Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(4-Chlorobenzoyl)(4-chlorophenyl)amino 3-(2-nitrophenyl)propanoate

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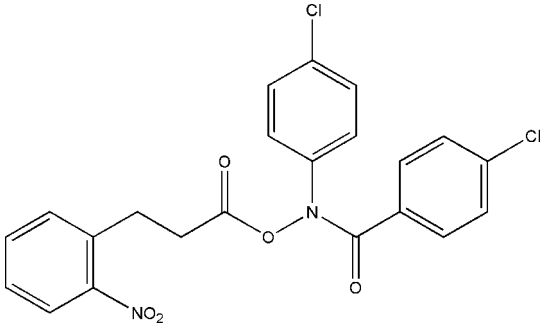
Received 28 February 2013; accepted 15 March 2013

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.113; data-to-parameter ratio = 16.4.

In the title hydroxamic acid derivate, $C_{22}H_{16}Cl_2N_2O_5$, the nitro-substituted benzene ring forms dihedral angles of 14.11 (15) and 16.08 (15)°, with the 4-chlorobenzoyl and 4-chlorophenyl benzene rings, respectively. The dihedral angle between the chloro-substituted benzene rings is 2.28 (13)°. In the crystal, molecules are linked by weak C—H···O hydrogen bonds, forming chains along [100].

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 related structures, see: Zhang *et al.* (2012); Ma *et al.* (2012).



Experimental

Crystal data

$C_{22}H_{16}Cl_2N_2O_5$ M_r = 459.27
Triclinic, $P\overline{1}$
a = 6.1710 (3) Å
b = 12.8881 (7) Å
c = 13.3490 (8) Å
α = 89.933 (5)°
β = 76.959 (5)°
γ = 82.114 (4)°
V = 1024.03 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 294 K
0.32 × 0.28 × 0.25 mm

Data collection

Agilent SuperNova (Dual, Cu at zero) Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.757, T_{max} = 1.000
7506 measured reflections
4578 independent reflections
3269 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.113
S = 1.02
4578 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.93	2.40	3.177 (2)	140
C17—H17B···O4^{ii}	0.97	2.55	3.515 (3)	171

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

This work was supported by the Natural Science Fund Projects of Gansu Province (0710RJZA124).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5593).

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supplementary materials

Acta Cryst. (2013). E**69**, o561 [doi:10.1107/S1600536813007174]

(4-Chlorobenzoyl)(4-chlorophenyl)amino 3-(2-nitrophenyl)propanoate

Yi-lan Ding and Chang-jiang Shao

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). We have performed the crystal structure determination of the title hydroxamic acid derivative.

The molecular structure of the title compound is shown in Fig. 1. The nitro-substituted benzene ring (C18-C23) forms dihedral angles of 14.11 (15) and 16.08 (15)°, with the p-chloro (C9-C14) and p-chloro-substituted (C1-C6) benzene rings, respectively. The dihedral angle between the two chloro-substituted benzene rings is 2.28 (13) °. In the crystal, molecules are linked by weak C—H···O hydrogen bonds to form chains along [100]. Closely related structures appear in the literature (Zhang *et al.*, 2012; Ma *et al.*, 2012).

