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(1*S**,2*S**)-1,2-Di-*tert*-butylglycol

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Key indicators: single-crystal X-ray study; T = 200 K; mean σ (C–C) = 0.003 Å; *R* factor = 0.041; *wR* factor = 0.109; data-to-parameter ratio = 12.7.

In the crystal structure of the title compound, $C_{10}H_{22}O_2$, cooperative chains of $O-H\cdots O$ hydrogen bonds are established by intra- as well as intermolecular interactions. These hydrogen bonds connect the molecules into infinite strands along [100], with a binary level graph-set descriptor $C_2^2(4)$. Excluding the H atoms on the hydroxy groups, the molecule shows non-crystallographic C_2 symmetry.

Related literature

The compound was synthesized according to a published procedure (Boehrer *et al.*, 1997). For the crystal structures of other ethane-1,2-diol derivatives with bulky substituents, see: Betz & Klüfers (2007); Allscher *et al.* (2008). For graph-set descriptors, see: Etter *et al.* (1990); Bernstein *et al.* (1995).



Experimental

Crystal data

 $\begin{array}{l} C_{10}H_{22}O_2\\ M_r = 174.28\\ \text{Orthorhombic, } P2_12_12\\ a = 9.7799 \ (3) \text{ \AA}\\ b = 16.3879 \ (7) \text{ \AA} \end{array}$

c = 6.9771 (3) Å V = 1118.23 (8) Å³ Z = 4 Mo K α radiation μ = 0.07 mm⁻¹ 1490 independent reflections

1253 reflections with $I > 2\sigma(I)$

 $0.30 \times 0.09 \times 0.02 \text{ mm}$

 $R_{\rm int} = 0.040$

T = 200 (2) K

Data collection

Nonius KappaCCD diffractometer Absorption correction: none 8640 measured reflections

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$	117 parameters
$vR(F^2) = 0.109$	H-atom parameters constrained
S = 1.05	$\Delta \rho_{\rm max} = 0.15 \ {\rm e} \ {\rm \AA}^{-3}$
490 reflections	$\Delta \rho_{\rm min} = -0.15 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	$D-{\rm H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$\begin{array}{c} \hline O1 - H811 \cdots O2^{i} \\ O2 - H821 \cdots O1 \end{array}$	0.84	1.93	2.7721 (16)	176
	0.84	1.97	2.5129 (16)	121

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 2$.

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2332).

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supporting information

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(1*S**,2*S**)-1,2-Di-*tert*-butylglycol

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S1. Comment

The title compound was synthesized as a potential chelating ligand with sterically demanding substituents on the carbon backbone to estimate the influence of steric pretense on coordination reactions with different central atoms.

In the molecule (Fig. 1) bond lengths and angles are found in the range apparent for other vicinal diols bearing sterically more demanding substituents (Betz & Klüfers, 2007, Allscher *et al.*, 2008). While the *tert*-butyl groups adopt a staggered conformation with respect to the hydroxy groups, the O atoms are present in a nearly eclipsed arrangement. The reason for this unfavourable conformation becomes evident when examining intermolecular contacts.

In the crystal structure, inter- and intramolecular hydrogen bonds are present which connect the molecules into strands along [1 0 0] (Fig. 2). The bulky hydrophobic *tert*-butyl groups encase this strand of hydroxyl groups. The hydrogen bonds form cooperative chains. In terms of graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995) the descriptor for these chains on the binary level is $C_{2}^{2}(4)$.

Excluding the H atoms on the hydroxy groups, the molecule shows non-crystallographic C_2 symmetry.

The molecular packing of the title compound is shown in Figure 3.

S2. Experimental

The title compound was prepared according to a published procedure (Boehrer *et al.*, 1997). Crystals suitable for X-ray studies were obtained upon recrystallization from boiling toluene.

S3. Refinement

Due to the absence of a strong anomalous scatterer, the absolute structure parameter, which is 0.982 with an estimated standard deviation of 1.241 for the unmerged data set, is meaningless. Thus 1056 Friedel opposites have been merged and the absolute configuration has been arbitrarily chosen.

Carbon-bound as well as oxygen-bound H atoms were placed in calculated positions (C—H 1.00 Å for CH-groups, C— H 0.98 Å for methyl groups and O—H 0.84 Å for hydroxy groups) and were included in the refinement in the riding model approximation, with U(H) set to $1.2U_{eq}(C)$ for the CH-groups and $1.5U_{eq}(C)$ for methyl groups and $1.5U_{eq}(O)$ for the hydroxy groups.



