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14-(4-Chlorophenyl)-14*H*-dibenzo[*a*,*j*]xanthene

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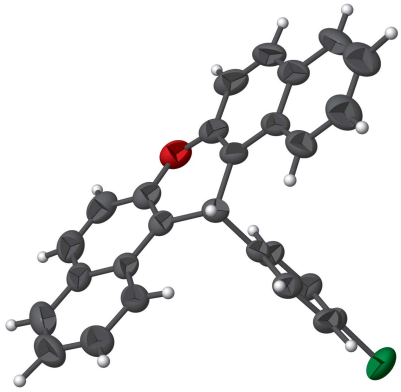
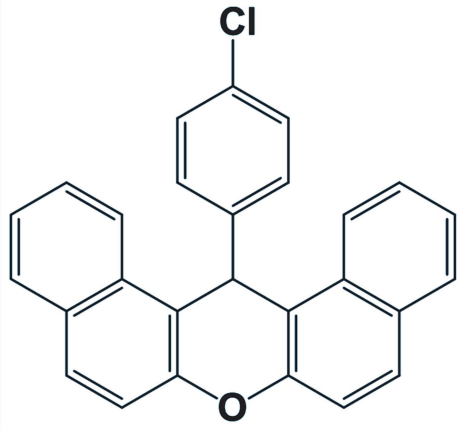
In the title compound, $C_{27}H_{17}ClO$, the xanthene fused-ring system adopts a shallow butterfly conformation [dihedral angle between the two halves of the ring system = 22.9 (1)°. The dihedral angle between the central heteroyclic ring and the pendant chlorophenyl group is 87.60 (8)°. In the crystal, molecules are linked by weak C—H···π interactions.

3D view



Chemical scheme



Structure description

The xanthene fused-ring building unit occurs in many natural alkaloids (Boente *et al.*, 1986; de la Fuente & Domínguez, 2007) and other biologically active compounds (Niu *et al.*, 2012). In the arena of materials, dibenzo[*a*,*j*]xanthene derivatives have been reported to be promising hole-transporting materials for organic optoelectronic devices (Martins *et al.*, 2017). Many reports on the synthesis of this class of compounds have been reported (Bartolomeu *et al.*, 2014; Mirjalili *et al.*, 2011). The present study of the title compound is a part of our work on the rapid synthesis of substituted dibenzo[*a*,*j*]xanthene derivatives as potential optical materials.

Fig. 1 shows the structure of the compound. The xanthene core has a shallow butterfly conformation with the angle between the planes of the naphthyl units (across the C6—O17 line) being 22.9 (1)°. The packing and the role of the different crystal symmetry operators in building it up are shown in Fig. 2*a*–*c*. The molecules are linked by weak C—H···π interaction and C—H···Cl hydrogen bonds (Table 1 and Fig. 2*d*).

Synthesis and crystallization

The title compound was synthesized by microwave irradiation of a mixture of 4-chlorobenzaldehyde (0.5 mmol) and 2-naphthol (1.0 mmol) in the presence of iodine (8 mol%) as cyclizing agent. After completion of the reaction, water and a few crystals of potassium iodide were added and the product was extracted with ethyl acetate. The crude

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

*Cg*2 and *Cg*4 are the centroids of the C2–C5/C28/C29 and C8–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H31···Cl1^{i}	0.98	3.00	3.547 (2)	116
C12—H121···*Cg*2^{ii}	0.93	2.90	3.649 (3)	138
C23—H231···*Cg*4^{iii}	0.98	3.00	3.740 (3)	134
C25—H251···*Cg*2^{iv}	1.02	2.97	3.942 (3)	160

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

product was purified by column chromatography and was dissolved in ethyl acetate. The solution was kept undisturbed for few days in an NMR tube to obtain colourless needles of the title compound, yield 85%, m.p. 265°C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ_H p.p.m.: 8.3 (*d*, *J* = 8.4 Hz, 2H, ArH), 7.83 (*d*,*J* = 8.0 Hz, 2H, ArH), 7.81 (*t*, *J* = 4.8 Hz, 2H, ArH), 7.80 (*d*, *J* = 8.8 Hz, 2H, ArH), 7.74 (*m*, 6H, ArH), 7.11 (*d*, *J* = 8.4 Hz, 2H, ArH), 6.458 (*s*,1*H*,CH). ^{13}C NMR ($CDCl_3$, 100 MHz) δ p.p.m.: 148.7, 143.4, 132.0, 131.2, 131.0, 129.4, 129.0, 128.9, 128.6, 126.9, 124.3, 122.4,118.0, 116.7, 37.3.

