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1-[6-Chloro-2-(phenanthren-9-yl)quinolin-4-yl]-pyrrolidin-2-one

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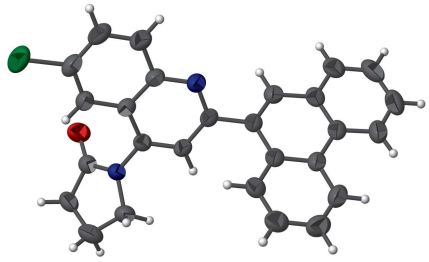
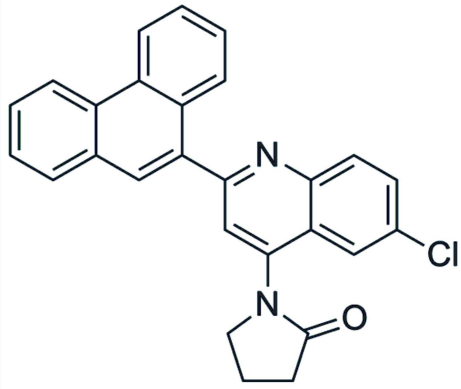
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{27}H_{19}ClN_2O$, the quinoline system is planar, with a maximum deviation from the mean plane of 0.003 Å for the N atom. This ring makes dihedral angles of 56.64 (5) and 49.26 (2)° with phenanthrene and pyrrolidine rings, respectively. The pyrrolidine ring adopts a twisted conformation. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming a two-dimensional network lying parallel to (010).

3D view



Chemical scheme



Structure description

A large number of natural products contain the quinoline and pyrrolidine heterocycles, and they are found in numerous commercial products, including pharmaceuticals, fragrances and dyes (Padwa *et al.*, 1999). Pyrrolidine derivatives are found to have anticonvulsant, antimicrobial and antifungal activities against various pathogens (Amal Raj *et al.*, 2003).

In the molecular structure of the title molecule (Fig. 1), the chlorobenzene ring belonging to the quinoline system adopts an almost planar conformation with a maximum deviation of 0.162 Å for Cl1. The pyrrolidine ring N1/C18–C21 adopts a twisted conformation with puckering parameters q_2 = 0.112 (3) Å and φ = 25.4 (15)°. This latter ring forms dihedral angles of 49.26 (2) and 49.27 (8)° with the quinoline and phenanthrene rings, respectively. The keto atom O1 in the 2-pyrrolidinone group deviates by 0.128 Å from the pyrrolidine mean plane.

In the crystal structure, molecules are linked *via* C—H···O intermolecular hydrogen bonds, forming a two-dimensional network lying parallel to the (010) plane (Table 1 and Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.45	3.358 (4)	164

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

Synthesis and crystallization

4-Chloroaniline (2.4 mmol), which was reacted with pyrene-1-carboxaldehyde (2.4 mmol) and *N*-vinyl-2-pyrrolidinone (2.5 mmol) in the presence of scandium(III) trifluoromethanesulfonate (5 mol %), in acetonitrile. This reaction was carried out at 80°C, and after completion, the reaction mixture was filtered and washed with acetonitrile. The overall yield was 85%. The product was dissolved in chloroform and heated for two minutes. The resulting solution was subjected to crystallization by slow evaporation of the solvent over two days, resulting in the formation of single crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

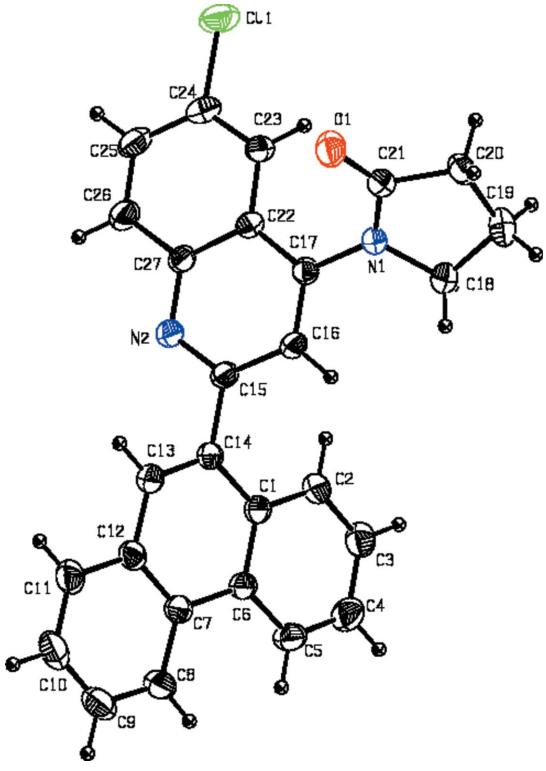

Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius.

