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5-(2-Hydroxy-5-methoxybenzoyl)-1-methyl-3-nitropyridin-2(1*H*)-one

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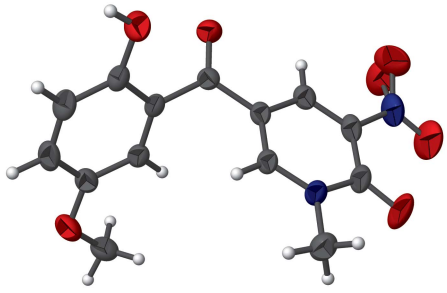
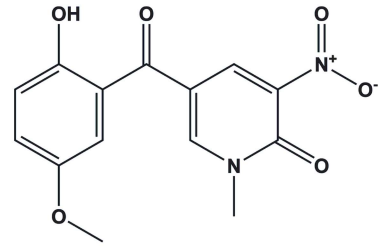
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{14}H_{12}N_2O_6$, the dihedral angle between the benzene and pyridine rings is 65.90 (7)°. The nitro group is disordered and tilted with respect to the mean plane of the pyridine ring by 21.5 (4) and 22.8 (5)°, for the major and minor components, respectively. In the crystal, molecules are linked by O—H···N hydrogen bonds, forming chains propagating along [10$\bar{1}$]. The chains are linked by C—H···O hydrogen bonds, forming a three-dimensional framework. The crystal packing is further stabilized by offset π–π stacking interactions [intercentroid distance = 3.6291 (9) Å]

3D view



Chemical scheme



Structure description

The pyridine skeleton is of great importance in clinically useful molecules having diverse biological activities (Patoliya *et al.*, 2015). Pyridine derivatives possess analgesic (Ajitkumar & Pandeya, 2011), anticancer (Hammam *et al.*, 2001), antimicrobial and antioxidative (Prachayasittikul *et al.*, 2008) activities. Pyridoxine, a derivative of pyridine, is an active neutraceutical found in the form of vitamin B3 (Chaubey *et al.*, 2011). Pyridine fused-ring systems act as chemotherapeutic agents (Kumar *et al.*, 2011). Picryl amino pyridines and their *N*-oxides possess antibacterial and antifungal (Badgujar *et al.*, 2010) activities. Pyridine congeners are associated with pesticidal, insecticidal and fungicidal properties (Pradhan *et al.*, 2012). As part of our studies in this area, we describe herein the synthesis and crystal structure of the title nitropyridine derivative.

In the title compound, Fig. 1, the dihedral angle between the benzene (C1–C6) and pyridine (N1/C8–C12) rings is 65.90 (7)°. Atom O6 of the nitro group is disordered, and the NO_2 groups are tilted with respect to the mean plane of the pyridine ring by 21.5 (4) and 22.8 (5)°, for the major (N2/O5/O6*A*) and minor (N2/O5/O6*B*) components,

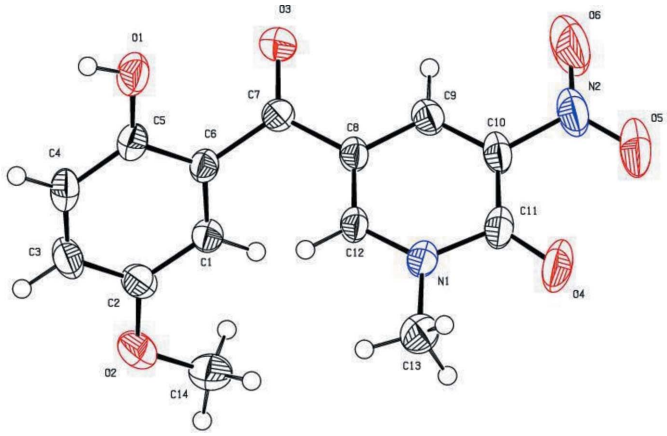


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

respectively. The methyl carbon atom C13 deviates from the plane of the pyridine ring by 0.070 (2) Å. The C14—O2—C2—C3 torsion angle of 178.54 (15)° indicates that the methoxy group (–O2—C14) is not quite coplanar with the phenol ring.

