IUCrData

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rac-3-(1,1-Dimethylethyl)-2,2,5,5-tetramethylhexane-3,4-diol

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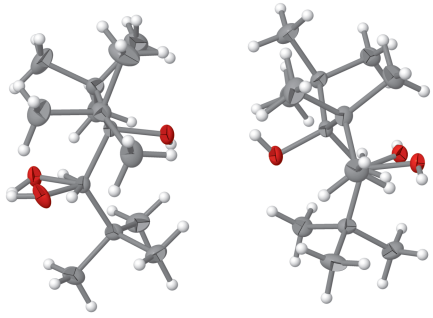
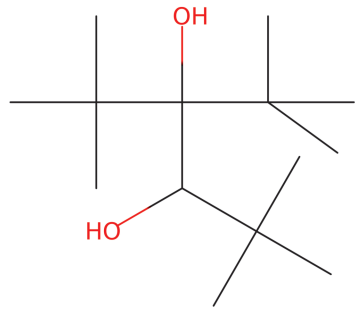
Structural data: full structural data are available from iucrdata.iucr.org

Two almost identical molecules in the asymmetric unit of the title compound, $C_{14}H_{30}O_2$, are linked by O—H···O hydrogen bonds into chains running parallel to the *a* axis. In both molecules, the hydroxy group and the H atom on the C atom to which it is attached are disordered. Bulky *tert*-butyl groups increase the bond angles at the nearby carbon atoms.

3D view



Chemical scheme



Structure description

The title compound, $C_{14}H_{30}O_2$ (Fig. 1), was prepared as an intermediate in a study on the synthesis (Detert *et al.*, 1992; Detert & Meier, 1997) and bromination of sterically demanding alkenes and strained alkynes (Chiappe *et al.*, 2002, 2003; Herges *et al.*, 2005). The title compound is starting material in the synthesis of tri-*t*-butylethene (Krebs *et al.*, 1983; Böhrer *et al.*, 1997) Eight molecules, four *A* molecules and four *B* molecules, fill the monoclinic unit cell. Molecules *A* and *B* are almost identical, both molecules showing disorder of O1 and the H atom on carbon C5. For molecule *A*, a ratio of approximately 90/10 was found, for *B* approximately 86/14. The most obvious difference between molecules *A* and *B* is the position of the disordered OH bonds: while these point 'outward' in *A*, they point 'inward' in *B*. The angle between the disordered positions of O1 in *A* is 51.8 (6)° and 68.0 (4)° in *B*. The voluminous *tert*-butyl groups widen the bond angles at the adjacent carbon atoms: C7*A*—C6*A*—C11*A* is 116.17 (12)°, C7*B*—C6*B*—C11*B* is 116.72 (13)° and C6*A*—C5*A*—C1*A* is 122.34 (14)°, C6*B*—C5*B*—C1*B* is 122.23 (12)°. Within the crystal, the molecules are arranged in chains along the *a*-axis direction. Molecules *A* and *B* alternate and they are connected through O—H···O hydrogen bonds (Table 1, Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
O2A—H2AO···O2B	0.75 (3)	2.27 (2)	2.8146 (16)	130 (2)
O1B—H1B···O1A^{i}	0.79 (3)	2.21 (3)	2.992 (2)	169 (3)
O1D—H1D···O1C^{i}	0.79 (4)	2.30 (6)	3.076 (14)	167 (19)

Symmetry code: (i) $x+1, y, z$.

Synthesis and crystallization

The diol was prepared according to the literature (Böhrer *et al.*, 1997) from pivaloin and *t*-butyllithium. Single crystals were obtained *via* slow evaporation of a solution in chloroform/2-propanol. ^{1}H-NMR (400 MHz, DMSO-d_6): δ = 4.25 (*d*, *J* = 8 Hz, 1 H, OH, H/D-exch.), 3.80 (*d*, *J* = 8 Hz, 1 H, OH, H/D-exch.), 3.14 (*s*, 1 H, 4-H), 1.18 (*s*, 9 H), 1.08 (*s*, 9 H), 1.02 (*s*, 9H); ^{13}C-NMR (100 MHz, DMSO-d$_6$): δ = 85.84, 81.36, 43.30, 42.94, 38–31, 32.12 (*bs*), 30.91, 29.74 (*bs*).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{30}O_2$
M_r	230.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	120
a, b, c (Å)	12.1595 (4), 17.8906 (4), 14.1682 (5)
β (°)	113.086 (3)
V (Å^3)	2835.33 (16)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.62 × 0.35 × 0.19
Data collection	
Diffractometer	Stoe *IPDS* 2T
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21718, 6774, 5738
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.660
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.065, 0.176, 1.06
No. of reflections	6774
No. of parameters	345
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.04, −0.32

Computer programs: *X-AREA WinXpose*, *X-AREA Recipe* and *X-AREA Integrate* (Stoe & Cie, 2020), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2009).

