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5-(4-Methoxybenzoyl)-6-(4-methoxyphenyl)-3-phenyl-3,4-dihydro-2*H*-1,3-oxazine-2,4-dione

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.154
Data-to-parameter ratio = 11.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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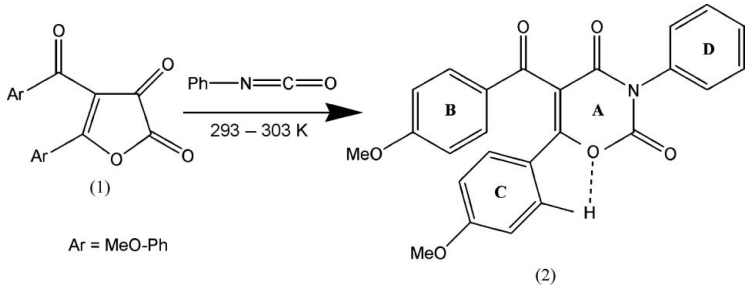
In the title compound, $C_{25}H_{19}NO_6$, the molecular structure is stabilized by intra- and intermolecular C—H···O hydrogen bonds. The intermolecular hydrogen bonds link the molecules into a herringbone-like dimer.

Comment

Oxazine derivatives have been shown to be antimicrobial agents (Bayomi *et al.*, 1985), fungicides (Player *et al.*, 1993), and also to exhibit some cytotoxic or antitumour activity (Eger & Frey, 1992; Mordarski *et al.*, 1970; Mordarski & Chylinska, 1971, 1972). In the light of this, we have synthesized and characterized the title compound, (2), and have determined its structure by X-ray analysis.



The molecular structure of (2) is illustrated in Fig. 1. The rings (*A*, *B*, *C* and *D*) are each essentially planar, with r.m.s. deviations of 0.031 (2), 0.019 (2), 0.017 (2) and 0.006 (2) Å, respectively. The dihedral angles between the rings are *A*/*B* = 64.31 (9)°, *A*/*C* = 19.49 (16)°, *A*/*D* = 82.31 (8)°, *B*/*C* = 62.22 (9)°, *B*/*D* = 61.61 (9)° and *C*/*D* = 63.73 (8)°. The bond lengths and angles are in agreement with reported literature values (Allen *et al.*, 1987).

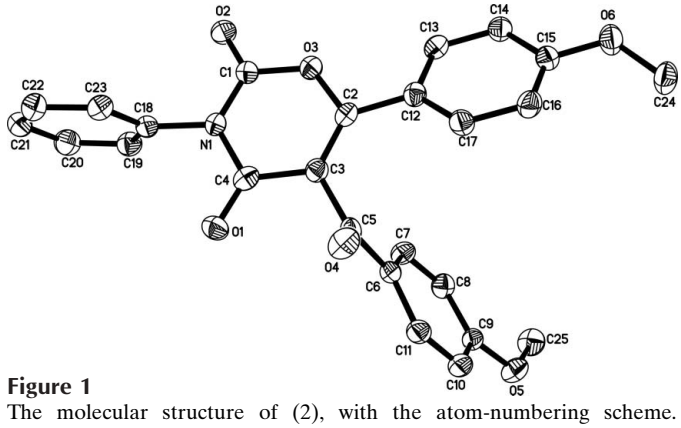


Figure 1
The molecular structure of (2), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted.

The structure is stabilized by intra- and intermolecular C—H···O hydrogen bonds (Table 1). In the crystal structure, the C—H···O intermolecular hydrogen bonds link the molecules into herringbone-like dimers which are stacked along the *b* axis (Fig. 2).

Experimental

Compound (1) was prepared from the cyclocondensation reaction that occurs between p,p′-dimethoxydibenzoylketene and oxalyl chloride (Hökelek *et al.*, 2002). Compound (2) was obtained from 1.0 g (2.96 mmol) (1) and 0.35 g (2.96 mmol) phenyl isocyanate in a 25 ml round-bottomed flask equipped with a calcium chloride tube. The mixture was heated at 393 K for 1 h. The cooled reaction mixture was triturated with dry diethyl ether and then recrystallized from *n*-butanol (yield 0.83 g, 65%, m.p. 480 K). IR (KBr, cm^{-1}): ν 1774 (C5—O4), 1690 (C4—O1), 1646 (C1—O2). ^{1}H NMR ($CDCl_3$): δ 7.95–6.81 (*m*, 13H, Ar—H), 3.84, 3.79 (*s*, 6H, CH3O); ^{13}C NMR ($CDCl_3$): δ 190.80 (C5—O4), 166.60 (C4—O1), 165.04 (C1—O2), 162.36–113.47 (C═C, aromatic and aliphatic), 57.52, 57.44 (CH_3O). Analysis calculated for $C_{40}H_{35}N_3O_5$: C 69.93, H 4.42, N 3.26%; found: C 69.80, H 4.51, N 3.14%.