In the crystal, molecules are linked by O—H···N hydrogen bonds, forming chains propagating along [10$\bar{1}$]; see Fig. 2 and Table 1. The chains are linked by C—H···O hydrogen bonds forming a three-dimensional framework (Table 1 and Fig. 3). The crystal packing also features offset π–π stacking interactions [$Cg1\cdots Cg2^{iii}$ = 3.6291 (9) Å, interplanar distance = 3.4403 (6) Å, slippage = 1.111 Å, $Cg1$ and $Cg2$ are the centroids of rings N1/C8—C12 and C1—C6, respectively, symmetry code: (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$]

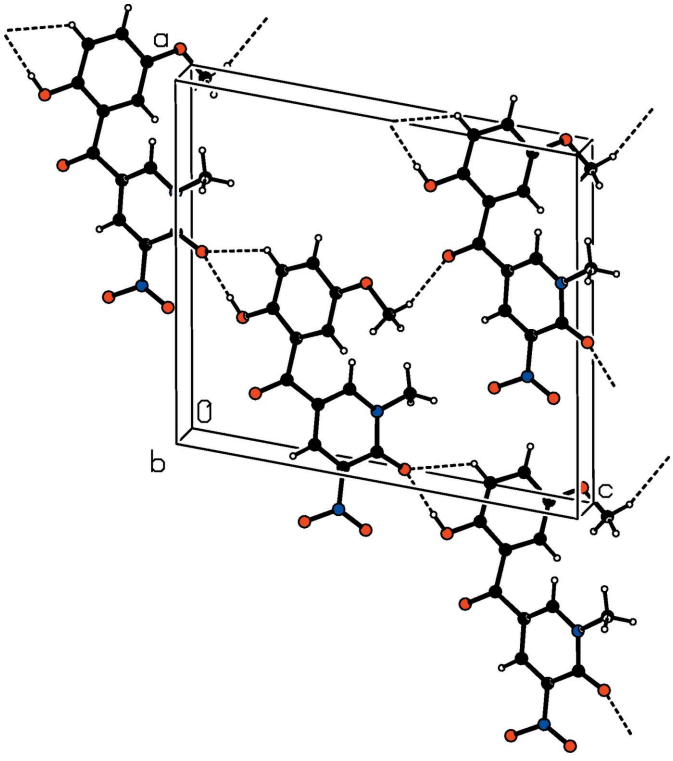


Figure 2
A partial view along the *b* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O4^{i}	0.83 (2)	1.87 (2)	2.6948 (17)	173 (2)
C4—H4···O4^{i}	0.93	2.56	3.233 (2)	129
C14—H14B···O3^{ii}	0.96	2.41	3.319 (2)	158

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

Synthesis and crystallization

A mixture of 6-methoxy-3-formylchromone (1 mmol), (*Z*)-*N*-methyl-1-(methylthio)-2-nitroethenamine (1 mmol), and indium trifluoromethanesulfonate (0.020 mmol) in ethanol (3 ml) were heated at reflux, and the resulting solution was stirred for 1 h. The consumption of the starting material was monitored by TLC. After completion of the reaction, the

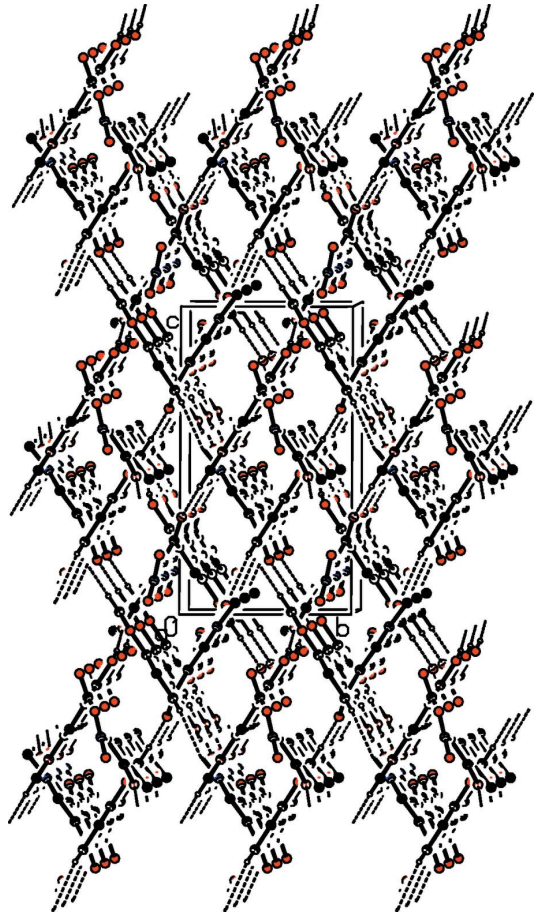


Figure 3
A view along the *a* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only the H atoms involved in hydrogen bonding are shown.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{12}N_2O_6$
M_r	304.26
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	12.5891 (4), 7.7739 (2), 14.1240 (4)
β (°)	100.466 (1)
V (Å^3)	1359.27 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.12
Crystal size (mm)	0.30 × 0.25 × 0.25
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.965, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10209, 2603, 2210
R_{int}	0.017
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.612
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.116, 1.07
No. of reflections	2603
No. of parameters	215
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