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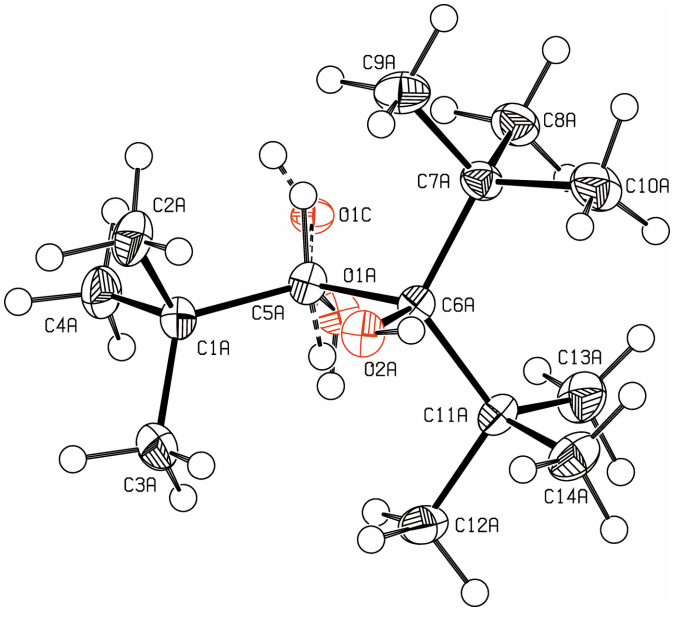

Figure 1
View of molecule *A* of the title compound. Displacement ellipsoids are drawn at the 50% probability level (Spek, 2009).

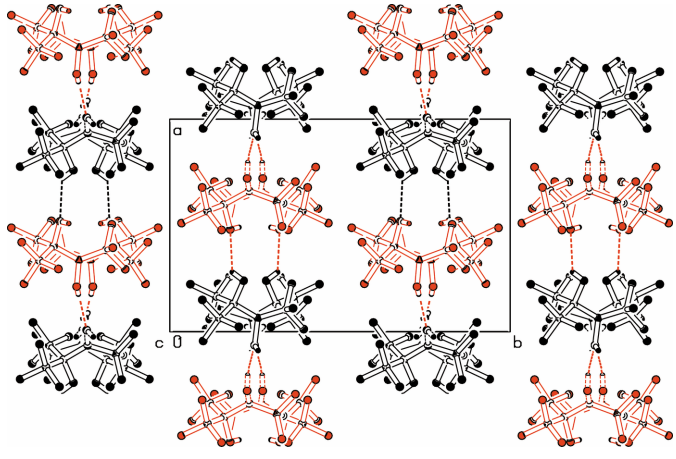

Figure 2
Part of the packing diagram. View along *c*-axis direction (Spek 2009). Independent molecules in different colors (*A*: black, *B*: red).

full crystallographic data

IUCrData (2026). **11**, x261176 [https://doi.org/10.1107/S2414314626011764]

rac-3-(1,1-Dimethylethyl)-2,2,5,5-tetramethylhexane-3,4-diol

Dieter Schollmeyer and Heiner Detert

rac-3-*tert*-Butyl-2,2,5,5-tetramethylhexane-3,4-diol

Crystal data

$C_{14}H_{30}O_2$
M_r = 230.38
Monoclinic, $P2_1/c$
a = 12.1595 (4) Å
b = 17.8906 (4) Å
c = 14.1682 (5) Å
β = 113.086 (3)°
V = 2835.33 (16) Å^3
Z = 8
$F(000)$ = 1040
D_x = 1.079 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 28708 reflections
θ = 2.8–28.5°
μ = 0.07 mm^{-1}
T = 120 K
Plate, colorless
0.62 × 0.35 × 0.19 mm

Data collection

Stoe IPDS 2T diffractometer
Detector resolution: 6.67 pixels mm^{-1}
rotation method, ω scans
21718 measured reflections
6774 independent reflections
5738 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 28.0°, θ_{min} = 2.9°
h = −16→16
k = −23→23
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.176
S = 1.06
6774 reflections
345 parameters
3 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 2.2754P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-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.

