	229-	75	10	10	9	2	8	9	297	287	235	165-	7	158	156	38	151	1	276	279	181	213-						
5	251	247	117	213-	11	18	19	5	19-	10	161	161	63	27-	5	65	39	23	23	3	128	124	66-	115-						
6	184	172	153-	79						11	163	161	103-	123-	9	54	54	26-	47	3	276	279	181	213-						
7	115	115	115	8	0	33	30	30	0	12	37	37	30	22																
8	153	146	129	60-	1	108	109	30	105	10	83	94	84-	0	84	97	67	0	4	60	61	57-	22							
9	27	25	18	21-	7	78	76	9-	75	14	45	45	44	11-	1	86	92	60	16	6	27	25	4	25-						
10	87	85	77-	51	3	86	82	75-	33						2	75	77	64-	42	7	55	52	46	24-						
11	66	66	66	66	4	160	179	81-	160-	0	740	740	0	0	3	18	14	3-	3-	8	90	100	30	96-						
12	74	74	74-	17-	5	82	82	60-	60-	1	164	169	128	111	4	48	50	32-	39-	9	165	169	101-	136-						
13	40	38	18-	33-	6	95	95	44	64	4	132	133	126-	92	5	33	35	16-	31	10	139	145	90-	113-						
14	34	34	13	31-	7	19	22	11	16	3	158	163	100-	6	93	93	81-	40	11	114	120	168	53-							
15	17	18	1	16	8	83	82	16-	60-	4	235	225	10	225	7	65	61	55	27-	12	34	36	35	8						
0	h	h	h	0	5	30	31	23-	21-	5	119	117	107-	47																
1	27	21	21	0	0	10	38	39	19	34	6	248	224	226	7-	0	560	60	60	0										
2	284	261	271	0	1	65	66	51-	40	0	90	94	60	21-	1	27	22	12-	18	0	2	32	32	0	0					
3	101	302	272-	132	0	205	209	209-	0	8	88	42	34-	86	4	32	32	21-	25-	1	212	216	15	216						
4	73	66	61	24-	1	54	56	47-	35	4	71	69	54-	38	3	57	55	13-	54-	2	220	215	193	95						
5	403	408	94	401-	6	100	96	61	73	10	201	195	73	4	33	32	32	1	3	151	149	149	9							
6	216	213	176-	121-	3	72	72	70-	16-	12	11	66	67	43	46	0	167	157	157	0	4	44	47	41	22-					
7	128	331	51-	327	4	32	29	11	46	12	35	30	14	27	0	167	157	157	0	4	132	131	97-	87						
8	186	184	166	81	7	11	11	11	11	11	42	42	40-	13	1	149	1023	278-	984-	0	4	32	37	27-	19					
9	208	198	56	171-	6	42	39	26-	30	14	49	47	46	6-	2	266	275	199-	190	7	184	186	111	186						
10	49	45	35	24	7	33	32	7-	31-	0	146	135	115	0	3	254	257	255	32	8	150	153	152	23						
11	128	125	68	104-	0	31	31	50	16	0	146	135	115	0	3	254	257	255	32	8	150	153	152	23						
12	68	66	22	62	4	30	31	26-	17-	1	300	291	172-	234	5	474	471	124	263-	10	19	18	15	10-						
13	66	63	22-	37	0	71	72	62	7	0	218	217	144-	162-	6	74	50	44-	11	11	40	38-	12-							
14	47	44	21	41-	1	40	38	30	43	4	70	66	65-	12-	8	208	215	215	2-											
0	299	316	316	0	1	125	127	127	0	5	105	104	25-	160	9	140	144	39	130-	0	35	41	41	0						
1	13	17	1-	1-	4	23	26	24	13	7	53	58	53-	23	11	108	109	98	47	2	132	142	91-	107-						
2	308	317	115-	296-	5	88	93	89	28-	8	175	170	30-	167-	12	115	123	52	112	3	267	268	76	257						
3	154	151	127-	83-	6	100	96	61	73	9	192	188	106-	0	15	17	17	3-	4	242	252	144-	207							
4	335	342	332-	82	7	81	81	42-	69	10	159	154	58-	126-	14	84	92	89	23-	5	80	84	77-	14-						
5	147	133	97-	91-	0	88	88	88	0	11	90	89	27	86																
6	128	118	108	51	0	88	88	88	0	12	81	76	70-	31	0	661	700	700	7	7	121	121	77-	74						

Table 5 (cont.)

