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N-(4-chlorobenzoyl)-*N*-(2-chlorophenyl)-*O*-[2-(2-nitrophenyl)acetyl]hydroxylamine

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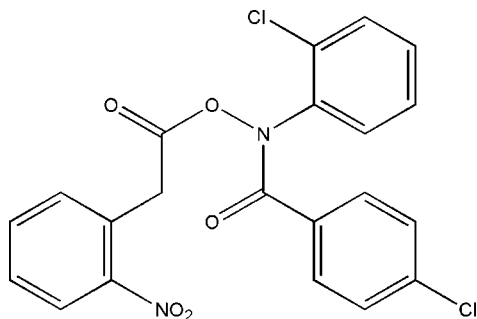
Received 20 September 2012; accepted 28 September 2012

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.054; wR factor = 0.069; data-to-parameter ratio = 13.5.

In the title hydroxamic acid derivate, $\text{C}_{21}\text{H}_{14}\text{N}_2\text{O}_5\text{Cl}_2$, the nitro-substituted benzene ring forms dihedral angles of $66.0(2)$ and $59.6(2)^\circ$, with the *p*-chloro and *o*-chloro-substituted benzene rings, respectively. The dihedral angle between the two chloro-substituted benzene rings is $64.2(2)$ Å. In the crystal, weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules along [010]. The crystal studied was an inversion twin with refined components in the ratio 0.60 (7):0.40 (7).

Related literature

For applications of hydroxamic acid derivatives, see: Noh *et al.* (2009); Zeng *et al.* (2003). For the synthesis, see: Ayyangark *et al.* (1986). For a related structure, see: Zhang *et al.* (2012).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{14}\text{Cl}_2\text{N}_2\text{O}_5$	$V = 1019(2)$ Å ³
$M_r = 445.24$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 12.366(14)$ Å	$\mu = 0.36$ mm ⁻¹
$b = 6.789(8)$ Å	$T = 296$ K
$c = 12.579(14)$ Å	$0.21 \times 0.20 \times 0.16$ mm
$\beta = 105.150(14)^\circ$	

Data collection

Bruker APEXII CCD diffractometer	5091 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3669 independent reflections
$T_{\min} = 0.929$, $T_{\max} = 0.945$	1821 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.069$	$\Delta\rho_{\text{max}} = 0.17$ e Å ⁻³
$S = 0.99$	$\Delta\rho_{\text{min}} = -0.16$ e Å ⁻³
3669 reflections	Absolute structure: Flack (1983),
271 parameters	1624 Friedel pairs
1 restraint	Flack parameter: 0.40 (7)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C5}-\text{H5}\cdots\text{O1}^i$	0.93	2.38	3.264 (7)	158
$\text{C15}-\text{H15B}\cdots\text{O1}^{ii}$	0.97	2.45	3.421 (6)	175

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); 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: LH5536).

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supporting information

Acta Cryst. (2012). E68, o3067 [doi:10.1107/S1600536812040883]

