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11-(4-Bromophenyl)-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) = 0.004 Å
R factor = 0.047
wR factor = 0.102
Data-to-parameter ratio = 17.8

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

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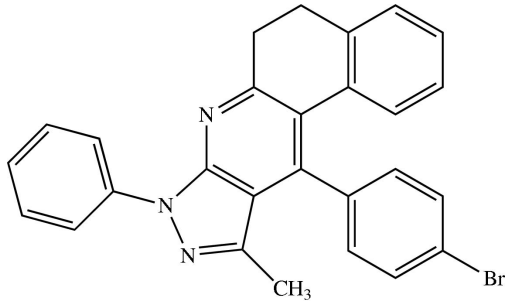
The title compound, $C_{27}H_{20}BrN_3$, is isostructural with the chloro analogue: the molecules are linked by two independent C—H···π(arene) hydrogen bonds into chains of edge-fused rings.

Comment

The title compound, (I) (Fig. 1), is isostructural with 11-(4-chlorophenyl)-10-methyl-8-phenyl-6,8-dihydro-5*H*-benzo[*f*]-pyrazolo[3,4-*b*]quinoline, (II) (Serrano *et al.*, 2005).



(I)

The bond lengths and angles, and the molecular conformation, for (I) are all virtually identical with those for (II). Two independent C—H···π(arene) hydrogen bonds (Table 1) link the molecules of (I) into a [101] chain of centrosymmetric edge-fused rings, just as in (II). There are no direction-specific interactions between adjacent chains: C—H···N and C—H···Br 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-bromobenzaldehyde (185.0 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.

Crystal data

$C_{27}H_{20}BrN_3$
M_r = 466.37
Triclinic, $P\overline{1}$
a = 7.0237 (3) Å
b = 12.8964 (7) Å
c = 13.3517 (7) Å
α = 106.630 (3)°
β = 101.423 (3)°
γ = 102.274 (3)°
V = 1088.18 (10) Å^3
Z = 2
D_x = 1.423 Mg m^{-3}
Mo Kα radiation
Cell parameters from 5001 reflections
θ = 3.1–27.7°
μ = 1.91 mm^{-1}
T = 120 (2) K
Plate, colourless
0.36 × 0.14 × 0.03 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.547, T_{max} = 0.945
223424 measured reflections
5001 independent reflections
3175 reflections with $I > 2\sigma(I)$
R_{int} = 0.085
θ_{max} = 27.7°
$h = -8 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.102
S = 1.03
5001 reflections
281 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C113—H113···*Cg*1^{i}	0.95	2.71	3.588 (3)	154
C115—H115···*Cg*2^{ii}	0.95	2.81	3.589 (3)	140

Symmetry codes: (i) $-x, 1-y, -z$; (ii) $1-x, 1-y, 1-z$. Note: *Cg*1 is the centroid of ring C81–C86, and *Cg*2 is the centroid of ring C1,C2,C3,C4,C4*A*,C11*B*

All H atoms were located in difference maps in fully ordered sites; they were then treated as riding atoms, with C—H distances 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.

