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(3a*RS*,9b*SR*)-3-(4-Chlorophenyl)-1-methyl-1,2,3,3a,4,9b-hexahydrochromeno[4,3-*b*]pyrrole-3a-carbonitrile

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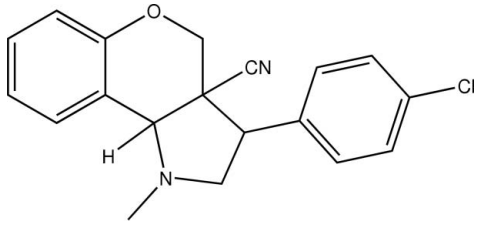
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.138; data-to-parameter ratio = 25.0.

In the molecule of the title compound, $C_{19}H_{17}ClN_2O$, the heterocyclic six-membered ring adopts a half-chair conformation, while the pyrrolidine ring has an envelope conformation. In the crystal structure, C—Cl$\cdots\pi$ [Cl$\cdots$centroid = 3.680 (2) Å] interactions and van der Waals forces are present.

Related literature

For general background, see: Caine (1993); Tidey (1992); Carlson (1993); Sokoloff *et al.* (1990); Wilner (1985); Biava *et al.* (2005); Fernandes *et al.* (2004); Borthwick *et al.* (2000); Jiang *et al.* (2004). For bond-length data, see: Allen *et al.* (1987). For puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Nardelli (1995).



Experimental

Crystal data

$C_{19}H_{17}ClN_2O$
M_r = 324.80
Monoclinic, $P2_1/c$
a = 8.8659 (4) Å
b = 7.6009 (3) Å
c = 24.2026 (10) Å
β = 97.701 (1)°
V = 1616.27 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 294 (2) K
0.28 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEX2 diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.935, T_{max} = 0.953
21338 measured reflections
5199 independent reflections
3858 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.138
S = 1.03
5199 reflections
208 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2395).

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supporting information

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(3a*RS*,9b*SR*)-3-(4-Chlorophenyl)-1-methyl-1,2,3,3a,4,9b-hexahydrochromeno[4,3-*b*]pyrrole-3a-carbonitrile

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S1. Comment

Chromenopyrrole compounds are used in the treatment of impulsive disorders (Caine, 1993), aggressiveness (Tidey, 1992), parkinson's disease (Carlson, 1993), psychoses, memory disorders (Sokoloff *et al.*, 1990), anxiety and depression (Wilner, 1985). Pyrrole derivatives have good invitro against mycobacteria and candidae (Biava *et al.*, 2005). These derivatives also possess anti-inflammatory (Fernandes *et al.*, 2004) and antiviral (Borthwick *et al.*, 2000) activities. It has also been shown that N-substituted pyrrole derivatives inhibit human immuno deficiency virus type-I (HIV-I) (Jiang *et al.*, 2004). In view of its medicinal importance, the crystal structure determination of the title compound, (I), was carried out.

In the molecule of (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The sum of bond angles around atom N1 [330.9 (4)°] indicates sp^3 hybridization. Rings A (C6—C11) and D (C13—C18) are, of course, planar and they are oriented at a dihedral angle of 46.7 (5)°. The heterocyclic ring B (O1/C4—C6/C11/C12) adopts a half-chair conformation with asymmetry parameters of ΔC_2(C4) = 0.028 (1) (Nardelli, 1995) and puckering parameters of q_2 = 0.778 (3) Å, q_3 = 0.054 (2) Å and φ = - 26.5 (2)° (Cremer & Pople, 1975). Atom C5 displaced by -0.645 (2) Å from the plane of the other five ring atoms. The pyrrolidine ring C (N1/C2—C4/C12) has an envelope conformation with asymmetry parameters of ΔC_s(N1) = 0.030 (1) (Nardelli, 1995) and puckering parameters of q_2 = 0.470 (1) Å and φ =175.3 (2)° (Cremer & Pople, 1975). Atom N1 displaced by -0.691 (2) Å from the plane of the other four ring atoms.

