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## Structure Reports

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**(2E)-3-(4-Bromophenyl)-1-(3-chlorophenyl)prop-2-en-1-one**Jerry P. Jasinski,<sup>a\*</sup> Ray J. Butcher,<sup>b</sup> B. Narayana,<sup>c</sup>  
K. Veena<sup>c</sup> and H. S. Yathirajan<sup>d</sup>

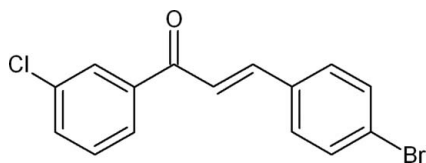
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Key indicators: single-crystal X-ray study;  $T = 110$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.058;  $wR$  factor = 0.164; data-to-parameter ratio = 14.9.

In the title compound,  $\text{C}_{15}\text{H}_{10}\text{BrClO}$ , the dihedral angle between mean planes of the bromo- and chloro-substituted benzene rings is  $46.2(2)^\circ$  compared to  $45.20(9)^\circ$  in the structure with the Cl substituent in the *meta* position of the aromatic ring. The dihedral angles between the mean plane of the prop-2-ene-1-one group and the mean planes of the 4-bromophenyl and 3-chlorophenyl rings are  $28.7(5)$  and  $24.2(4)^\circ$ , respectively. In the crystal, weak intermolecular  $\text{C}-\text{H}\cdots\pi$  interactions occur.

## Related literature

For a related structure, see: Ng *et al.* (2006).

## Experimental

## Crystal data

$\text{C}_{15}\text{H}_{10}\text{BrClO}$   
 $M_r = 321.59$

Triclinic,  $P\bar{1}$   
 $a = 5.9197(8)$  Å

$b = 7.3391(11)$  Å  
 $c = 14.8171(17)$  Å  
 $\alpha = 101.929(11)^\circ$   
 $\beta = 94.371(10)^\circ$   
 $\gamma = 93.299(11)^\circ$   
 $V = 626.22(15)$  Å<sup>3</sup>

$Z = 2$   
Cu  $K\alpha$  radiation  
 $\mu = 6.29$  mm<sup>-1</sup>  
 $T = 110$  K  
 $0.50 \times 0.21 \times 0.12$  mm

## Data collection

Oxford Diffraction Xcalibur diffractometer with a Ruby Gemini detector  
Absorption correction: analytical (*CrysAlis RED*; Oxford)

Diffraction, 2007)  
 $T_{\min} = 0.041$ ,  $T_{\max} = 0.344$   
3868 measured reflections  
2432 independent reflections  
2312 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.164$   
 $S = 1.07$   
2432 reflections

163 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 1.78$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.29$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C2A}-\text{H2AA}\cdots\text{Cg2}^{\text{i}}$	0.95	2.97	3.588 (4)	124
$\text{C5A}-\text{H5AA}\cdots\text{Cg2}^{\text{ii}}$	0.95	2.84	3.463 (4)	124
$\text{C12A}-\text{H12A}\cdots\text{Cg1}^{\text{iii}}$	0.95	2.83	3.527 (4)	131

Symmetry codes: (i)  $-x+1, -y+1, -z+1$ ; (ii)  $-x, -y, -z+1$ ; (iii)  $-x, -y+1, -z+1$ .  $\text{Cg1}$  is the centroid of the  $\text{C1A}-\text{C6A}$  ring and  $\text{Cg2}$  is the centroid of the  $\text{C10A}-\text{C15A}$  ring.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

KV thanksthe UGC for the sanction of a Junior Research Fellowship and for a SAP Chemical grant. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5130).

## References

- Ng, S.-L., Razak, I. A., Fun, H.-K., Shettigar, V., Patil, P. S. & Dharmaprakash, S. M. (2006). *Acta Cryst.* **E62**, o2175–o2177.  
Oxford Diffraction (2007). *CrysAlis PRO* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supporting information

*Acta Cryst.* (2010). E66, o158 [doi:10.1107/S1600536809053446]

**(2E)-3-(4-Bromophenyl)-1-(3-chlorophenyl)prop-2-en-1-one**

Jerry P. Jasinski, Ray J. Butcher, B. Narayana, K. Veena and H. S. Yathirajan

**S1. Comment**

In continuation of our interest in the synthesis and crystal structure determination of chalcones, the title chalcone,  $C_{15}H_{10}BrClO$ , is synthesized and its crystal structure is reported.

