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Crystal structure and Hirshfeld surface analysis of (*E*)-1-(2,4-dimethylfuran-3-yl)-3-phenylprop-2-en-1-one

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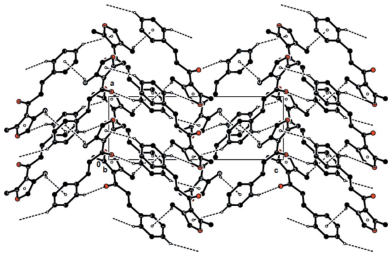
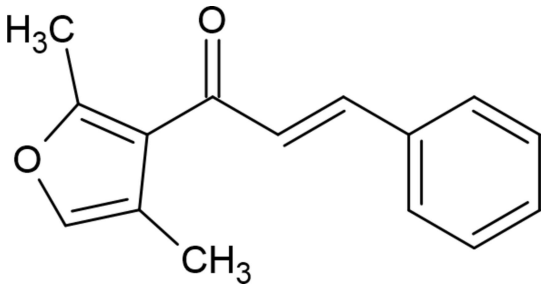
The title compound, $C_{15}H_{14}O_2$, adopts an *E* configuration about the C=C double bond. The furan ring is inclined to the phenyl ring by 12.03 (9)°. In the crystal, pairs of molecules are linked by C—H···O hydrogen bonds, forming dimers with $R_2^2(14)$ ring motifs. The molecules are connected *via* C—H···π interactions, forming a three dimensional network. No π–π interactions are observed.

1. Chemical context

Various C—C, C—N, C—S and C—O bond-formation reactions are keystones in organic synthesis. The application of such reactions has been expanded considerably, extending these approaches in different branches of chemistry, including green, medicinal, pharmaceutical and natural products chemistry, material science, supramolecular chemistry (Asadov *et al.*, 2003; Çelik *et al.*, 2023; Chalkha *et al.*, 2023; Gurbanov *et al.*, 2020; Zubkov *et al.*, 2018). α,β-Unsaturated ketones containing aryl–aryl or aryl–alkyl groups at both ends are known as chalcones or enones. There have been several important examples of enone derivatives used as target products and also as synthetic intermediates. Many natural compounds containing enone moieties, such as cyanthiwigin U, (+)-cepharamine, phorbol and grandisine G, have been the object of a total synthesis (Cuthbertson & Taylor, 2013; Kawamura *et al.*, 2016). These compounds have been obtained by many solvent-assisted or solvent-free methods. The enone moiety is a widespread structural motif of various synthetic biologically active compounds, possessing enzyme inhibitory, anticancer and antimicrobial activity (Poustforoosh *et al.*, 2022; Tapera *et al.*, 2022; Sarkı *et al.*, 2023).

In a continuation of our investigations in heterocyclic systems exhibiting biological activity and in the framework of ongoing structural studies (Maharramov *et al.*, 2021, 2022), we report herein the crystal structure and Hirshfeld surface analysis of the title compound, (*E*)-1-(2,4-dimethylfuran-3-yl)-3-phenylprop-2-en-1-one.





2. Structural commentary

As seen as Fig. 1, the title compound adopts an *E* configuration about the C=C double bond. The whole molecule is nearly planar. The furan ring (O1/C2–C5) is inclined to the phenyl ring (C9–C14) by 12.03 (9)°. The torsion angles are C2—C3—C6—O2 = 14.5 (2), C2—C3—C6—C7 = −164.79 (15), C3—C6—C7—C8 = −173.80 (15), C6—C7—C8—C9 = 179.30 (15) and C7—C8—C9—C10 = 172.52 (16)°. The geometrical parameter values of the the title compound are in agreement with those reported for similar compounds in the *Database survey* section.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, pairs of molecules are linked by C—H···O hydrogen bonds, forming dimers with $R_2^2(14)$ ring motifs (Bernstein *et al.*, 1995; Table 1; Figs. 2 and 3). The molecules are connected *via* C—H···π interactions, forming a three-dimensional network (Table 1; Fig. 4). No π–π interactions are observed.

CrystalExplorer17.5 (Spackman *et al.*, 2021) was used to compute Hirshfeld surfaces of the title molecule and two-dimensional fingerprints. The d_{norm} mappings for the title compound were performed in the range −0.1518 (red) to +1.1567 (blue) a.u. On the d_{norm} surfaces, bright-red spots indicate the locations of the C—H···O interactions and O···C/C···O contacts (Tables 1 and 2; Fig. 5*a*,*b*).

