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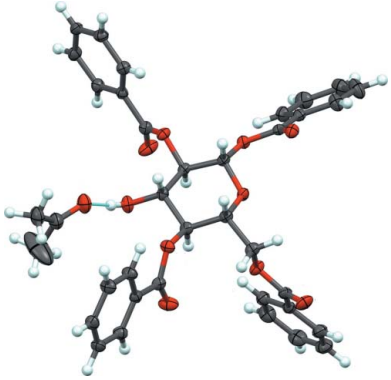
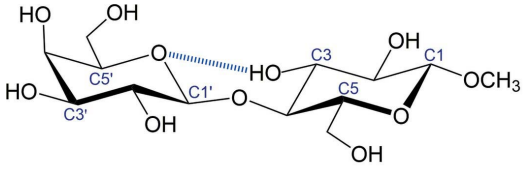
The crystal structures of 2,3,4,6-tetra-*O*-benzoyl-β-D-galactopyranosyl-(1→4)-1,2,6-tri-*O*-benzoyl-β-D-glucopyranose ethyl acetate hemisolvate, $C_{61}H_{50}O_{18}\cdot 0.5C_4H_8O_2$, and 1,2,4,6-tetra-*O*-benzoyl-β-D-glucopyranose acetone monosolvate, $C_{34}H_{28}O_{10}\cdot C_3H_6O$, were determined and compared to those of methyl β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside (methyl β-lactoside) and methyl β-D-glucopyranoside hemihydrate, $C_7H_{14}O_6\cdot 0.5H_2O$, to evaluate the effects of *O*-benzoylation on bond lengths, bond angles and torsion angles. In general, *O*-benzoylation exerts little effect on exo- and endocyclic C—C and endocyclic C—O bond lengths, but exocyclic C—O bonds involved in *O*-benzoylation are lengthened by 0.02–0.04 Å depending on the site of substitution. The conformation of the *O*-benzoyl side-chains is highly conserved, with the carbonyl O atom either eclipsing the H atom attached to a 2°-alcoholic C atom or bisecting the H—C—H bond angle of an 1°-alcoholic C atom. Of the three bonds that determine the side-chain geometry, the C—O bond involving the alcoholic C atom exhibits greater rotational variability than the remaining C—O and C—C bonds involving the carbonyl C atom. These findings are in good agreement with recent solution NMR studies of the *O*-acetyl side-chain conformation in saccharides.

1. Introduction

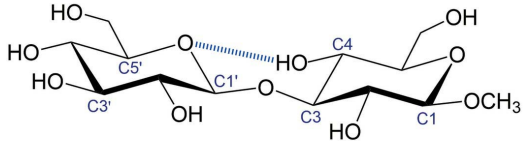
An interplay of noncovalent interactions controls the conformations of the *O*-glycosidic linkages of oligosaccharides in solution. These interactions, which include stereoelectronic effects (exo-anomeric) (Thøgersen *et al.*, 1982; Kirby, 1983; Alabugin, 2016; Juaristi & Cuevas, 1995), steric effects, hydrogen bonding (Kirschner & Woods, 2001; Corzana *et al.*, 2004; Battistel *et al.*, 2017; Zhang *et al.*, 2009) and electrostatic interactions, are superimposed on the inherent constraints on linkage conformation imposed by the covalent scaffold (*e.g.* bond lengths and angles). In β-(1→4) and β-(1→3) linkages, such as those found in methyl β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside [βGal-(1→4)-βGlcOCH$_3$], (I), and methyl β-D-glucopyranosyl-(1→3)-β-D-glucopyranoside [βGlc-(1→3)-βGlcOCH$_3$], (II), respectively, hydrogen bonding is commonly observed in crystal structures between contiguous residues (Scheme 1 shows the modes of inter-residue hydrogen bonding in β-linked disaccharides) (Stenutz *et al.*, 1999; Noguchi *et al.*, 1992). Only one linkage conformation allows this inter-residue hydrogen bonding in β-(1→4) linkages



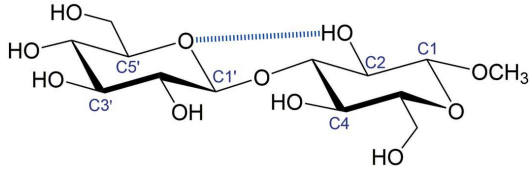
(Mode 1), but two linkage conformations are possible in β-(1→3) linkages (Modes 2 and 3), although only one has been observed to date (Mode 2) (Noguchi *et al.*, 1992). In contrast, experimental evidence for persistent inter-residue hydrogen bonding in aqueous solution has been difficult to obtain (Battistel *et al.*, 2017; Zhang *et al.*, 2009; Battistel *et al.*, 2013). The strength and persistence of this interaction, both of which determine its effect on conformational preference, is expected to depend in part on the nature of the solvent, with polar solvents reducing strength and/or persistence, and nonpolar solvents enhancing both properties (Ben-Tal *et al.*, 1997). With these thoughts in mind, we reasoned that optimal



Mode 1. β-(1→4)-linkage: βGal-(1→4)-βGlcOCH$_3$ (I)



Mode 2. β-(1→3)-linkage: βGlc-(1→3)-βGlcOCH$_3$ (IIa)



Mode 3. β-(1→3)-linkage: βGlc-(1→3)-βGlcOCH$_3$ (IIb)

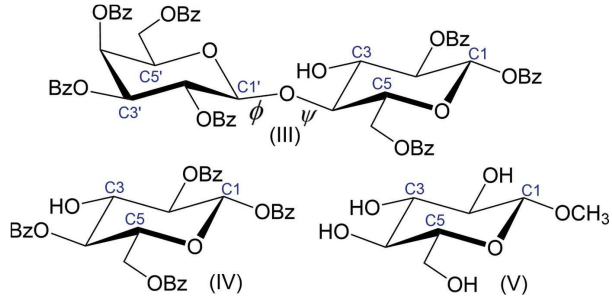
Scheme 1

conditions for inter-residue hydrogen bonding in solution might be achieved in a protected disaccharide derivative in which only the hydroxy group involved in the putative hydrogen bond is available, all others being protected to promote solubility in a nonpolar solvent. This model compound could then be used to test and/or develop experimental methods aimed at detecting the putative inter-residue hydrogen bond under solution conditions that favor its formation. A survey of the literature revealed a candidate with the desired structural features, namely 2,3,4,6-tetra-*O*-benzoyl-β-D-galactopyranosyl-(1→4)-1,2,6-tri-*O*-benzoyl-β-D-glucopyranose, (III) (β-lactose heptabenzoate) (Scheme 2). The lactose core of (III) has been shown from crystal structure studies to be predisposed towards inter-residue hydrogen bonding involving O3H (Glc) as the donor and O5′ (Gal) as the acceptor (Scheme 1) (Stenutz *et al.*, 1999). To confirm that similar hydrogen bonding occurs in (III) in the solid state, its crystal structure was determined and compared to that of (I). In an additional and related comparison, the crystal structure of 1,2,4,6-tetra-*O*-benzoyl-β-D-glucopyranose, (IV) (β-D-glucopyranose tetrabenzoate) (Scheme 2), was also determined, and its structural properties compared to that of methyl β-D-glucopyranoside hemihydrate, (V), and the βGlc*p* residue in (III). The crystal structure of (V) was redetermined at 120 K; the previously reported structure was determined at room temperature (Jeffrey & Takagi, 1977).

2. Experimental

2.1. Synthesis and crystallization

The crystal structure of (III) was determined on a sample prepared as described previously, with no significant modifications (Vazquez *et al.*, 1973). Lactose monohydrate (10 g, 27.8 mmol) was dissolved in an ice-cooled 20% *w*/*v* aqueous NaOH solution (480 ml) and benzoyl chloride (55 ml, 473 mmol) was added dropwise with efficient stirring. The solution was stirred for 1 h at room temperature, after which time the reaction mixture solidified. The reaction mixture was held at room temperature for an additional 1 h and then the solid was collected by vacuum filtration. The solid was washed with distilled water until the pH of the filtrate was neutral. The solid was extracted with boiling methanol (600 ml) and the extract was concentrated to a syrup *in vacuo* at 30 °C. The syrup was dissolved in hexane–ethyl acetate (1:1 *v*/*v*), which, upon standing at room temperature for several days, gave colorless blade-like crystals. The overall yield of (III) was ∼20%, which was close to the reported yield of 24%. The crystal structure of (IV) was determined on a sample prepared as described previously, with no significant modifications (Elsaidi *et al.*, 2015); the yield from this synthesis was ∼65%, starting from 1,2,5,6-di-*O*-isopropylidene-α-D-glucofuranose. The crystal structure of (V) was determined on a sample prepared from D-[1,3-$^{13}C_2$]glucose using Fischer glycosidation (Podlasek *et al.*, 1995).



Scheme 2

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Hydroxy H atoms were refined freely, while all other H atoms were included in geometrically calculated positions, with C—H = 1.00 (methyne), 0.99 (methylene), 0.95 (aromatic) or 0.98 Å (methyl) and U_{iso}(H) = 1.5U_{eq}(C) for methyl or 1.2U_{eq}(C) for all other H atoms bonded to C atoms. Residual density (0.46 e Å^{-3}) is located 1.17 Å from atom O8 in (III). Inspection of the very weak residual electron density (all 0.3 e Å^{-3} or less) suggests very minor disorder in the benzoyl group associated with atom O8. No attempt was made to model this further. Some structural analysis (Cremer–Pople analysis, some intermolecular interactions) was performed using *PLATON* (Spek, 2009).

Table 1
Experimental details.

	(III)	(IV)	(V)
Crystal data			
Chemical formula	$2C_{61}H_{50}O_{18}\cdot C_4H_8O_2$	$C_{34}H_{28}O_{10}\cdot C_3H_6O$	$2C_7H_{14}O_6\cdot H_2O$
M_r	2230.12	654.64	406.38
Crystal system, space group	Monoclinic, $P2_1$	Orthorhombic, $P2_12_12_1$	Tetragonal, $P4_12_12$
Temperature (K)	120	120	120
a, b, c (Å)	23.9979 (5), 8.8603 (2), 26.2562 (6)	5.6342 (2), 19.9711 (8), 29.6094 (11)	7.3482 (3), 7.3482 (3), 34.1260 (17)
α, β, γ (°)	90, 93.513 (1), 90	90, 90, 90	90, 90, 90
V (Å^3)	5572.3 (2)	3331.7 (2)	1842.67 (17)
Z	2	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.82	0.80	1.14
Crystal size (mm)	0.16 × 0.12 × 0.06	0.21 × 0.13 × 0.09	0.21 × 0.16 × 0.08
Data collection			
Diffractometer	Bruker APEXII	Bruker APEXII	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Numerical (*SADABS*; Krause *et al.*, 2015)	Numerical (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.634, 0.752	0.817, 0.864	0.862, 0.979
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	68691, 15912, 13858	55150, 6526, 6458	27800, 1797, 1786
R_{int}	0.048	0.031	0.034
θ_{max} (°)	59.0	72.2	71.8
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.556	0.618	0.616
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.130, 1.11	0.028, 0.073, 1.03	0.025, 0.067, 1.09
No. of reflections	15912	6526	1797
No. of parameters	1487	436	144
No. of restraints	1	0	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.22	0.16, −0.20	0.21, −0.19
Absolute structure	Flack x determined using 5615 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 2722 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 642 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.16 (6)	−0.08 (3)	0.03 (3)

Computer programs: *APEX2* (Bruker, 2015), *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

3. Results and discussion

Disaccharide (III) crystallized from ethyl acetate/hexane to give crystal *A* with an asymmetric unit containing two molecules of (III) and one molecule of ethyl acetate solvent (Fig. 1). A second crystalline form, crystal *B*, was also obtained with a standard cell containing one molecule of (III) and no solvent, but this crystal was very small and gave lower quality diffraction data (obtained at the Advanced Light Source) than crystal *A*. Diffraction data for crystal *B* have been deposited with the CDCC (CCDC deposition number 1879257; Turney *et al.*, 2018) and are not discussed here. The two molecules of (III) found in crystal *A* are denoted (III*a*) and (III*b*) in the following discussion.

Monosaccharides (IV) and (V) crystallized from acetone and water, respectively (Figs. 2 and 3). The crystal structure of (IV) contained one molecule of acetone in the lattice, and that of (V) contained half a water molecule.

Endocyclic and exocyclic C—C, endocyclic C—O, and *O*-glycosidic C—O bond lengths are minimally affected when multiple *O*-benzoyl groups are introduced into the structure of (I) to give (III) (Table 2). Potential steric crowding caused by proximal *O*-benzoyl groups in a pyranosyl ring does not appear to be manifested in longer endocyclic C—C and C—O bond lengths. In contrast, non-anomeric exocyclic C—O bonds are lengthened by ∼0.02 Å when involved in esterification, and this effect is more pronounced for anomeric C—O bonds (∼0.04 Å; see the C1—O1 bond length in Table 2). The C3—O3 bond length in (I) [1.421 (3) Å] is virtually identical to the average C3—O3 bond length in (III) (1.424 Å), as expected, since atom O3 is un-esterified in both structures. Exocyclic C—O bond-length elongation upon esterification presumably reflects the resonance properties of the ester bond, wherein the partial double-bond character of both C—O bonds involving the carbonyl carbon reduces electron density around the ester O atom and weakens the adjacent C—O bond. Steric crowding may also play a role in C—O bond elongation upon esterification, but the inter-residue C1′—O1′—C4 valence bond angle, a potential indicator of steric crowding, is less than 2° larger in (III) than in (I), indicating that crowding effects on the overall structure are small.

Table 2
Comparison of structural parameters in (I), (III*a*) and (III*b*).

Parameter	(I)	(III*a*)	(III*b*)
Bond lengths and internuclear distances (Å)			
C1—C2	1.516 (3)	1.498 (8)	1.522 (7)
C2—C3	1.519 (3)	1.524 (7)	1.510 (7)
C3—C4	1.531 (3)	1.529 (7)	1.532 (7)
C4—C5	1.530 (3)	1.531 (7)	1.524 (7)
C5—C6	1.508 (3)	1.509 (7)	1.493 (7)
C1′—C2′	1.527 (3)	1.522 (7)	1.522 (7)
C2′—C3′	1.531 (3)	1.508 (7)	1.521 (7)
C3′—C4′	1.521 (3)	1.503 (7)	1.508 (7)
C4′—C5′	1.521 (3)	1.524 (7)	1.524 (7)
C5′—C6′	1.511 (3)	1.494 (7)	1.506 (7)
C1—O1	1.384 (3)	1.437 (6)	1.413 (6)
C1—O5	1.413 (3)	1.398 (6)	1.414 (6)
C2—O2	1.418 (3)	1.442 (6)	1.440 (6)
C3—O3	1.421 (3)	1.413 (6)	1.434 (6)
C5—O5	1.428 (3)	1.440 (6)	1.441 (6)
C6—O6	1.424 (3)	1.447 (6)	1.453 (6)
C1′—O1′	1.387 (3)	1.376 (6)	1.389 (6)
C1′—O5′	1.425 (3)	1.442 (6)	1.430 (6)
C2′—O2′	1.414 (3)	1.429 (6)	1.440 (6)
C3′—O3′	1.422 (3)	1.438 (6)	1.441 (6)
C4′—O4′	1.423 (3)	1.451 (6)	1.443 (6)
C5′—O5′	1.432 (3)	1.438 (6)	1.437 (6)
C6′—O6′	1.426 (3)	1.451 (6)	1.450 (6)
C4—O1′	1.437 (3)	1.435 (6)	1.433 (6)
O1—CH_3	1.420 (4)		
O1—CO		1.369 (7)	1.374 (6)
O3···O5′	2.764 (2)	2.797 (5)	2.806 (5)
Bond angles (°)			
C1′—O1′—C4	116.22 (2)	116.97 (4)	117.92 (4)
C1—O1—CH_3	113.71 (2)		
C1—O1—CO		116.27 (4)	115.48 (4)
Torsion angles (°)			
C2—C1—O1—CH_3 (φ)	164.23 (2)		
C2—C1—O1—CO (φ)		102.31 (5)	108.33 (5)
O5—C1—O1—CH_3 (φ)	−77.35 (3)		
O5—C1—O1—CO (φ)		−139.21 (4)	−133.65 (4)
C2—C3—O3—H	−158.98	−134.24	−152.22
C1—C2—C3—C4	−44.22	−53.61 (5)	−53.42 (5)
C1′—C2′—C3′—C4′	−54.82	−52.55 (6)	−54.48 (6)
C1—O5—C5—C4	67.57	63.33 (5)	65.96 (5)
C1′—O5′—C5′—C4′	64.96	64.28 (5)	63.71 (5)
C2′—C1′—O1′—C4 (φ')	153.78 (2)	151.47 (4)	150.66 (4)
O5′—C1′—O1′—C4 (φ')	−88.44 (2)	−90.91 (5)	−91.97 (5)
C1′—O1′—C4—C3 (ψ')	78.42 (2)	64.87 (5)	66.00 (5)
C1′—O1′—C4—C5 (ψ')	−161.30 (2)	−174.84 (4)	−174.87 (4)
H1′—C1′—O1′—C4 (φ')	31.92	30.01	29.33
C1′—O1′—C4—H4 (ψ')	−43.65	−57.83	−57.32
O5—C5—C6—O6 (ω)	−4.60 (*gg*)	−65.78 (5) (*gg*)	−66.29 (5) (*gg*)
O5′—C5′—C6′—O6′ (ω')	57.26 (*gt*)	67.75 (5) (*gt*)	68.60 (5) (*gt*)

Note: *gg* is *gauche–gauche* and *gt* is *gauche–trans*.

Table 3
Comparison of structural parameters in (IV) and (V).

Parameter	Compound	
	(IV)	(V)
Bond lengths and internuclear distances (Å)		
C1—C2	1.517 (2)	1.525 (2)
C2—C3	1.524 (2)	1.521 (2)
C3—C4	1.524 (2)	1.532 (2)
C4—C5	1.526 (2)	1.527 (2)
C5—C6	1.509 (2)	1.519 (2)
C1—O1	1.420 (2)	1.379 (2)
C1—O5	1.411 (2)	1.439 (2)
C2—O2	1.441 (2)	1.428 (2)
C3—O3	1.416 (2)	1.424 (2)
C4—O4	1.449 (2)	1.427 (2)
C5—O5	1.427 (2)	1.441 (2)
C6—O6	1.440 (2)	1.419 (2)
O1—CH_3		1.440 (2)
O1—CO	1.359 (2)	
Bond angles (°)		
C1—O1—CH_3		112.44 (10)
C1—O1—CO	115.31 (11)	
Torsion angles (°)		
C2—C1—O1—CH_3		170.57 (11)
C2—C1—O1—CO	175.85 (11)	
O5—C1—O1—CH_3		−72.32 (13)
O5—C1—O1—CO	−68.08 (14)	
C2—C3—O3—H	−144.61	174.71
C1—C2—C3—C4	−53.21 (15)	−54.79 (13)
C1—O5—C5—C4	63.87 (15)	63.78 (13)
O5—C5—C6—O6 (ω)	−56.43 (15) (*gg*)	68.93 (13) (*gt*)

Note: *gg* is *gauche–gauche* and *gt* is *gauche–trans*.

The behaviors of the bond lengths in (I) and (III) are maintained in (IV) and (V) (Table 3). For example, the C1—O1 bond is 0.041 Å longer in (IV) than in (V), mimicking the behavior in (III) relative to (I). Likewise, the C2—O2, C4—O4 and C6—O6 bonds in (IV) are, on average, ∼0.02 Å longer than the corresponding bonds in (V). As observed in (I) and (III), the C3—O3 bond lengths in (IV) and (V) differ by less than 0.01 Å.

Glycosidic torsion angles φ and ψ in (III) (the definitions of φ and ψ are shown in Scheme 2) are affected differently by *O*-benzoylation. The φ torsion angle is virtually unchanged [for example, the C2′—C1′—O1′—C4 torsion angles in (I) and (III) (Table 2) vary by less than 3°]. In contrast, the effect of *O*-benzoylation on ψ is significant; for example, the C1′—O1′—C4—C3 torsion angle in (I) is ∼13° larger than the corresponding torsion angle in (III) (Table 2). These results suggest a greater malleability of ψ than of φ in response to multiple *O*-benzoylation, although this behavior is probably context dependent.

The effect of *O*-benzoylation on aldopyranosyl ring pucker is reflected in the Cremer–Pople values calculated for each ring in (I), (III*a*), (III*b*), (IV) and (V) (Table 4) (Cremer & Pople, 1975; Spek, 2009). The βGal*p* rings in (I) and (III) are less distorted than the βGlc*p* rings in these disaccharides, as reflected in the smaller values of θ (*i.e.* 2.7°–5.0° for βGal*p* and 6.9–12.0° for βGlc*p*). The range of ring distortion is modest in both βGal*p* and βGlc*p* rings, reflected in the 77° range in φ values for the former and 57° range for the latter. The βGal*p* rings, while less displaced conformationally from idealized $^4C_1$ chair conformers than the βGlc*p* rings, adopt a slightly broader range of distorted chair forms than the βGlc*p* rings. A comparison of the Cremer–Pople values for (IV) and (V) shows that *O*-benzoylation results in a reduction in θ, as observed between the βGlc*p* residues in (I) and (III). Thus, perhaps contrary to expectation, *O*-benzoylation renders the $^4C_1$ chair form of the βGlc*p* ring more ideal. The Cremer–Pople φ values for (IV), and (V) differ from those observed for the βGlc*p* rings in (III) and (I), respectively, indicating that context affects the direction of distortion. The βGlc*p* ring in (IV) is slightly distorted towards $^{3,0}B$, whereas the same ring in

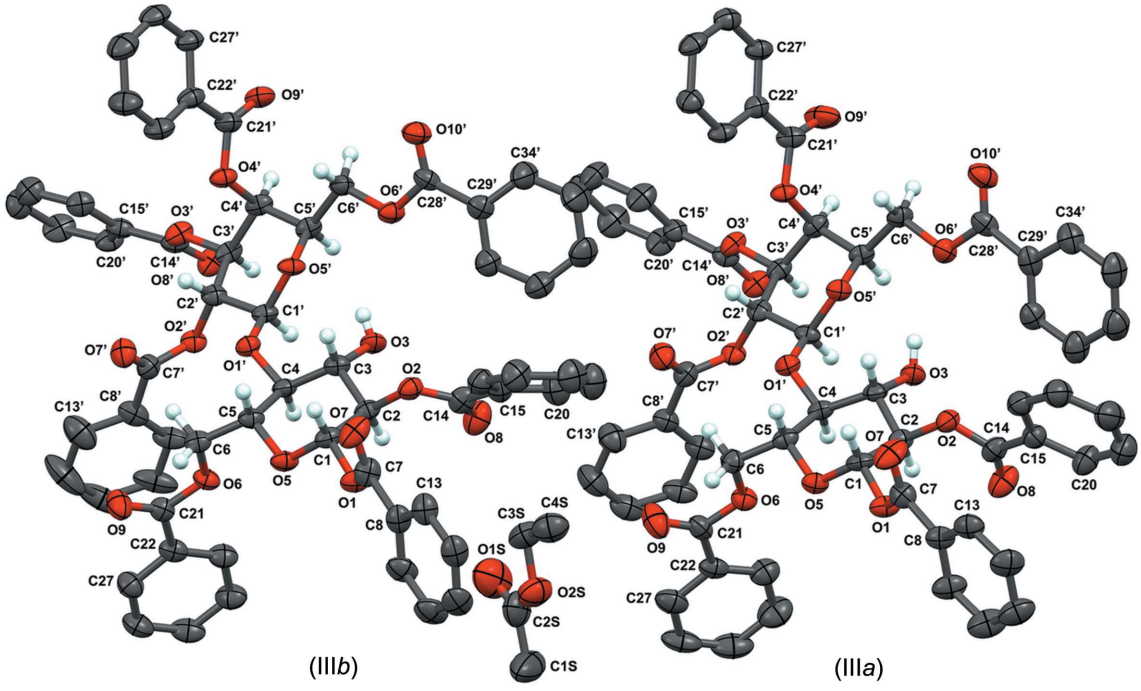


Figure 1
Labeling scheme for (III*a*) (right) and (III*b*) (left). Most H atoms have been omitted for clarity. Atomic displacement ellipsoids are represented at the 50% probability level and H atoms are represented as spheres of arbitrary radius.

