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7-Chloro-11a-phenyl-2,3,5,10,11,11a-hexahydro-1*H*-pyrrolo[2,1-*c*][1,4]-benzodiazepine-5,11-dione

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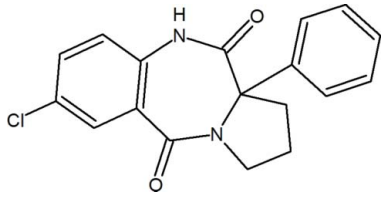
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.122; data-to-parameter ratio = 16.8.

The title compound, $C_{18}H_{15}ClN_2O_2$, is a potential human immunodeficiency virus type-1 (HIV-1) non-nucleoside reverse transcriptase inhibitor. The pyrrolidine ring adopts an envelope and the diazepine ring a boat conformation. In the crystal structure, two isomers (*R* and *S*) form centrosymmetric dimers *via* N—H···O hydrogen bonds.

Related literature

For details of the pharmacological properties of this family of compounds, see: De Clercq (1996). For the crystal structures of some analogues of the title compound, see: Karapetyan *et al.* (2002); Tamazyan *et al.* (2002, 2007). For reference structural data, see Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{15}ClN_2O_2$
M_r = 326.77
Triclinic, $P\overline{1}$
a = 8.9749 (18) Å
b = 9.2184 (18) Å
c = 9.912 (2) Å
α = 86.90 (3)°
β = 71.35 (3)°
γ = 88.27 (3)°
V = 775.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 293 (2) K
0.35 × 0.32 × 0.28 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
7347 measured reflections
4514 independent reflections
3148 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
3 standard reflections
frequency: 180 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.121
S = 1.02
4514 reflections
268 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O12^{i}	0.85 (2)	2.35 (2)	2.997 (2)	133 (2)

Symmetry code: (i) $-x+2, -y, -z+2$.

Data collection: *DATCOL* in *CAD-4* (Enraf–Nonius, 1988); cell refinement: *LS* in *CAD-4*; data reduction: *HELENA* (Spek, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2462).

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supporting information

Acta Cryst. (2008). E**64**, o587 [doi:10.1107/S160053680800408X]

7-Chloro-11a-phenyl-2,3,5,10,11,11a-hexahydro-1*H*-pyrrolo[2,1-*c*][1,4]benzodiazepine-5,11-dione

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S1. Comment

Interest in X-ray structural investigation of title compound, (I), Fig. 1, is stimulated by its potentially HIV-1 RT inhibition properties. These compounds belong to a family of non-nucleoside reverse transcriptase inhibitors (NNRTIs).

All intramolecular interatomic distances in molecule are in good agreement with their mean statistical values (Allen *et al.*, 1987). In the crystal structure dimers are formed by (*R* and S) optical isomers of molecules of (I) *via* O12···H4^{i}—N4^{i} and O12^{i}···H4—N4 double hydrogen bonding (Table 1, Fig.2).

S2. Experimental

A solution of 2-phenyl-2-pyrrolidinecarboxylic acid (0.01 mol) and 6-chloro-1,4-dihydro-2*H*-3,1-benzoxazine-2,4-dione (0.01 mol) in dry DMF (5 ml) was boiled for 4 h. After cooling in an ice bath the title compound formed as a colourless precipitate and was separated by filtration and washed with ethylacetate. The compound as synthesized was a racemic mixture. Crystals were grown from an ethanol solution of the compound.

S3. Refinement

Hydrogen atoms were located in a difference map and refined freely with isotropic thermal parameters.

