Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diethyl 2,5-diphenylfuran-3,4-dicarboxylate

Sheng-Li Hu,[a]* Yi-Cheng Le[b] and Ling Huang[a]

[a]Department of Chemistry & Environmental Engineering, Hubei Normal University, Huangshi 435002, People's Republic of China, and [b]712th Research Institute, CSIC, Wuhan 430064, People's Republic of China
Correspondence e-mail: hushengli168@126.com

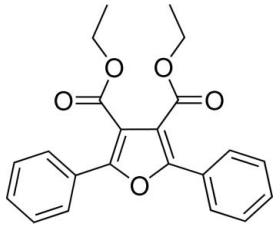
Received 20 October 2010; accepted 4 November 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.058; wR factor = 0.160; data-to-parameter ratio = 14.1.

In the title compound, $C_{22}H_{20}O_5$, the substituted benzene rings are twisted away from the furan ring, making dihedral angles of 54.91 (14) and 20.96 (15)° with the furan ring. The dihedral angle between the two benzene rings is 46.89 (13)°. One ethyl group of one ethoxycarbonyl unit is disordered over two sets of sites with occupancies of 0.56 (12) and 0.44 (12). In the crystal, weak intramolecular C—H···O hydrogen bonds link the molecules into chains along the c axis.

Related literature

For background to the applications of furan-3,4-dicarboxylic acid and its esters, see: Deshpande *et al.* (2002). For related structures, see: Hu & Wu (2005) Hu *et al.* (2005). For the synthesis, see: Wu *et al.* (1997).



Experimental

Crystal data

$C_{22}H_{20}O_5$
M_r = 364.38
Orthorhombic, *Pbca*
a = 11.9535 (8) Å
b = 17.0116 (12) Å
c = 18.9219 (14) Å
V = 3847.7 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.40 × 0.10 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.965, T_{max} = 0.993
19957 measured reflections
3778 independent reflections
1952 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.160
S = 1.01
3778 reflections
268 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O3	0.93	2.56	3.453 (4)	161

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We are grateful to Hubei Normal University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5048).

References

Bruker (2000). *SMART* and *SAINT* Bruker AXS Inc., Madison, Wisconsin, USA.
Deshpande, A. M., Natu, A. A. & Argade, N. P. (2002). *Synthesis*, **8**, 1010–1012.
Hu, S.-L., Wang, Z.-G. & Wu, A.-X. (2005). *Acta Cryst.* E**61**, o2801–o2803.
Hu, S.-L. & Wu, A.-X. (2005). *Acta Cryst.* E**61**, o2030–o2032.
Sheldrick, G. M. (1997). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wu, A., Wang, M. & Pan, X. (1997). *Synth. Commun.* **12**, 2087–2091.

supporting information

Acta Cryst. (2010). E**66**, o3116 [https://doi.org/10.1107/S1600536810045241]

Diethyl 2,5-diphenylfuran-3,4-dicarboxylate

Sheng-Li Hu, Yi-Cheng Le and Ling Huang

S1. Comment

Furan-3,4-dicarboxylic acid and its esters have been used as starting materials in the synthesis of several bioactive natural products and several pharmacologically useful molecules, preparation of complexes with rare earth metal ions and also as a potential dienes in Diels-Alder reactions for the synthesis of several novel heterocycles (Deshpande *et al.*, 2002). The crystal structures of some furan-3,4-dicarboxylic acid diethyl esters have been reported previously (Hu & Wu, 2005; Hu *et al.*, 2005). In this paper, we report the crystal structure of the title compound, (I). In compound (I), the C1–C6 and C11–C16 phenyl rings form dihedral angles of 54.91 (14) and 20.96 (15)°, respectively with the furan ring, Fig 1. The dihedral angle between the two benzene rings is 46.89 (13)°. In the crystal structure, weak intramolecular C4—H4···O3 hydrogen bonds link the molecules into chains along the *c* axis (Table 1 and Fig. 2).