Refinement. Hydrogen atoms of the methyl groups were placed at calculated positions and were refined in the riding-model approximation with C–H = 0.98Å, and with U_{iso}(H) = 1.5 U_{eq}(C). The methyl groups were allowed to rotate but not to tip. The coordinates of the tertiary H atoms were refined with U_{iso}(H) = 1.2 U_{eq}(C). The coordinates of the H atoms bonded to O were refined with U_{iso}(H) = 1.5 U_{eq}(O). The O-H bonds lengths were restrained to be equal and the $C_{tertiary}$-H bonds were also restrained to be equal.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1A	−0.06330 (11)	0.25098 (7)	0.18894 (11)	0.0221 (4)	0.901 (4)
H1A	−0.083 (2)	0.2411 (15)	0.132 (2)	0.033*	0.901 (4)
O1C	−0.0073 (10)	0.2443 (7)	0.2785 (9)	0.022 (3)	0.099 (4)
H1C	0.010 (6)	0.243 (13)	0.336 (3)	0.032*	0.099 (4)
O2A	0.24001 (10)	0.28345 (7)	0.21231 (9)	0.0227 (3)	
H2AO	0.280 (2)	0.3166 (14)	0.2160 (18)	0.034*	
C1A	0.10441 (15)	0.15915 (9)	0.22394 (13)	0.0229 (3)	
C2A	0.22558 (16)	0.14181 (10)	0.31120 (15)	0.0325 (4)	
H2A	0.246513	0.089381	0.306900	0.049*	
H2B	0.220104	0.150792	0.377450	0.049*	
H2C	0.287295	0.174203	0.304823	0.049*	
C3A	0.1102 (2)	0.13794 (10)	0.12150 (15)	0.0352 (4)	
H3A	0.032166	0.146917	0.065849	0.053*	
H3B	0.130951	0.084939	0.122563	0.053*	
H3C	0.171032	0.168369	0.110395	0.053*	
C4A	0.01221 (17)	0.10665 (10)	0.23986 (15)	0.0317 (4)	
H4A	−0.065090	0.111784	0.181947	0.048*	
H4B	0.003431	0.120048	0.303610	0.048*	
H4C	0.039839	0.054818	0.244115	0.048*	
C5A	0.06426 (13)	0.24129 (9)	0.23421 (12)	0.0196 (3)	
H5A	0.082078	0.244886	0.309223	0.023*	0.901 (4)
H5C	−0.000208	0.242256	0.163635	0.023*	0.099 (4)
C6A	0.13187 (13)	0.31289 (8)	0.21561 (11)	0.0175 (3)	
C7A	0.16604 (14)	0.36398 (9)	0.31558 (12)	0.0221 (3)	
C8A	0.05867 (16)	0.38281 (11)	0.34319 (14)	0.0292 (4)	
H8A	−0.002343	0.408962	0.285596	0.044*	
H8B	0.085154	0.414931	0.404089	0.044*	
H8C	0.024884	0.336533	0.357461	0.044*	
C9A	0.25910 (16)	0.32436 (12)	0.40900 (13)	0.0326 (4)	
H9A	0.225204	0.277710	0.422051	0.049*	
H9B	0.281098	0.356926	0.469239	0.049*	
H9C	0.330360	0.313171	0.395302	0.049*	
C10A	0.22336 (18)	0.43961 (11)	0.30743 (15)	0.0346 (4)	
H10A	0.289633	0.430861	0.285853	0.052*	
H10B	0.253526	0.464478	0.374418	0.052*	
H10C	0.163245	0.471387	0.256848	0.052*	
C11A	0.06378 (14)	0.35401 (9)	0.10749 (12)	0.0217 (3)	
C12A	0.02307 (17)	0.29724 (11)	0.01873 (13)	0.0299 (4)	
H12A	−0.009929	0.323972	−0.046837	0.045*	
H12B	−0.038378	0.264506	0.024923	0.045*	
H12C	0.091612	0.267099	0.021600	0.045*	
C13A	−0.04346 (16)	0.40210 (11)	0.09821 (15)	0.0329 (4)	
H13A	−0.082985	0.420072	0.027503	0.049*	
H13B	−0.016425	0.444898	0.144845	0.049*	
H13C	−0.099919	0.372260	0.116326	0.049*	

