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2-[(4-Chlorophenyl)(2-phenyl-1*H*-indol-3-yl)methyl]cyclohexan-1-one

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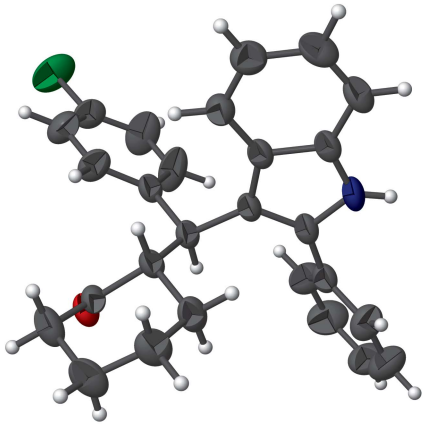
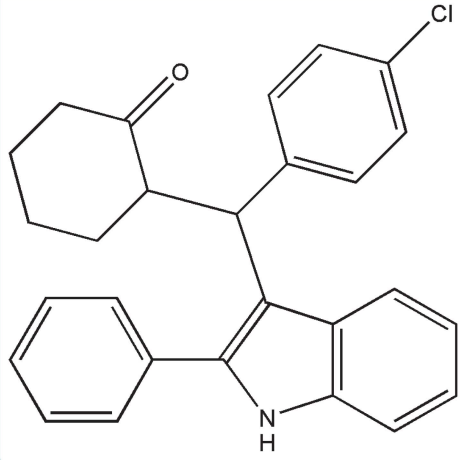
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{27}H_{24}ClNO$, the indole ring is almost orthogonal to the chlorophenyl ring and the mean plane of the cyclohexanone ring, making a dihedral angles of 82.11 (6) and 89.96 (4)°, respectively. In the crystal, a strong N—H···O hydrogen bond links the molecules, forming chains running along the *c* axis. The chains are linked by weak C—H···π interactions, forming layers parallel to the *ac* plane.

3D view



Chemical scheme



Structure description

Indole is a potent pharmacodynamic nucleus possessing properties such as anti-inflammatory, anti-cancer and antimicrobial activities (George *et al.*, 2008; El-Sawy *et al.*, 2009; Mandour *et al.*, 2007, 2010). Cyclohexanone is an aliphatic cyclic ketone (Fatima, *et al.*, 2014). Cyclohexanone derivatives have potent pharmacological activity in the treatment of broad spectrum of medical conditions (Puetz *et al.*, 2003). The cyclohexanone moiety constitutes an important structural feature in several anti-inflammatory, analgesic, local anaesthetic and antihistaminic drugs (Rajveer *et al.*, 2010; Fatima *et al.*, 2013). Cyclohexanone derivatives penetrate into the stratum corneum and alter the skin permeability of indomethacin by fluidizing or modifying the hard hydrophobic barrier of the corneum (Danyi *et al.*, 1989; Rizwana Begum *et al.*, 2012). Evaluation of bioactivities has shown cyclohexanone-containing analogues to exhibit anti-tumour properties and a wider anti-tumour spectrum than the acetone and cyclopentanone-containing analogues (Chen *et al.*, 2010).

The indole ring in the title compound (Fig. 1) is almost orthogonal to both the chlorophenyl ring and the mean plane of the cyclohexanone rings, making a dihedral angles of 82.11 (6) and 89.96 (4)°, respectively. Similarly the phenyl ring and cyclo-

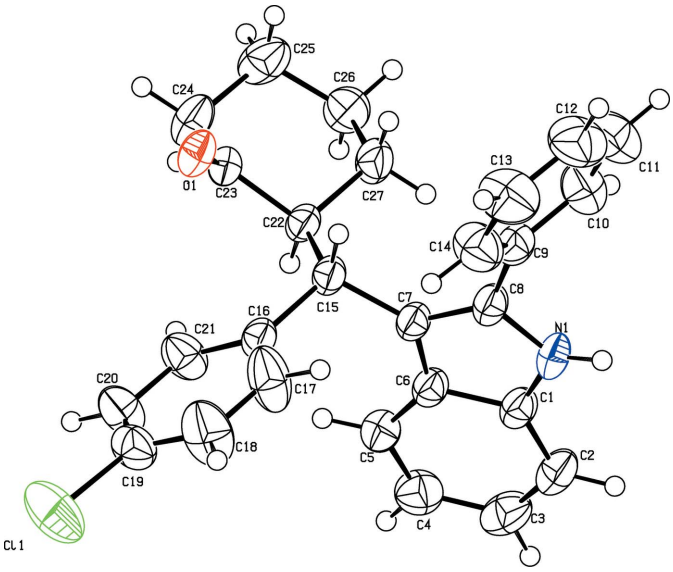


Figure 1
The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

hexanone mean plane are nearly orthogonal at a dihedral angle of 80.50 (8)°. The chlorophenyl ring is inclined to the phenyl and cyclohexanone rings by 43.57 (9) and 40.66 (9)°, respectively.