***N*-(4-chlorobenzoyl)-*N*-(2-chlorophenyl)-*O*-[2-(2-nitrophenyl)acetyl]hydroxylamine**

Jing Ma, Yi Ma and Dian He

S1. Comment

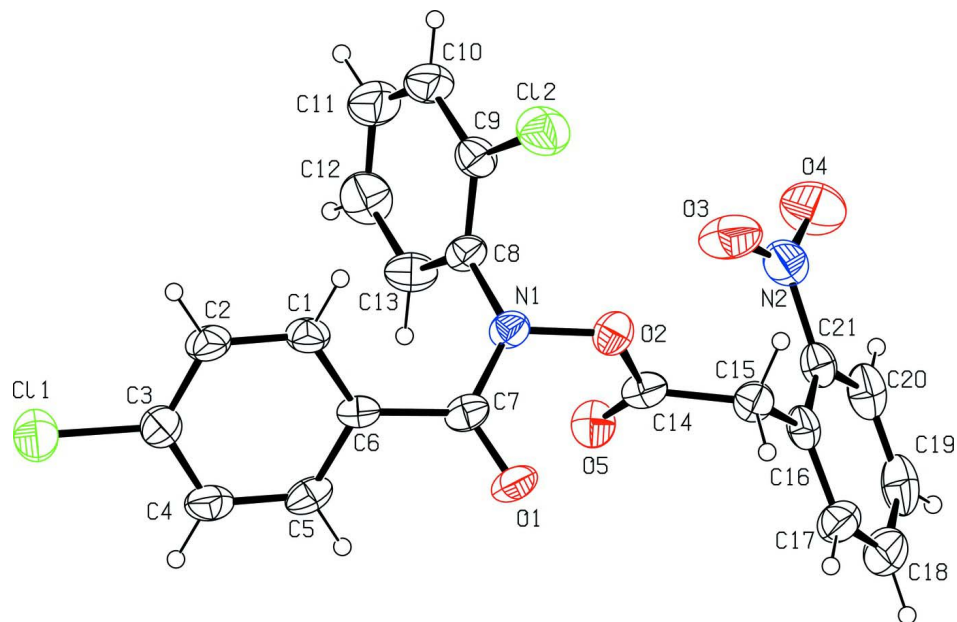
Hydroxamic acid derivatives have received considerable attention in recent years as the result of the discovery of their role in the biochemical toxicology of many drugs and other chemicals (Noh *et al.*, 2009; Zeng *et al.*, 2003). The molecular structure of the title compound is shown in Fig. 1. The nitro-substituted benzene ring (C16-C24) forms dihedral angles of 66.0 (2) and 59.6 (2)°, with the 4-chloro (C1-C6) and 2-chloro-substituted (C8-C13) benzene rings, respectively. The dihedral angle between the two chloro-substituted benzene rings (C1-6/C8-C13) is 64.2 (2)°. In the crystal, weak C—H···O hydrogen bonds link molecules along [010] (Fig. 2). The bond lengths and angles can be compared to those in *N*-(2-Chlorophenyl)-1-phenylformamido 3-(2-nitrophenyl)propanoate (Zhang *et al.*, 2012).

S2. Experimental

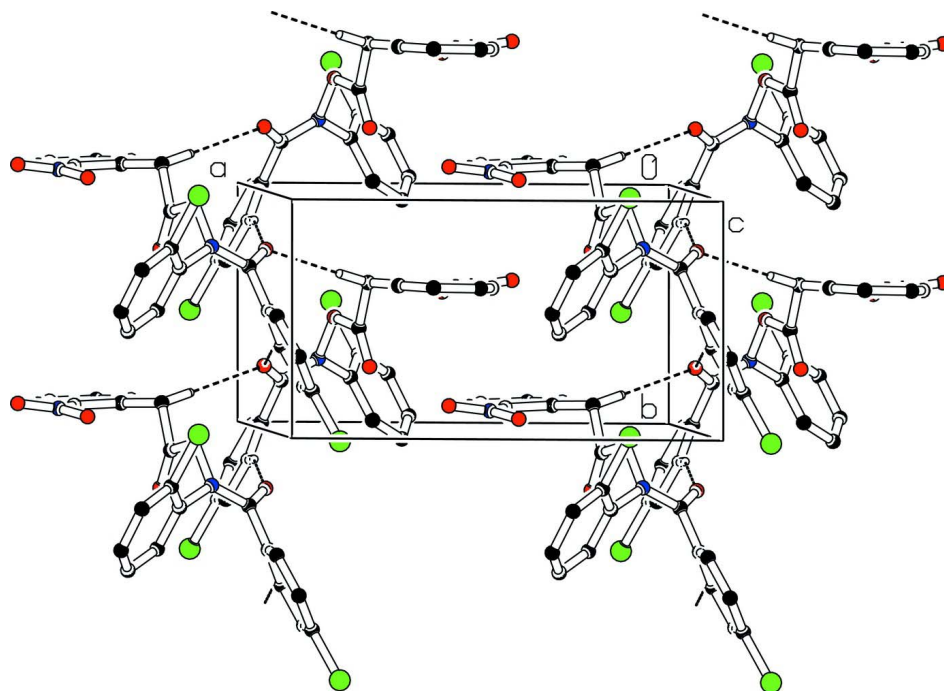
The title compound (I) was prepared according to the method described by Ayyangark *et al.* (1986). Crystals suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution of (I) in dichloromethane-methanol (1:3 *v/v*).