Crystal data

$C_{25}H_{19}NO_6$
M_r = 429.41
Monoclinic, $P2_1/c$
a = 10.950 (2) Å
b = 5.8163 (12) Å
c = 30.968 (6) Å
β = 91.010 (4)°
V = 1972.0 (7) Å^3
Z = 4
D_x = 1.446 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1626 reflections
θ = 4.5–50.4°
μ = 0.10 mm^{-1}
T = 150 (2) K
Needle, colourless
0.32 × 0.12 × 0.12 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.967, T_{max} = 0.988
13592 measured reflections
3456 independent reflections
2069 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 25.0°
$h = -13 \rightarrow 13$
$k = -6 \rightarrow 6$
$l = -36 \rightarrow 36$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.154
S = 0.98
3456 reflections
291 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O3	0.95	2.33	2.665 (4)	100
C14—H14···O2^{i}	0.95	2.45	3.384 (4)	168
C19—H19···O1^{ii}	0.95	2.47	3.231 (4)	137
C24—H24*A*···O2^{iii}	0.98	2.52	3.225 (4)	128

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $x, y-1, z$; (iii) $-x+2, -y+2, -z$.

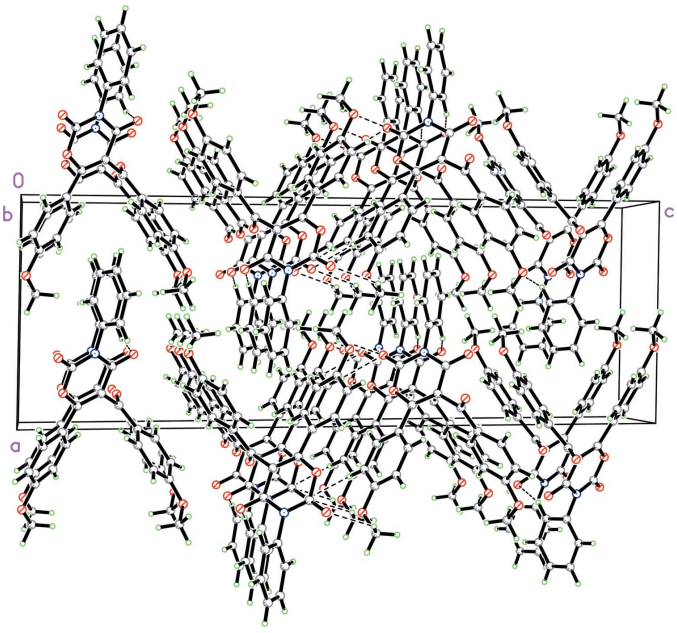


Figure 2
Packing diagram of (2); C—H···O hydrogen bonds are indicated by dashed lines.

H atoms were positioned geometrically [C—H = 0.95 (CH) and 0.98 Å (CH_3)] and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 (1.5 for methyl) times U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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supporting information

Acta Cryst. (2005). E**61**, o3910–o3911 [https://doi.org/10.1107/S1600536805034719]

