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Two polymorphs of *trans*-[3-(3-nitrophenyl)oxiran-2-yl](phenyl)methanone

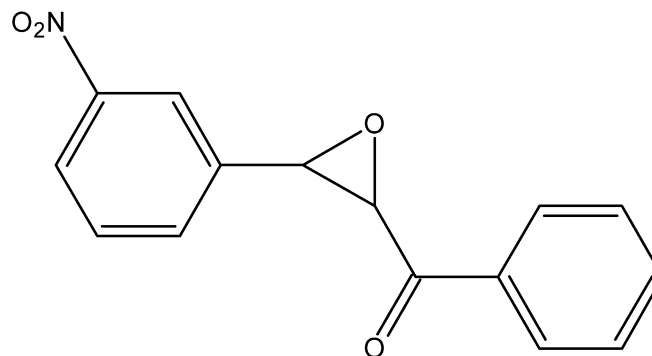
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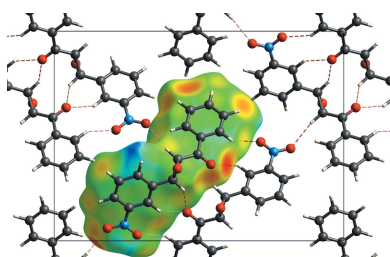
The title compound, C₁₅H₁₁NO₄, crystallizes in two polymorphic forms, centrosymmetric monoclinic and chiral orthorhombic. The geometry of the molecules in the two polymorphs is slightly different, possibly due to intermolecular interactions. There are no classical hydrogen bonding in these two structures. However, a number of C—H···O intermolecular interactions, involving both O atoms of the nitro as well the benzoyl groups, stabilize the crystal structures.

1. Chemical context

The title compound is a substituted chalcone oxide, a representative of a large group of organic compounds which are precursors for pharmaceutically significant flavonoids (Marais *et al.*, 2005). As for most biologically important molecules, chirality plays an important role in their reactions. These compounds can be also considered as isomers of substituted dibenzoylmethanes.



The simplest compound of this group, 1,3-diphenyl-2,3-epoxypropan-1-one (2-benzoyl-3-phenyloxirane, benzalacetophenone oxide) was isolated by Widman (1916) using Darzens condensation of benzaldehyde and bromoacetophenone in the presence of sodium ethoxide. When *m*-nitrobenzaldehyde was employed in this reaction, the title compound was obtained (Bodforss, 1916). The original publication mentioned the possibility of two different types of colorless crystals, both having the same melting point of 391 K. Later, a number of alternative synthetic routes were developed, including Claisen condensation of *m*-nitrobenzaldehyde with acetophenone with subsequent oxidation (Roth & Schwarz, 1961). The authors described the title compound as pale-yellow needles. A one-pot version of this synthesis was reported recently (Ngo *et al.*, 2014). Preparation of nitro-



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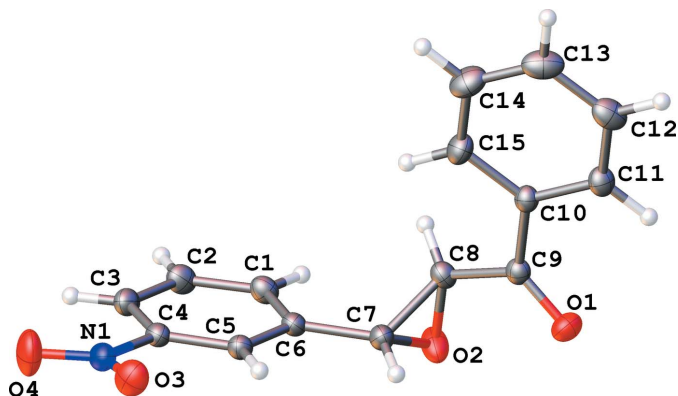


Figure 1
Numbering scheme of the title compound with 50% probability ellipsoids (monoclinic polymorph).

chalcone oxides seems to be one of the simplest condensation reactions and therefore attractive for use in undergraduate organic chemistry teaching laboratories. The interesting observation of possible polymorphism in the original publication encouraged us to conduct a structural study, exactly one hundred years after the first preparation of this compound had been reported.

2. Structural commentary

The title compound, $C_{15}H_{11}NO_4$, crystallizes in two polymorphic forms, centrosymmetric monoclinic (1) and chiral orthorhombic (2). Bond lengths and angles in the molecules of both polymorphs are very similar (Figs. 1 and 2). However, a molecular overlay (Fig. 3) reveals some difference in confor-

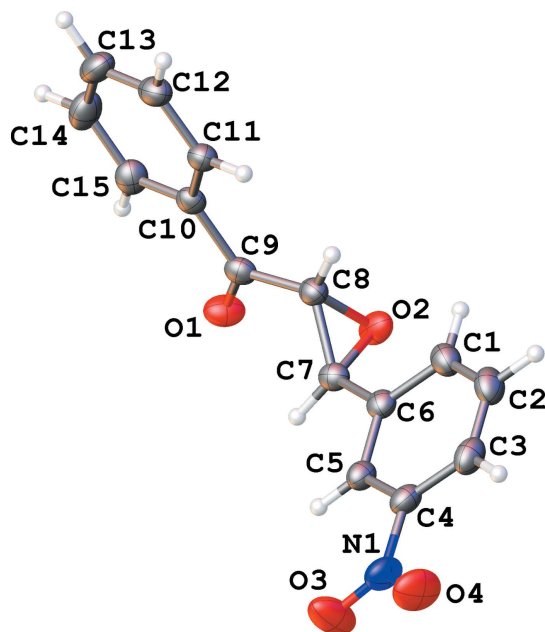


Figure 2
Numbering scheme of the title compound with 50% probability ellipsoids (orthorhombic polymorph).

Table 1
Angles between planes ($^{\circ}$).

Plane *A*: mean plane of the *m*-nitrophenyl benzene ring; plane *B*: oxirane ring; plane *C*: mean plane of the benzoyl benzene ring.

Planes	monoclinic polymorph	orthorhombic polymorph
<i>A/B</i>	99.78 (3)	97.97 (10)
<i>A/C</i>	102.36 (3)	66.21 (6)
<i>B/C</i>	55.53 (5)	75.54 (10)

mation, possibly because of different types of intermolecular interactions.

All atoms of the title polymorphs, except the oxirane ring hydrogen atoms, are located close to one of three planes: the benzene ring mean plane of the nitro-phenyl group (*A*), the oxirane ring plane (*B*), and the benzene ring plane of the benzoyl group (*C*). The largest deviations from these planes are -0.2003 (14) and 0.0457 (15) for O3 and O4 (monoclinic polymorph), 0.091 (4) and -0.189 (3) for O3 and O4 (orthorhombic), and 0.3398 (14) and 0.065 (3) for atom O1 in the monoclinic and the orthorhombic forms, respectively. Planes *A* and *B* are almost perpendicular in both polymorphs (Table 1). The angles between the two other planes differ significantly (Table 1).

