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Head-to-tail square-shaped cyclic hydrogen bonds leading to dimeric aggregates: 1,8-dibenzoyl-2,7-dihydroxynaphthalene and a comparison with its analogous benzoylnaphthalene

Saki Mohri,[a] Sayaka Yoshiwaka,[a] Katsuhiro Isozaki,[b] Noriyuki Yonezawa[a] and Akiko Okamoto[a]*

[a]Department of Organic and Polymer Materials Chemistry, Tokyo University of Agriculture & Technology (TUAT), Koganei, Tokyo 184-8588, Japan, and [b]International Research Center for Elements Science, Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan
Correspondence e-mail: aokamoto@cc.tuat.ac.jp

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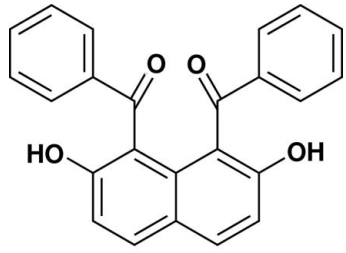
The title compound, $C_{24}H_{16}O_4$, crystallized with two independent molecules in the asymmetric unit. Both carbonyl groups in these molecules form intramolecular O—H···O=C hydrogen bonds with neighbouring hydroxy groups, affording six-membered cyclic structures. In the crystal, dimeric aggregates arise from two intermolecular O—H···O=C hydrogen bonds between both independent molecules, forming head-to-tail square-shaped cyclic ···O···H···O···H··· hydrogen bonds. These dimeric aggregates are connected into layers in the *bc* plane by intermolecular (naphthalene)C—H···O=C interactions. On the other hand, the analogous compound bearing methoxy groups at the 2- and 7-positions of the naphthalene ring, namely 1,8-dibenzoyl-2,7-dimethoxynaphthalene [Nakaema *et al.* (2008). *Acta Cryst.* E**64**, o807], forms a three-dimensional molecular network *via* C—H···O=C and π–π interactions between the benzoyl groups. These results show that the intramolecular O—H···O=C hydrogen bonds in the title compound control the orientations of the benzoyl groups and thus promote the formation of the cyclic intermolecular O—H···O=C interactions involving the same donor and acceptor groups in pairs of molecules.

Keywords: crystal structure; cyclic hydrogen bonds; 1,8-dibenzoyl-2,7-dihydroxynaphthalene; O—H···O=C hydrogen bonds.

1. Introduction

Molecules with noncoplanar aromatic rings, such as binaphthyl and biphenyl compounds, have been in the limelight because of their unique spatial shapes affording characteristic properties and various applications, *e.g.* optical and electronic properties, and the applications based on the properties for optically active polymers and catalysts, organic fluorescent dyes and light-emitting diodes (Alfonso *et al.*, 2007; Gasparrini *et al.*, 2008; Zhang *et al.*, 2011). *Peri*-substituted naphthalenes have also received much attention as characteristic structured aromatic core compounds for a variety of functional materials (Mei *et al.*, 2006; Shinamura *et al.*, 2010; Jiang *et al.*, 2010). Therefore, structural analyses have been actively performed (Gore *et al.*, 1980; Cohen *et al.*, 2004; Jing *et al.*, 2005). Recently, we have revealed that diaroylation at the 1- and 8-positions of naphthalene proceeds smoothly (Okamoto & Yonezawa, 2009; Okamoto *et al.*, 2011).



(I)

According to X-ray crystal structure studies, the resulting 1,8-diaroylated naphthalene derivatives, such as 1,8-dibenzoyl-2,7-dimethoxynaphthalene (Nakaema *et al.*, 2008), have a noncoplanar organization of the aromatic rings. Herein, the X-ray crystal structure of the title compound, 1,8-dibenzoyl-2,7-dihydroxynaphthalene, (I), is reported. The compound has hydroxy groups at the 2- and 7-positions of the naphthalene ring in place of the alkoxy groups of the above-mentioned compound. We report the single-crystal structure and the molecular packing of (I), and discuss the structure-determining factors through comparison with the analogous dimethoxy molecule.

2. Experimental

2.1. Synthesis and crystallization

To the solution of 1,8-dibenzoyl-2,7-diethoxynaphthalene (5.0 mmol, 2.1 g) and toluene (25 ml), $AlCl_3$ (25.0 mmol, 3.3 g) was added and the resulting solution stirred at 363 K for 1 h. The reaction mixture was poured into 2 *M* aqueous HCl and the mixture was extracted with $CHCl_3$. The combined extracts were washed with brine and dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure to give a cake of the crude material. The crude product was purified by recrystallization from chloroform and methanol (4:1 *v*/*v*). Single crystals suitable for X-ray diffraction were obtained by crystallization from toluene (48% isolated yield; m.p. 501.4–502.1 K). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.13 (2H, *d*, *J* = 8.9 Hz), 7.19 [4H, *d* (broad), *J* = 7.6 Hz], 7.30 (4H *t*, *J* = 7.6 Hz), 7.50 (2H, *t*, *J* = 7.6 Hz), 7.92 (2H, *d*, *J* = 8.9 Hz), 11.24 (2H, *s*). ^{13}C NMR (75 MHz, $CDCl_3$): δ 115.39, 117.13, 122.16, 128.17, 131.61, 132.82, 133.00, 136.38, 136.49, 161.99, 197.26. IR (KBr, cm^{-1}): 3441 (O—H), 1661 (C=O), 1595, 1513, 1451 (Ar,

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Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{16}O_4$
M_r	368.37
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	8.502 (3), 15.446 (5), 27.071 (10)
β (°)	96.226 (4)
V (Å^3)	3534 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.40 × 0.15 × 0.15
Data collection	
Diffractometer	Rigaku Saturn70 diffractometer
Absorption correction	Numerical (*NUMABS*; Higashi, 1999)
T_{min}, T_{max}	0.963, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23077, 6159, 4828
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.118, 1.09
No. of reflections	6159
No. of parameters	509
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.18

Computer programs: *CrystalClear* (Rigaku/MSC, 2006), *Il Milione* (Burla *et al.*, 2007), *SHELXL97* (Sheldrick, 2008) and *ORTEPIII* (Burnett & Johnson, 1996).

naphthalene). Elemental analysis calculated for $C_{24}H_{16}O_4$: C 78.25, H 4.38%; found: C 78.10, H 4.41%.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms could be located in difference Fourier maps, but were subsequently refined in optimized positions as riding atoms, with O—H = 0.84 Å and U_{iso}(H) = 1.5U_{eq}(O) for hydroxy H atoms, and C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms.

