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4-Chloro-*N*′-(3,5-dibromo-2-hydroxybenzylidene)benzohydrazide

Wei-Guang Zhang

College of Chemistry and Chemical Engineering, Qiqihar University, Qiqihar 161006, People's Republic of China
Correspondence e-mail: zhangweiguang1230@163.com

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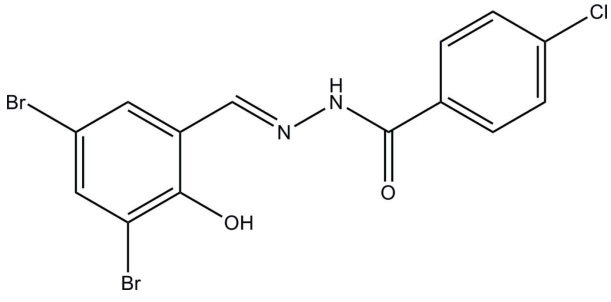
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.045; wR factor = 0.105; data-to-parameter ratio = 14.8.

The asymmetric unit of the title compound, $C_{14}H_9Br_2ClN_2O_2$, contains two independent molecules. Both molecules adopt an *E* configuration about the C=N bond. The dihedral angles between the benzene rings are 30.0 (2) and 51.6 (2)° in the two molecules. In the crystal, molecules are linked through N—H···O hydrogen bonds, forming chains along the *b* axis. In addition, there is an intramolecular O—H···N hydrogen bond in each molecule.

Related literature

For the biological properties of hydrazone compounds, see: Ajani *et al.* (2010); Angelusiu *et al.* (2010); Zhang *et al.* (2010); Horiuchi *et al.* (2009). For the crystal structures of similar hydrazone compounds, see: Ban (2010); Hussain *et al.* (2010); Shalash *et al.* (2010); Khaledi *et al.* (2009). For related structures reported recently by the author, see: Zhang (2011, 2012).



Experimental

Crystal data

$C_{14}H_9Br_2ClN_2O_2$
M_r = 432.50
Monoclinic, $C2/c$
a = 21.0503 (19) Å
b = 9.9895 (11) Å
c = 30.185 (2) Å
β = 101.836 (2)°
V = 6212.4 (10) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 5.40 mm^{-1}
T = 298 K
0.20 × 0.18 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.412, T_{max} = 0.461
21727 measured reflections
5775 independent reflections
2828 reflections with $I > 2\sigma(I)$
R_{int} = 0.093

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.105
S = 0.95
5775 reflections
389 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O2^{i}	0.90 (1)	1.95 (2)	2.827 (5)	166 (4)
N2—H2···O4	0.90 (1)	2.08 (2)	2.941 (5)	160 (4)
O3—H3···N3	0.82	1.87	2.569 (5)	143
O1—H1···N1	0.82	1.87	2.590 (5)	146

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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*.

Financial support from Qiqihar University is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5429).

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supplementary materials

Acta Cryst. (2012). E**68**, o1209 [doi:10.1107/S1600536812009786]

4-Chloro-*N*′-(3,5-dibromo-2-hydroxybenzylidene)benzohydrazide

Wei-Guang Zhang

Comment

Benzoylhydrazones are a kind of special Schiff bases bearing the –C(O)—NH—N═CH– group. Hydrazone compounds have received much attention for their excellent biological properties (Ajani *et al.*, 2010; Angelusiu *et al.*, 2010; Zhang *et al.*, 2010; Horiuchi *et al.*, 2009) as well as their crystal structures (Ban, 2010; Hussain *et al.*, 2010; Shalash *et al.*, 2010; Khaledi *et al.*, 2009). Recently, the author has reported some hydrazone compounds (Zhang, 2011; Zhang, 2012). In the present paper, the title new hydrazone compound, derived from the reaction of 3,5-dibromo-4-chlorobenzaldehyde with 4-chlorobenzohydrazide, is reported.