3. Supramolecular features

There are no classical hydrogen bonds in these two polymorphs. In the molecules, areas of negative electrostatic potential are located in the vicinity of all four oxygen atoms. Areas near hydrogen atoms are obviously positive, providing a tool for intermolecular interactions. This expectation is supported by the packing data. In both polymorphs, the two oxygen atoms O3 and O4 of the nitro group and oxygen atom O1 of the carbonyl group act as acceptors for $C-H \cdots O$ hydrogen bonds. Despite being relatively weak, such bonds play a significant role in intermolecular interactions (Desiraju & Steiner, 1999). Hydrogen atom H5 of the nitrophenyl group makes short contacts with the O1 oxygen of the carbonyl group in both cases. However, the short contacts involving the nitro group oxygen atoms O3 and O4 (Tables 2 and 3) are

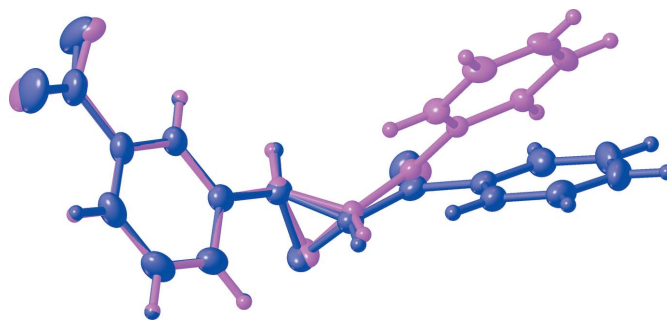


Figure 3
Overlay of the two polymorphic molecules (nitrophenyl group matching atoms). Pink: monoclinic (after inversion); purple: orthorhombic.

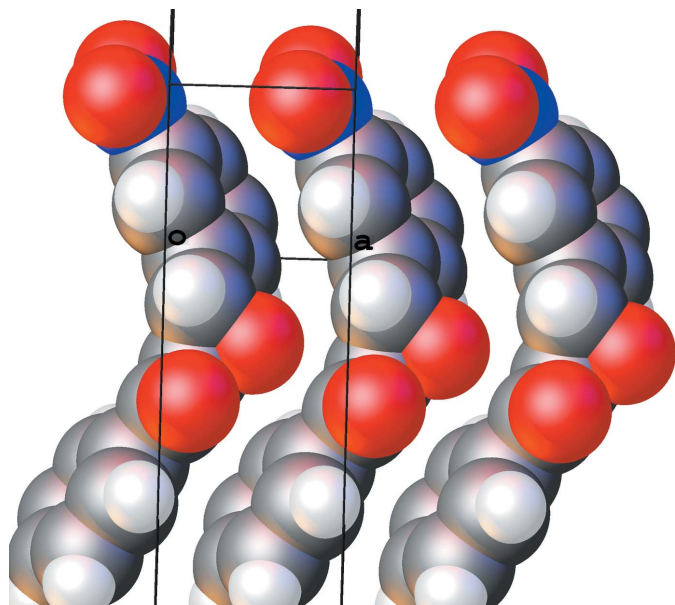


Figure 4
Packing diagram for the orthorhombic polymorph. One chain of molecules along the [100] axis is shown.

different in the two polymorphs. In the orthorhombic polymorph, the oxiran ring hydrogen atom H8 makes a short contact to one of the nitro group oxygen atoms. Another oxiran ring hydrogen atom makes a contact with carbonyl group oxygen O1 that is slightly longer than usual for C—H···O bonding [$D-H$ 1.000 (19), $H\cdots A$ 2.64 (2), $D\cdots A$ 3.419 (2) Å; $D-H\cdots A$ 134.7 (2)°]. There are a number of C—H··· π contacts that are on the long side of what is still considered to be an attractive interaction: $C12-H12\cdots C14(x, \frac{3}{2}-z, \frac{1}{2}+z)$ and $C1-H1\cdots C13(1-x, 1-y, 2-z)$ in the monoclinic form with C···C distances of 3.7870 (15) and 3.7637 (12) Å, respectively, and $C14-H14\cdots C2(\frac{1}{2}-x, 1-y, -0.5+z)$ in the orthorhombic form with a C···C distance of 3.731 (3) Å.

Table 2
Hydrogen-bond geometry (Å, °) for the monoclinic polymorph.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5\cdots O1^i$	0.962 (13)	2.335 (13)	3.2791 (11)	167.0 (11)
$C13-H13\cdots O3^{ii}$	0.945 (17)	2.490 (17)	3.3530 (13)	152.0 (13)
$C15-H15\cdots O4^{iii}$	0.992 (14)	2.381 (15)	3.2426 (13)	144.8 (12)

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

Table 3
Hydrogen-bond geometry (Å, °) for the orthorhombic polymorph.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5\cdots O1^i$	0.94 (1)	2.35 (1)	3.209 (2)	151 (1)
$C8-H8\cdots O4^{ii}$	0.96 (2)	2.49 (2)	3.401 (2)	158 (2)
$C15-H15\cdots O3^{iii}$	1.00 (1)	2.51 (2)	3.411 (2)	150 (1)

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

Without strong intermolecular bonding, the close-packing principle directs the assembly of molecules in the crystal. A multi-step approach to assembling is sometimes referred as the Kitaigorodskii Aufbau Principle (KAP) and may consist of the following sequence (Kitaigorodskii, 1961; Perlstein, 1994): (a) a single molecule or a number of molecules forming a unit; (b) units join up to form a chain; (c) chains assemble to make a 2D surface and (d) surfaces are stacked to form a crystal.

This sequence can be traced in the structure of the orthorhombic polymorph. Molecules of the title compound are stacked to form a chain along [100] axis (Fig. 4). An oxiran group forms a ‘wedge’ that fits into a concave ‘pocket’ between two phenyl rings of the next molecule. The interatomic distances between oxiran oxygen atom O2 and the corresponding carbon atoms are unusually short: $O2\cdots C7(1+x, y, z) = 3.113 (2)$, $O2\cdots C8(1+x, y, z) = 2.960 (2)$ and $O2\cdots C9(1+x, y, z) = 2.979 (2)$ Å. Two separate causes can make these short contacts possible: (i) dipole-dipole attraction of consecutive oxiran groups and (ii) close