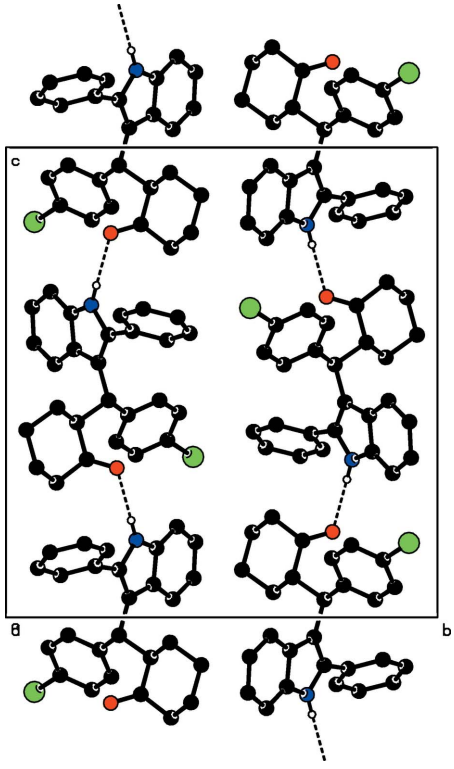


Figure 2
Crystal structure of title compound, showing the formation of chains running along the *c* axis generated by N—H···O hydrogen bonds.

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

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.83 (2)	2.08 (2)	2.8525 (18)	156 (2)
C10—H10···*Cg*^{ii}	0.93	2.96	3.562 (2)	124

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x-1, y, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{24}ClNO$
M_r	413.95
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	7.2562 (2), 16.4818 (5), 18.0306 (6)
β (°)	95.149 (2)
V (Å^3)	2147.67 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.35 × 0.21 × 0.16
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2004)
T_{min}, T_{max}	0.95, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23418, 4798, 3331
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.644
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.124, 1.04
No. of reflections	4798
No. of parameters	275
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.40

Computer programs: *APEX2* and *SAINT-Plus* (Bruker, 2009), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

In the crystal, a strong N—H···O hydrogen bond links the molecules, forming chains running along the *c* axis (Fig. 2 and Table 1). A weak C10—H10···π interaction generates chains running along the *a* axis. Together, these interactions generate a layered structure.

Synthesis and crystallization

A mixture of 2-(3-oxo-1,3-diarylpropyl)-1-cyclohexanones (1 mmol) and phenylhydrazine hydrochloride (3 mmol) in THF (10 ml) was refluxed for 3–4 h. After completion of the reaction (TLC), the mixture was poured into ice-cold water and the solid separated was filtered off. The product was separated by flash column using petroleum ether and ethyl-acetate (10:1 *v*/*v*) as eluant. The title compound was isolated as colourless plates.