Experimental

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

Refinement

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

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

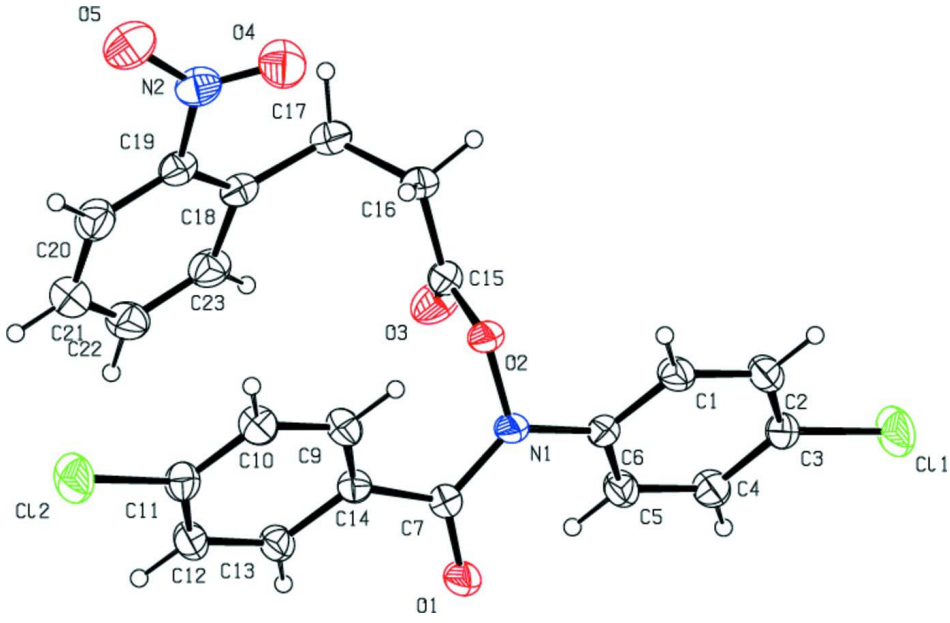

Figure 1

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

(4-Chlorobenzoyl)(4-chlorophenyl)amino 3-(2-nitrophenyl)propanoate

Crystal data

$C_{22}H_{16}Cl_2N_2O_5$
$M_r = 459.27$
Triclinic, $P\overline{1}$
$a = 6.1710$ (3) Å
$b = 12.8881$ (7) Å
$c = 13.3490$ (8) Å
$\alpha = 89.933$ (5)°
$\beta = 76.959$ (5)°
$\gamma = 82.114$ (4)°
$V = 1024.03$ (10) Å^3
$Z = 2$
$F(000) = 472$
$D_x = 1.489$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Cell parameters from 2661 reflections
$\theta = 3.1$–$28.4°$
$\mu = 0.36$ mm^{-1}
$T = 294$ K
Block, colourless
0.32 × 0.28 × 0.25 mm

Data collection

Agilent SuperNova (Dual, Cu at zero) Eos diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 16.0733 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.757$, $T_{max} = 1.000$
7506 measured reflections
4578 independent reflections
3269 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 28.5°$, $\theta_{min} = 3.1°$
$h = -8 \rightarrow 8$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.113$
$S = 1.02$
4578 reflections
280 parameters
0 restraints

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.2287P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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.

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.18649 (10)	0.33888 (6)	0.87407 (5)	0.0768 (2)
Cl2	1.31097 (10)	0.36534 (5)	0.04403 (5)	0.0728 (2)
O1	0.3913 (2)	0.46847 (10)	0.41480 (11)	0.0514 (4)
O2	0.6701 (2)	0.23063 (9)	0.47616 (10)	0.0446 (3)
O3	0.4204 (3)	0.15481 (12)	0.41153 (13)	0.0669 (5)
O4	1.2426 (3)	−0.06198 (14)	0.30600 (14)	0.0745 (5)
O5	1.4243 (3)	−0.09770 (15)	0.14952 (16)	0.0870 (6)
N1	0.5125 (3)	0.32286 (12)	0.48837 (13)	0.0488 (4)
N2	1.2639 (3)	−0.05271 (14)	0.21312 (17)	0.0567 (5)
C1	0.3969 (3)	0.28616 (15)	0.66805 (16)	0.0467 (5)
H1	0.5433	0.2555	0.6661	0.056*
C2	0.2353 (3)	0.28899 (16)	0.75827 (16)	0.0500 (5)
H2	0.2719	0.2603	0.8173	0.060*
C3	0.0195 (3)	0.33459 (15)	0.76041 (15)	0.0451 (5)
C4	−0.0374 (3)	0.37795 (15)	0.67448 (16)	0.0485 (5)
H4	−0.1837	0.4093	0.6772	0.058*
C5	0.1242 (3)	0.37473 (15)	0.58384 (15)	0.0475 (5)
H5	0.0866	0.4035	0.5250	0.057*
C6	0.3422 (3)	0.32880 (13)	0.58035 (14)	0.0402 (4)
C7	0.5349 (3)	0.39283 (14)	0.41068 (14)	0.0408 (4)
C9	0.9520 (3)	0.33060 (15)	0.32673 (15)	0.0455 (5)
H9	0.9773	0.3017	0.3877	0.055*
C10	1.1284 (3)	0.32752 (16)	0.24154 (16)	0.0487 (5)
H10	1.2719	0.2969	0.2450	0.058*
C11	1.0896 (3)	0.37022 (16)	0.15145 (16)	0.0475 (5)
C12	0.8791 (3)	0.41665 (16)	0.14499 (16)	0.0498 (5)
H12	0.8551	0.4451	0.0837	0.060*
C13	0.7042 (3)	0.42046 (15)	0.23050 (15)	0.0441 (4)
H13	0.5621	0.4529	0.2268	0.053*
C14	0.7361 (3)	0.37675 (13)	0.32217 (14)	0.0390 (4)
C15	0.5977 (3)	0.14812 (15)	0.43340 (15)	0.0451 (5)
C16	0.7738 (3)	0.05388 (14)	0.42254 (16)	0.0472 (5)
H16A	0.7454	0.0137	0.4845	0.057*
H16B	0.9199	0.0766	0.4152	0.057*