Figure 1

The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.



Figure 2

Hydrogen bonds in the crystal structure of the title compound, viewed along [0 0 1]. Underlying hydrogen bonds are not illustrated for clarity. Symmetry codes: $i_x + 1/2$, -y + 1/2, -z + 2; $i_x - 1/2$, -y + 1/2, -z + 2.



F(000) = 392 $D_x = 1.035 \text{ Mg m}^{-3}$

 $\theta = 3.1-27.5^{\circ}$ $\mu = 0.07 \text{ mm}^{-1}$ T = 200 KRod, colourless $0.30 \times 0.09 \times 0.02 \text{ mm}$

Mo *K* α radiation, $\lambda = 0.71073$ Å Cell parameters from 13560 reflections

Figure 3

The packing of the title compound, viewed along $[0\ 0\ -\ 1]$.

(1*S**,2*S**)-1,2-Di-*tert*-butylglycol

Crystal data
, С.,Н.,О.
M = 174.28
Orthorhombic $P_{2,2,2}$
Hall symbol: P 2 2ab
a = 9.7799 (3) Å
b = 16.3879(7) Å
c = 6.9771 (3) Å
V = 1118.23 (8) Å ³
Z = 4

Data collection

Nonius KappaCCD	1490 independent reflections
diffractometer	1253 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	$R_{\rm int} = 0.040$
MONTEL, graded multilayered X-ray optics	$\theta_{\rm max} = 27.5^{\circ}, \ \theta_{\rm min} = 3.2^{\circ}$
monochromator	$h = -12 \rightarrow 11$
CCD; rotation images; thick slices scans	$k = -19 \rightarrow 21$
8640 measured reflections	$l = -9 \rightarrow 8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from
$wR(F^2) = 0.109$	neighbouring sites
<i>S</i> = 1.05	H-atom parameters constrained
1490 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 0.0637P]$
117 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{\rm max} < 0.001$
Primary atom site location: structure-invariant	$\Delta ho_{ m max} = 0.15$ e Å ⁻³
direct methods	$\Delta ho_{\min} = -0.15 \text{ e} \text{ Å}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (A^2)

