

Crystal structure and Hirshfeld surface analysis of a chalcone derivative: (*E*)-3-(4-fluorophenyl)-1-(4-nitrophenyl)prop-2-en-1-one

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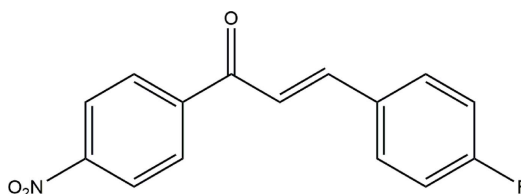
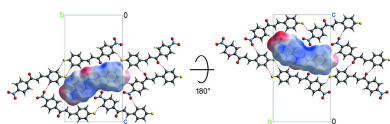
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The molecular structure of the title chalcone derivative, C₁₅H₁₀FNO₃, is nearly planar and the molecule adopts a *trans* configuration with respect to the C=C double bond. The nitro group is nearly coplanar with the attached benzene ring, which is nearly parallel to the second benzene ring. In the crystal, molecules are connected by pairs of weak intermolecular C—H···O hydrogen bonds into inversion dimers. The dimers are further linked by another C—H···O hydrogen bond and a C—H···F hydrogen bond into sheets parallel to (104). π – π interactions occur between the sheets, with a centroid–centroid distance of 3.8860 (11) Å. Hirshfeld surface analysis was used to investigate and quantify the intermolecular interactions.

1. Chemical context

Non-linear optics (NLO) is the study of interactions between intense light and matter, in which the dielectric polarization responds non-linearly to the electric field of the light. This non-linearity leads to frequency-mixing processes (second-, third- and high-harmonic generations), the optical Kerr effect *etc* (Boulanger & Zyss, 2006). Chalcone is one of the NLO materials and is known for its high NLO coefficients and good crystallizability (Prabhu *et al.*, 2013). Donor–acceptor substituted chalcone derivatives consist of two substituted phenyl rings covalently bonded to the ends of a α,β -unsaturated propenone bridge (C=C–C=O), which provides the necessary configuration for intramolecular charge transfer to show NLO properties (Fun *et al.*, 2011). However, organic chalcone derivatives with a low melting point are at a disadvantage for applications as optical instruments. In a continuation of our ongoing studies on non-linear optical properties of various chalcone derivatives (Chandra Shekhara Shetty *et al.*, 2017; Ekbote *et al.*, 2017; Kwong *et al.*, 2018), we report herein the synthesis, structure determination and Hirshfeld surface analysis of the title compound.



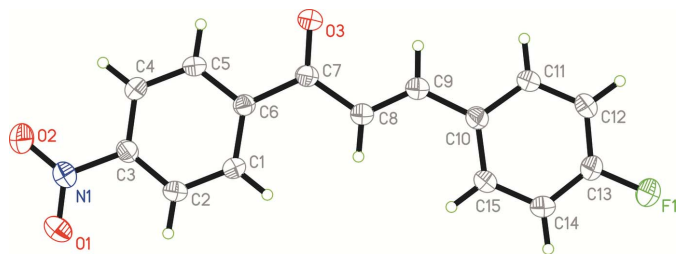


Figure 1
The molecular structure of the title compound with atom labels and 30% probability displacement ellipsoids.

2. Structural commentary

The asymmetric unit of the title chalcone derivative consists of a unique molecule, containing two *para*-substituted phenyl rings and an enone connecting bridge (Fig. 1). The molecule adopts a *trans* configuration with respect to the C8=C9 olefinic double bond, as indicated by the C7–C8–C9–C10 torsion angle of $-179.96(15)^\circ$. The C7=O3 carbonyl group adopts an *s-cis* configuration with respect to the C8=C9 double bond as indicated by O3–C7–C8–C9 torsion angle of $-0.8(3)^\circ$. The molecule (excluding H atoms) is nearly planar with a maximum deviation of $0.103(2)$ Å at atom O1 of the terminal nitro group. The nitro group is nearly coplanar with the attached C1–C6 benzene ring as indicated by the small dihedral angle of $7.9(2)^\circ$. The C1–C6 and C10–C15 benzene rings make a small dihedral angle of $4.27(8)^\circ$ with each other.