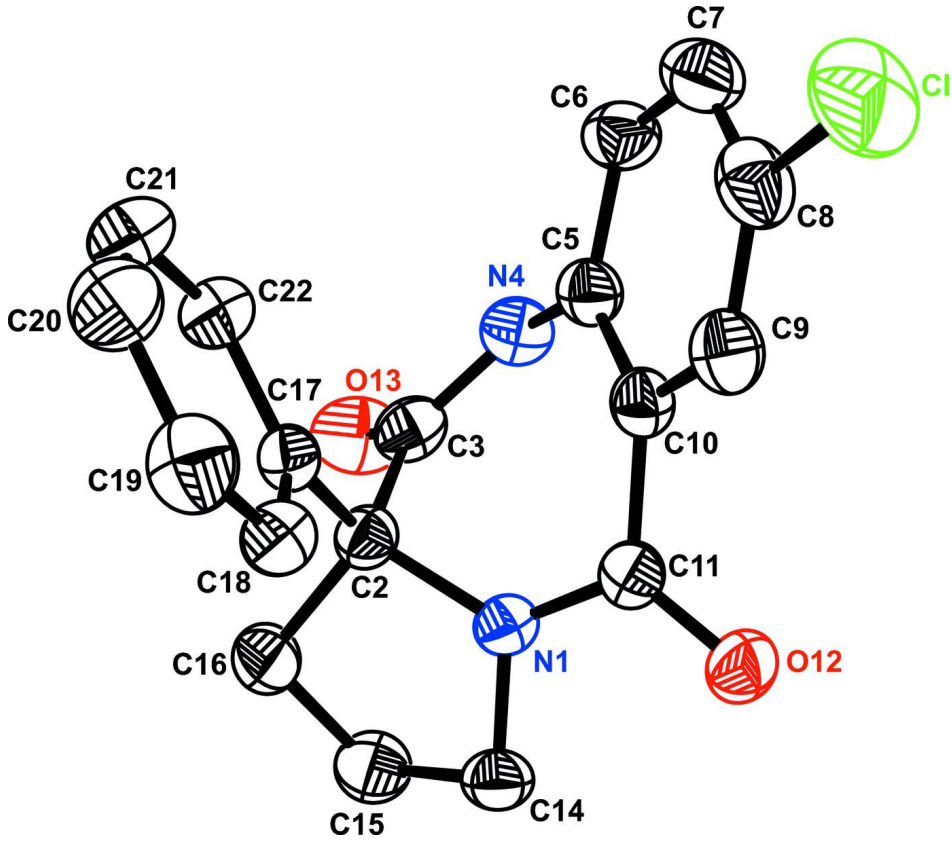

Figure 1

A view of molecule with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

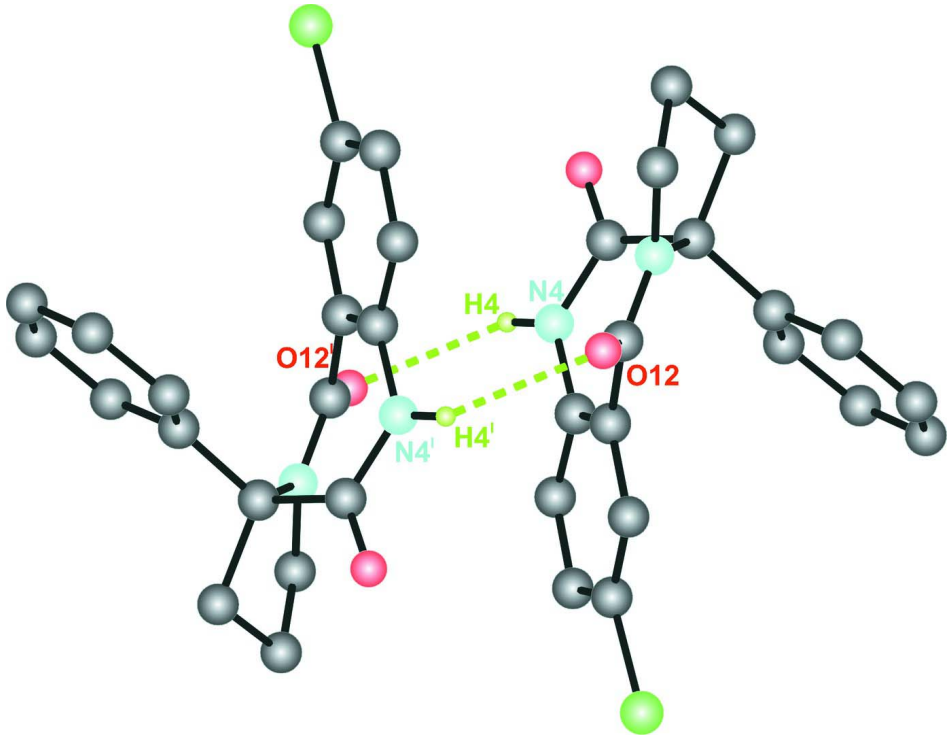

Figure 2

The formation dimers of molecules *via* hydrogen bonding. For clarity only those H atoms participating in hydrogen bonding are depicted. Symmetry code: (i) 2 - *x*, -*y*, 2 - *z*