O10.13030 (11)0.30082 (8)0.96003 (18)0.0402 (3)H8110.04760.29220.98570.060*O20.35411 (12)0.22582 (8)0.9762 (2)0.0437 (4)H8210.30540.25481.04840.066*C10.16231 (16)0.26595 (10)0.7782 (2)0.0330 (4)H10.07920.23710.72920.040*C20.27611 (16)0.20174 (10)0.8121 (2)0.0332 (4)C30.19990 (19)0.33399 (11)0.6353 (3)0.0393 (4)C40.0811 (2)0.39538 (13)0.6286 (3)0.0511 (6)C40.0811 (2)0.36550.60010.083*H42-0.00420.36650.60010.083*H430.09870.34600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34040.60870.077*H620.31880.39940.83700.077*H630.34660.42440.60870.103*H810.2740.09670.53940.103*H820.0760.11450.62180.103*H830.16340.01514 (15)0.9965 (4)0.0656 (7)H910.0986<		x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
H8110.04760.29220.98570.060*O20.35411 (12)0.22582 (8)0.9762 (2)0.0437 (4)H8210.30540.2558 (1)0.7762 (2)0.0330 (4)H10.07920.23710.7729 (2)0.0332 (4)H10.07920.23710.72920.040*C20.27611 (16)0.20174 (10)0.8121 (2)0.0332 (4)H20.33860.20350.69880.040*C30.19990 (19)0.33399 (11)0.6353 (3)0.0393 (4)C40.0811 (2)0.39538 (13)0.6286 (3)0.0551 (6)H410.07310.42280.75300.083*H42-0.00420.36650.60010.083*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.4049 (5)C80.1634 (3)0.8512 (14)0.6414 (4)0.6687 (7)H810.22740.09670.53940.103*H820.0760.53940.103*H830.14530.02640.64940.103*H910.0986 <td>01</td> <td>0.13030 (11)</td> <td>0.30082 (8)</td> <td>0.96003 (18)</td> <td>0.0402 (3)</td> <td></td>	01	0.13030 (11)	0.30082 (8)	0.96003 (18)	0.0402 (3)	
O2 0.35411 (12) 0.22582 (8) 0.9762 (2) 0.0437 (4) H821 0.3054 0.2548 1.0484 0.066* C1 0.16231 (16) 0.26595 (10) 0.7782 (2) 0.0300 (4) H1 0.0792 0.2371 0.7292 0.040* C2 0.27611 (16) 0.20174 (10) 0.8121 (2) 0.0332 (4) H2 0.3386 0.2035 0.6988 0.040* C3 0.19990 (19) 0.33399 (11) 0.6353 (3) 0.0593 (4) C4 0.0811 (2) 0.39538 (13) 0.6286 (3) 0.0551 (6) H41 0.0731 0.4228 0.7530 0.083* C5 0.2176 (3) 0.2976 (15) 0.4358 (3) 0.0628 (6) H51 0.2281 0.3422 0.3424 0.094* L52 0.1370 0.2653 0.4031 0.094* L6 0.3298 (2) 0.37869 (13) 0.6917 0.077* L6 0.3298 (2) 0.37869 (13) 0.6917 0.077*	H811	0.0476	0.2922	0.9857	0.060*	
H8210.30540.25481.04840.066*C10.16231 (16)0.26595 (10)0.7782 (2)0.0330 (4)H10.07920.23710.72920.040*C20.27611 (16)0.20174 (10)0.8121 (2)0.0332 (4)H20.33860.20350.69880.040*C30.19990 (19)0.33399 (11)0.6353 (3)0.0393 (4)C40.0811 (2)0.39538 (13)0.6286 (3)0.0551 (6)H410.07310.42280.60010.083*H42-0.00420.36650.60010.083*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.516 (5)H610.40750.34090.69170.077*H620.3180.39940.82700.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.4049 (5)C80.1634 (3)0.8512 (14)0.6441 (4)0.687 (7)H810.22740.90670.53940.103*H820.07760.53940.103*H830.14530.02640.64940.103*H830.14530.02640.64940.103*H940.99860.9985	O2	0.35411 (12)	0.22582 (8)	0.9762 (2)	0.0437 (4)	
C10.16231 (16)0.26595 (10)0.7782 (2)0.0330 (4)H10.07920.23710.72920.040*C20.27611 (16)0.20174 (10)0.8121 (2)0.0332 (4)H20.33860.20350.69880.040*C30.19990 (19)0.33399 (11)0.6553 (3)0.0393 (4)C40.0811 (2)0.39538 (13)0.6286 (3)0.0551 (6)H410.07310.42280.75300.083*H42-0.00420.36650.60010.083*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*L520.13700.26530.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.017*C70.22584 (18)0.11294 (12)0.8338 (3)0.4049 (5)C80.1634 (3)0.08612 (14)0.6414 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07660.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.098*H93 <td< td=""><td>H821</td><td>0.3054</td><td>0.2548</td><td>1.0484</td><td>0.066*</td><td></td></td<>	H821	0.3054	0.2548	1.0484	0.066*	
H10.07920.23710.72920.040*C20.27611 (16)0.20174 (10)0.8121 (2)0.0332 (4)H20.33860.20350.69880.040*C30.19990 (19)0.33399 (11)0.6535 (3)0.0393 (4)C40.0811 (2)0.39538 (13)0.6286 (3)0.0551 (6)H410.07310.42280.75300.083*H42-0.00420.36650.60010.83*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26320.43150.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.838 (3)0.0409 (5)C80.1634 (3)0.0812 (14)0.6414 (4)0.6687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*C90.1230 (2)0.1054 (15)0.9965 (4)0.0656 (7)H910.99860.47641.01380.998*H920.4070.13660.96530.098*H930.16340.12621.11500.098*H930.16340.12	C1	0.16231 (16)	0.26595 (10)	0.7782 (2)	0.0330 (4)	
C20.27611 (16)0.20174 (10)0.8121 (2)0.0332 (4)H20.33860.20350.69880.040*C30.19990 (19)0.33399 (11)0.6353 (3)0.0393 (4)C40.0811 (2)0.39538 (13)0.6286 (3)0.0551 (6)H410.07310.42280.75300.883*H42-0.00420.36650.60010.083*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.6286 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.0014*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.77*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40070.13660.96530.098*H930.16340.12621.11500.098*H940.3395 (2) <td>H1</td> <td>0.0792</td> <td>0.2371</td> <td>0.7292</td> <td>0.040*</td> <td></td>	H1	0.0792	0.2371	0.7292	0.040*	
H20.33860.20350.69880.040*C30.1990 (19)0.33399 (11)0.6353 (3)0.0393 (4)C40.0811 (2)0.39538 (13)0.6286 (3)0.0551 (6)H410.07310.42280.75300.083*H42-0.00420.36650.60010.83*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*L530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.4049 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*C90.1230 (2)0.0514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40070.13660.96530.098*H930.16340.12621.11500.9985H930.16340.12621.11500.098*H1010.38960.07400.99850.081*H1030.32040.056750.8	C2	0.27611 (16)	0.20174 (10)	0.8121 (2)	0.0332 (4)	
