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11-(4-Chlorophenyl)-10-methyl-8-phenyl-6,8-dihydro-5*H*-benzo[*f*]pyrazolo[3,4-*b*]-quinoline

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.110
Data-to-parameter ratio = 17.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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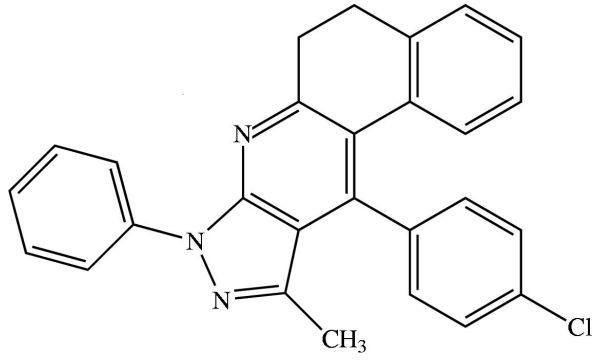
Molecules of the title compound, $C_{27}H_{20}ClN_3$, are linked by two independent C—H···π(arene) hydrogen bonds into chains of edge-fused rings.

Comment

Pyrazolo[3,4-*b*]quinolines are of interest as possible antiviral and antimalarial agents, and because of their other biological properties, such as parasiticidic, bactericidal, vasodilator and enzyme-inhibitory activity (Quiroga *et al.*, 2001). We have recently focused on the synthesis of fused heterocyclic systems containing the pyrazolo[3,4-*b*]quinoline moiety using multi-component cyclocondensation reactions under solvent-free conditions. We describe here the molecular and supramolecular structure of the title compound, (I), prepared using a three-component cyclocondensation involving 5-amino-3-methyl-1-phenylpyrazole, 2-tetralone and 4-chlorobenzaldehyde under solvent-free microwave irradiation.



(I)

Within the pyridine-type ring, the C—N bond lengths (Table 1) are very close to the mean value of 1.337 Å for bonds of this type (Allen *et al.*, 1987), and there is very strong bond fixation in the five-membered ring. The pyridine ring and the benzene ring containing atom C1 are not coplanar, and their planes make a dihedral angle of 25.5 (2)°. The carbocylic ring containing atoms C5 and C6 accordingly adopts a screw-boat conformation (Evans & Boeyens, 1989), with total puckering amplitude Q = 0.537 (2) Å, and ring-puckering parameters θ = 70.5 (2)° and φ = 92.5 (2)° (Cremer & Pople, 1975); the idealized values of the angular parameters for a screw-boat conformer are θ = 67.5° and φ = (60k + 30)°. The dihedral angle between the pyrazole-type ring and aryl ring C81–C86 is 28.1 (2)°, whereas that between the pyridine-type ring and aryl ring C111–C116 is 70.1 (2)°, possibly as a consequence of repulsive interactions between the H atoms bonded to C112 and C116 and those bonded to C101 and C1, respectively.