5	24	20	2-	19-	3	185	184	122	139	10	135	143	129-	61	0	60	60	60	0	8	108	110	10 ⁰	18	
6	44	39	28-	24-	4	24	12	12	4-	11	66	68	46-	51	1	226	223	223	12-	9	90	48	45	17	
7	76	75	74	-14	5	179	180	172-	52-	12	71	74	58	45	2	34	62	58-	23-	10	24	26	26-	0	
8	12	11	11	0	6	44	36	14-	33	13	67	73	73	12-	3	190	193	59-	183-	0	76	81	81-	0	
9	32	38	38-	0	7	57	56	20-	52	0	274	287	287	0	4	135	127	64-	110	0	76	81	81-	0	
10	14	71	55	46-	8	51	48	38	30	0	81	84	12	84-	6	32	24	23	8	2	91	92	54-	74-	
11	51	51	36	36-	9	64	64	46	45-	1	262	259	259-	7	149	147	145	27	3	83	88	8	87-		
12	10	7	7-	10	10	42	39	39-	4	2	262	259	259-	7	149	147	145	27	3	83	88	8	87-		
13	10	7	7-	10	10	42	39	39-	4	2	262	259	259-	7	149	147	145	27	3	83	88	8	87-		
14	90	89	24-	46	11	17	39	24-	29-	3	153	151	261	237	8	27	36	15	10	4	126	129	121-	51	
15	233	231	231-	0	17	74	73	10	73-	4	209	207	100-	176	7	154	150	111-	101-	5	24	23	71-	8-	
16	100	105	75-	75-	0	72	68	84	0	5	78	73	56-	48-	10	34	40	10	39	6	44	45	27-	51	
17	580	594	110-	58-	1	211	207	202-	45-	7	173	174	9-	174	12	32	33	33	5-	8	80	79	21-	76-	
18	315	120	108	57-	2	92	86	86-	35	8	80	109	43-	100-	13	59	61	57	20-	0	28	30	30	0	
19	4	285	278	286	3	52	53	34	41-	9	143	145	144	4	0	27	25	25-	0	1	24	22	22-	5-	
20	5	74	68	0	64-	4	155	161	4	161-	10	89	97	96-	11-	0	27	25	25-	0	1	24	22	22-	5-
21	174	171	171-	0	6	67	66	45-	46-	0	119	110	110-	0	5	17	15	12	9	6	28	28	22	17-	
22	10	173	171	171-	0	6	67	66	45-	46-	0	119	110	110-	0	5	17	15	12	9	6	28	28	22	17-
23	11	90	63	52-	54	10	81	62	28	35-	1	48	45	31	33-	8	81	82	37	50	7	13	11	8-	
24	12	106	104	93	47-	11	82	82	70-	42-	2	28	31	24-	18	7	130	143	91-	110-	0	20	24	0	
25	13	42	42	13	2-	8	362	365	365	0	4	87	77	76-	16	8	99	200	47-	88	1	49	50	41-	26-
26	16	28	28	28	2-	1	179	181	112	143	5	101	64	62	70-	10	105	106	103-	26-	2	95	93	34	84-
27	0	265	263	263	0	2	104	104	106	125-	6	106	110	105-	31-	11	80	79	41	67	3	40	77	70	32-
28	1	230	245	243-	43	5	81	81	94	58-	7	10	95	98	3-	48-	0	0	0	0	0	36	40	40	0
29	2	195	190	128	140-	4	120	115	53	102	6	67	47	2-	67	13	26	22	21-	8-	5	31	28	27-	4
30	3	172	168	143	23	5	223	224	107-	201	0	69	73	73-	1-	0	0	0	0	0	0	36	40	40	0
31	4	173	165	137-	43	6	222	224	107-	201	0	69	73	73-	1-	0	0	0	0	0	0	36	40	40	0
32	5	27	25	7-	24	7	35	33	18-	27	11	54	57	35	44-	1	264	268	63-	261	1	65	70	28-	64
