3,5-Dibromo-4-carbamoylbenzoic acid 2-propanol monosolvate

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In the title solvated crystal, $C_8H_5Br_2NO_3 \cdot C_3H_8O$, the acid molecules form inversion dimers by pairwise N—H⋯O hydrogen bonds between carbamoyl groups and the carboxyl and carbamoyl groups link to form head-to-tail inversion dimers. The 2-propanol hydroxyl group interposes between adjacent head-tail pairs, resulting in $C_3^3(10)$ chains of hydrogen bonds propagating along [100]. The molecules of 2-propanol are disordered over two sets of sites in a 0.598 (8):0.402 (8) ratio. The best-fit planes of the carbamoyl group and benzene ring are inclined by 88.26 (11)°. This is a greater inclination than was previously reported with CH_3, Cl, F or H in place of the Br atoms, although those analogues did not have a *para* carboxyl group.

3D view

Chemical scheme

Structure description

Although the structure of 2-bromobenzamide is reported twice (Izumi & Okamoto, 1972; Gulyás *et al.*, 2015) in the current version of the Cambridge Structural Database (version 5.42, Nov 2020; Groom *et al.*, 2016), no 2,6-dibromo- or 4-carboxylbenzamides were found. The title compound (I) is an example of both classes, and was accidentally prepared in an attempt to selectively hydrolyze the ester group of a cyano ester (II) (Fig. 1). The target was cyano acid (III), for a study in our laboratory involving co-crystals of (III) with anthracene (Noland *et al.*, 2017).

In the title crystal (Fig. 2), molecules of (I) form typical amide inversion dimers based on pairwise N1—H1A⋯O1 hydrogen bonds (Table 1; Fig. 3). The carboxyl groups do not homo-dimerize. Instead, they participate in amido-carboxy N1—H1B⋯O2 hydrogen bonding that forms head-to-tail inversion dimers about the center of the unit cell. The solvent molecule of 2-propanol interposes between H3A of the acid group and O1 of the amide group, forming an O3—H3A⋯O4—H4B⋯O1 hydrogen-bonded chain. Excluding amide dimerization, these hydrogen bonds collectively form $C_3^3(10)$ chains

Figure 1
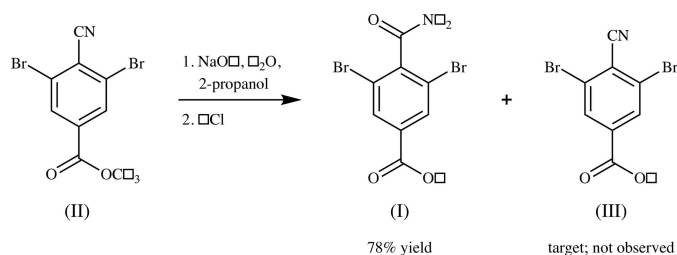The synthesis of (I).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O3—H3A⋯O4	0.84 (1)	1.74 (1)	2.580 (12)	174 (3)
O3—H3A⋯O4′	0.84 (1)	1.72 (2)	2.560 (19)	173 (3)
N1—H1A⋯O1^{i}	0.88 (1)	2.06 (1)	2.929 (2)	171 (3)
N1—H1B⋯O2^{ii}	0.88 (1)	2.08 (1)	2.931 (3)	164 (3)
O4—H4B⋯O1^{iii}	0.84 (1)	2.05 (3)	2.802 (11)	149 (5)
O4′—H4C⋯O1^{iii}	0.84 (1)	1.90 (5)	2.606 (18)	141 (7)

Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y+1, -z+1$.

propagating along [100]. The 2-propanol molecule is disordered over two sets of sites in a 0.598 (8):0.402 (8) ratio. The Br atoms and benzene ring do not participate in any short interactions.