7-Chloro-11*a*-phenyl-2,3,5,10,11,11*a*-hexahydro-1*H*- pyrrolo[2,1-*c*][1,4]benzodiazepine-5,11-dione

Crystal data

$C_{18}H_{15}ClN_2O_2$
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Hall symbol: -P 1
$a = 8.9749\ (18)$ Å
$b = 9.2184\ (18)$ Å
$c = 9.912\ (2)$ Å
$\alpha = 86.90\ (3)°$
$\beta = 71.35\ (3)°$
$\gamma = 88.27\ (3)°$
$V = 775.8\ (3)$ Å^3
$Z = 2$
$F(000) = 340$
$D_x = 1.399$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22 reflections
$\theta = 12.6–16.6°$
$\mu = 0.26$ mm^{-1}
$T = 293$ K
Prism, colourless
0.35 × 0.32 × 0.28 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\theta/2\theta$ scans
7347 measured reflections
4514 independent reflections
3148 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.2°$
$h = -12\rightarrow12$
$k = -12\rightarrow12$
$l = -13\rightarrow13$
3 standard reflections every 180 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.121$
$S = 1.02$
4514 reflections
268 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.2193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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}
C2	0.70626 (17)	0.27403 (17)	1.00932 (16)	0.0333 (3)
C3	0.66409 (19)	0.11255 (18)	1.04089 (17)	0.0389 (3)
C5	0.91077 (18)	0.04305 (16)	0.85230 (16)	0.0343 (3)
C6	0.9468 (2)	−0.05252 (19)	0.74145 (19)	0.0432 (4)
C7	1.0802 (2)	−0.0350 (2)	0.6255 (2)	0.0488 (4)
C8	1.1788 (2)	0.0798 (2)	0.61835 (19)	0.0470 (4)
C9	1.1492 (2)	0.1717 (2)	0.72885 (19)	0.0418 (4)
C10	1.01455 (17)	0.15430 (16)	0.84775 (16)	0.0332 (3)
C11	0.99809 (17)	0.25083 (15)	0.96767 (16)	0.0319 (3)
C14	0.8259 (2)	0.37447 (19)	1.17444 (18)	0.0391 (3)
C15	0.6494 (2)	0.3646 (2)	1.24567 (19)	0.0493 (4)
C16	0.5879 (2)	0.3677 (2)	1.11921 (19)	0.0448 (4)
C17	0.71935 (17)	0.32632 (16)	0.85722 (16)	0.0335 (3)
C18	0.8016 (2)	0.45256 (19)	0.79868 (18)	0.0405 (4)
C19	0.8104 (2)	0.5045 (2)	0.6632 (2)	0.0519 (4)
C20	0.7365 (3)	0.4332 (2)	0.5842 (2)	0.0571 (5)
C21	0.6523 (3)	0.3101 (2)	0.6421 (2)	0.0562 (5)
C22	0.6436 (2)	0.2556 (2)	0.7781 (2)	0.0439 (4)
Cl	1.33908 (7)	0.10803 (8)	0.46554 (6)	0.0735 (2)
H4	0.745 (2)	−0.072 (2)	0.987 (2)	0.052 (6)*
H6	0.874 (2)	−0.135 (2)	0.747 (2)	0.047 (5)*
H7	1.101 (3)	−0.097 (2)	0.551 (2)	0.062 (6)*
H9	1.219 (2)	0.246 (2)	0.725 (2)	0.049 (5)*
H18	0.851 (2)	0.504 (2)	0.853 (2)	0.048 (5)*
H19	0.864 (3)	0.590 (3)	0.625 (2)	0.065 (7)*