Refinement

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

Acknowledgements

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full crystallographic data

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Crystal data

$C_{27}H_{24}ClNO$
M_r = 413.95
Monoclinic, $P2_1/c$
a = 7.2562 (2) Å
b = 16.4818 (5) Å
c = 18.0306 (6) Å
β = 95.149 (2)°
V = 2147.67 (11) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.280 Mg m^{-3}
D_m = 1.28 Mg m^{-3}
D_m measured by floatation method
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7435 reflections
θ = 5.0–54.2°
μ = 0.20 mm^{-1}
T = 293 K
Plate, colourless
0.35 × 0.21 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.95, T_{max} = 0.96
23418 measured reflections
4798 independent reflections
3331 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.2°, θ_{min} = 2.3°
h = −9→9
k = −20→21
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
S = 1.04
4798 reflections
275 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.6834P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
H1	0.580 (3)	0.7097 (12)	−0.2067 (12)	0.055 (6)*
Cl1	1.35108 (9)	0.93406 (4)	0.15842 (4)	0.0884 (2)
O1	0.58279 (17)	0.75702 (7)	0.18216 (6)	0.0466 (3)
N1	0.6256 (2)	0.69785 (9)	−0.16453 (8)	0.0438 (4)
C1	0.7775 (2)	0.65094 (10)	−0.14730 (9)	0.0398 (4)
C2	0.8774 (3)	0.60370 (11)	−0.19316 (10)	0.0505 (5)
H2	0.8459	0.6013	−0.2443	0.061*
C3	1.0239 (3)	0.56090 (12)	−0.16037 (11)	0.0579 (5)
H3	1.0930	0.5284	−0.1897	0.069*
C4	1.0720 (3)	0.56496 (12)	−0.08374 (11)	0.0550 (5)
H4	1.1708	0.5342	−0.0628	0.066*
C5	0.9763 (2)	0.61330 (11)	−0.03885 (10)	0.0458 (4)
H5	1.0111	0.6162	0.0120	0.055*
C6	0.8261 (2)	0.65818 (10)	−0.07032 (8)	0.0376 (4)
C7	0.6973 (2)	0.71423 (10)	−0.04213 (8)	0.0368 (4)
C8	0.5782 (2)	0.73760 (10)	−0.10163 (8)	0.0394 (4)
C9	0.4177 (2)	0.79283 (11)	−0.10919 (9)	0.0429 (4)
C10	0.2496 (3)	0.76591 (13)	−0.14256 (11)	0.0596 (5)
H10	0.2358	0.7115	−0.1557	0.071*
C11	0.1022 (3)	0.81797 (17)	−0.15668 (14)	0.0749 (7)
H11	−0.0099	0.7984	−0.1787	0.090*
C12	0.1199 (3)	0.89791 (17)	−0.13854 (14)	0.0764 (7)
H12	0.0211	0.9333	−0.1490	0.092*
C13	0.2848 (3)	0.92597 (15)	−0.10471 (15)	0.0778 (7)
H13	0.2974	0.9804	−0.0918	0.093*
C14	0.4317 (3)	0.87357 (13)	−0.08986 (13)	0.0619 (5)
H14	0.5422	0.8931	−0.0664	0.074*
C15	0.6874 (2)	0.73783 (10)	0.03812 (8)	0.0365 (4)
H15	0.5848	0.7763	0.0393	0.044*
C16	0.8628 (2)	0.78262 (10)	0.06868 (8)	0.0383 (4)
C17	0.9042 (3)	0.85589 (14)	0.03785 (13)	0.0743 (7)
H17	0.8278	0.8754	−0.0023	0.089*
C18	1.0548 (4)	0.90128 (14)	0.06438 (14)	0.0794 (7)
H18	1.0792	0.9506	0.0421	0.095*
C19	1.1670 (3)	0.87422 (12)	0.12271 (11)	0.0517 (5)
C20	1.1358 (3)	0.80067 (13)	0.15377 (12)	0.0591 (5)
H20	1.2154	0.7810	0.1930	0.071*
C21	0.9837 (3)	0.75567 (12)	0.12616 (11)	0.0527 (5)
H21	0.9629	0.7054	0.1474	0.063*
C22	0.6399 (2)	0.66461 (10)	0.08515 (8)	0.0370 (4)
H22	0.7441	0.6266	0.0876	0.044*
C23	0.6033 (2)	0.68732 (11)	0.16372 (8)	0.0386 (4)
C24	0.5736 (3)	0.61723 (12)	0.21343 (10)	0.0563 (5)
H24A	0.5551	0.6364	0.2631	0.068*
H24B	0.6810	0.5819	0.2167	0.068*

