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Crystal structure of 3-(4-chlorophenoxy)-4-(2-nitrophenyl)azetidin-2-one with an unknown solvate

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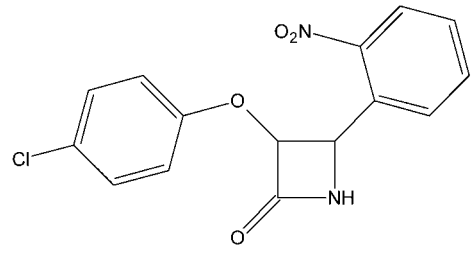
In the title compound, $C_{15}H_{11}ClN_2O_4$, the central β-lactam ring is approximately planar [maximum deviation = 0.044 (2) Å for the N atom from the mean plane] and subtends dihedral angles of 61.17 (11) and 40.21 (12) °, respectively, with the nitro and chlorobenzene rings. Both substituents lie to the same side of the β-lactam core. In the crystal, N—H···O hydrogen bonds link the molecules into $C(4)$ chains propagating in [010]. The chains are cross-linked by C—H···O and weak C—H···π interactions, generating a three-dimensional network. The solvent molecules were found to be highly disordered and their contribution to the scattering was removed with the SQUEEZE procedure in *PLATON* [Spek (2009). *Acta Cryst.* D**65**, 148–155], which indicated a solvent cavity of volume 318 Å^3 containing approximately 114 electrons. These solvent molecules are not considered in the given chemical formula and other crystal data.

Keywords: crystal structure; β-lactam ring; $C(4)$ chain; hydrogen bonding; N-unsubstituted 2-azetidinone; hydrogen bonds; C—H···π interactions.

CCDC reference: 1036035

1. Related literature

For the application of N-unsubstituted 2-azetidinones in the synthesis of β-lactam antibiotics, see: Cossio *et al.* (1987); Jarrahpour & Zarei (2007, 2008). For a related structure with a β-lactam ring, see: Butcher *et al.* (2011).



2. Experimental

2.1. Crystal data

$C_{15}H_{11}ClN_2O_4$
M_r = 318.71
Monoclinic, $P2_1/n$
a = 16.9505 (4) Å
b = 4.6517 (1) Å
c = 21.7167 (6) Å
β = 99.757 (1)°
V = 1687.56 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 K
0.30 × 0.20 × 0.15 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
16293 measured reflections
4358 independent reflections
3158 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.135
S = 1.04
4358 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

Cg2 is the centroid of the nitrobenzene ring (C4–C9).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.09	2.936 (2)	166
C8—H8···O3^{ii}	0.93	2.53	3.307 (2)	142
C15—H15···O2^{iii}	0.93	2.51	3.338 (2)	149
C3—H3···*Cg2*^{iv}	0.98	2.70	3.5118 (19)	141

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7322).

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supporting information

Acta Cryst. (2015). E**71**, o8–o9 [doi:10.1107/S2056989014025845]

Crystal structure of 3-(4-chlorophenoxy)-4-(2-nitrophenyl)azetidin-2-one with an unknown solvate

Sevim Türktekin Çelikesir, Mehmet Akkurt, Aliasghar Jarrahpour, Habib Allah Shafie and Ömer Çelik

S1. Comment

N-Unsubstituted 2-azetidinones offer major synthetic opportunities in the synthesis of *β*-lactam antibiotics such as the carbapenems, penams, monobactams, nocardicins, and the glutamine synthetase inhibitor, tabtoxin (Cossio, *et al.*, 1987) The application of N-unsubstituted 2-azetidinones in the semi-synthesis of the anticancer agents, Taxol and Taxotere has also been reported (Jarrahpour, *et al.*, 2007). N-Unsubstituted 2-azetidinones have been prepared by several methods. Among these methods, oxidative cleavage by ceric ammonium nitrate (CAN) of *p*-alkoxyphenyl moiety attached to the nitrogen of the *β*-lactam ring offers the most direct synthesis of N-unsubstituted *β*-lactams (Jarrahpour, *et al.*, 2008).

In the title compound (Fig. 1), the *β*-lactam ring is nearly planar with a maximum deviation of 0.044 (2) Å for N1 from the mean plane. The carboxyl O atom O1 attached to the *β*-lactam ring deviates by -0.137 (1) Å from the mean plane of the ring. The *β*-lactam ring makes dihedral angles of 61.17 (11) and 40.21 (12) ° with the nitro and choloro-benzene rings, respectively.