(III) shows a greater distortion towards the $^3S_1$ form. The βGlc*p* rings in (V) and (I) are distorted towards the $^3S_1$ and $^0S_2$ forms, respectively.

O-Benzoyl side-chain conformations in (III*a*) and (III*b*) were evaluated using two internuclear distances, *i.e.* r_1 and r_2, to characterize the conformation about the three rotatable bonds, *i.e.* θ_1, $\theta_{1'}$, and θ_2 (see Fig. 4 for the definition of r_1, r_2, θ_1, $\theta_{1'}$, and θ_2), in these side-chains. The values of r_1, which are determined by θ_1 and $\theta_{1'}$, average ~2.27 Å for 2°-OH benzoates and ~2.58 Å for 1°-OH benzoates (Table 5). For the former, the distances correspond to conformations about θ_1

Table 4
Cremer–Pople puckering parameters for aldopyranosyl residues in (I), (III*a*), (III*b*), (IV), and (V).

Compound/ residue	θ (°)	φ (°)	Q (Å)	q_2 (Å)	q_3 (Å)
(I): βGal*p*	4.7	28.2	0.5948	0.0485	0.5928
(I): βGlc*p*	12.0	341.5	0.5579	0.1159	0.5457
(III*a*): βGal*p*	5.0 (5)	347 (6)	0.575 (5)	0.053 (5)	0.573 (5)
(III*a*): βGlc*p*	7.8 (5)	38 (4)	0.595 (5)	0.080 (5)	0.590 (5)
(III*b*): βGal*p*	2.7 (5)	311 (9)	0.583 (5)	0.030 (5)	0.583 (5)
(III*b*): βGlc*p*	6.9 (5)	18 (4)	0.607 (5)	0.071 (5)	0.603 (5)
(IV): βGlc*p*	3.4 (2)	1 (3)	0.585 (2)	0.035 (2)	0.584 (2)
(V): βGlc*p*	7.5 (1)	41.9 (1)	0.604 (1)	0.079 (1)	0.599 (1)

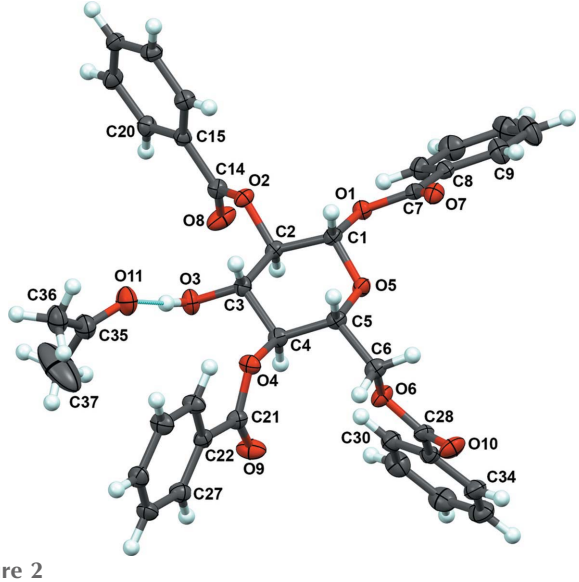


Figure 2
Labeling scheme for (IV). Atomic displacement ellipsoids are represented at the 50% probability level and H atoms are represented as spheres of arbitrary radius. The dashed line represents an intermolecular O—H···O hydrogen bond.

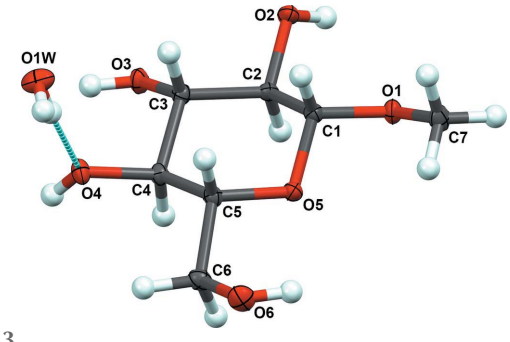


Figure 3
Labeling scheme for (V). Atomic displacement ellipsoids are represented at the 50% probability level and H atoms are represented as spheres of arbitrary radius. The dashed line represents an intermolecular O—H···O hydrogen bond.

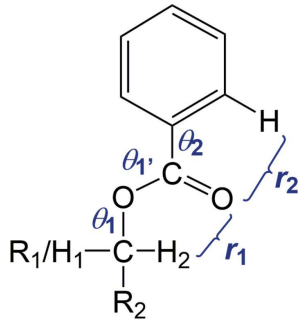


Figure 4
The internuclear distances, r_1 and r_2, used to characterize the *O*-benzoyl side-chain conformations in (III) and (IV). Distances r_1 and r_2 are sensitive to torsion angles θ_1 and $\theta_{1'}$, and θ_2, respectively. The pyranosyl ring C atom bearing the benzoylated O atom may bear two *R* groups (2°-OH) or one *R* group (1°-OH).

and $\theta_{1'}$ in which the carbonyl O atom eclipses the C—H bond; the latter occurs when the H—C_{alk}—O—C_{car} (θ_1) and C_{alk}—O—C_{car}═O_{car} ($\theta_{1'}$) torsion angles are close to, or equal to, 0°. The range of r_1 values appears to be greater for 1°-OH benzoates than for 2°-OH benzoates; in the former, the C═O bond bisects the H6*R*—C6—H6*S* bond angle, as reflected in the roughly equal r_1 values for the two diastereotopic C6 H atoms (Table 5). The greater range of r_1 for the 1°-OH benzoates, encoded in their standard deviations, presumably reflects a wider and flatter energy surface as θ_1 and/or $\theta_{1'}$ are rotated, compared to that for the 2°-OH benzoates. In contrast to r_1, the r_2 values, determined by the O_{car}═C_{car}—C_{ar}—C'_{ar} torsion angles, θ_2, are largely independent of the type of alcohol involved in esterification and exhibit less variability [2.543±0.032 and 2.551±0.039 Å in (III*a*) and (III*b*), respectively] (Table 5).

The behavior of the *O*-benzoyl side-chains in (IV) is similar to that found in (III) (Table 5). Preferred values of r_1 show greater variability on average than those of r_2. The average values of r_2 in (III) and (IV) are essentially identical, with similar standard deviations. However, r_1 for the *O*-benzoyl group at C1 of (IV) (2.537 Å) is significantly greater than that found in (III) (2.205 and 2.253 Å) due to an aberrant θ_1 (53°) compared to typical values of less than ±20°, while the average r_1 value for the O6-benzoyl group of (IV) is somewhat larger than those for the same groups in (III). These side-chain distortions at atoms C1 and C6 of (IV) are presumably caused by different packing forces in the crystals of (III) and (IV). In general, however, the conformational behaviors of the *O*-benzoyl side-chains in the crystal structures of (III) and (IV) mimic that of the *O*-acetyl side-chains observed in aqueous solutions of *O*-acetylated saccharides (Turney *et al.*, 2017).

An analysis of θ_1 and $\theta_{1'}$ values for the 2°-OH benzoyl side-chains in (III) and (IV) yields average values of −2.08±20.35° for θ_1 (H—C_{alk}—O—C_{car}) and 2.89±8.10° for $\theta_{1'}$ (C_{alk}—O—C_{car}═O_{car}). These findings point to unequal torsional properties of the two C—O bonds involving the ester O atom. The C_{alk}—O—C_{car}═O_{car} torsion angle is more constrained relative to the H—C_{alk}—O—C_{car} torsion angle. Thus, in most but not all cases, different values of r_1 are caused by different values of θ_1.

The crystal structure of (III) exhibits aromatic ring stacking involving the *O*-benzoyl groups attached to atoms O6 and O2′. This stacking is made possible by the *gg* exocyclic hydroxymethyl group conformation in the Glc residue, which allows the O6 benzoyl ring to be oriented nearly parallel to the O2′-benzoyl ring. While the two rings are not perfectly stacked, the interaction may indirectly influence the *O*-glycosidic linkage torsion angles, φ and ψ, in the crystal structure of (III), and potentially bias these angles in solution.

Structures (III*a*), (III*b*) and (IV) are largely devoid of free hydroxy H atoms that can potentially participate as donors or acceptors in intra- and intermolecular hydrogen bonding (Tables 6, 7 and 8). This situation differs significantly from that of (I), where extensive hydrogen bonding is observed involving hydroxyl H atoms as donors and hydroxyl, pyranosyl ring and/or glycosidic O atoms as acceptors. In (III*a*) and (III*b*), the carbonyl O atoms of the benzoyl side-chains often serve as single or dual hydrogen-bond acceptors, while the ester O atoms do so less often, but the participating donors in all cases are either C—H bonds in proximal pyranosyl rings or in proximal aromatic rings of benzoyl side-chains. The only conventional hydrogen bonds observed in (III*a*) and (III*b*) are those between O3H and O5′, where the O3···O5′ internuclear distances are ∼2.80 Å, a value similar to that observed in (I) [2.764 (2) Å] (Table 2). In (IV), hydroxyl group O3H serves as a donor in a hydrogen bond to the carbonyl O atom of an acetone solvent molecule in the crystal lattice. However, the hydroxyl O3H atom does not serve as a hydrogen-bond acceptor. The C2—C3—O3—H torsion angles in (I),

Table 5
Characterization of *O*-benzoyl ester side-chain conformations in (III) and (IV) using internuclear distances r_1 and r_2 (Fig. 4).

Substitution site	Internuclear distance (Å)					
	r_1 (III*a*)	r_1 (III*b*)	r_1 (IV)	r_2 (III*a*)	r_2 (III*b*)	r_2 (IV)
C1	2.253	2.205	2.537	2.535	2.549	2.512
C2	2.286	2.381	2.271	2.558	2.596	2.538
C4			2.333			2.569
C6[b]	2.439	2.445	2.518	2.503	2.507	2.565
	2.653	2.693	2.771			
C2′	2.325	2.330		2.601	2.611	
C3′	2.187	2.178		2.553	2.533	
C4′	2.252	2.271		2.521	2.517	
C6′[b]	2.601	2.597		2.528	2.547	
	2.604	2.575				
Avg±SD[a]	2.261±0.051[c]	2.273±0.085[c]	2.380±0.139[c]	2.543±0.032	2.551±0.039	2.546±0.027
	2.574±0.093[d]	2.578±0.102[d]	2.645±0.179[d]			

Notes: (*a*) SD = standard deviation; (*b*) the two values of r_1 shown are the internuclear distances between the ester carbonyl O atom and the two diastereotopic H atoms on C6 (H6*R* and H6*S*). (*c*) For 2°-OH benzoates. (*d*) For 1°-OH benzoates. See Fig. 4 for definitions of r_1 and r_2.

Table 6
Hydrogen-bond geometry (Å, °) for (III).

D—H···A	D—H	H···A	D···A	D—H···A
O3_1—H3O_1···O5′_1	0.79 (7)	2.32 (7)	2.797 (5)	120 (6)
O3_1—H3O_1···O6′_1	0.79 (7)	2.39 (7)	3.147 (6)	160 (6)
O3_2—H3O_2···O5′_2	0.73 (7)	2.19 (7)	2.806 (5)	142 (7)
O3_2—H3O_2···O6′_2	0.73 (7)	2.62 (7)	3.256 (5)	146 (6)

Table 7
Hydrogen-bond geometry (Å, °) for (IV).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O11	0.84	1.96	2.780 (2)	164

(III*a*), and (III*b*) are −159, −134, and −152°, respectively, which orient the O3H hydrogen towards O5′ in the three structures. The C2—C3—O3—H torsion angle is −145° in (IV) and 175° in (V), that is, in conformations not much different from those in (I) and (III). Thus, while inter-residue hydrogen bonding may bias the orientation of O3H in (I) and (III), hydrogen bonding may not be the sole factor dictating this orientation, given the C3—O3 bond torsion angles in (IV) and (V), where inter-residue hydrogen bonding cannot occur.

Despite the large number of aromatic rings in (III*a*) and (III*b*), there is a paucity of significant direction-specific inter- and intramolecular interactions, particularly π–π interactions. The shortest aromatic ring–aromatic ring distances observed in the two structures exceed 3.6 Å, which lie outside the range where relatively strong π-stacking interactions occur (Spek, 2009).

In summary, the crystal structures of (III) and (IV) have been determined, and the resulting structural data will be useful in future studies of the hydrogen-bonding properties of these molecules in solution using NMR spectroscopy and other analytical methods.

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Table 8
Hydrogen-bond geometry (Å, °) for (V).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···O5^{i}	0.83 (2)	2.12 (2)	2.952 (2)	172 (2)
O3—H3O···O2^{ii}	0.84 (3)	1.91 (3)	2.740 (2)	169 (2)
O4—H4O···O3^{ii}	0.84 (2)	1.85 (2)	2.679 (2)	172 (2)
O6—H6O···O1*W*^{iii}	0.86 (3)	2.12 (3)	2.944 (2)	160 (2)
O1*W*—H1*WA*···O4^{iv}	0.84 (2)	1.89 (2)	2.731 (2)	173 (2)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{3}{4}$; (ii) $x-\frac{1}{2}, -y+\frac{5}{2}, -z+\frac{3}{4}$; (iii) $x, y-1, z$; (iv) $y-1, x+1, -z+1$.

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supporting information

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O-Benzoyl side-chain conformations in 2,3,4,6-tetra-*O*-benzoyl-*β*-D-galacto-pyranosyl-(1→4)-1,2,6-tri-*O*-benzoyl-*β*-D-glucopyranose (ethyl acetate solvate) and 1,2,4,6-tetra-*O*-benzoyl-*β*-D-glucopyranose (acetone solvate)

Toby Turney, Qingfeng Pan, Wenhui Zhang, Allen G. Oliver and Anthony S. Serianni

Computing details

For all structures, data collection: *APEX2* (Bruker, 2015); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

2,3,4,6-Tetra-*O*-benzoyl-*β*-*D*-galactopyranosyl-(1→4)-1,2,6-tri-*O*-benzoyl-*β*-*D*-glucopyranose ethyl acetate hemisolvate (III)

Crystal data

$2C_{61}H_{50}O_{18}\cdot C_4H_8O_2$
M_r = 2230.12
Monoclinic, $P2_1$
a = 23.9979 (5) Å
b = 8.8603 (2) Å
c = 26.2562 (6) Å
β = 93.513 (1)°
V = 5572.3 (2) Å^3
Z = 2
$F(000)$ = 2336
D_x = 1.329 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9930 reflections
θ = 2.4–57.0°
μ = 0.82 mm^{-1}
T = 120 K
Blade, colorless
0.16 × 0.12 × 0.06 mm

Data collection

Bruker APEXII diffractometer
Radiation source: Incoatec micro-focus
Detector resolution: 8.33 pixels mm^{-1}
combination of ω and φ–scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.634, T_{max} = 0.752
68691 measured reflections
15912 independent reflections
13858 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 59.0°, θ_{min} = 1.7°
h = −26→26
k = −9→9
l = −28→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.130
S = 1.11
15912 reflections
1487 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 2.2199P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Absolute structure: Flack *x* determined using 5615 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.16 (6)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1_1	0.85594 (14)	−0.1830 (4)	0.55659 (15)	0.0371 (9)
O2_1	0.77338 (14)	−0.0691 (4)	0.61459 (14)	0.0372 (9)
O3_1	0.73839 (18)	0.2327 (4)	0.59165 (14)	0.0372 (9)
H3O_1	0.705 (3)	0.238 (7)	0.591 (2)	0.05 (2)*
O5_1	0.83948 (14)	0.0023 (4)	0.49731 (13)	0.0333 (8)
O6_1	0.86665 (15)	0.2680 (4)	0.44280 (14)	0.0357 (9)
O7_1	0.79418 (19)	−0.3742 (5)	0.55047 (17)	0.0585 (12)
O8_1	0.83919 (19)	0.0075 (5)	0.67409 (16)	0.0535 (11)
O9_1	0.8893 (2)	0.2840 (5)	0.36185 (18)	0.0625 (13)
C1_1	0.8144 (2)	−0.0811 (6)	0.5349 (2)	0.0346 (13)
H1_1	0.781619	−0.138652	0.519564	0.042*
C2_1	0.7965 (2)	0.0229 (6)	0.5758 (2)	0.0335 (12)
H2_1	0.829137	0.081692	0.590641	0.040*
C3_1	0.7517 (2)	0.1296 (6)	0.5532 (2)	0.0339 (12)
H3_1	0.717572	0.069903	0.542447	0.041*
C4_1	0.7734 (2)	0.2082 (5)	0.5065 (2)	0.0305 (12)
H4_1	0.802797	0.283331	0.517672	0.037*
C5_1	0.7977 (2)	0.0935 (6)	0.4703 (2)	0.0319 (12)
H5_1	0.766731	0.025429	0.457248	0.038*
C6_1	0.8234 (2)	0.1637 (6)	0.4249 (2)	0.0368 (13)
H6A_1	0.839492	0.083979	0.403873	0.044*
H6B_1	0.794397	0.217748	0.403578	0.044*
O1′_1	0.73017 (14)	0.2818 (4)	0.47550 (13)	0.0335 (8)
O2′_1	0.73105 (14)	0.5826 (4)	0.43640 (13)	0.0345 (8)
O3′_1	0.62427 (14)	0.7234 (4)	0.43493 (13)	0.0350 (9)
O4′_1	0.56144 (14)	0.4847 (3)	0.46937 (13)	0.0311 (8)
O5′_1	0.65583 (14)	0.3411 (4)	0.52118 (13)	0.0311 (8)
O6′_1	0.61436 (15)	0.3033 (4)	0.61635 (14)	0.0374 (9)
O7′_1	0.72748 (17)	0.4454 (5)	0.36413 (15)	0.0481 (10)
O8′_1	0.67386 (16)	0.9196 (4)	0.46755 (15)	0.0402 (9)
O9′_1	0.48860 (17)	0.5924 (6)	0.50503 (18)	0.0628 (13)
O10′_1	0.53380 (18)	0.2183 (4)	0.64377 (16)	0.0510 (11)
C1′_1	0.7035 (2)	0.4011 (5)	0.4971 (2)	0.0301 (12)

H1′_1	0.729188	0.454066	0.522598	0.036*
C2′_1	0.6833 (2)	0.5086 (6)	0.4547 (2)	0.0324 (12)
H2′_1	0.662687	0.452072	0.426411	0.039*
C3′_1	0.6464 (2)	0.6283 (5)	0.4757 (2)	0.0323 (12)
H3′_1	0.670113	0.692456	0.499744	0.039*
C4′_1	0.5996 (2)	0.5653 (5)	0.5047 (2)	0.0334 (12)
H4′_1	0.579438	0.648884	0.521371	0.040*
C5′_1	0.6245 (2)	0.4569 (5)	0.5450 (2)	0.0294 (12)
H5′_1	0.650381	0.514701	0.569007	0.035*
C6′_1	0.5823 (2)	0.3788 (6)	0.5752 (2)	0.0334 (12)
H6′A_1	0.556095	0.452513	0.588850	0.040*
H6′B_1	0.560734	0.304687	0.553715	0.040*
C7_1	0.8382 (2)	−0.3261 (6)	0.5667 (2)	0.0384 (13)
C8_1	0.8788 (2)	−0.4079 (6)	0.6012 (2)	0.0367 (13)
C9_1	0.9317 (2)	−0.3514 (7)	0.6153 (3)	0.0499 (16)
H9_1	0.943922	−0.259435	0.601113	0.060*
C10_1	0.9663 (3)	−0.4292 (7)	0.6499 (3)	0.0639 (19)
H10_1	1.002480	−0.391074	0.659121	0.077*
C11_1	0.9489 (3)	−0.5617 (8)	0.6712 (3)	0.0624 (19)
H11_1	0.972746	−0.613366	0.695648	0.075*
C12_1	0.8960 (3)	−0.6203 (7)	0.6568 (3)	0.0536 (17)
H12_1	0.883995	−0.712504	0.670992	0.064*
C13_1	0.8614 (3)	−0.5430 (6)	0.6219 (2)	0.0439 (14)
H13_1	0.825601	−0.582438	0.611934	0.053*
C14_1	0.8024 (2)	−0.0788 (6)	0.6603 (2)	0.0394 (13)
C15_1	0.7837 (2)	−0.2085 (6)	0.6912 (2)	0.0392 (13)
C16_1	0.7452 (2)	−0.3132 (6)	0.6714 (2)	0.0435 (14)
H16_1	0.729457	−0.302883	0.637459	0.052*
C17_1	0.7301 (3)	−0.4318 (7)	0.7011 (3)	0.0546 (17)
H17_1	0.703553	−0.503189	0.687660	0.065*
C18_1	0.7529 (3)	−0.4491 (9)	0.7503 (3)	0.065 (2)
H18_1	0.741592	−0.531071	0.770585	0.078*
C19_1	0.7919 (3)	−0.3476 (9)	0.7700 (3)	0.0648 (19)
H19_1	0.807953	−0.359664	0.803773	0.078*
C20_1	0.8076 (3)	−0.2278 (7)	0.7403 (2)	0.0514 (16)
H20_1	0.834841	−0.158200	0.753520	0.062*
C21_1	0.8981 (2)	0.3198 (6)	0.4058 (2)	0.0401 (14)
C22_1	0.9441 (2)	0.4236 (6)	0.4252 (2)	0.0380 (14)
C23_1	0.9504 (3)	0.4662 (6)	0.4749 (2)	0.0476 (15)
H23_1	0.924401	0.433810	0.498471	0.057*
C24_1	0.9957 (3)	0.5590 (8)	0.4911 (3)	0.0647 (19)
H24_1	1.001254	0.588553	0.525785	0.078*
C25_1	1.0322 (3)	0.6064 (8)	0.4551 (3)	0.067 (2)
H25_1	1.062763	0.669859	0.465490	0.081*
C26_1	1.0251 (3)	0.5637 (7)	0.4056 (3)	0.0587 (19)
H26_1	1.050612	0.596950	0.381685	0.070*
C27_1	0.9805 (2)	0.4712 (7)	0.3898 (3)	0.0508 (16)
H27_1	0.975177	0.441215	0.355087	0.061*

