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2-Methoxybenzohydrazide

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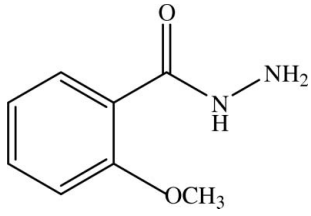
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.110; data-to-parameter ratio = 12.4.

The title compound, $C_8H_{10}N_2O_2$, crystallizes as two independent molecules linked by N—H···N and N—H···O hydrogen bonds into a linear chain running along the a axis of the monoclinic unit cell. The intra- and intermolecular hydrogen bonds are described as a two-ring $R_2^2(10)$ motif. The six-membered $R_1^1(6)$ rings formed by the intramolecular interactions are almost planar (r.m.s. deviations 0.06 and 0.08 Å). In one molecule, the aromatic and hydrogen-bonded rings are oriented at 4.8 (2)°, whereas in the other molecule these rings are oriented at 6.1 (4)°.

Related literature

For related structures, see: Ashiq *et al.* (2009); Kallel *et al.* (1992); Saraogi *et al.* (2002). For the biological activity of hydrazides, see: Ara *et al.* (2007); El-Emam *et al.* (2004); Maqsood *et al.* (2006). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_8H_{10}N_2O_2$
M_r = 166.18
Monoclinic, $P2_1/c$
a = 7.6486 (5) Å
b = 10.7123 (7) Å
c = 20.4781 (13) Å
β = 95.563 (3)°
V = 1669.95 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.22 × 0.19 × 0.11 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: none
15129 measured reflections
2938 independent reflections
1695 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.02
2938 reflections
237 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21N···O3^{i}	0.88 (2)	2.27 (2)	3.091 (3)	155 (2)
N3—H3N···N2^{ii}	0.87 (2)	2.44 (2)	3.111 (3)	134.2 (18)
N4—H41N···O3^{iii}	0.96 (2)	2.25 (3)	3.136 (3)	152.3 (19)
N4—H42N···O1^{iv}	0.87 (2)	2.26 (2)	3.055 (3)	153 (2)
N1—H1N···O2	0.89 (2)	1.98 (2)	2.655 (2)	130.8 (17)
N3—H3N···O4	0.86 (2)	2.01 (2)	2.653 (2)	129.9 (19)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2643).

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2-Methoxybenzohydrazide

Uzma Ashiq, Rifat Ara Jamal, Muhammad Nadeem Arshad, Zahida Tasneem Maqsood and Islam Ullah Khan

S1. Comment

Hydrazides are known to have different biological activities and have been used for the synthesis of various heterocyclic compounds (El-Emam *et al.*, 2004). In order to study the biological activity of 2-methoxybenzohydrazide, we undertook the synthesis of title compound and report its crystal structure in this paper. The title compound I was found to be antifungal (Maqsood *et al.*, 2006) and phytotoxic (Ara *et al.*, 2007). The unit cell contains two crystallographically unique molecules (Fig. 1). The structures of benzhydrazide (Kallel *et al.*, 1992), *para*-chloro (Saraogi *et al.*, 2002) and *para*-methoxy (Ashiq *et al.*, 2009), analogues of (I) have already been reported.

The molecular packing diagram (Fig. 2) shows the presence of intermolecular hydrogen bonds of N—H···N and N—H···O types (details are given in Table 1) results in the formation of two ring motifs with graphic notation $R_2^2(10)$ (Bernstein *et al.*, 1995), for each. Intramolecular interactions give rise six membered rings C (O2/C6/C1/C7/N1/H1N) and D (O4/C14/C9/C15/N3/H3N) $R_1^1(6)$ (Bernstein *et al.*, 1995), in each molecule. In one molecule, the A and C rings are oriented at 4.8 (2)°, whereas in the other molecule, the B and D rings are oriented at 6.1 (4)°.

S2. Experimental

All reagent-grade chemicals were obtained from Aldrich and Sigma Chemical companies and were used without further purification. To a solution of ethyl-2-methoxybenzoate (3.6 g, 20 mmol) in 75 ml e thanol, hydrazine hydrate (5.0 ml, 100 mmol) was added. The mixture was refluxed for 5 h and a solid was obtained upon removal of the solvent by rotary evaporation. The resulting solid was washed with hexane to afford 2-methoxybenzohydrazide (yield 78%) (Ara *et al.*, 2007). Colourless single crystals of (I) were obtained by slow evaporation of methanol solution at room temperature.

