

## 4-(4-Nitrophenyl)-3-phenoxyazetidin-2-one

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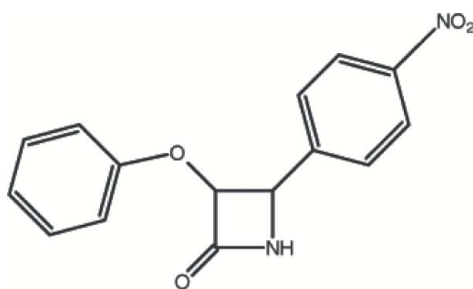
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.043;  $wR$  factor = 0.116; data-to-parameter ratio = 13.5.

The title compound,  $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_4$ , contains a nearly planar four-membered  $\beta$ -lactam ring, making dihedral angles of  $67.01$  (13) and  $75.21$  (11) $^\circ$  with the phenyl and the benzene rings, respectively. A single  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond links molecules into centrosymmetric dimers.

## Related literature

For related literature, see: Akkurt *et al.* (2006); Alcaide *et al.* (2007); Bernstein *et al.* (1995); Bruggink (2001); Cha *et al.* (2006); Chan *et al.* (1995); Coyne *et al.* (2007); Dobrowolski *et al.* (2004); Fukuyama *et al.* (1980); Georg (1993); Jarrahpour & Alvand (2007); Jarrahpour & Zarei (2006); Kamiya *et al.* (1982); Katritzky *et al.* (1996); Koster *et al.* (1982); Kronenthal *et al.* (1982); Morin & Gorman (1982); Pınar *et al.* (2006).



## Experimental

## Crystal data

 $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_4$   
 $M_r = 284.27$   
Triclinic,  $P\bar{1}$   
 $a = 6.1548$  (7) Å  
 $b = 9.8007$  (11) Å $c = 11.9296$  (13) Å  
 $\alpha = 80.552$  (9) $^\circ$   
 $\beta = 75.167$  (9) $^\circ$   
 $\gamma = 82.188$  (9) $^\circ$   
 $V = 682.86$  (14) Å<sup>3</sup> $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup> $T = 296$  K  
 $0.77 \times 0.41 \times 0.22$  mm

## Data collection

Stoe IPDS2 diffractometer  
Absorption correction: integration  
(*X-RED32*; Stoe & Cie, 2002)  
 $T_{\min} = 0.925$ ,  $T_{\max} = 0.978$ 5874 measured reflections  
2635 independent reflections  
2047 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.116$   
 $S = 1.03$   
2635 reflections  
195 parametersH atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.24$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O2}^i$	0.90 (2)	2.09 (2)	2.940 (2)	156.9 (18)
$\text{C9}-\text{H9}\cdots\text{O2}^{ii}$	0.98	2.45	3.383 (2)	159

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

Data collection: *X-Area* (Stoe & Cie, 2002); cell refinement: *X-Area*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2126).

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**supplementary materials**

*Acta Cryst.* (2007). E63, o3729–o3730 [ doi:10.1107/S1600536807038354 ]

#### 4-(4-Nitrophenyl)-3-phenoxyazetididin-2-one

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##### Comment

$\beta$ -Lactams are one of the best known and most extensively studied class of compounds due to their biological activity (Bruggink, 2001; Morin & Gorman, 1982; Katritzky *et al.*, 1996; Georg, 1993). The  $\beta$ -lactam class of drugs have revolutionized treatment in medicine (Coyne *et al.*, 2007). In the late 1970's and early 1980's, the first classes of the monocyclic  $\beta$ -lactam antibacterial agents were found in natural sources (Dobrowolski *et al.*, 2004). All  $\beta$ -lactams are based on a  $\beta$ -lactam ring responsible for the antibacterial activity and variable side chains that account for the major differences in their chemical and pharmacological properties (Cha *et al.*, 2006). Monocyclic  $\beta$ -lactams such as nocardicins (Kamiya *et al.*, 1982) and monobactams (Koster *et al.*, 1982) are of interest as they have been found to exhibit antibiotic properties. These compounds can be synthesized by various routes, although the preparation of a *N*-unsubstituted  $\beta$ -lactam is a common feature (Chan *et al.*, 1995). Apart from their clinical interest, the use of  $\beta$ -lactams as versatile synthons for the preparation of compounds of biological relevance, such as  $\alpha$ - and  $\beta$ -amino acids, alkaloids, heterocycles, and taxoids, has triggered a renewed interest in the building of new  $\beta$ -lactam systems (Alcaide *et al.*, 2007). In solution-phase syntheses, CAN has been utilized to remove the *p*-methoxyphenyl group from the amide nitrogen of  $\beta$ -lactams to generate corresponding *N*-unsubstituted analogs (Fukuyama *et al.*, 1980; Kronenthal *et al.*, 1982; Jarrahpour & Zarei, 2006). Jarrahpour and coworkers have synthesized some sugar-based monocyclic  $\beta$ -lactams (Jarrahpour & Alvand, 2007). We herein report on the crystal and molecular structures of the title compound, (I).