C7′_1	0.7499 (2)	0.5406 (6)	0.3912 (2)	0.0348 (13)
C8′_1	0.8010 (2)	0.6246 (6)	0.3790 (2)	0.0355 (13)
C9′_1	0.8323 (2)	0.7036 (6)	0.4160 (2)	0.0402 (14)
H9′_1	0.821216	0.706046	0.450124	0.048*
C10′_1	0.8803 (2)	0.7796 (6)	0.4032 (3)	0.0471 (15)
H10′_1	0.901849	0.833501	0.428689	0.056*
C11′_1	0.8966 (3)	0.7775 (6)	0.3544 (3)	0.0512 (17)
H11′_1	0.929198	0.830107	0.345904	0.061*
C12′_1	0.8654 (3)	0.6986 (8)	0.3175 (3)	0.0620 (19)
H12′_1	0.876562	0.697434	0.283359	0.074*
C13′_1	0.8183 (3)	0.6215 (7)	0.3297 (2)	0.0516 (16)
H13′_1	0.797481	0.565814	0.304165	0.062*
C14′_1	0.6428 (2)	0.8685 (6)	0.4347 (2)	0.0324 (12)
C15′_1	0.6197 (2)	0.9520 (6)	0.3890 (2)	0.0351 (13)
C16′_1	0.5828 (3)	0.8875 (6)	0.3525 (2)	0.0456 (15)
H16′_1	0.570275	0.786773	0.356763	0.055*
C17′_1	0.5640 (3)	0.9688 (7)	0.3100 (2)	0.0536 (17)
H17′_1	0.538462	0.924581	0.285251	0.064*
C18′_1	0.5828 (3)	1.1154 (7)	0.3035 (2)	0.0520 (17)
H18′_1	0.570467	1.171437	0.274068	0.062*
C19′_1	0.6193 (3)	1.1793 (7)	0.3400 (3)	0.0572 (18)
H19′_1	0.632038	1.279643	0.335497	0.069*
C20′_1	0.6375 (2)	1.1000 (6)	0.3826 (2)	0.0454 (15)
H20′_1	0.662111	1.145933	0.407680	0.055*
C21′_1	0.5058 (2)	0.5101 (6)	0.4733 (2)	0.0354 (13)
C22′_1	0.4705 (2)	0.4251 (6)	0.4357 (2)	0.0326 (12)
C23′_1	0.4927 (2)	0.3260 (6)	0.4010 (2)	0.0354 (13)
H23′_1	0.531828	0.309811	0.401391	0.042*
C24′_1	0.4568 (2)	0.2508 (7)	0.3656 (2)	0.0426 (14)
H24′_1	0.471331	0.183079	0.341698	0.051*
C25′_1	0.3992 (2)	0.2759 (6)	0.3657 (2)	0.0429 (14)
H25′_1	0.374593	0.225708	0.341505	0.051*
C26′_1	0.3781 (2)	0.3722 (6)	0.4003 (2)	0.0388 (14)
H26′_1	0.338961	0.387367	0.400405	0.047*
C27′_1	0.4131 (2)	0.4472 (6)	0.4350 (2)	0.0360 (13)
H27′_1	0.397985	0.514637	0.458737	0.043*
C28′_1	0.5837 (2)	0.2266 (5)	0.6490 (2)	0.0368 (13)
C29′_1	0.6191 (3)	0.1500 (6)	0.6908 (2)	0.0387 (14)
C30′_1	0.6760 (3)	0.1684 (6)	0.6974 (2)	0.0424 (14)
H30′_1	0.695045	0.230294	0.674589	0.051*
C31′_1	0.7052 (3)	0.0968 (7)	0.7371 (2)	0.0540 (17)
H31′_1	0.744369	0.111864	0.742268	0.065*
C32′_1	0.6780 (3)	0.0035 (7)	0.7693 (3)	0.0576 (18)
H32′_1	0.698680	−0.048336	0.795927	0.069*
C33′_1	0.6219 (3)	−0.0148 (7)	0.7633 (2)	0.0554 (18)
H33′_1	0.603162	−0.076702	0.786310	0.066*
C34′_1	0.5918 (3)	0.0569 (6)	0.7234 (2)	0.0463 (15)
H34′_1	0.552642	0.042074	0.718573	0.056*

O1_2	0.84604 (14)	0.2635 (4)	0.07633 (14)	0.0372 (9)
O2_2	0.75556 (15)	0.3668 (4)	0.12666 (14)	0.0362 (9)
O3_2	0.72191 (18)	0.6747 (4)	0.10155 (15)	0.0373 (9)
H3O_2	0.694 (3)	0.693 (8)	0.091 (2)	0.05 (2)*
O5_2	0.83283 (14)	0.4445 (4)	0.01627 (14)	0.0346 (8)
O6_2	0.86187 (14)	0.6982 (4)	−0.04511 (14)	0.0355 (9)
O7_2	0.78722 (19)	0.0664 (4)	0.06455 (16)	0.0526 (11)
O8_2	0.7913 (2)	0.4889 (5)	0.19624 (16)	0.0572 (12)
O9_2	0.88717 (18)	0.6898 (5)	−0.12596 (16)	0.0544 (11)
C1_2	0.8051 (2)	0.3589 (5)	0.0525 (2)	0.0327 (12)
H1_2	0.774381	0.297845	0.035271	0.039*
C2_2	0.7819 (2)	0.4649 (5)	0.0916 (2)	0.0320 (12)
H2_2	0.812649	0.523992	0.109682	0.038*
C3_2	0.7400 (2)	0.5692 (5)	0.0646 (2)	0.0307 (12)
H3_2	0.707218	0.508554	0.051119	0.037*
C4_2	0.7663 (2)	0.6480 (6)	0.0200 (2)	0.0326 (12)
H4_2	0.795383	0.721218	0.033243	0.039*
C5_2	0.7923 (2)	0.5314 (5)	−0.0140 (2)	0.0320 (12)
H5_2	0.761942	0.460475	−0.026164	0.038*
C6_2	0.8185 (2)	0.5899 (6)	−0.0602 (2)	0.0337 (12)
H6C_2	0.834769	0.505153	−0.078886	0.040*
H6D_2	0.789719	0.638969	−0.083259	0.040*
O2′_2	0.73415 (14)	1.0263 (4)	−0.05267 (13)	0.0330 (8)
O3′_2	0.62946 (15)	1.1682 (4)	−0.06736 (14)	0.0363 (9)
O1′_2	0.72620 (14)	0.7235 (4)	−0.01375 (13)	0.0315 (8)
O4′_2	0.56165 (14)	0.9299 (4)	−0.03920 (14)	0.0335 (8)
O5′_2	0.64768 (13)	0.7910 (3)	0.02464 (13)	0.0305 (8)
O6′_2	0.59142 (14)	0.7601 (4)	0.11354 (14)	0.0362 (9)
O7′_2	0.73943 (17)	0.8832 (4)	−0.12360 (15)	0.0461 (10)
O8′_2	0.66683 (16)	1.3712 (4)	−0.02683 (15)	0.0414 (10)
O9′_2	0.48279 (15)	1.0124 (4)	−0.00685 (16)	0.0441 (10)
O10′_2	0.50621 (17)	0.6740 (4)	0.12857 (16)	0.0464 (10)
C1′_2	0.6981 (2)	0.8465 (5)	0.0051 (2)	0.0303 (12)
H1′_2	0.721628	0.899199	0.032347	0.036*
C2′_2	0.6836 (2)	0.9521 (5)	−0.0395 (2)	0.0322 (12)
H2′_2	0.666308	0.895128	−0.069305	0.039*
C3′_2	0.6450 (2)	1.0771 (5)	−0.0233 (2)	0.0302 (12)
H3′_2	0.665622	1.141660	0.002780	0.036*
C4′_2	0.5938 (2)	1.0136 (5)	−0.0005 (2)	0.0327 (12)
H4′_2	0.570781	1.097410	0.012625	0.039*
C5′_2	0.6133 (2)	0.9093 (5)	0.0432 (2)	0.0320 (12)
H5′_2	0.635638	0.969146	0.069440	0.038*
C6′_2	0.5662 (2)	0.8321 (6)	0.0682 (2)	0.0338 (12)
H6′C_2	0.537723	0.906560	0.077421	0.041*
H6′D_2	0.548122	0.756185	0.044966	0.041*
C7_2	0.8306 (3)	0.1151 (6)	0.0813 (2)	0.0399 (14)
C8_2	0.8749 (3)	0.0234 (6)	0.1097 (2)	0.0399 (14)
C9_2	0.9289 (3)	0.0734 (7)	0.1183 (2)	0.0487 (16)

H9_2	0.939464	0.170079	0.106613	0.058*
C10_2	0.9680 (3)	−0.0190 (7)	0.1444 (3)	0.0563 (18)
H10_2	1.005705	0.013456	0.149538	0.068*
C11_2	0.9523 (3)	−0.1567 (7)	0.1626 (3)	0.0530 (17)
H11_2	0.979103	−0.218361	0.180801	0.064*
C12_2	0.8984 (3)	−0.2062 (6)	0.1549 (2)	0.0478 (16)
H12_2	0.887835	−0.301588	0.167774	0.057*
C13_2	0.8589 (3)	−0.1162 (6)	0.1280 (2)	0.0448 (15)
H13_2	0.821458	−0.149996	0.122320	0.054*
C14_2	0.7682 (3)	0.3798 (6)	0.1767 (2)	0.0419 (14)
C15_2	0.7510 (2)	0.2431 (6)	0.2057 (2)	0.0421 (14)
C16_2	0.7379 (2)	0.1106 (7)	0.1814 (2)	0.0453 (15)
H16_2	0.736603	0.105926	0.145234	0.054*
C17_2	0.7264 (3)	−0.0167 (7)	0.2093 (3)	0.0549 (17)
H17_2	0.717776	−0.109057	0.192165	0.066*
C18_2	0.7276 (3)	−0.0102 (8)	0.2617 (3)	0.0603 (18)
H18_2	0.720406	−0.098485	0.280807	0.072*
C19_2	0.7389 (3)	0.1229 (8)	0.2864 (3)	0.068 (2)
H19_2	0.738260	0.128164	0.322490	0.081*
C20_2	0.7515 (3)	0.2512 (8)	0.2585 (3)	0.0579 (17)
H20_2	0.760363	0.343434	0.275548	0.070*
C21_2	0.8943 (2)	0.7377 (6)	−0.0832 (2)	0.0342 (13)
C22_2	0.9409 (2)	0.8404 (6)	−0.0658 (2)	0.0367 (13)
C23_2	0.9492 (2)	0.8934 (6)	−0.0167 (2)	0.0424 (14)
H23_2	0.923454	0.867660	0.007982	0.051*
C24_2	0.9949 (3)	0.9843 (7)	−0.0027 (3)	0.0476 (15)
H24_2	1.001163	1.018654	0.031418	0.057*
C25_2	1.0311 (3)	1.0237 (6)	−0.0395 (3)	0.0492 (16)
H25_2	1.062235	1.086339	−0.030327	0.059*
C26_2	1.0231 (3)	0.9750 (7)	−0.0885 (3)	0.0517 (16)
H26_2	1.048343	1.003658	−0.113264	0.062*
C27_2	0.9779 (2)	0.8832 (7)	−0.1021 (2)	0.0450 (15)
H27_2	0.972048	0.849263	−0.136289	0.054*
C7′_2	0.7581 (2)	0.9813 (6)	−0.0953 (2)	0.0357 (13)
C8′_2	0.8099 (2)	1.0702 (6)	−0.1026 (2)	0.0400 (14)
C9′_2	0.8383 (2)	1.1442 (6)	−0.0632 (3)	0.0450 (15)
H9′_2	0.824807	1.139890	−0.029937	0.054*
C10′_2	0.8863 (3)	1.2252 (6)	−0.0712 (3)	0.062 (2)
H10′_2	0.906389	1.274716	−0.043732	0.075*
C11′_2	0.9043 (3)	1.2325 (8)	−0.1197 (4)	0.082 (3)
H11′_2	0.936668	1.289662	−0.125899	0.099*
C12′_2	0.8764 (4)	1.1586 (9)	−0.1593 (4)	0.089 (3)
H12′_2	0.889684	1.164618	−0.192620	0.107*
C13′_2	0.8293 (3)	1.0759 (7)	−0.1513 (3)	0.064 (2)
H13′_2	0.810251	1.023271	−0.178646	0.077*
C14′_2	0.6453 (2)	1.3151 (6)	−0.0647 (2)	0.0328 (12)
C15′_2	0.6330 (2)	1.3953 (6)	−0.1136 (2)	0.0338 (13)
C16′_2	0.6052 (2)	1.3274 (6)	−0.1553 (2)	0.0363 (13)

H16′_2	0.593069	1.225654	−0.153276	0.044*
C17′_2	0.5951 (3)	1.4085 (6)	−0.2001 (2)	0.0445 (15)
H17′_2	0.574988	1.363437	−0.228424	0.053*
C18′_2	0.6144 (3)	1.5559 (6)	−0.2033 (2)	0.0472 (15)
H18′_2	0.608488	1.610644	−0.234286	0.057*
C19′_2	0.6423 (2)	1.6229 (6)	−0.1615 (2)	0.0462 (15)
H19′_2	0.654971	1.724154	−0.163711	0.055*
C20′_2	0.6517 (2)	1.5443 (6)	−0.1169 (2)	0.0380 (13)
H20′_2	0.670772	1.590784	−0.088292	0.046*
C21′_2	0.5056 (2)	0.9384 (6)	−0.0379 (2)	0.0379 (13)
C22′_2	0.4760 (2)	0.8449 (6)	−0.0783 (2)	0.0363 (13)
C23′_2	0.5034 (2)	0.7502 (7)	−0.1100 (2)	0.0466 (15)
H23′_2	0.542897	0.741865	−0.106541	0.056*
C24′_2	0.4731 (3)	0.6672 (7)	−0.1467 (3)	0.0554 (17)
H24′_2	0.491944	0.600601	−0.168261	0.067*
C25′_2	0.4157 (3)	0.6807 (8)	−0.1523 (3)	0.0572 (18)
H25′_2	0.395260	0.625351	−0.178141	0.069*
C26′_2	0.3881 (2)	0.7745 (7)	−0.1203 (2)	0.0486 (16)
H26′_2	0.348538	0.781427	−0.123717	0.058*
C27′_2	0.4177 (2)	0.8593 (7)	−0.0829 (2)	0.0428 (14)
H27′_2	0.398845	0.925019	−0.061106	0.051*
C28′_2	0.5546 (2)	0.6892 (6)	0.1420 (2)	0.0348 (13)
C29′_2	0.5813 (2)	0.6338 (6)	0.1918 (2)	0.0374 (13)
C30′_2	0.6382 (3)	0.6363 (6)	0.2025 (2)	0.0437 (14)
H30′_2	0.662477	0.666165	0.177122	0.052*
C31′_2	0.6597 (3)	0.5948 (7)	0.2506 (2)	0.0493 (16)
H31′_2	0.698921	0.593118	0.257896	0.059*
C32′_2	0.6245 (3)	0.5562 (7)	0.2877 (3)	0.0557 (17)
H32′_2	0.639372	0.532260	0.321087	0.067*
C33′_2	0.5675 (3)	0.5520 (9)	0.2767 (3)	0.068 (2)
H33′_2	0.543078	0.523846	0.302163	0.082*
C34′_2	0.5467 (3)	0.5887 (8)	0.2287 (2)	0.0555 (17)
H34′_2	0.507569	0.582889	0.220660	0.067*
O1S_3	0.9572 (3)	0.5093 (7)	0.2217 (2)	0.0971 (19)
O2S_3	0.9617 (2)	0.2776 (6)	0.25283 (19)	0.0678 (13)
C1S_3	1.0440 (3)	0.4157 (14)	0.2566 (4)	0.109 (4)
H1SA_3	1.064301	0.445529	0.226973	0.164*
H1SB_3	1.057012	0.316195	0.268587	0.164*
H1SC_3	1.050817	0.489858	0.284009	0.164*
C2S_3	0.9847 (3)	0.4089 (10)	0.2424 (3)	0.072 (2)
C3S_3	0.9022 (3)	0.2583 (8)	0.2396 (3)	0.0619 (19)
H3SA_3	0.894147	0.271514	0.202423	0.074*
H3SB_3	0.880162	0.333027	0.257861	0.074*
C4S_3	0.8879 (3)	0.0979 (8)	0.2558 (3)	0.0653 (19)
H4SA_3	0.848624	0.076701	0.245812	0.098*
H4SB_3	0.894026	0.088477	0.292893	0.098*
H4SC_3	0.911728	0.025820	0.239047	0.098*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1_1	0.028 (2)	0.0242 (19)	0.059 (3)	−0.0011 (15)	−0.0023 (18)	0.0011 (16)
O2_1	0.033 (2)	0.040 (2)	0.038 (2)	−0.0008 (16)	−0.0048 (18)	0.0034 (17)
O3_1	0.033 (2)	0.040 (2)	0.039 (2)	0.0109 (18)	0.0039 (19)	−0.0010 (16)
O5_1	0.030 (2)	0.0254 (18)	0.045 (2)	0.0023 (15)	0.0042 (17)	−0.0014 (16)
O6_1	0.035 (2)	0.031 (2)	0.042 (2)	−0.0045 (16)	0.0030 (17)	−0.0010 (16)
O7_1	0.055 (3)	0.045 (3)	0.073 (3)	−0.022 (2)	−0.022 (2)	0.007 (2)
O8_1	0.064 (3)	0.038 (2)	0.056 (3)	−0.011 (2)	−0.017 (2)	0.0018 (19)
O9_1	0.075 (3)	0.064 (3)	0.050 (3)	−0.026 (2)	0.020 (2)	−0.008 (2)
C1_1	0.020 (3)	0.032 (3)	0.050 (4)	0.002 (2)	−0.004 (2)	−0.001 (2)
C2_1	0.028 (3)	0.029 (3)	0.043 (3)	−0.001 (2)	0.000 (2)	0.008 (2)
C3_1	0.021 (3)	0.041 (3)	0.040 (3)	−0.001 (2)	−0.002 (2)	−0.001 (2)
C4_1	0.023 (3)	0.025 (3)	0.042 (3)	0.001 (2)	−0.004 (2)	0.000 (2)
C5_1	0.029 (3)	0.026 (3)	0.041 (3)	−0.001 (2)	−0.004 (2)	−0.003 (2)
C6_1	0.036 (3)	0.040 (3)	0.035 (3)	−0.002 (2)	0.003 (3)	−0.003 (2)
O1′_1	0.029 (2)	0.033 (2)	0.038 (2)	−0.0003 (15)	−0.0028 (16)	−0.0013 (16)
O2′_1	0.031 (2)	0.034 (2)	0.038 (2)	−0.0088 (15)	0.0003 (17)	0.0007 (16)
O3′_1	0.036 (2)	0.0264 (19)	0.041 (2)	−0.0058 (15)	−0.0106 (17)	0.0066 (15)
O4′_1	0.023 (2)	0.0243 (18)	0.045 (2)	−0.0032 (14)	−0.0028 (16)	−0.0010 (15)
O5′_1	0.029 (2)	0.0234 (18)	0.041 (2)	0.0010 (14)	0.0034 (16)	0.0021 (15)
O6′_1	0.039 (2)	0.032 (2)	0.041 (2)	0.0038 (16)	0.0050 (18)	0.0092 (16)
O7′_1	0.048 (3)	0.055 (3)	0.042 (2)	−0.011 (2)	0.002 (2)	−0.006 (2)
O8′_1	0.044 (2)	0.026 (2)	0.049 (2)	−0.0056 (17)	−0.008 (2)	0.0011 (17)
O9′_1	0.035 (3)	0.077 (3)	0.076 (3)	0.010 (2)	0.000 (2)	−0.036 (3)
O10′_1	0.042 (3)	0.049 (3)	0.063 (3)	0.0031 (19)	0.018 (2)	0.017 (2)
C1′_1	0.024 (3)	0.025 (3)	0.042 (3)	−0.002 (2)	0.005 (2)	−0.004 (2)
C2′_1	0.030 (3)	0.030 (3)	0.037 (3)	−0.010 (2)	−0.002 (2)	−0.001 (2)
C3′_1	0.032 (3)	0.026 (3)	0.038 (3)	−0.005 (2)	−0.007 (2)	0.003 (2)
C4′_1	0.036 (3)	0.024 (3)	0.039 (3)	0.004 (2)	−0.005 (3)	−0.001 (2)
C5′_1	0.028 (3)	0.020 (3)	0.040 (3)	0.004 (2)	−0.001 (2)	−0.001 (2)
C6′_1	0.030 (3)	0.026 (3)	0.044 (3)	0.006 (2)	−0.001 (3)	0.006 (2)
C7_1	0.042 (4)	0.030 (3)	0.043 (3)	−0.004 (3)	0.004 (3)	−0.004 (2)
C8_1	0.034 (3)	0.023 (3)	0.052 (4)	0.003 (2)	0.002 (3)	−0.007 (2)
C9_1	0.041 (4)	0.031 (3)	0.076 (5)	0.005 (3)	−0.005 (3)	0.002 (3)
C10_1	0.053 (4)	0.040 (4)	0.096 (6)	−0.002 (3)	−0.014 (4)	−0.003 (4)
C11_1	0.051 (4)	0.051 (4)	0.083 (5)	0.009 (3)	−0.015 (4)	0.002 (4)
C12_1	0.050 (4)	0.035 (3)	0.076 (5)	0.010 (3)	0.002 (3)	0.011 (3)
C13_1	0.040 (4)	0.036 (3)	0.056 (4)	0.006 (3)	0.003 (3)	−0.007 (3)
C14_1	0.043 (4)	0.033 (3)	0.041 (4)	0.007 (3)	−0.005 (3)	−0.002 (3)
C15_1	0.039 (3)	0.040 (3)	0.039 (3)	0.002 (3)	0.003 (3)	0.002 (2)
C16_1	0.039 (3)	0.045 (3)	0.046 (4)	0.001 (3)	0.000 (3)	0.005 (3)
C17_1	0.049 (4)	0.056 (4)	0.059 (4)	0.001 (3)	0.005 (3)	0.011 (3)
C18_1	0.058 (5)	0.070 (5)	0.066 (5)	0.006 (4)	0.009 (4)	0.025 (4)
C19_1	0.065 (5)	0.080 (5)	0.048 (4)	0.000 (4)	−0.004 (4)	0.011 (4)
C20_1	0.058 (4)	0.048 (4)	0.046 (4)	−0.003 (3)	−0.008 (3)	0.007 (3)
C21_1	0.040 (3)	0.039 (3)	0.042 (4)	0.005 (3)	0.013 (3)	0.004 (3)