3. Results and discussion

There are two independent molecules (*A* and *B*) in the asymmetric unit of (I) which display intramolecular O—H···O=C hydrogen bonds between the hydroxy and carbonyl groups (Fig. 1). Each independent molecule has essentially the same noncoplanar organization of aromatic rings, as indicated by a least-squares fit of the two molecules (r.m.s. deviation = 0.003 Å). The dihedral angles between the planes of the benzene rings are 9.10 (11) (for molecule *A*) and 2.37 (10)° (for molecule *B*), and those between the planes of the benzene rings and the naphthalene system are 62.77 (10) and 56.43 (8)° (for molecule *A*), and 54.68 (8) and 54.74 (9)° (for molecule *B*).

In the crystal packing, the molecules are related only by noncrystallographic centres of inversion. Independent molecules *A* and *B* are connected into a supramolecular dimer *via* head-to-tail square-shaped cyclic hydrogen bonds involving two intermolecular C=O···H hydrogen bonds between the hydroxy H atoms and the carbonyl O atoms (Table 2 and

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*A*···O1	0.84	1.91	2.631 (2)	143
O4—H4*A*···O2	0.84	1.90	2.616 (2)	142
O4—H4*A*···O5^{i}	0.84	2.39	2.989 (2)	129
O7—H7*A*···O2^{ii}	0.84	2.26	2.843 (2)	126
O7—H7*A*···O5	0.84	1.92	2.635 (2)	143
O8—H8*A*···O6	0.84	1.83	2.557 (2)	144
C3—H3···O6	0.95	2.59	3.542 (3)	178
C21—H21···O4^{iii}	0.95	2.57	3.401 (3)	146

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

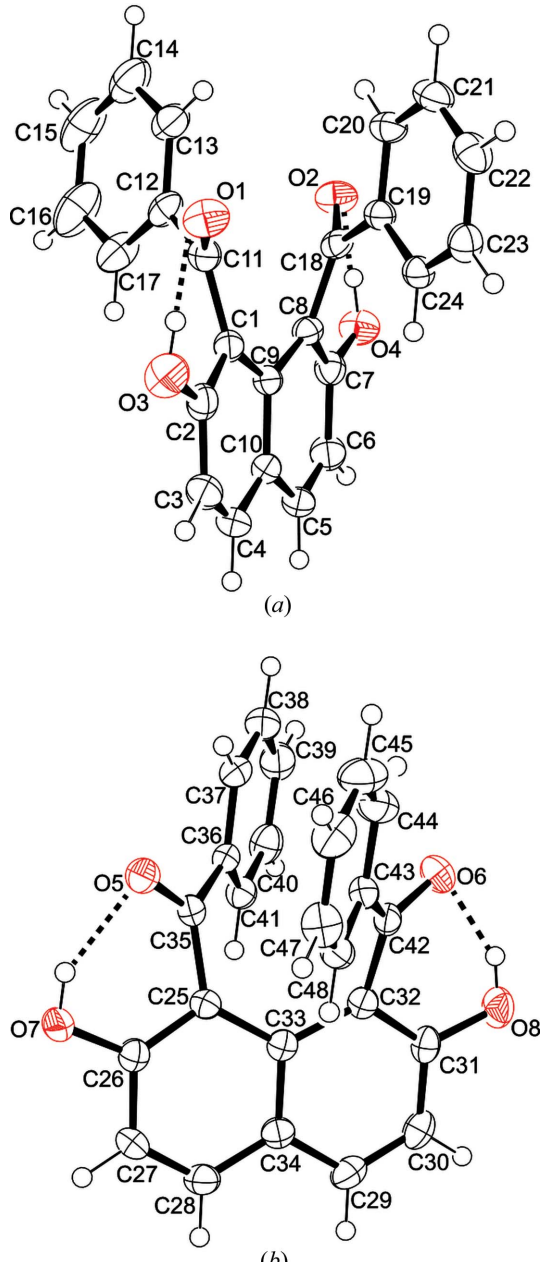

Figure 1
The molecular structure of the title compound, showing (*a*) molecule *A* and (*b*) molecule *B*, together with the atom-numbering schemes. Displacement ellipsoids are drawn at the 50% probability level.

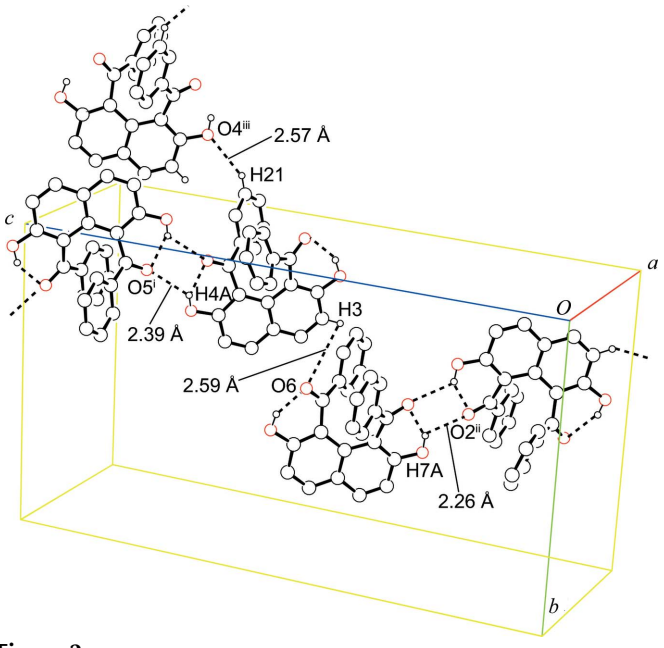

Figure 2
A partial view of the crystal packing of the title compound, showing the intermolecular O—H···O and C—H···O hydrogen bonds (see Table 1 for details). [Symmetry codes: (i) $x-1, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x+1, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.]