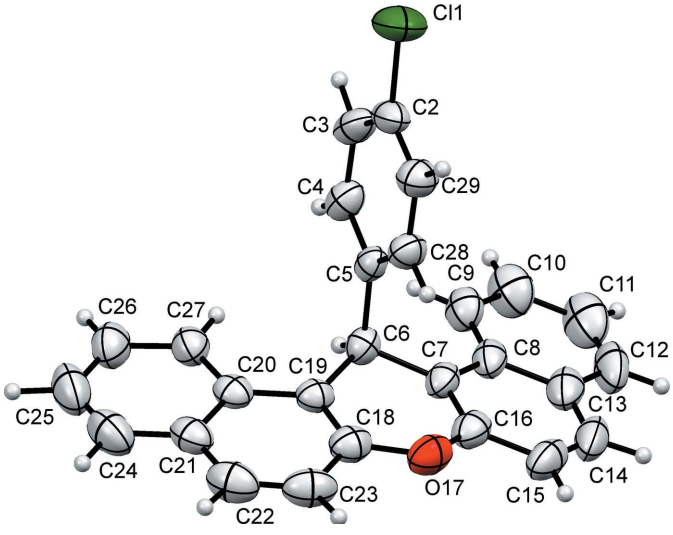


Figure 1
The molecular structure of the title compound with displacement ellipsoids at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{17}ClO$
M_r	392.88
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	296
a, *b*, *c* (Å)	14.0201 (7), 17.4488 (8), 7.8775 (3)
V (Å^3)	1927.10 (15)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.21
Crystal size (mm)	0.40 × 0.21 × 0.10
Data collection	
Diffractometer	Bruker SMART APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2010)
T_{min}, T_{max}	0.853, 1
No. of measured, independent and observed [$I > 2.0\sigma(I)$] reflections	34384, 4980, 4052
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.682
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.046, 0.053, 0.61
No. of reflections	4970
No. of parameters	264
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.41
Absolute structure	Flack (1983), 2260 Friedel-pairs
Absolute structure parameter	0.15 (5)

Computer programs: *APEX2* and *SAINT* (Bruker, 2010), *SUPERFLIP* (Palatinus & Chapuis, 2007), *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *CAMERON* (Watkin *et al.*, 2003), *ORTEP-3 for Windows* (Farrugia, 2012) and *CRYSTALS* (Betteridge *et al.*, 2003).