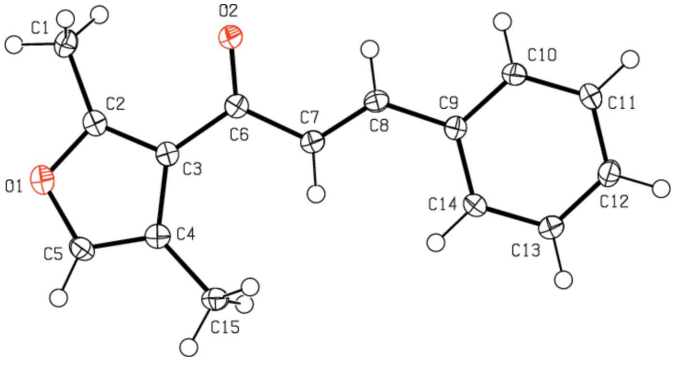


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

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

*Cg*1 and *Cg*2 are the centroids of the furan (O1/C2–C5) and phenyl (C9–C14) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O2^{i}	0.95	2.52	3.413 (2)	157
C12—H12···*Cg*1^{ii}	0.95	2.91	3.7339 (19)	146
C15—H15*B*···*Cg*2^{iii}	0.98	2.85	3.6366 (19)	137

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

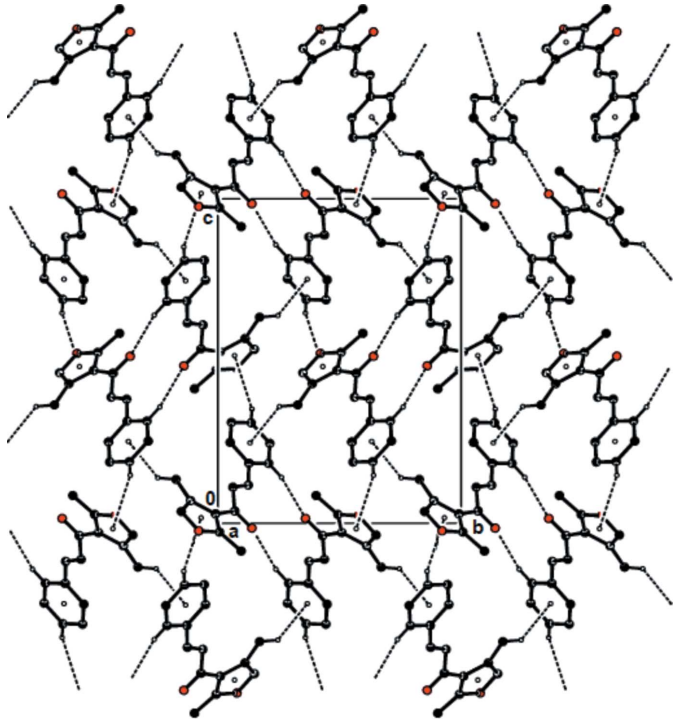


Figure 2
View of the C—H···O hydrogen bonds and C—H···π interactions of the title compound down the *a* axis. Only the H atoms involved in these interactions have been included.

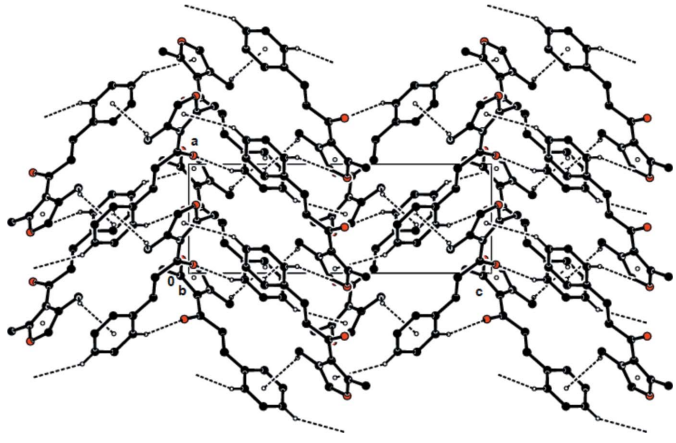


Figure 3
View of the C—H···O hydrogen bonds and C—H···π interactions of the title compound down the *b* axis. Only the H atoms involved in these interactions have been included.