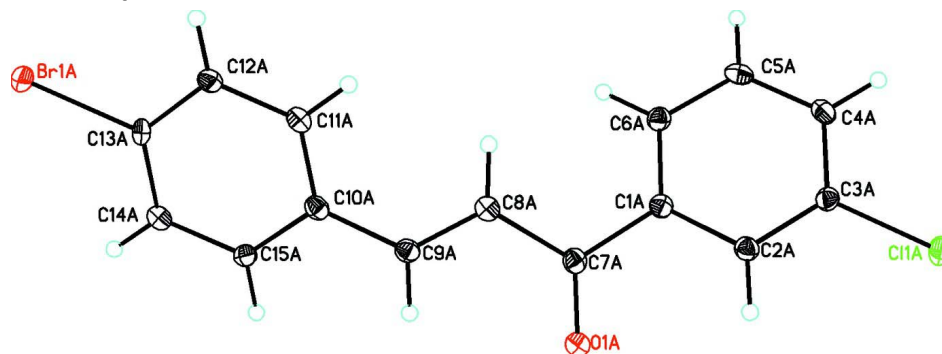
The title compound, (I), is a chalcone derivative with 4-bromophenyl and 3-chlorophenyl rings bonded at the opposite ends of a propenone group, the biologically active region (Fig.1). The dihedral angle between mean planes of the chloro and bromo substituted benzene rings is  $46.2(2)^\circ$  compared to  $45.20(9)^\circ$  (Ng *et al.* (2006)) and  $46.70(5)^\circ$  for a similar related molecule. The angles between the mean plane of the prop-2-ene-1-one group and the mean planes of the 4-bromophenyl and 3-chlorophenyl rings are  $28.7(5)^\circ$  and  $24.2(4)^\circ$  and respectively. This compares to  $20.66(1)^\circ$  and  $24.54(1)^\circ$  in the similar structure. While no classical hydrogen bonds are present, weak intermolecular C—H $\cdots$  $\pi$ -ring interactions are observed which contribute to the stability of crystal packing (Fig.2, Table 1).

**S2. Experimental**

50% KOH was added to a mixture of 3-chloroacetophenone (0.01 mol) and *p*-bromobenzaldehyde (0.01 mol) in 25 ml of ethanol (Scheme 2). The mixture was stirred for an hour at room temperature and the precipitate was collected by filtration and purified by recrystallization from ethanol. Single crystals were grown from ethyl acetate by slow evaporation method with the yield of the compound being 70% (m.p.412–414 K). Analytical data for  $C_{15}H_{10}BrClO$ : Found (Calculated): C %: 55.97 (56.02); H%: 3.09 (3.13).