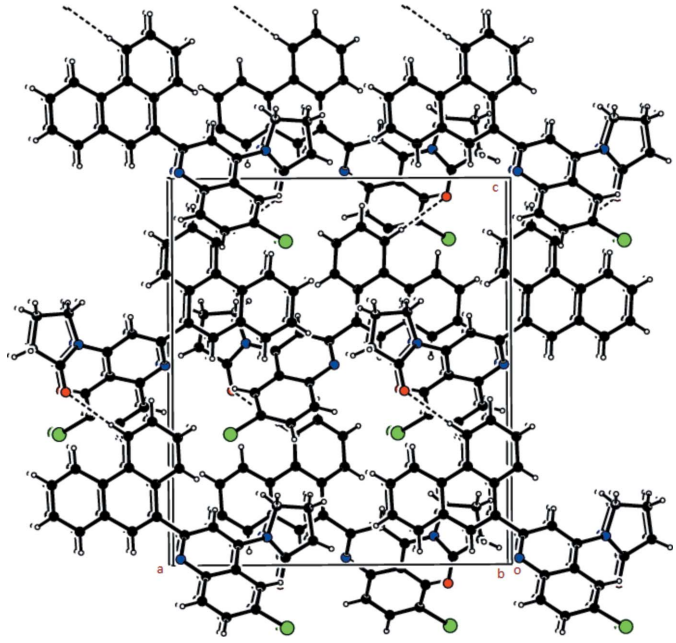

Figure 2
The molecular packing viewed down the *b* axis. The hydrogen bonds are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{19}ClN_2O$
M_r	422.89
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	293
a, b, c (Å)	14.824 (3), 8.2946 (17), 16.924 (3)
V (Å^3)	2081.0 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.25 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.952, 0.960
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8128, 3530, 2845
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.093, 1.06
No. of reflections	3530
No. of parameters	280
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.16
Absolute structure	Flack (1983)
Absolute structure parameter	0.11 (7)

Computer programs: *APEX2* (Bruker, 2008), *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL97* and *PLATON* (Spek, 2009).

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full crystallographic data

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Crystal data

$C_{27}H_{19}ClN_2O$
M_r = 422.89
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 14.824 (3) Å
b = 8.2946 (17) Å
c = 16.924 (3) Å
V = 2081.0 (7) Å^3
Z = 4
$F(000)$ = 880
D_x = 1.350 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2845 reflections
θ = 2.4–25.0°
μ = 0.21 mm^{-1}
T = 293 K
Block, colourless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.952, T_{max} = 0.960
8128 measured reflections
3530 independent reflections
2845 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −17→13
k = −9→9
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.06
3530 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.0804P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.11 (7)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	−0.05298 (16)	0.8783 (3)	0.71094 (14)	0.0444 (6)