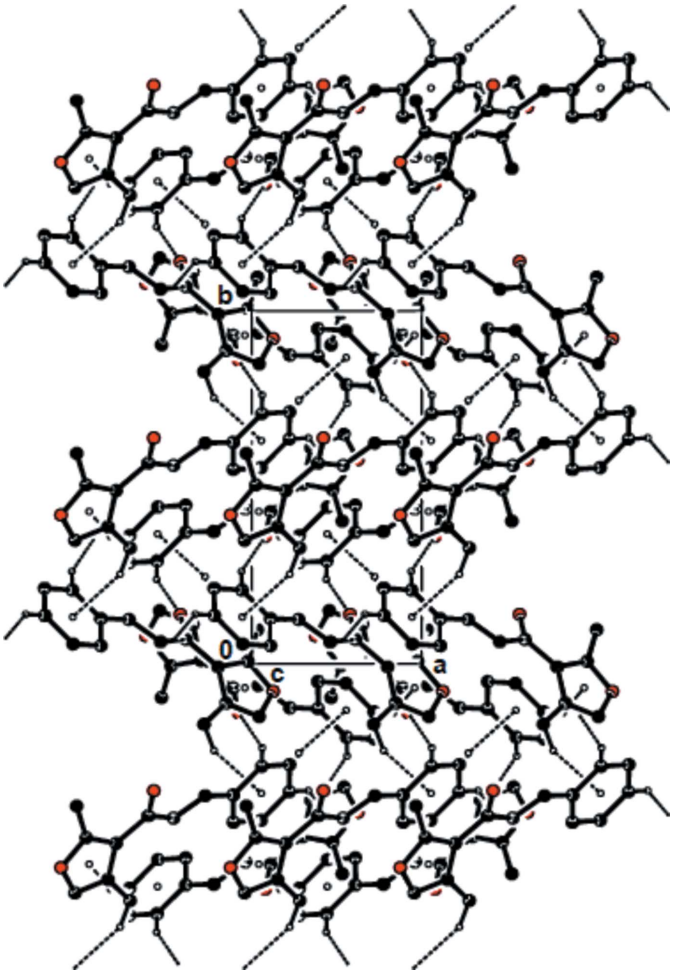


Figure 4
View of the C—H···O hydrogen bonds and C—H···π interactions of the title compound down the *c* axis. Only the H atoms involved in these interactions have been included.

The most important interatomic contact is H···H (51.1%; Fig. 6*b*) as it makes the highest contribution to the crystal packing. The C···H/H···C (Fig. 6*c*; 25.3%), O···H/H···O (Fig. 6*d*; 15.9%), C···C (5.1%) and O···C/C···O (2.5%) contacts have little directional influence on the molecular packing.

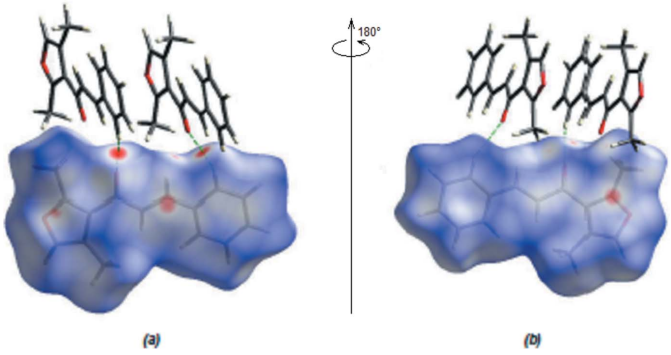


Figure 5
(*a*) Front and (*b*) back sides of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm}, with a fixed colour scale of −0.1518 to +1.1567 a.u.

Table 2
Summary of short interatomic contacts (Å) in the title compound.

H1*B*···H8	2.57	$-1+x, y, z$
H1*C*···H13	2.52	$\frac{3}{2}-x, 1-y, \frac{1}{2}+z$
H1*B*···H8	2.47	$-\frac{1}{2}+x, \frac{3}{2}-y, 1-z$
H1*A*···H10	2.39	$-\frac{3}{2}+x, \frac{3}{2}-y, 1-z$
C12···H5	2.94	$1-x, \frac{1}{2}+y, \frac{1}{2}-z$
H13···H1*A*	2.49	$\frac{1}{2}-x, 1-y, -\frac{1}{2}+z$
C15···H11	3.05	$2-x, -\frac{1}{2}+y, \frac{1}{2}-z$