S3. Refinement

The Hydrogen atoms bonded to aryl and methyl Carbon atoms were positioned geometrically, with C—H = 0.93 Å and C—H = 0.96 Å respectively. The thermal parameter of H-atoms of methyl group was taken 1.5 times of the parent C-atom, whereas for aromatic H-atoms it was taken 1.2 times of their parent atoms. Atoms H1N, H21N, H22N H3N, H41N, H42N with N–H= 0.86 (2)–0.96 (2)Å are located in a difference Fourier map and constrained to ride on their parent atom, with $U_{iso}(H) = 1.2U_{eq}(N)$.

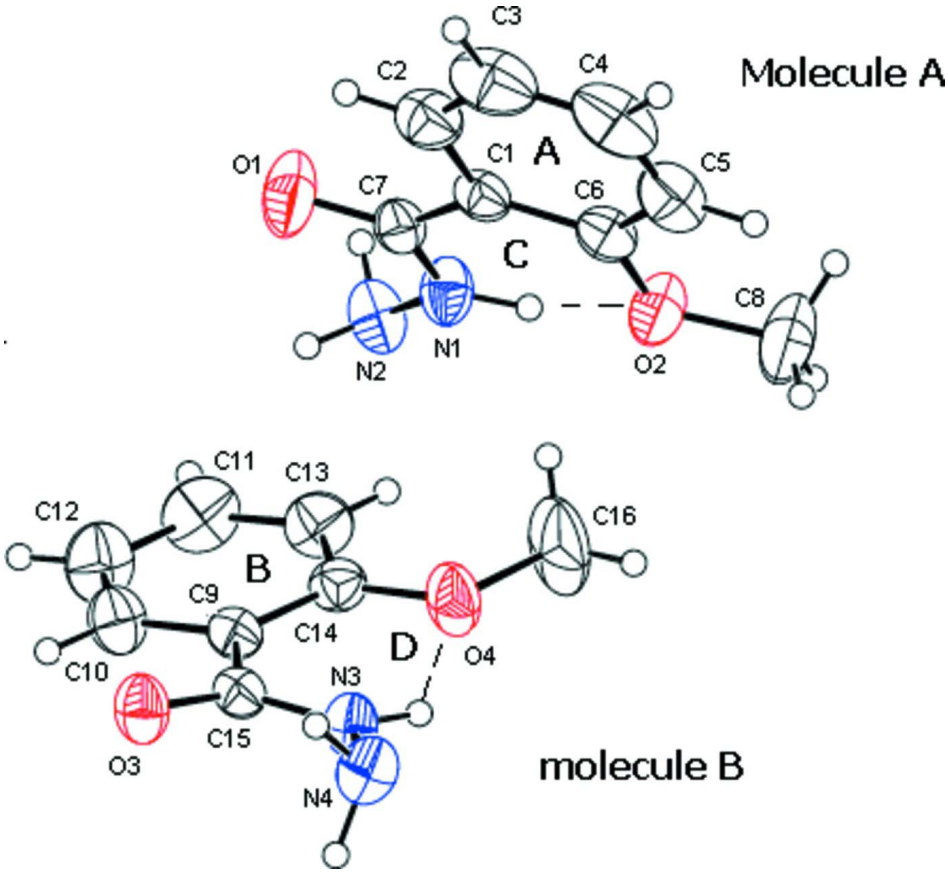

Figure 1

ORTEP plot of the title compound with the ellipsoids drawn at the 40% probability level, showing the atomic labels.

