



The structure of 9-(3-bromo-6-chloro-2-hydroxyphenyl)-10-(2-hydroxyethyl)-3,6-diphenyl-3,4,5,6,7,9-hexahydro-2*H*-acridine-1,8-dione

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In the structure of the title compound C₃₃H₂₉BrClNO₄, (I), the hexahydro-2*H*-acridine ring system has a hydroxyethyl substituent on the N atom and a 3-bromo-6-chloro-2-hydroxyphenyl substituent on the central C atom at the 9-position. An unusual feature of the molecule is that the substituents at the 3- and 5-positions of the outer cyclohexenone rings are phenyl rings rather than the more common dimethyl substituents. C atoms on both of the cyclohexenone rings are disordered over two sites. In the crystal structure, O—H···O, C—H···O and C—H···π(ring) hydrogen bonds combine with an Br—O and unusual C—Br···π(ring) halogen bonds to generate a three dimensional network with molecules stacked along the *a*-axis direction.

1. Chemical context

Acridine derivatives form an important class of heterocycles containing nitrogen with a broad range of pharmaceutical properties. These include compounds that are used as anti-inflammatory (Chen *et al.*, 2002), anti-cancer (Gamega *et al.*, 1999), anti-microbial (Kaya *et al.*, 2011), anti-tubercular (Aly & Abadi 2004; Tripathi *et al.*, 2006), anti-parasitic (Di Giorgio, *et al.*, 2005), anti-malarial (Kumar *et al.*, 2009; Tomar *et al.*, 2010), anti-viral (Gupta & Jaiswal, 2010; Tonelli *et al.*, 2011) and fungicidal agents (Srivastava & Nizamuddin, 2004). Furthermore, acridines are used as dyes, fluorescent materials for the visualization of biomolecules and in laser technologies (Niknam & Damya, 2009). In this context we report here the synthesis and crystal structure of the title acridine derivative.

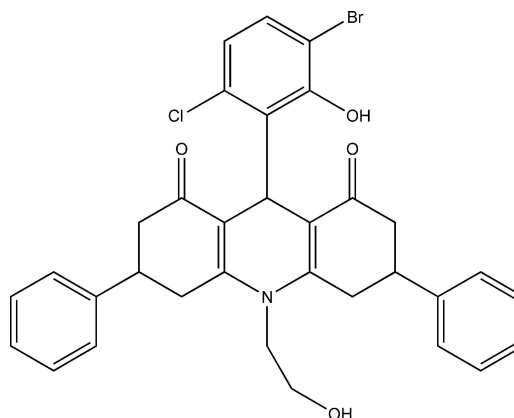
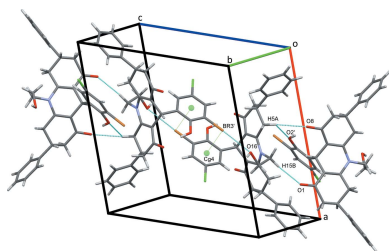


Table 1

Hydrogen-bond geometry (Å, °).

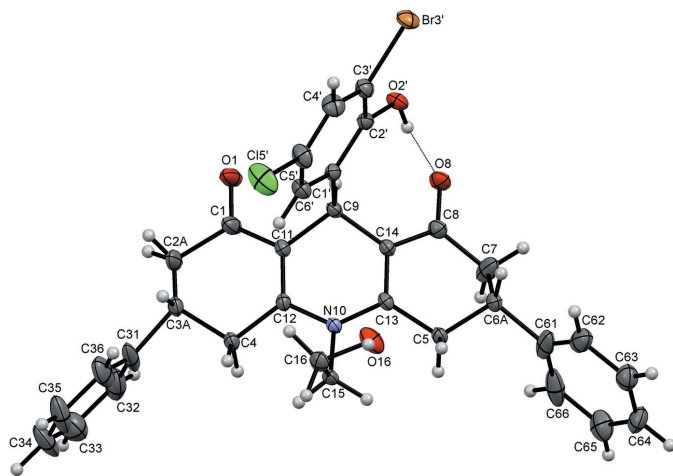
Cg7 and *Cg8* are the centroids of the C31–C36 and C61–C66 phenyl rings, respectively.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O2′—H2′ <i>O</i> ···O8	0.85 (3)	1.79 (3)	2.626 (2)	170 (3)
O16—H16 <i>O</i> ···O8 ⁱ	0.84 (4)	1.97 (4)	2.782 (2)	163 (4)
C15—H15 <i>A</i> ···O16 ⁱⁱ	0.99	2.68	3.622 (3)	159
C5—H5 <i>A</i> ···O8 ⁱⁱⁱ	0.99	2.69	3.669 (3)	172
C5—H5 <i>A</i> ···O2′ ⁱⁱⁱ	0.99	2.70	3.336 (3)	122
C15—H15 <i>B</i> ···O1 ⁱⁱⁱ	0.99	2.47	3.451 (3)	172
C34—H34···Cl5 ^{iv}	0.95	2.87	3.560 (3)	131
C16—H16 <i>B</i> ··· <i>Cg8</i> ⁱⁱ	0.99	2.66	3.529 (3)	147
C65—H65··· <i>Cg7</i> ^v	0.95	2.78	3.648 (4)	152

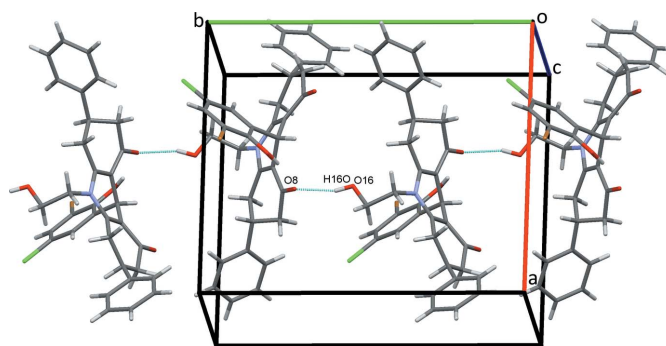
 Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z$; (iii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iv) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $x - 1, -y - \frac{1}{2}, z - \frac{1}{2}$.

2. Structural commentary

The title compound (I), consists of a hexahydro-2*H*-acridine ring system made up of a central dihydropyridine ring with an N-bound 2-hydroxyethyl substituent flanked by two cyclohexenone rings that carry phenyl substituents in the 3- and 5-positions, respectively (Fig. 1). The central C9 atom bears a 3-bromo-6-chloro-2-hydroxyphenyl substituent and the O2′ hydroxy group forms an intramolecular hydrogen bond to the adjacent O8 carbonyl oxygen enclosing an *S*(8) ring. The C2 and C3 atoms of one cyclohexenone are disordered over two sites as is the C6 atom of the corresponding cyclohexenone. Their occupancy ratios refine to 0.521 (10):0.479 (10) for C2,C3 and 0.746 (9):0.254 (9) for C6. Only details of the major disorder components will be considered here. The central C9,N10,C11–C14 ring adopts a half-chair conformation and is inclined to the adjacent C1–C4,C11,C12 and C5–C8,C13,C14 rings at angles of 7.11 (18) and 21.64 (10)°, respectively, so the hexahydro-2*H*-acridine unit is far from planar. The 3-bromo-6-chloro-2-hydroxyphenyl ring subtends an angle of 84.39 (6)°


Figure 1

The structure of (I) with ellipsoids drawn at the 50% probability level. For clarity only the major disorder components of the two cyclohexenone rings are shown. An intramolecular hydrogen bond is drawn as a dashed line.