Fig. 2). The dimeric aggregates are arranged in layers in the *bc* plane by C—H···O═C hydrogen bonds between the naphthalene rings and the carbonyl groups not involved in the formation of the square-shaped cyclic hydrogen bonds (C3—H3···O6; Table 2 and Fig. 2). Intermolecular C—H···O interactions between the benzene rings of the benzoyl groups and the hydroxy groups (C21—H21···O4^{iii}; Table 2 and Fig. 2) contribute to the stability of the molecular alignments along the *b* axis.

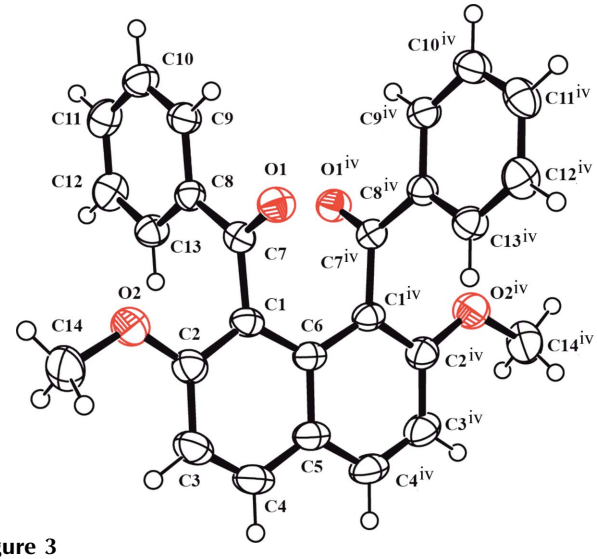

Figure 3
The molecular structure of 1,8-dibenzoyl-2,7-dimethoxynaphthalene (Nakaema *et al.*, 2008), showing the atom-labelling scheme and with displacement ellipsoids drawn at the 50% probability level [symmetry code: (iv) $-x, y, -z+\frac{1}{2}$].

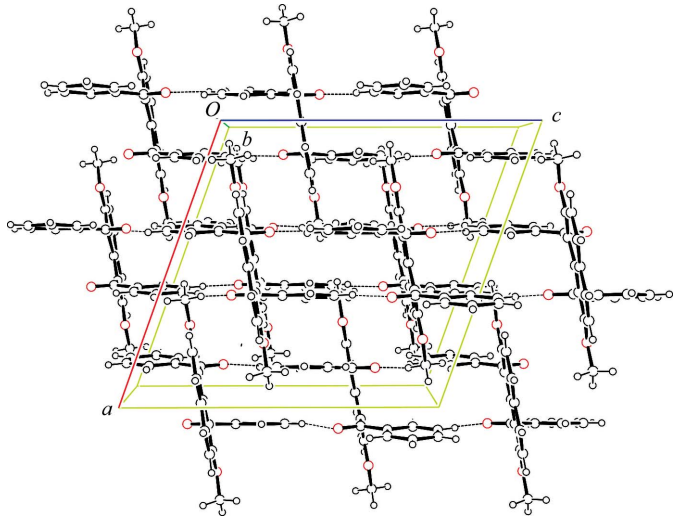

Figure 4
A partial packing diagram of compound (II), viewed down the *b* axis. The dashed lines indicate hydrogen bonds.

Several years ago, we published the crystal structure of a 1,8-dibenzoylnaphthalene analogue bearing methoxy groups at the 2- and 7-positions, namely 1,8-dibenzoyl-2,7-dimethoxynaphthalene, (II) (Nakaema *et al.*, 2008; Fig. 3). The molecules are located on twofold rotation axes. The molecular packing differs strikingly from that of (I). In the crystal of (II), a three-dimensional molecular network is formed by benzene and methyl C—H···O═C interactions and benzene–benzene π–π stacking interactions (Fig. 4). The dihedral angle between the planes of the benzene ring and the naphthalene system in (II) is larger than the corresponding values for (I) mentioned earlier.

The data indicate that intramolecular O—H···O═C hydrogen bonds constrain the orientations of the benzoyl groups in (I). The constrained benzoyl groups might be retarded the formation of three-dimensional molecular network through C—H···O and π–π interactions as the methoxy analogue (II). Consequently, the cyclic intermolecular O—H···O═C interactions involving the same donor and acceptor groups in pairs of molecules contribute to the stabilization of the molecular packing of (I).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG3312). Services for accessing these data are described at the back of the journal.

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supplementary materials

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Head-to-tail square-shaped cyclic hydrogen bonds leading to dimeric aggregates: 1,8-dibenzoyl-2,7-dihydroxynaphthalene and a comparison with its analogous benzoylnaphthalene

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Computing details

Data collection: *CrystalClear* (Rigaku/MSC, 2006); cell refinement: *CrystalClear* (Rigaku/MSC, 2006); data reduction: *CrystalClear* (Rigaku/MSC, 2006); program(s) used to solve structure: *Il Milione* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

1,8-Dibenzoyl-2,7-dihydroxynaphthalene

Crystal data

$C_{24}H_{16}O_4$
M_r = 368.37
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 8.502 (3) Å
b = 15.446 (5) Å
c = 27.071 (10) Å
β = 96.226 (4)°
V = 3534 (2) Å^3
Z = 8
$F(000)$ = 1536
D_x = 1.385 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71070 Å
Cell parameters from 9173 reflections
θ = 2.0–31.2°
μ = 0.09 mm^{-1}
T = 173 K
Block, colourless
0.40 × 0.15 × 0.15 mm

Data collection

Rigaku Saturn70 diffractometer
Radiation source: rotating anode
Graphite monochromator
Detector resolution: 7.314 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
T_{min} = 0.963, T_{max} = 0.986
23077 measured reflections
6159 independent reflections
4828 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 25.0°, θ_{min} = 3.0°
h = −7→10
k = −18→18
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.118
S = 1.09
6159 reflections
509 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.7407P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