3. Supramolecular features

In the crystal, molecules are connected by pairs of weak C–H...O hydrogen bonds (C11–H11A...O3ⁱⁱ; symmetry code as in Table 1) into inversion dimers with an $R_2^2(14)$ ring motif. These dimers are further linked by C–H...O and C–H...F hydrogen bonds (C15–H15A...O1ⁱⁱⁱ and C4–H4A...F1ⁱ; Table 1) into two-dimensional sheets parallel to (104) (Fig. 2).

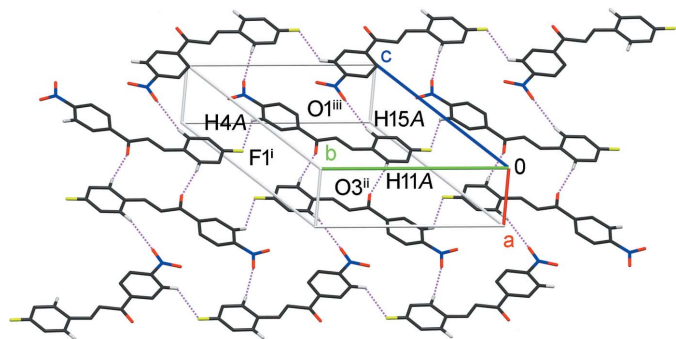


Figure 2
A partial packing diagram of the title compound, showing a two-dimensional sheet formed by C–H...O and C–H...F hydrogen bonds (dotted lines). H atoms not involved in hydrogen bonding are omitted for clarity. [Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 2, -y + 1, -z + 1$; (iii) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$]

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4–H4A...F1 ⁱ	0.93	2.53	3.183 (2)	128
C11–H11A...O3 ⁱⁱ	0.93	2.43	3.329 (2)	161
C15–H15A...O1 ⁱⁱⁱ	0.93	2.58	3.489 (2)	166

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

Weak π – π interactions occur between the sheets [$Cg1\cdots Cg1^{iv,v}$ and $Cg2\cdots Cg2^{iv,v} = 3.8860(11)$ Å, where $Cg1$ and $Cg2$ are the centroids of C1–C6 and C10–C15 benzene rings, respectively; symmetry codes: (iv) $x - 1, y, z$; (v) $x + 1, y, z$] (Fig. 3).

4. Hirshfeld surface analysis

The Hirshfeld surfaces mapped with normalized contact distance d_{norm} and electrostatic potentials, and the two-dimensional fingerprint plot were generated using *Crystal-Explorer* (Version 17.5; Spackman & Jayatilaka, 2009; Spackman & McKinnon, 2002; Spackman *et al.*, 2008; Turner *et al.*, 2017). The darkest red spots on the Hirshfeld surface mapped with d_{norm} [Fig. 4(a)] correspond to the C11–H11A...O3 hydrogen bond. The C4–H4A...F1 and C15–H15A...O1 hydrogen bonds are indicated as two pairs of lighter red spots on the d_{norm} surface. The H12A...F1 contact, with its H...F distance shorter than the sum of van der Waals radii by 0.01 Å, appears as two tiny red spots on the d_{norm} surface. The donor and acceptor of a hydrogen bond with positive and negative electrostatic potentials, respectively, are