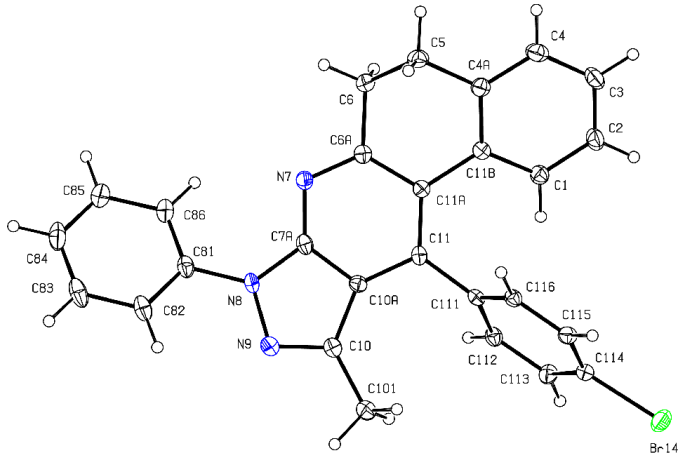


Figure 1
The molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

References

Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Hooft, R. W. W. (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
McArdle, P. (2003). *OSCAIL for Windows*. Version 10. Crystallography Centre, Chemistry Department, NUI Galway, Ireland.
Otwinowski, Z. & Minor, W (1997). *Methods in Enzymology*, Vol. 276, Macromolecular Crystallography, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Serrano, H., Quiroga, J., Cobo, J., Low, J. N. & Glidewell, C. (2005). *Acta Cryst.* E**61**, o1058–o1060.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

Acta Cryst. (2005). E**61**, o1702–o1703 [https://doi.org/10.1107/S1600536805014479]

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$\gamma = 102.274\ (3)°$
$V = 1088.18\ (10)$ Å^3
$Z = 2$
$F(000) = 476$
$D_x = 1.423$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5001 reflections
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$\mu = 1.91$ mm^{-1}
$T = 120$ K
Plate, colourless
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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)
$T_{min} = 0.547$, $T_{max} = 0.945$
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$\theta_{max} = 27.7°$, $\theta_{min} = 3.1°$
$h = -8\rightarrow9$
$k = -16\rightarrow16$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.102$
$S = 1.03$
5001 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
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br14	0.41479 (5)	0.13431 (3)	0.25854 (3)	0.03966 (13)
N7	0.2796 (3)	0.81718 (19)	0.26822 (18)	0.0255 (5)
N8	−0.0557 (3)	0.7067 (2)	0.15048 (19)	0.0270 (6)
N9	−0.1652 (3)	0.5942 (2)	0.10704 (19)	0.0285 (6)
C1	0.7765 (4)	0.6159 (2)	0.3633 (2)	0.0271 (7)
C2	0.9607 (4)	0.6214 (3)	0.4281 (3)	0.0330 (7)
C3	1.0668 (4)	0.7171 (3)	0.5171 (3)	0.0397 (8)
C4	0.9893 (4)	0.8088 (3)	0.5380 (2)	0.0355 (7)
C4A	0.8045 (4)	0.8053 (2)	0.4736 (2)	0.0277 (7)
C5	0.7231 (4)	0.9057 (2)	0.4936 (2)	0.0316 (7)
C6	0.6183 (4)	0.9125 (2)	0.3856 (2)	0.0285 (7)
C6A	0.4510 (4)	0.8058 (2)	0.3224 (2)	0.0244 (6)
C7A	0.1361 (4)	0.7190 (2)	0.2108 (2)	0.0252 (6)
C10	−0.0459 (4)	0.5364 (2)	0.1383 (2)	0.0252 (6)
C10A	0.1496 (4)	0.6113 (2)	0.2045 (2)	0.0224 (6)
C11	0.3307 (4)	0.6008 (2)	0.2637 (2)	0.0209 (6)
C11A	0.4864 (4)	0.7007 (2)	0.3226 (2)	0.0212 (6)
C11B	0.6911 (4)	0.7059 (2)	0.3862 (2)	0.0230 (6)
C81	−0.1493 (4)	0.7901 (2)	0.1331 (2)	0.0289 (7)
C82	−0.3588 (4)	0.7661 (3)	0.1102 (2)	0.0336 (7)
C83	−0.4501 (5)	0.8470 (3)	0.0925 (2)	0.0404 (8)
C84	−0.3341 (5)	0.9503 (3)	0.0971 (3)	0.0460 (9)
C85	−0.1276 (5)	0.9730 (3)	0.1203 (3)	0.0523 (10)
C86	−0.0334 (5)	0.8924 (3)	0.1375 (3)	0.0455 (9)
C101	−0.1264 (4)	0.4110 (2)	0.1040 (2)	0.0318 (7)
C111	0.3419 (4)	0.4862 (2)	0.2618 (2)	0.0218 (6)
C112	0.3481 (4)	0.4073 (2)	0.1668 (2)	0.0252 (6)
C113	0.3656 (4)	0.3019 (2)	0.1659 (2)	0.0268 (6)
C114	0.3778 (4)	0.2760 (2)	0.2600 (2)	0.0255 (6)
C115	0.3655 (4)	0.3515 (2)	0.3539 (2)	0.0253 (6)
C116	0.3482 (4)	0.4563 (2)	0.3542 (2)	0.0229 (6)
H1	0.7063	0.5497	0.3020	0.033*
H2	1.0147	0.5590	0.4113	0.040*
H3	1.1910	0.7200	0.5632	0.048*
H4	1.0640	0.8756	0.5977	0.043*
H5A	0.8356	0.9756	0.5350	0.038*
H5B	0.6255	0.8988	0.5373	0.038*
H6A	0.5621	0.9778	0.3986	0.034*
H6B	0.7175	0.9234	0.3435	0.034*
H10A	−0.1058	0.3878	0.1682	0.048*
H10B	−0.0546	0.3752	0.0544	0.048*
H10C	−0.2715	0.3875	0.0667	0.048*
H82	−0.4386	0.6951	0.1067	0.040*
H83	−0.5933	0.8314	0.0771	0.048*
H84	−0.3974	1.0052	0.0842	0.055*