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, last update November 2022; Groom *et al.*, 2016) for the '1-(furan-3-yl)-3-phenylprop-2-en-1-one' skeleton of the title compound yielded one hit, 1-(3-furyl)-3-[3-(trifluoromethyl)phenyl]prop-2-en-1-one (CSD refcode KUDNAA; Bąkowicz *et al.*, 2015). When the positions of the furan and phenyl rings are switched, 1-(3-chlorophenyl)-3-(3-furyl)prop-2-en-1-one (NUQFOW; Zingales *et al.* 2015), (*E*)-3-(2-furyl)-1-phenylprop-2-en-1-one (NOTCUW01; Vázquez-Vuelvas *et al.* 2015) are the most similar structures.

In KUDNAA, molecules are linked by intermolecular C—H···O interactions, forming zigzag chains with *C*(5) motifs

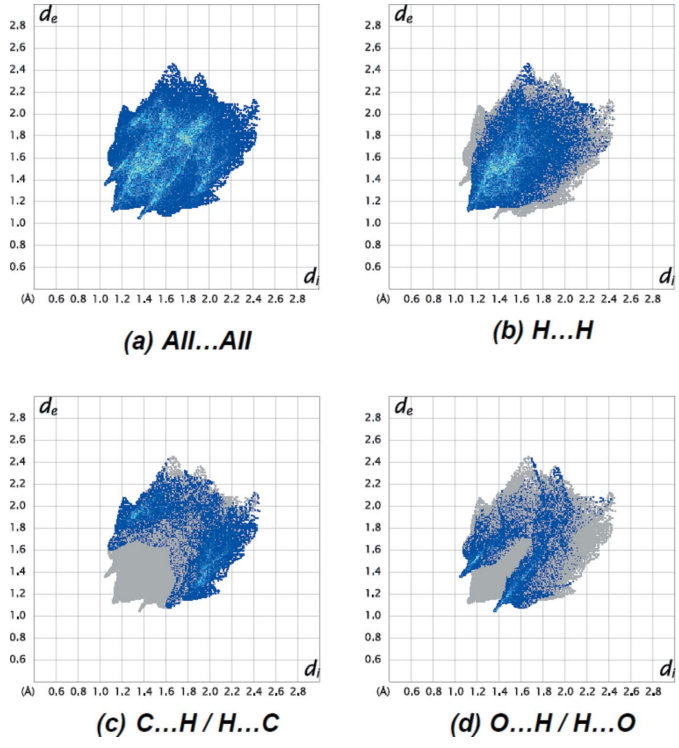


Figure 6
The two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C and (*d*) O···H/H···O interactions. [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

along the *b*-axis direction. In addition, molecules are connected by face-to-face π–π stacking interactions [centroid–centroid distances = 3.926 (3) and 3.925 (2) Å] between the opposing benzene and furan rings of the molecules along the *c*-axis direction. In NUQFOW, the molecule exhibits a non-planar geometry, the furan ring being inclined to the benzene ring by 50.52 (16)°. In the crystal of NUQFOW, molecules stack along the *a*-axis; however, there are no significant intermolecular interactions present. In NOTCUW01, the molecule also adopts an *E* configuration about the C═C double bond and the furan and phenyl rings are inclined to one another by 24.07 (7)°. In the crystal of NOTCUW01, molecules are connected by weak C—H···O hydrogen bonds and C—H···π interactions, forming ribbons extending along the *c*-axis direction.

5. Synthesis and crystallization

To a solution of 1-(2,4-dimethylfuran-3-yl)ethan-1-one (2 g, 14.5 mmol) in ethanol (10 mL), were added 10 mL of aqueous solution of sodium hydroxide (0.65 g, 16.3 mmol) and the mixture was stirred at room temperature for 2 h. Then benzaldehyde (1.73 g, 16.3 mmol) was added to the vigorously stirred reaction mixture and it was left overnight. The precipitated crystals were separated by filtration and recrystallized from an ethanol/water (1:1) solution (yield 90%; m.p. 349–350 K).