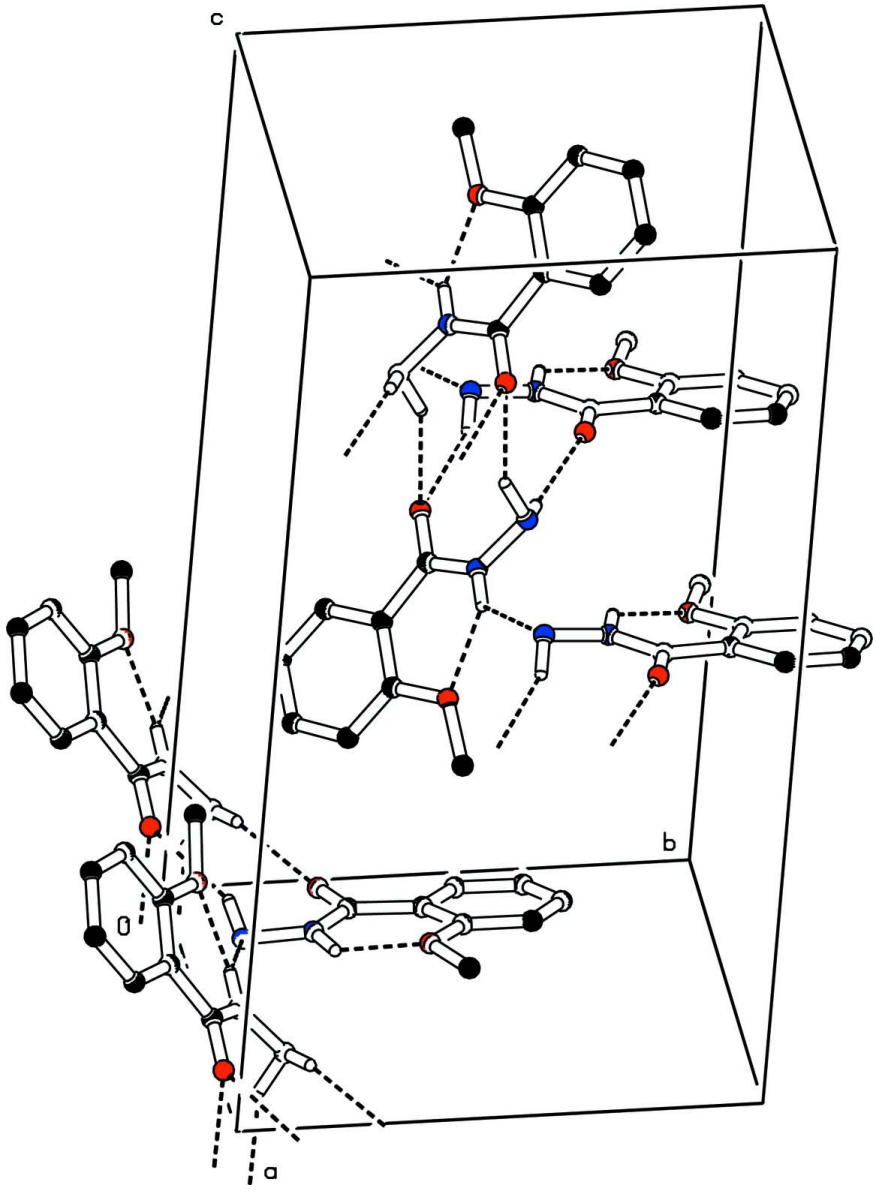

Figure 2

A unit cell packing diagram of (I) showing hydrogen bonds drawn by dashed lines. Hydrogen atoms not involved in H-bonding have been omitted.

2-Methoxybenzohydrazide

Crystal data

$C_8H_{10}N_2O_2$
M_r = 166.18
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.6486 (5) Å
b = 10.7123 (7) Å
c = 20.4781 (13) Å
β = 95.563 (3)°
V = 1669.95 (19) Å^3
Z = 8
F(000) = 704
D_x = 1.322 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2389 reflections
θ = 2.7–22.7°
μ = 0.10 mm^{-1}

T = 296 K
Needle, colourless

0.22 × 0.19 × 0.11 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
15129 measured reflections
2938 independent reflections

1695 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −9→9
k = −12→12
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.02
2938 reflections
237 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.2288P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Special details

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}
O1	0.1822 (2)	0.26307 (16)	0.04342 (10)	0.0827 (6)
O2	0.6697 (2)	0.39866 (15)	0.11303 (8)	0.0656 (5)
N2	0.4302 (3)	0.0831 (2)	0.06058 (12)	0.0615 (6)
N1	0.4586 (2)	0.21149 (17)	0.07266 (9)	0.0525 (5)
H1N	0.569 (3)	0.235 (2)	0.0811 (11)	0.063*
H21N	0.335 (3)	0.066 (2)	0.0792 (11)	0.063*
H22N	0.400 (3)	0.081 (2)	0.0191 (12)	0.063*
C1	0.3759 (3)	0.43070 (19)	0.07062 (10)	0.0437 (5)
C2	0.2404 (3)	0.5132 (2)	0.05221 (12)	0.0618 (7)
H2	0.1317	0.4815	0.0359	0.074*
C3	0.2614 (5)	0.6394 (3)	0.05727 (14)	0.0803 (9)
H3	0.1683	0.6925	0.0442	0.096*
C4	0.4197 (5)	0.6872 (3)	0.08160 (14)	0.0802 (9)
H4	0.4341	0.7732	0.0853	0.096*