C14A	0.14973 (17)	0.40455 (11)	0.07809 (15)	0.0336 (4)	
H14A	0.107962	0.423187	0.007977	0.050*	
H14B	0.219666	0.375385	0.082139	0.050*	
H14C	0.175659	0.446871	0.125666	0.050*	
O1B	0.78764 (11)	0.27368 (8)	0.31174 (11)	0.0240 (4)	0.861 (4)
H1B	0.821 (3)	0.2626 (17)	0.276 (2)	0.036*	0.861 (4)
O1D	0.7217 (8)	0.2729 (6)	0.1953 (7)	0.029 (3)	0.139 (4)
H1D	0.792 (3)	0.273 (11)	0.216 (15)	0.043*	0.139 (4)
O2B	0.48103 (10)	0.32248 (7)	0.26463 (10)	0.0241 (3)	
H2BO	0.491 (2)	0.2970 (14)	0.3070 (19)	0.036*	
C1B	0.61505 (15)	0.18659 (9)	0.26432 (13)	0.0231 (3)	
C2B	0.49518 (17)	0.17063 (10)	0.17502 (15)	0.0320 (4)	
H2D	0.504097	0.177553	0.109762	0.048*	
H2E	0.434263	0.205120	0.178493	0.048*	
H2F	0.470729	0.119058	0.179826	0.048*	
C3B	0.60474 (19)	0.16755 (10)	0.36557 (15)	0.0344 (4)	
H3D	0.543837	0.199410	0.374298	0.052*	
H3E	0.681923	0.176045	0.422469	0.052*	
H3F	0.581844	0.114974	0.364947	0.052*	
C4B	0.70593 (18)	0.13109 (10)	0.25303 (16)	0.0334 (4)	
H4D	0.676084	0.079960	0.250807	0.050*	
H4E	0.782593	0.136303	0.311660	0.050*	
H4F	0.716960	0.141675	0.189437	0.050*	
C5B	0.66290 (13)	0.26699 (9)	0.25474 (12)	0.0199 (3)	
H5B	0.654931	0.269121	0.181816	0.024*	0.861 (4)
H5D	0.732583	0.268422	0.322371	0.024*	0.139 (4)
C6B	0.59755 (13)	0.34123 (8)	0.26741 (11)	0.0178 (3)	
C7B	0.56779 (15)	0.38969 (9)	0.16587 (13)	0.0240 (3)	
C8B	0.67884 (18)	0.40496 (12)	0.14124 (16)	0.0370 (4)	
H8D	0.713798	0.357363	0.132765	0.056*	
H8E	0.737954	0.433212	0.197651	0.056*	
H8F	0.655164	0.434001	0.077676	0.056*	
C9B	0.47866 (17)	0.34786 (12)	0.07241 (13)	0.0334 (4)	
H9D	0.456646	0.379656	0.011433	0.050*	
H9E	0.406871	0.335484	0.084699	0.050*	
H9F	0.515627	0.301759	0.061528	0.050*	
C10B	0.5110 (2)	0.46557 (12)	0.16916 (18)	0.0448 (5)	
H10D	0.486821	0.490002	0.102131	0.067*	
H10E	0.569193	0.497079	0.221771	0.067*	
H10F	0.440693	0.458162	0.185682	0.067*	
C11B	0.66511 (15)	0.38317 (10)	0.37427 (13)	0.0258 (3)	
C12B	0.70489 (18)	0.32750 (12)	0.46434 (14)	0.0357 (4)	
H12D	0.634720	0.301547	0.466048	0.054*	
H12E	0.745250	0.354584	0.528899	0.054*	
H12F	0.760029	0.290921	0.455389	0.054*	
C13B	0.77441 (19)	0.42840 (14)	0.38320 (17)	0.0439 (5)	
H13D	0.830674	0.396300	0.367949	0.066*	
H13E	0.813097	0.448074	0.453092	0.066*	