compound obtained was purified by column chromatography to obtain pure product in good yield (78%). The purified compound was recrystallized from the mixed solvents of ethanol and DMSO-D_6. On slow evaporation of the solvents, block-like colourless crystals of the title compound were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atom O6 of the NO_2 group was split over two positions and refined with a fixed occupancy ratio of O6*A*:O6*B* = 0.6:0.4.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{14}H_{12}N_2O_6$
M_r = 304.26
Monoclinic, $P2_1/n$
a = 12.5891 (4) Å
b = 7.7739 (2) Å
c = 14.1240 (4) Å
β = 100.466 (1)°
V = 1359.27 (7) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.487 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2062 reflections
θ = 2.0–25.0°
μ = 0.12 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.25 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.965, T_{max} = 0.971
10209 measured reflections
2603 independent reflections
2210 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.8°, θ_{min} = 2.0°
h = −15→11
k = −9→9
l = −17→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.07
2603 reflections
215 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.5029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0065 (17)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.34903 (10)	0.35190 (18)	0.14070 (9)	0.0491 (4)	
H1O	0.3954 (19)	0.328 (3)	0.1083 (17)	0.073 (7)*	
O2	0.52579 (9)	0.72712 (18)	0.46370 (9)	0.0506 (3)	
O3	0.15540 (9)	0.52987 (17)	0.17871 (8)	0.0450 (3)	
O4	0.00621 (11)	0.1998 (2)	0.53725 (10)	0.0699 (5)	
O5	−0.17278 (12)	0.3564 (3)	0.44625 (13)	0.0941 (6)	
O6A	−0.1779 (5)	0.4205 (9)	0.2961 (4)	0.097 (2)	0.6
O6B	−0.1684 (7)	0.4936 (10)	0.3255 (5)	0.077 (2)	0.4
N1	0.15383 (10)	0.24178 (17)	0.47099 (9)	0.0345 (3)	
N2	−0.12793 (12)	0.3882 (2)	0.37995 (13)	0.0554 (4)	
C1	0.36915 (12)	0.5983 (2)	0.36290 (10)	0.0326 (3)	
H1	0.3237	0.6360	0.4037	0.039*	
C2	0.47843 (12)	0.6343 (2)	0.38467 (11)	0.0373 (4)	
C3	0.54549 (12)	0.5717 (2)	0.32474 (12)	0.0442 (4)	
H3	0.6192	0.5939	0.3394	0.053*	
C4	0.50445 (13)	0.4774 (2)	0.24408 (12)	0.0428 (4)	
H4	0.5509	0.4351	0.2054	0.051*	
C5	0.39424 (12)	0.4444 (2)	0.21954 (11)	0.0350 (4)	
C6	0.32676 (11)	0.50583 (19)	0.28016 (10)	0.0301 (3)	
C7	0.20704 (11)	0.48412 (19)	0.25570 (10)	0.0310 (3)	
C8	0.15132 (11)	0.40964 (19)	0.33026 (10)	0.0303 (3)	
C9	0.03961 (12)	0.4296 (2)	0.32247 (11)	0.0355 (4)	
H9	0.0005	0.4898	0.2707	0.043*	
C10	−0.01181 (12)	0.3610 (2)	0.39050 (12)	0.0387 (4)	
C11	0.04319 (13)	0.2634 (2)	0.47101 (12)	0.0406 (4)	
C12	0.20469 (11)	0.31358 (19)	0.40519 (10)	0.0310 (3)	
H12	0.2788	0.2975	0.4107	0.037*	
C13	0.21453 (15)	0.1356 (3)	0.54895 (13)	0.0497 (5)	
H13A	0.2888	0.1289	0.5417	0.075*	
H13B	0.1841	0.0220	0.5459	0.075*	
H13C	0.2102	0.1866	0.6100	0.075*	
C14	0.45551 (15)	0.7941 (3)	0.52332 (12)	0.0505 (5)	
H14A	0.4037	0.8696	0.4862	0.076*	
H14B	0.4970	0.8567	0.5759	0.076*	
H14C	0.4185	0.7010	0.5480	0.076*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0419 (7)	0.0648 (9)	0.0456 (7)	−0.0080 (6)	0.0214 (6)	−0.0176 (6)
O2	0.0350 (6)	0.0647 (8)	0.0491 (7)	−0.0081 (6)	−0.0002 (5)	−0.0084 (6)
O3	0.0360 (6)	0.0615 (8)	0.0359 (6)	−0.0013 (5)	0.0025 (5)	0.0080 (5)
O4	0.0531 (8)	0.0988 (12)	0.0680 (9)	0.0020 (8)	0.0378 (7)	0.0260 (8)
O5	0.0414 (8)	0.1529 (19)	0.0978 (13)	0.0083 (10)	0.0385 (8)	0.0166 (12)
O6A	0.0331 (16)	0.187 (7)	0.069 (3)	0.015 (3)	0.0041 (16)	−0.001 (3)