C3 0.19990 (19) 0.33399 (11) 0.6353 (3) 0.0393 (4) C4 0.0811 (2) 0.39538 (13) 0.6286 (3) 0.0551 (6) H41 0.0731 0.4228 0.7530 0.083* H42 -0.0042 0.3665 0.6001 0.083* H43 0.0987 0.4360 0.5285 0.083* C5 0.2176 (3) 0.29796 (15) 0.4358 (3) 0.0628 (6) H51 0.2281 0.3422 0.3424 0.094* H52 0.1370 0.2632 0.4335 0.094* H53 0.2992 0.2632 0.4335 0.094* H64 0.4075 0.3409 0.6917 0.077* H61 0.4075 0.3409 0.6917 0.077* H62 0.3188 0.3994 0.8270 0.077* H63 0.3466 0.4244 0.6087 0.103* C7 0.22584 (18) 0.11294 (12) 0.8338 (3) 0.4069 (5) C8 0.1634 (3) <t< td=""><td>H2</td><td>0.3386</td><td>0.2035</td><td>0.6988</td><td>0.040*</td><td></td></t<>	H2	0.3386	0.2035	0.6988	0.040*	
C40.0811 (2)0.39538 (13)0.6286 (3)0.0551 (6)H410.07310.42280.75300.083*H42-0.00420.36650.60010.083*H430.09870.43600.52850.0602*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.0409 (5)C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*H910.9860.04761.01380.098*H920.4070.13660.96530.098*H930.16340.12621.11500.098*H930.16340.12621.11500.098*H1010.38960.07400.98550.081*H1020.41760.06580.77330.081*	C3	0.19990 (19)	0.33399 (11)	0.6353 (3)	0.0393 (4)	
H410.07310.42280.75300.083*H42-0.00420.36650.60010.083*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.6687 (7)H810.22740.09670.53940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40070.13660.96530.098*H930.16340.12621.11500.998H930.16340.12621.11500.098*H930.16340.0572 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*	C4	0.0811 (2)	0.39538 (13)	0.6286 (3)	0.0551 (6)	
H42-0.00420.36650.60010.083*H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6411 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40470.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*	H41	0.0731	0.4228	0.7530	0.083*	
H430.09870.43600.52850.083*C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40470.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*	H42	-0.0042	0.3665	0.6001	0.083*	
C50.2176 (3)0.29796 (15)0.4358 (3)0.0628 (6)H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.6687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40070.13660.96530.098*H930.16340.12621.11500.998*H930.16340.12621.11500.098*H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H43	0.0987	0.4360	0.5285	0.083*	
H510.22810.34220.34240.094*H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.4070.13660.96530.098*H930.16340.12621.11500.098*H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	C5	0.2176 (3)	0.29796 (15)	0.4358 (3)	0.0628 (6)	
H520.13700.26530.40310.094*H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40770.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H51	0.2281	0.3422	0.3424	0.094*	
H530.29920.26320.43350.094*C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.0409 (5)C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H52	0.1370	0.2653	0.4031	0.094*	
C60.3298 (2)0.37869 (13)0.6961 (3)0.0516 (5)H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H53	0.2992	0.2632	0.4335	0.094*	
H610.40750.34090.69170.077*H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.66580.77330.081*H1030.32040.00150.87930.081*	C6	0.3298 (2)	0.37869 (13)	0.6961 (3)	0.0516 (5)	
H620.31880.39940.82700.077*H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40770.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H61	0.4075	0.3409	0.6917	0.077*	
H630.34660.42440.60870.077*C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.4070.13660.96530.098*H930.16340.12621.11500.998*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H62	0.3188	0.3994	0.8270	0.077*	
C70.22584 (18)0.11294 (12)0.8338 (3)0.0409 (5)C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.40770.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H63	0.3466	0.4244	0.6087	0.077*	
C80.1634 (3)0.08512 (14)0.6441 (4)0.0687 (7)H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.04070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	C7	0.22584 (18)	0.11294 (12)	0.8338 (3)	0.0409 (5)	
H810.22740.09670.53940.103*H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.04070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	C8	0.1634 (3)	0.08512 (14)	0.6441 (4)	0.0687 (7)	
H820.07760.11450.62180.103*H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.04070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H81	0.2274	0.0967	0.5394	0.103*	
H830.14530.02640.64940.103*C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.04070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H82	0.0776	0.1145	0.6218	0.103*	
C90.1230 (2)0.10514 (15)0.9965 (4)0.0656 (7)H910.09860.04761.01380.098*H920.04070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H83	0.1453	0.0264	0.6494	0.103*	
H910.09860.04761.01380.098*H920.04070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	C9	0.1230 (2)	0.10514 (15)	0.9965 (4)	0.0656 (7)	
H920.04070.13660.96530.098*H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H91	0.0986	0.0476	1.0138	0.098*	
H930.16340.12621.11500.098*C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H92	0.0407	0.1366	0.9653	0.098*	
C100.3495 (2)0.05872 (12)0.8749 (4)0.0542 (5)H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H93	0.1634	0.1262	1.1150	0.098*	
H1010.38960.07400.99850.081*H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	C10	0.3495 (2)	0.05872 (12)	0.8749 (4)	0.0542 (5)	
H1020.41760.06580.77330.081*H1030.32040.00150.87930.081*	H101	0.3896	0.0740	0.9985	0.081*	
H103 0.3204 0.0015 0.8793 0.081*	H102	0.4176	0.0658	0.7733	0.081*	
	H103	0.3204	0.0015	0.8793	0.081*	