33	6	71	59	44	39-	8	40	41	4-	48-	12	47	50	56-	7-	126	174	90-	149-	2	143	141	123	139-	
34	7	107	102	98-	39-	9	39	41	25	33-	13	12	14	14	7-	3	120	112	14	111	3	130	121	121-	0
35	8	70	72	64	32-	10	57	57	5-	57	0	73	74	74-	0	4	125	119	118-	16	4	128	125	46	110
36	9	78	81	75-	29	0	199	204	204-	0	1	15	7	4	0	5	79	83	62-	42	5	148	148	5	56-
37	11	100	103	86-	57-	1	86	86	38	78	2	85	83	20	81-	7	179	180	0	180	7	58	57	56	11-
38	12	81	72	22	20	8	81	81	81	13	9	94	95	46-	12	87	83	63	29	4	146	149	46	142	
39	13	57	58	4	58	3	5*	11	10-	5*	4	113	113	74-	85	9	54	51	40	31	4	146	149	46	142
40	14	58	53	37	38-	4	70	66	65-	13	5	74	76	3	78	10	141	138	122-	64-	10	99	102	63-	81-
41	0	26	28	28	0	6	125	128	120-	45	7	50	52	11-	50-	12	33	33	5-	33-	12	63	58	44-	37-
42	1	185	174	158	77-	7	41	41	38	17-	8	71	76	63	41	0	0	0	0	0	13	44	2	0	2-
43	2	30	38	21-	31-	8	14	14	4-	13	9	95	71	64	0	3	33	33	0	0	0	93	90	90	0
44	3	249	236	7	235-	9	40	43	20-	38	10	62	66	58-	31-	1	100	98	35	92-	0	93	90	90	0
45	4	218	208	173	111	10	10	10	10	10	11	33	33	17	27	2	70	62	35-	52	1	51	42	29	31-
46	5	100	104	88	82	0	80	83	0	0	12	33	36	17	36-	3	108	63	27	2	110	106	40-	98-	
47	6	101	99	44	53	1	67	69	24-	65-	0	72	79	75-	0	4	21	24	3-	24	3	55	63	0	83-
48	7	152	156	79	134-	2	90	64	52-	36	0	72	79	75-	0	4	21	24	3-	24	3	55	63	0	83-
49	8	133	128	127	127	7	71	74	27	1	11	9	97	85	66-	5	80	75	62-	42	4	140	139	3-	139
50	9	25	25	5-	25	4	47	44	35-	26-	2	108	111	95-	58-	7	26	24	2-	24-	6	96	93	26	89-
51	10	189	177	175	22-	6	61	61	45-	3	123	122	135	120-	7	149	148	7	120-	7	88	88	77	43	
52	11	89	89	89	89	6	46	46	46	46	91	30	85	4	43	48	40-	26	9	88	87	4	87-	20	146
53	12	91	91	91	91	7	70	71	30-	65-	5	62	60	54-	26	10	81	79	73-	31-	9	103	101	51	88
54	13	33	31	2-	31-	8	63	61	61	0	6	24	22	3	22	11	38	38	14-	11	30	28	10-	23-	
55	14	77	71	4-	70	0	63	61	61	0	7	32	33	17-	28	12	43	48	74-	44	11	86	86	12	63
56	0	81	80	80	0	1	15	12	10-	6-	8	79	79	59-	56	0	0	0	0	0	12	14	9	8	7
57	0	135	145	31-	142	3	24	29	12	26-	10	40	40	20-	34-	1	51	54	53-	0	0	5	10	10-	0
58	1	315	304	304	2-	4	61	60	14	59-	11	24	24	22-	10	2	234	232	60	224-	1	83	81	40-	67
59	3	108	105	105-	10	5	39	35	28-	22-	0	204	203	203	0	3	180	185	128	134-	2	248	250	167-	186-
60	4	80	73	21-	70-	0	86	92	82	0	0	105	106	47	95-	5	48	46	34-	31	3	260	268	90	253-