In the crystal structure, no significant intermolecular π–π interactions are observed between two chlorophenyl rings as their centroids are seperated by 4.1049 (9) Å. Weak intermolecular C—Cl···π interactions (Spek, 2003), with C16···*Cg*4 = 3.680 (2) Å and Cl1···*Cg*4 = 3.858 (8) Å [*Cg*4 denotes centroid of ring D] and van der Waals forces stabilize the crystal structure (Fig. 2).

S2. Experimental

For the preparation of the title compound, a solution of (*Z*)-2-((2-formyl- phenoxy)methyl)-3-(4-chlorophenyl)acrylonitrile (1 mmol) and sarcosine (1 mmol) in anhydrous methanol (10 ml) was refluxed. Completion of the reaction was evidenced by thin layer chromatography analysis. The solvent was removed in vacuum. The crude product was subjected to column chromatography on silica gel (100–200 mesh) using petroleum ether-ethylacetate (7:3) as the eluent. Compound was recrystallized from methanol.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H,

and x = 1.2 for all other H atoms.

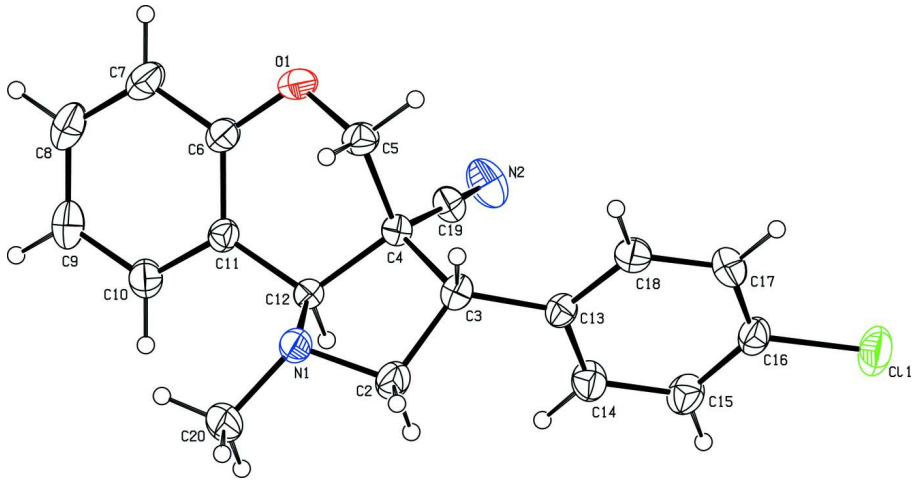

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

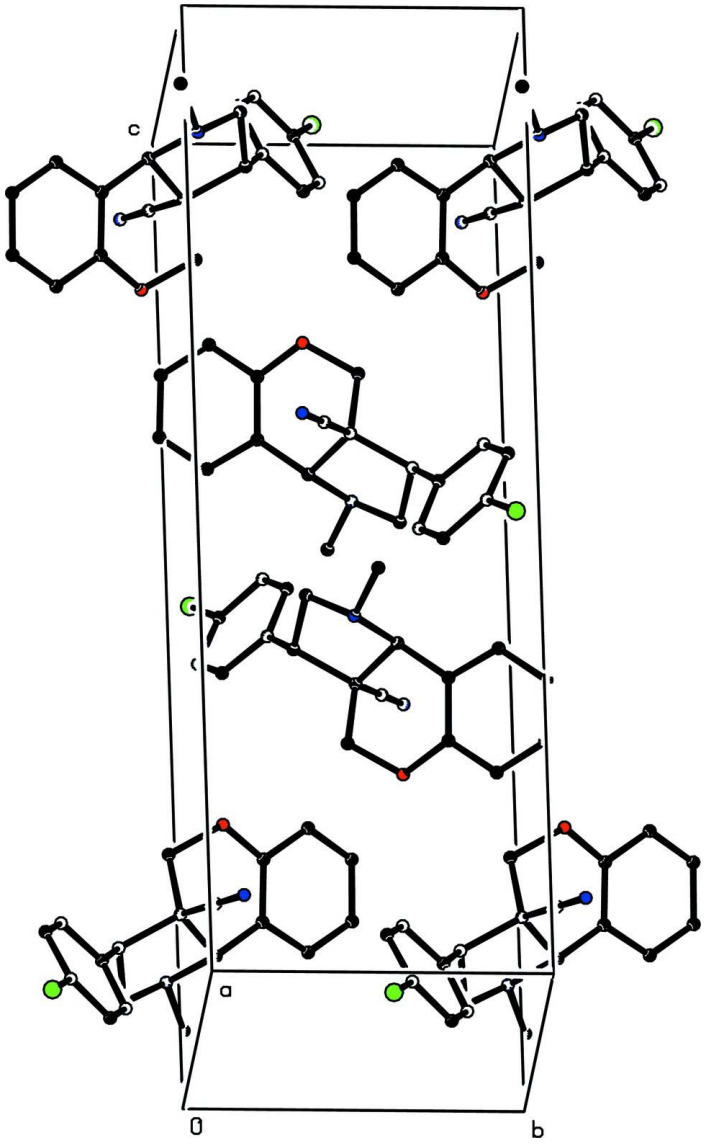

Figure 2

A packing diagram of (I). Hydrogen atoms are omited for clarity.

(3a*R*,9 b*S*)-3-(4-Chlorophenyl)-1-methyl-1,2,3,3a,4,9 b- hexahydrochromeno[4,3-*b*]pyrrole-3a-carbonitrile

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$b = 7.6009$ (3) Å
$c = 24.2026$ (10) Å
$\beta = 97.701$ (1)°
$V = 1616.27$ (12) Å^3
