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2-[4,5-Bis(4-bromophenyl)-1-(4-*tert*-butylphenyl)-1*H*-imidazol-2-yl]-4,6-dichlorophenol

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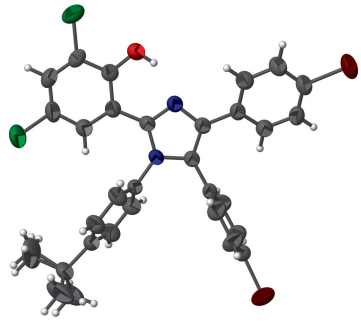
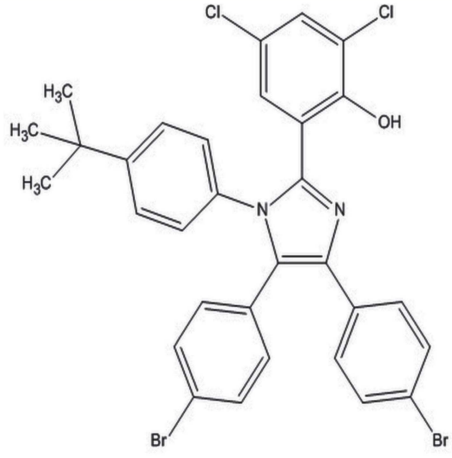
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{31}H_{24}Br_2Cl_2N_2O$, the dihedral angles subtended by the *tert*-butyl-phenyl, 4,6-dichlorophenol and 4-bromophenyl (×2) rings are 70.7 (3), 8.1 (3), 28.1 (3) and 84.2 (3)°, respectively. The orientations of the pendant rings may be related to intramolecular O—H···N and C—H···π interactions. One of the *tert*-butyl methyl groups is disordered over two sets of sites in a 0.54 (3):0.46 (3) ratio. In the crystal, a weak C—H···π interaction generates inversion dimers.

3D view



Chemical scheme



Structure description

Imidazole and its derivatives play an important role in natural product chemistry (*e.g.* Brown *et al.*, 1998; Forte *et al.*, 2009). As part of our studies in this area, we now report the synthesis and structure of the title compound, which consists of an imidazole ring bearing C4–C9 *tert*-butylphenyl, C14–C19 4,6-dichlorophenol and C2–C25 and C26–C31 4-bromophenyl rings (Fig. 1). The dihedral angles between the imidazole core and these four rings are 70.7 (3), 8.1 (3), 28.1 (3) and 84.2 (3)°, respectively. An intramolecular O—H···N hydrogen bond (Table 1) may help to establish the near-coplanarity of the imidazole and C14 rings and an intramolecular C—H···π interaction may help to establish the near-orthogonal relationship between the imidazole and C4 ring. The C11 *tert*-butyl methyl group is disordered over two sets of sites in a 0.54 (3):0.46 (3) ratio. In the crystal, a weak C—H···π interaction generates inversion dimers but there are no aromatic π–π stacking interactions (Fig. 2). A very weak C27—H27···N2 hydrogen bond is also present.

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

*Cg*2 and *Cg*4 are the centroids of the C4–C9 and C20–C25 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.82	1.81	2.542 (7)	148
C27—H27···N2^{i}	0.93	2.68	3.547 (6)	156
C15—H15···*Cg*2	0.93	2.76	3.621 (7)	154
C9—H9···*Cg*4^{ii}	0.93	2.85	3.641 (6)	144

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x+\frac{3}{2}, y+\frac{5}{2}, z$.

Synthesis and crystallization

1,2-Bis(4-bromophenyl)ethane-1,2-dione (10 mmol), 4-*tert*-butylaniline (10 mmol) and 3,5-dichloro-2-hydroxybenzaldehyde (10 mmol) along with ammonium acetate (10 mmol) in acetic acid (15 ml) were refluxed at room temperature for 6 h. The progress of the reaction was monitored by TLC (7:3 petroleum ether: ethyl acetate). On completion, the reaction mixture was poured onto ice-cold water, the obtained precipitate was filtered, dried and purified by column chromatography (7:3 petroleum ether: ethyl acetate), giving a yield of 80%. The compound was recrystallized from ethanol solution. 1*H*-NMR ($CDCl_3$): δ 1.26 (*s*, 9H), 6.07 (*s*, OH), 7.26–7.38 (*m*, 6H), 3.97–4.03 (*q*, 8H).