S3. Refinement

Hydrogen atoms were placed in calculated positions with C—H = 0.93 and 0.97 Å and included in a riding-model approximation with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

The molecular structure of the title compound with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radius.

**Figure 2**

Part of the crystal structure with weak hydrogen bonds shown as dashed lines.

N*-(4-chlorobenzoyl)-*N*-(2-chlorophenyl)-*O*-[2-(2-nitrophenyl)acetyl]hydroxylamineCrystal data*C₂₁H₁₄Cl₂N₂O₅ $M_r = 445.24$ Monoclinic, $P2_1$

Hall symbol: P 2yb

 $a = 12.366 (14) \text{ \AA}$ $b = 6.789 (8) \text{ \AA}$ $c = 12.579 (14) \text{ \AA}$ $\beta = 105.150 (14)^\circ$ $V = 1019 (2) \text{ \AA}^3$ $Z = 2$ $F(000) = 456$ $D_x = 1.450 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 985 reflections

 $\theta = 2.7\text{--}19.2^\circ$ $\mu = 0.36 \text{ mm}^{-1}$ $T = 296 \text{ K}$

Block, colorless

 $0.21 \times 0.20 \times 0.16 \text{ mm}$ *Data collection*

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.929$, $T_{\max} = 0.945$

5091 measured reflections

3669 independent reflections

1821 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.030$ $\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.7^\circ$ $h = -14 \rightarrow 14$ $k = -8 \rightarrow 8$ $l = -15 \rightarrow 14$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.054$ $wR(F^2) = 0.069$ $S = 0.99$

3669 reflections

271 parameters

1 restraint

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0117P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.17 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.16 \text{ e \AA}^{-3}$

Absolute structure: Flack (1983), 1624 Friedel

pairs

Absolute structure parameter: 0.40 (7)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0147 (3)	0.5015 (8)	0.8371 (3)	0.0556 (12)
H1	0.0422	0.4007	0.8869	0.067*
C2	-0.0321 (4)	0.6675 (7)	0.8709 (3)	0.0590 (13)
H2	-0.0363	0.6786	0.9434	0.071*
C3	-0.0720 (4)	0.8152 (6)	0.7973 (4)	0.0581 (14)

C4	-0.0663 (4)	0.8041 (7)	0.6904 (4)	0.0642 (15)
H4	-0.0935	0.9061	0.6414	0.077*
C5	-0.0194 (4)	0.6382 (7)	0.6562 (4)	0.0554 (13)
H5	-0.0148	0.6292	0.5838	0.067*
C6	0.0207 (3)	0.4855 (7)	0.7292 (3)	0.0439 (11)
C7	0.0602 (4)	0.3045 (7)	0.6835 (4)	0.0493 (13)
C8	0.2401 (3)	0.3019 (7)	0.8323 (4)	0.0487 (12)
C9	0.2722 (4)	0.2095 (7)	0.9344 (4)	0.0577 (13)
C10	0.3508 (4)	0.2985 (10)	1.0199 (5)	0.0814 (17)
H10	0.3720	0.2376	1.0884	0.098*
C11	0.3970 (4)	0.4729 (11)	1.0044 (5)	0.0906 (19)
H11	0.4484	0.5328	1.0628	0.109*
C12	0.3684 (4)	0.5626 (8)	0.9024 (5)	0.0831 (18)
H12	0.4026	0.6801	0.8915	0.100*
C13	0.2899 (4)	0.4789 (8)	0.8174 (4)	0.0640 (14)
H13	0.2697	0.5411	0.7492	0.077*
C14	0.2324 (3)	0.0798 (8)	0.6138 (4)	0.0493 (13)
C15	0.2469 (3)	-0.1148 (6)	0.5610 (3)	0.0523 (12)
H15A	0.2688	-0.2138	0.6182	0.063*
H15B	0.1754	-0.1543	0.5128	0.063*
C16	0.3330 (4)	-0.1087 (6)	0.4954 (4)	0.0494 (12)
C17	0.2956 (4)	-0.1148 (7)	0.3812 (4)	0.0669 (14)
H17	0.2190	-0.1217	0.3485	0.080*
C18	0.3679 (5)	-0.1107 (8)	0.3152 (4)	0.0791 (16)
H18	0.3406	-0.1116	0.2390	0.095*
C19	0.4823 (5)	-0.1054 (7)	0.3634 (5)	0.0778 (16)
H19	0.5320	-0.1053	0.3191	0.093*
C20	0.5227 (4)	-0.1003 (7)	0.4756 (5)	0.0690 (14)
H20	0.5994	-0.0966	0.5082	0.083*
C21	0.4474 (4)	-0.1006 (6)	0.5391 (4)	0.0511 (12)
Cl1	-0.13093 (10)	1.0228 (2)	0.84135 (10)	0.0924 (4)
Cl2	0.21125 (11)	-0.0100 (2)	0.95615 (10)	0.0868 (4)
N1	0.1548 (3)	0.2169 (6)	0.7465 (3)	0.0501 (9)
N2	0.4985 (4)	-0.0959 (6)	0.6589 (4)	0.0711 (13)
O1	0.0103 (2)	0.2380 (4)	0.5951 (2)	0.0622 (9)
O2	0.1866 (2)	0.0409 (4)	0.7008 (2)	0.0563 (8)
O3	0.4389 (3)	-0.0664 (6)	0.7204 (3)	0.0983 (14)
O4	0.5971 (3)	-0.1181 (7)	0.6925 (3)	0.1191 (16)
O5	0.2537 (2)	0.2392 (5)	0.5864 (2)	0.0613 (10)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.062 (3)	0.066 (3)	0.040 (3)	0.008 (3)	0.015 (2)	0.012 (3)
C2	0.068 (3)	0.077 (4)	0.035 (3)	0.006 (3)	0.017 (3)	0.005 (3)
C3	0.053 (3)	0.053 (3)	0.062 (4)	-0.007 (3)	0.005 (3)	-0.006 (3)
C4	0.068 (4)	0.065 (4)	0.048 (4)	-0.012 (3)	-0.006 (3)	0.005 (3)
C5	0.063 (4)	0.070 (4)	0.035 (3)	-0.020 (3)	0.016 (3)	-0.002 (3)