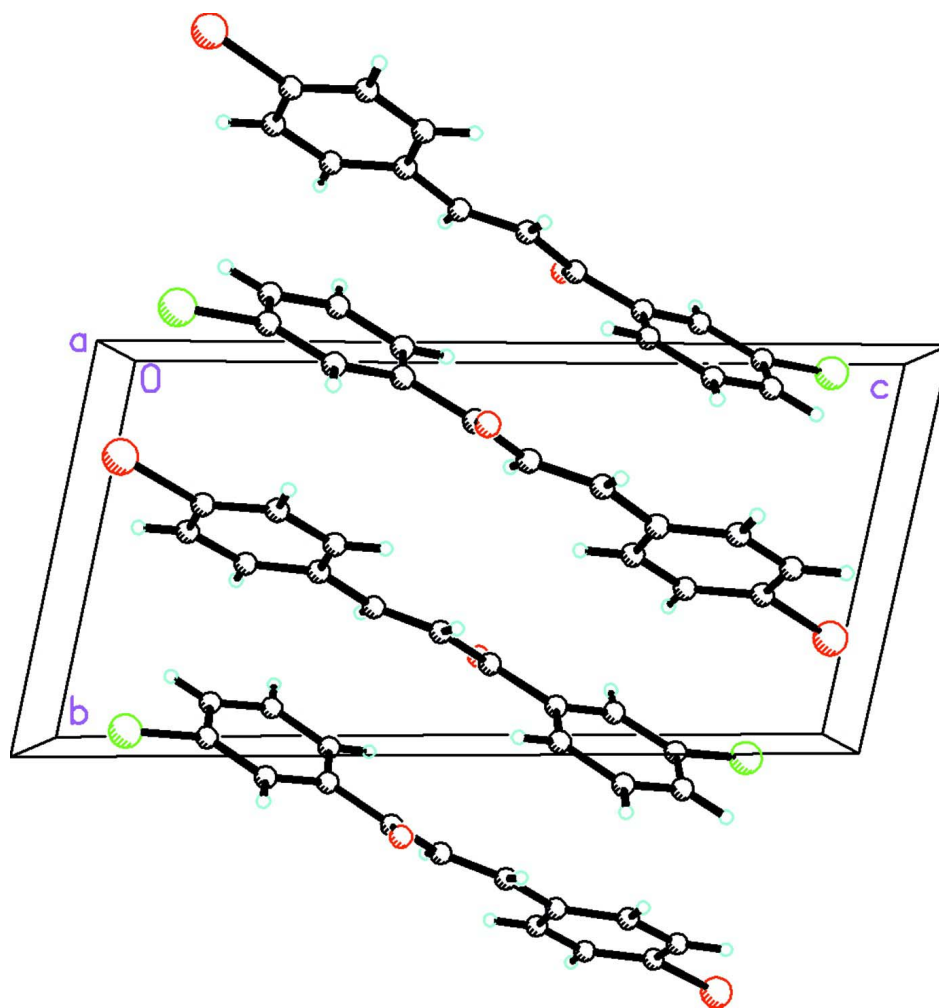
**S3. Refinement**

All of the H atoms were placed in calculated positions and then refined using the riding model with C—H = 0.95 Å, and with  $U_{iso}(H) = 1.17\text{--}1.21U_{eq}(C)$ .



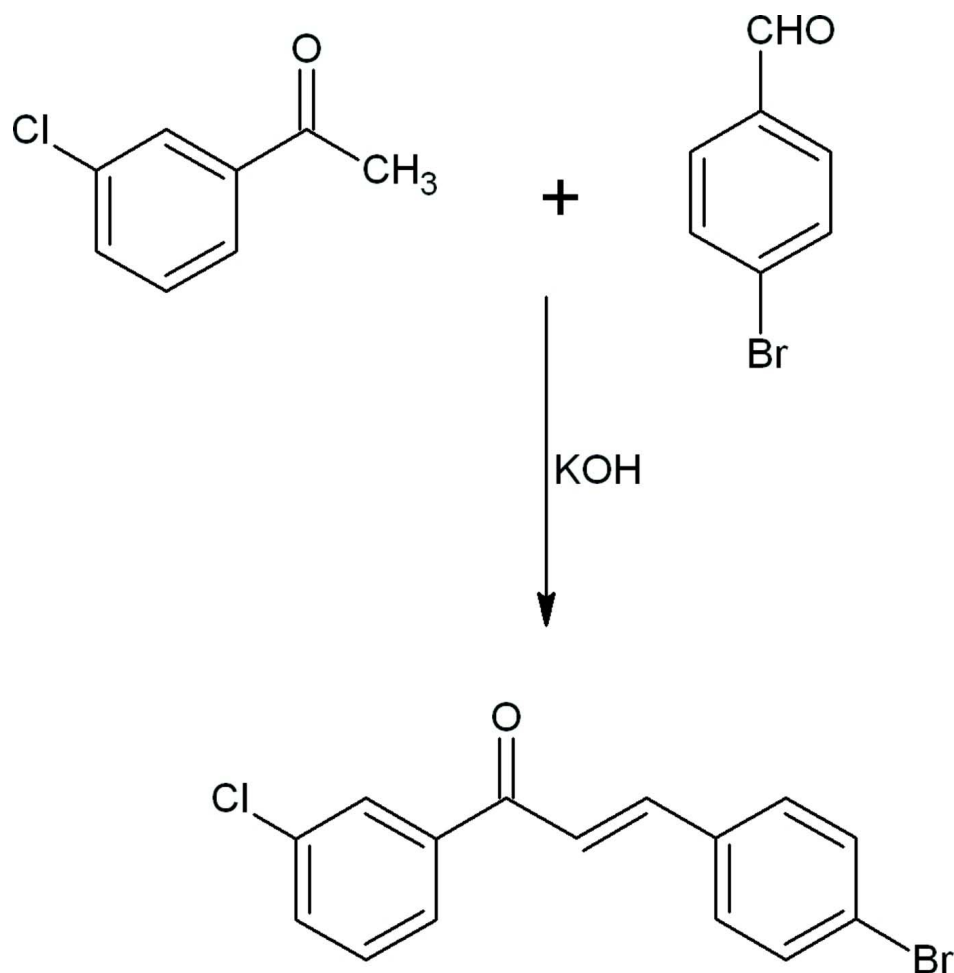
**Figure 1**

Molecular structure of the title compound,  $C_{15}H_{10}BrClO$ , showing the atom labeling scheme and 50% probability displacement ellipsoids.