All bond lengths and angles are comparable with those reported in a related structure (Butcher *et al.*, 2011).

In the crystal, molecules are linked into [010] *C*(4) chains by N—H···O hydrogen bonds. C—H···O hydrogen bonds (Fig. 2) and weak C—H···*π* interactions link the chains into a three-dimensional network (Table 1).

S2. Experimental

A solution of $(NH_4)_2Ce(NO_3)_6$ (CAN) (3.00 mmol) in water (15.00 ml) was added dropwise to a solution of *β*-lactam (1.00 mmol) in CH_3CN (30.00 ml) at room temperature and stirred for 45 min. Then water (30.00 ml) was added and the mixture was extracted with EtOAc (3 × 20 ml) and washed with 10% of $NaHCO_3$ (40 ml). The aqueous layer of $NaHCO_3$ was extracted again with EtOAc (15 ml), and all organic extracts were combined and washed successively with 10% $NaHSO_3$ (2×30 ml), 10% $NaHCO_3$ (20 ml), brine (20 ml) and then dried over sodium sulfate. After filtration and evaporation of the solvent in vacuo, the crude product was purified by column chromatography or recrystallization from hexane/EtOAc (4:6) solution to give colourless prisms (Yield 75%). Mp 350–352 K IR (KBr, cm^{-1}): 1774 (CO *β*-lactam), 3217 (NH). ^{1}H NMR (250 MHz, DMSO-d_6) *δ*(p.p.m.): 5.74 (H-3, d, 1H, J=5.5 Hz), 6.23 (H-4, d, 1H, J=5.5 Hz), 7.27–8.15 (aromatic H, m, 8H), 9.13 (NH, brs, 1H). ^{13}C NMR (62.9 MHz, DMSO-d_6) *δ*(p.p.m.): 54.60 (C-4), 83.18 (C-3), 117.5, 124.7, 125.9, 128.7, 128.9, 129.1, 132.8, 134.4, 147.4, 155.8 (aromatic carbons), 165.90 (CO, *β*- lactam). Analysis calculated for $C_{15}H_{11}ClN_2O_4$: C, 51.01; H, 2.85; N, 7.93%. Found: C, 51.03; H, 2.87; N, 7.91%.

S3. Refinement

C and N-bound H atoms were positioned geometrically (C—H = 0.93 - 0.98 Å and N—H =0.86 Å), and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C,*N*). The twenty two reflections were omitted owing to bad disagreement. The crystal

quality and data was not good enough. A region of disordered electron density, most probably disordered solvent molecules, occupying voids of *ca* 318 Å^3 for an electron count of 114, was removed with the SQUEEZE procedure in *PLATON* [Spek (2009). Acta Cryst. D65, 148–155] following unsuccessful attempts to model it as a plausible solvent molecule. Their formula mass and unit-cell characteristics were not taken into account during refinement.