C6	0.038 (3)	0.058 (3)	0.035 (3)	-0.005 (3)	0.007 (2)	0.007 (3)
C7	0.050 (3)	0.068 (4)	0.036 (3)	-0.006 (3)	0.022 (3)	0.003 (3)
C8	0.029 (3)	0.071 (4)	0.043 (3)	0.003 (3)	0.005 (3)	-0.008 (3)
C9	0.046 (3)	0.065 (3)	0.061 (3)	0.011 (3)	0.010 (3)	0.001 (3)
C10	0.067 (4)	0.103 (5)	0.061 (4)	0.024 (4)	-0.007 (3)	-0.005 (4)
C11	0.076 (4)	0.108 (6)	0.074 (4)	0.011 (5)	-0.006 (3)	-0.012 (5)
C12	0.055 (4)	0.083 (5)	0.104 (5)	-0.008 (4)	0.008 (3)	-0.004 (4)
C13	0.049 (3)	0.082 (4)	0.057 (3)	-0.009 (3)	0.007 (3)	0.012 (3)
C14	0.031 (3)	0.076 (4)	0.042 (3)	-0.004 (3)	0.011 (2)	0.000 (3)
C15	0.042 (3)	0.059 (3)	0.055 (3)	-0.001 (3)	0.010 (2)	-0.006 (3)
C16	0.040 (3)	0.042 (3)	0.068 (4)	0.007 (3)	0.017 (3)	-0.004 (3)
C17	0.067 (4)	0.082 (3)	0.051 (3)	0.009 (3)	0.013 (3)	-0.011 (3)
C18	0.101 (5)	0.082 (4)	0.063 (4)	0.014 (4)	0.036 (4)	-0.003 (3)
C19	0.083 (5)	0.055 (3)	0.114 (5)	0.009 (4)	0.059 (4)	-0.005 (4)
C20	0.050 (3)	0.050 (3)	0.110 (5)	-0.003 (3)	0.025 (3)	-0.012 (4)
C21	0.049 (3)	0.038 (3)	0.069 (4)	-0.001 (3)	0.019 (3)	0.000 (3)
Cl1	0.0909 (10)	0.0798 (10)	0.0966 (10)	0.0165 (10)	0.0068 (8)	-0.0179 (9)
Cl2	0.1014 (10)	0.0849 (11)	0.0788 (9)	0.0064 (10)	0.0320 (7)	0.0200 (9)
N1	0.040 (2)	0.065 (3)	0.044 (2)	0.003 (2)	0.009 (2)	-0.006 (2)
N2	0.060 (4)	0.059 (3)	0.083 (4)	-0.002 (3)	-0.002 (3)	-0.004 (3)
O1	0.057 (2)	0.088 (2)	0.0363 (19)	0.001 (2)	0.0039 (16)	-0.0121 (18)
O2	0.0591 (19)	0.060 (2)	0.0549 (19)	-0.0036 (19)	0.0230 (16)	-0.0048 (18)
O3	0.073 (3)	0.146 (4)	0.067 (3)	0.002 (3)	0.003 (2)	0.003 (3)
O4	0.056 (2)	0.155 (4)	0.124 (3)	0.012 (3)	-0.016 (2)	-0.003 (3)
O5	0.063 (2)	0.062 (2)	0.067 (2)	-0.006 (2)	0.0312 (18)	0.0019 (18)