Experimental. Spectroscopic data for the title compound: 1H NMR δ (300 MHz, CDCl3): 7.13 (2*H*, d, J = 8.9 Hz), 7.19 (4*H*, d, J=7.6 Hz), 7.30 (4*H*, t, J = 7.6 Hz), 7.50 (2*H*, tt, J = 7.6 Hz), 7.92 (2*H*, d, J = 8.9 Hz), 11.24(2*H*, s) p.p.m. 13 C NMR δ (75 MHz, CDCl3): 115.39, 117.13, 122.16, 128.17, 131.61, 132.82, 133.00, 136.38, 136.49, 161.99, 197.26 p.p.m. IR (KBr): 3441(–OH), 1661 (Cδb O), 1595, 1513, 1451 (Ar, naphthalene) cm-1. Elemental analysis: Calcd for C24H16O4; C 78.25, H 4.38. Found: C 78.10, H 4.41. m.p. = 501.4–502.1 K.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.59530 (16)	0.00535 (9)	0.56238 (5)	0.0397 (4)
O2	0.33352 (16)	0.08096 (8)	0.70315 (5)	0.0354 (3)
O3	0.70450 (18)	0.12871 (10)	0.50841 (5)	0.0454 (4)
H3A	0.6979	0.0774	0.5182	0.068*
O4	0.28594 (17)	0.24410 (9)	0.72288 (5)	0.0379 (4)
H4A	0.2677	0.1908	0.7248	0.057*
O5	1.16664 (16)	0.38740 (8)	0.29072 (5)	0.0343 (3)
O6	0.88873 (16)	0.33585 (9)	0.43501 (5)	0.0383 (4)
O7	1.23369 (16)	0.54805 (8)	0.26784 (5)	0.0342 (3)
H7A	1.2436	0.4940	0.2662	0.051*
O8	0.78121 (16)	0.46528 (9)	0.47975 (5)	0.0388 (4)
H8A	0.7869	0.4129	0.4717	0.058*
C1	0.5552 (2)	0.15430 (12)	0.57795 (7)	0.0261 (4)
C2	0.6448 (2)	0.18248 (13)	0.54094 (7)	0.0317 (5)
C3	0.6704 (3)	0.27101 (14)	0.53296 (8)	0.0402 (5)
H3	0.7307	0.2890	0.5072	0.048*
C4	0.6088 (3)	0.33053 (14)	0.56218 (8)	0.0403 (5)
H4	0.6211	0.3903	0.5553	0.048*
C5	0.4711 (2)	0.36949 (13)	0.63416 (8)	0.0374 (5)
H5	0.4903	0.4289	0.6281	0.045*
C6	0.3910 (2)	0.34717 (13)	0.67298 (8)	0.0375 (5)
H6	0.3509	0.3908	0.6930	0.045*
C7	0.3676 (2)	0.25929 (12)	0.68344 (7)	0.0301 (4)
C8	0.4339 (2)	0.19376 (11)	0.65670 (7)	0.0251 (4)
C9	0.5044 (2)	0.21635 (11)	0.61254 (7)	0.0262 (4)
C10	0.5268 (2)	0.30588 (12)	0.60257 (7)	0.0304 (4)
C11	0.5047 (2)	0.06209 (12)	0.57486 (7)	0.0281 (4)
C12	0.3372 (2)	0.03860 (12)	0.57922 (7)	0.0307 (4)
C13	0.3004 (3)	−0.04404 (14)	0.59417 (8)	0.0394 (5)
H13	0.3828	−0.0838	0.6043	0.047*
C14	0.1447 (3)	−0.06876 (18)	0.59444 (9)	0.0546 (7)
H14	0.1201	−0.1250	0.6055	0.066*
C15	0.0249 (3)	−0.01195 (19)	0.57867 (10)	0.0622 (8)

H15	−0.0824	−0.0291	0.5787	0.075*
C16	0.0608 (3)	0.07032 (18)	0.56283 (11)	0.0634 (8)
H16	−0.0219	0.1092	0.5515	0.076*
C17	0.2165 (3)	0.09592 (15)	0.56354 (9)	0.0452 (6)
H17	0.2410	0.1527	0.5533	0.054*
C18	0.4434 (2)	0.10713 (11)	0.68058 (7)	0.0266 (4)
C19	0.5934 (2)	0.05592 (11)	0.68426 (6)	0.0256 (4)
C20	0.5880 (2)	−0.03217 (12)	0.69564 (7)	0.0312 (4)
H20	0.4893	−0.0591	0.6992	0.037*
C21	0.7257 (3)	−0.08031 (13)	0.70180 (7)	0.0372 (5)
H21	0.7212	−0.1405	0.7088	0.045*
C22	0.8705 (3)	−0.04107 (13)	0.69773 (8)	0.0387 (5)
H22	0.9650	−0.0744	0.7018	0.046*
C23	0.8772 (2)	0.04705 (13)	0.68771 (7)	0.0342 (5)
H23	0.9764	0.0743	0.6856	0.041*
C24	0.7395 (2)	0.09493 (12)	0.68081 (7)	0.0281 (4)
H24	0.7445	0.1550	0.6736	0.034*
C25	1.0770 (2)	0.50749 (11)	0.33412 (7)	0.0239 (4)
C26	1.1526 (2)	0.56839 (12)	0.30663 (7)	0.0270 (4)
C27	1.1424 (2)	0.65782 (12)	0.31597 (7)	0.0319 (5)
H27	1.1923	0.6982	0.2963	0.038*
C28	1.0614 (2)	0.68587 (12)	0.35303 (7)	0.0320 (5)
H28	1.0491	0.7463	0.3578	0.038*
C29	0.9136 (2)	0.65890 (13)	0.42445 (7)	0.0324 (5)
H29	0.9099	0.7195	0.4301	0.039*
C30	0.8418 (2)	0.60489 (13)	0.45416 (7)	0.0329 (5)
H30	0.7822	0.6275	0.4789	0.039*
C31	0.8562 (2)	0.51460 (13)	0.44808 (7)	0.0284 (4)
C32	0.9476 (2)	0.47933 (12)	0.41317 (6)	0.0249 (4)
C33	1.0070 (2)	0.53647 (11)	0.37722 (6)	0.0236 (4)
C34	0.9944 (2)	0.62724 (12)	0.38497 (7)	0.0269 (4)
C35	1.0602 (2)	0.41899 (11)	0.31273 (7)	0.0253 (4)
C36	0.9068 (2)	0.37078 (11)	0.31184 (6)	0.0253 (4)
C37	0.9079 (2)	0.28096 (12)	0.30647 (7)	0.0311 (4)
H37	1.0052	0.2513	0.3050	0.037*
C38	0.7674 (3)	0.23492 (13)	0.30334 (8)	0.0390 (5)
H38	0.7686	0.1736	0.3006	0.047*
C39	0.6254 (3)	0.27830 (14)	0.30416 (8)	0.0409 (5)
H39	0.5290	0.2467	0.3019	0.049*
C40	0.6233 (2)	0.36775 (14)	0.30822 (7)	0.0369 (5)
H40	0.5255	0.3975	0.3082	0.044*
C41	0.7638 (2)	0.41366 (12)	0.31236 (7)	0.0291 (4)
H41	0.7623	0.4749	0.3156	0.035*
C42	0.9873 (2)	0.38596 (12)	0.41975 (7)	0.0272 (4)
C43	1.1500 (2)	0.35211 (12)	0.41585 (7)	0.0267 (4)
C44	1.1717 (3)	0.26267 (13)	0.41421 (8)	0.0389 (5)
H44	1.0824	0.2254	0.4128	0.047*
C45	1.3211 (3)	0.22773 (14)	0.41467 (9)	0.0474 (6)
H45	1.3345	0.1668	0.4132	0.057*