S2. Experimental

Compound (I) was synthesized according to the literature procedure (Wu *et al.*, 1997). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution at room temperature.

S3. Refinement

The C21/C22 ethyl group of an ethyl carboxylate unit is disordered over two positions with occupancies 0.56 (12)/0.44 (12). Suitable restraints were applied to the O—C and C—C distances involving the disordered atoms. The H atoms were placed in idealized positions and constrained to ride on their parent atoms,with C—H distances in the range 0.97–0.97 Å, and with U_{iso}(H) =1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for others. Each methyl group was allowed to rotate freely about its C—C bond.

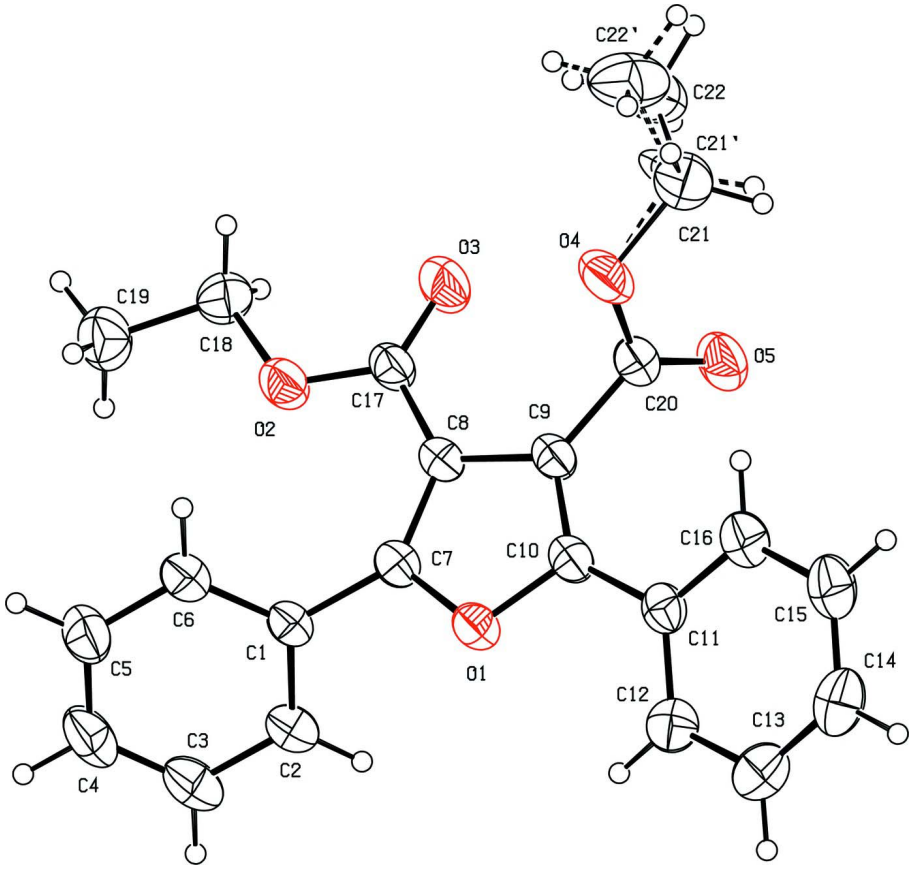


Figure 1

View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

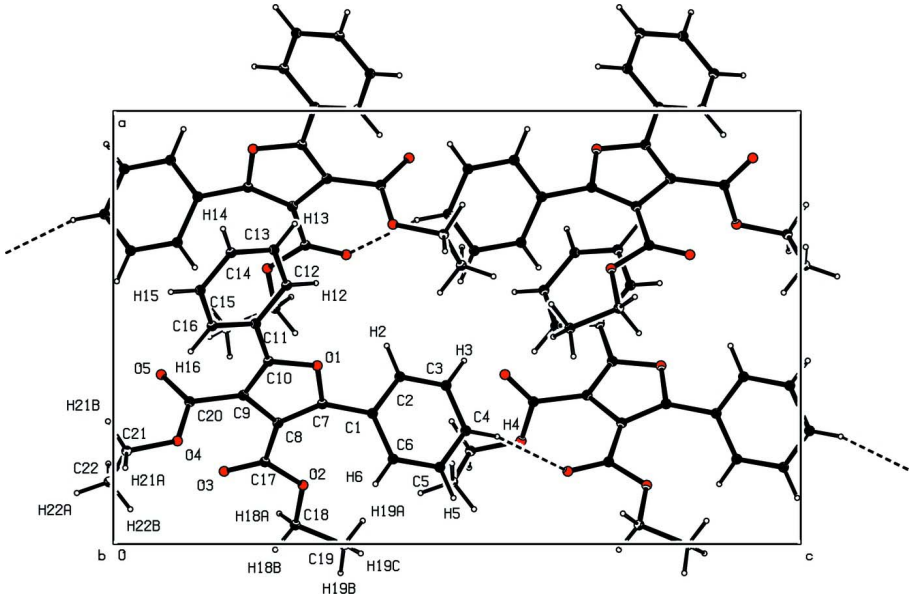


Figure 2

The molecular packing of (I), viewed along the *a* axis.

Diethyl 2,5-diphenylfuran-3,4-dicarboxylate

Crystal data

$C_{22}H_{20}O_5$
M_r = 364.38
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 11.9535 (8) Å
b = 17.0116 (12) Å
c = 18.9219 (14) Å
V = 3847.7 (5) Å^3
Z = 8
F(000) = 1536
D_x = 1.258 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 1354 reflections
θ = 2.3–16.5°
μ = 0.09 mm^{-1}