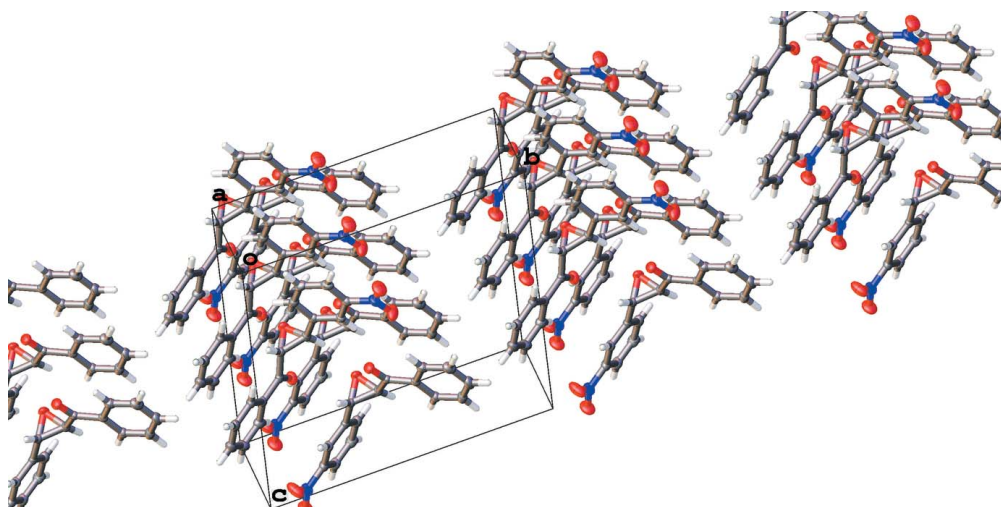


Figure 5
Packing diagram for the orthorhombic polymorph. Chains of molecules with one direction are stacked in the (001) plane.

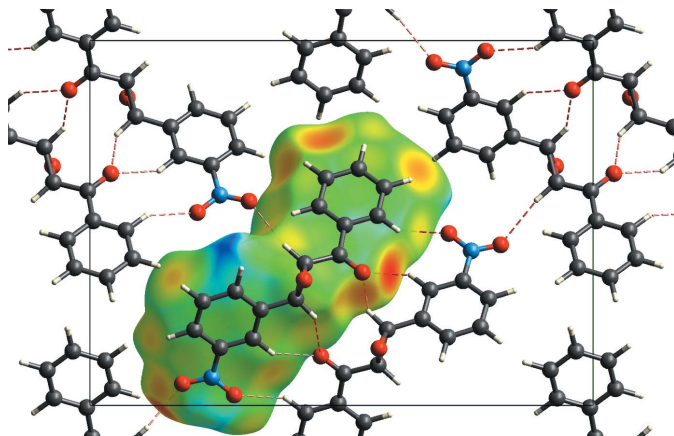


Figure 6
Packing diagram for the orthorhombic polymorph. View along the *a* axis. Hirshfeld surface shown for one molecule (calculated using *Crystal-Explorer*; Wolff *et al.*, 2012).

packing of recurrent flat benzoyl and nitrophenyl groups with the distances between their mean planes being 3.472 (2) and 3.493 (2), respectively. Because all these groups are parallel, there is no hydrogen bonding within the chain. At the next level, chains are packed in the (001) plane *via* a 2_1 symmetry operation, with all oxiran groups oriented in one direction (Fig. 5). Finally, chains are closely packed with the next 2_1 operation, forming a crystal with favorable hydrogen bonding (Fig. 6).

The monoclinic form of the title compound is possible only if the starting solution contains a racemic mixture. In the first step, two molecules are π -stacked *via* inversion centers *via* their nitrophenyl groups and two symmetric hydrogen bonds (Fig. 7). The distance between the parallel planes of these phenyl rings is 3.4115 (10), which is slightly longer than in

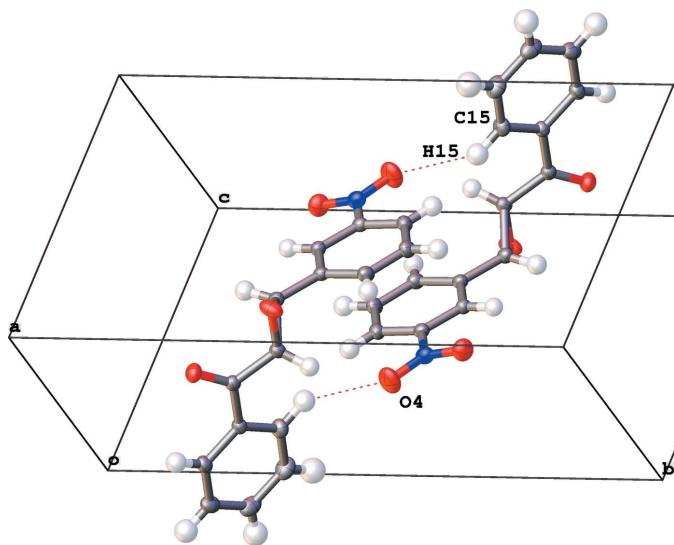


Figure 7
Packing of the monoclinic polymorph. Two molecules are related by inversion.

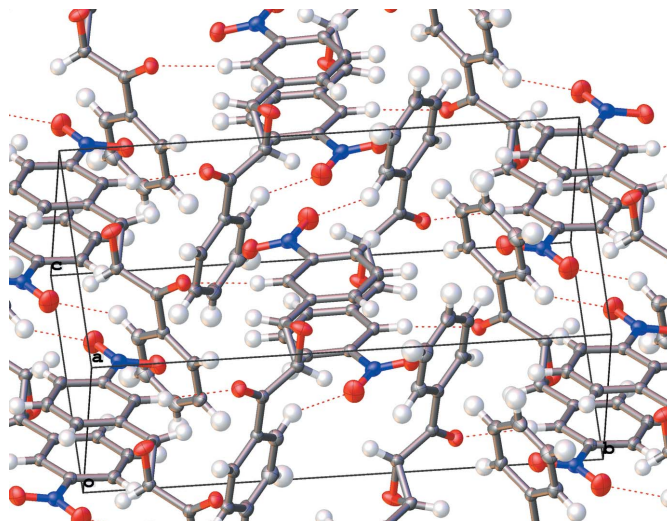


Figure 8
Packing diagram of the monoclinic polymorph. Molecules are assembled in the (100) plane.

polyaromatic hydrocarbons (3.38 Å; Kitaigorodskii, 1961) and indicates very close packing. These centrosymmetric units are assembled in the (100) plane *via* a system of hydrogen bonds