C46	1.4513 (3)	0.28168 (15)	0.41724 (8)	0.0431 (5)
H46	1.5543	0.2579	0.4172	0.052*
C47	1.4317 (2)	0.37000 (14)	0.41985 (8)	0.0384 (5)
H47	1.5216	0.4069	0.4221	0.046*
C48	1.2822 (2)	0.40531 (12)	0.41925 (7)	0.0300 (4)
H48	1.2698	0.4663	0.4212	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0404 (8)	0.0342 (8)	0.0473 (9)	0.0026 (7)	0.0166 (7)	−0.0063 (7)
O2	0.0376 (8)	0.0319 (8)	0.0399 (8)	−0.0025 (6)	0.0186 (7)	0.0004 (6)
O3	0.0493 (9)	0.0543 (10)	0.0355 (8)	−0.0099 (8)	0.0185 (7)	−0.0065 (7)
O4	0.0443 (9)	0.0315 (8)	0.0401 (8)	0.0052 (7)	0.0137 (7)	−0.0053 (7)
O5	0.0375 (8)	0.0308 (8)	0.0373 (8)	0.0012 (6)	0.0161 (7)	−0.0012 (6)
O6	0.0404 (8)	0.0361 (8)	0.0402 (8)	−0.0111 (7)	0.0132 (7)	0.0051 (7)
O7	0.0421 (8)	0.0287 (7)	0.0347 (8)	−0.0034 (6)	0.0170 (6)	0.0011 (6)
O8	0.0374 (8)	0.0478 (9)	0.0336 (8)	−0.0054 (7)	0.0153 (6)	0.0011 (7)
C1	0.0256 (10)	0.0285 (10)	0.0239 (9)	−0.0021 (8)	0.0016 (8)	0.0009 (8)
C2	0.0307 (10)	0.0401 (12)	0.0242 (10)	−0.0066 (9)	0.0022 (8)	−0.0001 (9)
C3	0.0469 (13)	0.0453 (13)	0.0285 (11)	−0.0149 (10)	0.0050 (10)	0.0080 (10)
C4	0.0502 (13)	0.0329 (12)	0.0357 (12)	−0.0131 (10)	−0.0050 (10)	0.0111 (10)
C5	0.0480 (13)	0.0216 (10)	0.0397 (12)	−0.0003 (9)	−0.0093 (10)	0.0038 (9)
C6	0.0468 (13)	0.0255 (11)	0.0389 (12)	0.0077 (9)	−0.0018 (10)	−0.0049 (9)
C7	0.0294 (10)	0.0311 (11)	0.0293 (10)	0.0032 (8)	0.0012 (8)	−0.0011 (8)
C8	0.0254 (9)	0.0217 (9)	0.0282 (10)	0.0000 (8)	0.0025 (8)	−0.0009 (8)
C9	0.0245 (9)	0.0244 (10)	0.0284 (10)	−0.0010 (8)	−0.0021 (8)	0.0029 (8)
C10	0.0340 (11)	0.0254 (10)	0.0297 (10)	−0.0032 (8)	−0.0057 (9)	0.0020 (8)
C11	0.0325 (11)	0.0284 (10)	0.0241 (10)	0.0006 (9)	0.0066 (8)	−0.0012 (8)
C12	0.0331 (11)	0.0311 (11)	0.0289 (10)	−0.0048 (9)	0.0076 (8)	−0.0112 (9)
C13	0.0475 (13)	0.0382 (12)	0.0333 (11)	−0.0131 (10)	0.0079 (10)	−0.0061 (9)
C14	0.0574 (16)	0.0649 (17)	0.0429 (14)	−0.0318 (14)	0.0114 (12)	−0.0089 (12)
C15	0.0408 (14)	0.086 (2)	0.0621 (17)	−0.0305 (15)	0.0159 (13)	−0.0271 (15)
C16	0.0314 (13)	0.0724 (19)	0.085 (2)	−0.0024 (12)	0.0013 (13)	−0.0304 (16)
C17	0.0357 (12)	0.0396 (13)	0.0596 (15)	−0.0046 (10)	0.0021 (11)	−0.0127 (11)
C18	0.0322 (10)	0.0234 (10)	0.0249 (10)	−0.0032 (8)	0.0061 (8)	−0.0060 (8)
C19	0.0341 (10)	0.0236 (10)	0.0197 (9)	−0.0007 (8)	0.0058 (8)	−0.0008 (7)
C20	0.0390 (11)	0.0259 (10)	0.0297 (10)	−0.0018 (9)	0.0090 (9)	0.0017 (8)
C21	0.0522 (14)	0.0248 (10)	0.0350 (11)	0.0057 (10)	0.0065 (10)	0.0043 (9)
C22	0.0414 (12)	0.0375 (12)	0.0369 (12)	0.0125 (10)	0.0034 (10)	0.0018 (10)
C23	0.0313 (11)	0.0406 (12)	0.0306 (11)	−0.0017 (9)	0.0032 (9)	0.0001 (9)
C24	0.0340 (11)	0.0270 (10)	0.0233 (10)	−0.0006 (8)	0.0036 (8)	0.0002 (8)
C25	0.0232 (9)	0.0229 (9)	0.0257 (9)	−0.0006 (7)	0.0031 (8)	0.0002 (8)
C26	0.0270 (10)	0.0288 (10)	0.0255 (10)	−0.0001 (8)	0.0047 (8)	0.0000 (8)
C27	0.0390 (11)	0.0249 (10)	0.0326 (11)	−0.0068 (9)	0.0074 (9)	0.0034 (8)
C28	0.0383 (11)	0.0236 (10)	0.0337 (11)	−0.0003 (8)	0.0024 (9)	−0.0013 (8)
C29	0.0353 (11)	0.0313 (11)	0.0302 (10)	0.0058 (9)	0.0010 (9)	−0.0065 (9)
C30	0.0291 (10)	0.0433 (12)	0.0269 (10)	0.0052 (9)	0.0059 (9)	−0.0053 (9)
C31	0.0235 (10)	0.0389 (12)	0.0227 (9)	−0.0020 (8)	0.0021 (8)	0.0008 (8)
C32	0.0218 (9)	0.0284 (10)	0.0247 (9)	−0.0020 (8)	0.0026 (8)	−0.0010 (8)