T = 293 K
Block, colorless
0.40 × 0.10 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.965, T_{max} = 0.993
19957 measured reflections
3778 independent reflections
1952 reflections with $I > 2\sigma(I)$
R_{int} = 0.081
θ_{max} = 26.0°, θ_{min} = 2.2°
h = −14→14
k = −18→20
l = −23→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.160
S = 1.01
3778 reflections
268 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.4808P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0010 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.8016 (2)	0.14397 (15)	0.62303 (14)	0.0490 (7)	
C2	0.8864 (3)	0.17700 (17)	0.58313 (15)	0.0605 (8)	
H2	0.9579	0.1817	0.6021	0.073*	
C3	0.8659 (4)	0.2028 (2)	0.51602 (17)	0.0791 (10)	
H3	0.9234	0.2252	0.4898	0.095*	
C4	0.7618 (4)	0.1959 (2)	0.48719 (18)	0.0840 (11)	
H4	0.7483	0.2141	0.4417	0.101*	
C5	0.6774 (3)	0.1621 (2)	0.52514 (18)	0.0820 (11)	
H5	0.6067	0.1569	0.5051	0.098*	
C6	0.6963 (3)	0.13579 (18)	0.59302 (16)	0.0665 (9)	
H6	0.6387	0.1126	0.6186	0.080*	
C7	0.8238 (2)	0.11805 (15)	0.69580 (14)	0.0492 (7)	
C8	0.7797 (2)	0.13356 (15)	0.76053 (14)	0.0482 (7)	
C9	0.8438 (2)	0.08957 (16)	0.81084 (14)	0.0502 (7)	
C10	0.9221 (2)	0.04934 (16)	0.77404 (14)	0.0523 (7)	
C11	1.0088 (2)	−0.00776 (16)	0.79305 (15)	0.0527 (7)	