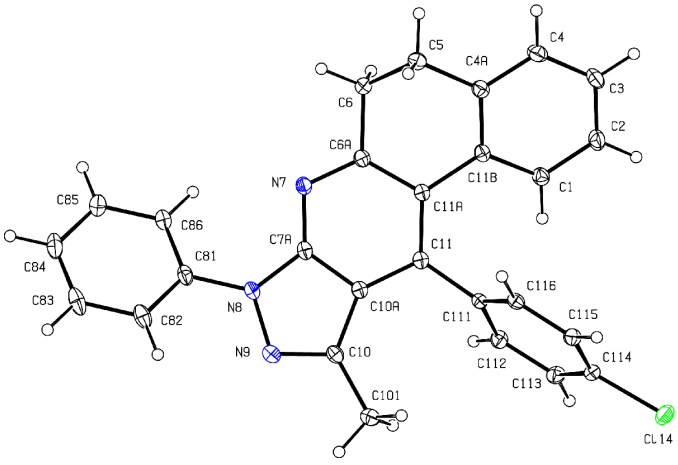


Figure 1
The molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

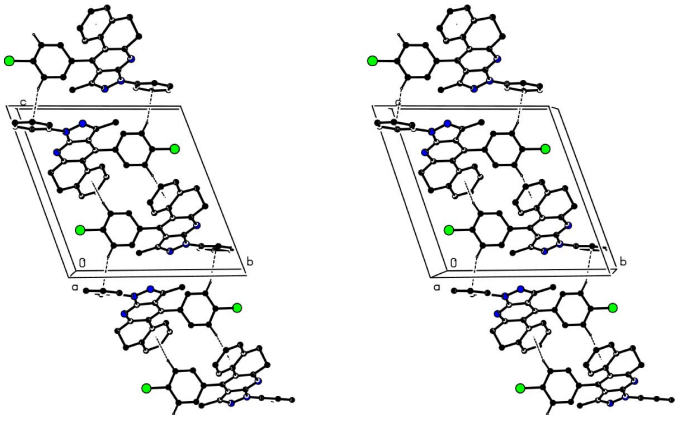


Figure 2
Stereoview of part of the crystal structure of compound (I), showing the formation of a chain of edge-fused rings along [101]. For the sake of clarity, the H atoms not involved in these motifs have been omitted.

The molecules of (I) are linked by two independent C—H···π(arene) hydrogen bonds into a chain of edge-fused rings. Aryl atom C113 in the molecule at (x, y, z) acts as donor to the phenyl ring C81–C86 in the molecule at ($-x$, $1-y$, $-z$), so forming a centrosymmetric ring, centred at $(0, \frac{1}{2}, 0)$. In a similar way, atom C115 at (x, y, z) acts as donor to the fused aryl ring, containing C1, in the molecule at ($1-x$, $1-y$, $1-z$), so generating a second centrosymmetric ring, centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Propagation by inversion of these two interactions then generates a chain of edge-fused centrosymmetric rings running parallel to the [101] direction (Fig. 2). There are no direction-specific interactions between adjacent chains: C—H···N and C—H···Cl hydrogen bonds, and aromatic π–π stacking interactions are all absent from the structure of (I).

Experimental

Equimolar amounts of 5-amino-3-methyl-1-phenylpyrazole (173 mg, 1.0 mmol), 2-tetralone (146 mg, 1.0 mmol) and 4-chlorobenzaldehyde (140.6 mg, 1.0 mmol) were placed in open Pyrex glass vessels and irradiated in a domestic microwave oven for 4 min at 600 W. The reaction mixture was then extracted with ethanol and, after removal of the solvent, the product was recrystallized from ethanol/dimethylformamide to give crystals suitable for single-crystal X-ray diffraction. Pale-green crystals (m.p. 467 K, yield 58%). MS: (30 eV) m/z (%) 279 (100, M^+), 264 (27).

Crystal data

$C_{27}H_{20}ClN_3$
$M_r = 421.91$
Triclinic, $P\overline{1}$
$a = 7.1270$ (1) Å
$b = 12.6300$ (4) Å
$c = 13.2847$ (4) Å
$\alpha = 107.3380$ (13)°
$\beta = 103.6230$ (17)°
$\gamma = 101.4230$ (18)°
$V = 1061.98$ (5) Å^3
$Z = 2$
$D_x = 1.319$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4871 reflections
$\theta = 3.0$–27.6°
$\mu = 0.20$ mm^{-1}
$T = 120$ (2) K
Plate, pale green
0.53 × 0.20 × 0.08 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.906$, $T_{max} = 0.984$
21 625 measured reflections
4871 independent reflections
3853 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.6°$
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.110$
$S = 1.08$
4871 reflections
281 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.2795P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected bond lengths (Å).