Geometric parameters (Å, °)

C1—C6	1.382 (5)	C12—C13	1.366 (5)
C1—C2	1.384 (6)	C12—H12	0.9300
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.366 (6)	C14—O5	1.186 (5)
C2—H2	0.9300	C14—O2	1.384 (5)
C3—C4	1.367 (5)	C14—C15	1.510 (6)
C3—C11	1.742 (5)	C15—C16	1.509 (5)
C4—C5	1.386 (5)	C15—H15A	0.9700
C4—H4	0.9300	C15—H15B	0.9700
C5—C6	1.388 (5)	C16—C21	1.379 (5)
C5—H5	0.9300	C16—C17	1.390 (5)
C6—C7	1.492 (6)	C17—C18	1.370 (6)
C7—O1	1.209 (5)	C17—H17	0.9300
C7—N1	1.367 (5)	C18—C19	1.386 (6)
C8—C13	1.385 (5)	C18—H18	0.9300
C8—C9	1.391 (5)	C19—C20	1.369 (6)
C8—N1	1.419 (5)	C19—H19	0.9300
C9—C10	1.386 (6)	C20—C21	1.378 (5)
C9—C12	1.724 (5)	C20—H20	0.9300
C10—C11	1.351 (6)	C21—N2	1.474 (6)

C10—H10	0.9300	N1—O2	1.426 (4)
C11—C12	1.381 (6)	N2—O4	1.191 (5)
C11—H11	0.9300	N2—O3	1.216 (4)
C6—C1—C2	120.0 (4)	C12—C13—H13	119.8
C6—C1—H1	120.0	C8—C13—H13	119.8
C2—C1—H1	120.0	O5—C14—O2	124.9 (5)
C3—C2—C1	119.8 (4)	O5—C14—C15	127.6 (4)
C3—C2—H2	120.1	O2—C14—C15	107.5 (4)
C1—C2—H2	120.1	C16—C15—C14	113.5 (4)
C2—C3—C4	121.5 (4)	C16—C15—H15A	108.9
C2—C3—C11	119.1 (4)	C14—C15—H15A	108.9
C4—C3—C11	119.4 (4)	C16—C15—H15B	108.9
C3—C4—C5	118.9 (4)	C14—C15—H15B	108.9
C3—C4—H4	120.5	H15A—C15—H15B	107.7
C5—C4—H4	120.5	C21—C16—C17	116.3 (4)
C4—C5—C6	120.5 (4)	C21—C16—C15	125.5 (4)
C4—C5—H5	119.7	C17—C16—C15	118.3 (4)
C6—C5—H5	119.7	C18—C17—C16	122.2 (5)
C1—C6—C5	119.3 (5)	C18—C17—H17	118.9
C1—C6—C7	123.4 (5)	C16—C17—H17	118.9
C5—C6—C7	117.2 (4)	C17—C18—C19	119.3 (5)
O1—C7—N1	121.7 (4)	C17—C18—H18	120.4
O1—C7—C6	121.5 (4)	C19—C18—H18	120.4
N1—C7—C6	116.8 (4)	C20—C19—C18	120.5 (5)
C13—C8—C9	119.1 (4)	C20—C19—H19	119.8
C13—C8—N1	121.2 (4)	C18—C19—H19	119.8
C9—C8—N1	119.6 (5)	C19—C20—C21	118.6 (5)
C10—C9—C8	119.5 (5)	C19—C20—H20	120.7
C10—C9—C12	120.1 (5)	C21—C20—H20	120.7
C8—C9—C12	120.4 (4)	C20—C21—C16	123.2 (5)
C11—C10—C9	120.5 (6)	C20—C21—N2	114.8 (5)
C11—C10—H10	119.7	C16—C21—N2	122.0 (4)
C9—C10—H10	119.7	C7—N1—C8	128.2 (4)
C10—C11—C12	120.3 (6)	C7—N1—O2	114.5 (3)
C10—C11—H11	119.8	C8—N1—O2	114.8 (3)
C12—C11—H11	119.8	O4—N2—O3	122.0 (5)
C13—C12—C11	120.1 (6)	O4—N2—C21	119.0 (5)
C13—C12—H12	120.0	O3—N2—C21	118.9 (4)
C11—C12—H12	120.0	C14—O2—N1	111.9 (3)
C12—C13—C8	120.4 (4)		
C6—C1—C2—C3	-0.1 (7)	C14—C15—C16—C17	-107.7 (5)
C1—C2—C3—C4	-0.5 (7)	C21—C16—C17—C18	-0.7 (7)
C1—C2—C3—C11	179.9 (3)	C15—C16—C17—C18	-179.7 (4)
C2—C3—C4—C5	0.4 (7)	C16—C17—C18—C19	1.6 (8)
C11—C3—C4—C5	-180.0 (3)	C17—C18—C19—C20	-1.3 (8)
C3—C4—C5—C6	0.3 (7)	C18—C19—C20—C21	0.0 (8)

