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4-Chloro-2-(6-nitro-1*H*-benzimidazol-2-yl)phenol *N*,*N*-dimethylformamide solvate

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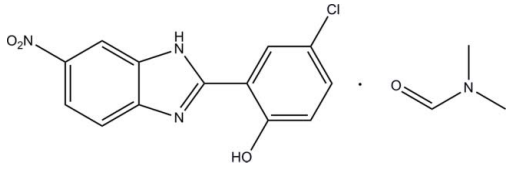
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.065; wR factor = 0.201; data-to-parameter ratio = 16.3.

In the title compound, $C_{13}H_8ClN_3O_3\cdot C_3H_7NO$, the benzimidazole and benzene rings make a dihedral angle of 0.63 (11)°. An intramolecular O—H···N hydrogen bond generates an S(6) ring motif. The solvent molecule is hydrogen-bonded to the benzimidazole molecule by intermolecular N—H···O and C—H···O hydrogen bonds, generating an $R_2^1(7)$ ring motif. In the crystal, the molecules are arranged into parallel layers perpendicular to the c axis and stabilized by weak π–π interactions [centroid–centroid distances in the range 3.4036 (18)–3.5878 (16) Å].

Related literature

For general background to and the biological activity of benzimidazole derivatives, see: Trivedi *et al.* (2006); White *et al.* (2004); Garuti *et al.* (2004). For related structures, see: Eltayeb *et al.* (2009); Yeap *et al.* (2009). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_8ClN_3O_3\cdot C_3H_7NO$
M_r = 362.77
Monoclinic, $C2/c$
a = 15.200 (2) Å
b = 18.355 (2) Å
c = 13.279 (3) Å
β = 119.232 (2)°
V = 3233.1 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 100 K
0.45 × 0.12 × 0.05 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.889, T_{max} = 0.987
14542 measured reflections
3719 independent reflections
2771 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.201
S = 1.07
3719 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1*O3*···N2	0.75	1.90	2.568 (4)	149
N1—H1*N1*···O4	0.89	1.86	2.736 (4)	167
C13—H13*A*···O4	0.93	2.58	3.472 (5)	161

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5046).

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supporting information

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4-Chloro-2-(6-nitro-1*H*-benzimidazol-2-yl)phenol *N*,*N*-dimethylformamide solvate

Abeer Mohamed Farag, Siang Guan Teoh, Hasnah Osman, Chin Sing Yeap and Hoong-Kun Fun

S1. Comment

Benzimidazole and its derivatives are widely used in biological systems (Trivedi *et al.*, 2006). Some derivatives of benzimidazole are used as inhibitors of the DNA-repair enzyme poly (ADP-ribose) polymerase-1 (PARP-1) (White *et al.*, 2004) and antiproliferative activities (Garuti *et al.*, 2004). In view of the biological importance of aforementioned benzimidazole, the crystal structure determination of the title compound was carried out and the result is presented here.

The asymmetric unit of title compound consists of one benzimidazole molecule and one dimethylformamide solvent (Fig. 1). The geometric parameters are comparable to those related structures (Eltayeb *et al.*, 2009; Yeap *et al.*, 2009). The molecular structure of the benzimidazole is essentially planar with the maximum deviation of 0.071 Å for atom O1. An intramolecular O3—H1O3···N2 hydrogen bond generate *S*(6) ring motif (Bernstein *et al.*, 1995). The solvent molecule is hydrogen-bonded to the benzimidazole molecule by intermolecular N1—H1N1···O4 and C13—H13A···O4 hydrogen bonds generating $R^1_2(7)$ ring motif. In the crystal packing, the molecules are arranged into parallel layers perpendicular to *c* axis and stabilized by weak $\pi\cdots\pi$ interactions [*Cg*1···*Cg*1^{i} of 3.4036 (18) Å, *Cg*1···*Cg*1^{ii} of 3.5247 (17) Å and *Cg*1···*Cg*2^{i} of 3.5878 (16) Å; (i) -*x*, *y*, 1/2 - *z*; (ii) -*x*, 1 - *y*, 1 - *z*. *Cg*1 and *Cg*2 are centroids of N1–C1–C6–N2–C7 and C1–C6 rings, respectively].

