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(4S)-4-[(R)-Chloro(4-nitrophenyl)methyl]-1,3-oxazolidin-2-one

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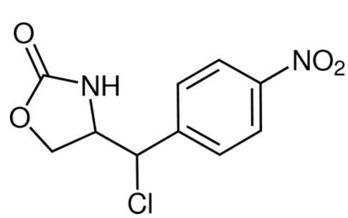
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.001 Å; R factor = 0.037; wR factor = 0.098; data-to-parameter ratio = 38.7.

In the title compound, $C_{10}H_9ClN_2O_4$, the oxazolidinone ring adopts a near-planar conformation, with mean and maximum deviations of 0.0204 (8) and 0.0328 (8) Å, respectively. The nitro group is twisted slightly from the plane of the benzene ring, making a dihedral angle of 6.79 (3)°. The dihedral angle between the mean oxazolidinone plane and the benzene ring is 56.21 (3)°. In the crystal, N—H⋯O hydrogen bonds and N—O⋯π interactions [O⋯centroid distances = 3.478 (1) and 3.238 (1) Å] dominate the packing, forming infinite zigzag chains along the b-axis direction. Neighbouring chains are linked together through C—H⋯O and C—H⋯Cl interactions. The absolute configuration of the two stereogenic centres was determined using the anomalous dispersion of the Cl atom.

Related literature

For the biological activity of oxazolidinone derivatives, see: Michalska *et al.* (2012); Mathur *et al.* (2013); Jindal *et al.* (2013). For related structures, see: Bach *et al.* (2001); Tsui *et al.* (2013). For detailed of the synthesis, see: Madesclaire *et al.* (2013).



Experimental

Crystal data

$C_{10}H_9ClN_2O_4$
M_r = 256.64
Monoclinic, $P2_1$
a = 7.2372 (1) Å
b = 6.6726 (1) Å
c = 11.7126 (2) Å
β = 106.715 (1)°
V = 541.71 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 296 K
0.52 × 0.49 × 0.34 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2012) T_{min} = 0.915, T_{max} = 1.000
12895 measured reflections
6114 independent reflections
5384 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
S = 1.06
6114 reflections
158 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Absolute structure: Flack (1983), 2348 Friedel pairs
Flack parameter: −0.03 (3)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3—H3⋯O15^{i}	0.77 (2)	2.32 (2)	3.095 (1)	179 (2)
C6—H6⋯O16^{ii}	0.98	2.46	3.309 (2)	145
C11—H11⋯Cl17^{iii}	0.93	2.83	3.582 (1)	139

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

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); 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, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2451).

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supplementary materials

Acta Cryst. (2013). E**69**, o783 [doi:10.1107/S1600536813010398]

(4*S*)-4-[(*R*)-Chloro(4-nitrophenyl)methyl]-1,3-oxazolidin-2-one

V. Gaumet, C. Denis, M. Madesclaire and V. P. Zaitsev

Comment

Oxazolidinones are a new class of synthetic antimicrobial agents. Linezolid is the first oxazolidinone approved for human use in the treatment of multidrug-resistant gram-positive bacterial infections (Michalska *et al.*, 2012; Mathur *et al.*, 2013). Linezolid may also offer novel disease modifying and symptomatic therapeutic potential for the treatment of anxiety disorders (Jindal *et al.*, 2013).

The molecular structure of the title compound (Fig. 1) reveals a planar oxazolidinone ring with a mean deviation of 0.0204 (8) Å, maximum deviation from planarity being 0.0328 (8) Å for atom C5. The dihedral angle between the mean oxazolidinone plane and the phenyl ring is 56.21 (3)°. The *p*-NO_2 group form a interplanar angle of 6.79° with the benzene ring. In the crystal, molecules are linked through N3—H3···O15 hydrogen bonds into infinite zigzag chains extending along the *b* axis (Table 1, Fig. 2). In chains, molecules are regularly arranged in head-to-tail sequence allowing N—O···π stacking interactions which reinforce the chain cohesion (Fig. 2 and 3). These stacking forces are characterized by two N13—O15···$C_g^{i, iv}$ [symmetry code: i: $-x + 1$, $y + 1/2$, $-z + 1$; iv: $-x + 1$, $y - 1/2$, $-z + 1$] interactions with distances of 3.478 (1) Å and 3.238 (1) Å between the O15 atom and centroid, C_g, of the (C7—C12) aromatic rings. Adjacent chains build the three dimensional network *via* C6—H6···O16 and C11—H11···Cl17 interactions (Table 1).