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{31}H_{24}Br_2Cl_2N_2O$
M_r	671.24
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	373
a, *b*, *c* (Å)	17.7619 (5), 12.7435 (4), 28.2194 (8)
β (°)	102.478 (2)
V (Å^3)	6236.5 (3)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	2.80
Crystal size (mm)	0.16 × 0.15 × 0.14
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 1998)
T_{min}, T_{max}	0.646, 0.676
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38305, 3839, 3305
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.064, 0.239, 1.15
No. of reflections	3839
No. of parameters	353
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.03, −0.53

Computer programs: *SMART* and *SAINT-Plus* (Bruker, 1998), *SHELXLT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *CAMERON* (Watkin *et al.*, 1996).

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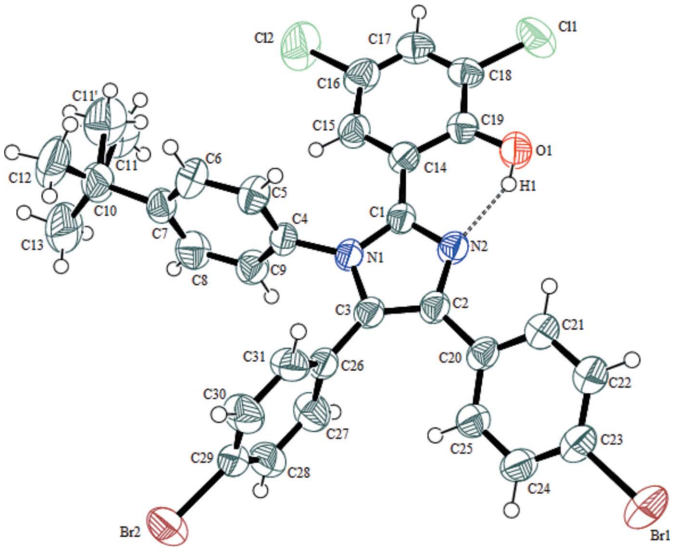

Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

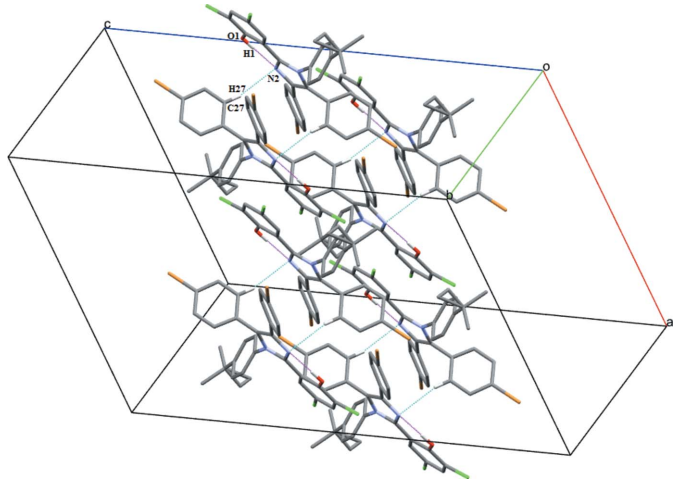

Figure 2
Unit-cell packing of the title compound showing intermolecular C—H···N interactions with dotted lines. H atoms not involved in hydrogen bonding have been excluded.

full crystallographic data

IUCrData (2019). **4**, x191672 [https://doi.org/10.1107/S2414314619016729]

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2-[4,5-Bis(4-bromophenyl)-1-(4-*tert*-butylphenyl)-1*H*-imidazol-2-yl]-4,6-dichlorophenol