Refinement

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

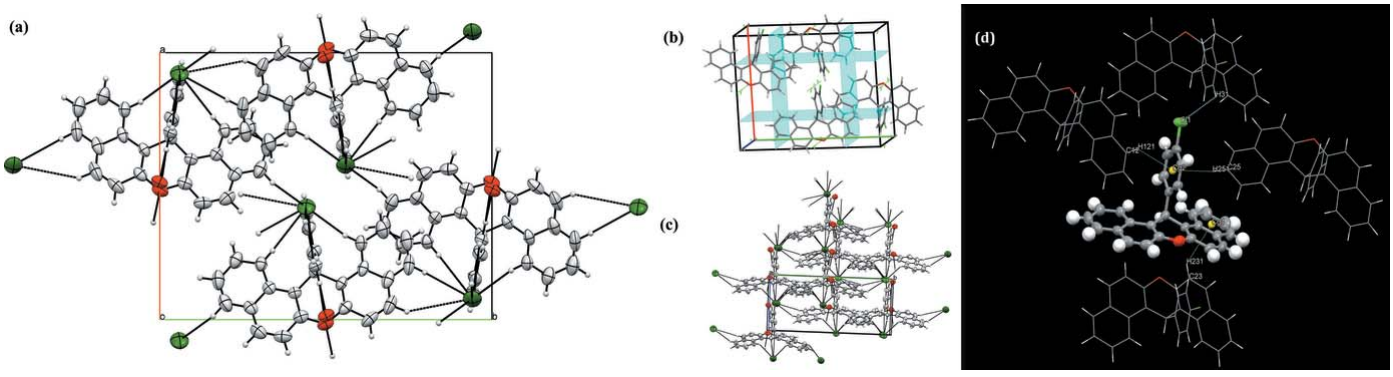


Figure 2
(*a*) A view of the crystal packing along [001]; (*b*) locations of the screw axis (green marker) and glide plane (blue planes) within the unit cell; (*c*) view of the molecular stacking (approximately along [100]); (*d*) packing diagram highlighting the C—H···π interactions (green dotted lines from the ring centroid to hydrogen) and Cl···H hydrogen bond (blue dotted line). All hanging interactions were removed for a clearer view.

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full crystallographic data

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Crystal data

$C_{27}H_{17}ClO$
M_r = 392.88
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 14.0201 (7) Å
b = 17.4488 (8) Å
c = 7.8775 (3) Å
V = 1927.10 (15) Å^3
Z = 4
$F(000)$ = 815.997
D_x = 1.354 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9942 reflections
θ = 2.8–24.1°
μ = 0.21 mm^{-1}
T = 296 K
Needle, colourless
0.40 × 0.21 × 0.10 mm

Data collection

BRUKER SMART APEXII diffractometer
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2010)
T_{min} = 0.853, T_{max} = 1
34384 measured reflections
4980 independent reflections
4052 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.034
θ_{max} = 29.0°, θ_{min} = 2.3°
h = −19→18
k = −23→23
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.053
S = 0.61
4970 reflections
264 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
H-atom parameters constrained
Method = Quasi-Unit *w*eights W = 1.0 or 1./4*F*sq
$(\Delta/\sigma)_{max}$ = 0.0002
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Extinction correction: Larson (1970), Equation 22
Extinction coefficient: 140 (3)
Absolute structure: Flack (1983), 2260 Friedel-pairs
Absolute structure parameter: 0.15 (5)

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems open-flow nitrogen cryostat (Cosier & Glazer, 1986) with a nominal stability of 0.1K.

Cosier, J. & Glazer, A.M., 1986. J. Appl. Cryst. 105-107.