C17	0.7776 (3)	−0.01623 (15)	0.32980 (16)	0.0479 (5)
H17A	0.8685	−0.0829	0.3345	0.057*
H17B	0.6260	−0.0296	0.3314	0.057*
C18	0.8705 (3)	0.03217 (14)	0.22905 (15)	0.0429 (4)
C19	1.0947 (3)	0.01729 (15)	0.17520 (16)	0.0450 (5)
C20	1.1712 (4)	0.06501 (18)	0.08326 (18)	0.0589 (6)
H20	1.3221	0.0522	0.0498	0.071*
C21	1.0231 (5)	0.13115 (18)	0.04204 (19)	0.0665 (6)
H21	1.0729	0.1647	−0.0188	0.080*
C22	0.8000 (4)	0.14722 (17)	0.09175 (19)	0.0640 (6)
H22	0.6982	0.1915	0.0639	0.077*
C23	0.7258 (4)	0.09832 (16)	0.18248 (18)	0.0542 (5)
H23	0.5735	0.1098	0.2139	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0613 (4)	0.0970 (5)	0.0541 (4)	0.0046 (3)	0.0148 (3)	0.0189 (3)
Cl2	0.0545 (3)	0.0921 (5)	0.0570 (4)	0.0001 (3)	0.0116 (3)	0.0122 (3)
O1	0.0516 (8)	0.0480 (8)	0.0467 (8)	0.0080 (6)	−0.0041 (7)	0.0103 (6)
O2	0.0459 (7)	0.0344 (7)	0.0468 (8)	0.0041 (5)	−0.0020 (6)	0.0021 (6)
O3	0.0497 (9)	0.0645 (10)	0.0839 (12)	0.0104 (7)	−0.0210 (9)	−0.0156 (9)
O4	0.0601 (10)	0.0904 (13)	0.0709 (13)	0.0111 (9)	−0.0239 (9)	0.0071 (10)
O5	0.0570 (10)	0.0872 (13)	0.0979 (15)	0.0279 (9)	−0.0008 (10)	−0.0043 (11)
N1	0.0554 (10)	0.0346 (8)	0.0430 (9)	0.0104 (7)	0.0065 (8)	0.0069 (7)
N2	0.0405 (9)	0.0541 (10)	0.0727 (14)	0.0027 (8)	−0.0128 (9)	−0.0007 (10)
C1	0.0417 (10)	0.0455 (10)	0.0475 (12)	0.0044 (8)	−0.0054 (9)	0.0090 (9)
C2	0.0524 (12)	0.0527 (12)	0.0411 (11)	0.0004 (9)	−0.0074 (9)	0.0115 (9)
C3	0.0450 (11)	0.0441 (10)	0.0399 (11)	−0.0027 (8)	0.0009 (9)	0.0033 (8)
C4	0.0391 (10)	0.0528 (12)	0.0491 (12)	0.0025 (9)	−0.0057 (9)	0.0069 (9)
C5	0.0474 (11)	0.0526 (11)	0.0400 (11)	0.0016 (9)	−0.0097 (9)	0.0079 (9)
C6	0.0452 (10)	0.0339 (9)	0.0366 (10)	−0.0018 (8)	−0.0013 (8)	0.0006 (7)
C7	0.0464 (10)	0.0388 (10)	0.0360 (10)	−0.0029 (8)	−0.0087 (8)	0.0018 (8)
C9	0.0461 (11)	0.0508 (11)	0.0412 (11)	−0.0072 (9)	−0.0134 (9)	0.0090 (9)
C10	0.0385 (10)	0.0549 (12)	0.0514 (12)	−0.0048 (9)	−0.0084 (9)	0.0070 (9)
C11	0.0426 (10)	0.0511 (11)	0.0437 (12)	−0.0063 (9)	0.0003 (9)	0.0011 (9)
C12	0.0523 (12)	0.0556 (12)	0.0385 (11)	−0.0022 (9)	−0.0075 (9)	0.0092 (9)
C13	0.0418 (10)	0.0475 (11)	0.0405 (11)	−0.0008 (8)	−0.0076 (9)	0.0061 (8)
C14	0.0425 (10)	0.0362 (9)	0.0384 (10)	−0.0066 (8)	−0.0088 (8)	0.0014 (7)
C15	0.0465 (11)	0.0416 (10)	0.0408 (11)	0.0017 (8)	−0.0016 (9)	0.0032 (8)
C16	0.0497 (11)	0.0379 (10)	0.0496 (12)	0.0045 (8)	−0.0086 (9)	0.0038 (8)
C17	0.0442 (10)	0.0376 (10)	0.0594 (13)	−0.0014 (8)	−0.0093 (10)	−0.0013 (9)
C18	0.0439 (10)	0.0349 (9)	0.0497 (12)	−0.0014 (8)	−0.0126 (9)	−0.0057 (8)
C19	0.0432 (10)	0.0400 (10)	0.0506 (12)	0.0010 (8)	−0.0120 (9)	−0.0043 (9)
C20	0.0560 (13)	0.0579 (13)	0.0571 (14)	−0.0051 (11)	−0.0024 (11)	−0.0039 (11)
C21	0.0851 (18)	0.0564 (13)	0.0553 (15)	−0.0061 (12)	−0.0128 (13)	0.0077 (11)
C22	0.0783 (17)	0.0532 (13)	0.0615 (16)	0.0066 (11)	−0.0276 (14)	0.0049 (11)
C23	0.0488 (11)	0.0522 (12)	0.0604 (14)	0.0063 (9)	−0.0179 (11)	−0.0040 (10)