Crystal data

$C_{31}H_{24}Br_2Cl_2N_2O$
M_r = 671.24
Monoclinic, $C2/c$
a = 17.7619 (5) Å
b = 12.7435 (4) Å
c = 28.2194 (8) Å
β = 102.478 (2)°
V = 6236.5 (3) Å^3
Z = 8
$F(000)$ = 2688
D_x = 1.430 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3839 reflections
θ = 2.0–22.0°
μ = 2.80 mm^{-1}
T = 373 K
Block, colorless
0.16 × 0.15 × 0.14 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1998)
T_{min} = 0.646, T_{max} = 0.676
38305 measured reflections
3839 independent reflections
3305 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −18→18
k = −13→13
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.239
S = 1.15
3839 reflections
353 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1772P)^2 + 7.3582P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 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}	Occ. (<1)
Br2	0.37961 (5)	0.94032 (8)	0.22600 (3)	0.0880 (4)	
Br1	0.23913 (4)	0.66001 (7)	−0.09750 (3)	0.0874 (4)	
Cl1	0.83979 (12)	0.86713 (16)	−0.08924 (7)	0.0808 (6)	
Cl2	0.93419 (14)	1.0667 (2)	0.07944 (9)	0.1126 (10)	
N1	0.6357 (3)	0.9183 (4)	0.07290 (16)	0.0441 (11)	
C1	0.6612 (3)	0.8957 (4)	0.03174 (19)	0.0438 (13)	
N2	0.6050 (3)	0.8543 (4)	−0.00143 (17)	0.0465 (12)	
C2	0.5402 (3)	0.8518 (4)	0.0183 (2)	0.0459 (14)	
C3	0.5576 (3)	0.8907 (4)	0.0646 (2)	0.0438 (13)	
C4	0.6785 (3)	0.9547 (4)	0.11935 (19)	0.0431 (13)	
C14	0.7370 (3)	0.9191 (4)	0.0217 (2)	0.0464 (14)	
C21	0.4692 (4)	0.7306 (5)	−0.0446 (2)	0.0558 (15)	
H21	0.516363	0.708611	−0.050285	0.067*	
C26	0.5132 (3)	0.9005 (4)	0.10235 (19)	0.0426 (13)	
C25	0.3960 (4)	0.8382 (5)	−0.0018 (2)	0.0555 (16)	
H25	0.394035	0.889568	0.021273	0.067*	
C29	0.4321 (3)	0.9217 (5)	0.1747 (2)	0.0520 (15)	
C23	0.3317 (4)	0.7187 (5)	−0.0614 (2)	0.0586 (16)	
C19	0.7511 (3)	0.8830 (4)	−0.0234 (2)	0.0467 (14)	
C20	0.4676 (3)	0.8068 (5)	−0.0095 (2)	0.0472 (14)	
C16	0.8641 (4)	0.9950 (5)	0.0397 (3)	0.0634 (18)	
C31	0.5155 (4)	0.8252 (5)	0.1367 (2)	0.0586 (16)	
H31	0.544710	0.764970	0.135677	0.070*	
C18	0.8229 (3)	0.9081 (5)	−0.0342 (2)	0.0525 (15)	
C15	0.7941 (4)	0.9753 (5)	0.0527 (2)	0.0556 (16)	
H15	0.785674	0.999713	0.082200	0.067*	
C7	0.7660 (4)	1.0275 (5)	0.2066 (2)	0.0523 (15)	
C5	0.7312 (4)	0.8902 (5)	0.1474 (2)	0.0548 (15)	
H5	0.737765	0.821949	0.137379	0.066*	
C30	0.4755 (4)	0.8365 (5)	0.1730 (3)	0.0649 (18)	
H30	0.478605	0.784616	0.196467	0.078*	
C24	0.3288 (4)	0.7958 (5)	−0.0271 (2)	0.0578 (16)	
H24	0.281729	0.818176	−0.021413	0.069*	
C27	0.4672 (4)	0.9865 (5)	0.1043 (2)	0.0644 (17)	
H27	0.463475	1.038139	0.080597	0.077*	
C6	0.7747 (4)	0.9267 (5)	0.1906 (2)	0.0579 (16)	
H6	0.810783	0.882507	0.209454	0.069*	
C9	0.6670 (4)	1.0540 (5)	0.1352 (2)	0.0553 (16)	
H9	0.629949	1.097589	0.116773	0.066*	
C28	0.4262 (4)	0.9985 (6)	0.1405 (3)	0.0646 (17)	
H28	0.395513	1.057269	0.141495	0.077*	
C17	0.8784 (4)	0.9612 (5)	−0.0025 (2)	0.0573 (16)	
H17	0.926012	0.974023	−0.009986	0.069*	
C8	0.7105 (4)	1.0880 (5)	0.1781 (3)	0.0633 (18)	
H8	0.702101	1.155354	0.188617	0.076*	