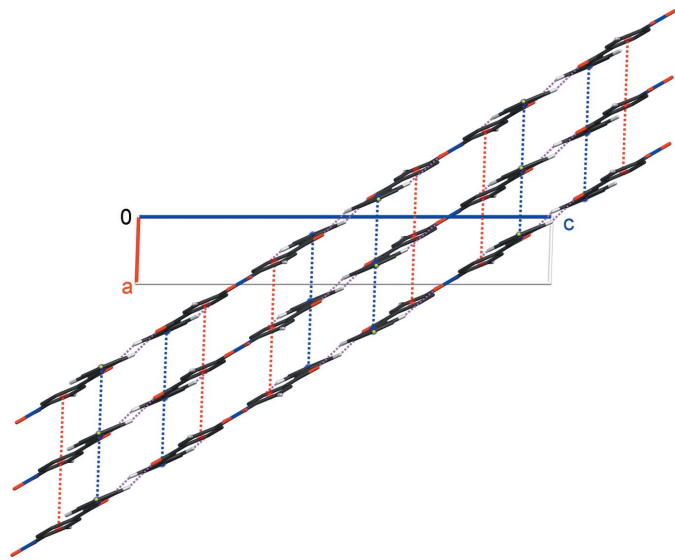


Figure 3
A partial packing diagram of the title compound, showing three separated sheets parallel to (104). The intermolecular π – π interactions between adjacent sheets are represented as red and blue dashed lines, involving $Cg1\cdots Cg1$ and $Cg2\cdots Cg2$, respectively. $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C10–C15 benzene rings, respectively.

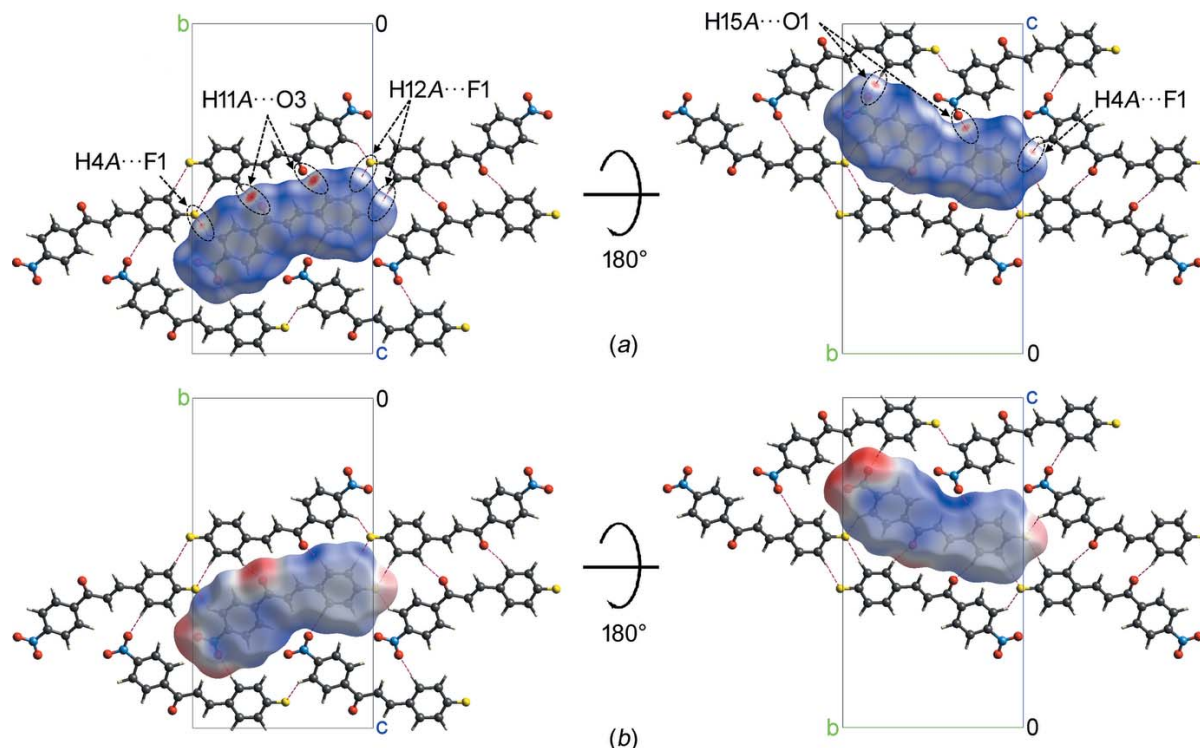


Figure 4
The Hirshfeld surfaces mapped with (a) d_{norm} and (b) electrostatic potential for the central molecule of the title compound surrounded by six neighbouring molecules.