C25	0.4033 (3)	0.57094 (13)	0.18092 (11)	0.0625 (6)
H25A	0.3876	0.5226	0.2103	0.075*
H25B	0.2944	0.6046	0.1834	0.075*
C26	0.4211 (3)	0.54718 (12)	0.10116 (11)	0.0574 (5)
H26A	0.3064	0.5225	0.0807	0.069*
H26B	0.5187	0.5071	0.0997	0.069*
C27	0.4647 (3)	0.61950 (12)	0.05341 (10)	0.0518 (5)
H27A	0.3607	0.6567	0.0502	0.062*
H27B	0.4816	0.6009	0.0034	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0660 (4)	0.0675 (4)	0.1272 (6)	−0.0240 (3)	−0.0165 (4)	−0.0153 (4)
O1	0.0624 (8)	0.0458 (7)	0.0319 (6)	−0.0011 (6)	0.0062 (5)	−0.0077 (5)
N1	0.0591 (9)	0.0482 (9)	0.0237 (7)	−0.0008 (7)	0.0005 (6)	0.0018 (6)
C1	0.0506 (10)	0.0387 (9)	0.0307 (8)	−0.0074 (8)	0.0069 (7)	0.0010 (7)
C2	0.0677 (12)	0.0499 (11)	0.0353 (9)	−0.0063 (9)	0.0128 (8)	−0.0064 (8)
C3	0.0654 (13)	0.0538 (12)	0.0576 (12)	0.0015 (10)	0.0234 (10)	−0.0109 (10)
C4	0.0514 (11)	0.0553 (12)	0.0587 (12)	0.0054 (9)	0.0073 (9)	−0.0003 (9)
C5	0.0468 (10)	0.0523 (11)	0.0381 (9)	−0.0023 (8)	0.0033 (7)	0.0016 (8)
C6	0.0446 (9)	0.0386 (9)	0.0299 (8)	−0.0075 (7)	0.0053 (7)	0.0006 (7)
C7	0.0425 (9)	0.0410 (9)	0.0271 (8)	−0.0068 (7)	0.0042 (6)	0.0002 (7)
C8	0.0498 (10)	0.0403 (9)	0.0282 (8)	−0.0065 (7)	0.0034 (7)	0.0009 (7)
C9	0.0487 (10)	0.0483 (11)	0.0318 (8)	−0.0021 (8)	0.0051 (7)	0.0049 (7)
C10	0.0588 (12)	0.0553 (12)	0.0621 (13)	−0.0078 (10)	−0.0080 (10)	0.0063 (10)
C11	0.0508 (13)	0.0830 (18)	0.0882 (17)	−0.0032 (12)	−0.0088 (11)	0.0132 (14)
C12	0.0561 (14)	0.0830 (19)	0.0900 (18)	0.0166 (12)	0.0053 (12)	0.0087 (14)
C13	0.0704 (16)	0.0594 (14)	0.1039 (19)	0.0119 (12)	0.0094 (14)	−0.0124 (13)
C14	0.0535 (11)	0.0577 (13)	0.0736 (14)	0.0011 (10)	0.0014 (10)	−0.0126 (11)
C15	0.0424 (9)	0.0398 (9)	0.0273 (8)	−0.0034 (7)	0.0027 (6)	−0.0036 (6)
C16	0.0460 (9)	0.0407 (9)	0.0285 (8)	−0.0052 (7)	0.0049 (7)	−0.0046 (7)
C17	0.0902 (16)	0.0610 (14)	0.0652 (14)	−0.0272 (12)	−0.0300 (12)	0.0218 (11)
C18	0.0933 (17)	0.0548 (14)	0.0851 (17)	−0.0304 (13)	−0.0195 (14)	0.0184 (12)
C19	0.0461 (10)	0.0468 (11)	0.0617 (12)	−0.0102 (8)	0.0015 (9)	−0.0111 (9)
C20	0.0454 (11)	0.0623 (13)	0.0670 (13)	−0.0062 (9)	−0.0102 (9)	0.0063 (10)
C21	0.0463 (10)	0.0480 (11)	0.0619 (12)	−0.0083 (8)	−0.0051 (9)	0.0099 (9)
C22	0.0422 (9)	0.0410 (9)	0.0284 (8)	−0.0047 (7)	0.0065 (6)	−0.0045 (7)
C23	0.0398 (9)	0.0467 (10)	0.0290 (8)	−0.0042 (7)	0.0016 (6)	−0.0044 (7)
C24	0.0831 (14)	0.0526 (12)	0.0344 (9)	−0.0065 (10)	0.0122 (9)	0.0017 (8)
C25	0.0803 (15)	0.0550 (13)	0.0557 (12)	−0.0161 (11)	0.0247 (11)	0.0027 (10)
C26	0.0618 (12)	0.0548 (12)	0.0564 (12)	−0.0208 (10)	0.0100 (9)	−0.0078 (9)
C27	0.0586 (11)	0.0599 (12)	0.0369 (9)	−0.0214 (9)	0.0039 (8)	−0.0082 (8)

Geometric parameters (Å, º)

Cl1—C19	1.7367 (18)	C14—H14	0.9300
O1—C23	1.209 (2)	C15—C16	1.531 (2)