C22_1	0.030 (3)	0.026 (3)	0.058 (4)	0.004 (2)	0.007 (3)	0.005 (3)
C23_1	0.047 (4)	0.041 (3)	0.055 (4)	−0.005 (3)	−0.003 (3)	0.000 (3)
C24_1	0.062 (5)	0.054 (4)	0.076 (5)	−0.014 (4)	−0.011 (4)	−0.005 (4)
C25_1	0.039 (4)	0.046 (4)	0.116 (7)	−0.009 (3)	−0.001 (4)	0.000 (4)
C26_1	0.033 (4)	0.038 (4)	0.107 (6)	−0.007 (3)	0.017 (4)	−0.002 (4)
C27_1	0.041 (4)	0.041 (4)	0.072 (5)	0.006 (3)	0.013 (3)	0.003 (3)
C7′_1	0.039 (3)	0.028 (3)	0.037 (3)	−0.003 (2)	−0.002 (3)	0.002 (2)
C8′_1	0.034 (3)	0.029 (3)	0.044 (3)	0.000 (2)	0.006 (3)	0.002 (2)
C9′_1	0.037 (3)	0.029 (3)	0.055 (4)	−0.002 (2)	0.008 (3)	−0.003 (3)
C10′_1	0.036 (3)	0.030 (3)	0.077 (5)	−0.005 (2)	0.011 (3)	−0.002 (3)
C11′_1	0.044 (4)	0.032 (3)	0.079 (5)	−0.001 (3)	0.018 (4)	0.012 (3)
C12′_1	0.063 (5)	0.063 (4)	0.063 (5)	−0.006 (4)	0.027 (4)	0.003 (4)
C13′_1	0.054 (4)	0.049 (4)	0.053 (4)	−0.012 (3)	0.010 (3)	0.000 (3)
C14′_1	0.029 (3)	0.024 (3)	0.045 (3)	−0.004 (2)	0.005 (3)	−0.001 (2)
C15′_1	0.032 (3)	0.032 (3)	0.041 (3)	−0.005 (2)	0.002 (3)	0.008 (2)
C16′_1	0.049 (4)	0.030 (3)	0.057 (4)	−0.014 (3)	−0.010 (3)	0.007 (3)
C17′_1	0.052 (4)	0.052 (4)	0.054 (4)	−0.008 (3)	−0.017 (3)	0.013 (3)
C18′_1	0.052 (4)	0.049 (4)	0.053 (4)	−0.007 (3)	−0.004 (3)	0.020 (3)
C19′_1	0.067 (5)	0.034 (3)	0.070 (5)	−0.015 (3)	−0.001 (4)	0.016 (3)
C20′_1	0.047 (4)	0.030 (3)	0.057 (4)	−0.017 (3)	−0.007 (3)	0.009 (3)
C21′_1	0.029 (3)	0.023 (3)	0.054 (4)	−0.002 (2)	0.000 (3)	0.001 (3)
C22′_1	0.031 (3)	0.027 (3)	0.040 (3)	−0.003 (2)	0.001 (2)	0.006 (2)
C23′_1	0.025 (3)	0.028 (3)	0.053 (4)	−0.004 (2)	−0.004 (3)	0.004 (2)
C24′_1	0.038 (4)	0.042 (3)	0.047 (4)	−0.007 (3)	0.002 (3)	0.000 (3)
C25′_1	0.033 (3)	0.040 (3)	0.053 (4)	−0.008 (3)	−0.012 (3)	0.005 (3)
C26′_1	0.031 (3)	0.034 (3)	0.051 (4)	−0.004 (2)	0.002 (3)	0.009 (3)
C27′_1	0.029 (3)	0.029 (3)	0.050 (4)	0.001 (2)	0.000 (3)	0.006 (2)
C28′_1	0.040 (4)	0.023 (3)	0.049 (4)	0.004 (2)	0.015 (3)	0.003 (2)
C29′_1	0.061 (4)	0.019 (3)	0.038 (3)	0.007 (2)	0.012 (3)	0.001 (2)
C30′_1	0.050 (4)	0.033 (3)	0.044 (4)	0.006 (3)	0.008 (3)	0.005 (3)
C31′_1	0.068 (5)	0.046 (4)	0.049 (4)	0.007 (3)	0.005 (3)	0.007 (3)
C32′_1	0.070 (5)	0.056 (4)	0.048 (4)	0.011 (4)	0.006 (4)	0.010 (3)
C33′_1	0.083 (6)	0.037 (3)	0.047 (4)	0.002 (3)	0.008 (4)	0.016 (3)
C34′_1	0.060 (4)	0.034 (3)	0.046 (4)	−0.006 (3)	0.008 (3)	−0.001 (3)
O1_2	0.033 (2)	0.0240 (19)	0.055 (2)	0.0037 (15)	−0.0001 (18)	0.0038 (16)
O2_2	0.033 (2)	0.034 (2)	0.041 (2)	−0.0010 (16)	−0.0025 (18)	0.0083 (16)
O3_2	0.030 (2)	0.040 (2)	0.042 (2)	0.0123 (18)	0.0011 (19)	0.0002 (17)
O5_2	0.027 (2)	0.0267 (19)	0.050 (2)	0.0029 (15)	0.0015 (17)	0.0033 (16)
O6_2	0.029 (2)	0.033 (2)	0.046 (2)	−0.0044 (15)	0.0075 (17)	−0.0009 (16)
O7_2	0.063 (3)	0.031 (2)	0.060 (3)	−0.013 (2)	−0.021 (2)	0.0052 (18)
O8_2	0.075 (3)	0.044 (3)	0.051 (3)	−0.004 (2)	−0.008 (2)	−0.002 (2)
O9_2	0.054 (3)	0.067 (3)	0.043 (3)	−0.022 (2)	0.009 (2)	−0.007 (2)
C1_2	0.027 (3)	0.023 (3)	0.047 (3)	−0.001 (2)	−0.004 (3)	0.005 (2)
C2_2	0.028 (3)	0.026 (3)	0.042 (3)	−0.002 (2)	−0.005 (2)	0.000 (2)
C3_2	0.026 (3)	0.023 (3)	0.043 (3)	0.000 (2)	0.000 (2)	−0.001 (2)
C4_2	0.021 (3)	0.037 (3)	0.040 (3)	0.002 (2)	−0.001 (2)	0.003 (2)
C5_2	0.026 (3)	0.026 (3)	0.044 (3)	−0.001 (2)	0.001 (2)	0.002 (2)
C6_2	0.031 (3)	0.025 (3)	0.044 (3)	−0.004 (2)	−0.001 (2)	−0.002 (2)

O2′_2	0.031 (2)	0.0261 (19)	0.042 (2)	−0.0076 (15)	0.0014 (17)	−0.0008 (15)
O3′_2	0.037 (2)	0.0207 (19)	0.050 (2)	−0.0048 (15)	−0.0076 (18)	0.0059 (15)
O1′_2	0.029 (2)	0.0259 (18)	0.039 (2)	0.0006 (15)	−0.0019 (16)	0.0019 (15)
O4′_2	0.026 (2)	0.0261 (18)	0.048 (2)	−0.0010 (15)	−0.0027 (17)	0.0037 (16)
O5′_2	0.0199 (18)	0.0220 (18)	0.050 (2)	−0.0014 (13)	0.0019 (16)	0.0038 (15)
O6′_2	0.029 (2)	0.031 (2)	0.048 (2)	0.0012 (15)	0.0010 (17)	0.0088 (17)
O7′_2	0.053 (3)	0.044 (2)	0.041 (2)	−0.0136 (19)	0.002 (2)	−0.0034 (19)
O8′_2	0.054 (3)	0.0215 (19)	0.047 (2)	−0.0091 (17)	−0.008 (2)	0.0023 (17)
O9′_2	0.029 (2)	0.046 (2)	0.056 (3)	0.0070 (18)	−0.0027 (19)	−0.001 (2)
O10′_2	0.032 (2)	0.049 (2)	0.059 (3)	−0.0003 (18)	0.006 (2)	0.0091 (19)
C1′_2	0.021 (3)	0.026 (3)	0.044 (3)	−0.001 (2)	−0.001 (2)	0.001 (2)
C2′_2	0.028 (3)	0.025 (3)	0.043 (3)	−0.005 (2)	0.001 (2)	0.004 (2)
C3′_2	0.031 (3)	0.013 (2)	0.046 (3)	−0.005 (2)	−0.008 (2)	0.007 (2)
C4′_2	0.030 (3)	0.020 (3)	0.046 (3)	0.003 (2)	−0.004 (2)	−0.002 (2)
C5′_2	0.033 (3)	0.020 (3)	0.042 (3)	0.004 (2)	−0.002 (2)	0.001 (2)
C6′_2	0.026 (3)	0.034 (3)	0.041 (3)	0.003 (2)	0.002 (2)	0.006 (2)
C7_2	0.053 (4)	0.022 (3)	0.044 (4)	−0.001 (3)	0.001 (3)	0.002 (2)
C8_2	0.054 (4)	0.027 (3)	0.039 (3)	0.008 (3)	0.006 (3)	0.000 (2)
C9_2	0.044 (4)	0.037 (3)	0.066 (4)	0.014 (3)	0.015 (3)	0.007 (3)
C10_2	0.047 (4)	0.048 (4)	0.076 (5)	0.018 (3)	0.017 (3)	0.010 (3)
C11_2	0.057 (4)	0.039 (4)	0.064 (4)	0.025 (3)	0.010 (3)	0.013 (3)
C12_2	0.067 (5)	0.029 (3)	0.048 (4)	0.010 (3)	0.010 (3)	0.003 (3)
C13_2	0.063 (4)	0.031 (3)	0.042 (3)	−0.001 (3)	0.006 (3)	−0.002 (2)
C14_2	0.049 (4)	0.029 (3)	0.047 (4)	0.006 (3)	−0.002 (3)	−0.001 (3)
C15_2	0.050 (4)	0.036 (3)	0.041 (4)	0.010 (3)	0.004 (3)	0.003 (3)
C16_2	0.043 (4)	0.047 (4)	0.045 (4)	0.000 (3)	0.000 (3)	0.007 (3)
C17_2	0.063 (4)	0.039 (3)	0.063 (5)	−0.010 (3)	0.003 (3)	0.014 (3)
C18_2	0.071 (5)	0.046 (4)	0.064 (5)	−0.004 (3)	0.006 (4)	0.019 (3)
C19_2	0.084 (6)	0.063 (5)	0.056 (5)	0.000 (4)	0.006 (4)	0.012 (4)
C20_2	0.072 (5)	0.048 (4)	0.054 (4)	0.003 (3)	0.009 (4)	−0.004 (3)
C21_2	0.036 (3)	0.025 (3)	0.041 (4)	−0.001 (2)	0.005 (3)	0.003 (2)
C22_2	0.034 (3)	0.023 (3)	0.053 (4)	0.001 (2)	0.007 (3)	0.000 (2)
C23_2	0.036 (3)	0.035 (3)	0.056 (4)	−0.007 (3)	0.004 (3)	0.001 (3)
C24_2	0.041 (4)	0.042 (3)	0.060 (4)	−0.005 (3)	0.000 (3)	−0.010 (3)
C25_2	0.037 (4)	0.033 (3)	0.077 (5)	−0.008 (3)	0.007 (3)	−0.003 (3)
C26_2	0.039 (4)	0.053 (4)	0.064 (5)	−0.008 (3)	0.016 (3)	0.000 (3)
C27_2	0.045 (4)	0.042 (3)	0.048 (4)	−0.007 (3)	0.009 (3)	0.003 (3)
C7′_2	0.038 (3)	0.032 (3)	0.037 (3)	−0.003 (2)	0.001 (3)	0.005 (3)
C8′_2	0.040 (3)	0.020 (3)	0.061 (4)	0.002 (2)	0.015 (3)	0.004 (3)
C9′_2	0.031 (3)	0.026 (3)	0.079 (5)	−0.005 (2)	0.009 (3)	−0.008 (3)
C10′_2	0.036 (4)	0.029 (3)	0.126 (7)	−0.002 (3)	0.025 (4)	−0.011 (4)
C11′_2	0.062 (5)	0.034 (4)	0.158 (9)	−0.009 (3)	0.062 (6)	−0.014 (5)
C12′_2	0.103 (7)	0.062 (5)	0.111 (7)	−0.016 (5)	0.075 (6)	−0.003 (5)
C13′_2	0.075 (5)	0.046 (4)	0.075 (5)	−0.010 (3)	0.032 (4)	−0.005 (3)
C14′_2	0.024 (3)	0.026 (3)	0.049 (4)	−0.002 (2)	0.002 (3)	−0.001 (2)
C15′_2	0.026 (3)	0.026 (3)	0.049 (4)	−0.001 (2)	0.005 (3)	−0.002 (2)
C16′_2	0.039 (3)	0.021 (3)	0.049 (4)	−0.002 (2)	0.001 (3)	0.001 (2)
C17′_2	0.050 (4)	0.033 (3)	0.050 (4)	−0.005 (3)	−0.002 (3)	−0.006 (3)

C18′_2	0.056 (4)	0.036 (3)	0.050 (4)	−0.006 (3)	0.003 (3)	0.010 (3)
C19′_2	0.047 (4)	0.021 (3)	0.069 (4)	−0.016 (2)	−0.005 (3)	0.007 (3)
C20′_2	0.032 (3)	0.030 (3)	0.051 (4)	−0.009 (2)	−0.004 (3)	0.003 (3)
C21′_2	0.026 (3)	0.038 (3)	0.050 (4)	0.002 (2)	0.001 (3)	0.006 (3)
C22′_2	0.028 (3)	0.031 (3)	0.049 (4)	−0.004 (2)	−0.005 (3)	0.010 (2)
C23′_2	0.030 (3)	0.050 (4)	0.059 (4)	−0.005 (3)	−0.005 (3)	−0.001 (3)
C24′_2	0.040 (4)	0.054 (4)	0.072 (5)	−0.008 (3)	−0.001 (3)	−0.007 (3)
C25′_2	0.045 (4)	0.061 (4)	0.064 (5)	−0.015 (3)	−0.011 (3)	0.007 (3)
C26′_2	0.028 (3)	0.052 (4)	0.065 (4)	−0.011 (3)	−0.009 (3)	0.015 (3)
C27′_2	0.027 (3)	0.047 (3)	0.054 (4)	−0.004 (3)	−0.003 (3)	0.012 (3)
C28′_2	0.031 (3)	0.028 (3)	0.047 (3)	0.001 (2)	0.013 (3)	0.003 (2)
C29′_2	0.040 (4)	0.027 (3)	0.046 (4)	0.004 (2)	0.005 (3)	0.002 (2)
C30′_2	0.046 (4)	0.039 (3)	0.046 (4)	−0.002 (3)	0.003 (3)	0.004 (3)
C31′_2	0.045 (4)	0.046 (4)	0.056 (4)	−0.002 (3)	−0.007 (3)	0.002 (3)
C32′_2	0.059 (5)	0.051 (4)	0.056 (4)	0.006 (3)	−0.004 (4)	0.018 (3)
C33′_2	0.060 (5)	0.080 (5)	0.065 (5)	−0.017 (4)	0.010 (4)	0.027 (4)
C34′_2	0.047 (4)	0.063 (4)	0.056 (4)	−0.007 (3)	0.001 (3)	0.024 (3)
O1S_3	0.102 (5)	0.078 (4)	0.113 (5)	0.007 (3)	0.021 (4)	0.037 (4)
O2S_3	0.057 (3)	0.066 (3)	0.079 (3)	0.006 (2)	−0.007 (3)	0.019 (3)
C1S_3	0.058 (6)	0.176 (11)	0.093 (7)	−0.025 (6)	−0.006 (5)	0.061 (7)
C2S_3	0.082 (6)	0.076 (6)	0.058 (5)	0.002 (5)	0.009 (4)	0.028 (4)
C3S_3	0.049 (4)	0.063 (4)	0.072 (5)	0.011 (3)	−0.010 (4)	0.002 (4)
C4S_3	0.058 (5)	0.054 (4)	0.084 (5)	0.007 (3)	−0.002 (4)	−0.005 (4)

Geometric parameters (Å, º)

O1_1—C7_1	1.368 (7)	O5_2—C5_2	1.440 (6)
O1_1—C1_1	1.437 (6)	O6_2—C21_2	1.350 (6)
O2_1—C14_1	1.353 (6)	O6_2—C6_2	1.453 (6)
O2_1—C2_1	1.440 (6)	O7_2—C7_2	1.187 (7)
O3_1—C3_1	1.412 (6)	O8_2—C14_2	1.212 (7)
O3_1—H3O_1	0.79 (7)	O9_2—C21_2	1.204 (6)
O5_1—C1_1	1.398 (6)	C1_2—C2_2	1.522 (7)
O5_1—C5_1	1.441 (6)	C1_2—H1_2	1.0000
O6_1—C21_1	1.347 (6)	C2_2—C3_2	1.509 (7)
O6_1—C6_1	1.447 (6)	C2_2—H2_2	1.0000
O7_1—C7_1	1.193 (7)	C3_2—C4_2	1.533 (7)
O8_1—C14_1	1.207 (7)	C3_2—H3_2	1.0000
O9_1—C21_1	1.202 (7)	C4_2—O1′_2	1.433 (6)
C1_1—C2_1	1.500 (7)	C4_2—C5_2	1.525 (7)
C1_1—H1_1	1.0000	C4_2—H4_2	1.0000
C2_1—C3_1	1.524 (7)	C5_2—C6_2	1.491 (7)
C2_1—H2_1	1.0000	C5_2—H5_2	1.0000
C3_1—C4_1	1.531 (7)	C6_2—H6C_2	0.9900
C3_1—H3_1	1.0000	C6_2—H6D_2	0.9900
C4_1—O1′_1	1.436 (6)	O2′_2—C7′_2	1.349 (6)
C4_1—C5_1	1.531 (7)	O2′_2—C2′_2	1.441 (6)
C4_1—H4_1	1.0000	O3′_2—C14′_2	1.356 (6)

C5_1—C6_1	1.508 (7)	O3′_2—C3′_2	1.440 (6)
C5_1—H5_1	1.0000	O1′_2—C1′_2	1.388 (6)
C6_1—H6A_1	0.9900	O4′_2—C21′_2	1.349 (6)
C6_1—H6B_1	0.9900	O4′_2—C4′_2	1.443 (6)
O1′_1—C1′_1	1.376 (6)	O5′_2—C1′_2	1.431 (6)
O2′_1—C7′_1	1.347 (6)	O5′_2—C5′_2	1.438 (6)
O2′_1—C2′_1	1.429 (6)	O6′_2—C28′_2	1.347 (6)
O3′_1—C14′_1	1.361 (6)	O6′_2—C6′_2	1.450 (6)
O3′_1—C3′_1	1.438 (6)	O7′_2—C7′_2	1.211 (6)
O4′_1—C21′_1	1.364 (6)	O8′_2—C14′_2	1.201 (6)
O4′_1—C4′_1	1.450 (6)	O9′_2—C21′_2	1.204 (7)
O5′_1—C5′_1	1.437 (6)	O10′_2—C28′_2	1.200 (6)
O5′_1—C1′_1	1.441 (6)	C1′_2—C2′_2	1.521 (7)
O6′_1—C28′_1	1.346 (6)	C1′_2—H1′_2	1.0000
O6′_1—C6′_1	1.451 (6)	C2′_2—C3′_2	1.521 (7)
O7′_1—C7′_1	1.208 (6)	C2′_2—H2′_2	1.0000
O8′_1—C14′_1	1.194 (6)	C3′_2—C4′_2	1.507 (7)
O9′_1—C21′_1	1.199 (7)	C3′_2—H3′_2	1.0000
O10′_1—C28′_1	1.199 (7)	C4′_2—C5′_2	1.523 (7)
C1′_1—C2′_1	1.522 (7)	C4′_2—H4′_2	1.0000
C1′_1—H1′_1	1.0000	C5′_2—C6′_2	1.506 (7)
C2′_1—C3′_1	1.508 (7)	C5′_2—H5′_2	1.0000
C2′_1—H2′_1	1.0000	C6′_2—H6′C_2	0.9900
C3′_1—C4′_1	1.503 (7)	C6′_2—H6′D_2	0.9900
C3′_1—H3′_1	1.0000	C7_2—C8_2	1.499 (8)
C4′_1—C5′_1	1.523 (7)	C8_2—C9_2	1.376 (8)
C4′_1—H4′_1	1.0000	C8_2—C13_2	1.389 (8)
C5′_1—C6′_1	1.493 (7)	C9_2—C10_2	1.393 (9)
C5′_1—H5′_1	1.0000	C9_2—H9_2	0.9500
C6′_1—H6′A_1	0.9900	C10_2—C11_2	1.372 (9)
C6′_1—H6′B_1	0.9900	C10_2—H10_2	0.9500
C7_1—C8_1	1.478 (8)	C11_2—C12_2	1.370 (9)
C8_1—C13_1	1.390 (8)	C11_2—H11_2	0.9500
C8_1—C9_1	1.394 (8)	C12_2—C13_2	1.396 (8)
C9_1—C10_1	1.376 (9)	C12_2—H12_2	0.9500
C9_1—H9_1	0.9500	C13_2—H13_2	0.9500
C10_1—C11_1	1.376 (10)	C14_2—C15_2	1.502 (8)
C10_1—H10_1	0.9500	C15_2—C16_2	1.363 (8)
C11_1—C12_1	1.403 (9)	C15_2—C20_2	1.387 (8)
C11_1—H11_1	0.9500	C16_2—C17_2	1.381 (8)
C12_1—C13_1	1.379 (8)	C16_2—H16_2	0.9500
C12_1—H12_1	0.9500	C17_2—C18_2	1.378 (9)
C13_1—H13_1	0.9500	C17_2—H17_2	0.9500
C14_1—C15_1	1.490 (8)	C18_2—C19_2	1.364 (10)
C15_1—C16_1	1.388 (8)	C18_2—H18_2	0.9500
C15_1—C20_1	1.389 (8)	C19_2—C20_2	1.395 (9)
C16_1—C17_1	1.371 (8)	C19_2—H19_2	0.9500
C16_1—H16_1	0.9500	C20_2—H20_2	0.9500