C6*A*—N7	1.3336 (18)	C10—C10*A*	1.436 (2)
N7—C7*A*	1.3415 (19)	C10*A*—C11	1.4055 (19)
C7*A*—N8	1.3730 (17)	C11—C11*A*	1.403 (2)
N8—N9	1.3791 (17)	C11*A*—C6*A*	1.4324 (19)
N9—C10	1.3190 (19)	C7*A*—C10*A*	1.398 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

*Cg*1 is the centroid of ring C81–C86, and *Cg*2 is the centroid of ring C1–C4/C4*A*/C11*B*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C113—H113···*Cg*1^{i}	0.95	2.65	3.5214 (16)	152
C115—H115···*Cg*2^{ii}	0.95	2.90	3.6403 (17)	136

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

All H atoms were located in difference maps in fully ordered sites; they were then treated as riding atoms, with C—H distances of 0.95 (aromatic), 0.98 (methyl) or 0.99 Å (CH$_2$), and with U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(C) for the methyl group.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. JC thanks the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. JQ and HS thank COLCIENCIAS and UNIVALLE (Universidad del Valle, Colombia) for financial support.

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supporting information

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$V = 1061.98\ (5)$ Å^3
$Z = 2$
$F(000) = 440$
$D_x = 1.319$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4871 reflections
$\theta = 3.0–27.6°$
$\mu = 0.20$ mm^{-1}
$T = 120$ K
Plate, pale green
0.53 × 0.20 × 0.08 mm

Data collection

Bruker–Nonius 95mm CCD camera on κ goniostat diffractometer
Radiation source: Bruker-Nonius FR91 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.906$, $T_{max} = 0.984$
21625 measured reflections
4871 independent reflections
3853 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.0°$
$h = -9\rightarrow9$
$k = -16\rightarrow16$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.110$
$S = 1.08$
4871 reflections
281 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.2795P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl14	0.41830 (6)	0.13253 (3)	0.25576 (3)	0.03150 (13)
N7	0.28893 (18)	0.82176 (10)	0.27569 (10)	0.0221 (3)
N8	−0.04974 (18)	0.71127 (11)	0.15444 (10)	0.0230 (3)
N9	−0.16306 (18)	0.59652 (11)	0.10792 (10)	0.0239 (3)
C1	0.7802 (2)	0.60892 (13)	0.36213 (13)	0.0230 (3)
C2	0.9656 (2)	0.61188 (14)	0.42735 (14)	0.0294 (4)
C3	1.0767 (2)	0.70935 (15)	0.52083 (15)	0.0332 (4)
C4	1.0043 (2)	0.80434 (14)	0.54597 (14)	0.0294 (4)
C4A	0.8184 (2)	0.80333 (13)	0.48129 (12)	0.0226 (3)
C5	0.7424 (2)	0.90812 (13)	0.50638 (13)	0.0263 (3)
C6	0.6306 (2)	0.91716 (12)	0.39763 (13)	0.0242 (3)
C6A	0.4606 (2)	0.80831 (12)	0.32939 (12)	0.0204 (3)
C7A	0.1426 (2)	0.72218 (13)	0.21502 (12)	0.0212 (3)
C10	−0.0445 (2)	0.53571 (13)	0.13762 (12)	0.0216 (3)
C10A	0.1534 (2)	0.61046 (12)	0.20561 (12)	0.0198 (3)
C11	0.3345 (2)	0.59779 (12)	0.26387 (11)	0.0186 (3)
C11A	0.4943 (2)	0.69932 (12)	0.32585 (11)	0.0187 (3)
C11B	0.6994 (2)	0.70225 (13)	0.38950 (12)	0.0199 (3)
C81	−0.1403 (2)	0.79824 (13)	0.13851 (12)	0.0249 (3)
C82	−0.3462 (2)	0.77830 (15)	0.11958 (13)	0.0289 (4)
C83	−0.4338 (3)	0.86323 (17)	0.10284 (14)	0.0350 (4)
C84	−0.3185 (3)	0.96645 (16)	0.10570 (14)	0.0375 (4)
C85	−0.1139 (3)	0.98489 (16)	0.12430 (16)	0.0425 (5)
C86	−0.0237 (2)	0.90067 (15)	0.14042 (16)	0.0369 (4)
C101	−0.1276 (2)	0.40710 (13)	0.09992 (14)	0.0281 (3)
C111	0.34498 (19)	0.48015 (12)	0.25989 (12)	0.0184 (3)
C112	0.3473 (2)	0.39855 (13)	0.16309 (12)	0.0225 (3)
C113	0.3674 (2)	0.29104 (13)	0.16129 (12)	0.0238 (3)
C114	0.3829 (2)	0.26520 (12)	0.25674 (12)	0.0218 (3)
C115	0.3725 (2)	0.34275 (13)	0.35236 (12)	0.0221 (3)
C116	0.3542 (2)	0.45043 (12)	0.35347 (12)	0.0198 (3)
H1	0.7064	0.5423	0.2976	0.028*
H2	1.0166	0.5472	0.4080	0.035*
H3	1.2017	0.7107	0.5672	0.040*
H4	1.0827	0.8719	0.6087	0.035*
H5A	0.8572	0.9788	0.5499	0.032*
H5B	0.6505	0.9014	0.5511	0.032*
H6A	0.5764	0.9846	0.4137	0.029*
H6B	0.7252	0.9291	0.3554	0.029*
H82	−0.4262	0.7077	0.1181	0.035*
H83	−0.5750	0.8501	0.0892	0.042*
H84	−0.3796	1.0243	0.0949	0.045*
H85	−0.0341	1.0557	0.1261	0.051*
H86	0.1170	0.9134	0.1527	0.044*
H10A	−0.2733	0.3843	0.0626	0.042*