S2. Experimental

5-Chloro-2-hydroxy benzaldehyde (0.626 g, 4 mmol) was added to the solution of 4-nitrobenzene-1,2-diamine (0.306 g, 2 mmol) in methanol (30 ml). The mixture was refluxed with stirring for 1 h. The resultant solid obtained was then filtered and washed with methanol. Orange plate-shaped single crystals of the title compound suitable for X-ray structure determination was obtained from DMF by slow evaporation at room temperature.

S3. Refinement

The O– and N-bound hydrogen atoms were located from difference Fourier map and refined using a riding model [U_{iso}(H) = 1.2U_{eq} (N) or 1.5U_{eq}(O)]. The rest of hydrogen atoms were positioned geometrically [C–H = 0.93 & 0.96 Å] and refined using a riding model [U_{iso}(H) = 1.2 & 1.5U_{eq}(C)]. A rotating-group model were applied for methyl groups.

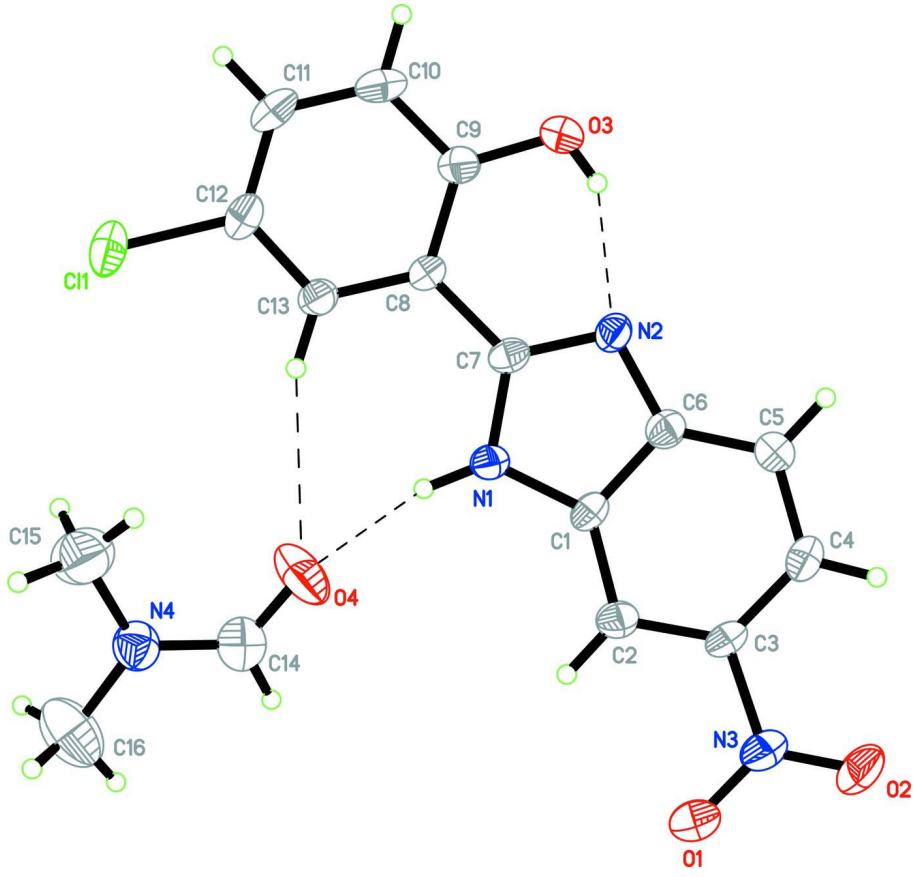

Figure 1

The molecular structure of title compound with atom labels and 50% probability ellipsoids for non-H atoms. Intramolecular hydrogen bonds are shown as dashed lines.