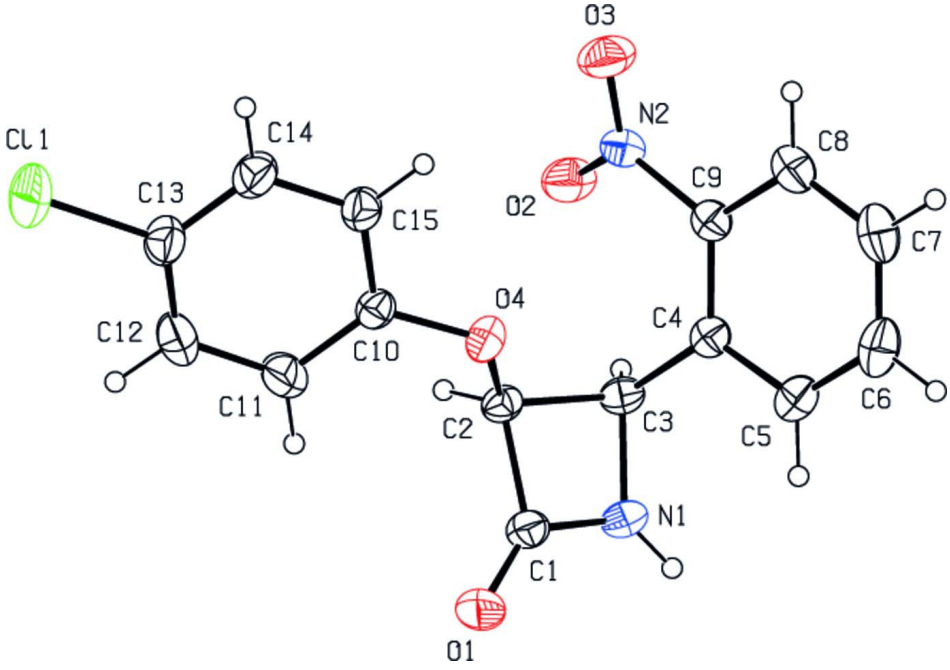

Figure 1

View of the title compound with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

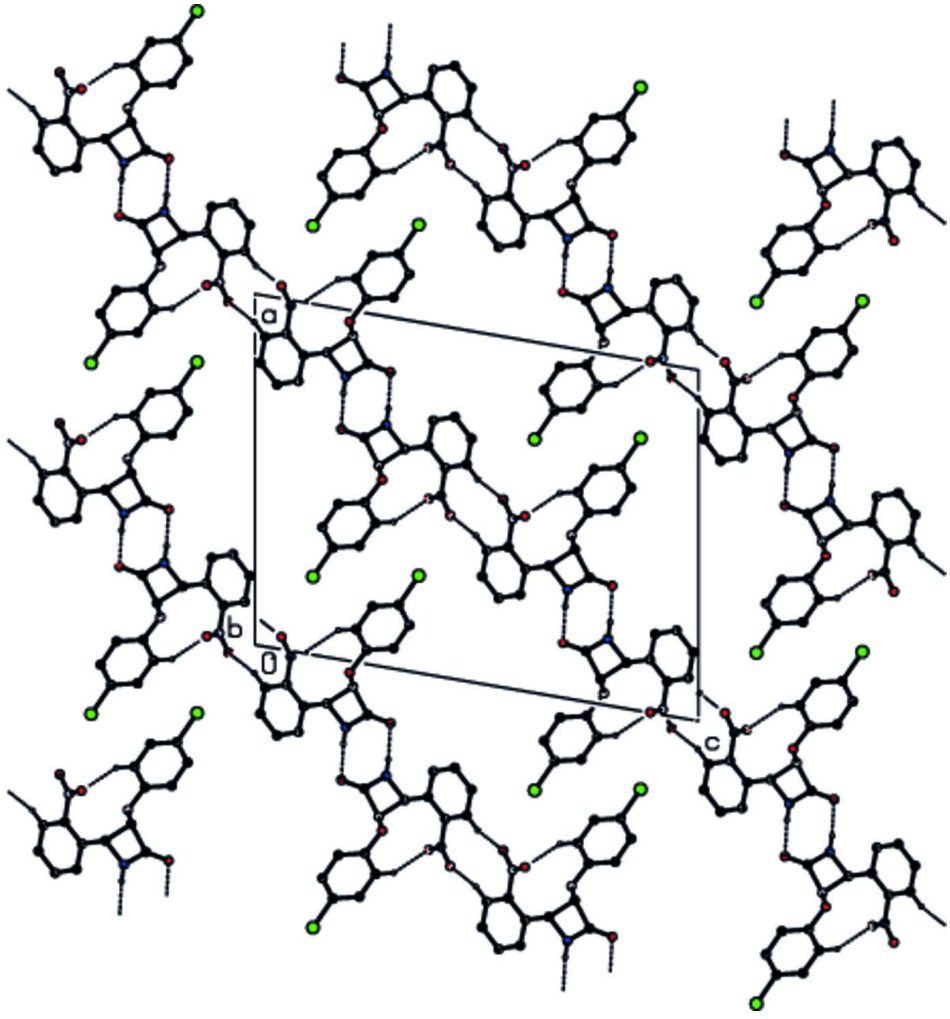

Figure 2

View of the hydrogen bonding of the title compound along *b* axis. Only H atoms involved in H bonding are shown.