The title coumpound exhibits structural similarities with related structures (Bach *et al.*, 2001; Tsui *et al.*, 2013).

Experimental

The title compound was obtained as a by-product from the reaction of 4-[hydroxy(4-nitrophenyl)methyl]-1,3-oxazolidin-2-one and benzenesulfonyl chloride with pyridine in chloroform. The synthesis process is described by Madesclaire *et al.* (2013). After isolation and purification by column chromatography, crystals suitable for X-ray analysis were obtained by slow evaporation from a mixture of ethyl acetate-cyclohexane (1:1 vol.) solution.

Refinement

H atoms were all found in a difference map, but those bonded to C were refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C) and C—H = 0.93–0.98 Å. The H atom bonded to N was freely refined. The highest peak and the deepest hole in the difference Fourier map are located 0.70 and 1.02 Å, respectively from C11 and C8 atoms. The absolute structure was determined on the basis of 2348 Friedel pairs.

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); 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, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

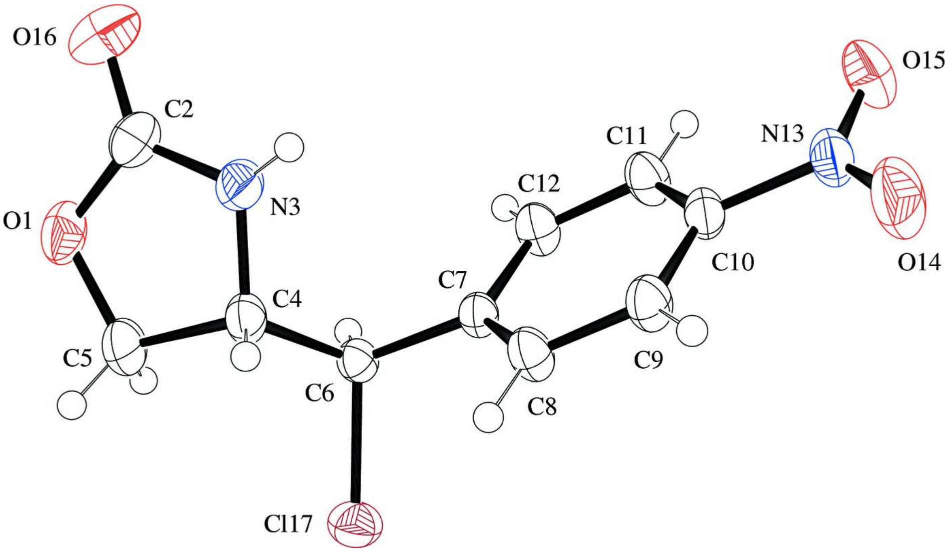

Figure 1

Molecular structure showing the atom labelling scheme and 50% probability displacement ellipsoids for non-H atoms.