C17_1—C18_1	1.380 (9)	C21_2—C22_2	1.491 (8)
C17_1—H17_1	0.9500	C22_2—C23_2	1.376 (8)
C18_1—C19_1	1.377 (10)	C22_2—C27_2	1.392 (8)
C18_1—H18_1	0.9500	C23_2—C24_2	1.392 (8)
C19_1—C20_1	1.384 (9)	C23_2—H23_2	0.9500
C19_1—H19_1	0.9500	C24_2—C25_2	1.382 (9)
C20_1—H20_1	0.9500	C24_2—H24_2	0.9500
C21_1—C22_1	1.502 (8)	C25_2—C26_2	1.360 (9)
C22_1—C23_1	1.357 (8)	C25_2—H25_2	0.9500
C22_1—C27_1	1.380 (8)	C26_2—C27_2	1.385 (8)
C23_1—C24_1	1.409 (9)	C26_2—H26_2	0.9500
C23_1—H23_1	0.9500	C27_2—H27_2	0.9500
C24_1—C25_1	1.392 (11)	C7′_2—C8′_2	1.495 (7)
C24_1—H24_1	0.9500	C8′_2—C9′_2	1.371 (8)
C25_1—C26_1	1.354 (10)	C8′_2—C13′_2	1.386 (9)
C25_1—H25_1	0.9500	C9′_2—C10′_2	1.386 (8)
C26_1—C27_1	1.392 (9)	C9′_2—H9′_2	0.9500
C26_1—H26_1	0.9500	C10′_2—C11′_2	1.370 (11)
C27_1—H27_1	0.9500	C10′_2—H10′_2	0.9500
C7′_1—C8′_1	1.487 (7)	C11′_2—C12′_2	1.369 (12)
C8′_1—C9′_1	1.381 (8)	C11′_2—H11′_2	0.9500
C8′_1—C13′_1	1.384 (8)	C12′_2—C13′_2	1.375 (10)
C9′_1—C10′_1	1.392 (8)	C12′_2—H12′_2	0.9500
C9′_1—H9′_1	0.9500	C13′_2—H13′_2	0.9500
C10′_1—C11′_1	1.361 (9)	C14′_2—C15′_2	1.480 (8)
C10′_1—H10′_1	0.9500	C15′_2—C16′_2	1.385 (8)
C11′_1—C12′_1	1.378 (9)	C15′_2—C20′_2	1.398 (7)
C11′_1—H11′_1	0.9500	C16′_2—C17′_2	1.385 (8)
C12′_1—C13′_1	1.376 (9)	C16′_2—H16′_2	0.9500
C12′_1—H12′_1	0.9500	C17′_2—C18′_2	1.391 (8)
C13′_1—H13′_1	0.9500	C17′_2—H17′_2	0.9500
C14′_1—C15′_1	1.486 (8)	C18′_2—C19′_2	1.385 (8)
C15′_1—C16′_1	1.389 (8)	C18′_2—H18′_2	0.9500
C15′_1—C20′_1	1.393 (8)	C19′_2—C20′_2	1.369 (8)
C16′_1—C17′_1	1.380 (8)	C19′_2—H19′_2	0.9500
C16′_1—H16′_1	0.9500	C20′_2—H20′_2	0.9500
C17′_1—C18′_1	1.388 (9)	C21′_2—C22′_2	1.493 (8)
C17′_1—H17′_1	0.9500	C22′_2—C23′_2	1.376 (8)
C18′_1—C19′_1	1.381 (9)	C22′_2—C27′_2	1.402 (8)
C18′_1—H18′_1	0.9500	C23′_2—C24′_2	1.383 (9)
C19′_1—C20′_1	1.368 (8)	C23′_2—H23′_2	0.9500
C19′_1—H19′_1	0.9500	C24′_2—C25′_2	1.382 (9)
C20′_1—H20′_1	0.9500	C24′_2—H24′_2	0.9500
C21′_1—C22′_1	1.470 (8)	C25′_2—C26′_2	1.381 (9)
C22′_1—C27′_1	1.391 (7)	C25′_2—H25′_2	0.9500
C22′_1—C23′_1	1.394 (7)	C26′_2—C27′_2	1.395 (8)
C23′_1—C24′_1	1.397 (8)	C26′_2—H26′_2	0.9500
C23′_1—H23′_1	0.9500	C27′_2—H27′_2	0.9500

C24′_1—C25′_1	1.400 (8)	C28′_2—C29′_2	1.504 (8)
C24′_1—H24′_1	0.9500	C29′_2—C34′_2	1.373 (8)
C25′_1—C26′_1	1.367 (8)	C29′_2—C30′_2	1.377 (8)
C25′_1—H25′_1	0.9500	C30′_2—C31′_2	1.383 (8)
C26′_1—C27′_1	1.371 (8)	C30′_2—H30′_2	0.9500
C26′_1—H26′_1	0.9500	C31′_2—C32′_2	1.371 (9)
C27′_1—H27′_1	0.9500	C31′_2—H31′_2	0.9500
C28′_1—C29′_1	1.509 (8)	C32′_2—C33′_2	1.381 (9)
C29′_1—C30′_1	1.376 (8)	C32′_2—H32′_2	0.9500
C29′_1—C34′_1	1.382 (8)	C33′_2—C34′_2	1.366 (9)
C30′_1—C31′_1	1.375 (8)	C33′_2—H33′_2	0.9500
C30′_1—H30′_1	0.9500	C34′_2—H34′_2	0.9500
C31′_1—C32′_1	1.376 (9)	O1S_3—C2S_3	1.216 (9)
C31′_1—H31′_1	0.9500	O2S_3—C2S_3	1.324 (9)
C32′_1—C33′_1	1.357 (9)	O2S_3—C3S_3	1.459 (8)
C32′_1—H32′_1	0.9500	C1S_3—C2S_3	1.450 (11)
C33′_1—C34′_1	1.388 (9)	C1S_3—H1SA_3	0.9800
C33′_1—H33′_1	0.9500	C1S_3—H1SB_3	0.9800
C34′_1—H34′_1	0.9500	C1S_3—H1SC_3	0.9800
O1_2—C7_2	1.374 (6)	C3S_3—C4S_3	1.528 (10)
O1_2—C1_2	1.413 (6)	C3S_3—H3SA_3	0.9900
O2_2—C14_2	1.336 (7)	C3S_3—H3SB_3	0.9900
O2_2—C2_2	1.440 (6)	C4S_3—H4SA_3	0.9800
O3_2—C3_2	1.434 (6)	C4S_3—H4SB_3	0.9800
O3_2—H3O_2	0.73 (7)	C4S_3—H4SC_3	0.9800
O5_2—C1_2	1.415 (6)		

C7_1—O1_1—C1_1	116.2 (4)	O2_2—C2_2—C3_2	111.3 (4)
C14_1—O2_1—C2_1	117.6 (4)	O2_2—C2_2—C1_2	104.6 (4)
C3_1—O3_1—H3O_1	107 (5)	C3_2—C2_2—C1_2	108.7 (4)
C1_1—O5_1—C5_1	109.1 (4)	O2_2—C2_2—H2_2	110.7
C21_1—O6_1—C6_1	114.0 (4)	C3_2—C2_2—H2_2	110.7
O5_1—C1_1—O1_1	107.1 (4)	C1_2—C2_2—H2_2	110.7
O5_1—C1_1—C2_1	109.6 (4)	O3_2—C3_2—C2_2	107.6 (4)
O1_1—C1_1—C2_1	108.9 (4)	O3_2—C3_2—C4_2	112.1 (4)
O5_1—C1_1—H1_1	110.4	C2_2—C3_2—C4_2	110.2 (4)
O1_1—C1_1—H1_1	110.4	O3_2—C3_2—H3_2	109.0
C2_1—C1_1—H1_1	110.4	C2_2—C3_2—H3_2	109.0
O2_1—C2_1—C1_1	107.4 (4)	C4_2—C3_2—H3_2	109.0
O2_1—C2_1—C3_1	109.5 (4)	O1′_2—C4_2—C5_2	103.8 (4)
C1_1—C2_1—C3_1	109.1 (4)	O1′_2—C4_2—C3_2	113.2 (4)
O2_1—C2_1—H2_1	110.3	C5_2—C4_2—C3_2	110.0 (4)
C1_1—C2_1—H2_1	110.3	O1′_2—C4_2—H4_2	109.9
C3_1—C2_1—H2_1	110.3	C5_2—C4_2—H4_2	109.9
O3_1—C3_1—C2_1	107.9 (4)	C3_2—C4_2—H4_2	109.9
O3_1—C3_1—C4_1	112.4 (4)	O5_2—C5_2—C6_2	109.4 (4)
C2_1—C3_1—C4_1	109.1 (4)	O5_2—C5_2—C4_2	109.0 (4)
O3_1—C3_1—H3_1	109.1	C6_2—C5_2—C4_2	116.7 (4)

C2_1—C3_1—H3_1	109.1	O5_2—C5_2—H5_2	107.1
C4_1—C3_1—H3_1	109.1	C6_2—C5_2—H5_2	107.1
O1′_1—C4_1—C3_1	113.0 (4)	C4_2—C5_2—H5_2	107.1
O1′_1—C4_1—C5_1	103.8 (4)	O6_2—C6_2—C5_2	109.7 (4)
C3_1—C4_1—C5_1	110.9 (4)	O6_2—C6_2—H6C_2	109.7
O1′_1—C4_1—H4_1	109.7	C5_2—C6_2—H6C_2	109.7
C3_1—C4_1—H4_1	109.7	O6_2—C6_2—H6D_2	109.7
C5_1—C4_1—H4_1	109.7	C5_2—C6_2—H6D_2	109.7
O5_1—C5_1—C6_1	108.3 (4)	H6C_2—C6_2—H6D_2	108.2
O5_1—C5_1—C4_1	110.2 (4)	C7′_2—O2′_2—C2′_2	118.2 (4)
C6_1—C5_1—C4_1	113.9 (4)	C14′_2—O3′_2—C3′_2	116.0 (4)
O5_1—C5_1—H5_1	108.1	C1′_2—O1′_2—C4_2	118.0 (4)
C6_1—C5_1—H5_1	108.1	C21′_2—O4′_2—C4′_2	116.4 (4)
C4_1—C5_1—H5_1	108.1	C1′_2—O5′_2—C5′_2	112.7 (4)
O6_1—C6_1—C5_1	109.2 (4)	C28′_2—O6′_2—C6′_2	113.9 (4)
O6_1—C6_1—H6A_1	109.8	O1′_2—C1′_2—O5′_2	107.3 (4)
C5_1—C6_1—H6A_1	109.8	O1′_2—C1′_2—C2′_2	107.6 (4)
O6_1—C6_1—H6B_1	109.8	O5′_2—C1′_2—C2′_2	109.2 (4)
C5_1—C6_1—H6B_1	109.8	O1′_2—C1′_2—H1′_2	110.9
H6A_1—C6_1—H6B_1	108.3	O5′_2—C1′_2—H1′_2	110.9
C1′_1—O1′_1—C4_1	117.0 (4)	C2′_2—C1′_2—H1′_2	110.9
C7′_1—O2′_1—C2′_1	119.2 (4)	O2′_2—C2′_2—C3′_2	105.7 (4)
C14′_1—O3′_1—C3′_1	116.8 (4)	O2′_2—C2′_2—C1′_2	108.0 (4)
C21′_1—O4′_1—C4′_1	116.9 (4)	C3′_2—C2′_2—C1′_2	110.4 (4)
C5′_1—O5′_1—C1′_1	112.2 (3)	O2′_2—C2′_2—H2′_2	110.9
C28′_1—O6′_1—C6′_1	114.9 (4)	C3′_2—C2′_2—H2′_2	110.9
O1′_1—C1′_1—O5′_1	107.4 (4)	C1′_2—C2′_2—H2′_2	110.9
O1′_1—C1′_1—C2′_1	108.4 (4)	O3′_2—C3′_2—C4′_2	110.6 (4)
O5′_1—C1′_1—C2′_1	109.0 (4)	O3′_2—C3′_2—C2′_2	108.4 (4)
O1′_1—C1′_1—H1′_1	110.6	C4′_2—C3′_2—C2′_2	111.3 (4)
O5′_1—C1′_1—H1′_1	110.6	O3′_2—C3′_2—H3′_2	108.8
C2′_1—C1′_1—H1′_1	110.6	C4′_2—C3′_2—H3′_2	108.8
O2′_1—C2′_1—C3′_1	107.5 (4)	C2′_2—C3′_2—H3′_2	108.8
O2′_1—C2′_1—C1′_1	107.9 (4)	O4′_2—C4′_2—C3′_2	109.0 (4)
C3′_1—C2′_1—C1′_1	109.9 (4)	O4′_2—C4′_2—C5′_2	110.1 (4)
O2′_1—C2′_1—H2′_1	110.5	C3′_2—C4′_2—C5′_2	107.8 (4)
C3′_1—C2′_1—H2′_1	110.5	O4′_2—C4′_2—H4′_2	109.9
C1′_1—C2′_1—H2′_1	110.5	C3′_2—C4′_2—H4′_2	109.9
O3′_1—C3′_1—C4′_1	109.9 (4)	C5′_2—C4′_2—H4′_2	109.9
O3′_1—C3′_1—C2′_1	109.7 (4)	O5′_2—C5′_2—C6′_2	106.1 (4)
C4′_1—C3′_1—C2′_1	113.4 (4)	O5′_2—C5′_2—C4′_2	110.1 (4)
O3′_1—C3′_1—H3′_1	107.9	C6′_2—C5′_2—C4′_2	113.6 (4)
C4′_1—C3′_1—H3′_1	107.9	O5′_2—C5′_2—H5′_2	109.0
C2′_1—C3′_1—H3′_1	107.9	C6′_2—C5′_2—H5′_2	109.0
O4′_1—C4′_1—C3′_1	108.8 (4)	C4′_2—C5′_2—H5′_2	109.0
O4′_1—C4′_1—C5′_1	109.8 (4)	O6′_2—C6′_2—C5′_2	105.7 (4)
C3′_1—C4′_1—C5′_1	108.2 (4)	O6′_2—C6′_2—H6′C_2	110.6
O4′_1—C4′_1—H4′_1	110.0	C5′_2—C6′_2—H6′C_2	110.6

C3′_1—C4′_1—H4′_1	110.0	O6′_2—C6′_2—H6′D_2	110.6
C5′_1—C4′_1—H4′_1	110.0	C5′_2—C6′_2—H6′D_2	110.6
O5′_1—C5′_1—C6′_1	106.9 (4)	H6′C_2—C6′_2—H6′D_2	108.7
O5′_1—C5′_1—C4′_1	110.0 (4)	O7_2—C7_2—O1_2	123.2 (5)
C6′_1—C5′_1—C4′_1	114.3 (4)	O7_2—C7_2—C8_2	124.5 (5)
O5′_1—C5′_1—H5′_1	108.5	O1_2—C7_2—C8_2	112.3 (5)
C6′_1—C5′_1—H5′_1	108.5	C9_2—C8_2—C13_2	120.4 (6)
C4′_1—C5′_1—H5′_1	108.5	C9_2—C8_2—C7_2	122.6 (5)
O6′_1—C6′_1—C5′_1	105.3 (4)	C13_2—C8_2—C7_2	116.9 (5)
O6′_1—C6′_1—H6′A_1	110.7	C8_2—C9_2—C10_2	119.5 (6)
C5′_1—C6′_1—H6′A_1	110.7	C8_2—C9_2—H9_2	120.3
O6′_1—C6′_1—H6′B_1	110.7	C10_2—C9_2—H9_2	120.3
C5′_1—C6′_1—H6′B_1	110.7	C11_2—C10_2—C9_2	120.1 (6)
H6′A_1—C6′_1—H6′B_1	108.8	C11_2—C10_2—H10_2	119.9
O7_1—C7_1—O1_1	122.7 (5)	C9_2—C10_2—H10_2	119.9
O7_1—C7_1—C8_1	125.4 (5)	C12_2—C11_2—C10_2	120.7 (6)
O1_1—C7_1—C8_1	111.8 (5)	C12_2—C11_2—H11_2	119.6
C13_1—C8_1—C9_1	119.7 (5)	C10_2—C11_2—H11_2	119.6
C13_1—C8_1—C7_1	117.3 (5)	C11_2—C12_2—C13_2	119.8 (6)
C9_1—C8_1—C7_1	122.9 (5)	C11_2—C12_2—H12_2	120.1
C10_1—C9_1—C8_1	119.9 (6)	C13_2—C12_2—H12_2	120.1
C10_1—C9_1—H9_1	120.1	C8_2—C13_2—C12_2	119.4 (6)
C8_1—C9_1—H9_1	120.1	C8_2—C13_2—H13_2	120.3
C11_1—C10_1—C9_1	120.7 (7)	C12_2—C13_2—H13_2	120.3
C11_1—C10_1—H10_1	119.6	O8_2—C14_2—O2_2	123.7 (5)
C9_1—C10_1—H10_1	119.6	O8_2—C14_2—C15_2	124.2 (6)
C10_1—C11_1—C12_1	119.8 (6)	O2_2—C14_2—C15_2	112.1 (5)
C10_1—C11_1—H11_1	120.1	C16_2—C15_2—C20_2	120.0 (6)
C12_1—C11_1—H11_1	120.1	C16_2—C15_2—C14_2	121.3 (5)
C13_1—C12_1—C11_1	119.6 (6)	C20_2—C15_2—C14_2	118.6 (5)
C13_1—C12_1—H12_1	120.2	C15_2—C16_2—C17_2	120.3 (6)
C11_1—C12_1—H12_1	120.2	C15_2—C16_2—H16_2	119.9
C12_1—C13_1—C8_1	120.3 (6)	C17_2—C16_2—H16_2	119.9
C12_1—C13_1—H13_1	119.8	C18_2—C17_2—C16_2	120.2 (6)
C8_1—C13_1—H13_1	119.8	C18_2—C17_2—H17_2	119.9
O8_1—C14_1—O2_1	123.5 (5)	C16_2—C17_2—H17_2	119.9
O8_1—C14_1—C15_1	124.3 (5)	C19_2—C18_2—C17_2	120.1 (6)
O2_1—C14_1—C15_1	112.1 (5)	C19_2—C18_2—H18_2	119.9
C16_1—C15_1—C20_1	119.5 (5)	C17_2—C18_2—H18_2	119.9
C16_1—C15_1—C14_1	121.8 (5)	C18_2—C19_2—C20_2	119.9 (7)
C20_1—C15_1—C14_1	118.6 (5)	C18_2—C19_2—H19_2	120.1
C17_1—C16_1—C15_1	119.5 (6)	C20_2—C19_2—H19_2	120.1
C17_1—C16_1—H16_1	120.3	C15_2—C20_2—C19_2	119.6 (6)
C15_1—C16_1—H16_1	120.3	C15_2—C20_2—H20_2	120.2
C16_1—C17_1—C18_1	121.0 (7)	C19_2—C20_2—H20_2	120.2
C16_1—C17_1—H17_1	119.5	O9_2—C21_2—O6_2	122.9 (5)
C18_1—C17_1—H17_1	119.5	O9_2—C21_2—C22_2	124.2 (5)
C19_1—C18_1—C17_1	120.1 (7)	O6_2—C21_2—C22_2	112.9 (5)

C19_1—C18_1—H18_1	119.9	C23_2—C22_2—C27_2	119.1 (5)
C17_1—C18_1—H18_1	119.9	C23_2—C22_2—C21_2	123.8 (5)
C18_1—C19_1—C20_1	119.4 (6)	C27_2—C22_2—C21_2	117.1 (5)
C18_1—C19_1—H19_1	120.3	C22_2—C23_2—C24_2	120.7 (6)
C20_1—C19_1—H19_1	120.3	C22_2—C23_2—H23_2	119.7
C19_1—C20_1—C15_1	120.6 (6)	C24_2—C23_2—H23_2	119.7
C19_1—C20_1—H20_1	119.7	C25_2—C24_2—C23_2	118.7 (6)
C15_1—C20_1—H20_1	119.7	C25_2—C24_2—H24_2	120.6
O9_1—C21_1—O6_1	122.0 (5)	C23_2—C24_2—H24_2	120.6
O9_1—C21_1—C22_1	124.7 (5)	C26_2—C25_2—C24_2	121.5 (6)
O6_1—C21_1—C22_1	113.3 (5)	C26_2—C25_2—H25_2	119.2
C23_1—C22_1—C27_1	121.6 (6)	C24_2—C25_2—H25_2	119.2
C23_1—C22_1—C21_1	122.2 (5)	C25_2—C26_2—C27_2	119.5 (6)
C27_1—C22_1—C21_1	116.2 (6)	C25_2—C26_2—H26_2	120.2
C22_1—C23_1—C24_1	119.4 (6)	C27_2—C26_2—H26_2	120.2
C22_1—C23_1—H23_1	120.3	C26_2—C27_2—C22_2	120.4 (6)
C24_1—C23_1—H23_1	120.3	C26_2—C27_2—H27_2	119.8
C25_1—C24_1—C23_1	118.6 (7)	C22_2—C27_2—H27_2	119.8
C25_1—C24_1—H24_1	120.7	O7′_2—C7′_2—O2′_2	124.1 (5)
C23_1—C24_1—H24_1	120.7	O7′_2—C7′_2—C8′_2	125.3 (5)
C26_1—C25_1—C24_1	121.3 (7)	O2′_2—C7′_2—C8′_2	110.5 (5)
C26_1—C25_1—H25_1	119.4	C9′_2—C8′_2—C13′_2	119.9 (6)
C24_1—C25_1—H25_1	119.4	C9′_2—C8′_2—C7′_2	122.3 (5)
C25_1—C26_1—C27_1	120.0 (7)	C13′_2—C8′_2—C7′_2	117.8 (6)
C25_1—C26_1—H26_1	120.0	C8′_2—C9′_2—C10′_2	120.8 (6)
C27_1—C26_1—H26_1	120.0	C8′_2—C9′_2—H9′_2	119.6
C22_1—C27_1—C26_1	119.1 (7)	C10′_2—C9′_2—H9′_2	119.6
C22_1—C27_1—H27_1	120.5	C11′_2—C10′_2—C9′_2	118.6 (7)
C26_1—C27_1—H27_1	120.5	C11′_2—C10′_2—H10′_2	120.7
O7′_1—C7′_1—O2′_1	123.4 (5)	C9′_2—C10′_2—H10′_2	120.7
O7′_1—C7′_1—C8′_1	124.4 (5)	C12′_2—C11′_2—C10′_2	121.1 (7)
O2′_1—C7′_1—C8′_1	112.2 (4)	C12′_2—C11′_2—H11′_2	119.4
C9′_1—C8′_1—C13′_1	119.1 (5)	C10′_2—C11′_2—H11′_2	119.4
C9′_1—C8′_1—C7′_1	121.5 (5)	C11′_2—C12′_2—C13′_2	120.4 (7)
C13′_1—C8′_1—C7′_1	119.4 (5)	C11′_2—C12′_2—H12′_2	119.8
C8′_1—C9′_1—C10′_1	119.8 (6)	C13′_2—C12′_2—H12′_2	119.8
C8′_1—C9′_1—H9′_1	120.1	C12′_2—C13′_2—C8′_2	119.1 (7)
C10′_1—C9′_1—H9′_1	120.1	C12′_2—C13′_2—H13′_2	120.4
C11′_1—C10′_1—C9′_1	120.7 (6)	C8′_2—C13′_2—H13′_2	120.4
C11′_1—C10′_1—H10′_1	119.7	O8′_2—C14′_2—O3′_2	123.0 (5)
C9′_1—C10′_1—H10′_1	119.7	O8′_2—C14′_2—C15′_2	124.9 (5)
C10′_1—C11′_1—C12′_1	119.7 (6)	O3′_2—C14′_2—C15′_2	112.1 (5)
C10′_1—C11′_1—H11′_1	120.2	C16′_2—C15′_2—C20′_2	120.1 (5)
C12′_1—C11′_1—H11′_1	120.2	C16′_2—C15′_2—C14′_2	122.5 (5)
C13′_1—C12′_1—C11′_1	120.3 (6)	C20′_2—C15′_2—C14′_2	117.4 (5)
C13′_1—C12′_1—H12′_1	119.8	C17′_2—C16′_2—C15′_2	119.8 (5)
C11′_1—C12′_1—H12′_1	119.8	C17′_2—C16′_2—H16′_2	120.1
C12′_1—C13′_1—C8′_1	120.4 (6)	C15′_2—C16′_2—H16′_2	120.1