C22	0.4018 (4)	0.6868 (5)	−0.0711 (2)	0.0605 (17)	
H22	0.403347	0.636937	−0.094918	0.073*	
C10	0.8204 (4)	1.0707 (6)	0.2521 (3)	0.074 (2)	
C13	0.7885 (7)	1.1621 (8)	0.2744 (3)	0.105 (3)	
H13A	0.783692	1.221159	0.252859	0.158*	
H13B	0.822629	1.179705	0.304664	0.158*	
H13C	0.738721	1.144285	0.280167	0.158*	
C12	0.8438 (6)	0.9853 (10)	0.2916 (3)	0.114 (4)	
H12A	0.798250	0.954386	0.298811	0.170*	
H12B	0.874070	1.016495	0.320452	0.170*	
H12C	0.873526	0.932020	0.279996	0.170*	
C11	0.888 (2)	1.133 (3)	0.2282 (14)	0.099 (7)	0.46 (3)
H11A	0.863919	1.184217	0.204867	0.148*	0.46 (3)
H11B	0.915147	1.082875	0.212585	0.148*	0.46 (3)
H11C	0.924449	1.167696	0.253678	0.148*	0.46 (3)
C11′	0.8959 (19)	1.086 (3)	0.2423 (11)	0.099 (7)	0.54 (3)
H11D	0.926404	1.128018	0.267490	0.148*	0.54 (3)
H11E	0.891222	1.120856	0.211635	0.148*	0.54 (3)
H11F	0.920299	1.019054	0.241150	0.148*	0.54 (3)
O1	0.7002 (3)	0.8310 (3)	−0.05618 (15)	0.0588 (11)	
H1	0.660977	0.821259	−0.045930	0.088*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br2	0.0757 (6)	0.1339 (8)	0.0630 (6)	0.0197 (5)	0.0340 (5)	0.0061 (4)
Br1	0.0554 (6)	0.1039 (7)	0.0923 (7)	−0.0211 (4)	−0.0076 (4)	−0.0165 (4)
Cl1	0.0874 (14)	0.0892 (12)	0.0797 (13)	−0.0099 (10)	0.0485 (11)	−0.0157 (10)
Cl2	0.0775 (14)	0.166 (2)	0.0940 (16)	−0.0665 (15)	0.0169 (12)	−0.0298 (15)
N1	0.041 (3)	0.054 (3)	0.035 (3)	−0.006 (2)	0.004 (2)	−0.001 (2)
C1	0.043 (3)	0.051 (3)	0.036 (3)	−0.001 (3)	0.004 (3)	0.000 (2)
N2	0.045 (3)	0.054 (3)	0.039 (3)	−0.006 (2)	0.006 (2)	0.005 (2)
C2	0.044 (3)	0.053 (3)	0.038 (3)	−0.001 (2)	0.004 (3)	0.005 (2)
C3	0.041 (3)	0.051 (3)	0.038 (3)	0.000 (3)	0.004 (2)	0.004 (2)
C4	0.042 (3)	0.052 (3)	0.035 (3)	−0.010 (3)	0.007 (3)	0.002 (2)
C14	0.044 (3)	0.050 (3)	0.044 (3)	−0.004 (3)	0.007 (3)	0.007 (3)
C21	0.052 (4)	0.059 (4)	0.056 (4)	0.000 (3)	0.009 (3)	−0.004 (3)
C26	0.037 (3)	0.051 (3)	0.038 (3)	−0.003 (3)	0.004 (2)	0.005 (3)
C25	0.051 (4)	0.067 (4)	0.047 (3)	−0.004 (3)	0.009 (3)	0.001 (3)
C29	0.043 (3)	0.071 (4)	0.041 (3)	0.001 (3)	0.008 (3)	0.003 (3)
C23	0.049 (4)	0.065 (4)	0.057 (4)	−0.012 (3)	0.000 (3)	0.005 (3)
C19	0.048 (3)	0.046 (3)	0.045 (3)	0.003 (3)	0.007 (3)	0.005 (3)
C20	0.041 (3)	0.058 (3)	0.040 (3)	−0.003 (3)	0.003 (3)	0.010 (3)
C16	0.047 (4)	0.072 (4)	0.068 (4)	−0.018 (3)	0.004 (3)	0.001 (4)
C31	0.052 (4)	0.061 (4)	0.065 (4)	0.011 (3)	0.017 (3)	0.005 (3)
C18	0.048 (4)	0.054 (3)	0.061 (4)	0.004 (3)	0.024 (3)	0.007 (3)
C15	0.052 (4)	0.064 (4)	0.050 (4)	−0.011 (3)	0.010 (3)	−0.003 (3)
C7	0.049 (4)	0.068 (4)	0.041 (3)	−0.016 (3)	0.012 (3)	−0.005 (3)