H20	0.745 (3)	0.481 (2)	0.482 (3)	0.064 (6)*
H21	0.599 (3)	0.259 (2)	0.595 (2)	0.058 (6)*
H22	0.584 (2)	0.174 (2)	0.816 (2)	0.051 (6)*
H14A	0.856 (2)	0.473 (2)	1.1500 (19)	0.040 (5)*
H15A	0.608 (3)	0.445 (3)	1.311 (2)	0.065 (6)*
H16A	0.596 (2)	0.467 (2)	1.080 (2)	0.052 (6)*
H14B	0.886 (2)	0.328 (2)	1.233 (2)	0.048 (5)*
H15B	0.623 (2)	0.270 (2)	1.301 (2)	0.054 (6)*
H16B	0.484 (3)	0.331 (2)	1.139 (2)	0.055 (6)*
N1	0.85316 (15)	0.29356 (14)	1.04452 (13)	0.0327 (3)
N4	0.77286 (16)	0.01605 (16)	0.96731 (15)	0.0390 (3)
O12	1.11592 (13)	0.28878 (12)	0.99545 (13)	0.0410 (3)
O13	0.54222 (16)	0.07208 (16)	1.12946 (15)	0.0604 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0302 (7)	0.0378 (8)	0.0323 (7)	−0.0007 (6)	−0.0102 (5)	−0.0035 (6)
C3	0.0373 (8)	0.0440 (9)	0.0352 (8)	−0.0102 (6)	−0.0106 (6)	−0.0001 (6)
C5	0.0389 (8)	0.0298 (7)	0.0351 (7)	0.0016 (6)	−0.0134 (6)	0.0008 (6)
C6	0.0543 (10)	0.0354 (8)	0.0433 (9)	0.0004 (7)	−0.0199 (8)	−0.0040 (7)
C7	0.0610 (11)	0.0468 (10)	0.0399 (9)	0.0125 (8)	−0.0178 (8)	−0.0093 (8)
C8	0.0423 (9)	0.0553 (11)	0.0373 (8)	0.0095 (8)	−0.0055 (7)	0.0000 (8)
C9	0.0352 (8)	0.0438 (9)	0.0437 (9)	0.0006 (7)	−0.0092 (7)	0.0006 (7)
C10	0.0324 (7)	0.0316 (7)	0.0359 (7)	0.0017 (5)	−0.0118 (6)	−0.0001 (6)
C11	0.0342 (7)	0.0263 (7)	0.0361 (7)	−0.0030 (5)	−0.0131 (6)	0.0040 (5)
C14	0.0480 (9)	0.0360 (8)	0.0367 (8)	0.0009 (7)	−0.0174 (7)	−0.0070 (7)
C15	0.0494 (10)	0.0602 (12)	0.0365 (9)	0.0050 (9)	−0.0102 (7)	−0.0112 (8)
C16	0.0394 (9)	0.0540 (11)	0.0407 (9)	0.0087 (8)	−0.0115 (7)	−0.0118 (8)
C17	0.0310 (7)	0.0363 (8)	0.0343 (7)	0.0047 (6)	−0.0119 (6)	−0.0050 (6)
C18	0.0417 (9)	0.0405 (9)	0.0418 (9)	−0.0001 (7)	−0.0168 (7)	−0.0032 (7)
C19	0.0563 (11)	0.0507 (11)	0.0463 (10)	−0.0007 (9)	−0.0147 (8)	0.0080 (8)
C20	0.0711 (13)	0.0641 (13)	0.0382 (9)	0.0087 (10)	−0.0213 (9)	−0.0014 (9)
C21	0.0687 (13)	0.0618 (12)	0.0508 (11)	0.0060 (10)	−0.0354 (10)	−0.0148 (9)
C22	0.0462 (9)	0.0440 (9)	0.0467 (9)	−0.0005 (7)	−0.0215 (8)	−0.0068 (8)
Cl	0.0554 (3)	0.0986 (5)	0.0498 (3)	0.0051 (3)	0.0065 (2)	−0.0053 (3)
N1	0.0349 (6)	0.0337 (6)	0.0318 (6)	−0.0002 (5)	−0.0134 (5)	−0.0037 (5)
N4	0.0418 (7)	0.0314 (7)	0.0417 (7)	−0.0078 (5)	−0.0106 (6)	0.0026 (6)
O12	0.0371 (6)	0.0362 (6)	0.0532 (7)	−0.0047 (4)	−0.0189 (5)	−0.0019 (5)
O13	0.0519 (8)	0.0631 (9)	0.0522 (8)	−0.0217 (7)	0.0050 (6)	−0.0049 (6)