C12′_1—C13′_1—H13′_1	119.8	C16′_2—C17′_2—C18′_2	119.8 (6)
C8′_1—C13′_1—H13′_1	119.8	C16′_2—C17′_2—H17′_2	120.1
O8′_1—C14′_1—O3′_1	123.0 (5)	C18′_2—C17′_2—H17′_2	120.1
O8′_1—C14′_1—C15′_1	125.4 (5)	C19′_2—C18′_2—C17′_2	120.1 (6)
O3′_1—C14′_1—C15′_1	111.6 (5)	C19′_2—C18′_2—H18′_2	120.0
C16′_1—C15′_1—C20′_1	119.4 (5)	C17′_2—C18′_2—H18′_2	120.0
C16′_1—C15′_1—C14′_1	122.9 (5)	C20′_2—C19′_2—C18′_2	120.4 (5)
C20′_1—C15′_1—C14′_1	117.7 (5)	C20′_2—C19′_2—H19′_2	119.8
C17′_1—C16′_1—C15′_1	120.4 (5)	C18′_2—C19′_2—H19′_2	119.8
C17′_1—C16′_1—H16′_1	119.8	C19′_2—C20′_2—C15′_2	119.8 (5)
C15′_1—C16′_1—H16′_1	119.8	C19′_2—C20′_2—H20′_2	120.1
C16′_1—C17′_1—C18′_1	119.7 (6)	C15′_2—C20′_2—H20′_2	120.1
C16′_1—C17′_1—H17′_1	120.1	O9′_2—C21′_2—O4′_2	122.9 (5)
C18′_1—C17′_1—H17′_1	120.1	O9′_2—C21′_2—C22′_2	124.5 (5)
C19′_1—C18′_1—C17′_1	119.7 (6)	O4′_2—C21′_2—C22′_2	112.5 (5)
C19′_1—C18′_1—H18′_1	120.2	C23′_2—C22′_2—C27′_2	121.0 (5)
C17′_1—C18′_1—H18′_1	120.2	C23′_2—C22′_2—C21′_2	122.9 (5)
C20′_1—C19′_1—C18′_1	120.9 (6)	C27′_2—C22′_2—C21′_2	116.1 (5)
C20′_1—C19′_1—H19′_1	119.5	C22′_2—C23′_2—C24′_2	119.7 (6)
C18′_1—C19′_1—H19′_1	119.5	C22′_2—C23′_2—H23′_2	120.1
C19′_1—C20′_1—C15′_1	119.9 (6)	C24′_2—C23′_2—H23′_2	120.1
C19′_1—C20′_1—H20′_1	120.1	C25′_2—C24′_2—C23′_2	120.3 (7)
C15′_1—C20′_1—H20′_1	120.1	C25′_2—C24′_2—H24′_2	119.9
O9′_1—C21′_1—O4′_1	122.2 (5)	C23′_2—C24′_2—H24′_2	119.9
O9′_1—C21′_1—C22′_1	124.7 (5)	C26′_2—C25′_2—C24′_2	120.1 (6)
O4′_1—C21′_1—C22′_1	113.1 (4)	C26′_2—C25′_2—H25′_2	120.0
C27′_1—C22′_1—C23′_1	119.9 (5)	C24′_2—C25′_2—H25′_2	120.0
C27′_1—C22′_1—C21′_1	117.8 (5)	C25′_2—C26′_2—C27′_2	120.6 (6)
C23′_1—C22′_1—C21′_1	122.3 (5)	C25′_2—C26′_2—H26′_2	119.7
C22′_1—C23′_1—C24′_1	119.4 (5)	C27′_2—C26′_2—H26′_2	119.7
C22′_1—C23′_1—H23′_1	120.3	C26′_2—C27′_2—C22′_2	118.2 (6)
C24′_1—C23′_1—H23′_1	120.3	C26′_2—C27′_2—H27′_2	120.9
C23′_1—C24′_1—C25′_1	119.5 (6)	C22′_2—C27′_2—H27′_2	120.9
C23′_1—C24′_1—H24′_1	120.3	O10′_2—C28′_2—O6′_2	123.0 (5)
C25′_1—C24′_1—H24′_1	120.3	O10′_2—C28′_2—C29′_2	124.9 (5)
C26′_1—C25′_1—C24′_1	120.3 (5)	O6′_2—C28′_2—C29′_2	112.0 (5)
C26′_1—C25′_1—H25′_1	119.8	C34′_2—C29′_2—C30′_2	119.8 (6)
C24′_1—C25′_1—H25′_1	119.8	C34′_2—C29′_2—C28′_2	117.6 (5)
C25′_1—C26′_1—C27′_1	120.6 (5)	C30′_2—C29′_2—C28′_2	122.5 (5)
C25′_1—C26′_1—H26′_1	119.7	C29′_2—C30′_2—C31′_2	119.4 (6)
C27′_1—C26′_1—H26′_1	119.7	C29′_2—C30′_2—H30′_2	120.3
C26′_1—C27′_1—C22′_1	120.3 (5)	C31′_2—C30′_2—H30′_2	120.3
C26′_1—C27′_1—H27′_1	119.9	C32′_2—C31′_2—C30′_2	120.2 (6)
C22′_1—C27′_1—H27′_1	119.9	C32′_2—C31′_2—H31′_2	119.9
O10′_1—C28′_1—O6′_1	122.7 (5)	C30′_2—C31′_2—H31′_2	119.9
O10′_1—C28′_1—C29′_1	124.7 (5)	C31′_2—C32′_2—C33′_2	120.2 (6)
O6′_1—C28′_1—C29′_1	112.7 (5)	C31′_2—C32′_2—H32′_2	119.9
C30′_1—C29′_1—C34′_1	119.8 (6)	C33′_2—C32′_2—H32′_2	119.9

C30′_1—C29′_1—C28′_1	123.3 (5)	C34′_2—C33′_2—C32′_2	119.3 (6)
C34′_1—C29′_1—C28′_1	116.9 (6)	C34′_2—C33′_2—H33′_2	120.4
C31′_1—C30′_1—C29′_1	119.8 (6)	C32′_2—C33′_2—H33′_2	120.4
C31′_1—C30′_1—H30′_1	120.1	C33′_2—C34′_2—C29′_2	121.0 (6)
C29′_1—C30′_1—H30′_1	120.1	C33′_2—C34′_2—H34′_2	119.5
C30′_1—C31′_1—C32′_1	120.2 (7)	C29′_2—C34′_2—H34′_2	119.5
C30′_1—C31′_1—H31′_1	119.9	C2S_3—O2S_3—C3S_3	117.9 (6)
C32′_1—C31′_1—H31′_1	119.9	C2S_3—C1S_3—H1SA_3	109.5
C33′_1—C32′_1—C31′_1	120.3 (6)	C2S_3—C1S_3—H1SB_3	109.5
C33′_1—C32′_1—H32′_1	119.8	H1SA_3—C1S_3—H1SB_3	109.5
C31′_1—C32′_1—H32′_1	119.8	C2S_3—C1S_3—H1SC_3	109.5
C32′_1—C33′_1—C34′_1	120.0 (6)	H1SA_3—C1S_3—H1SC_3	109.5
C32′_1—C33′_1—H33′_1	120.0	H1SB_3—C1S_3—H1SC_3	109.5
C34′_1—C33′_1—H33′_1	120.0	O1S_3—C2S_3—O2S_3	120.9 (8)
C29′_1—C34′_1—C33′_1	119.7 (6)	O1S_3—C2S_3—C1S_3	125.6 (8)
C29′_1—C34′_1—H34′_1	120.1	O2S_3—C2S_3—C1S_3	113.5 (7)
C33′_1—C34′_1—H34′_1	120.1	O2S_3—C3S_3—C4S_3	106.1 (5)
C7_2—O1_2—C1_2	115.5 (4)	O2S_3—C3S_3—H3SA_3	110.5
C14_2—O2_2—C2_2	119.7 (4)	C4S_3—C3S_3—H3SA_3	110.5
C3_2—O3_2—H3O_2	102 (5)	O2S_3—C3S_3—H3SB_3	110.5
C1_2—O5_2—C5_2	109.2 (4)	C4S_3—C3S_3—H3SB_3	110.5
C21_2—O6_2—C6_2	113.9 (4)	H3SA_3—C3S_3—H3SB_3	108.7
O1_2—C1_2—O5_2	106.0 (4)	C3S_3—C4S_3—H4SA_3	109.5
O1_2—C1_2—C2_2	110.1 (4)	C3S_3—C4S_3—H4SB_3	109.5
O5_2—C1_2—C2_2	109.2 (4)	H4SA_3—C4S_3—H4SB_3	109.5
O1_2—C1_2—H1_2	110.5	C3S_3—C4S_3—H4SC_3	109.5
O5_2—C1_2—H1_2	110.5	H4SA_3—C4S_3—H4SC_3	109.5
C2_2—C1_2—H1_2	110.5	H4SB_3—C4S_3—H4SC_3	109.5

C5_1—O5_1—C1_1—O1_1	173.3 (4)	C5_2—O5_2—C1_2—O1_2	172.9 (4)
C5_1—O5_1—C1_1—C2_1	−68.8 (5)	C5_2—O5_2—C1_2—C2_2	−68.5 (5)
C7_1—O1_1—C1_1—O5_1	−139.3 (4)	C14_2—O2_2—C2_2—C3_2	−114.4 (5)
C7_1—O1_1—C1_1—C2_1	102.2 (5)	C14_2—O2_2—C2_2—C1_2	128.4 (5)
C14_1—O2_1—C2_1—C1_1	111.1 (5)	O1_2—C1_2—C2_2—O2_2	−63.2 (5)
C14_1—O2_1—C2_1—C3_1	−130.5 (5)	O5_2—C1_2—C2_2—O2_2	−179.2 (4)
O5_1—C1_1—C2_1—O2_1	−177.3 (4)	O1_2—C1_2—C2_2—C3_2	177.8 (4)
O1_1—C1_1—C2_1—O2_1	−60.5 (5)	O5_2—C1_2—C2_2—C3_2	61.8 (5)
O5_1—C1_1—C2_1—C3_1	64.1 (5)	O2_2—C2_2—C3_2—O3_2	69.5 (5)
O1_1—C1_1—C2_1—C3_1	−179.1 (4)	C1_2—C2_2—C3_2—O3_2	−175.9 (4)
O2_1—C2_1—C3_1—O3_1	66.7 (5)	O2_2—C2_2—C3_2—C4_2	−168.1 (4)
C1_1—C2_1—C3_1—O3_1	−176.0 (4)	C1_2—C2_2—C3_2—C4_2	−53.4 (5)
O2_1—C2_1—C3_1—C4_1	−170.9 (4)	O3_2—C3_2—C4_2—O1′_2	−72.6 (6)
C1_1—C2_1—C3_1—C4_1	−53.6 (5)	C2_2—C3_2—C4_2—O1′_2	167.6 (4)
O3_1—C3_1—C4_1—O1′_1	−74.7 (5)	O3_2—C3_2—C4_2—C5_2	171.8 (4)
C2_1—C3_1—C4_1—O1′_1	165.6 (4)	C2_2—C3_2—C4_2—C5_2	52.0 (6)
O3_1—C3_1—C4_1—C5_1	169.2 (4)	C1_2—O5_2—C5_2—C6_2	−165.5 (4)
C2_1—C3_1—C4_1—C5_1	49.6 (6)	C1_2—O5_2—C5_2—C4_2	65.9 (5)
C1_1—O5_1—C5_1—C6_1	−171.3 (4)	O1′_2—C4_2—C5_2—O5_2	−178.5 (3)

C1_1—O5_1—C5_1—C4_1	63.5 (5)
O1′_1—C4_1—C5_1—O5_1	−175.9 (4)
C3_1—C4_1—C5_1—O5_1	−54.3 (5)
O1′_1—C4_1—C5_1—C6_1	62.2 (5)
C3_1—C4_1—C5_1—C6_1	−176.2 (4)
C21_1—O6_1—C6_1—C5_1	170.4 (4)
O5_1—C5_1—C6_1—O6_1	−65.7 (5)
C4_1—C5_1—C6_1—O6_1	57.3 (6)
C3_1—C4_1—O1′_1—C1′_1	64.9 (5)
C5_1—C4_1—O1′_1—C1′_1	−174.9 (4)
C4_1—O1′_1—C1′_1—O5′_1	−90.9 (5)
C4_1—O1′_1—C1′_1—C2′_1	151.4 (4)
C5′_1—O5′_1—C1′_1—O1′_1	−179.7 (4)
C5′_1—O5′_1—C1′_1—C2′_1	−62.5 (5)
C7′_1—O2′_1—C2′_1—C3′_1	−136.7 (4)
C7′_1—O2′_1—C2′_1—C1′_1	104.8 (5)
O1′_1—C1′_1—C2′_1—O2′_1	−71.5 (5)
O5′_1—C1′_1—C2′_1—O2′_1	171.8 (4)
O1′_1—C1′_1—C2′_1—C3′_1	171.5 (4)
O5′_1—C1′_1—C2′_1—C3′_1	54.9 (5)
C14′_1—O3′_1—C3′_1—C4′_1	122.9 (5)
C14′_1—O3′_1—C3′_1—C2′_1	−111.7 (5)
O2′_1—C2′_1—C3′_1—O3′_1	66.9 (5)
C1′_1—C2′_1—C3′_1—O3′_1	−176.0 (4)
O2′_1—C2′_1—C3′_1—C4′_1	−169.8 (4)
C1′_1—C2′_1—C3′_1—C4′_1	−52.7 (6)
C21′_1—O4′_1—C4′_1—C3′_1	−135.0 (4)
C21′_1—O4′_1—C4′_1—C5′_1	106.8 (5)
O3′_1—C3′_1—C4′_1—O4′_1	56.8 (5)
C2′_1—C3′_1—C4′_1—O4′_1	−66.4 (5)
O3′_1—C3′_1—C4′_1—C5′_1	176.0 (4)
C2′_1—C3′_1—C4′_1—C5′_1	52.8 (6)
C1′_1—O5′_1—C5′_1—C6′_1	−171.2 (4)
C1′_1—O5′_1—C5′_1—C4′_1	64.2 (5)
O4′_1—C4′_1—C5′_1—O5′_1	61.8 (5)
C3′_1—C4′_1—C5′_1—O5′_1	−56.8 (5)
O4′_1—C4′_1—C5′_1—C6′_1	−58.4 (6)
C3′_1—C4′_1—C5′_1—C6′_1	−177.0 (4)
C28′_1—O6′_1—C6′_1—C5′_1	179.1 (4)
O5′_1—C5′_1—C6′_1—O6′_1	67.8 (5)
C4′_1—C5′_1—C6′_1—O6′_1	−170.3 (4)
C1_1—O1_1—C7_1—O7_1	13.4 (8)
C1_1—O1_1—C7_1—C8_1	−164.4 (4)
O7_1—C7_1—C8_1—C13_1	−9.3 (9)
O1_1—C7_1—C8_1—C13_1	168.5 (5)
O7_1—C7_1—C8_1—C9_1	174.0 (6)
O1_1—C7_1—C8_1—C9_1	−8.2 (8)
C13_1—C8_1—C9_1—C10_1	−0.4 (9)
C3_2—C4_2—C5_2—O5_2	−57.1 (5)
O1′_2—C4_2—C5_2—C6_2	57.0 (6)
C3_2—C4_2—C5_2—C6_2	178.4 (4)
C21_2—O6_2—C6_2—C5_2	169.1 (4)
O5_2—C5_2—C6_2—O6_2	−66.2 (5)
C4_2—C5_2—C6_2—O6_2	58.0 (6)
C5_2—C4_2—O1′_2—C1′_2	−174.8 (4)
C3_2—C4_2—O1′_2—C1′_2	66.0 (5)
C4_2—O1′_2—C1′_2—O5′_2	−91.9 (5)
C4_2—O1′_2—C1′_2—C2′_2	150.7 (4)
C5′_2—O5′_2—C1′_2—O1′_2	−177.2 (4)
C5′_2—O5′_2—C1′_2—C2′_2	−60.8 (5)
C7′_2—O2′_2—C2′_2—C3′_2	−136.5 (4)
C7′_2—O2′_2—C2′_2—C1′_2	105.3 (5)
O1′_2—C1′_2—C2′_2—O2′_2	−73.6 (5)
O5′_2—C1′_2—C2′_2—O2′_2	170.2 (4)
O1′_2—C1′_2—C2′_2—C3′_2	171.3 (4)
O5′_2—C1′_2—C2′_2—C3′_2	55.1 (5)
C14′_2—O3′_2—C3′_2—C4′_2	119.7 (5)
C14′_2—O3′_2—C3′_2—C2′_2	−118.0 (5)
O2′_2—C2′_2—C3′_2—O3′_2	67.2 (5)
C1′_2—C2′_2—C3′_2—O3′_2	−176.3 (4)
O2′_2—C2′_2—C3′_2—C4′_2	−171.0 (4)
C1′_2—C2′_2—C3′_2—C4′_2	−54.5 (6)
C21′_2—O4′_2—C4′_2—C3′_2	−143.6 (4)
C21′_2—O4′_2—C4′_2—C5′_2	98.3 (5)
O3′_2—C3′_2—C4′_2—O4′_2	56.2 (5)
C2′_2—C3′_2—C4′_2—O4′_2	−64.4 (5)
O3′_2—C3′_2—C4′_2—C5′_2	175.7 (4)
C2′_2—C3′_2—C4′_2—C5′_2	55.2 (5)
C1′_2—O5′_2—C5′_2—C6′_2	−173.0 (4)
C1′_2—O5′_2—C5′_2—C4′_2	63.6 (5)
O4′_2—C4′_2—C5′_2—O5′_2	60.3 (5)
C3′_2—C4′_2—C5′_2—O5′_2	−58.6 (5)
O4′_2—C4′_2—C5′_2—C6′_2	−58.6 (6)
C3′_2—C4′_2—C5′_2—C6′_2	−177.5 (4)
C28′_2—O6′_2—C6′_2—C5′_2	177.8 (4)
O5′_2—C5′_2—C6′_2—O6′_2	68.5 (5)
C4′_2—C5′_2—C6′_2—O6′_2	−170.3 (4)
C1_2—O1_2—C7_2—O7_2	3.8 (8)
C1_2—O1_2—C7_2—C8_2	−176.5 (4)
O7_2—C7_2—C8_2—C9_2	164.8 (6)
O1_2—C7_2—C8_2—C9_2	−14.9 (8)
O7_2—C7_2—C8_2—C13_2	−16.0 (9)
O1_2—C7_2—C8_2—C13_2	164.3 (5)
C13_2—C8_2—C9_2—C10_2	1.8 (9)
C7_2—C8_2—C9_2—C10_2	−179.0 (6)
C8_2—C9_2—C10_2—C11_2	−2.0 (10)

C7_1—C8_1—C9_1—C10_1	176.2 (6)
C8_1—C9_1—C10_1—C11_1	−0.8 (10)
C9_1—C10_1—C11_1—C12_1	1.5 (11)
C10_1—C11_1—C12_1—C13_1	−1.0 (10)
C11_1—C12_1—C13_1—C8_1	−0.2 (9)
C9_1—C8_1—C13_1—C12_1	0.9 (8)
C7_1—C8_1—C13_1—C12_1	−175.9 (5)
C2_1—O2_1—C14_1—O8_1	16.2 (8)
C2_1—O2_1—C14_1—C15_1	−163.5 (4)
O8_1—C14_1—C15_1—C16_1	−173.2 (6)
O2_1—C14_1—C15_1—C16_1	6.5 (7)
O8_1—C14_1—C15_1—C20_1	3.9 (9)
O2_1—C14_1—C15_1—C20_1	−176.4 (5)
C20_1—C15_1—C16_1—C17_1	1.9 (9)
C14_1—C15_1—C16_1—C17_1	179.0 (5)
C15_1—C16_1—C17_1—C18_1	−0.4 (9)
C16_1—C17_1—C18_1—C19_1	−0.8 (11)
C17_1—C18_1—C19_1—C20_1	0.6 (11)
C18_1—C19_1—C20_1—C15_1	0.8 (10)
C16_1—C15_1—C20_1—C19_1	−2.1 (9)
C14_1—C15_1—C20_1—C19_1	−179.3 (6)
C6_1—O6_1—C21_1—O9_1	1.7 (7)
C6_1—O6_1—C21_1—C22_1	−177.9 (4)
O9_1—C21_1—C22_1—C23_1	176.7 (6)
O6_1—C21_1—C22_1—C23_1	−3.7 (7)
O9_1—C21_1—C22_1—C27_1	−4.6 (8)
O6_1—C21_1—C22_1—C27_1	175.1 (5)
C27_1—C22_1—C23_1—C24_1	−1.3 (9)
C21_1—C22_1—C23_1—C24_1	177.5 (6)
C22_1—C23_1—C24_1—C25_1	1.2 (10)
C23_1—C24_1—C25_1—C26_1	−0.7 (11)
C24_1—C25_1—C26_1—C27_1	0.2 (11)
C23_1—C22_1—C27_1—C26_1	0.8 (9)
C21_1—C22_1—C27_1—C26_1	−178.0 (5)
C25_1—C26_1—C27_1—C22_1	−0.3 (9)
C2′_1—O2′_1—C7′_1—O7′_1	2.1 (8)
C2′_1—O2′_1—C7′_1—C8′_1	−177.7 (4)
O7′_1—C7′_1—C8′_1—C9′_1	−163.8 (5)
O2′_1—C7′_1—C8′_1—C9′_1	16.0 (7)
O7′_1—C7′_1—C8′_1—C13′_1	15.0 (8)
O2′_1—C7′_1—C8′_1—C13′_1	−165.1 (5)
C13′_1—C8′_1—C9′_1—C10′_1	0.5 (8)
C7′_1—C8′_1—C9′_1—C10′_1	179.4 (5)
C8′_1—C9′_1—C10′_1—C11′_1	0.3 (8)
C9′_1—C10′_1—C11′_1—C12′_1	−0.4 (9)
C10′_1—C11′_1—C12′_1—C13′_1	−0.4 (10)
C11′_1—C12′_1—C13′_1—C8′_1	1.2 (10)
C9′_1—C8′_1—C13′_1—C12′_1	−1.3 (9)
C9_2—C10_2—C11_2—C12_2	1.0 (10)
C10_2—C11_2—C12_2—C13_2	0.2 (10)
C9_2—C8_2—C13_2—C12_2	−0.6 (8)
C7_2—C8_2—C13_2—C12_2	−179.9 (5)
C11_2—C12_2—C13_2—C8_2	−0.4 (9)
C2_2—O2_2—C14_2—O8_2	16.5 (8)
C2_2—O2_2—C14_2—C15_2	−162.9 (4)
O8_2—C14_2—C15_2—C16_2	−163.8 (6)
O2_2—C14_2—C15_2—C16_2	15.6 (8)
O8_2—C14_2—C15_2—C20_2	12.7 (9)
O2_2—C14_2—C15_2—C20_2	−167.9 (5)
C20_2—C15_2—C16_2—C17_2	−1.6 (9)
C14_2—C15_2—C16_2—C17_2	174.9 (6)
C15_2—C16_2—C17_2—C18_2	0.8 (10)
C16_2—C17_2—C18_2—C19_2	1.3 (11)
C17_2—C18_2—C19_2—C20_2	−2.4 (12)
C16_2—C15_2—C20_2—C19_2	0.4 (10)
C14_2—C15_2—C20_2—C19_2	−176.2 (6)
C18_2—C19_2—C20_2—C15_2	1.6 (11)
C6_2—O6_2—C21_2—O9_2	1.5 (7)
C6_2—O6_2—C21_2—C22_2	−176.0 (4)
O9_2—C21_2—C22_2—C23_2	−179.3 (6)
O6_2—C21_2—C22_2—C23_2	−1.8 (7)
O9_2—C21_2—C22_2—C27_2	0.4 (8)
O6_2—C21_2—C22_2—C27_2	177.8 (5)
C27_2—C22_2—C23_2—C24_2	−2.2 (9)
C21_2—C22_2—C23_2—C24_2	177.4 (5)
C22_2—C23_2—C24_2—C25_2	1.7 (9)
C23_2—C24_2—C25_2—C26_2	−0.4 (9)
C24_2—C25_2—C26_2—C27_2	−0.3 (10)
C25_2—C26_2—C27_2—C22_2	−0.3 (9)
C23_2—C22_2—C27_2—C26_2	1.5 (9)
C21_2—C22_2—C27_2—C26_2	−178.2 (5)
C2′_2—O2′_2—C7′_2—O7′_2	0.7 (7)
C2′_2—O2′_2—C7′_2—C8′_2	−179.8 (4)
O7′_2—C7′_2—C8′_2—C9′_2	−159.4 (6)
O2′_2—C7′_2—C8′_2—C9′_2	21.2 (7)
O7′_2—C7′_2—C8′_2—C13′_2	20.4 (8)
O2′_2—C7′_2—C8′_2—C13′_2	−159.1 (5)
C13′_2—C8′_2—C9′_2—C10′_2	0.0 (9)
C7′_2—C8′_2—C9′_2—C10′_2	179.8 (5)
C8′_2—C9′_2—C10′_2—C11′_2	1.3 (9)
C9′_2—C10′_2—C11′_2—C12′_2	−1.5 (11)
C10′_2—C11′_2—C12′_2—C13′_2	0.4 (13)
C11′_2—C12′_2—C13′_2—C8′_2	1.0 (12)
C9′_2—C8′_2—C13′_2—C12′_2	−1.2 (10)
C7′_2—C8′_2—C13′_2—C12′_2	179.0 (6)
C3′_2—O3′_2—C14′_2—O8′_2	−6.1 (7)