**Figure 2**

Packing diagram of the title compound, (I), viewed down the *a* axis.

**Figure 3**

The formation of the title compound.

**(2E)-3-(4-Bromophenyl)-1-(3-chlorophenyl)prop-2-en-1-one**

*Crystal data*

$C_{15}H_{10}BrClO$

$M_r = 321.59$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 5.9197$  (8) Å

$b = 7.3391$  (11) Å

$c = 14.8171$  (17) Å

$\alpha = 101.929$  (11)°

$\beta = 94.371$  (10)°

$\gamma = 93.299$  (11)°

$V = 626.22$  (15) Å<sup>3</sup>

$Z = 2$

$F(000) = 320$

$D_x = 1.706$  Mg m<sup>-3</sup>

Cu  $K\alpha$  radiation,  $\lambda = 1.54178$  Å

Cell parameters from 3370 reflections

$\theta = 6.1$ – $73.9$ °

$\mu = 6.29$  mm<sup>-1</sup>

$T = 110$  K

Plate, colorless

$0.50 \times 0.21 \times 0.12$  mm

*Data collection*

Oxford Diffraction Xcalibur

diffractometer with a Ruby Gemini detector

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.5081 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: analytical

(*CrysAlis RED*; Oxford Diffraction, 2007)

$T_{\min} = 0.041$ ,  $T_{\max} = 0.344$   
 3868 measured reflections  
 2432 independent reflections  
 2312 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

$\theta_{\max} = 74.0^\circ$ ,  $\theta_{\min} = 6.1^\circ$   
 $h = -7 \rightarrow 6$   
 $k = -9 \rightarrow 8$   
 $l = -18 \rightarrow 18$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.164$   
 $S = 1.07$   
 2432 reflections  
 163 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  
 $w = 1/[\sigma^2(F_o^2) + (0.1305P)^2 + 0.5925P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.78 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -1.29 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1A	-0.10431 (6)	0.72017 (5)	0.94001 (2)	0.0266 (2)
Cl1A	0.58277 (16)	-0.04318 (14)	0.11075 (6)	0.0269 (3)
O1A	0.7080 (5)	0.2207 (4)	0.47588 (19)	0.0270 (6)
C12A	-0.0341 (6)	0.5947 (5)	0.7495 (3)	0.0205 (7)
H12A	-0.1777	0.6408	0.7378	0.025*
C1A	0.3919 (6)	0.1019 (5)	0.3683 (3)	0.0195 (7)
C2A	0.5227 (6)	0.0801 (5)	0.2923 (3)	0.0214 (7)
H2AA	0.6756	0.1315	0.2992	0.026*
C11A	0.0849 (6)	0.5125 (5)	0.6764 (3)	0.0215 (7)
H11A	0.0215	0.5019	0.6146	0.026*
C5A	0.0776 (6)	-0.0794 (5)	0.2713 (3)	0.0232 (8)
H5AA	-0.0727	-0.1364	0.2645	0.028*
C10A	0.2967 (6)	0.4452 (5)	0.6929 (3)	0.0207 (7)
C8A	0.3490 (7)	0.2931 (6)	0.5299 (3)	0.0245 (8)
H8AA	0.1944	0.3044	0.5110	0.029*
C14A	0.2701 (6)	0.5451 (5)	0.8595 (3)	0.0229 (7)
H14A	0.3318	0.5556	0.9216	0.027*
C3A	0.4245 (6)	-0.0180 (5)	0.2068 (3)	0.0200 (7)
C15A	0.3894 (6)	0.4648 (5)	0.7854 (2)	0.0210 (7)
H15A	0.5352	0.4227	0.7974	0.025*