In (I) (Fig. 1), the four-membered  $\beta$ -lactam ring is nearly planar, with a maximum deviation of 0.013 (1) Å for atom N1. Within the lactam ring, the bond lengths are similar to those observed in our previous studies (Pinar *et al.*, 2006; Akkurt *et al.*, 2006). The four-membered  $\beta$ -lactam ring (N1/C7/C8/C9) in (I) makes dihedral angles of 67.01 (13) and 75.21 (11)°, respectively, with the C1...C6 phenyl and the C10...C15 benzene rings.

A single N—H...O hydrogen bond (Fig. 2) links molecules into centrosymmetric dimers, forming a  $R_2^2(8)$  motif (Bernstein *et al.*, 1995).

##### Experimental

Treatment of 1-(4-methoxyphenyl)-4-(4-nitrophenyl)-3-phenoxyazetididin-2-one with ceric ammonium nitrate (CAN) at 273 K in acetonitrile gave the title *N*-unsubstituted monocyclic  $\beta$ -lactam (Jarrahpour *et al.*, 2006). Compound (I) was recrystallized from dichloromethane to give light yellow single crystals. The IR spectrum showed the characteristic absorption of  $\beta$ -lactam carbonyl at 1755  $\text{cm}^{-1}$  and the lactam NH at 3383.9  $\text{cm}^{-1}$ . The  $^1\text{H}$  NMR spectrum showed the  $\beta$ -lactam H-4 proton as a doublet at 5.11 p.p.m. ( $J = 5.50$  Hz) and the H-3 proton also as a doublet at 5.71 p.p.m. ( $J = 5.50$  Hz), NH at 6.76 p.p.m. and aromatic H protons at 6.59–8.21 p.p.m.. The  $^{13}\text{C}$  NMR spectrum exhibited the following signals:  $\beta$ -lactam C-4 at 55.11,  $\beta$ -lactam C-3 at 88.76, aromatic carbons at 114.23–158.13, and CO of  $\beta$ -lactam at 167.56 p.p.m.. The mass spectrum showed the molecular ion at  $m/e$  284 and the base peak at  $m/e$  191.

## Refinement

The H atom bonded to N atoms was found in a difference map and refined freely. The C-bonded H atoms were included in idealized positions and refined using a riding model approximation with C—H bond lengths set to 0.93 (aromatic CH) or 0.98 Å (methine CH), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

## Figures

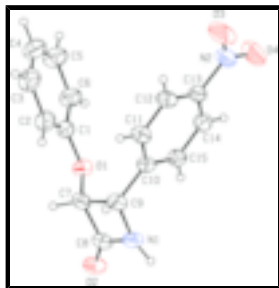


Fig. 1. An ORTEP drawing of the title compound, with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

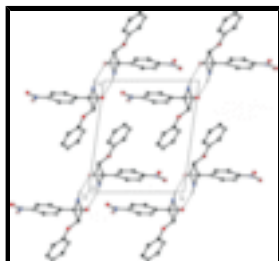


Fig. 2. View of the packing of (I), showing the formation of centrosymmetric dimers, down the *a* axis in the unit cell. For the sake of clarity, H atoms not involved in the motifs shown have been omitted.