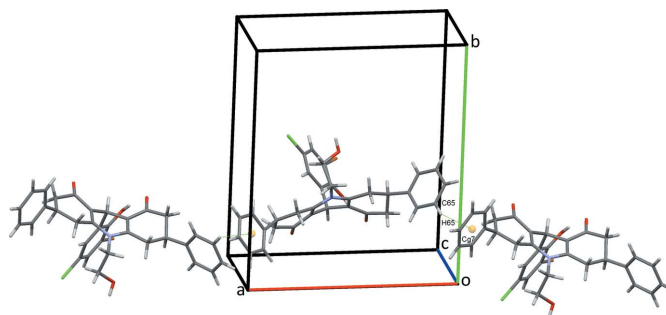

Figure 2

C(9) chains of molecules of (I) along *b*. In this and subsequent figures, hydrogen bonds are drawn as dashed lines.

to this central ring. The C1–C4,C11,C12 ring is best described as a severely flattened boat while the C5–C8,C13,C14 system is in a distorted half-chair conformation. The phenyl substituents on these outer cyclohexenone rings are inclined to their parent rings at angles of 76.87 (12)° for C31–C36 and 86.27 (8)° for C61–C66. The N-bound 2-hydroxyethyl substituent points away from the convex face of the hexahydro-2*H*-acridine system as does the 3-bromo-6-chloro-2-hydroxyphenyl substituent.

3. Supramolecular features

The crystal structure of (I) is supported by a full range of classical and non-classical hydrogen bonds and C—H··· π (ring) contacts, together with an intermolecular O···Br halogen bond and an unusual C—Br··· π (ring) contact. Classical O16—H16*O*···O8 hydrogen bonds, Table 1, form *C*(9) chains along the *b*-axis direction, linking the molecules in a head-to-tail fashion, Fig. 2. Chains also form along the *a*-axis direction through C65—H65···*Cg7* contacts, Fig. 3, Table 1. C15—H15*A*···O16 hydrogen bonds form inversion dimers that enclose $R_2^2(8)$ rings and are strengthened by C16—H16···*Cg8* interactions. Adjacent dimers are linked by C34—H34···Cl5′ hydrogen bonds, forming double chains of molecules along the *ab* diagonal, Fig. 4. The extensive series of contacts is completed with inversion dimers that also form


Figure 3

Chains of molecules of (I) along *a*. C—H··· π contacts are shown as dotted green lines with ring centroids shown as coloured spheres.

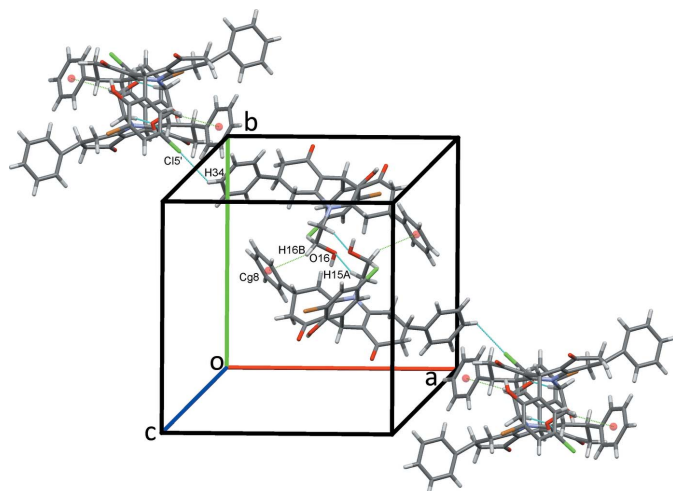


Figure 4
Double chains of molecules of (I) along the *ab* diagonal.

through $O16 \cdots Br3^v$ halogen bonds [$O \cdots Br = 3.0308$ (18) Å; symmetry code: (v) $1 - x, 1 - y, 1 - z$] (Cavallo *et al.*, 2016; Chifotides & Dunbar, 2013) and are supported by unusual $C3' - Br3^v \cdots Cg4^v$ contacts [$Br3^v \cdots Cg4 = 3.6991$ (10) Å, $C3' - Br3^v \cdots Cg4 = 83.89$ (7)°; $Cg4$ is the centroid of the $C1' - C6'$ benzene ring] (Matter *et al.*, 2009; Shukla *et al.*, 2017; Andleeb *et al.*, 2018). Both of these contacts are significantly shorter than the sum of the Br and O radii, 3.42 Å (Bondi, 1964) and that of the Br radius and an estimated half thickness of the benzene ring, 3.75 Å. The dimers are linked into chains running along the *ac* diagonal by a series of $C - H \cdots O$ hydrogen bonds generating $R_1^2(8)$ and $R_2^2(13)$ rings, with C5 acting as a bifurcated donor, Table 1, Fig. 5. Overall this plethora of intermolecular contacts combine to generate a complex three-dimensional network with molecules stacked along the *a*-axis direction, Fig. 6.

4. Database survey

A search of the Cambridge Structural Database (Version 5.39 Nov 2017 with three updates; Groom *et al.* 2016) for an acridine

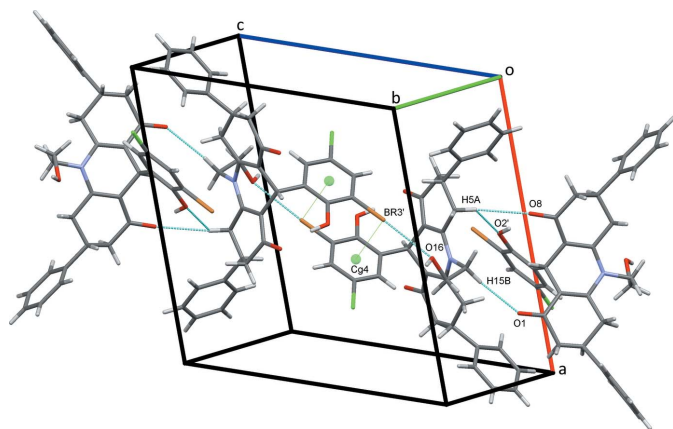


Figure 5
Chains of molecule of (I) formed by $C - H \cdots O$ hydrogen bonds, $C - Br \cdots \pi$ and $O \cdots Br$ contacts, dotted green lines.