C13A	0.0594 (7)	0.6090 (5)	0.8404 (2)	0.0200 (7)
C6A	0.1690 (6)	0.0229 (5)	0.3577 (3)	0.0214 (7)
H6AA	0.0799	0.0386	0.4091	0.026*
C7A	0.5018 (6)	0.2071 (5)	0.4605 (2)	0.0213 (7)
C9A	0.4280 (6)	0.3546 (5)	0.6187 (3)	0.0210 (7)
H9AA	0.5826	0.3381	0.6351	0.025*
C4A	0.2037 (6)	-0.0988 (5)	0.1951 (3)	0.0228 (7)
H4AA	0.1399	-0.1661	0.1360	0.027*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1A	0.0240 (3)	0.0339 (3)	0.0202 (3)	0.00673 (19)	0.00381 (18)	0.0001 (2)
C11A	0.0292 (5)	0.0316 (5)	0.0200 (5)	0.0051 (4)	0.0061 (3)	0.0036 (4)
O1A	0.0217 (13)	0.0343 (15)	0.0224 (14)	0.0029 (12)	0.0001 (10)	0.0010 (11)
C12A	0.0183 (16)	0.0213 (17)	0.0211 (17)	-0.0020 (13)	-0.0003 (13)	0.0044 (14)
C1A	0.0205 (17)	0.0196 (17)	0.0191 (17)	0.0030 (13)	0.0014 (13)	0.0057 (13)
C2A	0.0207 (17)	0.0211 (17)	0.0213 (17)	0.0032 (14)	-0.0002 (13)	0.0026 (14)
C11A	0.0230 (17)	0.0209 (17)	0.0195 (17)	-0.0015 (14)	-0.0015 (13)	0.0039 (13)
C5A	0.0174 (16)	0.0211 (17)	0.030 (2)	-0.0020 (13)	-0.0039 (14)	0.0061 (15)
C10A	0.0222 (18)	0.0199 (17)	0.0194 (17)	-0.0032 (14)	-0.0003 (14)	0.0050 (13)
C8A	0.0228 (18)	0.0278 (19)	0.0217 (18)	0.0016 (14)	0.0005 (14)	0.0033 (15)
C14A	0.0227 (18)	0.0233 (18)	0.0213 (17)	-0.0006 (14)	-0.0019 (14)	0.0036 (14)
C3A	0.0201 (17)	0.0211 (18)	0.0197 (17)	0.0058 (13)	0.0029 (13)	0.0047 (14)
C15A	0.0179 (16)	0.0258 (18)	0.0192 (17)	0.0022 (13)	0.0018 (13)	0.0045 (14)
C13A	0.0252 (18)	0.0181 (17)	0.0155 (17)	0.0027 (14)	0.0045 (14)	-0.0006 (13)
C6A	0.0208 (17)	0.0239 (18)	0.0208 (18)	0.0013 (14)	0.0034 (13)	0.0075 (14)
C7A	0.0239 (17)	0.0218 (17)	0.0187 (17)	0.0006 (14)	0.0017 (14)	0.0061 (14)
C9A	0.0203 (17)	0.0208 (17)	0.0218 (18)	-0.0003 (14)	0.0008 (14)	0.0055 (14)
C4A	0.0240 (18)	0.0218 (17)	0.0203 (17)	0.0035 (14)	-0.0043 (14)	0.0008 (14)

*Geometric parameters (Å, °)*

Br1A—C13A	1.896 (4)	C5A—H5AA	0.9500
C11A—C3A	1.747 (4)	C10A—C15A	1.413 (5)
O1A—C7A	1.219 (5)	C10A—C9A	1.463 (5)
C12A—C11A	1.388 (6)	C8A—C9A	1.339 (5)
C12A—C13A	1.398 (5)	C8A—C7A	1.487 (5)
C12A—H12A	0.9500	C8A—H8AA	0.9500
C1A—C6A	1.395 (5)	C14A—C13A	1.387 (5)
C1A—C2A	1.402 (5)	C14A—C15A	1.396 (5)
C1A—C7A	1.503 (5)	C14A—H14A	0.9500
C2A—C3A	1.387 (5)	C3A—C4A	1.387 (5)
C2A—H2AA	0.9500	C15A—H15A	0.9500
C11A—C10A	1.396 (5)	C6A—H6AA	0.9500
C11A—H11A	0.9500	C9A—H9AA	0.9500
C5A—C4A	1.388 (6)	C4A—H4AA	0.9500
C5A—C6A	1.395 (5)		