A dihedral angle of 88.26 (11)° is observed between the best-fit planes of the carbamoyl group (O1/N1/C1) and the benzene ring (C2–C7; Fig. 4). The corresponding angle is also shown for 2,4,6-trimethyl- (IV; Gdaniec *et al.*, 2004), 2,6-dichloro- (V; Mukherjee *et al.*, 2013), 2,6-difluoro- (VI; Rauf *et al.*, 2006), and unsubstituted (VII; Blake *et al.*, 1972) benza-
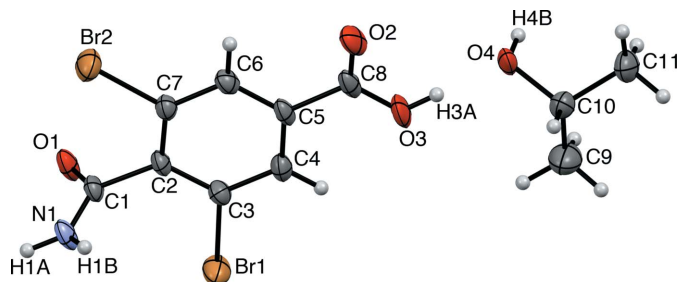
mides. Although none of these reported crystals contain a *para*-carboxyl group, crystal (I) fits the expected trend. The *ortho* Br atoms cause a carbamoyl inclination slightly larger than the inclination observed with *ortho* methyl groups, which is in turn larger than inclinations caused by *ortho* Cl, F, or H atoms.

Synthesis and crystallization

3,5-Dibromo-4-carbamoylbenzoic acid (I): a portion of compound (II) (589 mg, Fig. 1) taken from our prior study (Noland *et al.*, 2017) was placed in a round-bottomed flask with water (5 ml), 2-propanol (5 ml) and NaOH (186 mg). The resulting mixture was refluxed for 1 h, and then cooled to 290 K. Hydrochloric acid (6 *M*) was added dropwise until the pH of the mixture was less than 4. An off-white precipitate was collected by suction filtration, and then triturated with 2-propanol, giving a white powder (476 mg, 78%), m.p. 528–529 K. ^{1}H NMR (500 MHz, DMSO-d_6) δ 13.705 (*s*, 1H, H3*A*), 8.124 (*s*, 1H, H1*A* or H1*B*), 8.069 (*s*, 2H, H4*A*, H6*A*), 7.887 (*s*, 1H, H1*B* or H1*A*); ^{13}C NMR (126 MHz, DMSO-d_6) δ 166.8 (1 C, C1 or C8), 164.5 (1 C, C8 or C1), 144.3 (1 C, C5), 133.4 (1 C, C2), 132.0 (2 C, C4, C6), 119.7 (2 C, C3, C7); IR (KBr, cm^{-1}) 3442, 3314, 3185, 3088, 2921, 2487, 1719, 1648, 1604, 1542, 1371, 1270, 901, 743; MS (ESI, *m/z*) $[M − H]^{−}$ calculated for $C_8H_5{}^{81}Br^{79}BrNO_3$ 321.8543, found 321.8549.

Crystallization: a portion of the white powder was dissolved in refluxing 2-propanol and the resulting mixture was incrementally cooled to 268 K over 6 h. Crystals were collected by decantation, and then washed with 2-propanol.

Figure 2
The molecular structure of (I), with atomic numbering and displacement ellipsoids at the 50% probability level. For clarity, only the major disorder component of 2-propanol is shown.
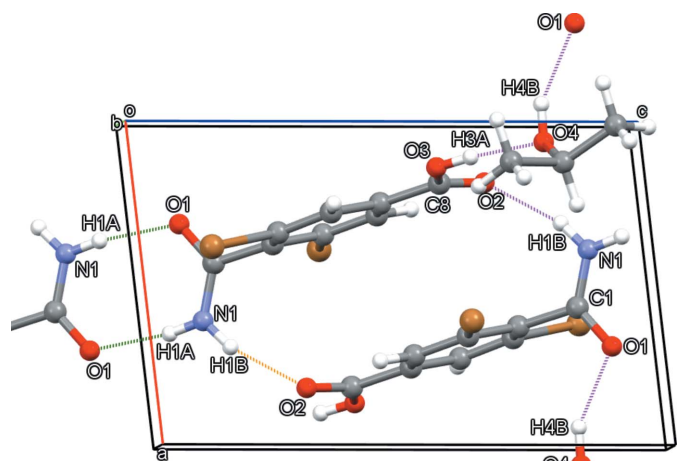