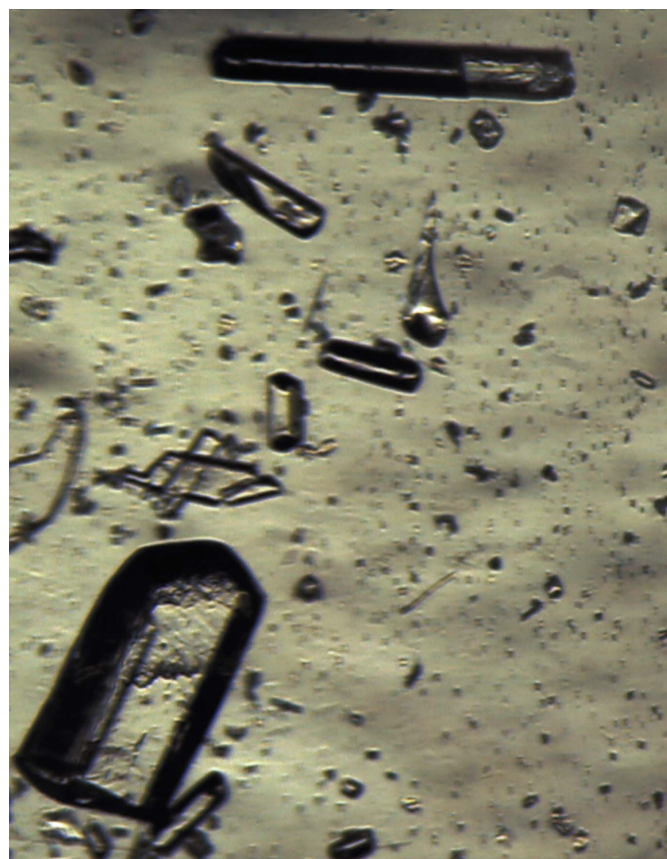


Figure 9
Crystals of different polymorphs in solution. Large blocks are monoclinic, needles are orthorhombic.

Table 4
Experimental details.

	monoclinic polymorph	orthorhombic polymorph
Crystal data		
Chemical formula	C ₁₅ H ₁₁ NO ₄	C ₁₅ H ₁₁ NO ₄
<i>M_r</i>	269.25	269.25
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Temperature (K)	173	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.8463 (5), 16.2514 (9), 10.2032 (6)	4.1615 (2), 14.7498 (6), 20.3168 (8)
α , β , γ (°)	90, 108.839 (2), 90	90, 90, 90
<i>V</i> (Å ³)	1231.35 (13)	1247.07 (9)
<i>Z</i>	4	4
Radiation type	Mo <i>K</i> α	Cu <i>K</i> α
μ (mm ⁻¹)	0.11	0.88
Crystal size (mm)	0.5 × 0.45 × 0.4	0.44 × 0.07 × 0.06
Data collection		
Diffractometer	Bruker PHOTON-100 CMOS	Bruker PHOTON-100 CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
<i>T</i> _{min} , <i>T</i> _{max}	0.942, 0.969	0.798, 0.950
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	60976, 5593, 4604	39306, 2640, 2435
<i>R</i> _{int}	0.031	0.037
(sin θ / λ) _{max} (Å ⁻¹)	0.820	0.636
Refinement		
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.044, 0.125, 1.06	0.029, 0.071, 1.06
No. of reflections	5593	2640
No. of parameters	225	197
H-atom treatment	All H-atom parameters refined	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.49, -0.23	0.13, -0.15
Absolute structure	–	Refined as an inversion twin
Absolute structure parameter	–	0.3 (2)

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *CrystalExplorer* (Spackman & Jayatilaka, 2009).

(Fig. 8). The stacking planar assemblies in the 3D crystal uses no additional hydrogen bonding.

The assembling sequence is mechanically more straightforward in the case of the chiral orthorhombic form, which results in favorable formation of the orthorhombic polymorph. The absence of an enantiomer requirement may also make it kinetically more favorable. These two factors can serve as a qualitative explanation of the preferred formation of the orthorhombic form upon crystallization from alcohols or from hexane. The monoclinic form has a slightly smaller cell volume (see Table 4) and, therefore, closer packing of molecules, an indication that the monoclinic form might be the thermodynamically slightly more stable of the polymorphs according to Burger and Ramberger's Density Rule (Burger & Ramberger, 1979*a,b*). Nevertheless, the packing of the two forms is significantly different and transition from one form to another requires dissolution of the crystal. This observation explains the kinetic stability of both forms at room temperature and at 173 K.

4. Database survey

There are sixteen reported chalcone oxide structures deposited in the Cambridge Structural Database (CSD Version 5.37; Groom *et al.*, 2016). Of these structures, six report hydroxy-

and methoxy-substituted molecules with strong intermolecular interactions. The closest to our study is [3-(4-nitrophenyl)oxiran-2-yl](phenyl)methanone (refcode COVKAB; Obregón-Mendoza *et al.*, 2014). In this case, the oxiran oxygen atom makes short contacts instead of the benzoyl group; the *p*-nitrophenyl ring is practically flat. The simplest unsubstituted chalcone oxide was recently reported (refcode TIBXIM; Zaidi *et al.*, 2007). In this structure, like in our case, only the benzoyl group oxygen atom makes short intermolecular contacts. Chains similar to those in the orthorhombic form of the title molecule are present in the chiral *P*2₁ crystal of [3-(4-chlorophenyl)oxiran-2-yl](phenyl)methanone (refcode QECFAF; Bakó *et al.*, 1999). However, the distances between oxiran oxygen atom and the subsequent carbon atoms are much longer than in the present case.

5. Synthesis and crystallization

The title compound was obtained *via* the classic route (Bodforss, 1916). Mass-spectrum (EI): 269 (*M*⁺, 20%), 105 (PhCO⁺, 100), 77 (Ph⁺, 60). Because all precursor compounds were non-chiral and synthetic conditions should not induce chirality, we expected to see a racemic product. Crystallization from hexane yielded colorless thin needles suitable for single-crystal investigation. X-ray diffraction data revealed the chiral

orthorhombic space group $P2_12_12_1$. Crystallization from ethanol produced better quality crystals of the same polymorph, one of which was used in this study. After two weeks of standing at 273 K, a number of large (up to 1 mm) crystals were observed in the remaining ethanol solution (Fig. 9). A suitable crystal was cut to dimensions appropriate for X-ray analysis. It turned out to be a monoclinic $P2_1/c$ polymorph of the same compound. Several crystals of different shape, also formed from the same solution, resulted to be of a benzoin admixture.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. The structure of the orthorhombic polymorph was refined as a two-component inversion twin. All hydrogen atoms in the monoclinic form were refined in isotropic approximation. In the orthorhombic form, the oxiran ring hydrogen atoms H7 and H8 were refined in isotropic approximation with $U_{\text{iso}} = 1.2U_{\text{iso}}(\text{C})$. All aromatic hydrogen atoms in this molecule were refined with riding coordinates and $U_{\text{iso}} = 1.2U_{\text{iso}}(\text{C})$.

For the monoclinic polymorph structure, positive residual density was observed at all bonds between non-hydrogen atoms, demonstrating the limitations of the atom-in-molecule approach for high-resolution structures of organic molecules.