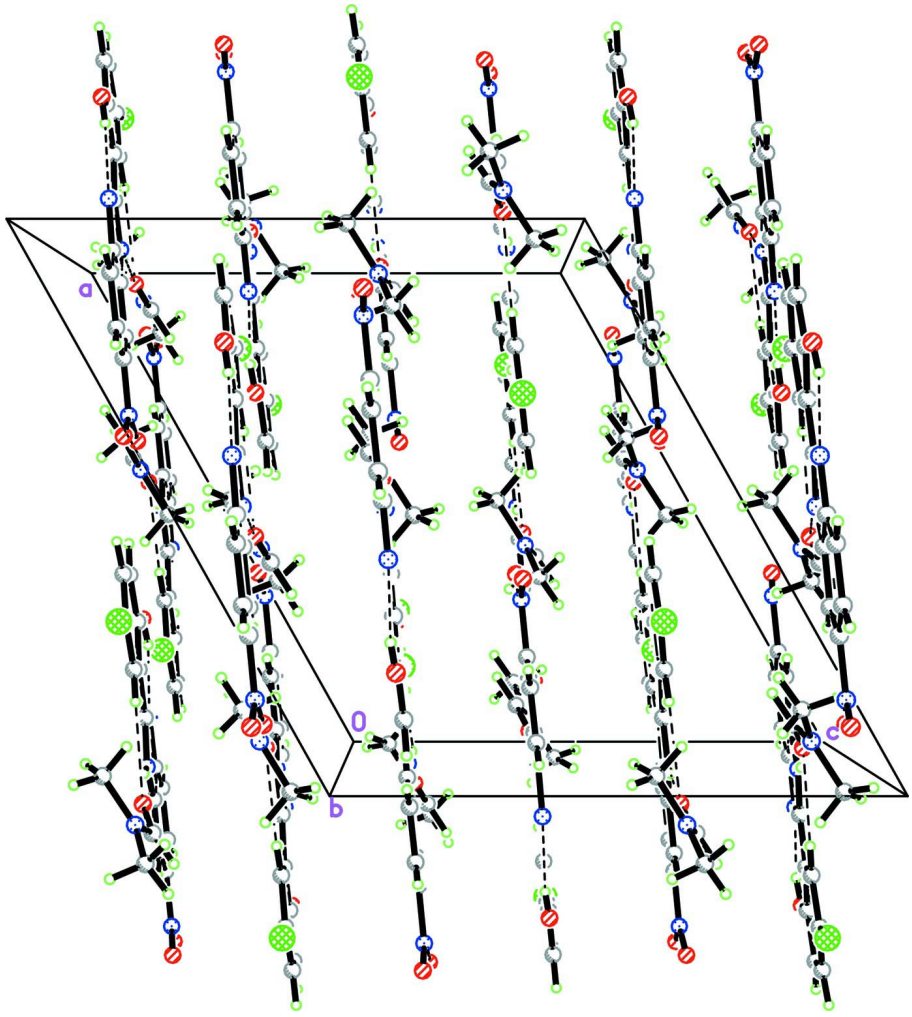

Figure 2

The crystal packing of title compound viewed down *b* axis, showing the molecules are arranged into parallel layers.

4-Chloro-2-(6-nitro-1*H*-benzimidazol-2-yl)phenol *N*,*N*-dimethylformamide solvate

Crystal data

$C_{13}H_8ClN_3O_3·C_3H_7NO$
M_r = 362.77
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 15.200 (2) Å
b = 18.355 (2) Å
c = 13.279 (3) Å
β = 119.232 (2)°
V = 3233.1 (9) Å^3
Z = 8

F(000) = 1504
D_x = 1.491 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3050 reflections
θ = 2.8–29.6°
μ = 0.27 mm^{-1}
T = 100 K
Plate, orange
0.45 × 0.12 × 0.05 mm

Data collection

Bruker 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} = 0.889, T_{max} = 0.987
14542 measured reflections
3719 independent reflections
2771 reflections with $I > 2\sigma(I)$

R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −19→19
k = −23→23
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.201
S = 1.07
3719 reflections
228 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0961P)^2 + 7.3038P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *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	−0.29053 (6)	0.25697 (4)	0.23736 (8)	0.0465 (3)
O1	0.37235 (16)	0.53844 (13)	0.5412 (2)	0.0418 (6)
O2	0.36636 (17)	0.65517 (14)	0.5483 (2)	0.0444 (6)
O3	−0.28130 (16)	0.57579 (11)	0.23880 (19)	0.0362 (5)
H1O3	−0.2293	0.5904	0.2591	0.054*
N1	−0.00189 (16)	0.46895 (13)	0.37354 (18)	0.0242 (5)
H1N1	0.0057	0.4209	0.3772	0.029*
N2	−0.08820 (17)	0.57321 (12)	0.33366 (19)	0.0245 (5)
N3	0.32588 (18)	0.59601 (15)	0.5240 (2)	0.0327 (6)
C1	0.06745 (19)	0.52535 (15)	0.4062 (2)	0.0227 (5)
C2	0.1718 (2)	0.52401 (16)	0.4543 (2)	0.0261 (6)
H2A	0.2085	0.4809	0.4719	0.031*
C3	0.21629 (19)	0.59173 (15)	0.4736 (2)	0.0250 (6)
C4	0.1634 (2)	0.65760 (16)	0.4484 (2)	0.0304 (6)
H4A	0.1978	0.7016	0.4629	0.036*
C5	0.0598 (2)	0.65720 (16)	0.4018 (2)	0.0287 (6)
H5A	0.0233	0.7004	0.3852	0.034*