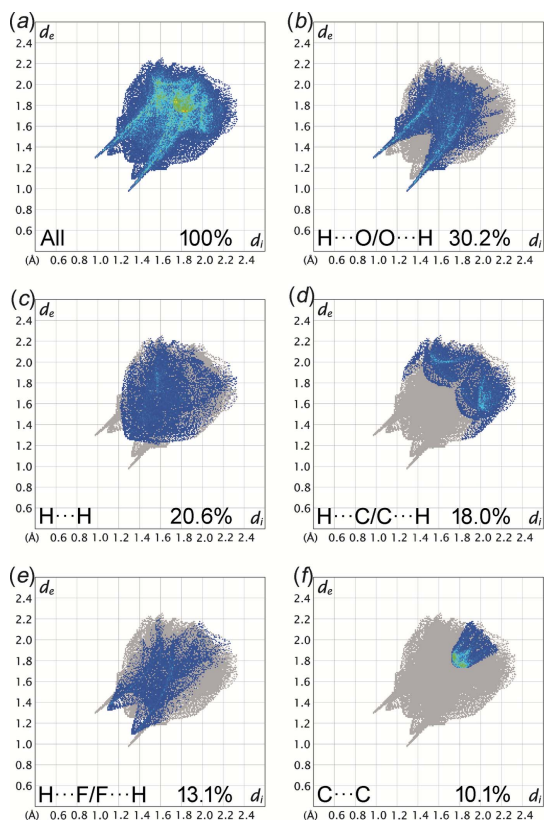


Figure 5
The two-dimensional fingerprint plots of the title compound for different intermolecular contacts and their percentage contributions to the Hirshfeld surface. d_i and d_e are the distances from the Hirshfeld surface to the nearest atom interior and exterior, respectively, to the surface.

represented as blue and red regions on the Hirshfeld surface mapped with electrostatic potential [Fig. 4(b)]. The electrostatic potential of the F atom is less negative as compared to the O atoms of nitro and carbonyl groups, as indicated by the lighter red region. The $\text{H}\cdots\text{O}/\text{O}\cdots\text{H}$ contacts are the most populated contacts and contribute 30.2% of the total intermolecular contacts, followed by $\text{H}\cdots\text{H}$ (20.6%), $\text{H}\cdots\text{C}/\text{C}\cdots\text{H}$ (18.0%), $\text{H}\cdots\text{F}/\text{F}\cdots\text{H}$ (13.1%) and $\text{C}\cdots\text{C}$ (10.1%) contacts (Fig. 5). The shortest $\text{H}\cdots\text{O}/\text{O}\cdots\text{H}$ and $\text{H}\cdots\text{F}/\text{F}\cdots\text{H}$ contacts are represented as the tips of the pseudo-mirrored sharp spikes and blunt peaks at $d_e + d_i \simeq 2.3$ and 2.4 Å, respectively, which correspond to the $\text{C11-H11A}\cdots\text{O3}$ and $\text{C4-H4A}\cdots\text{F1}$ hydrogen bonds. The characteristic ‘wings’ are missing in the fingerprint plot of $\text{H}\cdots\text{C}/\text{C}\cdots\text{H}$ contacts, indicating the absence of any significant $\text{C-H}\cdots\pi$ interactions in the crystal. The $\text{C}\cdots\text{C}$ contacts, including the intermolecular $\pi\text{-}\pi$ interactions, appear as a unique ‘triangle’ focused at $d_e \simeq d_i \simeq 1.8$ Å. The presence of significant $\pi\text{-}\pi$ interactions is supported by the unique pattern of red and blue ‘triangles’ on the shape-index surface (Fig. 6), and the flat regions on the curvedness surface (Fig. 7) of the benzene rings.

5. Database survey

The bond lengths and bond angles of the title compound are comparable with those in two similar structures, *viz.*, (*E*)-1-(4-nitrophenyl)-3-phenylprop-2-en-1-one (refcode BUDXOO; Jing, 2009a) and (*E*)-3-(4-fluorophenyl)-1-phenylprop-2-en-1-one (refcode BUDYOP; Jing, 2009b) found in the Cambridge