## 4-(4-Nitrophenyl)-3-phenoxyazetidin-2-one

### Crystal data

$\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_4$

$M_r = 284.27$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 6.1548\ (7)\ \text{\AA}$

$b = 9.8007\ (11)\ \text{\AA}$

$c = 11.9296\ (13)\ \text{\AA}$

$\alpha = 80.552\ (9)^\circ$

$\beta = 75.167\ (9)^\circ$

$\gamma = 82.188\ (9)^\circ$

$V = 682.86\ (14)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 296$

$D_x = 1.383\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3067 reflections

$\theta = 2.1\text{--}27.9^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Prism, light yellow

$0.77 \times 0.41 \times 0.22\ \text{mm}$

### Data collection

Stoe IPDS2  
diffractometer

2635 independent reflections

Monochromator: plane graphite	2047 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.032$
$T = 296$ K	$\theta_{\text{max}} = 26.0^\circ$
$\omega$ scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.925$ , $T_{\text{max}} = 0.978$	$k = -12 \rightarrow 12$
5874 measured reflections	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.1246P]$
$wR(F^2) = 0.116$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2635 reflections	$\Delta\rho_{\text{max}} = 0.19 \text{ e } \text{\AA}^{-3}$
195 parameters	$\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97, $FC^* = KFC[1 + 0.001XFC^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.028 (4)

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.43673 (18)	0.16127 (12)	0.32486 (10)	0.0569 (4)
O2	0.31243 (19)	-0.00746 (14)	0.15344 (12)	0.0669 (5)
O3	1.0921 (4)	0.7129 (2)	0.1750 (2)	0.1277 (10)
O4	0.7998 (4)	0.78343 (17)	0.11047 (19)	0.1150 (9)
N1	0.6469 (2)	0.09919 (15)	0.07432 (14)	0.0586 (5)
N2	0.9265 (4)	0.69132 (18)	0.14639 (16)	0.0798 (7)
C1	0.5052 (3)	0.19644 (19)	0.41665 (15)	0.0587 (6)
C2	0.6992 (4)	0.1401 (2)	0.44995 (19)	0.0765 (8)
C3	0.7471 (5)	0.1856 (3)	0.5453 (2)	0.1007 (11)
C4	0.6077 (7)	0.2836 (4)	0.6032 (2)	0.1137 (13)
C5	0.4185 (6)	0.3397 (3)	0.5681 (2)	0.1074 (13)
C6	0.3640 (4)	0.2961 (2)	0.47587 (18)	0.0797 (8)
C7	0.5801 (3)	0.06734 (16)	0.25548 (15)	0.0529 (5)
C8	0.4792 (3)	0.04325 (17)	0.15693 (16)	0.0540 (5)
C9	0.7757 (3)	0.12692 (17)	0.15498 (15)	0.0529 (5)
C10	0.8109 (2)	0.27613 (16)	0.15189 (14)	0.0467 (5)
C11	0.9911 (3)	0.30699 (18)	0.19038 (16)	0.0548 (5)
C12	1.0272 (3)	0.44190 (18)	0.19040 (16)	0.0587 (6)
C13	0.8818 (3)	0.54697 (17)	0.15168 (14)	0.0551 (5)