N1—C1	1.359 (2)	C15—C22	1.532 (2)
N1—C8	1.380 (2)	C15—H15	0.9800
N1—H1	0.82 (2)	C16—C21	1.371 (2)
C1—C2	1.387 (2)	C16—C17	1.374 (3)
C1—C6	1.406 (2)	C17—C18	1.374 (3)
C2—C3	1.365 (3)	C17—H17	0.9300
C2—H2	0.9300	C18—C19	1.347 (3)
C3—C4	1.396 (3)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.363 (3)
C4—C5	1.368 (3)	C20—C21	1.384 (3)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.395 (2)	C21—H21	0.9300
C5—H5	0.9300	C22—C23	1.511 (2)
C6—C7	1.439 (2)	C22—C27	1.538 (2)
C7—C8	1.371 (2)	C22—H22	0.9800
C7—C15	1.506 (2)	C23—C24	1.490 (2)
C8—C9	1.475 (2)	C24—C25	1.524 (3)
C9—C14	1.377 (3)	C24—H24A	0.9700
C9—C10	1.384 (3)	C24—H24B	0.9700
C10—C11	1.377 (3)	C25—C26	1.507 (3)
C10—H10	0.9300	C25—H25A	0.9700
C11—C12	1.361 (4)	C25—H25B	0.9700
C11—H11	0.9300	C26—C27	1.520 (3)
C12—C13	1.374 (3)	C26—H26A	0.9700
C12—H12	0.9300	C26—H26B	0.9700
C13—C14	1.379 (3)	C27—H27A	0.9700
C13—H13	0.9300	C27—H27B	0.9700

C1—N1—C8	109.83 (14)	C21—C16—C17	116.25 (17)
C1—N1—H1	126.5 (14)	C21—C16—C15	124.84 (15)
C8—N1—H1	122.5 (14)	C17—C16—C15	118.91 (16)
N1—C1—C2	129.78 (16)	C16—C17—C18	122.3 (2)
N1—C1—C6	107.69 (14)	C16—C17—H17	118.9
C2—C1—C6	122.53 (17)	C18—C17—H17	118.9
C3—C2—C1	117.42 (17)	C19—C18—C17	119.8 (2)
C3—C2—H2	121.3	C19—C18—H18	120.1
C1—C2—H2	121.3	C17—C18—H18	120.1
C2—C3—C4	121.29 (17)	C18—C19—C20	120.27 (18)
C2—C3—H3	119.4	C18—C19—Cl1	119.48 (16)
C4—C3—H3	119.4	C20—C19—Cl1	120.24 (16)
C5—C4—C3	121.23 (19)	C19—C20—C21	119.04 (19)
C5—C4—H4	119.4	C19—C20—H20	120.5
C3—C4—H4	119.4	C21—C20—H20	120.5
C4—C5—C6	119.18 (17)	C16—C21—C20	122.27 (18)
C4—C5—H5	120.4	C16—C21—H21	118.9
C6—C5—H5	120.4	C20—C21—H21	118.9
C5—C6—C1	118.30 (15)	C23—C22—C15	113.00 (13)
C5—C6—C7	134.86 (15)	C23—C22—C27	105.06 (13)

C1—C6—C7	106.84 (14)	C15—C22—C27	113.23 (14)
C8—C7—C6	106.73 (14)	C23—C22—H22	108.5
C8—C7—C15	126.73 (15)	C15—C22—H22	108.5
C6—C7—C15	126.41 (14)	C27—C22—H22	108.5
C7—C8—N1	108.87 (15)	O1—C23—C24	122.91 (15)
C7—C8—C9	133.06 (15)	O1—C23—C22	121.97 (15)
N1—C8—C9	118.06 (14)	C24—C23—C22	114.76 (15)
C14—C9—C10	117.52 (18)	C23—C24—C25	108.23 (16)
C14—C9—C8	122.23 (16)	C23—C24—H24A	110.1
C10—C9—C8	120.02 (17)	C25—C24—H24A	110.1
C11—C10—C9	121.3 (2)	C23—C24—H24B	110.1
C11—C10—H10	119.3	C25—C24—H24B	110.1
C9—C10—H10	119.3	H24A—C24—H24B	108.4
C12—C11—C10	120.3 (2)	C26—C25—C24	111.16 (15)
C12—C11—H11	119.9	C26—C25—H25A	109.4
C10—C11—H11	119.9	C24—C25—H25A	109.4
C11—C12—C13	119.5 (2)	C26—C25—H25B	109.4
C11—C12—H12	120.3	C24—C25—H25B	109.4
C13—C12—H12	120.3	H25A—C25—H25B	108.0
C12—C13—C14	120.2 (2)	C25—C26—C27	112.13 (16)
C12—C13—H13	119.9	C25—C26—H26A	109.2
C14—C13—H13	119.9	C27—C26—H26A	109.2
C9—C14—C13	121.2 (2)	C25—C26—H26B	109.2
C9—C14—H14	119.4	C27—C26—H26B	109.2
C13—C14—H14	119.4	H26A—C26—H26B	107.9
C7—C15—C16	111.14 (12)	C26—C27—C22	112.04 (15)
C7—C15—C22	111.15 (13)	C26—C27—H27A	109.2
C16—C15—C22	113.70 (13)	C22—C27—H27A	109.2
C7—C15—H15	106.8	C26—C27—H27B	109.2
C16—C15—H15	106.8	C22—C27—H27B	109.2
C22—C15—H15	106.8	H27A—C27—H27B	107.9