C12	1.0976 (3)	−0.02123 (18)	0.74782 (17)	0.0644 (8)	
H12	1.1025	0.0058	0.7052	0.077*	
C13	1.1795 (3)	−0.0752 (2)	0.7664 (2)	0.0765 (10)	
H13	1.2394	−0.0841	0.7361	0.092*	
C14	1.1728 (3)	−0.1154 (2)	0.8287 (2)	0.0823 (11)	
H14	1.2277	−0.1519	0.8404	0.099*	
C15	1.0860 (3)	−0.10230 (19)	0.87366 (19)	0.0791 (10)	
H15	1.0820	−0.1295	0.9162	0.095*	
C16	1.0039 (3)	−0.04870 (17)	0.85632 (16)	0.0664 (9)	
H16	0.9449	−0.0399	0.8873	0.080*	
C17	0.6899 (2)	0.18876 (18)	0.77946 (16)	0.0570 (8)	
C18	0.5443 (3)	0.27088 (19)	0.73529 (17)	0.0713 (9)	
H18A	0.5707	0.3181	0.7587	0.086*	
H18B	0.4872	0.2468	0.7645	0.086*	
C19	0.4984 (3)	0.2902 (2)	0.66417 (18)	0.0901 (11)	
H19A	0.5539	0.3179	0.6372	0.135*	
H19B	0.4332	0.3227	0.6694	0.135*	
H19C	0.4785	0.2426	0.6401	0.135*	
C20	0.8287 (3)	0.08891 (18)	0.88887 (16)	0.0598 (8)	
O1	0.91184 (16)	0.06707 (10)	0.70331 (9)	0.0542 (5)	
O2	0.63606 (18)	0.21673 (12)	0.72406 (10)	0.0703 (6)	
O3	0.66800 (19)	0.20603 (17)	0.83882 (12)	0.1034 (9)	
O4	0.7383 (2)	0.04851 (17)	0.90669 (11)	0.1010 (9)	
O5	0.89136 (19)	0.11776 (13)	0.93023 (11)	0.0773 (7)	
C22	0.6437 (8)	0.0896 (6)	1.0062 (4)	0.108 (3)	0.56
H22A	0.6858	0.1376	1.0073	0.163*	0.56
H22B	0.6179	0.0774	1.0530	0.163*	0.56
H22C	0.5806	0.0956	0.9753	0.163*	0.56
C21	0.7149 (11)	0.0258 (6)	0.9805 (5)	0.088 (4)	0.56