## supplementary materials

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C14	0.6991 (3)	0.52079 (18)	0.11567 (15)	0.0598 (6)
C15	0.6654 (3)	0.38471 (17)	0.11566 (15)	0.0549 (6)
H1	0.684 (3)	0.091 (2)	-0.0023 (19)	0.075 (6)*
H2	0.79660	0.07320	0.41010	0.0920*
H3	0.87740	0.14780	0.56940	0.1210*
H4	0.64140	0.31240	0.66680	0.1360*
H5	0.32430	0.40860	0.60680	0.1290*
H6	0.23200	0.33390	0.45360	0.0960*
H7	0.62810	-0.01890	0.30100	0.0630*
H9	0.91710	0.06610	0.14960	0.0640*
H11	1.08870	0.23500	0.21660	0.0660*
H12	1.14830	0.46180	0.21620	0.0700*
H14	0.60000	0.59340	0.09170	0.0720*
H15	0.54260	0.36560	0.09090	0.0660*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0555 (6)	0.0631 (7)	0.0574 (7)	-0.0073 (5)	-0.0158 (5)	-0.0182 (5)
O2	0.0579 (7)	0.0690 (8)	0.0845 (9)	-0.0143 (6)	-0.0215 (6)	-0.0274 (7)
O3	0.1617 (18)	0.0836 (12)	0.166 (2)	-0.0607 (12)	-0.0640 (16)	-0.0180 (12)
O4	0.1542 (17)	0.0467 (9)	0.1371 (17)	0.0001 (10)	-0.0286 (13)	-0.0104 (9)
N1	0.0623 (8)	0.0590 (9)	0.0615 (9)	-0.0137 (7)	-0.0132 (7)	-0.0248 (7)
N2	0.1102 (14)	0.0526 (10)	0.0743 (11)	-0.0222 (10)	-0.0060 (10)	-0.0157 (8)
C1	0.0706 (10)	0.0604 (10)	0.0480 (9)	-0.0262 (8)	-0.0115 (8)	-0.0039 (7)
C2	0.0866 (13)	0.0816 (14)	0.0718 (13)	-0.0252 (11)	-0.0342 (11)	-0.0021 (10)
C3	0.124 (2)	0.113 (2)	0.0853 (17)	-0.0509 (17)	-0.0543 (16)	0.0080 (15)
C4	0.177 (3)	0.121 (2)	0.0630 (15)	-0.071 (2)	-0.0369 (18)	-0.0102 (15)
C5	0.154 (3)	0.107 (2)	0.0636 (14)	-0.0338 (19)	-0.0079 (16)	-0.0303 (14)
C6	0.0971 (15)	0.0826 (14)	0.0591 (12)	-0.0178 (11)	-0.0053 (10)	-0.0225 (10)
C7	0.0549 (9)	0.0428 (8)	0.0668 (11)	-0.0061 (7)	-0.0212 (8)	-0.0124 (7)
C8	0.0528 (8)	0.0444 (8)	0.0711 (11)	-0.0040 (7)	-0.0185 (8)	-0.0210 (7)
C9	0.0474 (8)	0.0475 (9)	0.0691 (11)	-0.0023 (7)	-0.0169 (7)	-0.0199 (8)
C10	0.0433 (7)	0.0473 (8)	0.0512 (9)	-0.0043 (6)	-0.0088 (6)	-0.0156 (7)
C11	0.0444 (8)	0.0517 (9)	0.0726 (11)	-0.0020 (7)	-0.0184 (7)	-0.0158 (8)
C12	0.0522 (9)	0.0596 (10)	0.0701 (11)	-0.0150 (8)	-0.0137 (8)	-0.0190 (9)
C13	0.0673 (10)	0.0476 (9)	0.0493 (9)	-0.0132 (7)	-0.0035 (7)	-0.0140 (7)
C14	0.0720 (11)	0.0496 (9)	0.0580 (10)	0.0049 (8)	-0.0202 (8)	-0.0094 (7)
C15	0.0555 (9)	0.0563 (10)	0.0590 (10)	-0.0020 (7)	-0.0223 (7)	-0.0149 (8)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

O1—C1	1.377 (2)	C10—C15	1.382 (2)
O1—C7	1.402 (2)	C10—C11	1.389 (2)
O2—C8	1.212 (2)	C11—C12	1.370 (3)
O3—N2	1.209 (4)	C12—C13	1.371 (3)
O4—N2	1.208 (3)	C13—C14	1.370 (3)
N1—C8	1.339 (2)	C14—C15	1.377 (2)
N1—C9	1.471 (2)	C2—H2	0.9300