61	5	150	150	150	146	0	96	92	82	0	2	211	213	124	172-	6	48	44	40	19-	4	58	61	9	60-
62	6	36	36	36	35	1	189	188	125	141	2	211	213	124	172-	6	48	44	40	19-	4	58	61	9	60-
63	7	52	47	20-	43	2	73	80	78-	17-	3	109	112	76	83-	7	106	106	0	106	6	24	26	3-	26
64	8	283	280	280	0	3	212	229	163-	161	4	103	101	28	97	8	86	88	70	53	7	46	46	46	3-
65	9	214	206	115-	170	4	139	136	90-	120-	5	53	56	54-	15-	9	85	85	35	79-	8	77	81	80-	12-
66	10	142	138	126-	54-	5	85	89	32-	50	6	154	154	153	14-	10	84	85	83-	15-	9	113	116	84	80-
67	11	90	89	10-	87	6	65	12	3	12	7	8*	11	4	10-	11	27	37	35-	19	10	151	151	48-	155-
68	12	48	45	8	44	7	27	29	8	28	8	97	95	85	42-	12	46	48	33	34-	11	70	74	68	29-
69	13	63	58	49-	30	8	152	154	39	149	9	40	39	1	39-	0	0	0	0	0	12	49	50	48	14
70	0	36	34	14	0	10	218	222	168-	145-	0	73	72	37-	43	0	60	60	60	0	0	36	37	37-	0
71	1	134	137	86-	107	11	74	72	2-	72-	0	212	212	212-	0	2	31	33	4</						

Table 5 (cont.)

5	74	77	69-	36	8	57	57	55-	16	0	29	31	31	0	H ⁺	6	L ⁺	-4	0	41	38	38	0	
6	30	31	31	2-	9	41	41	38-	16-	1	59	7	0	6	0	42	42	42	0	1	32	29	19-	
7	46	86	39-	70	10	38	38	21-	31-	2	81	82	11-	81-	1	23	27	8-	25	2	70	71	60-	
8	41	35	2-	26-	11	70	70	25-	0	3	47	2	0	9	2	47	22	11	19	3	22	11	22-	
9	69	69	69	1-	0	H ⁺	7	L ⁺	4	4	71	70	36-	13	3	40	43	18-	34	4	32	36	35-	
10	27	27	27-	4	0	87	84	84	0	5	17	13	3-	13	4	98	97	91	32	5	88	80	78-	
11	01	01	01	19-	1	H ⁺	4	L ⁺	4	0	5	17	13	3-	13	4	98	97	91	32	5	88	80	78-
0	6 ⁺	10	10	0	1	35	32	7	31	1	42	40	35	21	7	42	43	30	16-	0	23	25	25-	
1	41	35	19	24	4	90	56	35-	65	2	14	15	13	7-	8	71	70	24-	66	1	31	29	29-	
2	56	55	37-	40-	5	64	61	58-	14-	0	52	51	51	0	6	90	84	48	60	0	23	25	25-	
3	41	51	27	43-	6	77	71	13	70	0	72	69	69-	0	0	56	55	55	0	3	25	28	27-	
4	21	14	11	9	7	45	47	47-	6	1	43	162	103	125	1	36	42	42	7	4	79	75	42-	
5	01	42	60-	16	8	07	65	61	22	2	135	140	134	15	2	24	18	16	9-	5	74	75	20	
6	17	11	9-	5-	9	78	74	23-	71-	3	56	53	38	37-	3	57	56	1	56-	0	3	25	28	
7	49	47	37	26-	10	73	24	2-	24-	4	63	68	42	53-	4	51	49	48-	6-	0	21	21	21	
8	23	45	10-	23	0	H ⁺	3	L ⁺	4	0	6	73	74	67-	33	6	85	83	41	72	2	33	11	
9	44	42	10	41-	0	34	27	27-	0	6	73	74	67-	33	6	85	83	41	72	2	33	11		
10	35	34	16	30-	1	59	60	38	52-	7	40	45	62	19-	7	18	17	17	1-	3	18	20	15-	
0	19	14	14	0	1	51	53	46-	26-	8	142	142	124	0	0	H ⁺	8	L ⁺	-4	0	35	37	37-	