O6B	0.035 (3)	0.108 (5)	0.091 (5)	0.021 (3)	0.018 (3)	0.035 (4)
N1	0.0333 (7)	0.0381 (7)	0.0343 (7)	−0.0014 (6)	0.0124 (5)	−0.0002 (6)
N2	0.0297 (8)	0.0688 (11)	0.0716 (11)	0.0007 (8)	0.0197 (8)	−0.0014 (9)
C1	0.0295 (7)	0.0369 (8)	0.0322 (7)	0.0008 (6)	0.0078 (6)	0.0033 (6)
C2	0.0317 (8)	0.0398 (9)	0.0386 (8)	−0.0022 (7)	0.0021 (6)	0.0050 (7)
C3	0.0249 (7)	0.0540 (10)	0.0543 (10)	−0.0024 (7)	0.0088 (7)	0.0061 (8)
C4	0.0329 (8)	0.0509 (10)	0.0494 (10)	0.0011 (7)	0.0200 (7)	0.0007 (8)
C5	0.0345 (8)	0.0374 (8)	0.0357 (8)	−0.0017 (7)	0.0137 (6)	0.0033 (6)
C6	0.0282 (7)	0.0328 (8)	0.0308 (7)	−0.0005 (6)	0.0096 (6)	0.0052 (6)
C7	0.0305 (7)	0.0329 (8)	0.0297 (7)	0.0001 (6)	0.0063 (6)	−0.0019 (6)
C8	0.0261 (7)	0.0334 (8)	0.0329 (8)	−0.0012 (6)	0.0096 (6)	−0.0056 (6)
C9	0.0287 (7)	0.0388 (8)	0.0394 (8)	0.0005 (6)	0.0067 (6)	−0.0035 (7)
C10	0.0260 (8)	0.0435 (9)	0.0493 (9)	−0.0020 (7)	0.0144 (7)	−0.0082 (7)
C11	0.0354 (8)	0.0470 (10)	0.0443 (9)	−0.0048 (7)	0.0202 (7)	−0.0037 (7)
C12	0.0265 (7)	0.0354 (8)	0.0334 (7)	−0.0009 (6)	0.0121 (6)	−0.0044 (6)
C13	0.0462 (10)	0.0589 (11)	0.0445 (10)	0.0003 (9)	0.0097 (8)	0.0139 (8)
C14	0.0500 (10)	0.0590 (12)	0.0400 (9)	−0.0072 (9)	0.0015 (8)	−0.0078 (8)

Geometric parameters (Å, º)

O1—C5	1.3602 (19)	C3—H3	0.9300
O1—H1O	0.83 (2)	C4—C5	1.392 (2)
O2—C2	1.3714 (19)	C4—H4	0.9300
O2—C14	1.426 (2)	C5—C6	1.395 (2)
O3—C7	1.2144 (18)	C6—C7	1.493 (2)
O4—C11	1.223 (2)	C7—C8	1.485 (2)
O5—N2	1.204 (2)	C8—C12	1.368 (2)
O6A—N2	1.261 (6)	C8—C9	1.399 (2)
O6B—N2	1.174 (8)	C9—C10	1.361 (2)
N1—C12	1.3421 (19)	C9—H9	0.9300
N1—C11	1.403 (2)	C10—C11	1.436 (2)
N1—C13	1.474 (2)	C12—H12	0.9300
N2—C10	1.458 (2)	C13—H13A	0.9600
C1—C2	1.383 (2)	C13—H13B	0.9600
C1—C6	1.393 (2)	C13—H13C	0.9600
C1—H1	0.9300	C14—H14A	0.9600
C2—C3	1.388 (2)	C14—H14B	0.9600
C3—C4	1.374 (2)	C14—H14C	0.9600
C5—O1—H1O	110.0 (16)	O3—C7—C6	121.85 (13)
C2—O2—C14	116.63 (12)	C8—C7—C6	117.83 (12)
C12—N1—C11	123.28 (13)	C12—C8—C9	117.83 (14)
C12—N1—C13	120.16 (13)	C12—C8—C7	122.20 (13)
C11—N1—C13	116.56 (13)	C9—C8—C7	119.90 (13)
O6B—N2—O5	116.3 (4)	C10—C9—C8	120.08 (15)
O5—N2—O6A	123.1 (3)	C10—C9—H9	120.0
O6B—N2—C10	118.4 (4)	C8—C9—H9	120.0
O5—N2—C10	119.62 (17)	C9—C10—C11	122.90 (14)