H21A	0.6762	−0.0243	0.9826	0.106*	0.56
H21B	0.7834	0.0223	1.0078	0.106*	0.56
C21′	0.7110 (15)	0.0659 (11)	0.9813 (5)	0.107 (6)	0.44
H21C	0.7015	0.1220	0.9882	0.128*	0.44
H21D	0.7700	0.0475	1.0123	0.128*	0.44
C22′	0.6045 (8)	0.0235 (7)	0.9961 (5)	0.116 (4)	0.44
H22D	0.5445	0.0479	0.9705	0.173*	0.44
H22E	0.5888	0.0255	1.0458	0.173*	0.44
H22F	0.6115	−0.0304	0.9815	0.173*	0.44

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0605 (18)	0.0467 (16)	0.0398 (16)	0.0013 (14)	0.0019 (14)	−0.0015 (13)
C2	0.072 (2)	0.0598 (19)	0.0498 (19)	−0.0033 (16)	0.0079 (16)	0.0032 (15)
C3	0.106 (3)	0.078 (2)	0.053 (2)	−0.002 (2)	0.013 (2)	0.0133 (17)
C4	0.124 (3)	0.081 (3)	0.047 (2)	0.024 (2)	−0.003 (2)	0.0108 (18)
C5	0.088 (3)	0.105 (3)	0.053 (2)	0.015 (2)	−0.012 (2)	−0.006 (2)
C6	0.068 (2)	0.083 (2)	0.0479 (19)	−0.0009 (17)	0.0025 (16)	−0.0035 (17)
C7	0.0581 (18)	0.0435 (16)	0.0458 (18)	−0.0024 (14)	−0.0003 (14)	0.0012 (13)
C8	0.0561 (18)	0.0496 (17)	0.0389 (16)	−0.0037 (14)	0.0023 (14)	0.0003 (13)
C9	0.0573 (17)	0.0552 (17)	0.0380 (16)	−0.0107 (15)	−0.0010 (14)	0.0001 (13)
C10	0.0598 (19)	0.0561 (19)	0.0411 (17)	−0.0076 (16)	−0.0020 (15)	0.0014 (14)
C11	0.0583 (19)	0.0511 (17)	0.0486 (18)	−0.0080 (15)	−0.0070 (15)	−0.0027 (14)
C12	0.065 (2)	0.059 (2)	0.069 (2)	−0.0058 (17)	−0.0023 (18)	0.0043 (16)
C13	0.063 (2)	0.073 (2)	0.093 (3)	−0.0019 (19)	−0.0025 (19)	−0.004 (2)
C14	0.077 (3)	0.070 (2)	0.100 (3)	0.0083 (19)	−0.024 (2)	0.002 (2)
C15	0.093 (3)	0.075 (2)	0.069 (2)	0.011 (2)	−0.018 (2)	0.0121 (18)
C16	0.078 (2)	0.064 (2)	0.057 (2)	0.0032 (18)	−0.0064 (17)	0.0031 (16)
C17	0.062 (2)	0.070 (2)	0.0397 (18)	−0.0095 (16)	−0.0018 (15)	−0.0039 (15)
C18	0.068 (2)	0.074 (2)	0.072 (2)	0.0157 (18)	0.0038 (18)	−0.0095 (17)
C19	0.099 (3)	0.096 (3)	0.075 (3)	0.025 (2)	−0.011 (2)	0.002 (2)
C20	0.064 (2)	0.070 (2)	0.0456 (19)	−0.0010 (17)	−0.0030 (17)	0.0004 (15)
O1	0.0654 (13)	0.0538 (12)	0.0434 (12)	0.0046 (10)	0.0026 (9)	0.0025 (9)
O2	0.0822 (15)	0.0820 (15)	0.0465 (13)	0.0269 (12)	0.0012 (11)	−0.0039 (11)
O3	0.0985 (18)	0.164 (3)	0.0481 (15)	0.0494 (17)	−0.0063 (13)	−0.0242 (15)
O4	0.0833 (17)	0.174 (3)	0.0456 (14)	−0.0452 (18)	0.0023 (12)	0.0138 (15)
O5	0.0858 (16)	0.0948 (17)	0.0513 (14)	−0.0113 (13)	−0.0116 (12)	−0.0124 (12)
C22	0.122 (8)	0.127 (8)	0.076 (6)	0.025 (6)	0.022 (5)	0.004 (5)
C21	0.081 (7)	0.103 (9)	0.081 (7)	−0.008 (5)	0.003 (5)	0.018 (5)
C21′	0.121 (12)	0.162 (17)	0.036 (6)	−0.034 (12)	0.029 (6)	−0.015 (8)
C22′	0.119 (9)	0.105 (9)	0.123 (9)	−0.006 (7)	0.049 (7)	0.033 (7)

Geometric parameters (Å, º)