N2—C13	1.466 (3)	C3—H3	0.9300
N1—H1	0.90 (2)	C4—H4	0.9300
C1—C6	1.375 (3)	C5—H5	0.9300
C1—C2	1.371 (3)	C6—H6	0.9300
C2—C3	1.398 (3)	C7—H7	0.9800
C3—C4	1.351 (5)	C9—H9	0.9800
C4—C5	1.354 (5)	C11—H11	0.9300
C5—C6	1.374 (4)	C12—H12	0.9300
C7—C8	1.526 (3)	C14—H14	0.9300
C7—C9	1.565 (3)	C15—H15	0.9300
C9—C10	1.500 (2)		
O1…O2	3.1236 (18)	C12…C14 <sup>vii</sup>	3.589 (3)
O1…N1	3.063 (2)	C14…C12 <sup>vii</sup>	3.589 (3)
O1…C15	3.202 (2)	C15…O1	3.202 (2)
O2…C9 <sup>i</sup>	3.383 (2)	C2…H7	2.7000
O2…O1	3.1236 (18)	C3…H7 <sup>ix</sup>	3.0400
O2…O3 <sup>ii</sup>	3.165 (3)	C4…H7 <sup>ix</sup>	3.0600
O2…N1 <sup>iii</sup>	2.940 (2)	C7…H2	2.5500
O3…O2 <sup>iv</sup>	3.165 (3)	C8…H1 <sup>iii</sup>	2.87 (2)
O4…C8 <sup>v</sup>	3.037 (3)	C8…H11 <sup>i</sup>	2.8500
O4…N1 <sup>v</sup>	3.103 (2)	C9…H2	3.0400
O1…H11 <sup>i</sup>	2.7300	C13…H5 <sup>x</sup>	2.9100
O2…H9 <sup>i</sup>	2.4500	H1…O2 <sup>iii</sup>	2.09 (2)
O2…H11 <sup>i</sup>	2.7000	H1…O3 <sup>vii</sup>	2.79 (2)
O2…H1 <sup>iii</sup>	2.09 (2)	H1…C8 <sup>iii</sup>	2.87 (2)
O3…H4 <sup>vi</sup>	2.7600	H2…C7	2.5500
O3…H12	2.4200	H2…C9	3.0400
O3…H1 <sup>vii</sup>	2.79 (2)	H2…H7	2.2200
O4…H14	2.4400	H4…O3 <sup>vi</sup>	2.7600
N1…O1	3.063 (2)	H5…C13 <sup>x</sup>	2.9100
N1…O4 <sup>viii</sup>	3.103 (2)	H7…C2	2.7000
N1…O2 <sup>iii</sup>	2.940 (2)	H7…H2	2.2200
N1…H15	2.6300	H7…C3 <sup>ix</sup>	3.0400
C1…C10	3.267 (2)	H7…C4 <sup>ix</sup>	3.0600
C2…C9	3.450 (3)	H9…O2 <sup>xi</sup>	2.4500
C2…C10	3.512 (3)	H9…H11	2.4200
C2…C11	3.432 (3)	H11…O1 <sup>xi</sup>	2.7300
C3…C7 <sup>ix</sup>	3.581 (3)	H11…O2 <sup>xi</sup>	2.7000
C5…C5 <sup>x</sup>	3.445 (4)	H11…C8 <sup>xi</sup>	2.8500
C7…C3 <sup>ix</sup>	3.581 (3)	H11…H9	2.4200
C8…O4 <sup>viii</sup>	3.037 (3)	H12…O3	2.4200
C9…C2	3.450 (3)	H14…O4	2.4400
C9…O2 <sup>xi</sup>	3.383 (2)	H14…H15 <sup>xii</sup>	2.5000