Acknowledgements

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supporting information

Acta Cryst. (2016). E72, 1054-1059 [https://doi.org/10.1107/S2056989016010239]

Two polymorphs of *trans*-[3-(3-nitrophenyl)oxiran-2-yl](phenyl)methanone

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Computing details

For both compounds, data collection: *APEX2* (Bruker, 2013); cell refinement: *S SAINT* (Bruker, 2013); data reduction: *S SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b). Molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *CrystalExplorer* (Spackman & Jayatilaka, 2009) for (1); *OLEX2* (Dolomanov *et al.*, 2009) for (2). For both compounds, software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

(1) [3-(3-Nitrophenyl)oxiran-2-yl](phenyl)methanone

Crystal data

$C_{15}H_{11}NO_4$

$M_r = 269.25$

Monoclinic, $P2_1/c$

$a = 7.8463$ (5) Å

$b = 16.2514$ (9) Å

$c = 10.2032$ (6) Å

$\beta = 108.839$ (2)°

$V = 1231.35$ (13) Å³

$Z = 4$

$F(000) = 560$

$D_x = 1.452$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9972 reflections

$\theta = 3.0$ – 30.6 °

$\mu = 0.11$ mm⁻¹

$T = 173$ K

Block, colourless

$0.5 \times 0.45 \times 0.4$ mm

Data collection

Bruker PHOTON-100 CMOS
diffractometer

Radiation source: sealedtube

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2014)

$T_{\min} = 0.942$, $T_{\max} = 0.969$

60976 measured reflections

5593 independent reflections

4604 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 35.6$ °, $\theta_{\min} = 3.0$ °

$h = -11 \rightarrow 12$

$k = -26 \rightarrow 25$

$l = -16 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.125$

$S = 1.06$

5593 reflections

225 parameters

0 restraints

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 0.211P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.49$ e Å⁻³

$\Delta\rho_{\min} = -0.23$ e Å⁻³

Special details

Experimental. SADABS-2014/5 (Bruker,2014/5) was used for absorption correction. wR2(int) was 0.0614 before and 0.0562 after correction. The Ratio of minimum to maximum transmission is 0.8403. The $\lambda/2$ correction factor is 0.00150.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.25037 (8)	0.71203 (4)	0.99764 (7)	0.02695 (13)
O2	0.10970 (8)	0.58236 (5)	0.82016 (7)	0.03095 (15)
O3	0.36177 (10)	0.64512 (4)	0.29974 (8)	0.03355 (15)
O4	0.32859 (13)	0.52785 (6)	0.19647 (8)	0.0453 (2)
N1	0.32668 (10)	0.57168 (5)	0.29372 (7)	0.02557 (14)
C1	0.21037 (11)	0.46686 (5)	0.63244 (8)	0.02330 (14)
H1	0.1830 (17)	0.4424 (8)	0.7101 (13)	0.031 (3)*
C2	0.22642 (12)	0.41642 (5)	0.52697 (9)	0.02570 (15)
H2	0.2120 (17)	0.3571 (8)	0.5326 (14)	0.033 (3)*
C3	0.26219 (11)	0.44992 (5)	0.41329 (8)	0.02357 (14)
H3	0.2706 (18)	0.4158 (8)	0.3413 (14)	0.032 (3)*
C4	0.28236 (9)	0.53439 (5)	0.40956 (7)	0.01988 (13)
C5	0.26492 (10)	0.58642 (5)	0.51200 (7)	0.01960 (13)
H5	0.2789 (16)	0.6449 (8)	0.5052 (13)	0.027 (3)*
C6	0.22844 (9)	0.55193 (5)	0.62477 (7)	0.01941 (13)
C7	0.21159 (10)	0.60861 (5)	0.73395 (8)	0.02193 (14)
H7	0.1953 (17)	0.6670 (8)	0.7099 (14)	0.032 (3)*
C8	0.29883 (10)	0.59190 (5)	0.88324 (8)	0.02108 (13)
H8	0.3656 (16)	0.5410 (8)	0.9094 (13)	0.029 (3)*
C9	0.35983 (10)	0.66437 (4)	0.97908 (7)	0.01953 (13)
C10	0.55753 (10)	0.67524 (4)	1.04317 (7)	0.01900 (12)
C11	0.62448 (11)	0.72792 (5)	1.15652 (8)	0.02299 (14)
H11	0.5381 (18)	0.7560 (9)	1.1946 (14)	0.033 (3)*
C12	0.80912 (12)	0.73856 (5)	1.21587 (10)	0.02919 (17)
H12	0.856 (2)	0.7750 (10)	1.2949 (15)	0.043 (4)*
C13	0.92704 (12)	0.69765 (6)	1.16210 (12)	0.0331 (2)
H13	1.053 (2)	0.7034 (10)	1.2027 (17)	0.048 (4)*
C14	0.86192 (12)	0.64582 (6)	1.04894 (12)	0.03278 (19)
H14	0.948 (2)	0.6188 (10)	1.0128 (17)	0.052 (4)*
C15	0.67737 (11)	0.63440 (5)	0.98993 (9)	0.02569 (15)
H15	0.6281 (19)	0.5978 (9)	0.9086 (15)	0.039 (3)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0250 (3)	0.0243 (3)	0.0327 (3)	0.0034 (2)	0.0109 (2)	-0.0014 (2)
O2	0.0229 (3)	0.0469 (4)	0.0248 (3)	-0.0096 (2)	0.0101 (2)	-0.0091 (3)

O3	0.0413 (4)	0.0311 (3)	0.0333 (3)	-0.0001 (3)	0.0191 (3)	0.0067 (3)
O4	0.0700 (6)	0.0447 (4)	0.0303 (4)	0.0012 (4)	0.0286 (4)	-0.0066 (3)
N1	0.0262 (3)	0.0311 (3)	0.0211 (3)	0.0044 (2)	0.0100 (2)	0.0018 (2)
C1	0.0259 (3)	0.0218 (3)	0.0206 (3)	-0.0013 (2)	0.0052 (3)	0.0019 (2)
C2	0.0295 (4)	0.0191 (3)	0.0257 (4)	-0.0018 (3)	0.0051 (3)	-0.0010 (3)
C3	0.0246 (3)	0.0219 (3)	0.0221 (3)	0.0010 (2)	0.0046 (3)	-0.0040 (3)
C4	0.0188 (3)	0.0226 (3)	0.0175 (3)	0.0021 (2)	0.0049 (2)	0.0002 (2)
C5	0.0207 (3)	0.0189 (3)	0.0184 (3)	0.0015 (2)	0.0053 (2)	0.0004 (2)
C6	0.0191 (3)	0.0211 (3)	0.0165 (3)	0.0017 (2)	0.0036 (2)	0.0002 (2)
C7	0.0234 (3)	0.0241 (3)	0.0180 (3)	0.0040 (2)	0.0062 (2)	0.0001 (2)
C8	0.0231 (3)	0.0205 (3)	0.0182 (3)	-0.0017 (2)	0.0048 (2)	-0.0002 (2)
C9	0.0221 (3)	0.0191 (3)	0.0178 (3)	-0.0001 (2)	0.0070 (2)	0.0009 (2)
C10	0.0213 (3)	0.0186 (3)	0.0183 (3)	-0.0012 (2)	0.0080 (2)	-0.0003 (2)
C11	0.0269 (3)	0.0198 (3)	0.0222 (3)	-0.0030 (2)	0.0079 (3)	-0.0021 (2)
C12	0.0297 (4)	0.0233 (3)	0.0294 (4)	-0.0077 (3)	0.0024 (3)	0.0009 (3)
C13	0.0221 (3)	0.0280 (4)	0.0459 (5)	-0.0042 (3)	0.0063 (3)	0.0093 (4)
C14	0.0257 (4)	0.0331 (4)	0.0447 (5)	0.0023 (3)	0.0186 (4)	0.0049 (4)
C15	0.0270 (3)	0.0270 (4)	0.0267 (4)	0.0007 (3)	0.0138 (3)	-0.0023 (3)