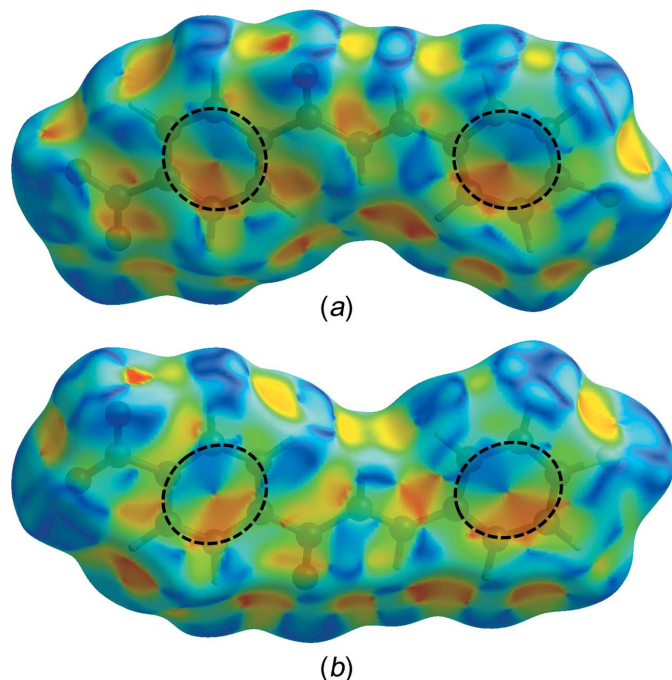


Figure 6
(a) Front and (b) rear views of the Hirshfeld surface mapped over shape-index for the title compound. The dashed-line circles highlight unique patterns of red and blue ‘triangles’.

Structural Database (Version 5.39; Groom *et al.*, 2016). The molecular conformations of these two structures are nearly planar, with small dihedral angles of 5.00 (6) and 10.60 (11)°, respectively, between the phenyl rings.

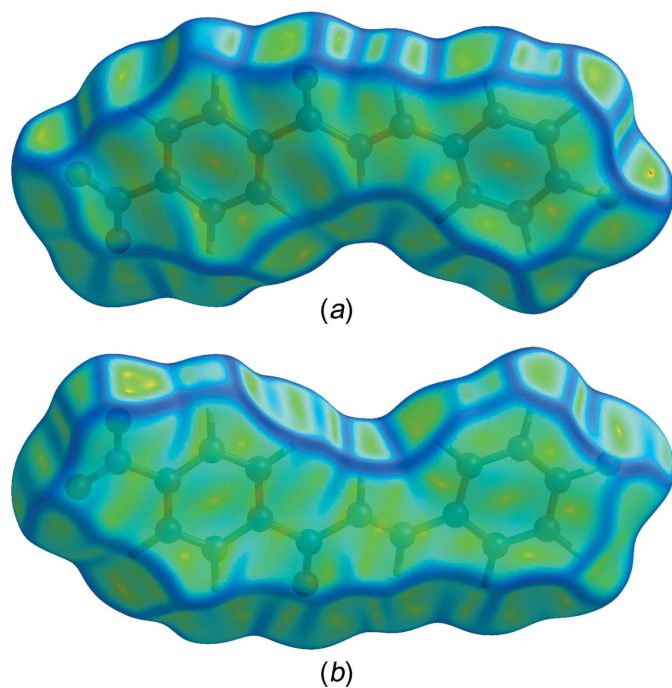


Figure 7
(a) Front and (b) rear views of the Hirshfeld surface mapped over curvedness.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₀ FNO ₃
<i>M_r</i>	271.24
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	3.8860 (5), 13.2324 (16), 24.199 (3)
β (°)	91.963 (2)
<i>V</i> (Å ³)	1243.6 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.11
Crystal size (mm)	0.49 × 0.35 × 0.31
Data collection	
Diffractometer	Bruker SMART APEXII DUO CCD area-detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2009)
<i>T_{min}</i> , <i>T_{max}</i>	0.794, 0.926
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	10823, 2418, 1922
<i>R_{int}</i>	0.026
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.617
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.043, 0.138, 1.04
No. of reflections	2418
No. of parameters	181
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.21, -0.17

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2013* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