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$h = -13 \rightarrow 13$
$k = -6 \rightarrow 6$
$l = -36 \rightarrow 36$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.154$
$S = 0.98$
3456 reflections
291 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
$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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}
N1	0.6735 (2)	0.7296 (4)	0.11287 (8)	0.0240 (6)
O1	0.67967 (19)	0.9619 (4)	0.17188 (7)	0.0298 (6)
O2	0.6885 (2)	0.4649 (4)	0.05875 (7)	0.0338 (6)
O3	0.83870 (19)	0.7146 (4)	0.06689 (7)	0.0289 (6)
O4	0.85931 (19)	1.3629 (4)	0.15074 (7)	0.0338 (6)
O5	1.3284 (2)	1.0185 (4)	0.25164 (7)	0.0333 (6)
O6	1.3438 (2)	1.0754 (4)	0.00958 (7)	0.0348 (6)
C1	0.7291 (3)	0.6242 (6)	0.07882 (10)	0.0267 (8)
C2	0.8967 (3)	0.8928 (5)	0.08885 (10)	0.0233 (7)
C3	0.8472 (3)	0.9798 (5)	0.12479 (10)	0.0234 (7)
C4	0.7289 (3)	0.8971 (5)	0.13949 (10)	0.0244 (7)
C5	0.9024 (3)	1.1690 (6)	0.15289 (10)	0.0238 (7)
C6	1.0064 (3)	1.1116 (5)	0.18196 (9)	0.0227 (7)
C7	1.0659 (3)	0.9017 (5)	0.18022 (10)	0.0268 (8)
H7	1.0331	0.7830	0.1624	0.032*
C8	1.1723 (3)	0.8613 (6)	0.20394 (10)	0.0276 (8)
H8	1.2121	0.7164	0.2023	0.033*
C9	1.2202 (3)	1.0334 (5)	0.22997 (10)	0.0242 (7)
C10	1.1577 (3)	1.2405 (5)	0.23456 (10)	0.0279 (8)
H10	1.1874	1.3542	0.2541	0.034*
C11	1.0519 (3)	1.2796 (5)	0.21046 (10)	0.0255 (8)
H11	1.0098	1.4215	0.2133	0.031*
C12	1.0107 (3)	0.9500 (5)	0.06736 (10)	0.0239 (7)
C13	1.0635 (3)	0.7939 (5)	0.03880 (10)	0.0259 (8)
H13	1.0234	0.6523	0.0328	0.031*
C14	1.1730 (3)	0.8423 (6)	0.01923 (10)	0.0272 (8)
H14	1.2072	0.7355	−0.0004	0.033*
C15	1.2328 (3)	1.0478 (5)	0.02836 (10)	0.0271 (8)
C16	1.1798 (3)	1.2093 (6)	0.05475 (10)	0.0288 (8)
H16	1.2188	1.3530	0.0597	0.035*
C17	1.0694 (3)	1.1609 (5)	0.07399 (10)	0.0272 (8)
H17	1.0330	1.2730	0.0920	0.033*
C18	0.5537 (3)	0.6412 (5)	0.12381 (10)	0.0247 (7)
C19	0.5450 (3)	0.4390 (5)	0.14677 (10)	0.0291 (8)
H19	0.6165	0.3620	0.1569	0.035*