H13F	0.750017	0.470003	0.334338	0.066*
C14B	0.57906 (19)	0.43522 (12)	0.40186 (17)	0.0404 (5)
H14D	0.552946	0.476524	0.352585	0.061*
H14E	0.620965	0.455292	0.471160	0.061*
H14F	0.509227	0.406526	0.399146	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0155 (6)	0.0266 (7)	0.0237 (7)	−0.0020 (5)	0.0073 (5)	−0.0004 (5)
O1C	0.022 (6)	0.027 (6)	0.020 (6)	−0.002 (4)	0.013 (5)	−0.002 (4)
O2A	0.0152 (5)	0.0256 (6)	0.0291 (6)	0.0006 (4)	0.0105 (4)	0.0010 (5)
C1A	0.0265 (8)	0.0176 (7)	0.0249 (8)	0.0006 (6)	0.0103 (6)	0.0009 (6)
C2A	0.0300 (9)	0.0253 (9)	0.0377 (10)	0.0065 (7)	0.0084 (8)	0.0089 (7)
C3A	0.0533 (12)	0.0234 (8)	0.0344 (10)	0.0061 (8)	0.0233 (9)	−0.0019 (7)
C4A	0.0373 (9)	0.0210 (8)	0.0369 (10)	−0.0056 (7)	0.0145 (8)	0.0020 (7)
C5A	0.0150 (7)	0.0200 (7)	0.0236 (7)	−0.0002 (5)	0.0074 (6)	0.0020 (6)
C6A	0.0148 (6)	0.0192 (7)	0.0191 (7)	0.0002 (5)	0.0073 (5)	0.0011 (5)
C7A	0.0226 (7)	0.0229 (8)	0.0215 (7)	−0.0043 (6)	0.0093 (6)	−0.0032 (6)
C8A	0.0324 (9)	0.0312 (9)	0.0273 (8)	0.0018 (7)	0.0153 (7)	−0.0038 (7)
C9A	0.0270 (9)	0.0430 (11)	0.0216 (8)	−0.0008 (8)	0.0030 (7)	−0.0022 (7)
C10A	0.0397 (10)	0.0318 (9)	0.0343 (10)	−0.0153 (8)	0.0166 (8)	−0.0084 (7)
C11A	0.0200 (7)	0.0228 (8)	0.0210 (7)	0.0007 (6)	0.0069 (6)	0.0054 (6)
C12A	0.0339 (9)	0.0346 (9)	0.0194 (8)	0.0018 (7)	0.0085 (7)	0.0015 (7)
C13A	0.0275 (9)	0.0352 (10)	0.0330 (9)	0.0099 (7)	0.0086 (7)	0.0056 (7)
C14A	0.0334 (9)	0.0376 (10)	0.0303 (9)	−0.0042 (8)	0.0130 (7)	0.0082 (7)
O1B	0.0137 (6)	0.0335 (8)	0.0236 (7)	0.0015 (5)	0.0061 (5)	−0.0011 (5)
O1D	0.026 (5)	0.041 (5)	0.027 (5)	0.010 (4)	0.019 (4)	0.003 (4)
O2B	0.0176 (5)	0.0264 (6)	0.0313 (6)	−0.0010 (4)	0.0128 (5)	0.0006 (5)
C1B	0.0247 (7)	0.0195 (7)	0.0259 (8)	−0.0004 (6)	0.0108 (6)	0.0000 (6)
C2B	0.0308 (9)	0.0241 (8)	0.0370 (10)	−0.0065 (7)	0.0090 (7)	−0.0062 (7)
C3B	0.0498 (11)	0.0251 (9)	0.0345 (10)	−0.0045 (8)	0.0230 (9)	0.0050 (7)
C4B	0.0366 (10)	0.0234 (8)	0.0414 (10)	0.0062 (7)	0.0165 (8)	0.0011 (7)
C5B	0.0169 (7)	0.0203 (7)	0.0234 (7)	−0.0005 (5)	0.0088 (6)	0.0004 (6)
C6B	0.0145 (6)	0.0191 (7)	0.0205 (7)	−0.0008 (5)	0.0076 (5)	−0.0012 (5)
C7B	0.0260 (8)	0.0226 (8)	0.0243 (8)	0.0043 (6)	0.0110 (6)	0.0050 (6)
C8B	0.0405 (10)	0.0420 (11)	0.0341 (10)	−0.0091 (8)	0.0206 (8)	0.0051 (8)
C9B	0.0286 (9)	0.0457 (11)	0.0216 (8)	0.0022 (8)	0.0051 (7)	0.0056 (7)
C10B	0.0604 (14)	0.0328 (10)	0.0456 (12)	0.0200 (10)	0.0255 (11)	0.0118 (9)
C11B	0.0222 (7)	0.0271 (8)	0.0249 (8)	−0.0012 (6)	0.0057 (6)	−0.0076 (6)
C12B	0.0342 (10)	0.0503 (12)	0.0201 (8)	−0.0071 (8)	0.0077 (7)	−0.0045 (8)
C13B	0.0367 (11)	0.0511 (13)	0.0399 (11)	−0.0219 (9)	0.0107 (9)	−0.0101 (9)
C14B	0.0411 (11)	0.0400 (11)	0.0393 (11)	0.0033 (9)	0.0149 (9)	−0.0120 (9)

Geometric parameters (Å, º)

O1A—C5A	1.4378 (18)	O1B—C5B	1.4165 (19)
O1A—H1A	0.77 (3)	O1B—H1B	0.79 (3)