The asymmetric unit of the title hydrazone compound contains two independent molecules, as shown in Fig. 1. Each of the molecules of the compound adopts an *E* configuration about the C═N double bond. The dihedral angles between the two substituted benzene rings are 30.0 (2)° [C1-C6/C9-C14] and 51.6 (2)° [C15-C20/C23-C28]. In the crystal, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1), forming chains along the *b* axis (Fig. 2). In addition, there is an intramolecular O—H···N hydrogen bond in each molecule.

Experimental

3,5-Dibromo-2-hydroxybenzaldehyde (0.280 g, 1 mmol) and 4-chlorobenzohydrazide (0.171 g, 1 mmol) were mixed in 50 ml methanol. The mixture was stirred and refluxed for 30 min and cooled to room temperature to give a colorless solution. Colorless block-shaped single crystals were obtained on slow evaporation of the solution in air.

Refinement

H2 and H4 were located in a difference Fourier map and refined with the N—H distances restrained to 0.90 (1) Å. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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* (Sheldrick, 2008).

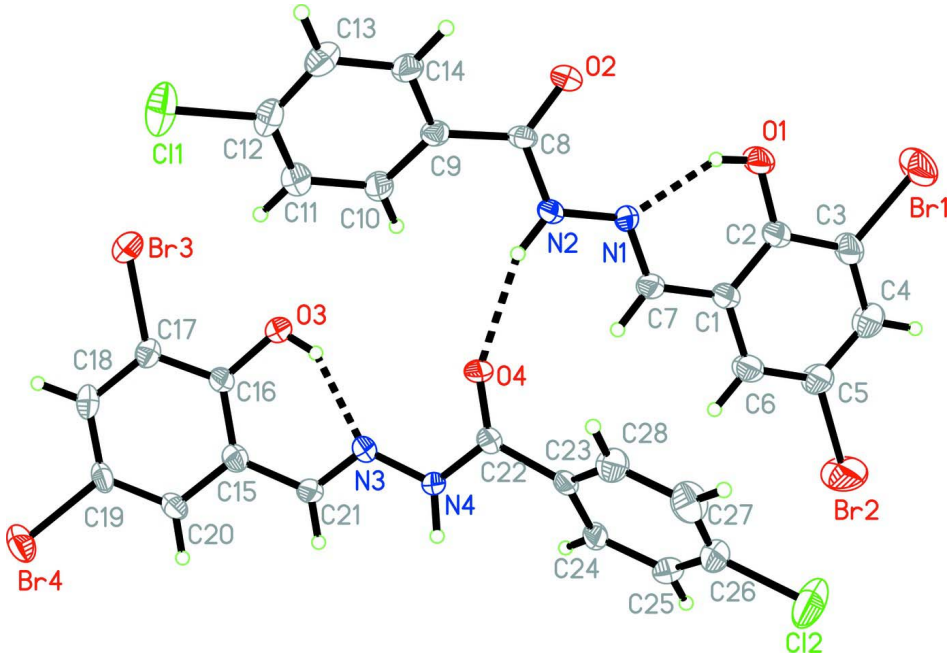

Figure 1

The asymmetric unit of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

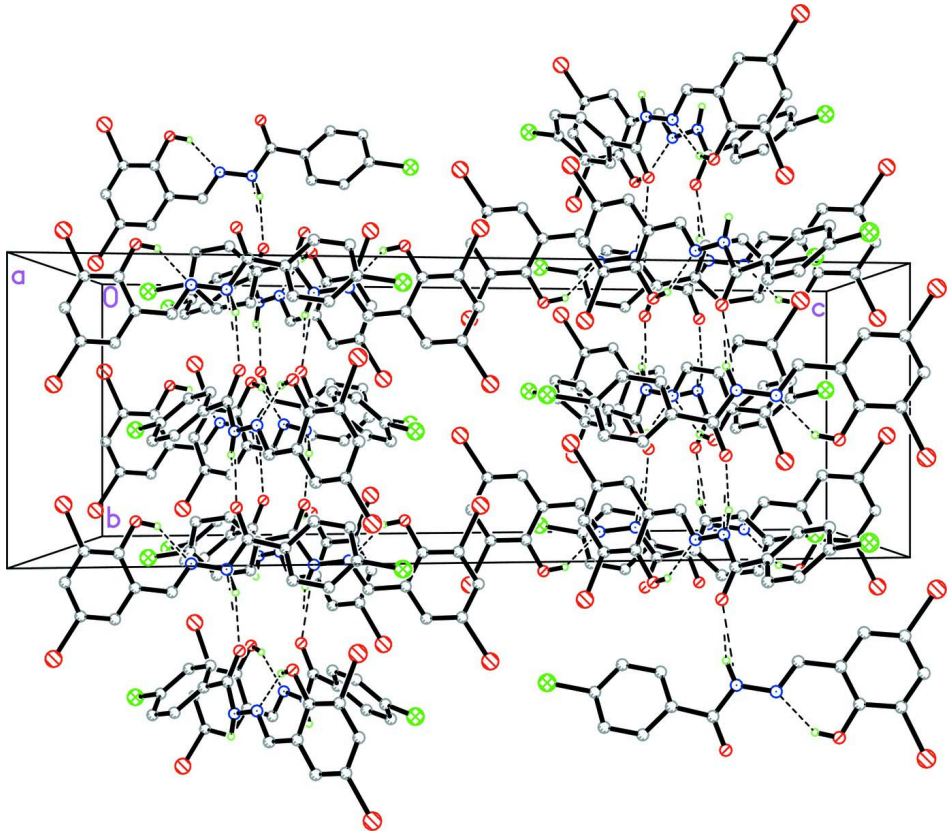

Figure 2

The molecular packing of the title compound viewed approximately along the *a* axis. Hydrogen bonds are shown as dashed lines. H-atoms not involved in hydrogen bonding have been omitted for clarity.

4-Chloro-*N*′-(3,5-dibromo-2-hydroxybenzylidene)benzohydrazide

Crystal data

$C_{14}H_9Br_2ClN_2O_2$
$M_r = 432.50$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 21.0503\ (19)$ Å
$b = 9.9895\ (11)$ Å
$c = 30.185\ (2)$ Å
$\beta = 101.836\ (2)°$
$V = 6212.4\ (10)$ Å^3
$Z = 16$
$F(000) = 3360$