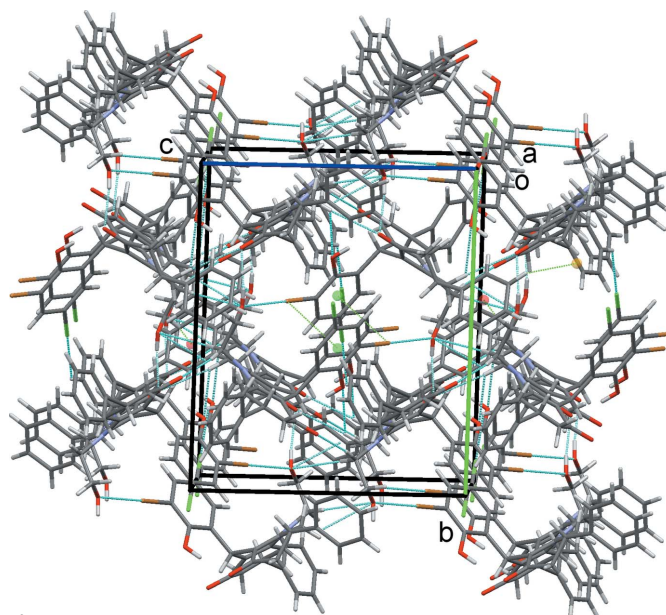


Figure 6
Overall packing of (I) viewed along the *a*-axis direction.

dine ring system with a phenyl or substituted benzene ring on the central C9 atom gave 94 hits, 76 of which represented unique occurrences. The majority of these, 58, have two methyl substituents at the 3- and 5-positions of the ring system. However, three instances reveal a pair of methyl substituents on the 3-position only, with the remaining 15 structures having no additional substitution on either of the cyclohexenone rings. Interestingly, no structures were observed with phenyl substituents at the 3- or the 3- and 5-positions of the hexahydro-2*H*-acridine ring system, emphasizing the uniqueness of the structure reported here. Refining the search to structures with CH_2CH substitution on the acridine N atom reduced the hits to seven, four of which have hydroxyethyl substituents on N10 (Mohamed *et al.*, 2013; Abdelhamid *et al.*, 2016, 2014, 2011). Only one of the entries has a 2-hydroxypropyl N10 substituent (Khalilov *et al.*, 2011), with pairs of methyl substituents on the 3- and 5-positions.

5. Synthesis and crystallization

The title compound was synthesized according to our previously reported method (Mohamed *et al.*, 2013). Crystals suitable for X-ray diffraction were obtained by the slow evaporation method using ethanol/acetone (5:1) as the solvent mixture. Yield, 79%; m.p. 451 K.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were refined using a riding model with $d(C - H) = 0.95$ Å for aromatic, 0.99 Å for methylene and 1.00 Å for methine H atoms, all with $U_{iso} = 1.2U_{eq}(C)$. The C2 and C3 atoms in the C1–C4, C11, C12 cyclohexenone ring and atom, C6, in the corresponding C5–C8, C13, C14 ring are disordered over two positions. Their

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₃₃ H ₂₉ BrClNO ₄
<i>M_r</i>	618.93
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.5669 (2), 15.4643 (2), 13.4979 (2)
β (°)	107.280 (1)
<i>V</i> (Å ³)	2903.39 (7)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	3.09
Crystal size (mm)	0.37 × 0.14 × 0.12
Data collection	
Diffraction	Agilent SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2014)
<i>T_{min}</i> , <i>T_{max}</i>	0.618, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	23967, 6076, 5714
<i>R_{int}</i>	0.045
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.631
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.040, 0.101, 1.07
No. of reflections	6076
No. of parameters	402
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.66, -0.57

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *TITAN* (Hunter & Simpson, 1999), *Mercury* (Macrae *et al.*, 2008), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009), *publCIF* (Westrip 2010) and *WinGX* (Farrugia 2012).

occupancies were refined to sum to unity with the disordered atoms of the different rings allowed to refine separately. The occupancies converged to ratios of 0.521 (10): 0.479 (10) for C2 and C3 and 0.746 (9): 0.254 (9) for C6. Positions of the hydrogen atoms on adjacent methylene groups and phenyl rings were assigned taking this disorder into account but a somewhat close H15A...H5C contact was still observed. One reflection with $F_o \gg F_c$, was omitted from the final refinement cycles.

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References

- Abdelhamid, A. A., Mohamed, S. K., Khalilov, A. N., Gurbanov, A. V. & Ng, S. W. (2011). *Acta Cryst.* **E67**, o744.
Abdelhamid, A. A., Mohamed, S. K. & Simpson, J. (2014). *Acta Cryst.* **E70**, 44–47.

- Abdelhamid, A. A., Mohamed, S. K. & Simpson, J. (2016). *IUCrData*, **1**, x152425.
Agilent (2014). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
Aly, E. I. & Abadi, A. H. (2004). *Arch. Pharm. Res.* **27**, 713–719.
Andleeb, H., Khan, I., Bauzá, A., Tahir, M. N., Simpson, J., Hameed, S. & Frontera, A. (2018). *Acta Cryst.* **C74**, 816–829.
Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
Cavallo, G., Metrangolo, P., Milani, R., Pilati, T., Priimagi, A., Resnati, G. & Terraneo, G. (2016). *Chem. Rev.* **116**, 2478–2601.
Chen, Y. L., Lu, C. M., Chen, I. L., Tsao, L. T. & Wang, J. P. (2002). *J. Med. Chem.* **45**, 4689–4694.
Chifotides, H. T. & Dunbar, K. R. (2013). *Acc. Chem. Res.* **46**, 894–906.
Di Giorgio, C., De Meo, M., Chiron, J., Delmas, F., Nikoyan, A., Jean, S., Dumenil, G., Timon-David, P. & Galy, J. P. (2005). *Bioorg. Med. Chem.* **13**, 5560–5568.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gamage, S. A., Spicer, J. A., Atwell, G. J., Finlay, G. J., Baguley, B. C. & Denny, W. A. (1999). *J. Med. Chem.* **42**, 2383–2393.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
Gupta, H. C. & Jaiswal, V. (2010). *Indian J. Heterocycl. Chem.* **19**, 409–410.
Hunter, K. A. & Simpson, J. (1999). *TITAN2000*. University of Otago, New Zealand.
Kaya, M., Yildırım, Y. & Çelik, G. Y. (2011). *Med. Chem. Res.* **20**, 293–299.
Khalilov, A. N., Abdelhamid, A. A., Gurbanov, A. V. & Ng, S. W. (2011). *Acta Cryst.* **E67**, o1146.
Kumar, A., Srivastava, K., Kumar, S. R., Puri, S. K. & Chauhan, M. S. (2009). *Bioorg. Med. Chem. Lett.* **19**, 6996–6999.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Matter, H., Nazaré, M., Güssregen, S., Will, D. W., Schreuder, H., Bauer, A., Urmann, M., Ritter, K., Wagner, M. & Wehner, V. (2009). *Angew. Chem. Int. Ed.* **48**, 2911–2916.
Mohamed, S. K., Akkurt, M., Horton, P. N., Abdelhamid, A. A. & Remaily, M. A. A. E. (2013). *Acta Cryst.* **E69**, o85–o86.
Niknam, K. & Damya, M. (2009). *Int. Chin. Chem. Soc.* **56**, 659–665.
Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
Shukla, R., Khan, I., Ibrar, A., Simpson, J. & Chopra, D. (2017). *CrystEngComm*, **19**, 3485–3498.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
Srivastava, A. & Nizamuddin, A. (2004). *Indian J. Heterocycl. Chem.* **13**, 261–264.
Tomar, V., Bhattacharjee, G., Kamaluddin, S. R., Rajakumar, S., Srivastava, K. & Puri, S. K. (2010). *Eur. J. Med. Chem.* **45**, 745–751.
Tonelli, M., Vettoretti, G., Tasso, B., Novelli, F., Boido, V., Sparatore, F., Busonera, B., Ouhtit, A., Farci, P., Blois, S., Giliberti, G. & La Colla, P. (2011). *Antiviral Res.* **91**, 133–141.
Tripathi, R. P., Verma, S. S., Pandey, J., Agarwal, K. C., Chaturvedi, V., Manju, Y. K., Srivastava, A. K., Gaikwad, A. & Sinha, S. (2006). *Bioorg. Med. Chem. Lett.* **16**, 5144–5147.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b) and TITAN (Hunter & Simpson, 1999); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015b), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009), *publCIF* (Westrip 2010) and *WinGX* (Farrugia 2012).