O1C—C5A	1.258 (11)	O1D—C5B	1.305 (8)
O1C—H1C	0.76 (3)	O1D—H1D	0.79 (4)
O2A—C6A	1.4341 (17)	O2B—C6B	1.4414 (18)
O2A—H2AO	0.75 (3)	O2B—H2BO	0.72 (3)
C1A—C3A	1.528 (2)	C1B—C3B	1.527 (2)
C1A—C2A	1.539 (2)	C1B—C2B	1.536 (2)
C1A—C4A	1.545 (2)	C1B—C4B	1.540 (2)
C1A—C5A	1.573 (2)	C1B—C5B	1.577 (2)
C2A—H2A	0.9800	C2B—H2D	0.9800
C2A—H2B	0.9800	C2B—H2E	0.9800
C2A—H2C	0.9800	C2B—H2F	0.9800
C3A—H3A	0.9800	C3B—H3D	0.9800
C3A—H3B	0.9800	C3B—H3E	0.9800
C3A—H3C	0.9800	C3B—H3F	0.9800
C4A—H4A	0.9800	C4B—H4D	0.9800
C4A—H4B	0.9800	C4B—H4E	0.9800
C4A—H4C	0.9800	C4B—H4F	0.9800
C5A—C6A	1.599 (2)	C5B—C6B	1.593 (2)
C5A—H5A	1.0000	C5B—H5B	1.0000
C5A—H5C	1.0000	C5B—H5D	1.0000
C6A—C7A	1.598 (2)	C6B—C7B	1.595 (2)
C6A—C11A	1.606 (2)	C6B—C11B	1.598 (2)
C7A—C9A	1.536 (2)	C7B—C10B	1.532 (3)
C7A—C8A	1.540 (2)	C7B—C9B	1.537 (2)
C7A—C10A	1.547 (2)	C7B—C8B	1.546 (2)
C8A—H8A	0.9800	C8B—H8D	0.9800
C8A—H8B	0.9800	C8B—H8E	0.9800
C8A—H8C	0.9800	C8B—H8F	0.9800
C9A—H9A	0.9800	C9B—H9D	0.9800
C9A—H9B	0.9800	C9B—H9E	0.9800
C9A—H9C	0.9800	C9B—H9F	0.9800
C10A—H10A	0.9800	C10B—H10D	0.9800
C10A—H10B	0.9800	C10B—H10E	0.9800
C10A—H10C	0.9800	C10B—H10F	0.9800
C11A—C13A	1.524 (2)	C11B—C13B	1.518 (3)
C11A—C12A	1.540 (2)	C11B—C12B	1.540 (3)
C11A—C14A	1.557 (2)	C11B—C14B	1.561 (3)
C12A—H12A	0.9800	C12B—H12D	0.9800
C12A—H12B	0.9800	C12B—H12E	0.9800
C12A—H12C	0.9800	C12B—H12F	0.9800
C13A—H13A	0.9800	C13B—H13D	0.9800
C13A—H13B	0.9800	C13B—H13E	0.9800
C13A—H13C	0.9800	C13B—H13F	0.9800
C14A—H14A	0.9800	C14B—H14D	0.9800
C14A—H14B	0.9800	C14B—H14E	0.9800
C14A—H14C	0.9800	C14B—H14F	0.9800
C5A—O1A—H1A	106.6 (19)	C5B—O1B—H1B	108 (2)

C5A—O1C—H1C	126 (5)	C5B—O1D—H1D	124 (10)
C6A—O2A—H2AO	106.4 (18)	C6B—O2B—H2BO	106 (2)
C3A—C1A—C2A	109.10 (15)	C3B—C1B—C2B	109.36 (15)
C3A—C1A—C4A	107.08 (15)	C3B—C1B—C4B	106.29 (15)
C2A—C1A—C4A	106.32 (14)	C2B—C1B—C4B	106.40 (14)
C3A—C1A—C5A	116.83 (14)	C3B—C1B—C5B	116.95 (14)
C2A—C1A—C5A	110.37 (13)	C2B—C1B—C5B	111.18 (13)
C4A—C1A—C5A	106.56 (13)	C4B—C1B—C5B	105.97 (13)
C1A—C2A—H2A	109.5	C1B—C2B—H2D	109.5
C1A—C2A—H2B	109.5	C1B—C2B—H2E	109.5
H2A—C2A—H2B	109.5	H2D—C2B—H2E	109.5
C1A—C2A—H2C	109.5	C1B—C2B—H2F	109.5
H2A—C2A—H2C	109.5	H2D—C2B—H2F	109.5
H2B—C2A—H2C	109.5	H2E—C2B—H2F	109.5
C1A—C3A—H3A	109.5	C1B—C3B—H3D	109.5
C1A—C3A—H3B	109.5	C1B—C3B—H3E	109.5
H3A—C3A—H3B	109.5	H3D—C3B—H3E	109.5
C1A—C3A—H3C	109.5	C1B—C3B—H3F	109.5
H3A—C3A—H3C	109.5	H3D—C3B—H3F	109.5
H3B—C3A—H3C	109.5	H3E—C3B—H3F	109.5
C1A—C4A—H4A	109.5	C1B—C4B—H4D	109.5
C1A—C4A—H4B	109.5	C1B—C4B—H4E	109.5
H4A—C4A—H4B	109.5	H4D—C4B—H4E	109.5
C1A—C4A—H4C	109.5	C1B—C4B—H4F	109.5
H4A—C4A—H4C	109.5	H4D—C4B—H4F	109.5
H4B—C4A—H4C	109.5	H4E—C4B—H4F	109.5
O1C—C5A—C1A	112.7 (6)	O1D—C5B—C1B	116.3 (5)
O1A—C5A—C1A	113.01 (13)	O1B—C5B—C1B	112.12 (13)
O1C—C5A—C6A	123.3 (6)	O1D—C5B—C6B	115.4 (4)
O1A—C5A—C6A	111.38 (12)	O1B—C5B—C6B	109.58 (13)
C1A—C5A—C6A	122.34 (12)	C1B—C5B—C6B	122.23 (12)
O1A—C5A—H5A	102.3	O1B—C5B—H5B	103.5
C1A—C5A—H5A	102.3	C1B—C5B—H5B	103.5
C6A—C5A—H5A	102.3	C6B—C5B—H5B	103.5
O1C—C5A—H5C	94.2	O1D—C5B—H5D	98.2
C1A—C5A—H5C	94.2	C1B—C5B—H5D	98.2
C6A—C5A—H5C	94.2	C6B—C5B—H5D	98.2
O2A—C6A—C7A	108.41 (12)	O2B—C6B—C5B	109.34 (12)
O2A—C6A—C5A	104.39 (12)	O2B—C6B—C7B	103.24 (12)
C7A—C6A—C5A	106.51 (12)	C5B—C6B—C7B	107.35 (12)
O2A—C6A—C11A	105.87 (12)	O2B—C6B—C11B	105.65 (12)
C7A—C6A—C11A	116.17 (12)	C5B—C6B—C11B	113.84 (12)
C5A—C6A—C11A	114.72 (12)	C7B—C6B—C11B	116.72 (13)
C9A—C7A—C8A	107.06 (14)	C10B—C7B—C9B	106.48 (16)
C9A—C7A—C10A	105.47 (14)	C10B—C7B—C8B	107.12 (16)
C8A—C7A—C10A	106.22 (14)	C9B—C7B—C8B	105.96 (15)
C9A—C7A—C6A	110.33 (13)	C10B—C7B—C6B	113.56 (14)
C8A—C7A—C6A	113.49 (13)	C9B—C7B—C6B	110.25 (14)