C33	0.0199 (9)	0.0269 (10)	0.0235 (9)	−0.0013 (8)	0.0003 (7)	−0.0006 (8)
C34	0.0254 (10)	0.0269 (10)	0.0280 (10)	0.0000 (8)	0.0014 (8)	−0.0016 (8)
C35	0.0299 (10)	0.0245 (10)	0.0219 (9)	0.0003 (8)	0.0051 (8)	0.0028 (8)
C36	0.0315 (10)	0.0248 (10)	0.0201 (9)	−0.0031 (8)	0.0048 (8)	−0.0017 (8)
C37	0.0376 (11)	0.0290 (10)	0.0272 (10)	−0.0035 (9)	0.0056 (9)	−0.0045 (8)
C38	0.0509 (14)	0.0320 (11)	0.0346 (11)	−0.0110 (10)	0.0067 (10)	−0.0033 (9)
C39	0.0427 (13)	0.0467 (13)	0.0327 (11)	−0.0183 (10)	0.0008 (10)	−0.0042 (10)
C40	0.0311 (11)	0.0493 (13)	0.0301 (11)	−0.0018 (10)	0.0028 (9)	−0.0019 (10)
C41	0.0323 (11)	0.0297 (10)	0.0247 (10)	−0.0013 (8)	0.0009 (8)	0.0001 (8)
C42	0.0321 (10)	0.0302 (10)	0.0196 (9)	−0.0077 (8)	0.0041 (8)	−0.0009 (8)
C43	0.0317 (10)	0.0259 (10)	0.0225 (9)	−0.0014 (8)	0.0024 (8)	0.0023 (8)
C44	0.0428 (13)	0.0294 (11)	0.0431 (13)	−0.0040 (9)	−0.0017 (10)	−0.0005 (9)
C45	0.0534 (15)	0.0327 (12)	0.0543 (15)	0.0080 (11)	−0.0019 (12)	−0.0057 (10)
C46	0.0385 (12)	0.0498 (14)	0.0401 (13)	0.0137 (11)	−0.0006 (10)	−0.0028 (10)
C47	0.0289 (11)	0.0469 (13)	0.0389 (12)	−0.0005 (9)	0.0011 (9)	0.0032 (10)
C48	0.0346 (11)	0.0271 (10)	0.0278 (10)	−0.0027 (8)	0.0006 (9)	0.0016 (8)

Geometric parameters (Å, º)

O1—C11	1.238 (2)	C21—H21	0.9500
O2—C18	1.238 (2)	C22—C23	1.390 (3)
O3—C2	1.349 (2)	C22—H22	0.9500
O3—H3A	0.8400	C23—C24	1.380 (3)
O4—C7	1.356 (2)	C23—H23	0.9500
O4—H4A	0.8400	C24—H24	0.9500
O5—C35	1.237 (2)	C25—C26	1.399 (3)
O6—C42	1.244 (2)	C25—C33	1.437 (2)
O7—C26	1.354 (2)	C25—C35	1.486 (2)
O7—H7A	0.8400	C26—C27	1.409 (3)
O8—C31	1.357 (2)	C27—C28	1.349 (3)
O8—H8A	0.8400	C27—H27	0.9500
C1—C2	1.392 (3)	C28—C34	1.414 (3)
C1—C9	1.439 (3)	C28—H28	0.9500
C1—C11	1.488 (3)	C29—C30	1.350 (3)
C2—C3	1.405 (3)	C29—C34	1.419 (3)
C3—C4	1.355 (3)	C29—H29	0.9500
C3—H3	0.9500	C30—C31	1.411 (3)
C4—C10	1.412 (3)	C30—H30	0.9500
C4—H4	0.9500	C31—C32	1.397 (3)
C5—C6	1.358 (3)	C32—C33	1.445 (2)
C5—C10	1.417 (3)	C32—C42	1.488 (3)
C5—H5	0.9500	C33—C34	1.424 (3)
C6—C7	1.405 (3)	C35—C36	1.500 (3)
C6—H6	0.9500	C36—C41	1.386 (3)
C7—C8	1.398 (3)	C36—C37	1.395 (3)
C8—C9	1.437 (3)	C37—C38	1.385 (3)
C8—C18	1.485 (3)	C37—H37	0.9500
C9—C10	1.426 (3)	C38—C39	1.383 (3)
C11—C12	1.487 (3)	C38—H38	0.9500
C12—C13	1.385 (3)	C39—C40	1.386 (3)

C12—C17	1.386 (3)	C39—H39	0.9500
C13—C14	1.379 (3)	C40—C41	1.383 (3)
C13—H13	0.9500	C40—H40	0.9500
C14—C15	1.377 (4)	C41—H41	0.9500
C14—H14	0.9500	C42—C43	1.493 (3)
C15—C16	1.386 (4)	C43—C48	1.387 (3)
C15—H15	0.9500	C43—C44	1.395 (3)
C16—C17	1.380 (3)	C44—C45	1.379 (3)
C16—H16	0.9500	C44—H44	0.9500
C17—H17	0.9500	C45—C46	1.381 (3)
C18—C19	1.495 (3)	C45—H45	0.9500
C19—C24	1.393 (3)	C46—C47	1.377 (3)
C19—C20	1.397 (3)	C46—H46	0.9500
C20—C21	1.381 (3)	C47—C48	1.382 (3)
C20—H20	0.9500	C47—H47	0.9500
C21—C22	1.388 (3)	C48—H48	0.9500