1	114	122	101-	68	4	31	32	24	22	10	26	24	2	24-	1	59	58	55-	18	1	82	84	30-	
2	63	63	31-	52-	4	29	27	10-	25	11	44	4	2	3	3	35	34	31-	14	2	92	88	72-	
3	36	35	26	71-	6	46	46	40-	32	7	42	40	38	10-	3	42	40	38	10-	3	78	73	16	
4	64	64	26-	54	7	75	78	77-	5	0	35	33	33	0	4	42	42	14-	39-	4	47	51	51-	
5	22	23	23	1-	8	32	3	16	25	1	44	144	151	31	5	18	11	1-	13-	5	15	21	15	
6	21	19	19	2	9	55	56	16-	53-	2	87	84	60-	60	6	38	37	5-	37	6	54	61	52-	
7	32	32	30-	12-	10	77	73	40	61-	3	17	13	2	13	0	H ⁺	9	L ⁺	-4	0	7	73	76	
8	24	25	5	24	0	H ⁺	4	L ⁺	4	4	50	49	48-	15	0	54	52	52	0	8	21	19	8-	
9	46	49	44	21	0	164	176	176	0	5	51	48	47	9-	2	14	11	5-	0	0	204	200	200	
0	41	41	41-	0	1	117	123	122	11	6	01	58	56-	5-	2	18	20	7-	19	0	704	700	700	
1	112	106	77-	75-	3	90	90	90-	1	8	38	39	38	3	0	H ⁺	0	L ⁺	5	1	49	49	38	
2	74	74	64-	37-	4	119	114	96-	70	4	67	68	18	66	0	42	45	45	0	3	36	36	24-	
3	57	54	21	40-	5	42	45	94-	14-	10	17	18	17	4-	1	75	80	52	61-	4	76	71	63	
4	15	16	0	16-	6	63	61	38	40-	11	53	50	50-	1-	2	38	40	29-	28-	5	18	21	20-	
5	51	52	31-	42-	7	65	66	98	32	0	H ⁺	3	L ⁺	-4	3	63	62	2	62-	6	71	70	66	
6	40	51	13	49	8	142	145	89	115-	0	15	142	142	0	4	37	34	3-	39	7	33	30	27-	
7	77	78	23-	75-	9	171	169	137-	98-	1	57	57	12	56	5	40	46	46-	5	0	58	53	53	
8	63	60	60	0	10	57	60	60-	5	2	144	140	136-	33-	6	46	49	18-	45	0	58	53	53	
9	65	61	45	55	0	44	49	28	5	0	3	19	8	1-	8	7	28	30	12	27-	1	133	132	
0	86	81	49	65-	1	71	73	16	71	5	86	82	87-	30-	0	H ⁺	1	L ⁺	5	4	22	23	15	
1	54	54	0	0-	2	179	181	161	83	6	21	19	14	13-	0	125	123	123	0	4	5	6	3-	
2	52	52	46	20-	3	111	126	69	106	7	45	48	42	23	1	21	21	15-	15-	5	77	80	29-	
3	90	88	86-	14	4	27	18	4	18	8	33	32	11-	30-	2	67	68	48-	48	6	42	43	38-	
4	88	11	L ⁺	-3	5	67	65	40-	22	9	43	46	43	17	3	13	15	13-	8-	7	72	69	61	
5	88	88	88-	0	6	101	101	3-	101	10	81	79	29	73-	4	26	26	9	26-	0	H ⁺	4	L ⁺	5
6	69	70	24	65	7	74	71	32	64	0	H ⁺	4	L ⁺	-4	0	6	44	2	1-	1-	0	68	69	69
7	422	275	275	0	8	91	92	80	13-	0	71	67	67	0	6	44	2	1-	1-	0	68	69	69	
8	135	134	45	126	9	48	46	45	18-	1	119	100	100-	82	7	14	17	17-	2-	43	39	27		
9	20	75	11	74-	0	16	16	16-	0	3	55	55	55-	0	0	H ⁺	2	L ⁺	5	4	18	20	20-	
0	122	114	40	112	1	97	98	96	24	4	65	66	63	63	0	127	117	117	0	5	43	45	38	
1	49	45	34	30	2	56	55	43-	48	5	29	28	15-	25-	1	73	75	47	58-	6	50	48	17-	
2	85	82	53-	63	3	26	25	25-	1	6	20	18	18-	4	2	28	29	21	20-	0	H ⁺	5	L ⁺	-5