C7′_1—C8′_1—C13′_1—C12′_1	179.8 (6)
C3′_1—O3′_1—C14′_1—O8′_1	−3.6 (7)
C3′_1—O3′_1—C14′_1—C15′_1	176.4 (4)
O8′_1—C14′_1—C15′_1—C16′_1	−178.6 (6)
O3′_1—C14′_1—C15′_1—C16′_1	1.4 (7)
O8′_1—C14′_1—C15′_1—C20′_1	3.1 (8)
O3′_1—C14′_1—C15′_1—C20′_1	−176.9 (5)
C20′_1—C15′_1—C16′_1—C17′_1	0.5 (9)
C14′_1—C15′_1—C16′_1—C17′_1	−177.9 (6)
C15′_1—C16′_1—C17′_1—C18′_1	0.7 (10)
C16′_1—C17′_1—C18′_1—C19′_1	−0.9 (10)
C17′_1—C18′_1—C19′_1—C20′_1	0.1 (11)
C18′_1—C19′_1—C20′_1—C15′_1	1.1 (10)
C16′_1—C15′_1—C20′_1—C19′_1	−1.3 (9)
C14′_1—C15′_1—C20′_1—C19′_1	177.1 (6)
C4′_1—O4′_1—C21′_1—O9′_1	−1.6 (7)
C4′_1—O4′_1—C21′_1—C22′_1	179.4 (4)
O9′_1—C21′_1—C22′_1—C27′_1	3.4 (8)
O4′_1—C21′_1—C22′_1—C27′_1	−177.5 (4)
O9′_1—C21′_1—C22′_1—C23′_1	−177.2 (6)
O4′_1—C21′_1—C22′_1—C23′_1	1.8 (7)
C27′_1—C22′_1—C23′_1—C24′_1	0.5 (8)
C21′_1—C22′_1—C23′_1—C24′_1	−178.8 (5)
C22′_1—C23′_1—C24′_1—C25′_1	−0.1 (8)
C23′_1—C24′_1—C25′_1—C26′_1	−0.6 (8)
C24′_1—C25′_1—C26′_1—C27′_1	0.9 (8)
C25′_1—C26′_1—C27′_1—C22′_1	−0.6 (8)
C23′_1—C22′_1—C27′_1—C26′_1	−0.1 (8)
C21′_1—C22′_1—C27′_1—C26′_1	179.2 (5)
C6′_1—O6′_1—C28′_1—O10′_1	1.7 (7)
C6′_1—O6′_1—C28′_1—C29′_1	179.8 (4)
O10′_1—C28′_1—C29′_1—C30′_1	−176.4 (5)
O6′_1—C28′_1—C29′_1—C30′_1	5.6 (7)
O10′_1—C28′_1—C29′_1—C34′_1	4.0 (8)
O6′_1—C28′_1—C29′_1—C34′_1	−174.1 (5)
C34′_1—C29′_1—C30′_1—C31′_1	−1.5 (8)
C28′_1—C29′_1—C30′_1—C31′_1	178.8 (5)
C29′_1—C30′_1—C31′_1—C32′_1	1.9 (9)
C30′_1—C31′_1—C32′_1—C33′_1	−2.2 (10)
C31′_1—C32′_1—C33′_1—C34′_1	2.1 (10)
C3′_2—O3′_2—C14′_2—C15′_2	173.8 (4)
O8′_2—C14′_2—C15′_2—C16′_2	−176.2 (5)
O3′_2—C14′_2—C15′_2—C16′_2	3.9 (7)
O8′_2—C14′_2—C15′_2—C20′_2	5.0 (8)
O3′_2—C14′_2—C15′_2—C20′_2	−174.8 (4)
C20′_2—C15′_2—C16′_2—C17′_2	−1.1 (8)
C14′_2—C15′_2—C16′_2—C17′_2	−179.8 (5)
C15′_2—C16′_2—C17′_2—C18′_2	2.0 (9)
C16′_2—C17′_2—C18′_2—C19′_2	−1.9 (9)
C17′_2—C18′_2—C19′_2—C20′_2	0.9 (10)
C18′_2—C19′_2—C20′_2—C15′_2	0.0 (9)
C16′_2—C15′_2—C20′_2—C19′_2	0.1 (8)
C14′_2—C15′_2—C20′_2—C19′_2	178.9 (5)
C4′_2—O4′_2—C21′_2—O9′_2	0.8 (7)
C4′_2—O4′_2—C21′_2—C22′_2	−178.4 (4)
O9′_2—C21′_2—C22′_2—C23′_2	−173.4 (6)
O4′_2—C21′_2—C22′_2—C23′_2	5.8 (7)
O9′_2—C21′_2—C22′_2—C27′_2	7.0 (8)
O4′_2—C21′_2—C22′_2—C27′_2	−173.8 (5)
C27′_2—C22′_2—C23′_2—C24′_2	−0.3 (9)
C21′_2—C22′_2—C23′_2—C24′_2	−179.8 (5)
C22′_2—C23′_2—C24′_2—C25′_2	0.9 (10)
C23′_2—C24′_2—C25′_2—C26′_2	−1.6 (10)
C24′_2—C25′_2—C26′_2—C27′_2	1.5 (10)
C25′_2—C26′_2—C27′_2—C22′_2	−0.9 (9)
C23′_2—C22′_2—C27′_2—C26′_2	0.2 (8)
C21′_2—C22′_2—C27′_2—C26′_2	179.8 (5)
C6′_2—O6′_2—C28′_2—O10′_2	7.0 (7)
C6′_2—O6′_2—C28′_2—C29′_2	−172.6 (4)
O10′_2—C28′_2—C29′_2—C34′_2	−13.1 (8)
O6′_2—C28′_2—C29′_2—C34′_2	166.5 (5)
O10′_2—C28′_2—C29′_2—C30′_2	171.2 (5)
O6′_2—C28′_2—C29′_2—C30′_2	−9.3 (7)
C34′_2—C29′_2—C30′_2—C31′_2	−0.8 (9)
C28′_2—C29′_2—C30′_2—C31′_2	174.9 (5)
C29′_2—C30′_2—C31′_2—C32′_2	−2.0 (9)
C30′_2—C31′_2—C32′_2—C33′_2	2.9 (10)
C31′_2—C32′_2—C33′_2—C34′_2	−0.9 (11)
C32′_2—C33′_2—C34′_2—C29′_2	−1.9 (11)
C30′_2—C29′_2—C34′_2—C33′_2	2.8 (10)

C30′_1—C29′_1—C34′_1—C33′_1	1.4 (8)	C28′_2—C29′_2—C34′_2—C33′_2	−173.1 (6)
C28′_1—C29′_1—C34′_1—C33′_1	−178.9 (5)	C3S_3—O2S_3—C2S_3—O1S_3	−1.1 (11)
C32′_1—C33′_1—C34′_1—C29′_1	−1.7 (9)	C3S_3—O2S_3—C2S_3—C1S_3	−179.5 (7)
C7_2—O1_2—C1_2—O5_2	−133.6 (4)	C2S_3—O2S_3—C3S_3—C4S_3	179.9 (6)
C7_2—O1_2—C1_2—C2_2	108.4 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3_1—H3*O*_1···O5′_1	0.79 (7)	2.32 (7)	2.797 (5)	120 (6)
O3_1—H3*O*_1···O6′_1	0.79 (7)	2.39 (7)	3.147 (6)	160 (6)
O3_2—H3*O*_2···O5′_2	0.73 (7)	2.19 (7)	2.806 (5)	142 (7)
O3_2—H3*O*_2···O6′_2	0.73 (7)	2.62 (7)	3.256 (5)	146 (6)

1,2,4,6-Tetra-*O*-benzoyl-*β*-*D*-glucopyranose acetone monosolvate (IV)

Crystal data

$C_{34}H_{28}O_{10}\cdot C_3H_6O$
$M_r = 654.64$
Orthorhombic, $P2_12_12_1$
$a = 5.6342$ (2) Å
$b = 19.9711$ (8) Å
$c = 29.6094$ (11) Å
$V = 3331.7$ (2) Å^3
$Z = 4$
$F(000) = 1376$
$D_x = 1.305$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 9756 reflections
$\theta = 3.7$–$72.1°$
$\mu = 0.80$ mm^{-1}
$T = 120$ K
Needle, colorless
0.21 × 0.13 × 0.09 mm

Data collection

Bruker APEXII diffractometer
Radiation source: Incoatec micro-focus
Detector resolution: 8.33 pixels mm^{-1}
combination of ω and φ–scans
Absorption correction: numerical (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.817$, $T_{max} = 0.864$
55150 measured reflections
6526 independent reflections
6458 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 72.2°$, $\theta_{min} = 2.7°$
$h = -6\rightarrow6$
$k = -24\rightarrow24$
$l = -36\rightarrow36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.073$
$S = 1.03$
6526 reflections
436 parameters
0 restraints
Primary atom site location: real-space vector search
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.4158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Absolute structure: Flack *x* determined using 2722 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.08 (3)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.71598 (19)	0.61168 (5)	0.67190 (3)	0.0214 (2)
O2	0.51227 (19)	0.51317 (5)	0.73044 (3)	0.0213 (2)
O3	0.1940 (2)	0.42653 (6)	0.68429 (4)	0.0281 (2)
H3	0.1978	0.3853	0.6900	0.042*
O4	0.3962 (2)	0.37642 (5)	0.60127 (4)	0.0232 (2)
O5	0.66468 (19)	0.54186 (5)	0.61282 (3)	0.0215 (2)
O6	0.4464 (2)	0.52909 (6)	0.53425 (3)	0.0256 (2)
O7	1.0761 (2)	0.61400 (6)	0.63814 (3)	0.0251 (2)
O8	0.1803 (2)	0.57306 (7)	0.74478 (4)	0.0355 (3)
O9	0.0840 (2)	0.39447 (6)	0.55505 (4)	0.0339 (3)
O10	0.5742 (2)	0.53514 (6)	0.46280 (4)	0.0323 (3)
C1	0.6951 (3)	0.54302 (7)	0.66012 (5)	0.0195 (3)
H1	0.8379	0.5168	0.6696	0.023*
C2	0.4708 (3)	0.51718 (7)	0.68248 (4)	0.0192 (3)
H2	0.3348	0.5479	0.6760	0.023*
C3	0.4149 (3)	0.44667 (7)	0.66592 (5)	0.0208 (3)
H3A	0.5416	0.4154	0.6766	0.025*
C4	0.4086 (3)	0.44620 (7)	0.61448 (5)	0.0208 (3)
H4	0.2671	0.4713	0.6031	0.025*
C5	0.6368 (3)	0.47582 (7)	0.59525 (5)	0.0208 (3)
H5	0.7749	0.4476	0.6046	0.025*
C6	0.6350 (3)	0.48287 (8)	0.54450 (5)	0.0238 (3)
H6A	0.7891	0.5005	0.5336	0.029*
H6B	0.6054	0.4390	0.5300	0.029*
C7	0.9167 (3)	0.64249 (8)	0.65719 (5)	0.0209 (3)
C8	0.9126 (3)	0.71557 (8)	0.66667 (5)	0.0240 (3)
C9	1.1059 (3)	0.75298 (9)	0.65200 (6)	0.0344 (4)
H9	1.2339	0.7316	0.6369	0.041*
C10	1.1118 (4)	0.82151 (10)	0.65945 (8)	0.0445 (5)
H10	1.2439	0.8471	0.6495	0.053*
C11	0.9252 (4)	0.85264 (9)	0.68140 (7)	0.0407 (4)
H11	0.9299	0.8996	0.6866	0.049*
C12	0.7315 (4)	0.81563 (9)	0.69585 (6)	0.0366 (4)
H12	0.6037	0.8373	0.7108	0.044*
C13	0.7236 (3)	0.74696 (8)	0.68851 (6)	0.0291 (3)
H13	0.5905	0.7216	0.6983	0.035*
C14	0.3477 (3)	0.54065 (7)	0.75764 (5)	0.0213 (3)
C15	0.3993 (3)	0.52627 (7)	0.80603 (5)	0.0201 (3)
C16	0.6103 (3)	0.49601 (8)	0.81988 (5)	0.0235 (3)

H16	0.7268	0.4836	0.7982	0.028*
C17	0.6491 (3)	0.48408 (8)	0.86556 (5)	0.0253 (3)
H17	0.7941	0.4645	0.8752	0.030*
C18	0.4763 (3)	0.50067 (8)	0.89711 (5)	0.0255 (3)
H18	0.5023	0.4916	0.9282	0.031*
C19	0.2661 (3)	0.53037 (8)	0.88333 (5)	0.0280 (3)
H19	0.1481	0.5416	0.9050	0.034*
C20	0.2280 (3)	0.54381 (8)	0.83777 (5)	0.0242 (3)
H20	0.0853	0.5649	0.8284	0.029*
C21	0.2212 (3)	0.35697 (8)	0.57317 (5)	0.0222 (3)
C22	0.2203 (3)	0.28273 (8)	0.56731 (5)	0.0218 (3)
C23	0.4016 (3)	0.24286 (8)	0.58459 (5)	0.0263 (3)
H23	0.5296	0.2627	0.6006	0.032*
C24	0.3942 (3)	0.17400 (8)	0.57828 (6)	0.0302 (3)
H24	0.5192	0.1468	0.5896	0.036*
C25	0.2053 (3)	0.14467 (8)	0.55555 (5)	0.0286 (3)
H25	0.1999	0.0975	0.5517	0.034*
C26	0.0243 (3)	0.18441 (9)	0.53847 (5)	0.0289 (3)
H26	−0.1051	0.1643	0.5230	0.035*
C27	0.0317 (3)	0.25358 (8)	0.54393 (5)	0.0264 (3)
H27	−0.0910	0.2808	0.5318	0.032*
C28	0.4428 (3)	0.55396 (8)	0.49223 (5)	0.0231 (3)
C29	0.2557 (3)	0.60598 (8)	0.48703 (5)	0.0237 (3)
C30	0.0917 (3)	0.61948 (8)	0.52115 (5)	0.0271 (3)
H30	0.1010	0.5965	0.5492	0.033*
C31	−0.0851 (3)	0.66670 (9)	0.51390 (7)	0.0355 (4)
H31	−0.1985	0.6755	0.5369	0.043*
C32	−0.0971 (4)	0.70125 (9)	0.47316 (7)	0.0397 (4)
H32	−0.2187	0.7334	0.4683	0.048*
C33	0.0697 (4)	0.68854 (9)	0.43959 (6)	0.0380 (4)
H33	0.0633	0.7126	0.4119	0.046*
C34	0.2455 (3)	0.64079 (9)	0.44633 (5)	0.0307 (3)
H34	0.3584	0.6319	0.4233	0.037*
O11	0.2960 (3)	0.29141 (6)	0.69577 (5)	0.0383 (3)
C35	0.1682 (3)	0.24299 (9)	0.69602 (6)	0.0349 (4)
C36	0.2618 (4)	0.17400 (9)	0.70283 (7)	0.0398 (4)
H36A	0.2532	0.1492	0.6743	0.060*
H36B	0.1664	0.1510	0.7258	0.060*
H36C	0.4272	0.1764	0.7129	0.060*
C37	−0.0913 (6)	0.24957 (19)	0.6894 (2)	0.1159 (18)
H37A	−0.1729	0.2409	0.7181	0.174*
H37B	−0.1445	0.2171	0.6668	0.174*
H37C	−0.1284	0.2950	0.6791	0.174*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0222 (5)	0.0199 (5)	0.0220 (5)	0.0000 (4)	0.0021 (4)	−0.0020 (4)

O2	0.0219 (5)	0.0242 (5)	0.0178 (5)	0.0048 (4)	0.0011 (4)	0.0010 (4)
O3	0.0287 (6)	0.0220 (5)	0.0337 (5)	−0.0030 (5)	0.0079 (5)	0.0023 (4)
O4	0.0250 (5)	0.0169 (5)	0.0277 (5)	0.0022 (4)	−0.0042 (4)	−0.0021 (4)
O5	0.0285 (5)	0.0182 (5)	0.0176 (4)	−0.0002 (4)	0.0014 (4)	0.0001 (4)
O6	0.0289 (6)	0.0288 (5)	0.0190 (5)	0.0077 (5)	0.0030 (4)	0.0028 (4)
O7	0.0232 (5)	0.0271 (5)	0.0249 (5)	0.0030 (4)	0.0016 (4)	0.0036 (4)
O8	0.0351 (7)	0.0487 (7)	0.0228 (5)	0.0217 (6)	0.0009 (5)	0.0009 (5)
O9	0.0341 (6)	0.0278 (6)	0.0398 (6)	0.0097 (5)	−0.0133 (5)	−0.0062 (5)
O10	0.0380 (7)	0.0403 (6)	0.0185 (5)	0.0095 (6)	0.0024 (5)	−0.0026 (4)
C1	0.0222 (6)	0.0185 (6)	0.0179 (6)	0.0021 (5)	0.0003 (5)	−0.0006 (5)
C2	0.0212 (7)	0.0197 (6)	0.0167 (6)	0.0028 (5)	0.0001 (5)	0.0010 (5)
C3	0.0218 (7)	0.0186 (6)	0.0219 (6)	0.0018 (6)	0.0018 (6)	0.0016 (5)
C4	0.0238 (7)	0.0165 (6)	0.0222 (6)	0.0030 (6)	−0.0010 (6)	−0.0011 (5)
C5	0.0238 (7)	0.0183 (6)	0.0203 (6)	0.0029 (6)	0.0003 (5)	−0.0023 (5)
C6	0.0265 (7)	0.0234 (7)	0.0215 (7)	0.0050 (6)	0.0006 (6)	−0.0014 (5)
C7	0.0209 (7)	0.0245 (7)	0.0174 (6)	−0.0008 (6)	−0.0036 (5)	0.0026 (5)
C8	0.0260 (7)	0.0239 (7)	0.0220 (6)	−0.0014 (6)	−0.0043 (6)	0.0027 (5)
C9	0.0283 (8)	0.0288 (8)	0.0462 (10)	−0.0021 (7)	0.0016 (8)	0.0034 (7)
C10	0.0371 (10)	0.0277 (9)	0.0687 (13)	−0.0086 (8)	−0.0016 (10)	0.0071 (8)
C11	0.0463 (11)	0.0211 (7)	0.0548 (11)	−0.0025 (8)	−0.0092 (9)	−0.0004 (7)
C12	0.0419 (10)	0.0280 (8)	0.0401 (9)	0.0048 (8)	−0.0007 (8)	−0.0046 (7)
C13	0.0312 (8)	0.0252 (7)	0.0308 (8)	−0.0001 (6)	0.0010 (7)	0.0000 (6)
C14	0.0216 (7)	0.0199 (6)	0.0222 (7)	0.0019 (5)	0.0012 (5)	−0.0010 (5)
C15	0.0218 (7)	0.0175 (6)	0.0210 (6)	−0.0012 (5)	0.0005 (6)	−0.0005 (5)
C16	0.0239 (7)	0.0231 (6)	0.0237 (7)	0.0024 (6)	0.0002 (6)	−0.0010 (5)
C17	0.0272 (8)	0.0237 (7)	0.0251 (7)	0.0015 (6)	−0.0045 (6)	0.0000 (6)
C18	0.0332 (8)	0.0242 (7)	0.0189 (6)	−0.0060 (6)	−0.0019 (6)	0.0009 (5)
C19	0.0303 (8)	0.0312 (8)	0.0223 (7)	−0.0026 (6)	0.0053 (6)	−0.0017 (6)
C20	0.0226 (7)	0.0256 (7)	0.0243 (7)	0.0010 (6)	0.0020 (6)	−0.0012 (6)
C21	0.0209 (7)	0.0245 (7)	0.0211 (6)	0.0038 (6)	0.0008 (6)	−0.0028 (6)
C22	0.0230 (7)	0.0230 (7)	0.0195 (6)	0.0001 (6)	0.0027 (5)	−0.0019 (5)
C23	0.0255 (7)	0.0231 (7)	0.0302 (7)	0.0016 (6)	−0.0045 (6)	−0.0032 (6)
C24	0.0331 (8)	0.0219 (7)	0.0355 (8)	0.0024 (7)	−0.0047 (7)	−0.0005 (6)
C25	0.0361 (8)	0.0224 (7)	0.0272 (7)	−0.0037 (7)	0.0014 (7)	−0.0025 (6)
C26	0.0299 (8)	0.0312 (8)	0.0255 (7)	−0.0074 (7)	−0.0022 (6)	−0.0041 (6)
C27	0.0237 (7)	0.0298 (8)	0.0256 (7)	0.0010 (6)	−0.0006 (6)	−0.0022 (6)
C28	0.0279 (7)	0.0242 (7)	0.0172 (6)	−0.0017 (6)	−0.0011 (6)	−0.0026 (5)
C29	0.0278 (8)	0.0212 (7)	0.0220 (6)	−0.0029 (6)	−0.0044 (6)	−0.0015 (5)
C30	0.0288 (8)	0.0241 (7)	0.0283 (7)	−0.0005 (7)	0.0000 (6)	0.0000 (6)
C31	0.0308 (9)	0.0308 (8)	0.0448 (9)	0.0035 (8)	0.0012 (8)	−0.0015 (7)
C32	0.0369 (10)	0.0294 (8)	0.0528 (11)	0.0056 (8)	−0.0117 (9)	0.0026 (8)
C33	0.0473 (11)	0.0308 (8)	0.0357 (8)	0.0002 (8)	−0.0134 (8)	0.0068 (7)
C34	0.0389 (9)	0.0292 (8)	0.0239 (7)	−0.0018 (7)	−0.0049 (7)	0.0014 (6)
O11	0.0435 (7)	0.0255 (6)	0.0458 (7)	−0.0043 (5)	0.0052 (6)	0.0050 (5)
C35	0.0348 (10)	0.0321 (9)	0.0378 (9)	−0.0051 (7)	0.0007 (7)	0.0040 (7)
C36	0.0462 (11)	0.0269 (8)	0.0463 (10)	−0.0079 (8)	0.0055 (9)	0.0034 (7)
C37	0.0391 (15)	0.0708 (19)	0.238 (6)	−0.0009 (14)	−0.028 (2)	0.024 (3)