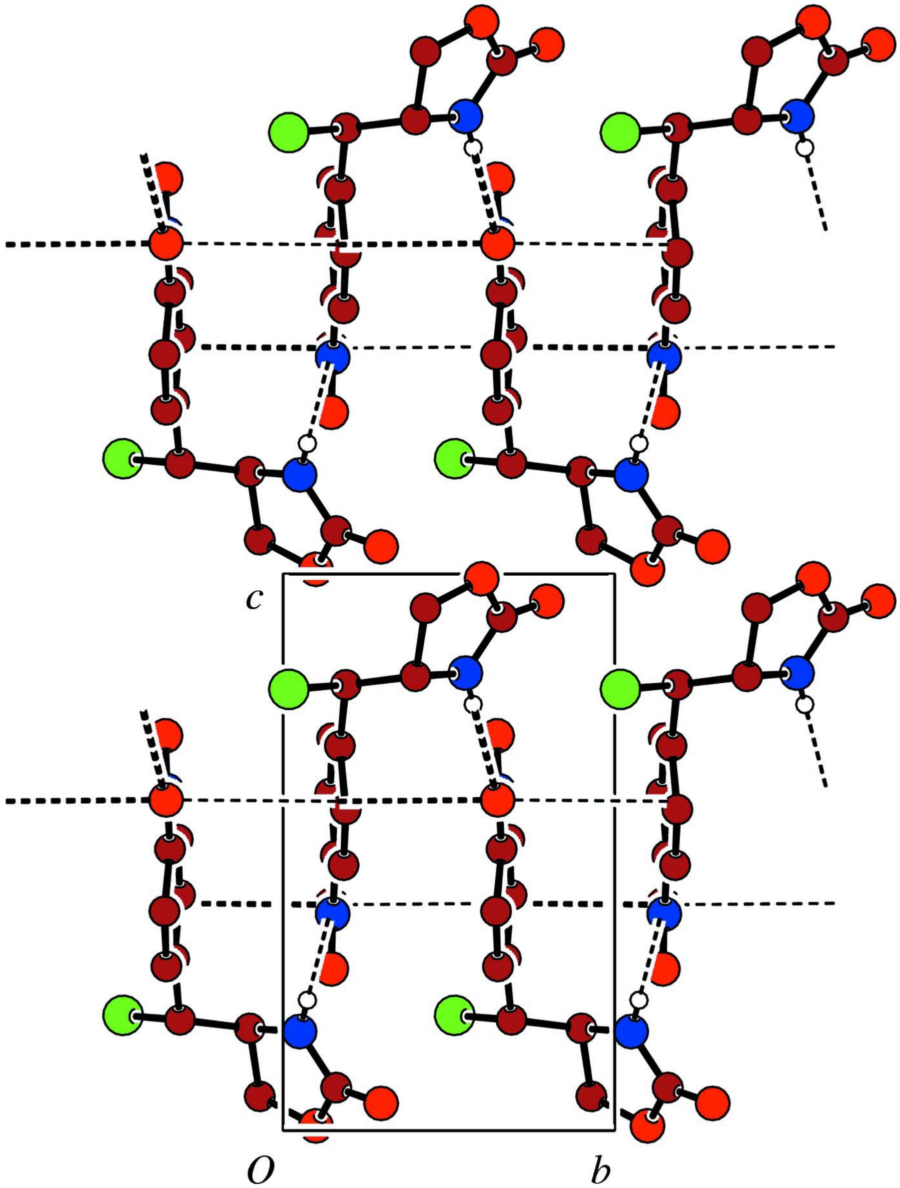

Figure 2

Projection along *a* axis, showing zigzag chain of $C_{10}H_9ClN_2O_4$ molecules connected by N—H···O hydrogen bonds and N—O···π interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