Refinement. The H atoms attached to carbon atoms were located in difference maps and refined as riding atoms in their as-found relative locations.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.42137 (5)	0.44109 (4)	−0.49033 (11)	0.0905
C2	0.35101 (15)	0.45059 (11)	−0.3081 (3)	0.0525
C3	0.39356 (14)	0.44159 (12)	−0.1537 (3)	0.0574
C4	0.33832 (12)	0.44586 (10)	−0.0064 (3)	0.0498
C5	0.24104 (11)	0.45958 (9)	−0.0168 (2)	0.0386
C6	0.17853 (13)	0.46716 (10)	0.1418 (2)	0.0421
C7	0.13553 (13)	0.54701 (11)	0.1471 (2)	0.0450
C8	0.19136 (16)	0.61195 (11)	0.1980 (3)	0.0500
C9	0.28621 (16)	0.60620 (11)	0.2561 (2)	0.0560
C10	0.3369 (2)	0.66973 (14)	0.3063 (3)	0.0747
C11	0.2959 (3)	0.74292 (15)	0.2984 (3)	0.0821
C12	0.2059 (3)	0.75021 (14)	0.2438 (3)	0.0776
C13	0.15026 (18)	0.68635 (12)	0.1914 (3)	0.0626
C14	0.0552 (2)	0.69352 (14)	0.1342 (3)	0.0734
C15	0.00195 (19)	0.63196 (14)	0.0875 (3)	0.0676
C16	0.04440 (15)	0.55834 (13)	0.0970 (2)	0.0531
O17	−0.01588 (9)	0.49912 (9)	0.04831 (19)	0.0608
C18	0.01068 (14)	0.42485 (12)	0.0923 (2)	0.0512
C19	0.10051 (13)	0.40635 (10)	0.1441 (2)	0.0415
C20	0.11915 (14)	0.32913 (10)	0.1936 (2)	0.0446
C21	0.04471 (16)	0.27372 (11)	0.1814 (3)	0.0533
C22	−0.04492 (17)	0.29705 (15)	0.1219 (3)	0.0675
C23	−0.06320 (15)	0.37023 (14)	0.0807 (3)	0.0640
H231	−0.1241	0.3856	0.0300	0.0765*
H221	−0.0936	0.2577	0.0994	0.0807*
C24	0.0624 (2)	0.19770 (13)	0.2329 (3)	0.0734
C25	0.1482 (2)	0.17598 (14)	0.2956 (3)	0.0773
C26	0.22213 (19)	0.22971 (12)	0.3076 (3)	0.0651
C27	0.20808 (16)	0.30473 (11)	0.2575 (2)	0.0520
H271	0.2583	0.3393	0.2605	0.0622*
H261	0.2849	0.2188	0.3669	0.0779*
H251	0.1567	0.1211	0.3386	0.0907*
H241	0.0128	0.1608	0.2309	0.0876*
H151	−0.0622	0.6373	0.0494	0.0807*
H141	0.0301	0.7435	0.1236	0.0901*
H121	0.1766	0.7974	0.2287	0.0959*
H111	0.3319	0.7883	0.3472	0.0967*
H101	0.4031	0.6629	0.3524	0.0904*
H91	0.3154	0.5576	0.2599	0.0665*
H61	0.2175	0.4624	0.2449	0.0468*
C28	0.20141 (14)	0.46887 (11)	−0.1766 (2)	0.0480
C29	0.25589 (15)	0.46442 (12)	−0.3222 (3)	0.0562
H291	0.2294	0.4713	−0.4303	0.0667*
H281	0.1359	0.4806	−0.1823	0.0578*
H41	0.3664	0.4380	0.0975	0.0603*