C2—C1—C6—C5	0.7 (6)	C19—C20—C21—C16	1.0 (7)
C2—C1—C6—C7	-174.2 (4)	C19—C20—C21—N2	179.7 (4)
C4—C5—C6—C1	-0.8 (6)	C17—C16—C21—C20	-0.6 (7)
C4—C5—C6—C7	174.4 (4)	C15—C16—C21—C20	178.3 (4)
C1—C6—C7—O1	134.5 (4)	C17—C16—C21—N2	-179.3 (4)
C5—C6—C7—O1	-40.6 (6)	C15—C16—C21—N2	-0.3 (7)
C1—C6—C7—N1	-45.1 (5)	O1—C7—N1—C8	159.2 (4)
C5—C6—C7—N1	139.9 (4)	C6—C7—N1—C8	-21.3 (6)
C13—C8—C9—C10	1.7 (6)	O1—C7—N1—O2	-1.6 (5)
N1—C8—C9—C10	-176.3 (4)	C6—C7—N1—O2	177.9 (3)
C13—C8—C9—C12	179.5 (3)	C13—C8—N1—C7	-49.9 (6)
N1—C8—C9—C12	1.5 (6)	C9—C8—N1—C7	128.1 (4)
C8—C9—C10—C11	-0.5 (7)	C13—C8—N1—O2	110.9 (4)
C12—C9—C10—C11	-178.4 (4)	C9—C8—N1—O2	-71.2 (5)
C9—C10—C11—C12	-1.5 (8)	C20—C21—N2—O4	-9.7 (7)
C10—C11—C12—C13	2.5 (8)	C16—C21—N2—O4	169.1 (5)
C11—C12—C13—C8	-1.3 (7)	C20—C21—N2—O3	169.2 (4)
C9—C8—C13—C12	-0.8 (6)	C16—C21—N2—O3	-12.1 (7)
N1—C8—C13—C12	177.2 (4)	O5—C14—O2—N1	7.0 (6)
O5—C14—C15—C16	23.1 (6)	C15—C14—O2—N1	-171.7 (3)
O2—C14—C15—C16	-158.2 (3)	C7—N1—O2—C14	74.1 (4)
C14—C15—C16—C21	73.3 (6)	C8—N1—O2—C14	-89.4 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C5—H5 \cdots O1 ⁱ	0.93	2.38	3.264 (7)	158
C15—H15B \cdots O1 ⁱⁱ	0.97	2.45	3.421 (6)	175

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