Geometric parameters (Å, °)

O1—C9	1.2159 (9)	C7—H7	0.978 (14)
O2—C7	1.4314 (10)	C7—C8	1.4796 (11)
O2—C8	1.4225 (10)	C8—H8	0.970 (13)
O3—N1	1.2220 (10)	C8—C9	1.5067 (11)
O4—N1	1.2254 (10)	C9—C10	1.4867 (10)
N1—C4	1.4664 (10)	C10—C11	1.3978 (10)
C1—H1	0.970 (13)	C10—C15	1.3964 (10)
C1—C2	1.3905 (12)	C11—H11	0.994 (13)
C1—C6	1.3945 (11)	C11—C12	1.3888 (12)
C2—H2	0.974 (14)	C12—H12	0.972 (15)
C2—C3	1.3895 (12)	C12—C13	1.3882 (15)
C3—H3	0.939 (13)	C13—H13	0.946 (16)
C3—C4	1.3838 (11)	C13—C14	1.3866 (16)
C4—C5	1.3851 (10)	C14—H14	0.969 (16)
C5—H5	0.962 (13)	C14—C15	1.3895 (13)
C5—C6	1.3902 (10)	C15—H15	0.992 (14)
C6—C7	1.4838 (10)		
C8—O2—C7	62.46 (5)	O2—C8—C7	59.07 (5)
O3—N1—O4	123.16 (8)	O2—C8—H8	115.1 (7)
O3—N1—C4	118.12 (7)	O2—C8—C9	116.43 (6)
O4—N1—C4	118.72 (8)	C7—C8—H8	118.0 (7)
C2—C1—H1	119.3 (8)	C7—C8—C9	117.97 (7)
C2—C1—C6	120.32 (7)	C9—C8—H8	117.3 (7)
C6—C1—H1	120.3 (8)	O1—C9—C8	120.45 (7)
C1—C2—H2	119.8 (8)	O1—C9—C10	123.02 (7)
C3—C2—C1	120.55 (7)	C10—C9—C8	116.50 (6)

C3—C2—H2	119.7 (8)	C11—C10—C9	119.79 (7)
C2—C3—H3	120.4 (8)	C15—C10—C9	120.69 (7)
C4—C3—C2	117.86 (7)	C15—C10—C11	119.52 (7)
C4—C3—H3	121.7 (8)	C10—C11—H11	118.9 (8)
C3—C4—N1	119.41 (7)	C12—C11—C10	119.83 (8)
C3—C4—C5	123.01 (7)	C12—C11—H11	121.3 (8)
C5—C4—N1	117.58 (7)	C11—C12—H12	120.1 (9)
C4—C5—H5	120.5 (8)	C13—C12—C11	120.17 (8)
C4—C5—C6	118.39 (7)	C13—C12—H12	119.8 (9)
C6—C5—H5	121.1 (7)	C12—C13—H13	121.1 (10)
C1—C6—C7	122.54 (7)	C14—C13—C12	120.44 (8)
C5—C6—C1	119.86 (7)	C14—C13—H13	118.5 (10)
C5—C6—C7	117.60 (7)	C13—C14—H14	118.5 (10)
O2—C7—C6	118.63 (7)	C13—C14—C15	119.62 (8)
O2—C7—H7	112.9 (8)	C15—C14—H14	121.9 (10)
O2—C7—C8	58.48 (5)	C10—C15—H15	118.7 (8)
C6—C7—H7	116.7 (8)	C14—C15—C10	120.42 (8)
C8—C7—C6	122.36 (7)	C14—C15—H15	120.8 (8)
C8—C7—H7	114.6 (8)		
O1—C9—C10—C11	17.50 (11)	C5—C6—C7—O2	156.24 (7)
O1—C9—C10—C15	-161.44 (8)	C5—C6—C7—C8	-134.82 (8)
O2—C7—C8—C9	-105.63 (8)	C6—C1—C2—C3	0.57 (12)
O2—C8—C9—O1	-1.28 (11)	C6—C7—C8—O2	-106.07 (8)
O2—C8—C9—C10	-178.97 (6)	C6—C7—C8—C9	148.30 (7)
O3—N1—C4—C3	-172.68 (7)	C7—O2—C8—C9	108.23 (7)
O3—N1—C4—C5	6.50 (11)	C7—C8—C9—O1	66.02 (10)
O4—N1—C4—C3	6.60 (11)	C7—C8—C9—C10	-111.67 (8)
O4—N1—C4—C5	-174.22 (8)	C8—O2—C7—C6	112.36 (7)
N1—C4—C5—C6	-178.05 (6)	C8—C9—C10—C11	-164.87 (7)
C1—C2—C3—C4	0.47 (12)	C8—C9—C10—C15	16.19 (10)
C1—C6—C7—O2	-24.23 (11)	C9—C10—C11—C12	-179.56 (7)
C1—C6—C7—C8	44.72 (11)	C9—C10—C15—C14	178.98 (8)
C2—C1—C6—C5	-0.81 (11)	C10—C11—C12—C13	0.61 (13)
C2—C1—C6—C7	179.66 (7)	C11—C10—C15—C14	0.05 (12)
C2—C3—C4—N1	177.80 (7)	C11—C12—C13—C14	-0.05 (14)
C2—C3—C4—C5	-1.33 (11)	C12—C13—C14—C15	-0.52 (14)
C3—C4—C5—C6	1.10 (11)	C13—C14—C15—C10	0.52 (14)
C4—C5—C6—C1	0.00 (10)	C15—C10—C11—C12	-0.61 (12)
C4—C5—C6—C7	179.55 (6)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C5—H5 \cdots O1 ⁱ	0.962 (13)	2.335 (13)	3.2791 (11)	167.0 (11)