3-(4-chlorophenoxy)-4-(2-nitrophenyl)azetidin-2-one

Crystal data

$C_{15}H_{11}ClN_2O_4$
M_r = 318.71
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 16.9505 (4) Å
b = 4.6517 (1) Å
c = 21.7167 (6) Å
β = 99.757 (1)°
V = 1687.56 (7) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.254 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6230 reflections
θ = 2.4–28.7°
μ = 0.24 mm^{-1}
T = 296 K
Prism, colourless
0.30 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
16293 measured reflections

4358 independent reflections
3158 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 28.8°$, $\theta_{min} = 1.7°$
$h = -21 \rightarrow 22$
$k = -6 \rightarrow 6$
$l = -28 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.135$
$S = 1.04$
4358 reflections
199 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2 + 0.3362P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.77735 (3)	0.02466 (16)	0.86934 (3)	0.0896 (2)
O1	0.34325 (8)	0.4694 (3)	0.80529 (6)	0.0684 (5)
O2	0.49880 (7)	0.6846 (3)	0.60857 (6)	0.0615 (5)
O3	0.53550 (8)	0.3225 (3)	0.55969 (6)	0.0686 (5)
O4	0.46717 (6)	0.2832 (2)	0.71337 (5)	0.0437 (3)
N1	0.30955 (8)	0.6612 (4)	0.70465 (6)	0.0523 (5)
N2	0.48444 (8)	0.4599 (3)	0.58069 (6)	0.0440 (4)
C1	0.35588 (9)	0.5438 (4)	0.75408 (7)	0.0462 (5)
C2	0.42874 (8)	0.5444 (3)	0.72098 (7)	0.0374 (4)
C3	0.36874 (9)	0.6469 (4)	0.66256 (7)	0.0399 (5)
C4	0.34857 (9)	0.4352 (3)	0.60981 (7)	0.0377 (4)
C5	0.27331 (10)	0.3099 (4)	0.59775 (8)	0.0503 (5)
C6	0.25251 (11)	0.1159 (5)	0.54958 (9)	0.0632 (7)
C7	0.30631 (13)	0.0396 (4)	0.51201 (9)	0.0625 (7)
C8	0.38224 (11)	0.1547 (4)	0.52289 (7)	0.0509 (6)
C9	0.40248 (9)	0.3484 (3)	0.57097 (7)	0.0387 (5)
C10	0.54003 (8)	0.2358 (3)	0.75211 (7)	0.0387 (4)
C11	0.55796 (12)	0.3387 (5)	0.81220 (8)	0.0661 (7)
C12	0.63188 (13)	0.2760 (6)	0.84797 (8)	0.0733 (8)
C13	0.68458 (10)	0.1055 (5)	0.82418 (8)	0.0559 (6)
C14	0.66690 (10)	0.0022 (4)	0.76469 (9)	0.0555 (6)
C15	0.59401 (9)	0.0697 (4)	0.72819 (8)	0.0470 (5)