Geometric parameters (Å, º)

O1—C7	1.3591 (19)	C16—C17	1.391 (2)
O1—C1	1.4197 (17)	C16—H16	0.9500
O2—C14	1.3451 (18)	C17—C18	1.389 (2)
O2—C2	1.4414 (16)	C17—H17	0.9500
O3—C3	1.4163 (18)	C18—C19	1.386 (2)
O3—H3	0.8400	C18—H18	0.9500
O4—C21	1.3473 (19)	C19—C20	1.392 (2)
O4—C4	1.4492 (16)	C19—H19	0.9500
O5—C1	1.4110 (16)	C20—H20	0.9500
O5—C5	1.4266 (17)	C21—C22	1.493 (2)
O6—C28	1.3399 (18)	C22—C23	1.393 (2)
O6—C6	1.4401 (19)	C22—C27	1.395 (2)
O7—C7	1.2036 (19)	C23—C24	1.388 (2)
O8—C14	1.206 (2)	C23—H23	0.9500
O9—C21	1.202 (2)	C24—C25	1.389 (2)
O10—C28	1.204 (2)	C24—H24	0.9500
C1—C2	1.517 (2)	C25—C26	1.388 (3)
C1—H1	1.0000	C25—H25	0.9500
C2—C3	1.5240 (19)	C26—C27	1.391 (2)
C2—H2	1.0000	C26—H26	0.9500
C3—C4	1.5235 (18)	C27—H27	0.9500
C3—H3A	1.0000	C28—C29	1.488 (2)
C4—C5	1.526 (2)	C29—C34	1.392 (2)
C4—H4	1.0000	C29—C30	1.395 (2)
C5—C6	1.5094 (18)	C30—C31	1.388 (2)
C5—H5	1.0000	C30—H30	0.9500
C6—H6A	0.9900	C31—C32	1.392 (3)
C6—H6B	0.9900	C31—H31	0.9500
C7—C8	1.486 (2)	C32—C33	1.391 (3)
C8—C9	1.390 (2)	C32—H32	0.9500
C8—C13	1.395 (2)	C33—C34	1.390 (3)
C9—C10	1.387 (3)	C33—H33	0.9500
C9—H9	0.9500	C34—H34	0.9500
C10—C11	1.383 (3)	O11—C35	1.206 (2)
C10—H10	0.9500	C35—C37	1.481 (4)
C11—C12	1.386 (3)	C35—C36	1.489 (3)
C11—H11	0.9500	C36—H36A	0.9800
C12—C13	1.389 (2)	C36—H36B	0.9800
C12—H12	0.9500	C36—H36C	0.9800
C13—H13	0.9500	C37—H37A	0.9800
C14—C15	1.4897 (19)	C37—H37B	0.9800
C15—C20	1.392 (2)	C37—H37C	0.9800
C15—C16	1.395 (2)		
C7—O1—C1	115.31 (11)	C15—C16—H16	120.2
C14—O2—C2	117.11 (11)	C18—C17—C16	120.21 (15)

C3—O3—H3	109.5	C18—C17—H17	119.9
C21—O4—C4	118.65 (11)	C16—C17—H17	119.9
C1—O5—C5	112.99 (11)	C19—C18—C17	120.18 (14)
C28—O6—C6	116.39 (12)	C19—C18—H18	119.9
O5—C1—O1	105.65 (11)	C17—C18—H18	119.9
O5—C1—C2	109.05 (12)	C18—C19—C20	119.97 (15)
O1—C1—C2	106.88 (11)	C18—C19—H19	120.0
O5—C1—H1	111.7	C20—C19—H19	120.0
O1—C1—H1	111.7	C15—C20—C19	119.94 (15)
C2—C1—H1	111.7	C15—C20—H20	120.0
O2—C2—C1	108.30 (11)	C19—C20—H20	120.0
O2—C2—C3	107.40 (11)	O9—C21—O4	124.49 (14)
C1—C2—C3	110.26 (11)	O9—C21—C22	124.36 (15)
O2—C2—H2	110.3	O4—C21—C22	111.15 (13)
C1—C2—H2	110.3	C23—C22—C27	120.15 (14)
C3—C2—H2	110.3	C23—C22—C21	121.50 (14)
O3—C3—C4	111.21 (12)	C27—C22—C21	118.34 (14)
O3—C3—C2	108.70 (12)	C24—C23—C22	119.67 (15)
C4—C3—C2	109.39 (11)	C24—C23—H23	120.2
O3—C3—H3A	109.2	C22—C23—H23	120.2
C4—C3—H3A	109.2	C23—C24—C25	120.38 (16)
C2—C3—H3A	109.2	C23—C24—H24	119.8
O4—C4—C3	106.08 (11)	C25—C24—H24	119.8
O4—C4—C5	108.22 (11)	C26—C25—C24	119.91 (15)
C3—C4—C5	110.57 (12)	C26—C25—H25	120.0
O4—C4—H4	110.6	C24—C25—H25	120.0
C3—C4—H4	110.6	C25—C26—C27	120.22 (15)
C5—C4—H4	110.6	C25—C26—H26	119.9
O5—C5—C6	106.11 (11)	C27—C26—H26	119.9
O5—C5—C4	108.36 (11)	C26—C27—C22	119.65 (15)
C6—C5—C4	113.72 (13)	C26—C27—H27	120.2
O5—C5—H5	109.5	C22—C27—H27	120.2
C6—C5—H5	109.5	O10—C28—O6	123.18 (15)
C4—C5—H5	109.5	O10—C28—C29	125.38 (14)
O6—C6—C5	105.94 (11)	O6—C28—C29	111.44 (13)
O6—C6—H6A	110.5	C34—C29—C30	120.20 (16)
C5—C6—H6A	110.5	C34—C29—C28	117.85 (15)
O6—C6—H6B	110.5	C30—C29—C28	121.95 (14)
C5—C6—H6B	110.5	C31—C30—C29	119.63 (15)
H6A—C6—H6B	108.7	C31—C30—H30	120.2
O7—C7—O1	123.86 (14)	C29—C30—H30	120.2
O7—C7—C8	124.34 (14)	C30—C31—C32	120.38 (18)
O1—C7—C8	111.79 (13)	C30—C31—H31	119.8
C9—C8—C13	120.09 (15)	C32—C31—H31	119.8
C9—C8—C7	117.17 (15)	C33—C32—C31	119.75 (17)
C13—C8—C7	122.72 (15)	C33—C32—H32	120.1
C10—C9—C8	119.96 (18)	C31—C32—H32	120.1
C10—C9—H9	120.0	C34—C33—C32	120.28 (16)

C8—C9—H9	120.0	C34—C33—H33	119.9
C11—C10—C9	120.02 (18)	C32—C33—H33	119.9
C11—C10—H10	120.0	C33—C34—C29	119.75 (17)
C9—C10—H10	120.0	C33—C34—H34	120.1
C10—C11—C12	120.25 (17)	C29—C34—H34	120.1
C10—C11—H11	119.9	O11—C35—C37	121.2 (2)
C12—C11—H11	119.9	O11—C35—C36	122.09 (19)
C11—C12—C13	120.23 (18)	C37—C35—C36	116.7 (2)
C11—C12—H12	119.9	C35—C36—H36A	109.5
C13—C12—H12	119.9	C35—C36—H36B	109.5
C12—C13—C8	119.45 (17)	H36A—C36—H36B	109.5
C12—C13—H13	120.3	C35—C36—H36C	109.5
C8—C13—H13	120.3	H36A—C36—H36C	109.5
O8—C14—O2	124.68 (13)	H36B—C36—H36C	109.5
O8—C14—C15	124.04 (14)	C35—C37—H37A	109.5
O2—C14—C15	111.28 (12)	C35—C37—H37B	109.5
C20—C15—C16	120.08 (14)	H37A—C37—H37B	109.5
C20—C15—C14	117.76 (14)	C35—C37—H37C	109.5
C16—C15—C14	122.16 (13)	H37A—C37—H37C	109.5
C17—C16—C15	119.60 (14)	H37B—C37—H37C	109.5
C17—C16—H16	120.2		

C5—O5—C1—O1	−179.08 (11)	C2—O2—C14—O8	−6.7 (2)
C5—O5—C1—C2	−64.51 (15)	C2—O2—C14—C15	173.67 (12)
C7—O1—C1—O5	−68.08 (14)	O8—C14—C15—C20	8.7 (2)
C7—O1—C1—C2	175.85 (11)	O2—C14—C15—C20	−171.64 (13)
C14—O2—C2—C1	130.92 (13)	O8—C14—C15—C16	−171.60 (16)
C14—O2—C2—C3	−110.01 (14)	O2—C14—C15—C16	8.1 (2)
O5—C1—C2—O2	175.05 (11)	C20—C15—C16—C17	−0.6 (2)
O1—C1—C2—O2	−71.18 (13)	C14—C15—C16—C17	179.73 (14)
O5—C1—C2—C3	57.80 (14)	C15—C16—C17—C18	1.6 (2)
O1—C1—C2—C3	171.57 (11)	C16—C17—C18—C19	−1.2 (2)
O2—C2—C3—O3	67.38 (14)	C17—C18—C19—C20	−0.2 (2)
C1—C2—C3—O3	−174.82 (11)	C16—C15—C20—C19	−0.8 (2)
O2—C2—C3—C4	−171.01 (11)	C14—C15—C20—C19	178.91 (14)
C1—C2—C3—C4	−53.21 (15)	C18—C19—C20—C15	1.2 (2)
C21—O4—C4—C3	126.65 (13)	C4—O4—C21—O9	6.4 (2)
C21—O4—C4—C5	−114.68 (14)	C4—O4—C21—C22	−173.81 (12)
O3—C3—C4—O4	−69.61 (14)	O9—C21—C22—C23	171.75 (16)
C2—C3—C4—O4	170.31 (11)	O4—C21—C22—C23	−8.1 (2)
O3—C3—C4—C5	173.28 (11)	O9—C21—C22—C27	−8.3 (2)
C2—C3—C4—C5	53.19 (15)	O4—C21—C22—C27	171.87 (13)
C1—O5—C5—C6	−173.65 (12)	C27—C22—C23—C24	0.3 (2)
C1—O5—C5—C4	63.87 (15)	C21—C22—C23—C24	−179.82 (15)
O4—C4—C5—O5	−172.82 (10)	C22—C23—C24—C25	−1.1 (3)
C3—C4—C5—O5	−57.04 (14)	C23—C24—C25—C26	0.9 (3)
O4—C4—C5—C6	69.46 (15)	C24—C25—C26—C27	0.2 (3)
C3—C4—C5—C6	−174.76 (12)	C25—C26—C27—C22	−1.0 (2)

C28—O6—C6—C5	166.40 (13)	C23—C22—C27—C26	0.8 (2)
O5—C5—C6—O6	−56.43 (15)	C21—C22—C27—C26	−179.12 (14)
C4—C5—C6—O6	62.59 (16)	C6—O6—C28—O10	6.6 (2)
C1—O1—C7—O7	−4.90 (19)	C6—O6—C28—C29	−174.32 (13)
C1—O1—C7—C8	173.92 (11)	O10—C28—C29—C34	−6.8 (2)
O7—C7—C8—C9	0.6 (2)	O6—C28—C29—C34	174.10 (14)
O1—C7—C8—C9	−178.22 (14)	O10—C28—C29—C30	172.22 (16)
O7—C7—C8—C13	179.42 (15)	O6—C28—C29—C30	−6.9 (2)
O1—C7—C8—C13	0.6 (2)	C34—C29—C30—C31	1.5 (2)
C13—C8—C9—C10	0.6 (3)	C28—C29—C30—C31	−177.49 (15)
C7—C8—C9—C10	179.42 (17)	C29—C30—C31—C32	−1.0 (3)
C8—C9—C10—C11	−0.1 (3)	C30—C31—C32—C33	−0.2 (3)
C9—C10—C11—C12	−0.3 (3)	C31—C32—C33—C34	1.0 (3)
C10—C11—C12—C13	0.2 (3)	C32—C33—C34—C29	−0.5 (3)
C11—C12—C13—C8	0.3 (3)	C30—C29—C34—C33	−0.8 (2)
C9—C8—C13—C12	−0.7 (2)	C28—C29—C34—C33	178.30 (15)
C7—C8—C13—C12	−179.46 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O11	0.84	1.96	2.780 (2)	164

Methyl *β*-*D*-glucopyranoside hemihydrate (V)

Crystal data

$2C_7H_{14}O_6·H_2O$
M_r = 406.38
Tetragonal, $P4_12_12$
a = 7.3482 (3) Å
c = 34.1260 (17) Å
V = 1842.67 (17) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.465 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 9836 reflections
θ = 5.2–71.9°
μ = 1.14 mm^{-1}
T = 120 K
Block, colorless
0.21 × 0.16 × 0.08 mm

Data collection

Bruker APEXII diffractometer
Radiation source: Incoatec micro-focus
Detector resolution: 8.33 pixels mm^{-1}
combination of ω and φ–scans
Absorption correction: numerical (SADABS; Krause *et al.*, 2015)
T_{min} = 0.862, T_{max} = 0.979
27800 measured reflections
1797 independent reflections
1786 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 71.8°, θ_{min} = 5.2°
h = −8→9
k = −9→9
l = −41→42

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.067
S = 1.09
1797 reflections
144 parameters
0 restraints
Primary atom site location: dual

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.3075P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Absolute structure: Flack *x* determined using 642 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.03 (3)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.71499 (14)	0.64312 (13)	0.41589 (3)	0.0148 (2)
O2	0.79300 (14)	0.97599 (14)	0.37803 (3)	0.0156 (2)
H2O	0.830 (3)	0.903 (3)	0.3610 (6)	0.039 (6)*
O3	0.49078 (14)	1.20829 (14)	0.36875 (3)	0.0163 (2)
H3O	0.426 (3)	1.301 (3)	0.3727 (6)	0.038 (6)*
O4	0.24036 (13)	1.20553 (14)	0.43537 (3)	0.0151 (2)
H4O	0.161 (3)	1.242 (3)	0.4196 (5)	0.021 (5)*
O5	0.43923 (13)	0.75034 (12)	0.43612 (3)	0.0131 (2)
O6	0.16468 (14)	0.71645 (16)	0.49750 (3)	0.0205 (2)
H6O	0.234 (3)	0.625 (4)	0.4923 (6)	0.041 (6)*
C1	0.62279 (18)	0.79966 (18)	0.42600 (4)	0.0126 (3)
H1	0.6839	0.8614	0.4486	0.015*
C2	0.61456 (19)	0.92624 (19)	0.39063 (4)	0.0125 (3)
H2	0.5490	0.8643	0.3687	0.015*
C3	0.51080 (19)	1.09652 (18)	0.40257 (4)	0.0128 (3)
H3	0.5821	1.1639	0.4229	0.015*
C4	0.32364 (18)	1.04683 (18)	0.41924 (4)	0.0124 (3)
H4	0.2453	0.9983	0.3977	0.015*
C5	0.33969 (19)	0.90353 (18)	0.45146 (4)	0.0128 (3)
H5	0.4057	0.9557	0.4745	0.015*
C6	0.15507 (19)	0.8322 (2)	0.46429 (4)	0.0160 (3)
H6A	0.0749	0.9366	0.4704	0.019*
H6B	0.0993	0.7644	0.4423	0.019*
C7	0.7541 (2)	0.52994 (19)	0.44928 (4)	0.0186 (3)
H7A	0.8212	0.4217	0.4407	0.028*
H7B	0.6398	0.4927	0.4617	0.028*
H7C	0.8279	0.5984	0.4681	0.028*
O1W	0.37693 (15)	1.37693 (15)	0.5000	0.0221 (3)
H1WA	0.322 (3)	1.327 (3)	0.5188 (5)	0.029 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0170 (5)	0.0121 (5)	0.0154 (4)	0.0039 (4)	0.0025 (4)	0.0015 (4)
O2	0.0133 (5)	0.0130 (5)	0.0203 (5)	−0.0014 (4)	0.0056 (4)	−0.0008 (4)
O3	0.0178 (5)	0.0135 (5)	0.0175 (5)	0.0037 (4)	0.0039 (4)	0.0048 (4)
O4	0.0161 (5)	0.0151 (5)	0.0141 (4)	0.0058 (4)	−0.0019 (4)	−0.0021 (4)
O5	0.0118 (5)	0.0122 (5)	0.0152 (4)	−0.0001 (3)	0.0022 (3)	−0.0003 (4)
O6	0.0207 (5)	0.0232 (5)	0.0176 (5)	0.0003 (4)	0.0041 (4)	0.0060 (4)
C1	0.0114 (6)	0.0120 (6)	0.0143 (6)	0.0006 (5)	0.0008 (5)	−0.0001 (5)
C2	0.0115 (6)	0.0121 (6)	0.0140 (6)	−0.0013 (5)	0.0013 (5)	0.0005 (5)
C3	0.0141 (6)	0.0118 (6)	0.0124 (5)	0.0001 (5)	0.0005 (5)	0.0005 (5)
C4	0.0133 (6)	0.0127 (6)	0.0113 (6)	0.0017 (5)	0.0002 (5)	−0.0008 (5)
C5	0.0132 (7)	0.0129 (6)	0.0124 (5)	0.0015 (5)	0.0004 (5)	−0.0010 (5)
C6	0.0143 (7)	0.0185 (7)	0.0151 (6)	−0.0006 (5)	0.0015 (5)	0.0021 (5)
C7	0.0196 (7)	0.0158 (7)	0.0203 (7)	0.0040 (5)	0.0033 (6)	0.0072 (5)
O1W	0.0254 (5)	0.0254 (5)	0.0153 (7)	−0.0094 (7)	0.0023 (4)	−0.0023 (4)

Geometric parameters (Å, º)

O1—C1	1.3789 (16)	O3—H3O	0.84 (3)
O1—C7	1.4399 (16)	O4—H4O	0.84 (2)
O2—C2	1.4275 (16)	O6—H6O	0.86 (3)
O3—C3	1.4241 (15)	C1—H1	1.0000
O4—C4	1.4273 (15)	C2—H2	1.0000
O5—C1	1.4387 (16)	C3—H3	1.0000
O5—C5	1.4409 (16)	C4—H4	1.0000
O6—C6	1.4187 (16)	C5—H5	1.0000
C1—C2	1.5252 (17)	C6—H6A	0.9900
C2—C3	1.5209 (18)	C6—H6B	0.9900
C3—C4	1.5324 (18)	C7—H7A	0.9800
C4—C5	1.5269 (17)	C7—H7B	0.9800
C5—C6	1.5188 (19)	C7—H7C	0.9800
O2—H2O	0.83 (2)	O1W—H1WA	0.84 (2)
C1—O1—C7	112.44 (10)	C2—C1—H1	110.5
C1—O5—C5	111.49 (10)	O2—C2—H2	109.5
O1—C1—O5	108.09 (11)	C3—C2—H2	109.5
O1—C1—C2	109.27 (10)	C1—C2—H2	109.5
O5—C1—C2	107.84 (11)	O3—C3—H3	109.3
O2—C2—C3	109.30 (11)	C2—C3—H3	109.3
O2—C2—C1	110.99 (11)	C4—C3—H3	109.3
C3—C2—C1	108.03 (10)	O4—C4—H4	109.2
O3—C3—C2	108.00 (10)	C5—C4—H4	109.2
O3—C3—C4	110.22 (11)	C3—C4—H4	109.2
C2—C3—C4	110.69 (11)	O5—C5—H5	109.8
O4—C4—C5	108.60 (10)	C6—C5—H5	109.8
O4—C4—C3	109.47 (11)	C4—C5—H5	109.8

C5—C4—C3	111.25 (11)	O6—C6—H6A	109.0
O5—C5—C6	106.77 (10)	C5—C6—H6A	109.0
O5—C5—C4	108.44 (10)	O6—C6—H6B	109.0
C6—C5—C4	112.12 (11)	C5—C6—H6B	109.0
O6—C6—C5	113.12 (11)	H6A—C6—H6B	107.8
C2—O2—H2O	110.3 (17)	O1—C7—H7A	109.5
C3—O3—H3O	113.4 (15)	O1—C7—H7B	109.5
C4—O4—H4O	108.1 (13)	H7A—C7—H7B	109.5
C6—O6—H6O	109.4 (15)	O1—C7—H7C	109.5
O1—C1—H1	110.5	H7A—C7—H7C	109.5
O5—C1—H1	110.5	H7B—C7—H7C	109.5
C7—O1—C1—O5	−72.32 (13)	O3—C3—C4—O4	−68.92 (13)
C7—O1—C1—C2	170.57 (11)	C2—C3—C4—O4	171.66 (10)
C5—O5—C1—O1	173.23 (9)	O3—C3—C4—C5	171.06 (10)
C5—O5—C1—C2	−68.74 (12)	C2—C3—C4—C5	51.64 (14)
O1—C1—C2—O2	−60.70 (14)	C1—O5—C5—C6	−175.22 (10)
O5—C1—C2—O2	−177.97 (10)	C1—O5—C5—C4	63.78 (13)
O1—C1—C2—C3	179.49 (11)	O4—C4—C5—O5	−174.60 (10)
O5—C1—C2—C3	62.22 (13)	C3—C4—C5—O5	−54.06 (14)
O2—C2—C3—O3	63.60 (13)	O4—C4—C5—C6	67.77 (13)
C1—C2—C3—O3	−175.53 (11)	C3—C4—C5—C6	−171.70 (11)
O2—C2—C3—C4	−175.65 (10)	O5—C5—C6—O6	68.93 (13)
C1—C2—C3—C4	−54.79 (13)	C4—C5—C6—O6	−172.45 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*O*···O5^{i}	0.83 (2)	2.12 (2)	2.952 (2)	172 (2)
O3—H3*O*···O2^{ii}	0.84 (3)	1.91 (3)	2.740 (2)	169 (2)
O4—H4*O*···O3^{ii}	0.84 (2)	1.85 (2)	2.679 (2)	172 (2)
O6—H6*O*···O1*W*^{iii}	0.86 (3)	2.12 (3)	2.944 (2)	160 (2)
O1*W*—H1*WA*···O4^{iv}	0.84 (2)	1.89 (2)	2.731 (2)	173 (2)

Symmetry codes: (i) *x*+1/2, −*y*+3/2, −*z*+3/4; (ii) *x*−1/2, −*y*+5/2, −*z*+3/4; (iii) *x*, *y*−1, *z*; (iv) *y*−1, *x*+1, −*z*+1.