H10B	−0.1019	0.3831	0.1643	0.042*
H10C	−0.0622	0.3696	0.0481	0.042*
H112	0.3351	0.4167	0.0978	0.027*
H113	0.3706	0.2358	0.0955	0.029*
H115	0.3777	0.3227	0.4162	0.027*
H116	0.3478	0.5046	0.4189	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl14	0.0414 (2)	0.0201 (2)	0.0309 (2)	0.01009 (16)	0.00622 (17)	0.00961 (16)
N7	0.0202 (6)	0.0235 (6)	0.0227 (6)	0.0084 (5)	0.0051 (5)	0.0085 (5)
N8	0.0184 (6)	0.0253 (7)	0.0238 (7)	0.0079 (5)	0.0025 (5)	0.0090 (5)
N9	0.0201 (6)	0.0271 (7)	0.0226 (7)	0.0059 (5)	0.0046 (5)	0.0083 (6)
C1	0.0193 (7)	0.0253 (8)	0.0259 (8)	0.0066 (6)	0.0080 (6)	0.0106 (6)
C2	0.0217 (8)	0.0319 (9)	0.0398 (10)	0.0126 (6)	0.0098 (7)	0.0169 (8)
C3	0.0189 (7)	0.0374 (10)	0.0402 (10)	0.0069 (7)	−0.0004 (7)	0.0181 (8)
C4	0.0246 (8)	0.0291 (8)	0.0273 (8)	0.0012 (6)	−0.0002 (6)	0.0109 (7)
C4A	0.0212 (7)	0.0250 (8)	0.0222 (7)	0.0051 (6)	0.0058 (6)	0.0112 (6)
C5	0.0264 (8)	0.0243 (8)	0.0223 (8)	0.0059 (6)	0.0023 (6)	0.0052 (6)
C6	0.0239 (7)	0.0201 (7)	0.0253 (8)	0.0065 (6)	0.0036 (6)	0.0071 (6)
C6A	0.0203 (7)	0.0231 (7)	0.0189 (7)	0.0071 (6)	0.0063 (6)	0.0084 (6)
C7A	0.0203 (7)	0.0257 (8)	0.0198 (7)	0.0096 (6)	0.0057 (6)	0.0099 (6)
C10	0.0195 (7)	0.0269 (8)	0.0185 (7)	0.0068 (6)	0.0055 (6)	0.0089 (6)
C10A	0.0203 (7)	0.0221 (7)	0.0180 (7)	0.0070 (6)	0.0066 (6)	0.0078 (6)
C11	0.0207 (7)	0.0226 (7)	0.0152 (7)	0.0079 (6)	0.0074 (5)	0.0082 (6)
C11A	0.0189 (7)	0.0214 (7)	0.0172 (7)	0.0071 (5)	0.0065 (5)	0.0077 (6)
C11B	0.0183 (7)	0.0241 (7)	0.0206 (7)	0.0070 (6)	0.0071 (6)	0.0113 (6)
C81	0.0255 (8)	0.0304 (8)	0.0184 (7)	0.0147 (6)	0.0029 (6)	0.0072 (6)
C82	0.0256 (8)	0.0468 (10)	0.0212 (8)	0.0182 (7)	0.0094 (6)	0.0156 (7)
C83	0.0301 (9)	0.0599 (12)	0.0258 (8)	0.0292 (8)	0.0116 (7)	0.0181 (8)
C84	0.0446 (10)	0.0421 (10)	0.0257 (9)	0.0301 (9)	0.0027 (7)	0.0074 (8)
C85	0.0382 (10)	0.0297 (9)	0.0513 (12)	0.0155 (8)	−0.0027 (8)	0.0126 (9)
C86	0.0247 (8)	0.0295 (9)	0.0507 (11)	0.0116 (7)	−0.0004 (7)	0.0135 (8)
C101	0.0221 (8)	0.0267 (8)	0.0304 (9)	0.0029 (6)	0.0034 (6)	0.0096 (7)
C111	0.0155 (6)	0.0193 (7)	0.0191 (7)	0.0045 (5)	0.0038 (5)	0.0069 (6)
C112	0.0259 (7)	0.0248 (8)	0.0174 (7)	0.0080 (6)	0.0055 (6)	0.0088 (6)
C113	0.0282 (8)	0.0215 (8)	0.0182 (7)	0.0075 (6)	0.0062 (6)	0.0033 (6)
C114	0.0217 (7)	0.0175 (7)	0.0235 (8)	0.0047 (6)	0.0035 (6)	0.0071 (6)
C115	0.0232 (7)	0.0231 (8)	0.0196 (7)	0.0044 (6)	0.0050 (6)	0.0101 (6)
C116	0.0183 (7)	0.0228 (7)	0.0159 (7)	0.0047 (6)	0.0045 (5)	0.0053 (6)