C2	0.01627 (17)	0.7975 (3)	0.75181 (15)	0.0508 (6)
H2	0.0666	0.7618	0.7240	0.061*
C3	0.01143 (19)	0.7702 (3)	0.83100 (16)	0.0596 (7)
H3	0.0578	0.7158	0.8567	0.072*
C4	−0.0630 (2)	0.8239 (4)	0.87318 (17)	0.0669 (8)
H4	−0.0653	0.8093	0.9276	0.080*
C5	−0.13266 (19)	0.8978 (3)	0.83552 (17)	0.0602 (7)
H5	−0.1828	0.9302	0.8645	0.072*
C6	−0.13060 (16)	0.9263 (3)	0.75391 (15)	0.0458 (6)
C7	−0.20672 (17)	0.9978 (3)	0.71181 (16)	0.0491 (6)
C8	−0.28684 (19)	1.0456 (4)	0.7507 (2)	0.0648 (8)
H8	−0.2921	1.0320	0.8050	0.078*
C9	−0.35642 (19)	1.1118 (4)	0.7090 (2)	0.0755 (9)
H9	−0.4086	1.1427	0.7354	0.091*
C10	−0.35063 (19)	1.1336 (4)	0.6281 (2)	0.0734 (9)
H10	−0.3985	1.1796	0.6006	0.088*
C11	−0.27442 (19)	1.0874 (3)	0.58848 (19)	0.0621 (7)
H11	−0.2708	1.1013	0.5340	0.075*
C12	−0.20145 (16)	1.0189 (3)	0.62972 (17)	0.0486 (6)
C13	−0.12090 (17)	0.9717 (3)	0.58905 (15)	0.0488 (6)
H13	−0.1178	0.9863	0.5346	0.059*
C14	−0.04928 (15)	0.9070 (3)	0.62676 (14)	0.0433 (6)
C15	0.03207 (16)	0.8673 (3)	0.57893 (13)	0.0422 (5)
C16	0.11754 (16)	0.9326 (3)	0.59887 (14)	0.0441 (6)
H16	0.1234	0.9978	0.6432	0.053*
C17	0.19117 (15)	0.8999 (3)	0.55315 (13)	0.0400 (5)
C18	0.30624 (17)	0.9863 (4)	0.65352 (15)	0.0564 (7)
H18A	0.3068	0.8833	0.6807	0.068*
H18B	0.2668	1.0596	0.6818	0.068*
C19	0.4006 (2)	1.0547 (4)	0.64752 (17)	0.0673 (8)
H19A	0.4068	1.1487	0.6812	0.081*
H19B	0.4448	0.9749	0.6636	0.081*
C20	0.41419 (16)	1.1001 (3)	0.56260 (15)	0.0556 (7)
H20A	0.4212	1.2159	0.5574	0.067*
H20B	0.4676	1.0480	0.5415	0.067*
C21	0.33183 (15)	1.0443 (3)	0.51965 (16)	0.0468 (6)
C22	0.18137 (15)	0.7916 (3)	0.48919 (13)	0.0408 (5)
C23	0.25435 (16)	0.7291 (3)	0.44529 (14)	0.0458 (6)
H23	0.3130	0.7622	0.4560	0.055*
C24	0.23791 (19)	0.6196 (3)	0.38689 (15)	0.0535 (7)
C25	0.1507 (2)	0.5708 (3)	0.36694 (15)	0.0614 (8)
H25	0.1415	0.4997	0.3252	0.074*
C26	0.07948 (19)	0.6280 (3)	0.40885 (15)	0.0584 (7)
H26	0.0213	0.5955	0.3958	0.070*
C27	0.09297 (16)	0.7365 (3)	0.47227 (13)	0.0435 (6)
Cl1	0.32930 (6)	0.53261 (10)	0.33873 (5)	0.0793 (3)
N1	0.27677 (13)	0.9669 (2)	0.57219 (11)	0.0426 (5)
N2	0.01915 (14)	0.7756 (2)	0.51683 (12)	0.0472 (5)