^{1}H NMR (300 MHz, DMSO-d_6, ppm): 2.1 (*s*, 3H, CH_3); 2.5 (*s*, 3H, CH_3); 7.2 (*d*, 1H, ═CH, $^3J_{H–H}$ = 15.8 Hz); 7.3 (*s*, 1H, fur.), 7.4 (*m*, 3H, arom.), 7.5 (*d*, 1H, ═CH, $^3J_{H–H}$ = 15.8 Hz); 7.8 (*m*, 2H, arom.). ^{13}C NMR (75 MHz, DMSO-d_6, ppm): 10.3 (CH_3), 15.0 (CH_3), 120.4 ($C_{quat.}$), 122.9 ($C_{quat.}$), 126.3 (═CH), 128.9 (CH, arom.), 129.4 (CH, arom.), 130.9 (CH, arom.), 134.8 ($C_{quat.}$), 139.0 (CH, furan), 142.8 (═CH), 158.2 ($C_{quat.}$), 187.7 (CO).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C-bound H atoms were placed at calculated positions and refined using a riding model, with C—H = 0.95 and 0.98 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Acknowledgements

Authors' contributions are as follows. Conceptualization, ANK and IGM; methodology, ANK, FNN and IGM; investigation, ANK, MA and AİS; writing (original draft), MA and ANK; writing (review and editing of the manuscript), MA and ANK; visualization, MA, ANK and IGM; funding acquisition, VNK, AB and ANK; resources, AB, VNK and RMR; supervision, ANK and MA.

Funding information

This paper was supported by Baku State University and the RUDN University Strategic Academic Leadership Program.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{14}O_2$
M_r	226.26
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, *b*, *c* (Å)	5.84787 (5), 12.18109 (9), 16.24568 (15)
V (Å^3)	1157.24 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.68
Crystal size (mm)	0.24 × 0.20 × 0.18
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.579, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12000, 2410, 2382
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.081, 1.06
No. of reflections	2410
No. of parameters	157
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.24
Absolute structure	Flack *x* determined using 940 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.16 (7)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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Ali N. Khalilov, Victor N. Khrustalev, Aida I. Samigullina, Mehmet Akkurt, Rovnag M. Rzayev, Ajaya Bhattarai and İbrahim G. Mamedov

Computing details

Data collection: *CrysAlis PRO* 1.171.41.117a (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* 1.171.41.117a (Rigaku OD, 2021); data reduction: *CrysAlis PRO* 1.171.41.117a (Rigaku OD, 2021); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

(*E*)-1-(2,4-Dimethylfuran-3-yl)-3-phenylprop-2-en-1-one

Crystal data

$C_{15}H_{14}O_2$
M_r = 226.26
Orthorhombic, $P2_12_12_1$
a = 5.84787 (5) Å
b = 12.18109 (9) Å
c = 16.24568 (15) Å
V = 1157.24 (2) Å^3
Z = 4
$F(000)$ = 480
D_x = 1.299 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 10780 reflections
θ = 4.5–77.7°
μ = 0.68 mm^{-1}
T = 100 K
Prism, colourless
0.24 × 0.20 × 0.18 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.579, T_{max} = 1.000
12000 measured reflections
2410 independent reflections
2382 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 77.8°, θ_{min} = 4.5°
h = −7→6
k = −15→15
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.081
S = 1.06
2410 reflections
157 parameters
0 restraints
Primary atom site location: difference Fourier map
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.3199P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0046 (4)
Absolute structure: Flack *x* determined using 940 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.16 (7)