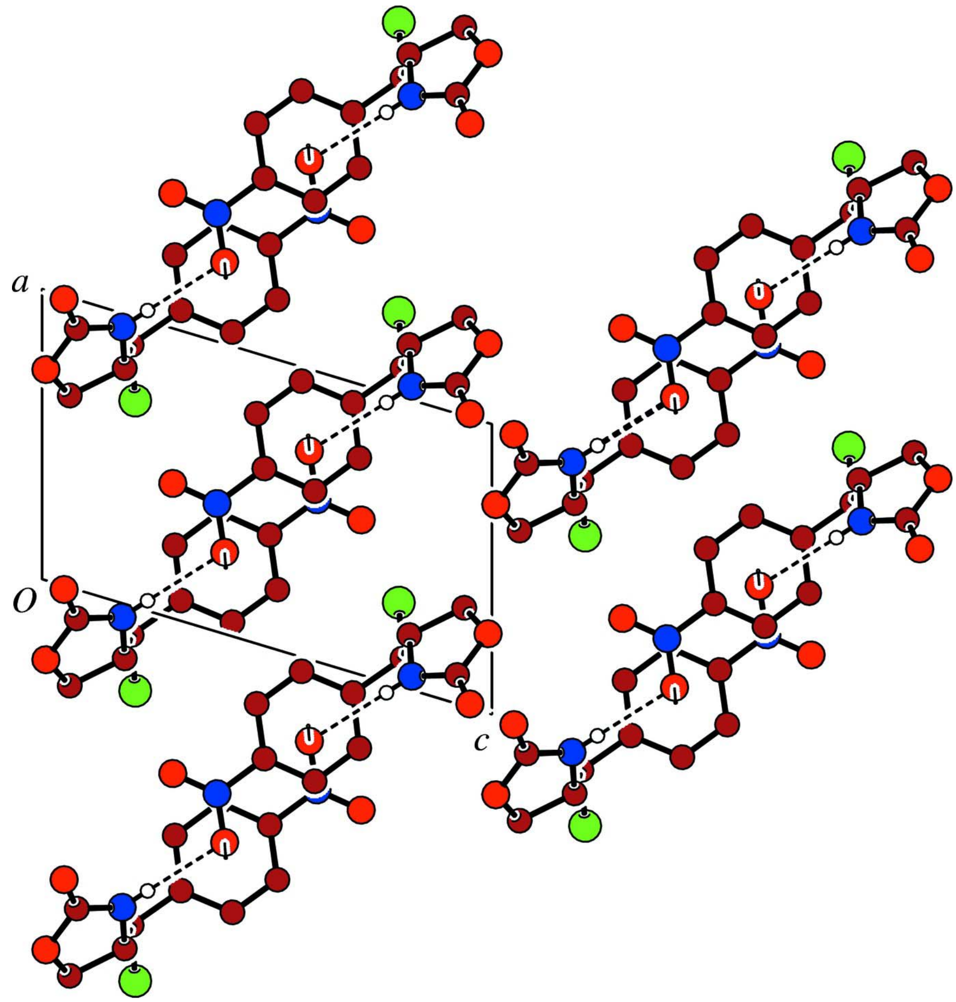

Figure 3

Projection along *b* axis, showing shift between adjacent chains. N—H···O hydrogen bonds and N—O···π interactions are represented as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

(4*S*)-4-[(*R*)-Chloro(4-nitrophenyl)methyl]-1,3-oxazolidin-2-one

Crystal data

$C_{10}H_9ClN_2O_4$	$F(000) = 264$
$M_r = 256.64$	$D_x = 1.573$ Mg m^{-3}
Monoclinic, $P2_1$	Melting point: 414 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.2372$ (1) Å	Cell parameters from 6817 reflections
$b = 6.6726$ (1) Å	$\theta = 4.0$–$39.2°$
$c = 11.7126$ (2) Å	$\mu = 0.36$ mm^{-1}
$\beta = 106.715$ (1)°	$T = 296$ K
$V = 541.71$ (1) Å^3	Block prism, colourless
$Z = 2$	0.52 × 0.49 × 0.34 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
$T_{min} = 0.915$, $T_{max} = 1.000$
12895 measured reflections
6114 independent reflections
5384 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 41.1°$, $\theta_{min} = 4.2°$
$h = -11 \rightarrow 13$
$k = -12 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.098$
$S = 1.06$
6114 reflections
158 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.0254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}
Absolute structure: Flack (1983), 2348 Friedel pairs
Flack parameter: −0.03 (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	−0.27342 (14)	1.09892 (14)	0.00860 (7)	0.04046 (18)
C2	−0.09939 (17)	1.16003 (16)	0.07729 (9)	0.03409 (18)
N3	−0.04803 (15)	1.04959 (14)	0.17795 (9)	0.0379 (2)
H3	0.035 (3)	1.073 (4)	0.234 (2)	0.064 (7)*
C4	−0.18727 (13)	0.89934 (14)	0.18369 (8)	0.02872 (15)
H4	−0.2438	0.9293	0.2484	0.034*
C5	−0.33823 (17)	0.9297 (2)	0.06159 (11)	0.0423 (2)
H5A	−0.3460	0.8116	0.0121	0.051*
H5B	−0.4646	0.9553	0.0716	0.051*
C6	−0.09944 (12)	0.68917 (13)	0.19899 (7)	0.02377 (12)
H6	−0.0574	0.6564	0.1288	0.029*
C7	0.07040 (11)	0.67131 (13)	0.30890 (7)	0.02336 (12)
C8	0.04894 (13)	0.68896 (17)	0.42314 (7)	0.02948 (16)
H8	−0.0736	0.7054	0.4323	0.035*
C9	0.20770 (14)	0.68227 (17)	0.52297 (7)	0.03020 (16)