C6	0.0120 (2)	0.59004 (15)	0.3807 (2)	0.0250 (6)
C7	−0.09359 (19)	0.50080 (15)	0.3299 (2)	0.0228 (5)
C8	−0.18949 (19)	0.46199 (14)	0.2832 (2)	0.0218 (5)
C9	−0.2793 (2)	0.50277 (16)	0.2409 (2)	0.0269 (6)
C10	−0.3707 (2)	0.46580 (18)	0.2000 (3)	0.0342 (7)
H10A	−0.4303	0.4923	0.1719	0.041*
C11	−0.3743 (2)	0.39127 (18)	0.2004 (2)	0.0339 (7)
H11A	−0.4355	0.3674	0.1750	0.041*
C12	−0.2861 (2)	0.35177 (17)	0.2390 (2)	0.0301 (6)
C13	−0.1943 (2)	0.38598 (15)	0.2804 (2)	0.0254 (6)
H13A	−0.1357	0.3586	0.3064	0.030*
O4	0.0524 (2)	0.32533 (15)	0.3936 (3)	0.0728 (9)
N4	0.0760 (2)	0.20375 (15)	0.4053 (2)	0.0374 (6)
C14	0.0997 (3)	0.2715 (2)	0.3954 (4)	0.0526 (9)
H14A	0.1575	0.2787	0.3892	0.063*
C15	−0.0141 (3)	0.1904 (3)	0.4121 (4)	0.0611 (11)
H15A	−0.0317	0.2334	0.4394	0.092*
H15B	−0.0026	0.1509	0.4645	0.092*
H15C	−0.0681	0.1779	0.3370	0.092*
C16	0.1378 (4)	0.1427 (2)	0.4137 (4)	0.0710 (13)
H16A	0.1942	0.1590	0.4061	0.106*
H16B	0.0989	0.1085	0.3534	0.106*
H16C	0.1616	0.1195	0.4873	0.106*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0443 (5)	0.0298 (4)	0.0618 (5)	−0.0138 (3)	0.0230 (4)	−0.0003 (3)
O1	0.0249 (11)	0.0443 (14)	0.0522 (13)	−0.0012 (10)	0.0157 (10)	−0.0013 (10)
O2	0.0298 (12)	0.0452 (14)	0.0561 (14)	−0.0158 (10)	0.0192 (10)	−0.0078 (11)
O3	0.0252 (10)	0.0291 (11)	0.0515 (13)	0.0043 (8)	0.0164 (10)	−0.0016 (9)
N1	0.0197 (11)	0.0250 (12)	0.0278 (11)	0.0006 (9)	0.0116 (9)	0.0019 (9)
N2	0.0230 (11)	0.0238 (12)	0.0279 (11)	−0.0039 (9)	0.0135 (9)	−0.0012 (9)
N3	0.0229 (12)	0.0402 (15)	0.0341 (12)	−0.0047 (11)	0.0133 (10)	−0.0033 (10)
C1	0.0209 (12)	0.0270 (14)	0.0217 (11)	−0.0059 (10)	0.0115 (10)	−0.0023 (10)
C2	0.0226 (13)	0.0301 (15)	0.0271 (12)	0.0008 (11)	0.0134 (10)	−0.0006 (10)
C3	0.0172 (12)	0.0326 (15)	0.0248 (12)	−0.0051 (10)	0.0101 (10)	−0.0024 (10)
C4	0.0292 (15)	0.0276 (15)	0.0334 (14)	−0.0087 (11)	0.0145 (11)	−0.0046 (11)
C5	0.0273 (14)	0.0251 (14)	0.0325 (14)	0.0016 (11)	0.0138 (11)	−0.0001 (11)
C6	0.0235 (13)	0.0276 (14)	0.0235 (12)	−0.0018 (11)	0.0112 (10)	−0.0020 (10)
C7	0.0196 (12)	0.0290 (14)	0.0217 (11)	−0.0008 (10)	0.0114 (10)	0.0009 (10)
C8	0.0187 (12)	0.0248 (14)	0.0219 (11)	−0.0025 (10)	0.0100 (10)	−0.0007 (9)
C9	0.0226 (13)	0.0294 (15)	0.0281 (13)	0.0011 (11)	0.0119 (11)	0.0008 (10)
C10	0.0186 (13)	0.0455 (19)	0.0371 (15)	0.0020 (12)	0.0124 (12)	−0.0009 (13)
C11	0.0227 (14)	0.0443 (18)	0.0328 (14)	−0.0118 (12)	0.0121 (11)	−0.0024 (12)
C12	0.0288 (14)	0.0309 (15)	0.0299 (13)	−0.0094 (12)	0.0138 (11)	−0.0005 (11)
C13	0.0213 (13)	0.0276 (14)	0.0264 (12)	−0.0011 (10)	0.0110 (10)	0.0019 (10)
O4	0.073 (2)	0.0341 (15)	0.099 (2)	0.0211 (14)	0.0322 (18)	0.0026 (14)