## supplementary materials

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C10...C2	3.512 (3)	H15...N1	2.6300
C10...C1	3.267 (2)	H15...H14 <sup>xiii</sup>	2.5000
C11...C2	3.432 (3)		
C1—O1—C7	118.37 (14)	N2—C13—C14	119.22 (17)
C8—N1—C9	96.21 (14)	N2—C13—C12	118.87 (18)
O3—N2—O4	122.8 (2)	C12—C13—C14	121.90 (16)
O3—N2—C13	118.55 (19)	C13—C14—C15	118.61 (17)
O4—N2—C13	118.6 (2)	C10—C15—C14	121.12 (17)
C9—N1—H1	133.2 (13)	C1—C2—H2	121.00
C8—N1—H1	127.4 (13)	C3—C2—H2	121.00
O1—C1—C6	115.25 (17)	C2—C3—H3	119.00
O1—C1—C2	124.64 (17)	C4—C3—H3	119.00
C2—C1—C6	120.10 (18)	C3—C4—H4	120.00
C1—C2—C3	118.4 (2)	C5—C4—H4	120.00
C2—C3—C4	121.3 (3)	C4—C5—H5	120.00
C3—C4—C5	119.6 (3)	C6—C5—H5	120.00
C4—C5—C6	120.8 (3)	C1—C6—H6	120.00
C1—C6—C5	119.8 (2)	C5—C6—H6	120.00
O1—C7—C8	111.02 (15)	O1—C7—H7	113.00
O1—C7—C9	117.47 (13)	C8—C7—H7	113.00
C8—C7—C9	85.24 (13)	C9—C7—H7	113.00
O2—C8—N1	133.27 (18)	N1—C9—H9	112.00
N1—C8—C7	92.45 (14)	C7—C9—H9	112.00
O2—C8—C7	134.29 (17)	C10—C9—H9	112.00
N1—C9—C10	116.21 (14)	C10—C11—H11	120.00
C7—C9—C10	116.46 (14)	C12—C11—H11	119.00
N1—C9—C7	86.05 (13)	C11—C12—H12	121.00
C11—C10—C15	118.48 (15)	C13—C12—H12	121.00
C9—C10—C11	119.25 (14)	C13—C14—H14	121.00
C9—C10—C15	122.23 (14)	C15—C14—H14	121.00
C10—C11—C12	121.01 (17)	C10—C15—H15	119.00
C11—C12—C13	118.85 (18)	C14—C15—H15	119.00
C7—O1—C1—C2	-3.9 (3)	C8—C7—C9—N1	1.65 (12)
C7—O1—C1—C6	175.69 (16)	C8—C7—C9—C10	119.04 (15)
C1—O1—C7—C8	-178.78 (14)	O1—C7—C8—N1	115.82 (15)
C1—O1—C7—C9	-83.06 (19)	O1—C7—C9—C10	7.8 (2)
C9—N1—C8—O2	-177.7 (2)	C9—C7—C8—O2	177.9 (2)
C8—N1—C9—C10	-119.51 (16)	C9—C7—C8—N1	-1.81 (13)
C9—N1—C8—C7	1.93 (14)	O1—C7—C9—N1	-109.59 (16)
C8—N1—C9—C7	-1.89 (13)	N1—C9—C10—C15	25.4 (2)
O3—N2—C13—C12	0.9 (3)	C7—C9—C10—C11	104.01 (19)
O4—N2—C13—C14	0.2 (3)	C7—C9—C10—C15	-73.7 (2)
O4—N2—C13—C12	178.9 (2)	N1—C9—C10—C11	-156.84 (16)
O3—N2—C13—C14	-177.8 (2)	C9—C10—C11—C12	-179.13 (16)
O1—C1—C6—C5	-179.2 (2)	C15—C10—C11—C12	-1.3 (3)
C6—C1—C2—C3	0.6 (3)	C9—C10—C15—C14	178.79 (16)
O1—C1—C2—C3	-179.8 (2)	C11—C10—C15—C14	1.0 (3)
C2—C1—C6—C5	0.4 (3)	C10—C11—C12—C13	0.0 (3)

C1—C2—C3—C4	-0.6 (4)	C11—C12—C13—N2	-177.11 (17)
C2—C3—C4—C5	-0.4 (5)	C11—C12—C13—C14	1.5 (3)
C3—C4—C5—C6	1.4 (5)	N2—C13—C14—C15	176.84 (16)
C4—C5—C6—C1	-1.4 (4)	C12—C13—C14—C15	-1.8 (3)
O1—C7—C8—O2	-64.5 (2)	C13—C14—C15—C10	0.5 (3)

Symmetry codes: (i)  $x-1, y, z$ ; (ii)  $x-1, y-1, z$ ; (iii)  $-x+1, -y, -z$ ; (iv)  $x+1, y+1, z$ ; (v)  $x, y+1, z$ ; (vi)  $-x+2, -y+1, -z+1$ ; (vii)  $-x+2, -y+1, -z$ ; (viii)  $x, y-1, z$ ; (ix)  $-x+1, -y, -z+1$ ; (x)  $-x+1, -y+1, -z+1$ ; (xi)  $x+1, y, z$ ; (xii)  $-x+1, -y+1, -z$ .