C20	0.4305 (3)	0.3499 (6)	0.15487 (11)	0.0340 (8)
H20	0.4231	0.2098	0.1704	0.041*
C21	0.3272 (3)	0.4636 (6)	0.14058 (11)	0.0358 (9)
H21	0.2489	0.4007	0.1460	0.043*
C22	0.3367 (3)	0.6701 (6)	0.11821 (11)	0.0359 (9)
H22	0.2652	0.7497	0.1089	0.043*
C23	0.4507 (3)	0.7586 (6)	0.10954 (10)	0.0296 (8)
H23	0.4583	0.8984	0.0940	0.035*
C24	1.4195 (3)	1.2633 (6)	0.02427 (12)	0.0368 (9)
H24A	1.3818	1.4093	0.0156	0.055*
H24B	1.5004	1.2505	0.0114	0.055*
H24C	1.4279	1.2578	0.0558	0.055*
C25	1.4026 (3)	0.8185 (6)	0.24371 (12)	0.0362 (9)
H25A	1.3620	0.6817	0.2551	0.054*
H25B	1.4824	0.8372	0.2581	0.054*
H25C	1.4138	0.8006	0.2126	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0209 (14)	0.0267 (15)	0.0244 (15)	−0.0043 (12)	0.0004 (12)	−0.0018 (12)
O1	0.0317 (13)	0.0315 (13)	0.0263 (13)	0.0015 (10)	0.0048 (11)	−0.0048 (10)
O2	0.0344 (14)	0.0349 (14)	0.0324 (13)	−0.0098 (11)	0.0033 (11)	−0.0135 (11)
O3	0.0269 (13)	0.0323 (13)	0.0277 (13)	−0.0080 (10)	0.0025 (10)	−0.0063 (10)
O4	0.0310 (13)	0.0254 (13)	0.0447 (15)	0.0073 (11)	−0.0069 (11)	−0.0064 (11)
O5	0.0312 (14)	0.0340 (14)	0.0342 (13)	−0.0002 (11)	−0.0091 (11)	−0.0036 (11)
O6	0.0283 (13)	0.0348 (14)	0.0418 (14)	−0.0050 (11)	0.0088 (11)	−0.0046 (11)
C1	0.0254 (18)	0.0309 (19)	0.0238 (17)	−0.0046 (16)	0.0016 (15)	−0.0019 (16)
C2	0.0208 (17)	0.0220 (18)	0.0269 (18)	−0.0008 (14)	−0.0041 (14)	−0.0010 (14)
C3	0.0214 (18)	0.0244 (18)	0.0245 (17)	0.0009 (14)	−0.0009 (14)	0.0002 (14)
C4	0.0265 (18)	0.0197 (18)	0.0268 (18)	0.0024 (14)	−0.0059 (15)	0.0007 (14)
C5	0.0177 (17)	0.0250 (19)	0.0290 (18)	0.0018 (14)	0.0044 (14)	−0.0017 (14)
C6	0.0222 (17)	0.0265 (18)	0.0195 (16)	−0.0037 (14)	0.0018 (14)	0.0009 (14)
C7	0.0307 (19)	0.0211 (18)	0.0285 (18)	−0.0032 (15)	−0.0004 (15)	−0.0053 (14)
C8	0.0271 (19)	0.0249 (18)	0.0310 (18)	−0.0002 (15)	0.0008 (15)	0.0005 (15)
C9	0.0215 (18)	0.0312 (19)	0.0200 (17)	−0.0030 (15)	−0.0016 (14)	0.0019 (14)
C10	0.0308 (19)	0.0256 (19)	0.0274 (18)	−0.0057 (15)	0.0015 (15)	−0.0048 (14)
C11	0.0286 (19)	0.0222 (18)	0.0257 (18)	−0.0020 (14)	0.0029 (15)	−0.0026 (14)
C12	0.0216 (18)	0.0247 (18)	0.0254 (18)	0.0004 (14)	−0.0013 (14)	0.0031 (14)
C13	0.0248 (18)	0.0248 (18)	0.0279 (18)	0.0002 (15)	−0.0045 (15)	−0.0004 (14)
C14	0.0268 (19)	0.0258 (19)	0.0290 (18)	−0.0005 (15)	0.0018 (15)	−0.0036 (15)
C15	0.0237 (18)	0.032 (2)	0.0254 (18)	−0.0003 (15)	0.0019 (15)	−0.0003 (15)
C16	0.0290 (19)	0.0244 (18)	0.0329 (19)	−0.0048 (15)	0.0002 (16)	−0.0010 (15)
C17	0.0290 (19)	0.0236 (18)	0.0292 (18)	−0.0014 (15)	0.0047 (15)	−0.0040 (15)
C18	0.0236 (18)	0.0272 (18)	0.0233 (17)	−0.0032 (15)	0.0017 (14)	−0.0045 (14)
C19	0.030 (2)	0.029 (2)	0.0283 (18)	0.0020 (16)	−0.0014 (15)	0.0009 (15)
C20	0.038 (2)	0.031 (2)	0.034 (2)	−0.0076 (17)	0.0034 (17)	−0.0014 (16)
C21	0.030 (2)	0.048 (2)	0.0293 (19)	−0.0078 (18)	0.0048 (16)	−0.0075 (17)

C22	0.026 (2)	0.049 (2)	0.033 (2)	0.0002 (17)	−0.0014 (16)	−0.0005 (18)
C23	0.0275 (19)	0.034 (2)	0.0271 (18)	0.0000 (16)	−0.0024 (15)	0.0001 (15)
C24	0.031 (2)	0.033 (2)	0.047 (2)	−0.0107 (16)	0.0038 (17)	−0.0006 (17)
C25	0.033 (2)	0.038 (2)	0.037 (2)	0.0059 (17)	−0.0059 (17)	0.0040 (17)

Geometric parameters (Å, º)