$Z = 4$
$F(000) = 680$
$D_x = 1.335$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7082 reflections
$\theta = 1.7$–25.0°
$\mu = 0.24$ mm^{-1}
$T = 294$ K
Prism, colourless
0.28 × 0.20 × 0.20 mm

Data collection

Bruker APEX2 kappa diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.935, T_{max} = 0.953
21338 measured reflections
5199 independent reflections
3858 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 31.2°, θ_{min} = 1.7°
h = −12→11
k = −10→11
l = −35→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.138
S = 1.04
5199 reflections
208 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 0.427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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}
Cl1	0.81942 (5)	−0.45073 (7)	0.00516 (2)	0.06969 (17)
O1	0.33531 (13)	0.11121 (15)	0.24679 (4)	0.0509 (3)
N1	0.07255 (13)	−0.04341 (16)	0.12043 (5)	0.0419 (3)
N2	0.57906 (16)	0.1425 (2)	0.13922 (7)	0.0626 (4)
C2	0.14526 (17)	−0.1758 (2)	0.08910 (6)	0.0484 (3)
H2A	0.1547	−0.1343	0.0518	0.058*
H2B	0.0876	−0.2846	0.0864	0.058*
C3	0.30137 (16)	−0.20196 (17)	0.12296 (5)	0.0388 (3)
H3	0.2894	−0.2909	0.1514	0.047*
C4	0.32937 (14)	−0.02060 (16)	0.15421 (5)	0.0336 (2)
C5	0.32588 (18)	−0.04940 (19)	0.21657 (5)	0.0434 (3)
H5A	0.2323	−0.1094	0.2219	0.052*
H5B	0.4103	−0.1245	0.2312	0.052*
C6	0.23237 (16)	0.23694 (18)	0.22598 (5)	0.0399 (3)
C7	0.20691 (19)	0.3728 (2)	0.26234 (6)	0.0511 (4)
H7	0.2563	0.3724	0.2988	0.061*