N4	0.0405 (15)	0.0347 (15)	0.0394 (14)	−0.0003 (11)	0.0214 (12)	−0.0028 (11)
C14	0.048 (2)	0.041 (2)	0.066 (2)	−0.0015 (17)	0.0258 (18)	0.0046 (17)
C15	0.048 (2)	0.070 (3)	0.064 (2)	−0.001 (2)	0.027 (2)	0.009 (2)
C16	0.092 (4)	0.051 (3)	0.078 (3)	0.023 (2)	0.049 (3)	0.000 (2)

Geometric parameters (Å, º)

Cl1—C12	1.741 (3)	C8—C13	1.397 (4)
O1—N3	1.229 (3)	C8—C9	1.411 (4)
O2—N3	1.212 (3)	C9—C10	1.396 (4)
O3—C9	1.341 (3)	C10—C11	1.369 (5)
O3—H1O3	0.7498	C10—H10A	0.9300
N1—C7	1.354 (3)	C11—C12	1.384 (4)
N1—C1	1.387 (3)	C11—H11A	0.9300
N1—H1N1	0.8875	C12—C13	1.376 (4)
N2—C7	1.331 (4)	C13—H13A	0.9300
N2—C6	1.370 (3)	O4—C14	1.216 (5)
N3—C3	1.463 (3)	N4—C14	1.319 (5)
C1—C2	1.391 (4)	N4—C16	1.431 (5)
C1—C6	1.399 (4)	N4—C15	1.437 (5)
C2—C3	1.378 (4)	C14—H14A	0.9300
C2—H2A	0.9300	C15—H15A	0.9600
C3—C4	1.399 (4)	C15—H15B	0.9600
C4—C5	1.383 (4)	C15—H15C	0.9600
C4—H4A	0.9300	C16—H16A	0.9600
C5—C6	1.388 (4)	C16—H16B	0.9600
C5—H5A	0.9300	C16—H16C	0.9600
C7—C8	1.461 (4)		
C9—O3—H1O3	110.0	O3—C9—C8	123.1 (2)
C7—N1—C1	106.1 (2)	C10—C9—C8	118.9 (3)
C7—N1—H1N1	122.1	C11—C10—C9	121.2 (3)
C1—N1—H1N1	131.8	C11—C10—H10A	119.4
C7—N2—C6	106.1 (2)	C9—C10—H10A	119.4
O2—N3—O1	123.4 (3)	C10—C11—C12	119.5 (3)
O2—N3—C3	119.1 (3)	C10—C11—H11A	120.3
O1—N3—C3	117.5 (2)	C12—C11—H11A	120.3
N1—C1—C2	130.7 (3)	C13—C12—C11	121.3 (3)
N1—C1—C6	106.4 (2)	C13—C12—Cl1	119.1 (2)
C2—C1—C6	122.9 (3)	C11—C12—Cl1	119.6 (2)
C3—C2—C1	114.6 (3)	C12—C13—C8	119.7 (3)
C3—C2—H2A	122.7	C12—C13—H13A	120.1
C1—C2—H2A	122.7	C8—C13—H13A	120.1
C2—C3—C4	124.2 (3)	C14—N4—C16	123.0 (4)
C2—C3—N3	118.6 (3)	C14—N4—C15	118.9 (3)
C4—C3—N3	117.1 (2)	C16—N4—C15	118.0 (4)
C5—C4—C3	119.9 (3)	O4—C14—N4	125.4 (4)
C5—C4—H4A	120.0	O4—C14—H14A	117.3