6. Synthesis and crystallization

4-Nitroacetophenone (1.65 g, 0.01 mol) and 4-fluorobenzaldehyde (1.24 g, 0.01 mol) were dissolved in methanol (20 ml). A catalytic amount of NaOH was added to the solution dropwise with vigorous stirring. The reaction mixture was stirred for about 6 h at room temperature. The progress of the reaction was monitored by TLC. The formed crude product was filtered, washed repeatedly with distilled water and recrystallized from ethanol to obtain the title chalcone derivative. Yellowish single-crystals suitable for X-ray diffraction were obtained from an acetone solution by slow evaporation at room temperature.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically (C–H = 0.93 Å) and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

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**Qin Ai Wong, Tze Shyang Chia, Huey Chong Kwong, C. S. Chidan Kumar, Ching Kheng Quah
and Md. Azharul Arafath**

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

(*E*)-3-(4-Fluorophenyl)-1-(4-nitrophenyl)prop-2-en-1-one

Crystal data

$C_{15}H_{10}FNO_3$

$M_r = 271.24$

Monoclinic, $P2_1/c$

$a = 3.8860$ (5) Å

$b = 13.2324$ (16) Å

$c = 24.199$ (3) Å

$\beta = 91.963$ (2)°

$V = 1243.6$ (3) Å³

$Z = 4$

$F(000) = 560$

$D_x = 1.449$ Mg m⁻³

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

Cell parameters from 4607 reflections

$\theta = 2.3$ – 30.4 °

$\mu = 0.11$ mm⁻¹

$T = 296$ K

Block, yellow

$0.49 \times 0.35 \times 0.31$ mm

Data collection

Bruker SMART APEXII DUO CCD area-detector

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.794$, $T_{\max} = 0.926$

10823 measured reflections

2418 independent reflections

1922 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 26.0$ °, $\theta_{\min} = 1.8$ °

$h = -4 \rightarrow 4$

$k = -16 \rightarrow 15$

$l = -29 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.138$

$S = 1.04$

2418 reflections

181 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.072P)^2 + 0.3042P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$$

Special details

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.7362 (4)	-0.01394 (9)	0.57883 (5)	0.0899 (5)
O1	-0.1032 (4)	0.85915 (12)	0.77829 (6)	0.0784 (5)
O2	0.0898 (6)	0.97163 (12)	0.72386 (8)	0.1026 (7)
O3	0.7296 (4)	0.61266 (9)	0.55381 (5)	0.0665 (4)
N1	0.0476 (4)	0.88363 (12)	0.73723 (6)	0.0578 (4)
C1	0.3037 (4)	0.63109 (12)	0.68456 (6)	0.0460 (4)
H1A	0.2995	0.5638	0.6955	0.055*
C2	0.1758 (4)	0.70499 (13)	0.71878 (6)	0.0479 (4)
H2A	0.0857	0.6880	0.7527	0.057*
C3	0.1848 (4)	0.80391 (12)	0.70162 (6)	0.0443 (4)
C4	0.3144 (5)	0.83206 (12)	0.65149 (7)	0.0502 (4)
H4A	0.3157	0.8995	0.6407	0.060*
C5	0.4418 (4)	0.75795 (12)	0.61790 (6)	0.0474 (4)
H5A	0.5311	0.7757	0.5841	0.057*
C6	0.4388 (4)	0.65682 (11)	0.63385 (6)	0.0397 (4)
C7	0.5886 (4)	0.58109 (12)	0.59466 (6)	0.0437 (4)
C8	0.5671 (4)	0.47246 (12)	0.60636 (7)	0.0465 (4)
H8A	0.4609	0.4501	0.6380	0.056*
C9	0.6995 (4)	0.40594 (13)	0.57171 (6)	0.0461 (4)
H9A	0.8020	0.4332	0.5409	0.055*
C10	0.7052 (4)	0.29630 (12)	0.57557 (6)	0.0441 (4)
C11	0.8374 (4)	0.24150 (13)	0.53176 (7)	0.0498 (4)
H11A	0.9211	0.2760	0.5015	0.060*
C12	0.8463 (5)	0.13763 (14)	0.53240 (8)	0.0573 (5)
H12A	0.9314	0.1015	0.5029	0.069*
C13	0.7264 (5)	0.08894 (13)	0.57778 (7)	0.0571 (5)
C14	0.5966 (5)	0.13871 (13)	0.62234 (7)	0.0571 (5)
H14A	0.5188	0.1032	0.6526	0.069*
C15	0.5851 (4)	0.24251 (13)	0.62076 (7)	0.0504 (4)
H15A	0.4958	0.2776	0.6503	0.061*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1376 (12)	0.0406 (6)	0.0943 (9)	0.0055 (6)	0.0442 (9)	0.0029 (6)
O1	0.1010 (11)	0.0756 (10)	0.0608 (8)	0.0045 (8)	0.0352 (8)	-0.0084 (7)