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Crystal data

C₃₃H₂₉BrClNO₄
M_r = 618.93
 Monoclinic, *P*2₁/*c*
a = 14.5669 (2) Å
b = 15.4643 (2) Å
c = 13.4979 (2) Å
 β = 107.280 (1)°
V = 2903.39 (7) Å³
Z = 4

F(000) = 1272
D_x = 1.416 Mg m⁻³
 Cu *K*α radiation, λ = 1.54184 Å
 Cell parameters from 16242 reflections
 θ = 4.2–76.6°
 μ = 3.09 mm⁻¹
T = 100 K
 Rectangular plate, pale yellow
 0.37 × 0.14 × 0.12 mm

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
 Radiation source: SuperNova (Cu) X-ray Source
 Detector resolution: 5.1725 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.618, *T_{max}* = 1.000

23967 measured reflections
 6076 independent reflections
 5714 reflections with *I* > 2σ(*I*)
R_{int} = 0.045
 θ_{\max} = 76.7°, θ_{\min} = 4.3°
h = -18→18
k = -19→14
l = -16→16

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.040
wR(*F*²) = 0.101

S = 1.07
 6076 reflections
 402 parameters
 0 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 3.2091P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.66 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.57 \text{ e } \text{\AA}^{-3}$

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.

Refinement. One reflection with $F_o \gg \gg F_c$ was omitted from the final refinement cycles.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.75525 (13)	0.16790 (13)	0.44418 (13)	0.0361 (4)	
C1	0.75604 (17)	0.20511 (17)	0.36498 (18)	0.0309 (5)	
C2A	0.8507 (4)	0.2118 (5)	0.3297 (4)	0.0302 (15)	0.521 (10)
H2A1	0.9018	0.2366	0.3886	0.036*	0.521 (10)
H2A2	0.8706	0.1521	0.3196	0.036*	0.521 (10)
C3A	0.8503 (3)	0.2523 (4)	0.2536 (4)	0.0197 (12)	0.521 (10)
H3A	0.8850	0.3059	0.2857	0.024*	0.521 (10)
C2B	0.8203 (4)	0.1718 (4)	0.3031 (5)	0.0198 (12)	0.479 (10)
H2B1	0.8869	0.1711	0.3503	0.024*	0.479 (10)
H2B2	0.8021	0.1109	0.2847	0.024*	0.479 (10)
C3B	0.8224 (4)	0.2130 (4)	0.2140 (5)	0.0240 (15)	0.479 (10)
H3B	0.7874	0.1693	0.1618	0.029*	0.479 (10)
C31	0.9137 (2)	0.2237 (2)	0.1795 (3)	0.0519 (9)	
C32	0.9205 (2)	0.1493 (2)	0.1268 (3)	0.0525 (9)	
H32	0.8802	0.1016	0.1290	0.063*	
C33	0.9860 (3)	0.1432 (2)	0.0700 (3)	0.0552 (8)	
H33	0.9902	0.0916	0.0334	0.066*	
C34	1.0447 (2)	0.2126 (2)	0.0674 (3)	0.0573 (9)	
H34	1.0896	0.2086	0.0289	0.069*	
C35	1.0389 (2)	0.2863 (2)	0.1194 (3)	0.0546 (9)	
H35	1.0792	0.3341	0.1170	0.065*	
C36	0.9734 (2)	0.2917 (2)	0.1762 (3)	0.0499 (8)	
H36A	0.9700	0.3432	0.2132	0.060*	0.521 (10)
H36B	0.9700	0.3432	0.2132	0.060*	0.479 (10)
C4	0.75926 (14)	0.29215 (14)	0.17397 (16)	0.0201 (4)	
H4A	0.7760	0.3489	0.1500	0.024*	0.521 (10)
H4B	0.7374	0.2537	0.1128	0.024*	0.521 (10)
H4C	0.8002	0.3445	0.1879	0.024*	0.479 (10)
H4D	0.7311	0.2870	0.0978	0.024*	0.479 (10)
C5	0.42495 (14)	0.37594 (13)	0.10511 (15)	0.0178 (4)	
H5A	0.4165	0.3450	0.0388	0.021*	0.746 (9)
H5B	0.4335	0.4381	0.0929	0.021*	0.746 (9)
H5C	0.433 (7)	0.370 (7)	0.025 (8)	0.021*	0.254 (9)