3	124	125	125	0	4	136	138	137-	12	7	55	55	54-	10	3	15	14	0	14-	0	87	89	89	
4	113	113	60	106	5	17	17	15-	15-	8	27	31	31-	5-	4	39	37	32-	30	1	23	20	37	
5	86	88	35	81-	6	17	21	18	10	9	42	47	25-	39	5	14	11	1	11-	2	61	61	36-	
6	39	39	39	7-	7	67	61	39	47	10	52	50	48-	13	6	15	8	0	8	3	24	21	20	
7	113	113	60	106	5	17	17	15-	15-	8	27	31	31-	5-	4	39	37	32-	30	1	23	20	37	
8	59	58	37-	45	0	37	36	16-	6-	0	55	53	53	0	7	55	54	39	38-	4	16	14	14	
9	130	134	134	0	0	24	27	27-	0	1	50	54	47-	26	0	59	10	10-	0	0	H ⁺	6	L ⁺	-5
0	74	81	59	55-	2	88	89	87	20-	3	98	98	59	78-	2	55	59	51	29	1	49	48	17-	
1	197	194	191-	51-	3	25	21	4	21-	4	60	61	38	47-	3	60	54	54	4-	2	51	46	32-	
2	64	66	17-	64	4	35	32	31	5	63	65	57-	31-	4	19	17	17	17	17	3	24	24	22-	
3	71	67	66-	13	5	84	81	3-	31-	6	24	23	5-	22	5	95	90	16	89-	4	42	40	36-	
4	95	95	95	77-	6	38	41	41-	3-	7	50	51	20	47-	6	32	35	32	13	0	H ⁺	7	L ⁺	-5
5	73	77	68	36	7	26	19	18	7-	8	15	13	6	12-	7	108	109	83	89	0	47	44	44	
6	69	71	65	27	9	101	105	85	62-	9	101	105	85	62-	0	H ⁺	4	L ⁺	5	0	0	0	0	0

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>i</i>	<i>j</i>	<i>D</i> (<i>ij</i>)	<i>i</i>	<i>j</i>	<i>k</i>	\angle (<i>ijk</i>)
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) <i>a</i>	2.666	C(6)	C(5)	O(5)	107.1 (3)
O(2)	O(3) <i>b</i>	2.686	C(

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>i</i>	<i>j</i>	<i>D</i> (<i>ij</i>)	<i>i</i>	<i>j</i>	<i>k</i>	\angle (<i>ijk</i>)
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') <i>a</i>	2.766	C(5')	C(4')	O(1)	106.4 (3)
O(2)	O(5') <i>b</i>	2.733	C(4')	C(5')	C(6')	113.6 (3)
O(3)	O(6') <i>c</i>	2.711	C(4')	C(5')	O(5')	109.2 (3)
O(3)	O(6') <i>b</i>	2.808	C(6')	C(5')	O(5')	106.4 (3)
O(4)	O(6') <i>c</i>	2.807	C(5')	C(6')	O(6')	111.8 (3)
O(4)	O(2') <i>d</i>	2.814				
O(5)	O(3')	2.767	C(1)	O(5)	C(5)	112.4 (2)
O(2')	O(6') <i>e</i>	2.789	C(1)	O(1)	C(4')	116.1 (2)
			C(1')	O(5')	C(5')	113.5 (3)

Symmetry code

-	<i>x</i>	<i>y</i>	<i>z</i>
<i>a</i>	- <i>x</i>	$-\frac{1}{2}+y$	- <i>z</i>
<i>b</i>	- <i>x</i>	$-\frac{1}{2}+y$	1- <i>z</i>
<i>c</i>	1- <i>x</i>	$-\frac{1}{2}+y$	1- <i>z</i>
<i>d</i>	1- <i>x</i>	$-\frac{1}{2}+y$	- <i>z</i>
<i>e</i>	- <i>x</i>	$\frac{1}{2}+y$	- <i>z</i>

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