Geometric parameters (Å, º)

Cl1—C3	1.7411 (19)	C10—C11	1.378 (3)
Cl2—C11	1.738 (2)	C10—H10	0.9300
O1—C7	1.216 (2)	C11—C12	1.374 (3)
O2—C15	1.379 (2)	C12—C13	1.378 (3)
O2—N1	1.4131 (18)	C12—H12	0.9300
O3—C15	1.187 (2)	C13—C14	1.389 (3)
O4—N2	1.224 (2)	C13—H13	0.9300
O5—N2	1.225 (2)	C15—C16	1.498 (3)
N1—C7	1.369 (2)	C16—C17	1.528 (3)
N1—C6	1.419 (2)	C16—H16A	0.9700
N2—C19	1.463 (3)	C16—H16B	0.9700
C1—C2	1.376 (3)	C17—C18	1.508 (3)
C1—C6	1.383 (3)	C17—H17A	0.9700
C1—H1	0.9300	C17—H17B	0.9700
C2—C3	1.374 (3)	C18—C19	1.395 (3)
C2—H2	0.9300	C18—C23	1.397 (3)
C3—C4	1.370 (3)	C19—C20	1.387 (3)
C4—C5	1.380 (3)	C20—C21	1.370 (3)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.384 (3)	C21—C22	1.374 (3)
C5—H5	0.9300	C21—H21	0.9300
C7—C14	1.500 (3)	C22—C23	1.379 (3)
C9—C10	1.382 (3)	C22—H22	0.9300
C9—C14	1.397 (3)	C23—H23	0.9300
C9—H9	0.9300		

C15—O2—N1	112.51 (14)	C12—C13—C14	121.23 (18)
C7—N1—O2	117.80 (15)	C12—C13—H13	119.4
C7—N1—C6	127.85 (16)	C14—C13—H13	119.4
O2—N1—C6	114.30 (14)	C13—C14—C9	118.39 (17)
O4—N2—O5	123.0 (2)	C13—C14—C7	115.43 (16)
O4—N2—C19	119.16 (18)	C9—C14—C7	125.93 (17)
O5—N2—C19	117.8 (2)	O3—C15—O2	122.88 (18)
C2—C1—C6	120.22 (18)	O3—C15—C16	127.89 (19)
C2—C1—H1	119.9	O2—C15—C16	109.23 (16)
C6—C1—H1	119.9	C15—C16—C17	112.10 (17)
C3—C2—C1	119.43 (19)	C15—C16—H16A	109.2
C3—C2—H2	120.3	C17—C16—H16A	109.2
C1—C2—H2	120.3	C15—C16—H16B	109.2
C4—C3—C2	121.17 (18)	C17—C16—H16B	109.2
C4—C3—Cl1	118.92 (15)	H16A—C16—H16B	107.9
C2—C3—Cl1	119.91 (16)	C18—C17—C16	112.42 (15)
C3—C4—C5	119.45 (18)	C18—C17—H17A	109.1
C3—C4—H4	120.3	C16—C17—H17A	109.1
C5—C4—H4	120.3	C18—C17—H17B	109.1
C4—C5—C6	120.08 (18)	C16—C17—H17B	109.1
C4—C5—H5	120.0	H17A—C17—H17B	107.9
C6—C5—H5	120.0	C19—C18—C23	114.77 (19)