O2	0.1626 (18)	0.0471 (9)	0.1018 (12)	0.0065 (9)	0.0579 (12)	-0.0095 (8)
O3	0.0962 (10)	0.0503 (7)	0.0550 (7)	-0.0027 (7)	0.0350 (7)	0.0017 (6)
N1	0.0665 (10)	0.0540 (10)	0.0534 (9)	0.0024 (7)	0.0107 (7)	-0.0086 (7)
C1	0.0552 (10)	0.0401 (9)	0.0430 (8)	-0.0028 (7)	0.0065 (7)	0.0049 (6)
C2	0.0546 (9)	0.0502 (10)	0.0395 (8)	-0.0036 (7)	0.0103 (7)	0.0030 (7)
C3	0.0465 (9)	0.0449 (9)	0.0417 (8)	-0.0009 (7)	0.0050 (7)	-0.0049 (7)
C4	0.0622 (10)	0.0374 (8)	0.0515 (9)	-0.0012 (7)	0.0107 (8)	0.0028 (7)
C5	0.0580 (10)	0.0443 (9)	0.0406 (8)	-0.0030 (7)	0.0110 (7)	0.0055 (7)
C6	0.0409 (8)	0.0398 (8)	0.0386 (8)	-0.0025 (6)	0.0027 (6)	0.0008 (6)
C7	0.0469 (9)	0.0449 (9)	0.0397 (8)	-0.0027 (7)	0.0056 (6)	0.0004 (6)
C8	0.0502 (9)	0.0438 (9)	0.0459 (8)	-0.0013 (7)	0.0098 (7)	0.0018 (7)
C9	0.0475 (9)	0.0464 (9)	0.0447 (8)	-0.0016 (7)	0.0061 (7)	0.0018 (7)
C10	0.0424 (8)	0.0450 (9)	0.0450 (8)	0.0008 (7)	0.0056 (7)	-0.0011 (7)
C11	0.0562 (10)	0.0493 (10)	0.0449 (9)	0.0016 (7)	0.0155 (7)	0.0020 (7)
C12	0.0689 (11)	0.0505 (10)	0.0538 (10)	0.0072 (8)	0.0206 (9)	-0.0059 (8)
C13	0.0689 (12)	0.0398 (9)	0.0634 (11)	0.0028 (8)	0.0151 (9)	0.0014 (8)
C14	0.0711 (12)	0.0503 (10)	0.0512 (10)	-0.0003 (8)	0.0194 (8)	0.0073 (8)
C15	0.0586 (10)	0.0494 (10)	0.0443 (9)	0.0032 (7)	0.0147 (7)	-0.0024 (7)

Geometric parameters (Å, °)