H5D	0.422 (8)	0.437 (7)	0.117 (8)	0.021*	0.254 (9)
C6A	0.33431 (18)	0.3641 (2)	0.1396 (2)	0.0195 (9)	0.746 (9)
H6A	0.3356	0.4086	0.1938	0.023*	0.746 (9)
C6B	0.3349 (5)	0.3168 (5)	0.0936 (6)	0.015 (2)	0.254 (9)
H6B	0.3341	0.2706	0.0415	0.019*	0.254 (9)
C61	0.24605 (17)	0.3823 (2)	0.0451 (2)	0.0420 (7)	
C62	0.20200 (18)	0.4592 (2)	0.0484 (2)	0.0396 (6)	
H62	0.2246	0.4951	0.1078	0.047*	
C63	0.12511 (18)	0.48598 (19)	-0.0327 (2)	0.0359 (5)	
H63	0.0953	0.5399	-0.0281	0.043*	
C64	0.09078 (17)	0.43614 (17)	-0.1202 (2)	0.0347 (6)	
H64	0.0377	0.4554	-0.1757	0.042*	
C65	0.13441 (19)	0.35737 (19)	-0.1267 (2)	0.0406 (6)	
H65	0.1118	0.3221	-0.1866	0.049*	
C66	0.21263 (19)	0.33072 (19)	-0.0430 (3)	0.0483 (8)	
H66A	0.2430	0.2770	-0.0466	0.058*	0.746 (9)
H66	0.2430	0.2770	-0.0466	0.058*	0.254 (9)
C7	0.33159 (18)	0.2777 (2)	0.1859 (2)	0.0424 (7)	
H7A	0.3299	0.2323	0.1337	0.051*	0.746 (9)
H7B	0.2729	0.2722	0.2081	0.051*	0.746 (9)
H7C	0.3036	0.2195	0.1671	0.051*	0.254 (9)
H7D	0.2846	0.3109	0.2107	0.051*	0.254 (9)
C8	0.41893 (15)	0.26609 (14)	0.27755 (16)	0.0217 (4)	
O8	0.41215 (11)	0.22515 (11)	0.35542 (12)	0.0253 (3)	
C9	0.59971 (14)	0.28147 (13)	0.35948 (15)	0.0164 (4)	
H9	0.5898	0.2278	0.3964	0.020*	
C11	0.67923 (14)	0.26478 (13)	0.31174 (15)	0.0169 (4)	
C12	0.67918 (13)	0.30368 (13)	0.22213 (15)	0.0165 (4)	
C13	0.51346 (14)	0.34248 (12)	0.18453 (15)	0.0156 (4)	
C14	0.50871 (14)	0.29899 (12)	0.27191 (15)	0.0162 (4)	
N10	0.60071 (11)	0.35389 (11)	0.16665 (13)	0.0159 (3)	
C15	0.61313 (14)	0.41375 (14)	0.08619 (15)	0.0186 (4)	
H15A	0.5504	0.4225	0.0328	0.022*	
H15B	0.6580	0.3879	0.0519	0.022*	
C16	0.65185 (15)	0.49977 (14)	0.13240 (17)	0.0236 (4)	
H16A	0.7049	0.4910	0.1973	0.028*	
H16B	0.6770	0.5327	0.0832	0.028*	
O16	0.57556 (13)	0.54592 (12)	0.15339 (15)	0.0336 (4)	
H16O	0.592 (3)	0.598 (3)	0.156 (3)	0.050*	
C1'	0.62288 (14)	0.35601 (13)	0.43787 (15)	0.0168 (4)	
C2'	0.57556 (14)	0.36228 (13)	0.51490 (15)	0.0179 (4)	
O2'	0.51146 (11)	0.30269 (10)	0.52679 (12)	0.0222 (3)	
H2'O	0.485 (2)	0.274 (2)	0.472 (3)	0.033*	
C3'	0.59615 (15)	0.43193 (14)	0.58369 (17)	0.0223 (4)	
Br3'	0.53322 (2)	0.44056 (2)	0.68754 (2)	0.02632 (9)	
C4'	0.66042 (17)	0.49627 (15)	0.57727 (18)	0.0278 (5)	
H4'	0.6733	0.5436	0.6243	0.033*	
C5'	0.70526 (16)	0.48948 (15)	0.50025 (19)	0.0275 (5)	

C15'	0.78601 (5)	0.56959 (4)	0.48926 (6)	0.04541 (18)
C6'	0.68789 (15)	0.42062 (15)	0.43232 (17)	0.0227 (4)
H6'	0.7206	0.4172	0.3811	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0387 (9)	0.0496 (11)	0.0255 (8)	0.0246 (8)	0.0179 (7)	0.0171 (8)
C1	0.0314 (12)	0.0418 (14)	0.0240 (11)	0.0176 (10)	0.0152 (9)	0.0099 (10)
C2A	0.023 (2)	0.042 (4)	0.029 (3)	0.017 (3)	0.012 (2)	0.013 (3)
C3A	0.0135 (19)	0.023 (3)	0.024 (2)	0.0011 (18)	0.0071 (17)	0.003 (2)
C2B	0.016 (2)	0.017 (3)	0.030 (3)	0.006 (2)	0.012 (2)	0.007 (2)
C3B	0.018 (2)	0.030 (3)	0.027 (3)	0.006 (2)	0.010 (2)	0.003 (2)
C31	0.0293 (13)	0.075 (2)	0.0634 (19)	0.0323 (14)	0.0320 (13)	0.0481 (17)
C32	0.0248 (12)	0.069 (2)	0.065 (2)	0.0031 (13)	0.0155 (13)	0.0302 (17)
C33	0.0555 (19)	0.060 (2)	0.059 (2)	0.0050 (16)	0.0308 (16)	0.0077 (16)
C34	0.0530 (18)	0.061 (2)	0.080 (2)	0.0205 (16)	0.0544 (18)	0.0245 (18)
C35	0.0339 (14)	0.0482 (17)	0.095 (3)	0.0124 (13)	0.0398 (16)	0.0261 (17)
C36	0.0411 (15)	0.0537 (18)	0.065 (2)	0.0271 (14)	0.0314 (15)	0.0204 (15)
C4	0.0152 (9)	0.0253 (10)	0.0218 (9)	0.0037 (8)	0.0087 (7)	0.0042 (8)
C5	0.0143 (8)	0.0203 (10)	0.0206 (9)	0.0000 (7)	0.0080 (7)	0.0028 (8)
C6A	0.0144 (12)	0.0235 (17)	0.0212 (15)	-0.0021 (10)	0.0062 (10)	0.0004 (13)
C6B	0.012 (3)	0.018 (5)	0.014 (4)	-0.007 (3)	0.000 (3)	-0.003 (3)
C61	0.0148 (10)	0.0588 (18)	0.0492 (16)	-0.0086 (11)	0.0047 (10)	0.0285 (14)
C62	0.0242 (11)	0.0598 (18)	0.0315 (13)	-0.0115 (12)	0.0034 (10)	0.0088 (12)
C63	0.0263 (11)	0.0403 (14)	0.0400 (14)	-0.0004 (10)	0.0083 (10)	0.0025 (11)
C64	0.0193 (10)	0.0414 (14)	0.0371 (13)	-0.0018 (10)	-0.0013 (9)	0.0055 (11)
C65	0.0288 (12)	0.0386 (14)	0.0549 (17)	-0.0125 (11)	0.0134 (12)	-0.0066 (12)
C66	0.0269 (12)	0.0332 (14)	0.093 (2)	0.0073 (11)	0.0301 (15)	0.0277 (15)
C7	0.0212 (11)	0.0646 (19)	0.0358 (13)	-0.0164 (12)	-0.0001 (10)	0.0226 (13)
C8	0.0201 (9)	0.0249 (10)	0.0208 (10)	-0.0044 (8)	0.0074 (8)	0.0022 (8)
O8	0.0240 (7)	0.0309 (8)	0.0232 (7)	-0.0077 (6)	0.0103 (6)	0.0049 (6)
C9	0.0170 (9)	0.0177 (9)	0.0170 (9)	0.0011 (7)	0.0088 (7)	0.0015 (7)
C11	0.0151 (8)	0.0192 (9)	0.0174 (9)	0.0023 (7)	0.0065 (7)	-0.0006 (7)
C12	0.0130 (8)	0.0186 (9)	0.0187 (9)	0.0015 (7)	0.0058 (7)	0.0004 (7)
C13	0.0154 (8)	0.0148 (9)	0.0185 (9)	-0.0001 (7)	0.0081 (7)	-0.0020 (7)
C14	0.0155 (8)	0.0170 (9)	0.0179 (9)	0.0007 (7)	0.0077 (7)	0.0004 (7)
N10	0.0138 (7)	0.0189 (8)	0.0168 (8)	0.0013 (6)	0.0073 (6)	0.0028 (6)
C15	0.0157 (8)	0.0253 (10)	0.0171 (9)	0.0025 (8)	0.0086 (7)	0.0050 (8)
C16	0.0208 (9)	0.0250 (10)	0.0267 (10)	-0.0020 (8)	0.0095 (8)	0.0062 (8)
O16	0.0374 (9)	0.0255 (8)	0.0458 (10)	-0.0031 (7)	0.0247 (8)	-0.0060 (8)
C1'	0.0166 (8)	0.0179 (9)	0.0164 (9)	0.0027 (7)	0.0057 (7)	0.0008 (7)
C2'	0.0176 (9)	0.0191 (9)	0.0178 (9)	0.0036 (7)	0.0067 (7)	0.0025 (7)
O2'	0.0257 (7)	0.0235 (7)	0.0217 (7)	-0.0039 (6)	0.0135 (6)	-0.0014 (6)
C3'	0.0227 (10)	0.0237 (10)	0.0224 (10)	0.0037 (8)	0.0096 (8)	0.0000 (8)
Br3'	0.03193 (14)	0.02757 (14)	0.02364 (13)	0.00358 (9)	0.01467 (9)	-0.00484 (8)
C4'	0.0295 (11)	0.0245 (11)	0.0296 (11)	-0.0018 (9)	0.0093 (9)	-0.0075 (9)
C5'	0.0247 (10)	0.0250 (11)	0.0354 (12)	-0.0065 (9)	0.0131 (9)	-0.0031 (9)