Special details

Experimental. CrysAlisPro 1.171.41.117a (Rigaku OD, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.1250 (2)	0.42159 (10)	0.52334 (8)	0.0225 (3)
O2	0.4218 (2)	0.63977 (10)	0.51486 (7)	0.0208 (3)
C1	−0.0327 (3)	0.59606 (14)	0.58548 (11)	0.0211 (4)
H1A	−0.1936	0.5903	0.6018	0.032*
H1B	−0.0064	0.6672	0.5590	0.032*
H1C	0.0647	0.5898	0.6343	0.032*
C2	0.0234 (3)	0.50662 (13)	0.52698 (10)	0.0174 (3)
C3	0.1991 (3)	0.49066 (13)	0.47138 (10)	0.0162 (3)
C4	0.1518 (3)	0.38801 (13)	0.43028 (10)	0.0183 (4)
C5	−0.0431 (3)	0.34981 (13)	0.46379 (11)	0.0197 (3)
H5	−0.1150	0.2828	0.4488	0.024*
C6	0.3897 (3)	0.56901 (13)	0.46209 (10)	0.0165 (3)
C7	0.5382 (3)	0.56193 (14)	0.38864 (10)	0.0184 (3)
H7	0.5012	0.5122	0.3456	0.022*
C8	0.7247 (3)	0.62533 (13)	0.38247 (10)	0.0169 (3)
H8	0.7528	0.6742	0.4269	0.020*
C9	0.8896 (3)	0.62758 (13)	0.31489 (10)	0.0162 (3)
C10	1.0585 (3)	0.70888 (13)	0.31532 (11)	0.0193 (3)
H10	1.0611	0.7615	0.3584	0.023*
C11	1.2225 (3)	0.71374 (14)	0.25365 (11)	0.0217 (4)
H11	1.3360	0.7695	0.2547	0.026*
C12	1.2207 (3)	0.63690 (14)	0.19019 (11)	0.0206 (4)
H12	1.3331	0.6400	0.1480	0.025*
C13	1.0538 (3)	0.55571 (14)	0.18888 (11)	0.0214 (4)
H13	1.0518	0.5033	0.1456	0.026*
C14	0.8901 (3)	0.55079 (14)	0.25044 (11)	0.0207 (3)
H14	0.7771	0.4948	0.2490	0.025*
C15	0.2820 (3)	0.32838 (14)	0.36480 (11)	0.0222 (4)
H15A	0.2637	0.3667	0.3122	0.033*
H15B	0.2231	0.2534	0.3598	0.033*

H15C	0.4444	0.3260	0.3796	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0189 (6)	0.0244 (6)	0.0242 (6)	−0.0017 (5)	0.0021 (5)	0.0025 (5)
O2	0.0195 (6)	0.0223 (6)	0.0207 (6)	−0.0032 (5)	0.0029 (5)	−0.0048 (5)
C1	0.0186 (7)	0.0235 (8)	0.0211 (8)	0.0027 (7)	0.0039 (7)	0.0001 (6)
C2	0.0161 (7)	0.0175 (7)	0.0187 (8)	0.0009 (6)	−0.0019 (6)	0.0034 (6)
C3	0.0155 (7)	0.0171 (7)	0.0161 (7)	0.0005 (6)	−0.0013 (6)	0.0017 (6)
C4	0.0190 (8)	0.0175 (8)	0.0184 (7)	0.0015 (6)	−0.0016 (6)	0.0009 (6)
C5	0.0190 (7)	0.0160 (7)	0.0241 (8)	−0.0030 (6)	−0.0008 (7)	−0.0005 (6)
C6	0.0155 (7)	0.0167 (7)	0.0172 (7)	0.0020 (6)	−0.0014 (6)	0.0011 (6)
C7	0.0189 (7)	0.0185 (7)	0.0177 (7)	−0.0006 (6)	0.0009 (6)	−0.0025 (6)
C8	0.0181 (7)	0.0154 (7)	0.0172 (7)	0.0021 (6)	−0.0007 (6)	−0.0011 (6)
C9	0.0155 (7)	0.0170 (7)	0.0160 (7)	0.0009 (6)	0.0002 (6)	0.0010 (6)
C10	0.0192 (8)	0.0182 (7)	0.0204 (8)	−0.0017 (7)	0.0003 (7)	−0.0035 (6)
C11	0.0192 (8)	0.0208 (8)	0.0250 (8)	−0.0056 (7)	0.0037 (7)	−0.0011 (7)
C12	0.0193 (8)	0.0224 (8)	0.0200 (8)	0.0008 (7)	0.0044 (7)	0.0006 (7)
C13	0.0225 (8)	0.0218 (8)	0.0199 (8)	−0.0018 (7)	0.0024 (7)	−0.0047 (7)
C14	0.0193 (7)	0.0201 (8)	0.0226 (8)	−0.0055 (7)	0.0023 (7)	−0.0042 (6)
C15	0.0222 (8)	0.0187 (8)	0.0258 (9)	−0.0009 (7)	0.0014 (7)	−0.0060 (7)

Geometric parameters (Å, º)