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ O2 <sup>iii</sup>	0.90 (2)	2.09 (2)	2.940 (2)	156.9 (18)
C9—H9 $\cdots$ O2 <sup>xi</sup>	0.98	2.45	3.383 (2)	159

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

Fig. 1

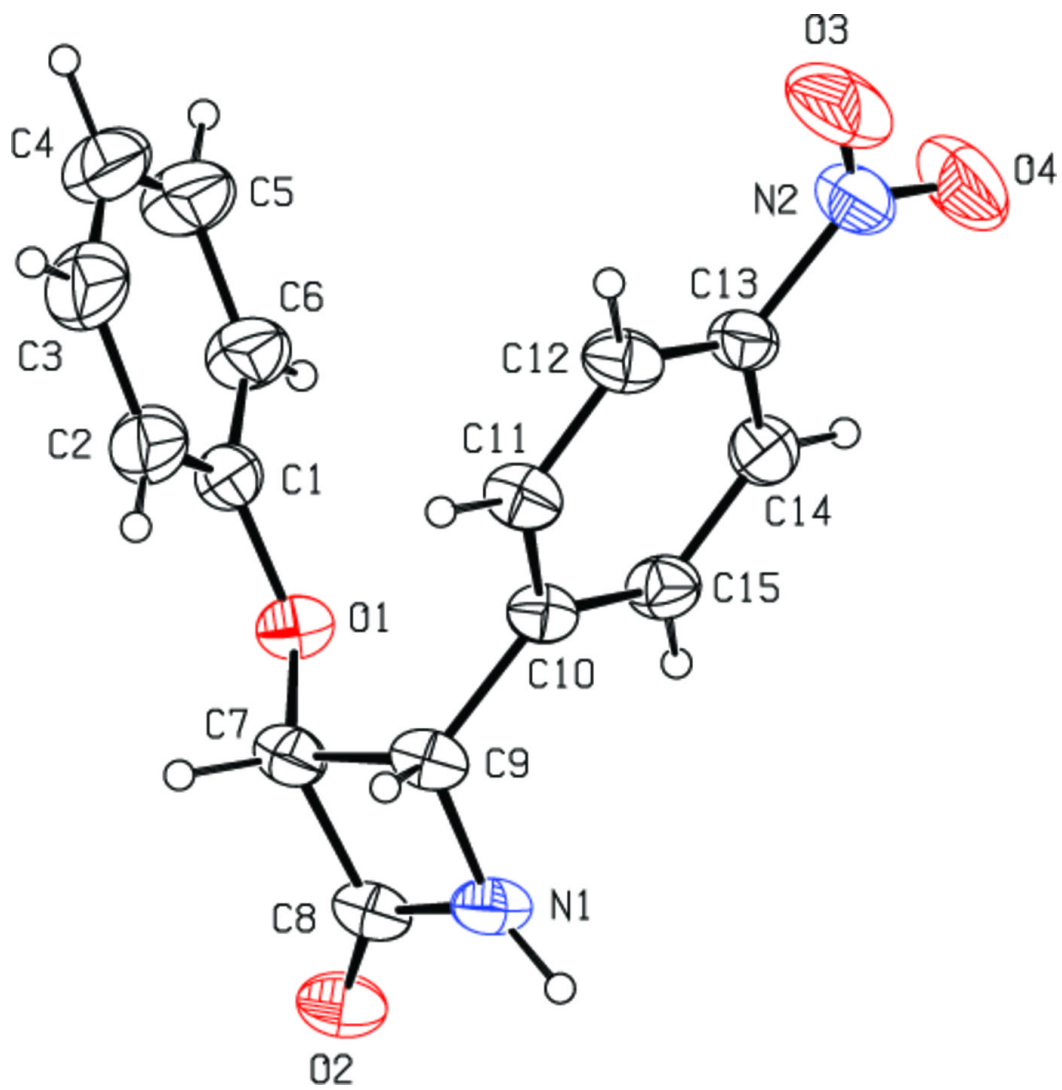


Fig. 2