$D_x = 1.850$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2652 reflections
$\theta = 2.3–24.3°$
$\mu = 5.40$ mm^{-1}
$T = 298$ K
Block, colorless
0.20 × 0.18 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.412$, $T_{max} = 0.461$
21727 measured reflections
5775 independent reflections
2828 reflections with $I > 2\sigma(I)$
$R_{int} = 0.093$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.2°$
$h = -25\rightarrow25$
$k = -12\rightarrow12$
$l = -36\rightarrow33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.105$
$S = 0.95$
5775 reflections
389 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.59984 (4)	−0.15649 (7)	0.50684 (2)	0.0893 (3)
Br2	0.60096 (5)	0.40530 (8)	0.51878 (3)	0.1266 (4)
Br3	0.16100 (3)	0.32156 (6)	0.13346 (2)	0.0621 (2)
Br4	0.13920 (3)	0.88180 (6)	0.11656 (2)	0.0662 (2)
Cl1	0.28553 (8)	0.0539 (2)	0.08490 (5)	0.0867 (6)
Cl2	0.69898 (8)	0.5736 (2)	0.42951 (6)	0.0988 (7)
N1	0.48103 (18)	0.0501 (4)	0.34395 (14)	0.0364 (10)
N2	0.4503 (2)	0.0679 (4)	0.29989 (14)	0.0393 (11)
N3	0.3518 (2)	0.5527 (4)	0.25814 (14)	0.0429 (11)
N4	0.4089 (2)	0.5744 (4)	0.28790 (15)	0.0452 (12)
O1	0.5259 (2)	−0.0988 (3)	0.41356 (11)	0.0564 (11)
H1	0.5103	−0.0831	0.3869	0.085*
O2	0.44485 (17)	−0.1529 (3)	0.28785 (12)	0.0522 (10)
O3	0.26677 (17)	0.3947 (3)	0.21220 (12)	0.0469 (9)
H3	0.3028	0.4132	0.2271	0.070*
O4	0.43685 (17)	0.3578 (3)	0.28369 (11)	0.0496 (10)
C1	0.5296 (2)	0.1408 (5)	0.41481 (18)	0.0409 (14)
C2	0.5433 (2)	0.0165 (5)	0.43546 (18)	0.0444 (14)
C3	0.5777 (3)	0.0117 (6)	0.48000 (19)	0.0544 (16)
C4	0.5949 (3)	0.1262 (6)	0.50448 (19)	0.0688 (19)
H4A	0.6173	0.1215	0.5344	0.083*
C5	0.5787 (3)	0.2482 (6)	0.4843 (2)	0.0661 (19)
C6	0.5472 (3)	0.2557 (5)	0.44034 (19)	0.0547 (16)
H6	0.5373	0.3392	0.4271	0.066*
C7	0.4980 (2)	0.1532 (5)	0.36838 (18)	0.0430 (14)