Geometric parameters (Å, º)

C1—C2	1.386 (2)	C81—C86	1.382 (2)
C1—C11B	1.402 (2)	C81—C82	1.386 (2)
C1—H1	0.95	C82—C83	1.390 (2)
C2—C3	1.387 (2)	C82—H82	0.95

C2—H2	0.95	C83—C84	1.381 (3)
C3—C4	1.380 (2)	C83—H83	0.95
C3—H3	0.95	C84—C85	1.379 (3)
C4—C4A	1.394 (2)	C84—H84	0.95
C4—H4	0.95	C85—C86	1.390 (2)
C4A—C11B	1.411 (2)	C85—H85	0.95
C4A—C5	1.504 (2)	C86—H86	0.95
C5—C6	1.525 (2)	C10—C101	1.495 (2)
C5—H5A	0.99	C101—H10A	0.98
C5—H5B	0.99	C101—H10B	0.98
C6—C6A	1.503 (2)	C101—H10C	0.98
C6—H6A	0.99	C11—C111	1.4883 (19)
C6—H6B	0.99	C11A—C11B	1.4937 (19)
C6A—N7	1.3336 (18)	C111—C116	1.393 (2)
N7—C7A	1.3415 (19)	C111—C112	1.394 (2)
C7A—N8	1.3730 (17)	C112—C113	1.387 (2)
N8—N9	1.3791 (17)	C112—H112	0.95
N9—C10	1.3190 (19)	C113—C114	1.386 (2)
C10—C10A	1.436 (2)	C113—H113	0.95
C10A—C11	1.4055 (19)	C114—C115	1.382 (2)
C11—C11A	1.403 (2)	C114—Cl14	1.7399 (14)
C11A—C6A	1.4324 (19)	C115—C116	1.388 (2)
C7A—C10A	1.398 (2)	C115—H115	0.95
N8—C81	1.4225 (18)	C116—H116	0.95