C5	0.060 (4)	0.048 (3)	0.052 (4)	−0.004 (3)	0.002 (3)	−0.003 (3)
C30	0.070 (5)	0.074 (4)	0.058 (4)	0.003 (4)	0.031 (4)	0.020 (3)
C24	0.040 (3)	0.076 (4)	0.057 (4)	−0.003 (3)	0.008 (3)	0.004 (3)
C27	0.076 (5)	0.065 (4)	0.054 (4)	0.007 (4)	0.017 (3)	0.012 (3)
C6	0.062 (4)	0.060 (4)	0.046 (4)	−0.007 (3)	−0.002 (3)	0.004 (3)
C9	0.060 (4)	0.051 (4)	0.053 (4)	0.005 (3)	0.008 (3)	0.000 (3)
C28	0.059 (4)	0.075 (4)	0.063 (4)	0.013 (3)	0.020 (3)	−0.004 (4)
C17	0.047 (4)	0.062 (4)	0.068 (4)	−0.006 (3)	0.023 (3)	0.005 (3)
C8	0.070 (4)	0.054 (4)	0.065 (4)	−0.006 (3)	0.012 (4)	−0.017 (3)
C22	0.053 (4)	0.066 (4)	0.059 (4)	−0.003 (3)	0.004 (3)	−0.009 (3)
C10	0.064 (4)	0.099 (5)	0.058 (4)	−0.028 (4)	0.010 (4)	−0.026 (4)
C13	0.117 (8)	0.107 (7)	0.081 (6)	−0.015 (5)	−0.001 (5)	−0.043 (5)
C12	0.110 (8)	0.145 (9)	0.065 (5)	0.013 (6)	−0.028 (5)	−0.028 (6)
C11	0.091 (10)	0.11 (2)	0.092 (16)	−0.072 (16)	0.019 (11)	−0.005 (12)
C11′	0.091 (10)	0.11 (2)	0.092 (16)	−0.072 (16)	0.019 (11)	−0.005 (12)
O1	0.057 (3)	0.071 (3)	0.048 (2)	−0.012 (2)	0.011 (2)	−0.008 (2)

Geometric parameters (Å, º)