H7	0.4896	0.2380	0.3558	0.052*
C8	0.4314 (2)	−0.0407 (5)	0.27356 (18)	0.0385 (13)
C9	0.3945 (2)	−0.0126 (5)	0.22721 (17)	0.0355 (13)
C10	0.3549 (2)	0.0978 (5)	0.21643 (18)	0.0464 (15)
H10	0.3515	0.1596	0.2389	0.056*
C11	0.3200 (3)	0.1184 (6)	0.1727 (2)	0.0550 (16)
H11	0.2930	0.1924	0.1657	0.066*
C12	0.3265 (3)	0.0269 (6)	0.13990 (18)	0.0499 (15)
C13	0.3631 (3)	−0.0858 (6)	0.1497 (2)	0.0564 (16)
H13	0.3650	−0.1487	0.1273	0.068*
C14	0.3976 (2)	−0.1056 (5)	0.19342 (19)	0.0460 (14)
H14	0.4231	−0.1818	0.2003	0.055*
C15	0.2601 (2)	0.6341 (5)	0.20665 (17)	0.0387 (13)
C16	0.2386 (2)	0.5064 (5)	0.19194 (17)	0.0373 (13)
C17	0.1875 (2)	0.4942 (5)	0.15544 (17)	0.0393 (13)
C18	0.1587 (2)	0.6050 (6)	0.13239 (17)	0.0460 (14)
H18	0.1263	0.5948	0.1066	0.055*
C19	0.1784 (3)	0.7297 (5)	0.14789 (17)	0.0421 (14)
C20	0.2292 (2)	0.7460 (5)	0.18405 (16)	0.0412 (14)
H20	0.2431	0.8316	0.1935	0.049*
C21	0.3177 (2)	0.6530 (5)	0.24191 (16)	0.0417 (14)
H21	0.3297	0.7386	0.2526	0.050*
C22	0.4500 (2)	0.4694 (5)	0.29903 (17)	0.0400 (14)
C23	0.5113 (3)	0.5008 (5)	0.33136 (16)	0.0351 (13)
C24	0.5150 (3)	0.5908 (5)	0.36667 (17)	0.0451 (15)
H24	0.4781	0.6385	0.3696	0.054*
C25	0.5719 (3)	0.6111 (5)	0.39751 (19)	0.0507 (15)
H25	0.5731	0.6693	0.4217	0.061*
C26	0.6262 (3)	0.5457 (6)	0.3924 (2)	0.0537 (16)
C27	0.6246 (3)	0.4561 (6)	0.3576 (2)	0.0648 (18)
H27	0.6620	0.4107	0.3545	0.078*
C28	0.5668 (3)	0.4343 (5)	0.32730 (18)	0.0510 (15)
H28	0.5656	0.3736	0.3038	0.061*
H2	0.440 (2)	0.150 (2)	0.2886 (14)	0.039 (15)*
H4	0.4239 (18)	0.6586 (17)	0.2928 (13)	0.028 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1524 (8)	0.0620 (5)	0.0432 (4)	0.0235 (5)	−0.0042 (4)	0.0114 (4)
Br2	0.2209 (11)	0.0680 (5)	0.0661 (6)	−0.0248 (6)	−0.0282 (6)	−0.0228 (4)
Br3	0.0642 (4)	0.0549 (4)	0.0575 (4)	−0.0059 (3)	−0.0101 (3)	−0.0099 (3)
Br4	0.0726 (5)	0.0615 (4)	0.0599 (4)	0.0200 (3)	0.0025 (3)	0.0202 (4)
Cl1	0.0802 (12)	0.1304 (16)	0.0417 (10)	−0.0018 (12)	−0.0056 (9)	0.0045 (10)
Cl2	0.0554 (11)	0.1279 (17)	0.0980 (15)	−0.0097 (11)	−0.0196 (10)	−0.0172 (13)
N1	0.043 (3)	0.033 (3)	0.029 (3)	−0.004 (2)	−0.002 (2)	0.005 (2)
N2	0.054 (3)	0.025 (3)	0.035 (3)	0.003 (2)	0.000 (2)	0.000 (2)
N3	0.051 (3)	0.032 (3)	0.040 (3)	0.001 (2)	−0.004 (2)	0.005 (2)
N4	0.048 (3)	0.026 (3)	0.050 (3)	−0.004 (2)	−0.016 (2)	0.003 (2)
O1	0.093 (3)	0.035 (2)	0.035 (2)	0.003 (2)	−0.001 (2)	0.0007 (18)