F1—C13	1.362 (2)	C7—C8	1.468 (2)
O1—N1	1.2147 (19)	C8—C9	1.331 (2)
O2—N1	1.221 (2)	C8—H8A	0.9300
O3—C7	1.2204 (19)	C9—C10	1.454 (2)
N1—C3	1.473 (2)	C9—H9A	0.9300
C1—C2	1.385 (2)	C10—C11	1.397 (2)
C1—C6	1.393 (2)	C10—C15	1.398 (2)
C1—H1A	0.9300	C11—C12	1.375 (2)
C2—C3	1.374 (2)	C11—H11A	0.9300
C2—H2A	0.9300	C12—C13	1.369 (3)
C3—C4	1.381 (2)	C12—H12A	0.9300
C4—C5	1.377 (2)	C13—C14	1.374 (2)
C4—H4A	0.9300	C14—C15	1.375 (2)
C5—C6	1.393 (2)	C14—H14A	0.9300
C5—H5A	0.9300	C15—H15A	0.9300
C6—C7	1.510 (2)		
O1—N1—O2	122.95 (16)	C9—C8—C7	120.02 (14)
O1—N1—C3	118.80 (16)	C9—C8—H8A	120.0
O2—N1—C3	118.24 (15)	C7—C8—H8A	120.0
C2—C1—C6	120.53 (14)	C8—C9—C10	128.67 (15)
C2—C1—H1A	119.7	C8—C9—H9A	115.7
C6—C1—H1A	119.7	C10—C9—H9A	115.7
C3—C2—C1	118.60 (14)	C11—C10—C15	118.08 (15)
C3—C2—H2A	120.7	C11—C10—C9	118.33 (14)
C1—C2—H2A	120.7	C15—C10—C9	123.59 (14)
C2—C3—C4	122.43 (15)	C12—C11—C10	121.34 (15)

C2—C3—N1	119.47 (14)	C12—C11—H11A	119.3
C4—C3—N1	118.09 (15)	C10—C11—H11A	119.3
C5—C4—C3	118.43 (15)	C13—C12—C11	118.06 (16)
C5—C4—H4A	120.8	C13—C12—H12A	121.0
C3—C4—H4A	120.8	C11—C12—H12A	121.0
C4—C5—C6	120.95 (14)	F1—C13—C12	118.38 (16)
C4—C5—H5A	119.5	F1—C13—C14	118.37 (16)
C6—C5—H5A	119.5	C12—C13—C14	123.25 (17)
C5—C6—C1	119.06 (14)	C13—C14—C15	118.00 (15)
C5—C6—C7	117.17 (13)	C13—C14—H14A	121.0
C1—C6—C7	123.78 (14)	C15—C14—H14A	121.0
O3—C7—C8	121.43 (15)	C14—C15—C10	121.26 (15)
O3—C7—C6	118.36 (14)	C14—C15—H15A	119.4
C8—C7—C6	120.20 (13)	C10—C15—H15A	119.4
C6—C1—C2—C3	0.0 (3)	C1—C6—C7—C8	6.1 (2)
C1—C2—C3—C4	0.4 (3)	O3—C7—C8—C9	-0.8 (3)
C1—C2—C3—N1	179.54 (15)	C6—C7—C8—C9	-179.99 (15)
O1—N1—C3—C2	-7.6 (2)	C7—C8—C9—C10	-179.96 (15)
O2—N1—C3—C2	172.67 (18)	C8—C9—C10—C11	175.31 (17)
O1—N1—C3—C4	171.54 (17)	C8—C9—C10—C15	-4.6 (3)
O2—N1—C3—C4	-8.2 (3)	C15—C10—C11—C12	0.8 (3)
C2—C3—C4—C5	-0.6 (3)	C9—C10—C11—C12	-179.15 (16)
N1—C3—C4—C5	-179.74 (15)	C10—C11—C12—C13	-1.0 (3)
C3—C4—C5—C6	0.3 (3)	C11—C12—C13—F1	-179.66 (17)
C4—C5—C6—C1	0.1 (3)	C11—C12—C13—C14	0.4 (3)
C4—C5—C6—C7	-179.16 (15)	F1—C13—C14—C15	-179.50 (17)
C2—C1—C6—C5	-0.3 (2)	C12—C13—C14—C15	0.5 (3)
C2—C1—C6—C7	178.91 (15)	C13—C14—C15—C10	-0.7 (3)
C5—C6—C7—O3	6.1 (2)	C11—C10—C15—C14	0.1 (3)
C1—C6—C7—O3	-173.10 (16)	C9—C10—C15—C14	-179.98 (16)
C5—C6—C7—C8	-174.65 (15)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4A \cdots F1 ⁱ	0.93	2.53	3.183 (2)	128
C11—H11A \cdots O3 ⁱⁱ	0.93	2.43	3.329 (2)	161
C15—H15A \cdots O1 ⁱⁱⁱ	0.93	2.58	3.489 (2)	166

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