Geometric parameters (Å, º)

C2—N1	1.4858 (19)	C14—C15	1.517 (3)
C2—C17	1.527 (2)	C14—H14A	0.956 (19)
C2—C3	1.538 (2)	C14—H14B	0.99 (2)
C2—C16	1.539 (2)	C15—C16	1.522 (3)
C3—O13	1.217 (2)	C15—H15A	0.99 (2)

C3—N4	1.356 (2)	C15—H15B	1.00 (2)
C5—C10	1.395 (2)	C16—H16A	0.97 (2)
C5—C6	1.396 (2)	C16—H16B	0.96 (2)
C5—N4	1.407 (2)	C17—C22	1.387 (2)
C6—C7	1.375 (3)	C17—C18	1.393 (2)
C6—H6	1.010 (19)	C18—C19	1.380 (3)
C7—C8	1.385 (3)	C18—H18	0.95 (2)
C7—H7	0.93 (2)	C19—C20	1.378 (3)
C8—C9	1.374 (3)	C19—H19	0.94 (2)
C8—Cl	1.7370 (19)	C20—C21	1.376 (3)
C9—C10	1.398 (2)	C20—H20	1.06 (2)
C9—H9	0.93 (2)	C21—C22	1.392 (3)
C10—C11	1.490 (2)	C21—H21	0.92 (2)
C11—O12	1.2391 (18)	C22—H22	0.92 (2)
C11—N1	1.340 (2)	N4—H4	0.85 (2)
C14—N1	1.472 (2)		

N1—C2—C17	113.17 (12)	C14—C15—C16	102.64 (15)
N1—C2—C3	106.65 (12)	C14—C15—H15A	111.5 (13)
C17—C2—C3	113.09 (13)	C16—C15—H15A	113.8 (13)
N1—C2—C16	101.84 (12)	C14—C15—H15B	110.0 (12)
C17—C2—C16	111.26 (13)	C16—C15—H15B	109.7 (12)
C3—C2—C16	110.18 (14)	H15A—C15—H15B	109.1 (18)
O13—C3—N4	121.24 (16)	C15—C16—C2	104.63 (14)
O13—C3—C2	122.47 (16)	C15—C16—H16A	107.3 (12)
N4—C3—C2	116.26 (13)	C2—C16—H16A	107.6 (12)
C10—C5—C6	119.46 (15)	C15—C16—H16B	115.7 (13)
C10—C5—N4	123.50 (14)	C2—C16—H16B	109.7 (13)
C6—C5—N4	116.96 (15)	H16A—C16—H16B	111.4 (18)
C7—C6—C5	120.84 (17)	C22—C17—C18	118.84 (15)
C7—C6—H6	119.9 (11)	C22—C17—C2	121.50 (15)
C5—C6—H6	119.3 (11)	C18—C17—C2	119.56 (14)
C6—C7—C8	119.40 (17)	C19—C18—C17	120.52 (17)
C6—C7—H7	120.2 (14)	C19—C18—H18	119.7 (12)
C8—C7—H7	120.4 (14)	C17—C18—H18	119.8 (12)
C9—C8—C7	120.77 (17)	C20—C19—C18	120.54 (19)
C9—C8—Cl	120.40 (15)	C20—C19—H19	119.1 (14)
C7—C8—Cl	118.82 (15)	C18—C19—H19	120.3 (14)
C8—C9—C10	120.23 (17)	C21—C20—C19	119.41 (18)
C8—C9—H9	120.2 (12)	C21—C20—H20	124.0 (12)
C10—C9—H9	119.6 (12)	C19—C20—H20	116.5 (12)
C5—C10—C9	119.18 (15)	C20—C21—C22	120.71 (19)
C5—C10—C11	123.97 (14)	C20—C21—H21	123.0 (13)
C9—C10—C11	116.69 (14)	C22—C21—H21	116.3 (14)
O12—C11—N1	121.43 (14)	C17—C22—C21	119.96 (18)
O12—C11—C10	120.38 (14)	C17—C22—H22	120.9 (13)
N1—C11—C10	118.18 (13)	C21—C22—H22	119.1 (13)
N1—C14—C15	103.15 (14)	C11—N1—C14	121.27 (13)