C5	0.5589 (4)	0.6088 (2)	0.10075 (12)	0.0669 (7)
H5	0.6664	0.6419	0.1174	0.080*
C6	0.5379 (3)	0.4812 (2)	0.09505 (10)	0.0486 (6)
C7	0.3323 (3)	0.2961 (2)	0.06103 (10)	0.0462 (6)
C8	0.8411 (3)	0.4463 (3)	0.13126 (16)	0.0977 (10)
H8A	0.8430	0.4878	0.1729	0.147*
H8B	0.8720	0.5045	0.0986	0.147*
H8C	0.9239	0.3787	0.1346	0.147*
O3	1.10200 (18)	0.94743 (13)	0.10222 (7)	0.0552 (4)
O4	0.64141 (19)	0.94752 (16)	0.19111 (7)	0.0652 (5)
N3	0.8244 (2)	1.01543 (17)	0.09341 (9)	0.0471 (5)
H3N	0.720 (3)	1.012 (2)	0.1063 (10)	0.057*
N4	0.8484 (3)	1.1070 (2)	0.04533 (11)	0.0558 (5)
H41N	0.862 (3)	1.062 (2)	0.0055 (12)	0.067*
H42N	0.950 (3)	1.140 (2)	0.0583 (11)	0.067*
C9	0.9165 (3)	0.85915 (19)	0.17588 (10)	0.0406 (5)
C10	1.0450 (3)	0.7726 (2)	0.19540 (11)	0.0572 (6)
H10	1.1445	0.7682	0.1728	0.069*
C11	1.0305 (4)	0.6926 (2)	0.24713 (13)	0.0740 (8)
H11	1.1178	0.6341	0.2587	0.089*
C12	0.8864 (4)	0.7004 (3)	0.28123 (13)	0.0738 (8)
H12	0.8768	0.6476	0.3168	0.089*
C13	0.7564 (3)	0.7843 (2)	0.26394 (11)	0.0615 (7)
H13	0.6591	0.7886	0.2878	0.074*
C14	0.7681 (3)	0.8634 (2)	0.21101 (10)	0.0459 (5)
C15	0.9534 (3)	0.94351 (18)	0.12070 (10)	0.0400 (5)
C16	0.4932 (4)	0.9605 (4)	0.22740 (15)	0.1152 (13)
H16A	0.4315	0.8825	0.2275	0.173*
H16B	0.4164	1.0236	0.2075	0.173*
H16C	0.5316	0.9842	0.2717	0.173*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0401 (10)	0.0727 (12)	0.1326 (16)	−0.0064 (9)	−0.0057 (10)	0.0055 (11)
O2	0.0463 (10)	0.0639 (11)	0.0838 (12)	−0.0039 (8)	−0.0079 (8)	−0.0035 (9)
N2	0.0550 (13)	0.0518 (14)	0.0805 (15)	−0.0044 (10)	0.0207 (12)	−0.0025 (12)
N1	0.0415 (11)	0.0404 (12)	0.0756 (14)	−0.0010 (10)	0.0055 (10)	−0.0032 (10)
C1	0.0458 (13)	0.0462 (14)	0.0409 (12)	0.0049 (11)	0.0136 (10)	0.0060 (10)
C2	0.0587 (15)	0.0638 (18)	0.0644 (16)	0.0143 (13)	0.0142 (12)	0.0144 (13)
C3	0.100 (2)	0.061 (2)	0.083 (2)	0.0307 (18)	0.0275 (18)	0.0185 (16)
C4	0.123 (3)	0.0454 (17)	0.079 (2)	0.0049 (19)	0.045 (2)	0.0001 (15)
C5	0.086 (2)	0.0551 (17)	0.0623 (17)	−0.0126 (15)	0.0217 (14)	−0.0100 (13)
C6	0.0554 (14)	0.0487 (15)	0.0436 (13)	0.0014 (12)	0.0136 (11)	0.0008 (11)
C7	0.0389 (13)	0.0556 (15)	0.0452 (13)	0.0005 (12)	0.0104 (10)	0.0047 (11)
C8	0.0504 (16)	0.114 (3)	0.124 (3)	−0.0211 (16)	−0.0132 (16)	−0.007 (2)
O3	0.0440 (9)	0.0614 (10)	0.0626 (10)	0.0031 (7)	0.0167 (7)	0.0124 (8)
O4	0.0523 (10)	0.0894 (13)	0.0575 (10)	0.0187 (9)	0.0243 (8)	0.0182 (9)