C2—O3—H3A	109.5	C23—C24—H24	119.7
C7—O4—H4A	109.5	C19—C24—H24	119.7
C26—O7—H7A	109.5	C26—C25—C33	118.50 (16)
C31—O8—H8A	109.5	C26—C25—C35	116.21 (16)
C2—C1—C9	119.10 (17)	C33—C25—C35	124.92 (16)
C2—C1—C11	115.86 (16)	O7—C26—C25	123.97 (17)
C9—C1—C11	124.69 (16)	O7—C26—C27	114.41 (16)
O3—C2—C1	123.45 (18)	C25—C26—C27	121.54 (17)
O3—C2—C3	115.02 (17)	C28—C27—C26	119.67 (17)
C1—C2—C3	121.41 (18)	C28—C27—H27	120.2
C4—C3—C2	119.62 (19)	C26—C27—H27	120.2
C4—C3—H3	120.2	C27—C28—C34	121.43 (18)
C2—C3—H3	120.2	C27—C28—H28	119.3
C3—C4—C10	121.60 (19)	C34—C28—H28	119.3
C3—C4—H4	119.2	C30—C29—C34	121.54 (18)
C10—C4—H4	119.2	C30—C29—H29	119.2
C6—C5—C10	121.30 (18)	C34—C29—H29	119.2
C6—C5—H5	119.3	C29—C30—C31	119.41 (18)
C10—C5—H5	119.4	C29—C30—H30	120.3
C5—C6—C7	119.68 (19)	C31—C30—H30	120.3
C5—C6—H6	120.2	O8—C31—C32	122.84 (18)
C7—C6—H6	120.2	O8—C31—C30	115.40 (17)
O4—C7—C8	123.51 (17)	C32—C31—C30	121.71 (17)
O4—C7—C6	114.94 (17)	C31—C32—C33	118.57 (17)
C8—C7—C6	121.41 (18)	C31—C32—C42	115.64 (16)
C7—C8—C9	118.88 (17)	C33—C32—C42	125.53 (16)
C7—C8—C18	115.65 (16)	C34—C33—C25	118.09 (16)
C9—C8—C18	124.97 (16)	C34—C33—C32	117.69 (16)
C10—C9—C8	117.98 (17)	C25—C33—C32	124.22 (16)
C10—C9—C1	117.86 (17)	C28—C34—C29	120.01 (17)
C8—C9—C1	124.16 (16)	C28—C34—C33	119.92 (17)
C4—C10—C5	120.37 (18)	C29—C34—C33	120.06 (17)

C4—C10—C9	119.71 (18)	O5—C35—C25	120.45 (16)
C5—C10—C9	119.88 (18)	O5—C35—C36	118.50 (16)
O1—C11—C12	118.62 (17)	C25—C35—C36	120.63 (16)
O1—C11—C1	120.57 (17)	C41—C36—C37	119.49 (17)
C12—C11—C1	120.18 (16)	C41—C36—C35	121.66 (16)
C13—C12—C17	119.67 (19)	C37—C36—C35	118.66 (17)
C13—C12—C11	119.78 (18)	C38—C37—C36	120.10 (19)
C17—C12—C11	120.21 (18)	C38—C37—H37	119.9
C14—C13—C12	120.3 (2)	C36—C37—H37	119.9
C14—C13—H13	119.9	C39—C38—C37	119.92 (19)
C12—C13—H13	119.9	C39—C38—H38	120.0
C15—C14—C13	120.0 (2)	C37—C38—H38	120.0
C15—C14—H14	120.0	C38—C39—C40	120.19 (19)
C13—C14—H14	120.0	C38—C39—H39	119.9
C14—C15—C16	120.0 (2)	C40—C39—H39	119.9
C14—C15—H15	120.0	C41—C40—C39	119.93 (19)
C16—C15—H15	120.0	C41—C40—H40	120.0
C17—C16—C15	120.1 (2)	C39—C40—H40	120.0
C17—C16—H16	119.9	C40—C41—C36	120.32 (18)
C15—C16—H16	119.9	C40—C41—H41	119.8
C16—C17—C12	119.9 (2)	C36—C41—H41	119.8
C16—C17—H17	120.1	O6—C42—C32	119.38 (17)
C12—C17—H17	120.1	O6—C42—C43	117.92 (17)
O2—C18—C8	120.07 (17)	C32—C42—C43	122.08 (15)
O2—C18—C19	118.57 (16)	C48—C43—C44	118.68 (18)
C8—C18—C19	120.77 (16)	C48—C43—C42	122.54 (17)
C24—C19—C20	119.16 (17)	C44—C43—C42	118.39 (17)
C24—C19—C18	121.83 (16)	C45—C44—C43	120.8 (2)
C20—C19—C18	118.79 (17)	C45—C44—H44	119.6
C21—C20—C19	120.20 (19)	C43—C44—H44	119.6
C21—C20—H20	119.9	C44—C45—C46	119.8 (2)
C19—C20—H20	119.9	C44—C45—H45	120.1
C20—C21—C22	120.19 (19)	C46—C45—H45	120.1
C20—C21—H21	119.9	C47—C46—C45	120.0 (2)
C22—C21—H21	119.9	C47—C46—H46	120.0
C21—C22—C23	119.90 (19)	C45—C46—H46	120.0
C21—C22—H22	120.0	C46—C47—C48	120.4 (2)
C23—C22—H22	120.0	C46—C47—H47	119.8
C24—C23—C22	119.95 (19)	C48—C47—H47	119.8
C24—C23—H23	120.0	C47—C48—C43	120.31 (19)
C22—C23—H23	120.0	C47—C48—H48	119.8
C23—C24—C19	120.56 (18)	C43—C48—H48	119.8
C9—C1—C2—O3	176.55 (17)	C33—C25—C26—O7	174.45 (16)
C11—C1—C2—O3	−9.9 (3)	C35—C25—C26—O7	−12.2 (3)
C9—C1—C2—C3	−7.7 (3)	C33—C25—C26—C27	−9.1 (3)
C11—C1—C2—C3	165.83 (18)	C35—C25—C26—C27	164.32 (17)
O3—C2—C3—C4	176.95 (19)	O7—C26—C27—C28	178.54 (18)
C1—C2—C3—C4	0.9 (3)	C25—C26—C27—C28	1.7 (3)