H85	−0.0478	1.0444	0.1248	0.063*
H86	0.1097	0.9080	0.1522	0.055*
H112	0.3403	0.4258	0.1024	0.030*
H113	0.3692	0.2481	0.1012	0.032*
H115	0.3690	0.3316	0.4174	0.030*
H116	0.3405	0.5088	0.4187	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br14	0.0560 (2)	0.02559 (19)	0.0352 (2)	0.01541 (15)	0.00394 (15)	0.01040 (14)
N7	0.0255 (13)	0.0257 (14)	0.0253 (13)	0.0099 (11)	0.0047 (11)	0.0084 (11)
N8	0.0226 (12)	0.0298 (14)	0.0298 (14)	0.0122 (11)	0.0019 (11)	0.0118 (12)
N9	0.0244 (13)	0.0304 (15)	0.0294 (14)	0.0081 (11)	0.0047 (11)	0.0099 (12)
C1	0.0244 (15)	0.0284 (17)	0.0296 (17)	0.0081 (13)	0.0084 (13)	0.0104 (14)
C2	0.0241 (16)	0.0384 (19)	0.0405 (19)	0.0139 (14)	0.0083 (14)	0.0162 (16)
C3	0.0215 (16)	0.045 (2)	0.050 (2)	0.0054 (15)	−0.0015 (15)	0.0230 (18)
C4	0.0334 (17)	0.0335 (18)	0.0306 (18)	−0.0012 (14)	−0.0009 (14)	0.0122 (15)
C4A	0.0295 (16)	0.0273 (16)	0.0263 (16)	0.0053 (13)	0.0061 (13)	0.0125 (14)
C5	0.0345 (17)	0.0258 (16)	0.0269 (17)	0.0040 (13)	0.0020 (14)	0.0053 (13)
C6	0.0294 (16)	0.0240 (16)	0.0288 (17)	0.0070 (13)	0.0038 (13)	0.0074 (13)
C6A	0.0258 (15)	0.0264 (16)	0.0221 (15)	0.0082 (13)	0.0075 (13)	0.0090 (13)
C7A	0.0250 (15)	0.0325 (17)	0.0216 (16)	0.0116 (13)	0.0061 (13)	0.0122 (14)
C10	0.0237 (15)	0.0299 (16)	0.0242 (16)	0.0089 (13)	0.0082 (13)	0.0106 (13)
C10A	0.0232 (15)	0.0237 (15)	0.0184 (15)	0.0054 (12)	0.0045 (12)	0.0062 (12)
C11	0.0233 (14)	0.0264 (15)	0.0175 (14)	0.0122 (12)	0.0079 (12)	0.0088 (12)
C11A	0.0222 (14)	0.0235 (15)	0.0196 (15)	0.0062 (12)	0.0069 (12)	0.0093 (12)
C11B	0.0225 (14)	0.0259 (16)	0.0215 (15)	0.0058 (12)	0.0071 (12)	0.0098 (13)
C81	0.0317 (17)	0.0357 (18)	0.0220 (16)	0.0177 (14)	0.0051 (13)	0.0099 (14)
C82	0.0309 (17)	0.052 (2)	0.0260 (17)	0.0216 (15)	0.0089 (14)	0.0171 (15)
C83	0.0382 (18)	0.069 (3)	0.0233 (17)	0.0323 (18)	0.0090 (15)	0.0168 (17)
C84	0.059 (2)	0.050 (2)	0.0327 (19)	0.0386 (19)	0.0032 (17)	0.0092 (17)
C85	0.050 (2)	0.035 (2)	0.065 (3)	0.0171 (17)	−0.0050 (19)	0.0173 (19)
C86	0.0362 (18)	0.037 (2)	0.063 (2)	0.0182 (16)	0.0017 (17)	0.0191 (18)
C101	0.0249 (15)	0.0323 (18)	0.0368 (18)	0.0068 (13)	0.0060 (14)	0.0126 (15)
C111	0.0158 (13)	0.0250 (15)	0.0223 (15)	0.0048 (11)	0.0029 (12)	0.0072 (13)
C112	0.0260 (15)	0.0297 (17)	0.0202 (15)	0.0095 (13)	0.0042 (12)	0.0095 (13)
C113	0.0328 (16)	0.0261 (16)	0.0208 (15)	0.0118 (13)	0.0069 (13)	0.0052 (13)
C114	0.0224 (15)	0.0229 (15)	0.0277 (16)	0.0046 (12)	0.0028 (12)	0.0078 (13)
C115	0.0265 (15)	0.0257 (16)	0.0217 (15)	0.0035 (13)	0.0039 (12)	0.0099 (13)
C116	0.0219 (14)	0.0258 (16)	0.0194 (15)	0.0076 (12)	0.0044 (12)	0.0056 (12)