O1—C2	1.352 (2)	C8—C9	1.461 (2)
O1—C5	1.389 (2)	C8—H8	0.9500
O2—C6	1.230 (2)	C9—C10	1.399 (2)
C1—C2	1.482 (2)	C9—C14	1.404 (2)
C1—H1A	0.9800	C10—C11	1.388 (2)
C1—H1B	0.9800	C10—H10	0.9500
C1—H1C	0.9800	C11—C12	1.392 (2)
C2—C3	1.382 (2)	C11—H11	0.9500
C3—C4	1.444 (2)	C12—C13	1.390 (2)
C3—C6	1.475 (2)	C12—H12	0.9500
C4—C5	1.346 (2)	C13—C14	1.385 (2)
C4—C15	1.496 (2)	C13—H13	0.9500
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.478 (2)	C15—H15A	0.9800
C7—C8	1.340 (2)	C15—H15B	0.9800
C7—H7	0.9500	C15—H15C	0.9800
C2—O1—C5	106.96 (13)	C7—C8—H8	116.4
C2—C1—H1A	109.5	C9—C8—H8	116.4
C2—C1—H1B	109.5	C10—C9—C14	118.27 (15)
H1A—C1—H1B	109.5	C10—C9—C8	118.39 (14)
C2—C1—H1C	109.5	C14—C9—C8	123.32 (15)
H1A—C1—H1C	109.5	C11—C10—C9	120.97 (15)

H1B—C1—H1C	109.5	C11—C10—H10	119.5
O1—C2—C3	109.92 (14)	C9—C10—H10	119.5
O1—C2—C1	116.68 (14)	C10—C11—C12	120.04 (16)
C3—C2—C1	133.39 (16)	C10—C11—H11	120.0
C2—C3—C4	106.33 (14)	C12—C11—H11	120.0
C2—C3—C6	122.53 (15)	C13—C12—C11	119.66 (16)
C4—C3—C6	131.14 (15)	C13—C12—H12	120.2
C5—C4—C3	105.95 (15)	C11—C12—H12	120.2
C5—C4—C15	123.41 (16)	C14—C13—C12	120.33 (15)
C3—C4—C15	130.63 (15)	C14—C13—H13	119.8
C4—C5—O1	110.84 (14)	C12—C13—H13	119.8
C4—C5—H5	124.6	C13—C14—C9	120.75 (16)
O1—C5—H5	124.6	C13—C14—H14	119.6
O2—C6—C3	119.83 (15)	C9—C14—H14	119.6
O2—C6—C7	120.92 (15)	C4—C15—H15A	109.5
C3—C6—C7	119.25 (14)	C4—C15—H15B	109.5
C8—C7—C6	120.31 (15)	H15A—C15—H15B	109.5
C8—C7—H7	119.8	C4—C15—H15C	109.5
C6—C7—H7	119.8	H15A—C15—H15C	109.5
C7—C8—C9	127.15 (15)	H15B—C15—H15C	109.5

C5—O1—C2—C3	−0.31 (17)	C2—C3—C6—C7	−164.79 (15)
C5—O1—C2—C1	178.43 (14)	C4—C3—C6—C7	15.8 (3)
O1—C2—C3—C4	0.56 (18)	O2—C6—C7—C8	6.9 (2)
C1—C2—C3—C4	−177.90 (17)	C3—C6—C7—C8	−173.80 (15)
O1—C2—C3—C6	−179.00 (14)	C6—C7—C8—C9	179.30 (15)
C1—C2—C3—C6	2.5 (3)	C7—C8—C9—C10	172.52 (16)
C2—C3—C4—C5	−0.59 (18)	C7—C8—C9—C14	−8.9 (3)
C6—C3—C4—C5	178.92 (17)	C14—C9—C10—C11	0.1 (3)
C2—C3—C4—C15	−179.55 (17)	C8—C9—C10—C11	178.70 (16)
C6—C3—C4—C15	0.0 (3)	C9—C10—C11—C12	−0.1 (3)
C3—C4—C5—O1	0.42 (18)	C10—C11—C12—C13	0.2 (3)
C15—C4—C5—O1	179.47 (15)	C11—C12—C13—C14	−0.2 (3)
C2—O1—C5—C4	−0.08 (18)	C12—C13—C14—C9	0.2 (3)
C2—C3—C6—O2	14.5 (2)	C10—C9—C14—C13	−0.1 (3)
C4—C3—C6—O2	−164.92 (16)	C8—C9—C14—C13	−178.66 (16)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the furan (O1/C2–C5) and phenyl (C9–C14) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2	0.95	2.44	2.792 (2)	102
C10—H10···O2^{i}	0.95	2.52	3.413 (2)	157
C12—H12···*Cg*1^{ii}	0.95	2.91	3.7339 (19)	146
C15—H15*B*···*Cg*2^{iii}	0.98	2.85	3.6366 (19)	137

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