C15'	0.0475 (4)	0.0350 (3)	0.0624 (4)	-0.0218 (3)	0.0296 (3)	-0.0141 (3)
C6'	0.0211 (9)	0.0255 (10)	0.0245 (10)	-0.0003 (8)	0.0110 (8)	-0.0004 (8)

Geometric parameters (Å, °)

O1—C1	1.217 (3)	C61—C66	1.394 (5)
C1—C11	1.464 (3)	C62—C63	1.377 (4)
C1—C2B	1.518 (5)	C62—H62	0.9500
C1—C2A	1.590 (6)	C63—C64	1.374 (4)
C2A—C3A	1.202 (7)	C63—H63	0.9500
C2A—H2A1	0.9900	C64—C65	1.389 (4)
C2A—H2A2	0.9900	C64—H64	0.9500
C3A—C4	1.564 (5)	C65—C66	1.407 (4)
C3A—C31	1.612 (5)	C65—H65	0.9500
C3A—H3A	1.0000	C66—H66A	0.9500
C2B—C3B	1.369 (7)	C66—H66	0.9500
C2B—H2B1	0.9900	C7—C8	1.499 (3)
C2B—H2B2	0.9900	C7—H7A	0.9900
C3B—C4	1.531 (5)	C7—H7B	0.9900
C3B—C31	1.543 (5)	C7—H7C	0.9900
C3B—H3B	1.0000	C7—H7D	0.9900
C31—C32	1.372 (6)	C8—O8	1.256 (3)
C31—C36	1.373 (5)	C8—C14	1.426 (3)
C32—C33	1.393 (4)	C9—C11	1.506 (2)
C32—H32	0.9500	C9—C14	1.516 (3)
C33—C34	1.379 (5)	C9—C1'	1.533 (3)
C33—H33	0.9500	C9—H9	1.0000
C34—C35	1.355 (5)	C11—C12	1.351 (3)
C34—H34	0.9500	C12—N10	1.401 (2)
C35—C36	1.393 (4)	C13—N10	1.374 (2)
C35—H35	0.9500	C13—C14	1.377 (3)
C36—H36A	0.9500	N10—C15	1.478 (2)
C36—H36B	0.9500	C15—C16	1.506 (3)
C4—C12	1.505 (3)	C15—H15A	0.9900
C4—H4A	0.9900	C15—H15B	0.9900
C4—H4B	0.9900	C16—O16	1.418 (3)
C4—H4C	0.9900	C16—H16A	0.9900
C4—H4D	0.9900	C16—H16B	0.9900
C5—C13	1.503 (3)	O16—Br3 ^{ti}	3.0308 (18)
C5—C6A	1.536 (3)	O16—H16O	0.84 (4)
C5—C6B	1.568 (7)	C1'—C6'	1.394 (3)
C5—H5A	0.9900	C1'—C2'	1.411 (3)
C5—H5B	0.9900	C2'—O2'	1.355 (3)
C5—H5C	1.12 (11)	C2'—C3'	1.395 (3)
C5—H5D	0.96 (10)	O2'—H2'O	0.85 (3)
C6A—C7	1.481 (4)	C3'—C4'	1.386 (3)
C6A—C61	1.544 (3)	C3'—Br3'	1.894 (2)
C6A—H6A	1.0000	C4'—C5'	1.386 (3)