Geometric parameters (Å, º)

C1—C2	1.381 (4)	C83—C84	1.383 (5)
C1—C11B	1.403 (4)	C83—H83	0.95
C1—H1	0.95	C84—C85	1.369 (5)
C2—C3	1.383 (4)	C84—H84	0.95

C2—H2	0.95	C85—C86	1.393 (4)
C3—C4	1.385 (4)	C85—H85	0.95
C3—H3	0.95	C86—H86	0.95
C4—C4A	1.392 (4)	N9—C10	1.318 (3)
C4—H4	0.95	C10—C10A	1.438 (4)
C4A—C11B	1.407 (4)	C10—C101	1.494 (4)
C4A—C5	1.501 (4)	C101—H10A	0.98
C5—C6	1.520 (4)	C101—H10B	0.98
C5—H5A	0.99	C101—H10C	0.98
C5—H5B	0.99	C10A—C11	1.413 (4)
C6—C6A	1.497 (4)	C11—C11A	1.398 (4)
C6—H6A	0.99	C11—C111	1.490 (4)
C6—H6B	0.99	C111—C116	1.390 (4)
C6A—N7	1.336 (3)	C111—C112	1.397 (4)
C6A—C11A	1.429 (4)	C112—C113	1.387 (4)
N7—C7A	1.342 (3)	C112—H112	0.95
C7A—N8	1.376 (3)	C113—C114	1.381 (4)
C7A—C10A	1.392 (4)	C113—H113	0.95
N8—N9	1.379 (3)	C114—C115	1.381 (4)
N8—C81	1.423 (3)	C114—Br14	1.894 (3)
C81—C86	1.373 (4)	C115—C116	1.382 (4)
C81—C82	1.388 (4)	C115—H115	0.95
C82—C83	1.385 (4)	C116—H116	0.95
C82—H82	0.95	C11A—C11B	1.495 (4)