C10A—C7A—C6A	113.73 (13)	C8B—C7B—C6B	112.98 (14)
C7A—C8A—H8A	109.5	C7B—C8B—H8D	109.5
C7A—C8A—H8B	109.5	C7B—C8B—H8E	109.5
H8A—C8A—H8B	109.5	H8D—C8B—H8E	109.5
C7A—C8A—H8C	109.5	C7B—C8B—H8F	109.5
H8A—C8A—H8C	109.5	H8D—C8B—H8F	109.5
H8B—C8A—H8C	109.5	H8E—C8B—H8F	109.5
C7A—C9A—H9A	109.5	C7B—C9B—H9D	109.5
C7A—C9A—H9B	109.5	C7B—C9B—H9E	109.5
H9A—C9A—H9B	109.5	H9D—C9B—H9E	109.5
C7A—C9A—H9C	109.5	C7B—C9B—H9F	109.5
H9A—C9A—H9C	109.5	H9D—C9B—H9F	109.5
H9B—C9A—H9C	109.5	H9E—C9B—H9F	109.5
C7A—C10A—H10A	109.5	C7B—C10B—H10D	109.5
C7A—C10A—H10B	109.5	C7B—C10B—H10E	109.5
H10A—C10A—H10B	109.5	H10D—C10B—H10E	109.5
C7A—C10A—H10C	109.5	C7B—C10B—H10F	109.5
H10A—C10A—H10C	109.5	H10D—C10B—H10F	109.5
H10B—C10A—H10C	109.5	H10E—C10B—H10F	109.5
C13A—C11A—C12A	108.17 (14)	C13B—C11B—C12B	107.18 (15)
C13A—C11A—C14A	106.89 (14)	C13B—C11B—C14B	108.19 (16)
C12A—C11A—C14A	101.48 (14)	C12B—C11B—C14B	101.66 (15)
C13A—C11A—C6A	116.39 (13)	C13B—C11B—C6B	115.92 (15)
C12A—C11A—C6A	110.93 (13)	C12B—C11B—C6B	111.05 (14)
C14A—C11A—C6A	111.85 (13)	C14B—C11B—C6B	111.80 (14)
C11A—C12A—H12A	109.5	C11B—C12B—H12D	109.5
C11A—C12A—H12B	109.5	C11B—C12B—H12E	109.5
H12A—C12A—H12B	109.5	H12D—C12B—H12E	109.5
C11A—C12A—H12C	109.5	C11B—C12B—H12F	109.5
H12A—C12A—H12C	109.5	H12D—C12B—H12F	109.5
H12B—C12A—H12C	109.5	H12E—C12B—H12F	109.5
C11A—C13A—H13A	109.5	C11B—C13B—H13D	109.5
C11A—C13A—H13B	109.5	C11B—C13B—H13E	109.5
H13A—C13A—H13B	109.5	H13D—C13B—H13E	109.5
C11A—C13A—H13C	109.5	C11B—C13B—H13F	109.5
H13A—C13A—H13C	109.5	H13D—C13B—H13F	109.5
H13B—C13A—H13C	109.5	H13E—C13B—H13F	109.5
C11A—C14A—H14A	109.5	C11B—C14B—H14D	109.5
C11A—C14A—H14B	109.5	C11B—C14B—H14E	109.5
H14A—C14A—H14B	109.5	H14D—C14B—H14E	109.5
C11A—C14A—H14C	109.5	C11B—C14B—H14F	109.5
H14A—C14A—H14C	109.5	H14D—C14B—H14F	109.5
H14B—C14A—H14C	109.5	H14E—C14B—H14F	109.5
C3A—C1A—C5A—O1C	137.6 (6)	C3B—C1B—C5B—O1D	149.9 (5)
C2A—C1A—C5A—O1C	−97.0 (6)	C2B—C1B—C5B—O1D	−83.6 (5)
C4A—C1A—C5A—O1C	18.1 (6)	C4B—C1B—C5B—O1D	31.6 (5)
C3A—C1A—C5A—O1A	81.10 (18)	C3B—C1B—C5B—O1B	74.30 (19)