C3—C4—H4A	120.0	N4—C14—H14A	117.3
C4—C5—C6	117.6 (3)	N4—C15—H15A	109.5
C4—C5—H5A	121.2	N4—C15—H15B	109.5
C6—C5—H5A	121.2	H15A—C15—H15B	109.5
N2—C6—C5	130.4 (3)	N4—C15—H15C	109.5
N2—C6—C1	108.9 (2)	H15A—C15—H15C	109.5
C5—C6—C1	120.8 (2)	H15B—C15—H15C	109.5
N2—C7—N1	112.6 (2)	N4—C16—H16A	109.5
N2—C7—C8	122.2 (2)	N4—C16—H16B	109.5
N1—C7—C8	125.2 (2)	H16A—C16—H16B	109.5
C13—C8—C9	119.4 (2)	N4—C16—H16C	109.5
C13—C8—C7	121.8 (2)	H16A—C16—H16C	109.5
C9—C8—C7	118.8 (2)	H16B—C16—H16C	109.5
O3—C9—C10	118.0 (3)		

C7—N1—C1—C2	−179.0 (3)	C6—N2—C7—C8	−179.2 (2)
C7—N1—C1—C6	0.6 (3)	C1—N1—C7—N2	−0.9 (3)
N1—C1—C2—C3	178.8 (2)	C1—N1—C7—C8	179.1 (2)
C6—C1—C2—C3	−0.8 (4)	N2—C7—C8—C13	−179.5 (2)
C1—C2—C3—C4	0.2 (4)	N1—C7—C8—C13	0.4 (4)
C1—C2—C3—N3	−180.0 (2)	N2—C7—C8—C9	−0.2 (4)
O2—N3—C3—C2	−175.2 (3)	N1—C7—C8—C9	179.8 (2)
O1—N3—C3—C2	3.6 (4)	C13—C8—C9—O3	−178.9 (2)
O2—N3—C3—C4	4.6 (4)	C7—C8—C9—O3	1.7 (4)
O1—N3—C3—C4	−176.6 (2)	C13—C8—C9—C10	1.7 (4)
C2—C3—C4—C5	0.5 (4)	C7—C8—C9—C10	−177.7 (2)
N3—C3—C4—C5	−179.3 (2)	O3—C9—C10—C11	−179.4 (3)
C3—C4—C5—C6	−0.7 (4)	C8—C9—C10—C11	0.0 (4)
C7—N2—C6—C5	178.3 (3)	C9—C10—C11—C12	−1.9 (4)
C7—N2—C6—C1	−0.4 (3)	C10—C11—C12—C13	2.1 (4)
C4—C5—C6—N2	−178.5 (3)	C10—C11—C12—Cl1	−178.9 (2)
C4—C5—C6—C1	0.1 (4)	C11—C12—C13—C8	−0.4 (4)
N1—C1—C6—N2	−0.1 (3)	Cl1—C12—C13—C8	−179.4 (2)
C2—C1—C6—N2	179.5 (2)	C9—C8—C13—C12	−1.5 (4)
N1—C1—C6—C5	−179.0 (2)	C7—C8—C13—C12	177.9 (2)
C2—C1—C6—C5	0.6 (4)	C16—N4—C14—O4	−176.2 (4)
C6—N2—C7—N1	0.8 (3)	C15—N4—C14—O4	1.6 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1*O3*···N2	0.75	1.90	2.568 (4)	149
N1—H1*N*1···O4	0.89	1.86	2.736 (4)	167
C13—H13*A*···O4	0.93	2.58	3.472 (5)	161