H31	0.4631	0.4339	−0.1510	0.0692*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0832 (4)	0.0975 (5)	0.0909 (4)	0.0033 (4)	0.0486 (4)	0.0036 (4)
C2	0.0583 (14)	0.0418 (11)	0.0575 (12)	−0.0032 (10)	0.0252 (11)	−0.0022 (11)
C3	0.0360 (11)	0.0498 (13)	0.0865 (17)	−0.0012 (10)	0.0105 (11)	−0.0150 (12)
C4	0.0424 (11)	0.0476 (11)	0.0594 (12)	0.0034 (9)	−0.0046 (10)	−0.0093 (11)
C5	0.0357 (10)	0.0311 (9)	0.0491 (11)	0.0013 (8)	−0.0018 (8)	−0.0044 (9)
C6	0.0449 (11)	0.0408 (10)	0.0405 (11)	0.0050 (9)	−0.0021 (8)	−0.0026 (9)
C7	0.0536 (12)	0.0419 (12)	0.0394 (11)	0.0128 (9)	0.0049 (9)	−0.0008 (9)
C8	0.0719 (14)	0.0398 (11)	0.0384 (10)	0.0114 (11)	0.0111 (10)	0.0008 (9)
C9	0.0712 (15)	0.0424 (12)	0.0545 (12)	0.0005 (11)	0.0016 (11)	−0.0066 (10)
C10	0.095 (2)	0.0604 (16)	0.0690 (16)	−0.0117 (15)	−0.0041 (15)	−0.0122 (13)
C11	0.123 (3)	0.0550 (16)	0.0678 (17)	−0.0101 (17)	0.0063 (17)	−0.0167 (14)
C12	0.128 (3)	0.0348 (12)	0.0703 (16)	0.0099 (16)	0.0237 (18)	−0.0007 (12)
C13	0.0924 (19)	0.0497 (13)	0.0456 (12)	0.0178 (13)	0.0176 (13)	0.0033 (11)
C14	0.107 (2)	0.0504 (14)	0.0633 (16)	0.0345 (15)	0.0264 (15)	0.0132 (12)
C15	0.0720 (16)	0.0778 (17)	0.0530 (13)	0.0381 (14)	0.0086 (11)	0.0146 (12)
C16	0.0582 (13)	0.0574 (13)	0.0437 (11)	0.0146 (12)	0.0062 (9)	0.0008 (11)
O17	0.0489 (8)	0.0754 (9)	0.0579 (9)	0.0158 (8)	−0.0042 (8)	0.0039 (8)
C18	0.0491 (12)	0.0642 (15)	0.0402 (11)	0.0059 (11)	0.0013 (9)	−0.0003 (10)
C19	0.0414 (10)	0.0498 (11)	0.0333 (10)	0.0023 (9)	0.0024 (8)	−0.0004 (9)
C20	0.0503 (12)	0.0500 (11)	0.0336 (10)	−0.0023 (10)	0.0067 (9)	−0.0037 (9)
C21	0.0579 (14)	0.0571 (13)	0.0449 (12)	−0.0095 (11)	0.0116 (11)	−0.0032 (11)
C22	0.0643 (16)	0.0761 (17)	0.0620 (16)	−0.0216 (14)	0.0075 (12)	−0.0140 (13)
C23	0.0445 (12)	0.0964 (19)	0.0510 (13)	−0.0026 (13)	−0.0015 (10)	−0.0089 (13)
C24	0.090 (2)	0.0611 (16)	0.0694 (18)	−0.0232 (15)	0.0155 (14)	−0.0003 (13)
C25	0.115 (2)	0.0465 (14)	0.0704 (17)	−0.0047 (16)	0.0155 (16)	0.0081 (13)
C26	0.0816 (18)	0.0576 (15)	0.0561 (14)	0.0121 (13)	0.0042 (13)	0.0099 (12)
C27	0.0613 (14)	0.0463 (12)	0.0484 (12)	0.0019 (11)	0.0060 (11)	0.0026 (10)
C28	0.0405 (10)	0.0547 (12)	0.0488 (11)	0.0079 (10)	0.0018 (10)	0.0024 (10)
C29	0.0563 (13)	0.0629 (13)	0.0494 (12)	0.0067 (11)	0.0070 (10)	0.0038 (12)

Geometric parameters (Å, º)

Cl1—C2	1.7496 (19)	C14—H141	0.944
C2—C3	1.364 (3)	C15—C16	1.418 (3)
C2—C29	1.360 (3)	C15—H151	0.953
C3—C4	1.397 (3)	C16—O17	1.389 (2)
C3—H31	0.985	O17—C18	1.392 (2)
C4—C5	1.387 (2)	C18—C19	1.363 (2)
C4—H41	0.919	C18—C23	1.411 (3)
C5—C6	1.532 (2)	C19—C20	1.427 (2)
C5—C28	1.386 (3)	C20—C21	1.426 (2)
C6—C7	1.519 (3)	C20—C27	1.410 (3)
C6—C19	1.524 (3)	C21—C22	1.402 (3)

C6—H61	0.983	C21—C24	1.409 (3)
C7—C8	1.435 (3)	C22—C23	1.342 (3)
C7—C16	1.352 (3)	C22—H221	0.985
C8—C9	1.410 (3)	C23—H231	0.981
C8—C13	1.421 (3)	C24—C25	1.355 (3)
C9—C10	1.375 (3)	C24—H241	0.947
C9—H91	0.943	C25—C26	1.401 (3)
C10—C11	1.401 (3)	C25—H251	1.022
C10—H101	1.005	C26—C27	1.381 (3)
C11—C12	1.339 (4)	C26—H261	1.014
C11—H111	1.014	C27—H271	0.928
C12—C13	1.422 (3)	C28—C29	1.380 (3)
C12—H121	0.927	C28—H281	0.942
C13—C14	1.412 (3)	C29—H291	0.937
C14—C15	1.359 (3)		