C6B—C7	1.398 (8)	C4'—H4'	0.9500
C6B—C61	1.620 (8)	C5'—C6'	1.379 (3)
C6B—H6B	1.0000	C5'—C15'	1.745 (2)
C61—C62	1.358 (5)	C6'—H6'	0.9500
O1—C1—C11	121.6 (2)	C62—C61—C6B	149.5 (4)
O1—C1—C2B	119.4 (3)	C66—C61—C6B	91.3 (4)
C11—C1—C2B	116.8 (2)	C61—C62—C63	121.2 (3)
O1—C1—C2A	122.0 (2)	C61—C62—H62	119.4
C11—C1—C2A	114.6 (3)	C63—C62—H62	119.4
C3A—C2A—C1	120.4 (4)	C64—C63—C62	121.1 (3)
C3A—C2A—H2A1	107.2	C64—C63—H63	119.4
C1—C2A—H2A1	107.2	C62—C63—H63	119.4
C3A—C2A—H2A2	107.2	C63—C64—C65	119.3 (2)
C1—C2A—H2A2	107.2	C63—C64—H64	120.3
H2A1—C2A—H2A2	106.9	C65—C64—H64	120.3
C2A—C3A—C4	125.5 (4)	C64—C65—C66	118.9 (3)
C2A—C3A—C31	122.0 (4)	C64—C65—H65	120.6
C4—C3A—C31	101.9 (3)	C66—C65—H65	120.6
C2A—C3A—H3A	100.8	C61—C66—C65	120.8 (3)
C4—C3A—H3A	100.8	C61—C66—H66A	119.6
C31—C3A—H3A	100.8	C65—C66—H66A	119.6
C3B—C2B—C1	120.3 (4)	C61—C66—H66	119.6
C3B—C2B—H2B1	107.3	C65—C66—H66	119.6
C1—C2B—H2B1	107.3	C6B—C7—C8	122.8 (3)
C3B—C2B—H2B2	107.3	C6A—C7—C8	109.5 (2)
C1—C2B—H2B2	107.3	C6A—C7—H7A	109.8
H2B1—C2B—H2B2	106.9	C8—C7—H7A	109.8
C2B—C3B—C4	120.9 (4)	C6A—C7—H7B	109.8
C2B—C3B—C31	124.2 (4)	C8—C7—H7B	109.8
C4—C3B—C31	106.8 (3)	H7A—C7—H7B	108.2
C2B—C3B—H3B	99.5	C6B—C7—H7C	106.6
C4—C3B—H3B	99.5	C8—C7—H7C	106.6
C31—C3B—H3B	99.5	C6B—C7—H7D	106.6
C32—C31—C36	118.7 (3)	C8—C7—H7D	106.6
C32—C31—C3B	105.5 (4)	H7C—C7—H7D	106.6
C36—C31—C3B	134.7 (4)	O8—C8—C14	121.73 (19)
C32—C31—C3A	134.0 (3)	O8—C8—C7	119.51 (19)
C36—C31—C3A	107.2 (4)	C14—C8—C7	118.70 (19)
C31—C32—C33	120.6 (3)	C11—C9—C14	107.62 (15)
C31—C32—H32	119.7	C11—C9—C1'	112.62 (16)
C33—C32—H32	119.7	C14—C9—C1'	111.48 (16)
C34—C33—C32	119.4 (3)	C11—C9—H9	108.3
C34—C33—H33	120.3	C14—C9—H9	108.3
C32—C33—H33	120.3	C1'—C9—H9	108.3
C35—C34—C33	120.5 (3)	C12—C11—C1	121.16 (18)
C35—C34—H34	119.7	C12—C11—C9	120.74 (17)
C33—C34—H34	119.7	C1—C11—C9	118.10 (17)

C34—C35—C36	119.6 (3)	C11—C12—N10	120.59 (17)
C34—C35—H35	120.2	C11—C12—C4	122.66 (18)
C36—C35—H35	120.2	N10—C12—C4	116.67 (17)
C31—C36—C35	121.1 (3)	N10—C13—C14	119.85 (18)
C31—C36—H36A	119.5	N10—C13—C5	118.23 (17)
C35—C36—H36A	119.5	C14—C13—C5	121.89 (17)
C31—C36—H36B	119.5	C13—C14—C8	120.01 (18)
C35—C36—H36B	119.5	C13—C14—C9	120.03 (17)
C12—C4—C3B	113.8 (2)	C8—C14—C9	119.87 (17)
C12—C4—C3A	111.0 (2)	C13—N10—C12	119.05 (16)
C12—C4—H4A	109.4	C13—N10—C15	122.07 (16)
C3A—C4—H4A	109.4	C12—N10—C15	118.77 (15)
C12—C4—H4B	109.4	N10—C15—C16	111.18 (16)
C3A—C4—H4B	109.4	N10—C15—H15A	109.4
H4A—C4—H4B	108.0	C16—C15—H15A	109.4
C12—C4—H4C	108.8	N10—C15—H15B	109.4
C3B—C4—H4C	108.8	C16—C15—H15B	109.4
C12—C4—H4D	108.8	H15A—C15—H15B	108.0
C3B—C4—H4D	108.8	O16—C16—C15	107.94 (17)
H4C—C4—H4D	107.7	O16—C16—H16A	110.1
C13—C5—C6A	112.05 (17)	C15—C16—H16A	110.1
C13—C5—C6B	112.7 (3)	O16—C16—H16B	110.1
C13—C5—H5A	109.2	C15—C16—H16B	110.1
C6A—C5—H5A	109.2	H16A—C16—H16B	108.4
C13—C5—H5B	109.2	C16—O16—Br3 ⁱ	141.43 (14)
C6A—C5—H5B	109.2	C16—O16—H16O	105 (3)
H5A—C5—H5B	107.9	Br3 ⁱ —O16—H16O	96 (3)
C13—C5—H5C	110 (5)	C6'—C1'—C2'	118.60 (19)
C6B—C5—H5C	100 (5)	C6'—C1'—C9	121.04 (18)
C13—C5—H5D	107 (6)	C2'—C1'—C9	120.31 (17)
C6B—C5—H5D	120 (6)	O2'—C2'—C3'	117.75 (18)
H5C—C5—H5D	106 (8)	O2'—C2'—C1'	123.03 (18)
C7—C6A—C5	111.7 (2)	C3'—C2'—C1'	119.20 (19)
C7—C6A—C61	113.1 (2)	C2'—O2'—H2'O	114 (2)
C5—C6A—C61	107.9 (2)	C4'—C3'—C2'	121.9 (2)
C7—C6A—H6A	108.0	C4'—C3'—Br3'	118.69 (16)
C5—C6A—H6A	108.0	C2'—C3'—Br3'	119.43 (16)
C61—C6A—H6A	108.0	C5'—C4'—C3'	118.0 (2)
C7—C6B—C5	114.4 (5)	C5'—C4'—H4'	121.0
C7—C6B—C61	113.3 (5)	C3'—C4'—H4'	121.0
C5—C6B—C61	102.7 (5)	C6'—C5'—C4'	121.5 (2)
C7—C6B—H6B	108.7	C6'—C5'—C15'	119.15 (18)
C5—C6B—H6B	108.7	C4'—C5'—C15'	119.32 (18)
C61—C6B—H6B	108.7	C5'—C6'—C1'	120.7 (2)
C62—C61—C66	118.7 (2)	C5'—C6'—H6'	119.6
C62—C61—C6A	114.7 (3)	C1'—C6'—H6'	119.6
C66—C61—C6A	126.5 (3)		