O6A—N2—C10	116.4 (3)	C9—C10—N2	117.90 (15)
C2—C1—C6	120.33 (14)	C11—C10—N2	119.20 (15)
C2—C1—H1	119.8	O4—C11—N1	117.87 (16)
C6—C1—H1	119.8	O4—C11—C10	128.61 (16)
O2—C2—C1	123.73 (15)	N1—C11—C10	113.53 (13)
O2—C2—C3	117.28 (14)	N1—C12—C8	122.26 (13)
C1—C2—C3	118.98 (15)	N1—C12—H12	118.9
C4—C3—C2	120.92 (14)	C8—C12—H12	118.9
C4—C3—H3	119.5	N1—C13—H13A	109.5
C2—C3—H3	119.5	N1—C13—H13B	109.5
C3—C4—C5	120.85 (15)	H13A—C13—H13B	109.5
C3—C4—H4	119.6	N1—C13—H13C	109.5
C5—C4—H4	119.6	H13A—C13—H13C	109.5
O1—C5—C4	123.47 (14)	H13B—C13—H13C	109.5
O1—C5—C6	118.19 (13)	O2—C14—H14A	109.5
C4—C5—C6	118.33 (14)	O2—C14—H14B	109.5
C1—C6—C5	120.55 (13)	H14A—C14—H14B	109.5
C1—C6—C7	117.98 (13)	O2—C14—H14C	109.5
C5—C6—C7	121.38 (13)	H14A—C14—H14C	109.5
O3—C7—C8	120.28 (13)	H14B—C14—H14C	109.5

C14—O2—C2—C1	−2.5 (2)	C12—C8—C9—C10	2.9 (2)
C14—O2—C2—C3	178.54 (15)	C7—C8—C9—C10	179.79 (14)
C6—C1—C2—O2	178.76 (14)	C8—C9—C10—C11	−1.4 (2)
C6—C1—C2—C3	−2.2 (2)	C8—C9—C10—N2	178.91 (15)
O2—C2—C3—C4	179.98 (15)	O6B—N2—C10—C9	−14.6 (5)
C1—C2—C3—C4	0.9 (2)	O5—N2—C10—C9	−167.08 (19)
C2—C3—C4—C5	1.0 (3)	O6A—N2—C10—C9	22.9 (4)
C3—C4—C5—O1	−179.97 (16)	O6B—N2—C10—C11	165.7 (4)
C3—C4—C5—C6	−1.5 (2)	O5—N2—C10—C11	13.2 (3)
C2—C1—C6—C5	1.7 (2)	O6A—N2—C10—C11	−156.8 (4)
C2—C1—C6—C7	−174.70 (14)	C12—N1—C11—O4	−176.21 (16)
O1—C5—C6—C1	178.72 (14)	C13—N1—C11—O4	3.1 (2)
C4—C5—C6—C1	0.2 (2)	C12—N1—C11—C10	3.6 (2)
O1—C5—C6—C7	−5.0 (2)	C13—N1—C11—C10	−177.08 (14)
C4—C5—C6—C7	176.48 (14)	C9—C10—C11—O4	178.07 (19)
C1—C6—C7—O3	123.47 (16)	N2—C10—C11—O4	−2.3 (3)
C5—C6—C7—O3	−52.9 (2)	C9—C10—C11—N1	−1.7 (2)
C1—C6—C7—C8	−54.42 (19)	N2—C10—C11—N1	177.93 (14)
C5—C6—C7—C8	129.20 (15)	C11—N1—C12—C8	−2.3 (2)
O3—C7—C8—C12	161.23 (15)	C13—N1—C12—C8	178.38 (15)
C6—C7—C8—C12	−20.9 (2)	C9—C8—C12—N1	−1.1 (2)
O3—C7—C8—C9	−15.5 (2)	C7—C8—C12—N1	−177.92 (13)
C6—C7—C8—C9	162.38 (14)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O4^{i}	0.83 (2)	1.87 (2)	2.6948 (17)	173 (2)
C4—H4···O4^{i}	0.93	2.56	3.233 (2)	129
C14—H14*B*···O3^{ii}	0.96	2.41	3.319 (2)	158

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