C1—C2	1.384 (4)	C15—C16	1.379 (4)
C1—C6	1.387 (4)	C15—H15	0.9300
C1—C7	1.470 (4)	C16—H16	0.9300

C2—C3	1.366 (4)	C17—O3	1.190 (3)
C2—H2	0.9300	C17—O2	1.319 (3)
C3—C4	1.364 (5)	C18—O2	1.448 (3)
C3—H3	0.9300	C18—C19	1.491 (4)
C4—C5	1.365 (5)	C18—H18A	0.9700
C4—H4	0.9300	C18—H18B	0.9700
C5—C6	1.379 (4)	C19—H19A	0.9600
C5—H5	0.9300	C19—H19B	0.9600
C6—H6	0.9300	C19—H19C	0.9600
C7—C8	1.359 (3)	C20—O5	1.189 (3)
C7—O1	1.371 (3)	C20—O4	1.324 (4)
C8—C9	1.433 (4)	O4—C21	1.475 (8)
C8—C17	1.470 (4)	O4—C21′	1.479 (8)
C9—C10	1.353 (4)	C22—C21	1.462 (9)
C9—C20	1.487 (4)	C22—H22A	0.9600
C10—O1	1.378 (3)	C22—H22B	0.9600
C10—C11	1.465 (4)	C22—H22C	0.9600
C11—C12	1.383 (4)	C21—H21A	0.9700
C11—C16	1.386 (4)	C21—H21B	0.9700
C12—C13	1.387 (4)	C21′—C22′	1.490 (10)
C12—H12	0.9300	C21′—H21C	0.9700
C13—C14	1.365 (5)	C21′—H21D	0.9700
C13—H13	0.9300	C22′—H22D	0.9600
C14—C15	1.360 (5)	C22′—H22E	0.9600
C14—H14	0.9300	C22′—H22F	0.9600

C2—C1—C6	118.8 (3)	C15—C16—C11	120.5 (3)
C2—C1—C7	120.0 (3)	C15—C16—H16	119.7
C6—C1—C7	121.2 (3)	C11—C16—H16	119.7
C3—C2—C1	120.4 (3)	O3—C17—O2	123.6 (3)
C3—C2—H2	119.8	O3—C17—C8	123.2 (3)
C1—C2—H2	119.8	O2—C17—C8	113.1 (2)
C4—C3—C2	120.5 (3)	O2—C18—C19	106.7 (3)
C4—C3—H3	119.7	O2—C18—H18A	110.4
C2—C3—H3	119.7	C19—C18—H18A	110.4
C3—C4—C5	120.0 (3)	O2—C18—H18B	110.4
C3—C4—H4	120.0	C19—C18—H18B	110.4
C5—C4—H4	120.0	H18A—C18—H18B	108.6
C4—C5—C6	120.4 (3)	C18—C19—H19A	109.5
C4—C5—H5	119.8	C18—C19—H19B	109.5
C6—C5—H5	119.8	H19A—C19—H19B	109.5
C5—C6—C1	119.8 (3)	C18—C19—H19C	109.5
C5—C6—H6	120.1	H19A—C19—H19C	109.5
C1—C6—H6	120.1	H19B—C19—H19C	109.5
C8—C7—O1	109.1 (2)	O5—C20—O4	124.1 (3)
C8—C7—C1	135.7 (3)	O5—C20—C9	125.0 (3)
O1—C7—C1	115.2 (2)	O4—C20—C9	110.8 (3)
C7—C8—C9	106.8 (2)	C7—O1—C10	107.9 (2)

C7—C8—C17	128.8 (3)	C17—O2—C18	118.8 (2)
C9—C8—C17	124.2 (2)	C20—O4—C21	122.1 (6)
C10—C9—C8	107.0 (2)	C20—O4—C21′	108.6 (5)
C10—C9—C20	126.2 (3)	C21—O4—C21′	26.8 (8)
C8—C9—C20	126.8 (3)	C22—C21—O4	103.4 (7)
C9—C10—O1	109.1 (2)	C22—C21—H21A	111.1
C9—C10—C11	134.3 (3)	O4—C21—H21A	111.1
O1—C10—C11	116.5 (2)	C22—C21—H21B	111.1
C12—C11—C16	118.9 (3)	O4—C21—H21B	111.1
C12—C11—C10	120.1 (3)	H21A—C21—H21B	109.1
C16—C11—C10	121.0 (3)	O4—C21′—C22′	105.7 (8)
C11—C12—C13	119.7 (3)	O4—C21′—H21C	110.6
C11—C12—H12	120.2	C22′—C21′—H21C	110.6
C13—C12—H12	120.2	O4—C21′—H21D	110.6
C14—C13—C12	120.6 (3)	C22′—C21′—H21D	110.6
C14—C13—H13	119.7	H21C—C21′—H21D	108.7
C12—C13—H13	119.7	C21′—C22′—H22D	109.5
C15—C14—C13	120.2 (3)	C21′—C22′—H22E	109.5
C15—C14—H14	119.9	H22D—C22′—H22E	109.5
C13—C14—H14	119.9	C21′—C22′—H22F	109.5
C14—C15—C16	120.1 (3)	H22D—C22′—H22F	109.5
C14—C15—H15	119.9	H22E—C22′—H22F	109.5
C16—C15—H15	119.9		