Br2—C29	1.899 (6)	C18—C17	1.361 (9)
Br1—C23	1.891 (6)	C15—H15	0.9300
Cl1—C18	1.725 (6)	C7—C8	1.368 (10)
Cl2—C16	1.743 (6)	C7—C6	1.380 (9)
N1—C1	1.365 (7)	C7—C10	1.532 (9)
N1—C3	1.400 (7)	C5—C6	1.375 (9)
N1—C4	1.443 (7)	C5—H5	0.9300
C1—N2	1.321 (7)	C30—H30	0.9300
C1—C14	1.466 (8)	C24—H24	0.9300
N2—C2	1.383 (7)	C27—C28	1.386 (10)
C2—C3	1.369 (8)	C27—H27	0.9300
C2—C20	1.473 (8)	C6—H6	0.9300
C3—C26	1.462 (8)	C9—C8	1.359 (10)
C4—C5	1.364 (9)	C9—H9	0.9300
C4—C9	1.371 (8)	C28—H28	0.9300
C14—C15	1.388 (9)	C17—H17	0.9300
C14—C19	1.424 (8)	C8—H8	0.9300
C21—C22	1.385 (9)	C22—H22	0.9300
C21—C20	1.391 (9)	C10—C11′	1.44 (3)
C21—H21	0.9300	C10—C13	1.493 (12)
C26—C31	1.359 (9)	C10—C12	1.550 (14)
C26—C27	1.375 (9)	C10—C11	1.70 (3)
C25—C24	1.362 (9)	C13—H13A	0.9600
C25—C20	1.395 (9)	C13—H13B	0.9600
C25—H25	0.9300	C13—H13C	0.9600
C29—C30	1.338 (9)	C12—H12A	0.9600
C29—C28	1.362 (9)	C12—H12B	0.9600
C23—C24	1.387 (10)	C12—H12C	0.9600
C23—C22	1.393 (9)	C11—H11A	0.9600

C19—O1	1.323 (7)	C11—H11B	0.9600
C19—C18	1.410 (8)	C11—H11C	0.9600
C16—C17	1.339 (10)	C11′—H11D	0.9600
C16—C15	1.395 (9)	C11′—H11E	0.9600
C31—C30	1.373 (9)	C11′—H11F	0.9600
C31—H31	0.9300	O1—H1	0.8200

C1—N1—C3	107.6 (4)	C31—C30—H30	119.7
C1—N1—C4	129.4 (5)	C25—C24—C23	119.1 (6)
C3—N1—C4	122.8 (5)	C25—C24—H24	120.5
N2—C1—N1	110.4 (5)	C23—C24—H24	120.5
N2—C1—C14	121.9 (5)	C26—C27—C28	121.9 (6)
N1—C1—C14	127.5 (5)	C26—C27—H27	119.1
C1—N2—C2	106.9 (5)	C28—C27—H27	119.1
C3—C2—N2	109.9 (5)	C5—C6—C7	121.6 (6)
C3—C2—C20	129.8 (5)	C5—C6—H6	119.2
N2—C2—C20	120.2 (5)	C7—C6—H6	119.2
C2—C3—N1	105.2 (5)	C8—C9—C4	119.3 (6)
C2—C3—C26	132.9 (5)	C8—C9—H9	120.3
N1—C3—C26	121.9 (5)	C4—C9—H9	120.3
C5—C4—C9	119.9 (6)	C29—C28—C27	118.1 (6)
C5—C4—N1	119.6 (5)	C29—C28—H28	121.0
C9—C4—N1	120.5 (5)	C27—C28—H28	121.0
C15—C14—C19	119.0 (5)	C16—C17—C18	119.7 (6)
C15—C14—C1	124.0 (5)	C16—C17—H17	120.2
C19—C14—C1	117.0 (5)	C18—C17—H17	120.2
C22—C21—C20	121.2 (6)	C9—C8—C7	122.8 (6)
C22—C21—H21	119.4	C9—C8—H8	118.6
C20—C21—H21	119.4	C7—C8—H8	118.6
C31—C26—C27	117.5 (6)	C21—C22—C23	118.8 (6)
C31—C26—C3	121.4 (5)	C21—C22—H22	120.6
C27—C26—C3	121.1 (5)	C23—C22—H22	120.6
C24—C25—C20	122.0 (6)	C11′—C10—C13	115.5 (14)
C24—C25—H25	119.0	C11′—C10—C7	109.4 (13)
C20—C25—H25	119.0	C13—C10—C7	114.0 (7)
C30—C29—C28	120.9 (6)	C11′—C10—C12	96.7 (16)
C30—C29—Br2	120.8 (5)	C13—C10—C12	108.1 (7)
C28—C29—Br2	118.3 (5)	C7—C10—C12	111.9 (6)
C24—C23—C22	120.9 (6)	C13—C10—C11	99.7 (17)
C24—C23—Br1	119.8 (5)	C7—C10—C11	102.0 (13)
C22—C23—Br1	119.2 (5)	C12—C10—C11	120.7 (17)
O1—C19—C18	118.4 (5)	C10—C13—H13A	109.5
O1—C19—C14	124.1 (5)	C10—C13—H13B	109.5
C18—C19—C14	117.5 (5)	H13A—C13—H13B	109.5
C21—C20—C25	118.0 (5)	C10—C13—H13C	109.5
C21—C20—C2	120.1 (5)	H13A—C13—H13C	109.5
C25—C20—C2	121.9 (5)	H13B—C13—H13C	109.5
C17—C16—C15	121.8 (6)	C10—C12—H12A	109.5