C2—C3—C4—C10	3.8 (3)	C26—C27—C28—C34	4.0 (3)
C10—C5—C6—C7	2.5 (3)	C34—C29—C30—C31	4.3 (3)
C5—C6—C7—O4	−179.88 (18)	C29—C30—C31—O8	179.54 (17)
C5—C6—C7—C8	4.2 (3)	C29—C30—C31—C32	2.3 (3)
O4—C7—C8—C9	173.87 (17)	O8—C31—C32—C33	172.72 (16)
C6—C7—C8—C9	−10.5 (3)	C30—C31—C32—C33	−10.2 (3)
O4—C7—C8—C18	−13.8 (3)	O8—C31—C32—C42	−12.8 (3)
C6—C7—C8—C18	161.77 (18)	C30—C31—C32—C42	164.26 (17)
C7—C8—C9—C10	10.1 (3)	C26—C25—C33—C34	10.5 (3)
C18—C8—C9—C10	−161.39 (17)	C35—C25—C33—C34	−162.23 (17)
C7—C8—C9—C1	−170.43 (17)	C26—C25—C33—C32	−169.88 (17)
C18—C8—C9—C1	18.0 (3)	C35—C25—C33—C32	17.4 (3)
C2—C1—C9—C10	9.7 (3)	C31—C32—C33—C34	11.4 (2)
C11—C1—C9—C10	−163.18 (17)	C42—C32—C33—C34	−162.44 (17)
C2—C1—C9—C8	−169.70 (17)	C31—C32—C33—C25	−168.17 (17)
C11—C1—C9—C8	17.4 (3)	C42—C32—C33—C25	18.0 (3)
C3—C4—C10—C5	176.50 (19)	C27—C28—C34—C29	178.29 (18)
C3—C4—C10—C9	−1.5 (3)	C27—C28—C34—C33	−2.2 (3)
C6—C5—C10—C4	179.50 (19)	C30—C29—C34—C28	176.80 (18)
C6—C5—C10—C9	−2.6 (3)	C30—C29—C34—C33	−2.7 (3)
C8—C9—C10—C4	174.14 (17)	C25—C33—C34—C28	−5.1 (3)
C1—C9—C10—C4	−5.3 (3)	C32—C33—C34—C28	175.24 (17)
C8—C9—C10—C5	−3.8 (3)	C25—C33—C34—C29	174.34 (17)
C1—C9—C10—C5	176.71 (17)	C32—C33—C34—C29	−5.3 (3)
C2—C1—C11—O1	39.0 (3)	C26—C25—C35—O5	37.0 (3)
C9—C1—C11—O1	−147.85 (19)	C33—C25—C35—O5	−150.10 (18)
C2—C1—C11—C12	−131.72 (18)	C26—C25—C35—C36	−135.40 (17)
C9—C1—C11—C12	41.4 (3)	C33—C25—C35—C36	37.5 (3)
O1—C11—C12—C13	32.3 (3)	O5—C35—C36—C41	−147.62 (18)
C1—C11—C12—C13	−156.76 (17)	C25—C35—C36—C41	24.9 (3)
O1—C11—C12—C17	−141.0 (2)	O5—C35—C36—C37	27.4 (2)
C1—C11—C12—C17	29.9 (3)	C25—C35—C36—C37	−160.11 (17)
C17—C12—C13—C14	−1.3 (3)	C41—C36—C37—C38	−2.1 (3)
C11—C12—C13—C14	−174.66 (19)	C35—C36—C37—C38	−177.20 (17)
C12—C13—C14—C15	1.6 (3)	C36—C37—C38—C39	1.8 (3)
C13—C14—C15—C16	−0.4 (4)	C37—C38—C39—C40	−0.1 (3)
C14—C15—C16—C17	−1.0 (4)	C38—C39—C40—C41	−1.2 (3)
C15—C16—C17—C12	1.3 (4)	C39—C40—C41—C36	0.8 (3)
C13—C12—C17—C16	−0.1 (3)	C37—C36—C41—C40	0.8 (3)
C11—C12—C17—C16	173.2 (2)	C35—C36—C41—C40	175.74 (17)
C7—C8—C18—O2	39.3 (3)	C31—C32—C42—O6	35.6 (2)
C9—C8—C18—O2	−148.98 (18)	C33—C32—C42—O6	−150.32 (18)
C7—C8—C18—C19	−131.77 (18)	C31—C32—C42—C43	−135.17 (18)
C9—C8—C18—C19	40.0 (3)	C33—C32—C42—C43	38.9 (3)
O2—C18—C19—C24	−150.29 (18)	O6—C42—C43—C48	−153.20 (18)
C8—C18—C19—C24	20.9 (3)	C32—C42—C43—C48	17.7 (3)
O2—C18—C19—C20	24.2 (3)	O6—C42—C43—C44	19.6 (3)
C8—C18—C19—C20	−164.63 (17)	C32—C42—C43—C44	−169.47 (17)
C24—C19—C20—C21	−2.0 (3)	C48—C43—C44—C45	−1.6 (3)

C18—C19—C20—C21	−176.70 (17)	C42—C43—C44—C45	−174.72 (19)
C19—C20—C21—C22	1.3 (3)	C43—C44—C45—C46	0.6 (3)
C20—C21—C22—C23	0.4 (3)	C44—C45—C46—C47	0.7 (3)
C21—C22—C23—C24	−1.3 (3)	C45—C46—C47—C48	−0.9 (3)
C22—C23—C24—C19	0.6 (3)	C46—C47—C48—C43	−0.2 (3)
C20—C19—C24—C23	1.1 (3)	C44—C43—C48—C47	1.4 (3)
C18—C19—C24—C23	175.56 (16)	C42—C43—C48—C47	174.21 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O1	0.84	1.91	2.631 (2)	143
O4—H4*A*···O2	0.84	1.90	2.616 (2)	142
O4—H4*A*···O5^{i}	0.84	2.39	2.989 (2)	129
O7—H7*A*···O2^{ii}	0.84	2.26	2.843 (2)	126
O7—H7*A*···O5	0.84	1.92	2.635 (2)	143
O8—H8*A*···O6	0.84	1.83	2.557 (2)	144
C3—H3···O6	0.95	2.59	3.542 (3)	178
C21—H21···O4^{iii}	0.95	2.57	3.401 (3)	146

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