N3	0.0421 (11)	0.0499 (12)	0.0506 (11)	0.0010 (9)	0.0107 (9)	0.0135 (9)
N4	0.0528 (12)	0.0576 (14)	0.0571 (13)	−0.0035 (10)	0.0063 (10)	0.0184 (11)
C9	0.0446 (12)	0.0366 (12)	0.0410 (12)	−0.0033 (10)	0.0069 (10)	−0.0014 (10)
C10	0.0569 (15)	0.0503 (15)	0.0657 (16)	0.0051 (12)	0.0131 (12)	0.0071 (13)
C11	0.081 (2)	0.0605 (17)	0.0807 (19)	0.0116 (14)	0.0108 (16)	0.0273 (15)
C12	0.089 (2)	0.0649 (18)	0.0679 (18)	−0.0072 (16)	0.0074 (16)	0.0266 (15)
C13	0.0641 (17)	0.0711 (18)	0.0512 (15)	−0.0101 (14)	0.0149 (12)	0.0114 (13)
C14	0.0463 (13)	0.0507 (14)	0.0406 (13)	−0.0027 (11)	0.0039 (10)	0.0005 (11)
C15	0.0416 (12)	0.0389 (12)	0.0401 (12)	−0.0015 (10)	0.0079 (10)	−0.0031 (10)
C16	0.078 (2)	0.184 (4)	0.093 (2)	0.051 (2)	0.0534 (18)	0.039 (2)

Geometric parameters (Å, º)

O1—C7	1.222 (2)	O3—C15	1.233 (2)
O2—C6	1.364 (3)	O4—C14	1.356 (2)
O2—C8	1.423 (3)	O4—C16	1.421 (3)
N2—N1	1.410 (3)	N3—C15	1.331 (3)
N2—H21N	0.88 (2)	N3—N4	1.414 (2)
N2—H22N	0.86 (2)	N3—H3N	0.87 (2)
N1—C7	1.329 (3)	N4—H41N	0.96 (2)
N1—H1N	0.88 (2)	N4—H42N	0.87 (2)
C1—C2	1.386 (3)	C9—C10	1.382 (3)
C1—C6	1.399 (3)	C9—C14	1.403 (3)
C1—C7	1.488 (3)	C9—C15	1.495 (3)
C2—C3	1.364 (4)	C10—C11	1.375 (3)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.364 (4)	C11—C12	1.363 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.383 (4)	C12—C13	1.362 (3)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.380 (3)	C13—C14	1.385 (3)
C5—H5	0.9300	C13—H13	0.9300
C8—H8A	0.9600	C16—H16A	0.9600
C8—H8B	0.9600	C16—H16B	0.9600
C8—H8C	0.9600	C16—H16C	0.9600
C6—O2—C8	118.5 (2)	C14—O4—C16	119.39 (19)
N1—N2—H21N	104.3 (15)	C15—N3—N4	123.54 (18)
N1—N2—H22N	102.9 (16)	C15—N3—H3N	120.8 (14)
H21N—N2—H22N	105 (2)	N4—N3—H3N	115.5 (15)
C7—N1—N2	122.49 (19)	N3—N4—H41N	105.8 (14)
C7—N1—H1N	120.3 (15)	N3—N4—H42N	104.1 (15)
N2—N1—H1N	116.3 (15)	H41N—N4—H42N	107 (2)
C2—C1—C6	117.6 (2)	C10—C9—C14	117.5 (2)
C2—C1—C7	115.5 (2)	C10—C9—C15	116.33 (18)
C6—C1—C7	126.91 (19)	C14—C9—C15	126.12 (19)
C3—C2—C1	122.1 (3)	C11—C10—C9	122.2 (2)
C3—C2—H2	118.9	C11—C10—H10	118.9