O1—C1—C2A—C3A	-176.6 (5)	O1—C1—C11—C9	1.9 (4)
C11—C1—C2A—C3A	-11.9 (8)	C2B—C1—C11—C9	164.9 (4)
C1—C2A—C3A—C4	-8.1 (10)	C2A—C1—C11—C9	-162.9 (4)
C1—C2A—C3A—C31	-146.2 (6)	C14—C9—C11—C12	31.2 (3)
O1—C1—C2B—C3B	-179.8 (5)	C1'—C9—C11—C12	-92.0 (2)
C11—C1—C2B—C3B	16.9 (7)	C14—C9—C11—C1	-148.5 (2)
C1—C2B—C3B—C4	-1.0 (9)	C1'—C9—C11—C1	88.2 (2)
C1—C2B—C3B—C31	143.5 (6)	C1—C11—C12—N10	173.7 (2)
C2B—C3B—C31—C32	85.6 (7)	C9—C11—C12—N10	-6.1 (3)
C4—C3B—C31—C32	-125.8 (4)	C1—C11—C12—C4	-3.0 (3)
C2B—C3B—C31—C36	-106.7 (6)	C9—C11—C12—C4	177.19 (18)
C4—C3B—C31—C36	41.9 (7)	C3B—C4—C12—C11	18.4 (4)
C2A—C3A—C31—C32	55.6 (8)	C3A—C4—C12—C11	-15.3 (4)
C4—C3A—C31—C32	-90.6 (4)	C3B—C4—C12—N10	-158.5 (4)
C2A—C3A—C31—C36	-121.9 (6)	C3A—C4—C12—N10	167.9 (3)
C4—C3A—C31—C36	91.9 (4)	C6A—C5—C13—N10	-176.0 (2)
C36—C31—C32—C33	-0.7 (5)	C6B—C5—C13—N10	145.0 (4)
C3B—C31—C32—C33	169.3 (3)	C6A—C5—C13—C14	6.0 (3)
C3A—C31—C32—C33	-178.0 (3)	C6B—C5—C13—C14	-33.0 (4)
C31—C32—C33—C34	0.3 (5)	N10—C13—C14—C8	-162.73 (19)
C32—C33—C34—C35	-0.1 (6)	C5—C13—C14—C8	15.3 (3)
C33—C34—C35—C36	0.3 (6)	N10—C13—C14—C9	13.7 (3)
C32—C31—C36—C35	0.9 (5)	C5—C13—C14—C9	-168.33 (17)
C3B—C31—C36—C35	-165.5 (4)	O8—C8—C14—C13	179.0 (2)
C3A—C31—C36—C35	178.9 (3)	C7—C8—C14—C13	1.7 (3)
C34—C35—C36—C31	-0.8 (5)	O8—C8—C14—C9	2.6 (3)
C2B—C3B—C4—C12	-15.9 (7)	C7—C8—C14—C9	-174.7 (2)
C31—C3B—C4—C12	-165.8 (3)	C11—C9—C14—C13	-35.1 (2)
C2A—C3A—C4—C12	21.5 (7)	C1'—C9—C14—C13	88.9 (2)
C31—C3A—C4—C12	166.1 (3)	C11—C9—C14—C8	141.31 (19)
C13—C5—C6A—C7	-43.4 (3)	C1'—C9—C14—C8	-94.7 (2)
C13—C5—C6A—C61	-168.4 (2)	C14—C13—N10—C12	15.8 (3)
C13—C5—C6B—C7	34.3 (7)	C5—C13—N10—C12	-162.27 (17)
C13—C5—C6B—C61	157.5 (3)	C14—C13—N10—C15	-167.96 (18)
C7—C6A—C61—C62	130.3 (3)	C5—C13—N10—C15	14.0 (3)
C5—C6A—C61—C62	-105.7 (3)	C11—C12—N10—C13	-20.0 (3)
C7—C6A—C61—C66	-53.9 (4)	C4—C12—N10—C13	156.96 (18)
C5—C6A—C61—C66	70.1 (3)	C11—C12—N10—C15	163.66 (19)
C7—C6B—C61—C62	73.4 (8)	C4—C12—N10—C15	-19.4 (3)
C5—C6B—C61—C62	-50.6 (9)	C13—N10—C15—C16	97.4 (2)
C7—C6B—C61—C66	-116.4 (5)	C12—N10—C15—C16	-86.4 (2)
C5—C6B—C61—C66	119.6 (4)	N10—C15—C16—O16	-75.8 (2)
C66—C61—C62—C63	0.7 (4)	C15—C16—O16—Br3 ^h	80.6 (3)
C6A—C61—C62—C63	176.9 (2)	C11—C9—C1'—C6'	24.5 (3)
C6B—C61—C62—C63	169.5 (6)	C14—C9—C1'—C6'	-96.6 (2)
C61—C62—C63—C64	-0.5 (4)	C11—C9—C1'—C2'	-158.07 (18)
C62—C63—C64—C65	0.1 (4)	C14—C9—C1'—C2'	80.8 (2)
C63—C64—C65—C66	0.2 (4)	C6'—C1'—C2'—O2'	-179.77 (18)

C62—C61—C66—C65	-0.4 (4)	C9—C1'—C2'—O2'	2.7 (3)
C6A—C61—C66—C65	-176.1 (2)	C6'—C1'—C2'—C3'	-0.9 (3)
C6B—C61—C66—C65	-174.8 (3)	C9—C1'—C2'—C3'	-178.40 (18)
C64—C65—C66—C61	0.0 (4)	O2'—C2'—C3'—C4'	-179.7 (2)
C5—C6B—C7—C8	-20.7 (8)	C1'—C2'—C3'—C4'	1.3 (3)
C61—C6B—C7—C8	-138.1 (4)	O2'—C2'—C3'—Br3'	-0.8 (3)
C5—C6A—C7—C8	58.8 (3)	C1'—C2'—C3'—Br3'	-179.80 (15)
C61—C6A—C7—C8	-179.2 (2)	C2'—C3'—C4'—C5'	-0.6 (3)
C6B—C7—C8—O8	-175.2 (5)	Br3'—C3'—C4'—C5'	-179.42 (18)
C6A—C7—C8—O8	143.9 (2)	C3'—C4'—C5'—C6'	-0.7 (4)
C6B—C7—C8—C14	2.2 (6)	C3'—C4'—C5'—C15'	179.59 (18)
C6A—C7—C8—C14	-38.7 (3)	C4'—C5'—C6'—C1'	1.2 (4)
O1—C1—C11—C12	-177.9 (2)	C15'—C5'—C6'—C1'	-179.13 (17)
C2B—C1—C11—C12	-14.9 (5)	C2'—C1'—C6'—C5'	-0.4 (3)
C2A—C1—C11—C12	17.3 (5)	C9—C1'—C6'—C5'	177.2 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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

Cg7 and Cg8 are the centroids of the C31–C36 and C61–C66 phenyl rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2'—H2'O \cdots O8	0.85 (3)	1.79 (3)	2.626 (2)	170 (3)
O16—H16O \cdots O8 ⁱⁱ	0.84 (4)	1.97 (4)	2.782 (2)	163 (4)
C15—H15A \cdots O16 ⁱⁱⁱ	0.99	2.68	3.622 (3)	159
C5—H5A \cdots O8 ^{iv}	0.99	2.69	3.669 (3)	172
C5—H5A \cdots O2' ^{iv}	0.99	2.70	3.336 (3)	122
C15—H15B \cdots O1 ^{iv}	0.99	2.47	3.451 (3)	172
C34—H34 \cdots C15' ^v	0.95	2.87	3.560 (3)	131
C16—H16B \cdots Cg8 ⁱⁱⁱ	0.99	2.66	3.529 (3)	147
C65—H65 \cdots Cg7 ^{vi}	0.95	2.78	3.648 (4)	152

Symmetry codes: (ii) $-x+1, y+1/2, -z+1/2$; (iii) $-x+1, -y+1, -z$; (iv) $x, -y+1/2, z-1/2$; (v) $-x+2, y-1/2, -z+1/2$; (vi) $x-1, -y-1/2, z-3/2$.