C13—H13···O3 ⁱⁱ	0.945 (17)	2.490 (17)	3.3530 (13)	152.0 (13)
C15—H15···O4 ⁱⁱⁱ	0.992 (14)	2.381 (15)	3.2426 (13)	144.8 (12)

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

(2) [3-(3-Nitrophenyl)oxiran-2-yl](phenyl)methanone

Crystal data

$C_{15}H_{11}NO_4$	$D_x = 1.434 \text{ Mg m}^{-3}$
$M_r = 269.25$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
Orthorhombic, $P2_12_12_1$	Cell parameters from 9668 reflections
$a = 4.1615 (2) \text{ \AA}$	$\theta = 3.7\text{--}77.7^\circ$
$b = 14.7498 (6) \text{ \AA}$	$\mu = 0.88 \text{ mm}^{-1}$
$c = 20.3168 (8) \text{ \AA}$	$T = 173 \text{ K}$
$V = 1247.07 (9) \text{ \AA}^3$	Needle, colourless
$Z = 4$	$0.44 \times 0.07 \times 0.06 \text{ mm}$
$F(000) = 560$	

Data collection

Bruker PHOTON-100 CMOS diffractometer	2640 independent reflections
Radiation source: sealedtube	2435 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.037$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$\theta_{\text{max}} = 78.6^\circ, \theta_{\text{min}} = 3.7^\circ$
$T_{\text{min}} = 0.798, T_{\text{max}} = 0.950$	$h = -5 \rightarrow 5$
39306 measured reflections	$k = -18 \rightarrow 18$
	$l = -23 \rightarrow 22$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.1972P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.071$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
2640 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
197 parameters	Absolute structure: Refined as an inversion twin
0 restraints	Absolute structure parameter: 0.3 (2)
Hydrogen site location: mixed	

Special details

Experimental. SADABS-2014/5 (Bruker,2014/5) was used for absorption correction. $wR2(\text{int})$ was 0.0614 before and 0.0562 after correction. The Ratio of minimum to maximum transmission is 0.8403. The $\lambda/2$ correction factor is 0.00150.

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.

Refinement. Refined as a 2-component inversion twin.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.6417 (4)	0.36468 (8)	0.45872 (6)	0.0372 (3)
O2	0.9762 (3)	0.34403 (8)	0.57437 (6)	0.0356 (3)
O3	0.2003 (5)	0.02869 (10)	0.71337 (7)	0.0606 (5)

O4	0.2482 (5)	0.05976 (11)	0.81622 (7)	0.0567 (5)
N1	0.2991 (5)	0.07647 (11)	0.75797 (7)	0.0395 (4)
C1	0.8151 (5)	0.31290 (13)	0.71103 (9)	0.0335 (4)
H1	0.934 (3)	0.3678 (12)	0.7004 (3)	0.040*
C2	0.7899 (5)	0.28508 (14)	0.77607 (9)	0.0383 (5)
H2	0.894 (2)	0.3214 (8)	0.8115 (8)	0.046*
C3	0.6211 (5)	0.20742 (13)	0.79219 (10)	0.0363 (4)
H3	0.6010 (7)	0.1885 (4)	0.8363 (10)	0.044*
C4	0.4826 (5)	0.15840 (12)	0.74146 (8)	0.0306 (4)
C5	0.5055 (4)	0.18379 (11)	0.67600 (8)	0.0273 (4)
H5	0.411 (2)	0.1484 (8)	0.6426 (7)	0.033*
C6	0.6718 (4)	0.26278 (11)	0.66071 (8)	0.0268 (4)
C7	0.6967 (4)	0.29204 (11)	0.59069 (8)	0.0264 (3)
H7	0.633 (5)	0.2466 (13)	0.5566 (9)	0.032*
C8	0.6695 (4)	0.38876 (11)	0.57279 (9)	0.0272 (3)
H8	0.635 (5)	0.4318 (13)	0.6078 (9)	0.033*
C9	0.5571 (4)	0.41215 (12)	0.50441 (8)	0.0266 (4)
C10	0.3543 (4)	0.49418 (11)	0.49357 (8)	0.0257 (4)
C11	0.2260 (4)	0.54583 (11)	0.54460 (9)	0.0281 (4)
H11	0.2629 (9)	0.5280 (4)	0.5902 (9)	0.034*
C12	0.0454 (5)	0.62269 (12)	0.53064 (10)	0.0354 (4)
H12	-0.050 (2)	0.6595 (8)	0.5677 (8)	0.043*
C13	-0.0041 (5)	0.64890 (14)	0.46594 (10)	0.0411 (5)
H13	-0.129 (3)	0.7042 (14)	0.4561 (3)	0.049*
C14	0.1213 (5)	0.59745 (14)	0.41521 (10)	0.0425 (5)
H14	0.0836 (10)	0.6162 (4)	0.3684 (11)	0.051*
C15	0.2985 (5)	0.52018 (13)	0.42860 (9)	0.0340 (4)
H15	0.3863 (19)	0.4831 (8)	0.3917 (8)	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0483 (8)	0.0309 (7)	0.0324 (7)	0.0018 (6)	0.0107 (6)	-0.0037 (5)
O2	0.0210 (6)	0.0352 (7)	0.0505 (8)	0.0011 (5)	0.0039 (6)	0.0093 (6)
O3	0.0981 (14)	0.0469 (9)	0.0369 (8)	-0.0287 (10)	-0.0071 (8)	0.0088 (6)
O4	0.0853 (14)	0.0539 (9)	0.0308 (8)	-0.0030 (9)	0.0051 (7)	0.0159 (6)
N1	0.0533 (11)	0.0351 (9)	0.0302 (9)	0.0034 (8)	-0.0007 (7)	0.0098 (6)
C1	0.0293 (9)	0.0336 (10)	0.0376 (10)	0.0009 (8)	-0.0035 (8)	-0.0067 (7)
C2	0.0380 (11)	0.0436 (11)	0.0333 (11)	0.0052 (9)	-0.0082 (8)	-0.0118 (8)
C3	0.0408 (11)	0.0420 (11)	0.0260 (9)	0.0123 (9)	-0.0045 (7)	-0.0017 (7)
C4	0.0354 (9)	0.0280 (9)	0.0285 (9)	0.0077 (8)	-0.0014 (7)	0.0029 (6)
C5	0.0324 (9)	0.0265 (8)	0.0231 (8)	0.0045 (8)	-0.0014 (7)	-0.0011 (6)
C6	0.0248 (9)	0.0258 (8)	0.0297 (9)	0.0047 (7)	0.0003 (7)	-0.0017 (6)
C7	0.0235 (8)	0.0248 (8)	0.0307 (9)	0.0007 (7)	0.0038 (7)	-0.0003 (6)
C8	0.0243 (8)	0.0245 (8)	0.0327 (9)	0.0005 (7)	-0.0011 (7)	-0.0014 (7)
C9	0.0261 (9)	0.0240 (9)	0.0298 (9)	-0.0046 (7)	0.0044 (7)	-0.0009 (6)
C10	0.0252 (8)	0.0236 (8)	0.0282 (9)	-0.0054 (7)	0.0014 (7)	0.0015 (6)
C11	0.0290 (9)	0.0242 (8)	0.0312 (9)	-0.0018 (7)	-0.0015 (7)	-0.0004 (6)