Figure 3
Hydrogen bonding in the crystal of (I), viewed along [010]. For clarity, the minor component and the lower-left molecule of 2-propanol are omitted from the unit cell. The dashed green lines represent amide dimerization. The dashed magenta lines represent the hydrogen bonds that form chains along [100]. The dashed orange line and its magenta counterpart (O2⋯N1) illustrate head-to-tail dimerization.
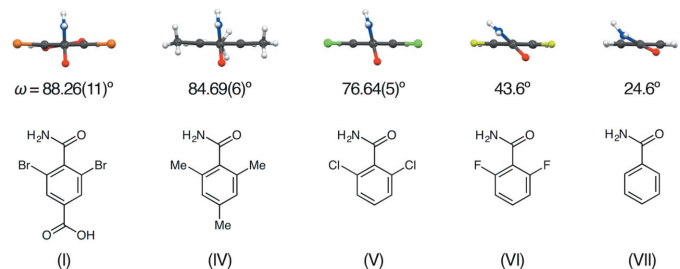

Figure 4
Substituted benzamides, in their crystals, viewed along carbamoyl group *ipso* bonds. The listed dihedral angles (ω) are between the best-fit planes of the respective benzene rings and carbamoyl groups.

Refinement

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

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_5Br_2NO_3 \cdot C_3H_8O$
M_r	383.04
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	173
a, b, c (Å)	7.2866 (5), 8.5212 (6), 12.1832 (8)
α, β, γ (°)	71.376 (1), 81.745 (1), 83.682 (1)
V (Å^3)	707.76 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.73
Crystal size (mm)	$0.40 \times 0.38 \times 0.16$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.486, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8139, 3128, 2683
R_{int}	0.021
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.645
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.026, 0.065, 1.04
No. of reflections	3128
No. of parameters	201
No. of restraints	151
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.63, −0.90

Computer programs: *APEX3* and *SAINT* (Bruker, 2018), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

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full crystallographic data

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Crystal data

$C_8H_5Br_2NO_3 \cdot C_3H_8O$
$M_r = 383.04$
Triclinic, $P\bar{1}$
$a = 7.2866\ (5)$ Å
$b = 8.5212\ (6)$ Å
$c = 12.1832\ (8)$ Å
$\alpha = 71.376\ (1)°$
$\beta = 81.745\ (1)°$
$\gamma = 83.682\ (1)°$
$V = 707.76\ (8)$ Å^3
$Z = 2$

$F(000) = 376$
$D_x = 1.797$ Mg m^{-3}
Melting point: 528 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2971 reflections
$\theta = 2.6–27.3°$
$\mu = 5.73$ mm^{-1}
$T = 173$ K
Block, colourless
$0.40 \times 0.38 \times 0.16$ mm

Data collection

Bruker APEXII CCD
  diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan
  (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.486$, $T_{max} = 0.746$
8139 measured reflections

3128 independent reflections
2683 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.3°$, $\theta_{min} = 1.8°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.065$
$S = 1.04$
3128 reflections
201 parameters
151 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent
  and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.5063P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.90$ 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.

Angle of C2/C3/C4/C5/C6/C7 vs. N1/C1/O1 below Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

6.9373 (0.0020) x - 1.2809 (0.0074) y + 2.6193 (0.0107) z = 5.8890 (0.0086)

* 0.0044 (0.0015) C2 * -0.0085 (0.0016) C3 * 0.0048 (0.0015) C4 * 0.0030 (0.0015) C5 * -0.0070 (0.0015) C6 * 0.0033 (0.0015) C7

Rms deviation of fitted atoms = 0.0055

1.3629 (0.0122) x + 7.5482 (0.0167) y + 8.7867 (0.0367) z = 9.5168 (0.0262)

Angle to previous plane (with approximate esd) = 88.256 (0.113)

* 0.0000 (0.0000) N1 * 0.0000 (0.0000) C1 * 0.0000 (0.0000) O1

Rms deviation of fitted atoms = 0.0000

Refinement. A direct-methods solution was calculated, followed by full-matrix least squares / difference Fourier cycles. All H atoms were placed in calculated positions (C—H = 0.95–1.00 Å, N—H = 0.88 Å, O—H = 0.84 Å) and refined as riding atoms with $U_{iso}(H)$ set to 1.2 or $1.5U_{eq}(C/N/O)$.