O1	0.31649 (13)	1.0648 (3)	0.45001 (12)	0.0693 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0415 (13)	0.0449 (12)	0.0469 (14)	−0.0090 (11)	0.0008 (12)	−0.0090 (11)
C2	0.0424 (14)	0.0554 (14)	0.0545 (17)	−0.0058 (11)	−0.0011 (12)	−0.0031 (13)
C3	0.0571 (16)	0.0645 (16)	0.0574 (18)	−0.0103 (13)	−0.0070 (15)	0.0063 (14)
C4	0.073 (2)	0.081 (2)	0.0466 (16)	−0.0090 (17)	0.0010 (15)	0.0048 (15)
C5	0.0574 (16)	0.0721 (17)	0.0512 (16)	−0.0089 (14)	0.0143 (15)	−0.0093 (15)
C6	0.0419 (14)	0.0497 (13)	0.0457 (14)	−0.0072 (11)	0.0045 (12)	−0.0101 (11)
C7	0.0423 (15)	0.0498 (14)	0.0551 (16)	−0.0099 (11)	0.0040 (12)	−0.0169 (11)
C8	0.0445 (16)	0.0788 (19)	0.0711 (19)	−0.0060 (15)	0.0093 (15)	−0.0211 (16)
C9	0.0409 (16)	0.084 (2)	0.101 (3)	0.0031 (15)	0.0036 (18)	−0.0272 (19)
C10	0.0451 (17)	0.0728 (18)	0.102 (3)	0.0040 (14)	−0.0187 (18)	−0.0194 (18)
C11	0.0505 (16)	0.0644 (16)	0.0714 (19)	−0.0024 (14)	−0.0104 (15)	−0.0170 (15)
C12	0.0405 (14)	0.0461 (13)	0.0591 (18)	−0.0027 (11)	−0.0023 (13)	−0.0129 (11)
C13	0.0459 (14)	0.0544 (14)	0.0460 (14)	−0.0059 (12)	−0.0007 (12)	−0.0088 (12)
C14	0.0384 (13)	0.0463 (12)	0.0451 (14)	−0.0070 (10)	0.0018 (11)	−0.0092 (11)
C15	0.0441 (13)	0.0446 (12)	0.0379 (13)	−0.0044 (10)	0.0042 (11)	−0.0057 (10)
C16	0.0448 (14)	0.0488 (13)	0.0387 (14)	−0.0046 (11)	0.0022 (11)	−0.0099 (10)
C17	0.0397 (13)	0.0415 (12)	0.0387 (13)	−0.0025 (10)	−0.0011 (11)	0.0006 (10)
C18	0.0489 (15)	0.0770 (17)	0.0431 (16)	−0.0007 (13)	−0.0066 (12)	−0.0028 (13)
C19	0.0555 (16)	0.0774 (18)	0.069 (2)	−0.0070 (14)	−0.0211 (15)	0.0002 (16)
C20	0.0377 (13)	0.0622 (16)	0.0669 (18)	−0.0006 (12)	−0.0045 (13)	−0.0085 (13)
C21	0.0421 (14)	0.0539 (14)	0.0446 (15)	−0.0002 (11)	0.0003 (12)	0.0003 (12)
C22	0.0450 (14)	0.0426 (12)	0.0349 (12)	−0.0002 (10)	0.0024 (11)	0.0008 (11)
C23	0.0440 (14)	0.0525 (13)	0.0409 (13)	0.0034 (11)	0.0040 (11)	−0.0004 (12)
C24	0.0660 (18)	0.0543 (14)	0.0402 (14)	0.0061 (13)	0.0126 (13)	−0.0003 (12)
C25	0.077 (2)	0.0652 (17)	0.0418 (16)	−0.0102 (15)	0.0101 (14)	−0.0149 (13)
C26	0.0604 (17)	0.0667 (16)	0.0483 (16)	−0.0136 (14)	0.0046 (14)	−0.0148 (14)
C27	0.0474 (15)	0.0477 (12)	0.0352 (13)	−0.0044 (11)	0.0021 (11)	−0.0034 (11)
Cl1	0.0815 (5)	0.0924 (5)	0.0641 (5)	0.0260 (4)	0.0160 (4)	−0.0179 (4)
N1	0.0360 (10)	0.0531 (11)	0.0388 (12)	−0.0023 (9)	−0.0029 (9)	−0.0026 (9)
N2	0.0433 (11)	0.0564 (11)	0.0419 (11)	−0.0084 (9)	0.0028 (10)	−0.0062 (10)
O1	0.0604 (12)	0.0985 (15)	0.0491 (13)	−0.0232 (11)	−0.0054 (10)	0.0164 (11)

Geometric parameters (Å, º)

C1—C2	1.408 (3)	C16—C17	1.365 (3)
C1—C6	1.418 (3)	C16—H16	0.9300
C1—C14	1.445 (3)	C17—C22	1.414 (3)
C2—C3	1.361 (3)	C17—N1	1.422 (3)
C2—H2	0.9300	C18—N1	1.453 (3)
C3—C4	1.388 (4)	C18—C19	1.513 (4)
C3—H3	0.9300	C18—H18A	0.9700
C4—C5	1.359 (4)	C18—H18B	0.9700
C4—H4	0.9300	C19—C20	1.499 (4)