N1—C14—H14A	110.2 (11)	C11—N1—C2	126.30 (12)
C15—C14—H14A	110.6 (11)	C14—N1—C2	112.36 (12)
N1—C14—H14B	109.6 (11)	C3—N4—C5	128.71 (14)
C15—C14—H14B	112.6 (11)	C3—N4—H4	113.7 (14)
H14A—C14—H14B	110.4 (15)	C5—N4—H4	116.9 (14)
N1—C2—C3—O13	118.43 (17)	C3—C2—C17—C22	23.3 (2)
C17—C2—C3—O13	−116.54 (18)	C16—C2—C17—C22	−101.29 (18)
C16—C2—C3—O13	8.7 (2)	N1—C2—C17—C18	−38.96 (19)
N1—C2—C3—N4	−59.63 (17)	C3—C2—C17—C18	−160.38 (14)
C17—C2—C3—N4	65.40 (18)	C16—C2—C17—C18	75.00 (18)
C16—C2—C3—N4	−169.39 (14)	C22—C17—C18—C19	−1.4 (2)
C10—C5—C6—C7	−2.5 (2)	C2—C17—C18—C19	−177.78 (16)
N4—C5—C6—C7	−179.40 (15)	C17—C18—C19—C20	0.7 (3)
C5—C6—C7—C8	−0.6 (3)	C18—C19—C20—C21	0.6 (3)
C6—C7—C8—C9	3.3 (3)	C19—C20—C21—C22	−1.2 (3)
C6—C7—C8—Cl	−175.46 (14)	C18—C17—C22—C21	0.8 (3)
C7—C8—C9—C10	−2.9 (3)	C2—C17—C22—C21	177.10 (16)
Cl—C8—C9—C10	175.88 (13)	C20—C21—C22—C17	0.5 (3)
C6—C5—C10—C9	2.9 (2)	O12—C11—N1—C14	−6.6 (2)
N4—C5—C10—C9	179.60 (14)	C10—C11—N1—C14	172.75 (13)
C6—C5—C10—C11	−172.22 (14)	O12—C11—N1—C2	170.27 (13)
N4—C5—C10—C11	4.5 (2)	C10—C11—N1—C2	−10.4 (2)
C8—C9—C10—C5	−0.3 (2)	C15—C14—N1—C11	−165.56 (14)
C8—C9—C10—C11	175.20 (15)	C15—C14—N1—C2	17.18 (18)
C5—C10—C11—O12	141.38 (15)	C17—C2—N1—C11	−50.6 (2)
C9—C10—C11—O12	−33.9 (2)	C3—C2—N1—C11	74.38 (18)
C5—C10—C11—N1	−38.0 (2)	C16—C2—N1—C11	−170.11 (15)
C9—C10—C11—N1	146.80 (14)	C17—C2—N1—C14	126.50 (14)
N1—C14—C15—C16	−34.22 (19)	C3—C2—N1—C14	−108.52 (14)
C14—C15—C16—C2	39.5 (2)	C16—C2—N1—C14	6.98 (17)
N1—C2—C16—C15	−28.50 (18)	O13—C3—N4—C5	172.76 (16)
C17—C2—C16—C15	−149.37 (15)	C2—C3—N4—C5	−9.1 (2)
C3—C2—C16—C15	84.38 (18)	C10—C5—N4—C3	43.9 (2)
N1—C2—C17—C22	144.75 (15)	C6—C5—N4—C3	−139.36 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O12^{i}	0.85 (2)	2.35 (2)	2.997 (2)	133 (2)

Symmetry code: (i) −*x*+2, −*y*, −*z*+2.