H1	0.26120	0.72420	0.69920	0.0630*
H2	0.46700	0.69550	0.73710	0.0450*
H3	0.38230	0.83720	0.64800	0.0480*
H5	0.23580	0.35770	0.62280	0.0600*
H6	0.20140	0.03640	0.54260	0.0760*
H7	0.29160	−0.08920	0.47930	0.0750*
H8	0.41950	0.10220	0.49800	0.0610*
H11	0.52090	0.44930	0.82870	0.0790*
H12	0.64530	0.35050	0.88810	0.0880*
H14	0.70350	−0.11280	0.74870	0.0670*
H15	0.58190	0.00190	0.68740	0.0560*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0624 (3)	0.1234 (6)	0.0723 (3)	0.0190 (3)	−0.0193 (3)	0.0066 (3)
O1	0.0550 (7)	0.1050 (12)	0.0494 (7)	−0.0149 (7)	0.0209 (6)	0.0013 (7)
O2	0.0577 (7)	0.0584 (9)	0.0733 (8)	−0.0162 (6)	0.0251 (6)	−0.0204 (7)
O3	0.0539 (7)	0.0755 (10)	0.0824 (9)	0.0055 (7)	0.0291 (7)	−0.0164 (8)
O4	0.0356 (5)	0.0379 (7)	0.0547 (6)	0.0017 (5)	−0.0002 (4)	−0.0061 (5)
N1	0.0371 (7)	0.0678 (11)	0.0547 (8)	0.0115 (7)	0.0153 (6)	−0.0048 (7)
N2	0.0467 (7)	0.0474 (9)	0.0407 (6)	−0.0008 (6)	0.0152 (5)	0.0008 (6)
C1	0.0378 (8)	0.0556 (11)	0.0471 (8)	−0.0065 (7)	0.0130 (6)	−0.0086 (8)
C2	0.0338 (7)	0.0349 (9)	0.0448 (7)	−0.0034 (6)	0.0107 (6)	−0.0054 (6)
C3	0.0388 (7)	0.0364 (9)	0.0468 (8)	0.0046 (6)	0.0139 (6)	0.0006 (7)
C4	0.0385 (7)	0.0336 (8)	0.0408 (7)	0.0029 (6)	0.0058 (6)	0.0060 (6)
C5	0.0383 (8)	0.0536 (11)	0.0582 (9)	0.0017 (7)	0.0057 (7)	0.0038 (8)
C6	0.0496 (10)	0.0607 (13)	0.0722 (12)	−0.0118 (9)	−0.0102 (9)	0.0016 (10)
C7	0.0732 (13)	0.0551 (12)	0.0522 (9)	−0.0058 (10)	−0.0093 (9)	−0.0082 (9)
C8	0.0623 (10)	0.0483 (11)	0.0408 (8)	0.0036 (9)	0.0051 (7)	−0.0030 (7)
C9	0.0431 (8)	0.0354 (9)	0.0375 (7)	0.0016 (7)	0.0065 (6)	0.0032 (6)
C10	0.0348 (7)	0.0390 (9)	0.0424 (7)	−0.0039 (6)	0.0069 (6)	0.0008 (6)
C11	0.0613 (11)	0.0918 (17)	0.0446 (9)	0.0206 (11)	0.0075 (8)	−0.0113 (10)
C12	0.0692 (12)	0.1051 (19)	0.0405 (9)	0.0120 (12)	−0.0056 (8)	−0.0085 (10)
C13	0.0451 (9)	0.0680 (13)	0.0511 (9)	0.0025 (9)	−0.0021 (7)	0.0074 (9)
C14	0.0402 (8)	0.0628 (13)	0.0621 (10)	0.0075 (8)	0.0050 (7)	−0.0067 (9)
C15	0.0396 (8)	0.0516 (11)	0.0481 (8)	−0.0014 (7)	0.0030 (6)	−0.0101 (8)

Geometric parameters (Å, º)

Cl1—C13	1.7474 (18)	C8—C9	1.378 (2)
O1—C1	1.218 (2)	C10—C15	1.366 (2)
O2—N2	1.2118 (19)	C10—C11	1.375 (2)
O3—N2	1.2245 (19)	C11—C12	1.389 (3)
O4—C2	1.4016 (17)	C12—C13	1.360 (3)
O4—C10	1.3891 (18)	C13—C14	1.363 (3)
N1—C1	1.335 (2)	C14—C15	1.386 (2)
N1—C3	1.469 (2)	C2—H2	0.9800

N2—C9	1.464 (2)	C3—H3	0.9800
C1—C2	1.531 (2)	C5—H5	0.9300
N1—H1	0.8600	C6—H6	0.9300
C2—C3	1.560 (2)	C7—H7	0.9300
C3—C4	1.505 (2)	C8—H8	0.9300
C4—C5	1.387 (2)	C11—H11	0.9300
C4—C9	1.404 (2)	C12—H12	0.9300
C5—C6	1.381 (3)	C14—H14	0.9300
C6—C7	1.370 (3)	C15—H15	0.9300
C7—C8	1.377 (3)		