O2	0.065 (3)	0.028 (2)	0.058 (3)	−0.0016 (19)	−0.002 (2)	0.0050 (19)
O3	0.054 (3)	0.034 (2)	0.046 (3)	−0.0019 (18)	−0.0069 (19)	−0.0033 (18)
O4	0.072 (3)	0.024 (2)	0.045 (2)	−0.0014 (18)	−0.009 (2)	−0.0068 (17)
C1	0.047 (3)	0.032 (3)	0.042 (4)	0.002 (3)	0.007 (3)	0.001 (3)
C2	0.052 (4)	0.033 (3)	0.047 (4)	0.003 (3)	0.006 (3)	0.000 (3)
C3	0.074 (4)	0.050 (4)	0.036 (4)	0.004 (3)	0.002 (3)	0.009 (3)
C4	0.097 (5)	0.069 (5)	0.030 (4)	−0.006 (4)	−0.010 (3)	−0.010 (4)
C5	0.099 (5)	0.051 (4)	0.038 (4)	−0.007 (4)	−0.011 (4)	−0.007 (3)
C6	0.079 (5)	0.038 (4)	0.045 (4)	−0.004 (3)	0.006 (3)	0.003 (3)
C7	0.054 (4)	0.033 (3)	0.040 (4)	−0.008 (3)	0.003 (3)	0.005 (3)
C8	0.040 (3)	0.023 (3)	0.050 (4)	−0.001 (3)	0.005 (3)	−0.001 (3)
C9	0.029 (3)	0.032 (3)	0.046 (4)	−0.003 (3)	0.007 (3)	−0.002 (3)
C10	0.053 (4)	0.041 (3)	0.042 (4)	0.007 (3)	0.000 (3)	−0.006 (3)
C11	0.057 (4)	0.049 (4)	0.054 (4)	0.006 (3)	0.000 (3)	0.001 (3)
C12	0.044 (4)	0.069 (4)	0.035 (4)	−0.011 (3)	0.003 (3)	0.001 (3)
C13	0.058 (4)	0.059 (4)	0.048 (4)	−0.007 (3)	0.004 (3)	−0.016 (3)
C14	0.044 (4)	0.038 (3)	0.052 (4)	0.005 (3)	0.001 (3)	−0.012 (3)
C15	0.043 (3)	0.039 (3)	0.035 (3)	0.003 (3)	0.009 (3)	0.003 (3)
C16	0.043 (3)	0.030 (3)	0.037 (3)	0.004 (3)	0.004 (3)	0.001 (3)
C17	0.037 (3)	0.046 (3)	0.034 (3)	0.003 (3)	0.004 (3)	−0.005 (3)
C18	0.045 (4)	0.062 (4)	0.028 (3)	0.008 (3)	0.001 (3)	0.004 (3)
C19	0.051 (4)	0.044 (4)	0.029 (3)	0.010 (3)	0.003 (3)	0.010 (3)
C20	0.049 (4)	0.033 (3)	0.041 (4)	0.005 (3)	0.009 (3)	0.009 (3)
C21	0.055 (4)	0.033 (3)	0.035 (3)	−0.008 (3)	0.003 (3)	0.003 (3)
C22	0.049 (4)	0.034 (3)	0.033 (3)	−0.002 (3)	0.000 (3)	0.006 (3)
C23	0.047 (4)	0.027 (3)	0.029 (3)	0.002 (3)	0.003 (3)	0.006 (2)
C24	0.052 (4)	0.031 (3)	0.045 (4)	0.010 (3)	−0.009 (3)	−0.006 (3)
C25	0.057 (4)	0.037 (3)	0.053 (4)	−0.007 (3)	0.000 (3)	−0.005 (3)
C26	0.042 (4)	0.056 (4)	0.058 (4)	−0.005 (3)	−0.001 (3)	0.005 (3)
C27	0.055 (4)	0.071 (5)	0.071 (5)	0.015 (4)	0.020 (4)	0.003 (4)
C28	0.058 (4)	0.054 (4)	0.042 (4)	−0.001 (3)	0.010 (3)	−0.003 (3)