C11A—C12A—C13A	119.4 (3)	C15A—C14A—H14A	120.7
C11A—C12A—H12A	120.3	C2A—C3A—C4A	122.0 (3)
C13A—C12A—H12A	120.3	C2A—C3A—C11A	119.4 (3)
C6A—C1A—C2A	120.2 (3)	C4A—C3A—C11A	118.6 (3)
C6A—C1A—C7A	121.8 (3)	C14A—C15A—C10A	121.1 (3)
C2A—C1A—C7A	117.9 (3)	C14A—C15A—H15A	119.5
C3A—C2A—C1A	118.7 (3)	C10A—C15A—H15A	119.5
C3A—C2A—H2AA	120.7	C14A—C13A—C12A	121.5 (3)
C1A—C2A—H2AA	120.7	C14A—C13A—Br1A	119.2 (3)
C12A—C11A—C10A	120.8 (3)	C12A—C13A—Br1A	119.3 (3)
C12A—C11A—H11A	119.6	C1A—C6A—C5A	119.6 (3)
C10A—C11A—H11A	119.6	C1A—C6A—H6AA	120.2
C4A—C5A—C6A	120.7 (3)	C5A—C6A—H6AA	120.2
C4A—C5A—H5AA	119.6	O1A—C7A—C8A	122.6 (3)
C6A—C5A—H5AA	119.6	O1A—C7A—C1A	120.2 (3)
C11A—C10A—C15A	118.7 (4)	C8A—C7A—C1A	117.2 (3)
C11A—C10A—C9A	123.1 (3)	C8A—C9A—C10A	125.6 (4)
C15A—C10A—C9A	118.2 (3)	C8A—C9A—H9AA	117.2
C9A—C8A—C7A	120.4 (4)	C10A—C9A—H9AA	117.2
C9A—C8A—H8AA	119.8	C3A—C4A—C5A	118.8 (3)
C7A—C8A—H8AA	119.8	C3A—C4A—H4AA	120.6
C13A—C14A—C15A	118.5 (3)	C5A—C4A—H4AA	120.6
C13A—C14A—H14A	120.7		
C6A—C1A—C2A—C3A	1.2 (5)	C7A—C1A—C6A—C5A	-177.6 (3)
C7A—C1A—C2A—C3A	179.4 (3)	C4A—C5A—C6A—C1A	-1.9 (6)
C13A—C12A—C11A—C10A	-0.4 (6)	C9A—C8A—C7A—O1A	-14.5 (6)
C12A—C11A—C10A—C15A	-0.9 (6)	C9A—C8A—C7A—C1A	166.1 (4)
C12A—C11A—C10A—C9A	179.0 (3)	C6A—C1A—C7A—O1A	155.6 (4)
C1A—C2A—C3A—C4A	-1.7 (5)	C2A—C1A—C7A—O1A	-22.6 (5)
C1A—C2A—C3A—C11A	178.8 (3)	C6A—C1A—C7A—C8A	-25.0 (5)
C13A—C14A—C15A—C10A	-1.3 (6)	C2A—C1A—C7A—C8A	156.8 (3)
C11A—C10A—C15A—C14A	1.7 (6)	C7A—C8A—C9A—C10A	178.5 (3)
C9A—C10A—C15A—C14A	-178.1 (3)	C11A—C10A—C9A—C8A	-13.4 (6)
C15A—C14A—C13A—C12A	0.0 (6)	C15A—C10A—C9A—C8A	166.4 (4)
C15A—C14A—C13A—Br1A	-179.5 (3)	C2A—C3A—C4A—C5A	0.4 (5)
C11A—C12A—C13A—C14A	0.8 (6)	C11A—C3A—C4A—C5A	179.8 (3)
C11A—C12A—C13A—Br1A	-179.7 (3)	C6A—C5A—C4A—C3A	1.4 (6)
C2A—C1A—C6A—C5A	0.6 (5)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

Cg1 is the centroid of the C1A—C6A ring and Cg2 is the centroid of the C10A—C15A ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2A—H2AA $\cdots$ Cg2 <sup>i</sup>	0.95	2.97	3.588 (4)	124

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C5A—H5AA...Cg2 <sup>ii</sup>	0.95	2.84	3.463 (4)	124
C12A—H12A...Cg1 <sup>iii</sup>	0.95	2.83	3.527 (4)	131

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