C17—C16—Cl2	119.6 (5)	C10—C12—H12B	109.5
C15—C16—Cl2	118.5 (5)	H12A—C12—H12B	109.5
C26—C31—C30	121.1 (6)	C10—C12—H12C	109.5
C26—C31—H31	119.5	H12A—C12—H12C	109.5
C30—C31—H31	119.5	H12B—C12—H12C	109.5
C17—C18—C19	122.1 (6)	C10—C11—H11A	109.5
C17—C18—Cl1	120.1 (5)	C10—C11—H11B	109.5
C19—C18—Cl1	117.9 (5)	H11A—C11—H11B	109.5
C14—C15—C16	119.9 (6)	C10—C11—H11C	109.5
C14—C15—H15	120.1	H11A—C11—H11C	109.5
C16—C15—H15	120.1	H11B—C11—H11C	109.5
C8—C7—C6	116.7 (6)	C10—C11′—H11D	109.5
C8—C7—C10	122.2 (6)	C10—C11′—H11E	109.5
C6—C7—C10	121.0 (6)	H11D—C11′—H11E	109.5
C4—C5—C6	119.6 (6)	C10—C11′—H11F	109.5
C4—C5—H5	120.2	H11D—C11′—H11F	109.5
C6—C5—H5	120.2	H11E—C11′—H11F	109.5
C29—C30—C31	120.5 (6)	C19—O1—H1	109.5
C29—C30—H30	119.7		