C2—C1—C11B	121.4 (3)	C83—C84—H84	120.1
C2—C1—H1	119.3	C84—C85—C86	120.6 (3)
C11B—C1—H1	119.3	C84—C85—H85	119.7
C1—C2—C3	120.4 (3)	C86—C85—H85	119.7
C1—C2—H2	119.8	C81—C86—C85	119.4 (3)
C3—C2—H2	119.8	C81—C86—H86	120.3
C2—C3—C4	119.0 (3)	C85—C86—H86	120.3
C2—C3—H3	120.5	C10—N9—N8	107.3 (2)
C4—C3—H3	120.5	N9—C10—C10A	110.3 (2)
C3—C4—C4A	121.5 (3)	N9—C10—C101	119.1 (2)
C3—C4—H4	119.2	C10A—C10—C101	130.6 (3)
C4A—C4—H4	119.2	C10—C101—H10A	109.5
C4—C4A—C11B	119.6 (3)	C10—C101—H10B	109.5
C4—C4A—C5	121.7 (3)	H10A—C101—H10B	109.5
C11B—C4A—C5	118.7 (2)	C10—C101—H10C	109.5
C4A—C5—C6	109.6 (2)	H10A—C101—H10C	109.5
C4A—C5—H5A	109.8	H10B—C101—H10C	109.5
C6—C5—H5A	109.8	C7A—C10A—C11	118.5 (2)
C4A—C5—H5B	109.8	C7A—C10A—C10	105.0 (2)
C6—C5—H5B	109.8	C11—C10A—C10	136.4 (3)
H5A—C5—H5B	108.2	C11A—C11—C10A	116.8 (2)
C6A—C6—C5	109.5 (2)	C11A—C11—C111	124.5 (2)
C6A—C6—H6A	109.8	C10A—C11—C111	118.7 (2)

C5—C6—H6A	109.8	C116—C111—C112	118.9 (3)
C6A—C6—H6B	109.8	C116—C111—C11	120.9 (2)
C5—C6—H6B	109.8	C112—C111—C11	120.2 (2)
H6A—C6—H6B	108.2	C113—C112—C111	120.3 (2)
N7—C6A—C11A	125.1 (2)	C113—C112—H112	119.9
N7—C6A—C6	116.3 (2)	C111—C112—H112	119.9
C11A—C6A—C6	118.5 (2)	C114—C113—C112	119.5 (3)
C6A—N7—C7A	114.1 (2)	C114—C113—H113	120.3
N7—C7A—N8	126.1 (2)	C112—C113—H113	120.3
N7—C7A—C10A	126.7 (2)	C115—C114—C113	121.2 (3)
N8—C7A—C10A	107.2 (2)	C115—C114—Br14	120.2 (2)
C7A—N8—N9	110.2 (2)	C113—C114—Br14	118.6 (2)
C7A—N8—C81	130.0 (2)	C114—C115—C116	119.0 (2)
N9—N8—C81	119.8 (2)	C114—C115—H115	120.5
C86—C81—C82	120.6 (3)	C116—C115—H115	120.5
C86—C81—N8	120.2 (3)	C115—C116—C111	121.1 (3)
C82—C81—N8	119.3 (3)	C115—C116—H116	119.5
C83—C82—C81	119.3 (3)	C111—C116—H116	119.5
C83—C82—H82	120.4	C11—C11A—C6A	118.7 (2)
C81—C82—H82	120.4	C11—C11A—C11B	124.4 (2)
C84—C83—C82	120.4 (3)	C6A—C11A—C11B	116.9 (2)
C84—C83—H83	119.8	C1—C11B—C4A	117.9 (2)
C82—C83—H83	119.8	C1—C11B—C11A	123.1 (2)
C85—C84—C83	119.7 (3)	C4A—C11B—C11A	119.0 (2)
C85—C84—H84	120.1		