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$	Occ. (<1)
Br1	0.61784 (4)	0.53550 (3)	0.84990 (2)	0.04348 (9)	
Br2	0.61751 (4)	0.03664 (3)	0.63196 (2)	0.04169 (9)	
O1	0.6947 (2)	0.0875 (2)	0.90019 (14)	0.0332 (4)	
O2	0.8164 (3)	0.6055 (2)	0.30554 (14)	0.0405 (4)	
O3	0.8603 (3)	0.7832 (2)	0.39910 (15)	0.0416 (4)	
H3A	0.891 (4)	0.846 (3)	0.3317 (11)	0.050*	
N1	0.3942 (3)	0.1688 (3)	0.87692 (17)	0.0327 (4)	
H1A	0.355 (4)	0.097 (3)	0.9439 (12)	0.039*	
H1B	0.312 (3)	0.227 (3)	0.8307 (19)	0.039*	
C1	0.5730 (3)	0.1757 (3)	0.84327 (18)	0.0252 (4)	
C2	0.6307 (3)	0.3004 (3)	0.72637 (17)	0.0241 (4)	
C3	0.6625 (3)	0.4624 (3)	0.71657 (19)	0.0265 (4)	
C4	0.7250 (3)	0.5743 (3)	0.61079 (19)	0.0278 (5)	
H4A	0.748438	0.683825	0.606128	0.033*	
C5	0.7527 (3)	0.5239 (3)	0.51214 (18)	0.0264 (5)	
C6	0.7196 (3)	0.3647 (3)	0.51800 (19)	0.0276 (5)	
H6A	0.737311	0.331352	0.449673	0.033*	
C7	0.6603 (3)	0.2545 (3)	0.62524 (19)	0.0256 (4)	
C8	0.8134 (3)	0.6414 (3)	0.3944 (2)	0.0308 (5)	
O4	0.9365 (13)	0.9719 (9)	0.1879 (11)	0.0313 (15)	0.598 (8)
H4B	1.0530 (14)	0.964 (8)	0.184 (5)	0.047*	0.598 (8)
C9	0.872 (3)	1.205 (2)	0.2603 (12)	0.060 (2)	0.598 (8)
H9A	0.820755	1.320374	0.241438	0.091*	0.598 (8)
H9B	1.000209	1.198652	0.278449	0.091*	0.598 (8)
H9C	0.796644	1.135893	0.327854	0.091*	0.598 (8)
C10	0.8716 (7)	1.1441 (5)	0.1583 (4)	0.0345 (13)	0.598 (8)
H10A	0.739971	1.152928	0.141246	0.041*	0.598 (8)
C11	0.9845 (12)	1.2460 (14)	0.0493 (7)	0.0429 (18)	0.598 (8)