C1—C2—H2	118.9	C9—C10—H10	118.9
C2—C3—C4	119.6 (3)	C12—C11—C10	119.1 (2)
C2—C3—H3	120.2	C12—C11—H11	120.4
C4—C3—H3	120.2	C10—C11—H11	120.4
C3—C4—C5	120.4 (3)	C13—C12—C11	120.9 (2)
C3—C4—H4	119.8	C13—C12—H12	119.6
C5—C4—H4	119.8	C11—C12—H12	119.6
C6—C5—C4	119.9 (3)	C12—C13—C14	120.4 (2)
C6—C5—H5	120.1	C12—C13—H13	119.8
C4—C5—H5	120.1	C14—C13—H13	119.8
O2—C6—C5	122.8 (2)	O4—C14—C13	122.9 (2)
O2—C6—C1	116.9 (2)	O4—C14—C9	117.24 (18)
C5—C6—C1	120.3 (2)	C13—C14—C9	119.9 (2)
O1—C7—N1	120.0 (2)	O3—C15—N3	121.28 (19)
O1—C7—C1	120.8 (2)	O3—C15—C9	119.98 (19)
N1—C7—C1	119.20 (19)	N3—C15—C9	118.72 (17)
O2—C8—H8A	109.5	O4—C16—H16A	109.5
O2—C8—H8B	109.5	O4—C16—H16B	109.5
H8A—C8—H8B	109.5	H16A—C16—H16B	109.5
O2—C8—H8C	109.5	O4—C16—H16C	109.5
H8A—C8—H8C	109.5	H16A—C16—H16C	109.5
H8B—C8—H8C	109.5	H16B—C16—H16C	109.5

C6—C1—C2—C3	0.1 (3)	C14—C9—C10—C11	0.0 (3)
C7—C1—C2—C3	−179.1 (2)	C15—C9—C10—C11	177.5 (2)
C1—C2—C3—C4	−0.5 (4)	C9—C10—C11—C12	−1.3 (4)
C2—C3—C4—C5	0.4 (4)	C10—C11—C12—C13	1.2 (4)
C3—C4—C5—C6	0.2 (4)	C11—C12—C13—C14	0.2 (4)
C8—O2—C6—C5	−7.4 (3)	C16—O4—C14—C13	3.1 (3)
C8—O2—C6—C1	173.2 (2)	C16—O4—C14—C9	−176.4 (2)
C4—C5—C6—O2	−180.0 (2)	C12—C13—C14—O4	179.1 (2)
C4—C5—C6—C1	−0.7 (3)	C12—C13—C14—C9	−1.5 (3)
C2—C1—C6—O2	179.89 (18)	C10—C9—C14—O4	−179.18 (19)
C7—C1—C6—O2	−1.1 (3)	C15—C9—C14—O4	3.7 (3)
C2—C1—C6—C5	0.5 (3)	C10—C9—C14—C13	1.3 (3)
C7—C1—C6—C5	179.5 (2)	C15—C9—C14—C13	−175.8 (2)
N2—N1—C7—O1	5.1 (3)	N4—N3—C15—O3	−4.7 (3)
N2—N1—C7—C1	−175.71 (19)	N4—N3—C15—C9	173.79 (19)
C2—C1—C7—O1	−6.0 (3)	C10—C9—C15—O3	−11.5 (3)
C6—C1—C7—O1	175.0 (2)	C14—C9—C15—O3	165.7 (2)
C2—C1—C7—N1	174.84 (19)	C10—C9—C15—N3	169.98 (19)
C6—C1—C7—N1	−4.2 (3)	C14—C9—C15—N3	−12.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21*N*···O3^{i}	0.88 (2)	2.27 (2)	3.091 (3)	155 (2)
N3—H3*N*···N2^{ii}	0.87 (2)	2.44 (2)	3.111 (3)	134.2 (18)

N4—H41*N*···O3^{iii}	0.96 (2)	2.25 (3)	3.136 (3)	152.3 (19)
N4—H42*N*···O1^{iv}	0.87 (2)	2.26 (2)	3.055 (3)	153 (2)
N1—H1*N*···O2	0.89 (2)	1.98 (2)	2.655 (2)	130.8 (17)
N3—H3*N*···O4	0.86 (2)	2.01 (2)	2.653 (2)	129.9 (19)

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