C1—C6—C5	119.65 (18)	C19—C18—C17	125.79 (18)
C1—C6—N1	118.58 (17)	C23—C18—C17	119.44 (18)
C5—C6—N1	121.76 (17)	C20—C19—C18	123.28 (19)
O1—C7—N1	119.37 (17)	C20—C19—N2	115.92 (19)
O1—C7—C14	120.50 (17)	C18—C19—N2	120.79 (18)
N1—C7—C14	120.13 (16)	C21—C20—C19	119.6 (2)
C10—C9—C14	120.58 (18)	C21—C20—H20	120.2
C10—C9—H9	119.7	C19—C20—H20	120.2
C14—C9—H9	119.7	C20—C21—C22	119.1 (2)
C11—C10—C9	119.39 (18)	C20—C21—H21	120.4
C11—C10—H10	120.3	C22—C21—H21	120.4
C9—C10—H10	120.3	C21—C22—C23	120.6 (2)
C12—C11—C10	121.25 (18)	C21—C22—H22	119.7
C12—C11—Cl2	119.40 (16)	C23—C22—H22	119.7
C10—C11—Cl2	119.35 (16)	C22—C23—C18	122.5 (2)
C11—C12—C13	119.15 (19)	C22—C23—H23	118.7
C11—C12—H12	120.4	C18—C23—H23	118.7
C13—C12—H12	120.4		

C15—O2—N1—C7	−92.94 (19)	C10—C9—C14—C13	−0.8 (3)
C15—O2—N1—C6	84.64 (19)	C10—C9—C14—C7	−174.88 (17)
C6—C1—C2—C3	−0.1 (3)	O1—C7—C14—C13	−27.1 (3)
C1—C2—C3—C4	−0.5 (3)	N1—C7—C14—C13	153.69 (17)
C1—C2—C3—Cl1	−179.90 (15)	O1—C7—C14—C9	147.14 (19)
C2—C3—C4—C5	0.7 (3)	N1—C7—C14—C9	−32.1 (3)
Cl1—C3—C4—C5	−179.79 (15)	N1—O2—C15—O3	−1.3 (3)
C3—C4—C5—C6	−0.5 (3)	N1—O2—C15—C16	179.71 (14)
C2—C1—C6—C5	0.2 (3)	O3—C15—C16—C17	32.6 (3)
C2—C1—C6—N1	−178.98 (17)	O2—C15—C16—C17	−148.51 (16)
C4—C5—C6—C1	0.1 (3)	C15—C16—C17—C18	71.5 (2)
C4—C5—C6—N1	179.25 (17)	C16—C17—C18—C19	92.1 (2)
C7—N1—C6—C1	−148.3 (2)	C16—C17—C18—C23	−87.9 (2)
O2—N1—C6—C1	34.4 (2)	C23—C18—C19—C20	0.9 (3)
C7—N1—C6—C5	32.5 (3)	C17—C18—C19—C20	−179.16 (19)
O2—N1—C6—C5	−144.76 (17)	C23—C18—C19—N2	−178.00 (17)
O2—N1—C7—O1	173.77 (16)	C17—C18—C19—N2	2.0 (3)
C6—N1—C7—O1	−3.4 (3)	O4—N2—C19—C20	149.1 (2)
O2—N1—C7—C14	−7.0 (3)	O5—N2—C19—C20	−29.2 (3)
C6—N1—C7—C14	175.80 (17)	O4—N2—C19—C18	−31.9 (3)
C14—C9—C10—C11	−0.2 (3)	O5—N2—C19—C18	149.7 (2)
C9—C10—C11—C12	0.6 (3)	C18—C19—C20—C21	0.6 (3)
C9—C10—C11—Cl2	−179.47 (15)	N2—C19—C20—C21	179.52 (19)
C10—C11—C12—C13	0.1 (3)	C19—C20—C21—C22	−1.3 (3)
Cl2—C11—C12—C13	−179.89 (15)	C20—C21—C22—C23	0.6 (3)
C11—C12—C13—C14	−1.1 (3)	C21—C22—C23—C18	1.0 (3)
C12—C13—C14—C9	1.5 (3)	C19—C18—C23—C22	−1.7 (3)
C12—C13—C14—C7	176.16 (17)	C17—C18—C23—C22	178.38 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.93	2.40	3.177 (2)	140
C17—H17*B*···O4^{ii}	0.97	2.55	3.515 (3)	171

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*−1, *y*, *z*.