Geometric parameters (Å, º)

Br1—C3	1.882 (5)	C9—C10	1.380 (6)
Br2—C5	1.888 (6)	C9—C14	1.391 (6)
Br3—C17	1.890 (5)	C10—C11	1.389 (7)
Br4—C19	1.888 (5)	C10—H10	0.9300
Cl1—C12	1.727 (5)	C11—C12	1.374 (7)
Cl2—C26	1.724 (6)	C11—H11	0.9300
N1—C7	1.274 (5)	C12—C13	1.363 (7)
N1—N2	1.366 (5)	C13—C14	1.383 (7)
N2—C8	1.356 (6)	C13—H13	0.9300
N2—H2	0.897 (10)	C14—H14	0.9300
N3—C21	1.271 (5)	C15—C16	1.396 (6)
N3—N4	1.362 (5)	C15—C20	1.398 (6)
N4—C22	1.357 (6)	C15—C21	1.452 (7)
N4—H4	0.900 (10)	C16—C17	1.379 (6)
O1—C2	1.341 (5)	C17—C18	1.379 (6)
O1—H1	0.8200	C18—C19	1.364 (7)

O2—C8	1.213 (5)	C18—H18	0.9300
O3—C16	1.349 (5)	C19—C20	1.373 (7)
O3—H3	0.8200	C20—H20	0.9300
O4—C22	1.217 (5)	C21—H21	0.9300
C1—C6	1.390 (6)	C22—C23	1.484 (6)
C1—C2	1.393 (6)	C23—C28	1.371 (7)
C1—C7	1.428 (7)	C23—C24	1.384 (6)
C2—C3	1.390 (7)	C24—C25	1.374 (7)
C3—C4	1.370 (7)	C24—H24	0.9300
C4—C5	1.374 (7)	C25—C26	1.352 (7)
C4—H4A	0.9300	C25—H25	0.9300
C5—C6	1.357 (7)	C26—C27	1.376 (7)
C6—H6	0.9300	C27—C28	1.380 (7)
C7—H7	0.9300	C27—H27	0.9300
C8—C9	1.482 (6)	C28—H28	0.9300