H9	0.1936	0.6931	0.5992	0.036*
C10	0.38832 (12)	0.65896 (14)	0.50598 (7)	0.02706 (14)
C11	0.41443 (13)	0.64207 (18)	0.39412 (9)	0.03193 (17)
H11	0.5374	0.6270	0.3855	0.038*
C12	0.25405 (13)	0.64796 (18)	0.29494 (8)	0.02991 (16)
H12	0.2691	0.6363	0.2190	0.036*
N13	0.55799 (13)	0.64956 (14)	0.61094 (8)	0.03406 (16)
O14	0.53442 (16)	0.6452 (3)	0.70939 (8)	0.0556 (3)
O15	0.71821 (13)	0.6472 (2)	0.59423 (9)	0.0488 (2)
O16	−0.0129 (2)	1.29556 (17)	0.04888 (10)	0.0528 (3)
Cl17	−0.28820 (3)	0.51760 (4)	0.20713 (2)	0.03492 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0460 (4)	0.0391 (4)	0.0291 (3)	0.0070 (3)	−0.0005 (3)	0.0078 (3)
C2	0.0433 (5)	0.0272 (4)	0.0324 (4)	0.0033 (4)	0.0119 (4)	0.0008 (3)
N3	0.0380 (4)	0.0299 (4)	0.0352 (4)	−0.0064 (3)	−0.0062 (3)	0.0051 (3)
C4	0.0271 (4)	0.0286 (3)	0.0258 (3)	0.0025 (3)	0.0002 (3)	0.0024 (3)
C5	0.0337 (5)	0.0426 (5)	0.0383 (5)	−0.0012 (4)	−0.0092 (4)	0.0089 (4)
C6	0.0232 (3)	0.0272 (3)	0.0201 (3)	0.0001 (2)	0.0049 (2)	0.0002 (2)
C7	0.0223 (3)	0.0262 (3)	0.0209 (3)	0.0023 (2)	0.0051 (2)	0.0020 (2)
C8	0.0229 (3)	0.0433 (5)	0.0221 (3)	0.0036 (3)	0.0063 (2)	0.0017 (3)
C9	0.0285 (4)	0.0399 (4)	0.0210 (3)	0.0030 (3)	0.0052 (3)	0.0024 (3)
C10	0.0248 (3)	0.0277 (3)	0.0250 (3)	0.0037 (3)	0.0013 (2)	0.0025 (3)
C11	0.0225 (3)	0.0415 (5)	0.0311 (4)	0.0062 (3)	0.0067 (3)	0.0010 (3)
C12	0.0256 (3)	0.0409 (4)	0.0239 (3)	0.0057 (3)	0.0083 (2)	0.0008 (3)
N13	0.0301 (3)	0.0315 (3)	0.0330 (4)	0.0043 (3)	−0.0029 (3)	0.0024 (3)
O14	0.0484 (5)	0.0801 (8)	0.0293 (4)	0.0045 (5)	−0.0032 (3)	0.0063 (5)
O15	0.0270 (3)	0.0631 (6)	0.0483 (5)	0.0074 (4)	−0.0018 (3)	0.0020 (5)
O16	0.0723 (7)	0.0370 (4)	0.0576 (6)	−0.0051 (4)	0.0321 (5)	0.0057 (4)
Cl17	0.03212 (10)	0.03645 (11)	0.03473 (10)	−0.00833 (9)	0.00727 (7)	−0.00087 (8)

Geometric parameters (Å, º)

O1—C2	1.3480 (15)	C7—C12	1.3938 (12)
O1—C5	1.4310 (16)	C7—C8	1.3956 (11)
C2—O16	1.2004 (15)	C8—C9	1.3844 (13)
C2—N3	1.3487 (14)	C8—H8	0.9300
N3—C4	1.4367 (14)	C9—C10	1.3863 (13)
N3—H3	0.77 (2)	C9—H9	0.9300
C4—C6	1.5288 (12)	C10—C11	1.3811 (13)
C4—C5	1.5431 (13)	C10—N13	1.4679 (11)
C4—H4	0.9800	C11—C12	1.3866 (13)
C5—H5A	0.9700	C11—H11	0.9300
C5—H5B	0.9700	C12—H12	0.9300
C6—C7	1.5073 (11)	N13—O14	1.2136 (14)
C6—Cl17	1.8058 (9)	N13—O15	1.2303 (13)
C6—H6	0.9800		