C2—O4—C10	116.71 (11)	C10—C11—C12	119.42 (18)
C1—N1—C3	96.38 (13)	C11—C12—C13	119.89 (18)
O2—N2—O3	122.79 (14)	Cl1—C13—C14	119.24 (15)
O2—N2—C9	118.87 (13)	Cl1—C13—C12	119.92 (14)
O3—N2—C9	118.34 (13)	C12—C13—C14	120.82 (17)
O1—C1—N1	132.86 (15)	C13—C14—C15	119.57 (17)
O1—C1—C2	135.24 (15)	C10—C15—C14	120.02 (16)
N1—C1—C2	91.90 (12)	O4—C2—H2	112.00
C1—N1—H1	132.00	C1—C2—H2	112.00
C3—N1—H1	132.00	C3—C2—H2	112.00
O4—C2—C1	118.81 (12)	N1—C3—H3	112.00
O4—C2—C3	114.90 (12)	C2—C3—H3	112.00
C1—C2—C3	85.17 (11)	C4—C3—H3	112.00
N1—C3—C2	85.85 (11)	C4—C5—H5	119.00
C2—C3—C4	116.85 (14)	C6—C5—H5	119.00
N1—C3—C4	114.34 (14)	C5—C6—H6	120.00
C3—C4—C9	123.94 (14)	C7—C6—H6	120.00
C3—C4—C5	120.12 (14)	C6—C7—H7	120.00
C5—C4—C9	115.94 (14)	C8—C7—H7	120.00
C4—C5—C6	121.75 (16)	C7—C8—H8	120.00
C5—C6—C7	120.68 (18)	C9—C8—H8	120.00
C6—C7—C8	119.63 (18)	C10—C11—H11	120.00
C7—C8—C9	119.33 (16)	C12—C11—H11	120.00
N2—C9—C8	116.69 (14)	C11—C12—H12	120.00
C4—C9—C8	122.66 (15)	C13—C12—H12	120.00
N2—C9—C4	120.65 (13)	C13—C14—H14	120.00
C11—C10—C15	120.23 (15)	C15—C14—H14	120.00
O4—C10—C11	123.40 (14)	C10—C15—H15	120.00
O4—C10—C15	116.34 (13)	C14—C15—H15	120.00

C10—O4—C2—C3	156.31 (12)	C2—C3—C4—C9	−70.06 (19)
C2—O4—C10—C11	32.5 (2)	C3—C4—C9—N2	1.0 (2)
C2—O4—C10—C15	−149.62 (14)	C3—C4—C9—C8	−179.81 (15)
C10—O4—C2—C1	−105.11 (15)	C3—C4—C5—C6	179.68 (17)
C3—N1—C1—C2	6.71 (14)	C9—C4—C5—C6	−1.2 (2)
C3—N1—C1—O1	−173.8 (2)	C5—C4—C9—N2	−178.08 (14)
C1—N1—C3—C2	−6.60 (14)	C5—C4—C9—C8	1.1 (2)

C1—N1—C3—C4	111.06 (16)	C4—C5—C6—C7	0.3 (3)
O3—N2—C9—C4	158.62 (14)	C5—C6—C7—C8	0.8 (3)
O2—N2—C9—C8	158.71 (15)	C6—C7—C8—C9	−0.9 (3)
O3—N2—C9—C8	−20.7 (2)	C7—C8—C9—C4	−0.1 (2)
O2—N2—C9—C4	−22.0 (2)	C7—C8—C9—N2	179.17 (15)
N1—C1—C2—C3	−6.30 (14)	O4—C10—C11—C12	178.78 (18)
N1—C1—C2—O4	−122.13 (15)	C15—C10—C11—C12	1.0 (3)
O1—C1—C2—O4	58.4 (3)	O4—C10—C15—C14	−177.37 (15)
O1—C1—C2—C3	174.2 (2)	C11—C10—C15—C14	0.6 (3)
O4—C2—C3—N1	125.34 (13)	C10—C11—C12—C13	−2.4 (3)
C1—C2—C3—N1	5.73 (12)	C11—C12—C13—Cl1	−179.60 (18)
C1—C2—C3—C4	−109.51 (14)	C11—C12—C13—C14	2.2 (4)
O4—C2—C3—C4	10.09 (19)	Cl1—C13—C14—C15	−178.84 (15)
N1—C3—C4—C9	−168.11 (14)	C12—C13—C14—C15	−0.6 (3)
C2—C3—C4—C5	108.95 (17)	C13—C14—C15—C10	−0.8 (3)
N1—C3—C4—C5	10.9 (2)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the nitrobenzene ring (C4–C9).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.09	2.936 (2)	166
C8—H8···O3^{ii}	0.93	2.53	3.307 (2)	142
C15—H15···O2^{iii}	0.93	2.51	3.338 (2)	149
C3—H3···*Cg*2^{iv}	0.98	2.70	3.5118 (19)	141

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