C12	0.0317 (10)	0.0278 (9)	0.0468 (11)	-0.0004 (8)	-0.0017 (8)	-0.0033 (8)
C13	0.0361 (10)	0.0307 (10)	0.0565 (13)	0.0032 (9)	-0.0058 (9)	0.0116 (8)
C14	0.0397 (11)	0.0480 (12)	0.0399 (11)	-0.0015 (9)	-0.0056 (9)	0.0167 (9)
C15	0.0333 (10)	0.0381 (10)	0.0304 (9)	-0.0040 (8)	0.0009 (8)	0.0042 (7)

Geometric parameters (Å, °)

O1—C9	1.215 (2)	C7—H7	1.000 (19)
O2—C7	1.432 (2)	C7—C8	1.477 (2)
O2—C8	1.437 (2)	C8—H8	0.964 (19)
O3—N1	1.219 (2)	C8—C9	1.506 (2)
O4—N1	1.227 (2)	C9—C10	1.491 (2)
N1—C4	1.468 (2)	C10—C11	1.393 (2)
C1—H1	0.97 (2)	C10—C15	1.394 (2)
C1—C2	1.388 (3)	C11—H11	0.974 (19)
C1—C6	1.395 (2)	C11—C12	1.389 (2)
C2—H2	1.00 (2)	C12—H12	1.01 (2)
C2—C3	1.383 (3)	C12—C13	1.386 (3)
C3—H3	0.94 (2)	C13—H13	0.99 (2)
C3—C4	1.385 (3)	C13—C14	1.382 (3)
C4—C5	1.385 (2)	C14—H14	1.00 (2)
C5—H5	0.943 (19)	C14—C15	1.385 (3)
C5—C6	1.390 (2)	C15—H15	1.00 (2)
C6—C7	1.490 (2)		
C7—O2—C8	61.95 (10)	O2—C8—C7	58.85 (11)
O3—N1—O4	122.84 (18)	O2—C8—H8	114.7 (13)
O3—N1—C4	118.77 (15)	O2—C8—C9	113.67 (14)
O4—N1—C4	118.38 (16)	C7—C8—H8	117.8 (11)
C2—C1—H1	119.7	C7—C8—C9	118.19 (15)
C2—C1—C6	120.58 (18)	C9—C8—H8	118.9 (12)
C6—C1—H1	119.7	O1—C9—C8	118.87 (16)
C1—C2—H2	119.7	O1—C9—C10	121.25 (15)
C3—C2—C1	120.59 (18)	C10—C9—C8	119.85 (14)
C3—C2—H2	119.7	C11—C10—C9	123.41 (15)
C2—C3—H3	121.1	C11—C10—C15	119.37 (16)
C2—C3—C4	117.87 (18)	C15—C10—C9	117.21 (15)
C4—C3—H3	121.1	C10—C11—H11	119.9
C3—C4—N1	118.44 (16)	C12—C11—C10	120.11 (16)
C3—C4—C5	123.03 (18)	C12—C11—H11	119.9
C5—C4—N1	118.52 (16)	C11—C12—H12	119.9
C4—C5—H5	120.8	C13—C12—C11	120.10 (18)
C4—C5—C6	118.39 (16)	C13—C12—H12	119.9
C6—C5—H5	120.8	C12—C13—H13	120.1
C1—C6—C7	121.08 (16)	C14—C13—C12	119.89 (19)
C5—C6—C1	119.53 (16)	C14—C13—H13	120.1
C5—C6—C7	119.39 (15)	C13—C14—H14	119.8
O2—C7—C6	115.65 (15)	C13—C14—C15	120.43 (18)

O2—C7—H7	114.4 (12)	C15—C14—H14	119.8
O2—C7—C8	59.20 (10)	C10—C15—H15	120.0
C6—C7—H7	116.7 (11)	C14—C15—C10	120.09 (18)
C8—C7—C6	120.63 (15)	C14—C15—H15	120.0
C8—C7—H7	117.2 (11)		
O1—C9—C10—C11	173.70 (17)	C5—C6—C7—O2	-151.82 (15)
O1—C9—C10—C15	-7.5 (2)	C5—C6—C7—C8	140.25 (17)
O2—C7—C8—C9	102.02 (17)	C6—C1—C2—C3	-0.3 (3)
O2—C8—C9—O1	29.4 (2)	C6—C7—C8—O2	103.45 (18)
O2—C8—C9—C10	-148.64 (14)	C6—C7—C8—C9	-154.53 (16)
O3—N1—C4—C3	-173.69 (19)	C7—O2—C8—C9	-109.74 (16)
O3—N1—C4—C5	7.2 (3)	C7—C8—C9—O1	-36.7 (2)
O4—N1—C4—C3	7.3 (3)	C7—C8—C9—C10	145.30 (17)
O4—N1—C4—C5	-171.84 (18)	C8—O2—C7—C6	-111.82 (17)
N1—C4—C5—C6	178.22 (17)	C8—C9—C10—C11	-8.3 (2)
C1—C2—C3—C4	0.7 (3)	C8—C9—C10—C15	170.47 (16)
C1—C6—C7—O2	27.6 (2)	C9—C10—C11—C12	178.49 (17)
C1—C6—C7—C8	-40.4 (3)	C9—C10—C15—C14	-177.84 (17)
C2—C1—C6—C5	-0.7 (3)	C10—C11—C12—C13	-0.9 (3)
C2—C1—C6—C7	179.91 (18)	C11—C10—C15—C14	1.0 (3)
C2—C3—C4—N1	-179.20 (17)	C11—C12—C13—C14	1.3 (3)
C2—C3—C4—C5	-0.1 (3)	C12—C13—C14—C15	-0.6 (3)
C3—C4—C5—C6	-0.8 (3)	C13—C14—C15—C10	-0.6 (3)
C4—C5—C6—C1	1.2 (3)	C15—C10—C11—C12	-0.3 (3)
C4—C5—C6—C7	-179.36 (16)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C5—H5...O1 ⁱ	0.94 (1)	2.35 (1)	3.209 (2)	151 (1)
C8—H8...O4 ⁱⁱ	0.96 (2)	2.49 (2)	3.401 (2)	158 (2)
C15—H15...O3 ⁱⁱⁱ	1.00 (1)	2.51 (2)	3.411 (2)	150 (1)

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