C3—N1—C1—N2	−1.0 (6)	C14—C19—C18—C17	2.4 (9)
C4—N1—C1—N2	173.7 (5)	O1—C19—C18—Cl1	−0.9 (7)
C3—N1—C1—C14	174.4 (5)	C14—C19—C18—Cl1	−178.7 (4)
C4—N1—C1—C14	−10.9 (9)	C19—C14—C15—C16	−0.4 (9)
N1—C1—N2—C2	1.3 (6)	C1—C14—C15—C16	−179.1 (6)
C14—C1—N2—C2	−174.4 (5)	C17—C16—C15—C14	0.1 (10)
C1—N2—C2—C3	−1.0 (6)	Cl2—C16—C15—C14	179.5 (5)
C1—N2—C2—C20	−178.2 (5)	C9—C4—C5—C6	−2.5 (9)
N2—C2—C3—N1	0.4 (6)	N1—C4—C5—C6	176.8 (5)
C20—C2—C3—N1	177.3 (5)	C28—C29—C30—C31	0.4 (11)
N2—C2—C3—C26	−176.0 (6)	Br2—C29—C30—C31	−177.7 (5)
C20—C2—C3—C26	0.8 (10)	C26—C31—C30—C29	1.1 (11)
C1—N1—C3—C2	0.4 (6)	C20—C25—C24—C23	0.3 (9)
C4—N1—C3—C2	−174.8 (5)	C22—C23—C24—C25	−1.8 (10)
C1—N1—C3—C26	177.3 (5)	Br1—C23—C24—C25	−179.2 (5)
C4—N1—C3—C26	2.1 (8)	C31—C26—C27—C28	1.8 (10)
C1—N1—C4—C5	−67.3 (8)	C3—C26—C27—C28	−178.3 (6)
C3—N1—C4—C5	106.7 (6)	C4—C5—C6—C7	0.4 (10)
C1—N1—C4—C9	112.0 (7)	C8—C7—C6—C5	2.0 (10)
C3—N1—C4—C9	−74.0 (7)	C10—C7—C6—C5	−173.7 (6)
N2—C1—C14—C15	170.8 (6)	C5—C4—C9—C8	2.2 (9)
N1—C1—C14—C15	−4.1 (9)	N1—C4—C9—C8	−177.2 (6)
N2—C1—C14—C19	−7.9 (8)	C30—C29—C28—C27	−0.8 (10)
N1—C1—C14—C19	177.2 (5)	Br2—C29—C28—C27	177.4 (5)
C2—C3—C26—C31	93.4 (8)	C26—C27—C28—C29	−0.4 (11)
N1—C3—C26—C31	−82.5 (7)	C15—C16—C17—C18	1.5 (10)
C2—C3—C26—C27	−86.5 (8)	Cl2—C16—C17—C18	−178.0 (5)
N1—C3—C26—C27	97.6 (7)	C19—C18—C17—C16	−2.8 (10)

C15—C14—C19—O1	−178.4 (5)	Cl1—C18—C17—C16	178.3 (5)
C1—C14—C19—O1	0.4 (8)	C4—C9—C8—C7	0.3 (10)
C15—C14—C19—C18	−0.8 (8)	C6—C7—C8—C9	−2.3 (10)
C1—C14—C19—C18	178.0 (5)	C10—C7—C8—C9	173.3 (7)
C22—C21—C20—C25	−0.1 (9)	C20—C21—C22—C23	−1.4 (10)
C22—C21—C20—C2	179.8 (6)	C24—C23—C22—C21	2.3 (10)
C24—C25—C20—C21	0.6 (9)	Br1—C23—C22—C21	179.7 (5)
C24—C25—C20—C2	−179.2 (5)	C8—C7—C10—C11′	−105.9 (17)
C3—C2—C20—C21	−150.0 (6)	C6—C7—C10—C11′	69.6 (17)
N2—C2—C20—C21	26.6 (8)	C8—C7—C10—C13	25.1 (10)
C3—C2—C20—C25	29.9 (9)	C6—C7—C10—C13	−159.5 (7)
N2—C2—C20—C25	−153.5 (5)	C8—C7—C10—C12	148.2 (7)
C27—C26—C31—C30	−2.2 (10)	C6—C7—C10—C12	−36.3 (9)
C3—C26—C31—C30	177.9 (6)	C8—C7—C10—C11	−81.4 (18)
O1—C19—C18—C17	−179.9 (6)	C6—C7—C10—C11	94.0 (18)

Hydrogen-bond geometry (Å, º)

*Cg*2 and *Cg*4 are the centroids of the C4–C9 and C20–C25 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.82	1.81	2.542 (7)	148
C27—H27···N2^{i}	0.93	2.68	3.547 (6)	156
C15—H15···*Cg*2	0.93	2.76	3.621 (7)	154
C9—H9···*Cg*4^{ii}	0.93	2.85	3.641 (6)	144

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*; (ii) *x*+3/2, *y*+5/2, *z*.