C8	0.1087 (2)	0.5073 (2)	0.24431 (8)	0.0579 (4)
H8	0.0908	0.5970	0.2688	0.069*
C9	0.0368 (2)	0.5099 (2)	0.19038 (8)	0.0577 (4)
H9	−0.0294	0.6011	0.1783	0.069*
C10	0.06331 (17)	0.3757 (2)	0.15411 (6)	0.0468 (3)
H10	0.0161	0.3795	0.1174	0.056*
C11	0.15891 (14)	0.23538 (17)	0.17135 (5)	0.0352 (3)
C12	0.19023 (14)	0.09239 (17)	0.13132 (5)	0.0335 (2)
H12	0.2081	0.1458	0.0959	0.040*
C13	0.42773 (15)	−0.26473 (16)	0.09160 (5)	0.0366 (3)
C14	0.44773 (19)	−0.2015 (2)	0.03930 (6)	0.0487 (3)
H14	0.3799	−0.1188	0.0220	0.058*
C15	0.56716 (19)	−0.2597 (2)	0.01243 (6)	0.0502 (4)
H15	0.5793	−0.2168	−0.0227	0.060*
C16	0.66710 (16)	−0.3812 (2)	0.03828 (6)	0.0443 (3)
C17	0.64861 (19)	−0.4491 (2)	0.08934 (7)	0.0525 (4)
H17	0.7159	−0.5332	0.1061	0.063*
C18	0.52856 (18)	−0.3910 (2)	0.11562 (6)	0.0469 (3)
H18	0.5153	−0.4377	0.1502	0.056*
C19	0.47093 (15)	0.06885 (18)	0.14530 (6)	0.0405 (3)
C20	−0.07204 (18)	0.0173 (3)	0.09117 (8)	0.0615 (5)
H20A	−0.1149	0.1038	0.1134	0.092*
H20B	−0.1407	−0.0804	0.0846	0.092*
H20C	−0.0560	0.0685	0.0562	0.092*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0478 (2)	0.0821 (3)	0.0832 (3)	0.0010 (2)	0.0237 (2)	−0.0308 (2)
O1	0.0589 (6)	0.0565 (6)	0.0342 (5)	0.0075 (5)	−0.0052 (4)	−0.0084 (4)
N1	0.0318 (5)	0.0495 (7)	0.0443 (6)	−0.0025 (5)	0.0050 (4)	−0.0124 (5)
N2	0.0406 (7)	0.0581 (8)	0.0890 (11)	−0.0015 (6)	0.0083 (7)	0.0112 (8)
C2	0.0416 (7)	0.0525 (8)	0.0515 (8)	−0.0031 (6)	0.0073 (6)	−0.0189 (7)
C3	0.0421 (7)	0.0355 (6)	0.0402 (6)	0.0001 (5)	0.0110 (5)	−0.0038 (5)
C4	0.0324 (6)	0.0360 (6)	0.0325 (5)	0.0017 (5)	0.0049 (4)	−0.0006 (4)
C5	0.0511 (8)	0.0443 (7)	0.0341 (6)	0.0052 (6)	0.0028 (5)	0.0021 (5)
C6	0.0395 (7)	0.0438 (7)	0.0371 (6)	−0.0040 (5)	0.0083 (5)	−0.0069 (5)
C7	0.0539 (9)	0.0562 (9)	0.0450 (7)	−0.0103 (7)	0.0130 (6)	−0.0184 (6)
C8	0.0607 (10)	0.0504 (8)	0.0675 (10)	−0.0045 (7)	0.0269 (8)	−0.0207 (8)
C9	0.0559 (10)	0.0471 (8)	0.0736 (11)	0.0119 (7)	0.0217 (8)	−0.0053 (7)
C10	0.0446 (7)	0.0477 (8)	0.0490 (7)	0.0076 (6)	0.0096 (6)	−0.0002 (6)
C11	0.0326 (6)	0.0383 (6)	0.0357 (6)	−0.0011 (5)	0.0088 (5)	−0.0031 (5)
C12	0.0316 (5)	0.0396 (6)	0.0294 (5)	0.0025 (5)	0.0043 (4)	−0.0021 (4)
C13	0.0407 (7)	0.0325 (6)	0.0372 (6)	0.0011 (5)	0.0073 (5)	−0.0031 (5)
C14	0.0540 (8)	0.0475 (8)	0.0468 (7)	0.0123 (7)	0.0146 (6)	0.0108 (6)
C15	0.0550 (9)	0.0543 (8)	0.0442 (7)	0.0015 (7)	0.0177 (6)	0.0032 (6)
C16	0.0371 (7)	0.0453 (7)	0.0517 (7)	−0.0033 (6)	0.0100 (6)	−0.0168 (6)
C17	0.0453 (8)	0.0535 (9)	0.0573 (9)	0.0148 (7)	0.0016 (6)	0.0003 (7)