C2—C1—C11B	121.33 (15)	C83—C84—H84	120.3
C2—C1—H1	119.3	C84—C85—C86	120.47 (18)
C11B—C1—H1	119.3	C84—C85—H85	119.8
C1—C2—C3	119.97 (15)	C86—C85—H85	119.8
C1—C2—H2	120.0	C81—C86—C85	119.52 (16)
C3—C2—H2	120.0	C81—C86—H86	120.2
C4—C3—C2	119.51 (14)	C85—C86—H86	120.2
C4—C3—H3	120.2	C10—N9—N8	107.06 (12)
C2—C3—H3	120.2	N9—C10—C10A	110.55 (13)
C3—C4—C4A	121.42 (15)	N9—C10—C101	119.21 (13)
C3—C4—H4	119.3	C10A—C10—C101	130.24 (13)
C4A—C4—H4	119.3	C10—C101—H10A	109.5
C4—C4A—C11B	119.43 (14)	C10—C101—H10B	109.5
C4—C4A—C5	121.47 (14)	H10A—C101—H10B	109.5
C11B—C4A—C5	119.10 (13)	C10—C101—H10C	109.5
C4A—C5—C6	109.32 (13)	H10A—C101—H10C	109.5
C4A—C5—H5A	109.8	H10B—C101—H10C	109.5
C6—C5—H5A	109.8	C7A—C10A—C11	118.41 (13)
C4A—C5—H5B	109.8	C7A—C10A—C10	104.91 (12)
C6—C5—H5B	109.8	C11—C10A—C10	136.58 (13)
H5A—C5—H5B	108.3	C11A—C11—C10A	117.00 (13)
C6A—C6—C5	110.02 (12)	C11A—C11—C111	123.84 (12)
C6A—C6—H6A	109.7	C10A—C11—C111	119.12 (12)

C5—C6—H6A	109.7	C11—C11A—C6A	118.51 (12)
C6A—C6—H6B	109.7	C11—C11A—C11B	124.46 (13)
C5—C6—H6B	109.7	C6A—C11A—C11B	117.03 (12)
H6A—C6—H6B	108.2	C1—C11B—C4A	118.14 (13)
N7—C6A—C11A	125.12 (13)	C1—C11B—C11A	122.97 (13)
N7—C6A—C6	116.43 (12)	C4A—C11B—C11A	118.89 (13)
C11A—C6A—C6	118.45 (12)	C116—C111—C112	119.07 (13)
C6A—N7—C7A	114.21 (12)	C116—C111—C11	120.28 (12)
N7—C7A—N8	126.25 (13)	C112—C111—C11	120.65 (12)
N7—C7A—C10A	126.71 (13)	C113—C112—C111	120.52 (13)
N8—C7A—C10A	106.98 (12)	C113—C112—H112	119.7
C7A—N8—N9	110.50 (11)	C111—C112—H112	119.7
C7A—N8—C81	129.74 (13)	C114—C113—C112	119.14 (14)
N9—N8—C81	119.72 (12)	C114—C113—H113	120.4
C86—C81—C82	120.67 (14)	C112—C113—H113	120.4
C86—C81—N8	119.98 (14)	C115—C114—C113	121.44 (13)
C82—C81—N8	119.34 (14)	C115—C114—Cl14	119.59 (11)
C81—C82—C83	118.94 (16)	C113—C114—Cl14	118.97 (12)
C81—C82—H82	120.5	C114—C115—C116	118.87 (14)
C83—C82—H82	120.5	C114—C115—H115	120.6
C84—C83—C82	120.90 (16)	C116—C115—H115	120.6
C84—C83—H83	119.5	C115—C116—C111	120.88 (13)
C82—C83—H83	119.5	C115—C116—H116	119.6
C85—C84—C83	119.49 (16)	C111—C116—H116	119.6
C85—C84—H84	120.3		