H11A	0.979250	1.201108	−0.014763	0.064*	0.598 (8)
H11B	1.113936	1.241251	0.064208	0.064*	0.598 (8)
H11C	0.933135	1.361577	0.028151	0.064*	0.598 (8)
O4′	0.978 (2)	0.9791 (14)	0.1997 (18)	0.0313 (15)	0.402 (8)
H4C	1.049 (8)	0.954 (10)	0.146 (5)	0.047*	0.402 (8)
C9′	0.883 (5)	1.202 (4)	0.2791 (18)	0.060 (2)	0.402 (8)
H9D	0.887410	1.321374	0.265058	0.091*	0.402 (8)
H9E	0.938938	1.140568	0.350651	0.091*	0.402 (8)
H9F	0.753869	1.174455	0.287647	0.091*	0.402 (8)
C10′	0.9900 (11)	1.1550 (7)	0.1784 (5)	0.0304 (17)	0.402 (8)
H10B	1.123331	1.176385	0.174482	0.036*	0.402 (8)
C11′	0.9228 (19)	1.250 (2)	0.0639 (10)	0.0429 (18)	0.402 (8)
H11D	0.793361	1.227577	0.065230	0.064*	0.402 (8)
H11E	1.000083	1.215842	0.001592	0.064*	0.402 (8)
H11F	0.931011	1.369041	0.049729	0.064*	0.402 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0693 (2)	0.03621 (15)	0.02540 (13)	−0.00969 (12)	0.00169 (12)	−0.01126 (10)
Br2	0.05996 (18)	0.02835 (13)	0.03767 (15)	−0.01118 (11)	−0.00300 (12)	−0.00992 (11)
O1	0.0278 (8)	0.0364 (9)	0.0226 (8)	−0.0049 (7)	−0.0010 (6)	0.0086 (7)
O2	0.0473 (10)	0.0395 (10)	0.0201 (8)	0.0044 (8)	0.0024 (7)	0.0058 (7)
O3	0.0468 (10)	0.0323 (9)	0.0294 (9)	−0.0094 (8)	0.0080 (8)	0.0101 (7)
N1	0.0295 (10)	0.0359 (11)	0.0200 (10)	−0.0038 (8)	0.0008 (8)	0.0080 (8)
C1	0.0314 (11)	0.0240 (10)	0.0155 (10)	−0.0062 (9)	0.0000 (8)	0.0007 (8)
C2	0.0260 (10)	0.0237 (10)	0.0170 (10)	−0.0044 (8)	−0.0003 (8)	0.0016 (8)
C3	0.0309 (11)	0.0270 (11)	0.0186 (10)	−0.0023 (9)	−0.0007 (8)	−0.0039 (8)
C4	0.0284 (11)	0.0238 (10)	0.0259 (11)	−0.0044 (9)	−0.0024 (9)	0.0005 (9)
C5	0.0221 (10)	0.0276 (11)	0.0195 (10)	−0.0012 (8)	0.0004 (8)	0.0053 (8)
C6	0.0295 (11)	0.0299 (11)	0.0184 (10)	0.0003 (9)	−0.0010 (8)	−0.0022 (9)
C7	0.0281 (11)	0.0231 (10)	0.0218 (10)	−0.0033 (8)	−0.0011 (8)	−0.0019 (8)
C8	0.0222 (10)	0.0311 (12)	0.0246 (11)	0.0025 (9)	0.0016 (9)	0.0080 (9)
O4	0.026 (4)	0.0233 (10)	0.034 (3)	−0.0051 (17)	0.008 (3)	0.0027 (10)
C9	0.091 (4)	0.0453 (19)	0.042 (4)	−0.0020 (19)	0.009 (4)	−0.016 (3)
C10	0.036 (3)	0.027 (2)	0.035 (2)	0.0005 (17)	−0.0004 (19)	−0.0050 (17)
C11	0.059 (6)	0.0292 (15)	0.032 (2)	−0.001 (4)	0.000 (3)	0.0010 (18)
O4′	0.026 (4)	0.0233 (10)	0.034 (3)	−0.0051 (17)	0.008 (3)	0.0027 (10)
C9′	0.091 (4)	0.0453 (19)	0.042 (4)	−0.0020 (19)	0.009 (4)	−0.016 (3)
C10′	0.039 (4)	0.020 (3)	0.030 (3)	−0.007 (2)	−0.009 (2)	−0.001 (2)
C11′	0.059 (6)	0.0292 (15)	0.032 (2)	−0.001 (4)	0.000 (3)	0.0010 (18)

Geometric parameters (Å, º)

Br1—C3	1.893 (2)	C9—C10	1.492 (10)
Br2—C7	1.890 (2)	C9—H9A	0.9800
O1—C1	1.236 (3)	C9—H9B	0.9800
O2—C8	1.213 (3)	C9—H9C	0.9800