C8—N1—C1—C2	−176.83 (17)	C12—C13—C14—C9	0.8 (4)
C8—N1—C1—C6	2.17 (19)	C8—C7—C15—C16	−120.19 (18)
N1—C1—C2—C3	−178.67 (18)	C6—C7—C15—C16	64.5 (2)
C6—C1—C2—C3	2.5 (3)	C8—C7—C15—C22	112.10 (18)
C1—C2—C3—C4	−0.4 (3)	C6—C7—C15—C22	−63.2 (2)
C2—C3—C4—C5	−1.4 (3)	C7—C15—C16—C21	−117.57 (19)
C3—C4—C5—C6	1.1 (3)	C22—C15—C16—C21	8.7 (2)
C4—C5—C6—C1	0.8 (2)	C7—C15—C16—C17	63.3 (2)
C4—C5—C6—C7	−179.46 (18)	C22—C15—C16—C17	−170.40 (18)
N1—C1—C6—C5	178.23 (15)	C21—C16—C17—C18	−2.1 (4)
C2—C1—C6—C5	−2.7 (2)	C15—C16—C17—C18	177.1 (2)
N1—C1—C6—C7	−1.56 (18)	C16—C17—C18—C19	−0.2 (4)
C2—C1—C6—C7	177.53 (15)	C17—C18—C19—C20	2.4 (4)
C5—C6—C7—C8	−179.35 (18)	C17—C18—C19—Cl1	−177.2 (2)
C1—C6—C7—C8	0.40 (18)	C18—C19—C20—C21	−2.2 (3)
C5—C6—C7—C15	−3.3 (3)	Cl1—C19—C20—C21	177.40 (16)

C1—C6—C7—C15	176.45 (15)	C17—C16—C21—C20	2.3 (3)
C6—C7—C8—N1	0.90 (18)	C15—C16—C21—C20	−176.89 (17)
C15—C7—C8—N1	−175.13 (15)	C19—C20—C21—C16	−0.2 (3)
C6—C7—C8—C9	179.73 (17)	C7—C15—C22—C23	−172.32 (13)
C15—C7—C8—C9	3.7 (3)	C16—C15—C22—C23	61.37 (18)
C1—N1—C8—C7	−1.94 (19)	C7—C15—C22—C27	−53.01 (19)
C1—N1—C8—C9	179.03 (14)	C16—C15—C22—C27	−179.32 (14)
C7—C8—C9—C14	59.1 (3)	C15—C22—C23—O1	12.0 (2)
N1—C8—C9—C14	−122.20 (19)	C27—C22—C23—O1	−111.93 (18)
C7—C8—C9—C10	−126.7 (2)	C15—C22—C23—C24	−174.64 (15)
N1—C8—C9—C10	52.1 (2)	C27—C22—C23—C24	61.44 (19)
C14—C9—C10—C11	0.7 (3)	O1—C23—C24—C25	111.76 (19)
C8—C9—C10—C11	−173.87 (19)	C22—C23—C24—C25	−61.5 (2)
C9—C10—C11—C12	0.6 (4)	C23—C24—C25—C26	54.5 (2)
C10—C11—C12—C13	−1.3 (4)	C24—C25—C26—C27	−53.6 (2)
C11—C12—C13—C14	0.6 (4)	C25—C26—C27—C22	55.8 (2)
C10—C9—C14—C13	−1.4 (3)	C23—C22—C27—C26	−56.3 (2)
C8—C9—C14—C13	173.03 (19)	C15—C22—C27—C26	179.95 (15)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.83 (2)	2.08 (2)	2.8525 (18)	156 (2)
C10—H10···*Cg*^{ii}	0.93	2.96	3.562 (2)	124

Symmetry codes: (i) x, $-y+3/2$, $z-1/2$; (ii) $x-1$, y, z.