C7—N1—N2	118.6 (4)	C12—C13—H13	120.4
C8—N2—N1	119.3 (4)	C14—C13—H13	120.4
C8—N2—H2	119 (3)	C13—C14—C9	120.6 (5)
N1—N2—H2	121 (3)	C13—C14—H14	119.7
C21—N3—N4	118.8 (4)	C9—C14—H14	119.7
C22—N4—N3	118.2 (4)	C16—C15—C20	119.2 (5)
C22—N4—H4	120 (3)	C16—C15—C21	121.3 (5)
N3—N4—H4	119 (3)	C20—C15—C21	119.3 (5)
C2—O1—H1	109.5	O3—C16—C17	119.2 (5)
C16—O3—H3	109.5	O3—C16—C15	121.9 (4)
C6—C1—C2	118.7 (5)	C17—C16—C15	119.0 (5)
C6—C1—C7	119.3 (5)	C18—C17—C16	121.5 (5)
C2—C1—C7	121.9 (5)	C18—C17—Br3	119.2 (4)
O1—C2—C3	118.8 (5)	C16—C17—Br3	119.1 (4)
O1—C2—C1	122.3 (5)	C19—C18—C17	119.3 (5)
C3—C2—C1	118.9 (5)	C19—C18—H18	120.4
C4—C3—C2	121.3 (5)	C17—C18—H18	120.4
C4—C3—Br1	119.9 (4)	C18—C19—C20	120.9 (5)
C2—C3—Br1	118.8 (4)	C18—C19—Br4	119.5 (4)
C3—C4—C5	119.1 (5)	C20—C19—Br4	119.5 (4)
C3—C4—H4A	120.4	C19—C20—C15	120.1 (5)
C5—C4—H4A	120.4	C19—C20—H20	119.9
C6—C5—C4	120.6 (5)	C15—C20—H20	119.9
C6—C5—Br2	120.6 (5)	N3—C21—C15	120.1 (5)
C4—C5—Br2	118.8 (4)	N3—C21—H21	120.0
C5—C6—C1	121.2 (5)	C15—C21—H21	120.0
C5—C6—H6	119.4	O4—C22—N4	122.0 (5)
C1—C6—H6	119.4	O4—C22—C23	122.9 (5)
N1—C7—C1	121.1 (5)	N4—C22—C23	115.1 (5)
N1—C7—H7	119.5	C28—C23—C24	118.0 (5)
C1—C7—H7	119.5	C28—C23—C22	118.8 (5)
O2—C8—N2	120.8 (5)	C24—C23—C22	123.2 (5)
O2—C8—C9	123.4 (5)	C25—C24—C23	121.3 (5)

N2—C8—C9	115.8 (4)	C25—C24—H24	119.3
C10—C9—C14	118.6 (5)	C23—C24—H24	119.3
C10—C9—C8	123.3 (5)	C26—C25—C24	119.5 (5)
C14—C9—C8	118.1 (5)	C26—C25—H25	120.2
C9—C10—C11	121.2 (5)	C24—C25—H25	120.2
C9—C10—H10	119.4	C25—C26—C27	120.8 (5)
C11—C10—H10	119.4	C25—C26—Cl2	120.5 (5)
C12—C11—C10	118.4 (5)	C27—C26—Cl2	118.8 (5)
C12—C11—H11	120.8	C26—C27—C28	119.3 (6)
C10—C11—H11	120.8	C26—C27—H27	120.3
C13—C12—C11	121.9 (5)	C28—C27—H27	120.3
C13—C12—Cl1	119.1 (5)	C23—C28—C27	121.0 (5)
C11—C12—Cl1	119.0 (5)	C23—C28—H28	119.5
C12—C13—C14	119.3 (5)	C27—C28—H28	119.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O2^{i}	0.90 (1)	1.95 (2)	2.827 (5)	166 (4)
N2—H2···O4	0.90 (1)	2.08 (2)	2.941 (5)	160 (4)
O3—H3···N3	0.82	1.87	2.569 (5)	143
O1—H1···N1	0.82	1.87	2.590 (5)	146

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