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	<i>U</i> ²³
01	0.0321 (6)	0.0536 (8)	0.0349 (6)	0.0056 (6)	0.0041 (5)	-0.0067 (6)
O2	0.0344 (6)	0.0518 (8)	0.0448 (7)	0.0046 (5)	-0.0136 (6)	-0.0073 (6)
C1	0.0260 (7)	0.0416 (9)	0.0314 (8)	0.0013 (7)	-0.0020 (7)	-0.0047 (7)
C2	0.0251 (7)	0.0428 (9)	0.0317 (8)	0.0007 (7)	-0.0004 (6)	-0.0032 (7)
C3	0.0397 (9)	0.0446 (10)	0.0334 (9)	0.0051 (8)	-0.0020 (8)	0.0026 (8)
C4	0.0548 (11)	0.0537 (12)	0.0568 (12)	0.0140 (10)	-0.0059 (11)	0.0094 (11)
C5	0.0841 (15)	0.0716 (15)	0.0327 (10)	0.0129 (13)	0.0028 (10)	0.0025 (10)
C6	0.0452 (11)	0.0493 (11)	0.0602 (13)	-0.0051 (9)	0.0029 (10)	0.0121 (10)
C7	0.0341 (9)	0.0374 (9)	0.0513 (11)	0.0025 (7)	0.0012 (8)	-0.0015 (8)
C8	0.0733 (15)	0.0485 (12)	0.0843 (18)	-0.0004 (12)	-0.0263 (14)	-0.0208 (12)
C9	0.0580 (13)	0.0499 (12)	0.0889 (18)	-0.0016 (10)	0.0295 (12)	0.0095 (12)
C10	0.0463 (10)	0.0435 (11)	0.0729 (14)	0.0087 (9)	-0.0010 (11)	0.0023 (11)