C11B—C1—C2—C3	−1.1 (2)	C101—C10—C10A—C7A	−178.83 (15)
C1—C2—C3—C4	−2.2 (3)	N9—C10—C10A—C11	176.65 (16)
C2—C3—C4—C4A	2.0 (3)	C101—C10—C10A—C11	−2.7 (3)
C3—C4—C4A—C11B	1.4 (2)	C7A—C10A—C11—C11A	−1.42 (19)
C3—C4—C4A—C5	−177.96 (15)	C10—C10A—C11—C11A	−177.13 (16)
C4—C4A—C5—C6	143.03 (15)	C7A—C10A—C11—C111	176.61 (13)
C11B—C4A—C5—C6	−36.33 (19)	C10—C10A—C11—C111	0.9 (2)
C4A—C5—C6—C6A	57.48 (16)	C10A—C11—C11A—C6A	2.45 (19)
C5—C6—C6A—N7	140.28 (13)	C111—C11—C11A—C6A	−175.48 (13)
C5—C6—C6A—C11A	−40.26 (18)	C10A—C11—C11A—C11B	−177.73 (13)
C11A—C6A—N7—C7A	−0.1 (2)	C111—C11—C11A—C11B	4.4 (2)
C6—C6A—N7—C7A	179.29 (13)	N7—C6A—C11A—C11	−1.8 (2)
C6A—N7—C7A—N8	178.03 (14)	C6—C6A—C11A—C11	178.82 (13)
C6A—N7—C7A—C10A	1.3 (2)	N7—C6A—C11A—C11B	178.38 (13)
N7—C7A—N8—N9	−176.39 (14)	C6—C6A—C11A—C11B	−1.02 (19)
C10A—C7A—N8—N9	0.84 (16)	C2—C1—C11B—C4A	4.4 (2)
N7—C7A—N8—C81	1.4 (2)	C2—C1—C11B—C11A	−175.73 (14)
C10A—C7A—N8—C81	178.62 (14)	C4—C4A—C11B—C1	−4.5 (2)
C7A—N8—C81—C86	30.1 (2)	C5—C4A—C11B—C1	174.84 (13)
N9—N8—C81—C86	−152.28 (15)	C4—C4A—C11B—C11A	175.61 (13)
C7A—N8—C81—C82	−150.81 (15)	C5—C4A—C11B—C11A	−5.0 (2)
N9—N8—C81—C82	26.8 (2)	C11—C11A—C11B—C1	25.6 (2)

C86—C81—C82—C83	−0.2 (2)	C6A—C11A—C11B—C1	−154.57 (14)
N8—C81—C82—C83	−179.27 (14)	C11—C11A—C11B—C4A	−154.55 (14)
C81—C82—C83—C84	−0.5 (2)	C6A—C11A—C11B—C4A	25.28 (19)
C82—C83—C84—C85	0.7 (3)	C11A—C11—C111—C116	68.91 (18)
C83—C84—C85—C86	−0.2 (3)	C10A—C11—C111—C116	−108.97 (15)
C82—C81—C86—C85	0.7 (3)	C11A—C11—C111—C112	−110.59 (16)
N8—C81—C86—C85	179.73 (16)	C10A—C11—C111—C112	71.52 (18)
C84—C85—C86—C81	−0.5 (3)	C116—C111—C112—C113	−2.8 (2)
C7A—N8—N9—C10	−0.49 (16)	C11—C111—C112—C113	176.71 (13)
C81—N8—N9—C10	−178.53 (13)	C111—C112—C113—C114	0.7 (2)
N8—N9—C10—C10A	−0.05 (16)	C112—C113—C114—C115	2.0 (2)
N8—N9—C10—C101	179.41 (13)	C112—C113—C114—Cl14	−177.44 (11)
N7—C7A—C10A—C11	−0.6 (2)	C113—C114—C115—C116	−2.6 (2)
N8—C7A—C10A—C11	−177.78 (12)	Cl14—C114—C115—C116	176.87 (10)
N7—C7A—C10A—C10	176.39 (14)	C114—C115—C116—C111	0.4 (2)
N8—C7A—C10A—C10	−0.82 (15)	C112—C111—C116—C115	2.2 (2)
N9—C10—C10A—C7A	0.55 (16)	C11—C111—C116—C115	−177.29 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C113—H113···*Cg*1^{i}	0.95	2.65	3.5214 (16)	152
C115—H115···*Cg*2^{ii}	0.95	2.90	3.6403 (17)	136

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