C2A—C1A—C5A—O1A	−153.53 (14)	C2B—C1B—C5B—O1B	−159.12 (14)
C4A—C1A—C5A—O1A	−38.49 (18)	C4B—C1B—C5B—O1B	−43.92 (18)
C3A—C1A—C5A—C6A	−56.4 (2)	C3B—C1B—C5B—C6B	−58.9 (2)
C2A—C1A—C5A—C6A	68.95 (19)	C2B—C1B—C5B—C6B	67.72 (19)
C4A—C1A—C5A—C6A	−176.01 (14)	C4B—C1B—C5B—C6B	−177.08 (14)
O1C—C5A—C6A—O2A	152.5 (6)	O1D—C5B—C6B—O2B	138.7 (5)
O1A—C5A—C6A—O2A	−150.07 (12)	O1B—C5B—C6B—O2B	−147.00 (13)
C1A—C5A—C6A—O2A	−11.94 (18)	C1B—C5B—C6B—O2B	−12.82 (19)
O1C—C5A—C6A—C7A	37.9 (7)	O1D—C5B—C6B—C7B	27.4 (5)
O1A—C5A—C6A—C7A	95.34 (14)	O1B—C5B—C6B—C7B	101.66 (14)
C1A—C5A—C6A—C7A	−126.53 (15)	C1B—C5B—C6B—C7B	−124.16 (15)
O1C—C5A—C6A—C11A	−92.1 (7)	O1D—C5B—C6B—C11B	−103.4 (5)
O1A—C5A—C6A—C11A	−34.67 (18)	O1B—C5B—C6B—C11B	−29.12 (18)
C1A—C5A—C6A—C11A	103.46 (16)	C1B—C5B—C6B—C11B	105.06 (16)
O2A—C6A—C7A—C9A	−45.28 (17)	O2B—C6B—C7B—C10B	67.99 (18)
C5A—C6A—C7A—C9A	66.55 (16)	C5B—C6B—C7B—C10B	−176.55 (15)
C11A—C6A—C7A—C9A	−164.28 (13)	C11B—C6B—C7B—C10B	−47.4 (2)
O2A—C6A—C7A—C8A	−165.43 (13)	O2B—C6B—C7B—C9B	−51.41 (16)
C5A—C6A—C7A—C8A	−53.60 (16)	C5B—C6B—C7B—C9B	64.06 (16)
C11A—C6A—C7A—C8A	75.57 (17)	C11B—C6B—C7B—C9B	−166.79 (14)
O2A—C6A—C7A—C10A	72.99 (17)	O2B—C6B—C7B—C8B	−169.76 (14)
C5A—C6A—C7A—C10A	−175.18 (14)	C5B—C6B—C7B—C8B	−54.29 (17)
C11A—C6A—C7A—C10A	−46.01 (19)	C11B—C6B—C7B—C8B	74.86 (18)
O2A—C6A—C11A—C13A	−169.49 (14)	O2B—C6B—C11B—C13B	−162.80 (16)
C7A—C6A—C11A—C13A	−49.12 (19)	C5B—C6B—C11B—C13B	77.22 (19)
C5A—C6A—C11A—C13A	75.97 (18)	C7B—C6B—C11B—C13B	−48.8 (2)
O2A—C6A—C11A—C12A	66.28 (16)	O2B—C6B—C11B—C12B	74.59 (16)
C7A—C6A—C11A—C12A	−173.35 (13)	C5B—C6B—C11B—C12B	−45.39 (18)
C5A—C6A—C11A—C12A	−48.26 (17)	C7B—C6B—C11B—C12B	−171.37 (14)
O2A—C6A—C11A—C14A	−46.24 (17)	O2B—C6B—C11B—C14B	−38.18 (19)
C7A—C6A—C11A—C14A	74.13 (17)	C5B—C6B—C11B—C14B	−158.17 (15)
C5A—C6A—C11A—C14A	−160.78 (14)	C7B—C6B—C11B—C14B	75.85 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*A*—H2*AO*···O2*B*	0.75 (3)	2.27 (2)	2.8146 (16)	130 (2)
O1*B*—H1*B*···O1*A*^{i}	0.79 (3)	2.21 (3)	2.992 (2)	169 (3)
O1*D*—H1*D*···O1*C*^{i}	0.79 (4)	2.30 (6)	3.076 (14)	167 (19)

Symmetry code: (i) *x*+1, *y*, *z*.