C6—C1—C2—C3	1.6 (4)	C11—C12—C13—C14	0.3 (5)
C7—C1—C2—C3	−178.6 (3)	C12—C13—C14—C15	−0.6 (5)
C1—C2—C3—C4	−0.4 (5)	C13—C14—C15—C16	0.5 (5)
C2—C3—C4—C5	−0.8 (5)	C14—C15—C16—C11	0.0 (5)
C3—C4—C5—C6	0.8 (5)	C12—C11—C16—C15	−0.4 (4)
C4—C5—C6—C1	0.4 (5)	C10—C11—C16—C15	180.0 (3)
C2—C1—C6—C5	−1.5 (4)	C7—C8—C17—O3	−169.1 (3)
C7—C1—C6—C5	178.7 (3)	C9—C8—C17—O3	5.6 (5)
C2—C1—C7—C8	124.2 (4)	C7—C8—C17—O2	11.2 (4)
C6—C1—C7—C8	−56.0 (5)	C9—C8—C17—O2	−174.0 (2)
C2—C1—C7—O1	−53.9 (3)	C10—C9—C20—O5	69.8 (4)
C6—C1—C7—O1	125.9 (3)	C8—C9—C20—O5	−109.1 (4)
O1—C7—C8—C9	−0.1 (3)	C10—C9—C20—O4	−107.2 (3)
C1—C7—C8—C9	−178.2 (3)	C8—C9—C20—O4	73.8 (4)
O1—C7—C8—C17	175.3 (2)	C8—C7—O1—C10	0.9 (3)
C1—C7—C8—C17	−2.8 (5)	C1—C7—O1—C10	179.4 (2)
C7—C8—C9—C10	−0.6 (3)	C9—C10—O1—C7	−1.3 (3)
C17—C8—C9—C10	−176.3 (2)	C11—C10—O1—C7	177.2 (2)
C7—C8—C9—C20	178.5 (3)	O3—C17—O2—C18	−0.6 (5)
C17—C8—C9—C20	2.8 (4)	C8—C17—O2—C18	179.0 (2)
C8—C9—C10—O1	1.2 (3)	C19—C18—O2—C17	−178.4 (3)
C20—C9—C10—O1	−178.0 (3)	O5—C20—O4—C21	−8.8 (6)
C8—C9—C10—C11	−176.9 (3)	C9—C20—O4—C21	168.3 (5)
C20—C9—C10—C11	4.0 (5)	O5—C20—O4—C21′	17.0 (11)

C9—C10—C11—C12	−160.6 (3)	C9—C20—O4—C21′	−166.0 (10)
O1—C10—C11—C12	21.5 (4)	C20—O4—C21—C22	93.6 (10)
C9—C10—C11—C16	19.1 (5)	C21′—O4—C21—C22	27.6 (18)
O1—C10—C11—C16	−158.9 (3)	C20—O4—C21′—C22′	175.9 (12)
C16—C11—C12—C13	0.2 (4)	C21—O4—C21′—C22′	−58.8 (17)
C10—C11—C12—C13	179.8 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O3	0.93	2.56	3.453 (4)	161