C18	0.0507 (8)	0.0507 (8)	0.0388 (6)	0.0079 (6)	0.0043 (6)	0.0037 (6)
C19	0.0346 (6)	0.0396 (7)	0.0467 (7)	0.0047 (5)	0.0031 (5)	0.0015 (5)
C20	0.0334 (7)	0.0812 (12)	0.0671 (10)	0.0026 (7)	−0.0031 (7)	−0.0231 (9)

Geometric parameters (Å, º)

C2—N1	1.4610 (18)	C10—C11	1.3909 (19)
C2—C3	1.524 (2)	C10—H10	0.9300
C2—H2A	0.9700	C11—C12	1.5063 (17)
C2—H2B	0.9700	C12—N1	1.4662 (17)
C3—C13	1.5122 (18)	C12—H12	0.9800
C3—C4	1.5760 (18)	C13—C18	1.3852 (19)
C3—H3	0.9800	C13—C14	1.3873 (18)
C4—C19	1.4684 (18)	C14—C15	1.387 (2)
C4—C5	1.5296 (17)	C14—H14	0.9300
C4—C12	1.5438 (17)	C15—C16	1.372 (2)
C5—O1	1.4197 (17)	C15—H15	0.9300
C5—H5A	0.9700	C16—C17	1.369 (2)
C5—H5B	0.9700	C16—Cl1	1.7423 (14)
C6—O1	1.3700 (18)	C17—C18	1.384 (2)
C6—C11	1.3935 (18)	C17—H17	0.9300
C6—C7	1.3945 (19)	C18—H18	0.9300
C7—C8	1.376 (3)	C19—N2	1.1368 (19)
C7—H7	0.9300	C20—N1	1.454 (2)
C8—C9	1.374 (3)	C20—H20A	0.9600
C8—H8	0.9300	C20—H20B	0.9600
C9—C10	1.386 (2)	C20—H20C	0.9600
C9—H9	0.9300		

C6—O1—C5	114.84 (10)	C8—C9—H9	120.2
C20—N1—C2	112.77 (11)	C10—C9—H9	120.2
C20—N1—C12	115.08 (13)	C9—C10—C11	121.50 (14)
C2—N1—C12	103.02 (10)	C11—C10—H10	119.2
N1—C2—C3	104.05 (11)	C10—C11—C6	117.81 (12)
N1—C2—H2A	110.9	C10—C11—C12	121.18 (12)
C3—C2—H2A	110.9	C6—C11—C12	120.89 (11)
N1—C2—H2B	110.9	N1—C12—C11	115.81 (10)
C3—C2—H2B	110.9	N1—C12—C4	100.84 (10)
H2A—C2—H2B	109.0	C11—C12—C4	112.20 (10)
C13—C3—C2	116.85 (11)	N1—C12—H12	109.2
C13—C3—C4	115.92 (11)	C11—C12—H12	109.2
C2—C3—C4	102.55 (11)	C4—C12—H12	109.2
C13—C3—H3	107.0	C18—C13—C14	117.95 (13)
C2—C3—H3	107.0	C18—C13—C3	119.19 (12)
C4—C3—H3	107.0	C14—C13—C3	122.86 (12)
C19—C4—C5	109.99 (11)	C15—C14—C13	121.09 (14)
C19—C4—C12	110.32 (10)	C15—C14—H14	119.5
C5—C4—C12	108.23 (10)	C13—C14—H14	119.5