Atomic displacement parameters $(Å^2)$

Geometric parameters (Å, °)

01—C1	1.426 (2)	С5—Н53	0.980
O1—H811	0.840	C6—H61	0.980
O2—C2	1.431 (2)	С6—Н62	0.980
O2—H821	0.840	С6—Н63	0.980
C1—C3	1.540 (3)	С7—С9	1.522 (3)
C1—C2	1.550(2)	С7—С8	1.527 (3)
C1—H1	1.000	C7—C10	1.528 (3)
С2—С7	1.543 (3)	C8—H81	0.980
С2—Н2	1.000	C8—H82	0.980
С3—С5	1.522 (3)	C8—H83	0.980
С3—С6	1.527 (3)	С9—Н91	0.980
C3—C4	1.538 (2)	С9—Н92	0.980
C4—H41	0.980	С9—Н93	0.980
C4—H42	0.980	C10—H101	0.980
C4—H43	0.980	C10—H102	0.980
С5—Н51	0.980	C10—H103	0.980
С5—Н52	0.980		
C1—O1—H811	109.5	H52—C5—H53	109.5
С2—О2—Н821	109.5	C3—C6—H61	109.5
O1—C1—C3	109.77 (14)	C3—C6—H62	109.5
O1—C1—C2	107.08 (13)	H61—C6—H62	109.5
C3—C1—C2	114.77 (13)	С3—С6—Н63	109.5
01—C1—H1	108.3	H61—C6—H63	109.5
C3—C1—H1	108.3	H62—C6—H63	109.5
C2—C1—H1	108.3	C9—C7—C8	110.91 (18)
O2—C2—C7	110.58 (14)	C9—C7—C10	109.53 (17)
O2—C2—C1	108.52 (13)	C8—C7—C10	107.79 (17)
C7—C2—C1	115.24 (14)	C9—C7—C2	111.26 (16)
O2—C2—H2	107.4	C8—C7—C2	108.91 (16)

107.4	C10—C7—C2	108.35 (14)
107.4	С7—С8—Н81	109.5
110.22 (19)	С7—С8—Н82	109.5
108.20 (17)	H81—C8—H82	109.5
108.86 (16)	С7—С8—Н83	109.5
109.78 (16)	H81—C8—H83	109.5
111.47 (15)	H82—C8—H83	109.5
108.22 (14)	С7—С9—Н91	109.5
109.5	С7—С9—Н92	109.5
109.5	Н91—С9—Н92	109.5
109.5	С7—С9—Н93	109.5
109.5	Н91—С9—Н93	109.5
109.5	Н92—С9—Н93	109.5
109.5	С7—С10—Н101	109.5
109.5	С7—С10—Н102	109.5
109.5	H101—C10—H102	109.5
109.5	С7—С10—Н103	109.5
109.5	H101-C10-H103	109.5
109.5	H102—C10—H103	109.5
-28.26 (17)	01—C1—C3—C4	-55.45 (18)
93.86 (17)	C2—C1—C3—C4	-176.09 (15)
96.34 (17)	O2—C2—C7—C9	66.46 (19)
-141.55 (15)	C1—C2—C7—C9	-57.1 (2)
-173.34 (16)	O2—C2—C7—C8	-170.99 (15)
66.0 (2)	C1—C2—C7—C8	65.5 (2)
64.23 (18)	O2—C2—C7—C10	-54.00 (19)
-56.4 (2)	C1—C2—C7—C10	-177.51 (16)
	107.4 107.4 $110.22 (19)$ $108.20 (17)$ $108.86 (16)$ $109.78 (16)$ $111.47 (15)$ $108.22 (14)$ 109.5 100.5	107.4 $C10-C7-C2$ 107.4 $C7-C8-H81$ $110.22 (19)$ $C7-C8-H81$ $108.20 (17)$ $H81-C8-H82$ $108.86 (16)$ $C7-C8-H83$ $109.78 (16)$ $H81-C8-H83$ $111.47 (15)$ $H82-C8-H83$ $108.22 (14)$ $C7-C9-H91$ 109.5 $C7-C9-H92$ 109.5 $C7-C9-H92$ 109.5 $C7-C9-H93$ 109.5 $H91-C9-H93$ 109.5 $H91-C9-H93$ 109.5 $H92-C9-H93$ 109.5 $C7-C10-H101$ 109.5 $C7-C10-H102$ 109.5 $C7-C10-H103$ 109.5 $H101-C10-H102$ 109.5 $H102-C10-H103$

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···· A	D—H···A
O1—H811…O2 ⁱ	0.84	1.93	2.7721 (16)	176
O2—H821…O1	0.84	1.97	2.5129 (16)	121

Symmetry code: (i) x-1/2, -y+1/2, -z+2.