N1—C1	1.371 (4)	C12—C17	1.398 (4)
N1—C4	1.407 (4)	C12—C13	1.400 (4)
N1—C18	1.455 (4)	C13—C14	1.382 (4)
O1—C4	1.207 (4)	C13—H13	0.9500
O2—C1	1.197 (4)	C14—C15	1.390 (4)
O3—C1	1.368 (4)	C14—H14	0.9500
O3—C2	1.387 (3)	C15—C16	1.380 (4)
O4—C5	1.224 (4)	C16—C17	1.386 (4)
O5—C9	1.355 (4)	C16—H16	0.9500
O5—C25	1.443 (4)	C17—H17	0.9500
O6—C15	1.366 (4)	C18—C19	1.379 (4)
O6—C24	1.441 (4)	C18—C23	1.385 (4)
C2—C3	1.345 (4)	C19—C20	1.384 (4)
C2—C12	1.463 (4)	C19—H19	0.9500
C3—C4	1.461 (4)	C20—C21	1.376 (5)
C3—C5	1.521 (4)	C20—H20	0.9500
C5—C6	1.478 (4)	C21—C22	1.391 (5)
C6—C7	1.385 (4)	C21—H21	0.9500
C6—C11	1.402 (4)	C22—C23	1.380 (4)
C7—C8	1.386 (4)	C22—H22	0.9500
C7—H7	0.9500	C23—H23	0.9500
C8—C9	1.383 (4)	C24—H24A	0.9800
C8—H8	0.9500	C24—H24B	0.9800
C9—C10	1.394 (4)	C24—H24C	0.9800
C10—C11	1.386 (4)	C25—H25A	0.9800
C10—H10	0.9500	C25—H25B	0.9800
C11—H11	0.9500	C25—H25C	0.9800
C1—N1—C4	124.6 (3)	C12—C13—H13	119.5
C1—N1—C18	115.8 (3)	C13—C14—C15	119.7 (3)
C4—N1—C18	119.3 (3)	C13—C14—H14	120.2
C1—O3—C2	123.4 (2)	C15—C14—H14	120.2
C9—O5—C25	117.3 (2)	O6—C15—C16	124.0 (3)
C15—O6—C24	117.8 (3)	O6—C15—C14	115.7 (3)
O2—C1—O3	118.5 (3)	C16—C15—C14	120.3 (3)
O2—C1—N1	125.4 (3)	C15—C16—C17	119.7 (3)
O3—C1—N1	116.0 (3)	C15—C16—H16	120.1
C3—C2—O3	119.9 (3)	C17—C16—H16	120.1
C3—C2—C12	130.5 (3)	C16—C17—C12	121.2 (3)
O3—C2—C12	109.5 (3)	C16—C17—H17	119.4
C2—C3—C4	120.4 (3)	C12—C17—H17	119.4

C2—C3—C5	125.7 (3)	C19—C18—C23	121.5 (3)
C4—C3—C5	113.9 (3)	C19—C18—N1	119.5 (3)
O1—C4—N1	120.6 (3)	C23—C18—N1	119.0 (3)
O1—C4—C3	124.6 (3)	C18—C19—C20	118.9 (3)
N1—C4—C3	114.9 (3)	C18—C19—H19	120.5
O4—C5—C6	122.2 (3)	C20—C19—H19	120.5
O4—C5—C3	119.1 (3)	C21—C20—C19	120.3 (3)
C6—C5—C3	118.6 (3)	C21—C20—H20	119.9
C7—C6—C11	118.5 (3)	C19—C20—H20	119.9
C7—C6—C5	122.2 (3)	C20—C21—C22	120.4 (3)
C11—C6—C5	119.1 (3)	C20—C21—H21	119.8
C6—C7—C8	121.3 (3)	C22—C21—H21	119.8
C6—C7—H7	119.3	C23—C22—C21	119.7 (3)
C8—C7—H7	119.3	C23—C22—H22	120.2
C9—C8—C7	119.5 (3)	C21—C22—H22	120.2
C9—C8—H8	120.3	C22—C23—C18	119.2 (3)
C7—C8—H8	120.3	C22—C23—H23	120.4
O5—C9—C8	124.2 (3)	C18—C23—H23	120.4
O5—C9—C10	115.6 (3)	O6—C24—H24A	109.5
C8—C9—C10	120.2 (3)	O6—C24—H24B	109.5
C11—C10—C9	119.6 (3)	H24A—C24—H24B	109.5
C11—C10—H10	120.2	O6—C24—H24C	109.5
C9—C10—H10	120.2	H24A—C24—H24C	109.5
C10—C11—C6	120.6 (3)	H24B—C24—H24C	109.5
C10—C11—H11	119.7	O5—C25—H25A	109.5
C6—C11—H11	119.7	O5—C25—H25B	109.5
C17—C12—C13	117.9 (3)	H25A—C25—H25B	109.5
C17—C12—C2	121.8 (3)	O5—C25—H25C	109.5
C13—C12—C2	120.3 (3)	H25A—C25—H25C	109.5
C14—C13—C12	121.1 (3)	H25B—C25—H25C	109.5
C14—C13—H13	119.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O3	0.95	2.33	2.665 (4)	100
C14—H14···O2^{i}	0.95	2.45	3.384 (4)	168
C19—H19···O1^{ii}	0.95	2.47	3.231 (4)	137
C24—H24*A*···O2^{iii}	0.98	2.52	3.225 (4)	128

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