C19—C4—C3	114.67 (11)	C16—C15—C14	119.20 (13)
C5—C4—C3	109.00 (10)	C16—C15—H15	120.4
C12—C4—C3	104.33 (10)	C14—C15—H15	120.4
O1—C5—C4	112.18 (11)	C17—C16—C15	121.16 (13)
O1—C5—H5A	109.2	C17—C16—Cl1	119.66 (12)
C4—C5—H5A	109.2	C15—C16—Cl1	119.18 (12)
O1—C5—H5B	109.2	C16—C17—C18	119.15 (14)
C4—C5—H5B	109.2	C16—C17—H17	120.4
H5A—C5—H5B	107.9	C18—C17—H17	120.4
O1—C6—C11	123.13 (11)	C17—C18—C13	121.41 (14)
O1—C6—C7	116.14 (12)	C17—C18—H18	119.3
C11—C6—C7	120.70 (14)	C13—C18—H18	119.3
C8—C7—C6	119.94 (14)	N2—C19—C4	177.88 (17)
C8—C7—H7	120.0	N1—C20—H20A	109.5
C6—C7—H7	120.0	N1—C20—H20B	109.5
C9—C8—C7	120.36 (14)	H20A—C20—H20B	109.5
C9—C8—H8	119.8	N1—C20—H20C	109.5
C7—C8—H8	119.8	H20A—C20—H20C	109.5
C8—C9—C10	119.64 (16)	H20B—C20—H20C	109.5

N1—C2—C3—C13	−153.76 (12)	C3—C4—C12—N1	31.53 (11)
N1—C2—C3—C4	−25.83 (14)	C19—C4—C12—C11	−80.99 (13)
C13—C3—C4—C19	4.02 (16)	C5—C4—C12—C11	39.40 (14)
C2—C3—C4—C19	−124.49 (12)	C3—C4—C12—C11	155.38 (10)
C13—C3—C4—C5	−119.76 (12)	C2—C3—C13—C18	−138.60 (14)
C2—C3—C4—C5	111.72 (12)	C4—C3—C13—C18	100.27 (15)
C13—C3—C4—C12	124.80 (12)	C2—C3—C13—C14	41.3 (2)
C2—C3—C4—C12	−3.72 (13)	C4—C3—C13—C14	−79.83 (17)
C19—C4—C5—O1	59.31 (15)	C18—C13—C14—C15	−1.5 (2)
C12—C4—C5—O1	−61.28 (15)	C3—C13—C14—C15	178.56 (14)
C3—C4—C5—O1	−174.18 (11)	C13—C14—C15—C16	−0.2 (3)
O1—C6—C7—C8	178.08 (14)	C14—C15—C16—C17	1.7 (2)
C11—C6—C7—C8	−0.2 (2)	C14—C15—C16—Cl1	−178.65 (13)
C6—C7—C8—C9	−0.8 (2)	C15—C16—C17—C18	−1.3 (2)
C7—C8—C9—C10	0.2 (3)	Cl1—C16—C17—C18	179.04 (12)
C8—C9—C10—C11	1.5 (3)	C16—C17—C18—C13	−0.5 (2)
C9—C10—C11—C6	−2.4 (2)	C14—C13—C18—C17	1.9 (2)
C9—C10—C11—C12	−178.46 (14)	C3—C13—C18—C17	−178.16 (14)
O1—C6—C11—C10	−176.39 (13)	C3—C2—N1—C20	172.67 (14)
C7—C6—C11—C10	1.7 (2)	C3—C2—N1—C12	47.99 (14)
O1—C6—C11—C12	−0.3 (2)	C11—C12—N1—C20	66.39 (15)
C7—C6—C11—C12	177.82 (12)	C4—C12—N1—C20	−172.28 (11)
C10—C11—C12—N1	−80.29 (16)	C11—C12—N1—C2	−170.45 (11)
C6—C11—C12—N1	103.76 (14)	C4—C12—N1—C2	−49.13 (12)
C10—C11—C12—C4	164.69 (12)	C11—C6—O1—C5	−20.14 (19)
C6—C11—C12—C4	−11.26 (17)	C7—C6—O1—C5	161.65 (13)
C19—C4—C12—N1	155.17 (10)	C4—C5—O1—C6	51.71 (16)
C5—C4—C12—N1	−84.44 (12)		