C2—O1—C5	110.26 (8)	C4—C6—H6	109.0
O16—C2—O1	122.33 (11)	Cl17—C6—H6	109.0
O16—C2—N3	128.27 (12)	C12—C7—C8	119.65 (7)
O1—C2—N3	109.38 (9)	C12—C7—C6	118.66 (7)
C2—N3—C4	113.67 (9)	C8—C7—C6	121.59 (7)
C2—N3—H3	126.1 (18)	C9—C8—C7	120.85 (8)
C4—N3—H3	119.1 (18)	C9—C8—H8	119.6
N3—C4—C6	111.84 (8)	C7—C8—H8	119.6
N3—C4—C5	100.62 (8)	C8—C9—C10	118.05 (8)
C6—C4—C5	112.87 (8)	C8—C9—H9	121.0
N3—C4—H4	110.4	C10—C9—H9	121.0
C6—C4—H4	110.4	C11—C10—C9	122.49 (8)
C5—C4—H4	110.4	C11—C10—N13	118.76 (8)
O1—C5—C4	105.81 (9)	C9—C10—N13	118.74 (8)
O1—C5—H5A	110.6	C10—C11—C12	118.85 (8)
C4—C5—H5A	110.6	C10—C11—H11	120.6
O1—C5—H5B	110.6	C12—C11—H11	120.6
C4—C5—H5B	110.6	C11—C12—C7	120.10 (8)
H5A—C5—H5B	108.7	C11—C12—H12	119.9
C7—C6—C4	112.46 (7)	C7—C12—H12	119.9
C7—C6—Cl17	110.38 (6)	O14—N13—O15	123.18 (10)
C4—C6—Cl17	107.00 (6)	O14—N13—C10	118.97 (9)
C7—C6—H6	109.0	O15—N13—C10	117.84 (9)

C5—O1—C2—O16	177.34 (12)	Cl17—C6—C7—C8	−53.58 (10)
C5—O1—C2—N3	−3.94 (14)	C12—C7—C8—C9	−0.42 (15)
O16—C2—N3—C4	179.45 (12)	C6—C7—C8—C9	−176.72 (9)
O1—C2—N3—C4	0.83 (14)	C7—C8—C9—C10	0.44 (15)
C2—N3—C4—C6	122.37 (10)	C8—C9—C10—C11	−0.12 (16)
C2—N3—C4—C5	2.29 (13)	C8—C9—C10—N13	−179.40 (9)
C2—O1—C5—C4	5.25 (13)	C9—C10—C11—C12	−0.22 (17)
N3—C4—C5—O1	−4.35 (12)	N13—C10—C11—C12	179.06 (10)
C6—C4—C5—O1	−123.69 (10)	C10—C11—C12—C7	0.23 (17)
N3—C4—C6—C7	57.76 (10)	C8—C7—C12—C11	0.08 (16)
C5—C4—C6—C7	170.37 (8)	C6—C7—C12—C11	176.48 (10)
N3—C4—C6—Cl17	179.12 (6)	C11—C10—N13—O14	−173.10 (13)
C5—C4—C6—Cl17	−68.26 (9)	C9—C10—N13—O14	6.21 (16)
C4—C6—C7—C12	−110.50 (10)	C11—C10—N13—O15	7.17 (15)
Cl17—C6—C7—C12	130.09 (8)	C9—C10—N13—O15	−173.52 (11)
C4—C6—C7—C8	65.84 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O15^{i}	0.77 (2)	2.32 (2)	3.095 (1)	179 (2)
C6—H6···O16^{ii}	0.98	2.46	3.309 (2)	145
C11—H11···Cl17^{iii}	0.93	2.83	3.582 (1)	139

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1; (ii) −*x*, *y*−1/2, −*z*; (iii) *x*+1, *y*, *z*.