C5—C6	1.402 (4)	C19—H19A	0.9700
C5—H5	0.9300	C19—H19B	0.9700
C6—C7	1.461 (4)	C20—C21	1.495 (3)
C7—C12	1.402 (4)	C20—H20A	0.9700
C7—C8	1.414 (4)	C20—H20B	0.9700
C8—C9	1.365 (5)	C21—O1	1.212 (3)
C8—H8	0.9300	C21—N1	1.367 (3)
C9—C10	1.384 (4)	C22—C23	1.411 (3)
C9—H9	0.9300	C22—C27	1.417 (3)
C10—C11	1.368 (4)	C23—C24	1.364 (4)
C10—H10	0.9300	C23—H23	0.9300
C11—C12	1.407 (4)	C24—C25	1.396 (4)
C11—H11	0.9300	C24—Cl1	1.738 (3)
C12—C13	1.433 (4)	C25—C26	1.357 (4)
C13—C14	1.350 (3)	C25—H25	0.9300
C13—H13	0.9300	C26—C27	1.415 (3)
C14—C15	1.489 (3)	C26—H26	0.9300
C15—N2	1.311 (3)	C27—N2	1.368 (3)
C15—C16	1.419 (3)		

C2—C1—C6	118.2 (2)	C15—C16—H16	119.9
C2—C1—C14	122.3 (2)	C16—C17—C22	118.5 (2)
C6—C1—C14	119.4 (2)	C16—C17—N1	120.5 (2)
C3—C2—C1	121.6 (3)	C22—C17—N1	120.9 (2)
C3—C2—H2	119.2	N1—C18—C19	104.8 (2)
C1—C2—H2	119.2	N1—C18—H18A	110.8
C2—C3—C4	119.7 (3)	C19—C18—H18A	110.8
C2—C3—H3	120.2	N1—C18—H18B	110.8
C4—C3—H3	120.2	C19—C18—H18B	110.8
C5—C4—C3	120.5 (3)	H18A—C18—H18B	108.9
C5—C4—H4	119.7	C20—C19—C18	106.4 (2)
C3—C4—H4	119.7	C20—C19—H19A	110.4
C4—C5—C6	121.4 (3)	C18—C19—H19A	110.4
C4—C5—H5	119.3	C20—C19—H19B	110.4
C6—C5—H5	119.3	C18—C19—H19B	110.4
C5—C6—C1	118.4 (2)	H19A—C19—H19B	108.6
C5—C6—C7	122.2 (2)	C21—C20—C19	106.2 (2)
C1—C6—C7	119.4 (2)	C21—C20—H20A	110.5
C12—C7—C8	118.2 (3)	C19—C20—H20A	110.5
C12—C7—C6	119.4 (2)	C21—C20—H20B	110.5
C8—C7—C6	122.4 (3)	C19—C20—H20B	110.5
C9—C8—C7	120.5 (3)	H20A—C20—H20B	108.7
C9—C8—H8	119.8	O1—C21—N1	125.9 (2)
C7—C8—H8	119.8	O1—C21—C20	125.6 (2)
C8—C9—C10	121.1 (3)	N1—C21—C20	108.5 (2)
C8—C9—H9	119.4	C23—C22—C17	123.9 (2)
C10—C9—H9	119.4	C23—C22—C27	118.9 (2)
C11—C10—C9	119.9 (3)	C17—C22—C27	117.0 (2)

C11—C10—H10	120.0	C24—C23—C22	119.3 (2)
C9—C10—H10	120.0	C24—C23—H23	120.4
C10—C11—C12	120.3 (3)	C22—C23—H23	120.4
C10—C11—H11	119.8	C23—C24—C25	122.2 (2)
C12—C11—H11	119.8	C23—C24—Cl1	118.5 (2)
C7—C12—C11	119.9 (3)	C25—C24—Cl1	119.2 (2)
C7—C12—C13	119.2 (2)	C26—C25—C24	119.5 (2)
C11—C12—C13	120.8 (3)	C26—C25—H25	120.2
C14—C13—C12	122.5 (2)	C24—C25—H25	120.2
C14—C13—H13	118.8	C25—C26—C27	120.6 (3)
C12—C13—H13	118.8	C25—C26—H26	119.7
C13—C14—C1	120.1 (2)	C27—C26—H26	119.7
C13—C14—C15	117.9 (2)	N2—C27—C26	117.1 (2)
C1—C14—C15	122.0 (2)	N2—C27—C22	123.5 (2)
N2—C15—C16	122.9 (2)	C26—C27—C22	119.3 (2)
N2—C15—C14	116.5 (2)	C21—N1—C17	124.7 (2)
C16—C15—C14	120.63 (19)	C21—N1—C18	112.6 (2)
C17—C16—C15	120.2 (2)	C17—N1—C18	121.7 (2)
C17—C16—H16	119.9	C15—N2—C27	117.5 (2)