O3—C8	1.311 (3)	C10—C11	1.517 (8)
O3—H3A	0.839 (3)	C10—H10A	1.0000
N1—C1	1.311 (3)	C11—H11A	0.9800
N1—H1A	0.880 (3)	C11—H11B	0.9800
N1—H1B	0.880 (3)	C11—H11C	0.9800
C1—C2	1.515 (3)	O4′—C10′	1.448 (11)
C2—C3	1.389 (3)	O4′—H4C	0.840 (3)
C2—C7	1.390 (3)	C9′—C10′	1.497 (13)
C3—C4	1.385 (3)	C9′—H9D	0.9800
C4—C5	1.382 (3)	C9′—H9E	0.9800
C4—H4A	0.9500	C9′—H9F	0.9800
C5—C6	1.381 (3)	C10′—C11′	1.492 (12)
C5—C8	1.501 (3)	C10′—H10B	1.0000
C6—C7	1.385 (3)	C11′—H11D	0.9800
C6—H6A	0.9500	C11′—H11E	0.9800
O4—C10	1.437 (8)	C11′—H11F	0.9800
O4—H4B	0.840 (3)		
C8—O3—H3A	110 (2)	H9A—C9—H9C	109.5
C1—N1—H1A	119.3 (18)	H9B—C9—H9C	109.5
C1—N1—H1B	121.2 (18)	O4—C10—C9	109.7 (8)
H1A—N1—H1B	119 (2)	O4—C10—C11	110.9 (7)
O1—C1—N1	124.32 (19)	C9—C10—C11	112.8 (10)
O1—C1—C2	118.97 (19)	O4—C10—H10A	107.8
N1—C1—C2	116.71 (19)	C9—C10—H10A	107.8
C3—C2—C7	117.58 (19)	C11—C10—H10A	107.8
C3—C2—C1	121.60 (19)	C10—C11—H11A	109.5
C7—C2—C1	120.79 (19)	C10—C11—H11B	109.5
C4—C3—C2	121.8 (2)	H11A—C11—H11B	109.5
C4—C3—Br1	118.38 (17)	C10—C11—H11C	109.5
C2—C3—Br1	119.85 (16)	H11A—C11—H11C	109.5
C5—C4—C3	118.9 (2)	H11B—C11—H11C	109.5
C5—C4—H4A	120.5	C10′—O4′—H4C	106 (6)
C3—C4—H4A	120.5	C10′—C9′—H9D	109.5
C6—C5—C4	121.02 (19)	C10′—C9′—H9E	109.5
C6—C5—C8	117.7 (2)	H9D—C9′—H9E	109.5
C4—C5—C8	121.3 (2)	C10′—C9′—H9F	109.5
C5—C6—C7	118.9 (2)	H9D—C9′—H9F	109.5
C5—C6—H6A	120.6	H9E—C9′—H9F	109.5
C7—C6—H6A	120.6	O4′—C10′—C9′	108.5 (13)
C6—C7—C2	121.8 (2)	O4′—C10′—C11′	109.7 (10)
C6—C7—Br2	118.33 (17)	C9′—C10′—C11′	113.5 (14)
C2—C7—Br2	119.82 (15)	O4′—C10′—H10B	108.3
O2—C8—O3	124.9 (2)	C9′—C10′—H10B	108.3
O2—C8—C5	122.0 (2)	C11′—C10′—H10B	108.3
O3—C8—C5	113.2 (2)	C10′—C11′—H11D	109.5
C10—O4—H4B	109 (5)	C10′—C11′—H11E	109.5
C10—C9—H9A	109.5	H11D—C11′—H11E	109.5

C10—C9—H9B	109.5	C10′—C11′—H11F	109.5
H9A—C9—H9B	109.5	H11D—C11′—H11F	109.5
C10—C9—H9C	109.5	H11E—C11′—H11F	109.5
O1—C1—C2—C3	−91.0 (3)	C4—C5—C6—C7	−0.9 (3)
N1—C1—C2—C3	89.3 (3)	C8—C5—C6—C7	−178.9 (2)
O1—C1—C2—C7	86.7 (3)	C5—C6—C7—C2	0.9 (3)
N1—C1—C2—C7	−93.0 (3)	C5—C6—C7—Br2	−179.53 (16)
C7—C2—C3—C4	−1.3 (3)	C3—C2—C7—C6	0.1 (3)
C1—C2—C3—C4	176.4 (2)	C1—C2—C7—C6	−177.6 (2)
C7—C2—C3—Br1	178.09 (16)	C3—C2—C7—Br2	−179.40 (16)
C1—C2—C3—Br1	−4.2 (3)	C1—C2—C7—Br2	2.8 (3)
C2—C3—C4—C5	1.3 (3)	C6—C5—C8—O2	7.2 (3)
Br1—C3—C4—C5	−178.05 (16)	C4—C5—C8—O2	−170.8 (2)
C3—C4—C5—C6	−0.2 (3)	C6—C5—C8—O3	−173.2 (2)
C3—C4—C5—C8	177.7 (2)	C4—C5—C8—O3	8.9 (3)

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H3A⋯O4	0.84 (1)	1.74 (1)	2.580 (12)	174 (3)
O3—H3A⋯O4′	0.84 (1)	1.72 (2)	2.560 (19)	173 (3)
N1—H1A⋯O1[i]	0.88 (1)	2.06 (1)	2.929 (2)	171 (3)
N1—H1B⋯O2[ii]	0.88 (1)	2.08 (1)	2.931 (3)	164 (3)
O4—H4B⋯O1[iii]	0.84 (1)	2.05 (3)	2.802 (11)	149 (5)
O4′—H4C⋯O1[iii]	0.84 (1)	1.90 (5)	2.606 (18)	141 (7)

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