Cl1—C2—C3	118.32 (16)	C14—C15—H151	121.8
Cl1—C2—C29	120.18 (18)	C16—C15—H151	120.1
C3—C2—C29	121.47 (19)	C15—C16—C7	123.0 (2)
C2—C3—C4	119.48 (18)	C15—C16—O17	113.84 (19)
C2—C3—H31	117.9	C7—C16—O17	123.15 (19)
C4—C3—H31	122.6	C16—O17—C18	117.46 (14)
C3—C4—C5	120.4 (2)	O17—C18—C19	122.84 (18)
C3—C4—H41	119.7	O17—C18—C23	114.62 (18)
C5—C4—H41	120.0	C19—C18—C23	122.54 (19)
C4—C5—C6	121.96 (18)	C6—C19—C18	119.65 (17)
C4—C5—C28	117.91 (19)	C6—C19—C20	121.97 (16)
C6—C5—C28	120.10 (15)	C18—C19—C20	118.35 (17)
C5—C6—C7	109.18 (15)	C19—C20—C21	119.20 (17)
C5—C6—C19	111.12 (14)	C19—C20—C27	122.99 (17)
C7—C6—C19	110.71 (15)	C21—C20—C27	117.80 (17)
C5—C6—H61	110.4	C20—C21—C22	118.80 (19)
C7—C6—H61	106.1	C20—C21—C24	119.4 (2)
C19—C6—H61	109.3	C22—C21—C24	121.8 (2)
C6—C7—C8	121.05 (16)	C21—C22—C23	121.9 (2)
C6—C7—C16	120.09 (18)	C21—C22—H221	118.6
C8—C7—C16	118.81 (19)	C23—C22—H221	119.2
C7—C8—C9	123.31 (18)	C18—C23—C22	119.1 (2)
C7—C8—C13	119.34 (19)	C18—C23—H231	118.8
C9—C8—C13	117.3 (2)	C22—C23—H231	121.7
C8—C9—C10	121.5 (2)	C21—C24—C25	121.6 (2)
C8—C9—H91	119.0	C21—C24—H241	120.4
C10—C9—H91	119.5	C25—C24—H241	117.9
C9—C10—C11	120.7 (3)	C24—C25—C26	119.6 (2)
C9—C10—H101	119.1	C24—C25—H251	119.1
C11—C10—H101	120.1	C26—C25—H251	121.2
C10—C11—C12	119.1 (3)	C25—C26—C27	120.6 (2)
C10—C11—H111	119.4	C25—C26—H261	123.2

C12—C11—H111	121.1	C27—C26—H261	115.6
C11—C12—C13	122.4 (3)	C20—C27—C26	120.9 (2)
C11—C12—H121	122.9	C20—C27—H271	119.0
C13—C12—H121	114.5	C26—C27—H271	120.0
C12—C13—C8	118.9 (2)	C5—C28—C29	121.77 (18)
C12—C13—C14	122.8 (2)	C5—C28—H281	117.3
C8—C13—C14	118.4 (2)	C29—C28—H281	120.8
C13—C14—C15	122.3 (2)	C28—C29—C2	119.0 (2)
C13—C14—H141	117.5	C28—C29—H291	121.9
C15—C14—H141	120.1	C2—C29—H291	119.0
C14—C15—C16	118.1 (2)		

Hydrogen-bond geometry (Å, º)

*Cg*2 and *Cg*4 are the centroids of the C2–C5/C28/C29 and C8–C13 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H31···Cl1^{i}	0.98	3.00	3.547 (2)	116
C12—H121···*Cg*2^{ii}	0.93	2.90	3.649 (3)	138
C23—H231···*Cg*4^{iii}	0.98	3.00	3.740 (3)	134
C25—H251···*Cg*2^{iv}	1.02	2.97	3.942 (3)	160

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