C6—C1—C2—C3	−2.3 (3)	C14—C15—C16—C17	−177.8 (2)
C14—C1—C2—C3	−179.4 (2)	C15—C16—C17—C22	−4.2 (3)
C1—C2—C3—C4	−0.5 (4)	C15—C16—C17—N1	179.1 (2)
C2—C3—C4—C5	2.6 (4)	N1—C18—C19—C20	10.3 (3)
C3—C4—C5—C6	−1.9 (4)	C18—C19—C20—C21	−5.0 (3)
C4—C5—C6—C1	−1.0 (4)	C19—C20—C21—O1	177.2 (3)
C4—C5—C6—C7	176.7 (2)	C19—C20—C21—N1	−2.6 (3)
C2—C1—C6—C5	3.0 (3)	C16—C17—C22—C23	−169.9 (2)
C14—C1—C6—C5	−179.8 (2)	N1—C17—C22—C23	6.8 (3)
C2—C1—C6—C7	−174.8 (2)	C16—C17—C22—C27	6.1 (3)
C14—C1—C6—C7	2.4 (3)	N1—C17—C22—C27	−177.2 (2)
C5—C6—C7—C12	−178.2 (2)	C17—C22—C23—C24	177.1 (2)
C1—C6—C7—C12	−0.4 (3)	C27—C22—C23—C24	1.1 (3)
C5—C6—C7—C8	1.1 (4)	C22—C23—C24—C25	2.3 (4)
C1—C6—C7—C8	178.8 (2)	C22—C23—C24—Cl1	−175.13 (18)
C12—C7—C8—C9	−0.6 (4)	C23—C24—C25—C26	−3.0 (4)
C6—C7—C8—C9	−179.9 (3)	Cl1—C24—C25—C26	174.4 (2)
C7—C8—C9—C10	0.0 (5)	C24—C25—C26—C27	0.2 (4)
C8—C9—C10—C11	0.5 (5)	C25—C26—C27—N2	−173.4 (2)
C9—C10—C11—C12	−0.5 (4)	C25—C26—C27—C22	3.2 (4)
C8—C7—C12—C11	0.6 (4)	C23—C22—C27—N2	172.5 (2)
C6—C7—C12—C11	179.9 (2)	C17—C22—C27—N2	−3.7 (3)
C8—C7—C12—C13	179.8 (2)	C23—C22—C27—C26	−3.8 (3)
C6—C7—C12—C13	−0.9 (3)	C17—C22—C27—C26	180.0 (2)
C10—C11—C12—C7	0.0 (4)	O1—C21—N1—C17	−1.1 (4)
C10—C11—C12—C13	−179.3 (2)	C20—C21—N1—C17	178.7 (2)
C7—C12—C13—C14	0.1 (3)	O1—C21—N1—C18	−170.0 (3)
C11—C12—C13—C14	179.4 (2)	C20—C21—N1—C18	9.9 (3)

C12—C13—C14—C1	1.9 (3)	C16—C17—N1—C21	−130.9 (2)
C12—C13—C14—C15	−178.1 (2)	C22—C17—N1—C21	52.5 (3)
C2—C1—C14—C13	173.9 (2)	C16—C17—N1—C18	37.0 (3)
C6—C1—C14—C13	−3.1 (3)	C22—C17—N1—C18	−139.6 (2)
C2—C1—C14—C15	−6.2 (3)	C19—C18—N1—C21	−12.8 (3)
C6—C1—C14—C15	176.8 (2)	C19—C18—N1—C17	178.0 (2)
C13—C14—C15—N2	−53.4 (3)	C16—C15—N2—C27	3.2 (3)
C1—C14—C15—N2	126.6 (2)	C14—C15—N2—C27	−179.5 (2)
C13—C14—C15—C16	123.9 (2)	C26—C27—N2—C15	175.4 (2)
C1—C14—C15—C16	−56.0 (3)	C22—C27—N2—C15	−0.9 (3)
N2—C15—C16—C17	−0.6 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.45	3.358 (4)	164

Symmetry code: (i) −*x*, −*y*+2, *z*+1/2.