C11B—C1—C2—C3	−0.7 (4)	C101—C10—C10A—C7A	−178.8 (3)
C1—C2—C3—C4	−2.3 (5)	N9—C10—C10A—C11	176.4 (3)
C2—C3—C4—C4A	2.1 (5)	C101—C10—C10A—C11	−2.9 (5)
C3—C4—C4A—C11B	1.2 (4)	C7A—C10A—C11—C11A	−1.7 (4)
C3—C4—C4A—C5	−177.9 (3)	C10—C10A—C11—C11A	−177.2 (3)
C4—C4A—C5—C6	142.4 (3)	C7A—C10A—C11—C111	176.9 (2)
C11B—C4A—C5—C6	−36.7 (3)	C10—C10A—C11—C111	1.4 (5)
C4A—C5—C6—C6A	58.3 (3)	C11A—C11—C111—C116	67.7 (3)
C5—C6—C6A—N7	140.1 (2)	C10A—C11—C111—C116	−110.7 (3)
C5—C6—C6A—C11A	−41.0 (3)	C11A—C11—C111—C112	−111.7 (3)
C11A—C6A—N7—C7A	−0.3 (4)	C10A—C11—C111—C112	69.8 (3)
C6—C6A—N7—C7A	178.5 (2)	C116—C111—C112—C113	−1.7 (4)
C6A—N7—C7A—N8	178.0 (3)	C11—C111—C112—C113	177.8 (2)
C6A—N7—C7A—C10A	0.9 (4)	C111—C112—C113—C114	−0.3 (4)
N7—C7A—N8—N9	−176.9 (2)	C112—C113—C114—C115	2.3 (4)
C10A—C7A—N8—N9	0.7 (3)	C112—C113—C114—Br14	−176.98 (19)
N7—C7A—N8—C81	0.2 (5)	C113—C114—C115—C116	−2.4 (4)
C10A—C7A—N8—C81	177.8 (3)	Br14—C114—C115—C116	176.94 (19)
C7A—N8—C81—C86	27.9 (5)	C114—C115—C116—C111	0.4 (4)
N9—N8—C81—C86	−155.2 (3)	C112—C111—C116—C115	1.6 (4)
C7A—N8—C81—C82	−152.9 (3)	C11—C111—C116—C115	−177.8 (2)
N9—N8—C81—C82	24.0 (4)	C10A—C11—C11A—C6A	2.2 (4)

C86—C81—C82—C83	−0.4 (4)	C111—C11—C11A—C6A	−176.3 (2)
N8—C81—C82—C83	−179.6 (3)	C10A—C11—C11A—C11B	−177.4 (2)
C81—C82—C83—C84	0.3 (4)	C111—C11—C11A—C11B	4.1 (4)
C82—C83—C84—C85	−0.6 (5)	N7—C6A—C11A—C11	−1.2 (4)
C83—C84—C85—C86	1.1 (5)	C6—C6A—C11A—C11	−180.0 (2)
C82—C81—C86—C85	0.9 (5)	N7—C6A—C11A—C11B	178.4 (2)
N8—C81—C86—C85	−180.0 (3)	C6—C6A—C11A—C11B	−0.4 (4)
C84—C85—C86—C81	−1.2 (6)	C2—C1—C11B—C4A	3.9 (4)
C7A—N8—N9—C10	−0.4 (3)	C2—C1—C11B—C11A	−176.0 (2)
C81—N8—N9—C10	−177.8 (2)	C4—C4A—C11B—C1	−4.1 (4)
N8—N9—C10—C10A	−0.1 (3)	C5—C4A—C11B—C1	175.1 (2)
N8—N9—C10—C101	179.3 (2)	C4—C4A—C11B—C11A	175.8 (2)
N7—C7A—C10A—C11	0.1 (4)	C5—C4A—C11B—C11A	−5.1 (4)
N8—C7A—C10A—C11	−177.5 (2)	C11—C11A—C11B—C1	24.6 (4)
N7—C7A—C10A—C10	176.9 (3)	C6A—C11A—C11B—C1	−155.0 (2)
N8—C7A—C10A—C10	−0.7 (3)	C11—C11A—C11B—C4A	−155.3 (3)
N9—C10—C10A—C7A	0.5 (3)	C6A—C11A—C11B—C4A	25.1 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C113—H113···*Cg*1^{i}	0.95	2.71	3.588 (3)	154
C115—H115···*Cg*2^{ii}	0.95	2.81	3.589 (3)	140

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